wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 06:21 am BST

PDB ID	:	2AXT
Title	:	Crystal Structure of Photosystem II from Thermosynechococcus elongatus
Authors	:	Loll, B.; Kern, J.; Saenger, W.; Zouni, A.; Biesiadka, J.
Deposited on	:	2005-09-06
Resolution	:	3.00 Å(reported)

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

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

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

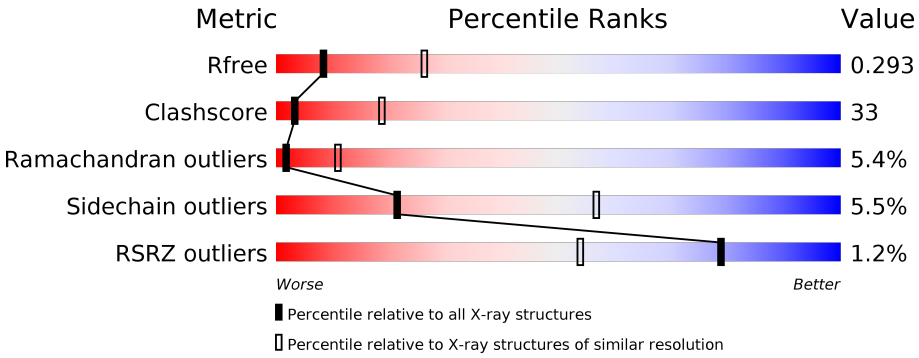
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	42% 48% 6%
1	a	344	% 88% 9%
2	B	510	55% 36% 5%
2	b	510	89% 6%
3	C	473	% 40% 48% 6% 5%
3	c	473	% 85% 10% 5%

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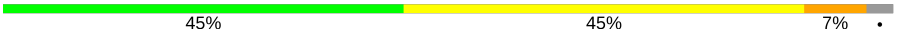
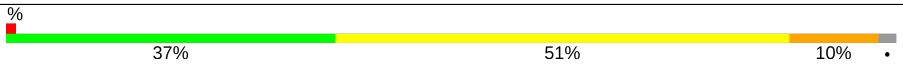
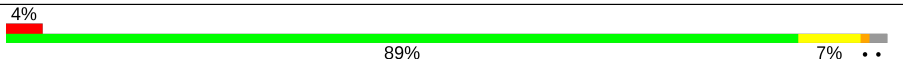
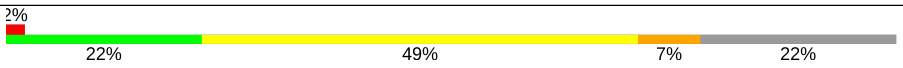
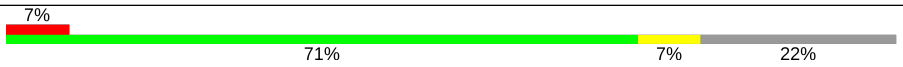
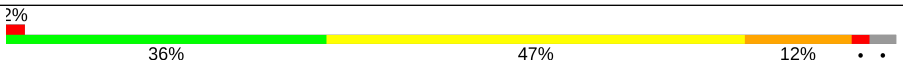
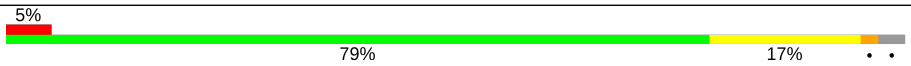
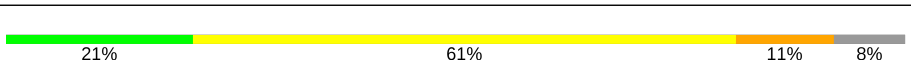
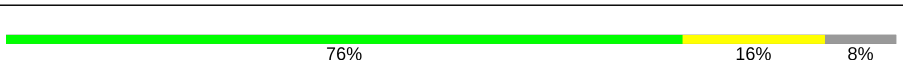
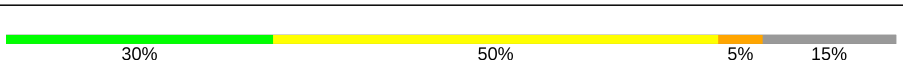
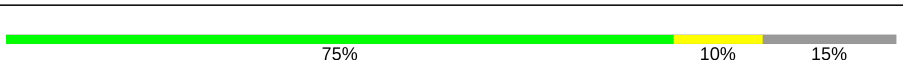
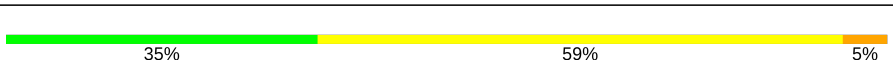
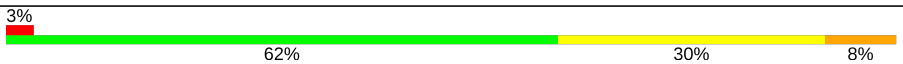
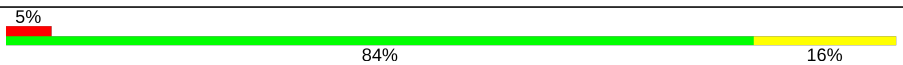
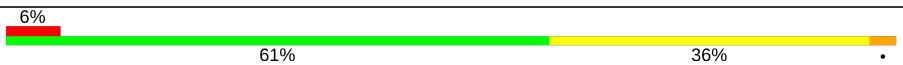
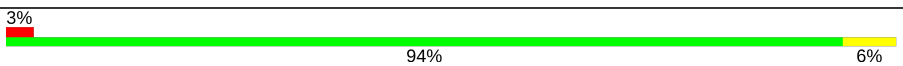
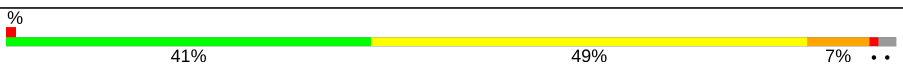
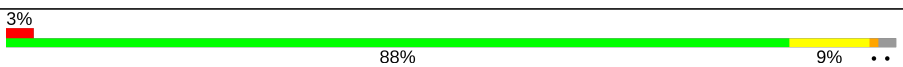
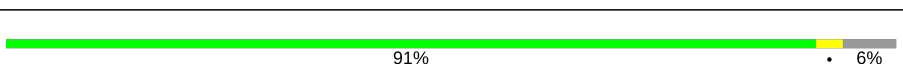
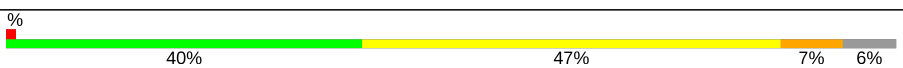
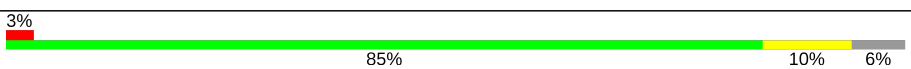
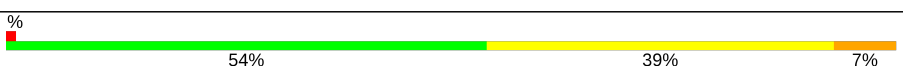
Mol	Chain	Length	Quality of chain
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	247	
13	o	247	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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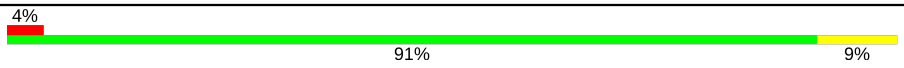
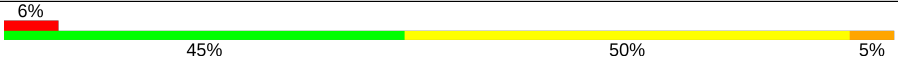
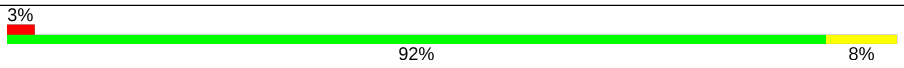
Mol	Chain	Length	Quality of chain
16	v	137	
17	X	129	
17	x	129	
18	Z	62	
18	z	62	

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
20	CLA	A	558	X	-	-	-
20	CLA	A	559	X	-	-	-
20	CLA	A	560	X	-	-	-
20	CLA	A	563	X	-	-	-
20	CLA	B	511	X	-	-	X
20	CLA	B	512	X	-	-	-
20	CLA	B	513	X	-	-	-
20	CLA	B	514	X	-	-	-
20	CLA	B	515	X	-	-	-
20	CLA	B	516	X	-	-	-
20	CLA	B	517	X	-	-	-
20	CLA	B	518	X	-	-	-
20	CLA	B	519	X	-	-	-
20	CLA	B	520	X	-	-	-
20	CLA	B	521	X	-	-	-
20	CLA	B	522	X	-	-	-
20	CLA	B	523	X	-	-	-
20	CLA	B	524	X	-	-	-
20	CLA	B	525	X	-	-	-
20	CLA	B	526	X	-	-	-
20	CLA	C	491	X	-	-	-
20	CLA	C	492	X	-	-	-
20	CLA	C	493	X	-	-	-
20	CLA	C	494	X	-	-	-
20	CLA	C	495	X	-	-	-
20	CLA	C	496	X	-	-	-
20	CLA	C	497	X	-	-	-
20	CLA	C	498	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	499	X	-	-	-
20	CLA	C	500	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	D	354	X	-	-	-
20	CLA	D	355	X	-	-	-
20	CLA	a	5558	X	-	-	-
20	CLA	a	5559	X	-	-	-
20	CLA	a	5560	X	-	-	-
20	CLA	a	5563	X	-	-	-
20	CLA	b	5511	X	-	-	-
20	CLA	b	5512	X	-	-	-
20	CLA	b	5513	X	-	-	-
20	CLA	b	5514	X	-	-	-
20	CLA	b	5515	X	-	-	-
20	CLA	b	5516	X	-	-	-
20	CLA	b	5517	X	-	-	-
20	CLA	b	5518	X	-	-	-
20	CLA	b	5519	X	-	-	-
20	CLA	b	5520	X	-	-	-
20	CLA	b	5521	X	-	-	-
20	CLA	b	5522	X	-	-	-
20	CLA	b	5523	X	-	-	-
20	CLA	b	5524	X	-	-	-
20	CLA	b	5525	X	-	-	-
20	CLA	b	5526	X	-	-	-
20	CLA	c	5491	X	-	-	-
20	CLA	c	5492	X	-	-	-
20	CLA	c	5493	X	-	-	-
20	CLA	c	5494	X	-	-	-
20	CLA	c	5495	X	-	-	-
20	CLA	c	5496	X	-	-	-
20	CLA	c	5497	X	-	-	-
20	CLA	c	5498	X	-	-	-
20	CLA	c	5499	X	-	-	-
20	CLA	c	5500	X	-	-	-
20	CLA	c	5501	X	-	-	-
20	CLA	c	5502	X	-	-	-
20	CLA	c	5503	X	-	-	-
20	CLA	d	5354	X	-	-	-
20	CLA	d	5355	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	BCR	x	5130	-	-	-	X
27	LMT	A	569	-	-	-	X
27	LMT	t	5217	-	-	-	X
29	UNK	C	489	-	-	-	X
30	DGD	C	507	X	-	-	-
30	DGD	C	508	X	-	-	-
30	DGD	C	509	X	-	-	-
30	DGD	H	208	X	-	-	-
30	DGD	c	5507	X	-	-	-
30	DGD	c	5508	X	-	-	-
30	DGD	c	5509	X	-	-	-
30	DGD	h	5208	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			
1	a	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			
2	b	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			
3	c	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			
4	d	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total 646	C 424	N 101	O 121	0	0	0
5	e	82	Total 646	C 424	N 101	O 121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total 278	C 189	N 46	O 42	S 1	0	0	0
6	f	35	Total 278	C 189	N 46	O 42	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total 492	C 330	N 77	O 83	S 2	0	0	0
7	h	64	Total 492	C 330	N 77	O 83	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total 286	C 195	N 45	O 45	S 1	0	0	0
8	i	35	Total 286	C 195	N 45	O 45	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total 240	C 164	N 35	O 40	S 1	0	0	0
9	j	34	Total 240	C 164	N 35	O 40	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 289	C 201	N 42	O 46	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total 289	C 201	N 42	O 46	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total 276	C 181	N 41	O 53	S 1	0	0	0
12	m	36	Total 276	C 181	N 41	O 53	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total 1772	C 1113	N 295	O 360	S 4	0	0	0
13	o	242	Total 1772	C 1113	N 295	O 360	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total 254	C 179	N 36	O 37	S 2	0	0	0
14	t	30	Total 254	C 179	N 36	O 37	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total 775	C 492	N 130	O 153	0	0	0
15	u	98	Total 775	C 492	N 130	O 153	0	0	0

- 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	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Unassigned subunits.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	X	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			

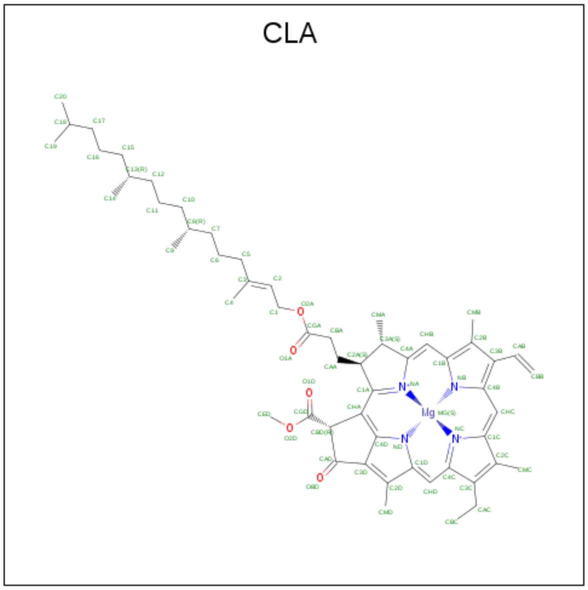
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			
18	z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			

- Molecule 19 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N O 55 45 1 4 5	0	0
20	B	1	Total C Mg N O 41 33 1 4 3	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	b	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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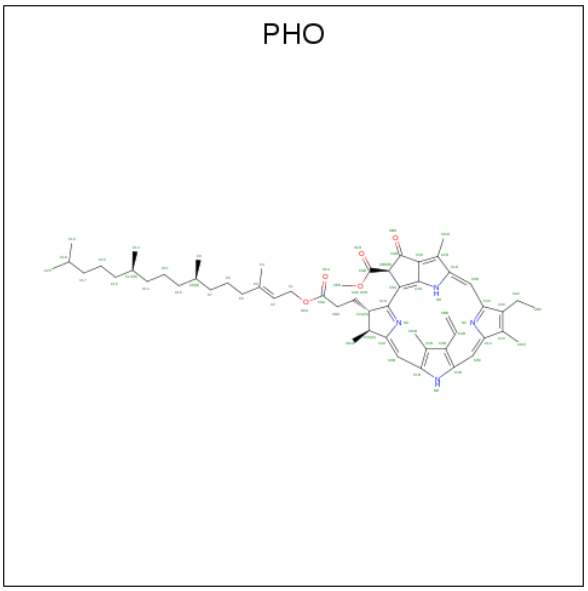
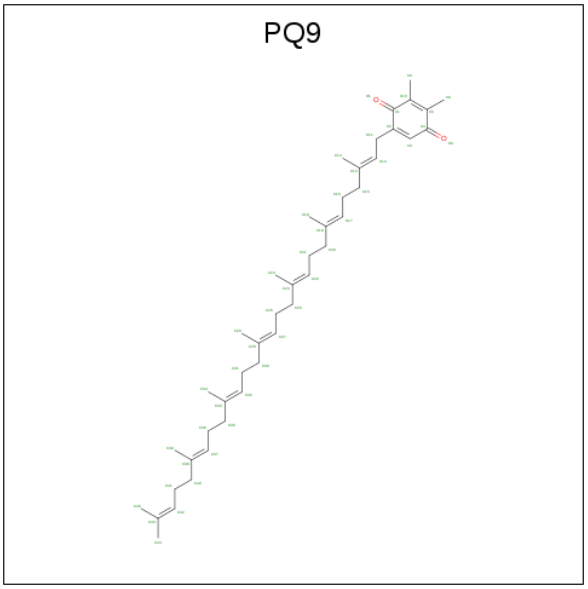
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



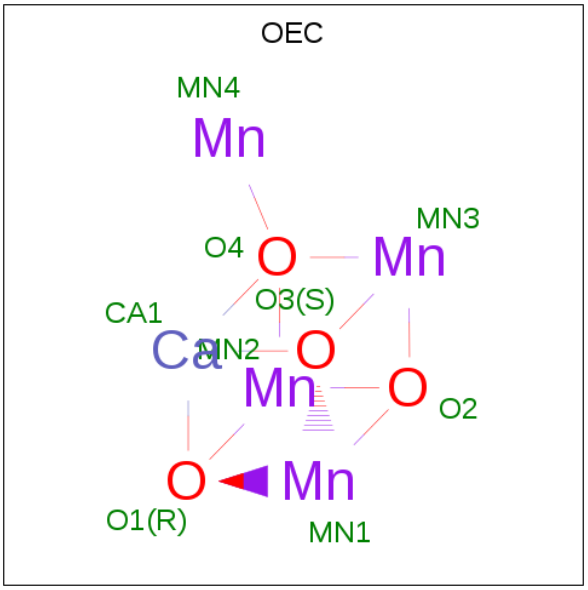
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 22 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: $C_{43}H_{64}O_2$).



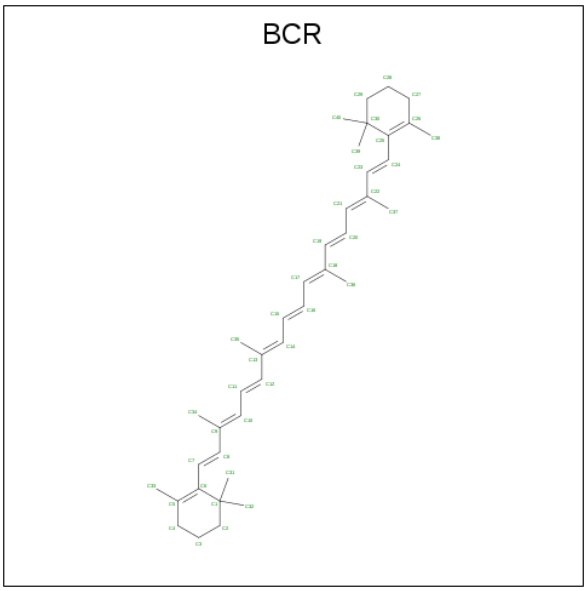
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O 30 28 2	0	0
22	D	1	Total C O 30 28 2	0	0
22	a	1	Total C O 30 28 2	0	0
22	d	1	Total C O 30 28 2	0	0

- Molecule 23 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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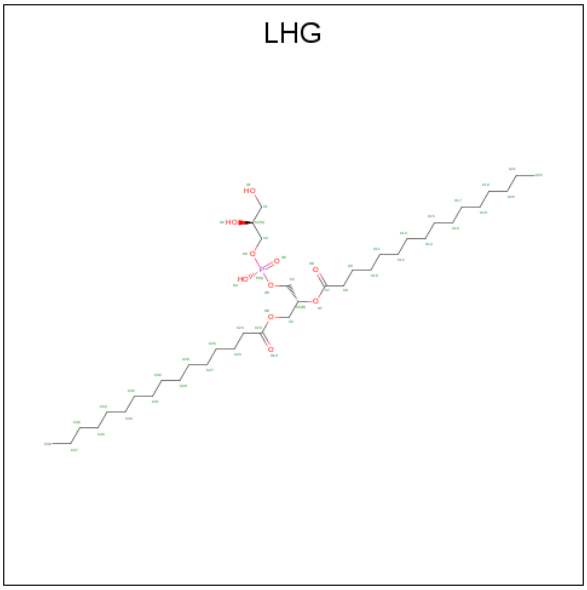
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

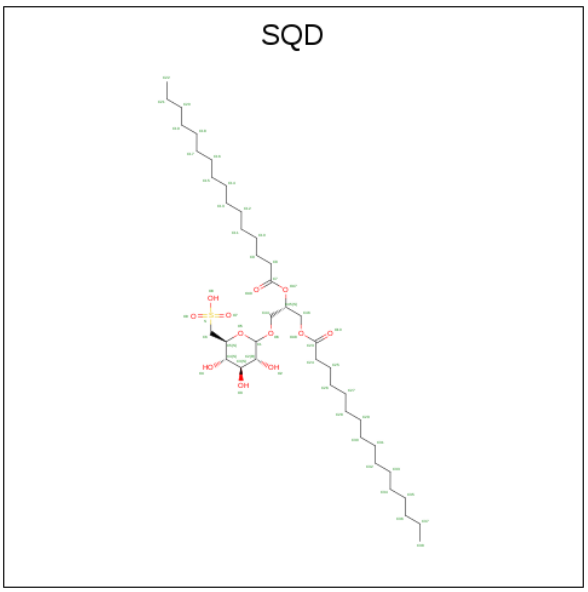
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 39 28 10 1	0	0
25	a	1	Total C O P 39 28 10 1	0	0

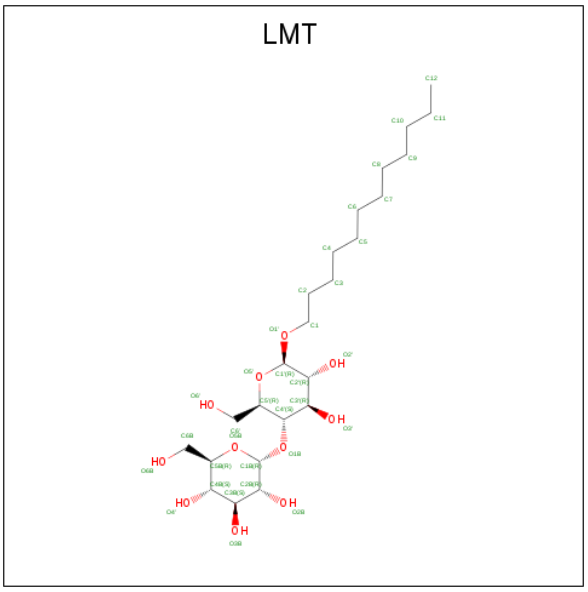
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



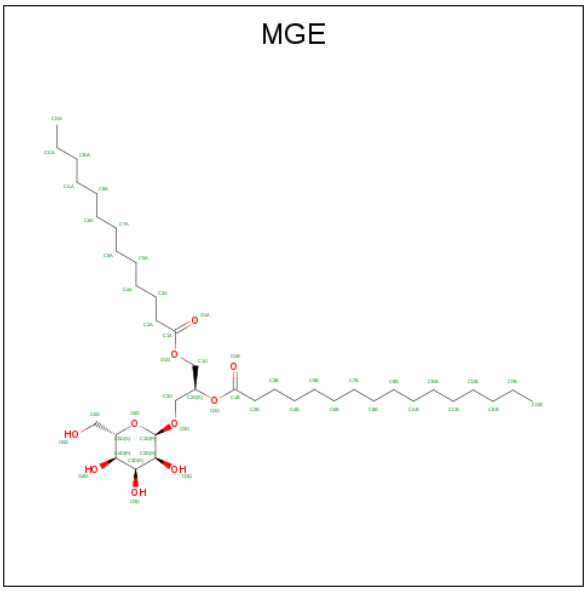
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	T	1	Total	C	O	0	0
			35	24	11		
27	a	1	Total	C	O	0	0
			35	24	11		
27	m	1	Total	C	O	0	0
			35	24	11		
27	t	1	Total	C	O	0	0
			35	24	11		

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: $C_{38}H_{72}O_{10}$).

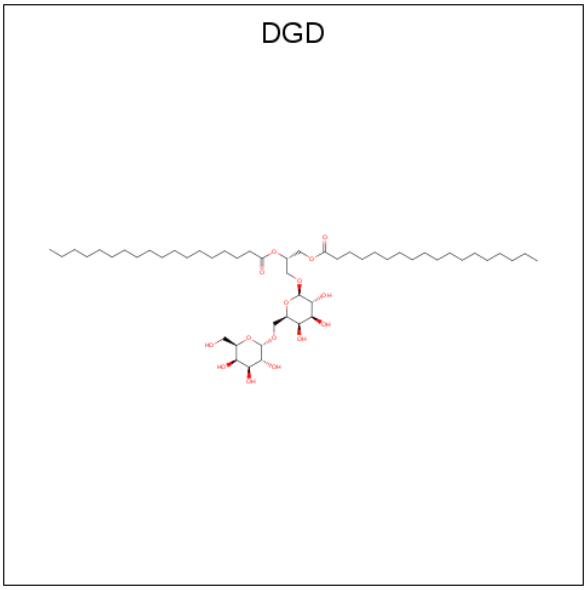


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B	1	Total C O 48 38 10	0	0
28	D	1	Total C O 47 37 10	0	0
28	D	1	Total C O 41 31 10	0	0
28	D	1	Total C O 48 38 10	0	0
28	I	1	Total C O 48 38 10	0	0
28	L	1	Total C O 48 38 10	0	0
28	b	1	Total C O 48 38 10	0	0
28	d	1	Total C O 47 37 10	0	0
28	d	1	Total C O 41 31 10	0	0
28	d	1	Total C O 48 38 10	0	0
28	i	1	Total C O 48 38 10	0	0
28	l	1	Total C O 48 38 10	0	0

- Molecule 29 is UNKNOWN (three-letter code: UNK) (formula: $C_4H_9NO_2$).

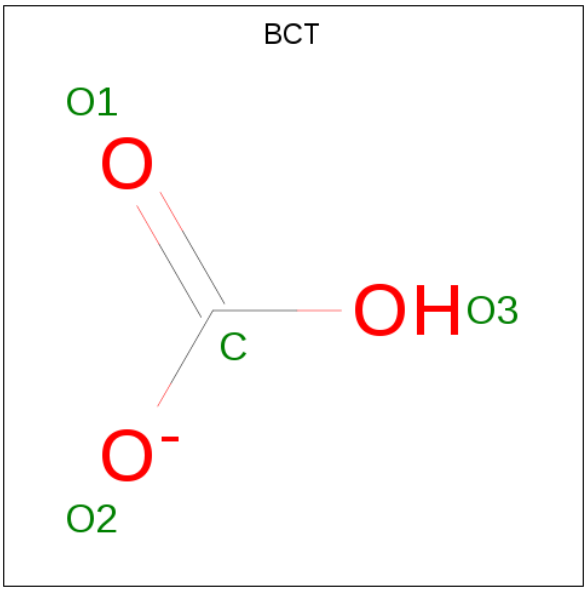
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	C	17	Total C 152 152	0	0
29	c	17	Total C 152 152	0	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



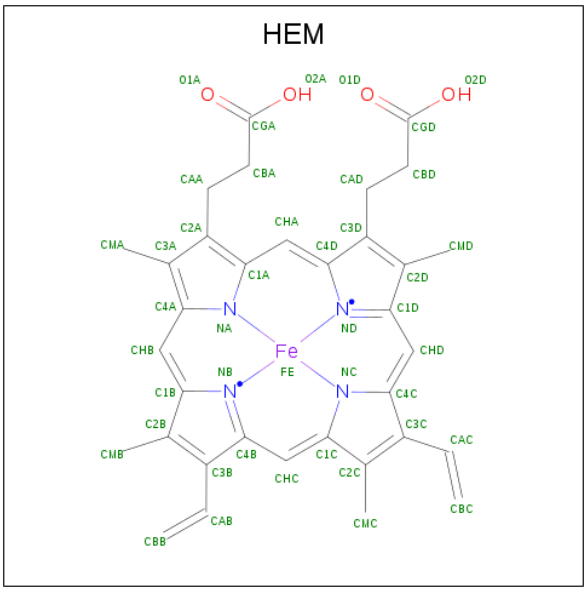
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	C	1	Total C O 53 38 15	0	0
30	C	1	Total C O 47 32 15	0	0
30	C	1	Total C O 57 42 15	0	0
30	H	1	Total C O 54 39 15	0	0
30	c	1	Total C O 53 38 15	0	0
30	c	1	Total C O 47 32 15	0	0
30	c	1	Total C O 57 42 15	0	0
30	h	1	Total C O 54 39 15	0	0

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



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

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



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

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

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

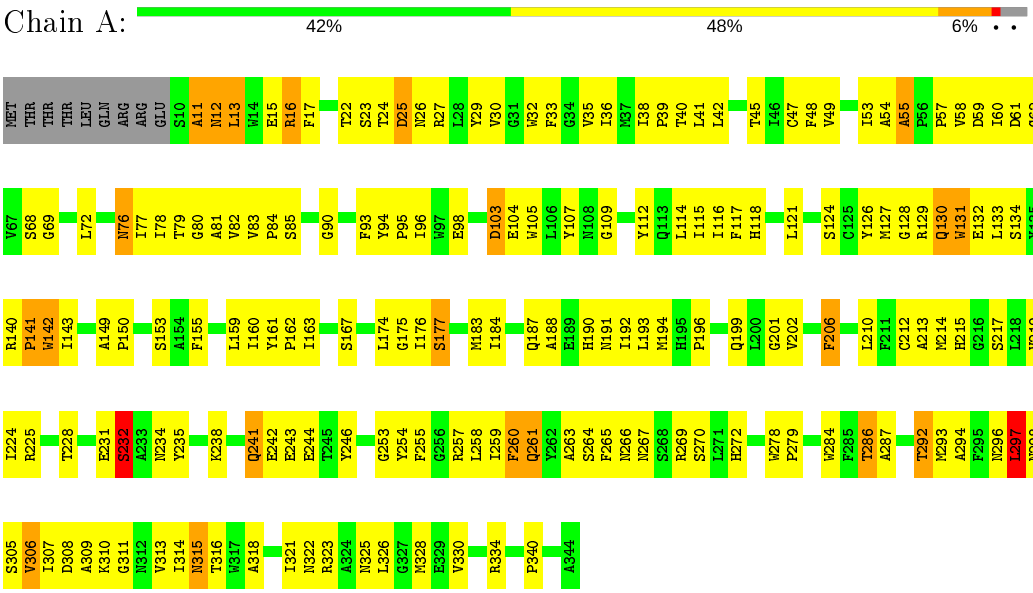
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	K	1	Total	Ca	0	0
			1	1		
33	k	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

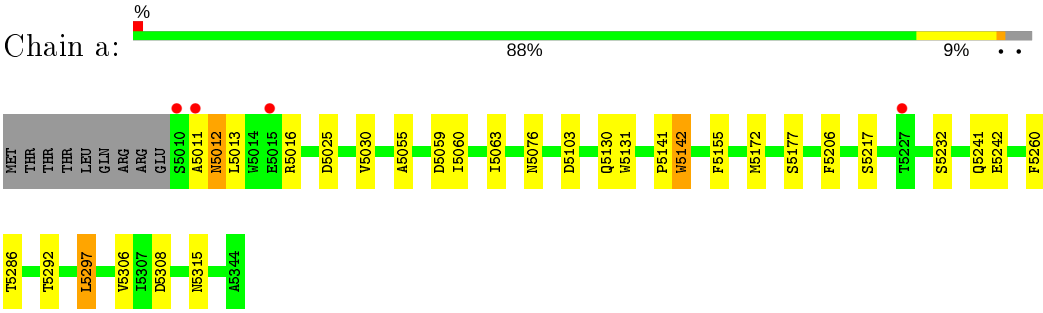
- Molecule 1: Photosystem Q(B) protein

Chain A:



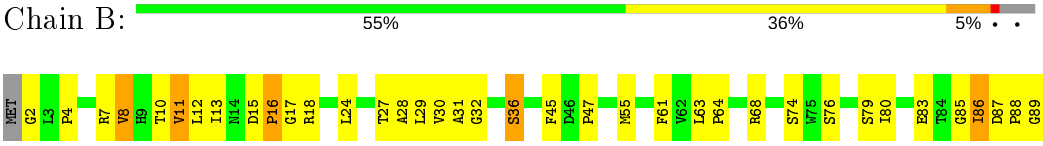
- Molecule 1: Photosystem Q(B) protein

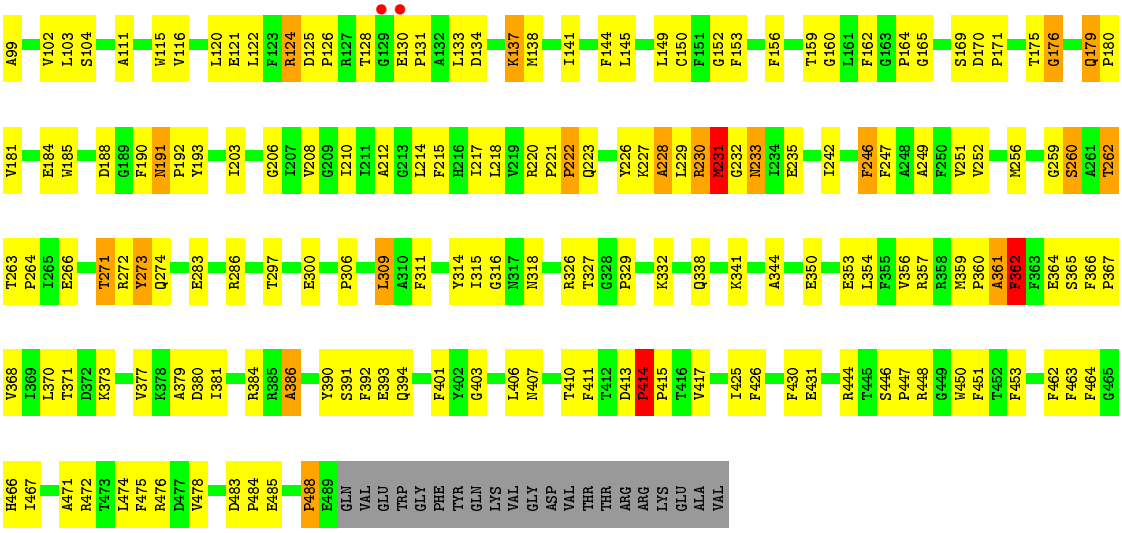
Chain a:



- Molecule 2: CP47 protein

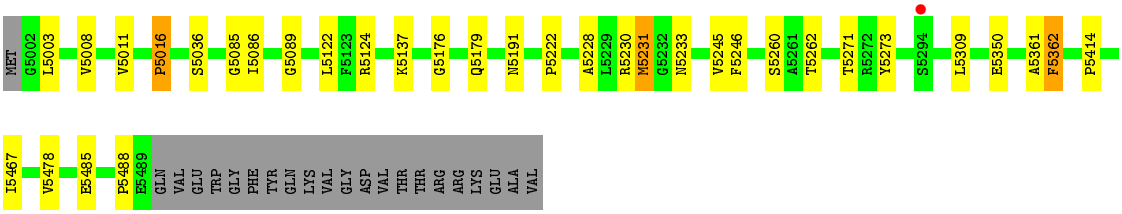
Chain B:





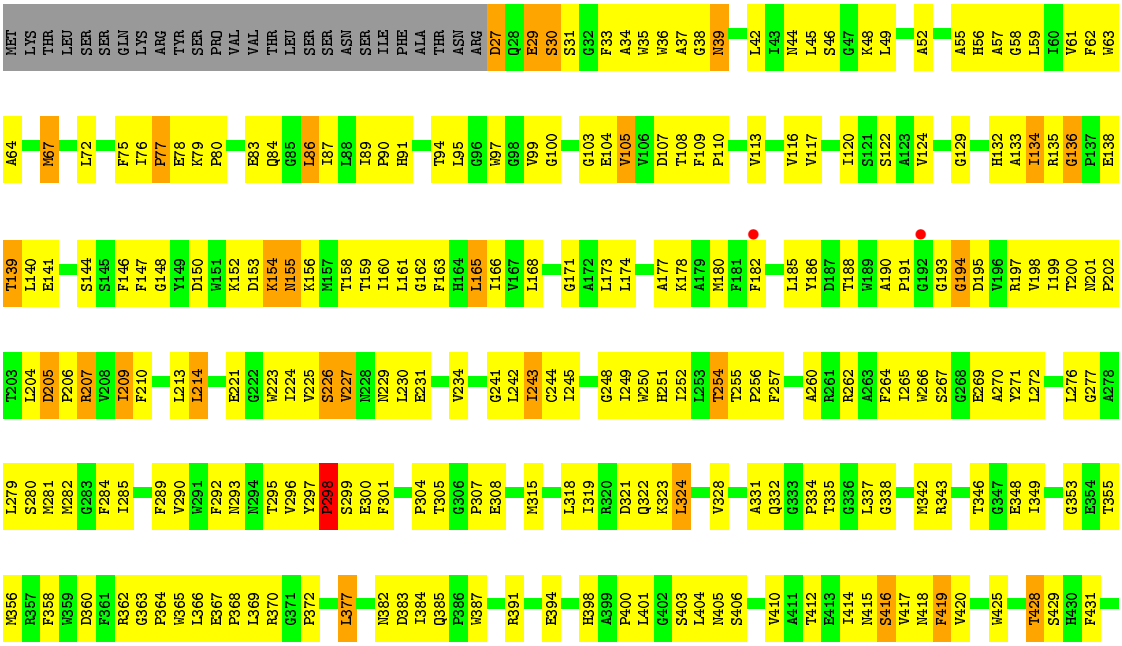
• Molecule 2: CP47 protein

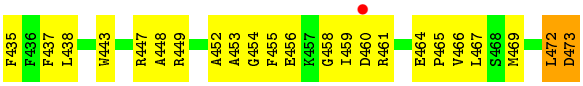
Chain b:



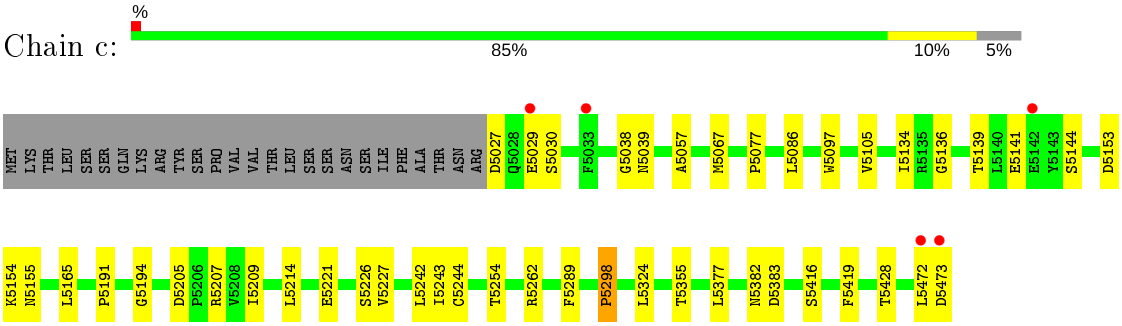
• Molecule 3: photosystem II CP43 protein

Chain C:

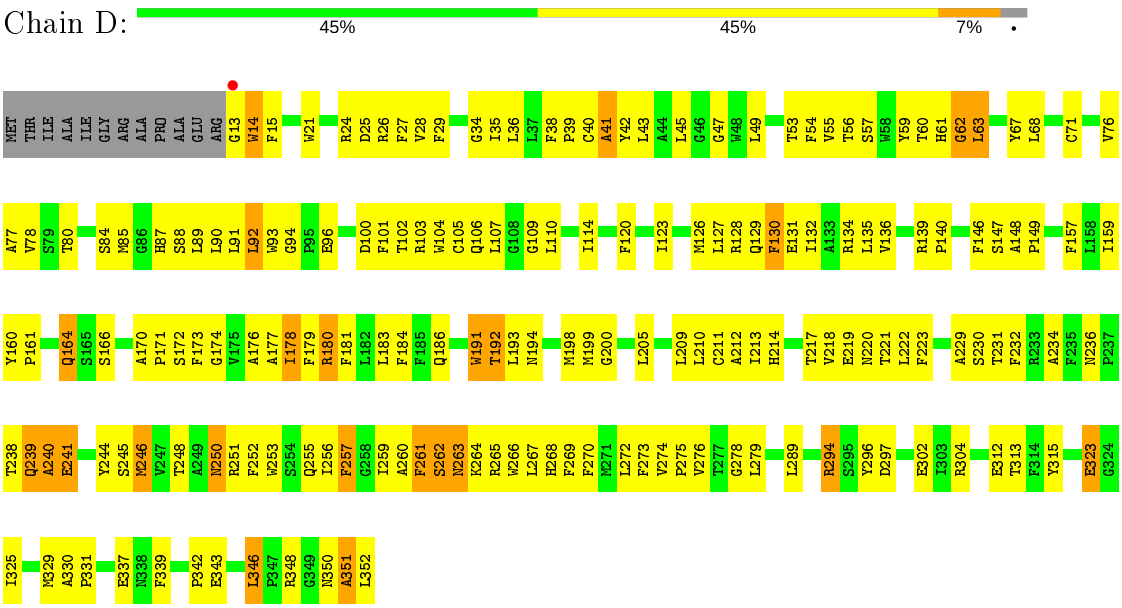




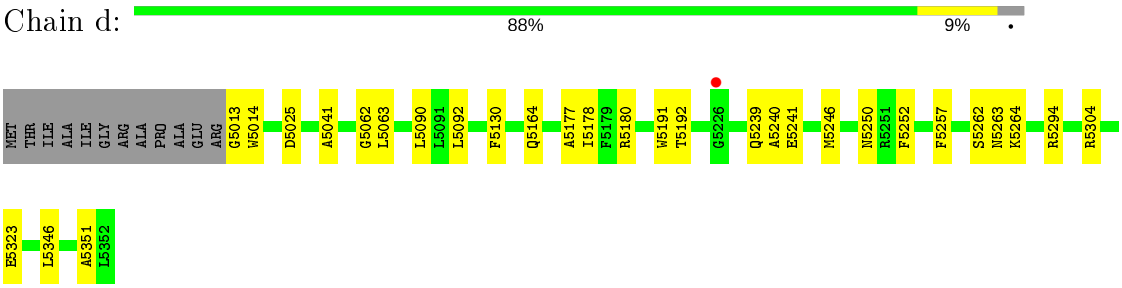
• Molecule 3: photosystem II CP43 protein



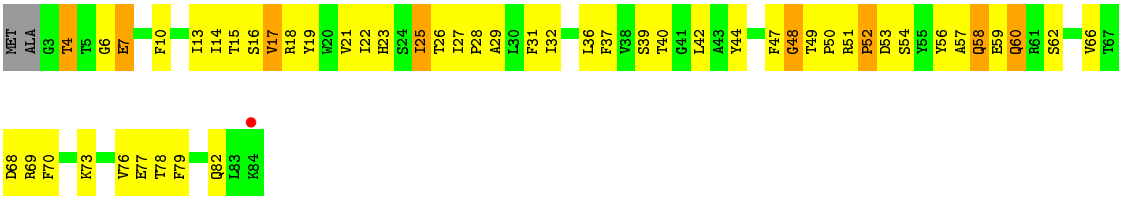
• Molecule 4: photosystem II reaction center D2 protein



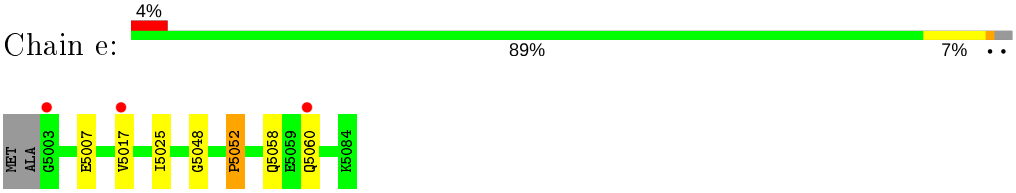
• Molecule 4: photosystem II reaction center D2 protein



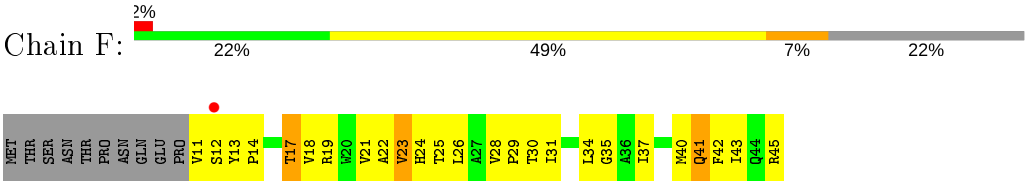
• Molecule 5: Cytochrome b559 alpha subunit



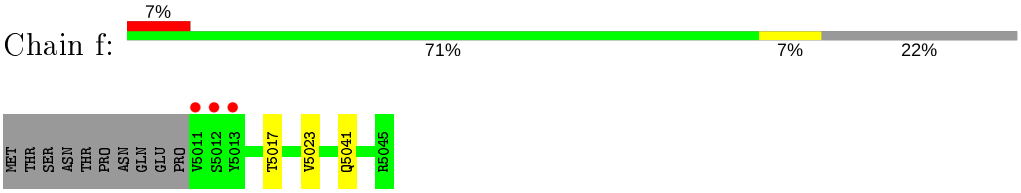
- Molecule 5: Cytochrome b559 alpha subunit



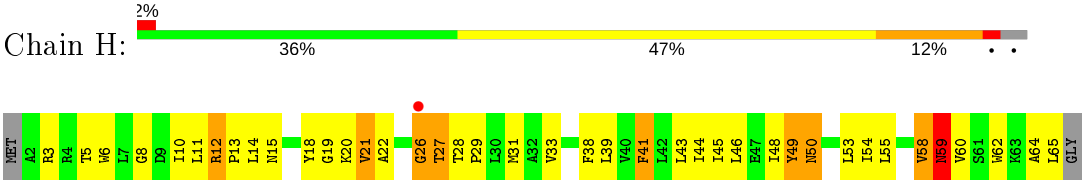
- Molecule 6: Cytochrome b559 beta subunit



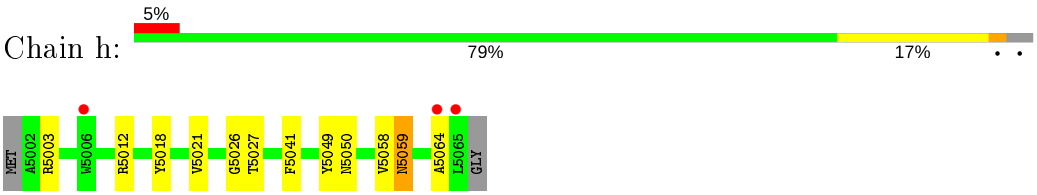
- Molecule 6: Cytochrome b559 beta subunit



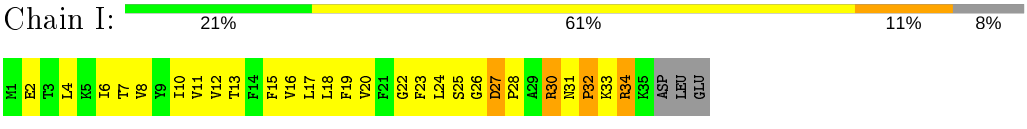
- Molecule 7: Photosystem II reaction center H protein



- Molecule 7: Photosystem II reaction center H protein

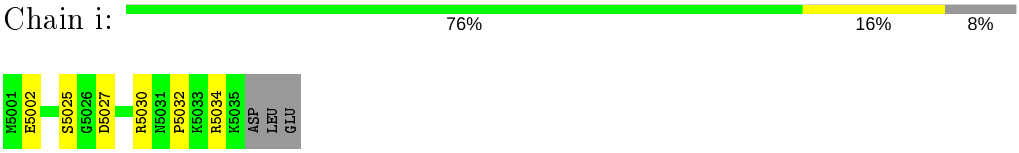


- Molecule 8: Photosystem II reaction center I protein



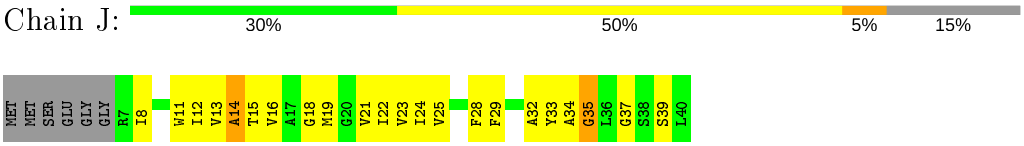
• Molecule 8: Photosystem II reaction center I protein

Chain i:



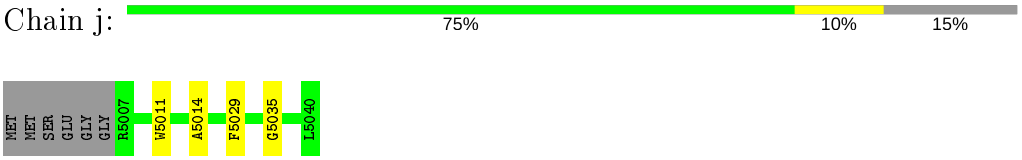
• Molecule 9: Photosystem II reaction center J protein

Chain J:



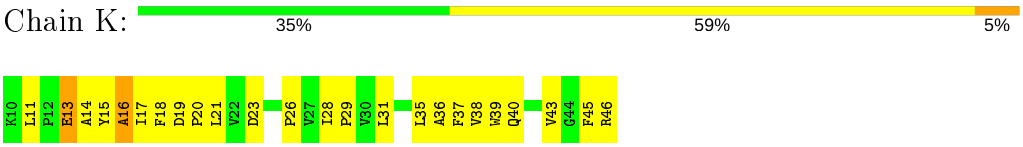
• Molecule 9: Photosystem II reaction center J protein

Chain j:



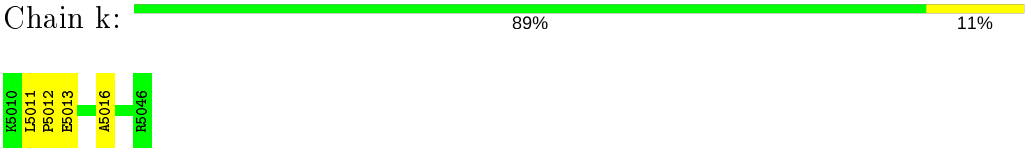
• Molecule 10: Photosystem II reaction center protein K

Chain K:



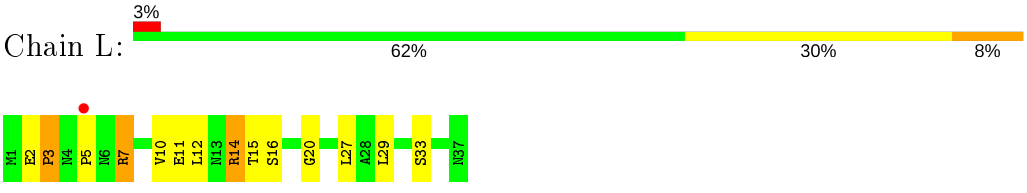
• Molecule 10: Photosystem II reaction center protein K

Chain k:



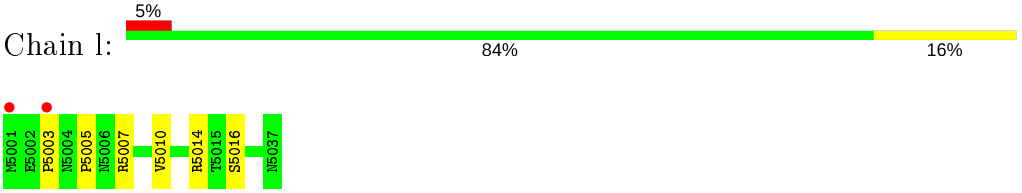
• Molecule 11: Photosystem II reaction center L protein

Chain L:



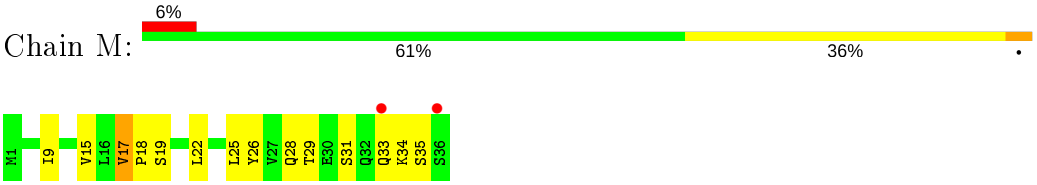
• Molecule 11: Photosystem II reaction center L protein

Chain l:



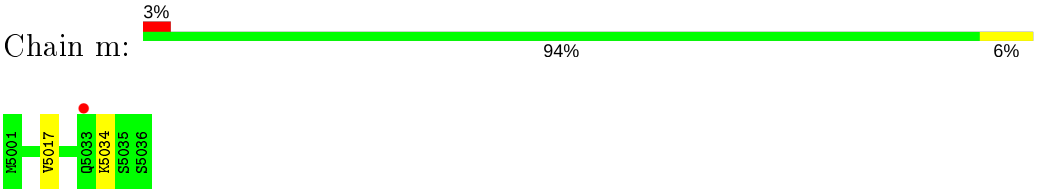
• Molecule 12: Photosystem II reaction center M protein

Chain M:



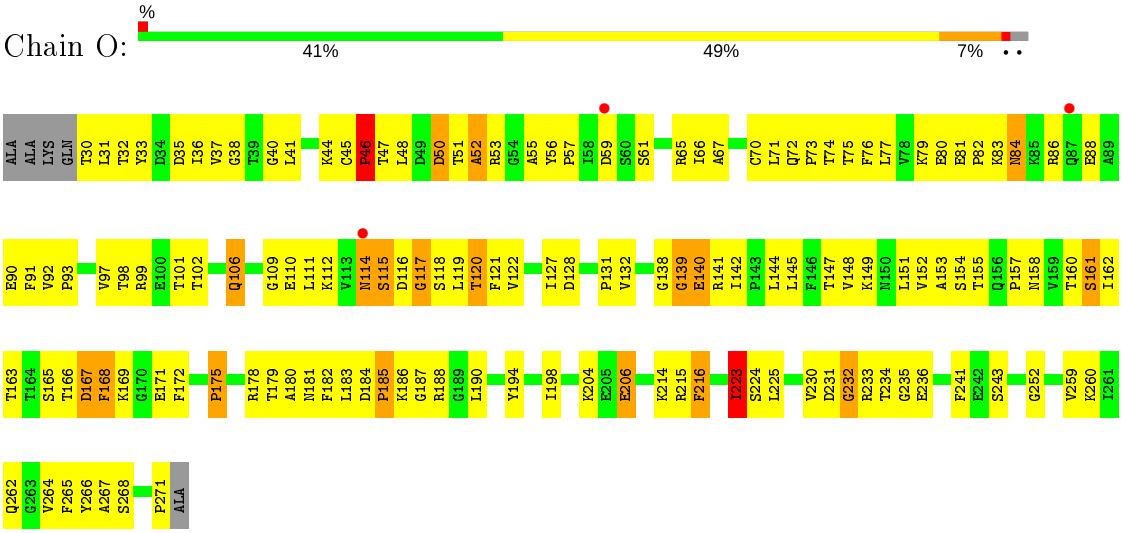
• Molecule 12: Photosystem II reaction center M protein

Chain m:



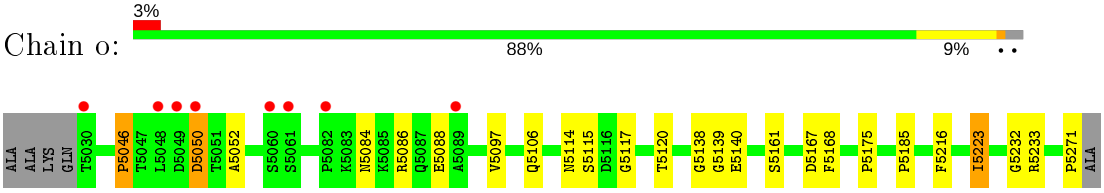
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



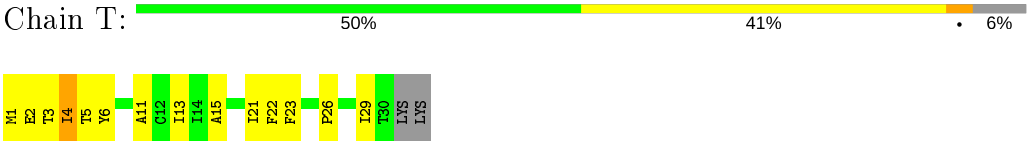
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



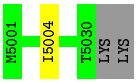
• Molecule 14: Photosystem II reaction center T protein

Chain T:



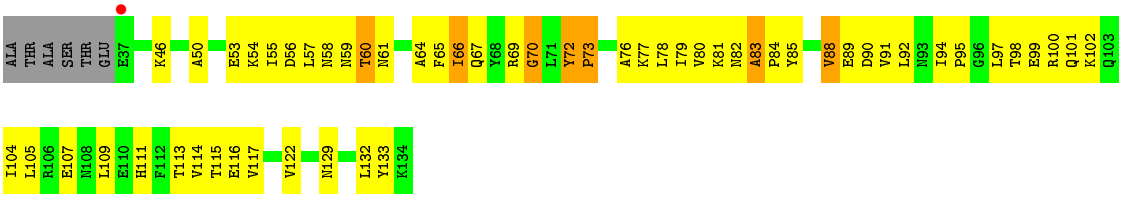
• Molecule 14: Photosystem II reaction center T protein

Chain t:



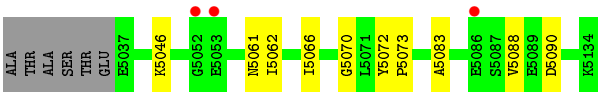
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



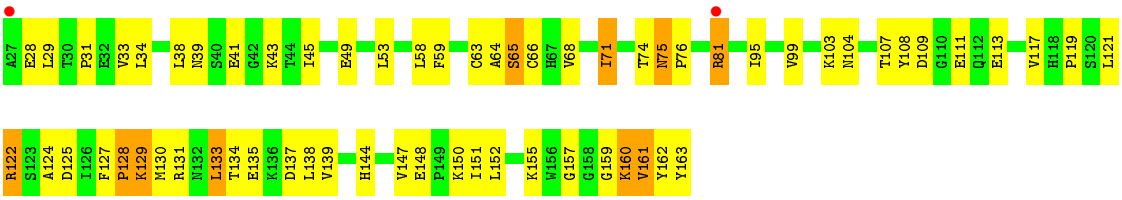
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



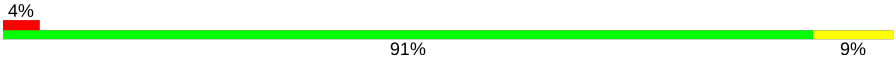
• Molecule 16: Cytochrome c-550

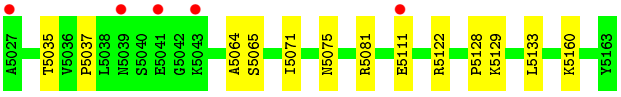
Chain V:



• Molecule 16: Cytochrome c-550

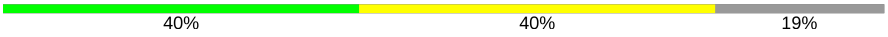
Chain v:

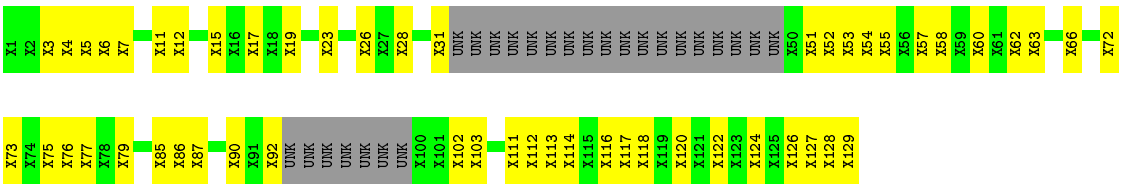




• Molecule 17: Unassigned subunits

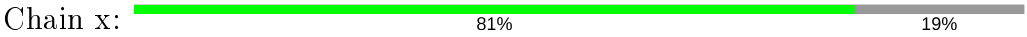
Chain X:





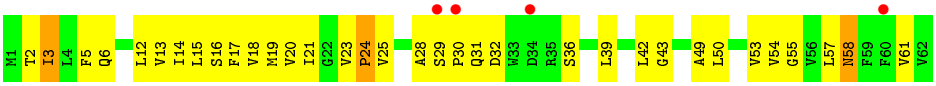
• Molecule 17: Unassigned subunits

Chain x:



• Molecule 18: Photosystem II reaction center Z protein

Chain Z:



• Molecule 18: Photosystem II reaction center Z protein

Chain z:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 81.7 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.286 0.241 , 0.293	Depositor DCC
R_{free} test set	1908 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: LHG, PHO, MGE, DGD, CA, LMT, CLA, BCT, FE2, PQ9, OEC, HEM, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.62	0/2708	0.72	1/3694 (0.0%)
1	a	0.62	0/2708	0.74	2/3694 (0.1%)
2	B	0.57	0/3935	0.69	0/5366
2	b	0.56	0/3935	0.70	1/5366 (0.0%)
3	C	0.54	0/3533	0.71	0/4815
3	c	0.57	0/3533	0.72	0/4815
4	D	0.62	1/2791 (0.0%)	0.70	0/3806
4	d	0.60	1/2791 (0.0%)	0.71	0/3806
5	E	0.59	0/665	0.76	0/911
5	e	0.63	0/665	0.77	0/911
6	F	0.66	0/287	0.67	0/392
6	f	0.67	0/287	0.63	0/392
7	H	0.55	0/505	0.73	0/692
7	h	0.55	0/505	0.75	0/692
8	I	0.65	0/293	0.69	0/395
8	i	0.62	0/293	0.69	0/395
9	J	0.57	0/246	0.72	0/335
9	j	0.56	0/246	0.72	0/335
10	K	0.63	0/299	0.72	0/412
10	k	0.74	0/299	0.73	0/412
11	L	0.64	0/308	0.75	0/419
11	l	0.67	0/308	0.74	0/419
12	M	0.71	0/279	0.73	0/379
12	m	0.73	0/279	0.73	0/379
13	O	0.61	0/1803	0.78	2/2461 (0.1%)
13	o	0.60	0/1803	0.77	3/2461 (0.1%)
14	T	0.70	0/263	0.72	0/356
14	t	0.71	0/263	0.72	0/356
15	U	0.62	0/786	0.77	0/1066
15	u	0.60	0/786	0.76	0/1066
16	V	0.58	0/1085	0.71	0/1473
16	v	0.60	0/1085	0.71	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
18	Z	0.66	0/451	0.67	0/620
18	z	0.74	0/451	0.70	0/620
All	All	0.60	2/40474 (0.0%)	0.72	9/55184 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	5013	GLY	N-CA	5.43	1.54	1.46
4	D	13	GLY	N-CA	5.12	1.53	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	271	PRO	CA-C-O	7.17	137.40	120.20
1	a	5297	LEU	N-CA-C	-5.78	95.40	111.00
1	A	297	LEU	N-CA-C	-5.56	96.00	111.00
13	o	5271	PRO	CA-C-O	5.23	132.76	120.20
1	a	5142	TRP	N-CA-C	5.22	125.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	TYR	Sidechain
2	b	5273	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2517	223	0
1	a	2623	0	2517	0	0
2	B	3800	0	3637	261	0
2	b	3800	0	3637	0	0
3	C	3421	0	3326	301	0
3	c	3421	0	3326	0	0
4	D	2696	0	2591	237	0
4	d	2696	0	2591	0	0
5	E	646	0	616	52	0
5	e	646	0	616	0	0
6	F	278	0	279	30	0
6	f	278	0	279	0	0
7	H	492	0	495	48	0
7	h	492	0	495	0	0
8	I	286	0	308	31	0
8	i	286	0	305	0	0
9	J	240	0	242	26	0
9	j	240	0	242	0	0
10	K	289	0	294	48	0
10	k	289	0	294	0	0
11	L	301	0	309	24	0
11	l	301	0	306	0	0
12	M	276	0	288	18	0
12	m	276	0	285	0	0
13	O	1772	0	1664	155	0
13	o	1772	0	1664	0	0
14	T	254	0	257	26	0
14	t	254	0	254	0	0
15	U	775	0	771	60	0
15	u	775	0	771	0	0
16	V	1064	0	1072	65	0
16	v	1064	0	1072	0	0
17	X	687	0	268	57	0
17	x	687	0	268	0	0
18	Z	442	0	460	37	0
18	z	442	0	457	0	0
19	A	1	0	0	0	0
19	a	1	0	0	0	0
20	A	250	0	265	15	0
20	B	1007	0	1088	74	0
20	C	774	0	783	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	D	115	0	111	8	0
20	a	250	0	265	0	0
20	b	1007	0	1088	0	0
20	c	774	0	783	0	0
20	d	115	0	111	0	0
21	A	128	0	148	12	0
21	a	128	0	148	0	0
22	A	30	0	37	2	0
22	D	30	0	37	7	0
22	a	30	0	37	0	0
22	d	30	0	37	0	0
23	A	5	0	0	0	0
23	a	5	0	0	0	0
24	A	40	0	56	1	0
24	B	120	0	168	6	0
24	C	120	0	168	20	0
24	D	40	0	56	4	0
24	H	40	0	56	3	0
24	T	40	0	56	5	0
24	X	40	0	56	9	0
24	a	40	0	56	0	0
24	b	120	0	168	0	0
24	c	120	0	168	0	0
24	d	40	0	56	0	0
24	h	40	0	56	0	0
24	t	40	0	56	0	0
24	x	40	0	56	0	0
25	A	39	0	51	4	0
25	a	39	0	51	0	0
26	A	80	0	92	0	0
26	L	47	0	60	0	0
26	a	26	0	15	0	0
26	d	54	0	77	0	0
26	t	47	0	60	0	0
27	A	35	0	46	0	0
27	M	35	0	46	0	0
27	T	35	0	46	3	0
27	a	35	0	46	0	0
27	m	35	0	46	0	0
27	t	35	0	46	0	0
28	B	48	0	72	1	0
28	D	136	0	194	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	I	48	0	72	1	0
28	L	48	0	72	2	0
28	b	48	0	72	0	0
28	d	136	0	194	0	0
28	i	48	0	72	0	0
28	l	48	0	72	0	0
29	C	152	0	17	2	0
29	c	152	0	17	0	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	0	0
30	h	54	0	66	0	0
31	D	4	0	0	0	0
31	d	4	0	0	0	0
32	F	43	0	30	3	0
32	V	43	0	30	2	0
32	f	43	0	30	0	0
32	v	43	0	30	0	0
33	K	1	0	0	0	0
33	k	1	0	0	0	0
All	All	48254	0	47107	1538	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 33.

The worst 5 of 1538 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)
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:CD	17:X:26:UNK:NE2	1.33	1.41
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14
13:O:223:ILE:HG23	13:O:243:SER:HB3	1.31	1.12
15:U:113:THR:HG22	15:U:114:VAL:H	1.15	1.07

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	279 (84%)	39 (12%)	15 (4%)	2	14
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	2	12
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	3	17
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	3	20
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	2	10
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	1	10
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	2	14
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	3	16
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	1	5
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	1	5
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	8
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	8
7	H	62/66 (94%)	45 (73%)	11 (18%)	6 (10%)	0	2
7	h	62/66 (94%)	44 (71%)	12 (19%)	6 (10%)	0	2
8	I	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	4	24
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	4	24
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	0	3
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	0	3
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	10
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	3
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	10
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	1	3
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	1	9
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	1	9
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	1 5
14	T	28/32 (88%)	24 (86%)	4 (14%)	0	100 100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100 100
15	U	96/104 (92%)	71 (74%)	18 (19%)	7 (7%)	1 5
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	1 5
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2 12
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	2 12
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1 6
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	1 6
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	2 11

5 of 269 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	269/280 (96%)	251 (93%)	18 (7%)	16 49
1	a	269/280 (96%)	252 (94%)	17 (6%)	18 51
2	B	378/407 (93%)	361 (96%)	17 (4%)	27 64
2	b	378/407 (93%)	360 (95%)	18 (5%)	25 62
3	C	341/374 (91%)	320 (94%)	21 (6%)	18 52
3	c	341/374 (91%)	320 (94%)	21 (6%)	18 52
4	D	273/283 (96%)	259 (95%)	14 (5%)	24 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	d	273/283 (96%)	258 (94%)	15 (6%)	21 57
5	E	68/73 (93%)	65 (96%)	3 (4%)	28 65
5	e	68/73 (93%)	66 (97%)	2 (3%)	42 76
6	F	27/39 (69%)	26 (96%)	1 (4%)	34 70
6	f	27/39 (69%)	26 (96%)	1 (4%)	34 70
7	H	50/55 (91%)	42 (84%)	8 (16%)	2 12
7	h	50/55 (91%)	43 (86%)	7 (14%)	3 16
8	I	32/35 (91%)	27 (84%)	5 (16%)	2 13
8	i	32/35 (91%)	27 (84%)	5 (16%)	2 13
9	J	22/28 (79%)	21 (96%)	1 (4%)	27 64
9	j	22/28 (79%)	21 (96%)	1 (4%)	27 64
10	K	29/30 (97%)	28 (97%)	1 (3%)	37 72
10	k	29/30 (97%)	28 (97%)	1 (3%)	37 72
11	L	34/35 (97%)	31 (91%)	3 (9%)	10 36
11	l	34/35 (97%)	31 (91%)	3 (9%)	10 36
12	M	32/33 (97%)	32 (100%)	0	100 100
12	m	32/33 (97%)	32 (100%)	0	100 100
13	O	181/208 (87%)	171 (94%)	10 (6%)	21 57
13	o	181/208 (87%)	172 (95%)	9 (5%)	24 60
14	T	26/29 (90%)	25 (96%)	1 (4%)	33 69
14	t	26/29 (90%)	25 (96%)	1 (4%)	33 69
15	U	83/89 (93%)	80 (96%)	3 (4%)	35 70
15	u	83/89 (93%)	80 (96%)	3 (4%)	35 70
16	V	117/117 (100%)	113 (97%)	4 (3%)	37 72
16	v	117/117 (100%)	111 (95%)	6 (5%)	24 60
18	Z	43/52 (83%)	42 (98%)	1 (2%)	50 80
18	z	43/52 (83%)	42 (98%)	1 (2%)	50 80
All	All	4010/4334 (92%)	3788 (94%)	222 (6%)	21 57

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	O	216	PHE

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Mol	Chain	Res	Type
1	a	5286	THR
13	o	5106	GLN
15	U	46	LYS
1	a	5013	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
13	O	130	GLN
1	a	5165	GLN
13	o	5106	GLN
15	U	108	ASN
1	a	5012	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 180 ligands modelled in this entry, 34 are unknown and 4 are monoatomic - leaving 142 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	$\#\|Z\|>2$
20	CLA	B	522	-	59,73,73	1.33	6 (10%)	67,113,113	1.91	10 (14%)
20	CLA	C	503	3	44,58,73	1.89	8 (18%)	49,95,113	2.31	12 (24%)
20	CLA	b	5517	-	59,73,73	1.56	7 (11%)	67,113,113	2.03	12 (17%)
20	CLA	B	512	2	59,73,73	1.30	5 (8%)	67,113,113	1.88	14 (20%)
20	CLA	c	5495	-	59,73,73	1.72	9 (15%)	67,113,113	2.12	16 (23%)
20	CLA	b	5526	-	59,73,73	1.57	11 (18%)	67,113,113	2.03	14 (20%)
27	LMT	T	217	-	36,36,36	1.40	6 (16%)	47,47,47	1.02	4 (8%)
28	MGE	D	358	-	47,47,48	1.22	5 (10%)	55,55,56	0.97	3 (5%)
20	CLA	b	5522	-	59,73,73	1.37	6 (10%)	67,113,113	1.93	9 (13%)
20	CLA	C	495	-	59,73,73	1.56	8 (13%)	67,113,113	2.07	15 (22%)
20	CLA	d	5354	4	59,73,73	1.26	8 (13%)	67,113,113	1.88	13 (19%)
20	CLA	c	5492	3	54,68,73	1.37	9 (16%)	61,107,113	2.10	12 (19%)
20	CLA	B	518	2	59,73,73	1.47	7 (11%)	67,113,113	2.07	11 (16%)
21	PHO	A	562	-	67,69,69	1.05	6 (8%)	85,99,99	1.49	14 (16%)
27	LMT	A	569	-	36,36,36	1.53	6 (16%)	47,47,47	1.07	1 (2%)
20	CLA	c	5497	-	59,73,73	1.36	8 (13%)	67,113,113	1.99	14 (20%)
27	LMT	M	5216	-	36,36,36	1.46	8 (22%)	47,47,47	0.91	2 (4%)
24	BCR	d	5357	-	41,41,41	1.97	8 (19%)	56,56,56	2.28	21 (37%)
20	CLA	a	5559	-	59,73,73	1.17	5 (8%)	67,113,113	1.86	10 (14%)
24	BCR	B	529	-	41,41,41	1.81	8 (19%)	56,56,56	2.17	20 (35%)
30	DGD	H	208	-	55,55,67	1.48	10 (18%)	69,69,81	1.53	8 (11%)
21	PHO	A	561	-	67,69,69	1.03	4 (5%)	85,99,99	1.44	14 (16%)
20	CLA	c	5503	3	44,58,73	1.93	9 (20%)	49,95,113	2.31	10 (20%)
20	CLA	c	5494	-	40,54,73	1.48	6 (15%)	44,90,113	2.29	11 (25%)
28	MGE	L	210	-	48,48,48	0.98	3 (6%)	56,56,56	1.17	4 (7%)
31	BCT	d	5353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	C	496	3	59,73,73	1.52	10 (16%)	67,113,113	2.01	14 (20%)
20	CLA	B	520	-	59,73,73	1.32	9 (15%)	67,113,113	1.91	14 (20%)
22	PQ9	A	564	-	30,30,45	0.87	1 (3%)	38,39,57	1.50	8 (21%)
20	CLA	C	494	-	40,54,73	1.58	6 (15%)	44,90,113	2.46	11 (25%)
22	PQ9	D	356	-	30,30,45	0.89	1 (3%)	38,39,57	1.67	9 (23%)
28	MGE	d	5360	-	41,41,48	1.20	6 (14%)	49,49,56	1.05	4 (8%)
24	BCR	b	5527	-	41,41,41	1.54	8 (19%)	56,56,56	1.95	14 (25%)
20	CLA	C	491	3	59,73,73	1.31	7 (11%)	67,113,113	1.83	9 (13%)
30	DGD	C	508	-	48,48,67	1.44	9 (18%)	62,62,81	1.70	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	b	5520	-	59,73,73	1.40	9 (15%)	67,113,113	1.90	13 (19%)
20	CLA	C	500	-	59,73,73	1.37	8 (13%)	67,113,113	1.91	12 (17%)
20	CLA	C	493	3	59,73,73	1.33	7 (11%)	67,113,113	2.03	14 (20%)
20	CLA	b	5514	2	59,73,73	1.47	6 (10%)	67,113,113	2.09	13 (19%)
32	HEM	V	552	16	27,50,50	1.99	9 (33%)	17,82,82	2.28	5 (29%)
24	BCR	T	5104	-	41,41,41	1.53	8 (19%)	56,56,56	2.26	22 (39%)
20	CLA	B	519	-	59,73,73	1.64	7 (11%)	67,113,113	1.95	13 (19%)
20	CLA	D	354	4	59,73,73	1.23	7 (11%)	67,113,113	1.83	12 (17%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.12	5 (8%)
26	SQD	A	5212	-	25,26,54	2.80	12 (48%)	34,37,65	2.72	11 (32%)
20	CLA	B	516	-	59,73,73	1.53	7 (11%)	67,113,113	2.05	12 (17%)
24	BCR	B	527	-	41,41,41	1.71	8 (19%)	56,56,56	2.03	16 (28%)
20	CLA	b	5512	2	59,73,73	1.26	7 (11%)	67,113,113	1.85	13 (19%)
20	CLA	B	513	2	59,73,73	1.37	8 (13%)	67,113,113	1.93	14 (20%)
24	BCR	c	5505	-	41,41,41	1.95	8 (19%)	56,56,56	2.09	18 (32%)
20	CLA	c	5499	-	41,55,73	1.65	10 (24%)	45,91,113	2.28	12 (26%)
30	DGD	h	5208	-	55,55,67	1.39	9 (16%)	69,69,81	1.55	9 (13%)
20	CLA	A	560	-	59,73,73	1.34	6 (10%)	67,113,113	1.97	14 (20%)
20	CLA	d	5355	-	44,58,73	1.76	8 (18%)	49,95,113	2.27	11 (22%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.47	6 (8%)
21	PHO	a	5561	-	67,69,69	1.04	5 (7%)	85,99,99	1.38	11 (12%)
27	LMT	m	216	-	36,36,36	1.46	7 (19%)	47,47,47	0.98	3 (6%)
20	CLA	B	525	-	59,73,73	1.34	7 (11%)	67,113,113	1.99	11 (16%)
20	CLA	c	5500	-	59,73,73	1.32	7 (11%)	67,113,113	1.92	14 (20%)
20	CLA	b	5518	2	59,73,73	1.50	6 (10%)	67,113,113	2.06	17 (25%)
22	PQ9	d	5356	-	30,30,45	0.81	0	38,39,57	1.66	6 (15%)
24	BCR	A	566	-	41,41,41	1.58	8 (19%)	56,56,56	2.09	21 (37%)
24	BCR	x	5130	-	41,41,41	1.95	10 (24%)	56,56,56	2.47	23 (41%)
26	SQD	L	5213	-	46,47,54	2.70	24 (52%)	55,58,65	2.44	13 (23%)
26	SQD	d	5358	-	53,54,54	2.44	27 (50%)	62,65,65	2.57	19 (30%)
20	CLA	B	524	2	50,64,73	1.57	5 (10%)	56,102,113	2.23	11 (19%)
20	CLA	B	515	-	59,73,73	1.31	9 (15%)	67,113,113	1.98	15 (22%)
32	HEM	f	5051	5,6	27,50,50	1.99	8 (29%)	17,82,82	2.64	8 (47%)
20	CLA	b	5525	-	59,73,73	1.28	6 (10%)	67,113,113	2.02	11 (16%)
24	BCR	b	5528	-	41,41,41	1.70	6 (14%)	56,56,56	2.00	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	C	502	-	45,59,73	1.93	11 (24%)	50,96,113	2.33	12 (24%)
24	BCR	C	505	-	41,41,41	1.92	9 (21%)	56,56,56	2.08	16 (28%)
20	CLA	a	5558	1	59,73,73	1.32	9 (15%)	67,113,113	1.78	12 (17%)
20	CLA	B	511	-	35,49,73	2.21	12 (34%)	38,84,113	2.34	10 (26%)
20	CLA	B	526	-	59,73,73	1.53	12 (20%)	67,113,113	2.01	13 (19%)
28	MGE	D	360	-	48,48,48	0.92	4 (8%)	56,56,56	1.11	4 (7%)
24	BCR	c	5504	-	41,41,41	2.12	6 (14%)	56,56,56	2.13	22 (39%)
20	CLA	b	5519	-	59,73,73	1.48	9 (15%)	67,113,113	1.96	13 (19%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.17	6 (10%)
28	MGE	I	201	-	48,48,48	1.10	5 (10%)	56,56,56	1.08	4 (7%)
20	CLA	b	5516	-	59,73,73	1.59	7 (11%)	67,113,113	2.09	12 (17%)
27	LMT	t	5217	-	36,36,36	1.45	5 (13%)	47,47,47	0.99	3 (6%)
24	BCR	a	5566	-	41,41,41	1.65	8 (19%)	56,56,56	2.09	22 (39%)
20	CLA	b	5513	2	59,73,73	1.31	8 (13%)	67,113,113	1.89	14 (20%)
30	DGD	C	507	-	54,54,67	1.36	8 (14%)	68,68,81	1.48	6 (8%)
20	CLA	c	5502	-	45,59,73	1.95	8 (17%)	50,96,113	2.33	12 (24%)
22	PQ9	a	5564	-	30,30,45	0.91	1 (3%)	38,39,57	1.46	8 (21%)
20	CLA	b	5523	-	59,73,73	1.23	7 (11%)	67,113,113	2.06	13 (19%)
20	CLA	a	5563	-	49,63,73	1.63	9 (18%)	55,101,113	1.97	11 (20%)
25	LHG	A	567	-	38,38,48	1.94	5 (13%)	41,44,54	1.50	4 (9%)
30	DGD	c	5509	-	58,58,67	1.35	9 (15%)	72,72,81	1.39	5 (6%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.02	3 (6%)
28	MGE	l	5210	-	48,48,48	0.89	3 (6%)	56,56,56	1.14	4 (7%)
26	SQD	a	212	-	25,26,54	3.06	14 (56%)	34,37,65	2.83	13 (38%)
30	DGD	c	5508	-	48,48,67	1.48	9 (18%)	62,62,81	1.74	11 (17%)
24	BCR	C	504	-	41,41,41	1.84	7 (17%)	56,56,56	2.16	22 (39%)
32	HEM	v	5552	16	27,50,50	2.17	8 (29%)	17,82,82	2.36	6 (35%)
20	CLA	b	5515	-	59,73,73	1.30	10 (16%)	67,113,113	1.95	15 (22%)
31	BCT	D	353	19	0,3,3	0.00	-	0,3,3	0.00	-
20	CLA	c	5493	3	59,73,73	1.48	7 (11%)	67,113,113	2.01	15 (22%)
24	BCR	h	5107	-	41,41,41	1.99	8 (19%)	56,56,56	2.24	25 (44%)
26	SQD	A	568	-	53,54,54	2.46	28 (52%)	62,65,65	2.61	19 (30%)
24	BCR	b	5529	-	41,41,41	1.69	8 (19%)	56,56,56	2.09	18 (32%)
20	CLA	B	523	-	59,73,73	1.29	6 (10%)	67,113,113	2.01	12 (17%)
20	CLA	c	5496	-	59,73,73	1.50	10 (16%)	67,113,113	1.96	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	b	5511	-	35,49,73	2.19	10 (28%)	38,84,113	2.42	10 (26%)
20	CLA	C	498	3	59,73,73	1.40	6 (10%)	67,113,113	1.97	11 (16%)
30	DGD	C	509	-	58,58,67	1.12	6 (10%)	72,72,81	1.40	6 (8%)
20	CLA	A	563	-	49,63,73	1.47	8 (16%)	55,101,113	2.08	15 (27%)
20	CLA	b	5521	2	59,73,73	1.27	6 (10%)	67,113,113	1.99	14 (20%)
24	BCR	B	528	-	41,41,41	1.88	6 (14%)	56,56,56	1.96	14 (25%)
24	BCR	H	107	-	41,41,41	2.09	7 (17%)	56,56,56	2.23	24 (42%)
20	CLA	A	559	-	59,73,73	1.17	6 (10%)	67,113,113	1.84	9 (13%)
20	CLA	A	558	1	59,73,73	1.29	6 (10%)	67,113,113	1.86	14 (20%)
32	HEM	F	51	5,6	27,50,50	2.00	8 (29%)	17,82,82	2.65	6 (35%)
20	CLA	B	517	-	59,73,73	1.56	6 (10%)	67,113,113	2.13	14 (20%)
26	SQD	t	213	-	46,47,54	2.70	23 (50%)	55,58,65	2.54	15 (27%)
20	CLA	a	5560	-	59,73,73	1.45	8 (13%)	67,113,113	1.97	12 (17%)
28	MGE	d	5361	-	48,48,48	1.04	4 (8%)	56,56,56	1.05	2 (3%)
20	CLA	C	501	3	59,73,73	1.64	8 (13%)	67,113,113	2.06	11 (16%)
24	BCR	C	506	-	41,41,41	1.73	9 (21%)	56,56,56	2.18	21 (37%)
24	BCR	c	5506	-	41,41,41	1.93	9 (21%)	56,56,56	2.10	20 (35%)
27	LMT	a	5568	-	36,36,36	1.45	6 (16%)	47,47,47	1.09	1 (2%)
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	0.97	3 (5%)
25	LHG	a	5567	-	38,38,48	1.98	5 (13%)	41,44,54	1.45	4 (9%)
20	CLA	D	355	-	44,58,73	1.77	8 (18%)	49,95,113	2.29	11 (22%)
24	BCR	D	357	-	41,41,41	1.92	9 (21%)	56,56,56	2.22	20 (35%)
20	CLA	C	499	-	41,55,73	1.66	9 (21%)	45,91,113	2.33	13 (28%)
23	OEC	A	565	1,3	0,0,13	0.00	-	-		
20	CLA	b	5524	2	50,64,73	1.46	6 (12%)	56,102,113	2.10	10 (17%)
24	BCR	X	130	-	41,41,41	1.91	10 (24%)	56,56,56	2.49	23 (41%)
20	CLA	c	5498	3	59,73,73	1.65	8 (13%)	67,113,113	2.01	10 (14%)
20	CLA	c	5491	3	59,73,73	1.51	8 (13%)	67,113,113	2.04	10 (14%)
23	OEC	a	5565	1,3	0,0,13	0.00	-	-		
20	CLA	B	521	2	59,73,73	1.34	9 (15%)	67,113,113	2.07	13 (19%)
20	CLA	C	492	3	54,68,73	1.42	10 (18%)	61,107,113	2.09	14 (22%)
20	CLA	c	5501	3	59,73,73	1.61	8 (13%)	67,113,113	2.05	10 (14%)
20	CLA	C	497	-	59,73,73	1.36	7 (11%)	67,113,113	2.12	12 (17%)
24	BCR	t	104	-	41,41,41	1.65	10 (24%)	56,56,56	2.22	22 (39%)
21	PHO	a	5562	-	67,69,69	1.06	6 (8%)	85,99,99	1.49	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	MGE	i	5201	-	48,48,48	1.25	8 (16%)	56,56,56	1.09	4 (7%)
20	CLA	B	514	2	59,73,73	1.47	7 (11%)	67,113,113	2.05	12 (17%)

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
20	CLA	b	5526	-	3/3/20/25	11/37/135/135	-
20	CLA	C	503	3	3/3/17/25	5/19/117/135	-
20	CLA	b	5517	-	3/3/20/25	14/37/135/135	-
20	CLA	B	512	2	3/3/20/25	14/37/135/135	-
20	CLA	c	5495	-	3/3/20/25	16/37/135/135	-
20	CLA	B	522	-	3/3/20/25	13/37/135/135	-
27	LMT	T	217	-	-	1/21/61/61	0/2/2/2
28	MGE	D	358	-	-	14/42/62/63	0/1/1/1
20	CLA	b	5522	-	3/3/20/25	12/37/135/135	-
20	CLA	C	495	-	3/3/20/25	16/37/135/135	-
20	CLA	d	5354	4	3/3/20/25	10/37/135/135	-
20	CLA	c	5492	3	3/3/19/25	10/31/129/135	-
20	CLA	B	518	2	3/3/20/25	15/37/135/135	-
21	PHO	A	562	-	-	10/53/103/103	0/5/6/6
27	LMT	A	569	-	-	1/21/61/61	0/2/2/2
20	CLA	c	5497	-	3/3/20/25	7/37/135/135	-
27	LMT	M	5216	-	-	2/21/61/61	0/2/2/2
24	BCR	d	5357	-	-	3/29/63/63	0/2/2/2
20	CLA	a	5559	-	3/3/20/25	17/37/135/135	-
24	BCR	B	529	-	-	4/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	c	5503	3	3/3/17/25	5/19/117/135	-
28	MGE	L	210	-	-	24/43/63/63	0/1/1/1
20	CLA	C	496	3	3/3/20/25	14/37/135/135	-
20	CLA	b	5524	2	3/3/18/25	9/27/125/135	-
22	PQ9	D	356	-	-	11/23/43/61	0/1/1/1
20	CLA	C	494	-	3/3/16/25	7/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PQ9	A	564	-	-	8/23/43/61	0/1/1/1
28	MGE	d	5360	-	-	18/36/56/63	0/1/1/1
30	DGD	C	508	-	3/3/13/13	14/36/76/95	0/2/2/2
20	CLA	C	491	3	3/3/20/25	8/37/135/135	-
24	BCR	b	5527	-	-	1/29/63/63	0/2/2/2
20	CLA	B	524	2	3/3/18/25	10/27/125/135	-
20	CLA	C	500	-	3/3/20/25	12/37/135/135	-
20	CLA	C	493	3	3/3/20/25	12/37/135/135	-
20	CLA	b	5514	2	3/3/20/25	12/37/135/135	-
32	HEM	V	552	16	-	0/6/54/54	-
24	BCR	b	5528	-	-	1/29/63/63	0/2/2/2
20	CLA	B	519	-	3/3/20/25	13/37/135/135	-
20	CLA	D	354	4	3/3/20/25	11/37/135/135	-
28	MGE	b	5530	-	-	21/43/63/63	0/1/1/1
26	SQD	A	5212	-	-	6/19/39/69	0/1/1/1
20	CLA	B	516	-	3/3/20/25	13/37/135/135	-
24	BCR	B	527	-	-	1/29/63/63	0/2/2/2
20	CLA	b	5512	2	3/3/20/25	13/37/135/135	-
20	CLA	B	513	2	3/3/20/25	11/37/135/135	-
24	BCR	c	5505	-	-	3/29/63/63	0/2/2/2
20	CLA	c	5499	-	3/3/16/25	7/16/114/135	-
30	DGD	h	5208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	A	560	-	3/3/20/25	10/37/135/135	-
20	CLA	d	5355	-	3/3/17/25	9/19/117/135	-
30	DGD	c	5507	-	3/3/13/13	20/42/82/95	0/2/2/2
21	PHO	a	5561	-	-	16/53/103/103	0/5/6/6
27	LMT	m	216	-	-	2/21/61/61	0/2/2/2
20	CLA	b	5521	2	3/3/20/25	8/37/135/135	-
20	CLA	c	5500	-	3/3/20/25	12/37/135/135	-
20	CLA	b	5518	2	3/3/20/25	14/37/135/135	-
22	PQ9	d	5356	-	-	11/23/43/61	0/1/1/1
24	BCR	A	566	-	-	4/29/63/63	0/2/2/2
24	BCR	x	5130	-	-	4/29/63/63	0/2/2/2
26	SQD	L	5213	-	-	20/42/62/69	0/1/1/1
26	SQD	d	5358	-	-	23/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	5520	-	3/3/20/25	15/37/135/135	-
20	CLA	B	515	-	3/3/20/25	18/37/135/135	-
32	HEM	f	5051	5,6	-	0/6/54/54	-
20	CLA	B	521	2	3/3/20/25	7/37/135/135	-
24	BCR	T	5104	-	-	4/29/63/63	0/2/2/2
20	CLA	C	502	-	3/3/17/25	9/21/119/135	-
24	BCR	C	505	-	-	3/29/63/63	0/2/2/2
20	CLA	a	5558	1	3/3/20/25	10/37/135/135	-
20	CLA	B	511	-	3/3/15/25	2/8/106/135	-
20	CLA	B	526	-	3/3/20/25	12/37/135/135	-
28	MGE	D	360	-	-	23/43/63/63	0/1/1/1
24	BCR	c	5504	-	-	5/29/63/63	0/2/2/2
20	CLA	b	5519	-	3/3/20/25	12/37/135/135	-
28	MGE	B	530	-	-	21/43/63/63	0/1/1/1
28	MGE	I	201	-	-	23/43/63/63	0/1/1/1
20	CLA	b	5516	-	3/3/20/25	14/37/135/135	-
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2
24	BCR	a	5566	-	-	4/29/63/63	0/2/2/2
20	CLA	b	5513	2	3/3/20/25	10/37/135/135	-
24	BCR	t	104	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5502	-	3/3/17/25	9/21/119/135	-
22	PQ9	a	5564	-	-	8/23/43/61	0/1/1/1
20	CLA	b	5523	-	3/3/20/25	15/37/135/135	-
20	CLA	a	5563	-	3/3/18/25	5/25/123/135	-
25	LHG	A	567	-	-	17/43/43/53	-
30	DGD	c	5509	-	3/3/13/13	19/46/86/95	0/2/2/2
28	MGE	D	359	-	-	18/36/56/63	0/1/1/1
28	MGE	l	5210	-	-	24/43/63/63	0/1/1/1
26	SQD	a	212	-	-	6/19/39/69	0/1/1/1
30	DGD	c	5508	-	3/3/13/13	16/36/76/95	0/2/2/2
24	BCR	C	504	-	-	5/29/63/63	0/2/2/2
32	HEM	v	5552	16	-	0/6/54/54	-
20	CLA	b	5515	-	3/3/20/25	18/37/135/135	-
20	CLA	c	5494	-	3/3/16/25	7/15/113/135	-
20	CLA	c	5493	3	3/3/20/25	12/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	h	5107	-	-	4/29/63/63	0/2/2/2
26	SQD	A	568	-	-	23/49/69/69	0/1/1/1
24	BCR	b	5529	-	-	3/29/63/63	0/2/2/2
20	CLA	B	523	-	3/3/20/25	16/37/135/135	-
20	CLA	c	5496	-	3/3/20/25	14/37/135/135	-
20	CLA	b	5511	-	3/3/15/25	2/8/106/135	-
20	CLA	C	498	3	3/3/20/25	20/37/135/135	-
30	DGD	C	509	-	3/3/13/13	20/46/86/95	0/2/2/2
20	CLA	A	563	-	3/3/18/25	5/25/123/135	-
20	CLA	B	525	-	3/3/20/25	13/37/135/135	-
24	BCR	B	528	-	-	2/29/63/63	0/2/2/2
24	BCR	H	107	-	-	4/29/63/63	0/2/2/2
20	CLA	A	559	-	3/3/20/25	17/37/135/135	-
20	CLA	A	558	1	3/3/20/25	8/37/135/135	-
32	HEM	F	51	5,6	-	0/6/54/54	-
20	CLA	B	517	-	3/3/20/25	14/37/135/135	-
26	SQD	t	213	-	-	19/42/62/69	0/1/1/1
20	CLA	a	5560	-	3/3/20/25	10/37/135/135	-
28	MGE	d	5361	-	-	23/43/63/63	0/1/1/1
20	CLA	C	501	3	3/3/20/25	14/37/135/135	-
24	BCR	C	506	-	-	4/29/63/63	0/2/2/2
24	BCR	c	5506	-	-	4/29/63/63	0/2/2/2
27	LMT	a	5568	-	-	3/21/61/61	0/2/2/2
28	MGE	d	5359	-	-	14/42/62/63	0/1/1/1
25	LHG	a	5567	-	-	16/43/43/53	-
20	CLA	D	355	-	3/3/17/25	9/19/117/135	-
24	BCR	D	357	-	-	3/29/63/63	0/2/2/2
20	CLA	C	499	-	3/3/16/25	7/16/114/135	-
21	PHO	A	561	-	-	16/53/103/103	0/5/6/6
20	CLA	B	520	-	3/3/20/25	18/37/135/135	-
24	BCR	X	130	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5498	3	3/3/20/25	19/37/135/135	-
20	CLA	c	5491	3	3/3/20/25	7/37/135/135	-
23	OEC	a	5565	1,3	-	-	0/1/0/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	5525	-	3/3/20/25	14/37/135/135	-
20	CLA	C	492	3	3/3/19/25	10/31/129/135	-
20	CLA	c	5501	3	3/3/20/25	13/37/135/135	-
20	CLA	C	497	-	3/3/20/25	7/37/135/135	-
30	DGD	C	507	-	3/3/13/13	20/42/82/95	0/2/2/2
21	PHO	a	5562	-	-	10/53/103/103	0/5/6/6
28	MGE	i	5201	-	-	22/43/63/63	0/1/1/1
20	CLA	B	514	2	3/3/20/25	12/37/135/135	-

The worst 5 of 1085 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5495	CLA	MG-NA	8.38	2.26	2.06
26	A	568	SQD	C4-C3	8.18	1.73	1.52
26	t	213	SQD	C4-C3	8.14	1.73	1.52
20	B	517	CLA	MG-NA	8.14	2.25	2.06
26	a	212	SQD	C4-C3	8.11	1.73	1.52

The worst 5 of 1635 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	c	5501	CLA	C4A-NA-C1A	13.09	112.59	106.71
20	b	5514	CLA	C4A-NA-C1A	13.03	112.56	106.71
20	C	501	CLA	C4A-NA-C1A	12.97	112.54	106.71
20	B	514	CLA	C4A-NA-C1A	12.87	112.49	106.71
20	B	524	CLA	C4A-NA-C1A	12.65	112.39	106.71

5 of 234 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	b	5526	CLA	NC
20	b	5526	CLA	ND
20	b	5526	CLA	NA
20	C	503	CLA	NC
20	C	503	CLA	ND

5 of 1497 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	b	5526	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	b	5526	CLA	C1-C2-C3-C4
20	b	5526	CLA	C1-C2-C3-C5
20	C	503	CLA	C1A-C2A-CAA-CBA
20	C	503	CLA	C1-C2-C3-C4

There are no ring outliers.

63 monomers are involved in 246 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	522	CLA	4	0
20	C	503	CLA	1	0
20	B	512	CLA	2	0
27	T	217	LMT	3	0
28	D	358	MGE	2	0
20	C	495	CLA	9	0
20	B	518	CLA	11	0
21	A	562	PHO	5	0
24	B	529	BCR	2	0
30	H	208	DGD	3	0
21	A	561	PHO	7	0
28	L	210	MGE	2	0
20	C	496	CLA	2	0
20	B	520	CLA	6	0
22	A	564	PQ9	2	0
20	C	494	CLA	2	0
22	D	356	PQ9	7	0
20	C	491	CLA	4	0
30	C	508	DGD	2	0
20	C	500	CLA	3	0
20	C	493	CLA	7	0
32	V	552	HEM	2	0
24	T	5104	BCR	5	0
20	B	519	CLA	5	0
20	D	354	CLA	5	0
20	B	516	CLA	6	0
24	B	527	BCR	2	0
20	B	513	CLA	8	0
20	A	560	CLA	1	0
20	B	525	CLA	4	0
24	A	566	BCR	1	0
20	B	524	CLA	4	0
20	B	515	CLA	12	0

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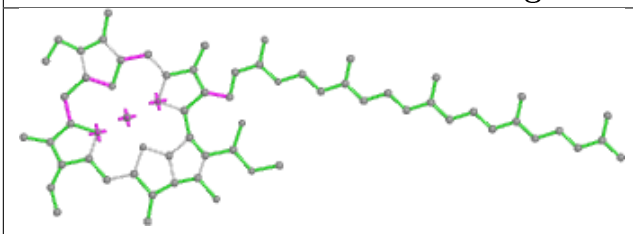
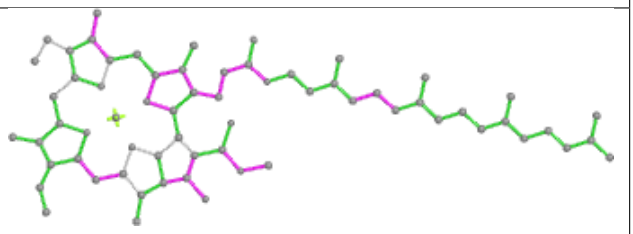
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	502	CLA	2	0
24	C	505	BCR	6	0
20	B	511	CLA	1	0
20	B	526	CLA	2	0
28	D	360	MGE	7	0
28	B	530	MGE	1	0
28	I	201	MGE	1	0
30	C	507	DGD	6	0
25	A	567	LHG	4	0
28	D	359	MGE	1	0
24	C	504	BCR	7	0
20	B	523	CLA	2	0
20	C	498	CLA	6	0
30	C	509	DGD	10	0
24	B	528	BCR	2	0
24	H	107	BCR	3	0
20	A	559	CLA	5	0
20	A	558	CLA	10	0
32	F	51	HEM	3	0
20	B	517	CLA	9	0
20	C	501	CLA	13	0
24	C	506	BCR	7	0
20	D	355	CLA	3	0
24	D	357	BCR	4	0
20	C	499	CLA	2	0
24	X	130	BCR	9	0
20	B	521	CLA	2	0
20	C	492	CLA	2	0
20	C	497	CLA	5	0
20	B	514	CLA	5	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.

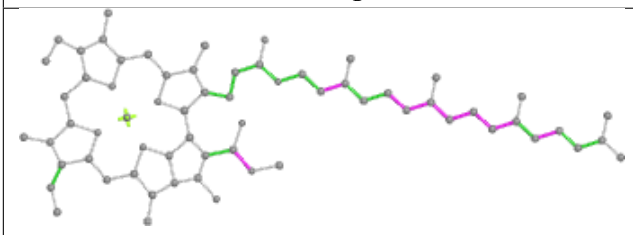
Ligand CLA B 522



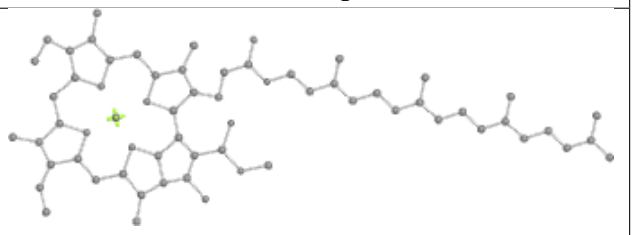
Bond lengths



Bond angles

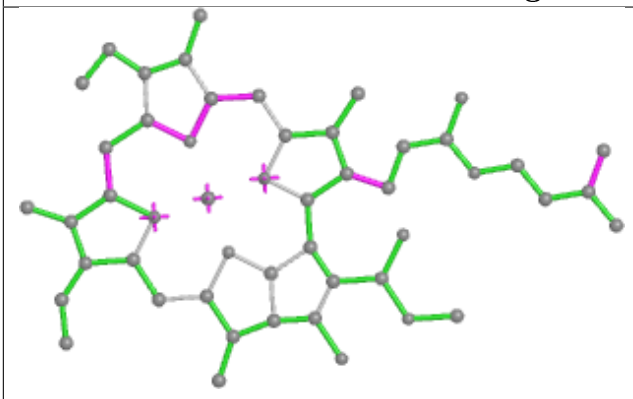


Torsions

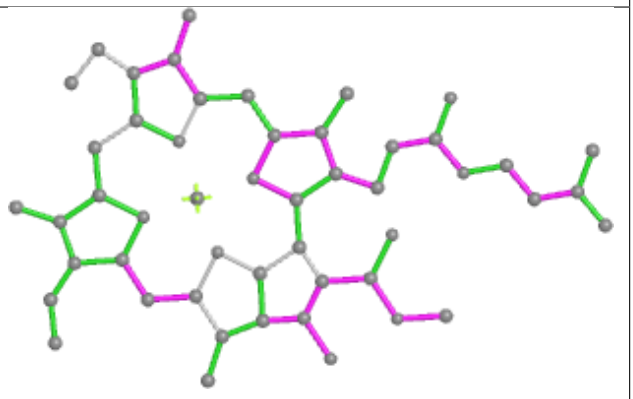


Rings

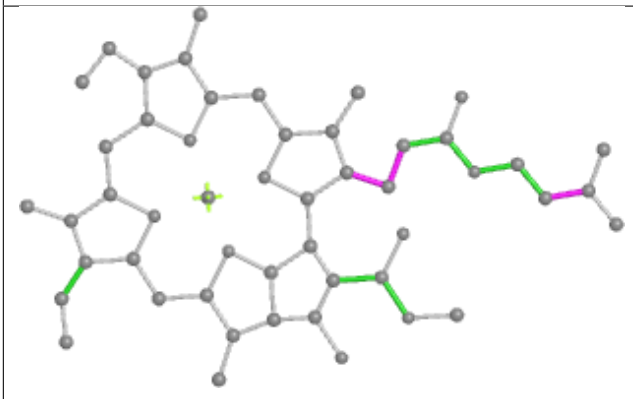
Ligand CLA C 503



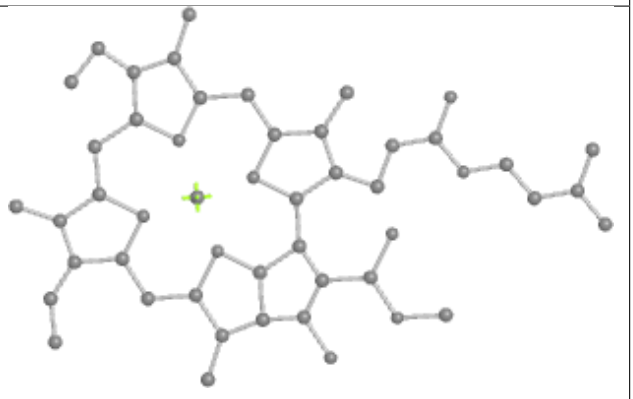
Bond lengths



Bond angles

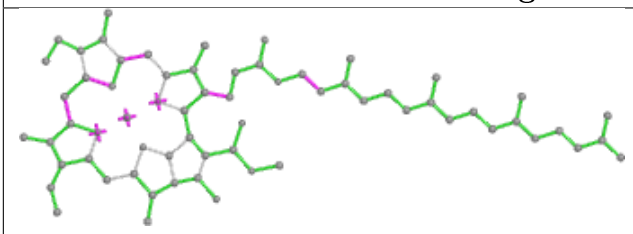


Torsions

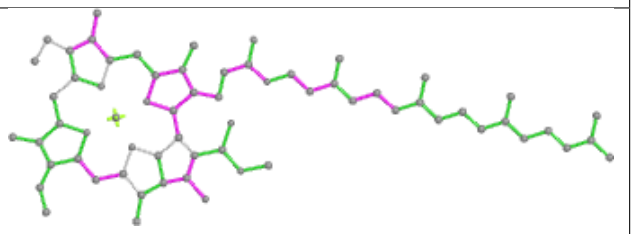


Rings

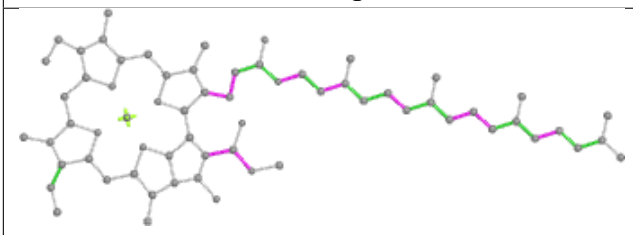
Ligand CLA b 5517



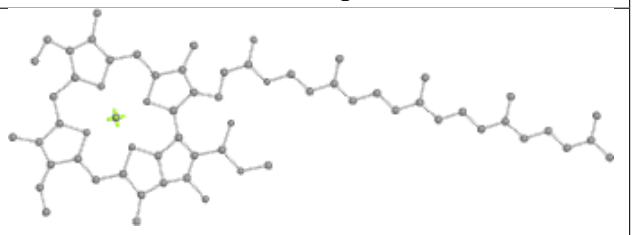
Bond lengths



Bond angles

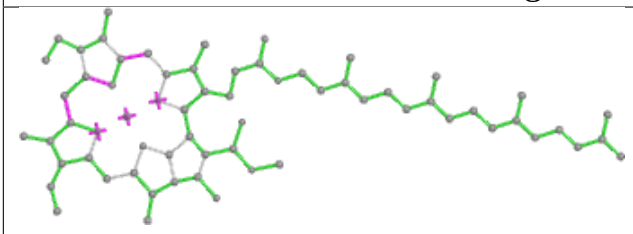


Torsions

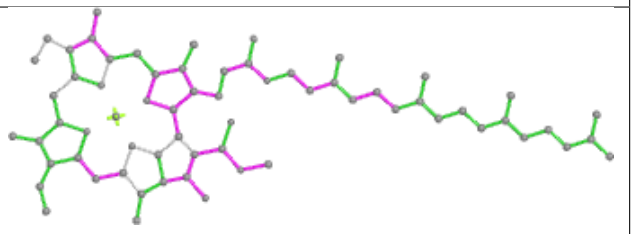


Rings

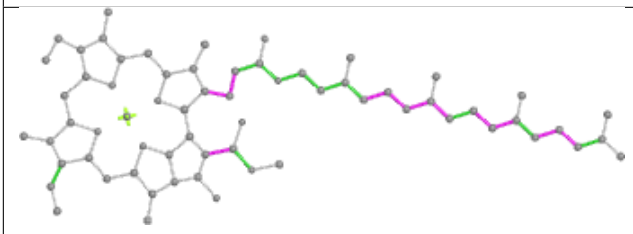
Ligand CLA B 512



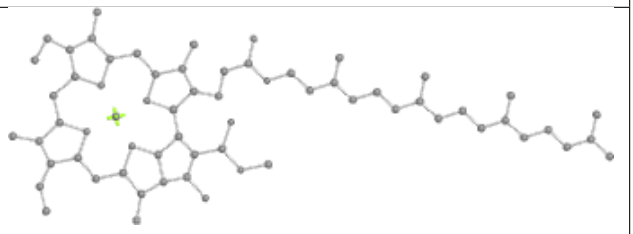
Bond lengths



Bond angles

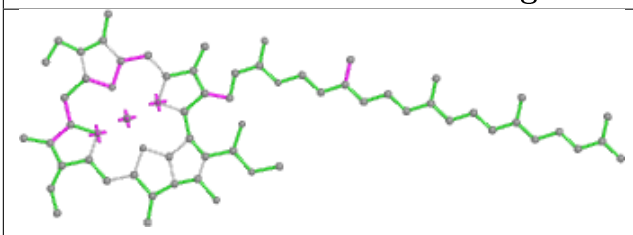


Torsions

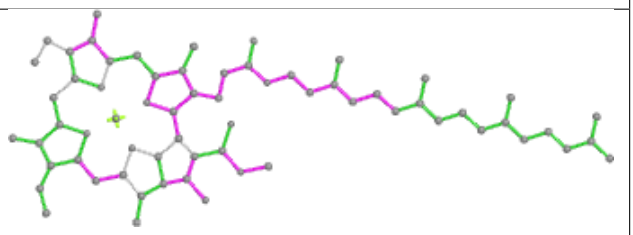


Rings

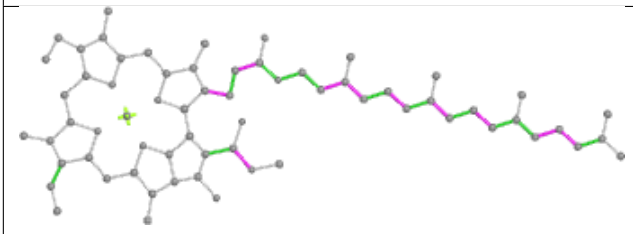
Ligand CLA c 5495



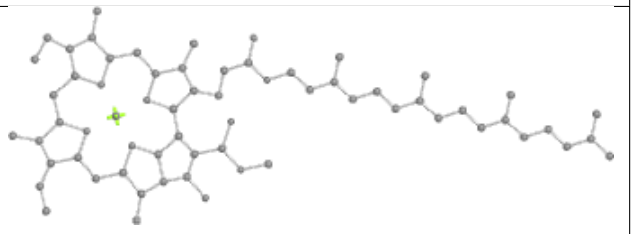
Bond lengths



Bond angles

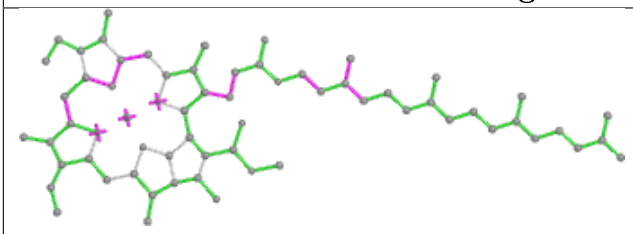


Torsions

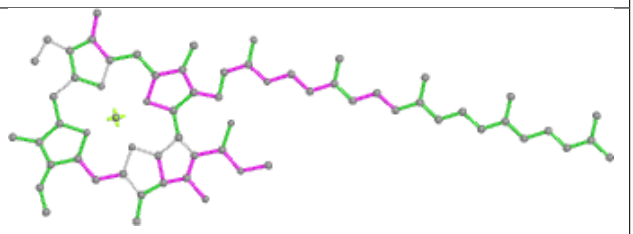


Rings

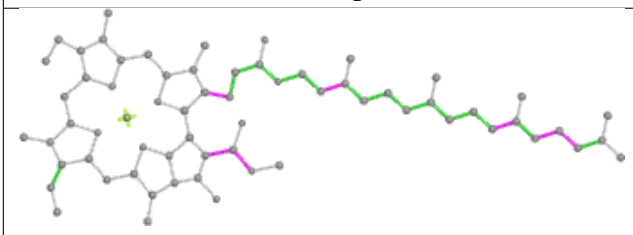
Ligand CLA b 5526



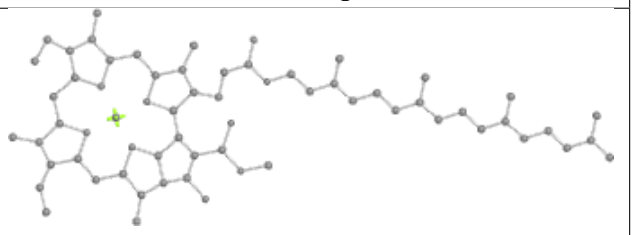
Bond lengths



Bond angles

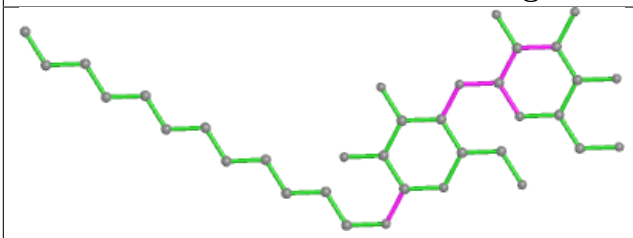


Torsions

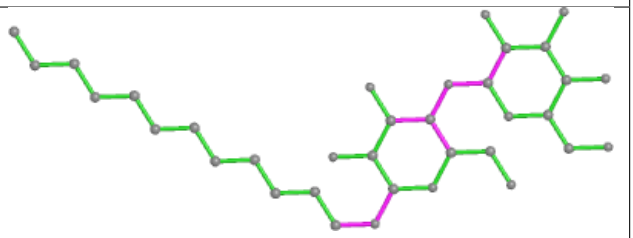


Rings

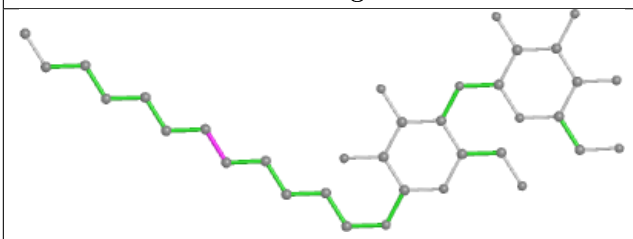
Ligand LMT T 217



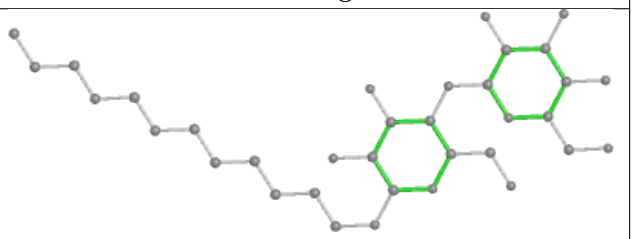
Bond lengths



Bond angles

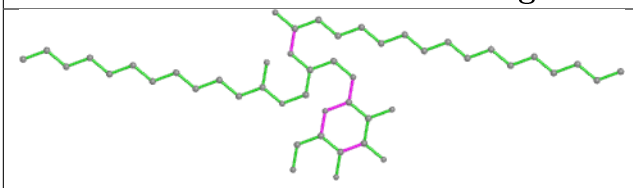


Torsions

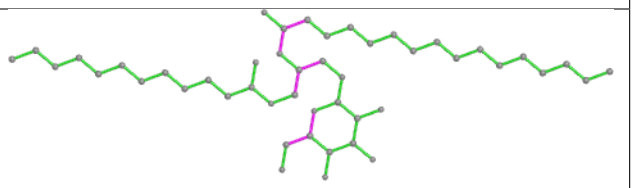


Rings

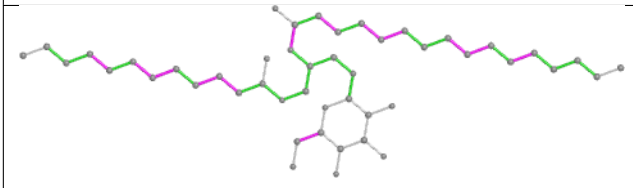
Ligand MGE D 358



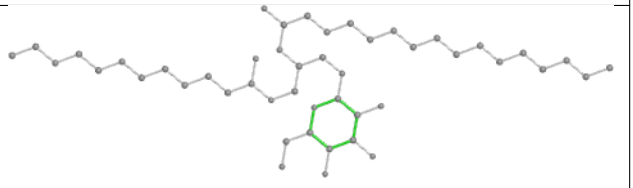
Bond lengths



Bond angles

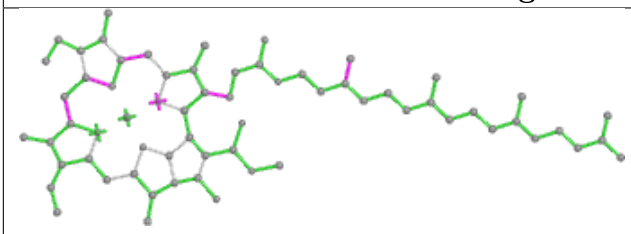


Torsions

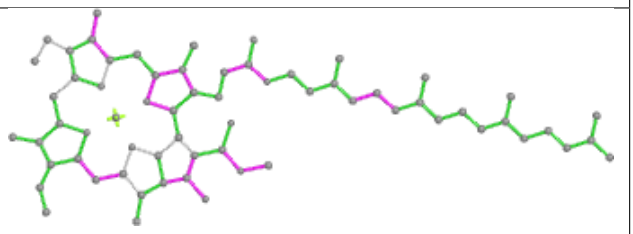


Rings

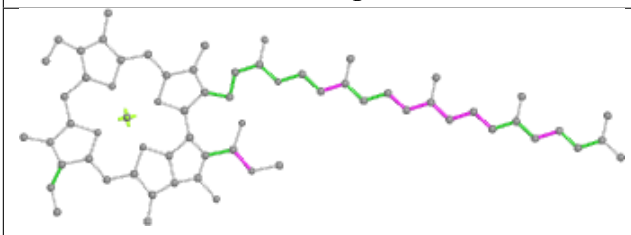
Ligand CLA b 5522



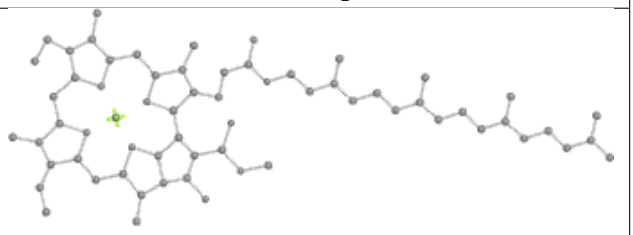
Bond lengths



Bond angles

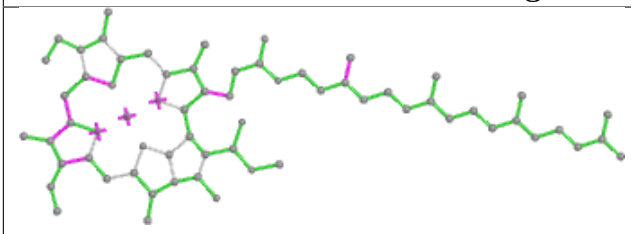


Torsions

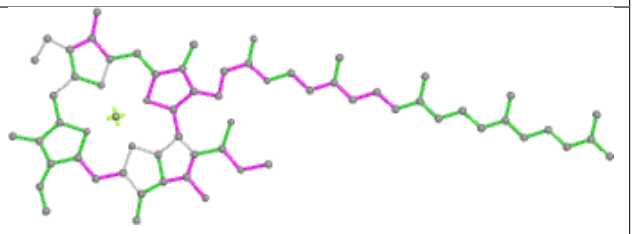


Rings

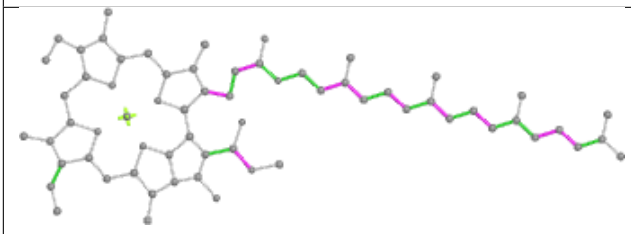
Ligand CLA C 495



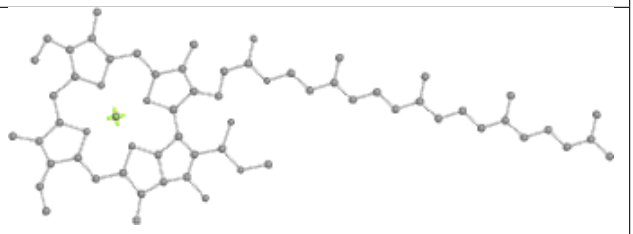
Bond lengths



Bond angles

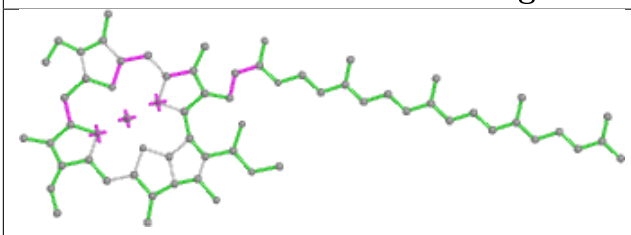


Torsions

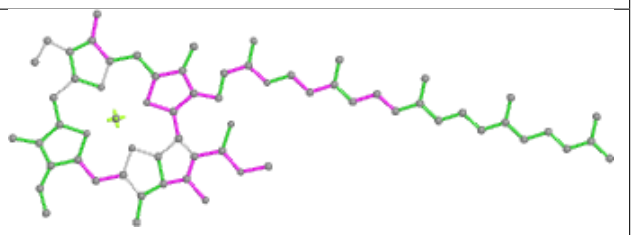


Rings

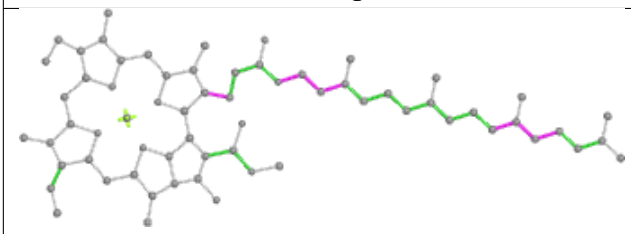
Ligand CLA d 5354



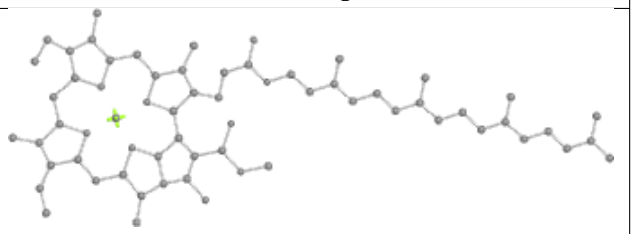
Bond lengths



Bond angles

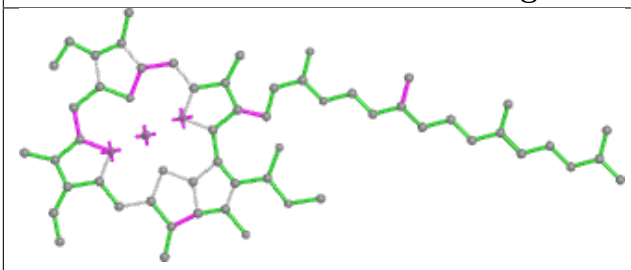


Torsions

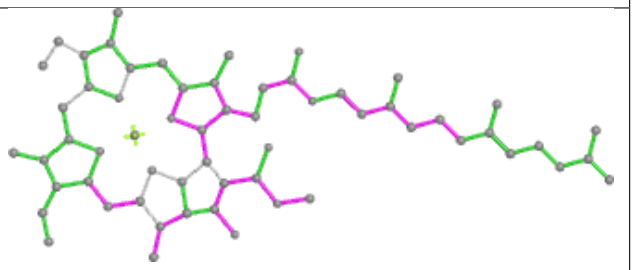


Rings

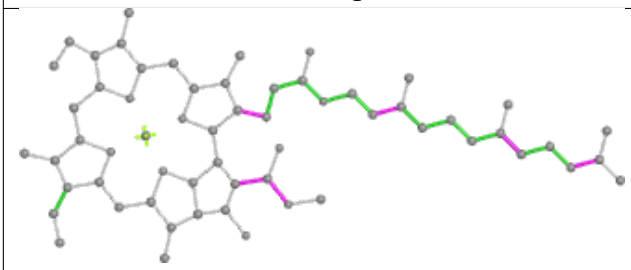
Ligand CLA c 5492



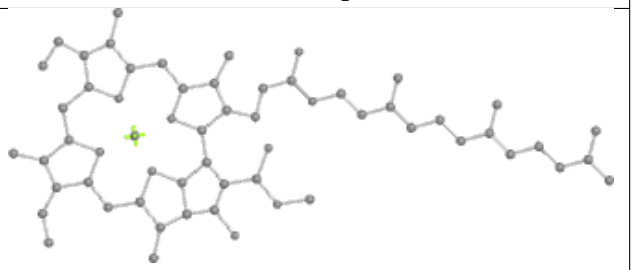
Bond lengths



Bond angles

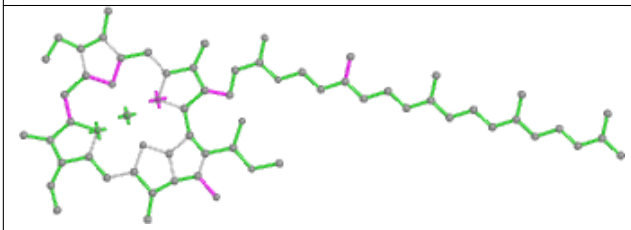


Torsions

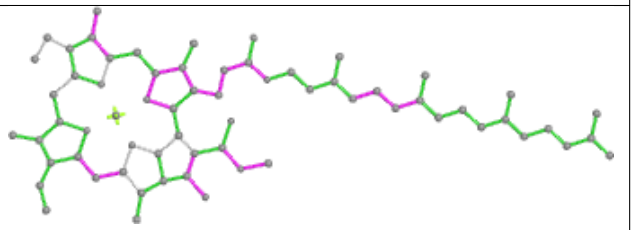


Rings

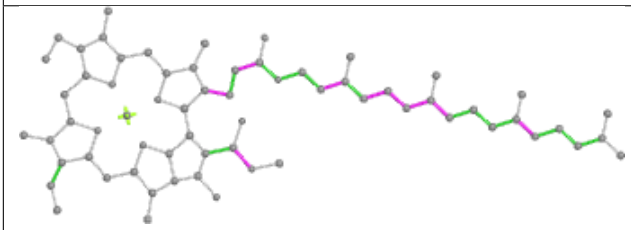
Ligand CLA B 518



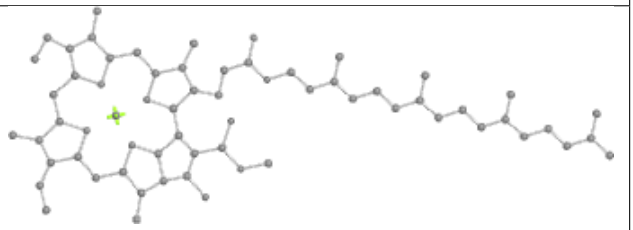
Bond lengths



Bond angles

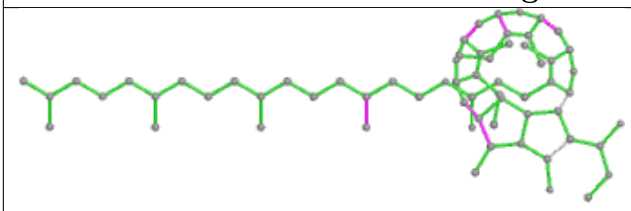


Torsions

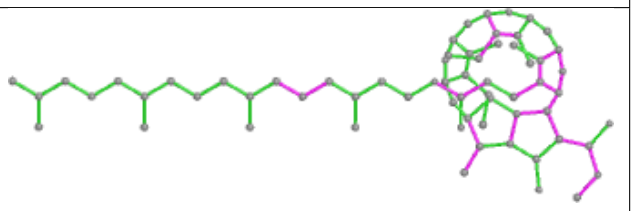


Rings

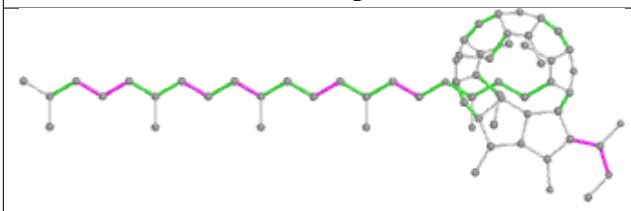
Ligand PHO A 562



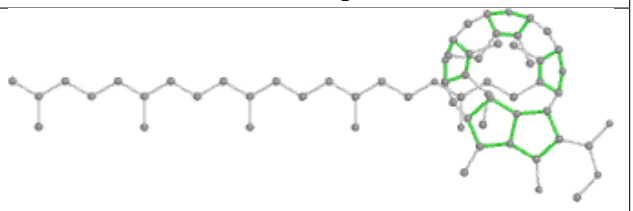
Bond lengths



Bond angles

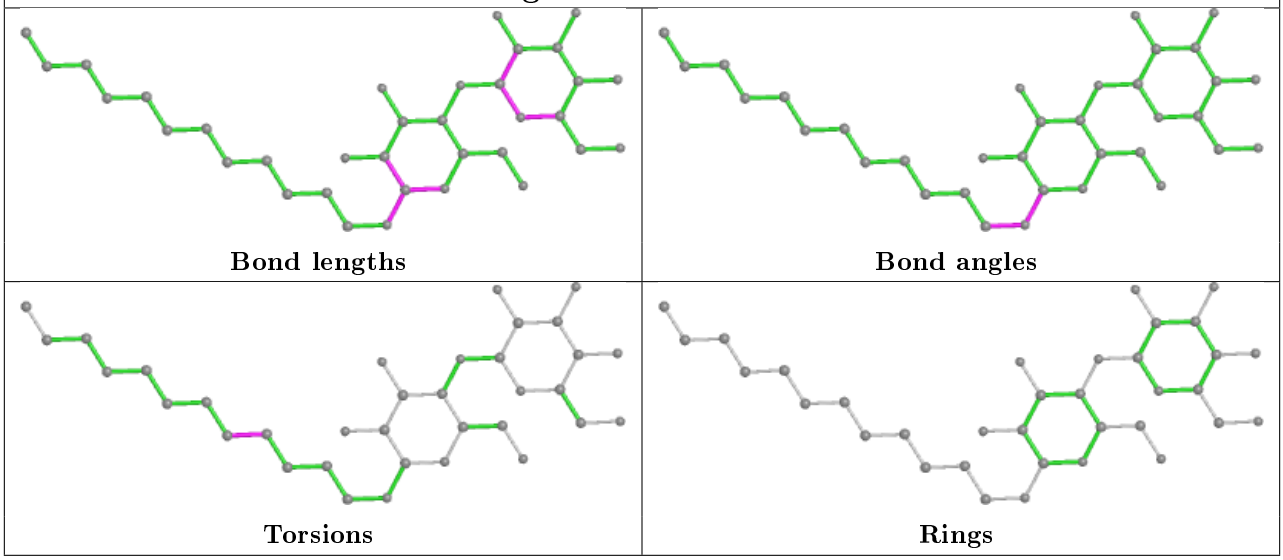


Torsions

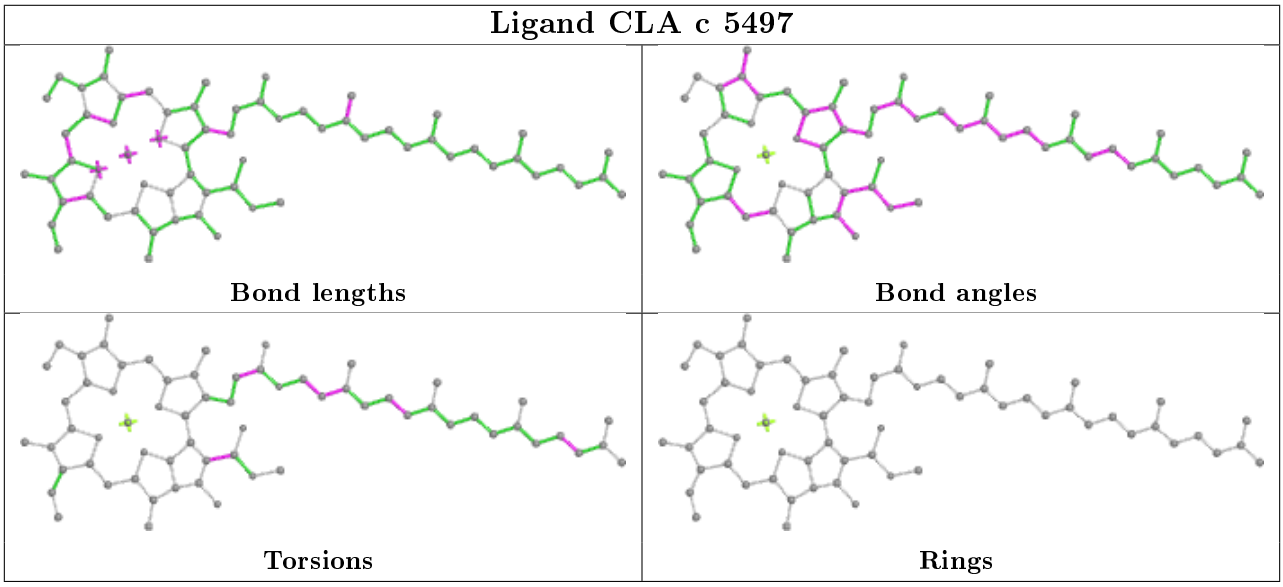


Rings

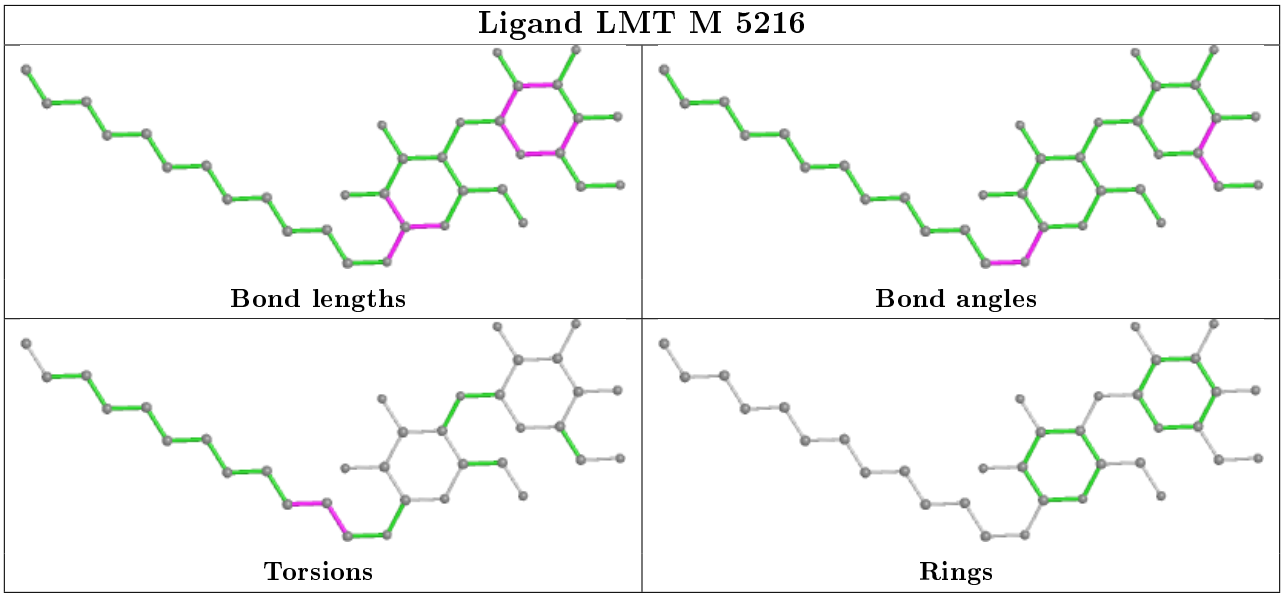
Ligand LMT A 569



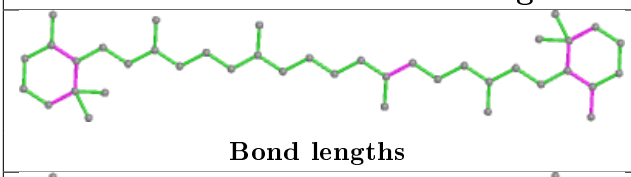
Ligand CLA c 5497

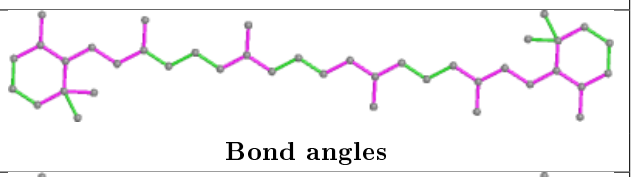


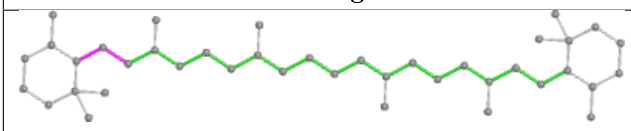
Ligand LMT M 5216

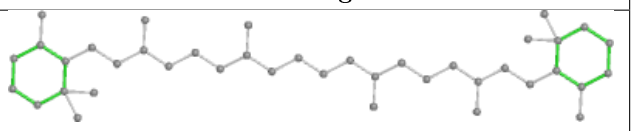


Ligand BCR d 5357

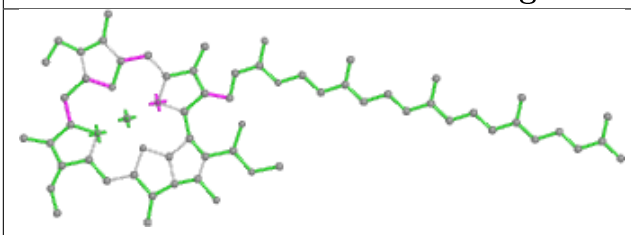

Bond lengths

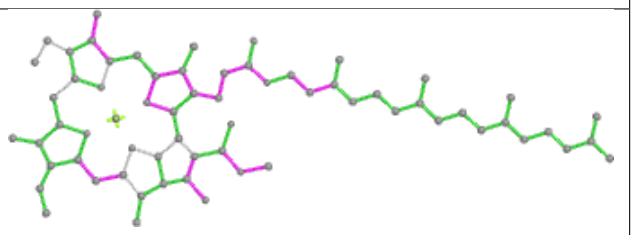

Bond angles

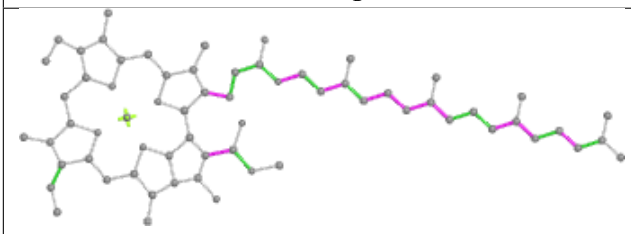

Torsions

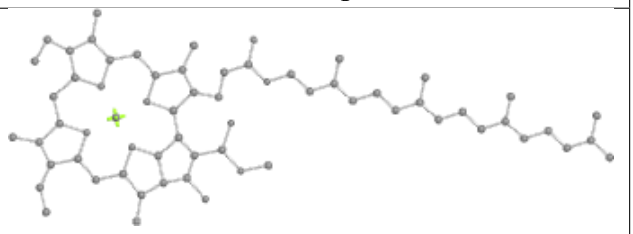

Rings

Ligand CLA a 5559

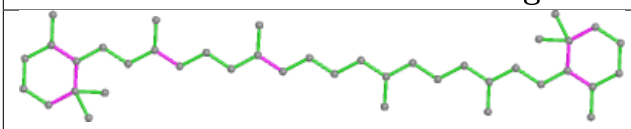

Bond lengths

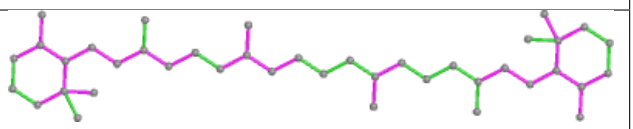

Bond angles

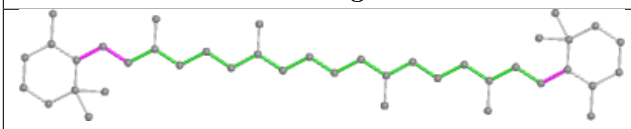

Torsions

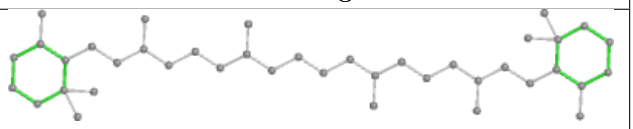

Rings

Ligand BCR B 529

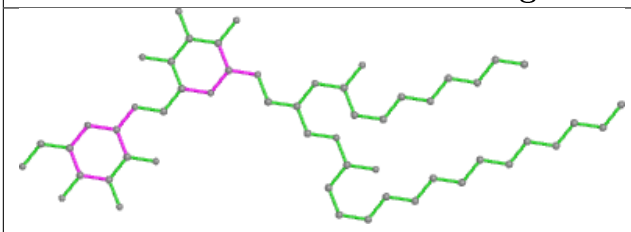

Bond lengths


Bond angles

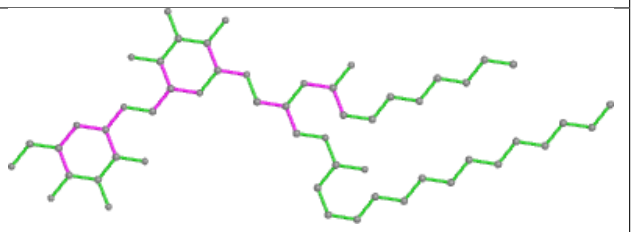

Torsions


Rings

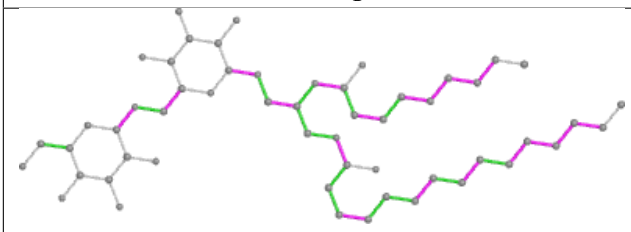
Ligand DGD H 208



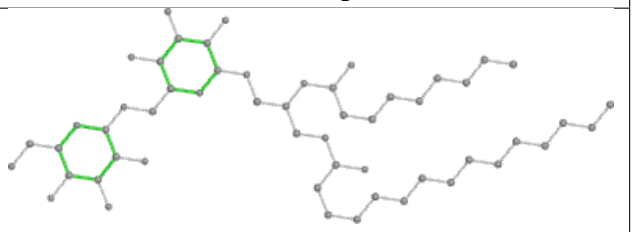
Bond lengths



Bond angles

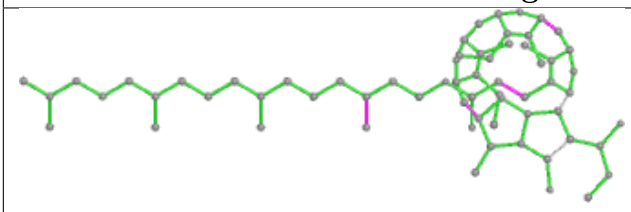


Torsions

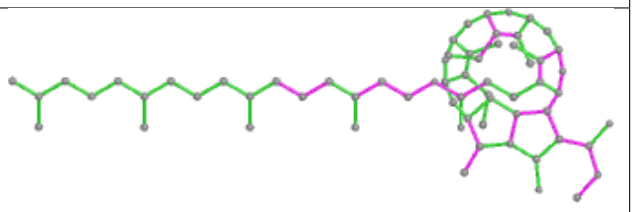


Rings

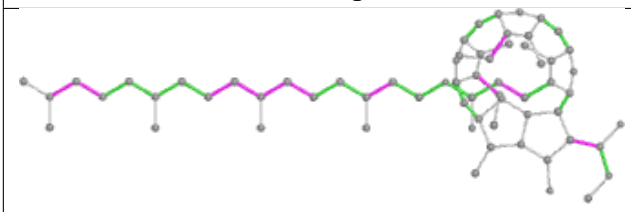
Ligand PHO A 561



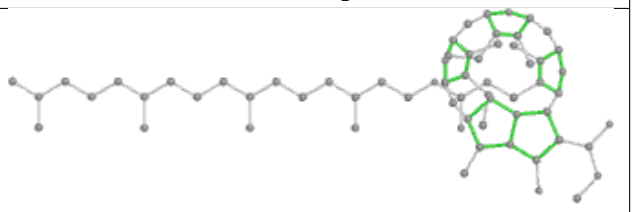
Bond lengths



Bond angles

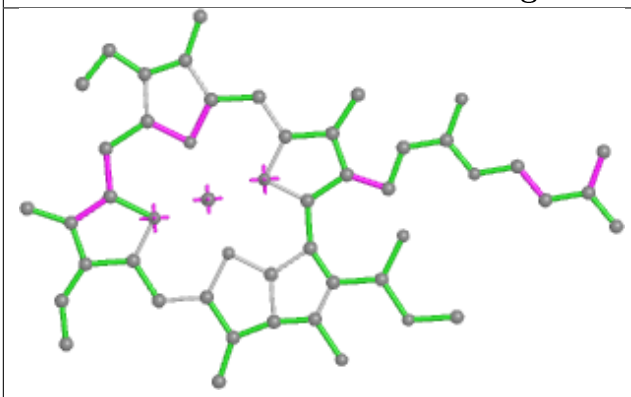


Torsions

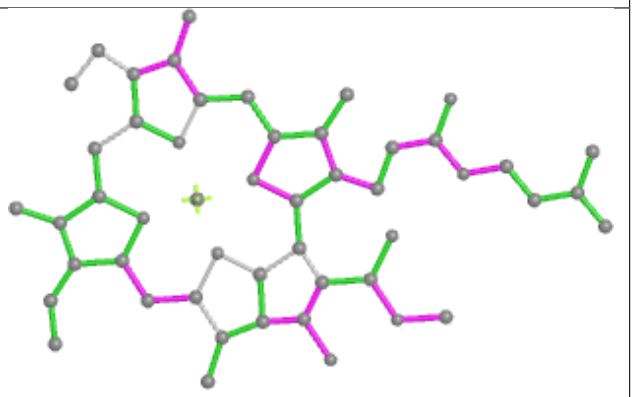


Rings

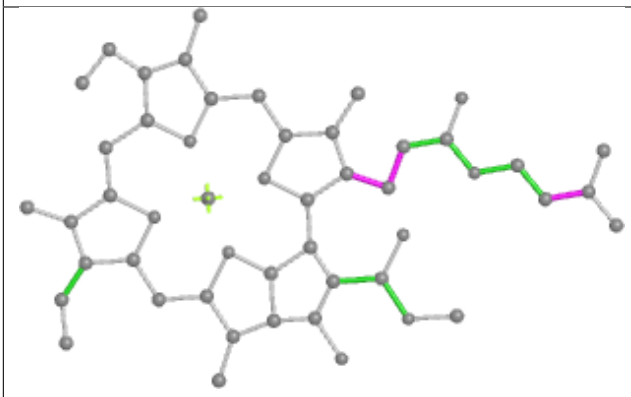
Ligand CLA c 5503



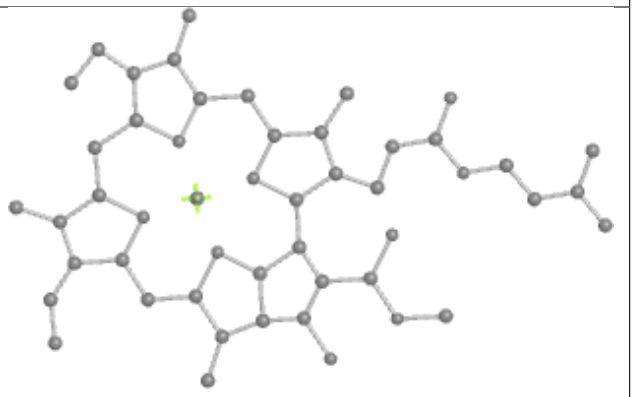
Bond lengths



Bond angles

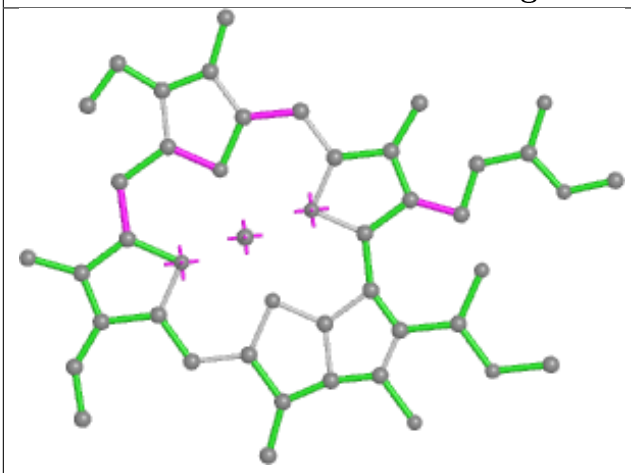


Torsions

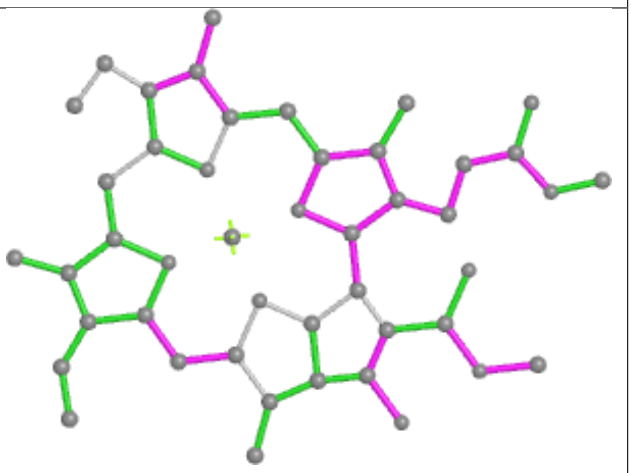


Rings

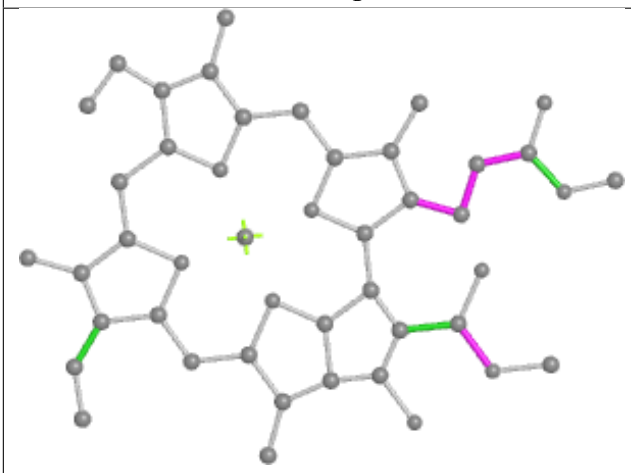
Ligand CLA c 5494



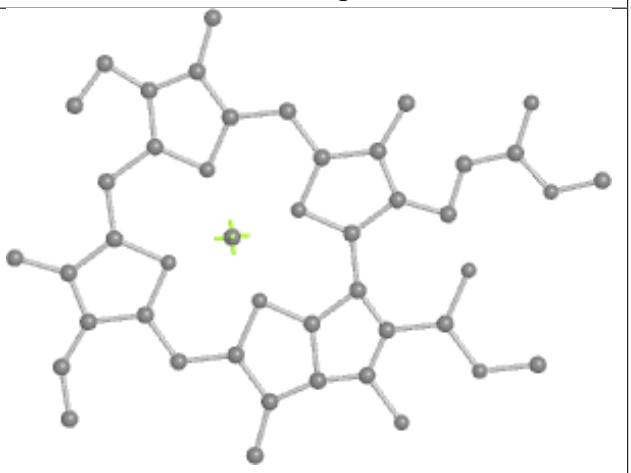
Bond lengths



Bond angles

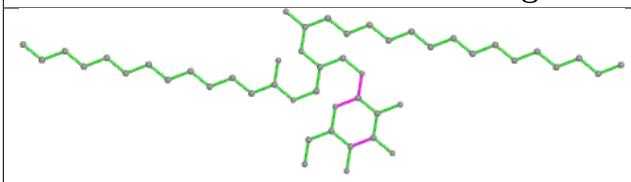


Torsions

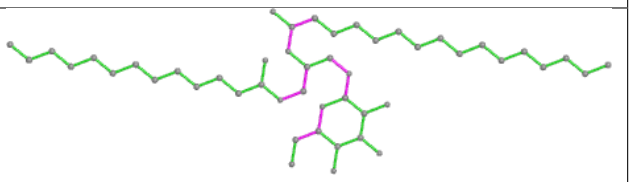


Rings

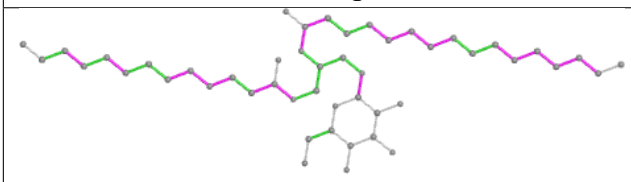
Ligand MGE L 210



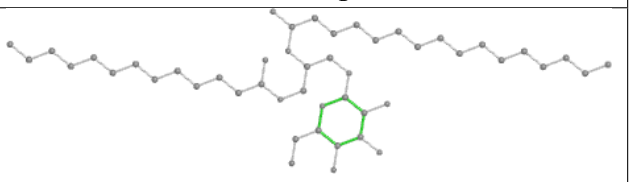
Bond lengths



Bond angles

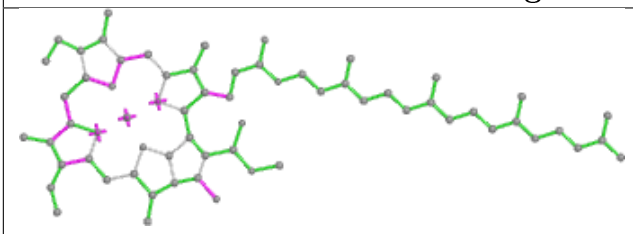


Torsions

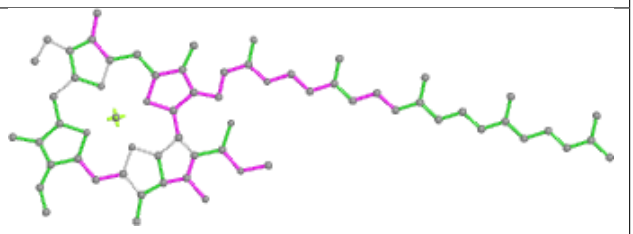


Rings

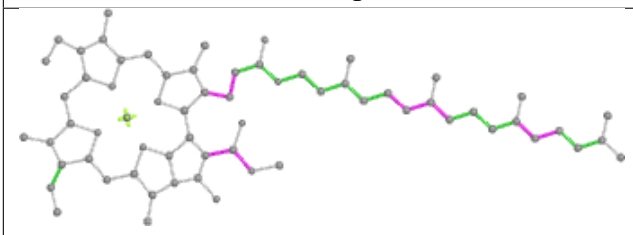
Ligand CLA C 496



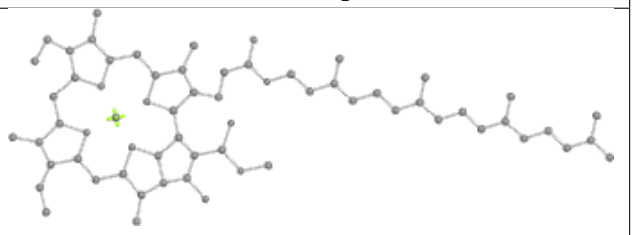
Bond lengths



Bond angles

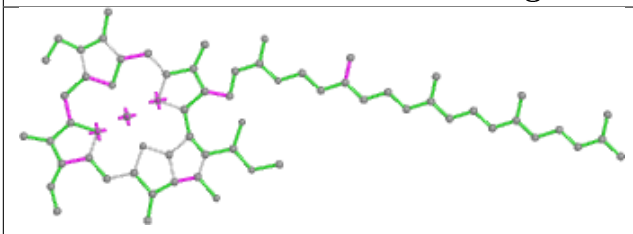


Torsions

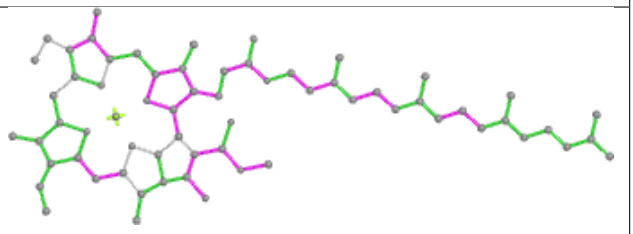


Rings

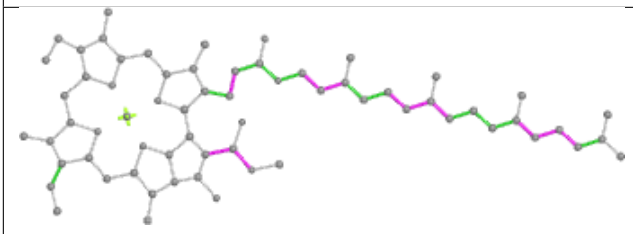
Ligand CLA B 520



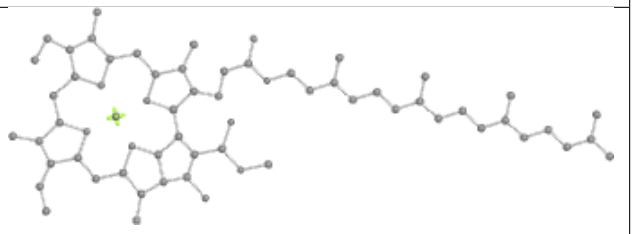
Bond lengths



Bond angles

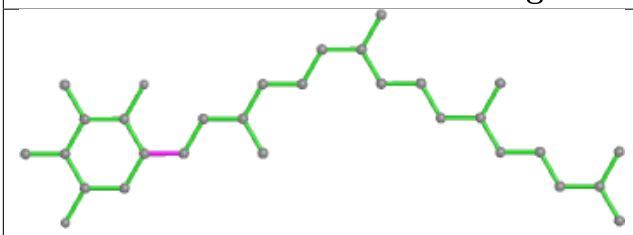


Torsions

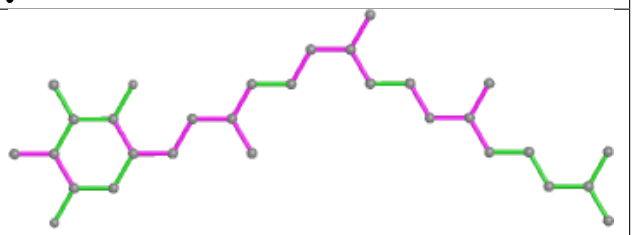


Rings

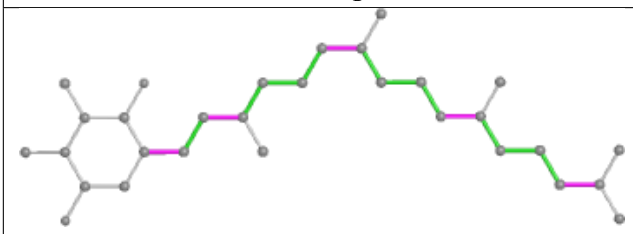
Ligand PQ9 A 564



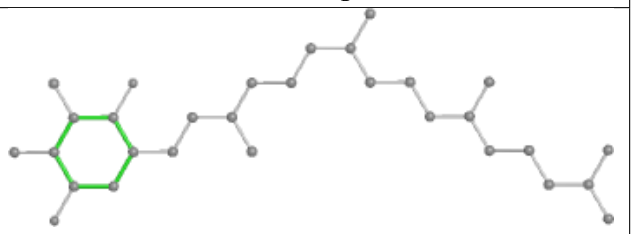
Bond lengths



Bond angles

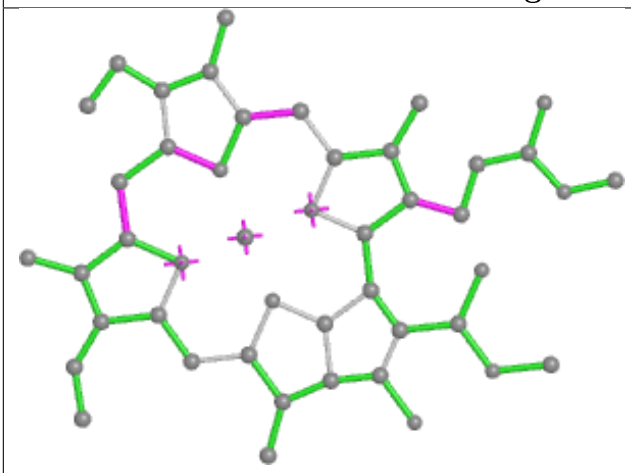


Torsions

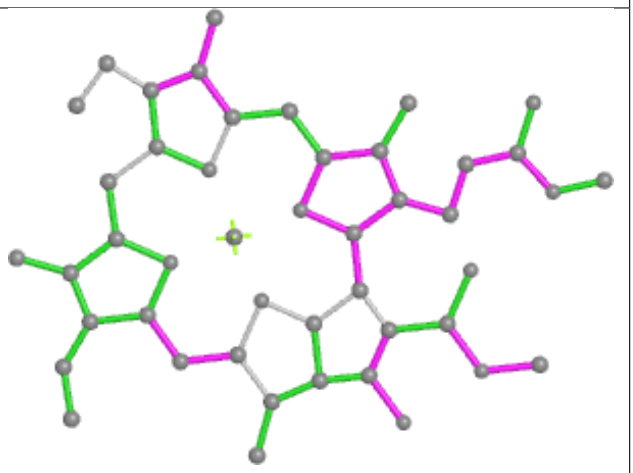


Rings

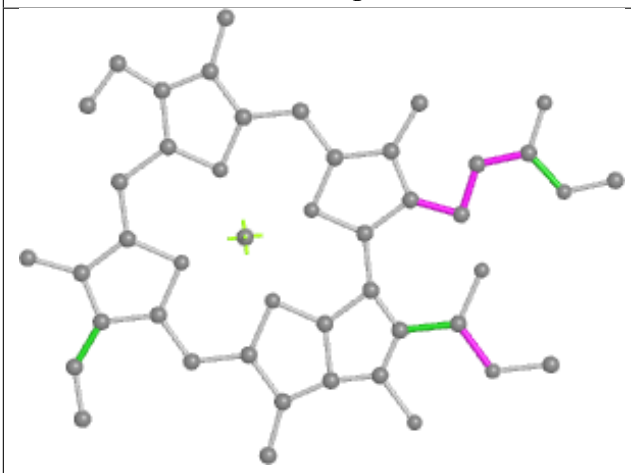
Ligand CLA C 494



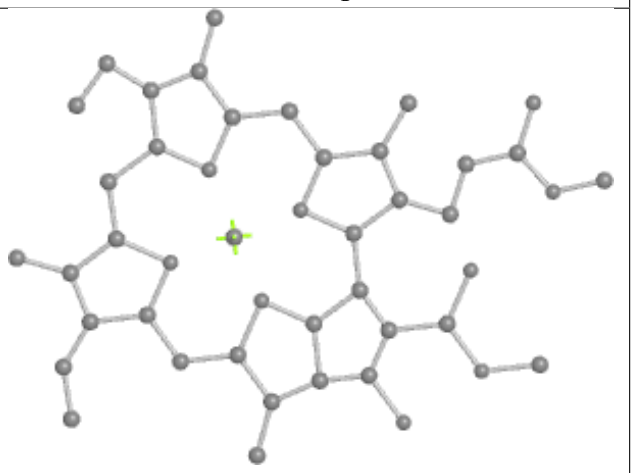
Bond lengths



Bond angles

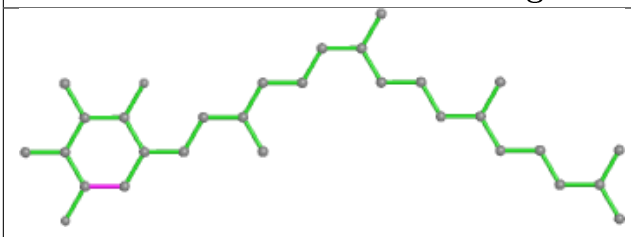


Torsions

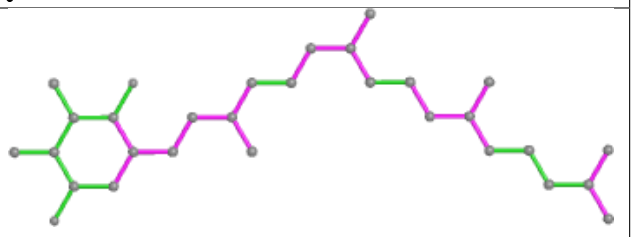


Rings

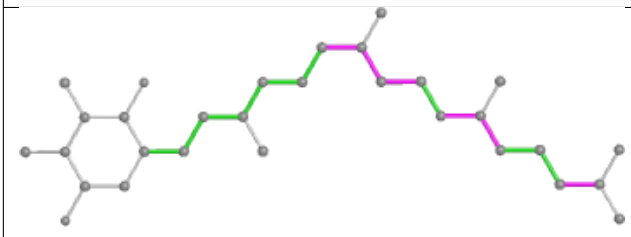
Ligand PQ9 D 356



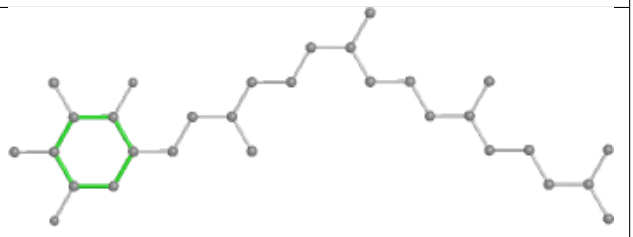
Bond lengths



Bond angles

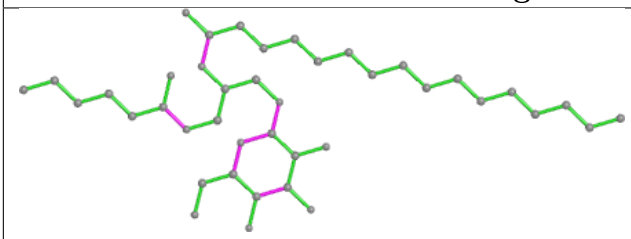


Torsions

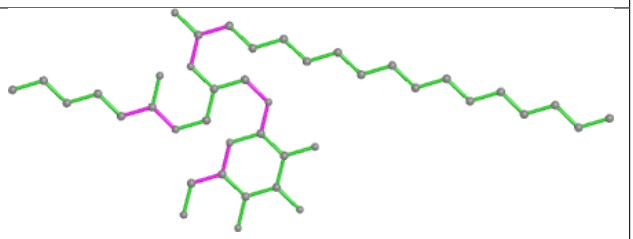


Rings

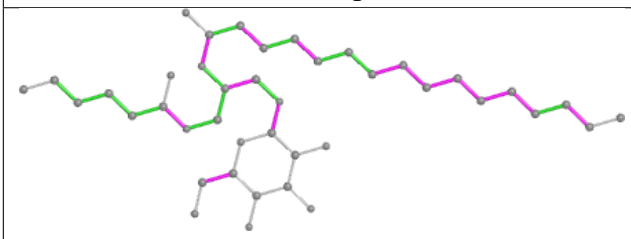
Ligand MGE d 5360



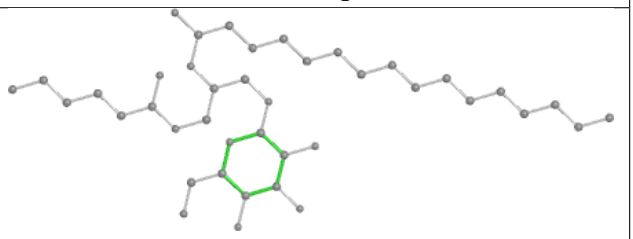
Bond lengths



Bond angles

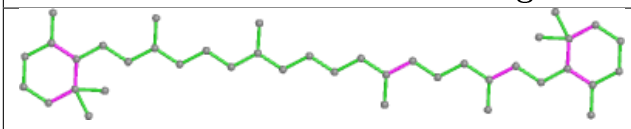


Torsions

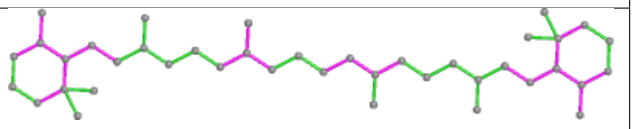


Rings

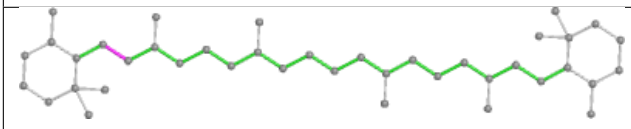
Ligand BCR b 5527



Bond lengths



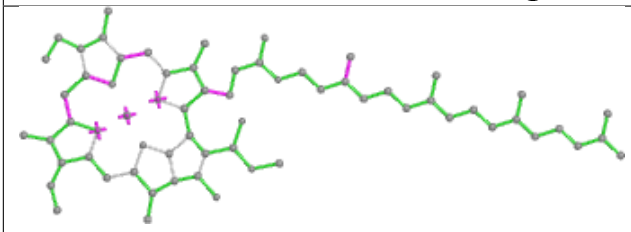
Bond angles



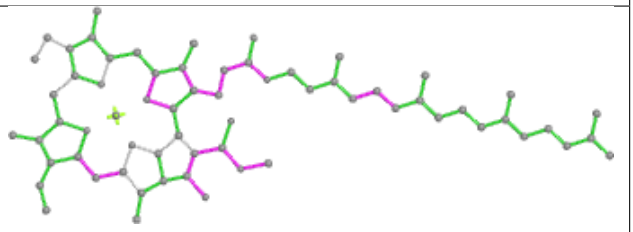
Torsions

Rings

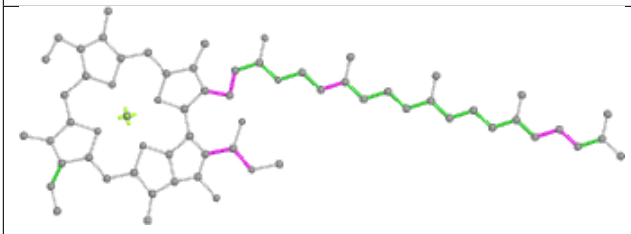
Ligand CLA C 491



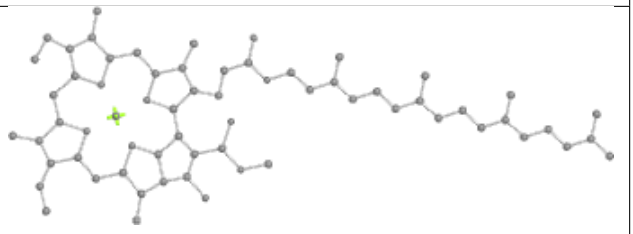
Bond lengths



Bond angles

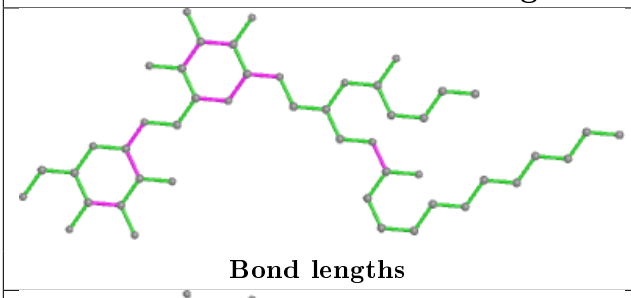


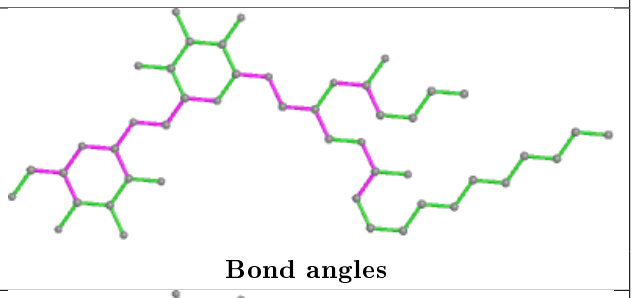
Torsions

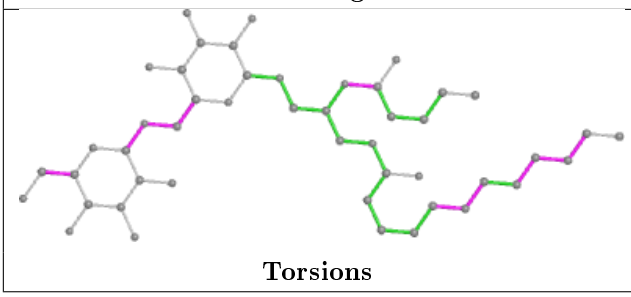


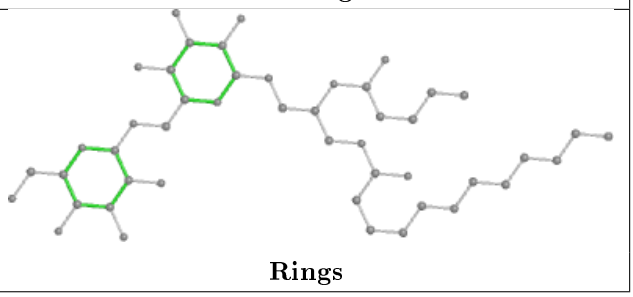
Rings

Ligand DGD C 508

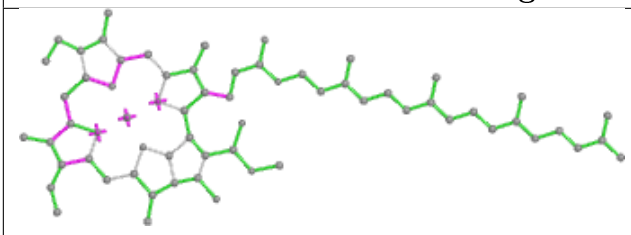

Bond lengths

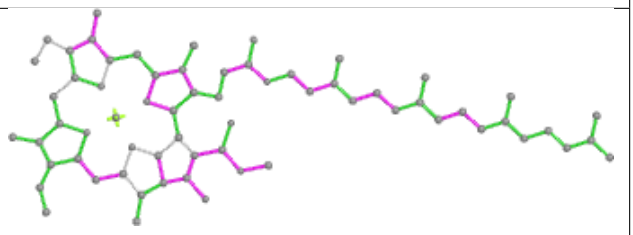

Bond angles

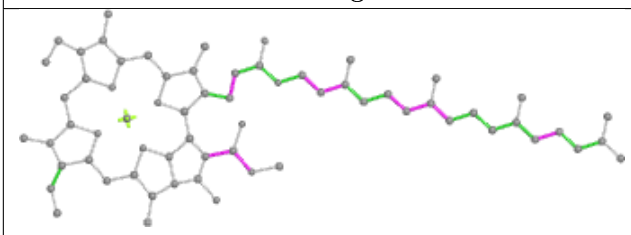

Torsions

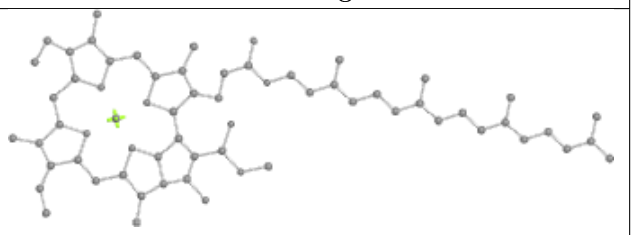

Rings

Ligand CLA b 5520

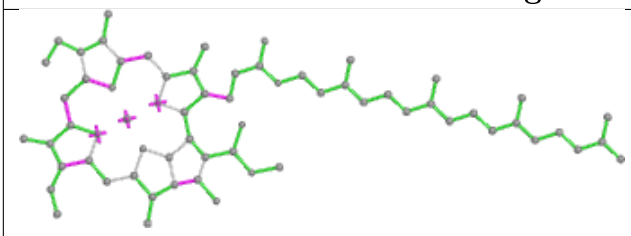

Bond lengths

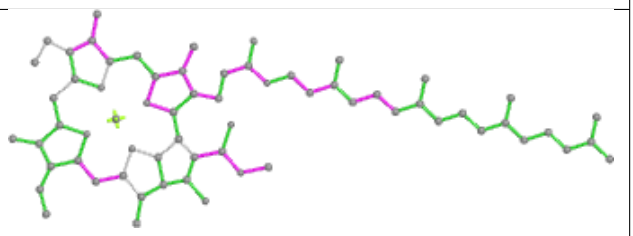

Bond angles

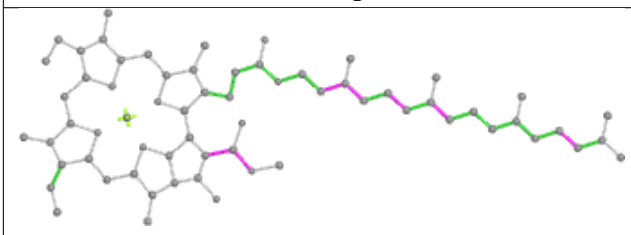

Torsions

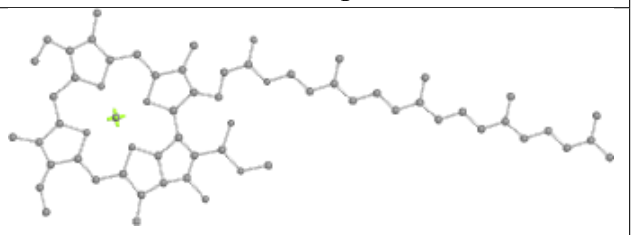

Rings

Ligand CLA C 500

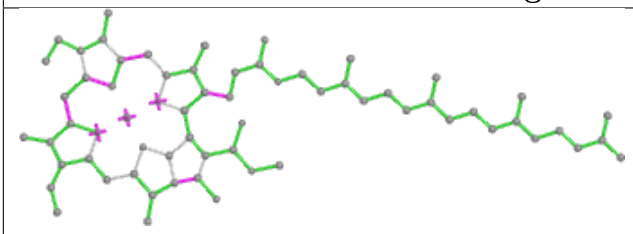

Bond lengths


Bond angles

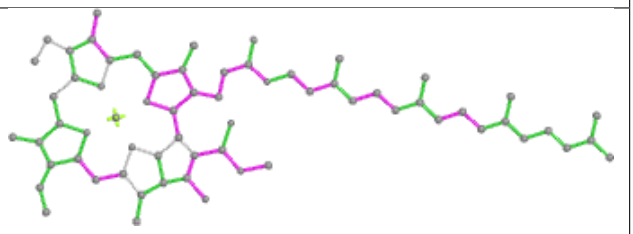

Torsions


Rings

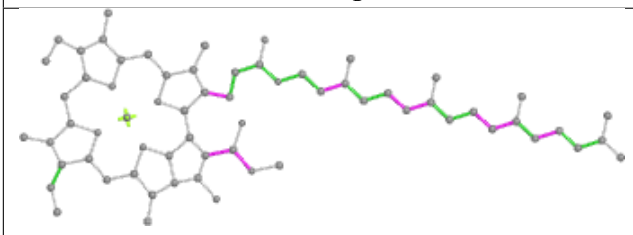
Ligand CLA C 493



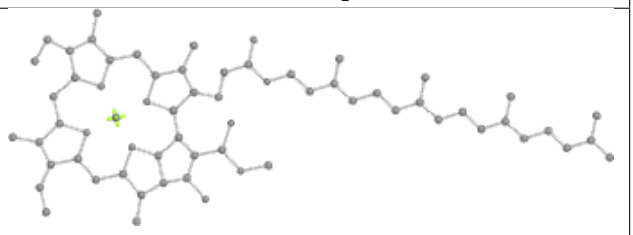
Bond lengths



Bond angles

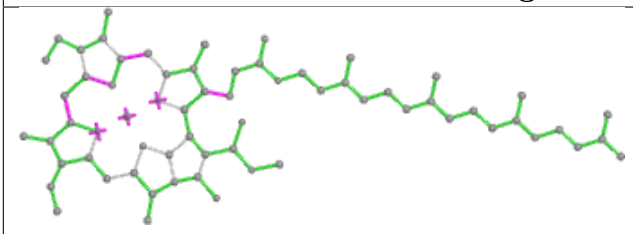


Torsions

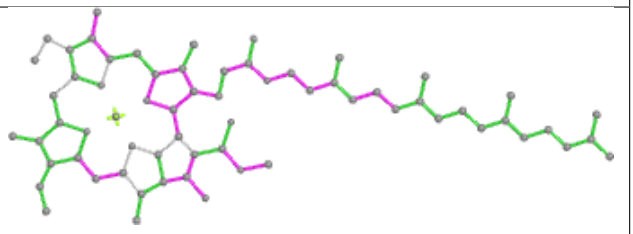


Rings

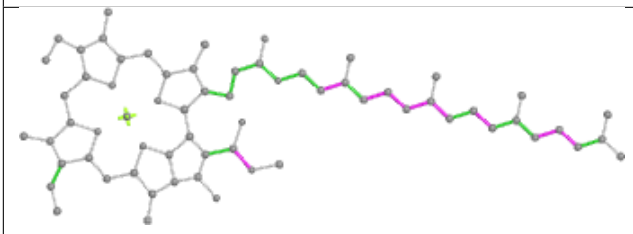
Ligand CLA b 5514



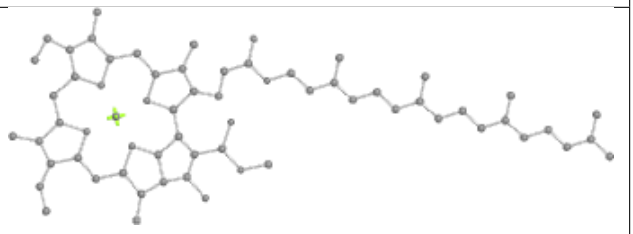
Bond lengths



Bond angles

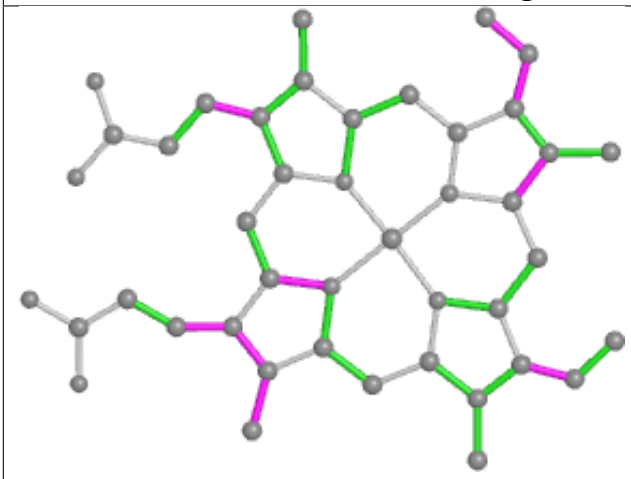


Torsions

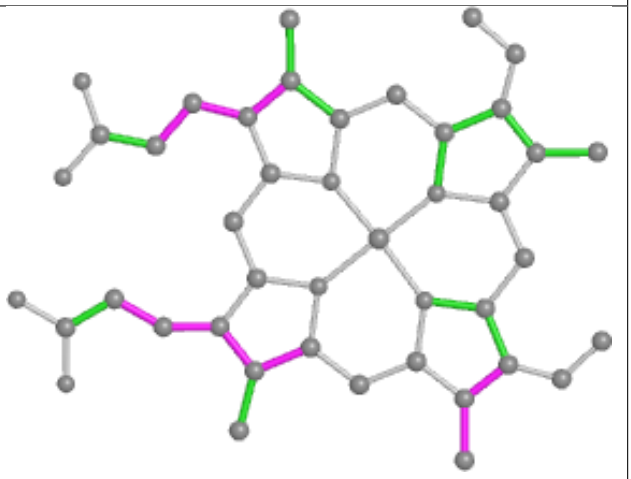


Rings

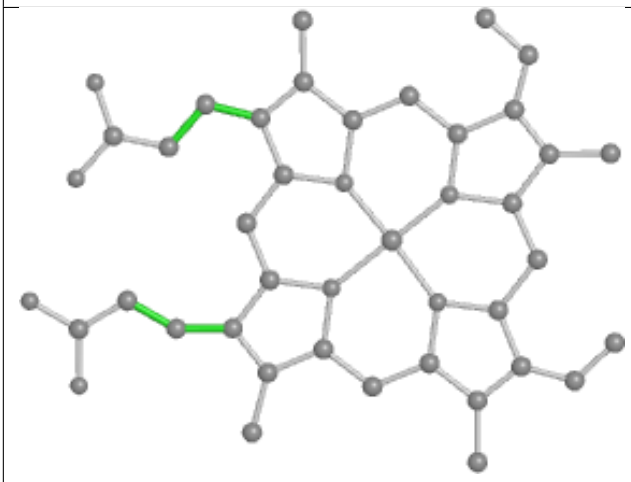
Ligand HEM V 552



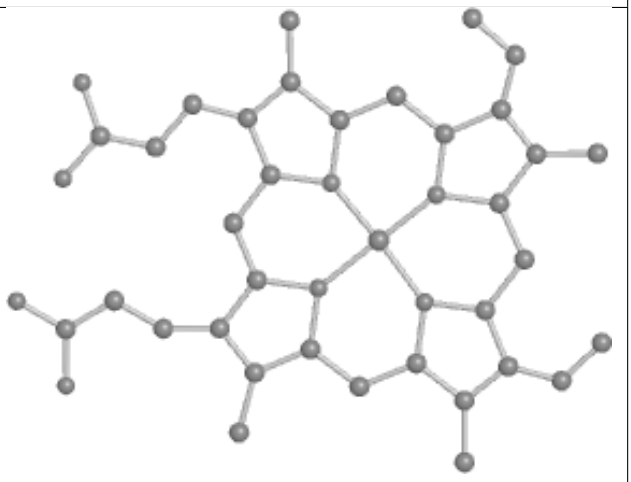
Bond lengths



Bond angles

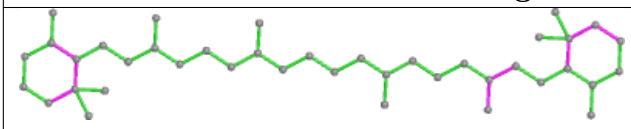


Torsions

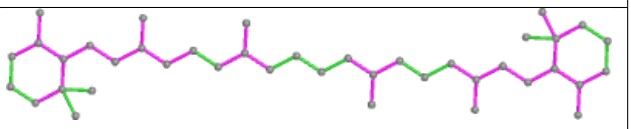


Rings

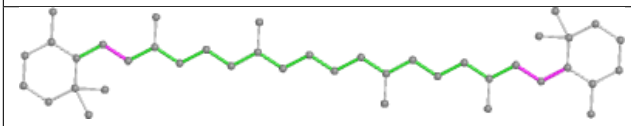
Ligand BCR T 5104



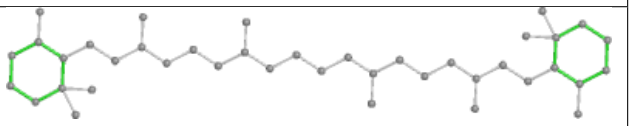
Bond lengths



Bond angles

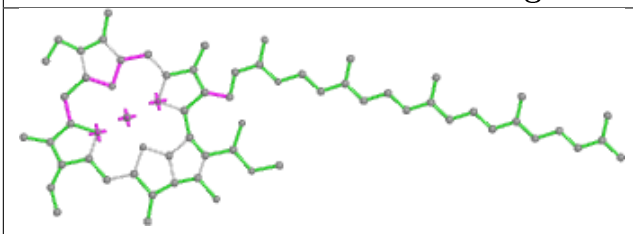


Torsions

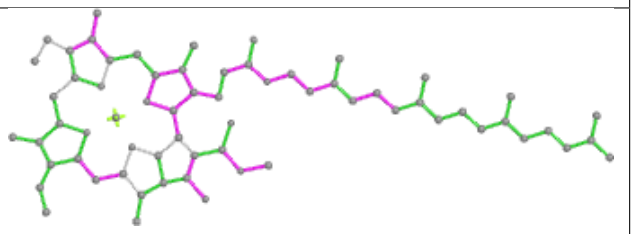


Rings

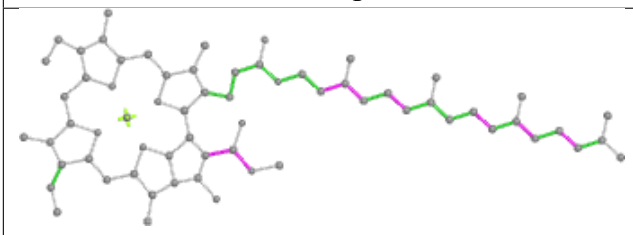
Ligand CLA B 519



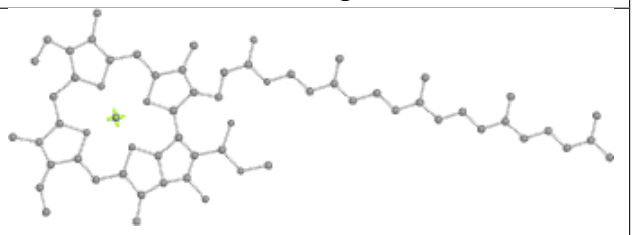
Bond lengths



Bond angles

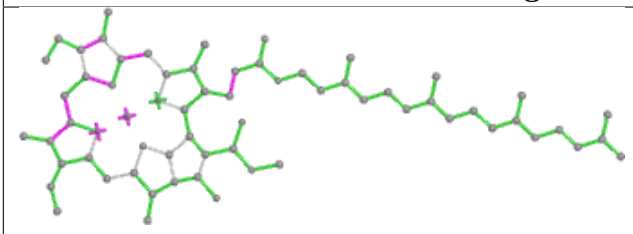


Torsions

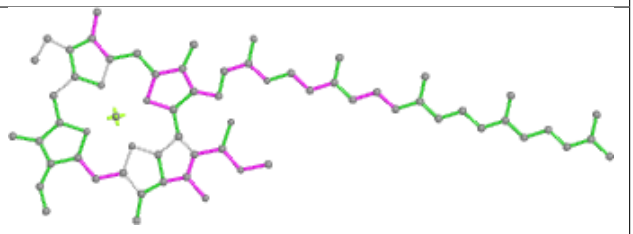


Rings

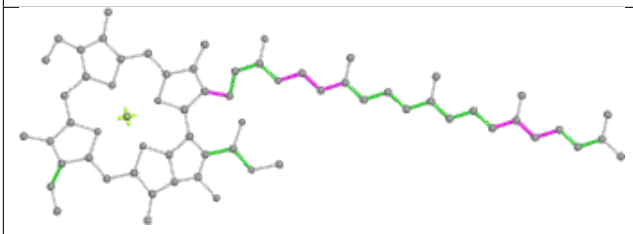
Ligand CLA D 354



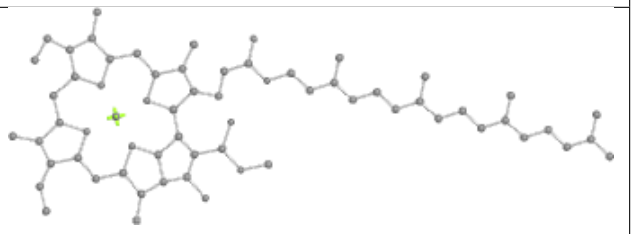
Bond lengths



Bond angles

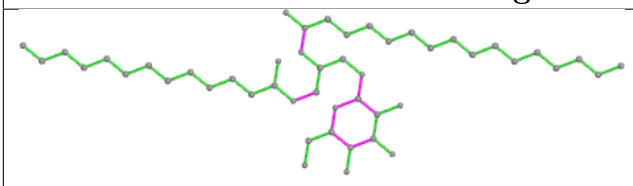


Torsions

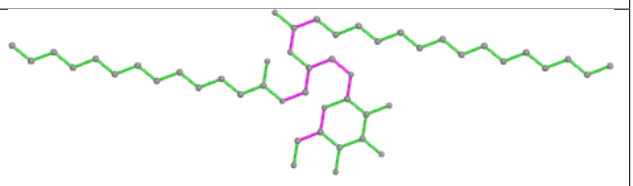


Rings

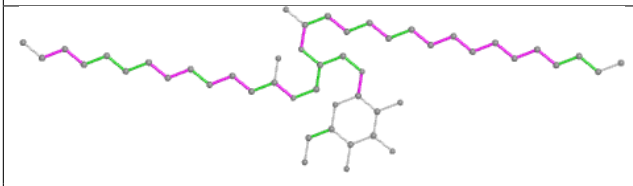
Ligand MGE b 5530



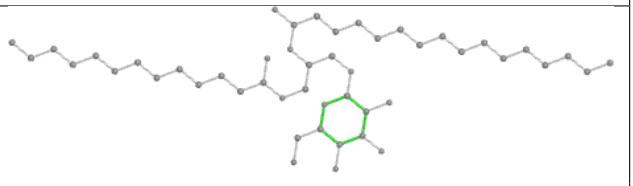
Bond lengths



Bond angles

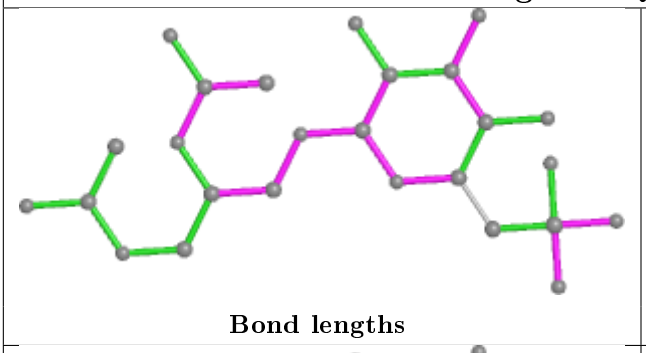


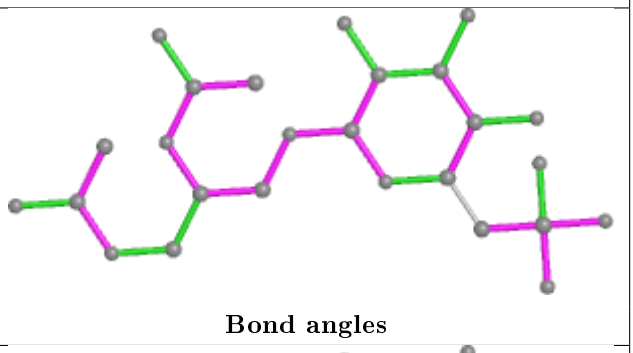
Torsions

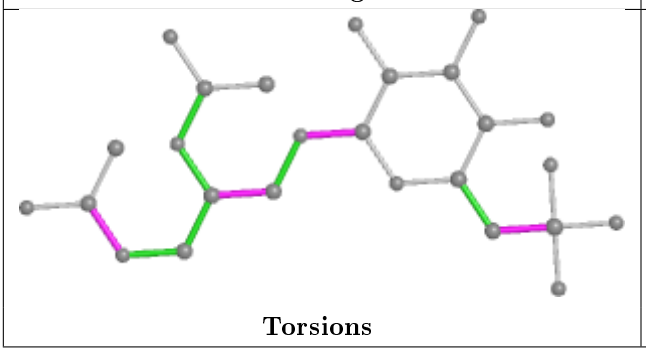


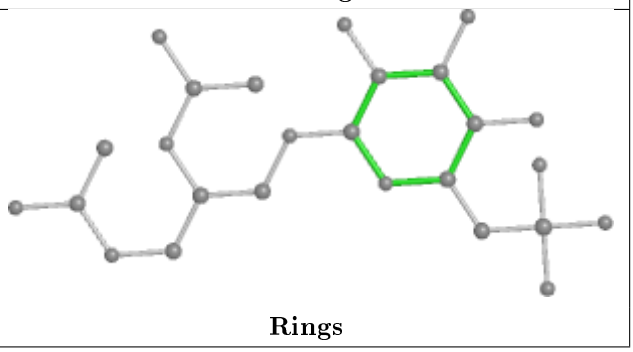
Rings

Ligand SQD A 5212

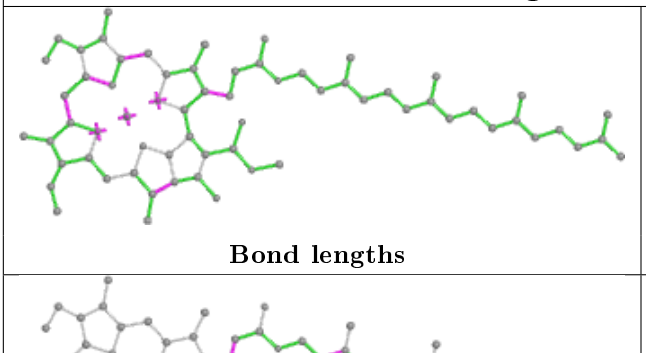

Bond lengths

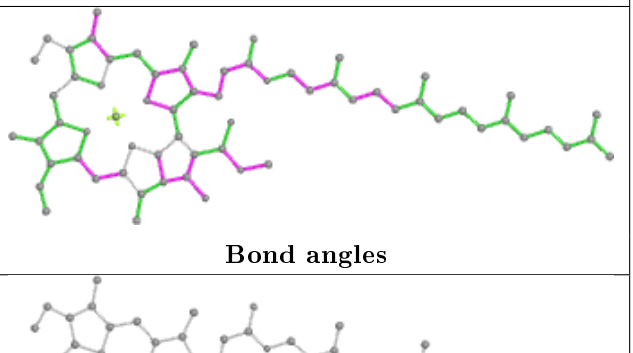

Bond angles

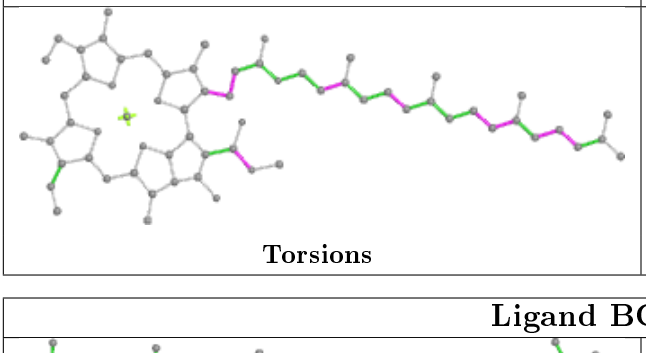

Torsions

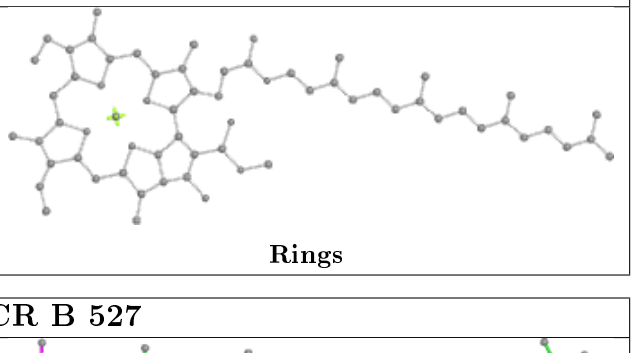

Rings

Ligand CLA B 516

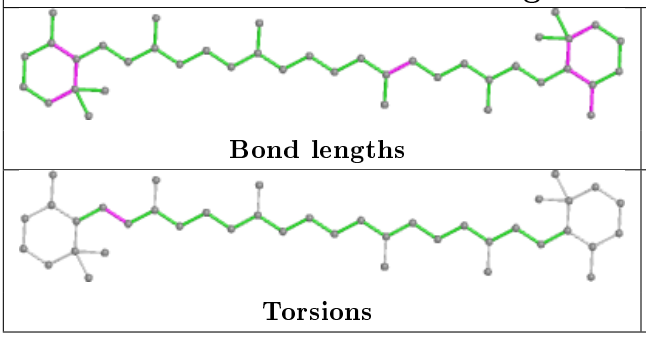

Bond lengths

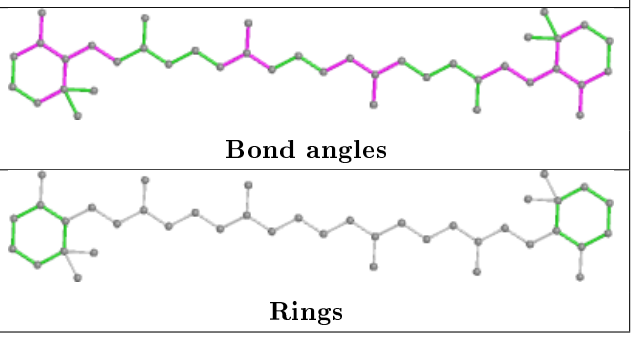

Bond angles


Torsions


Rings

Ligand BCR B 527

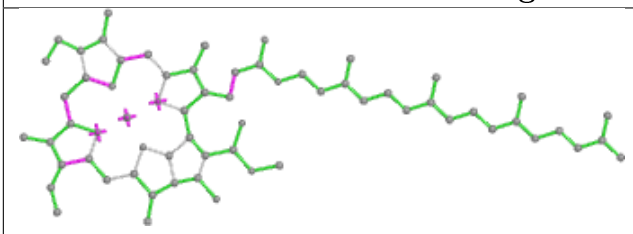

Bond lengths


Bond angles

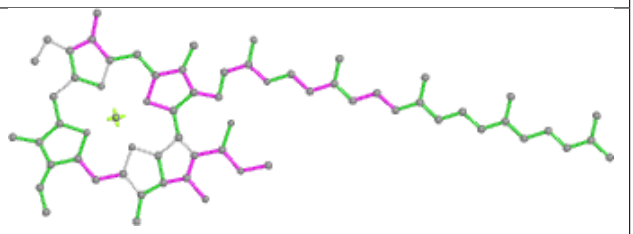
Torsions

Rings

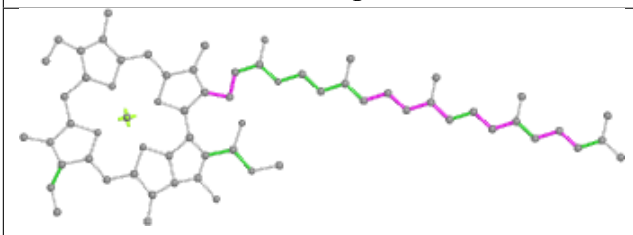
Ligand CLA b 5512



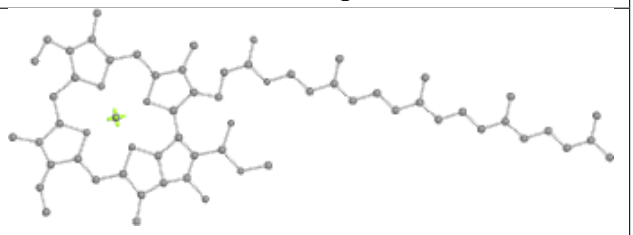
Bond lengths



Bond angles

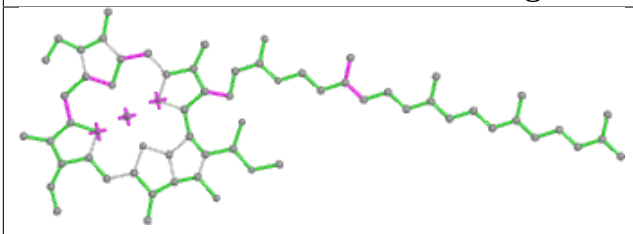


Torsions

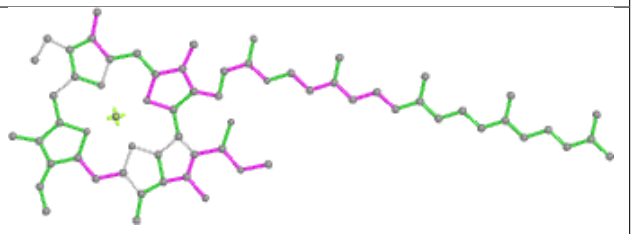


Rings

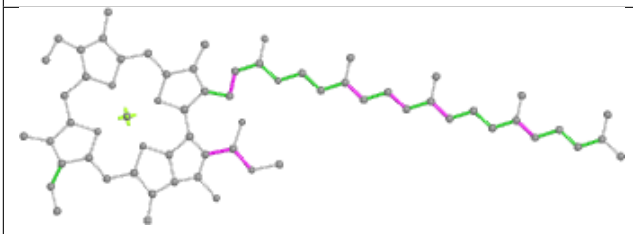
Ligand CLA B 513



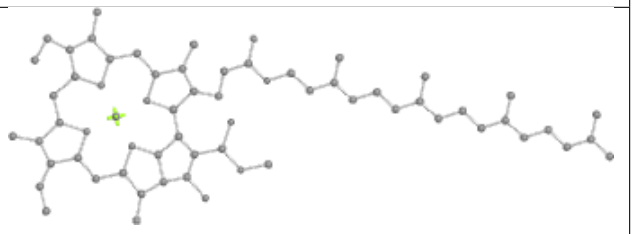
Bond lengths



Bond angles

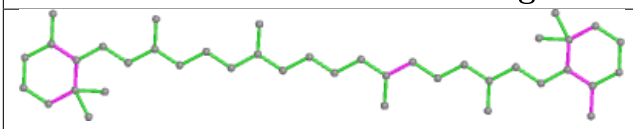


Torsions

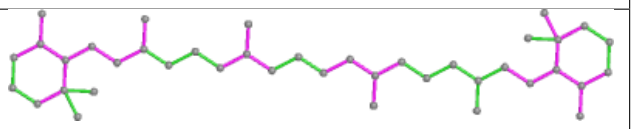


Rings

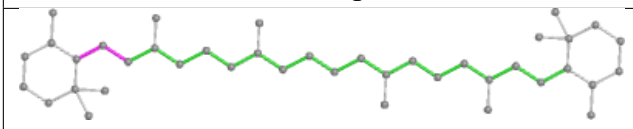
Ligand BCR c 5505



Bond lengths



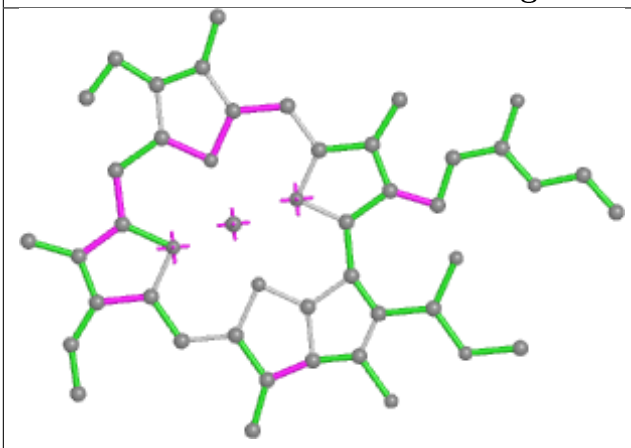
Bond angles



Torsions

Rings

Ligand CLA c 5499



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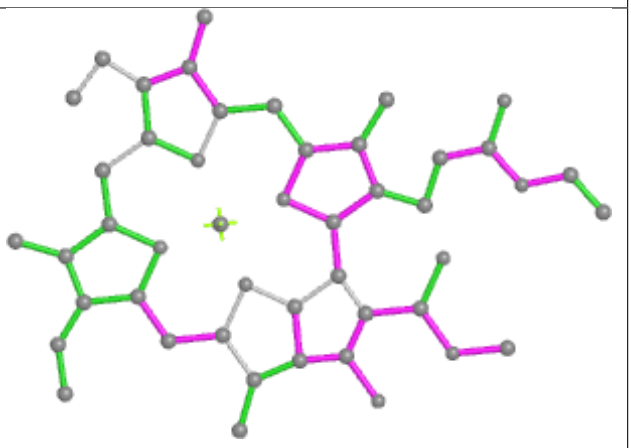
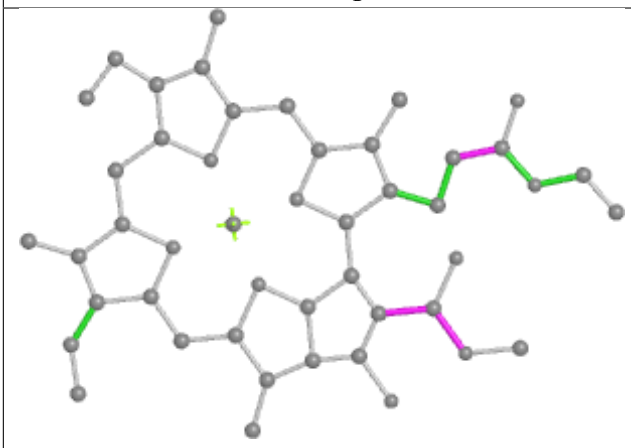
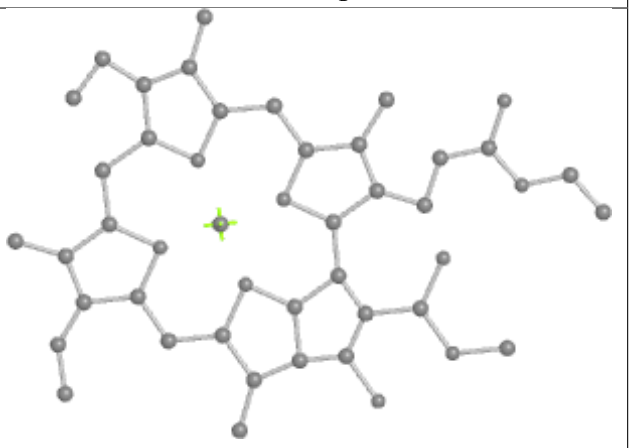


Bond angles

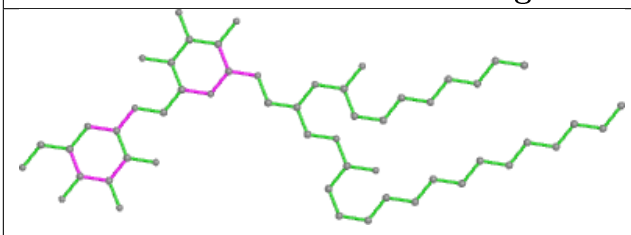


Torsions



Rings

Ligand DGD h 5208



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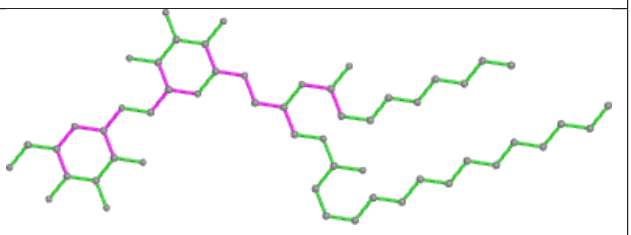
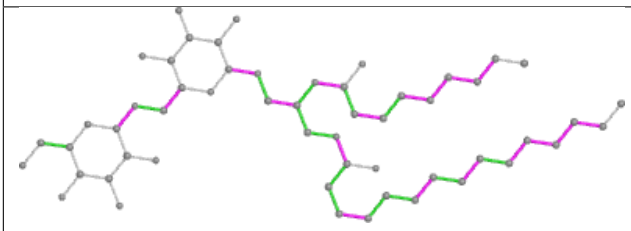
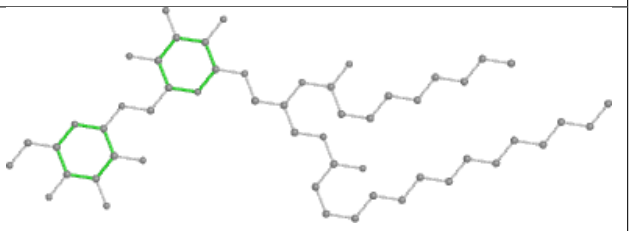


Bond angles

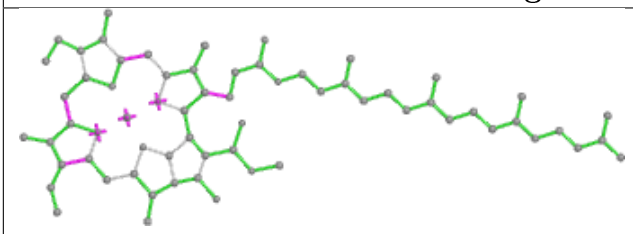


Torsions

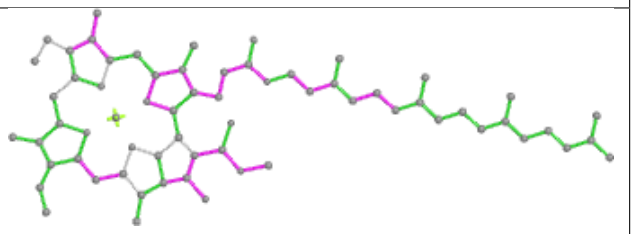


Rings

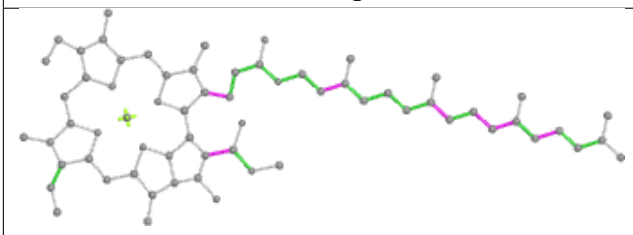
Ligand CLA A 560



Bond lengths



Bond angles



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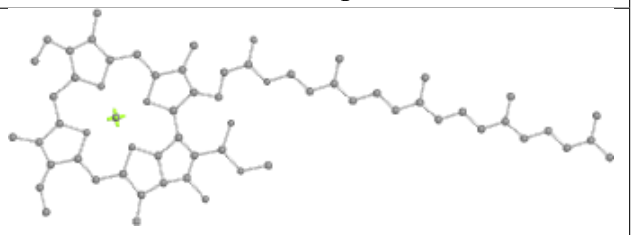
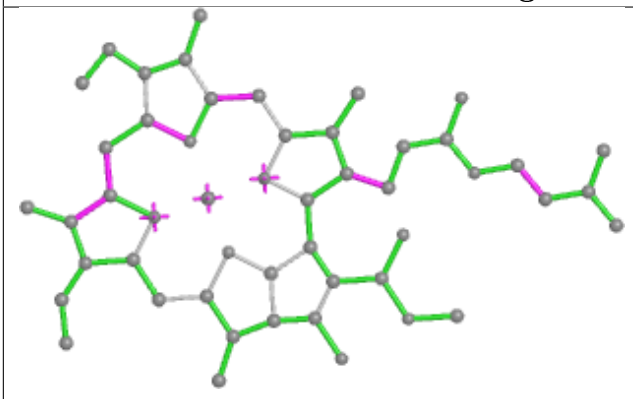


Rings

Ligand CLA d 5355



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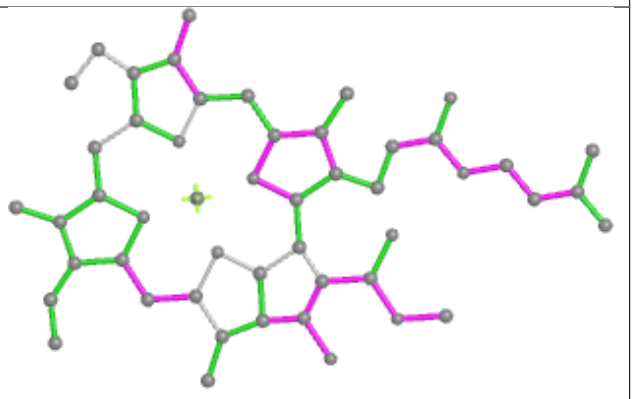
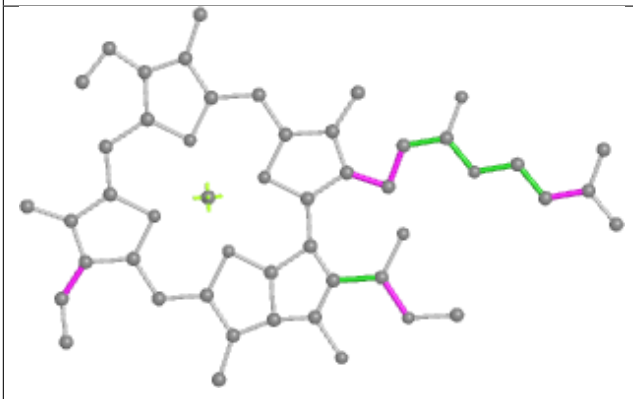


Bond angles



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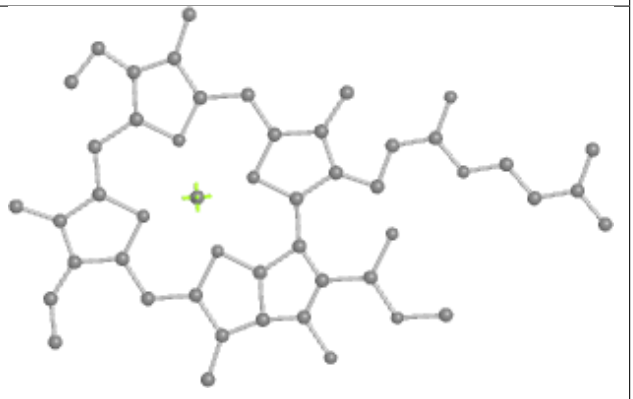
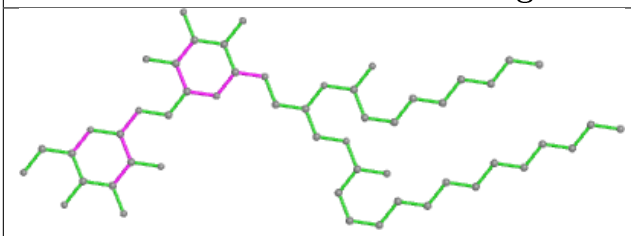
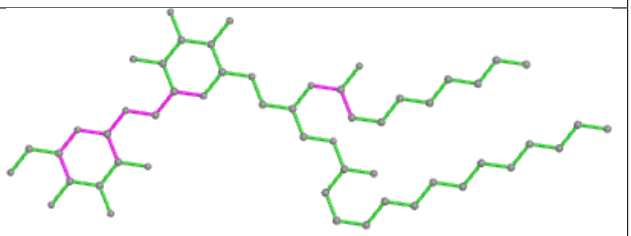


Rings

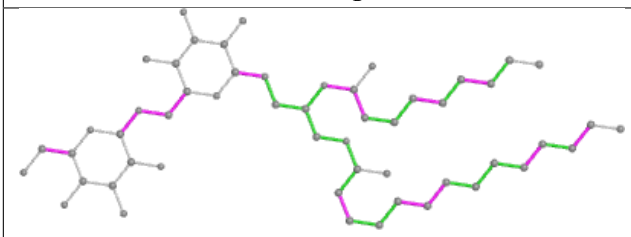
Ligand DGD c 5507



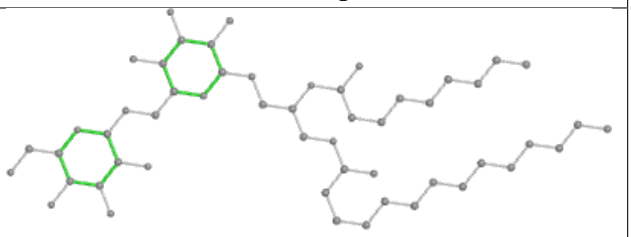
Bond lengths



Bond angles

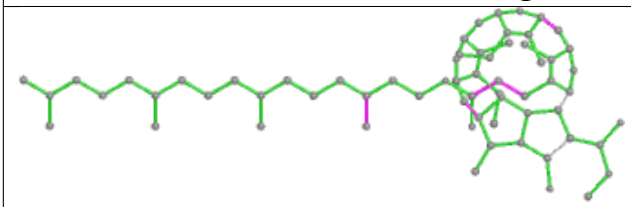


Torsions



Rings

Ligand PHO a 5561



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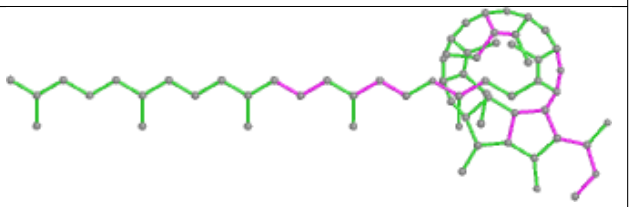
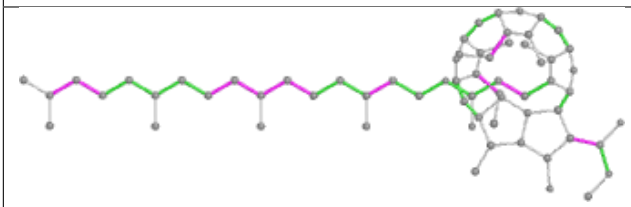


Bond angles



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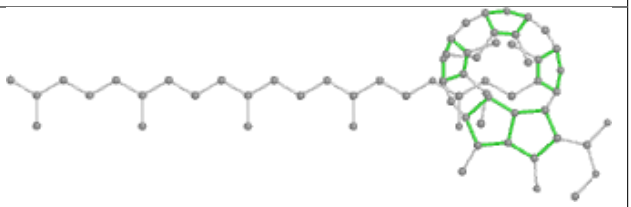
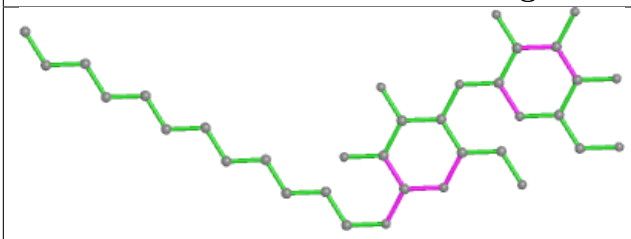


Rings

Ligand LMT m 216



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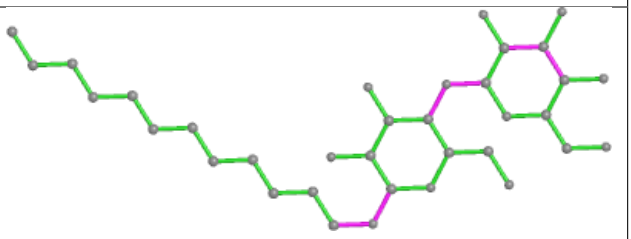
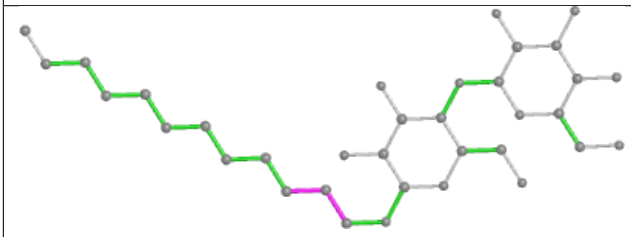
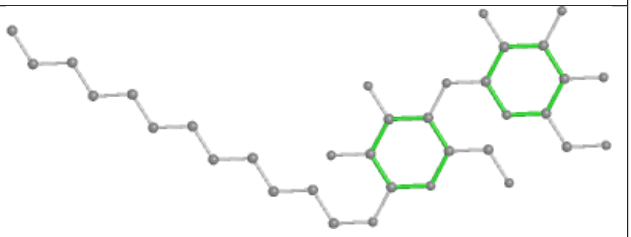


Bond angles

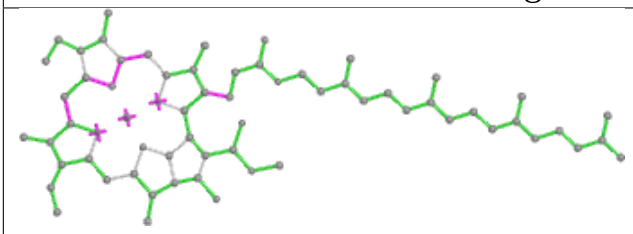


Torsions

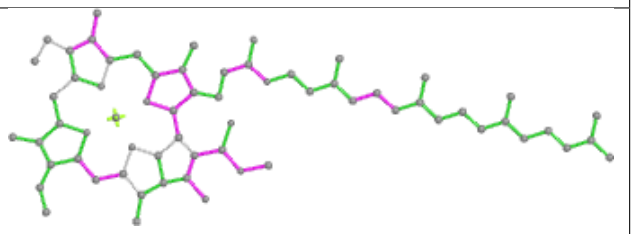


Rings

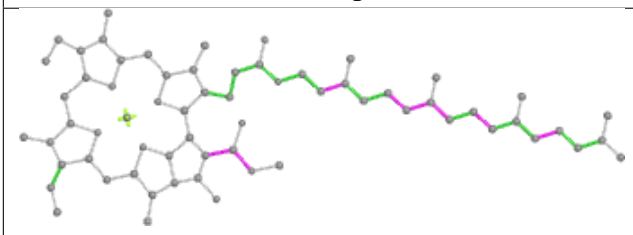
Ligand CLA B 525



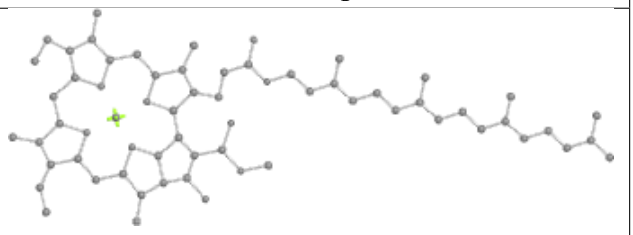
Bond lengths



Bond angles

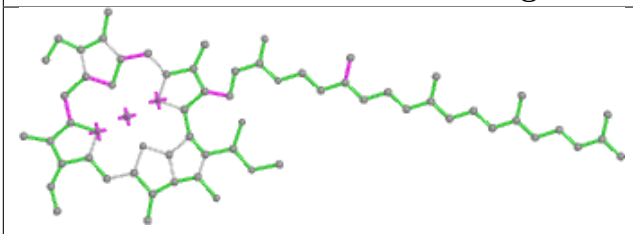


Torsions

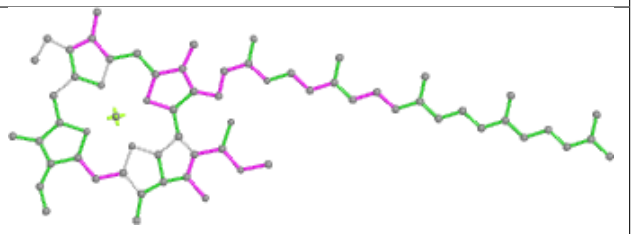


Rings

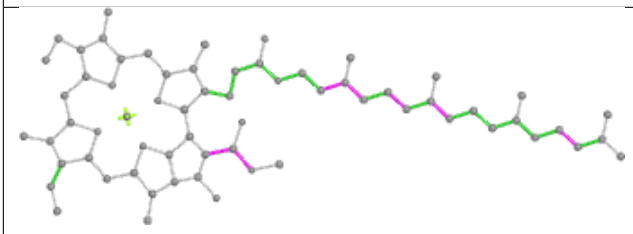
Ligand CLA c 5500



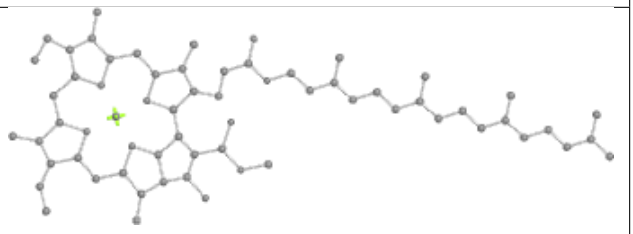
Bond lengths



Bond angles

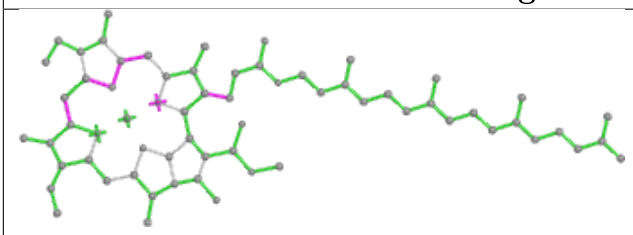


Torsions

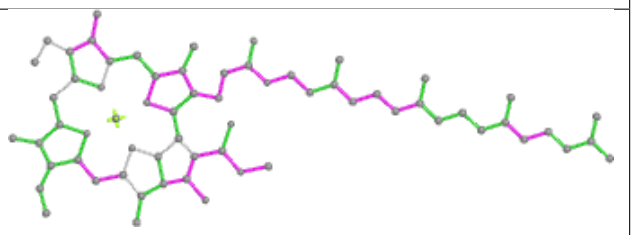


Rings

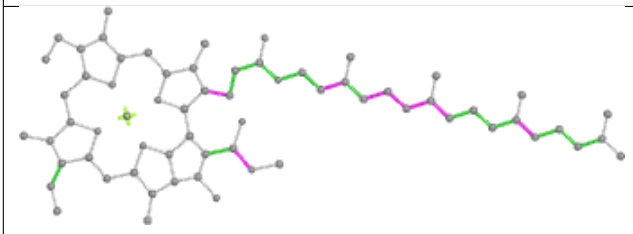
Ligand CLA b 5518



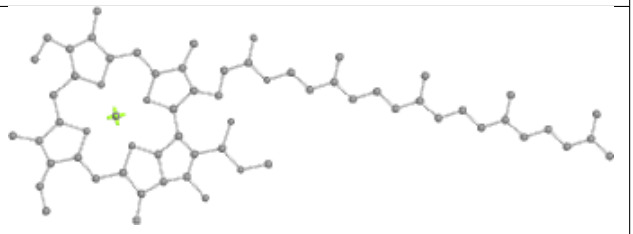
Bond lengths



Bond angles

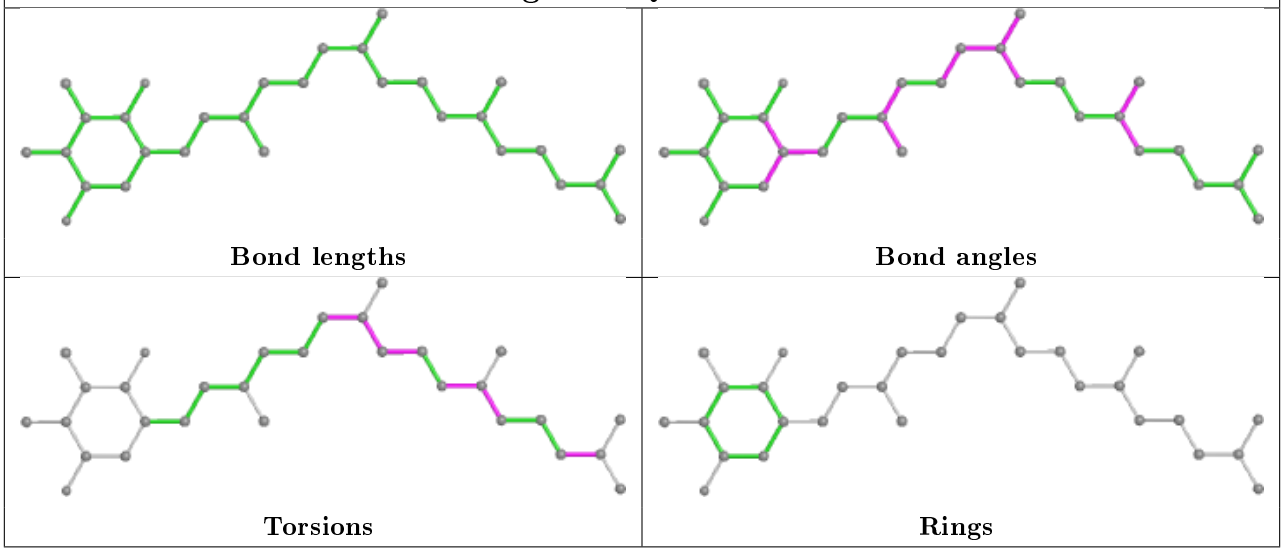


Torsions

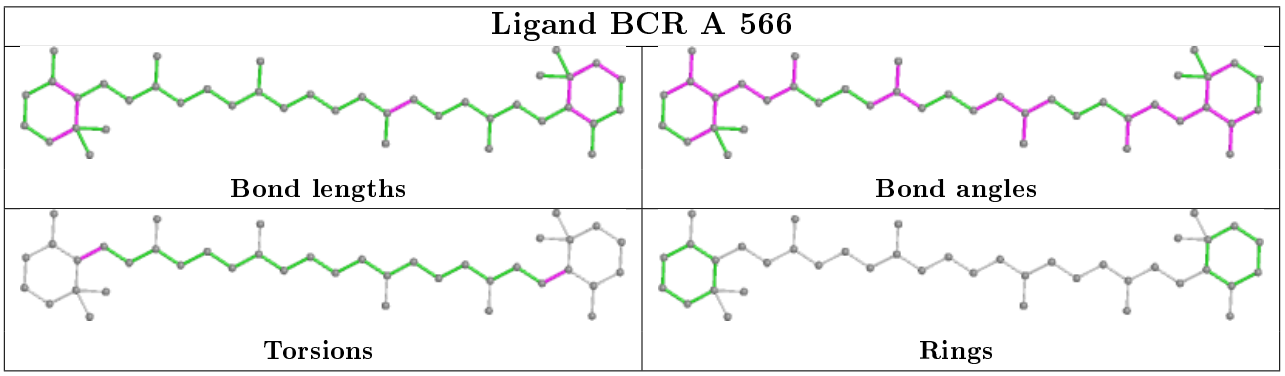


Rings

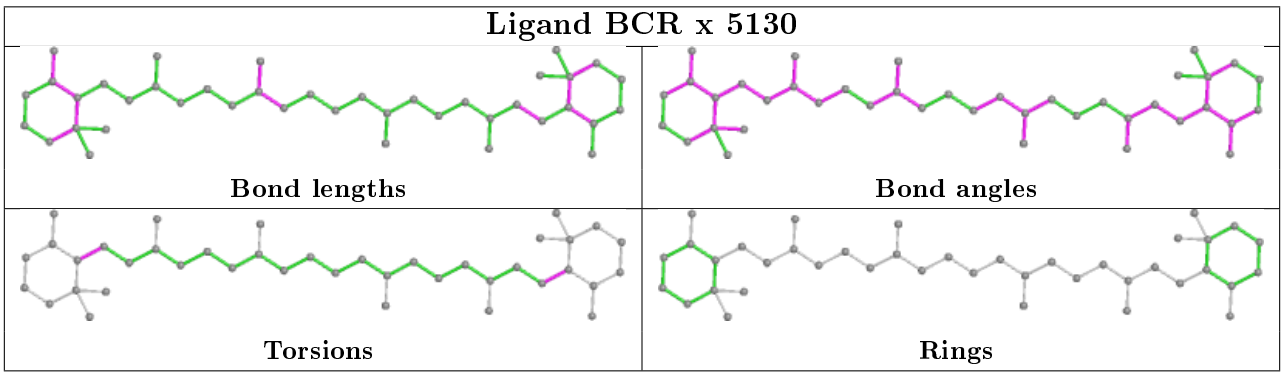
Ligand PQ9 d 5356



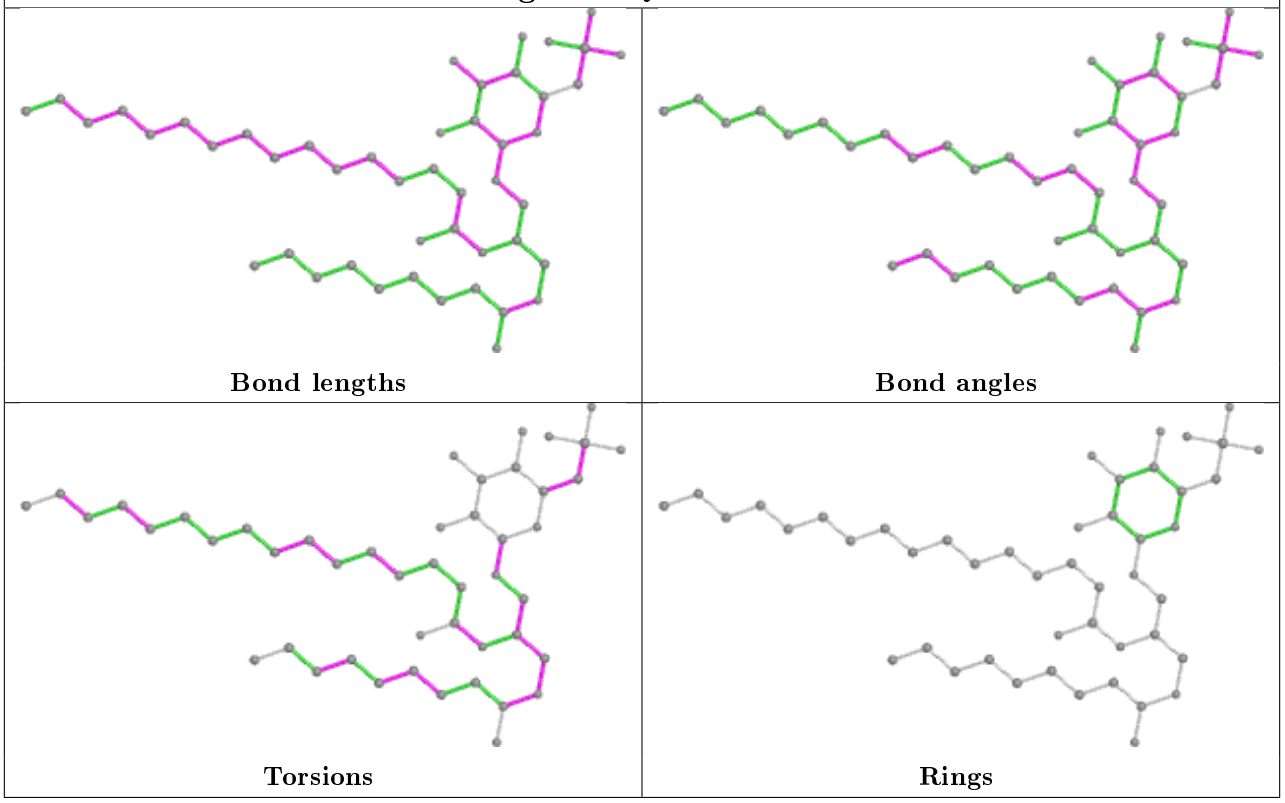
Ligand BCR A 566



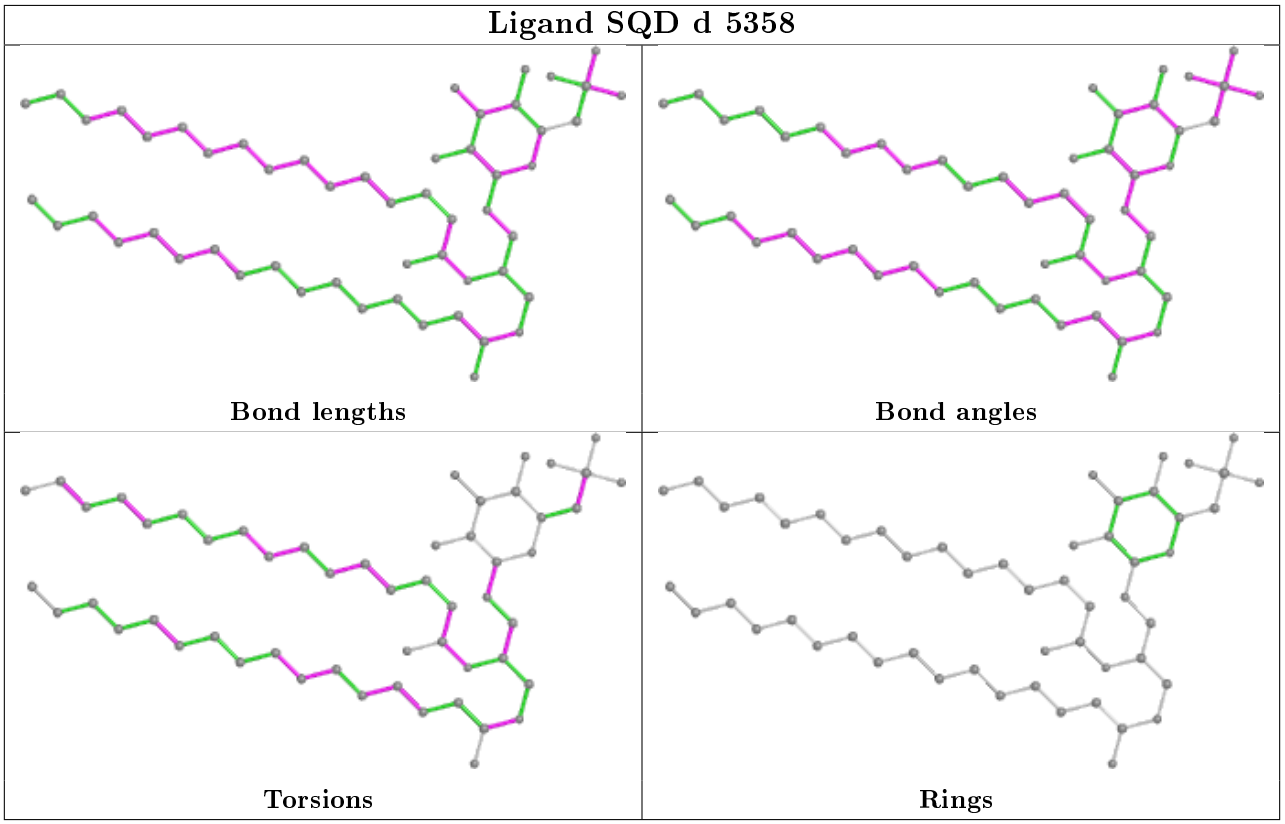
Ligand BCR x 5130



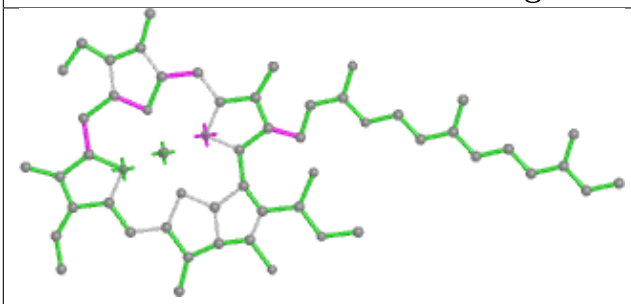
Ligand SQD L 5213



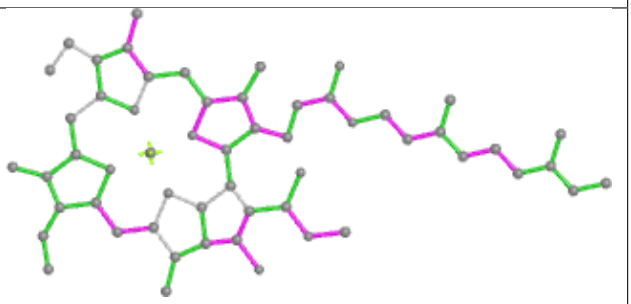
Ligand SQD d 5358



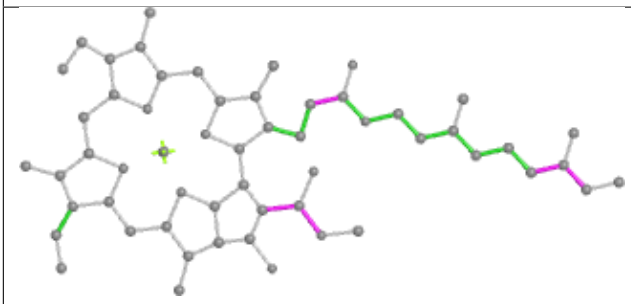
Ligand CLA B 524



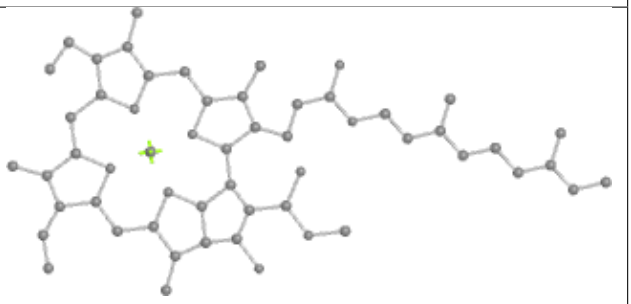
Bond lengths



Bond angles

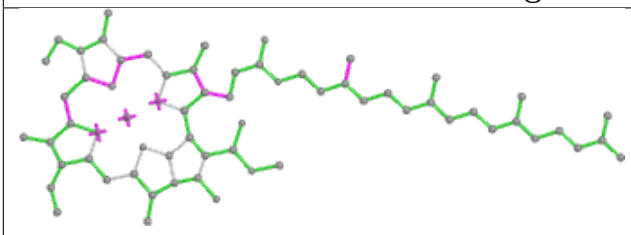


Torsions

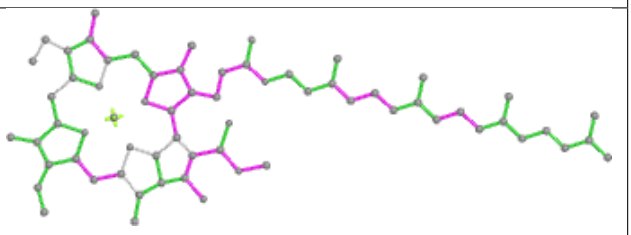


Rings

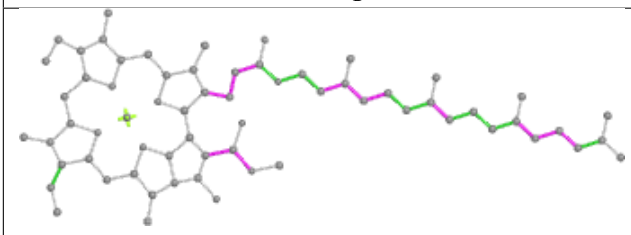
Ligand CLA B 515



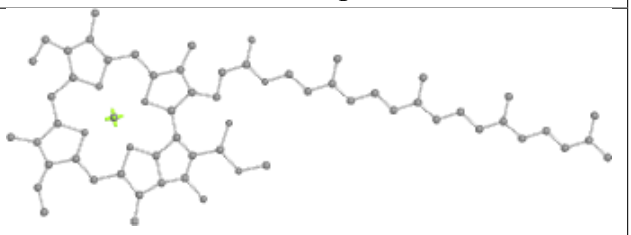
Bond lengths



Bond angles

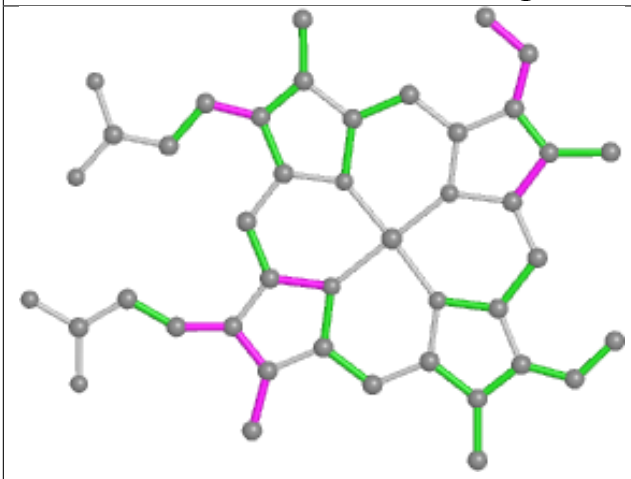


Torsions

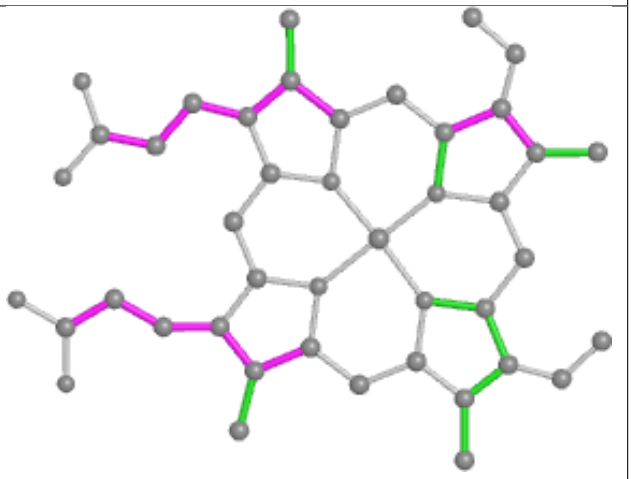


Rings

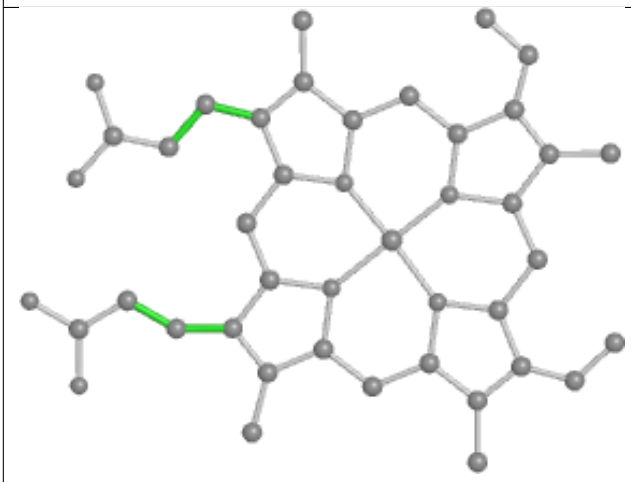
Ligand HEM f 5051



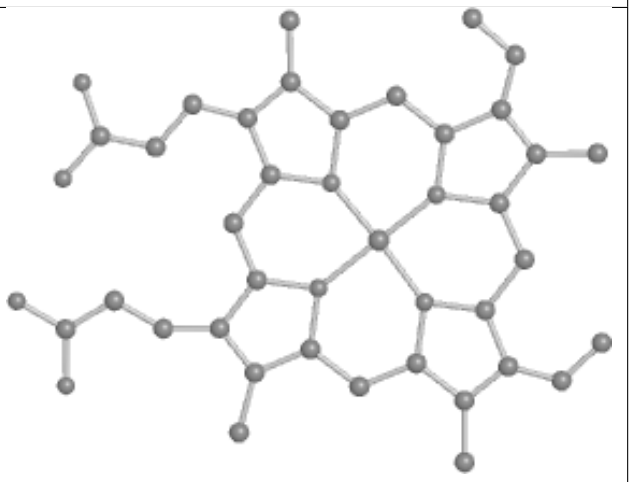
Bond lengths



Bond angles

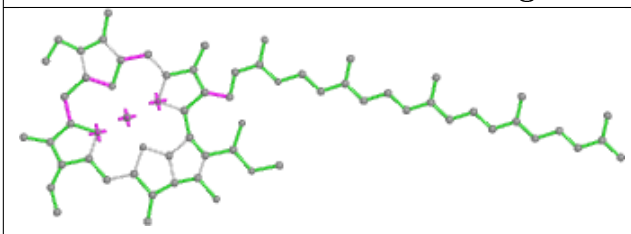


Torsions

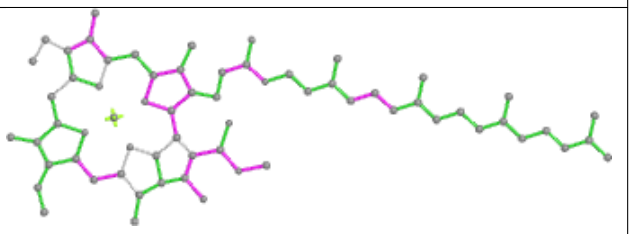


Rings

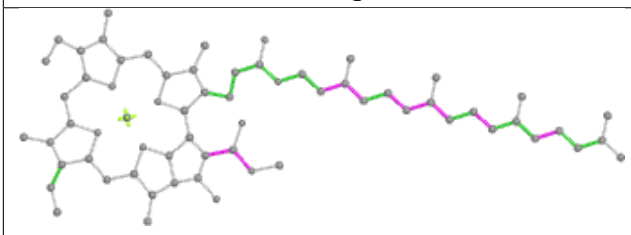
Ligand CLA b 5525



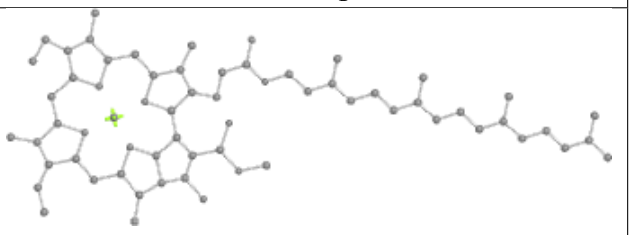
Bond lengths



Bond angles

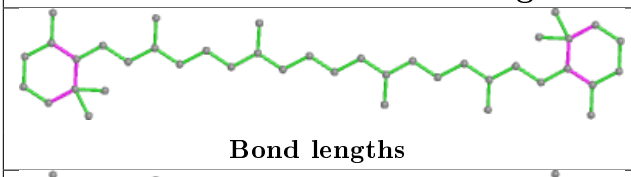


Torsions



Rings

Ligand BCR b 5528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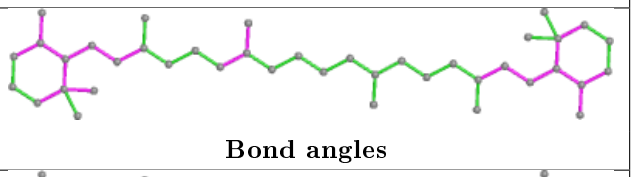
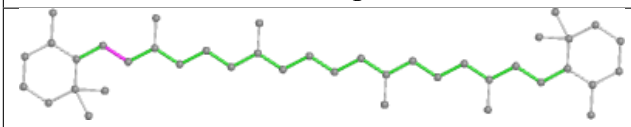
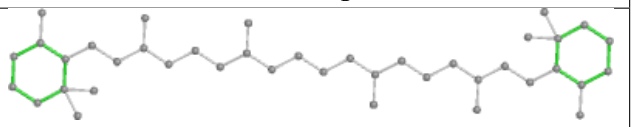
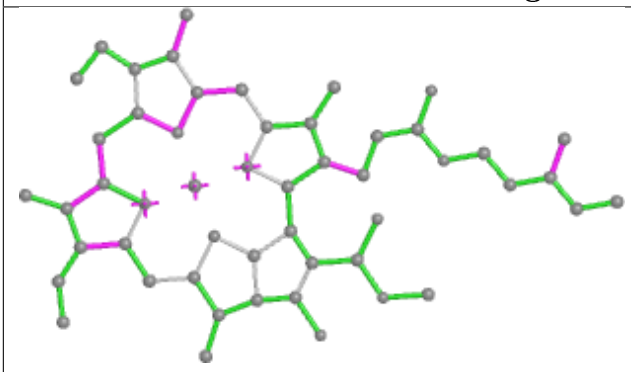

Bond angles


Torsions


Rings

Ligand CLA C 502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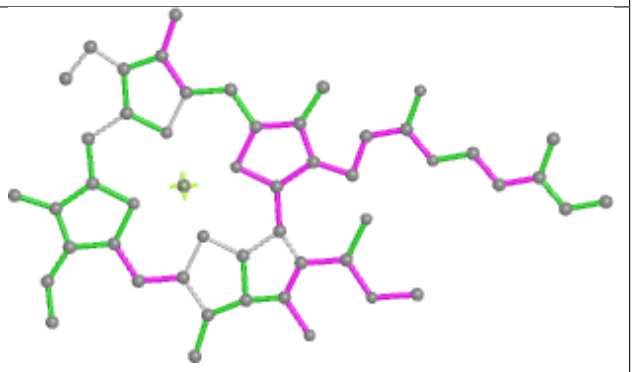
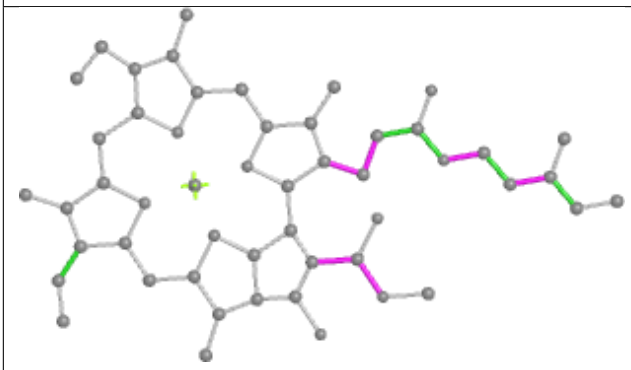
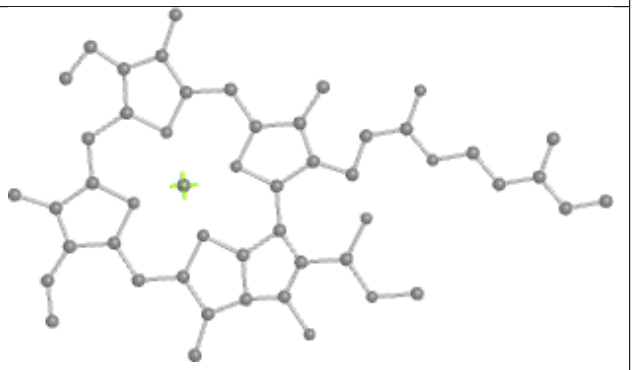
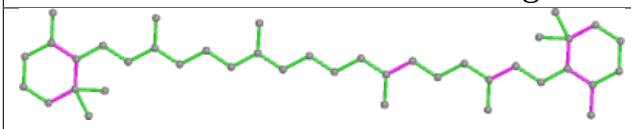
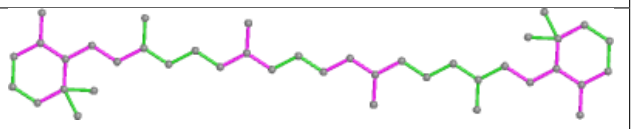

Bond angles

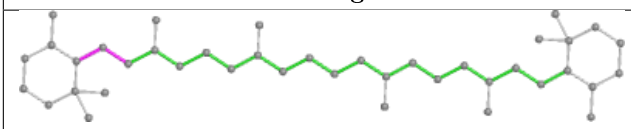

Torsions

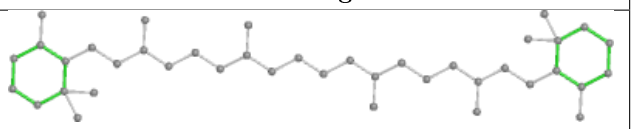

Rings

Ligand BCR C 505

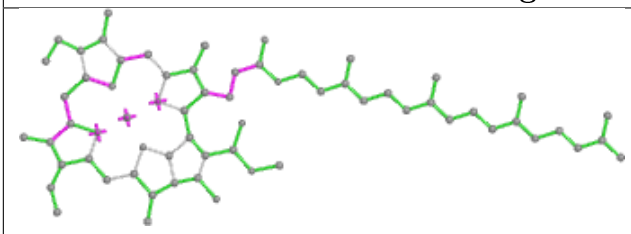

Bond lengths


Bond angles

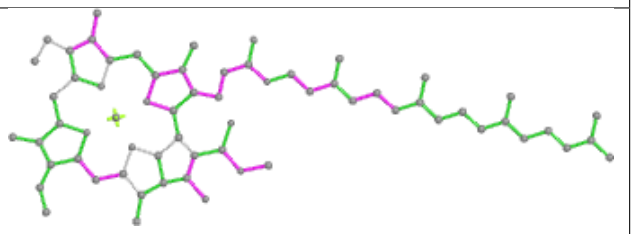

Torsions


Rings

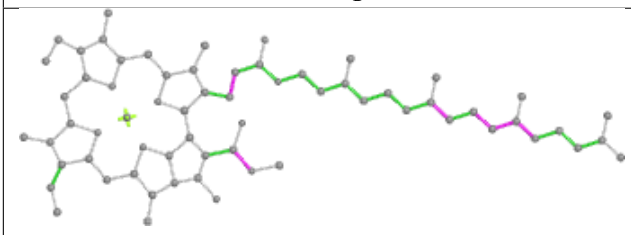
Ligand CLA a 5558



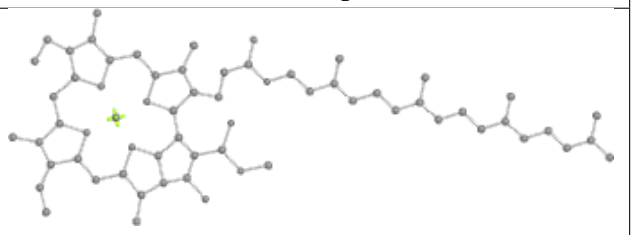
Bond lengths



Bond angles

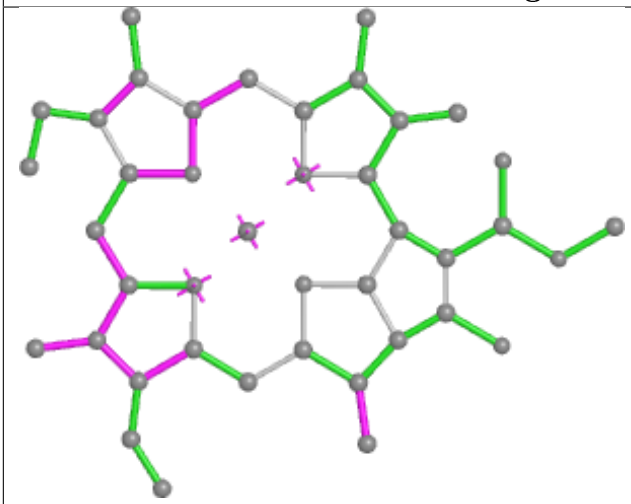


Torsions



Rings

Ligand CLA B 511



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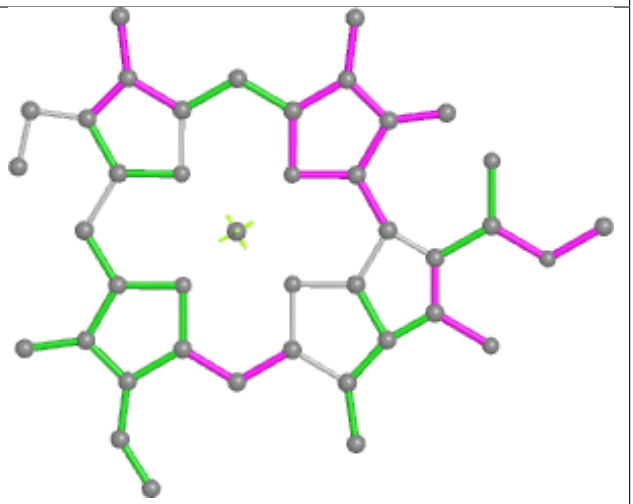
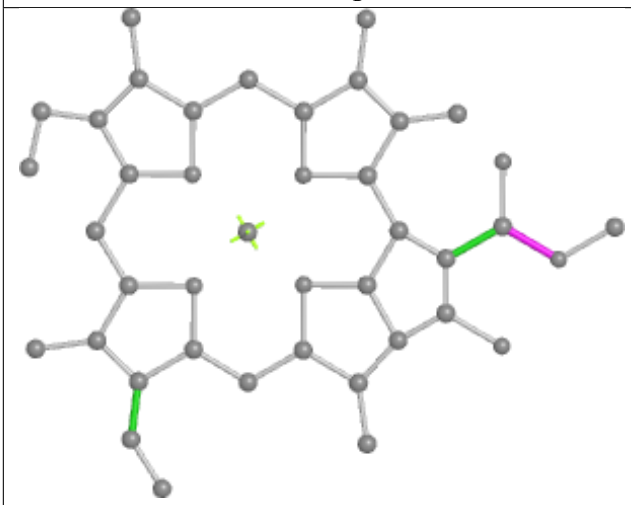


Bond angles



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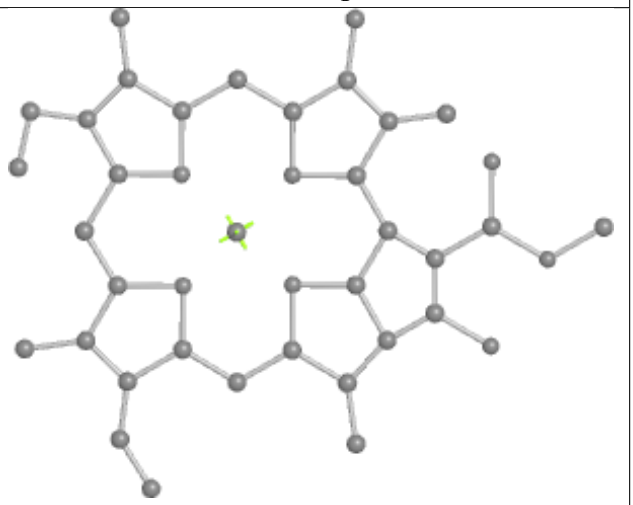
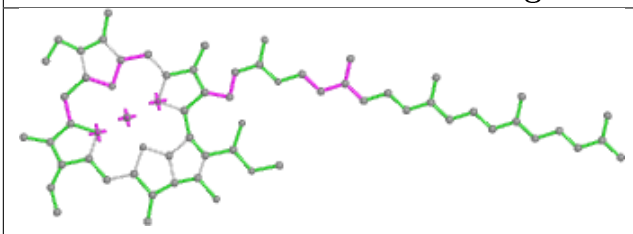
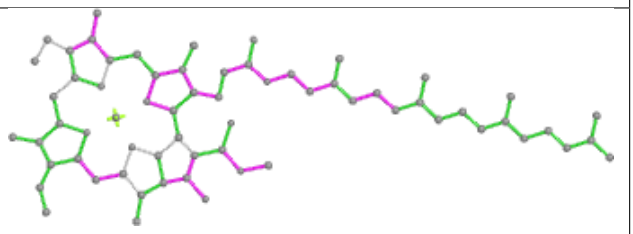


Rings

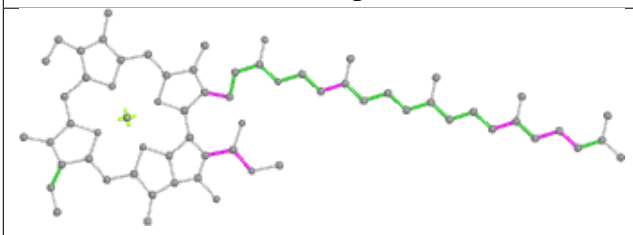
Ligand CLA B 526



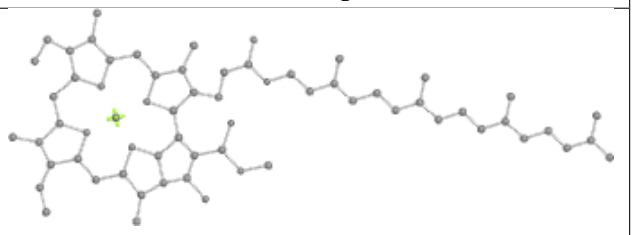
Bond lengths



Bond angles

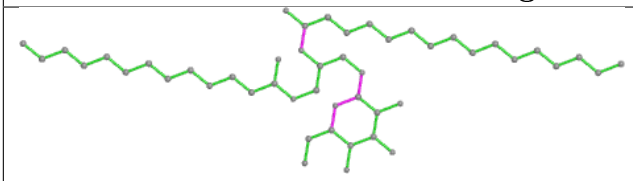


Torsions

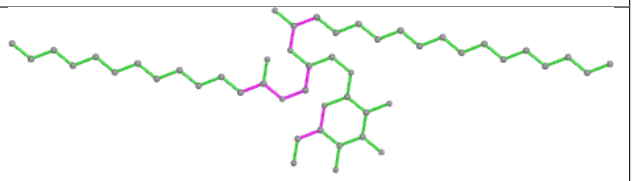


Rings

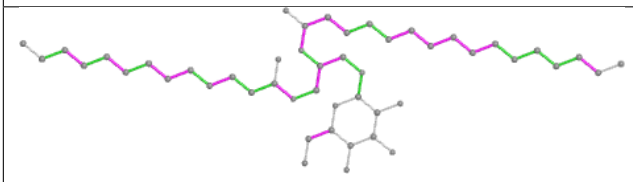
Ligand MGE D 360



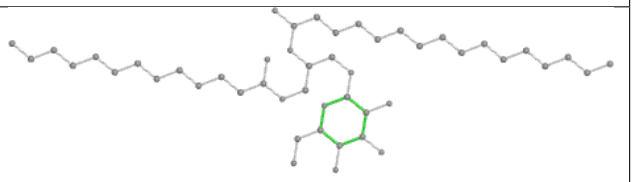
Bond lengths



Bond angles

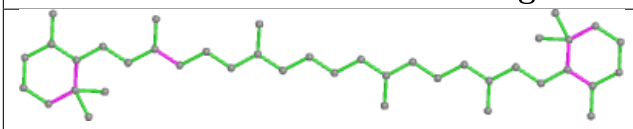


Torsions



Rings

Ligand BCR c 5504



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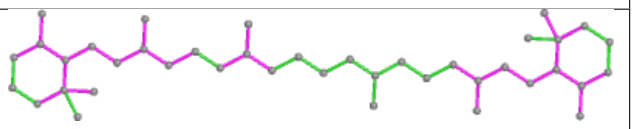
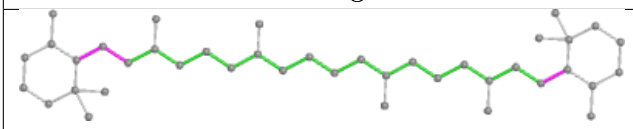


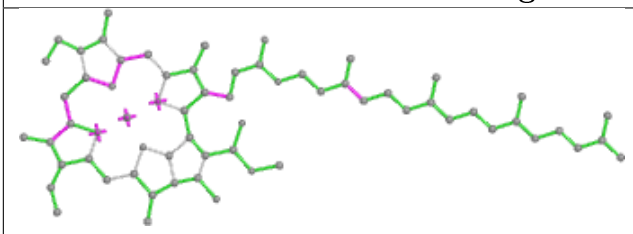
Bond angles



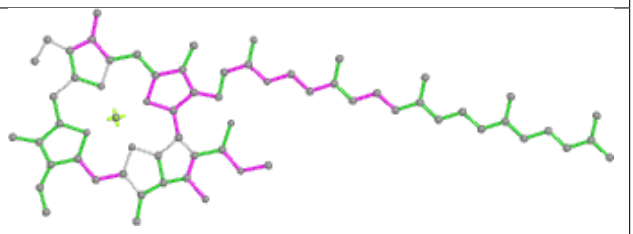
Torsions

Rings

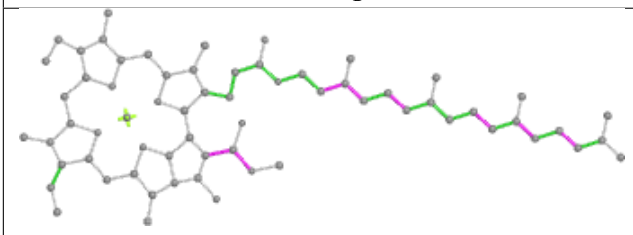
Ligand CLA b 5519



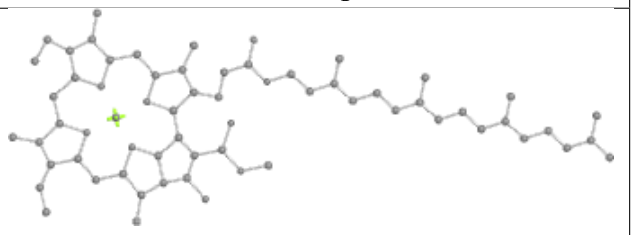
Bond lengths



Bond angles

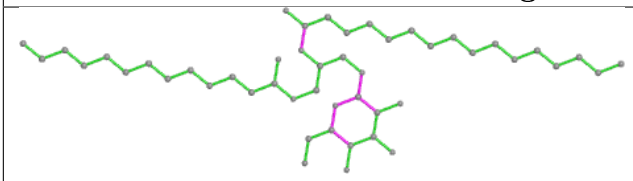


Torsions

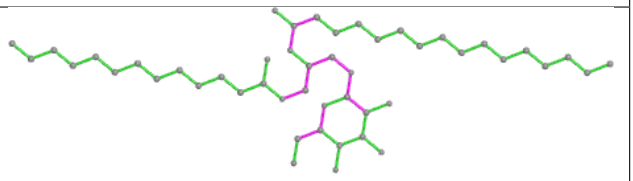


Rings

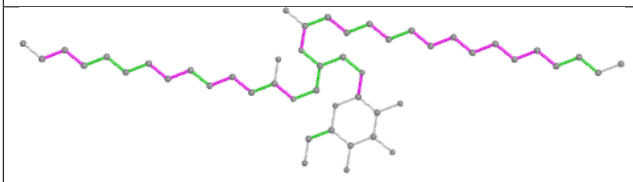
Ligand MGE B 530



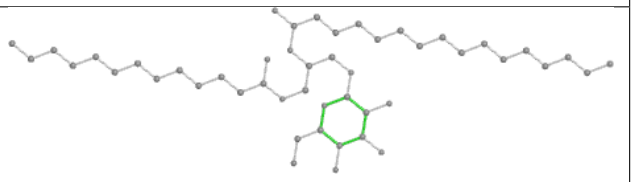
Bond lengths



Bond angles

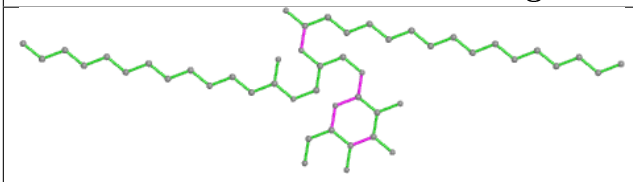


Torsions

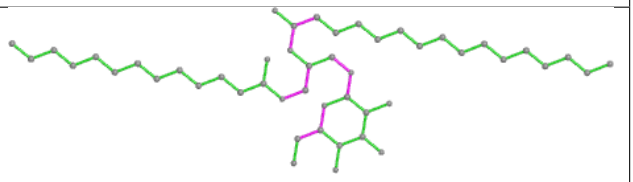


Rings

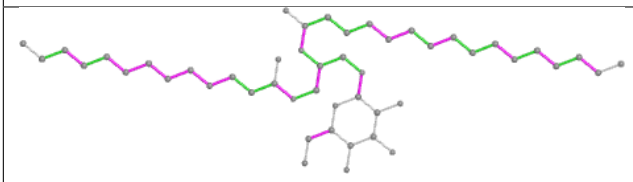
Ligand MGE I 201



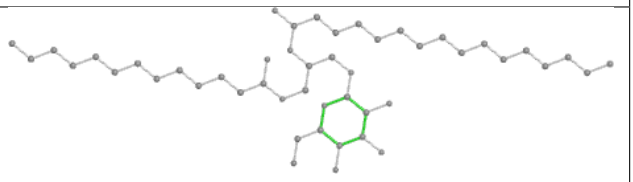
Bond lengths



Bond angles

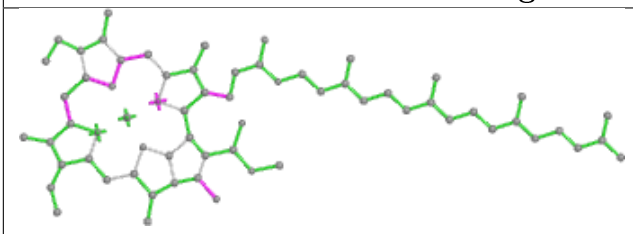


Torsions

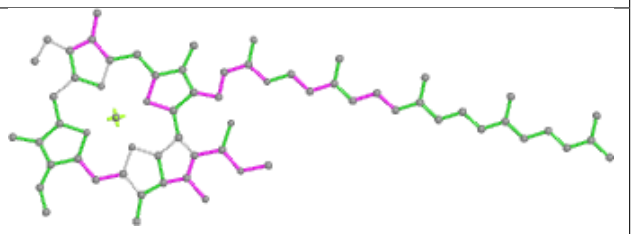


Rings

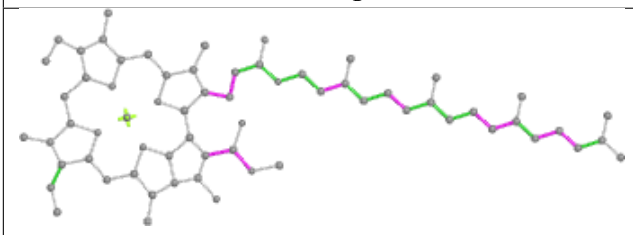
Ligand CLA b 5516



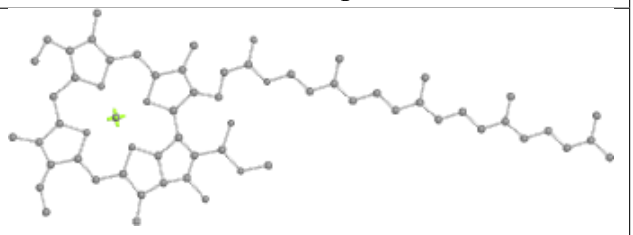
Bond lengths



Bond angles

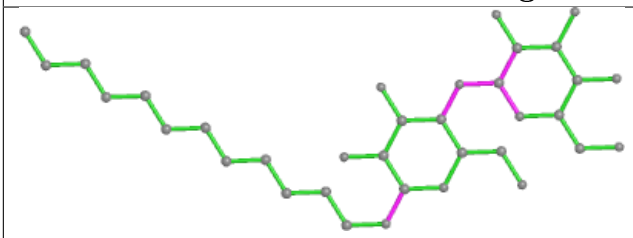


Torsions

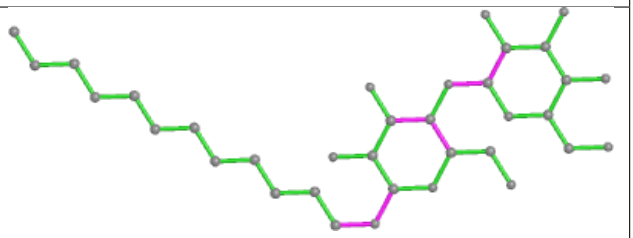


Rings

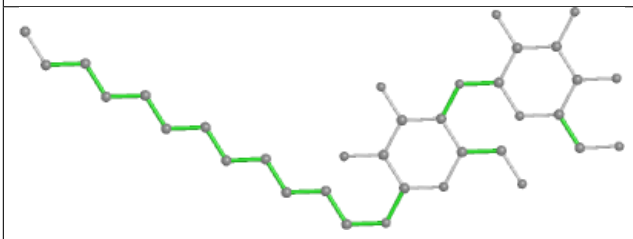
Ligand LMT t 5217



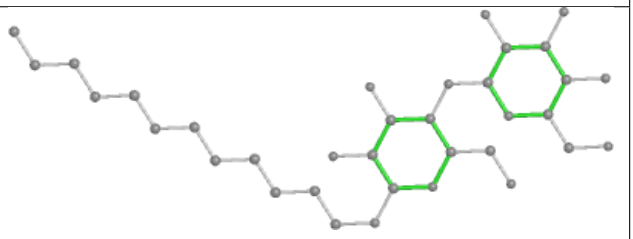
Bond lengths



Bond angles

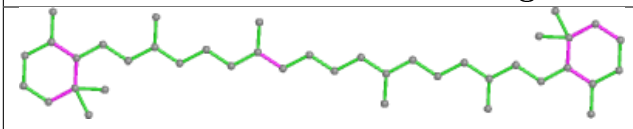


Torsions

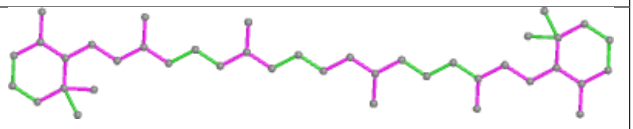


Rings

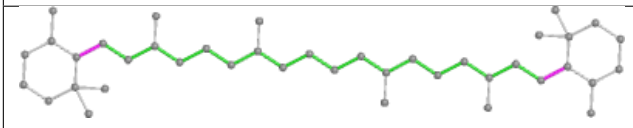
Ligand BCR a 5566



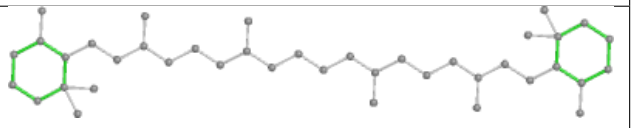
Bond lengths



Bond angles

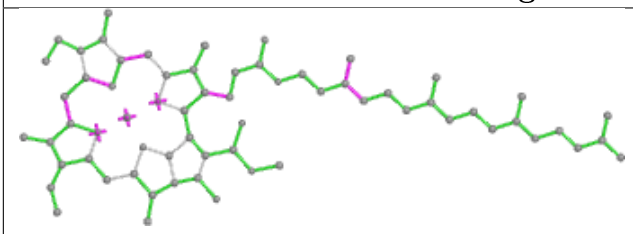


Torsions

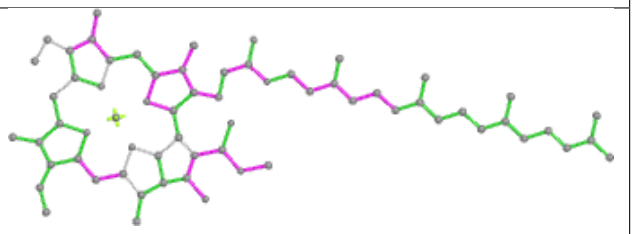


Rings

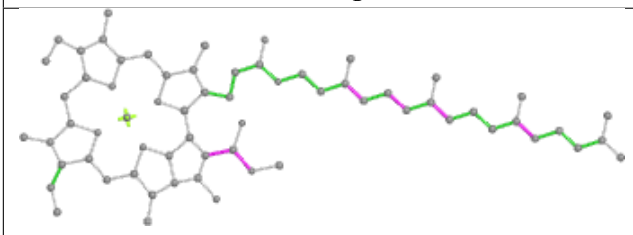
Ligand CLA b 5513



Bond lengths



Bond angles



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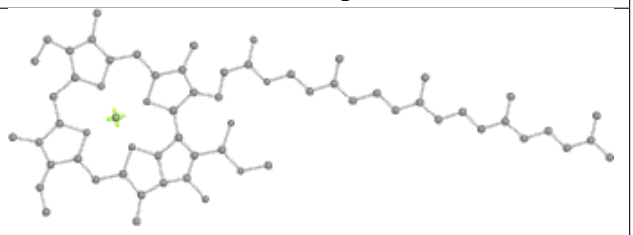
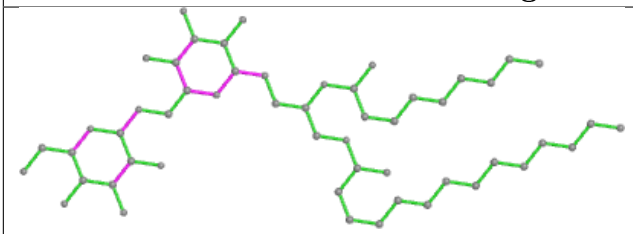
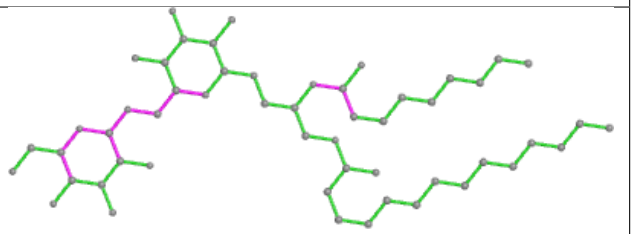


Rings

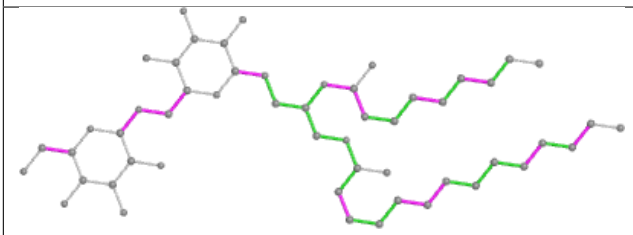
Ligand DGD C 507



Bond lengths



Bond angles



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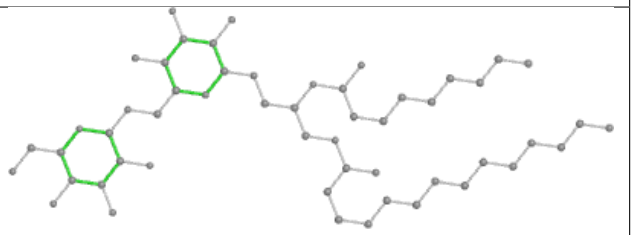
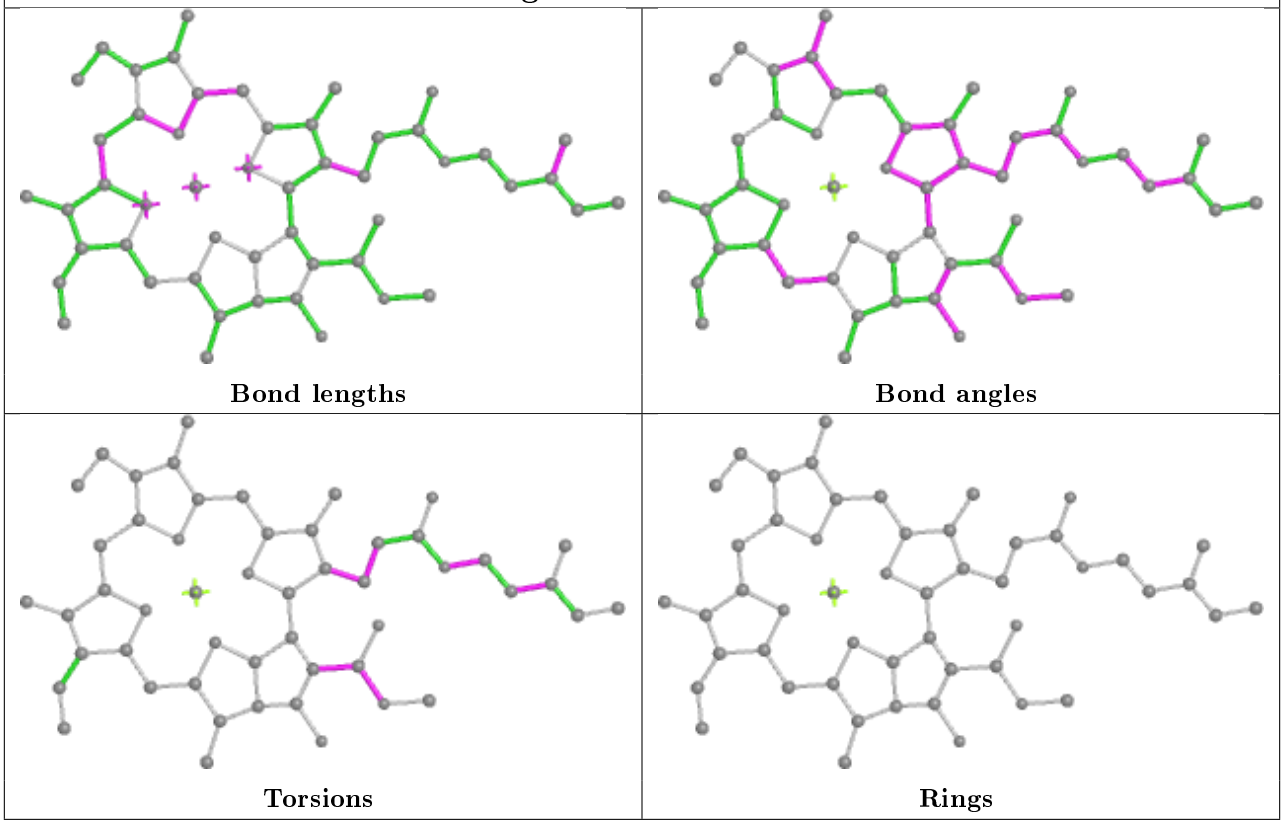
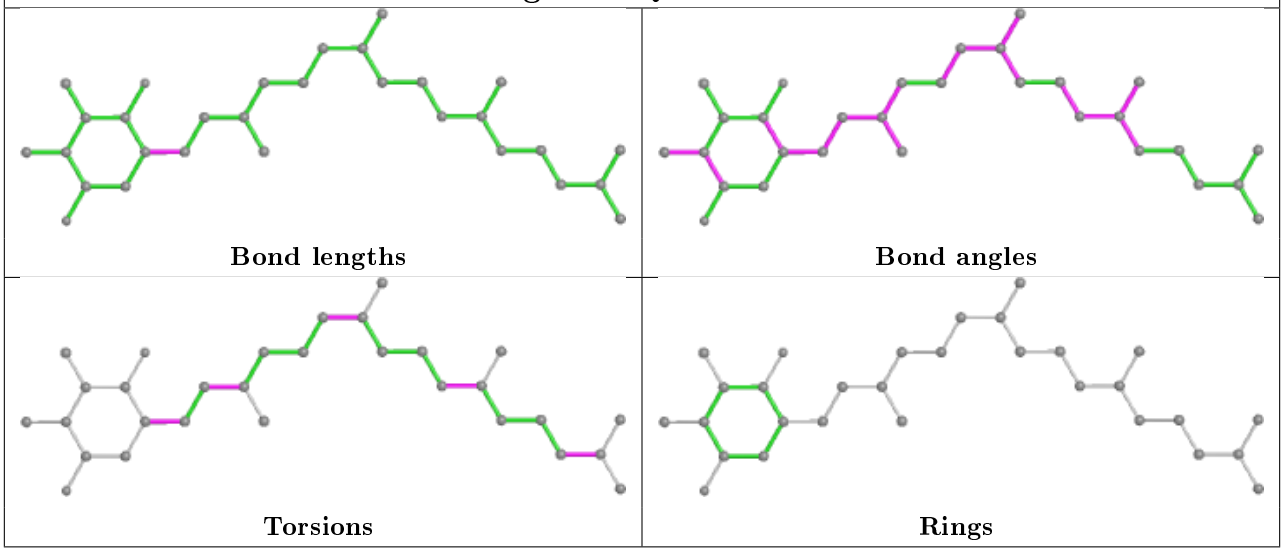


Rings

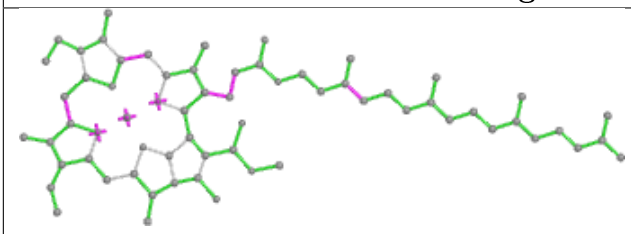
Ligand CLA c 5502



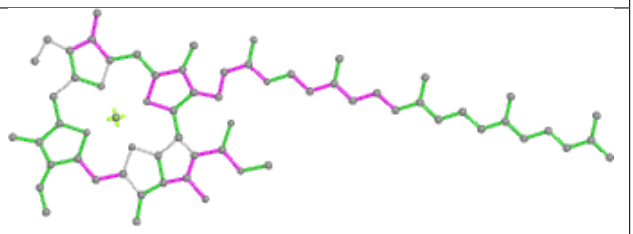
Ligand PQ9 a 5564



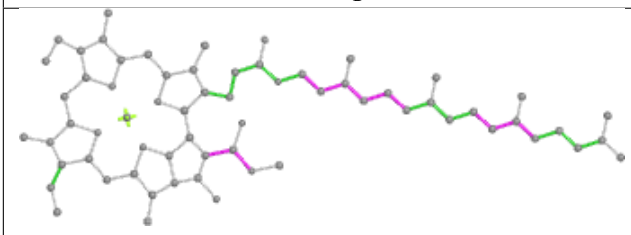
Ligand CLA b 5523



Bond lengths



Bond angles



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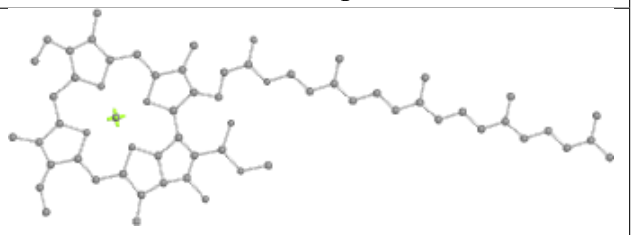
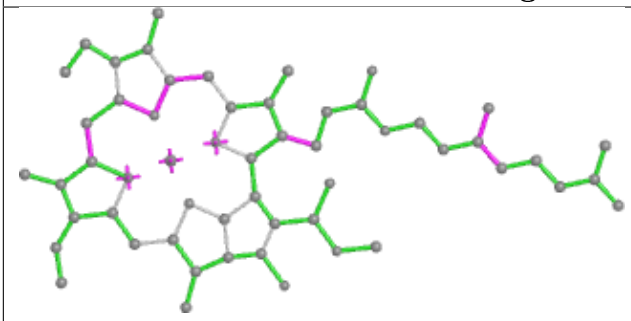
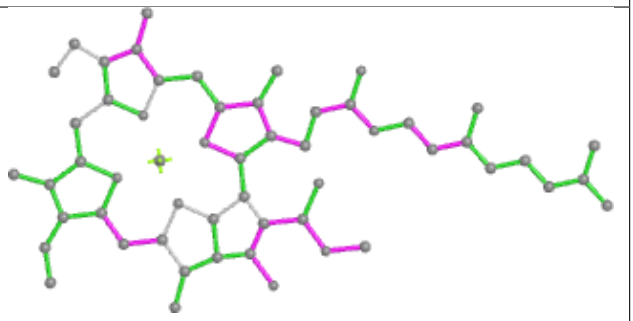


Rings

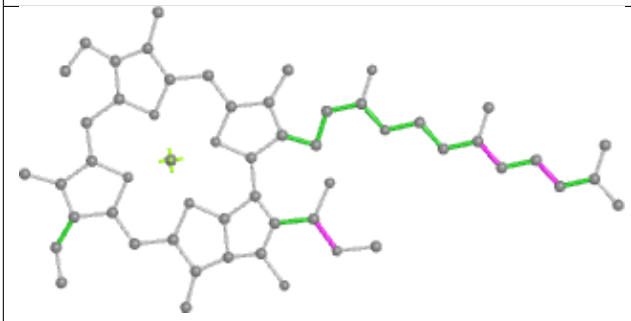
Ligand CLA a 5563



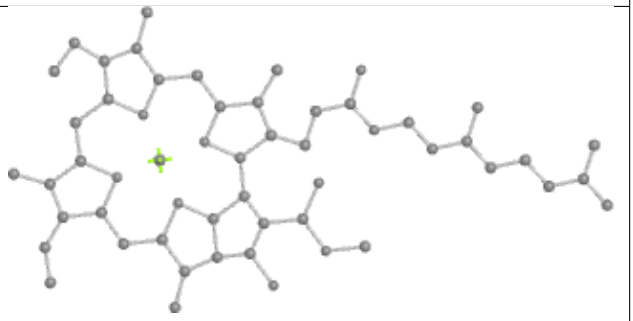
Bond lengths



Bond angles

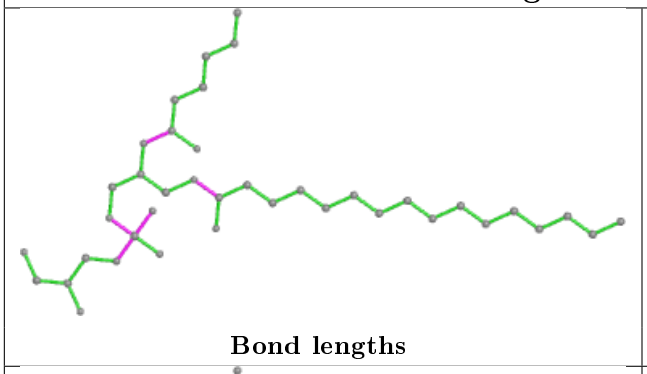


Torsions



Rings

Ligand LHG A 567



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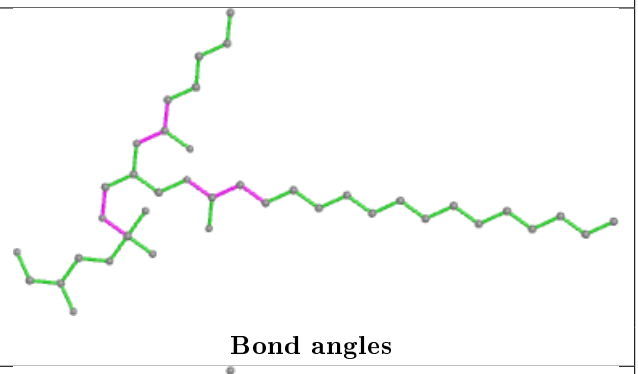
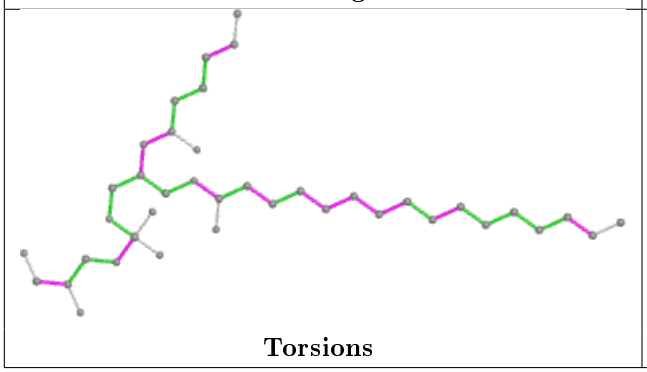


Bond angles



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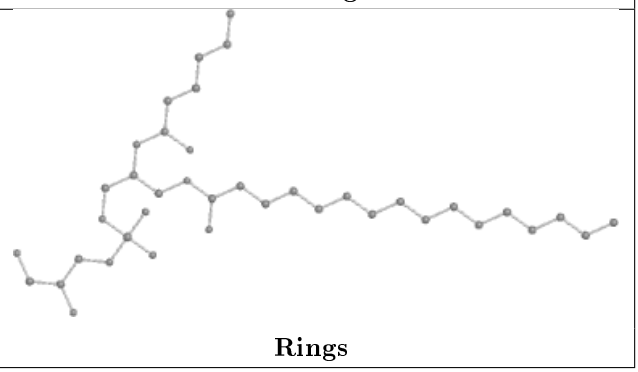
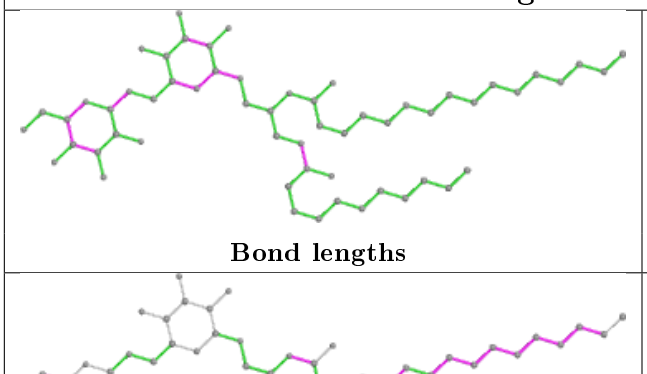
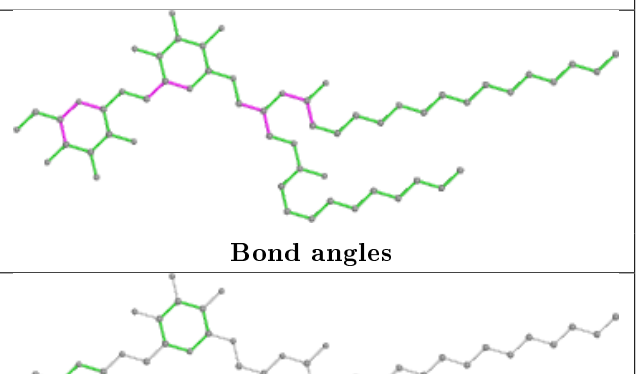


Rings

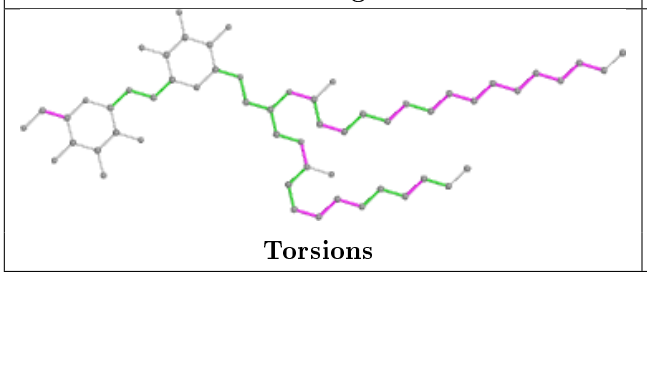
Ligand DGD c 5509



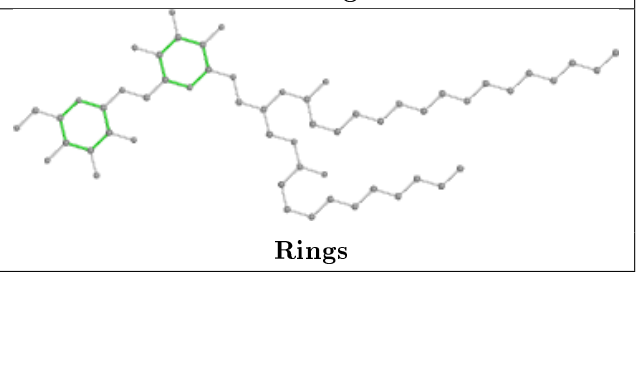
Bond lengths



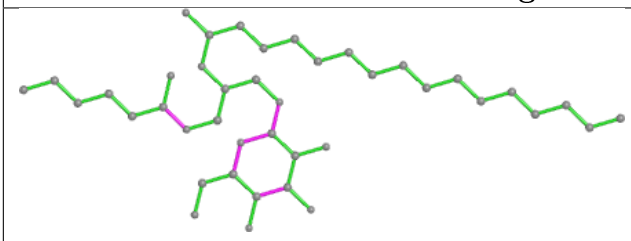
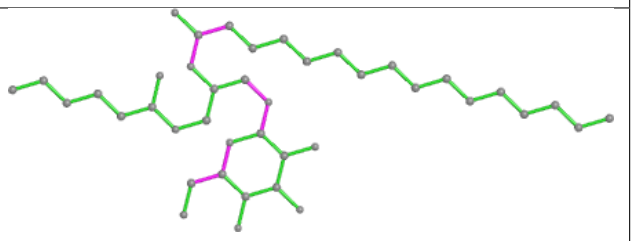
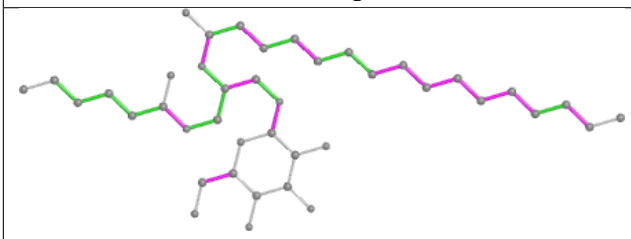
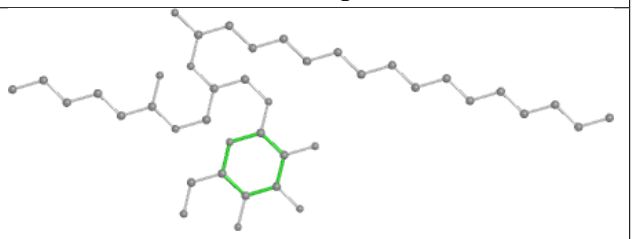
Bond angles

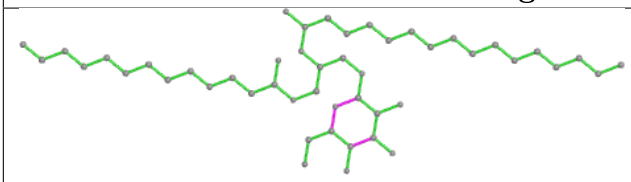
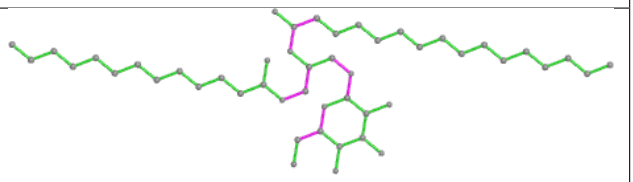
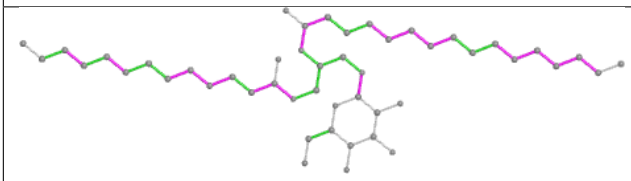
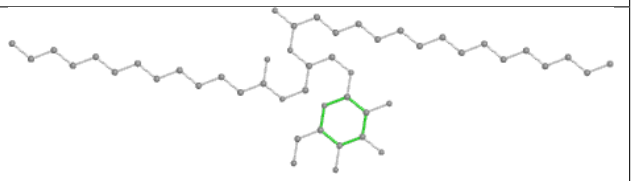


Torsions

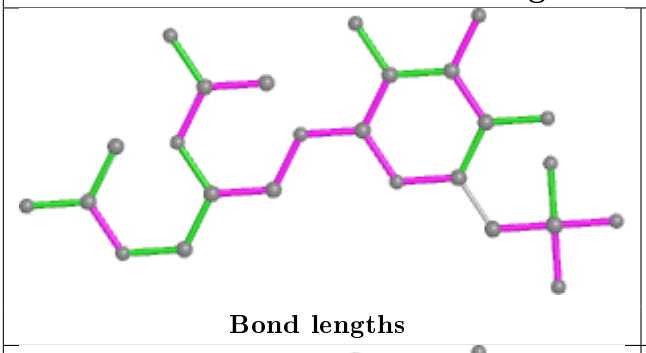


Rings

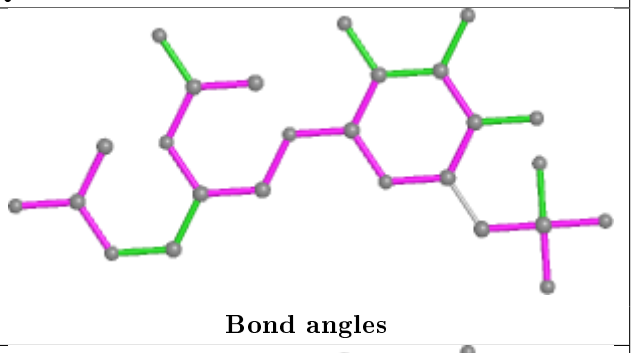
Ligand MGE D 359	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand MGE l 5210	
	
Bond lengths	Bond angles
	
Torsions	Rings

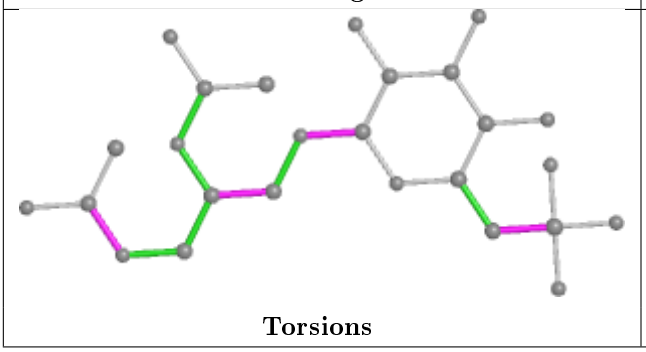
Ligand SQD a 212



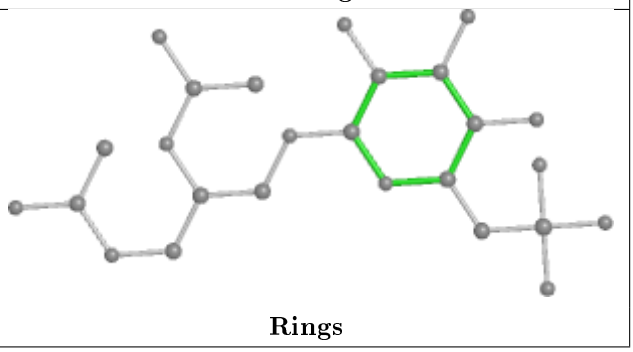
Bond lengths



Bond angles

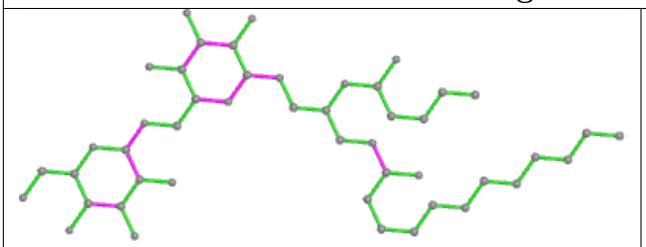


Torsions

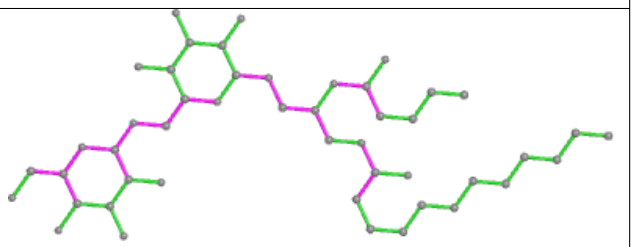


Rings

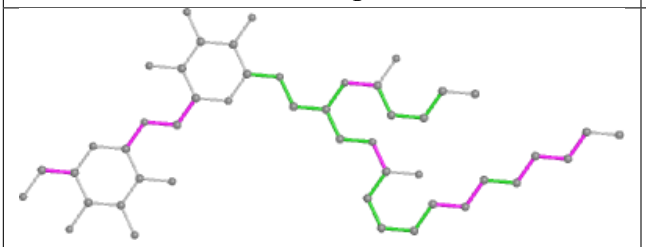
Ligand DGD c 5508



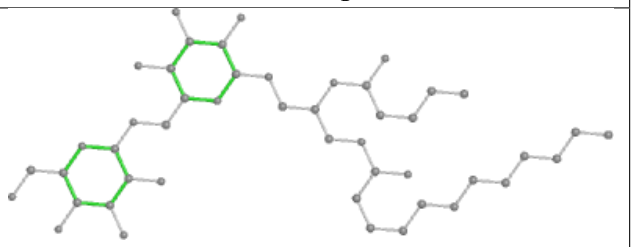
Bond lengths



Bond angles

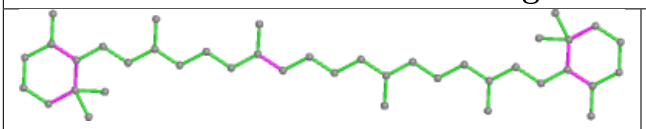


Torsions

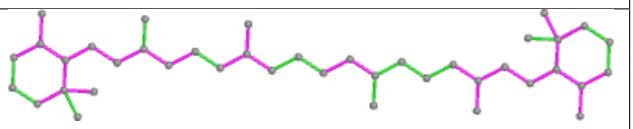


Rings

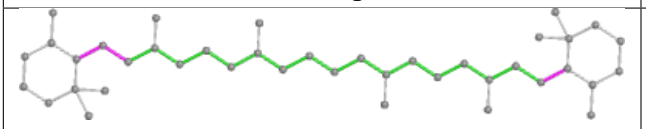
Ligand BCR C 504



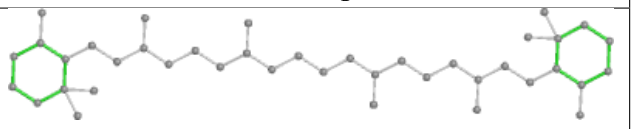
Bond lengths



Bond angles

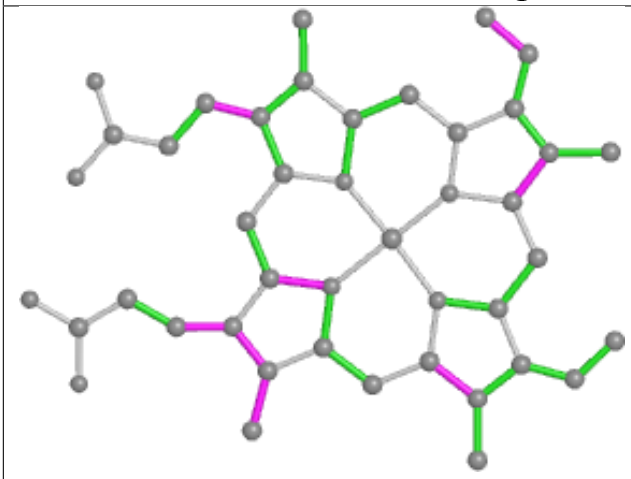


Torsions

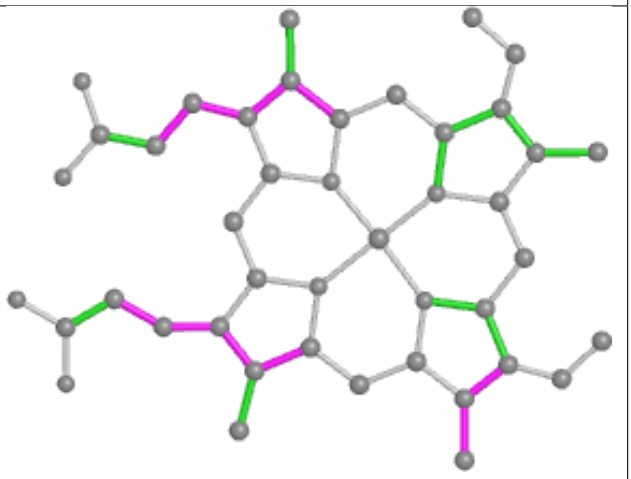


Rings

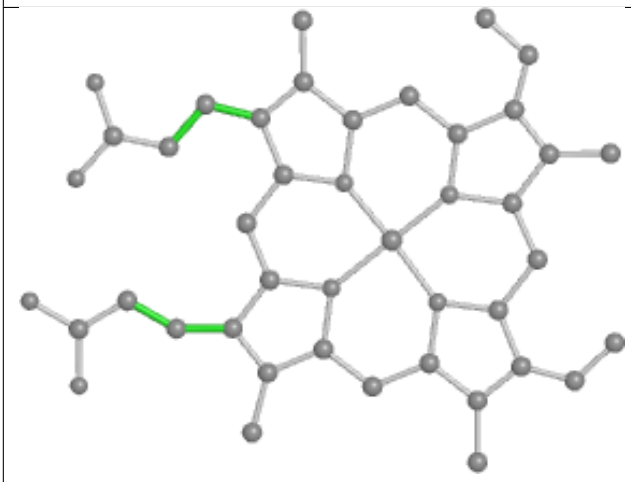
Ligand HEM v 5552



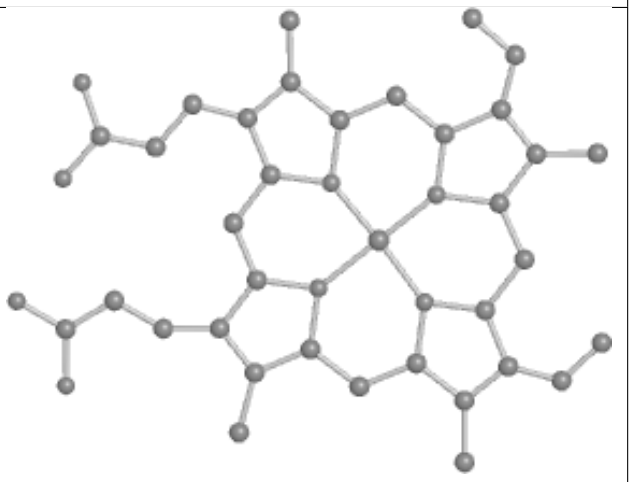
Bond lengths



Bond angles

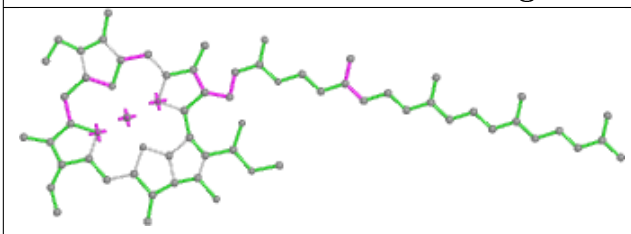


Torsions

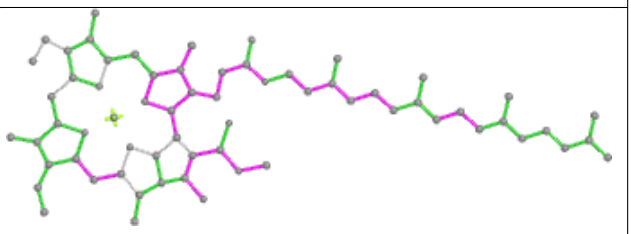


Rings

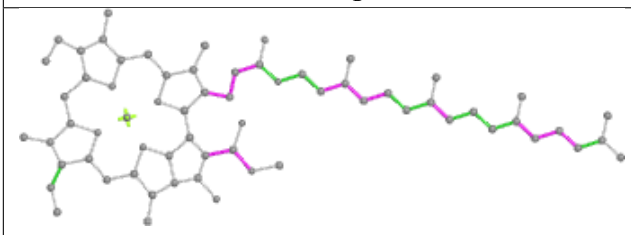
Ligand CLA b 5515



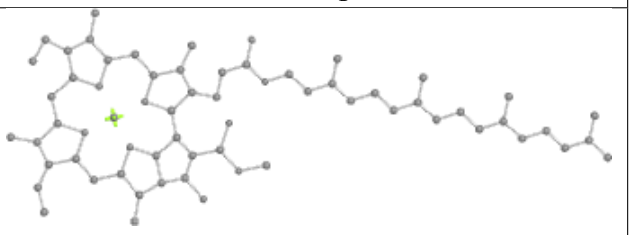
Bond lengths



Bond angles

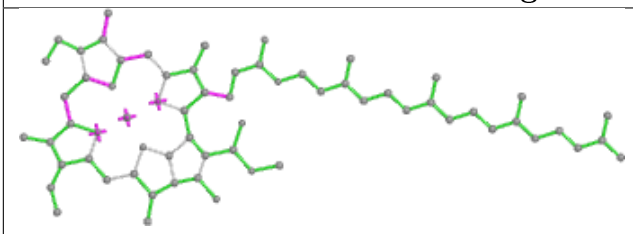


Torsions

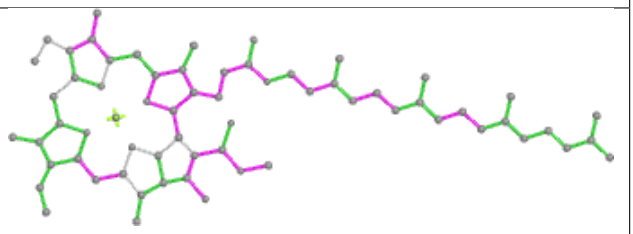


Rings

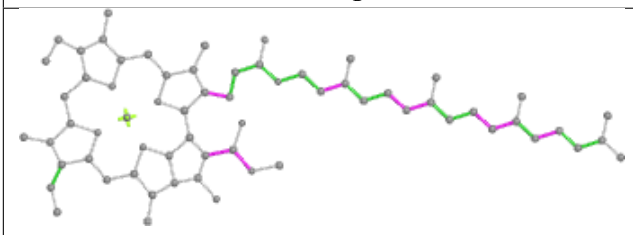
Ligand CLA c 5493



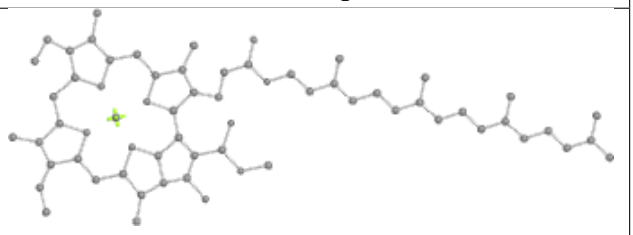
Bond lengths



Bond angles

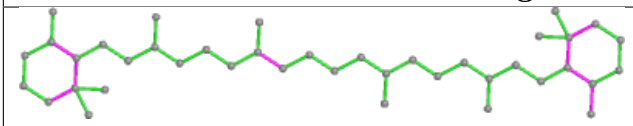


Torsions

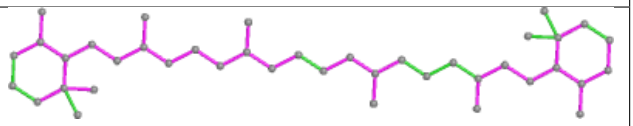


Rings

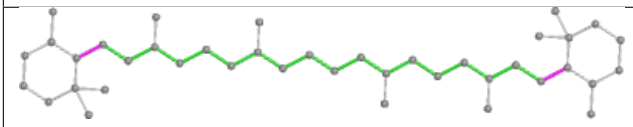
Ligand BCR h 5107



Bond lengths



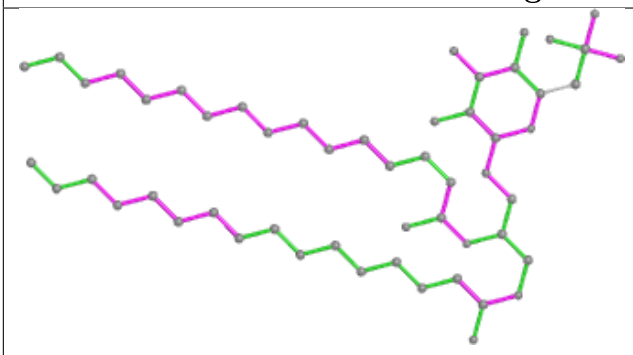
Bond angles



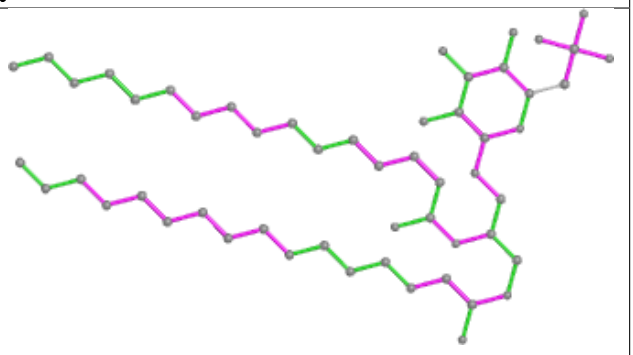
Torsions

Rings

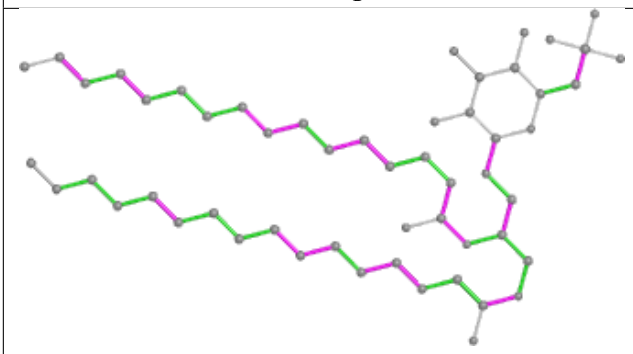
Ligand SQD A 568



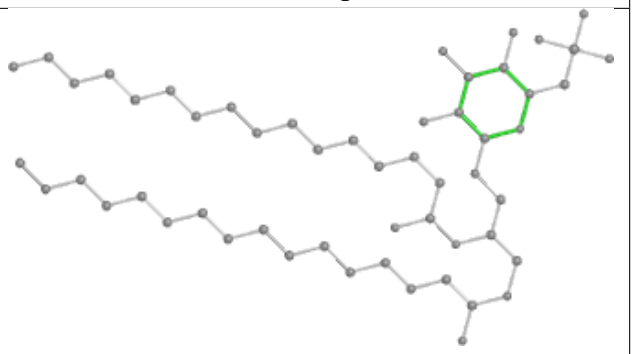
Bond lengths



Bond angles

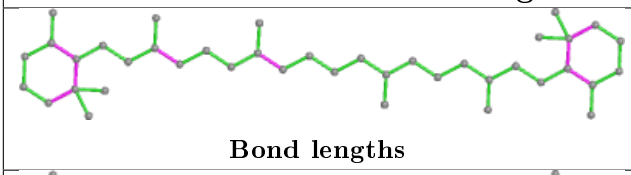


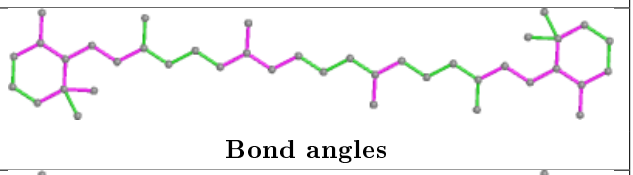
Torsions

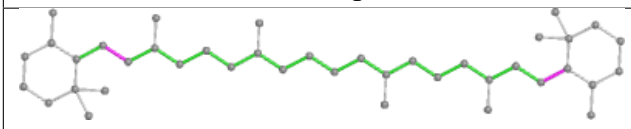


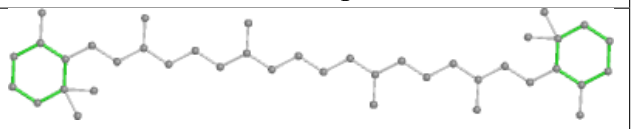
Rings

Ligand BCR b 5529

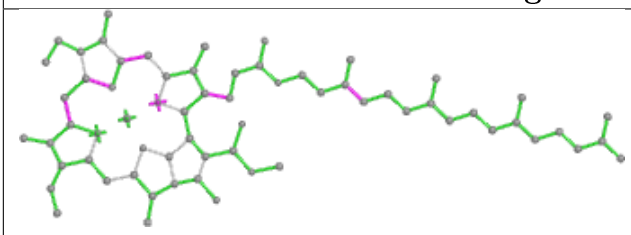

Bond lengths

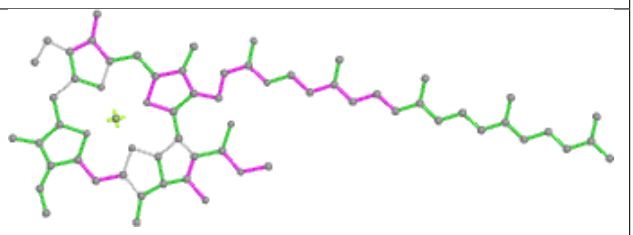

Bond angles

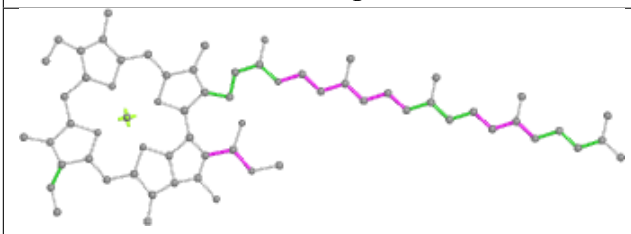

Torsions

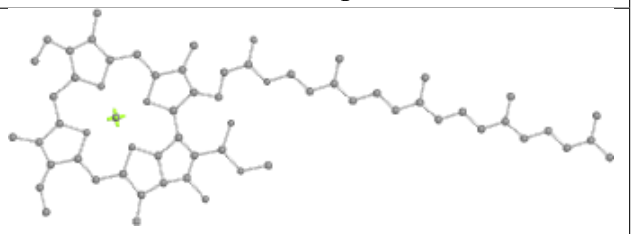

Rings

Ligand CLA B 523

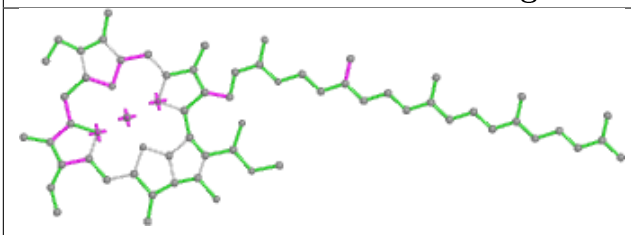

Bond lengths

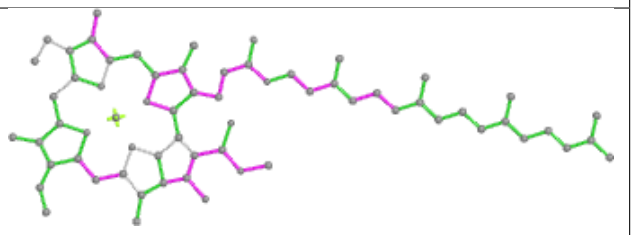

Bond angles

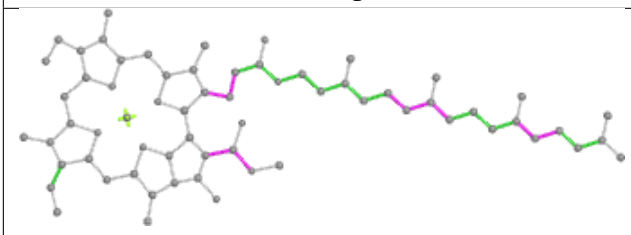

Torsions

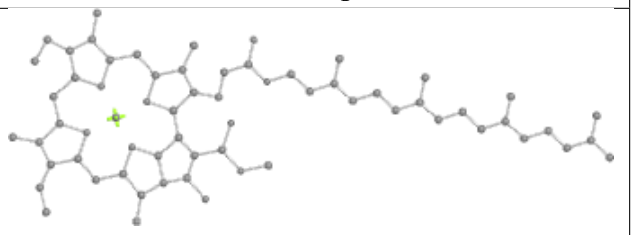

Rings

Ligand CLA c 5496

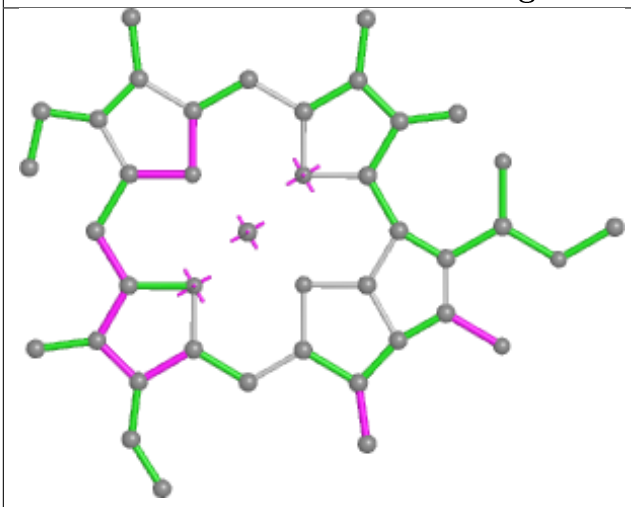

Bond lengths


Bond angles

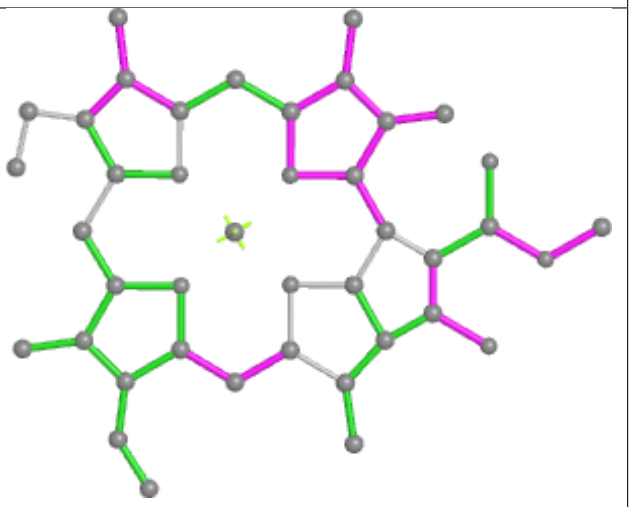

Torsions


Rings

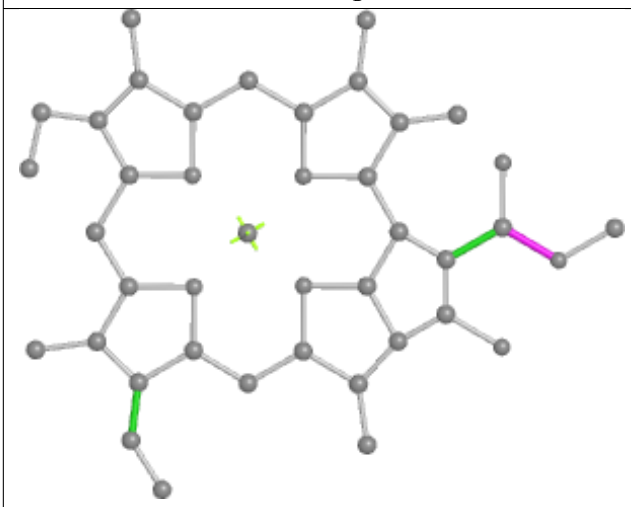
Ligand CLA b 5511



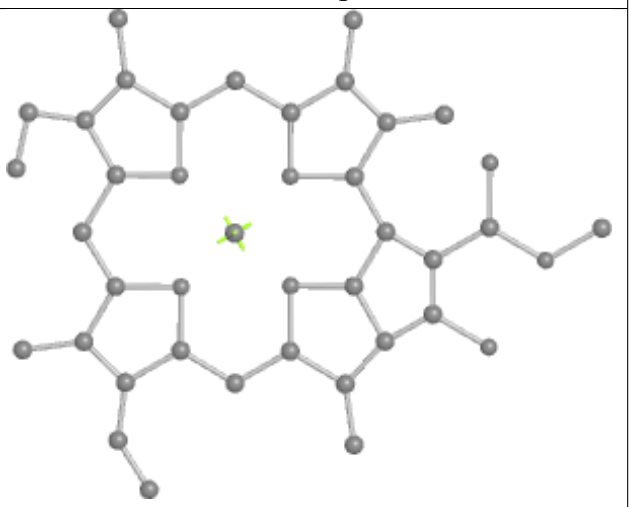
Bond lengths



Bond angles

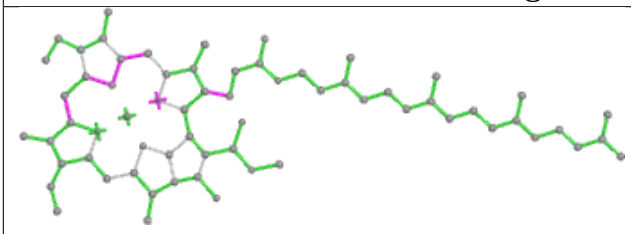


Torsions

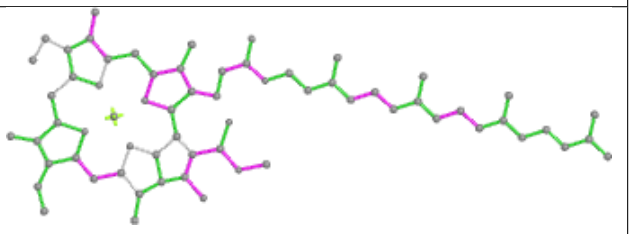


Rings

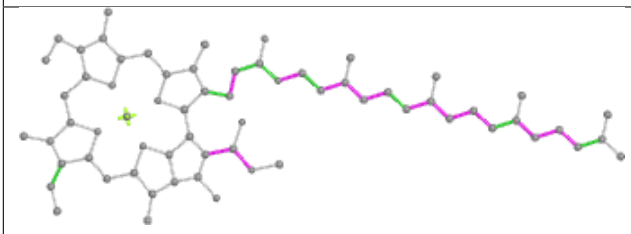
Ligand CLA C 498



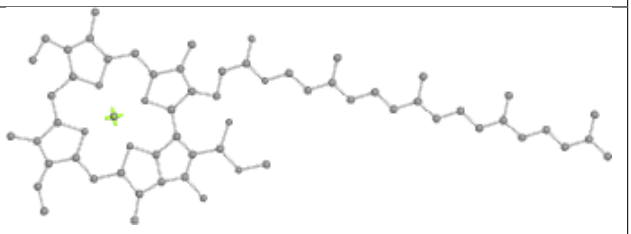
Bond lengths



Bond angles

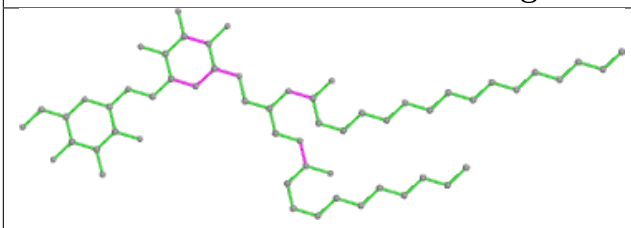


Torsions

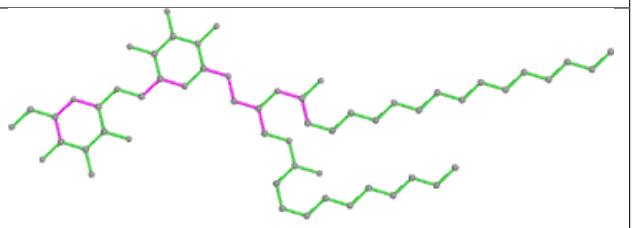


Rings

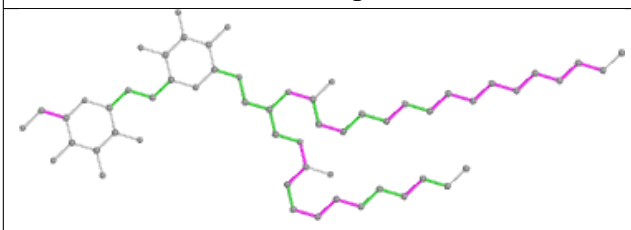
Ligand DGD C 509



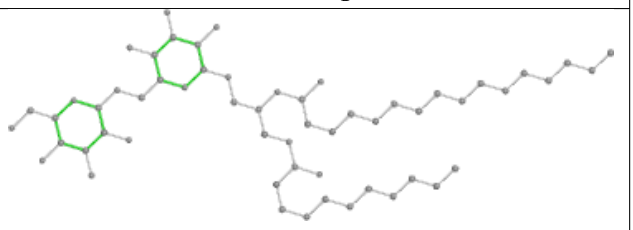
Bond lengths



Bond angles

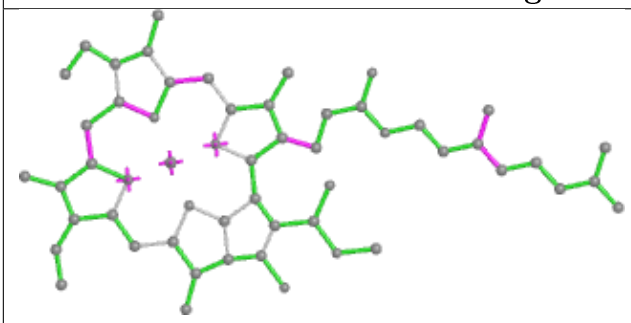


Torsions

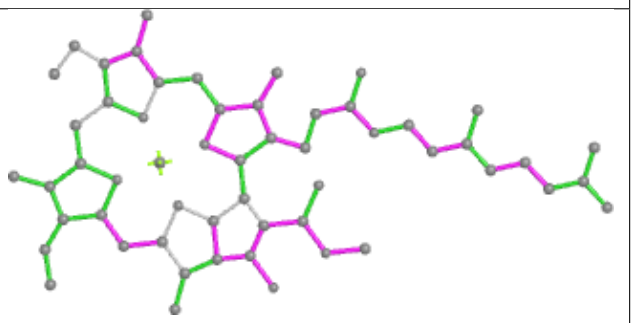


Rings

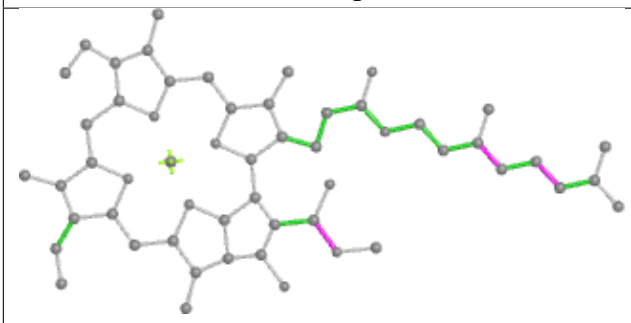
Ligand CLA A 563



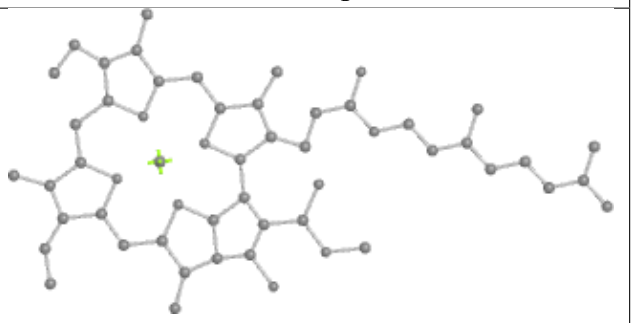
Bond lengths



Bond angles

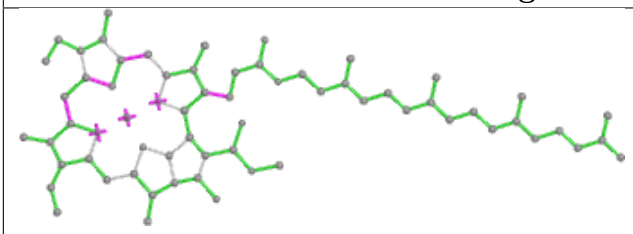


Torsions

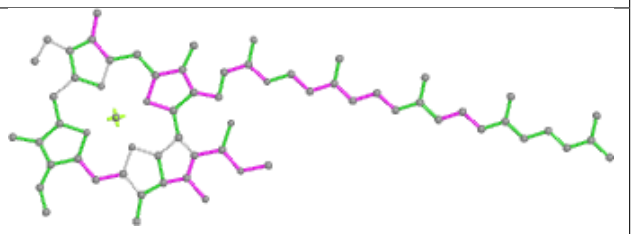


Rings

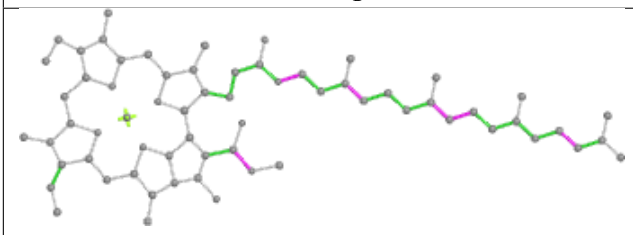
Ligand CLA b 5521



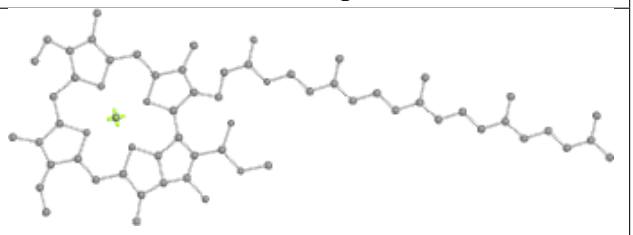
Bond lengths



Bond angles

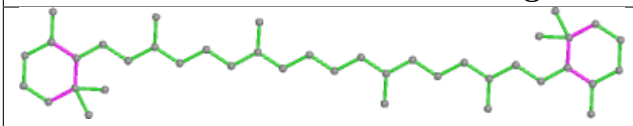


Torsions

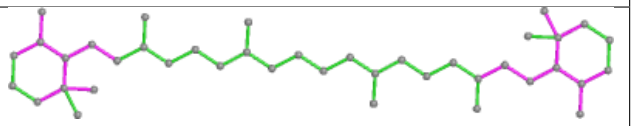


Rings

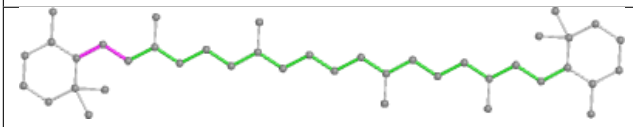
Ligand BCR B 528



Bond lengths



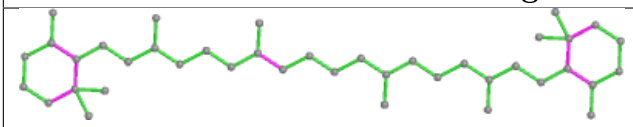
Bond angles



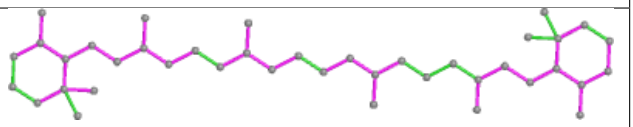
Torsions

Rings

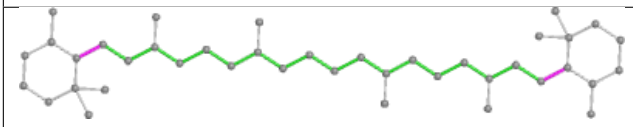
Ligand BCR H 107



Bond lengths



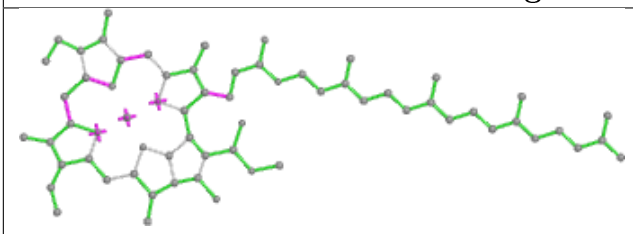
Bond angles



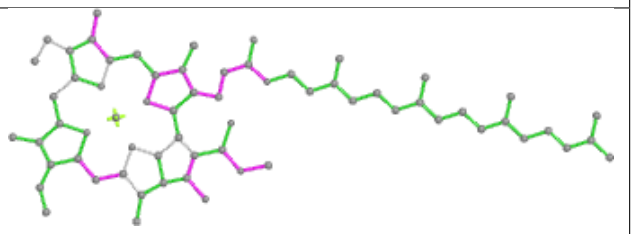
Torsions

Rings

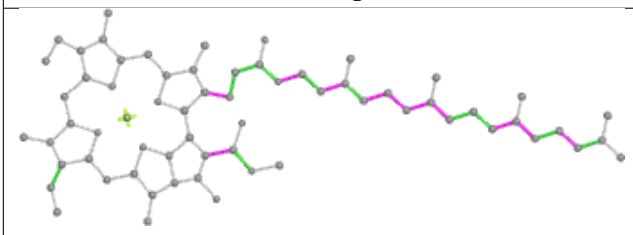
Ligand CLA A 559



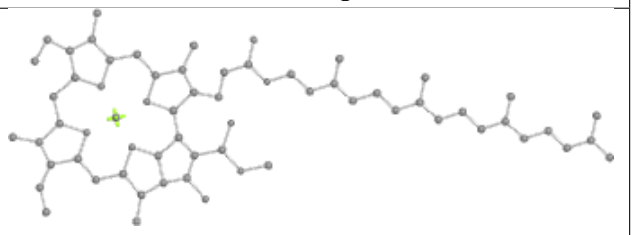
Bond lengths



Bond angles

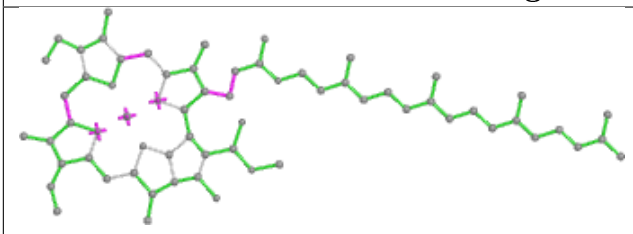


Torsions

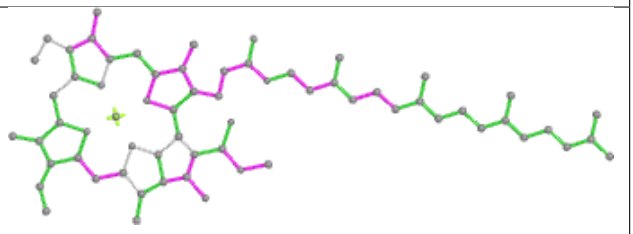


Rings

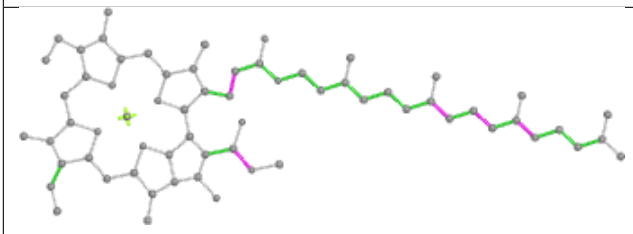
Ligand CLA A 558



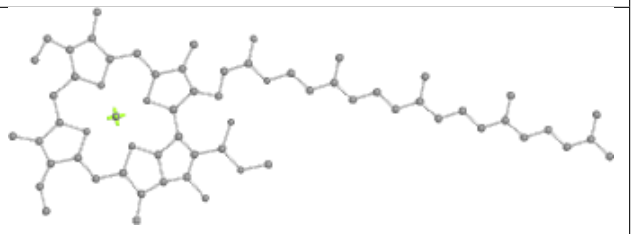
Bond lengths



Bond angles

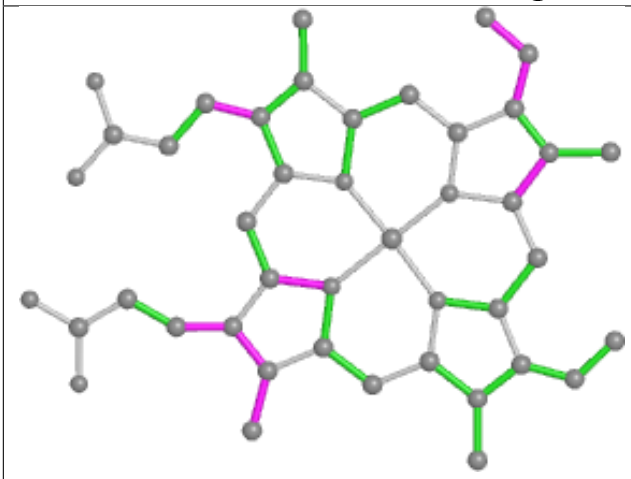


Torsions

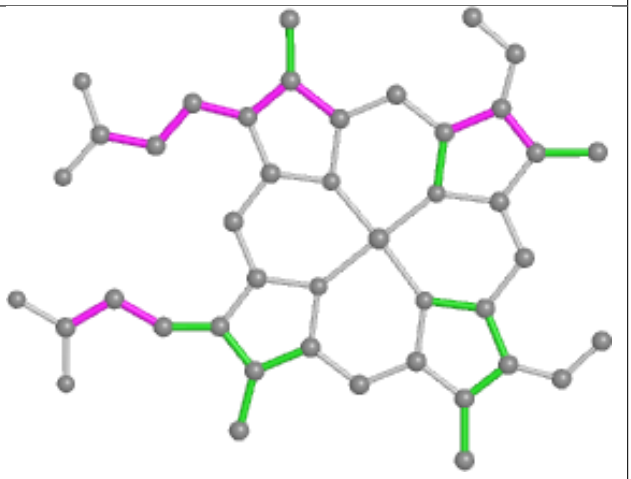


Rings

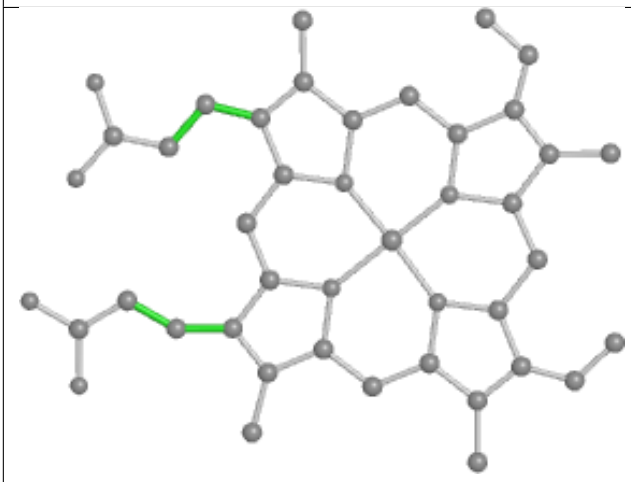
Ligand HEM F 51



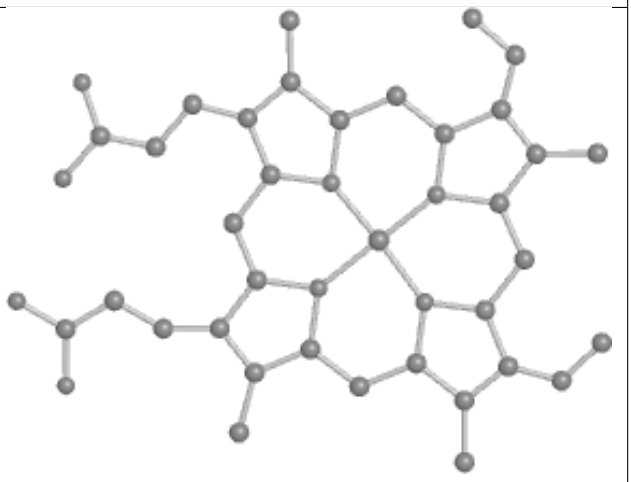
Bond lengths



Bond angles

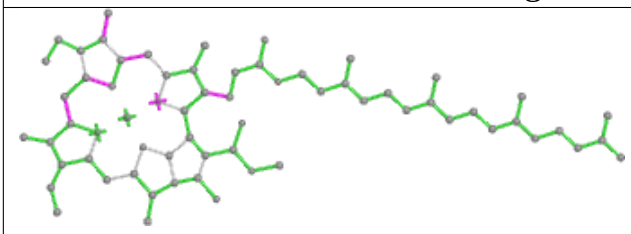


Torsions

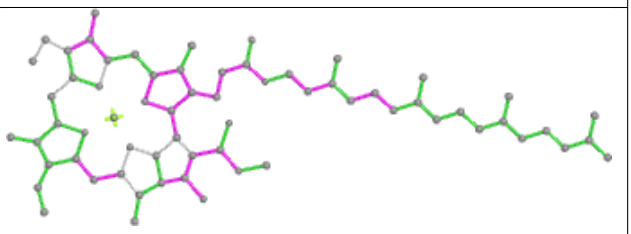


Rings

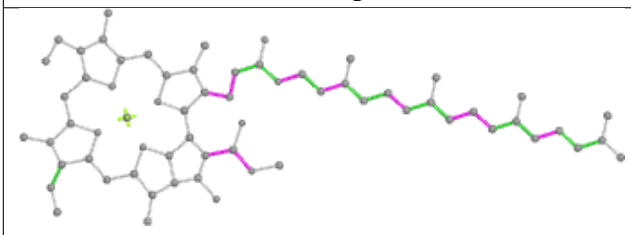
Ligand CLA B 517



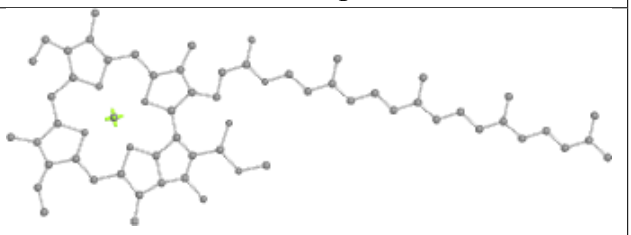
Bond lengths



Bond angles

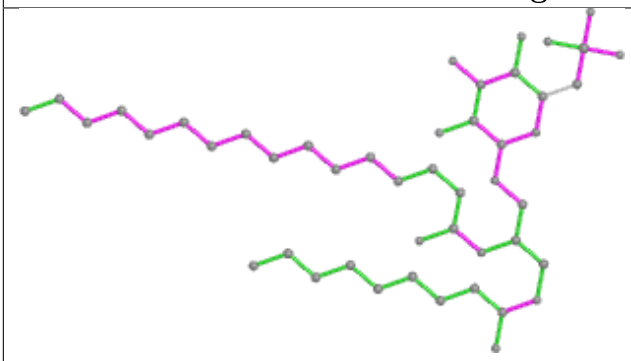


Torsions

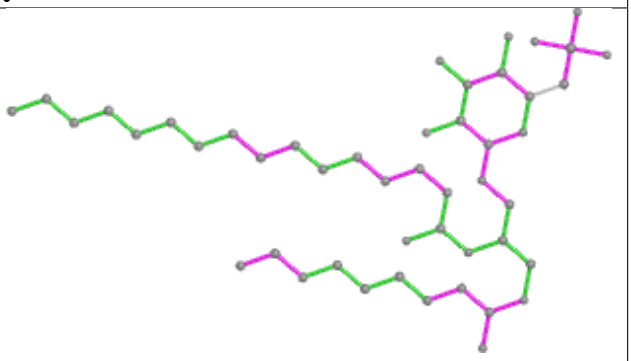


Rings

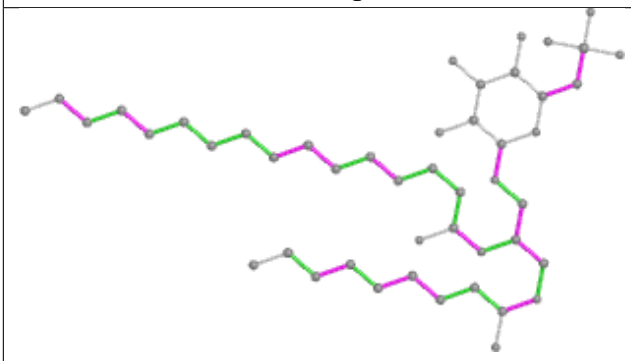
Ligand SQD t 213



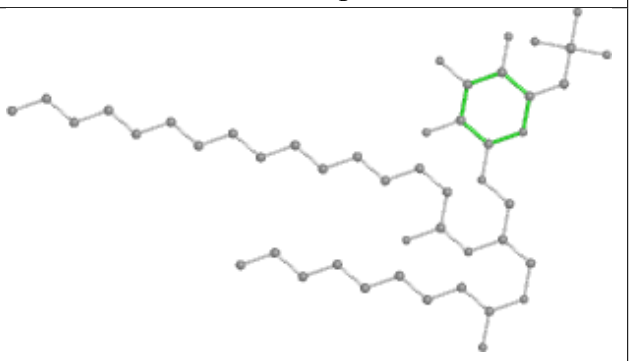
Bond lengths



Bond angles

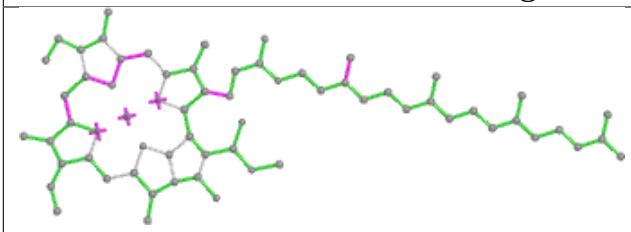


Torsions

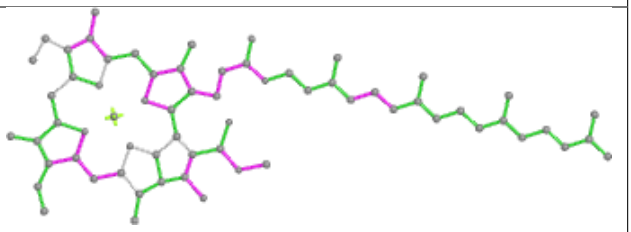


Rings

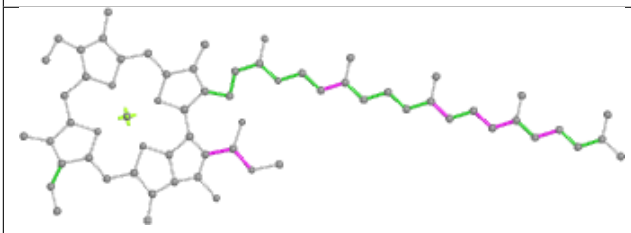
Ligand CLA a 5560



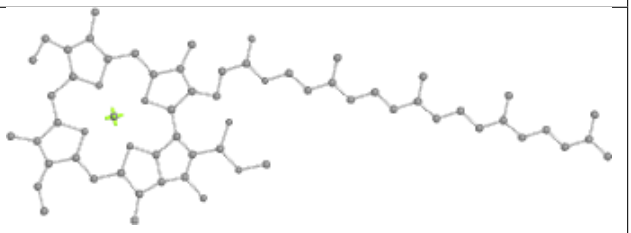
Bond lengths



Bond angles

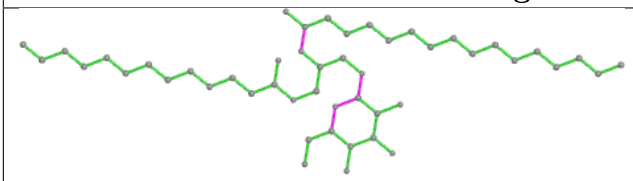


Torsions

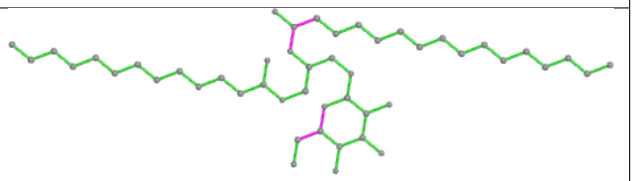


Rings

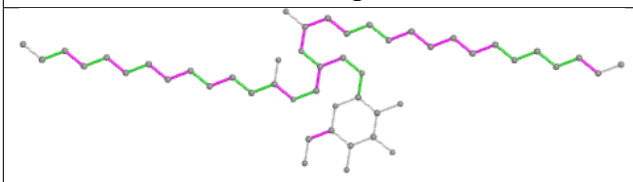
Ligand MGE d 5361



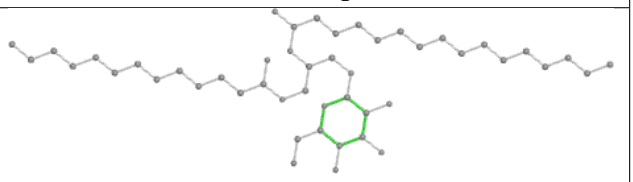
Bond lengths



Bond angles

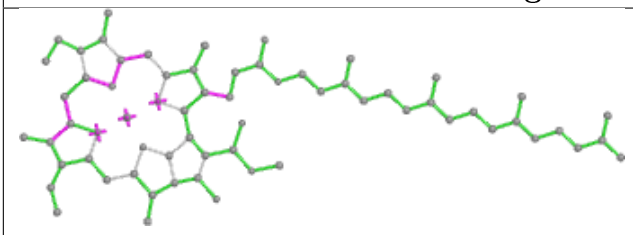


Torsions

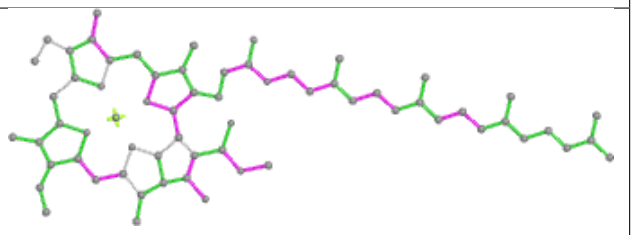


Rings

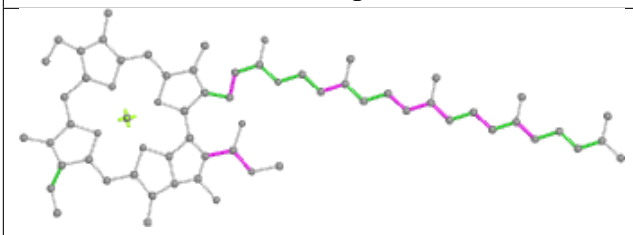
Ligand CLA C 501



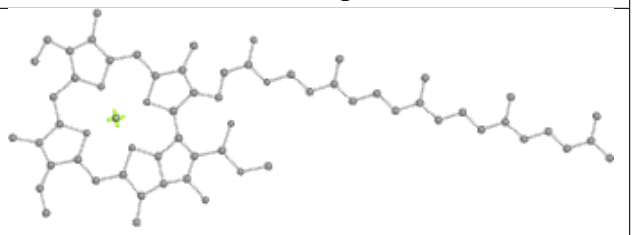
Bond lengths



Bond angles

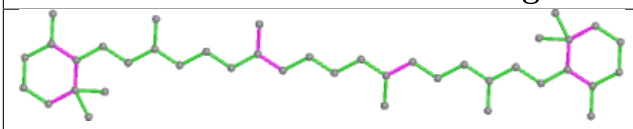


Torsions

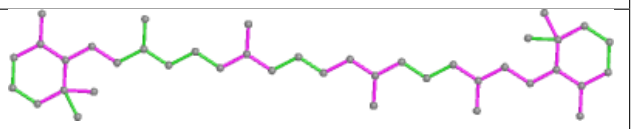


Rings

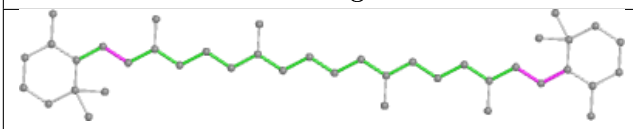
Ligand BCR C 506



Bond lengths



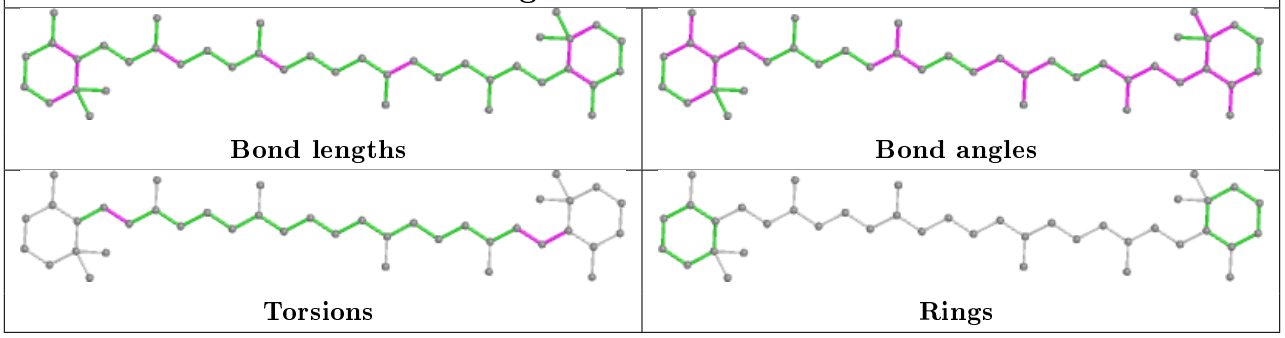
Bond angles



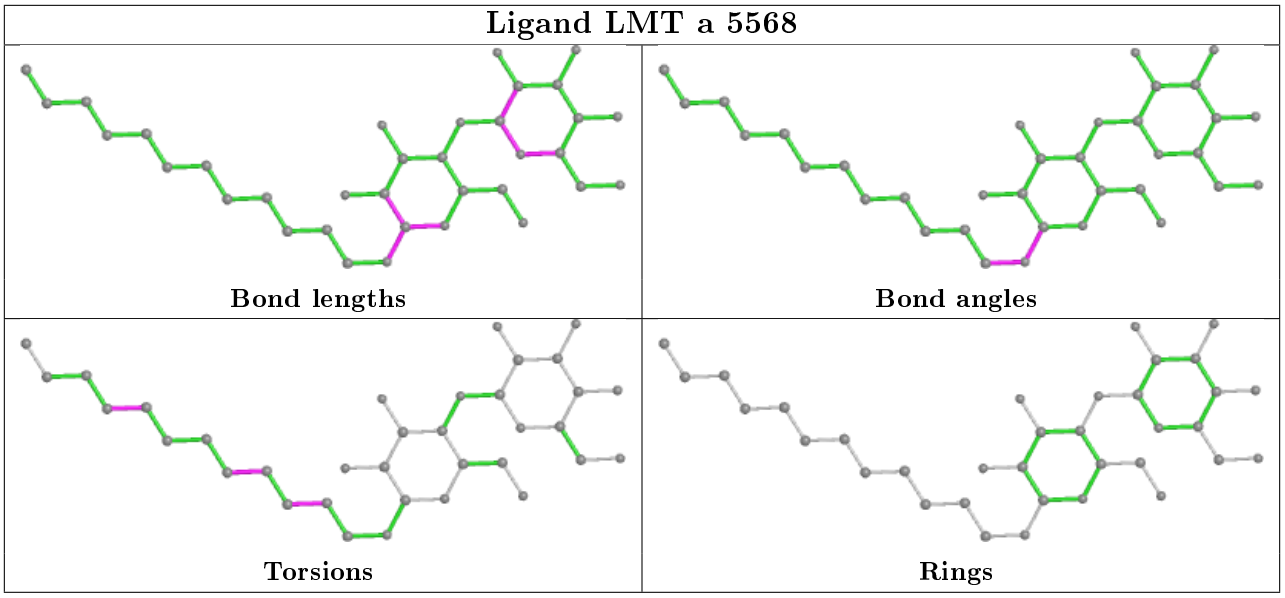
Torsions

Rings

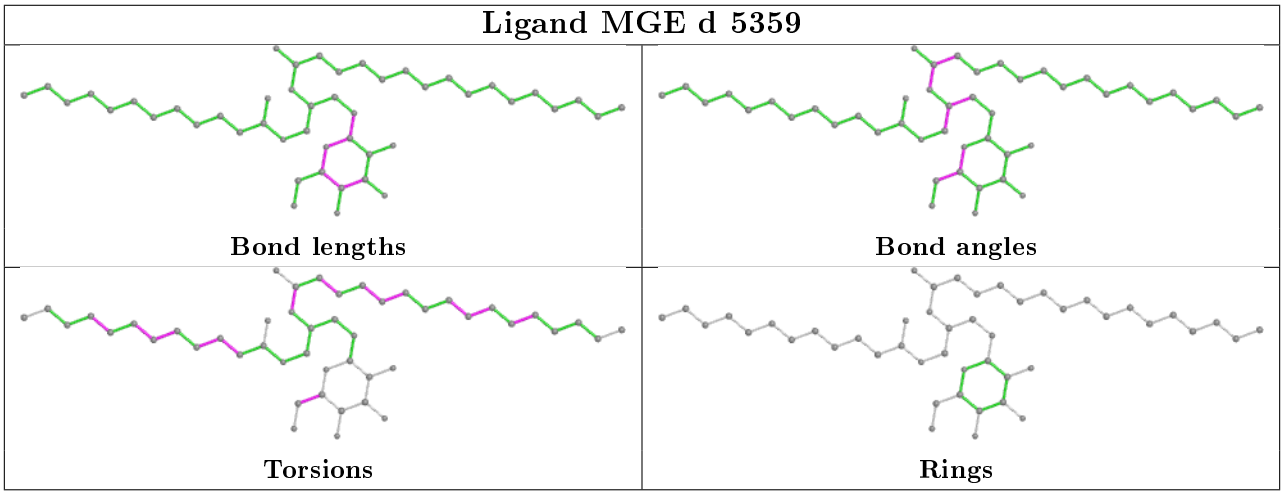
Ligand BCR c 5506



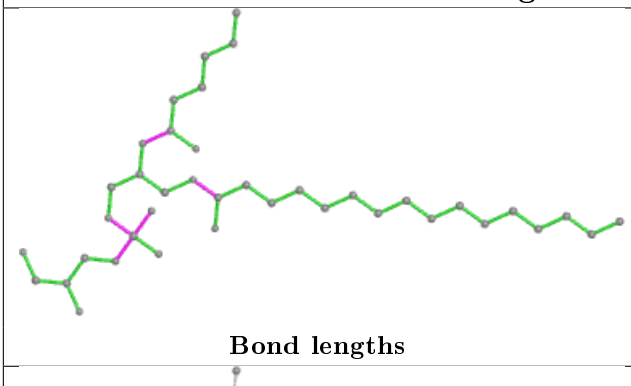
Ligand LMT a 5568



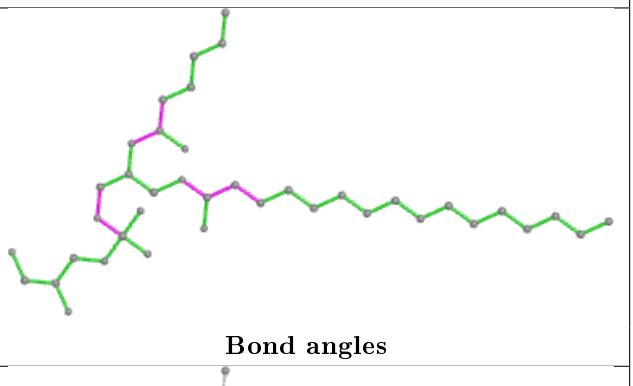
Ligand MGE d 5359



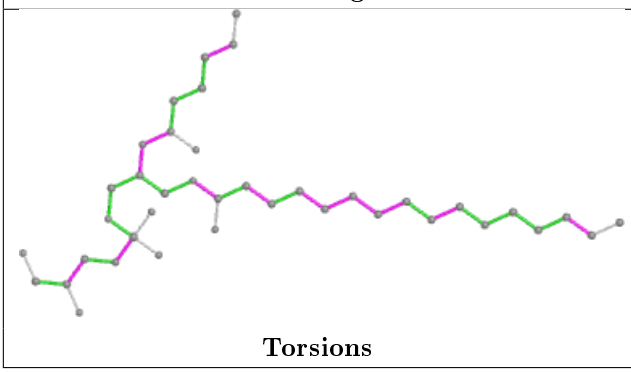
Ligand LHG a 5567



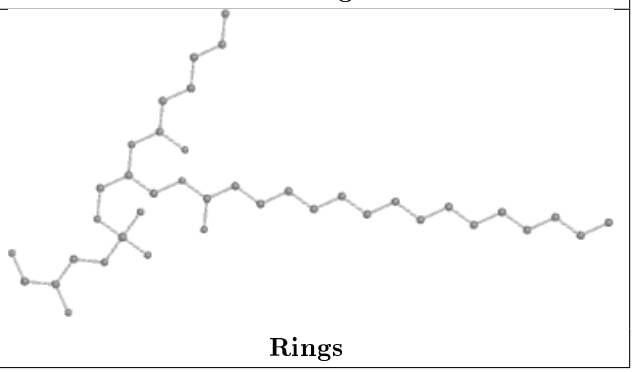
Bond lengths



Bond angles

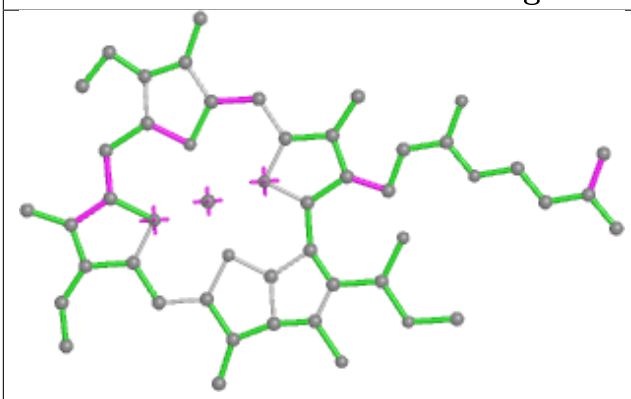


Torsions

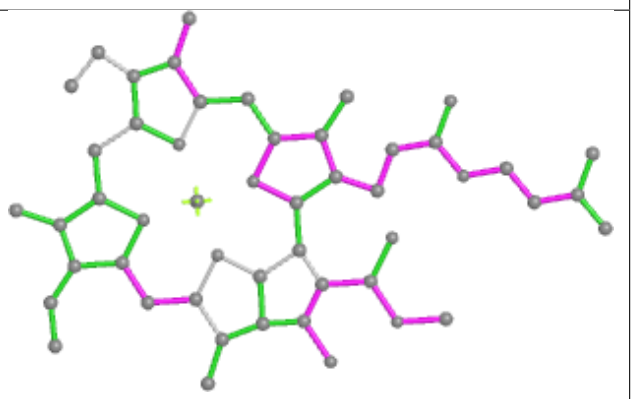


Rings

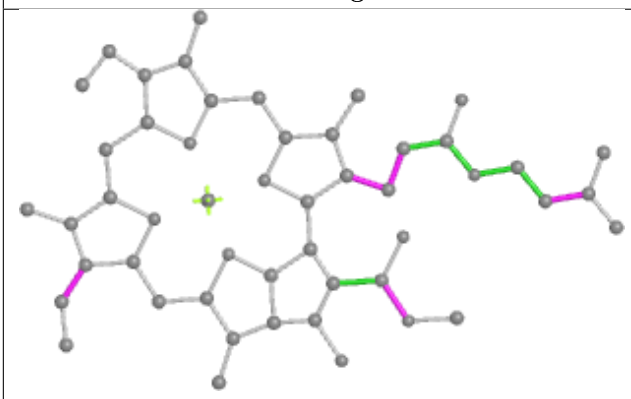
Ligand CLA D 355



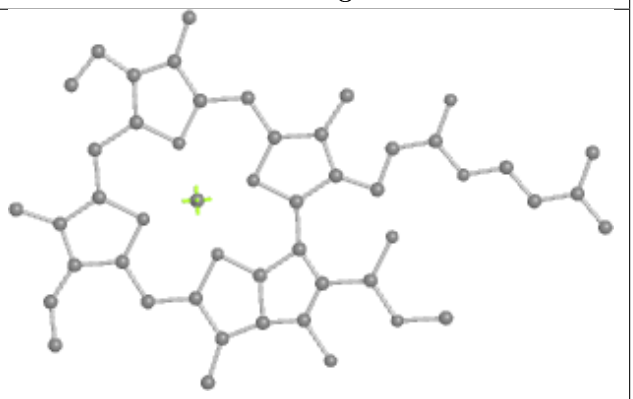
Bond lengths



Bond angles

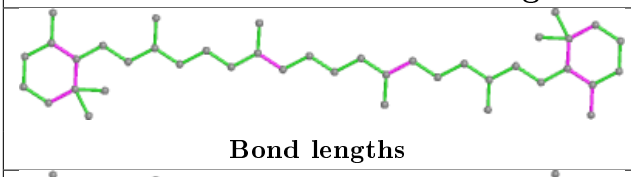


Torsions

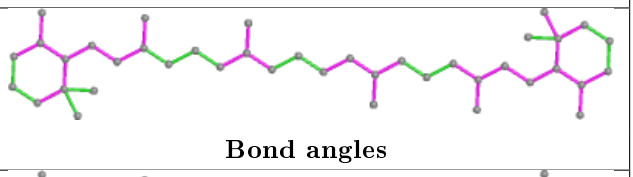


Rings

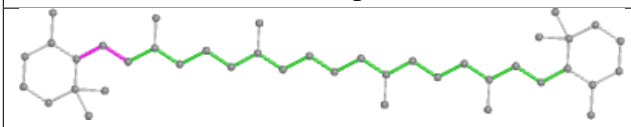
Ligand BCR D 357



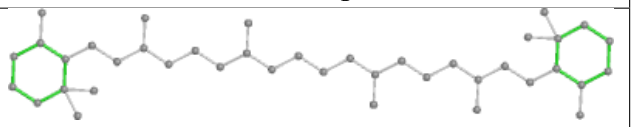
Bond lengths



Bond angles

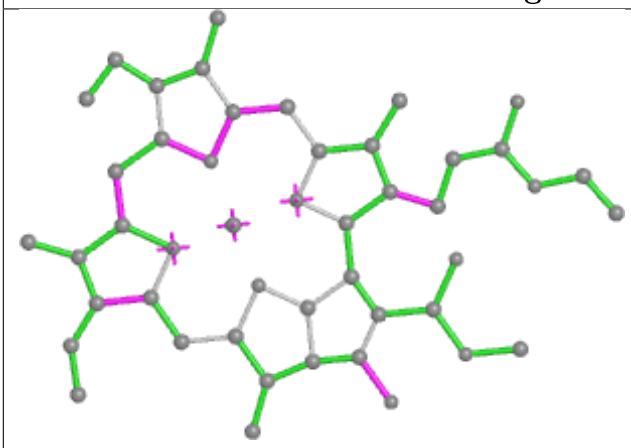


Torsions

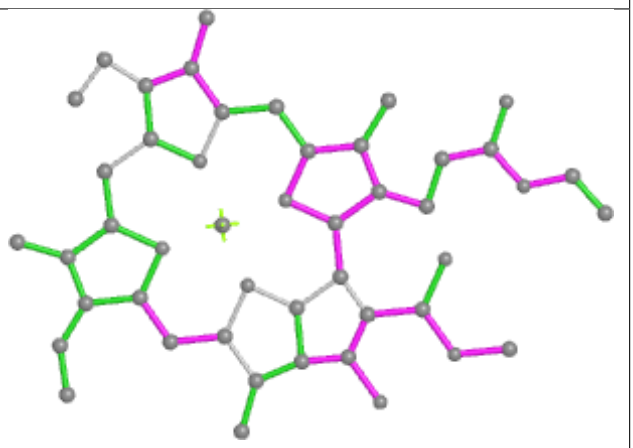


Rings

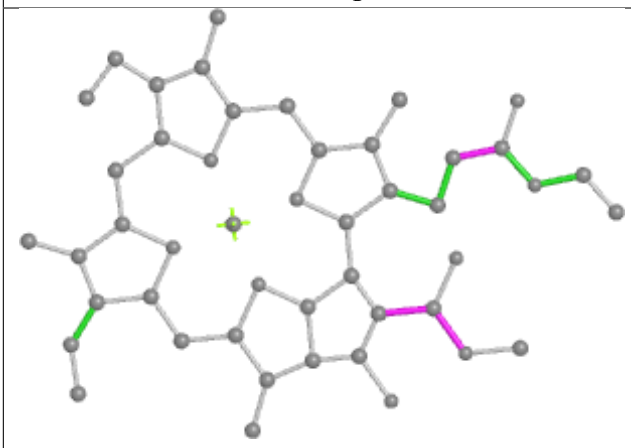
Ligand CLA C 499



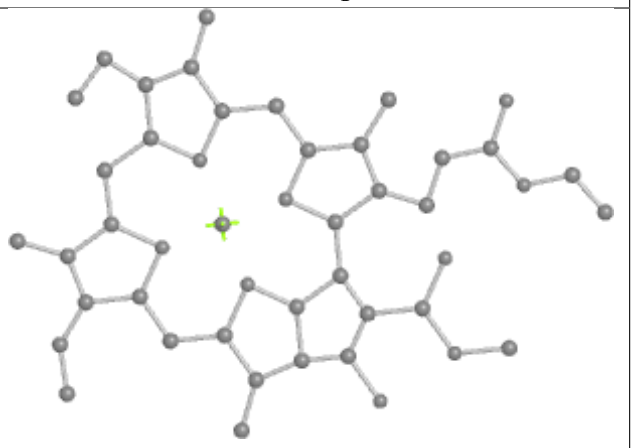
Bond lengths



Bond angles

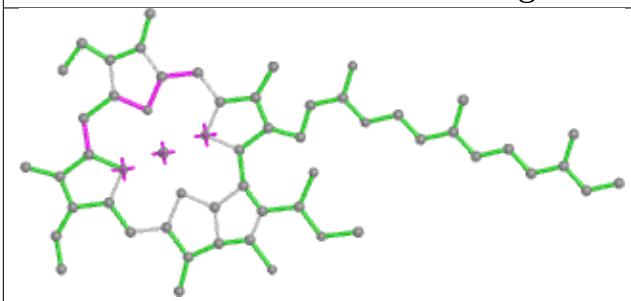


Torsions

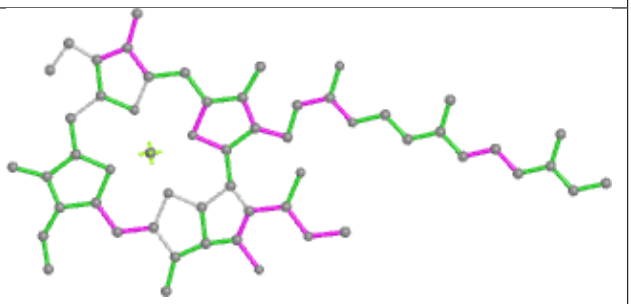


Rings

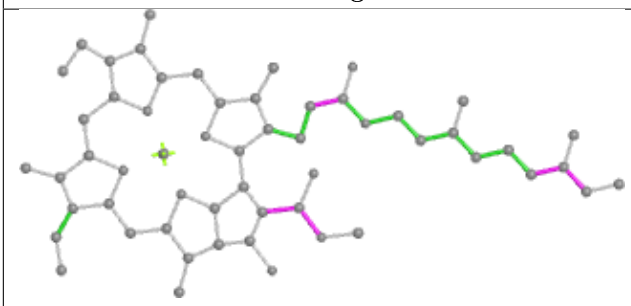
Ligand CLA b 5524



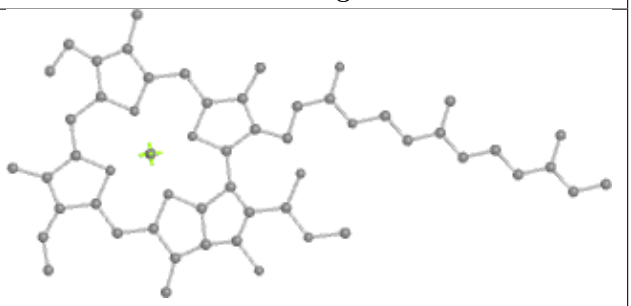
Bond lengths



Bond angles

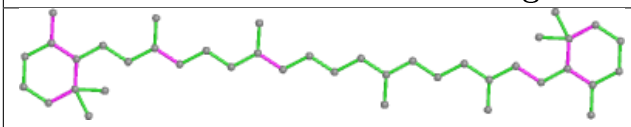


Torsions

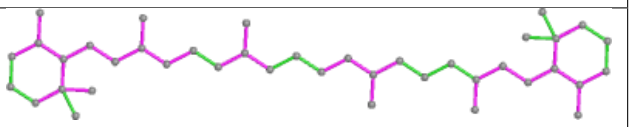


Rings

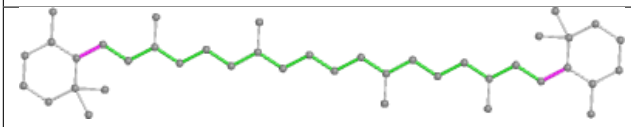
Ligand BCR X 130



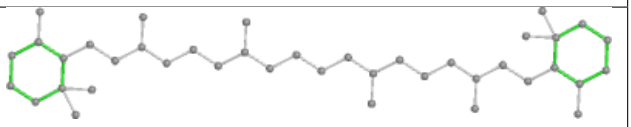
Bond lengths



Bond angles

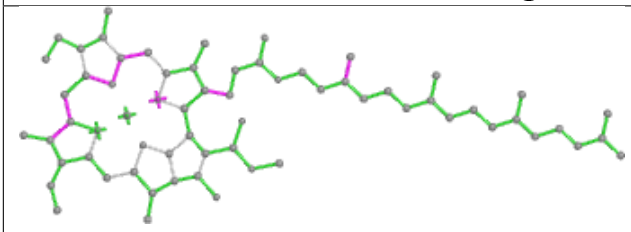


Torsions

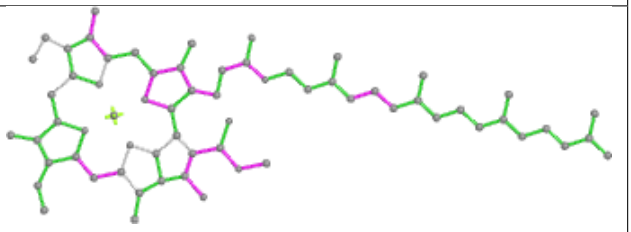


Rings

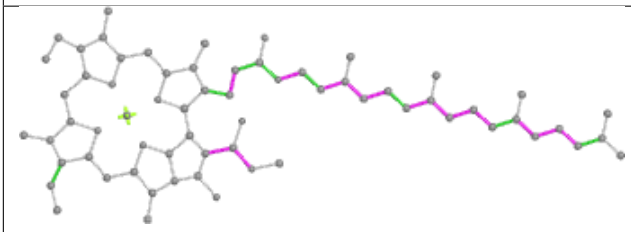
Ligand CLA c 5498



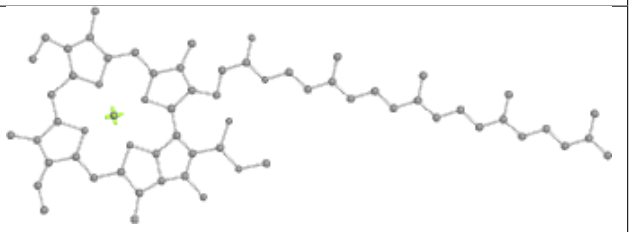
Bond lengths



Bond angles

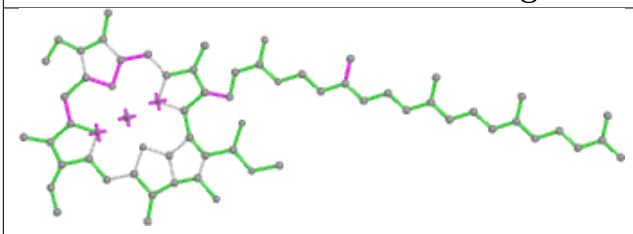


Torsions

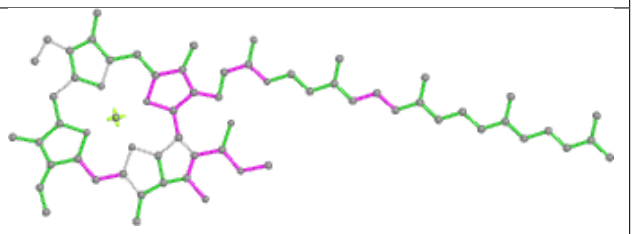


Rings

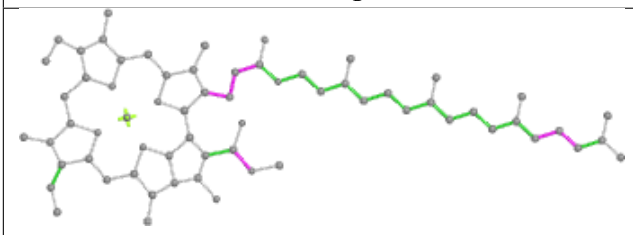
Ligand CLA c 5491



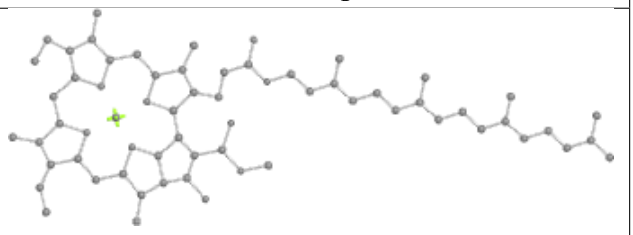
Bond lengths



Bond angles

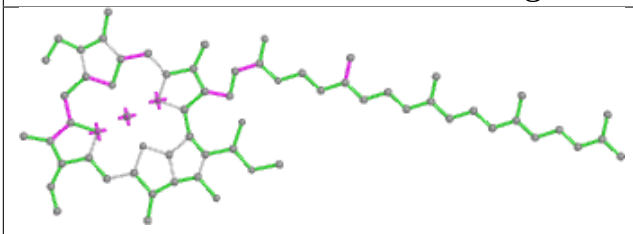


Torsions

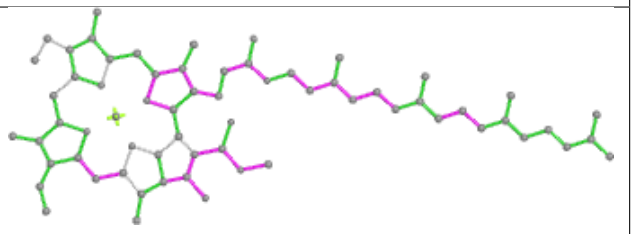


Rings

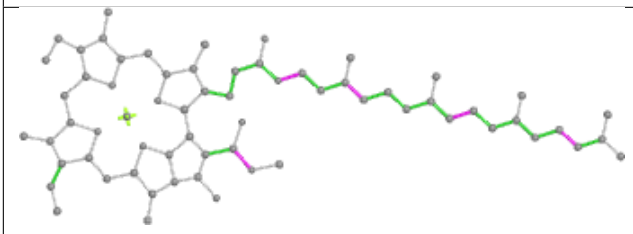
Ligand CLA B 521



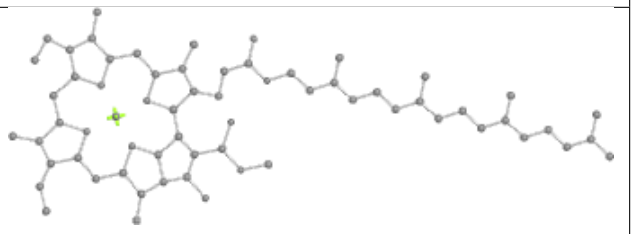
Bond lengths



Bond angles

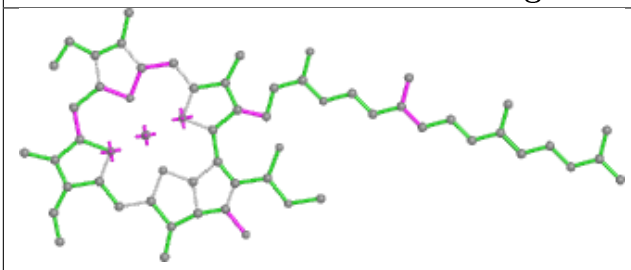


Torsions

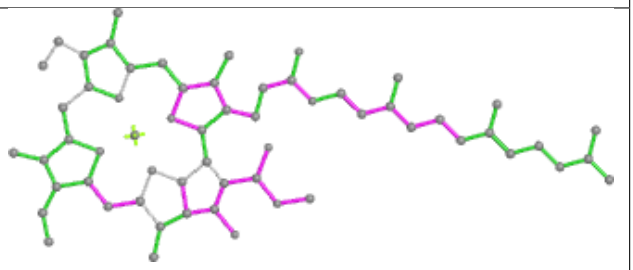


Rings

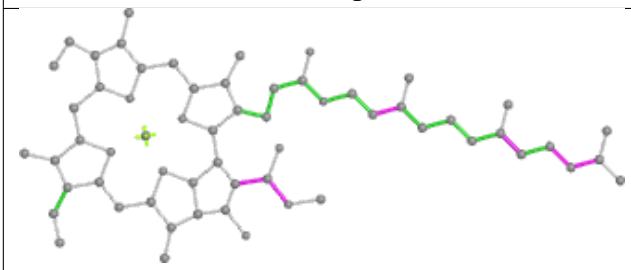
Ligand CLA C 492



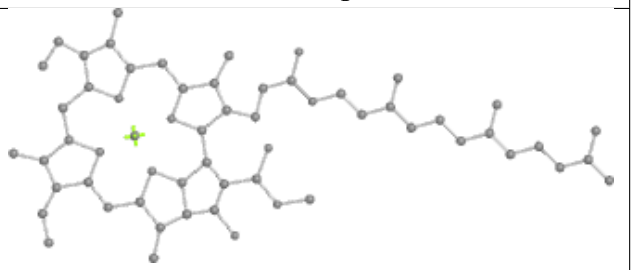
Bond lengths



Bond angles

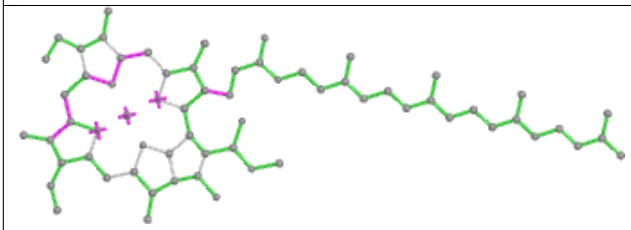


Torsions

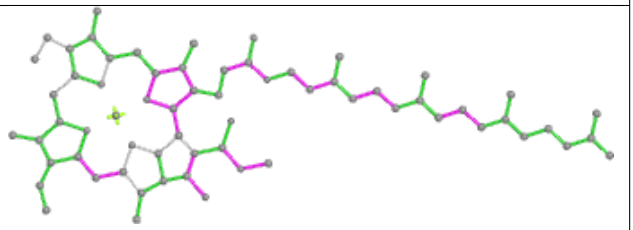


Rings

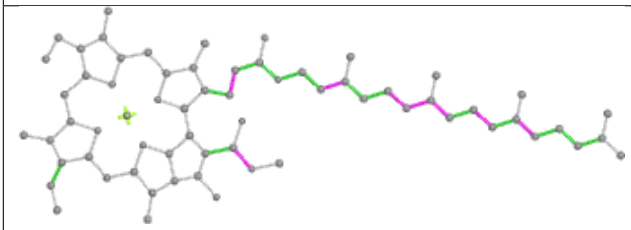
Ligand CLA c 5501



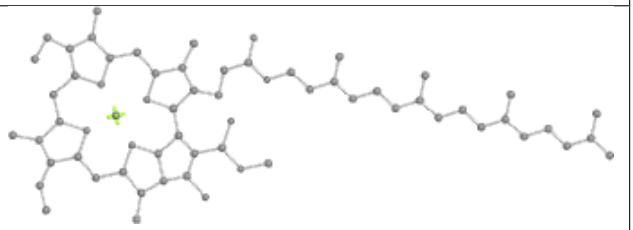
Bond lengths



Bond angles

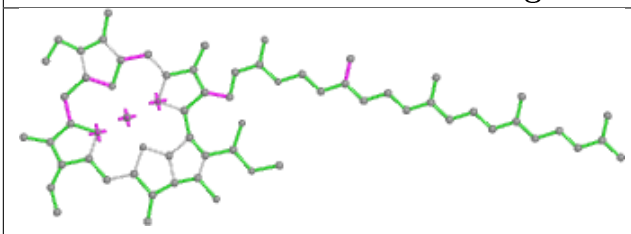


Torsions

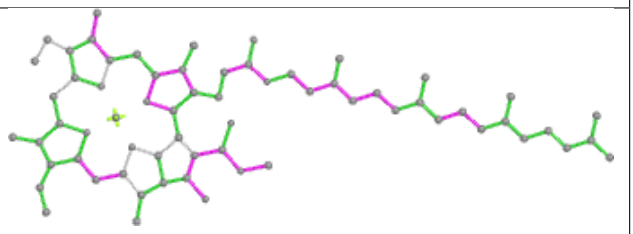


Rings

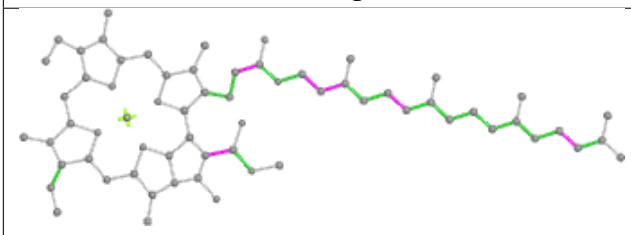
Ligand CLA C 497



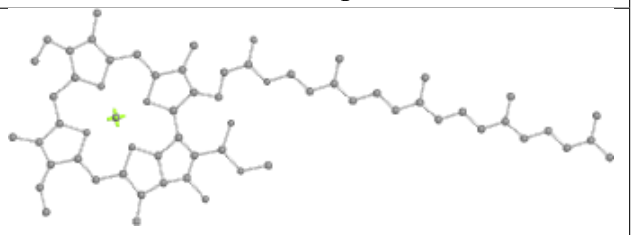
Bond lengths



Bond angles

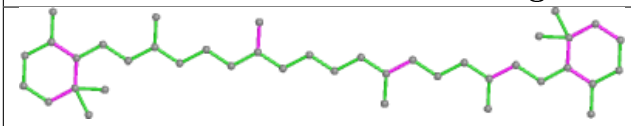


Torsions

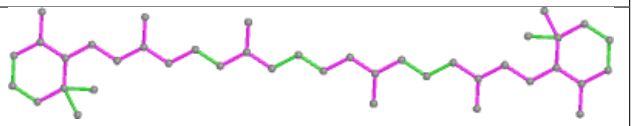


Rings

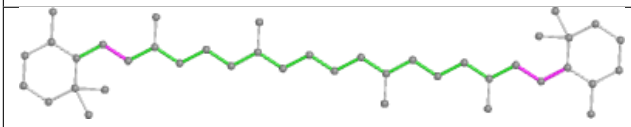
Ligand BCR t 104



Bond lengths



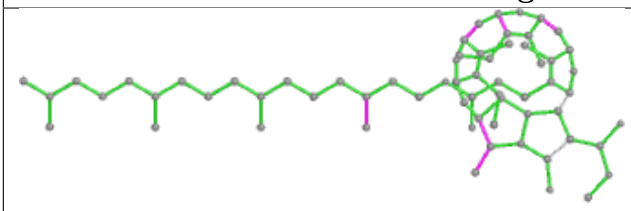
Bond angles



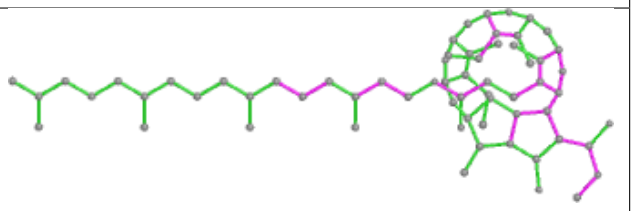
Torsions

Rings

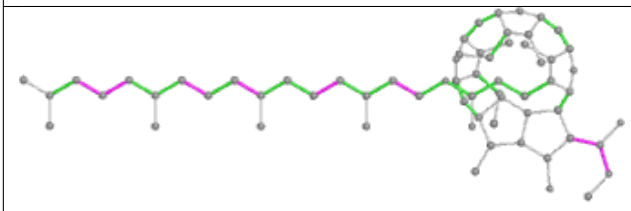
Ligand PHO a 5562



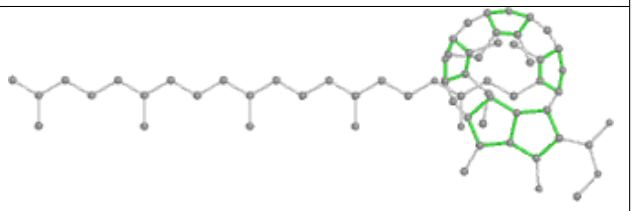
Bond lengths



Bond angles

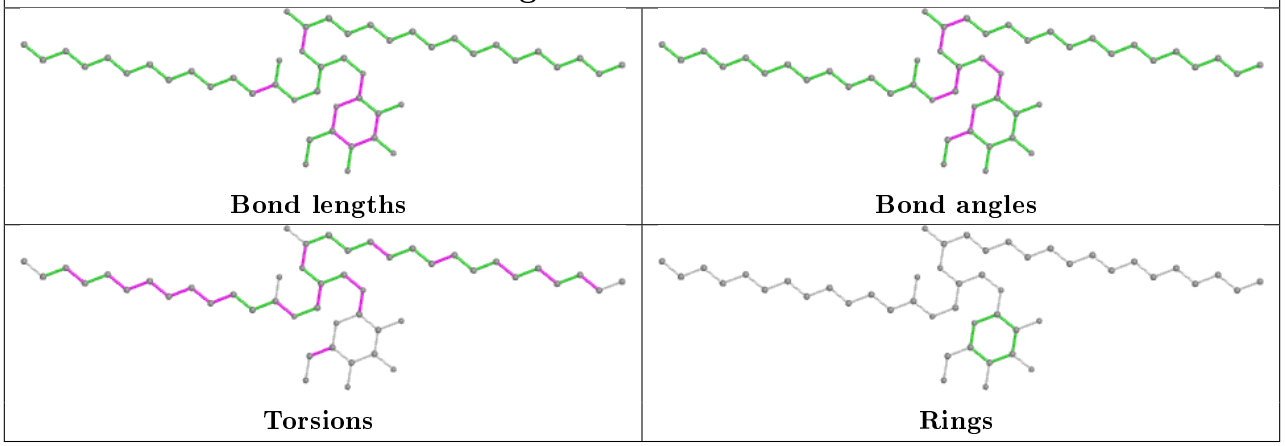


Torsions

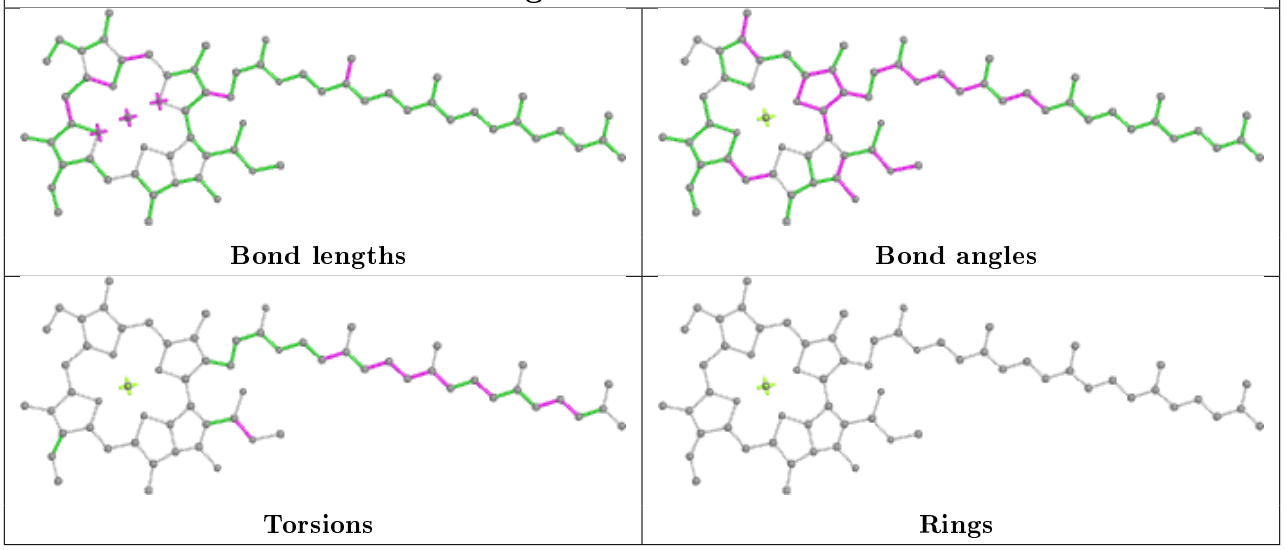


Rings

Ligand MGE i 5201



Ligand CLA B 514



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	335/344 (97%)	-0.59	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.53	4 (1%) 79 54	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.53	2 (0%) 92 79	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.50	1 (0%) 95 87	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.52	3 (0%) 87 69	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.35	5 (1%) 80 56	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.62	1 (0%) 94 84	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.57	1 (0%) 94 84	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.20	1 (1%) 79 54	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.01	3 (3%) 41 17	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.25	1 (2%) 51 23	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.11	3 (8%) 10 3	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.37	1 (1%) 72 44	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.19	3 (4%) 31 11	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.47	0 100 100	57, 65, 80, 88	0
8	i	35/38 (92%)	-0.34	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.60	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.52	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.53	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.40	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.15	1 (2%) 54 26	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.36	2 (5%) 25 9	45, 57, 86, 91	0
12	M	36/36 (100%)	-0.42	2 (5%) 24 8	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.34	1 (2%) 53 25	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	242/247 (97%)	-0.39	3 (1%) 79 54	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.30	8 (3%) 46 20	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.48	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.73	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.39	1 (1%) 82 59	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.42	3 (3%) 49 21	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.48	2 (1%) 73 46	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.24	5 (3%) 42 17	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.25	4 (6%) 18 5	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.20	2 (3%) 47 20	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.45	63 (1%) 79 54	35, 66, 85, 101	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	c	5473	ASP	4.5
1	a	5010	SER	4.4
13	o	5049	ASP	4.3
4	D	13	GLY	4.2
11	l	5001	MET	4.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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
20	CLA	b	5511	41/65	0.64	0.39	88,92,95,96	0
27	LMT	t	5217	35/35	0.69	0.45	76,95,104,105	0
29	UNK	c	5478	11/-	0.70	0.40	76,79,81,81	0
29	UNK	c	5490	4/-	0.71	0.33	91,92,92,92	0
29	UNK	C	481	13/-	0.72	0.37	61,64,68,69	0
27	LMT	A	569	35/35	0.73	0.47	80,89,92,93	0
20	CLA	B	511	41/65	0.73	0.41	88,90,92,98	0
29	UNK	C	475	12/-	0.73	0.32	68,69,72,73	0
29	UNK	c	5475	12/-	0.74	0.35	74,78,84,84	0
27	LMT	T	217	35/35	0.75	0.32	83,93,96,97	0
28	MGE	d	5359	47/48	0.76	0.30	72,81,96,98	0
22	PQ9	A	564	30/45	0.77	0.37	54,57,63,64	30
24	BCR	c	5506	40/40	0.77	0.32	75,81,86,86	0
24	BCR	x	5130	40/40	0.78	0.44	77,81,85,86	0
27	LMT	M	5216	35/35	0.78	0.31	58,83,90,90	0
20	CLA	b	5526	65/65	0.79	0.28	66,71,92,95	0
29	UNK	C	489	7/-	0.79	0.42	75,76,77,78	0
29	UNK	c	5489	7/-	0.79	0.39	73,73,74,74	0
26	SQD	d	5358	54/54	0.79	0.29	74,85,106,107	0
26	SQD	a	212	26/54	0.79	0.26	82,94,101,103	0
20	CLA	B	526	65/65	0.80	0.28	71,82,97,98	0
26	SQD	L	5213	47/54	0.80	0.27	52,85,106,108	0
29	UNK	c	5476	9/-	0.80	0.32	58,60,62,62	0
28	MGE	D	358	47/48	0.81	0.24	65,72,79,81	0
27	LMT	m	216	35/35	0.81	0.28	62,87,89,91	0
24	BCR	C	505	40/40	0.81	0.43	75,81,91,92	0
29	UNK	C	486	8/-	0.81	0.36	55,56,59,60	0
29	UNK	C	476	9/-	0.81	0.29	61,62,63,64	0
27	LMT	a	5568	35/35	0.81	0.43	79,92,94,96	0
20	CLA	b	5516	65/65	0.81	0.28	62,66,84,86	0
26	SQD	A	5212	26/54	0.81	0.23	75,100,107,107	0
24	BCR	d	5357	40/40	0.82	0.37	61,72,86,88	0
20	CLA	B	516	65/65	0.82	0.27	61,76,92,97	0
24	BCR	H	107	40/40	0.82	0.30	77,83,88,89	0
20	CLA	c	5496	65/65	0.82	0.27	79,83,95,97	0
29	UNK	c	5485	5/-	0.83	0.41	68,69,69,70	0
26	SQD	A	568	54/54	0.84	0.32	76,82,90,90	0
20	CLA	C	496	65/65	0.84	0.26	71,78,88,89	0
20	CLA	a	5563	55/65	0.84	0.32	59,65,102,103	0
24	BCR	B	528	40/40	0.84	0.25	54,68,74,75	0
29	UNK	C	478	11/-	0.84	0.24	58,65,66,66	0
29	UNK	c	5484	5/-	0.84	0.52	69,69,70,72	0
24	BCR	h	5107	40/40	0.85	0.28	74,79,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	SQD	t	213	47/54	0.85	0.27	61,95,116,117	0
29	UNK	C	479	11/-	0.85	0.26	58,64,67,67	0
20	CLA	C	503	50/65	0.85	0.27	83,86,88,94	0
20	CLA	c	5503	50/65	0.85	0.28	88,91,92,93	0
29	UNK	C	482	13/-	0.85	0.25	64,66,67,67	0
24	BCR	X	130	40/40	0.85	0.32	68,71,80,81	0
20	CLA	c	5498	65/65	0.85	0.25	81,90,93,93	0
28	MGE	i	5201	48/48	0.85	0.27	67,83,88,90	0
29	UNK	c	5479	11/-	0.85	0.24	76,77,77,77	0
30	DGD	c	5509	57/66	0.86	0.28	67,72,77,78	0
29	UNK	C	487	7/-	0.86	0.24	49,52,52,53	0
29	UNK	C	488	5/-	0.86	0.17	41,45,47,47	0
24	BCR	c	5504	40/40	0.86	0.29	73,80,88,89	0
24	BCR	b	5529	40/40	0.86	0.35	69,72,74,74	0
20	CLA	d	5355	50/65	0.86	0.23	74,77,80,81	0
29	UNK	C	484	5/-	0.86	0.21	47,51,52,53	0
28	MGE	D	359	41/48	0.87	0.23	60,67,76,79	0
20	CLA	B	519	65/65	0.87	0.26	73,82,85,87	0
20	CLA	c	5502	51/65	0.87	0.23	93,96,97,98	0
29	UNK	c	5481	13/-	0.87	0.22	60,62,66,66	0
28	MGE	I	201	48/48	0.87	0.22	73,81,89,90	0
20	CLA	C	498	65/65	0.88	0.22	64,74,98,101	0
20	CLA	A	563	55/65	0.88	0.26	43,49,75,78	0
24	BCR	T	5104	40/40	0.88	0.25	67,71,78,79	0
22	PQ9	a	5564	30/45	0.88	0.32	51,55,62,62	30
24	BCR	c	5505	40/40	0.88	0.31	84,87,91,92	0
29	UNK	c	5483	13/-	0.88	0.26	71,75,80,82	0
29	UNK	c	5487	7/-	0.88	0.20	57,57,58,58	0
20	CLA	C	502	51/65	0.88	0.21	74,80,83,84	0
24	BCR	C	506	40/40	0.88	0.22	68,72,79,80	0
29	UNK	C	483	13/-	0.89	0.23	61,68,78,78	0
28	MGE	L	210	48/48	0.89	0.24	59,68,73,75	0
30	DGD	c	5507	53/66	0.89	0.23	66,74,90,91	0
20	CLA	b	5519	65/65	0.89	0.24	70,75,80,81	0
20	CLA	C	501	65/65	0.89	0.25	70,78,83,85	0
29	UNK	c	5474	15/-	0.89	0.24	39,50,56,56	0
28	MGE	B	530	48/48	0.89	0.19	55,64,70,72	0
29	UNK	c	5477	7/-	0.89	0.34	67,68,70,70	0
20	CLA	c	5497	65/65	0.89	0.24	66,82,84,87	0
29	UNK	c	5486	8/-	0.89	0.30	63,64,65,66	0
29	UNK	C	474	15/-	0.89	0.18	26,37,40,40	0
24	BCR	D	357	40/40	0.89	0.26	61,66,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	MGE	d	5360	41/48	0.89	0.21	68,72,78,80	0
29	UNK	C	485	5/-	0.89	0.24	57,59,61,61	0
24	BCR	B	529	40/40	0.89	0.25	62,69,80,80	0
20	CLA	c	5501	65/65	0.89	0.26	82,91,94,95	0
20	CLA	C	497	65/65	0.89	0.24	74,78,80,82	0
30	DGD	C	507	53/66	0.89	0.25	55,66,86,88	0
29	UNK	c	5480	7/-	0.89	0.26	65,66,66,67	0
24	BCR	a	5566	40/40	0.90	0.25	59,75,78,79	0
20	CLA	B	520	65/65	0.90	0.23	62,67,76,79	0
25	LHG	a	5567	39/49	0.90	0.26	65,68,74,80	0
29	UNK	c	5482	13/-	0.90	0.19	60,61,71,72	0
20	CLA	a	5560	65/65	0.90	0.22	62,68,100,101	0
28	MGE	d	5361	48/48	0.90	0.21	61,68,78,83	0
28	MGE	l	5210	48/48	0.90	0.21	59,69,78,81	0
30	DGD	H	208	54/66	0.90	0.20	61,69,75,76	0
20	CLA	c	5493	65/65	0.90	0.21	67,81,86,86	0
20	CLA	b	5520	65/65	0.90	0.24	63,72,74,76	0
28	MGE	b	5530	48/48	0.90	0.18	59,64,71,73	0
30	DGD	C	508	47/66	0.91	0.19	61,71,80,83	0
20	CLA	A	560	65/65	0.91	0.21	49,57,86,88	0
20	CLA	B	512	65/65	0.91	0.24	68,75,78,79	0
20	CLA	D	355	50/65	0.91	0.22	63,65,68,70	0
22	PQ9	D	356	30/45	0.91	0.21	49,67,80,83	0
29	UNK	C	480	7/-	0.91	0.22	35,36,38,38	0
28	MGE	D	360	48/48	0.91	0.20	52,60,63,68	0
24	BCR	B	527	40/40	0.91	0.18	58,65,68,69	0
20	CLA	c	5491	65/65	0.91	0.20	70,78,81,86	0
30	DGD	C	509	57/66	0.91	0.20	52,60,69,70	0
20	CLA	c	5495	65/65	0.91	0.21	74,81,86,88	0
24	BCR	t	104	40/40	0.91	0.20	65,72,84,85	0
21	PHO	a	5562	64/64	0.91	0.22	70,75,81,82	0
30	DGD	c	5508	47/66	0.91	0.18	66,76,82,84	0
24	BCR	C	504	40/40	0.91	0.27	57,64,70,70	0
24	BCR	b	5527	40/40	0.92	0.19	58,63,72,72	0
22	PQ9	d	5356	30/45	0.92	0.20	51,57,66,66	0
20	CLA	b	5525	65/65	0.92	0.20	71,77,80,82	0
24	BCR	A	566	40/40	0.92	0.24	50,57,64,66	0
20	CLA	c	5499	47/65	0.92	0.20	60,69,76,78	0
29	UNK	c	5488	5/-	0.92	0.21	59,59,59,60	0
25	LHG	A	567	39/49	0.92	0.23	57,73,79,81	0
20	CLA	C	495	65/65	0.92	0.21	58,68,74,76	0
20	CLA	b	5512	65/65	0.92	0.23	68,72,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	c	5500	65/65	0.92	0.20	64,69,82,83	0
20	CLA	b	5524	56/65	0.93	0.18	63,68,89,91	0
20	CLA	B	515	65/65	0.93	0.21	55,66,71,72	0
20	CLA	c	5492	60/65	0.93	0.17	57,61,83,84	0
24	BCR	b	5528	40/40	0.93	0.17	61,64,72,73	0
30	DGD	h	5208	54/66	0.93	0.17	57,68,73,75	0
20	CLA	B	522	65/65	0.93	0.21	54,65,75,77	0
20	CLA	B	518	65/65	0.93	0.19	53,64,79,79	0
20	CLA	B	525	65/65	0.93	0.20	67,84,91,92	0
20	CLA	c	5494	46/65	0.93	0.16	72,77,86,88	0
20	CLA	B	514	65/65	0.93	0.21	59,64,82,83	0
20	CLA	B	524	56/65	0.93	0.19	67,72,77,80	0
20	CLA	b	5514	65/65	0.94	0.18	41,51,74,75	0
33	CA	k	5056	1/1	0.94	0.19	119,119,119,119	0
20	CLA	b	5515	65/65	0.94	0.21	46,51,74,76	0
21	PHO	a	5561	64/64	0.94	0.18	51,55,66,68	0
20	CLA	b	5521	65/65	0.94	0.15	48,57,63,64	0
20	CLA	b	5522	65/65	0.94	0.20	60,66,75,76	0
21	PHO	A	562	64/64	0.94	0.17	47,53,63,66	0
20	CLA	B	513	65/65	0.94	0.18	56,61,67,67	0
32	HEM	f	5051	43/43	0.94	0.28	80,84,97,101	0
20	CLA	b	5513	65/65	0.94	0.20	54,61,84,90	0
20	CLA	C	500	65/65	0.94	0.16	59,63,73,74	0
20	CLA	C	493	65/65	0.94	0.18	67,71,77,79	0
20	CLA	C	499	47/65	0.95	0.17	57,60,66,69	0
21	PHO	A	561	64/64	0.95	0.16	32,52,55,59	0
20	CLA	B	523	65/65	0.95	0.16	47,56,73,74	0
20	CLA	C	494	46/65	0.95	0.15	59,66,68,72	0
20	CLA	d	5354	65/65	0.95	0.17	39,47,64,65	0
20	CLA	a	5559	65/65	0.95	0.15	42,49,60,60	0
19	FE2	A	557	1/1	0.95	0.05	60,60,60,60	0
20	CLA	B	521	65/65	0.95	0.17	58,63,66,68	0
20	CLA	C	492	60/65	0.95	0.17	53,58,76,77	0
20	CLA	C	491	65/65	0.95	0.18	63,70,77,79	0
20	CLA	b	5518	65/65	0.95	0.17	60,64,69,75	0
20	CLA	b	5523	65/65	0.95	0.15	45,52,74,75	0
20	CLA	a	5558	65/65	0.95	0.16	41,50,55,61	0
20	CLA	b	5517	65/65	0.95	0.15	54,58,66,71	0
20	CLA	D	354	65/65	0.95	0.16	35,43,63,66	0
32	HEM	F	51	43/43	0.95	0.25	78,84,92,95	0
23	OEC	a	5565	5/9	0.96	0.13	63,64,71,87	0
20	CLA	A	558	65/65	0.96	0.14	41,46,50,51	0

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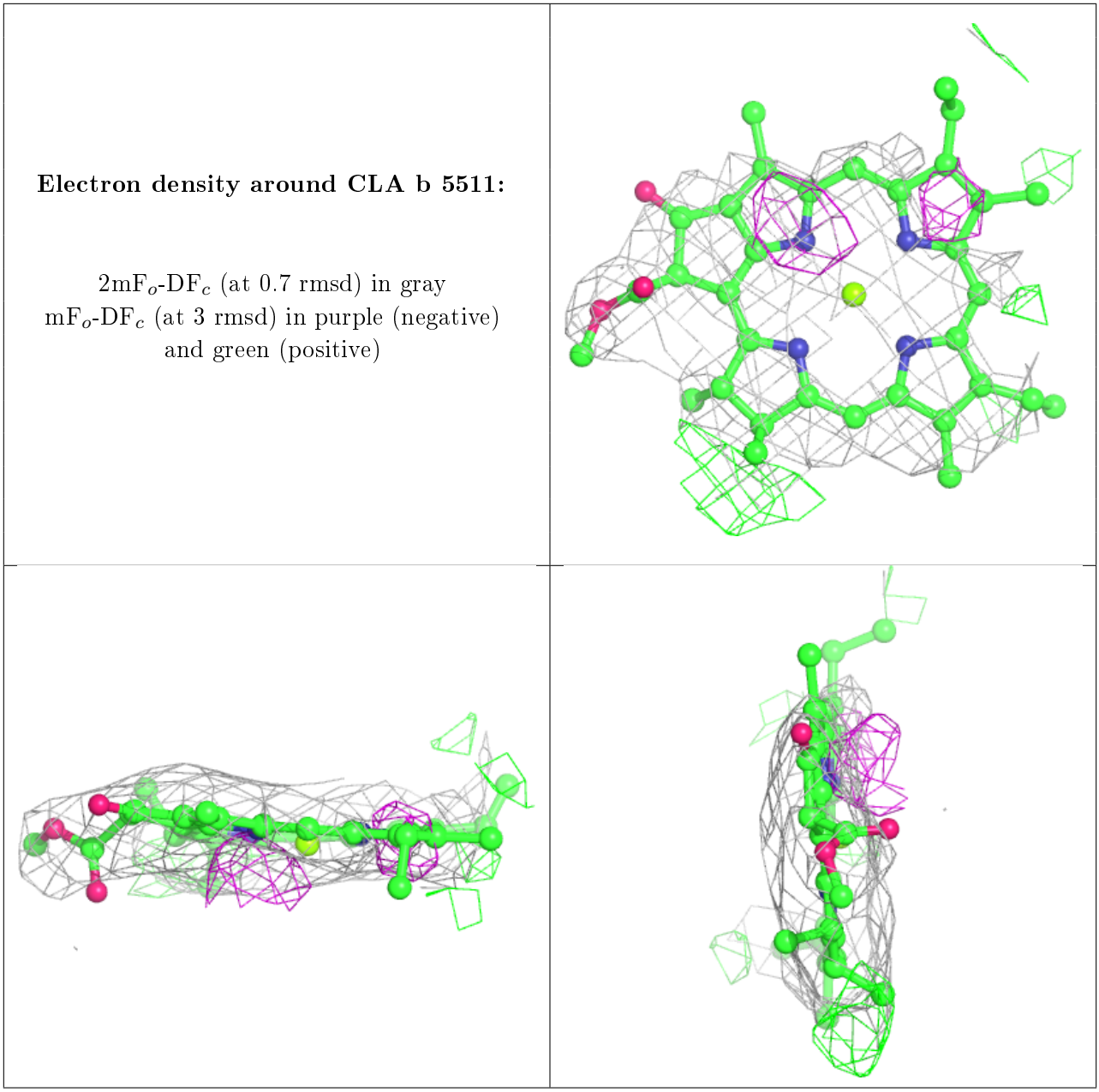
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	UNK	C	490	4/-	0.96	0.15	67,67,68,68	0
29	UNK	C	477	7/-	0.96	0.16	47,49,51,51	0
23	OEC	A	565	5/9	0.96	0.13	62,63,65,66	0
20	CLA	B	517	65/65	0.96	0.14	37,44,56,57	0
33	CA	K	56	1/1	0.96	0.09	119,119,119,119	0
32	HEM	v	5552	43/43	0.96	0.21	65,67,70,70	0
20	CLA	A	559	65/65	0.96	0.14	39,43,49,52	0
31	BCT	D	353	4/4	0.96	0.18	72,73,73,74	0
32	HEM	V	552	43/43	0.97	0.18	37,54,58,59	0
31	BCT	d	5353	4/4	0.98	0.15	75,75,76,77	0
19	FE2	a	5557	1/1	1.00	0.11	75,75,75,75	0

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

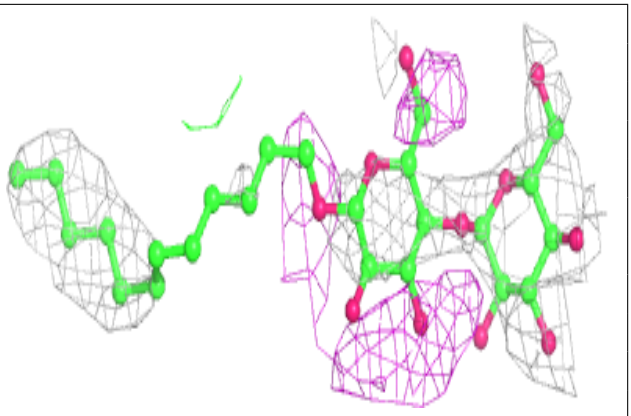
Electron density around CLA b 5511:

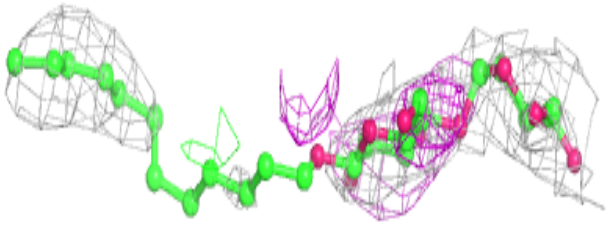
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

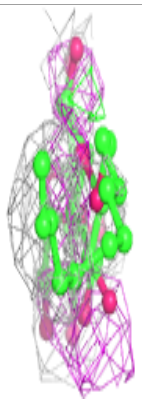


Electron density around LMT t 5217:

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

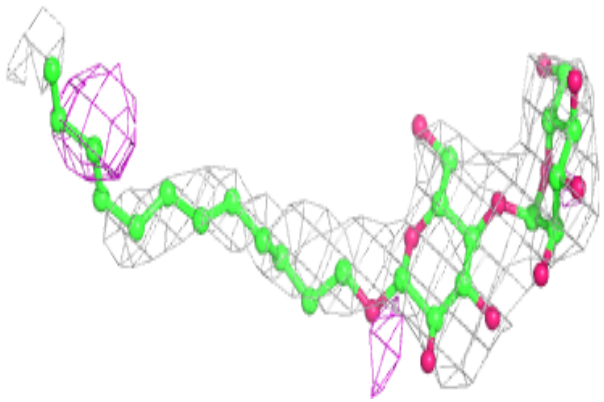


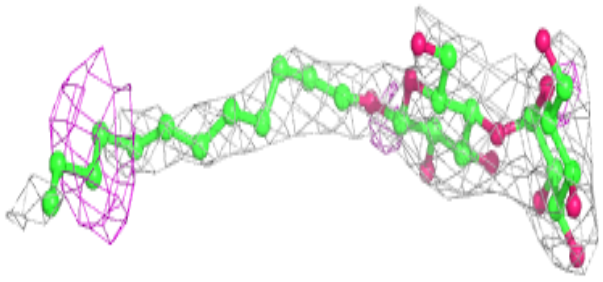


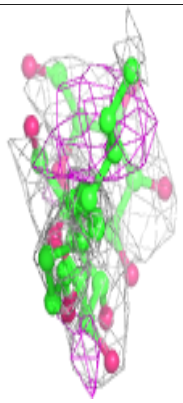


Electron density around LMT A 569:

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

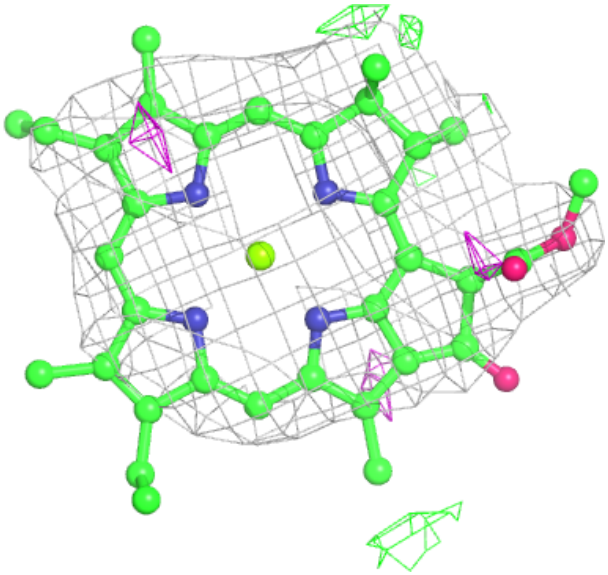


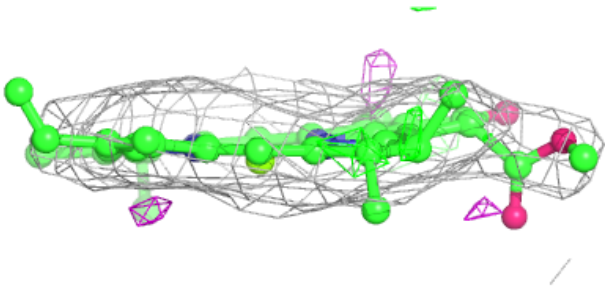


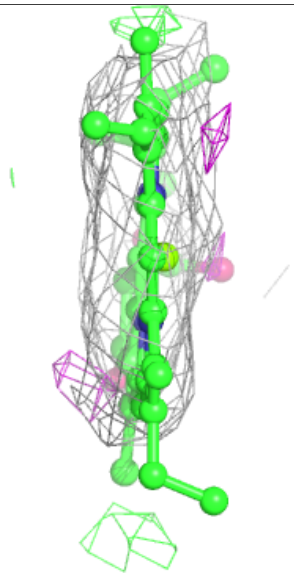


Electron density around CLA B 511:

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

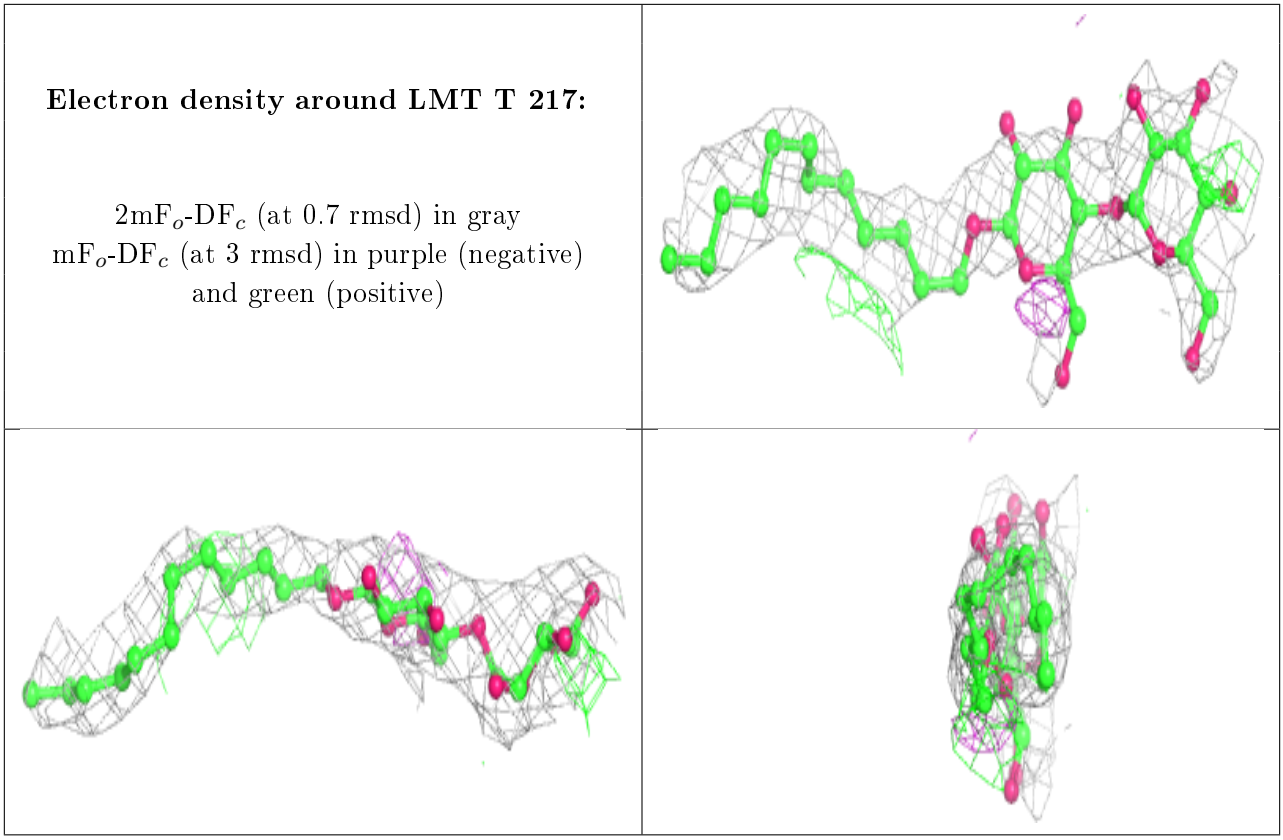






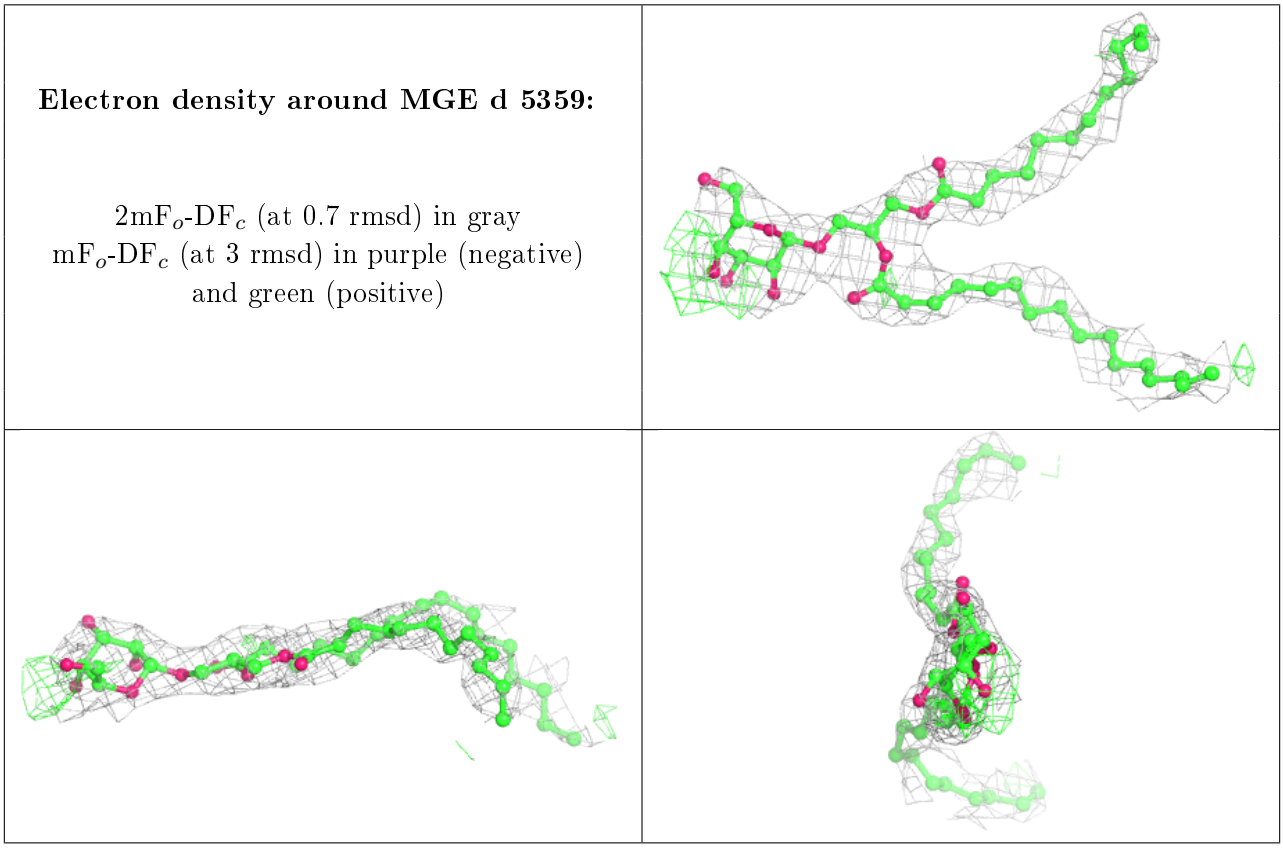
Electron density around LMT T 217:

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



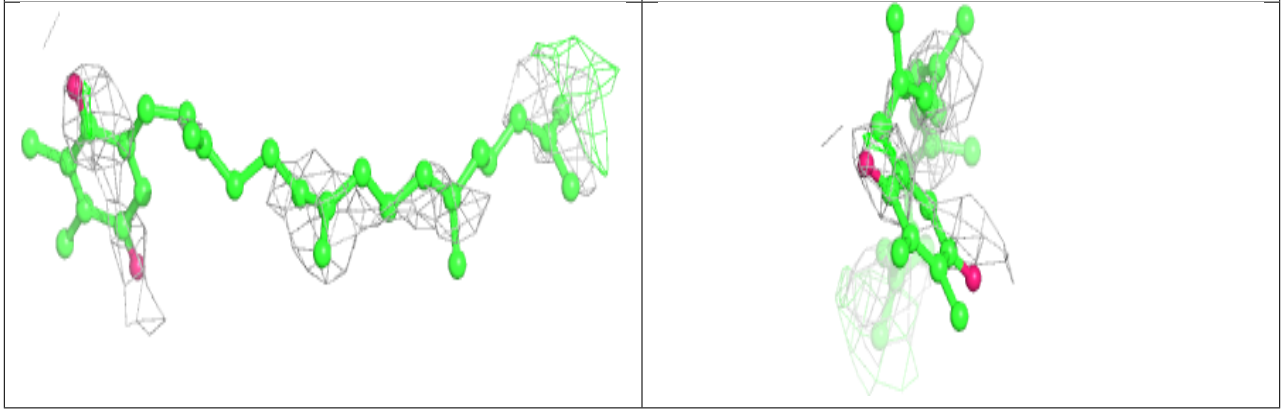
Electron density around MGE d 5359:

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



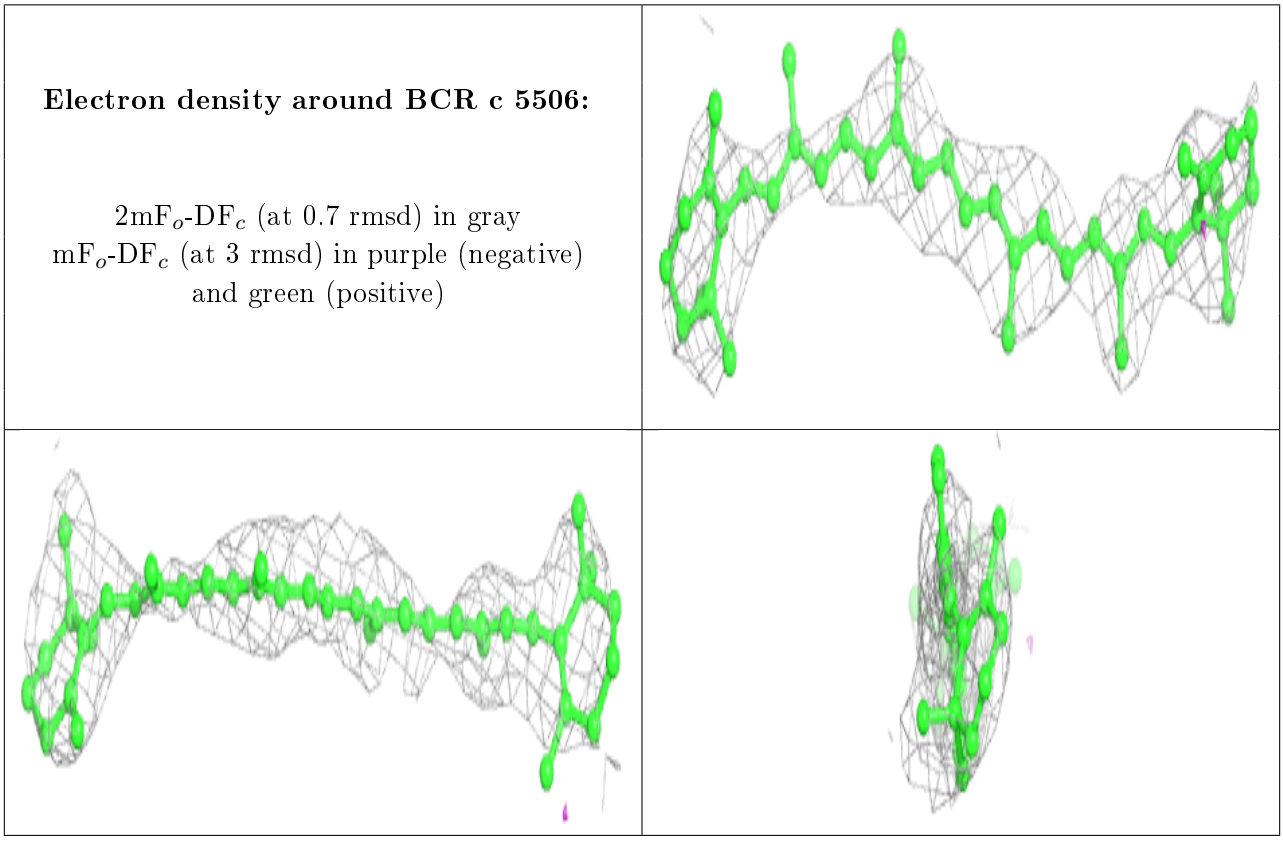
Electron density around PQ9 A 564:

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



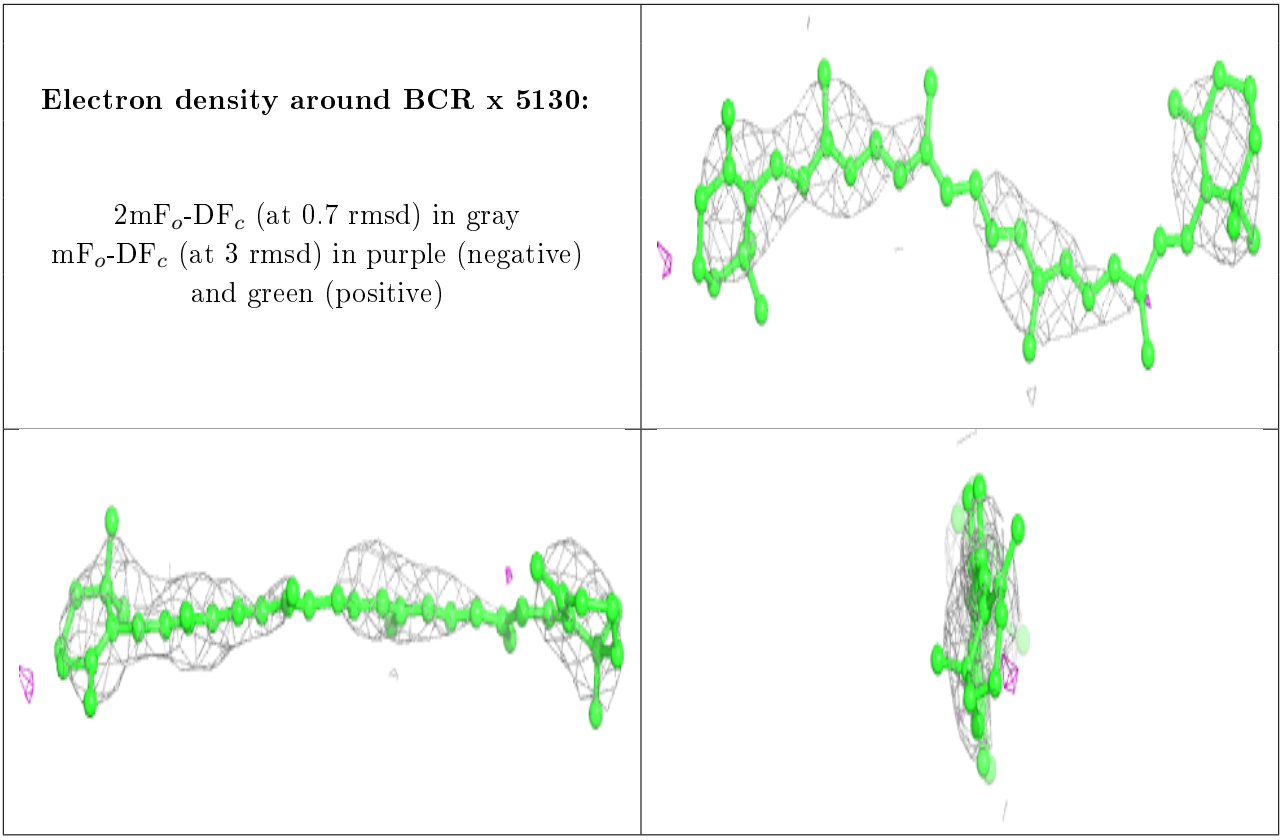
Electron density around BCR c 5506:

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



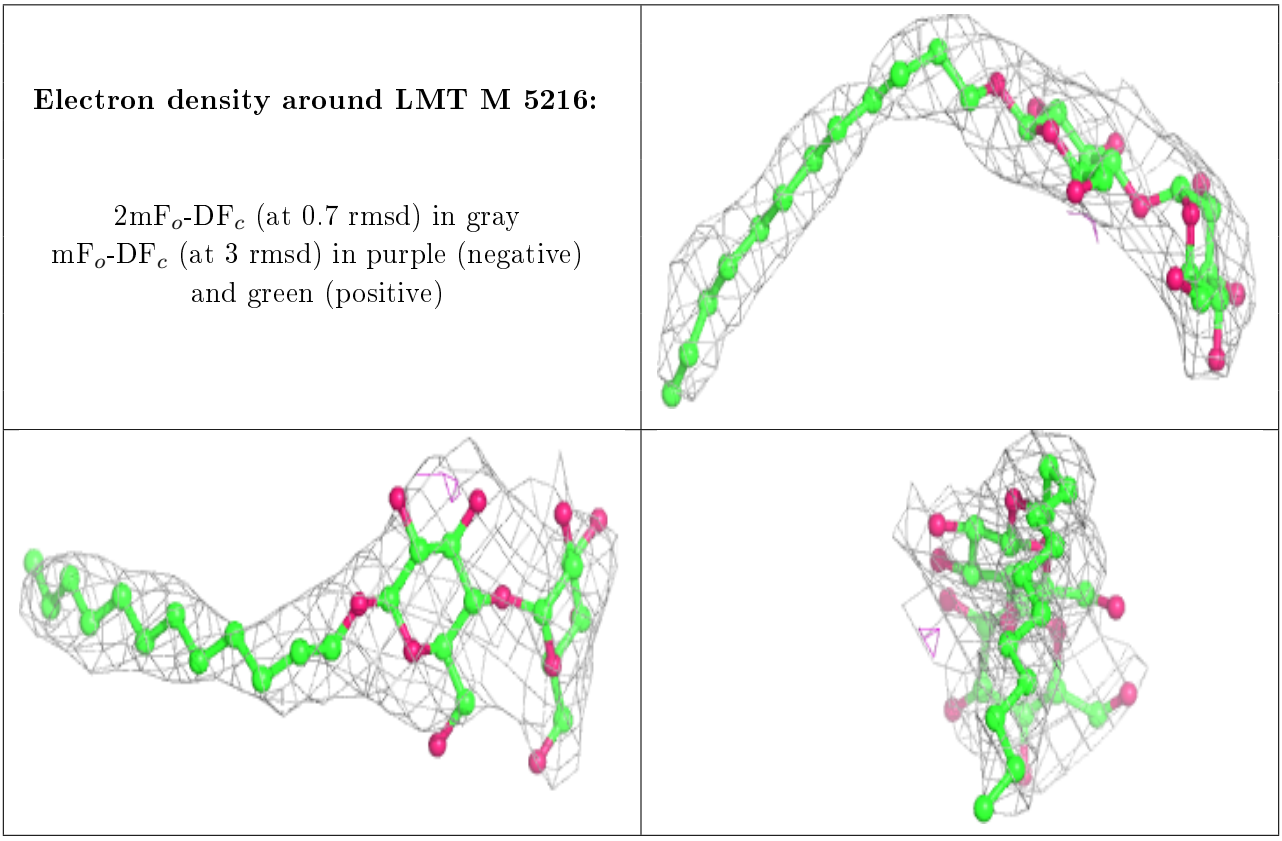
Electron density around BCR x 5130:

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



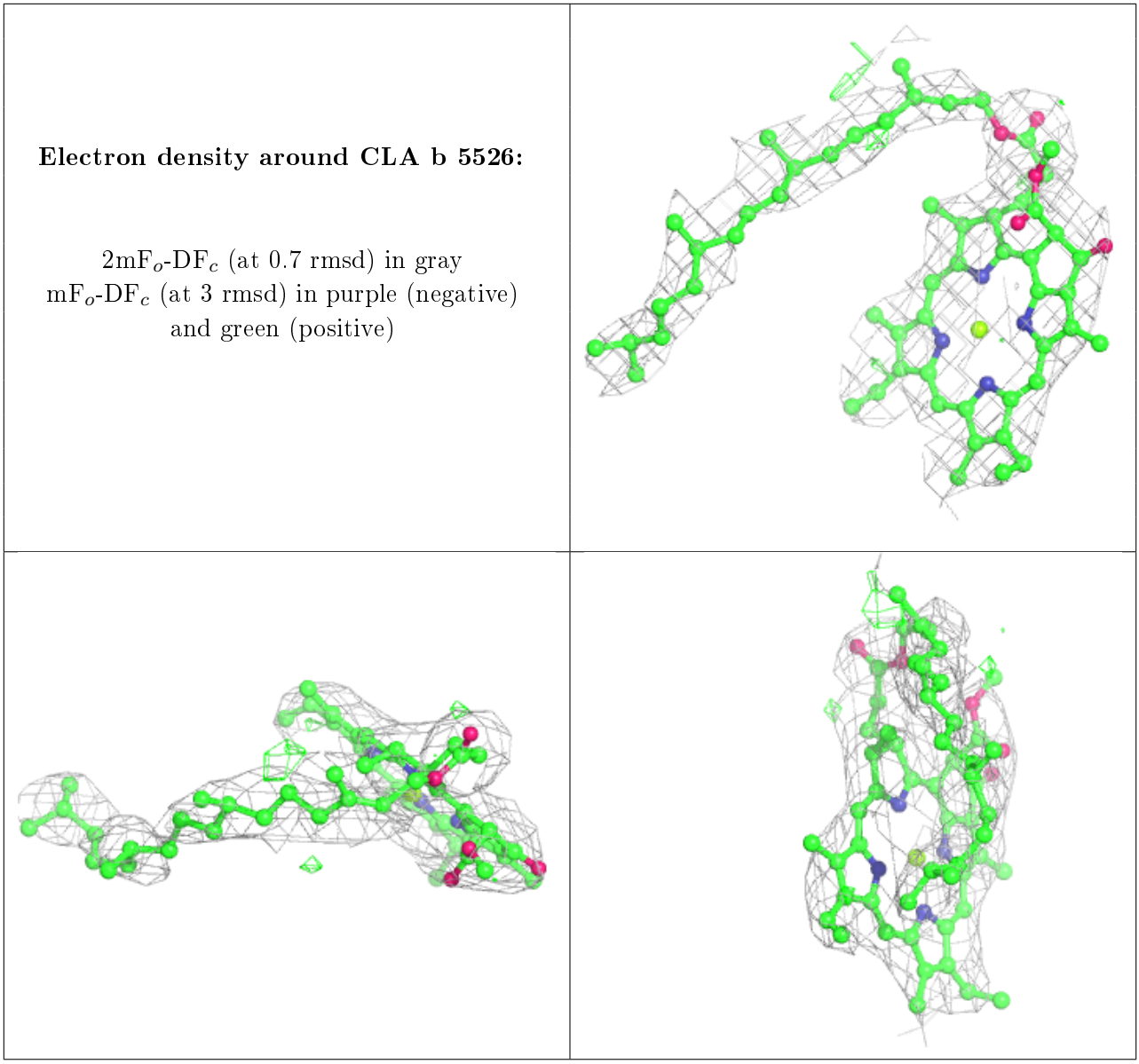
Electron density around LMT M 5216:

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



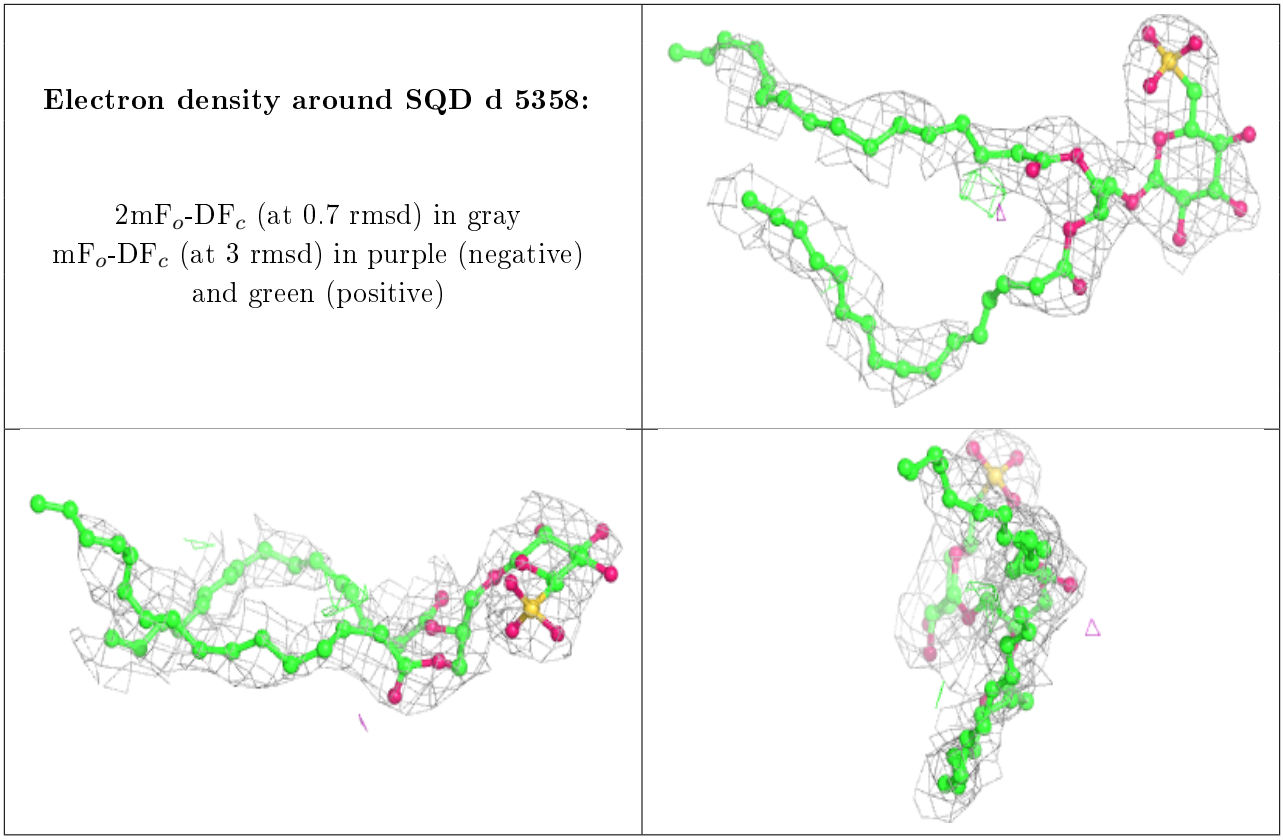
Electron density around CLA b 5526:

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



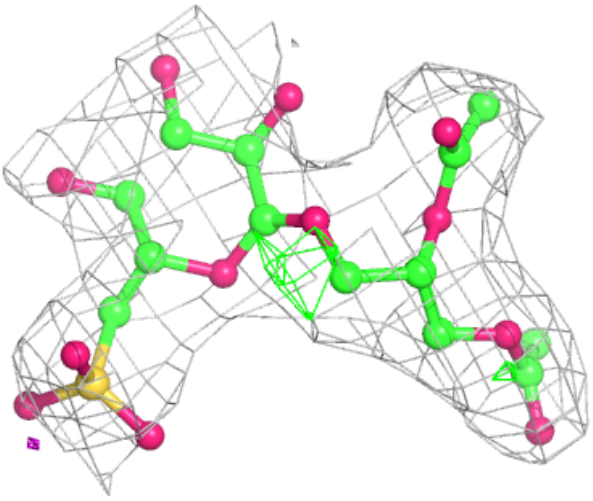
Electron density around SQD d 5358:

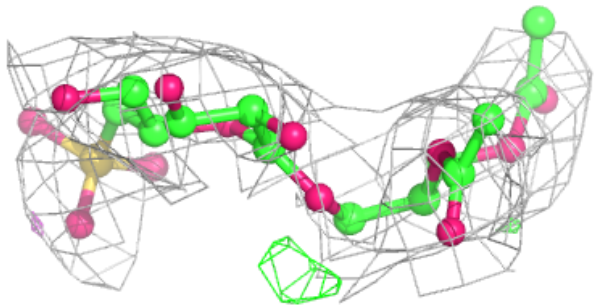
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

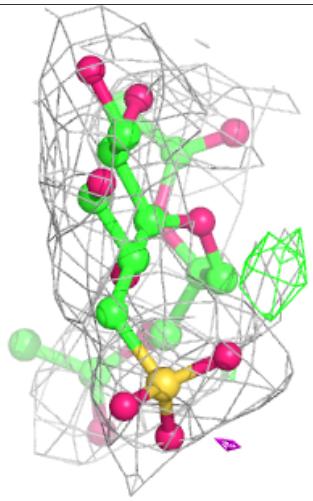


Electron density around SQD a 212:

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

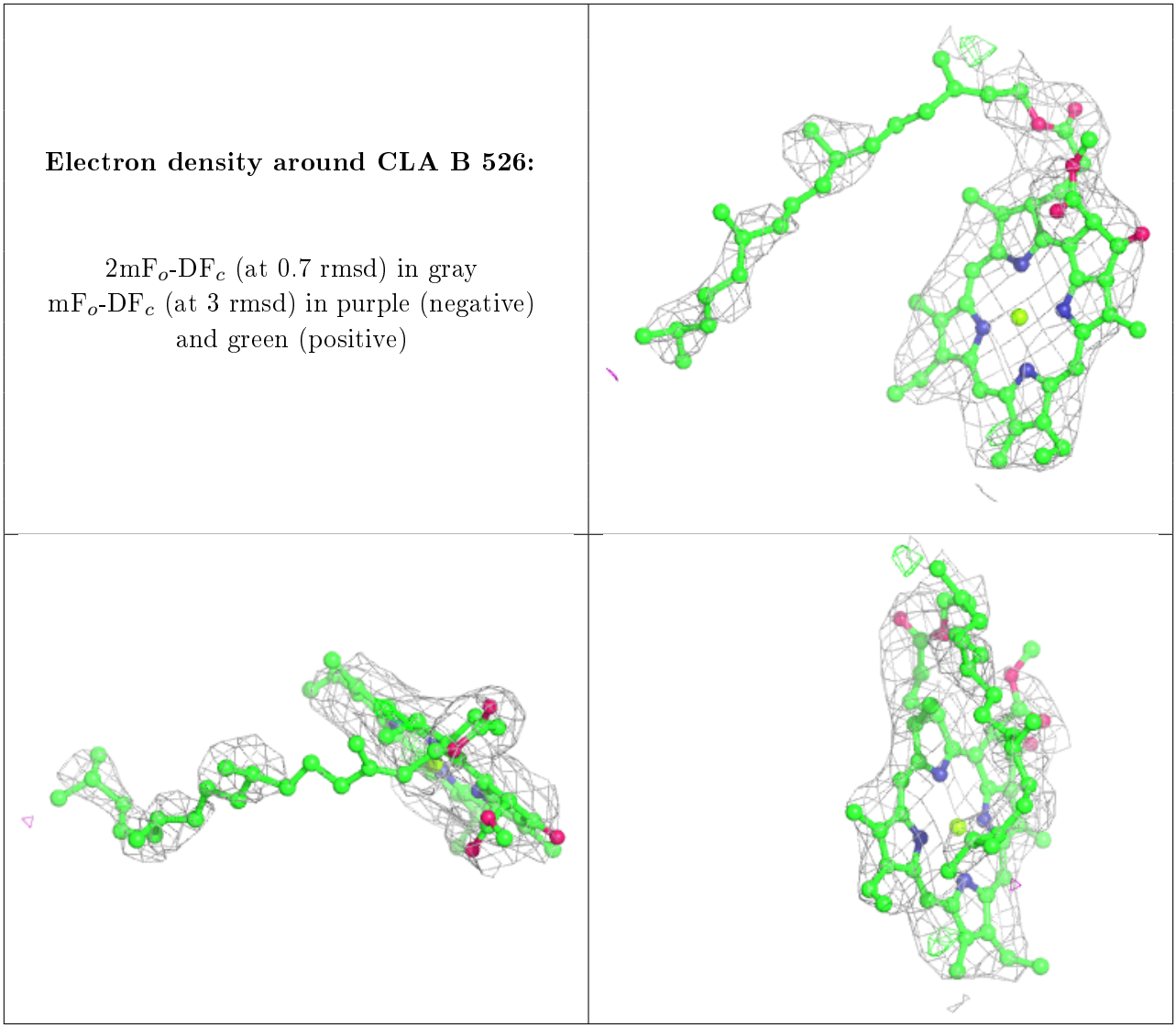






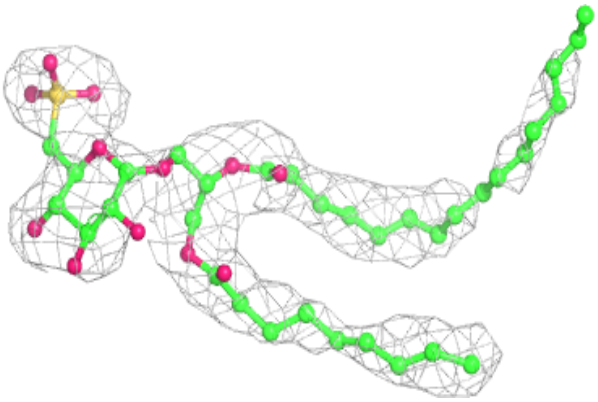
Electron density around CLA B 526:

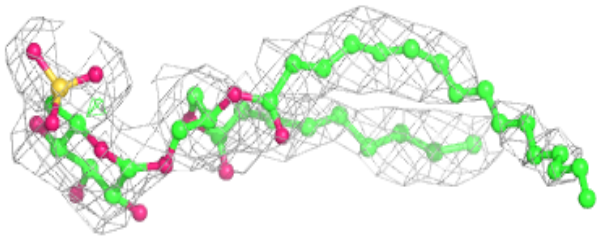
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

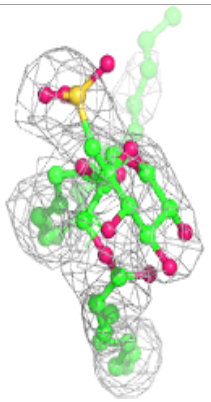


Electron density around SQD L 5213:

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

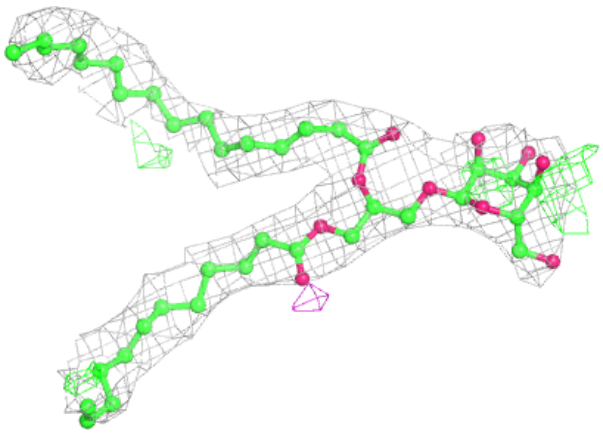


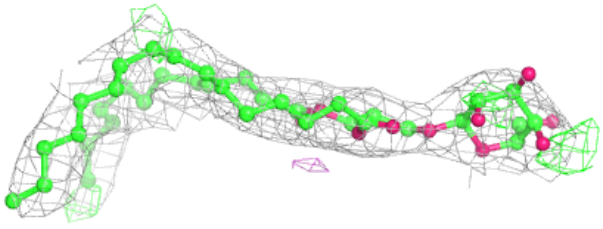


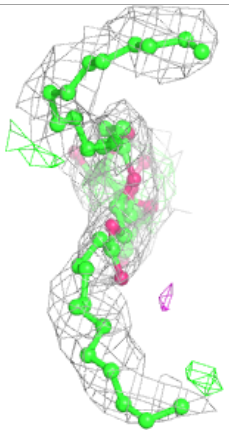


Electron density around MGE D 358:

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

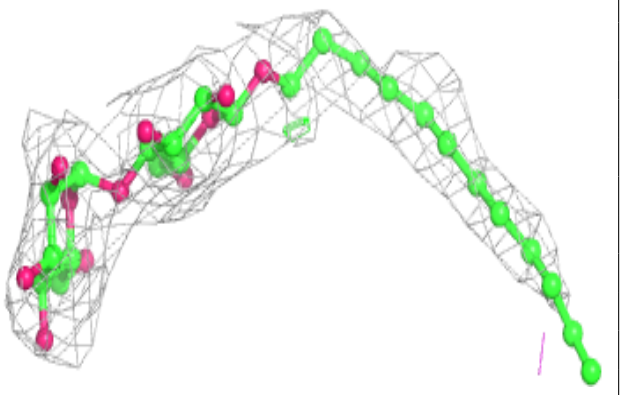


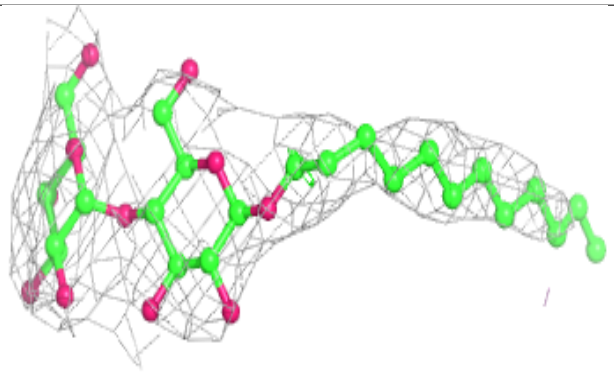


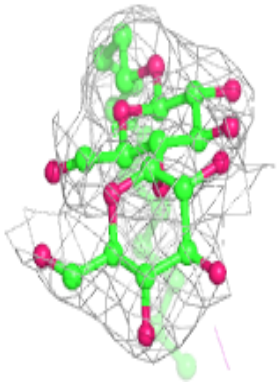


Electron density around LMT m 216:

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

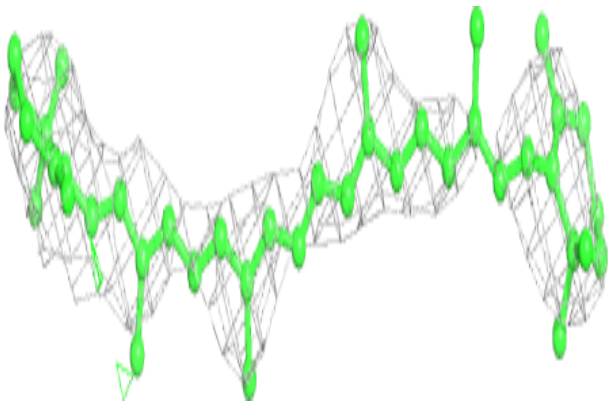


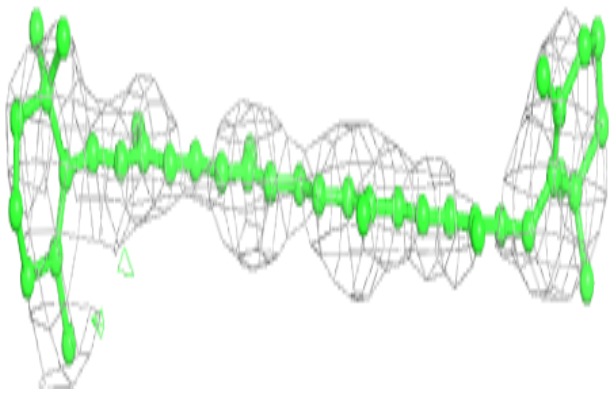


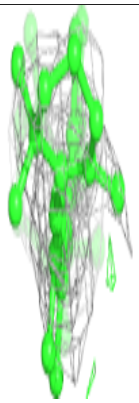


Electron density around BCR C 505:

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

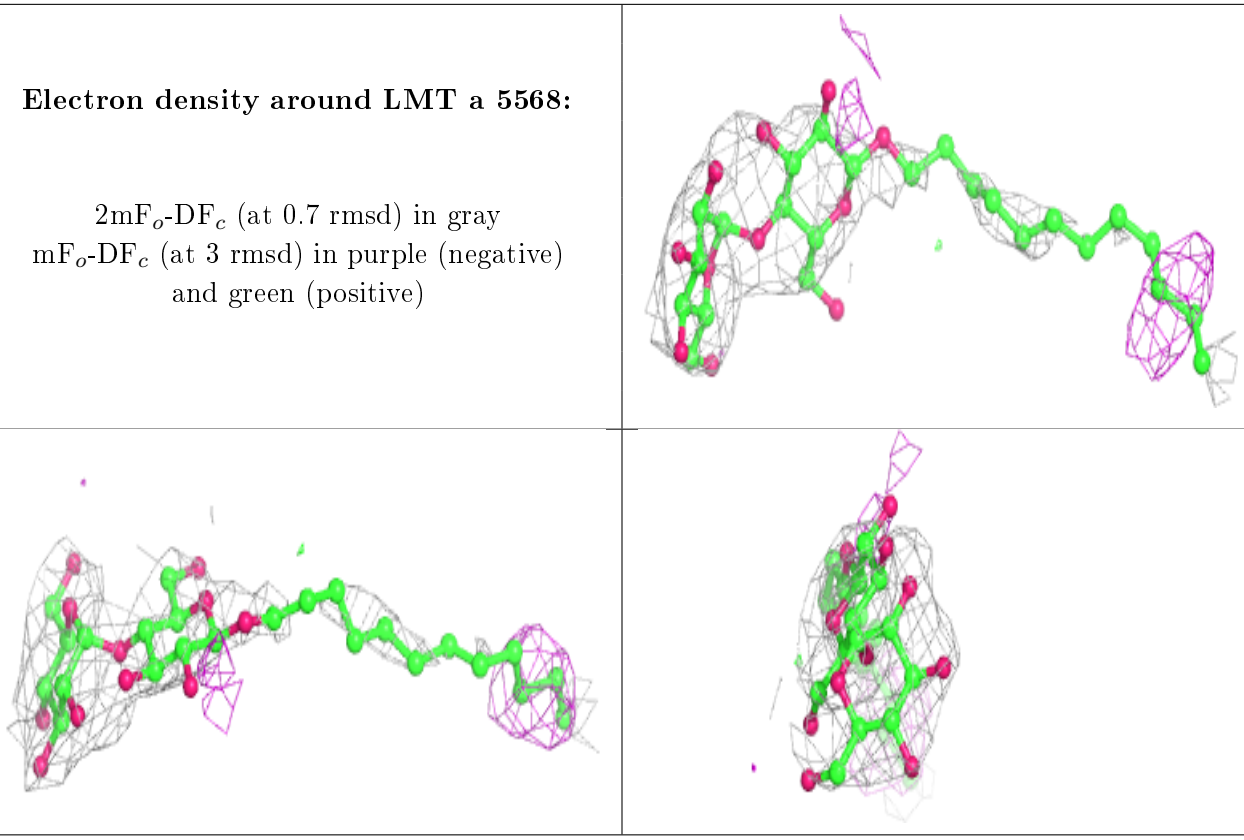






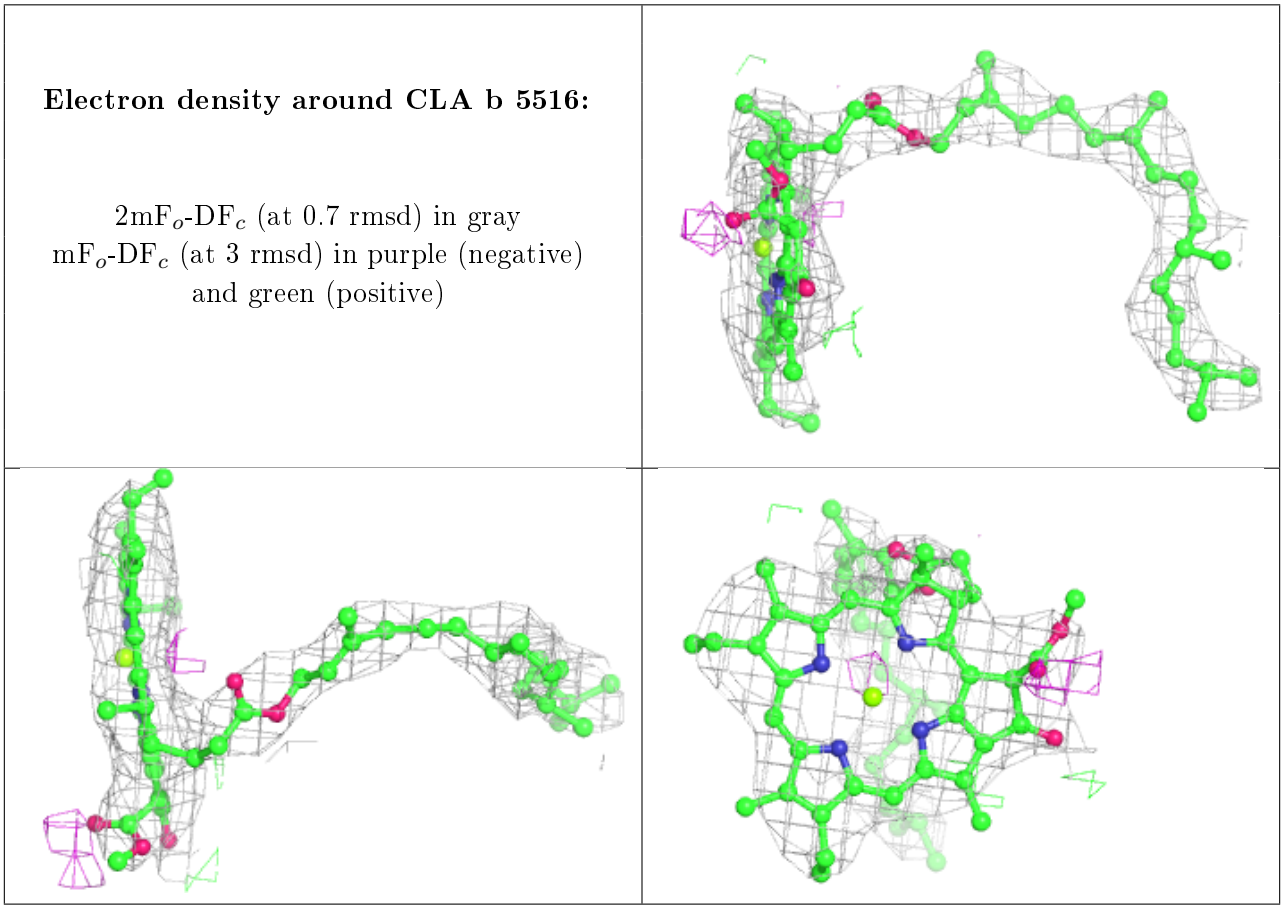
Electron density around LMT a 5568:

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



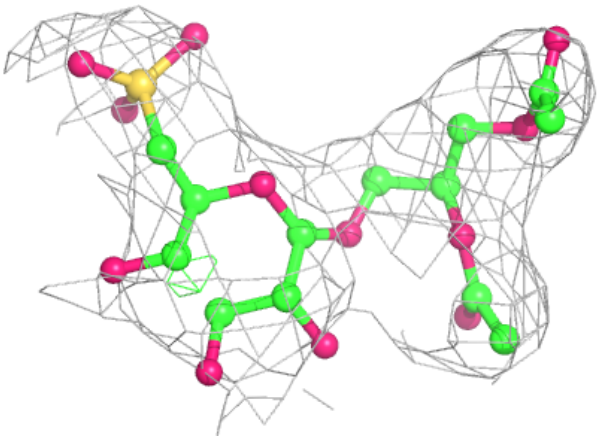
Electron density around CLA b 5516:

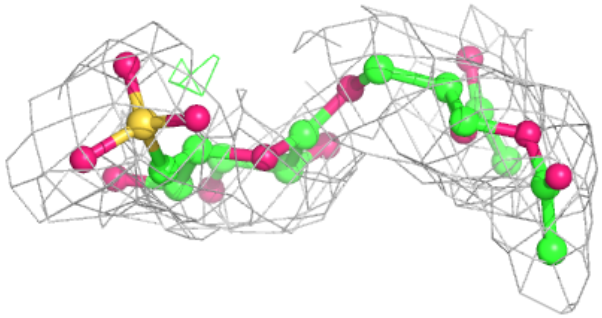
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

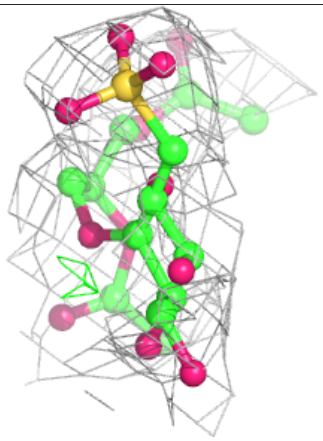


Electron density around SQD A 5212:

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

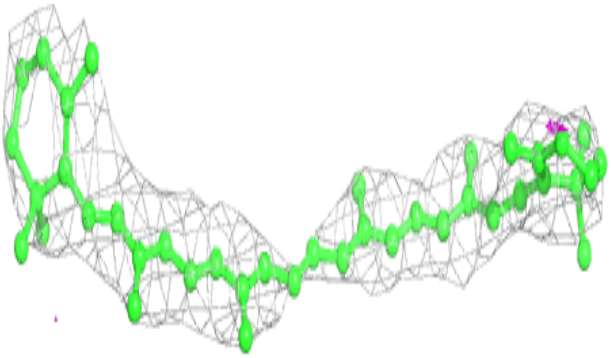


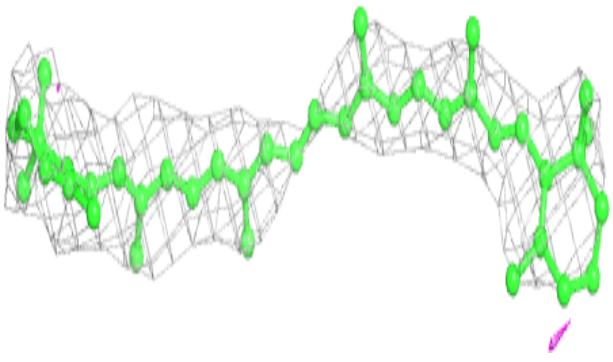


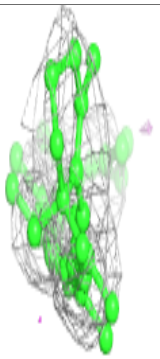


Electron density around BCR d 5357:

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

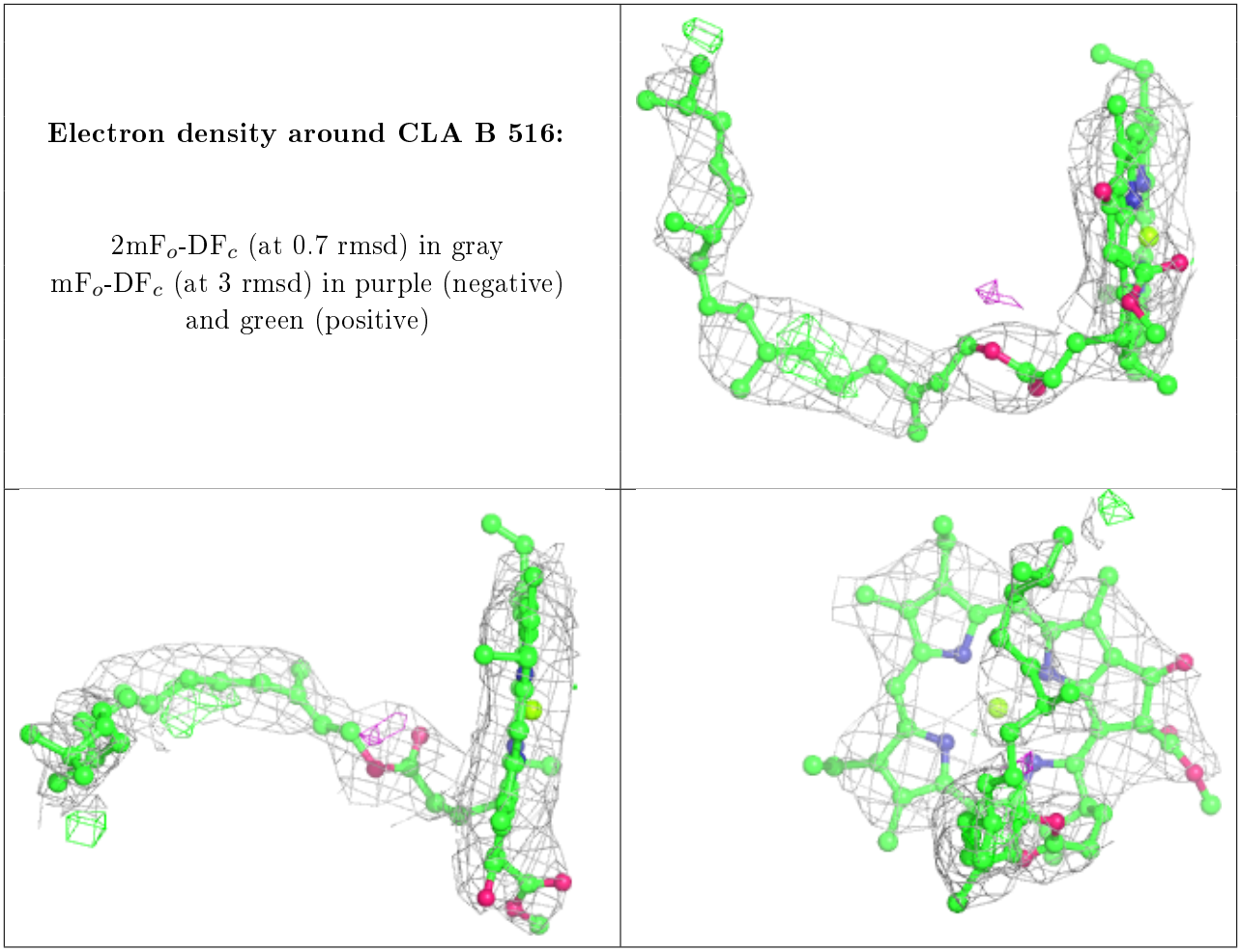






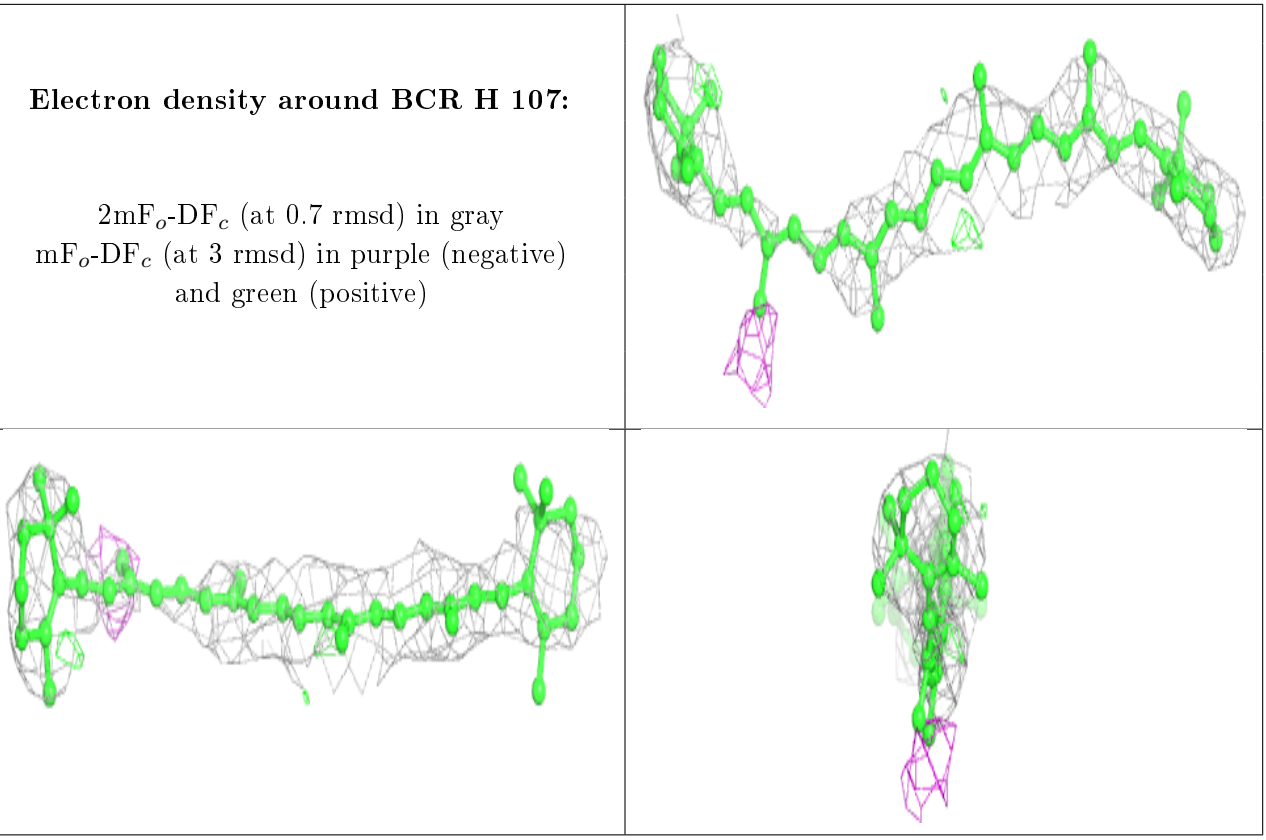
Electron density around CLA B 516:

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



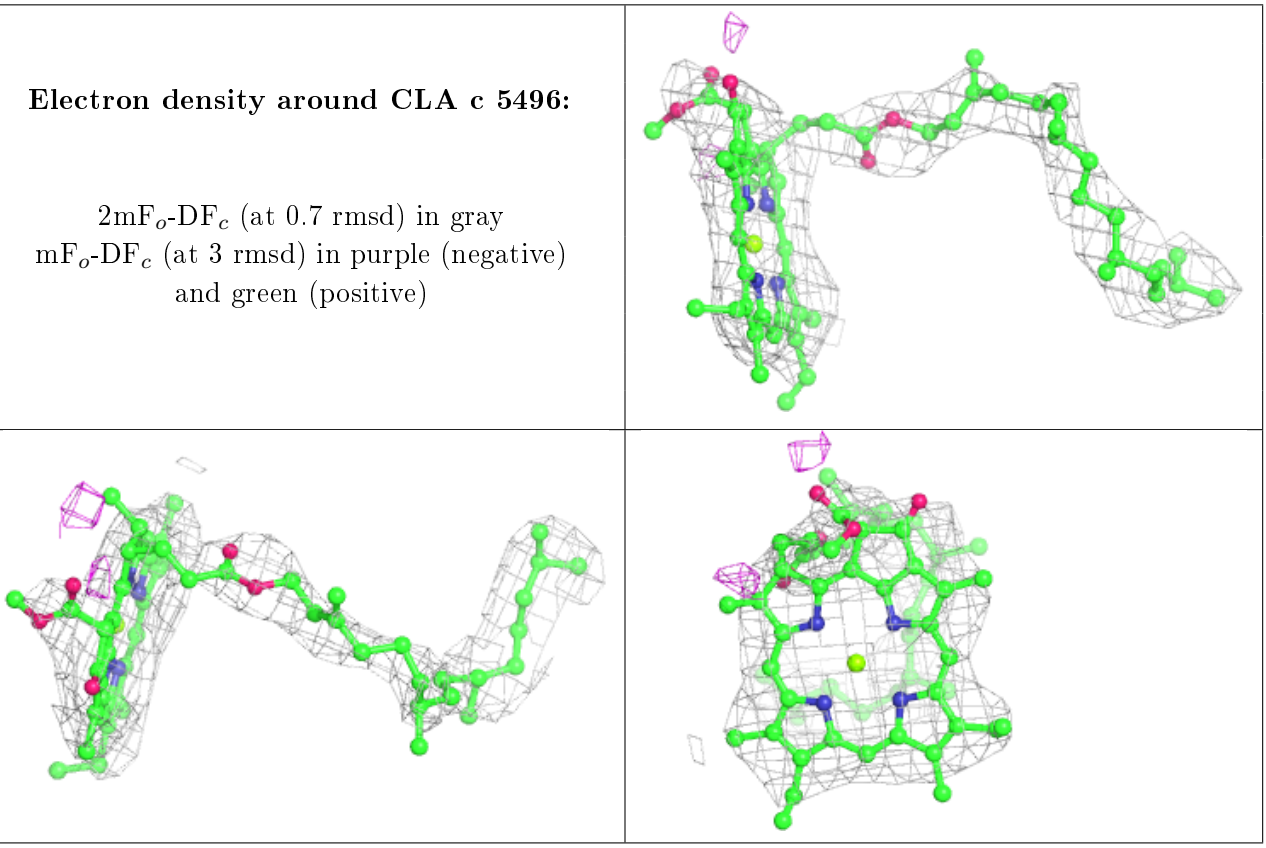
Electron density around BCR H 107:

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



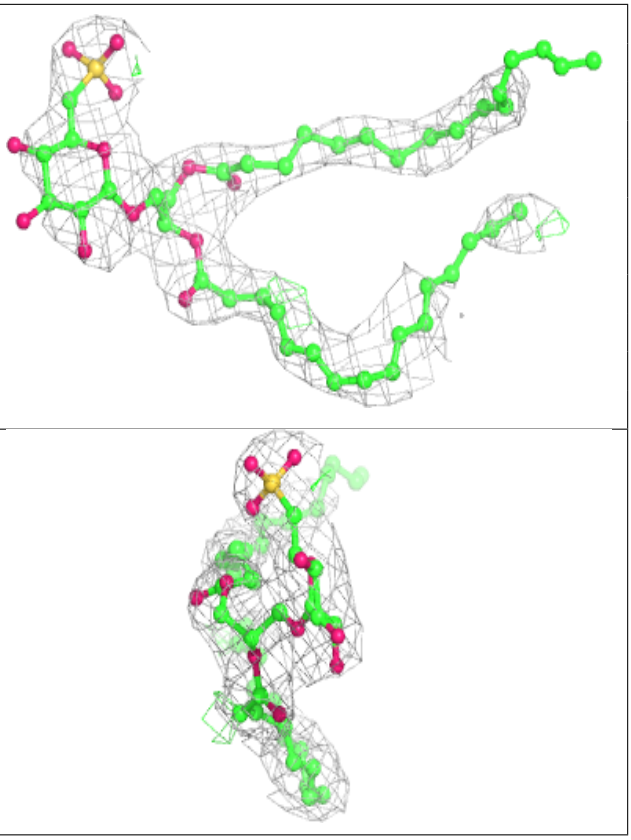
Electron density around CLA c 5496:

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



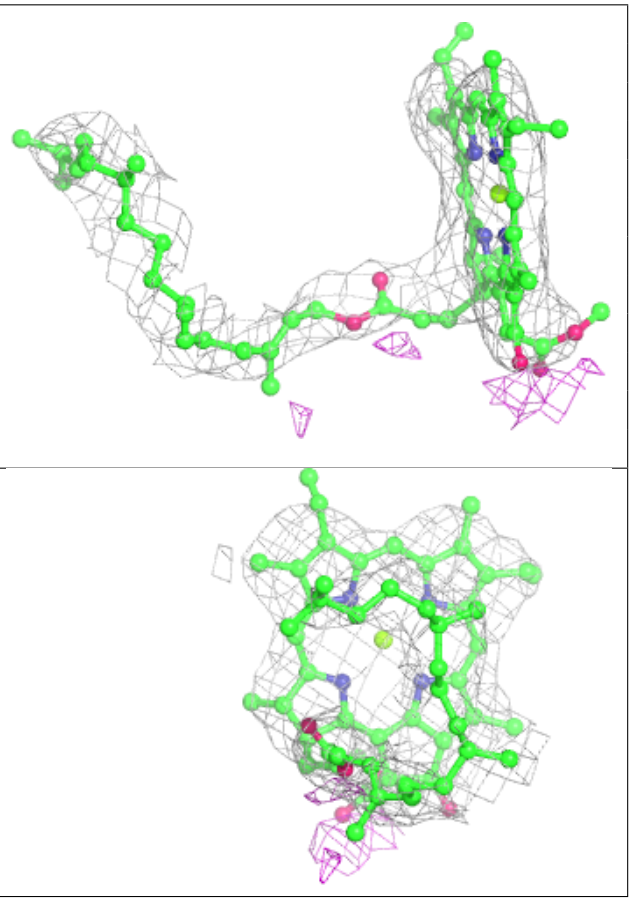
Electron density around SQD A 568:

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



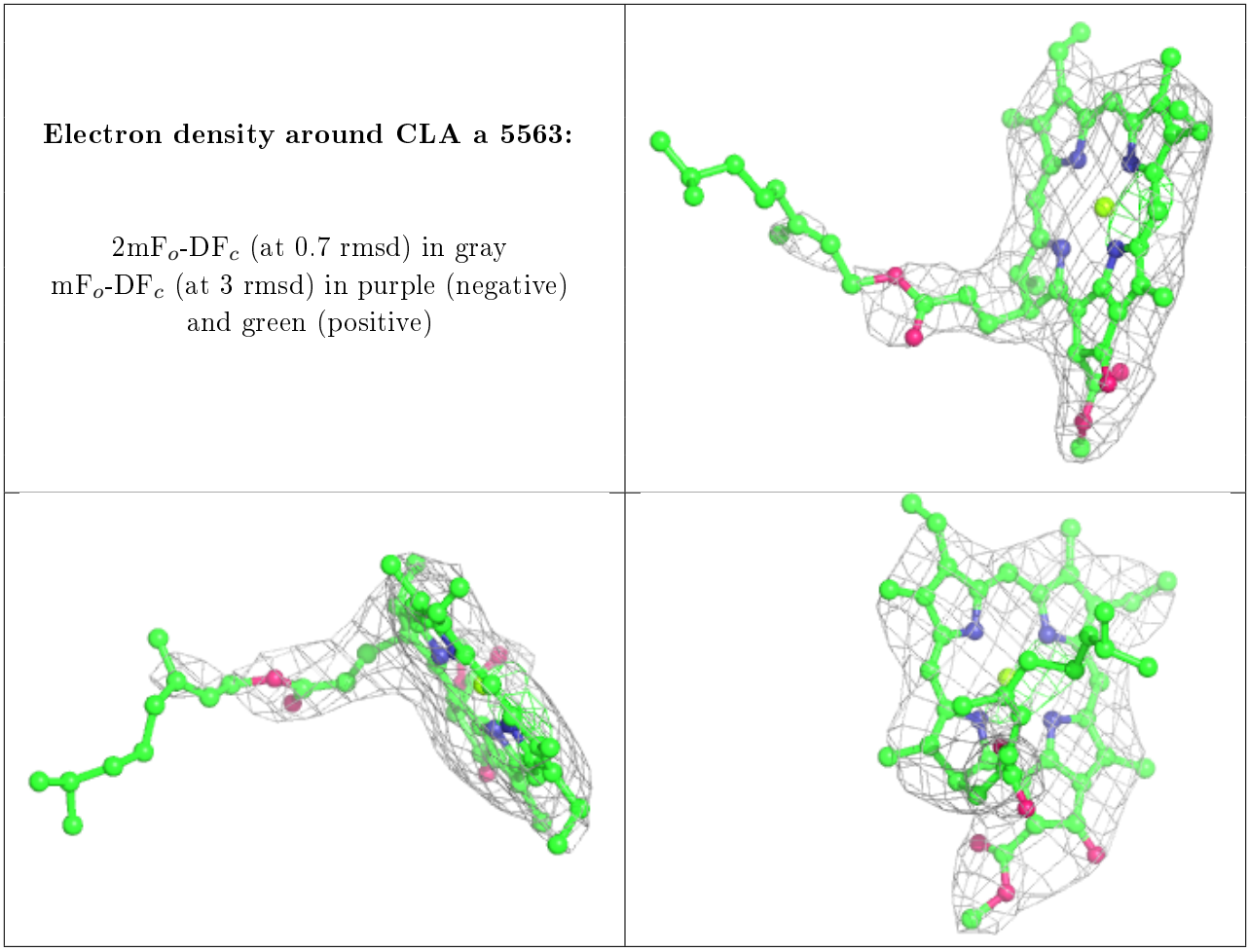
Electron density around CLA C 496:

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



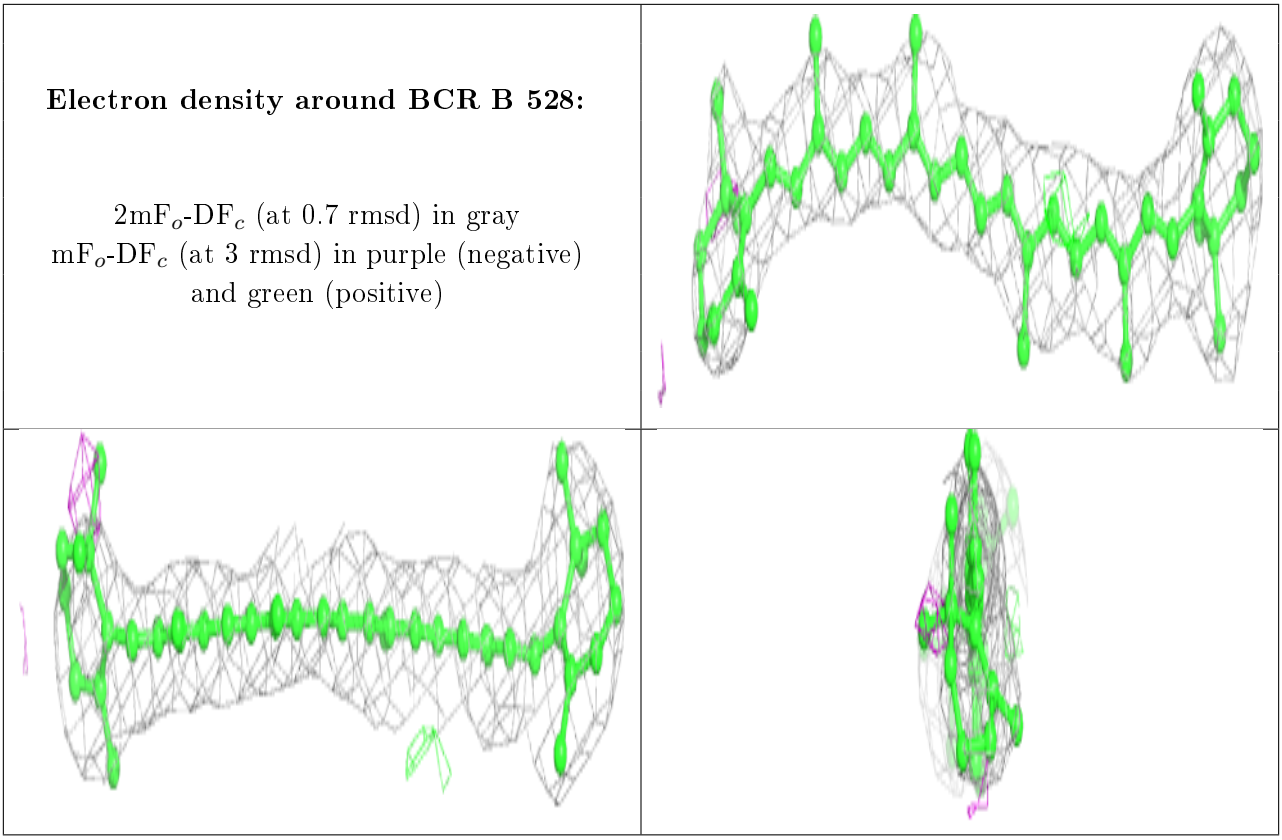
Electron density around CLA a 5563:

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



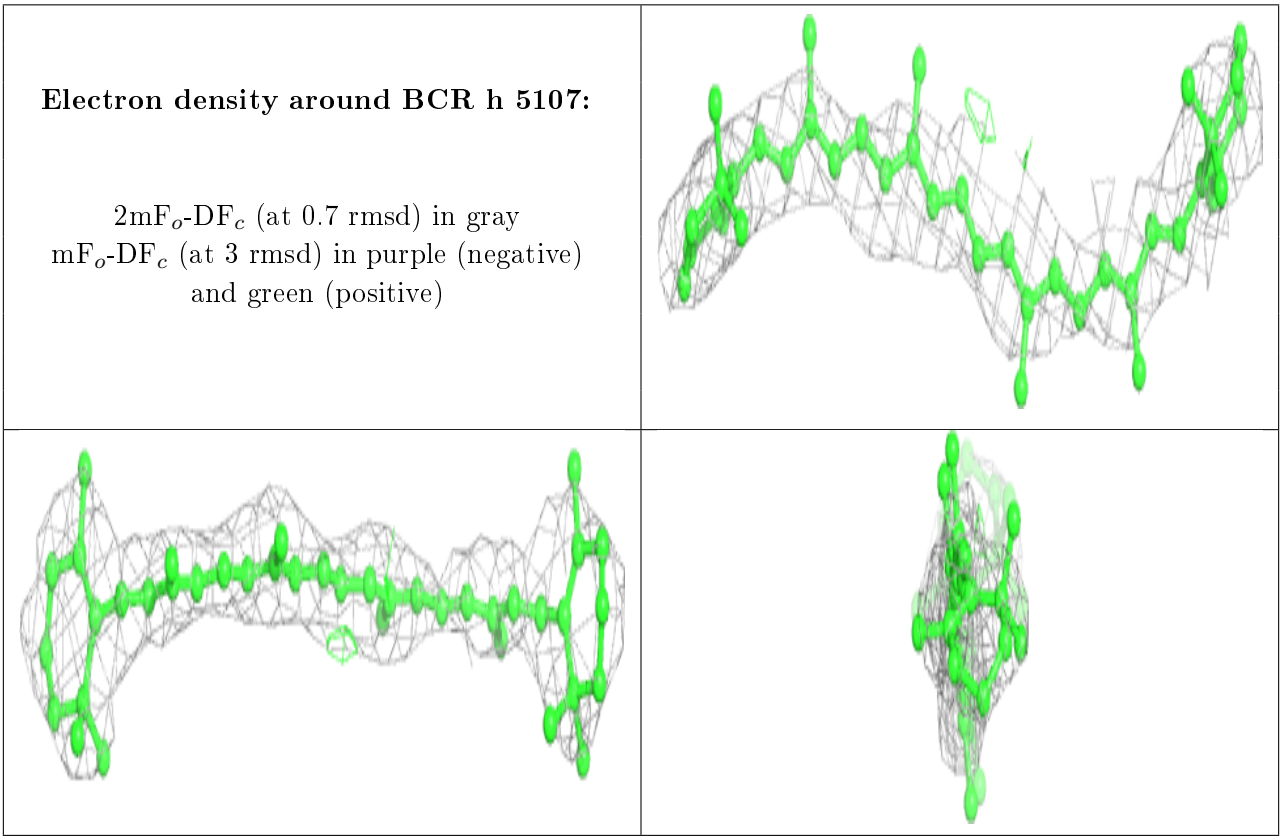
Electron density around BCR B 528:

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



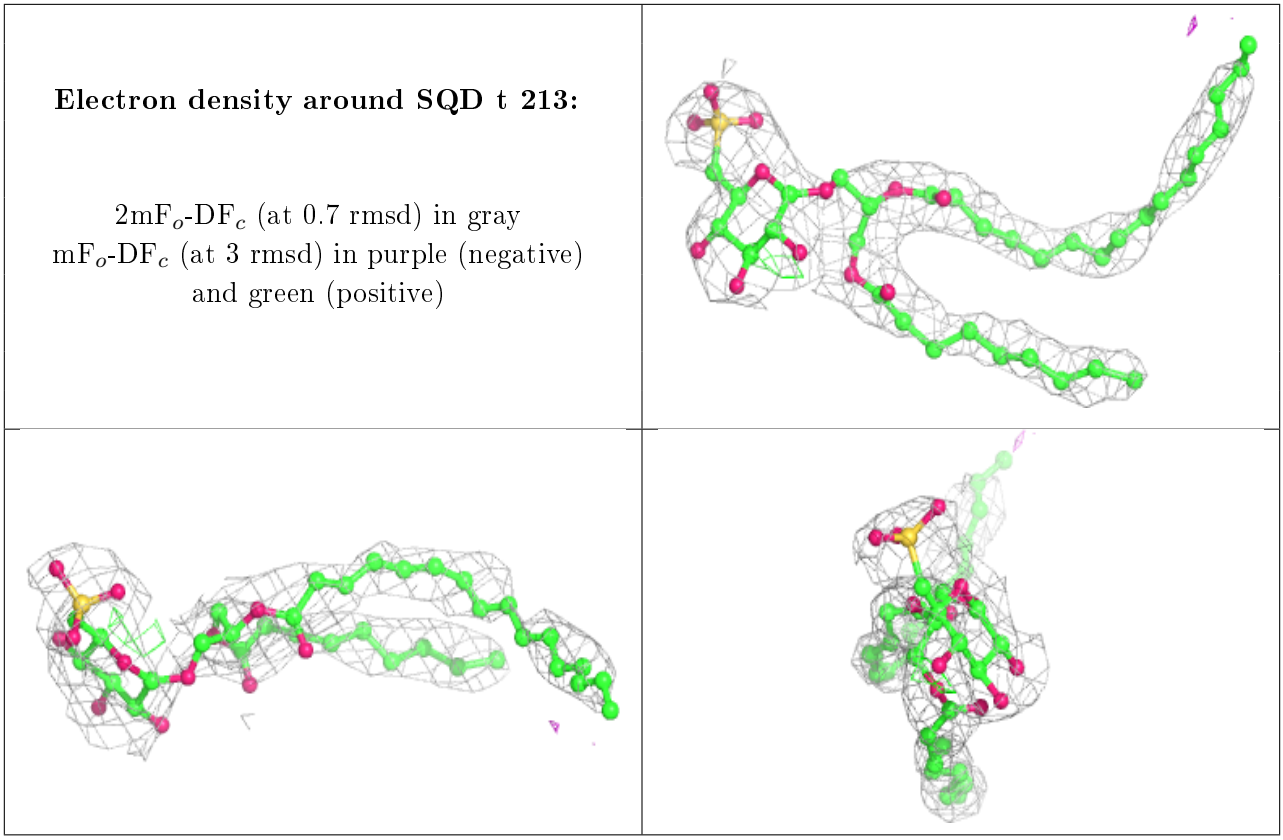
Electron density around BCR h 5107:

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



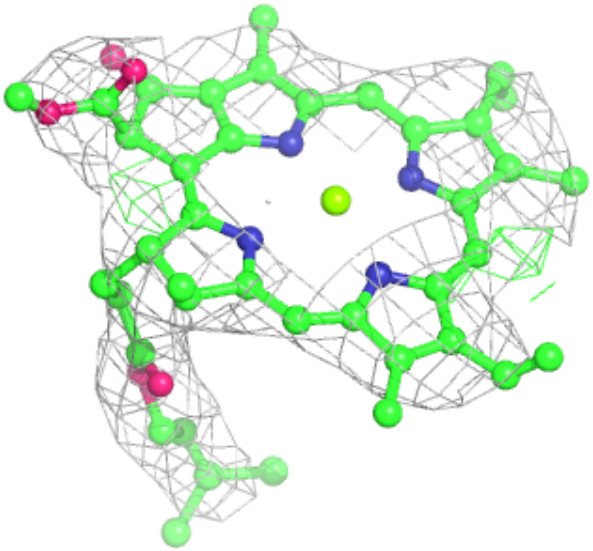
Electron density around SQD t 213:

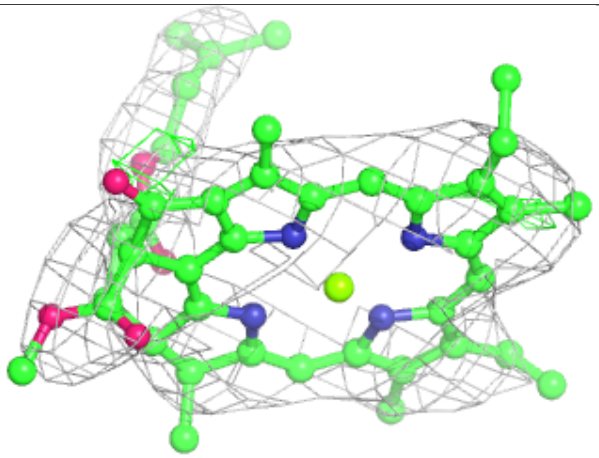
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

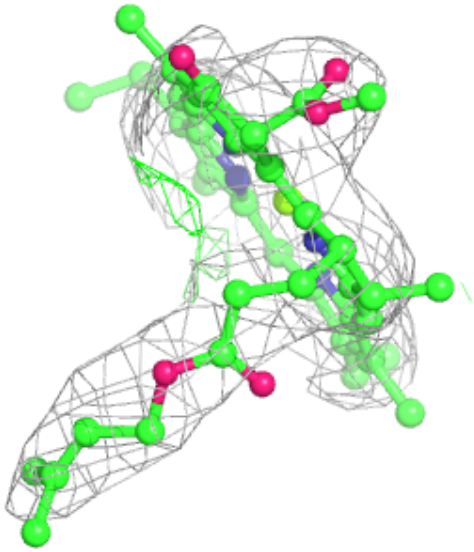


Electron density around CLA C 503:

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

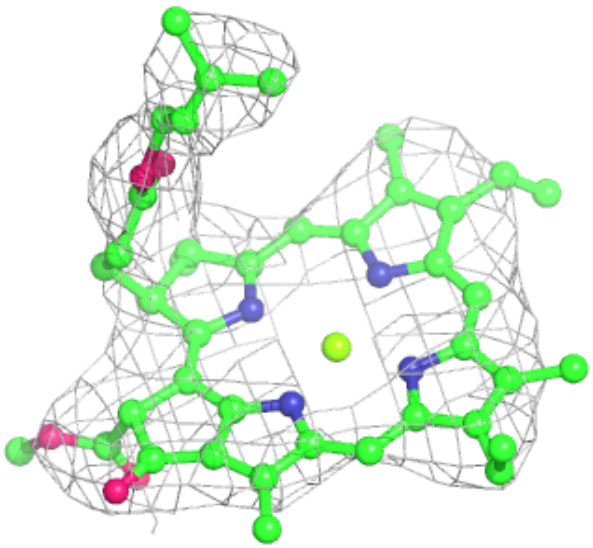


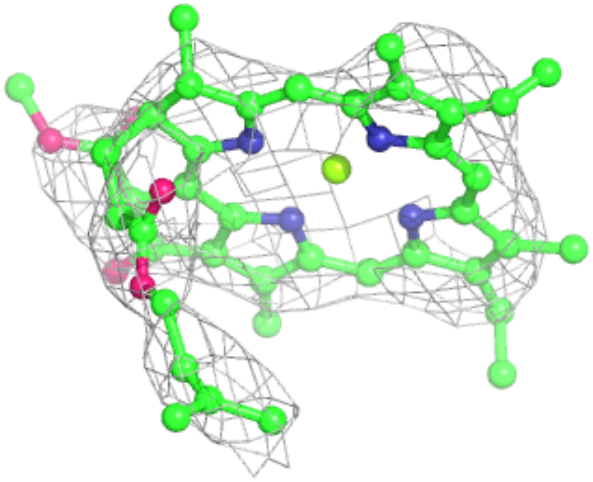


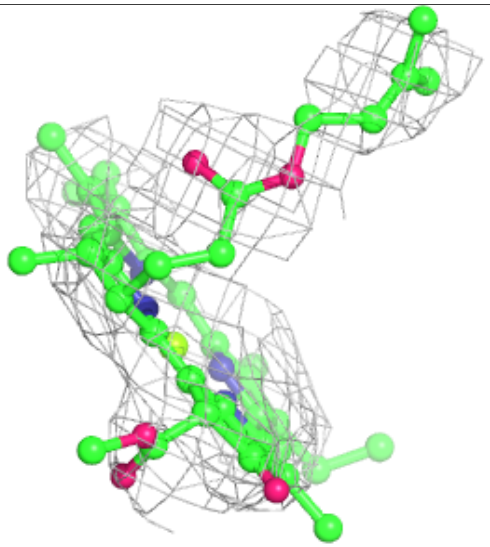


Electron density around CLA c 5503:

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

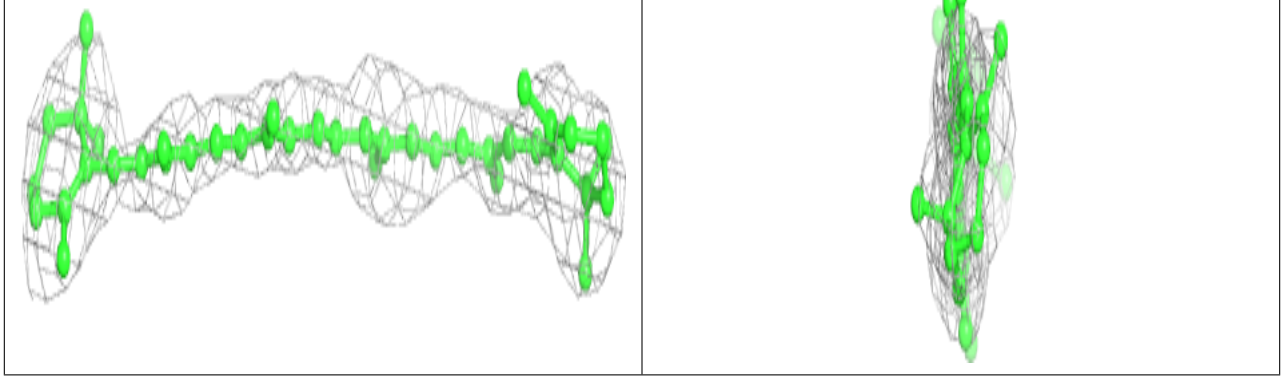






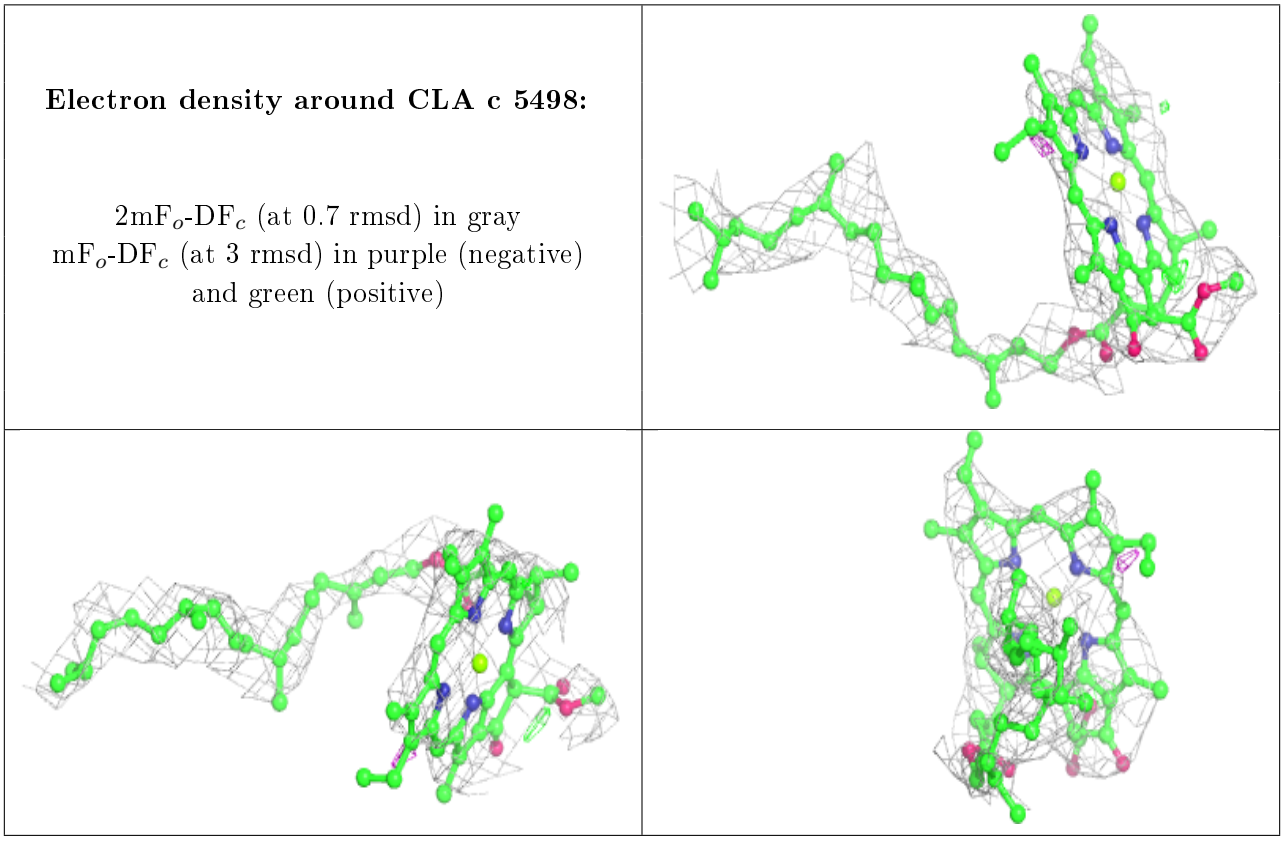
Electron density around BCR X 130:

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



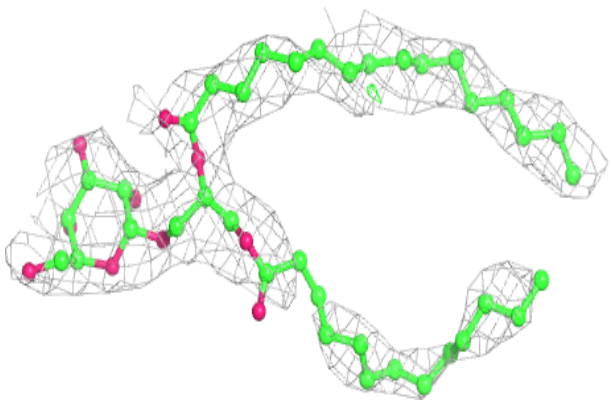
Electron density around CLA c 5498:

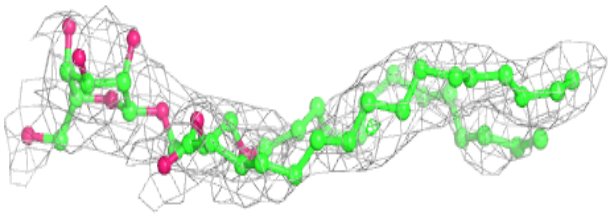
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

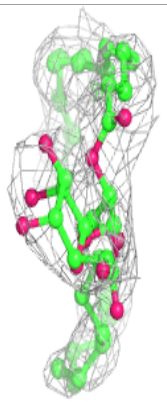


Electron density around MGE i 5201:

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

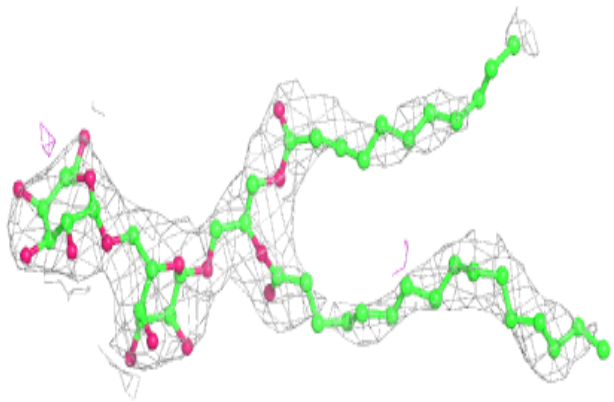


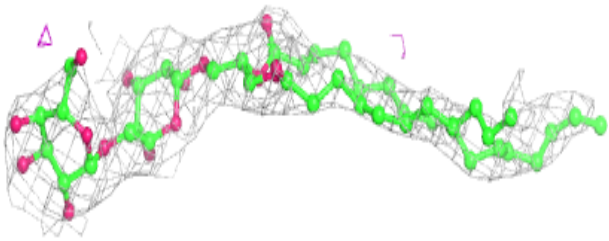


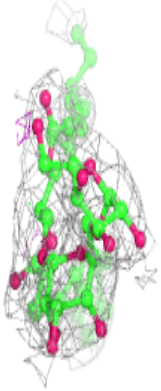


Electron density around DGD c 5509:

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

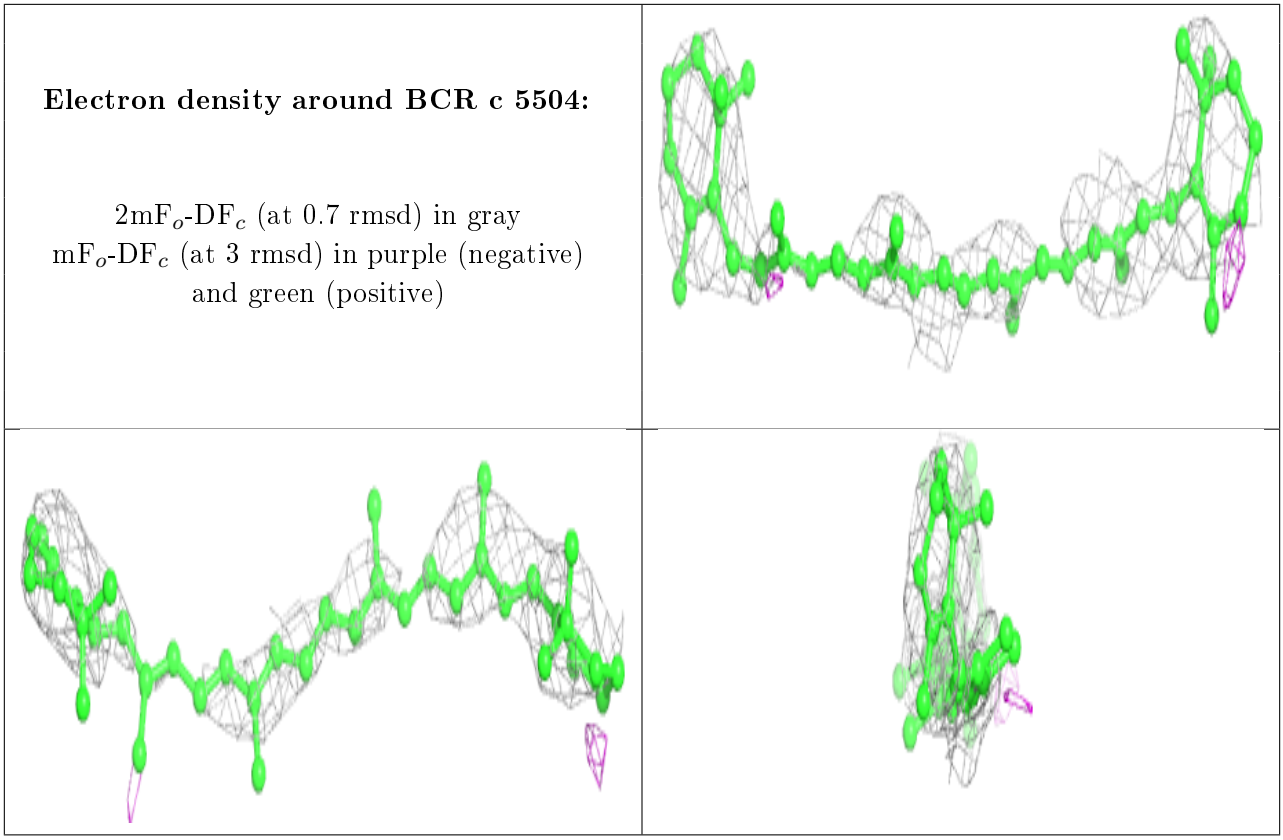






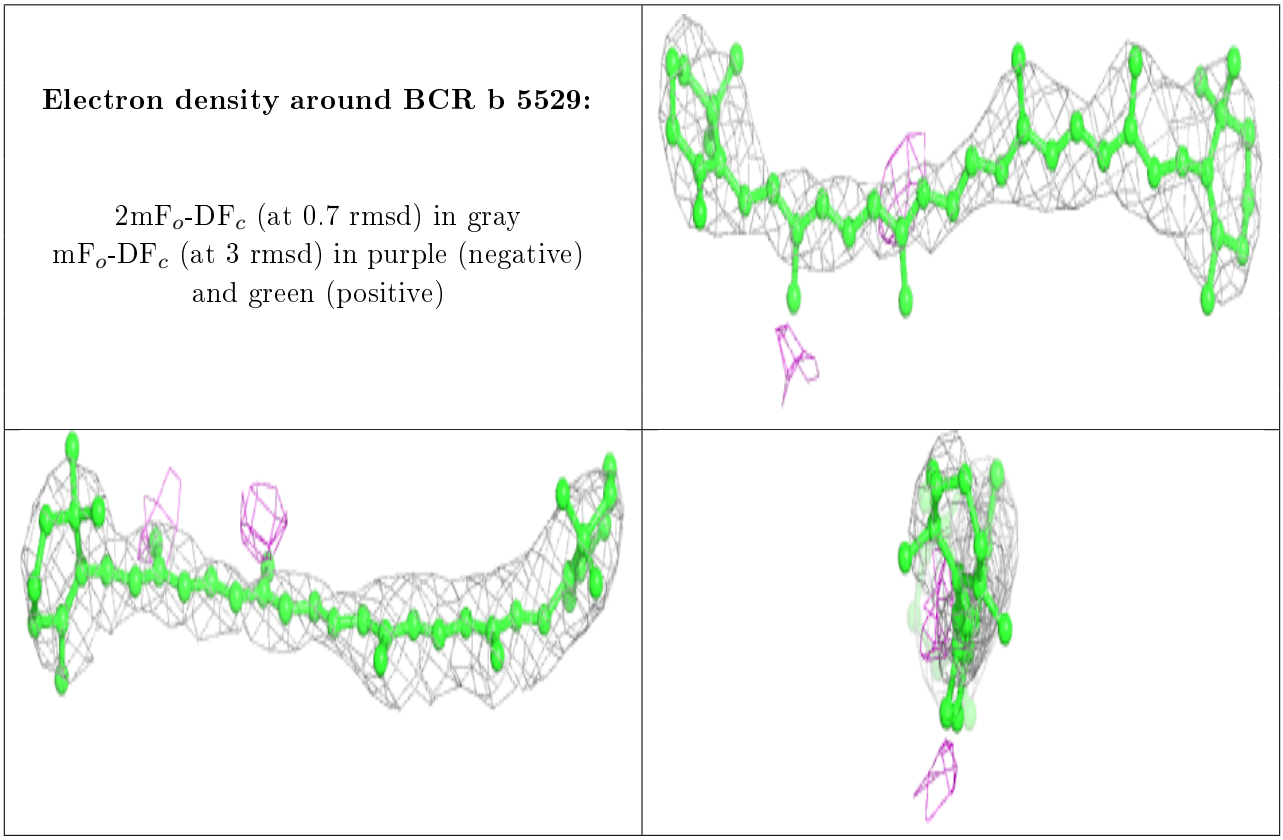
Electron density around BCR c 5504:

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



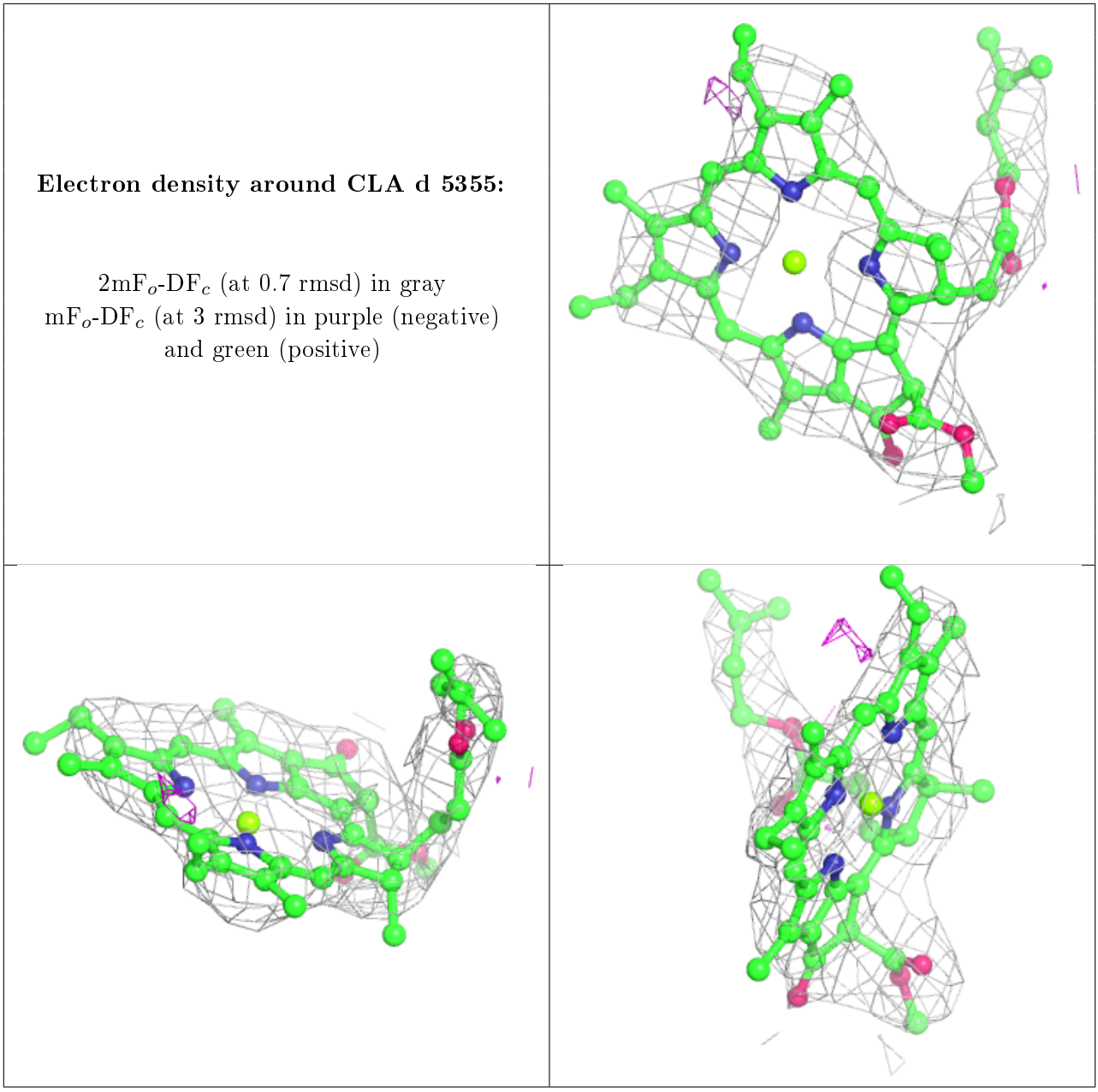
Electron density around BCR b 5529:

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



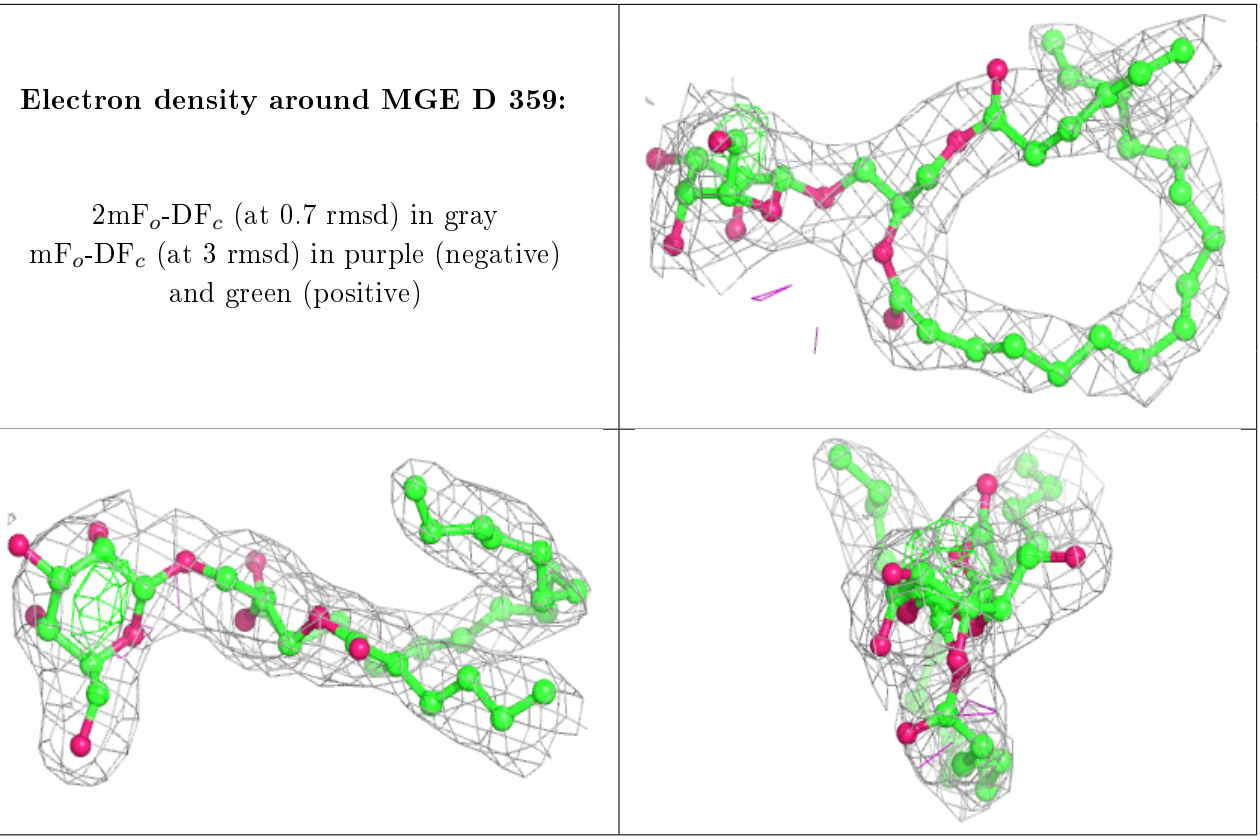
Electron density around CLA d 5355:

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



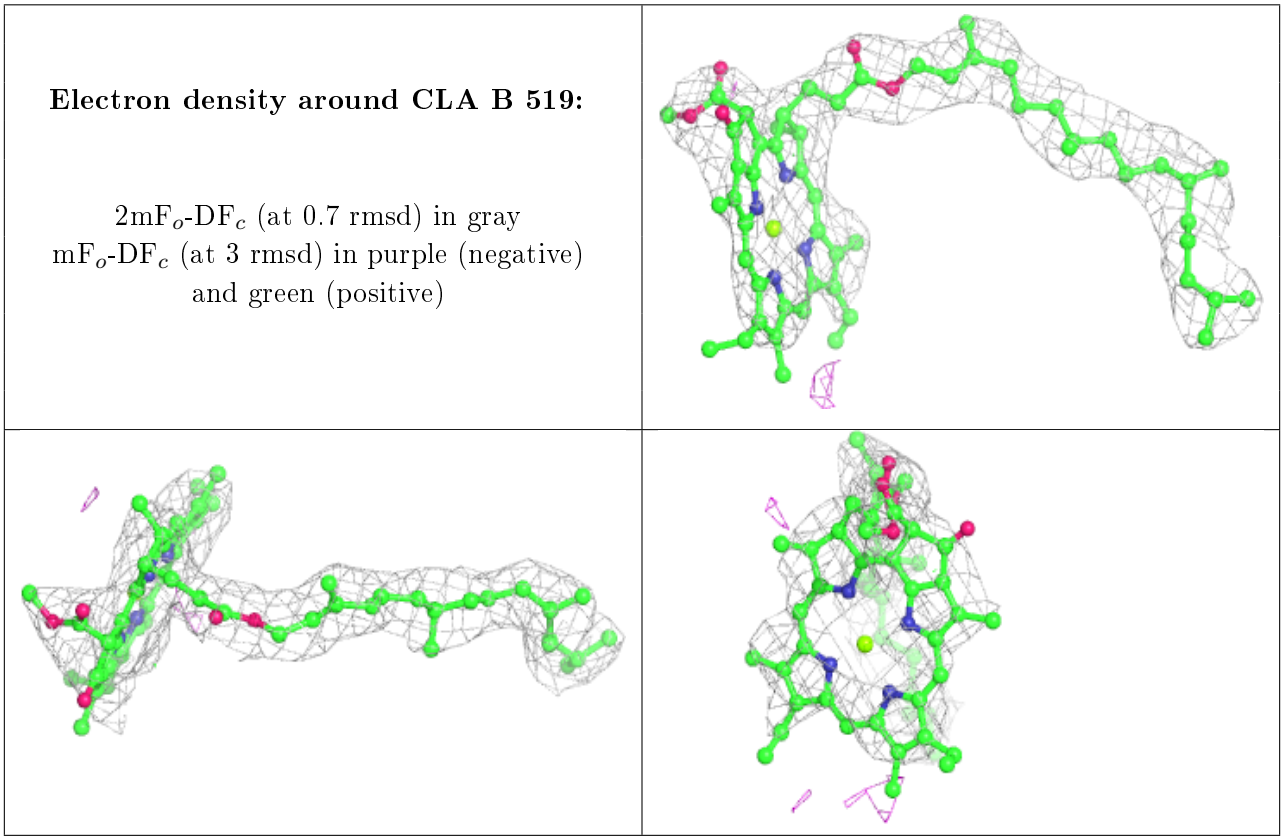
Electron density around MGE D 359:

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



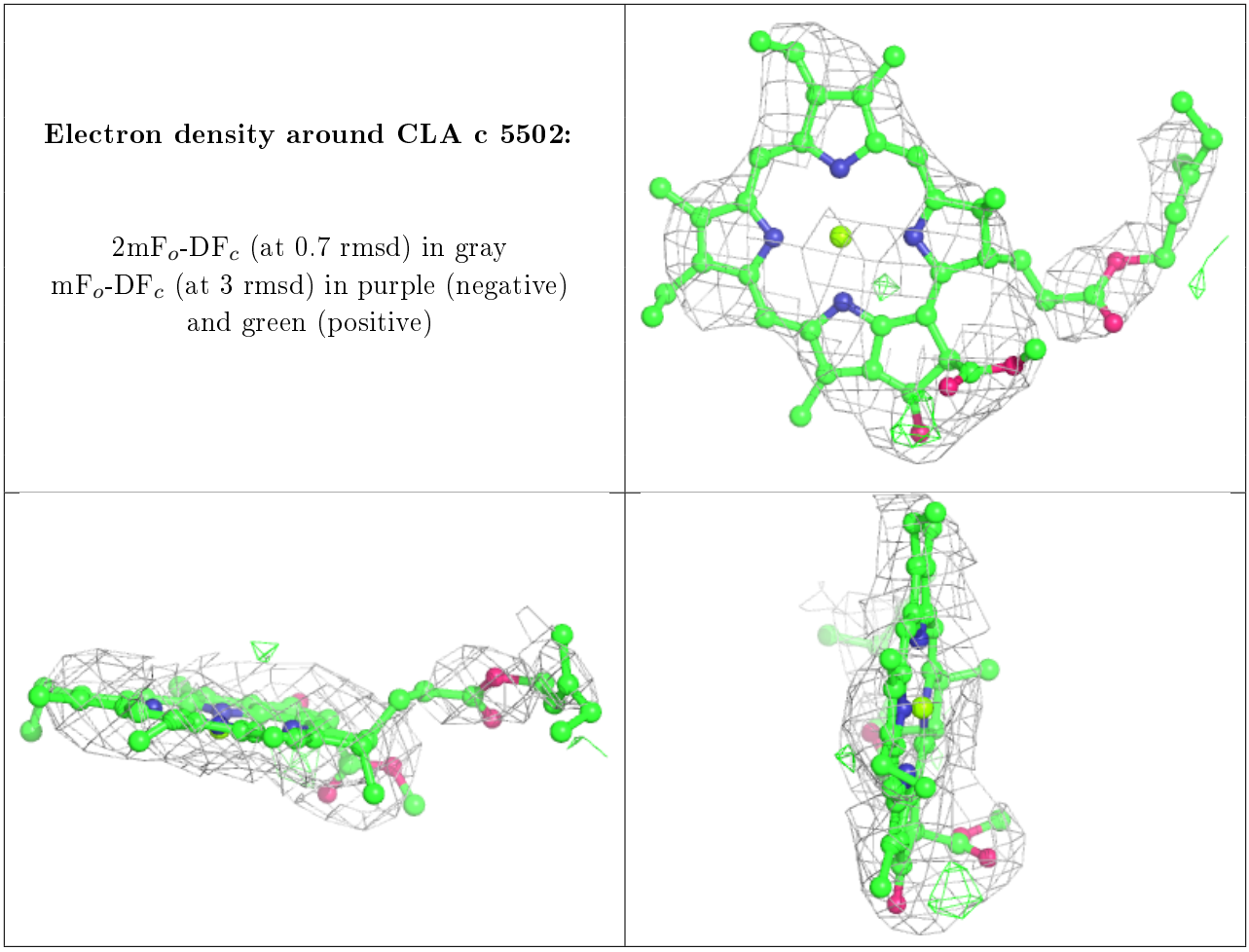
Electron density around CLA B 519:

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



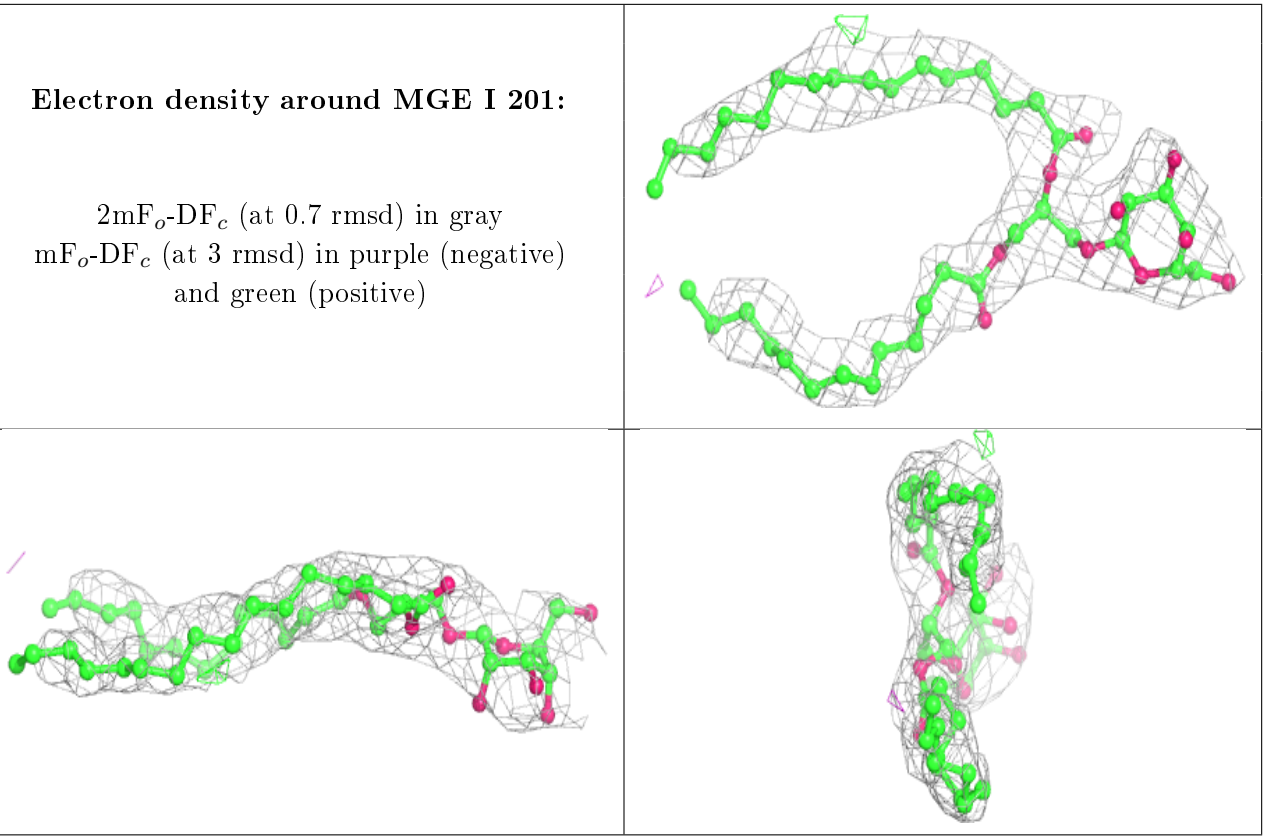
Electron density around CLA c 5502:

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



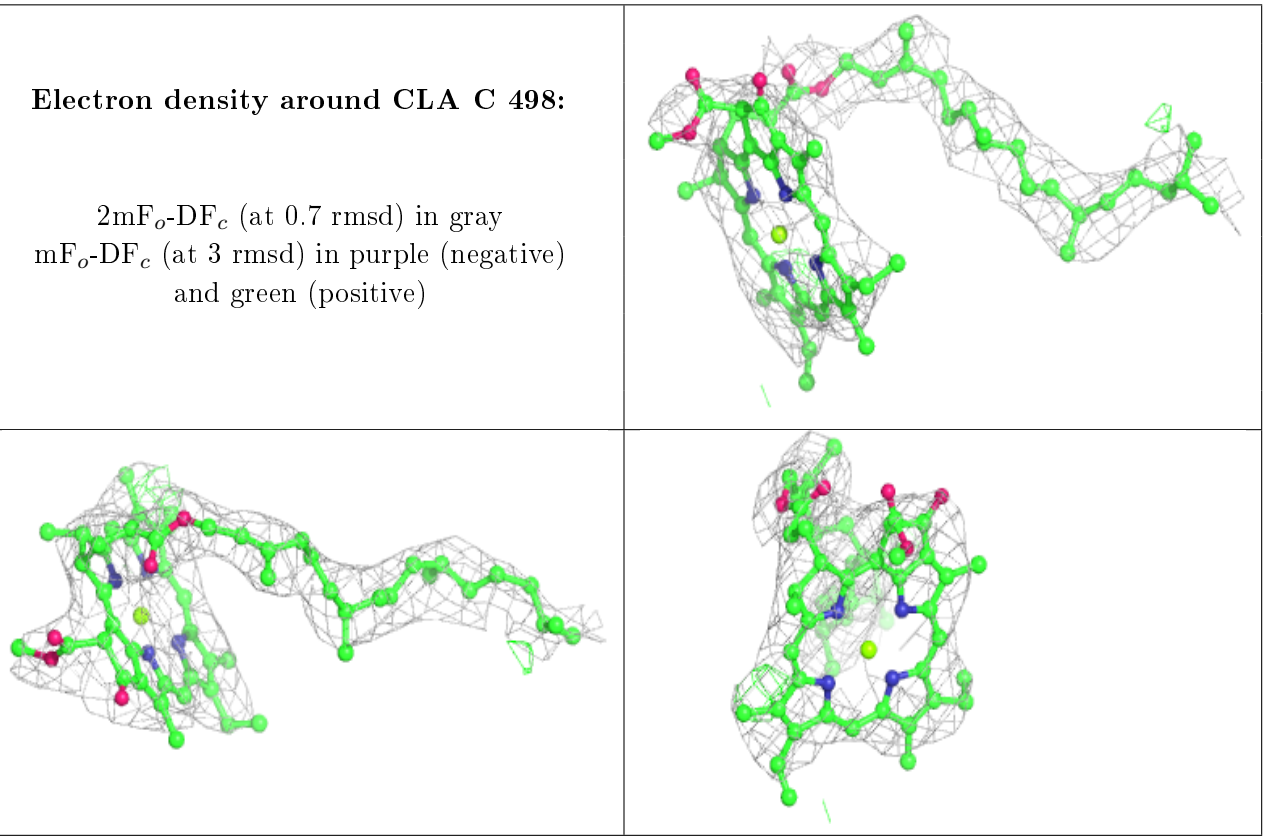
Electron density around MGE I 201:

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



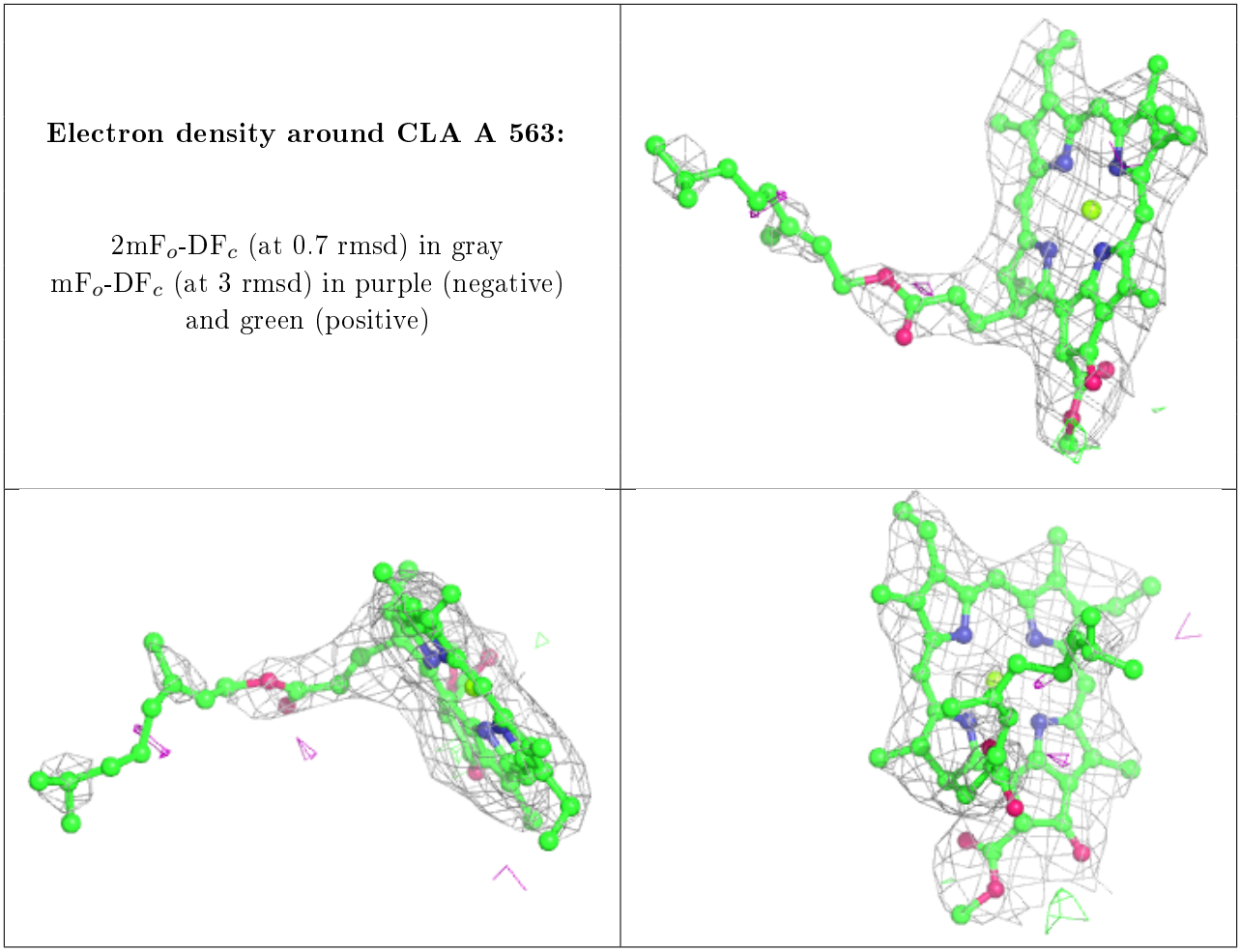
Electron density around CLA C 498:

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



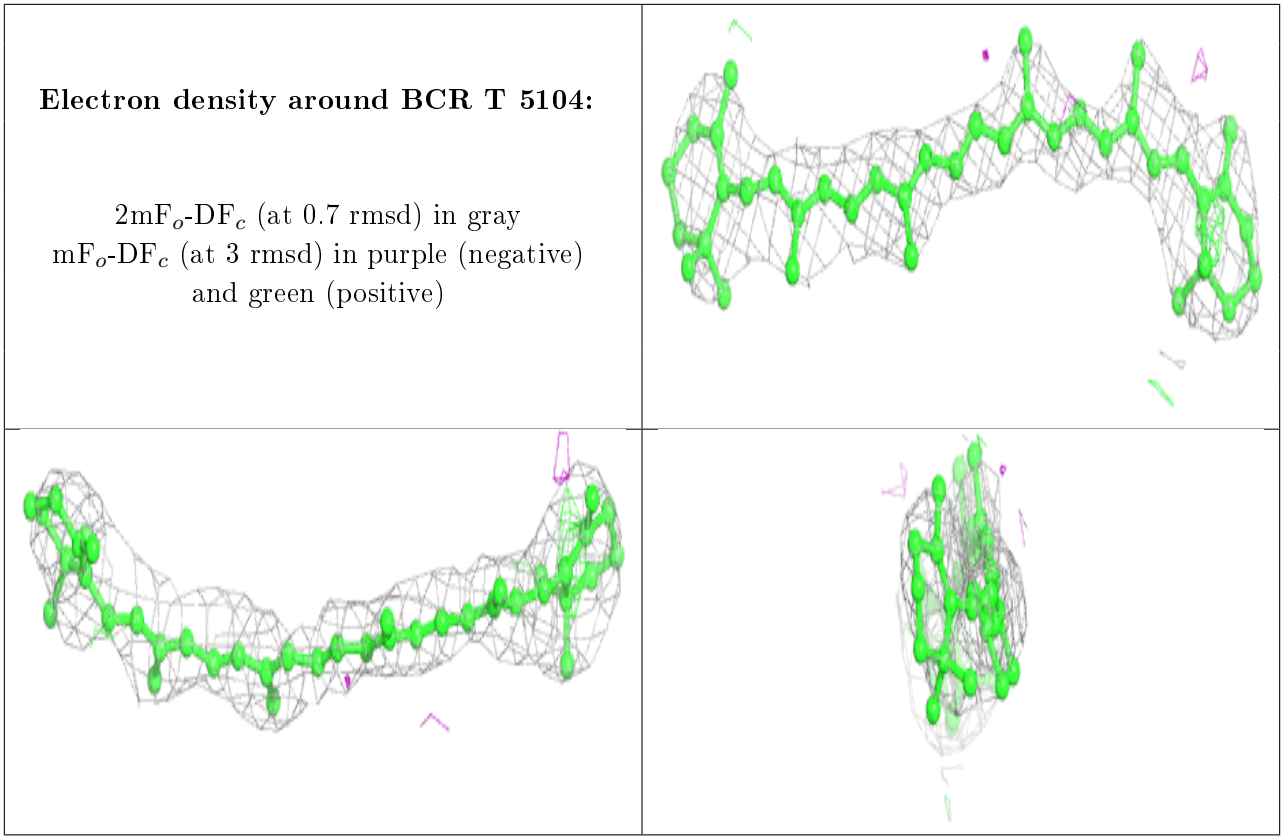
Electron density around CLA A 563:

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



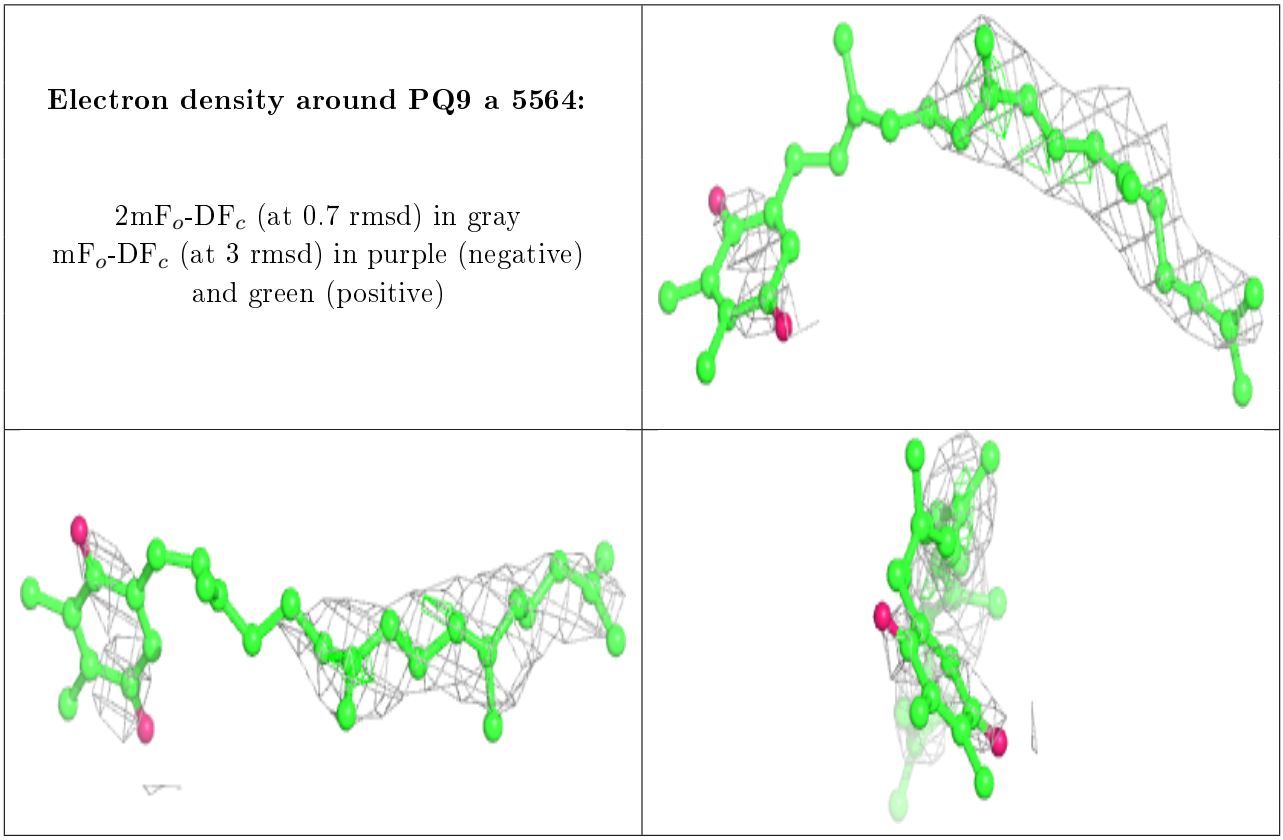
Electron density around BCR T 5104:

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



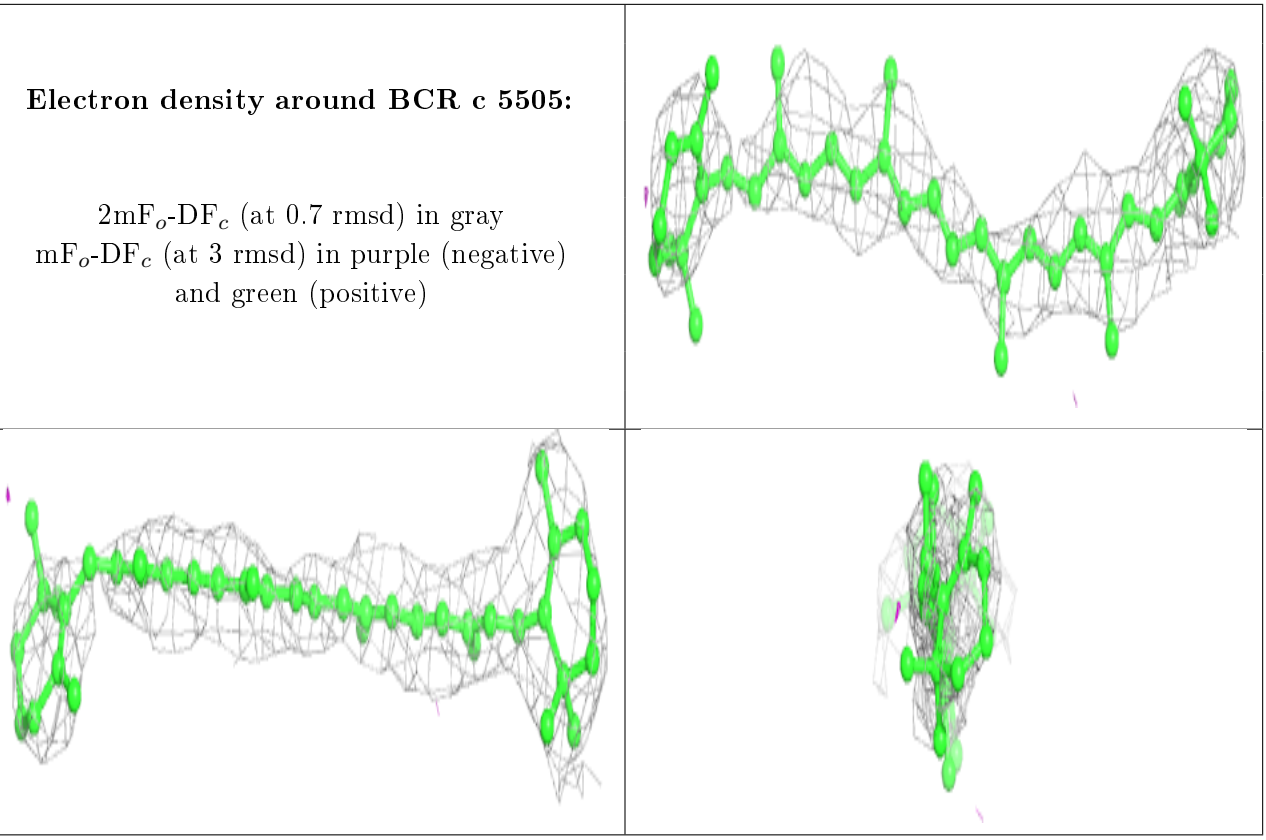
Electron density around PQ9 a 5564:

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



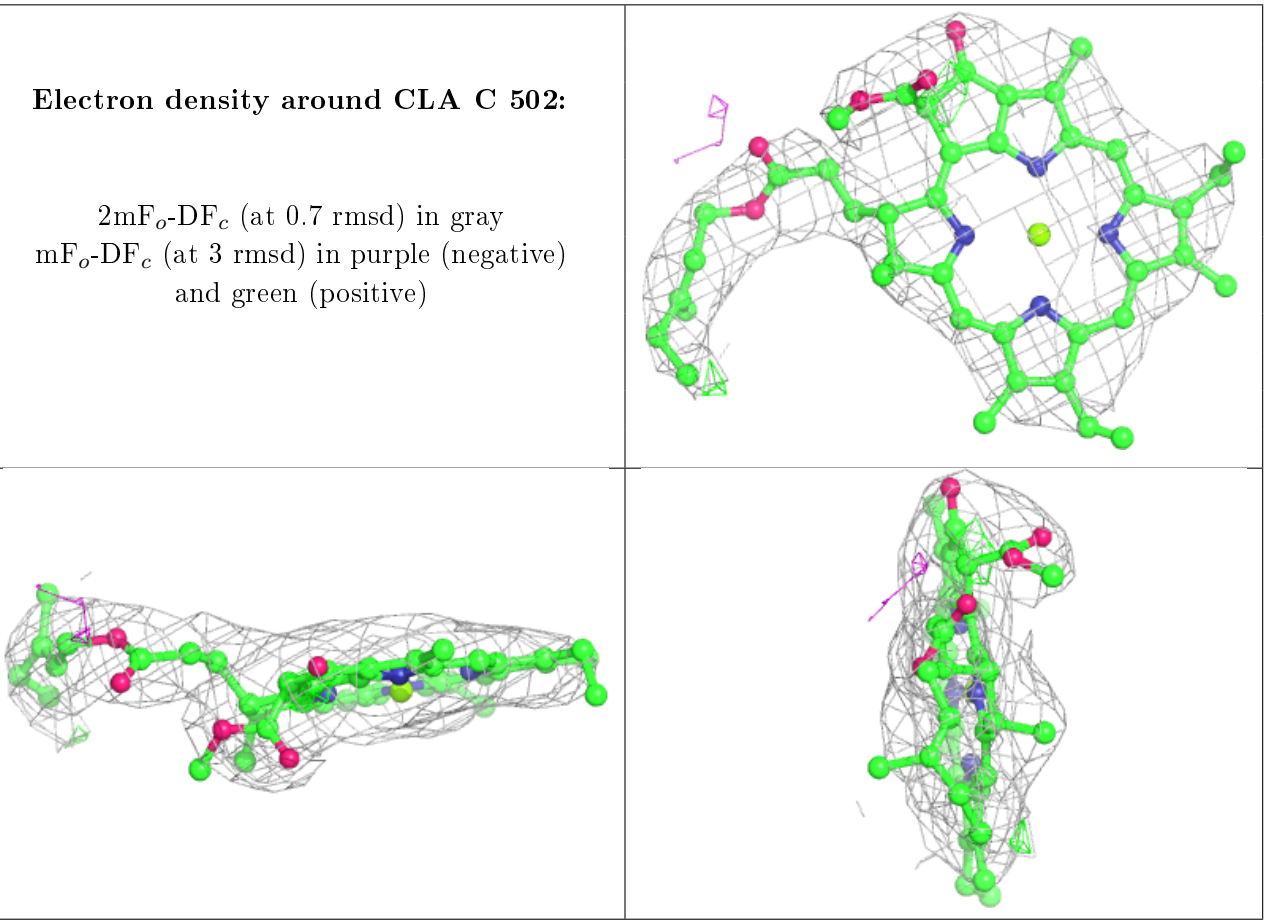
Electron density around BCR c 5505:

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



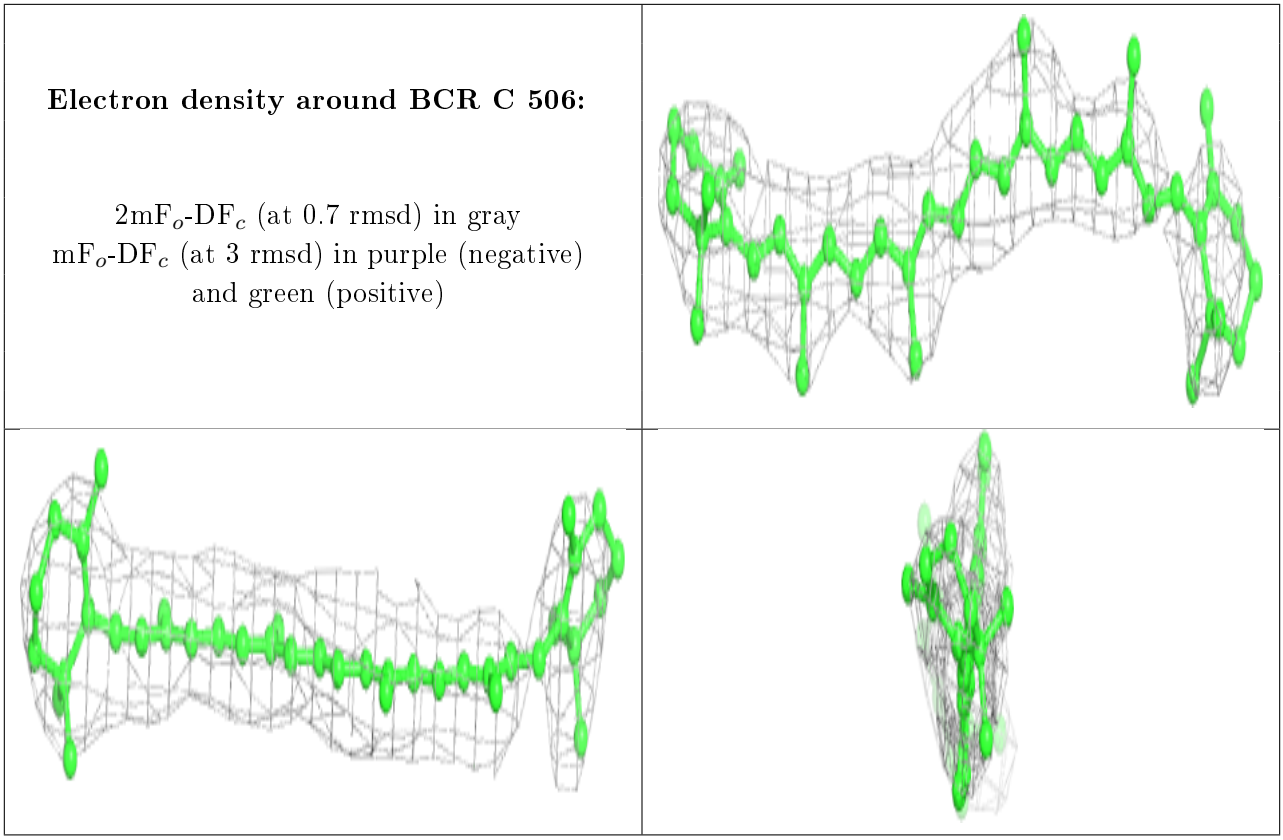
Electron density around CLA C 502:

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



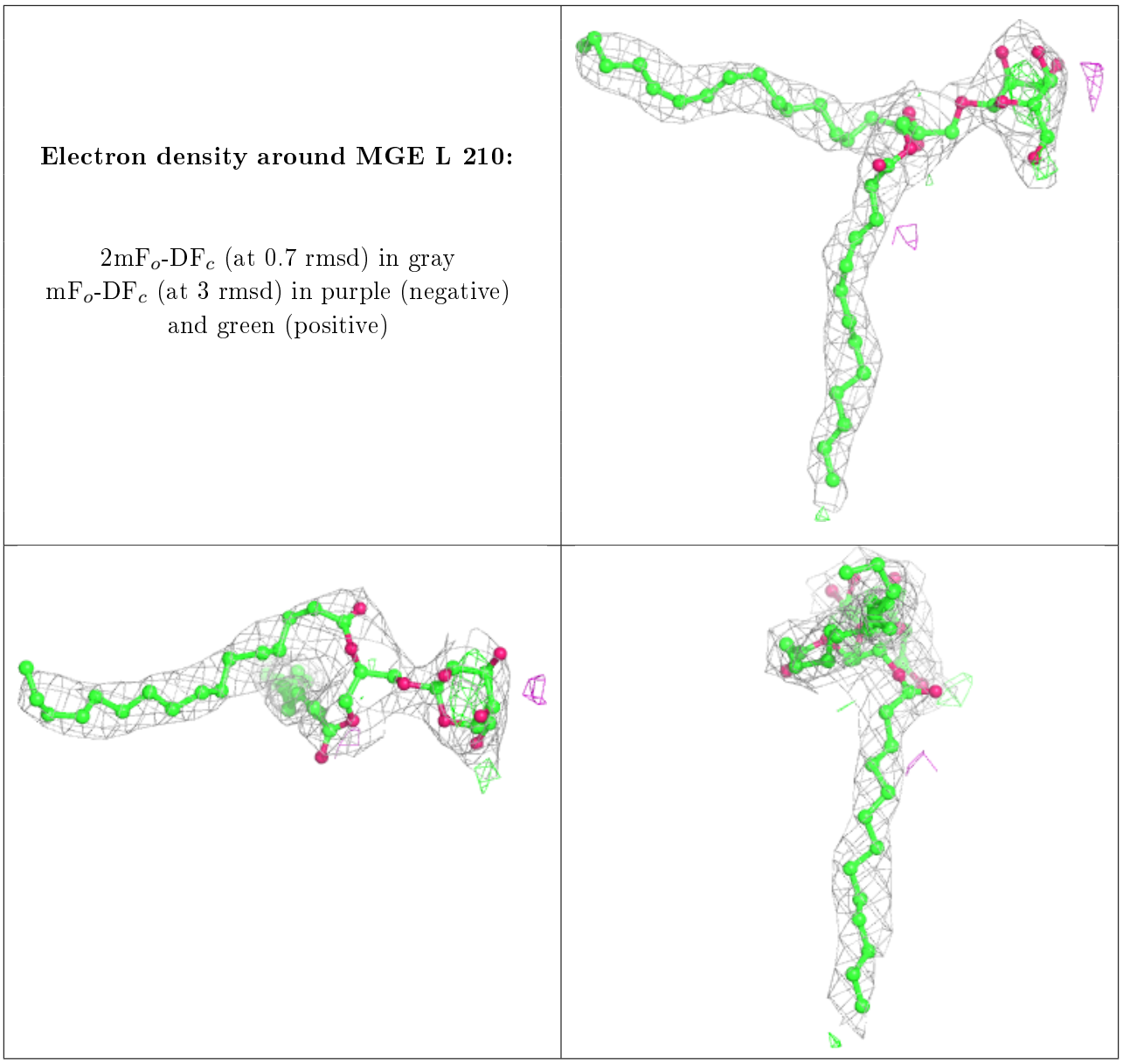
Electron density around BCR C 506:

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



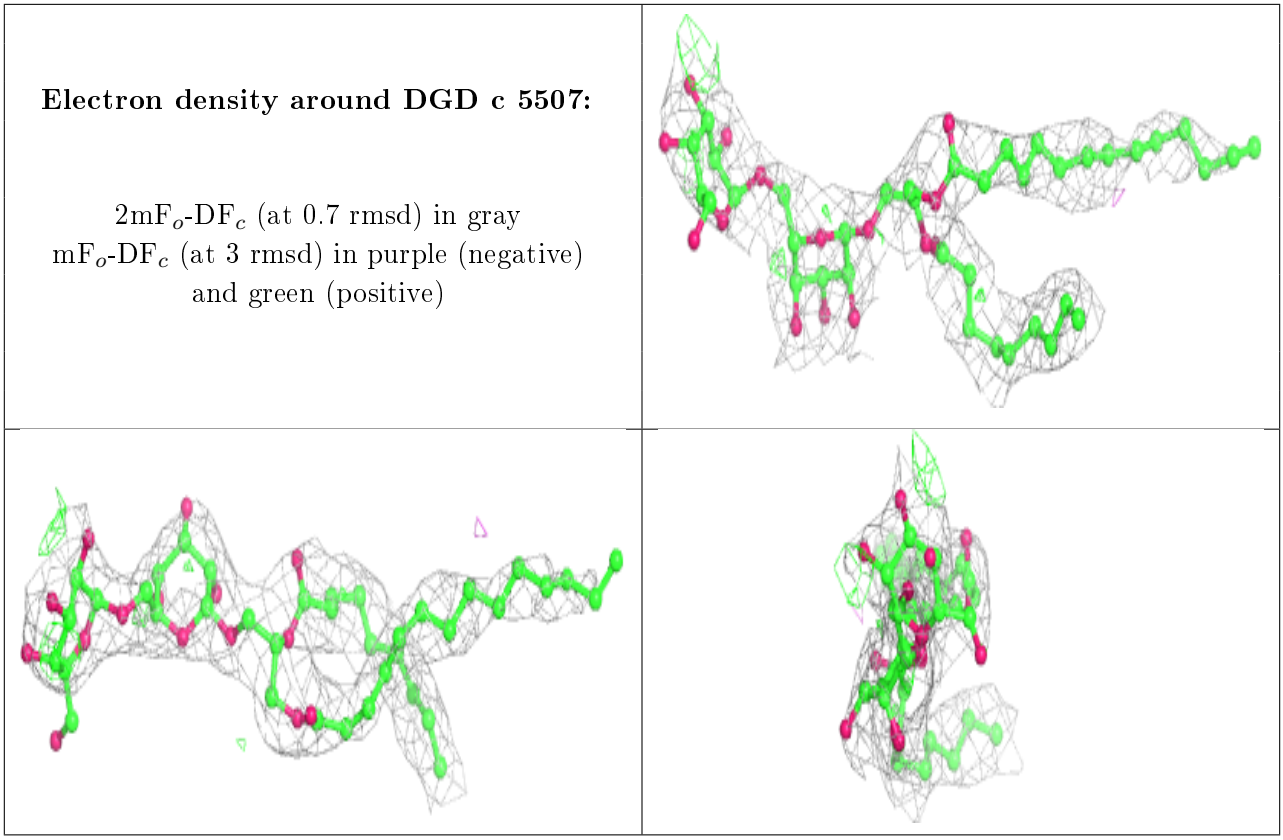
Electron density around MGE L 210:

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



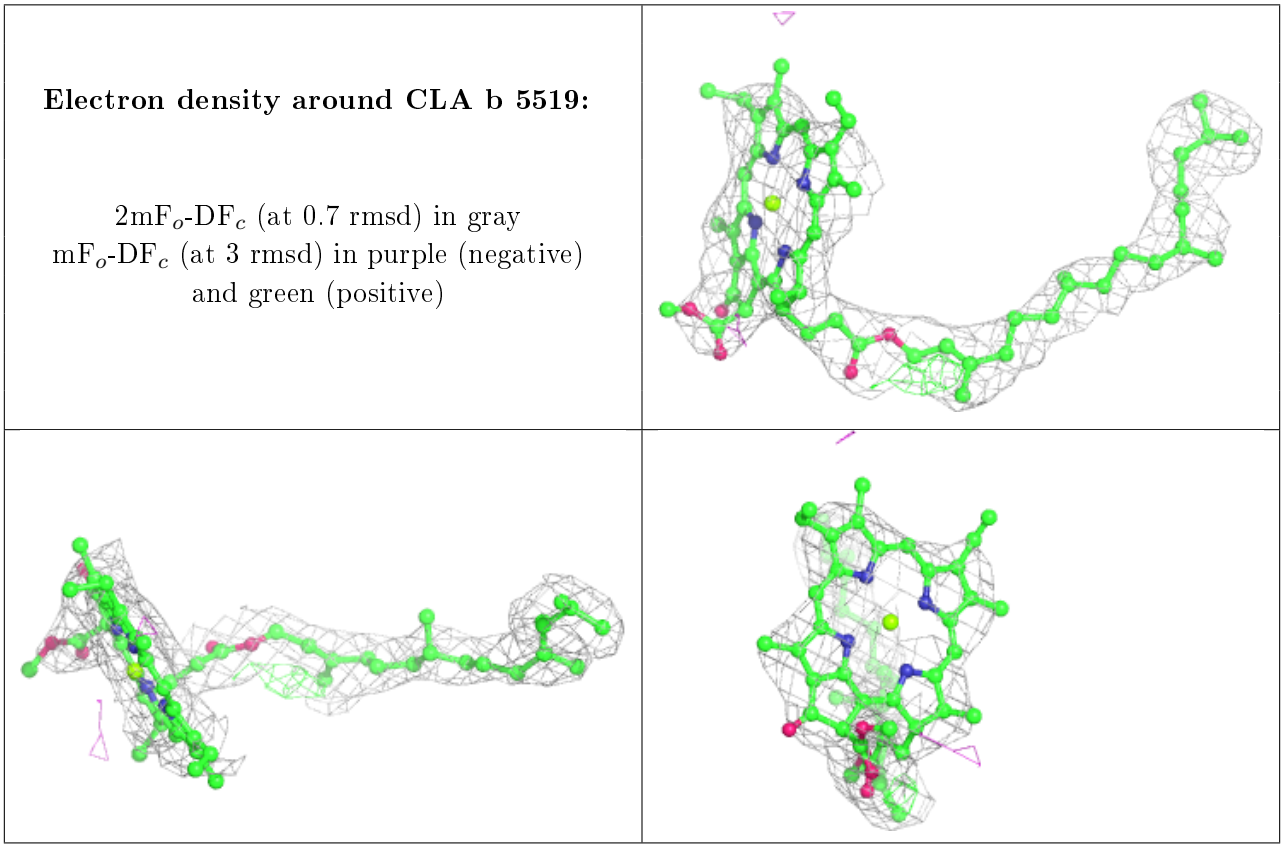
Electron density around DGD c 5507:

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



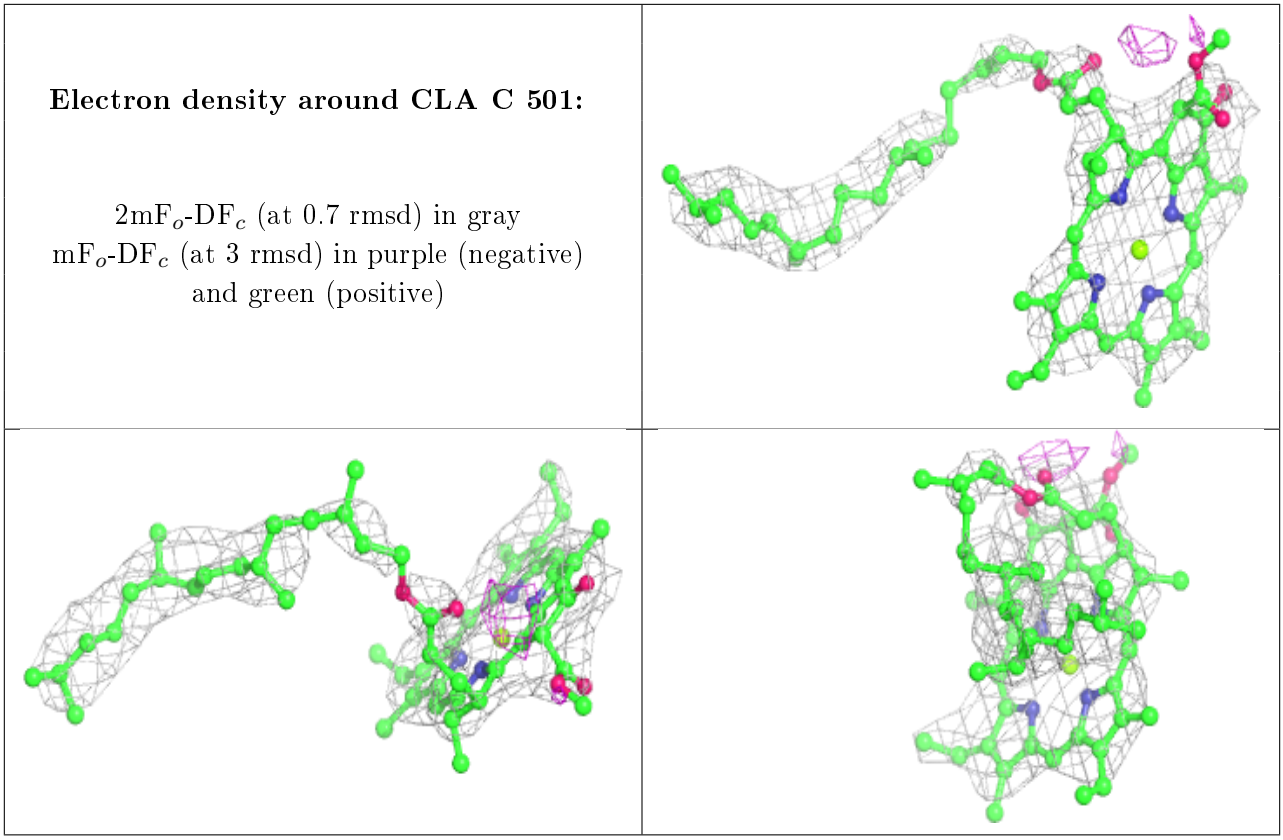
Electron density around CLA b 5519:

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



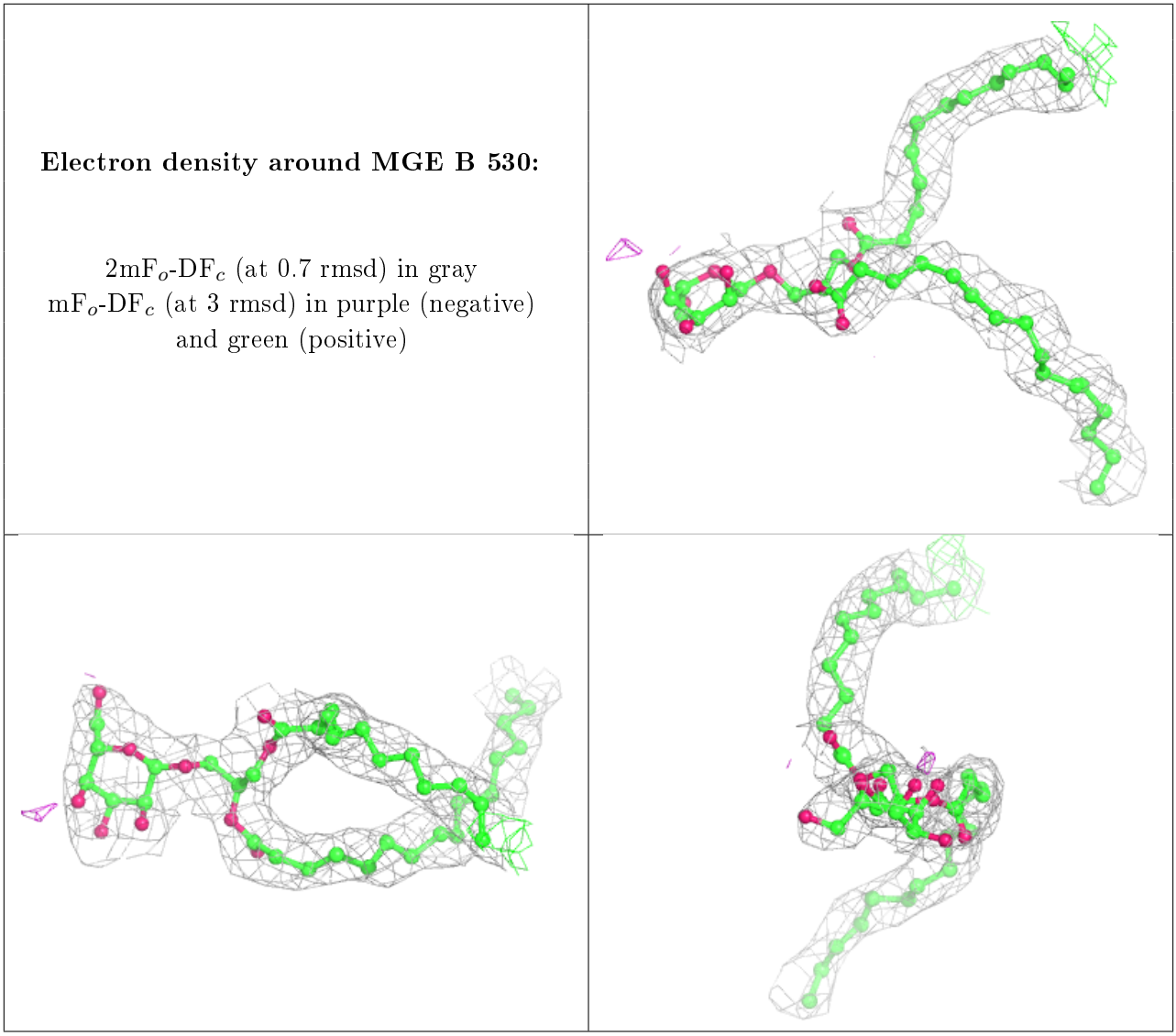
Electron density around CLA C 501:

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



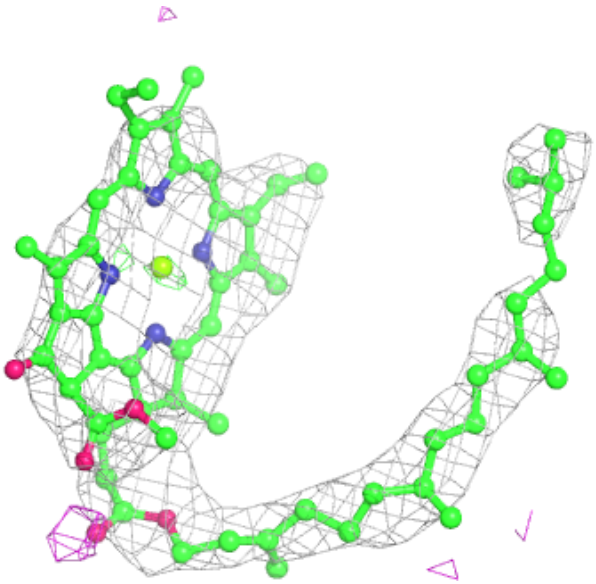
Electron density around MGE B 530:

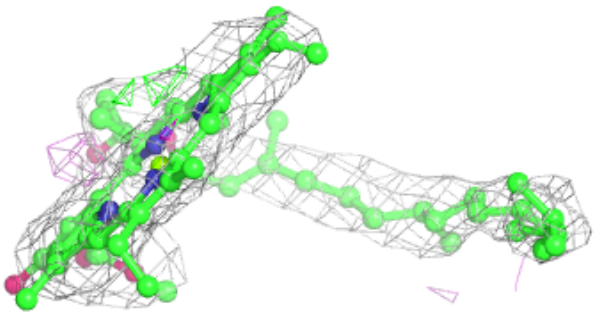
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

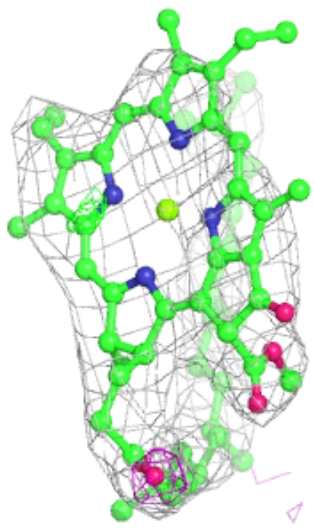


Electron density around CLA c 5497:

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

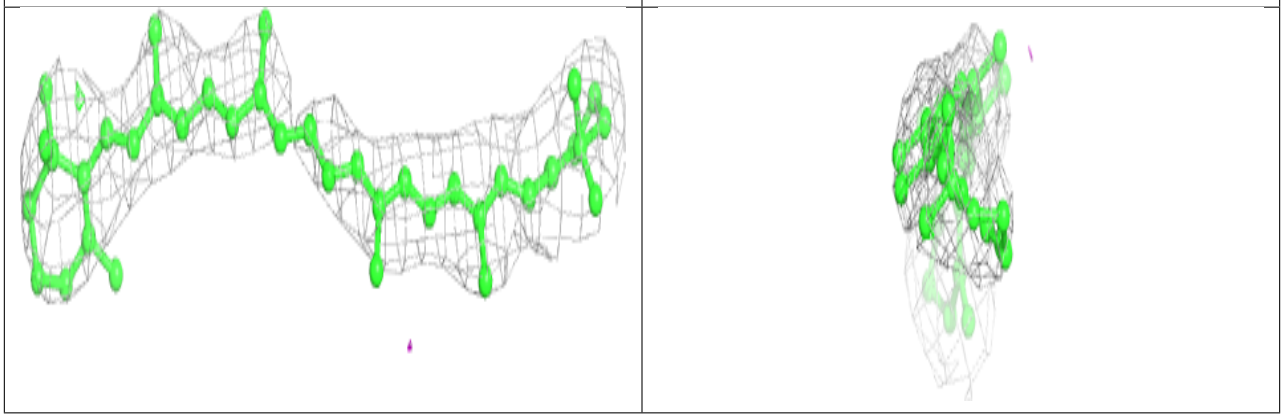






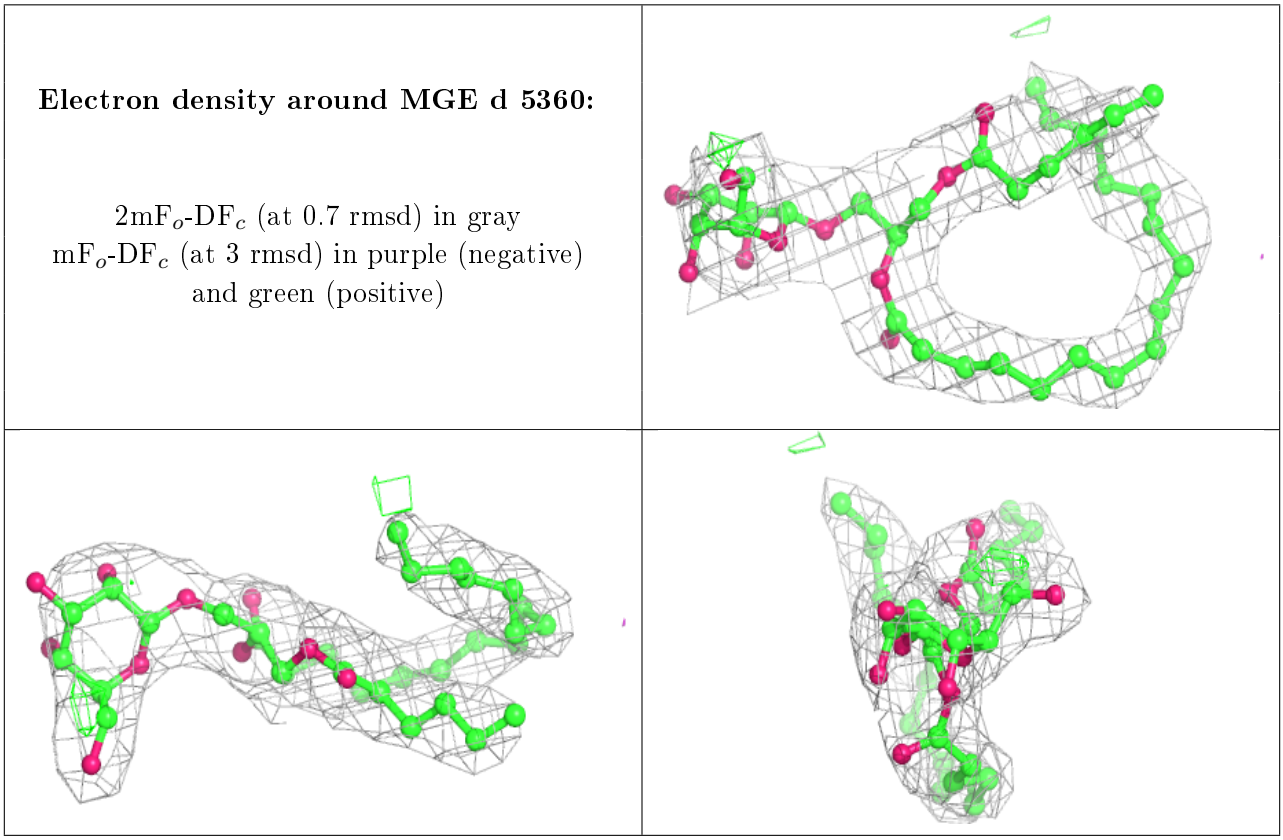
Electron density around BCR D 357:

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



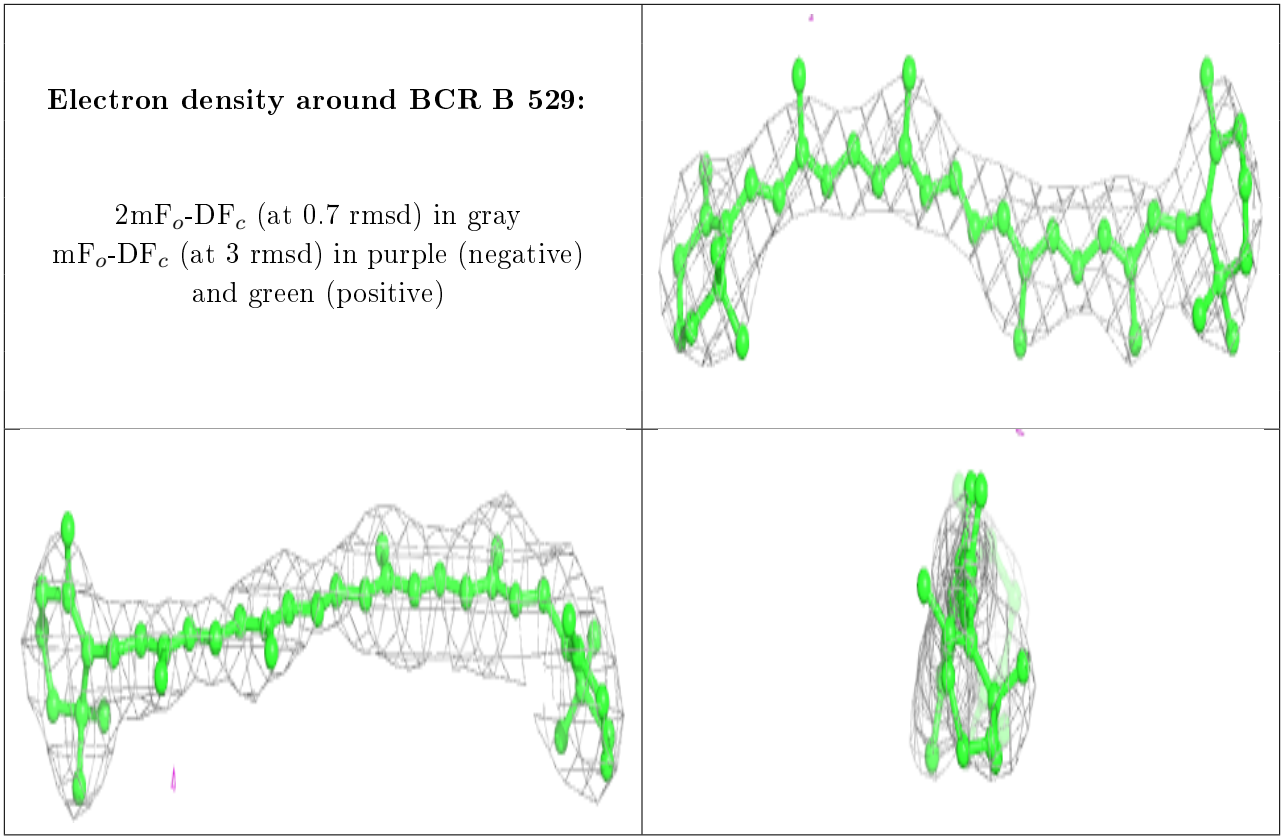
Electron density around MGE d 5360:

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



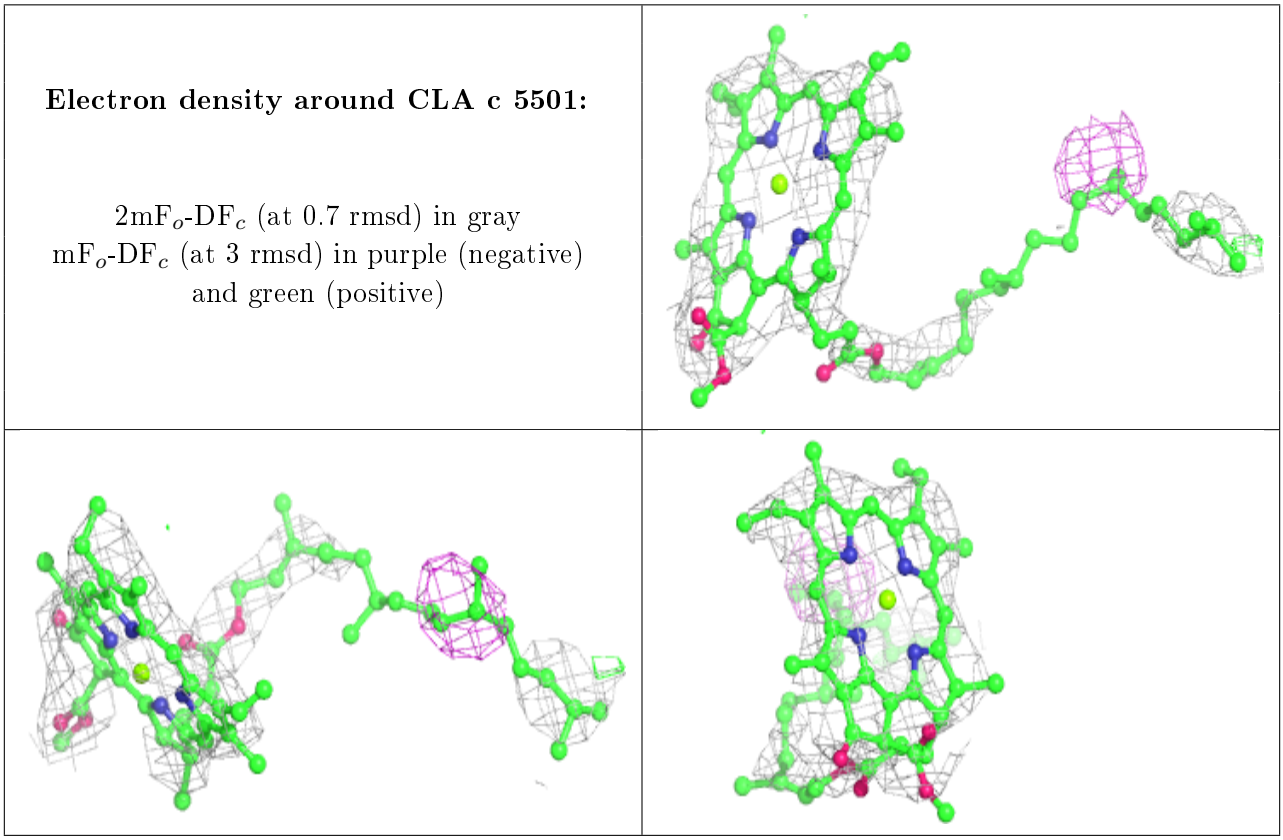
Electron density around BCR B 529:

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



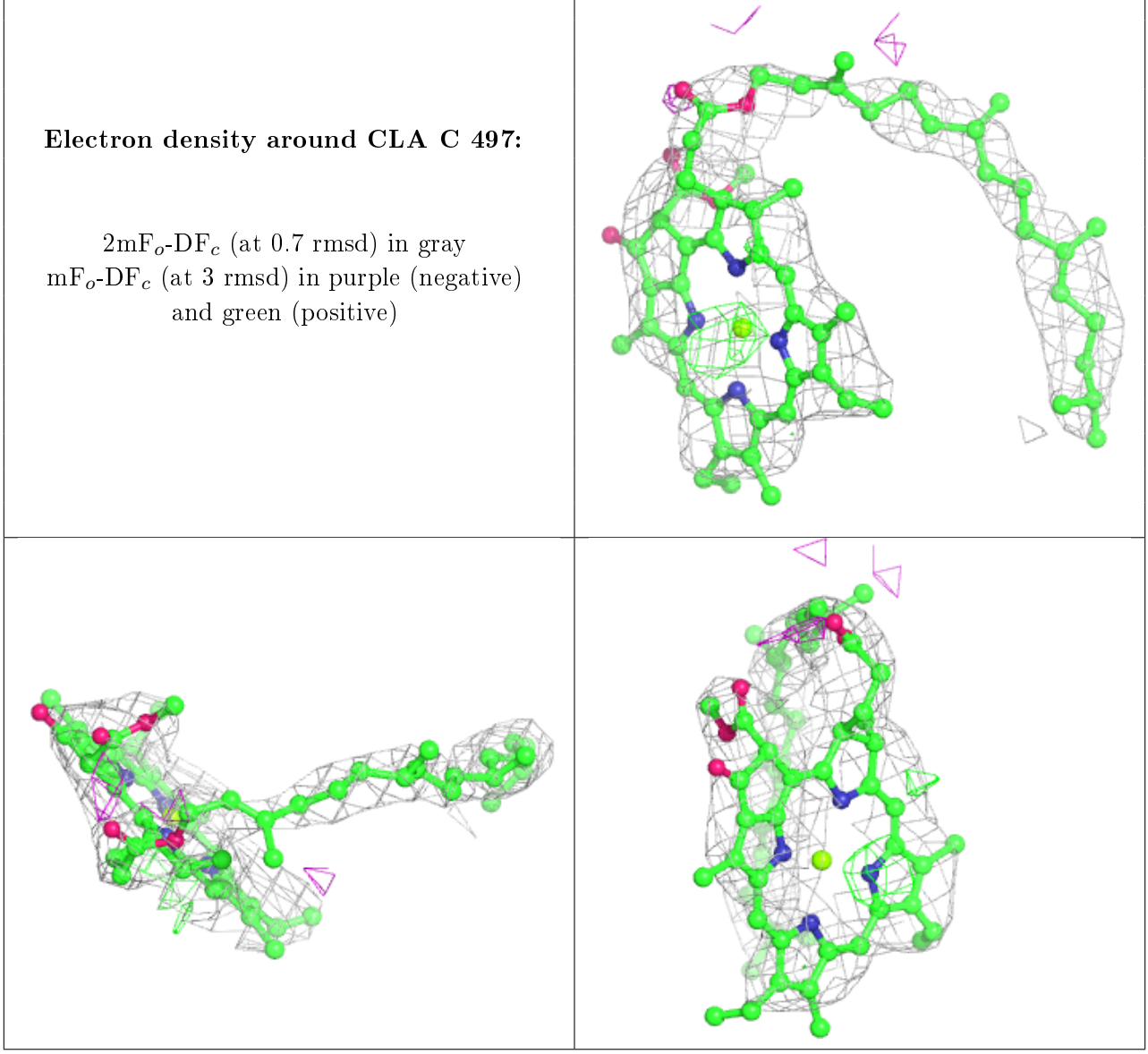
Electron density around CLA c 5501:

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



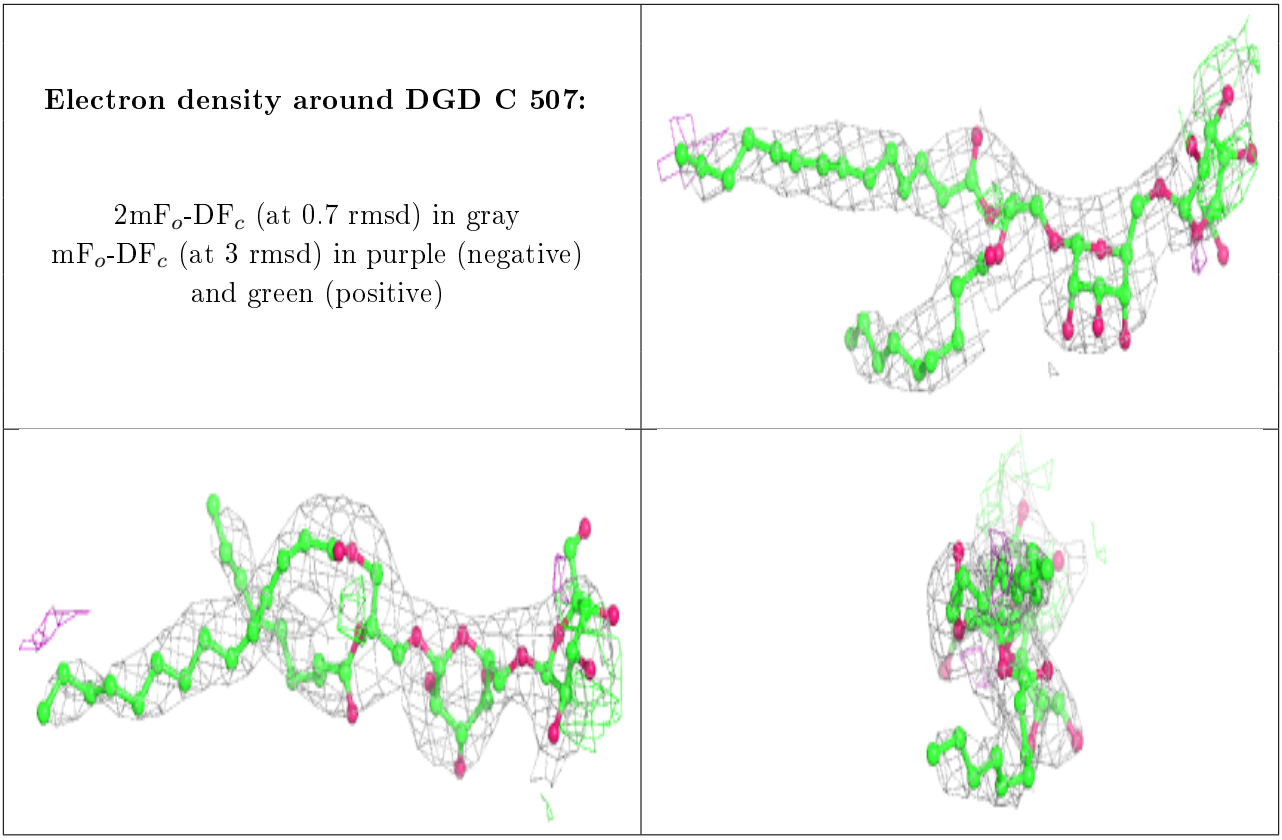
Electron density around CLA C 497:

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



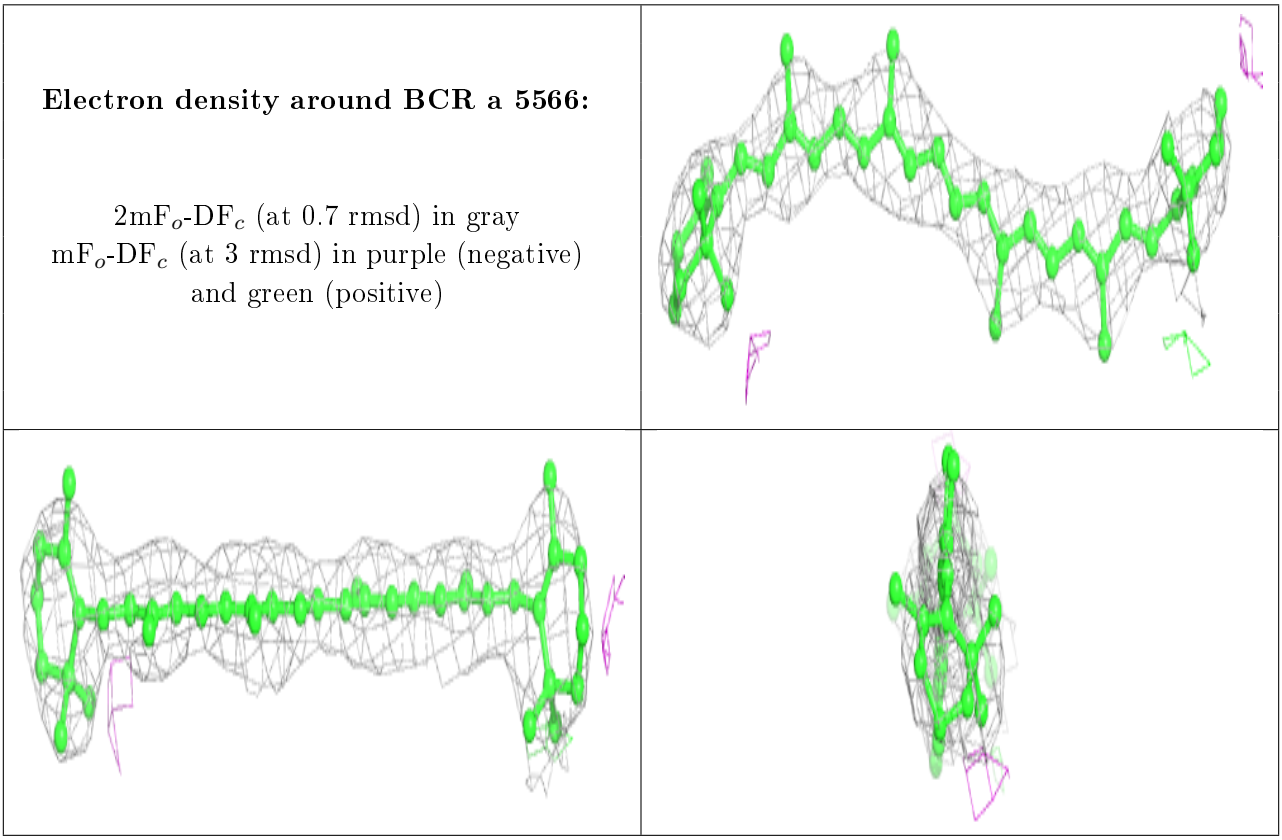
Electron density around DGD C 507:

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



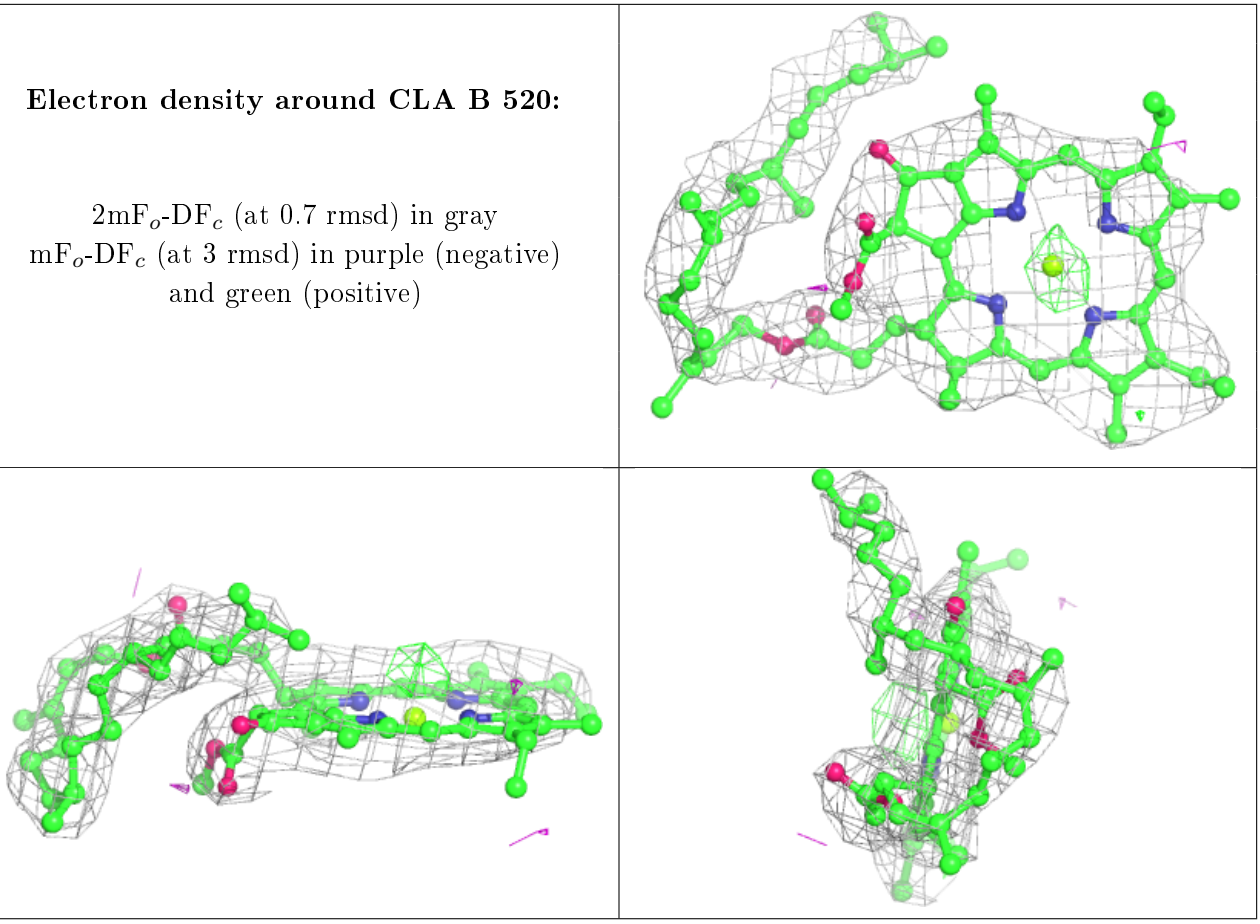
Electron density around BCR a 5566:

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



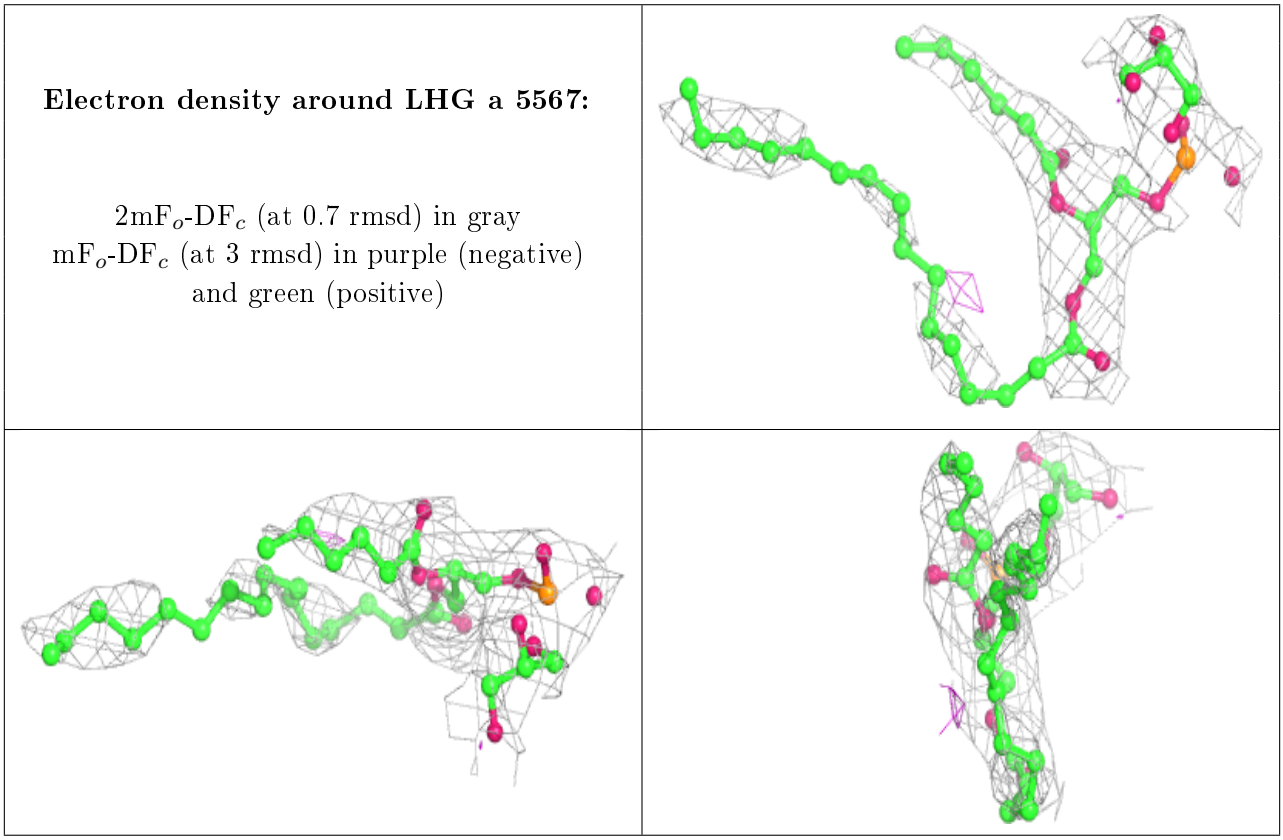
Electron density around CLA B 520:

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



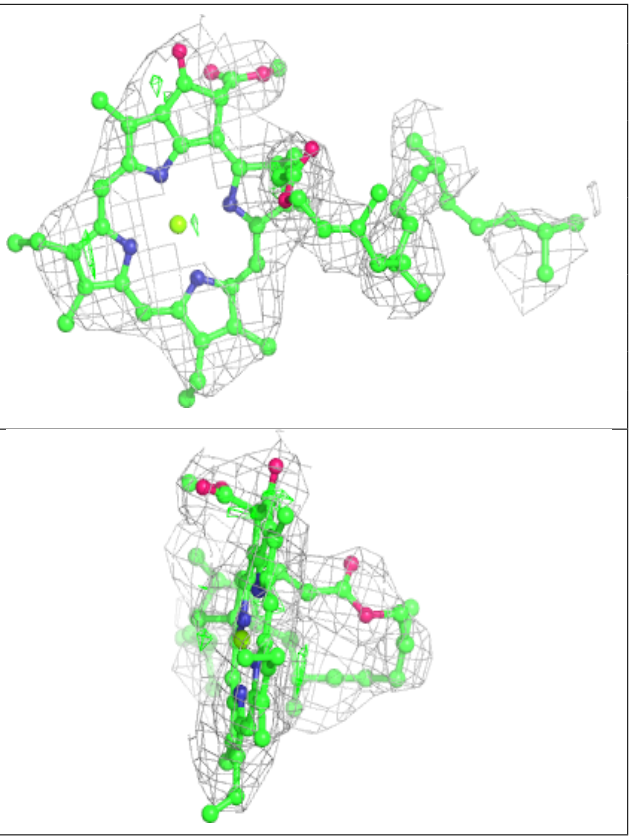
Electron density around LHG a 5567:

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



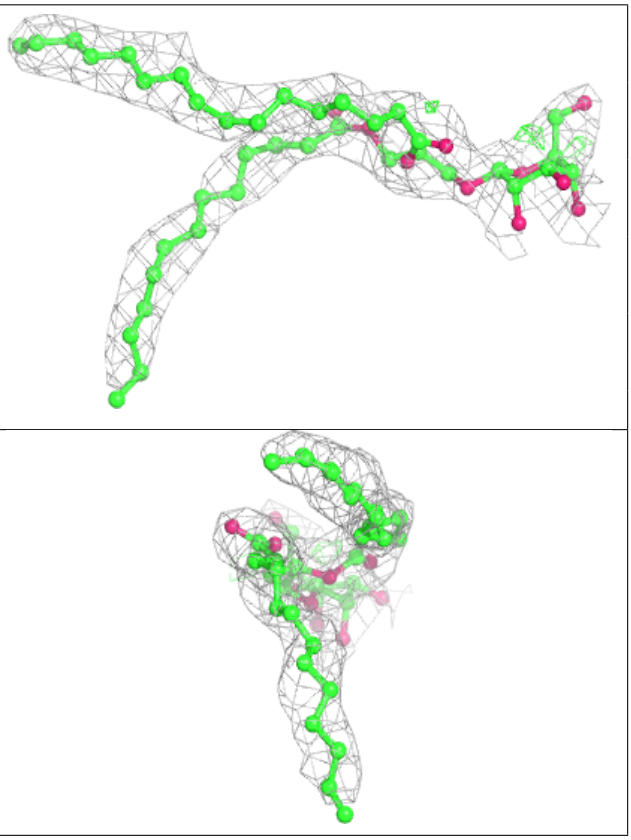
Electron density around CLA a 5560:

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



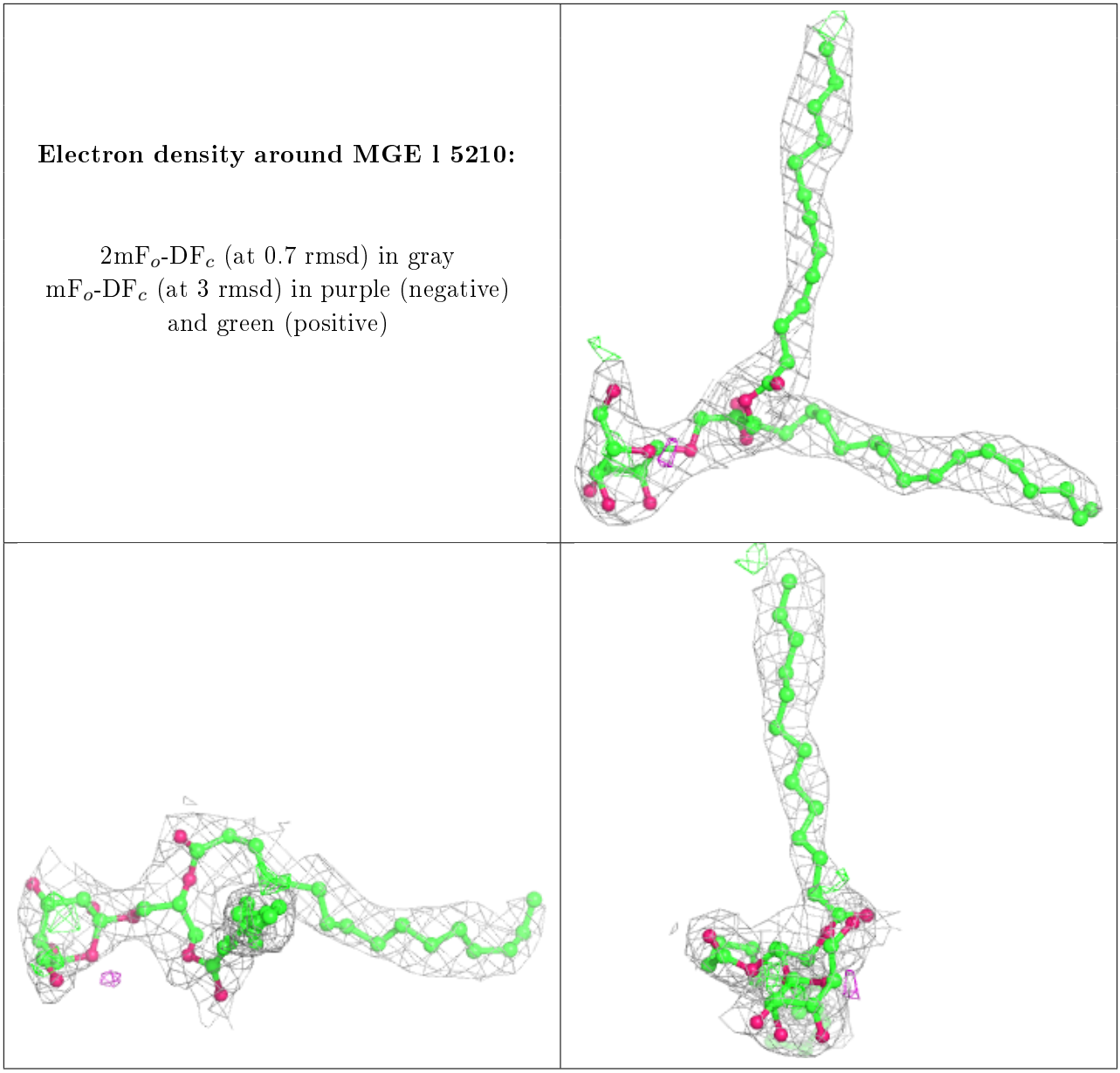
Electron density around MGE d 5361:

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



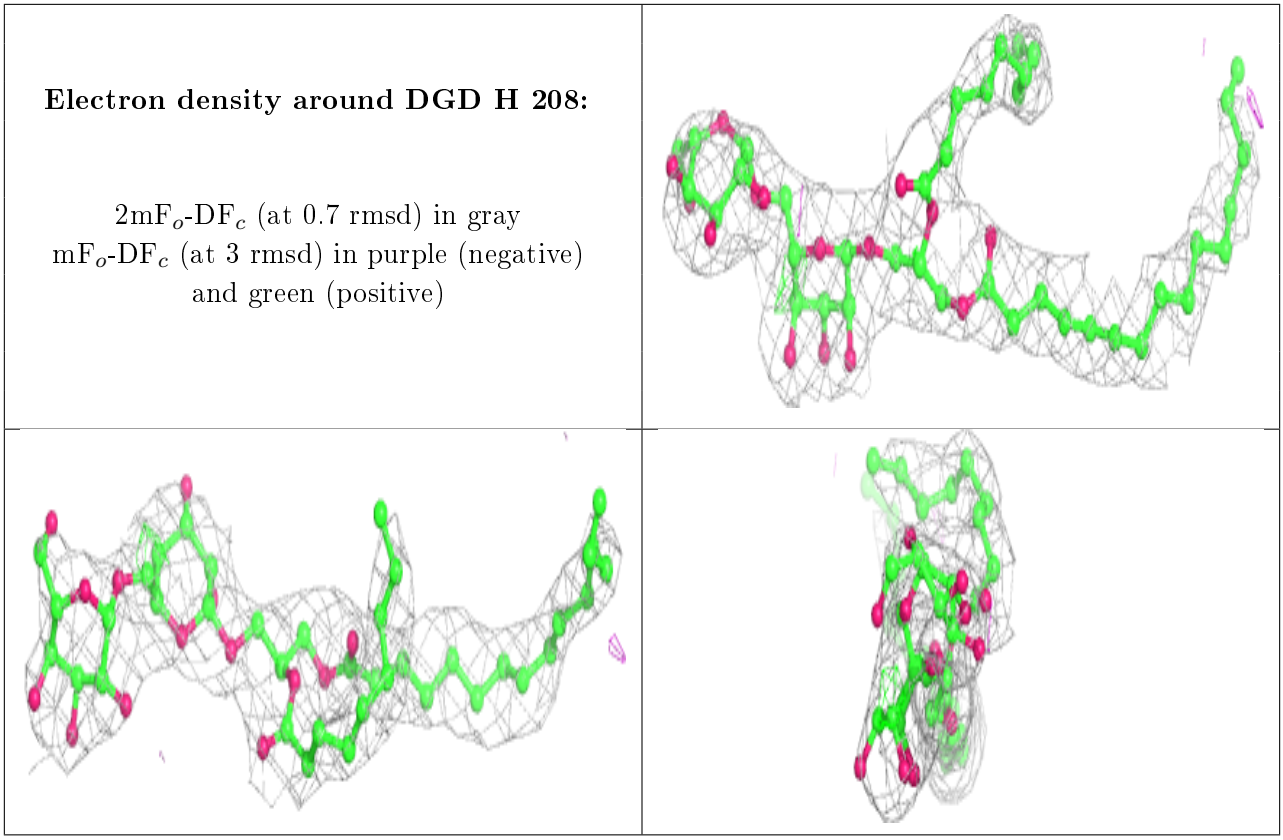
Electron density around MGE l 5210:

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



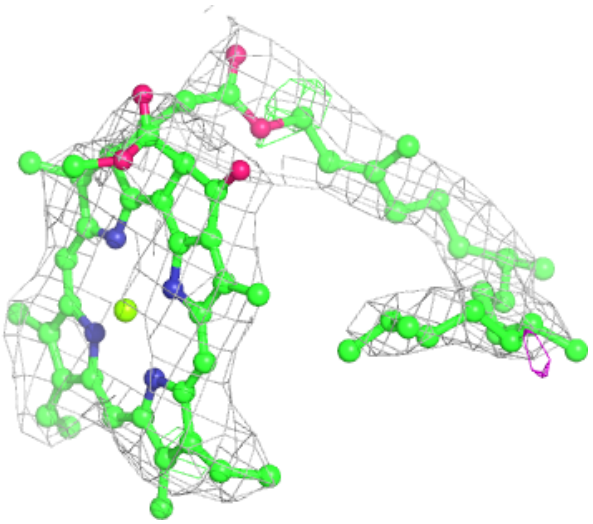
Electron density around DGD H 208:

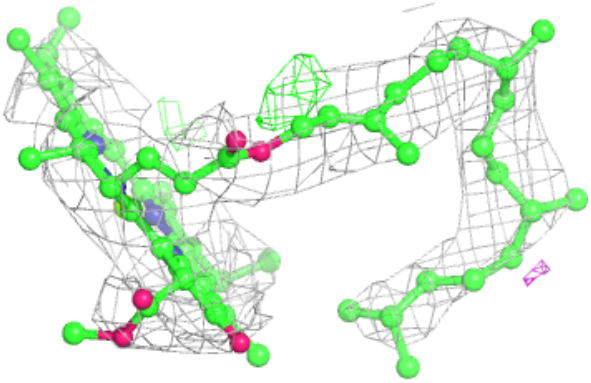
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

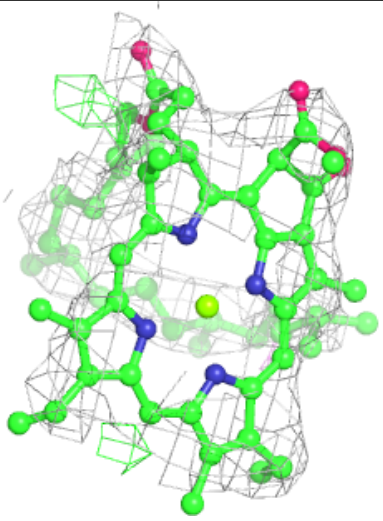


Electron density around CLA c 5493:

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

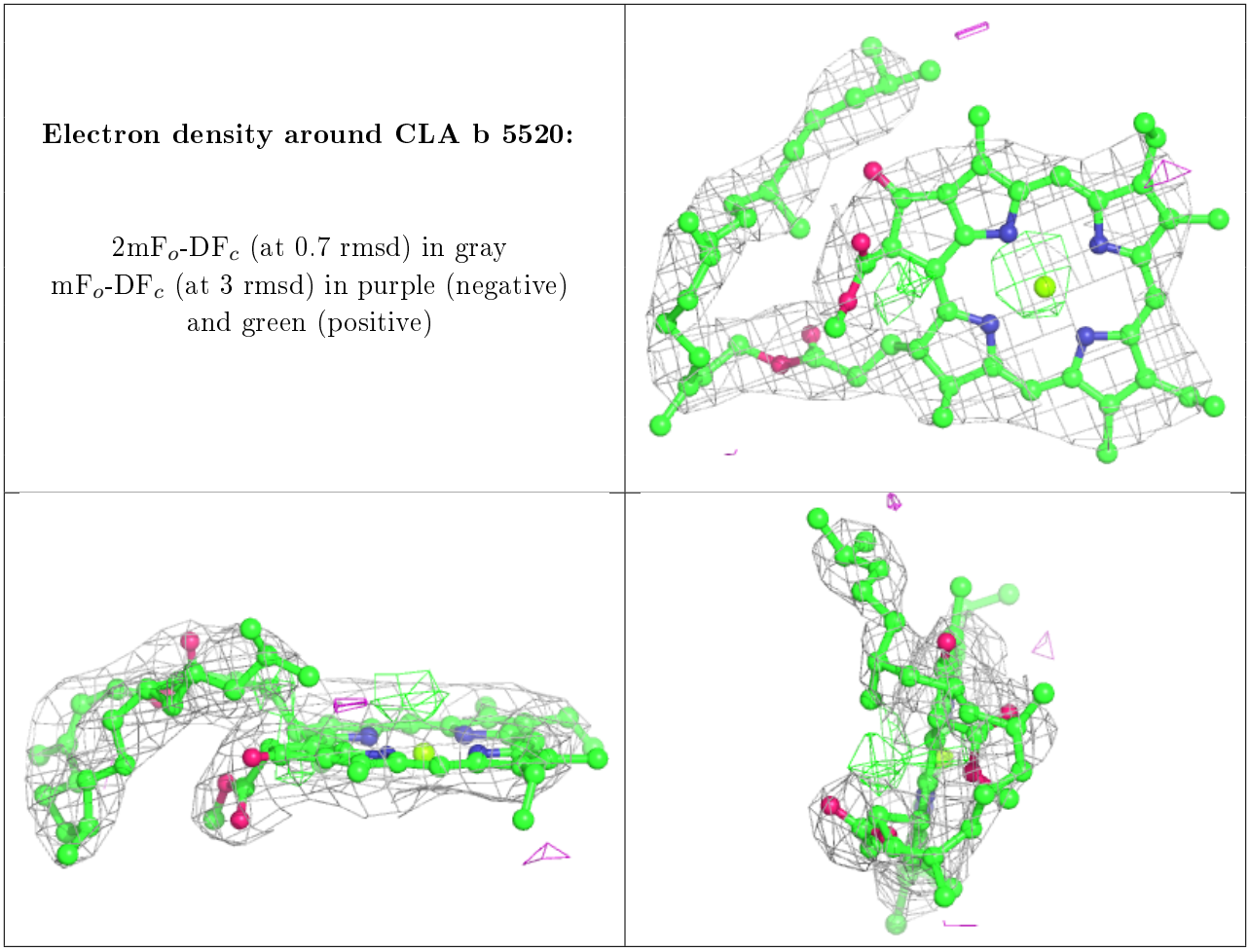






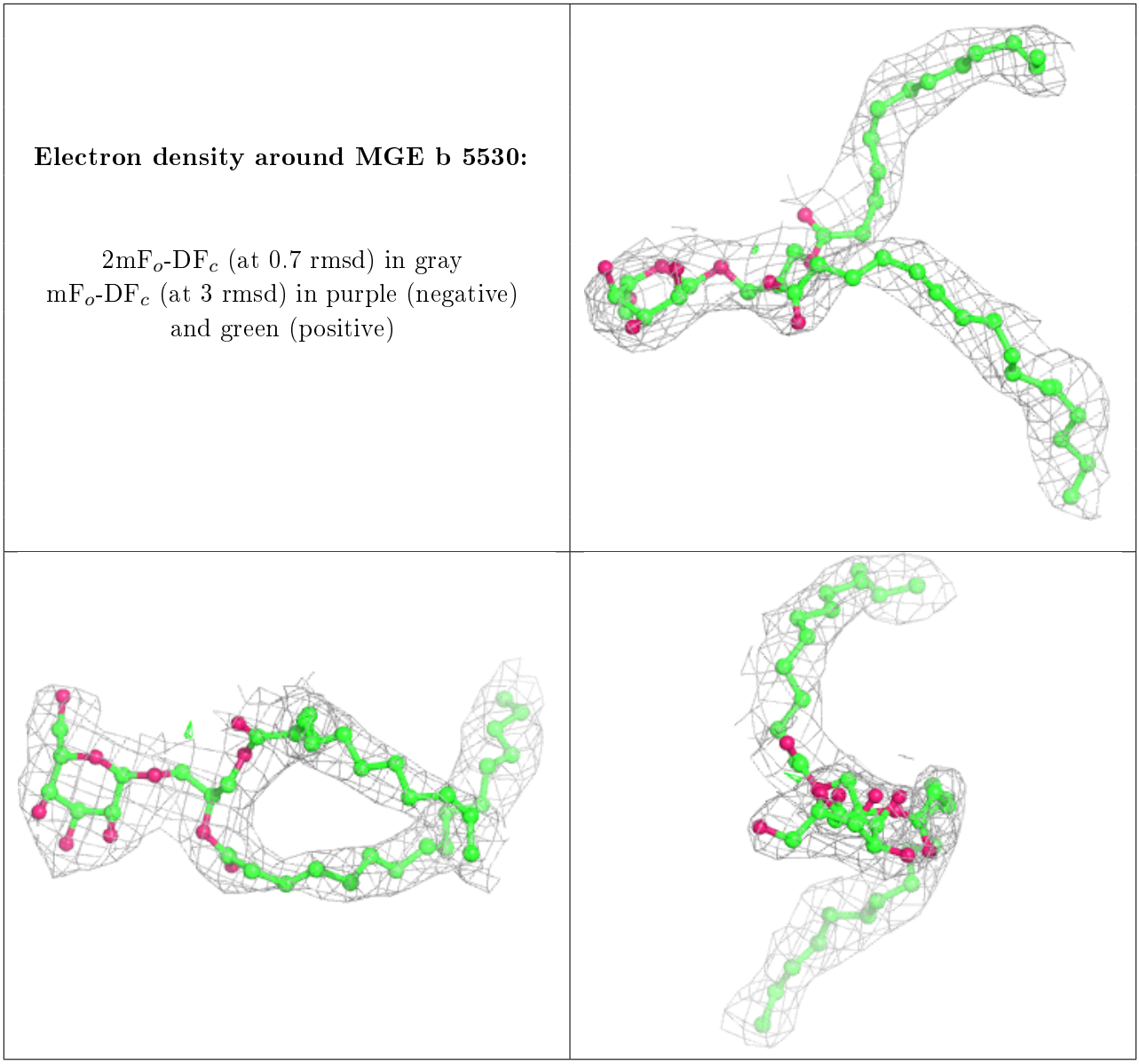
Electron density around CLA b 5520:

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



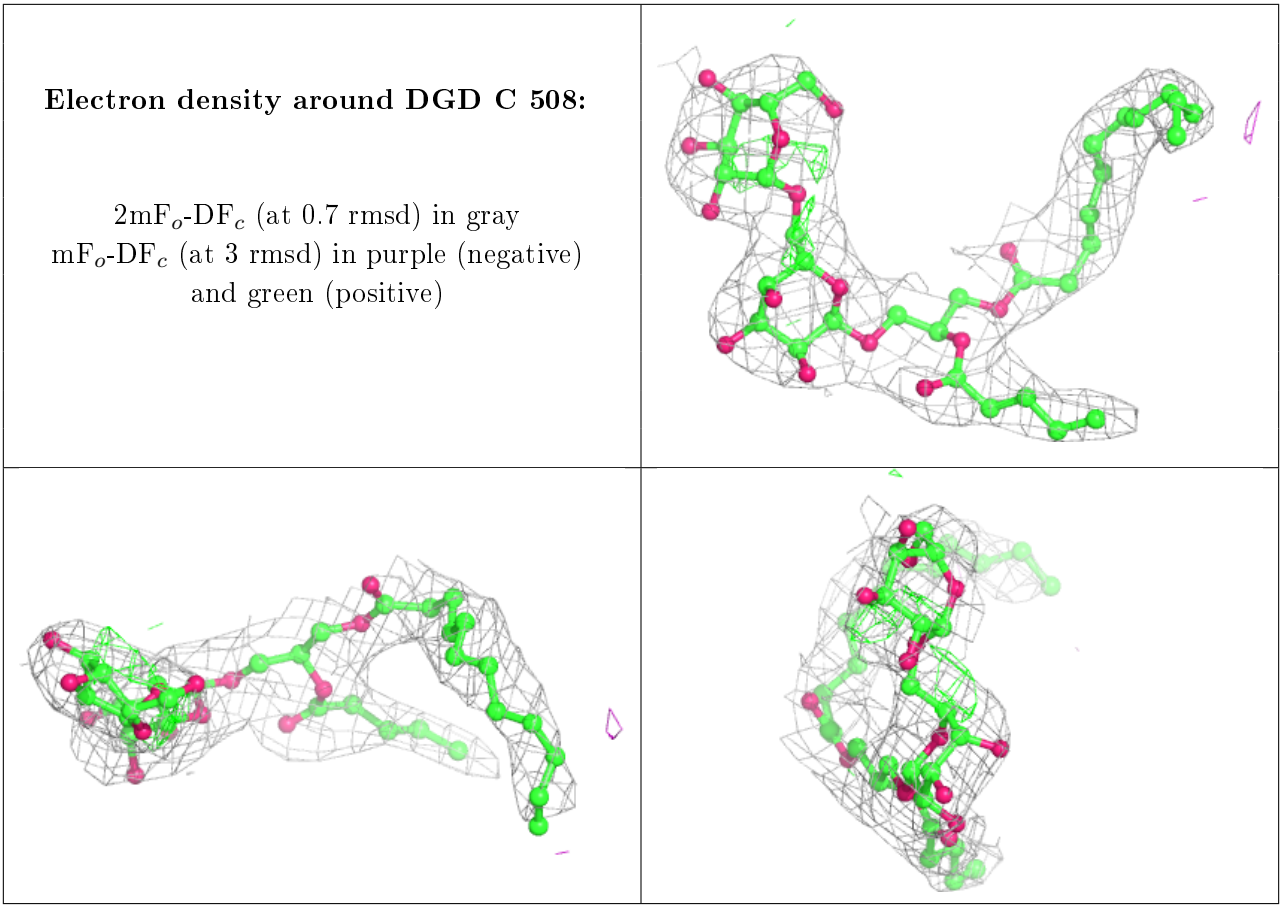
Electron density around MGE b 5530:

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



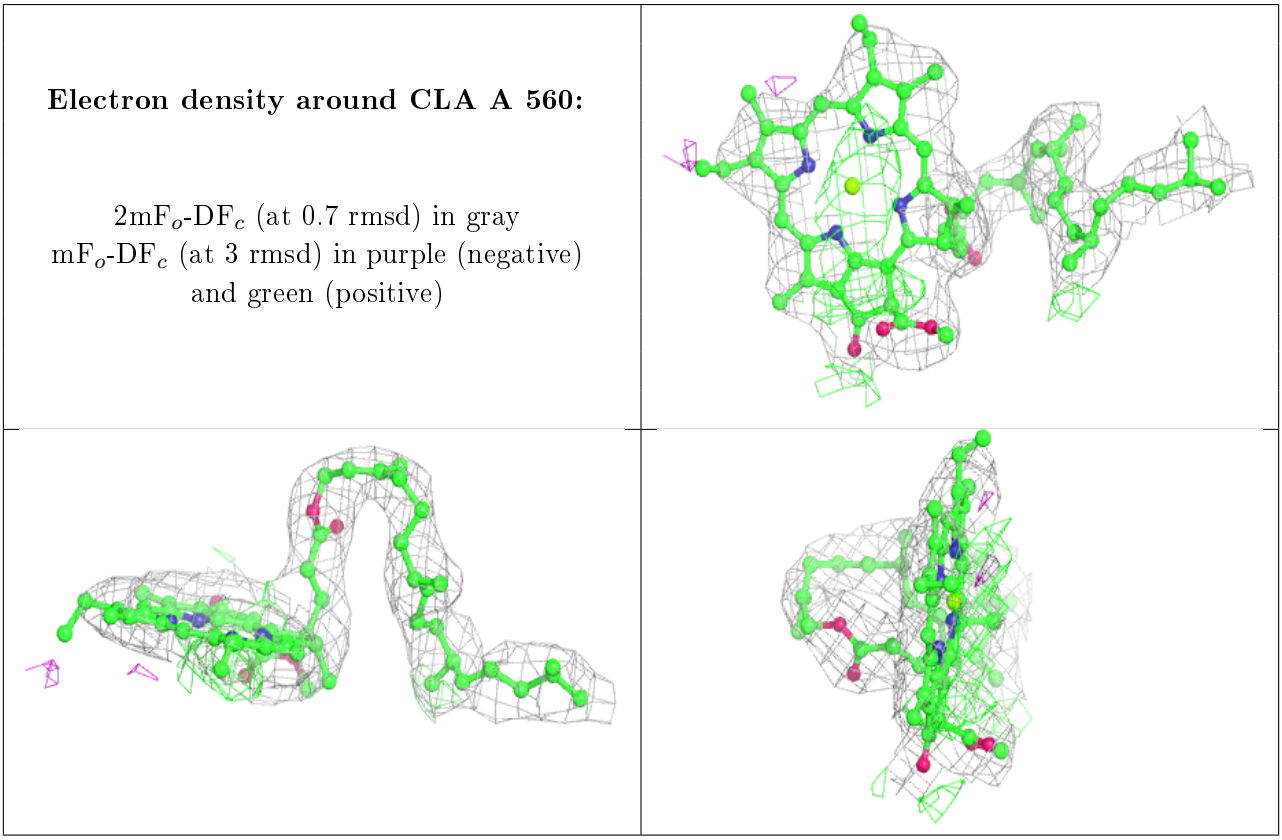
Electron density around DGD C 508:

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



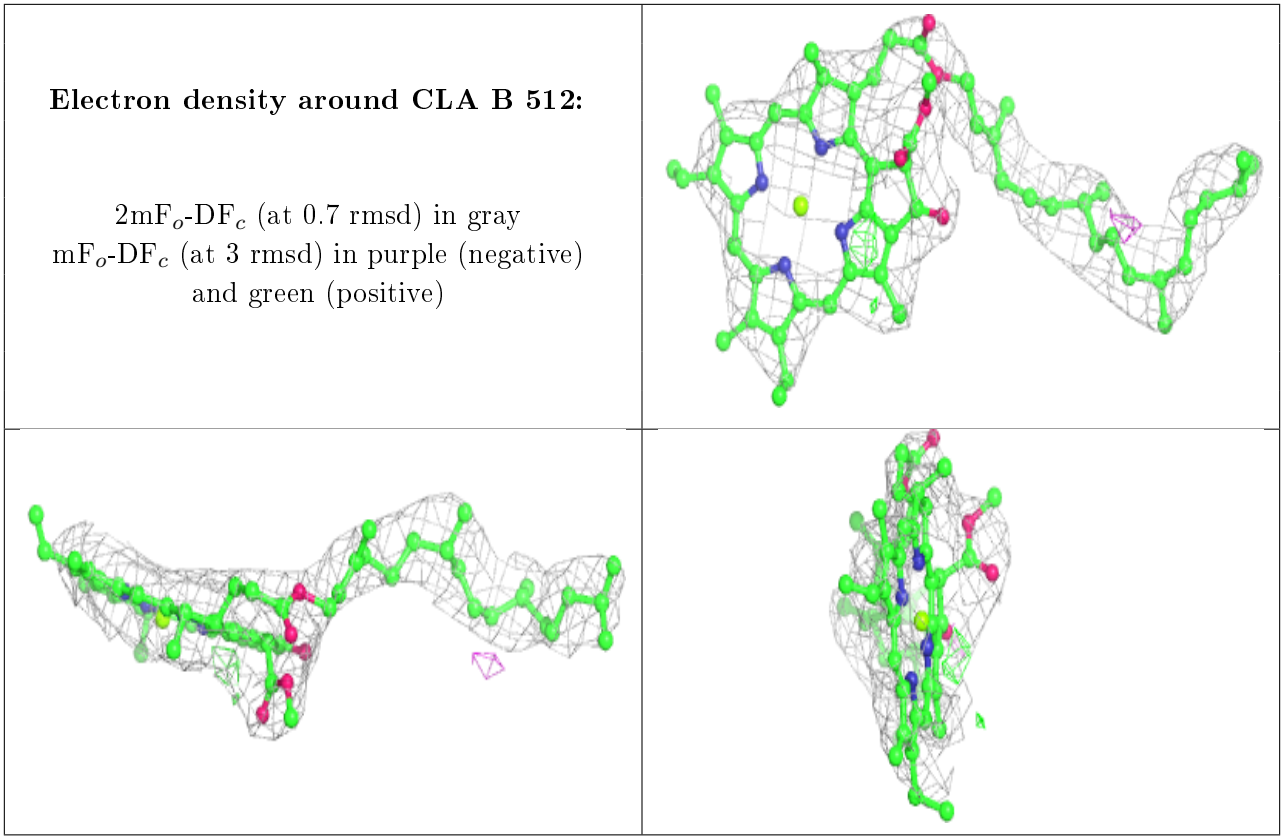
Electron density around CLA A 560:

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



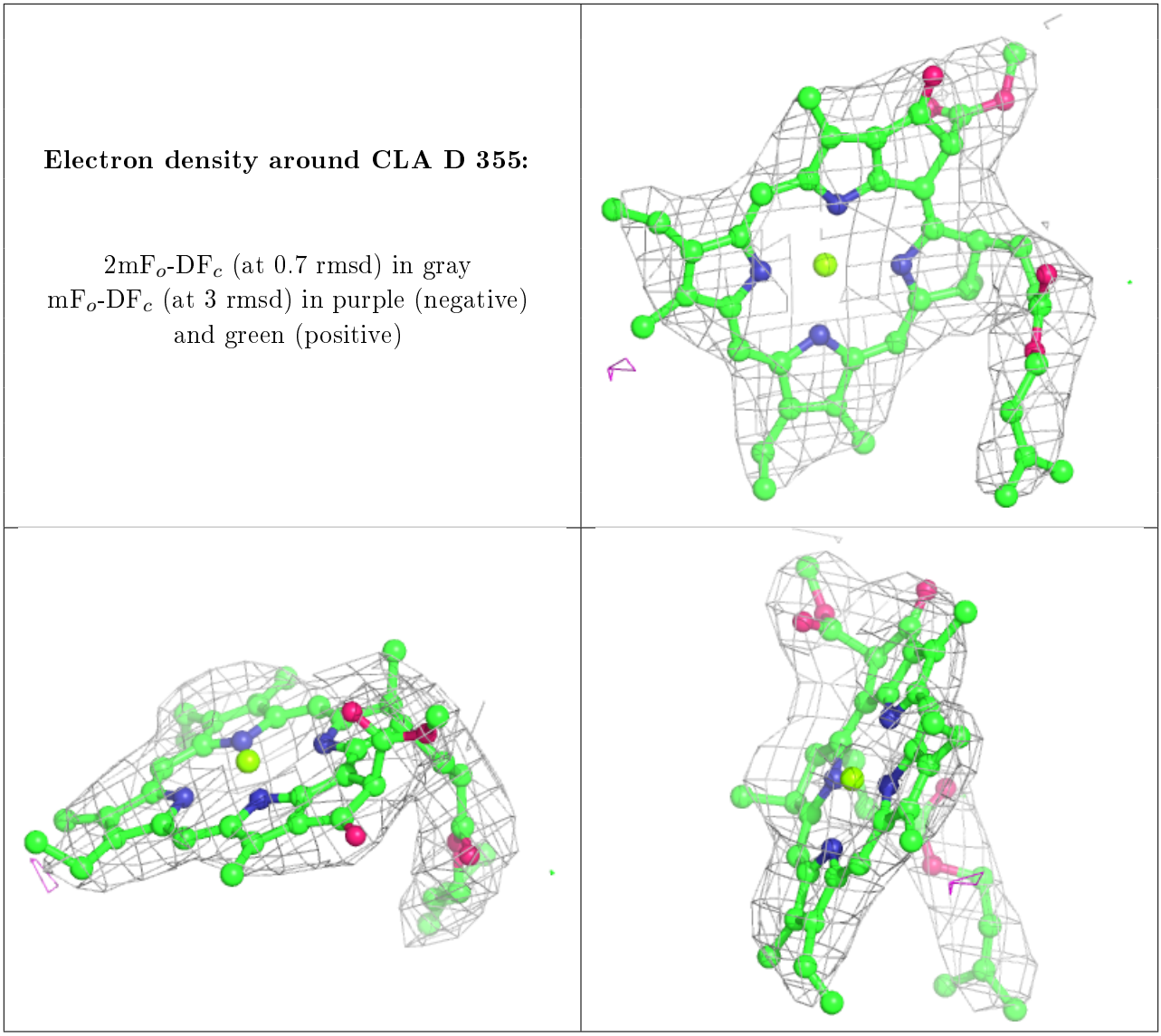
Electron density around CLA B 512:

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



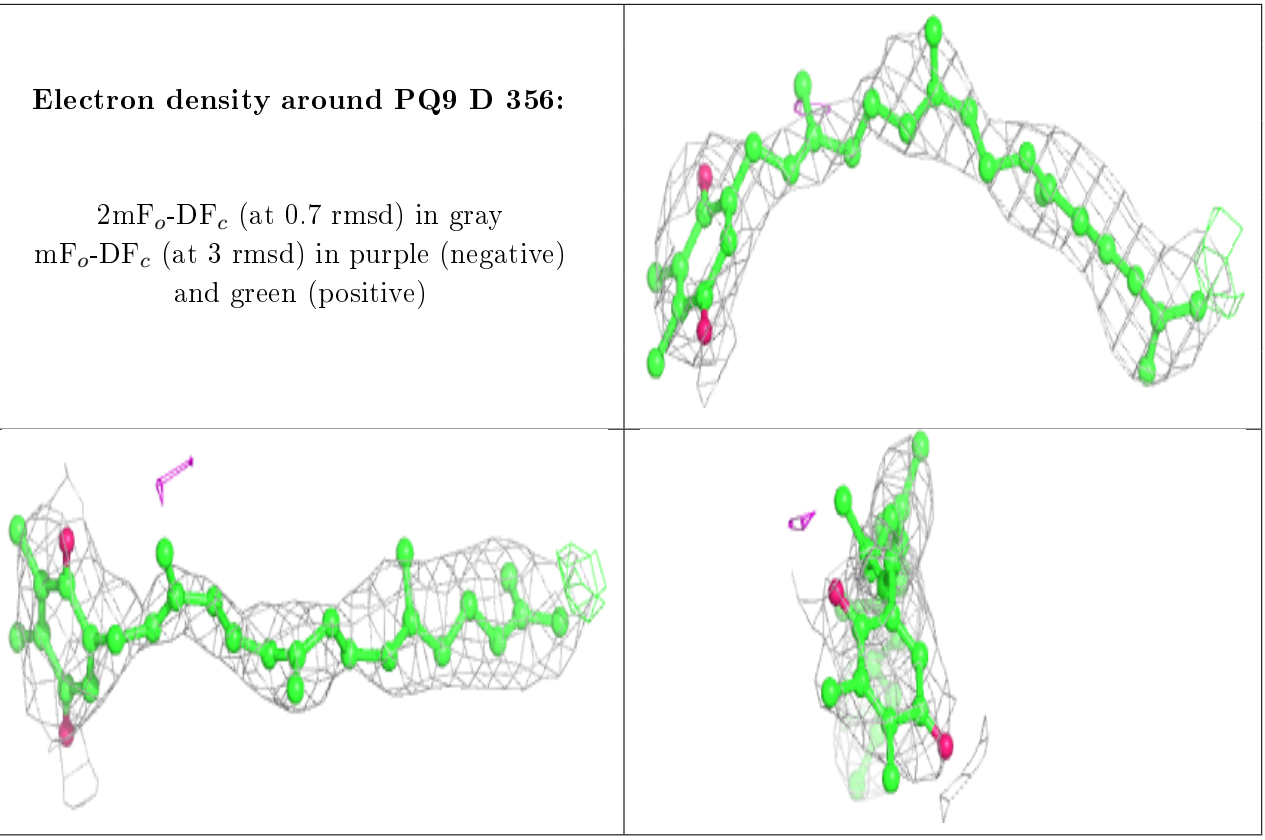
Electron density around CLA D 355:

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



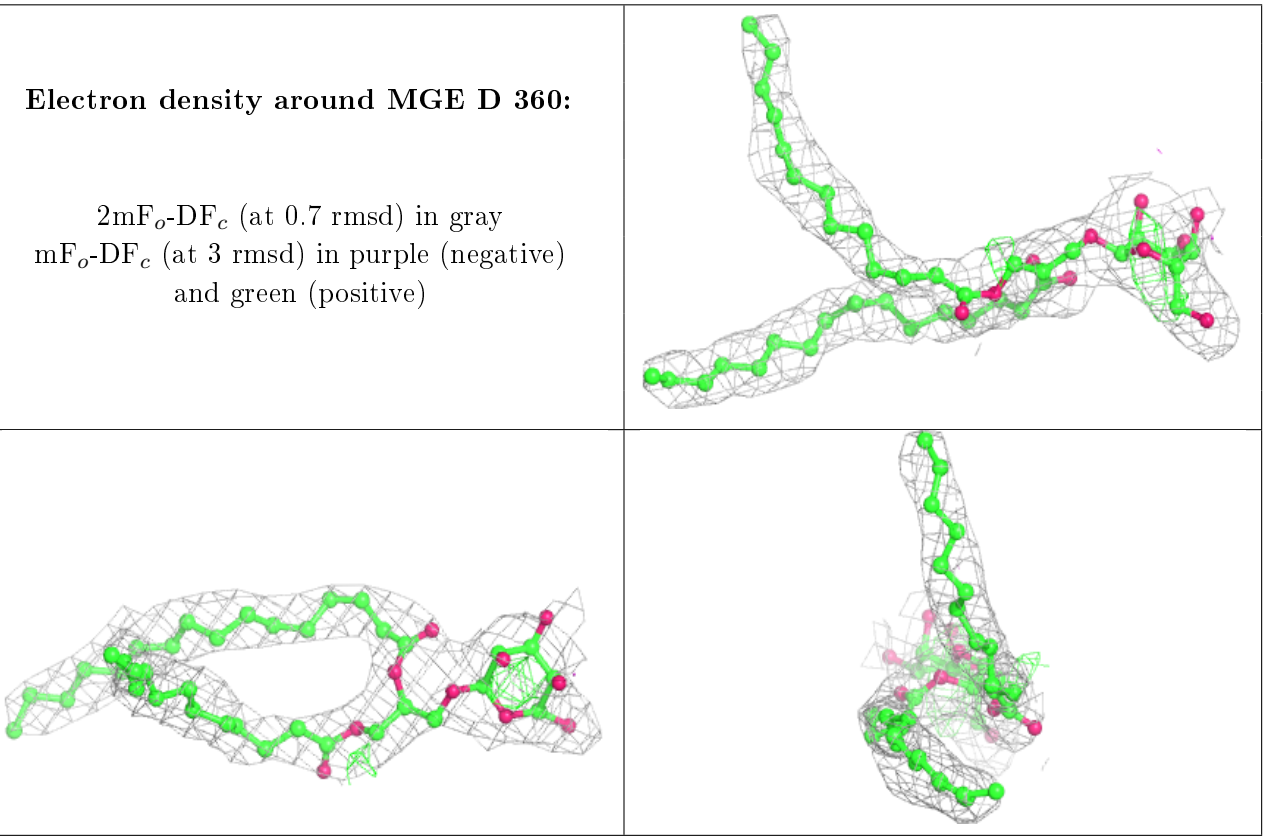
Electron density around PQ9 D 356:

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



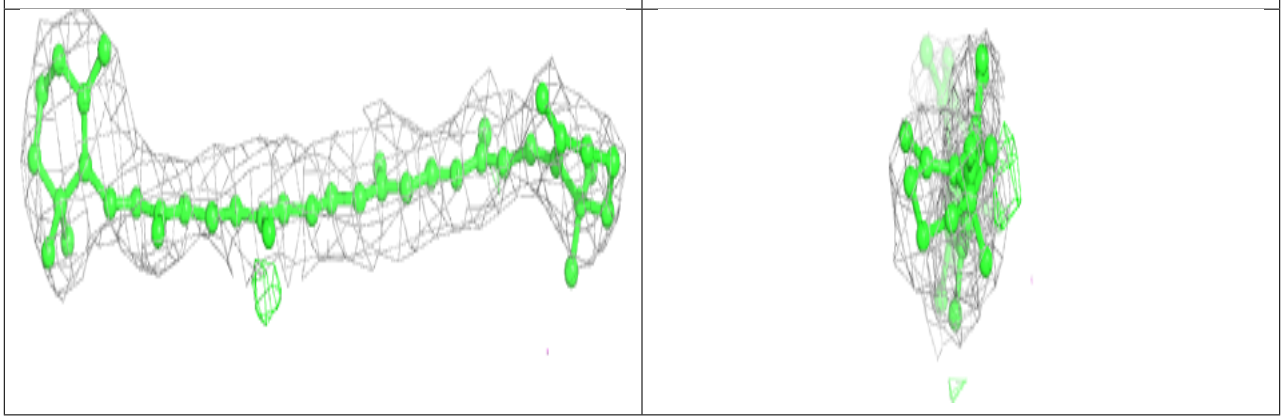
Electron density around MGE D 360:

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



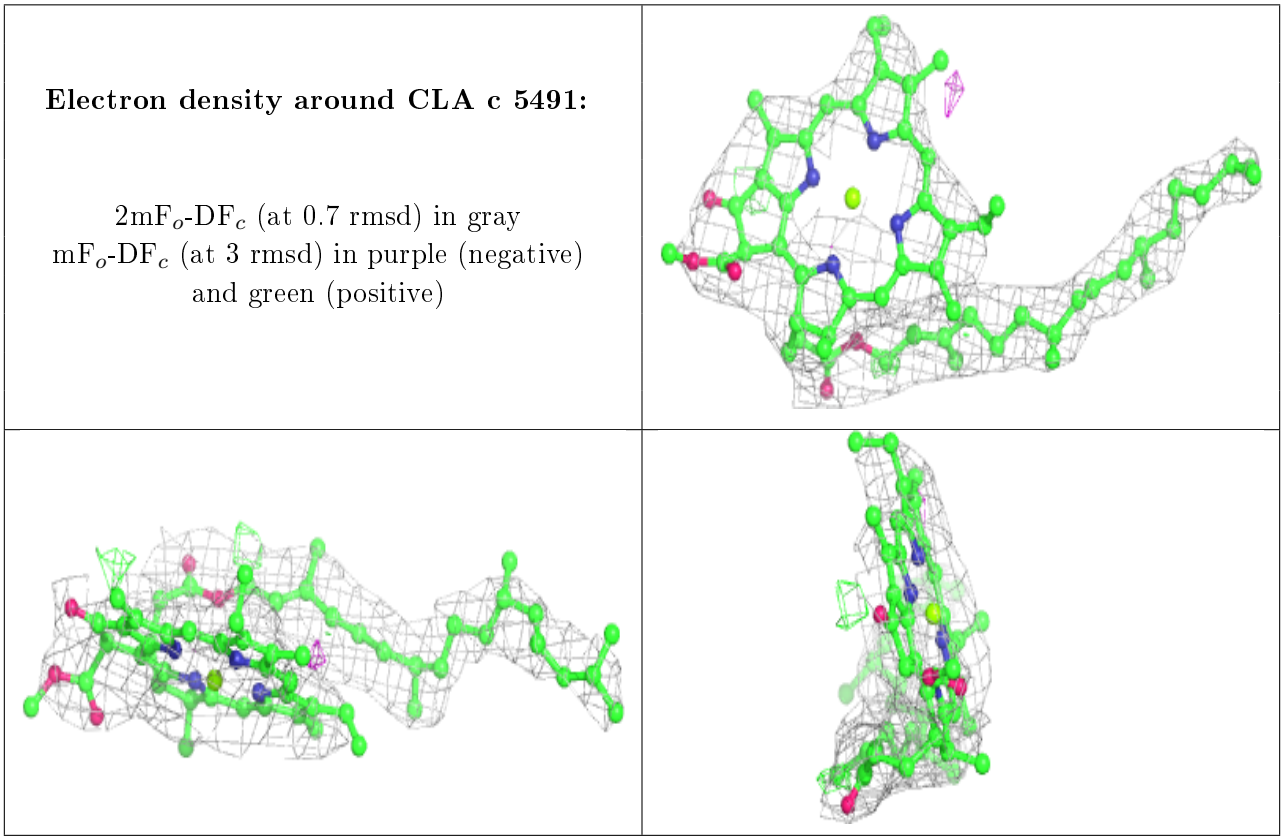
Electron density around BCR B 527:

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



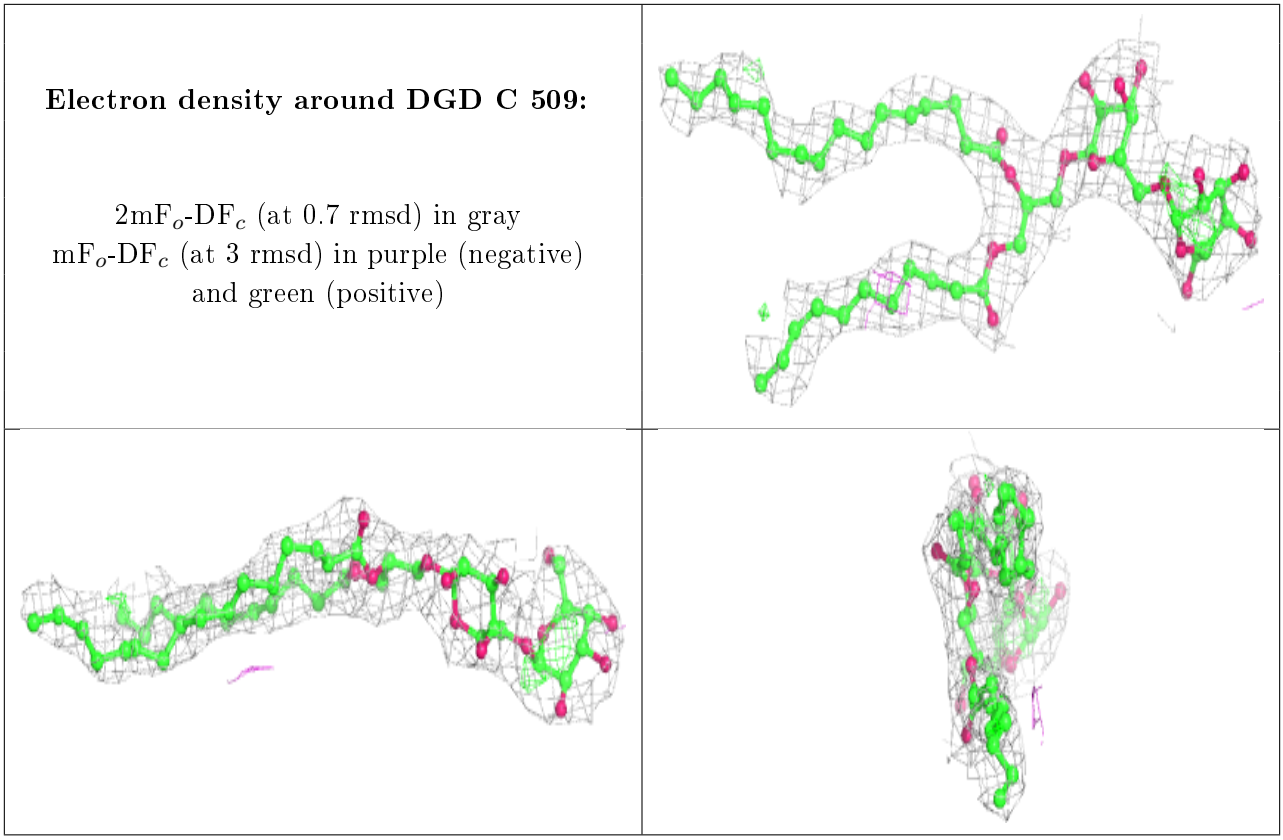
Electron density around CLA c 5491:

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



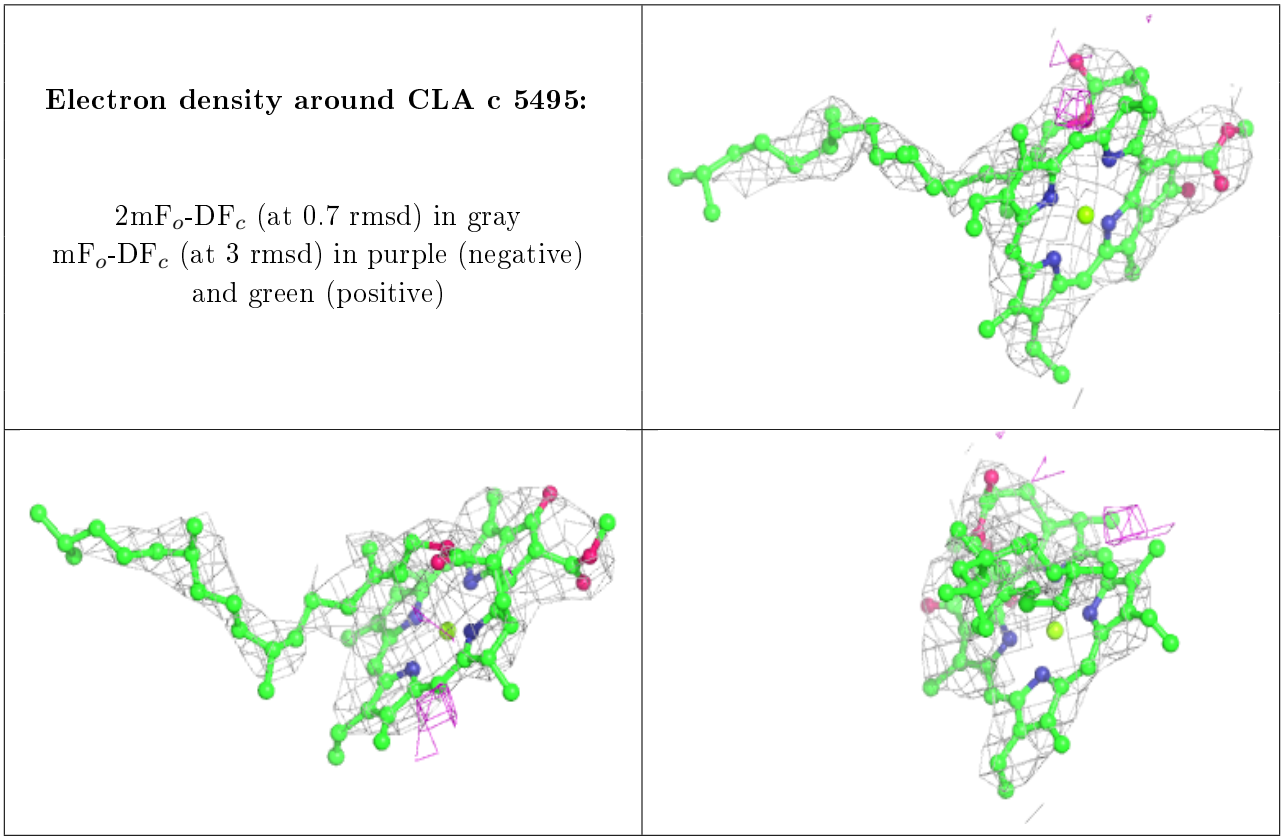
Electron density around DGD C 509:

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



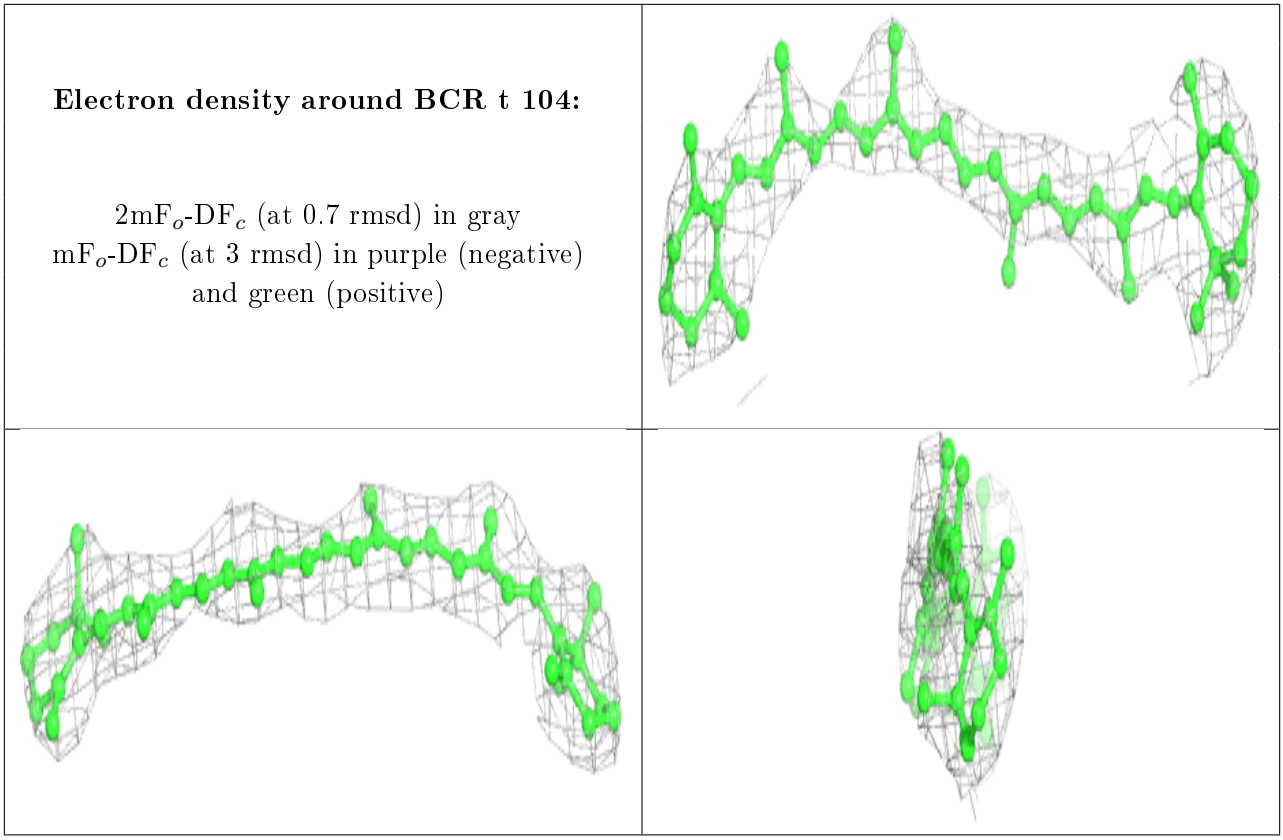
Electron density around CLA c 5495:

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



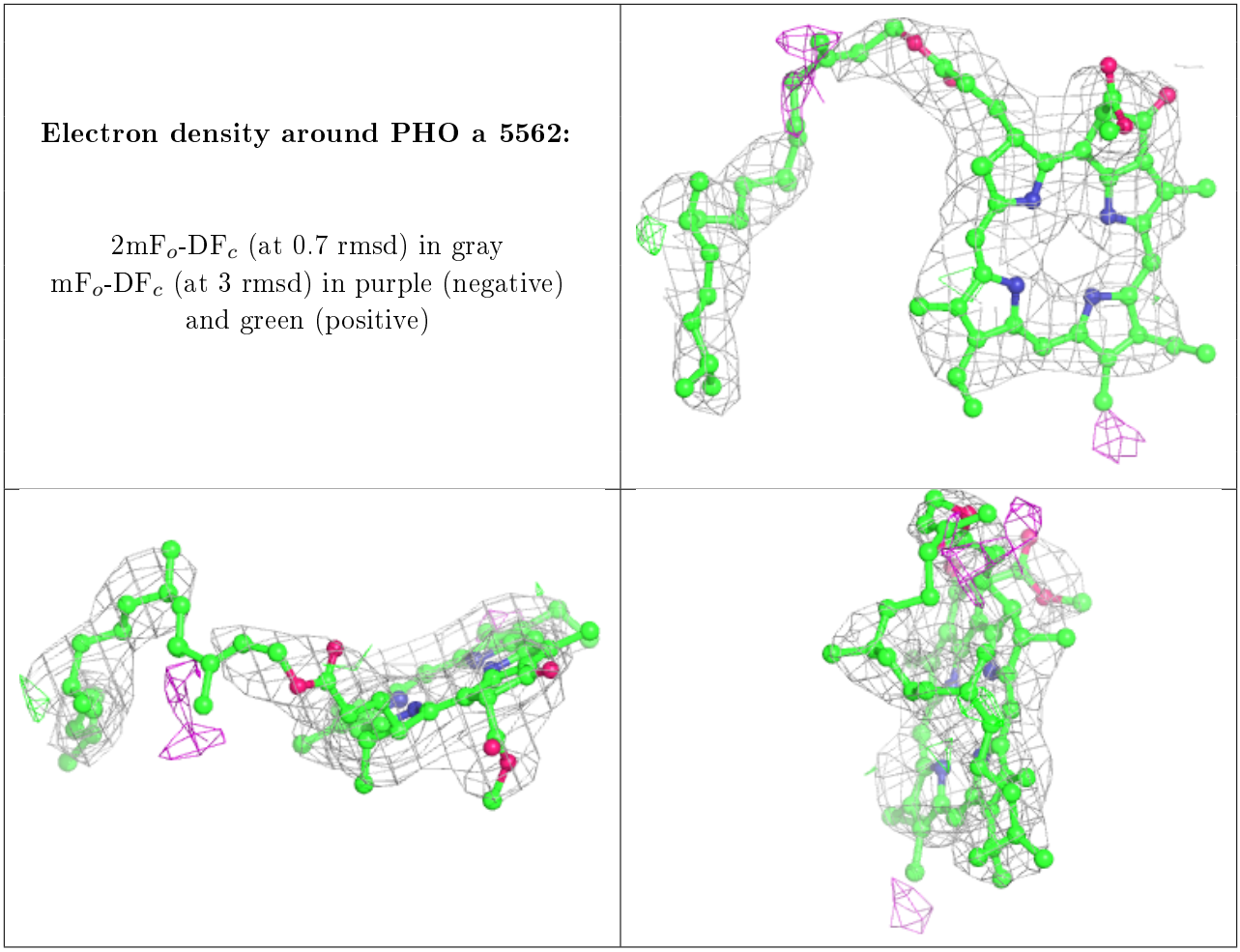
Electron density around BCR t 104:

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



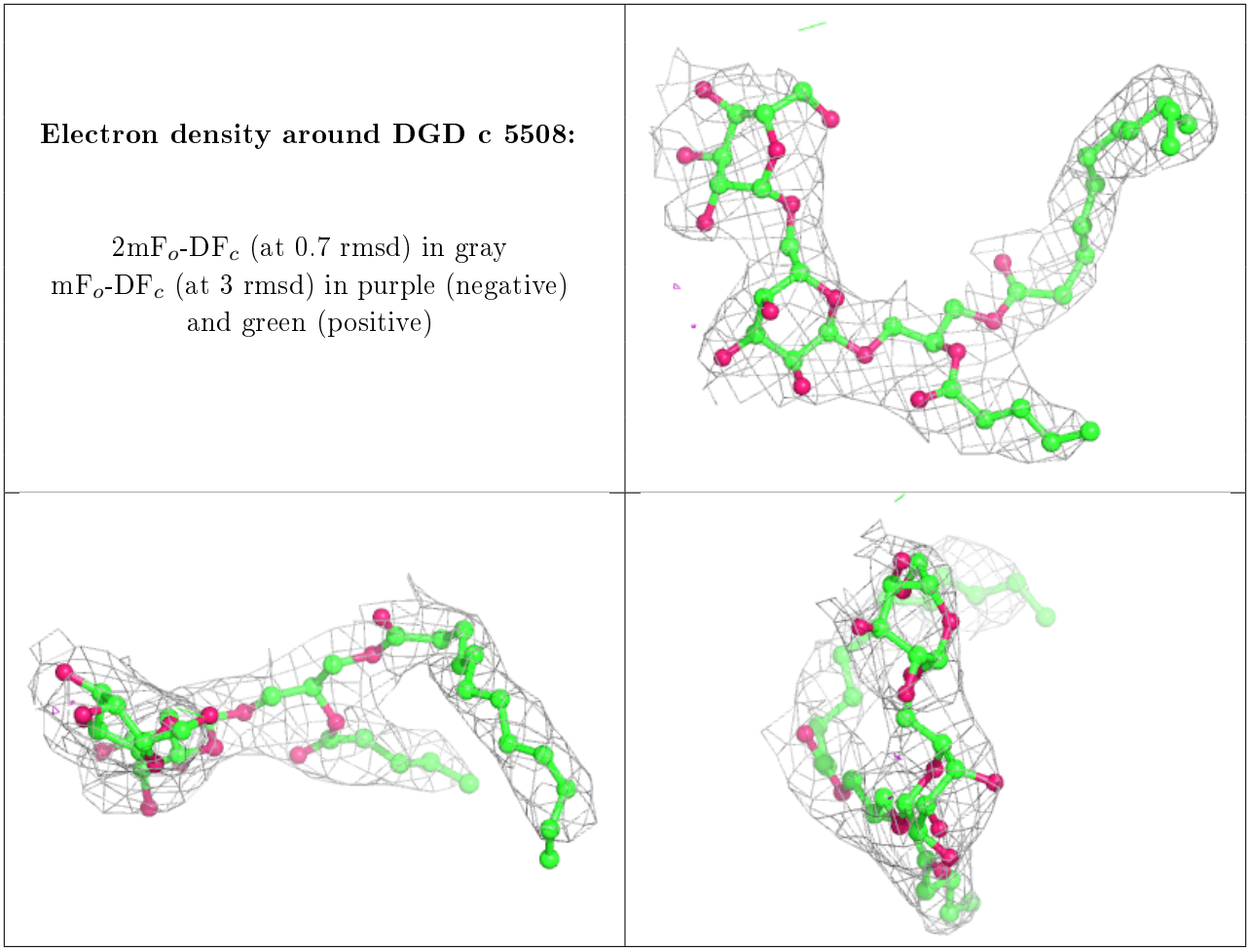
Electron density around PHO a 5562:

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



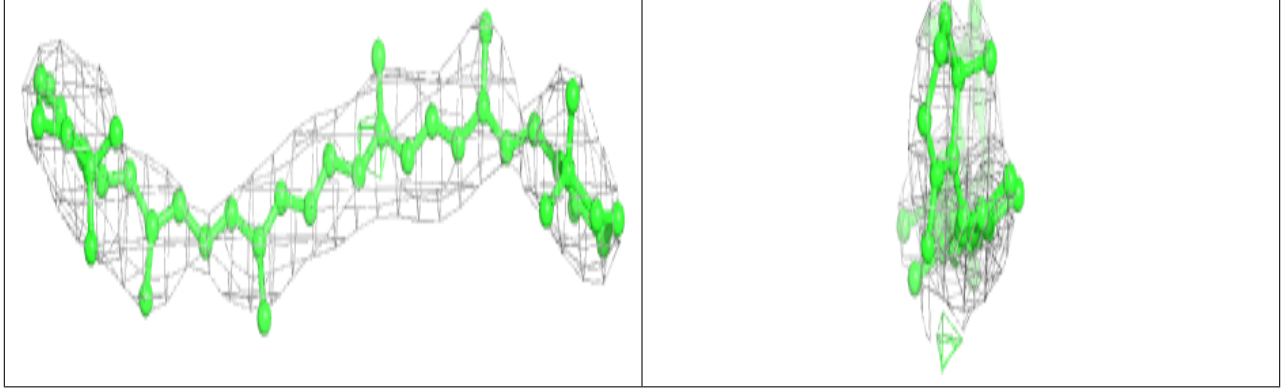
Electron density around DGD c 5508:

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



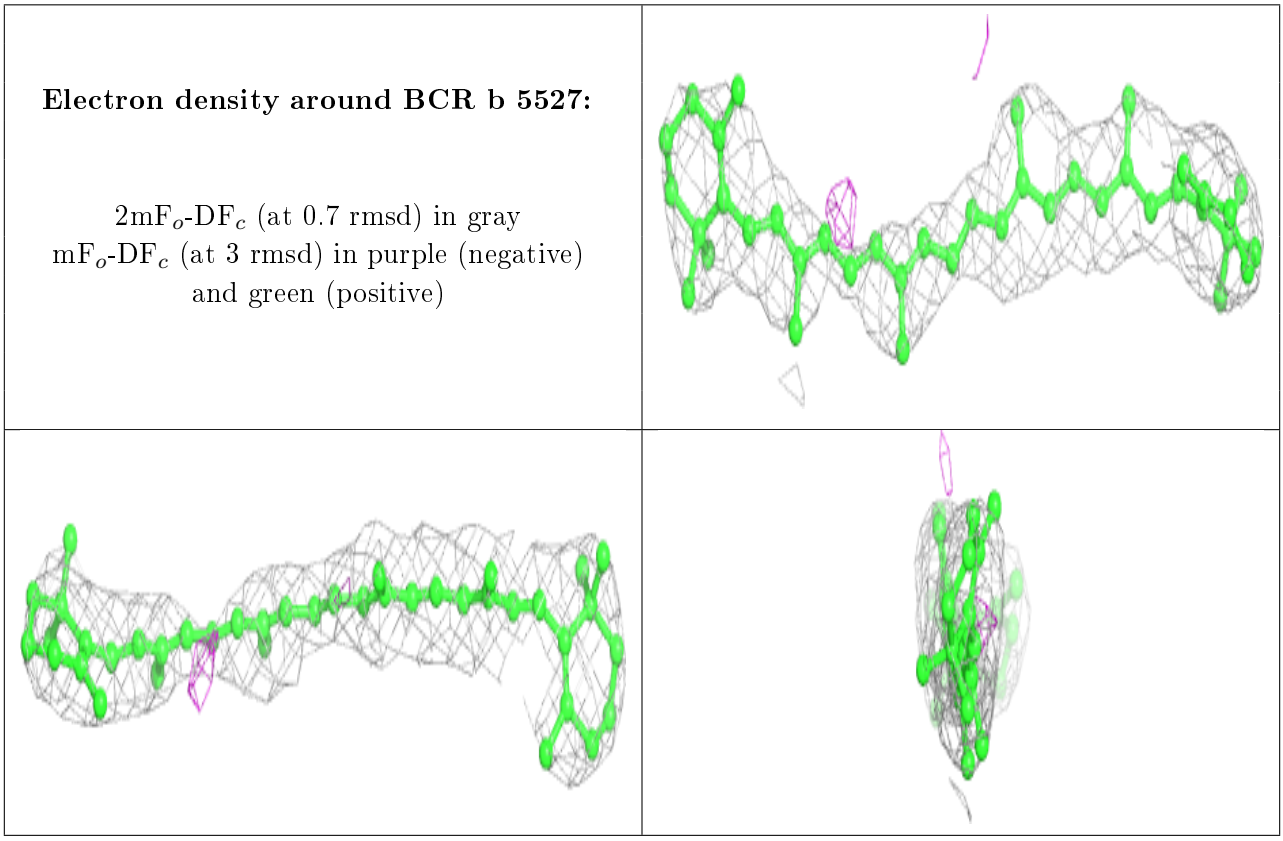
Electron density around BCR C 504:

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



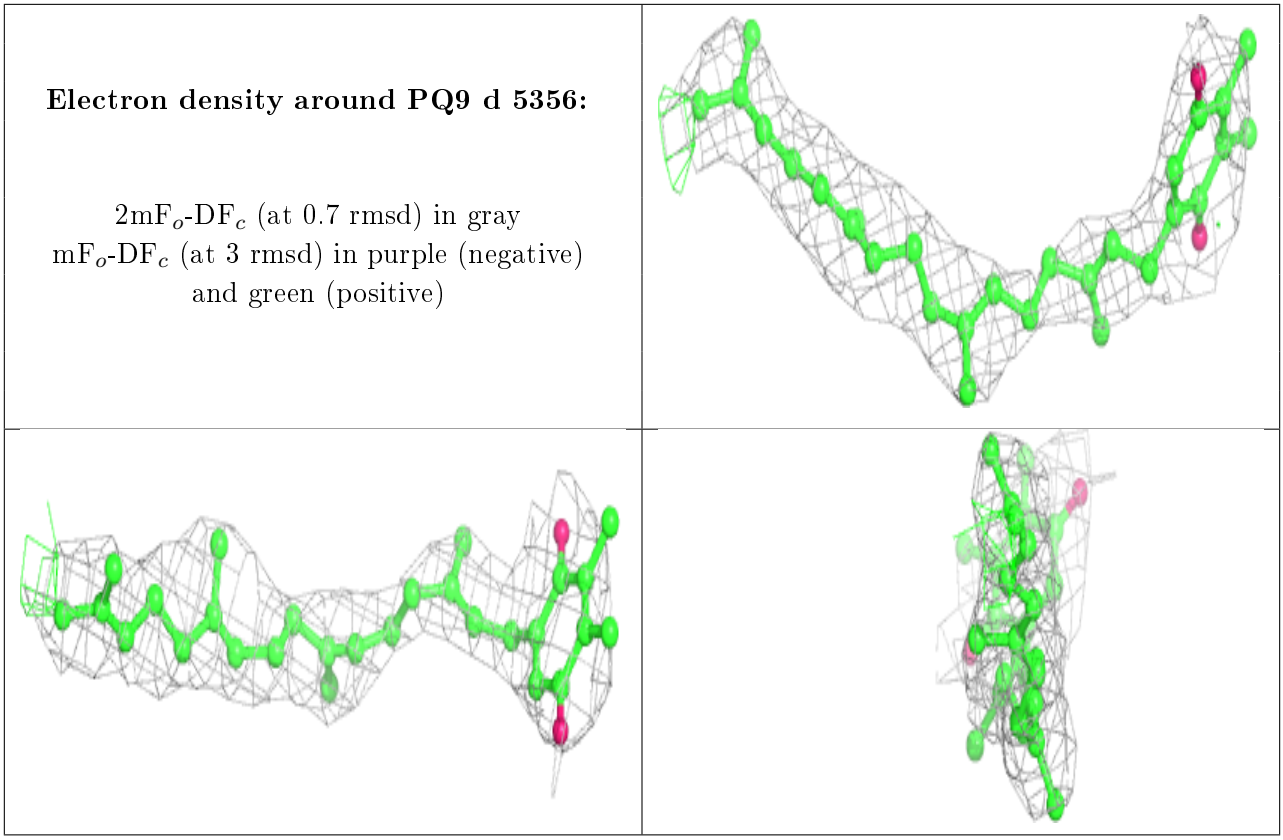
Electron density around BCR b 5527:

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



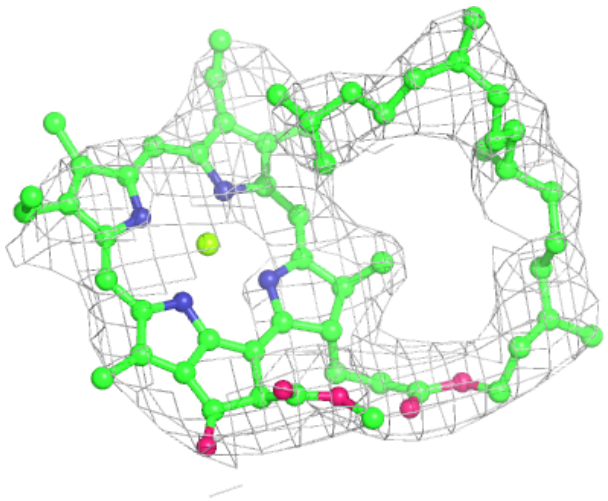
Electron density around PQ9 d 5356:

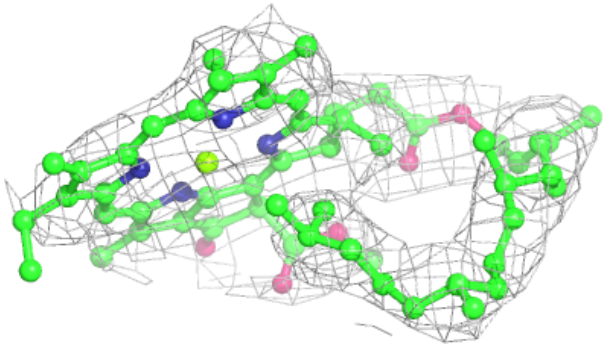
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

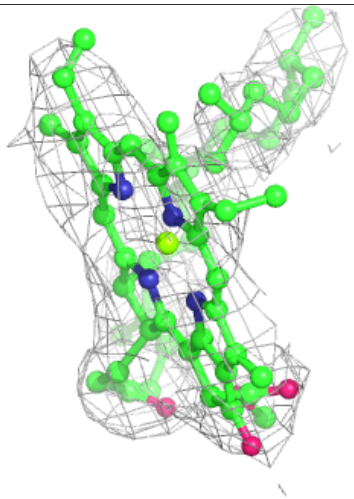


Electron density around CLA b 5525:

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

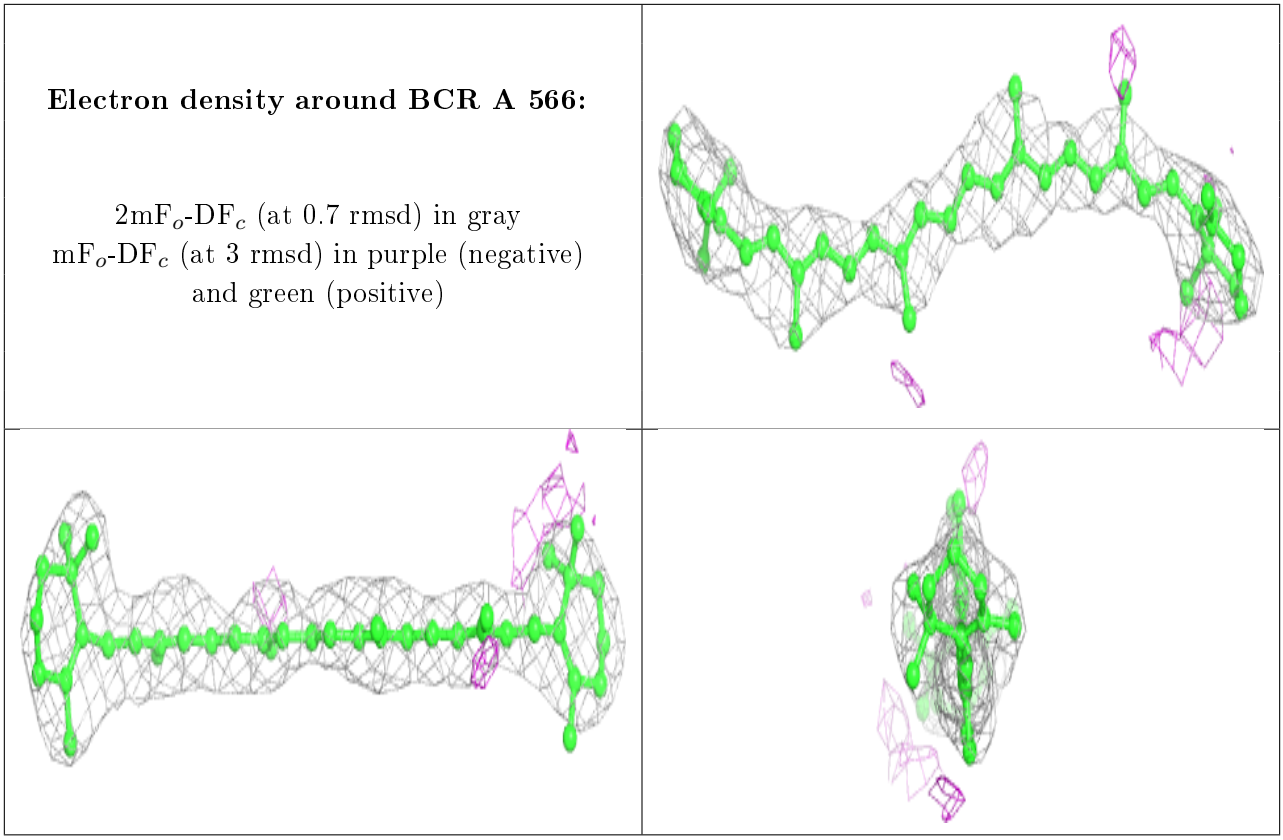






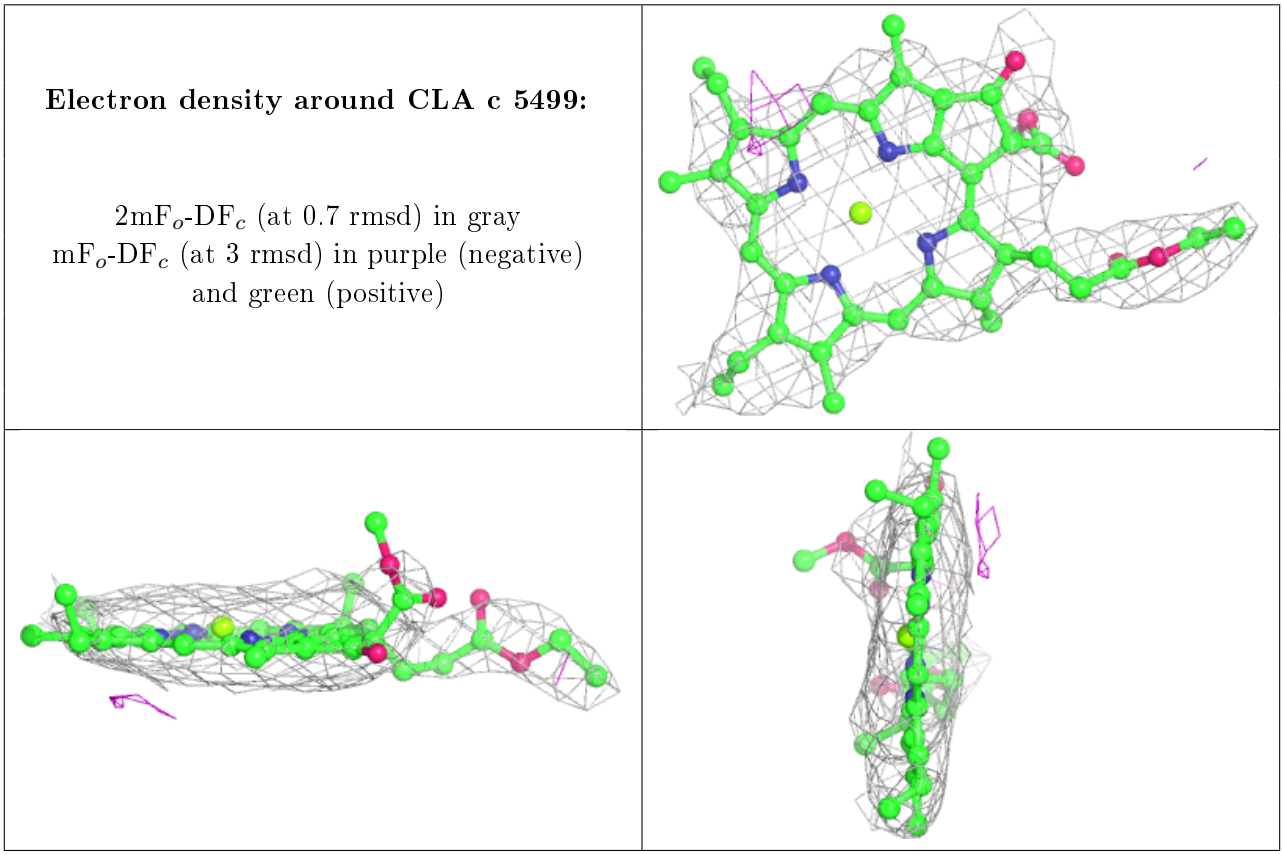
Electron density around BCR A 566:

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



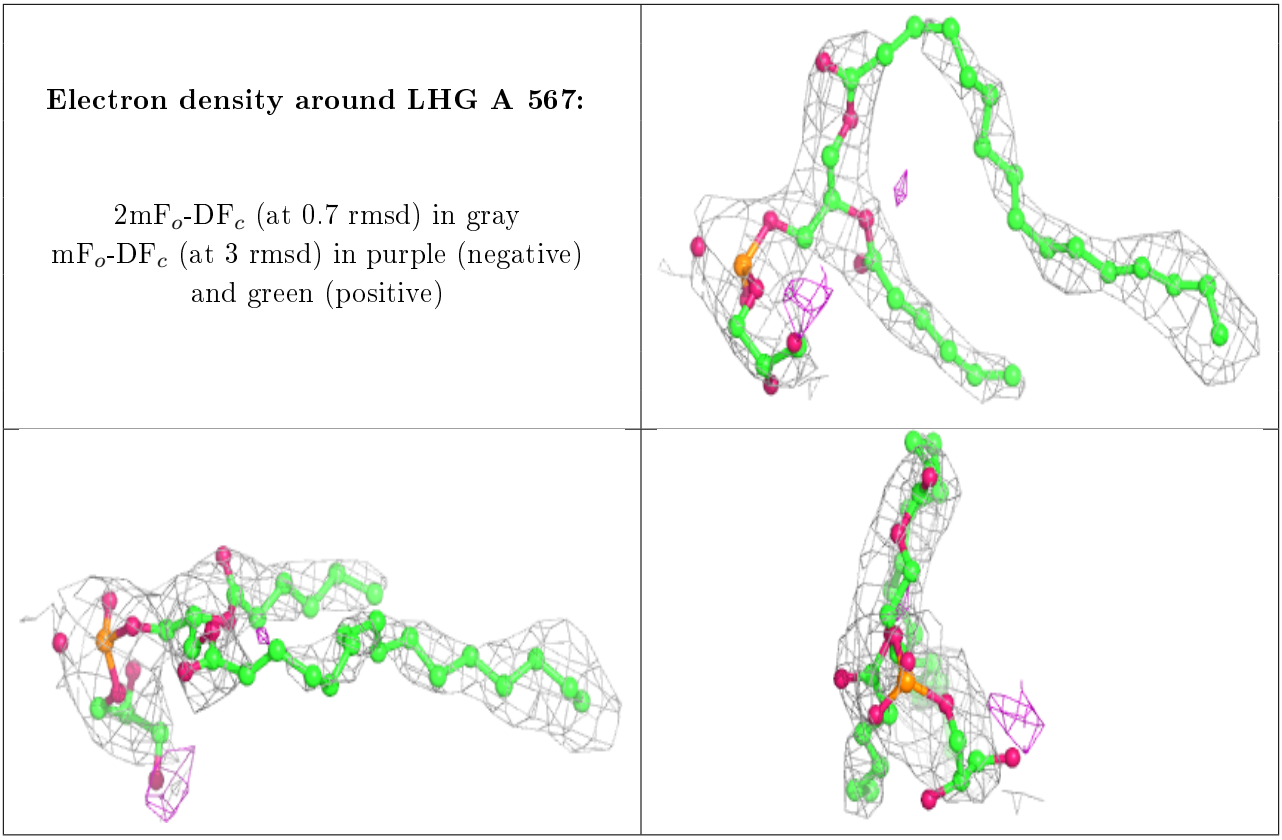
Electron density around CLA c 5499:

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



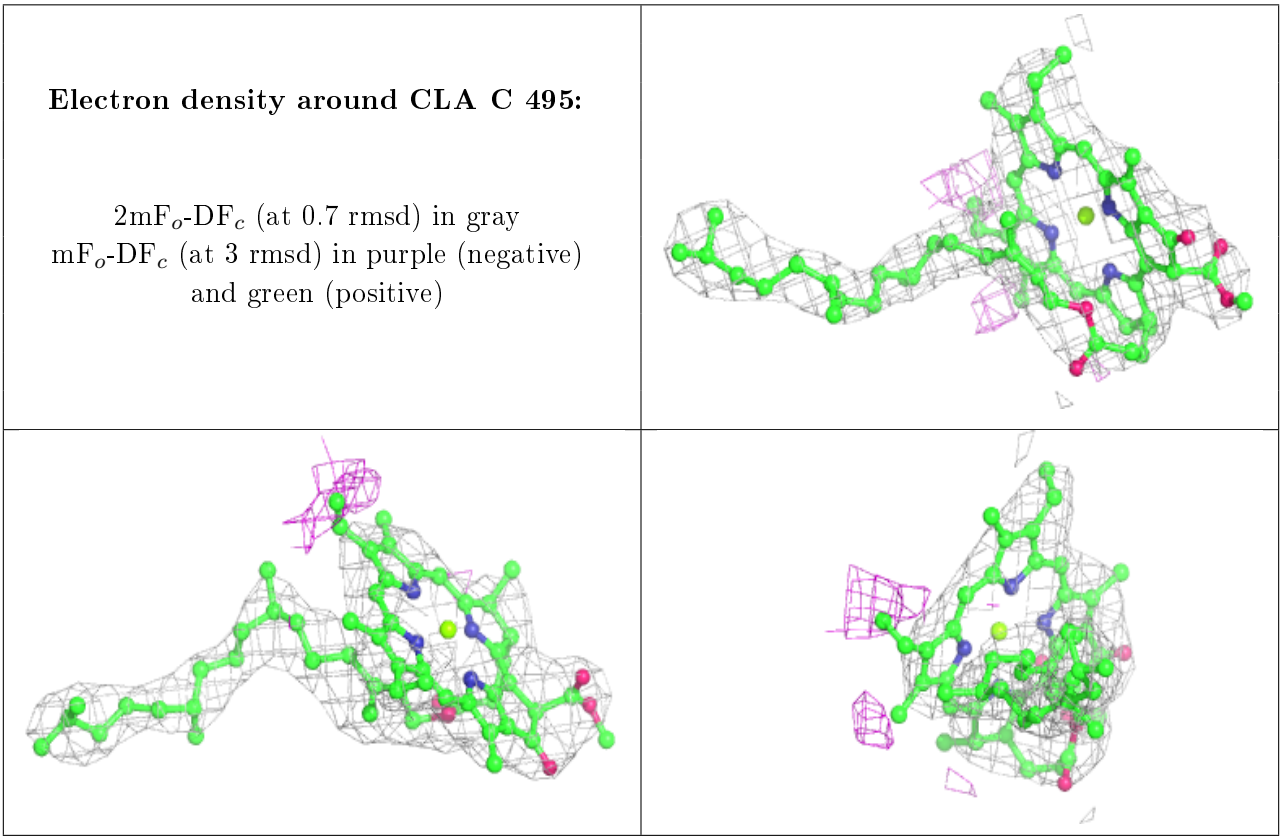
Electron density around LHG A 567:

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



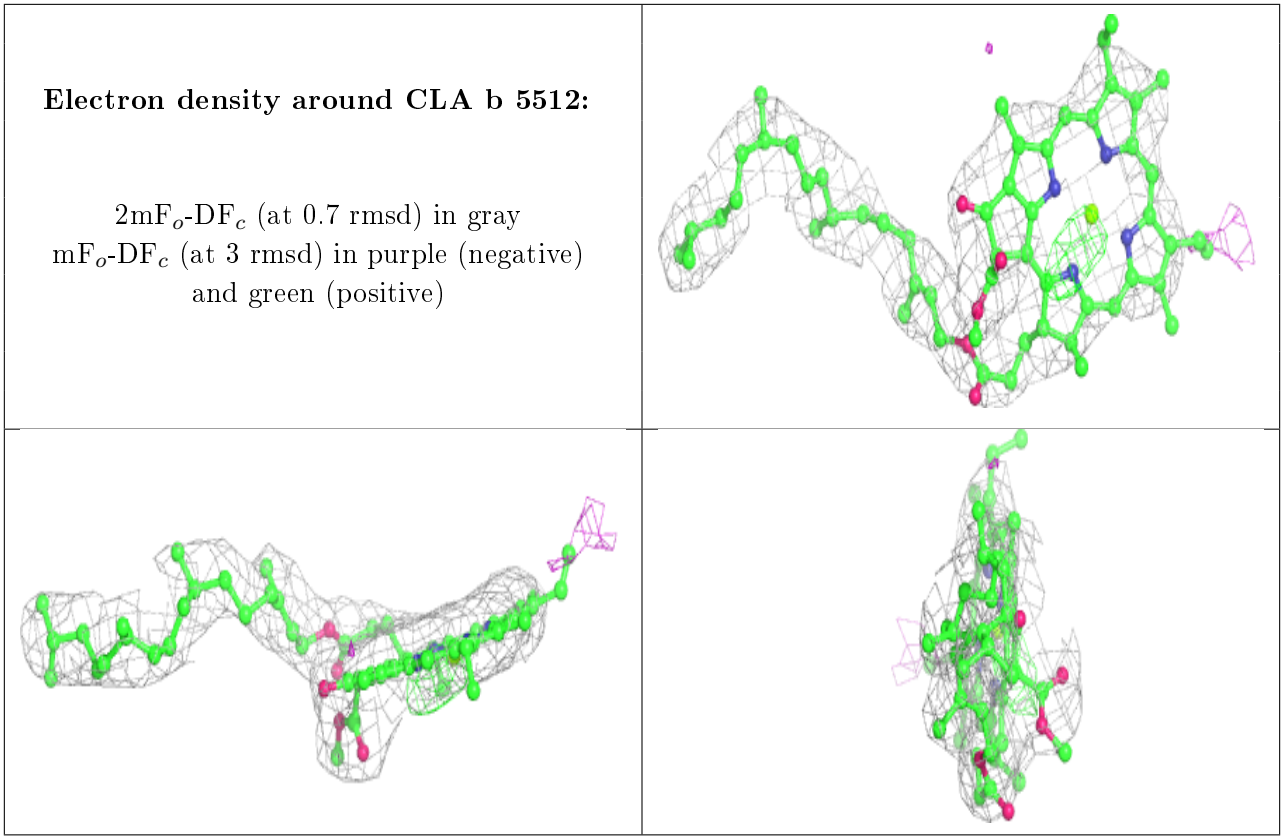
Electron density around CLA C 495:

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



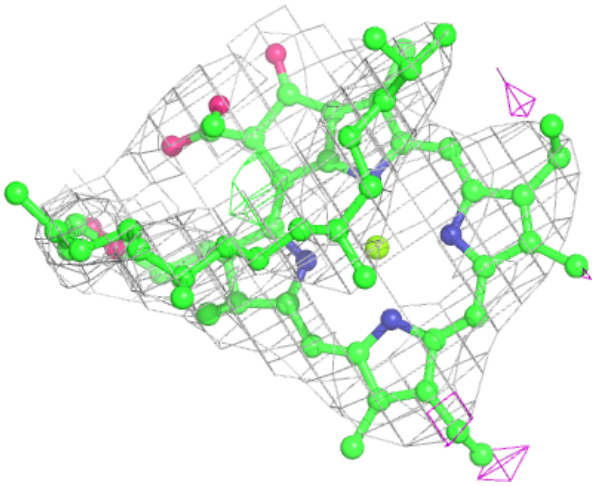
Electron density around CLA b 5512:

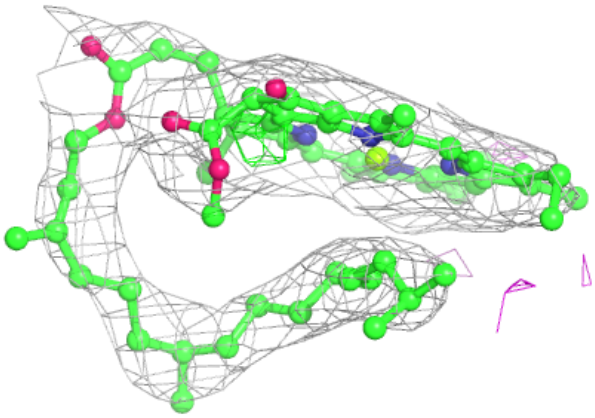
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

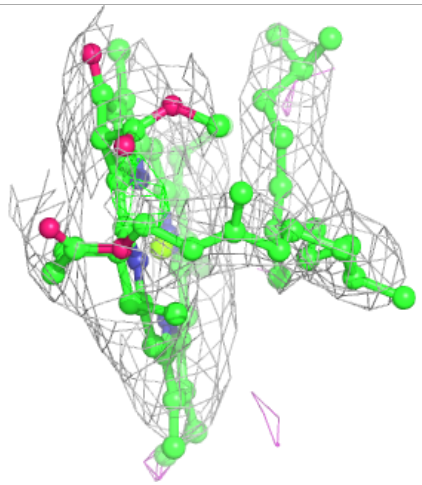


Electron density around CLA c 5500:

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

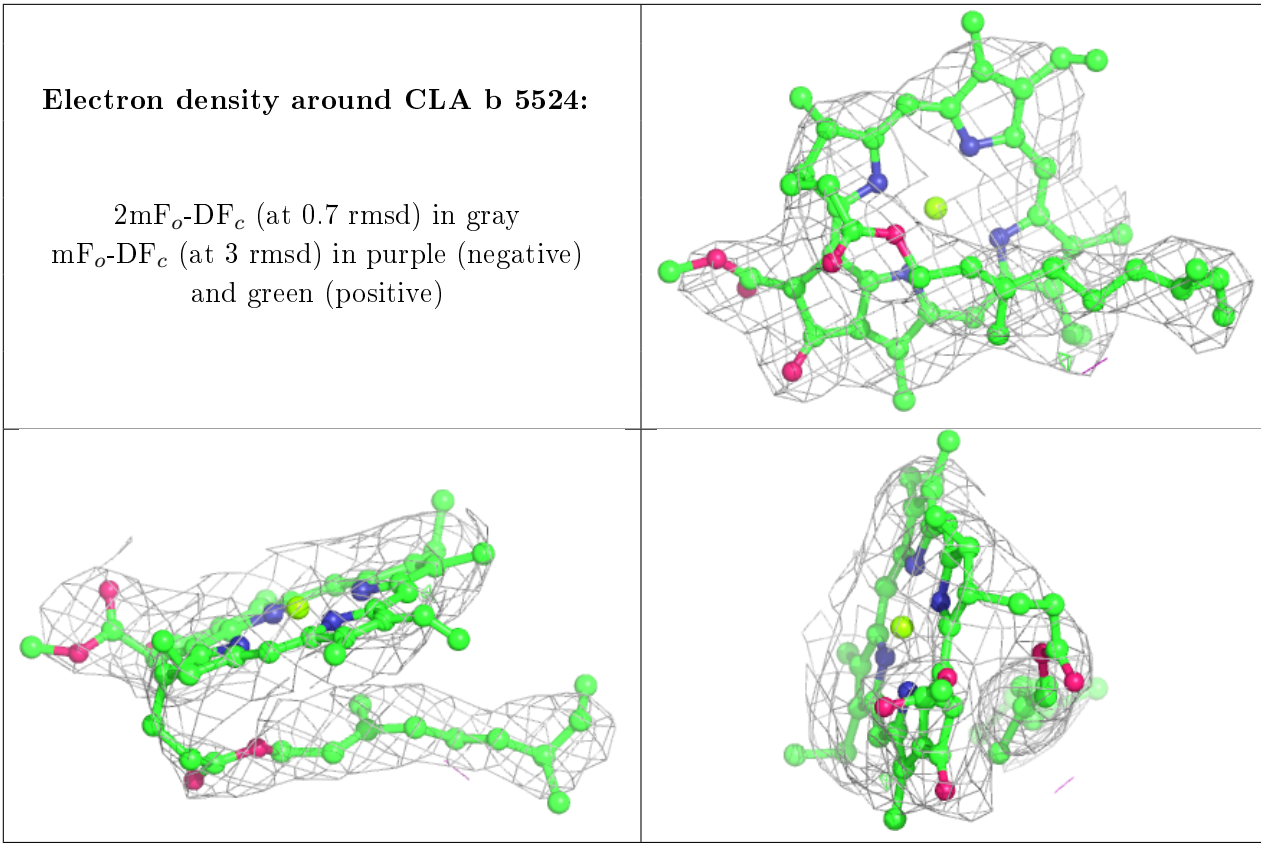






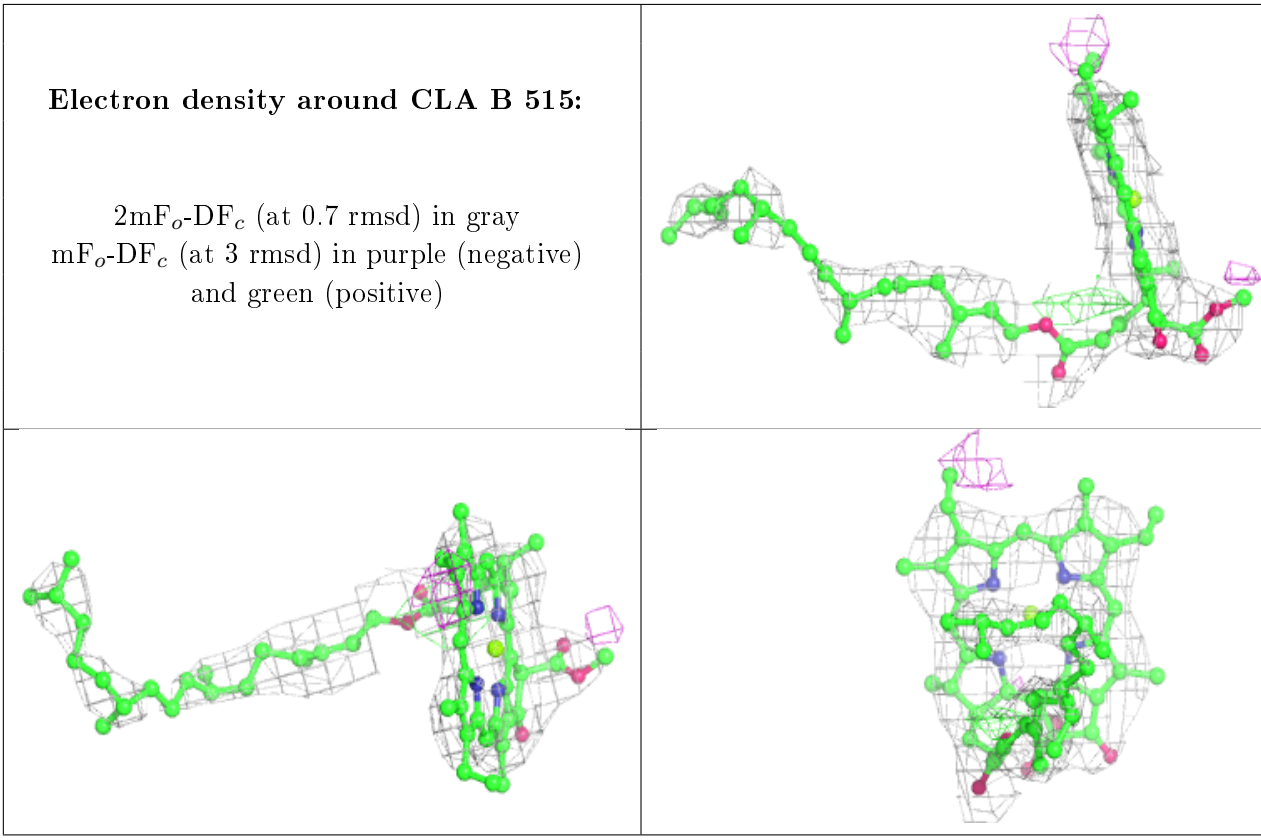
Electron density around CLA b 5524:

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



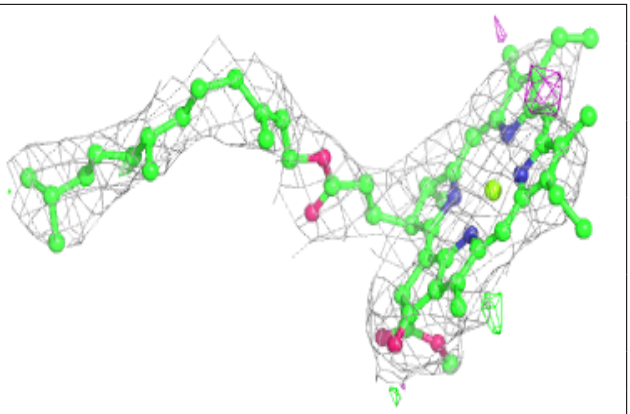
Electron density around CLA B 515:

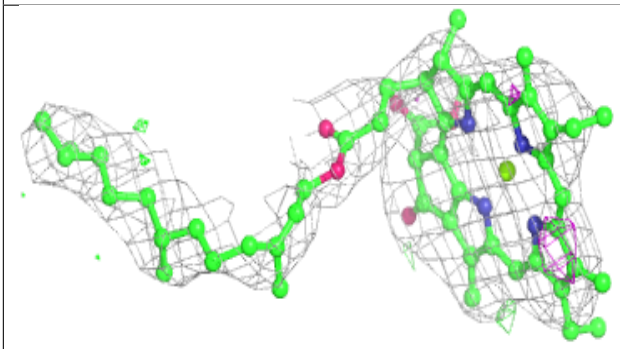
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

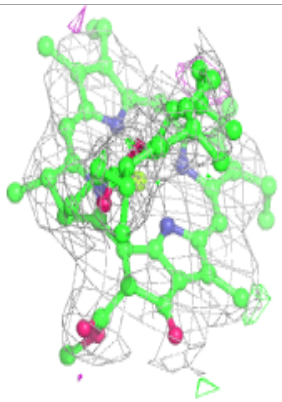


Electron density around CLA c 5492:

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

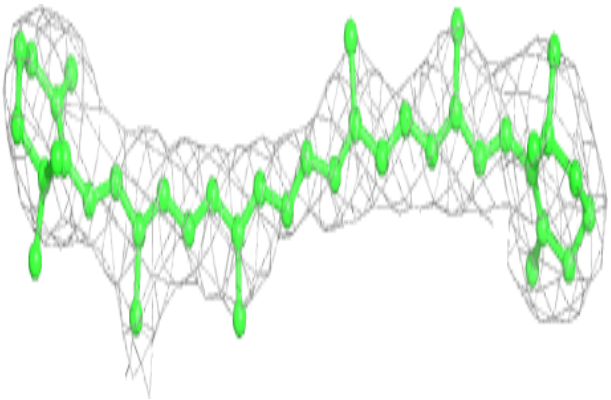


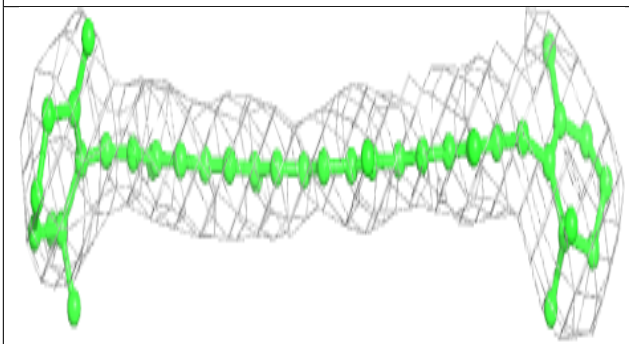




Electron density around BCR b 5528:

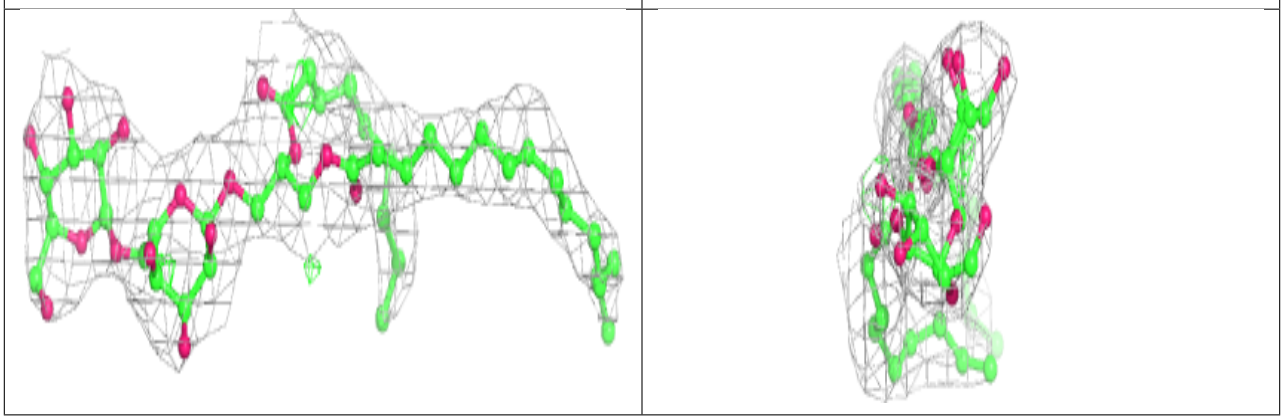
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





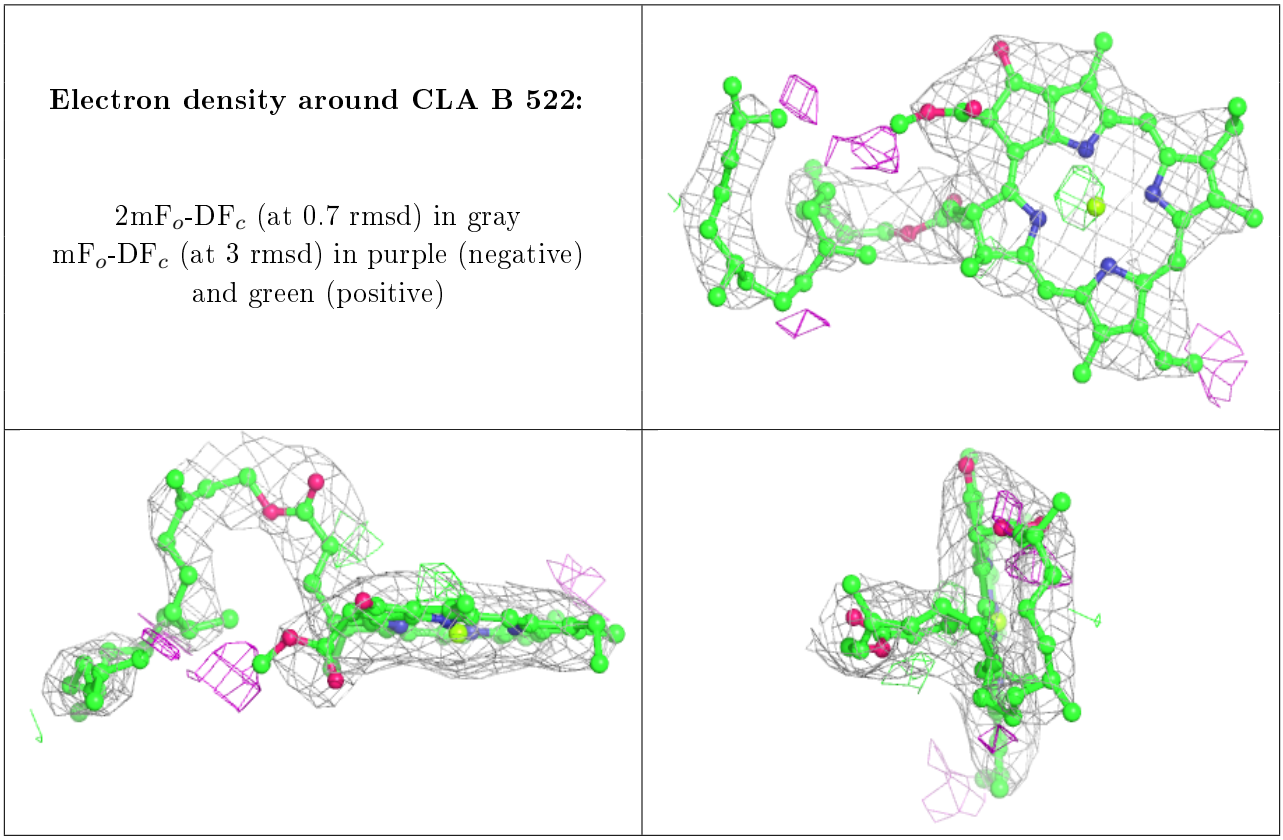
Electron density around DGD h 5208:

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



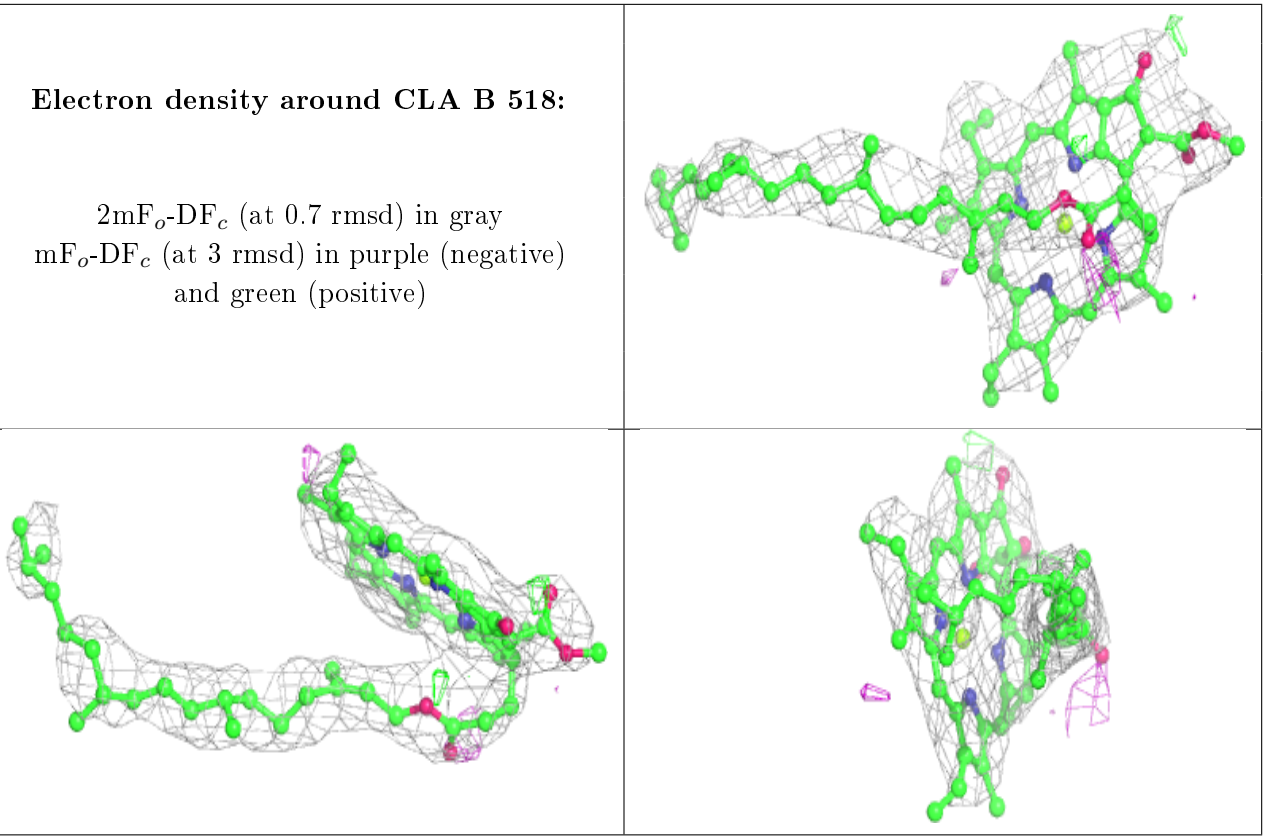
Electron density around CLA B 522:

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



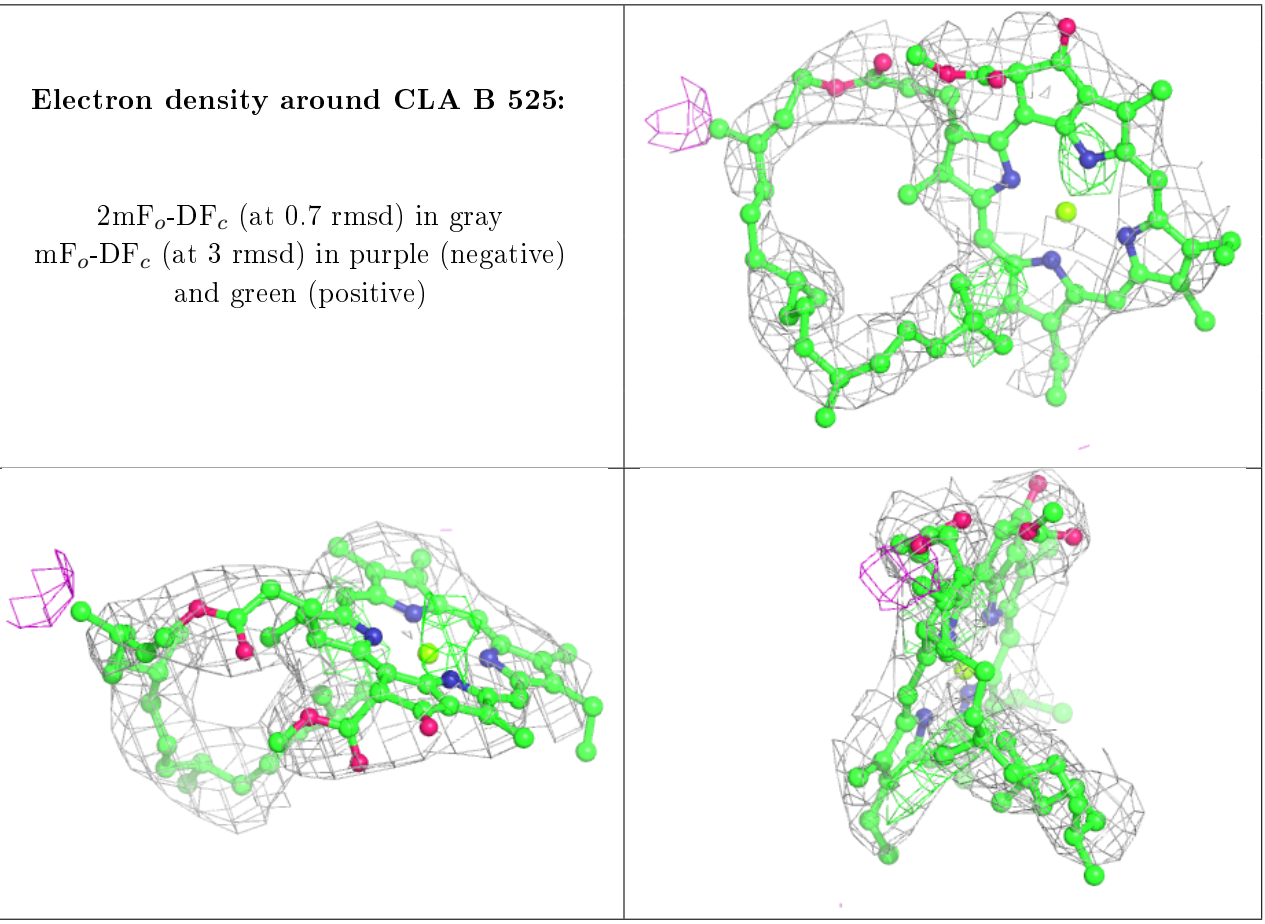
Electron density around CLA B 518:

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



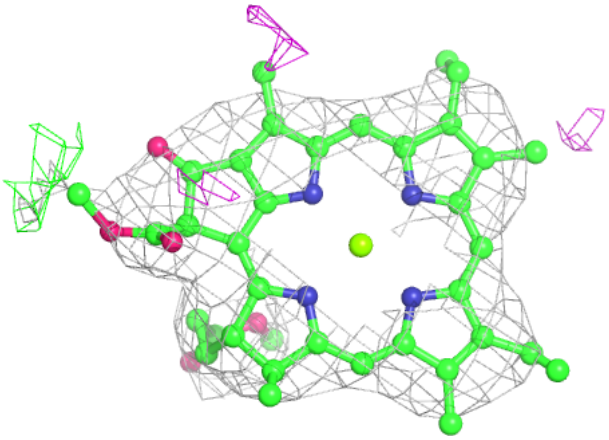
Electron density around CLA B 525:

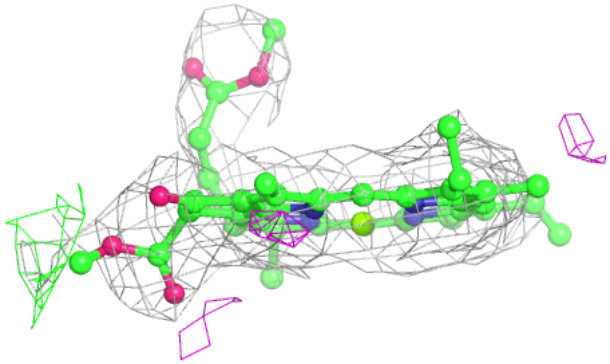
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

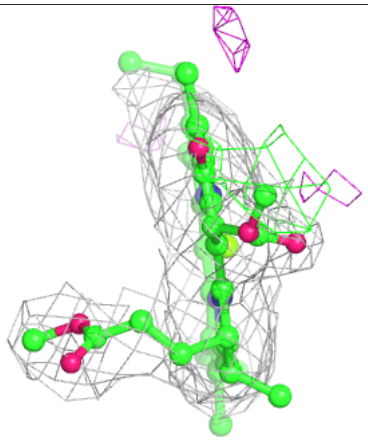


Electron density around CLA c 5494:

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

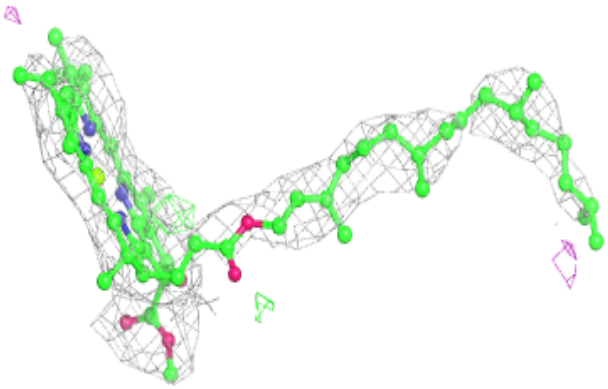


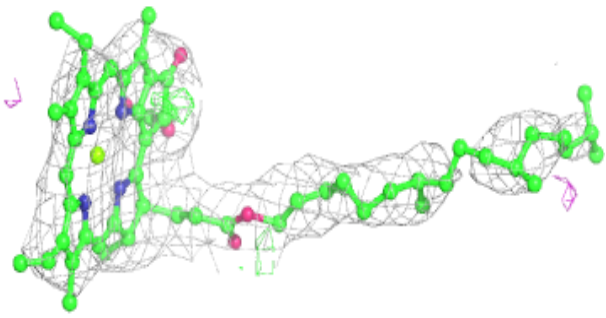


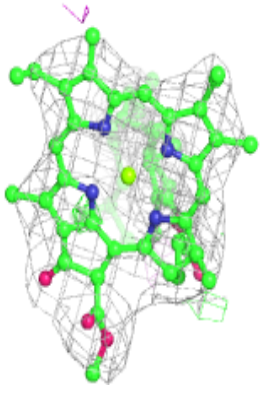


Electron density around CLA B 514:

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

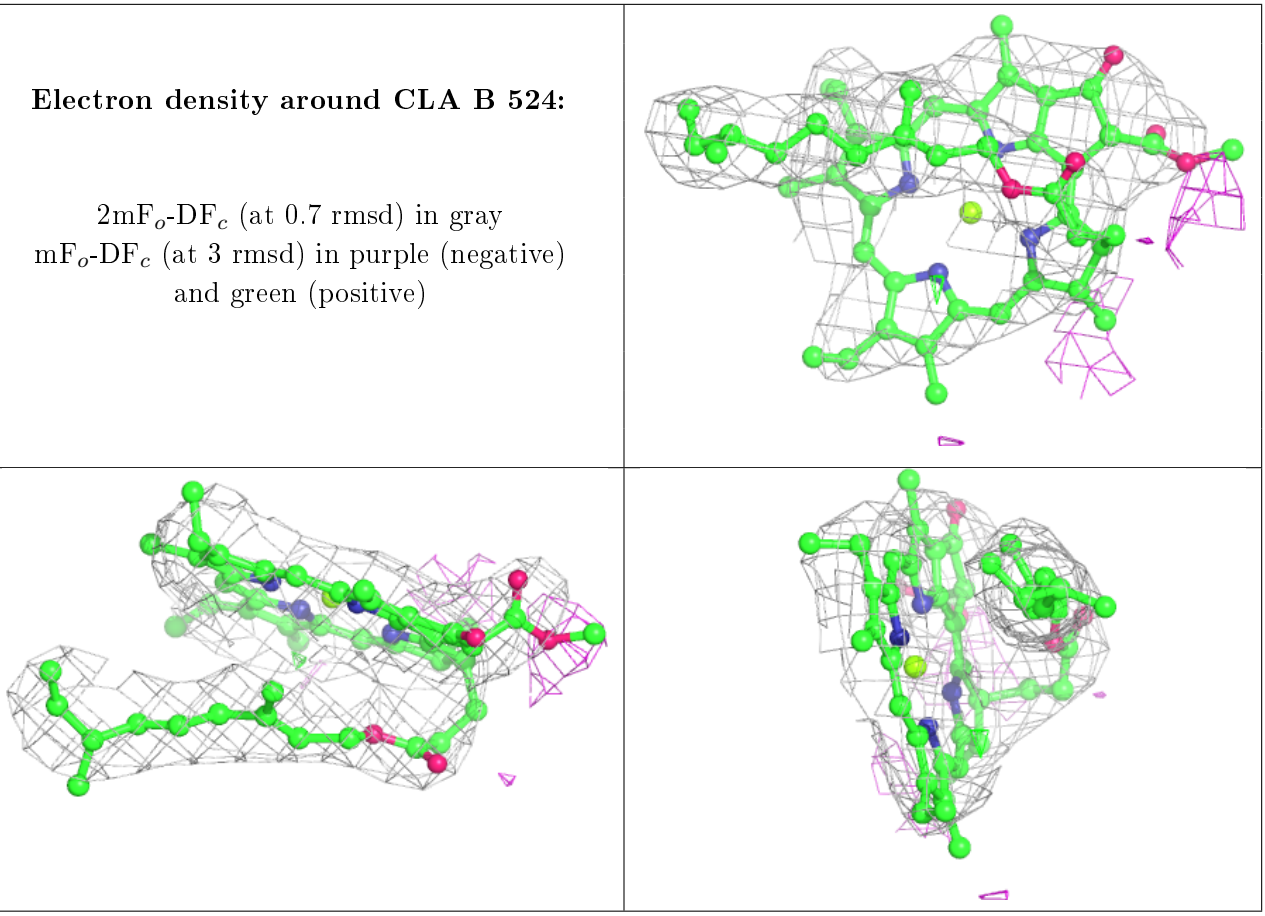






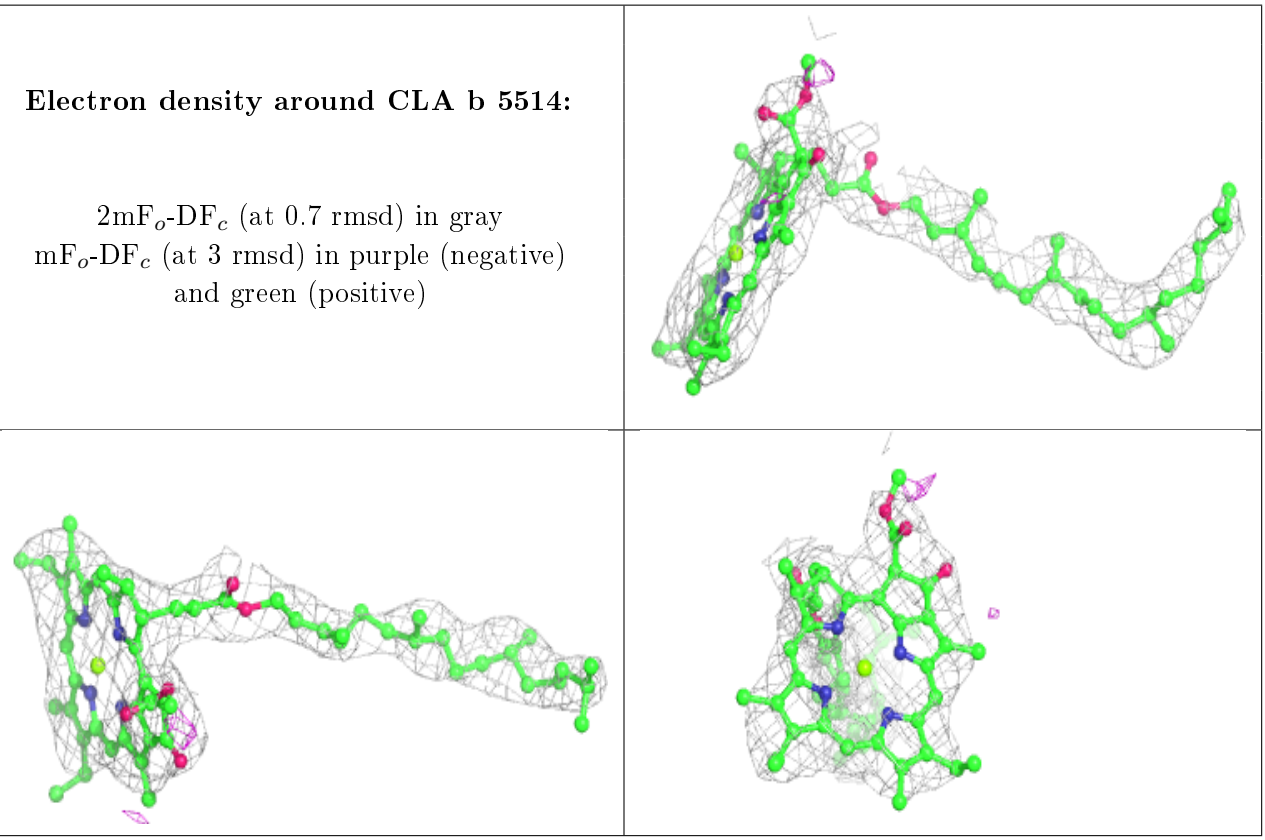
Electron density around CLA B 524:

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



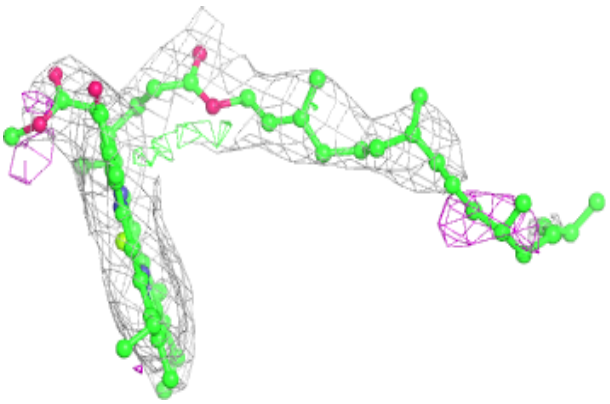
Electron density around CLA b 5514:

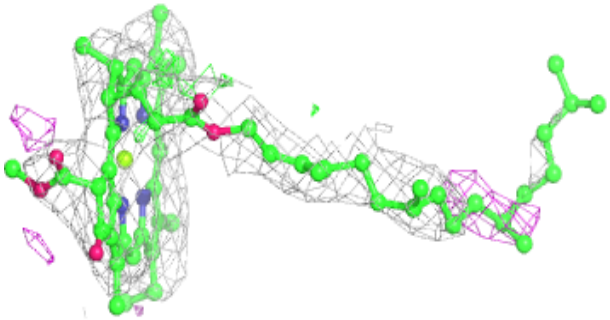
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

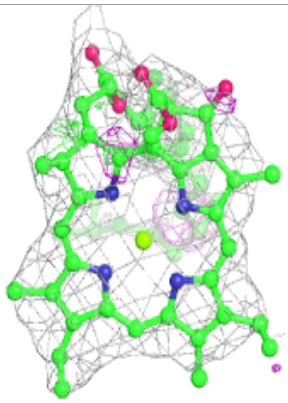


Electron density around CLA b 5515:

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

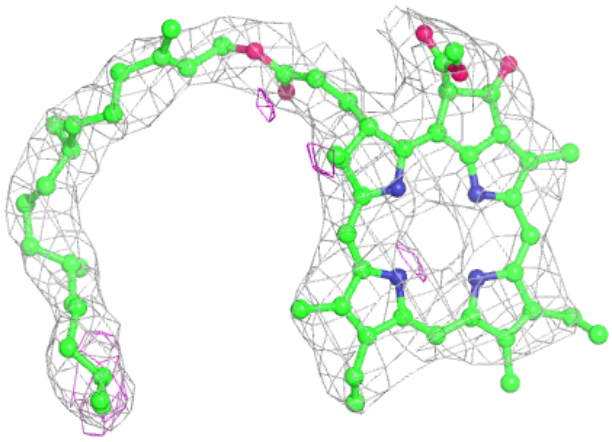


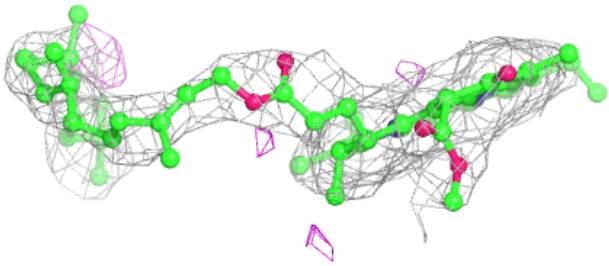


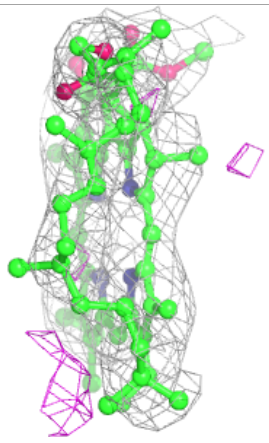


Electron density around PHO a 5561:

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

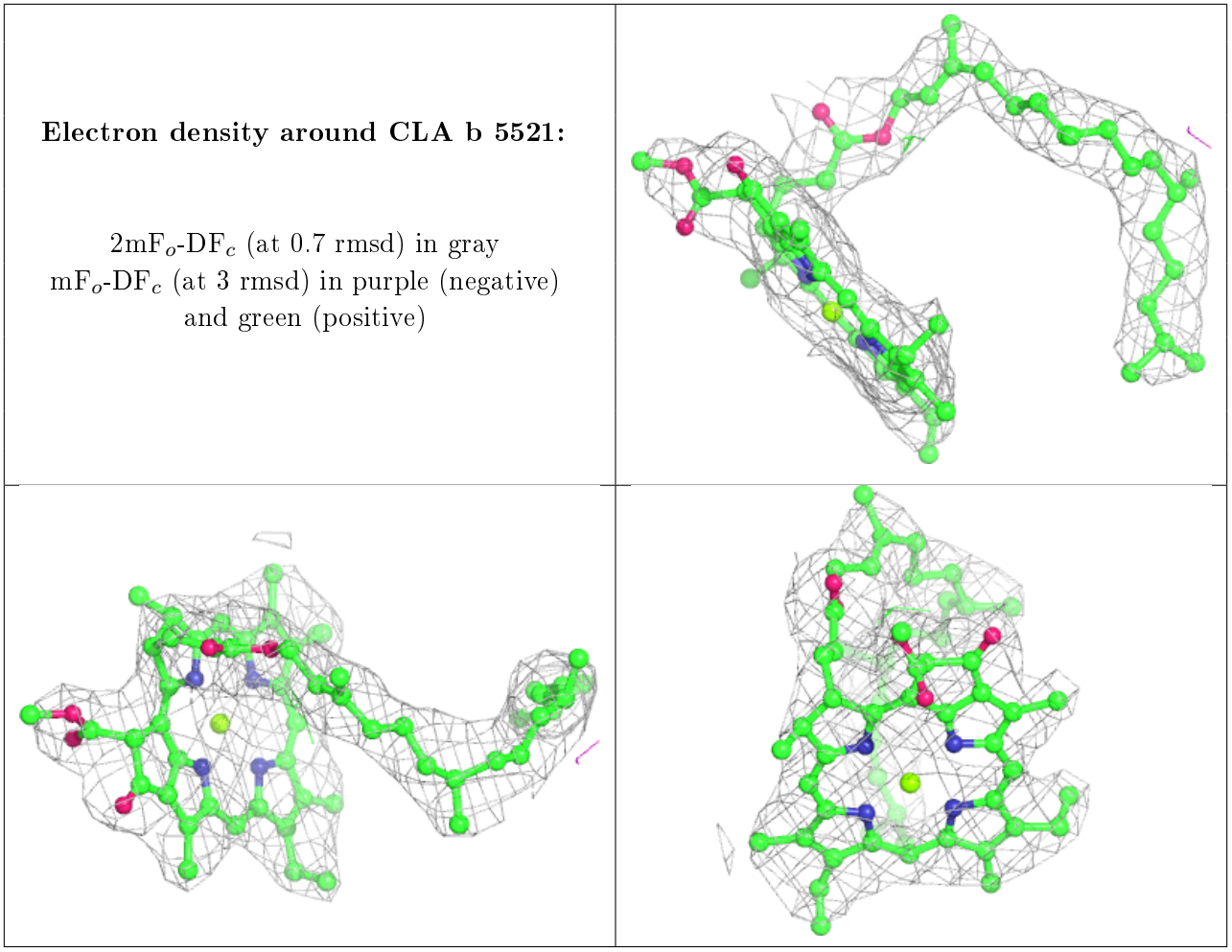






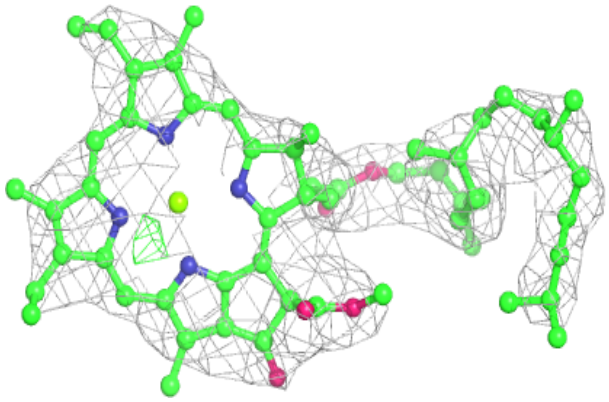
Electron density around CLA b 5521:

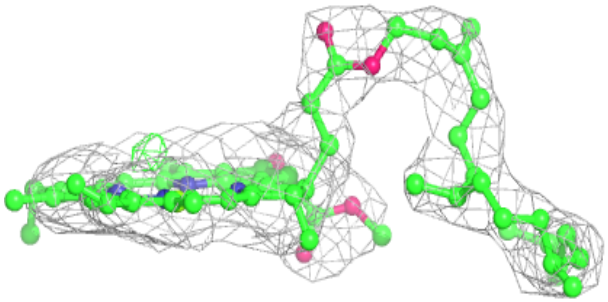
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

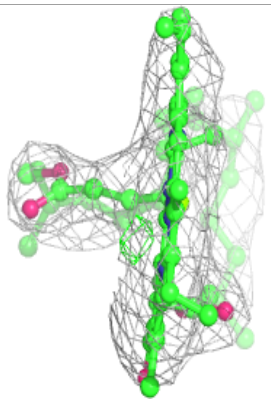


Electron density around CLA b 5522:

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

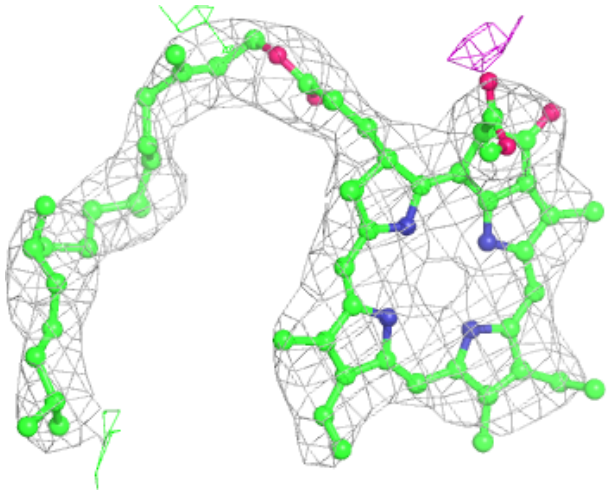


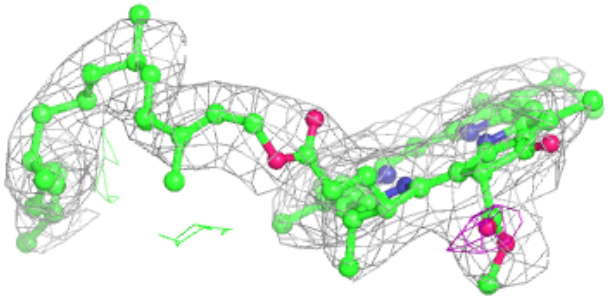


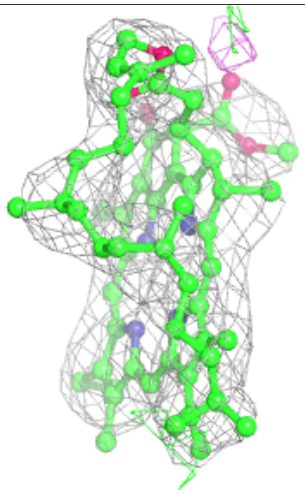


Electron density around PHO A 562:

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

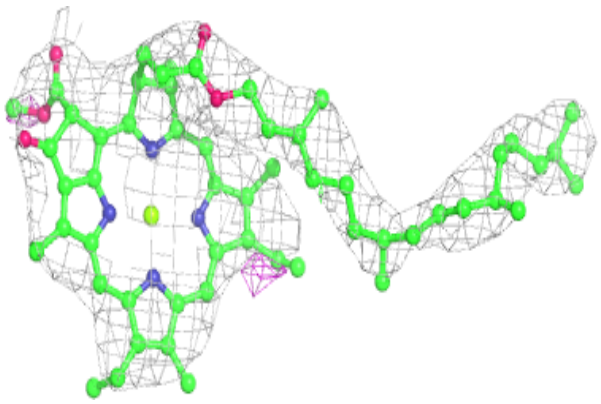


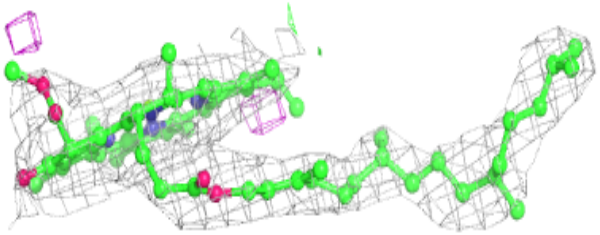


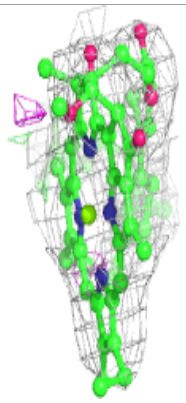


Electron density around CLA B 513:

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

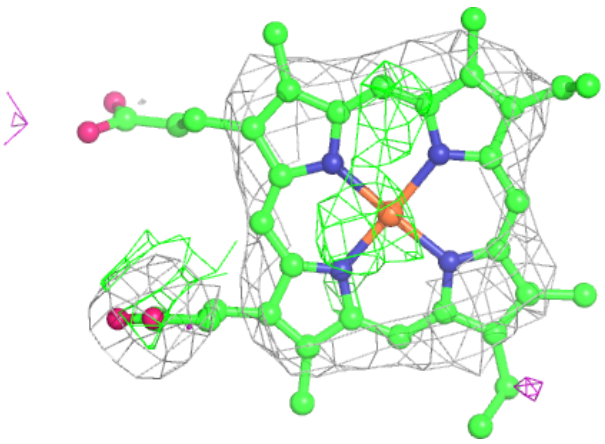


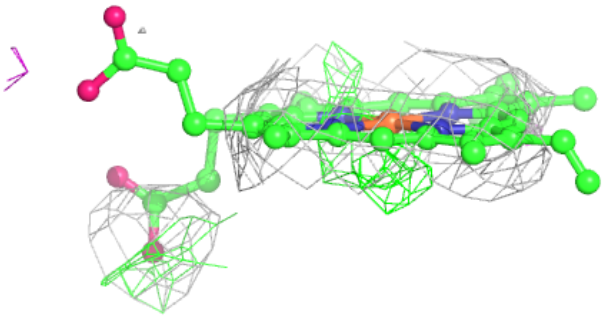


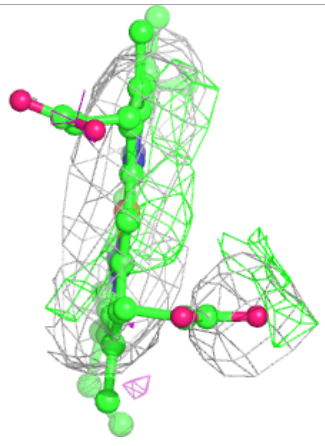


Electron density around HEM f 5051:

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

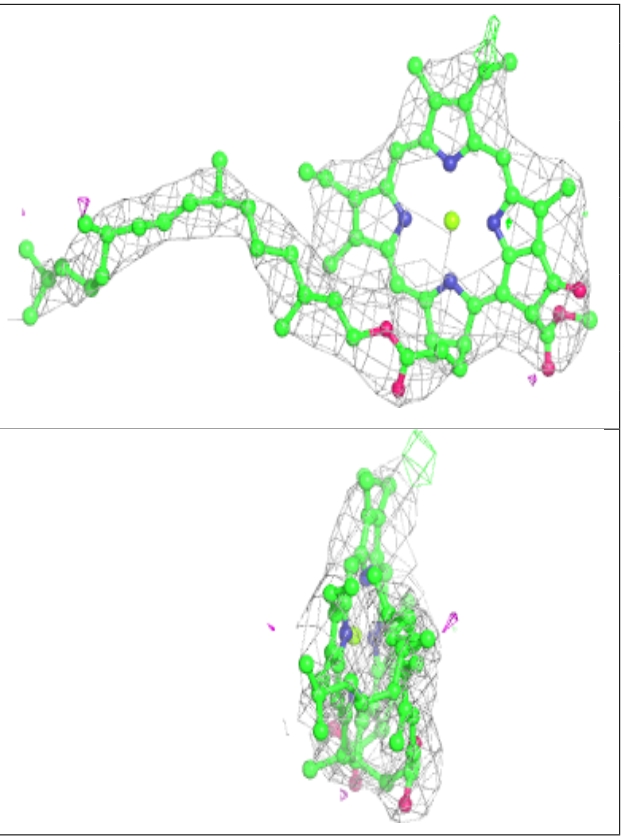


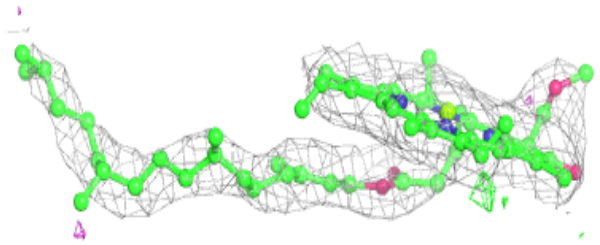




Electron density around CLA b 5513:

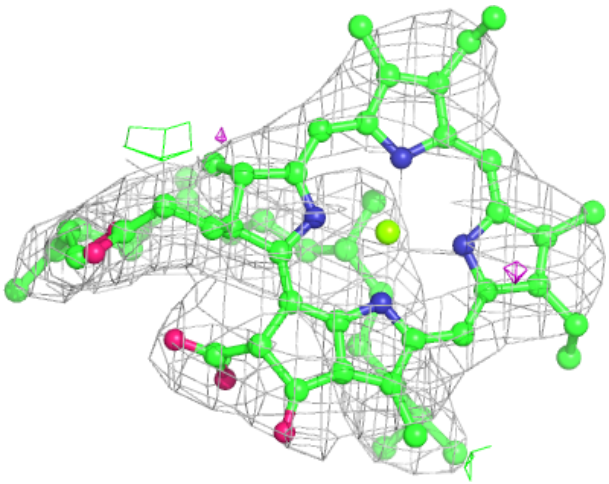
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

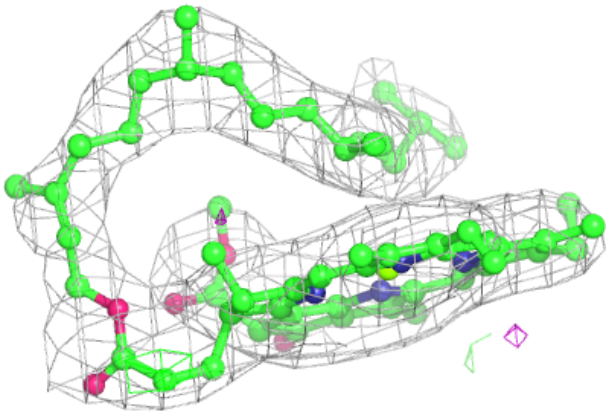


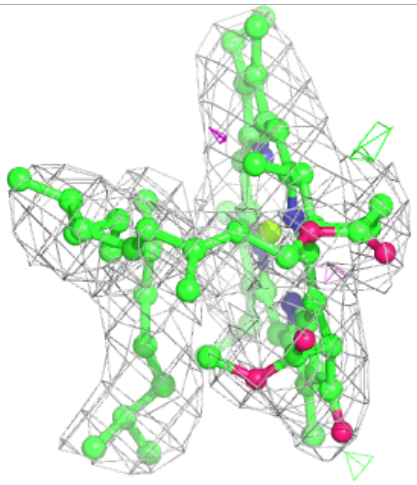


Electron density around CLA C 500:

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

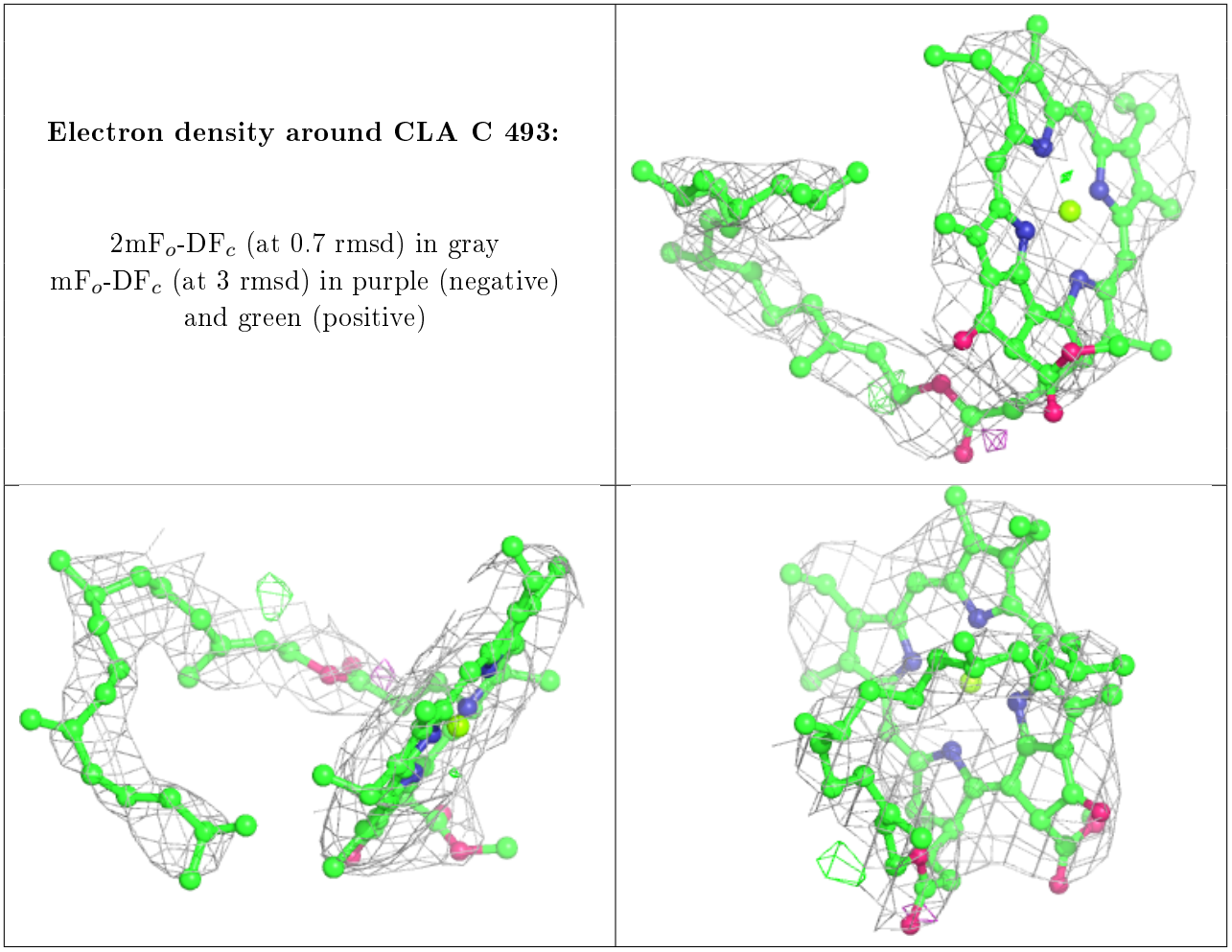






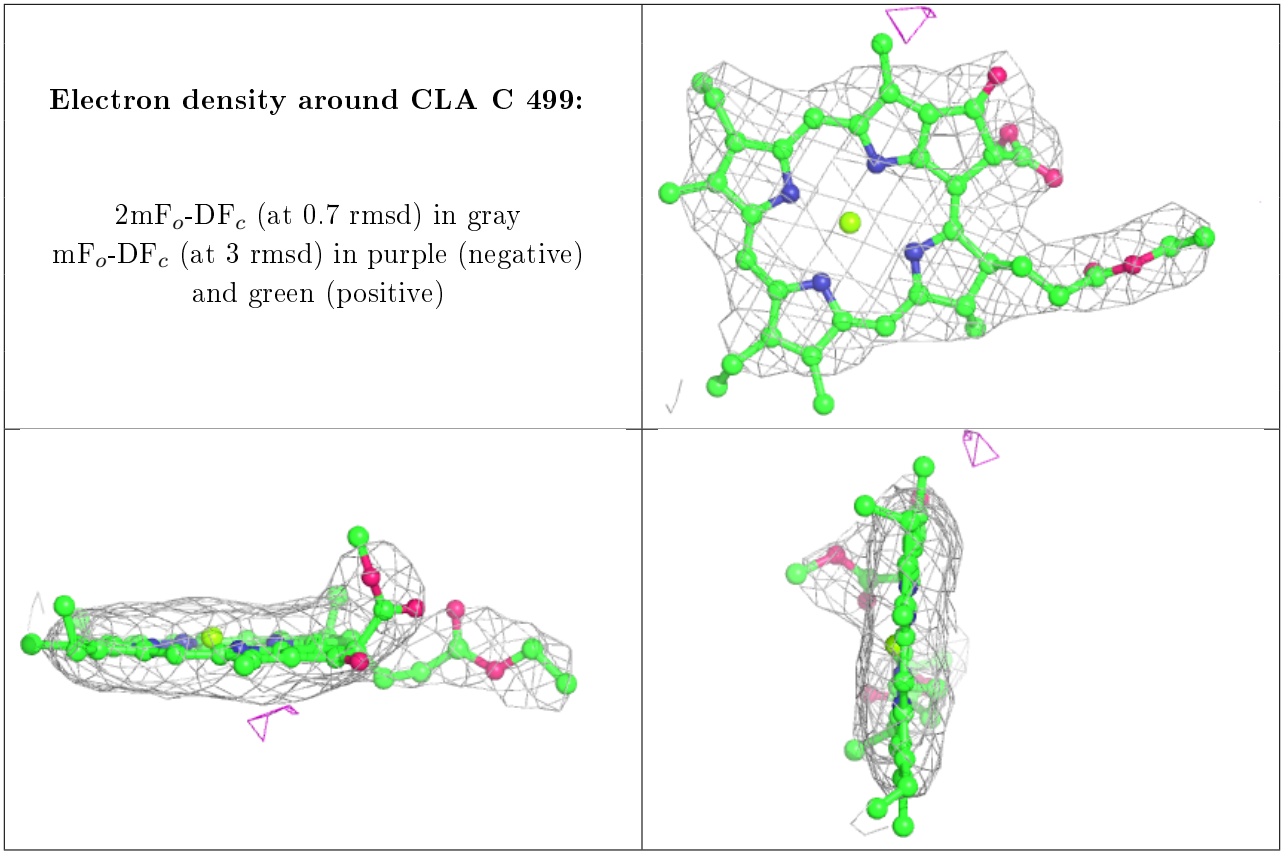
Electron density around CLA C 493:

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



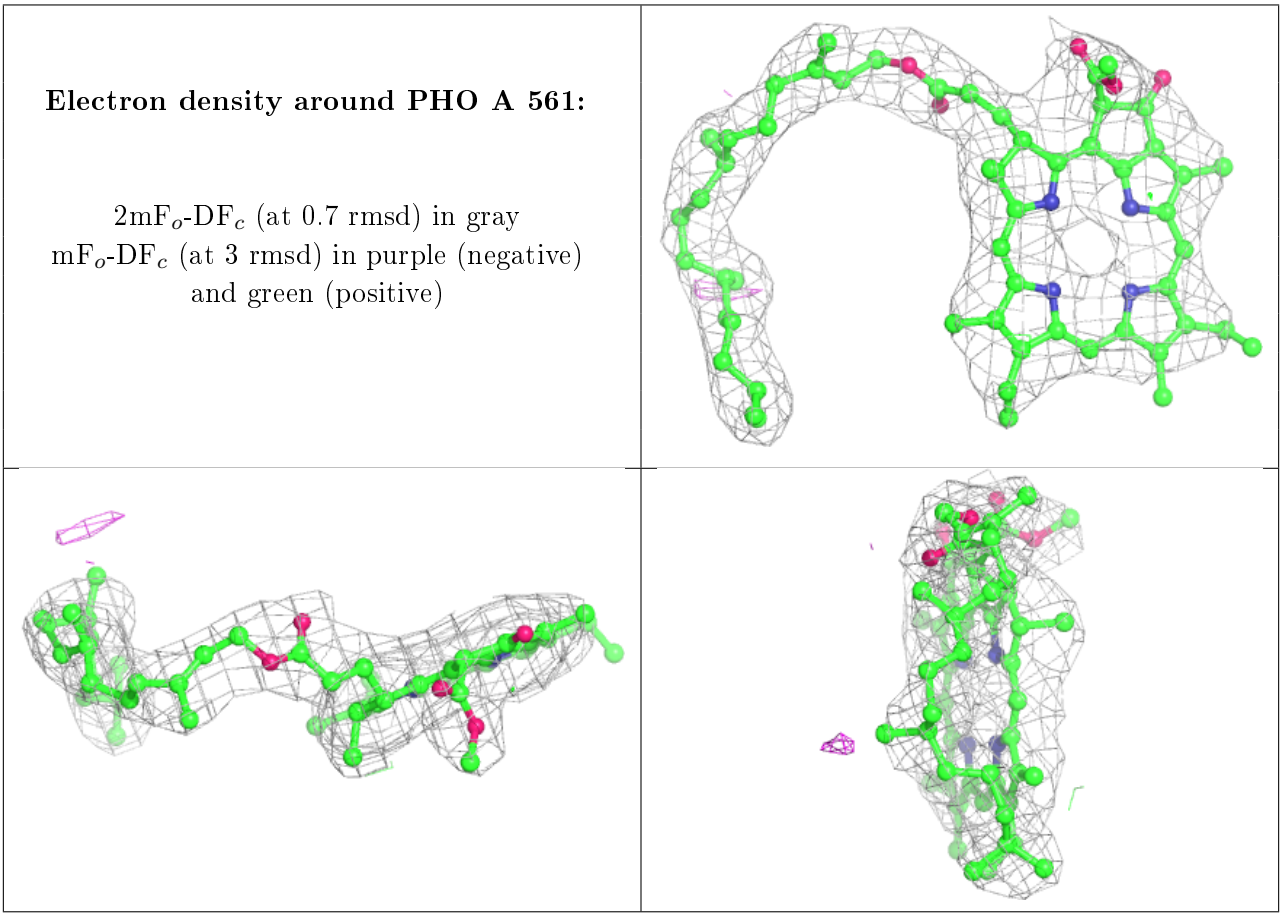
Electron density around CLA C 499:

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



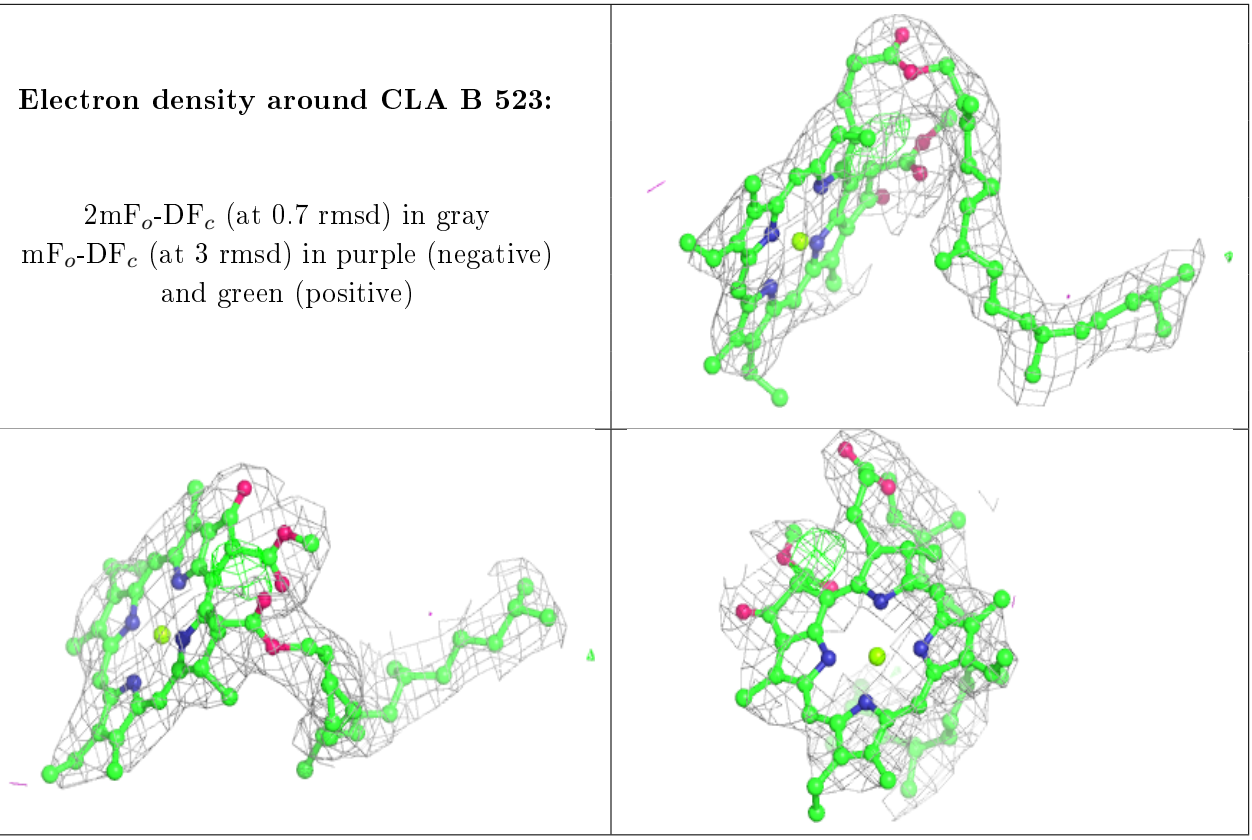
Electron density around PHO A 561:

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



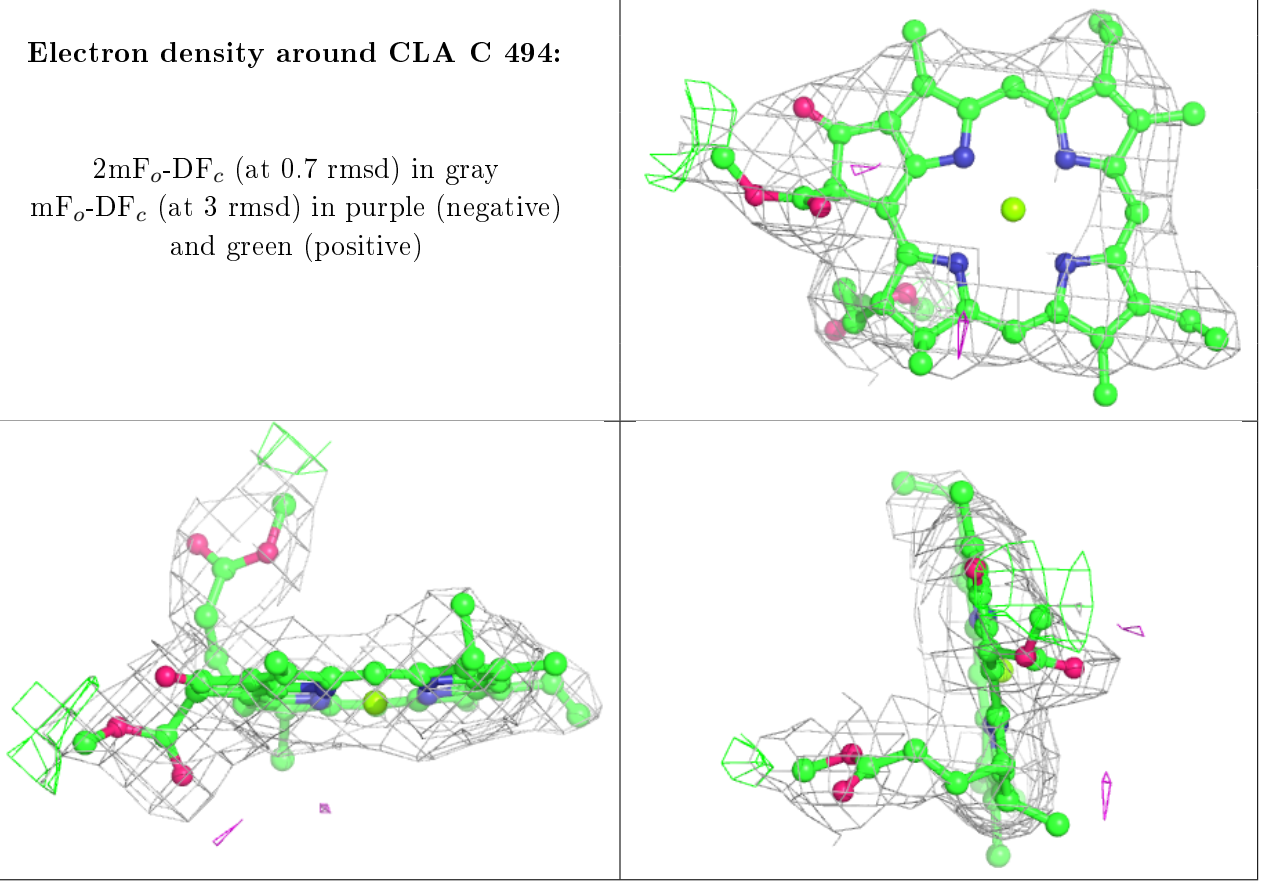
Electron density around CLA B 523:

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



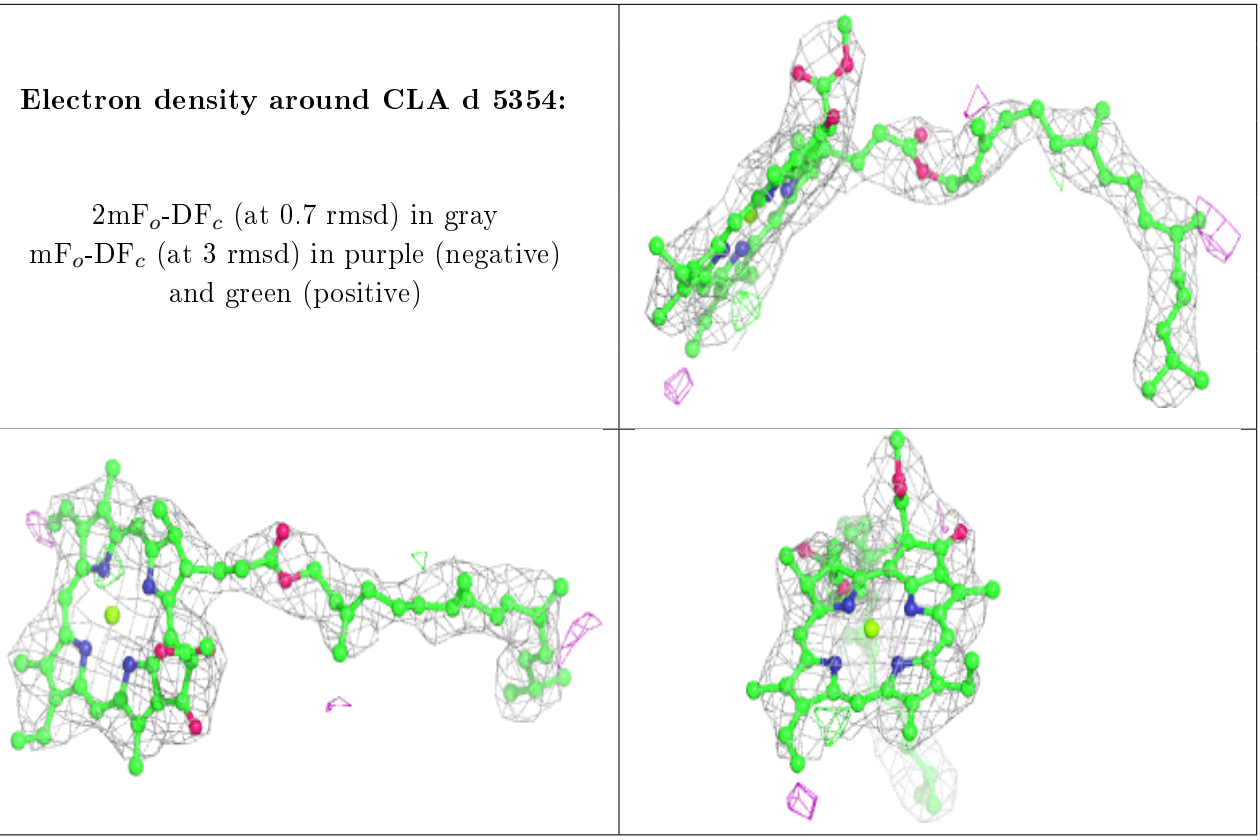
Electron density around CLA C 494:

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



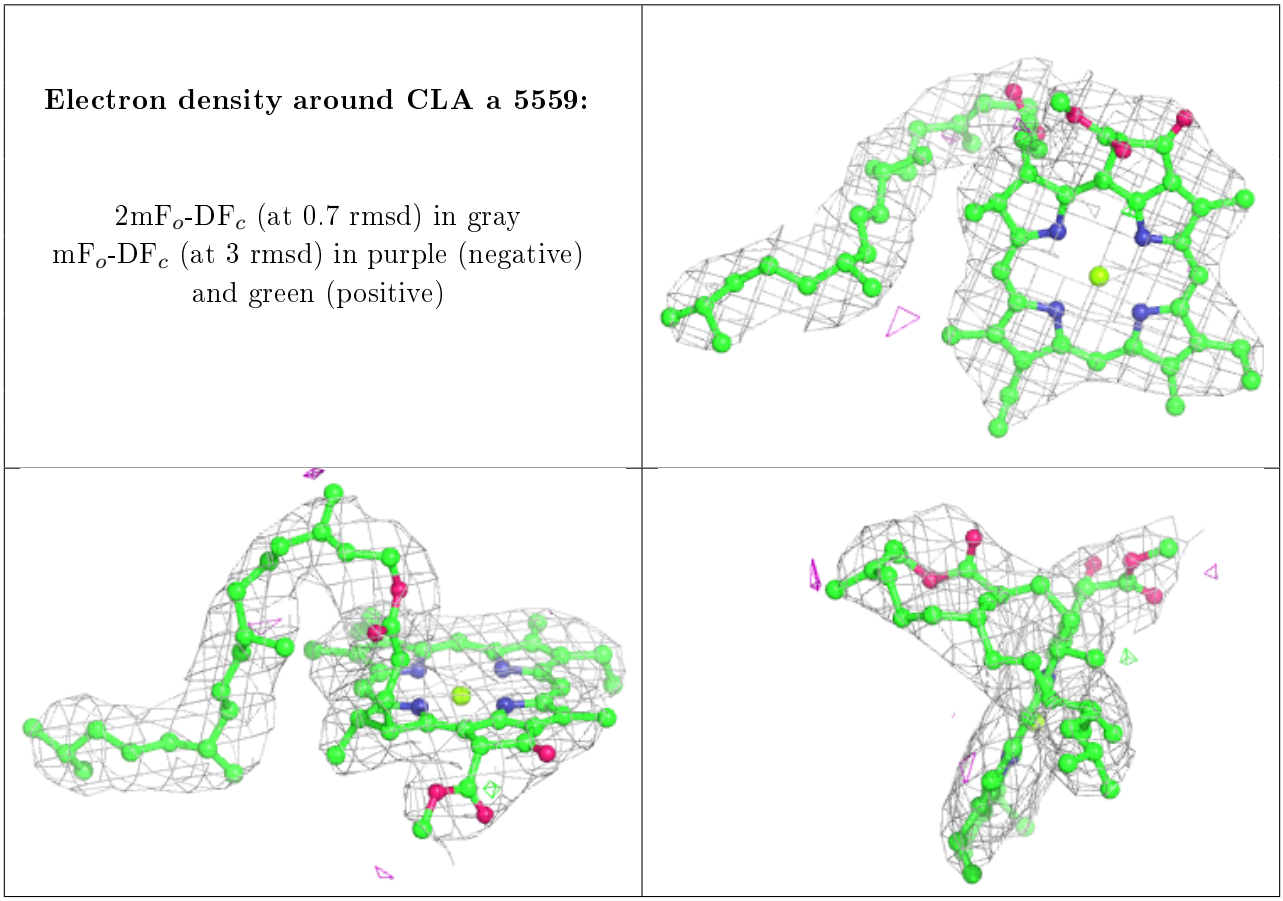
Electron density around CLA d 5354:

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



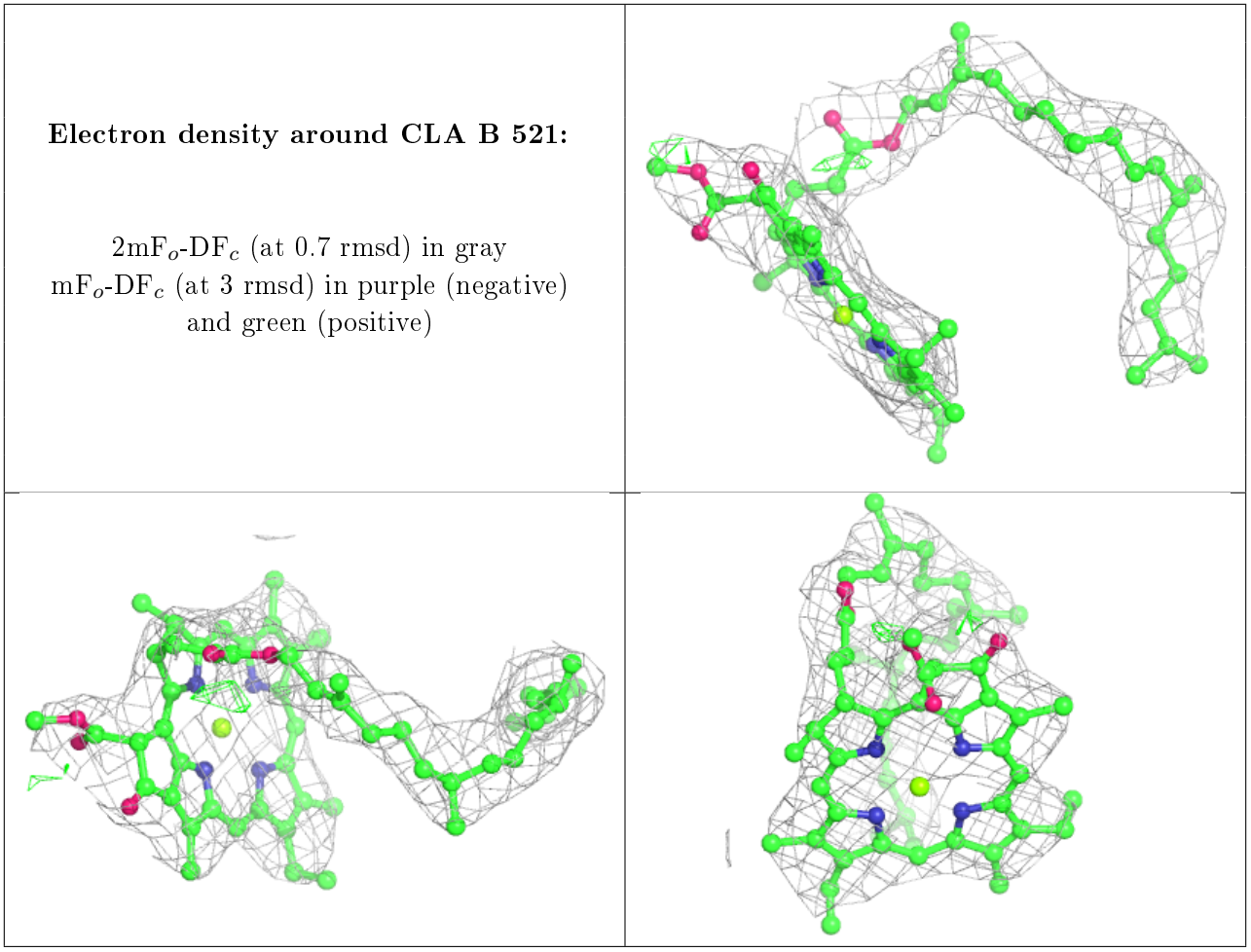
Electron density around CLA a 5559:

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



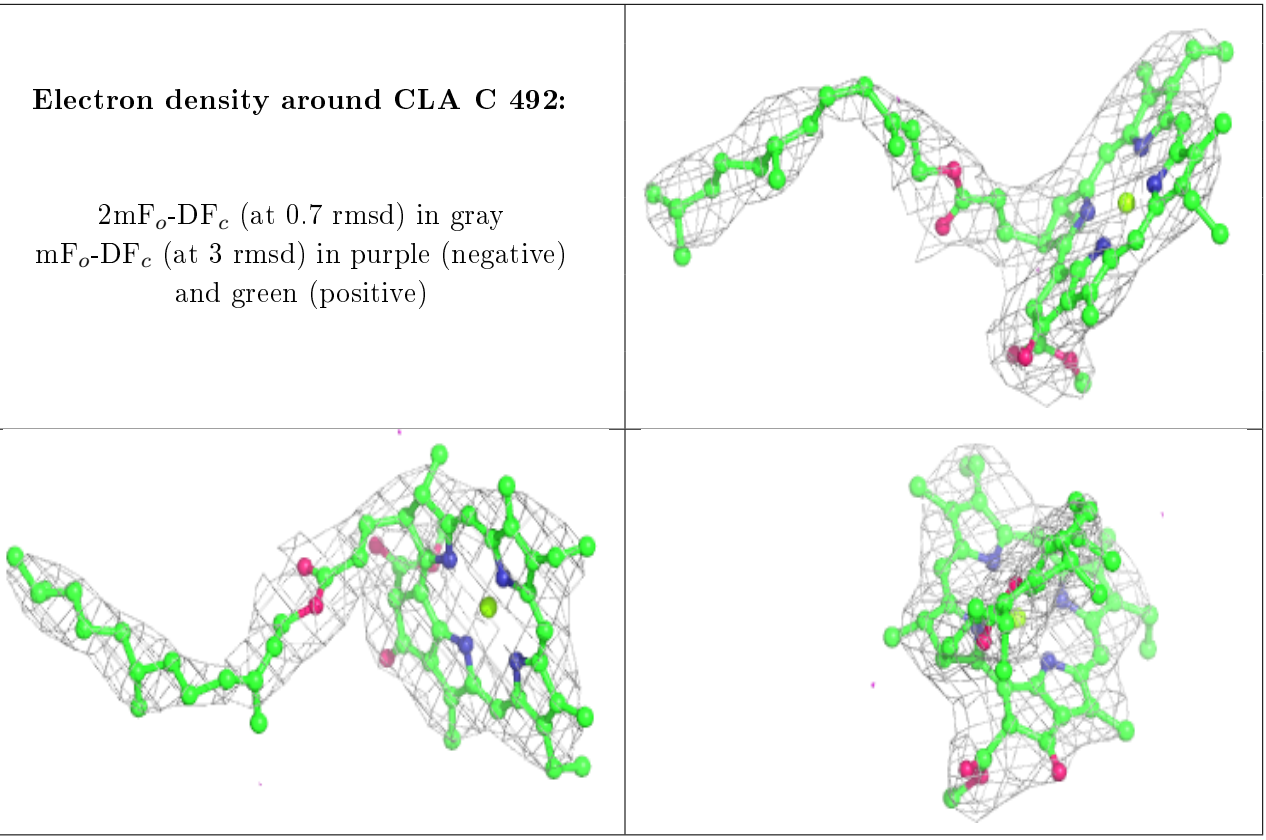
Electron density around CLA B 521:

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



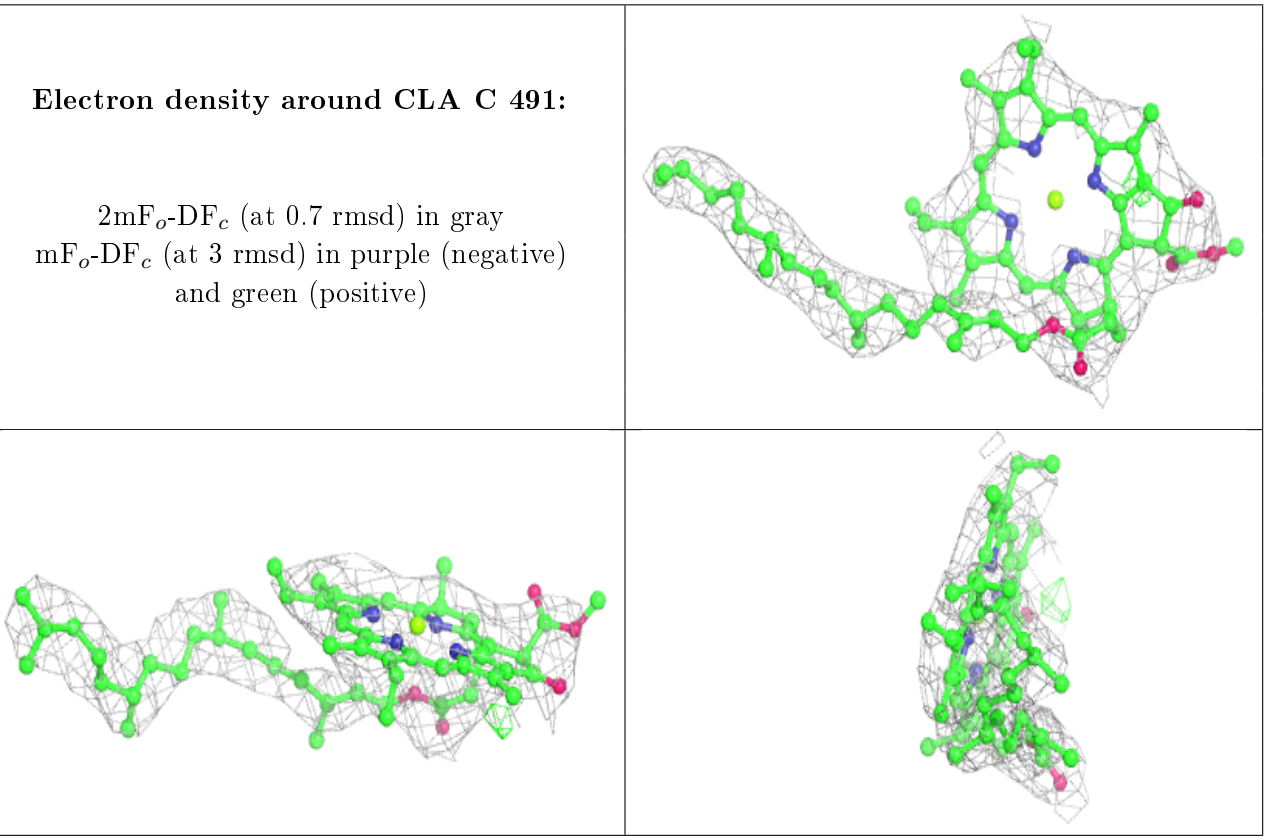
Electron density around CLA C 492:

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



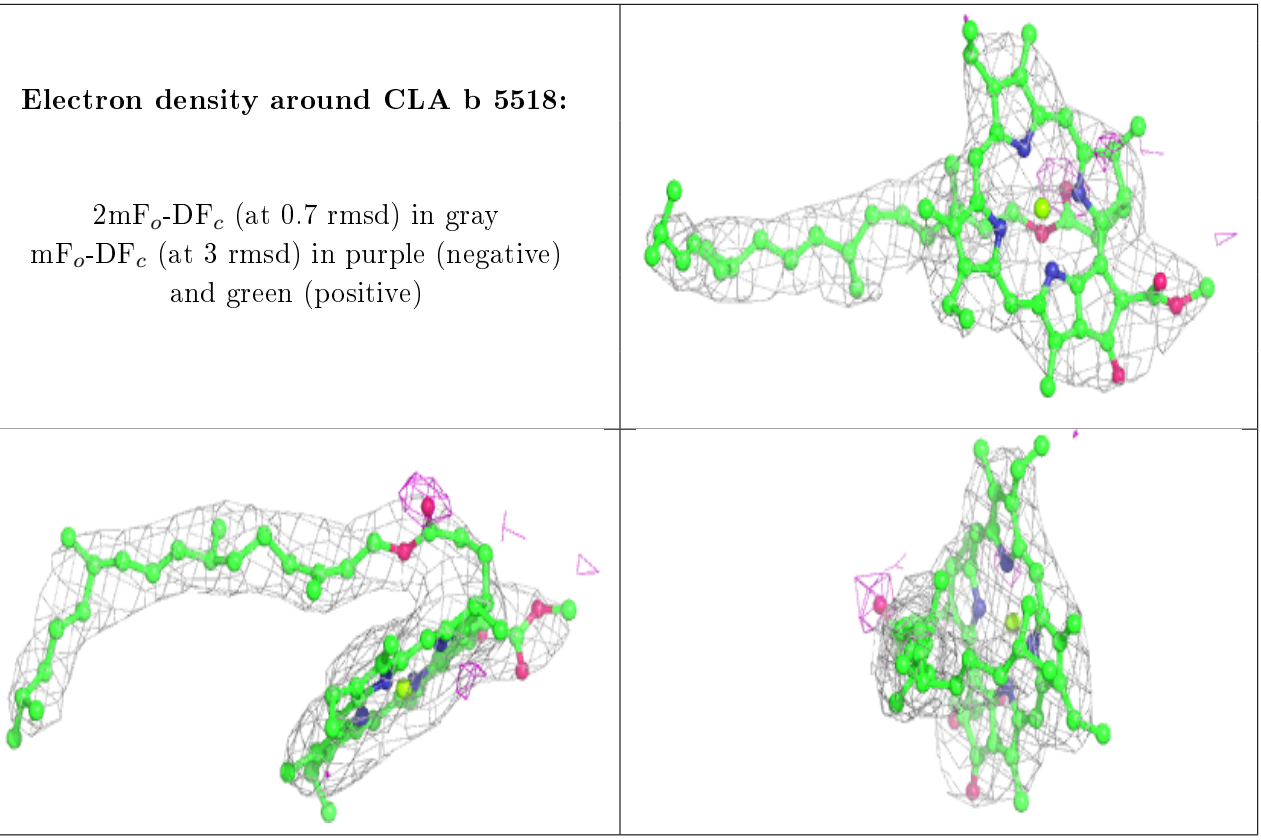
Electron density around CLA C 491:

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



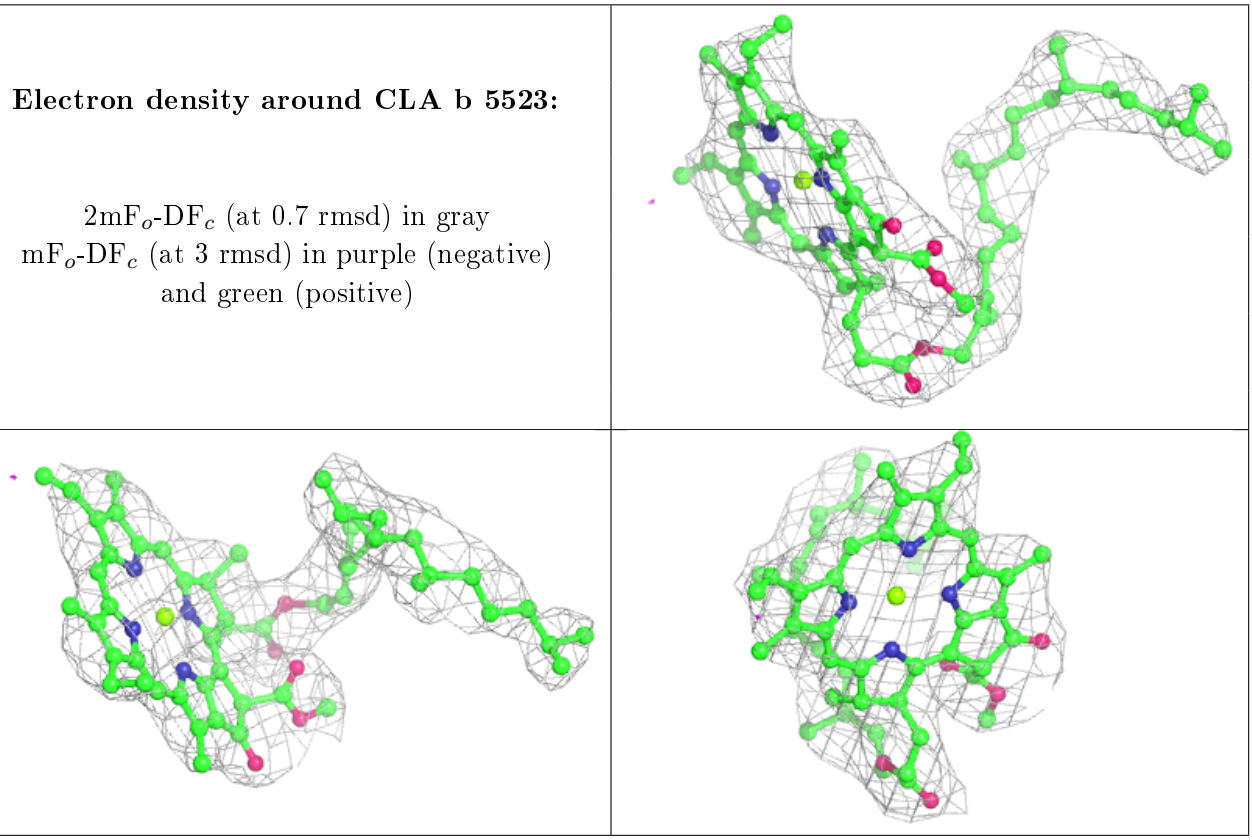
Electron density around CLA b 5518:

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



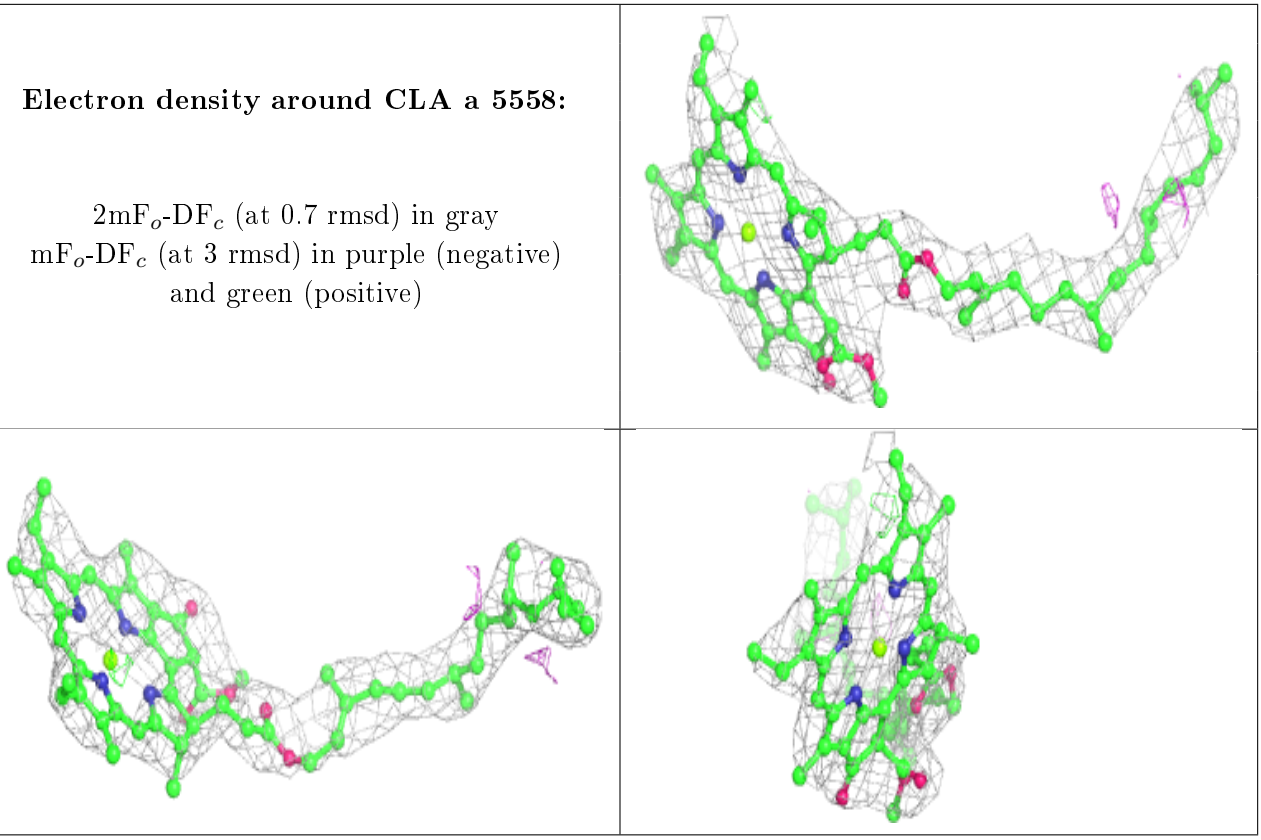
Electron density around CLA b 5523:

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



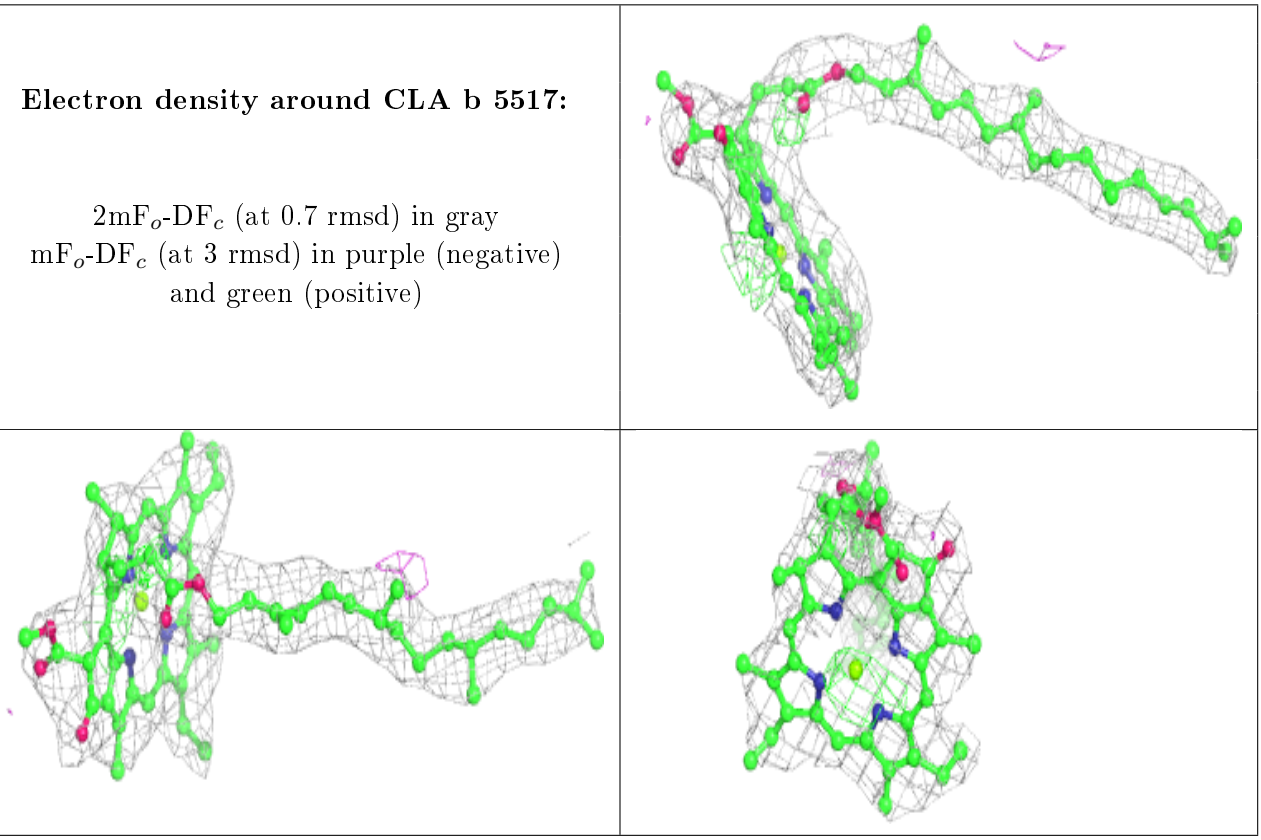
Electron density around CLA a 5558:

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



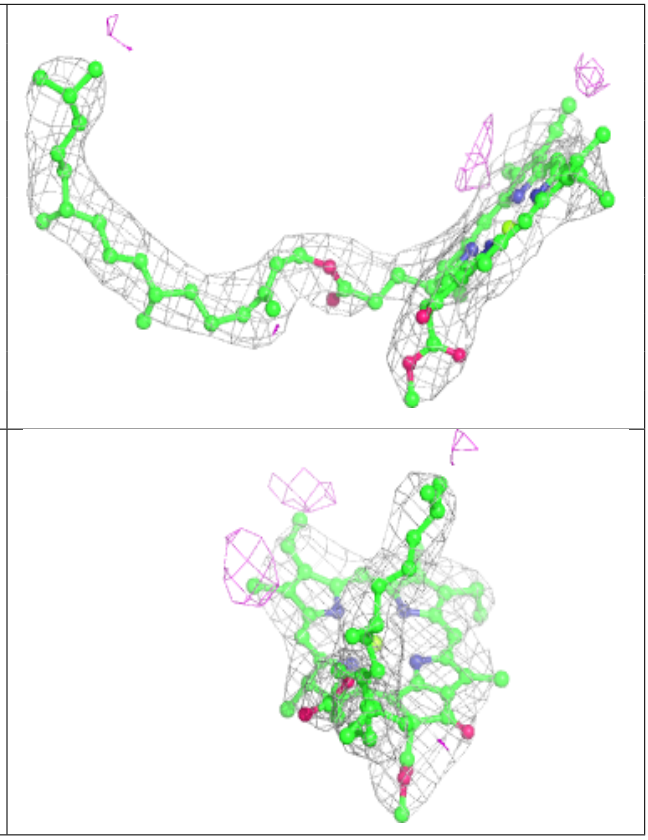
Electron density around CLA b 5517:

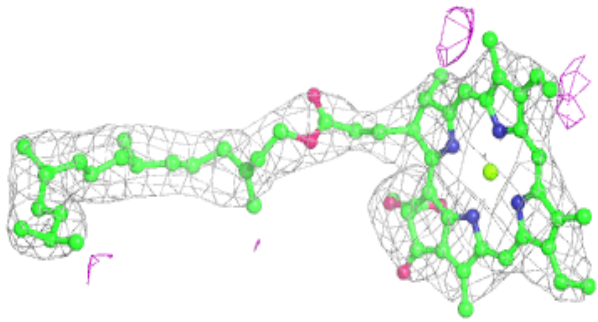
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA D 354:

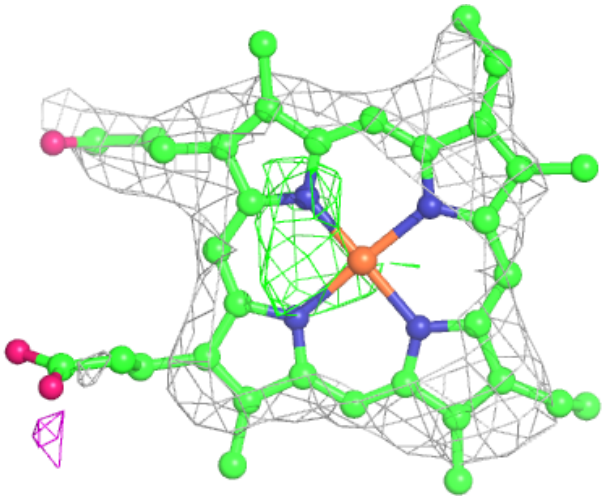
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

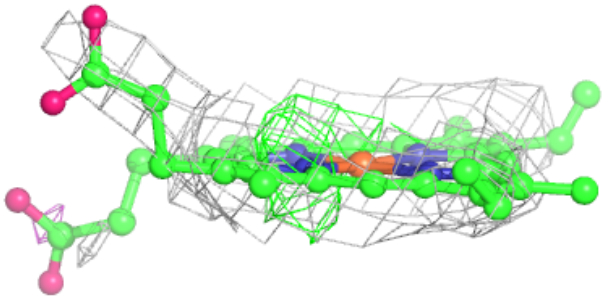


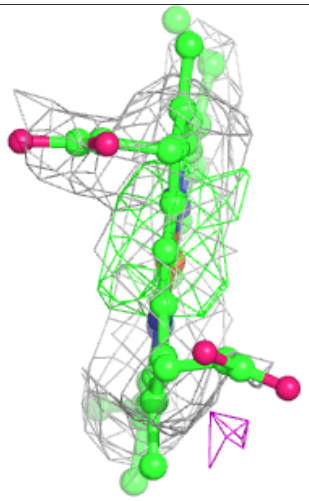


Electron density around HEM F 51:

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

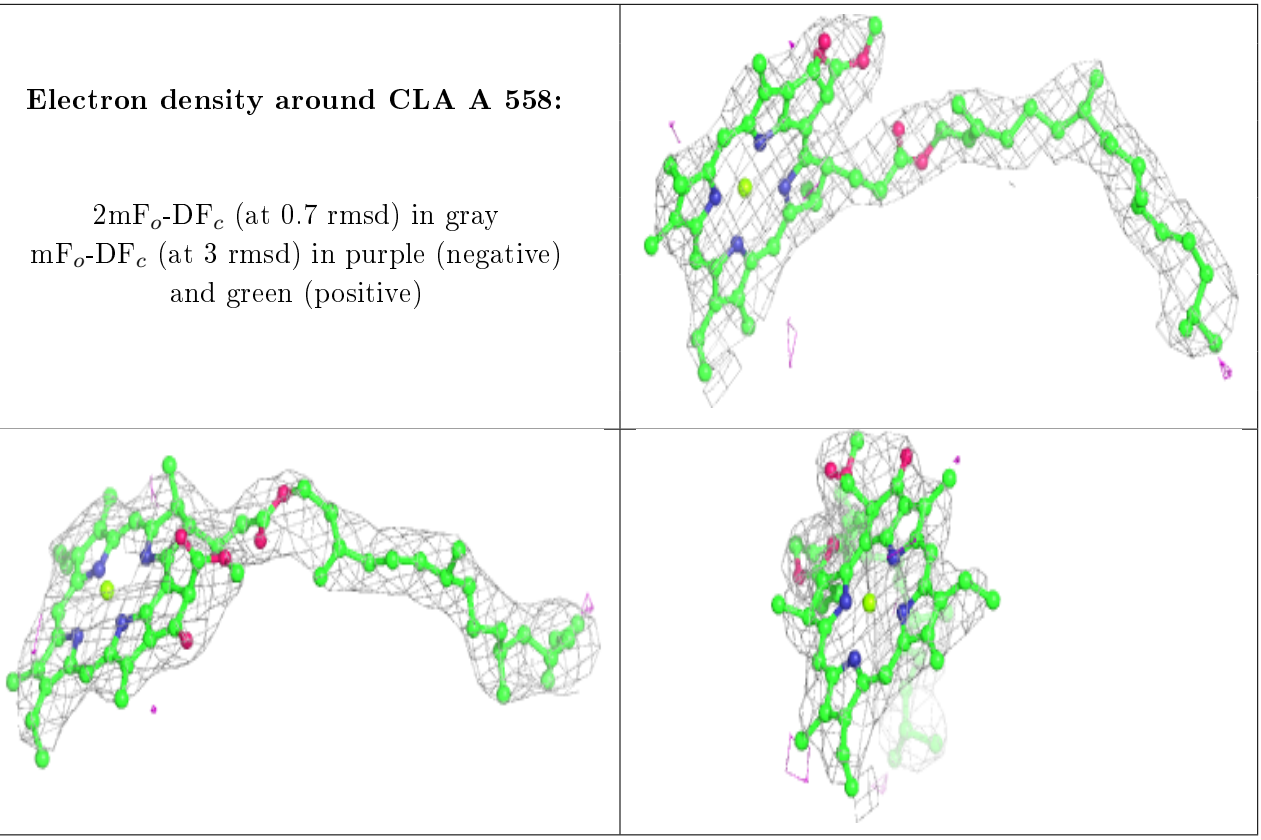






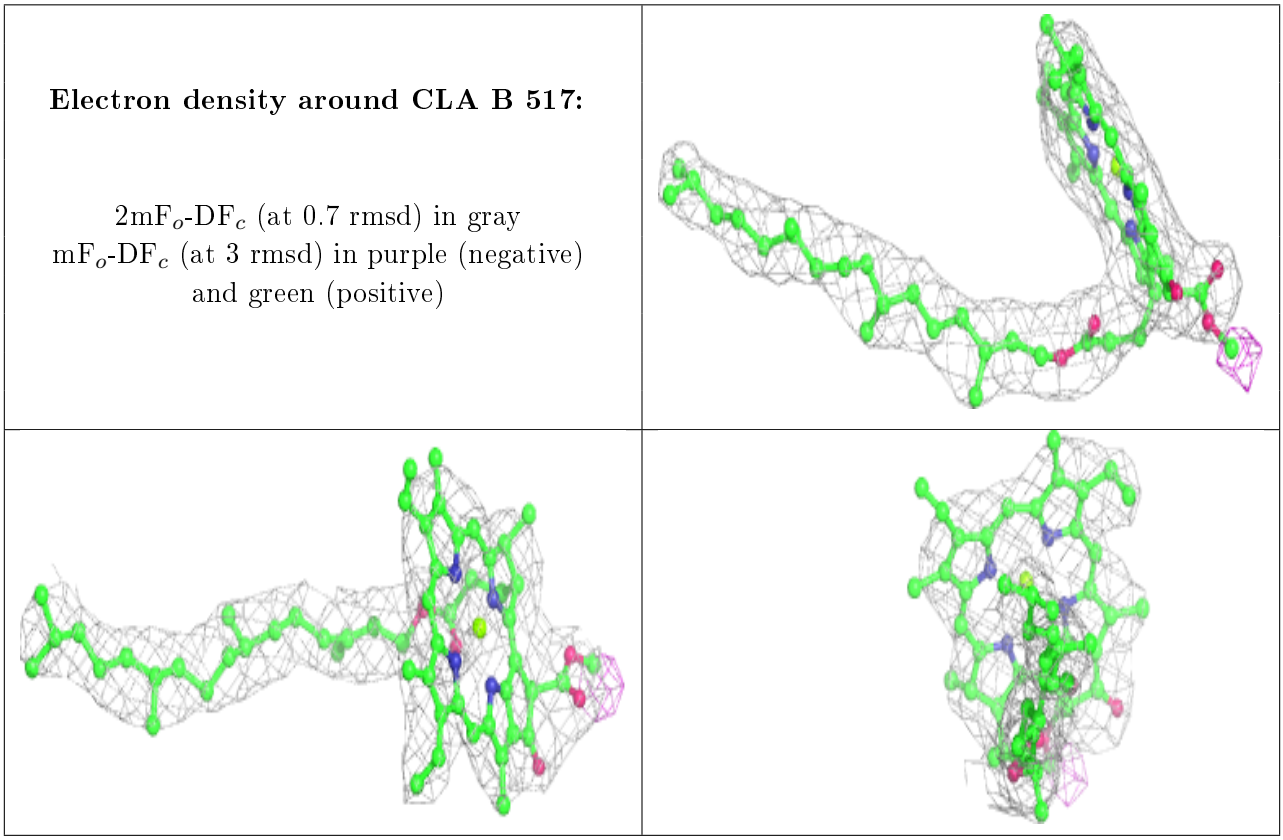
Electron density around CLA A 558:

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



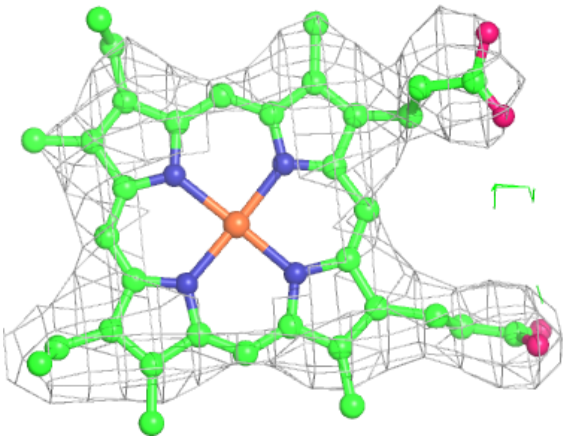
Electron density around CLA B 517:

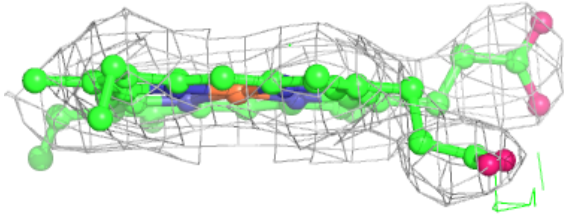
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

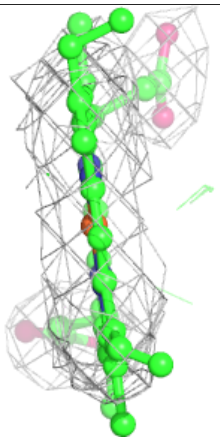


Electron density around HEM v 5552:

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

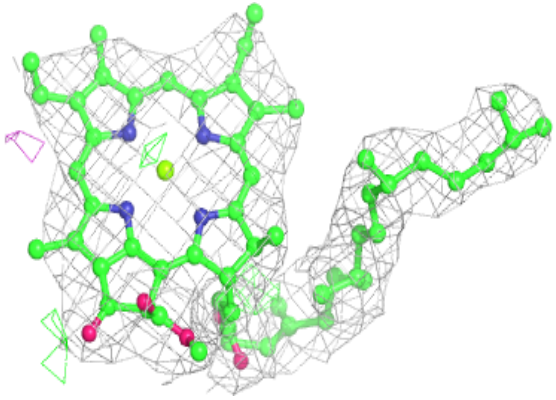


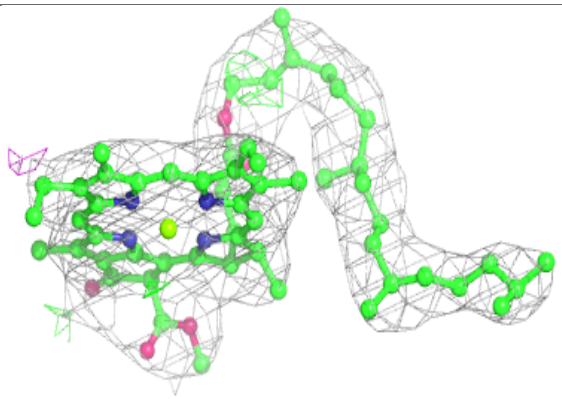




Electron density around CLA A 559:

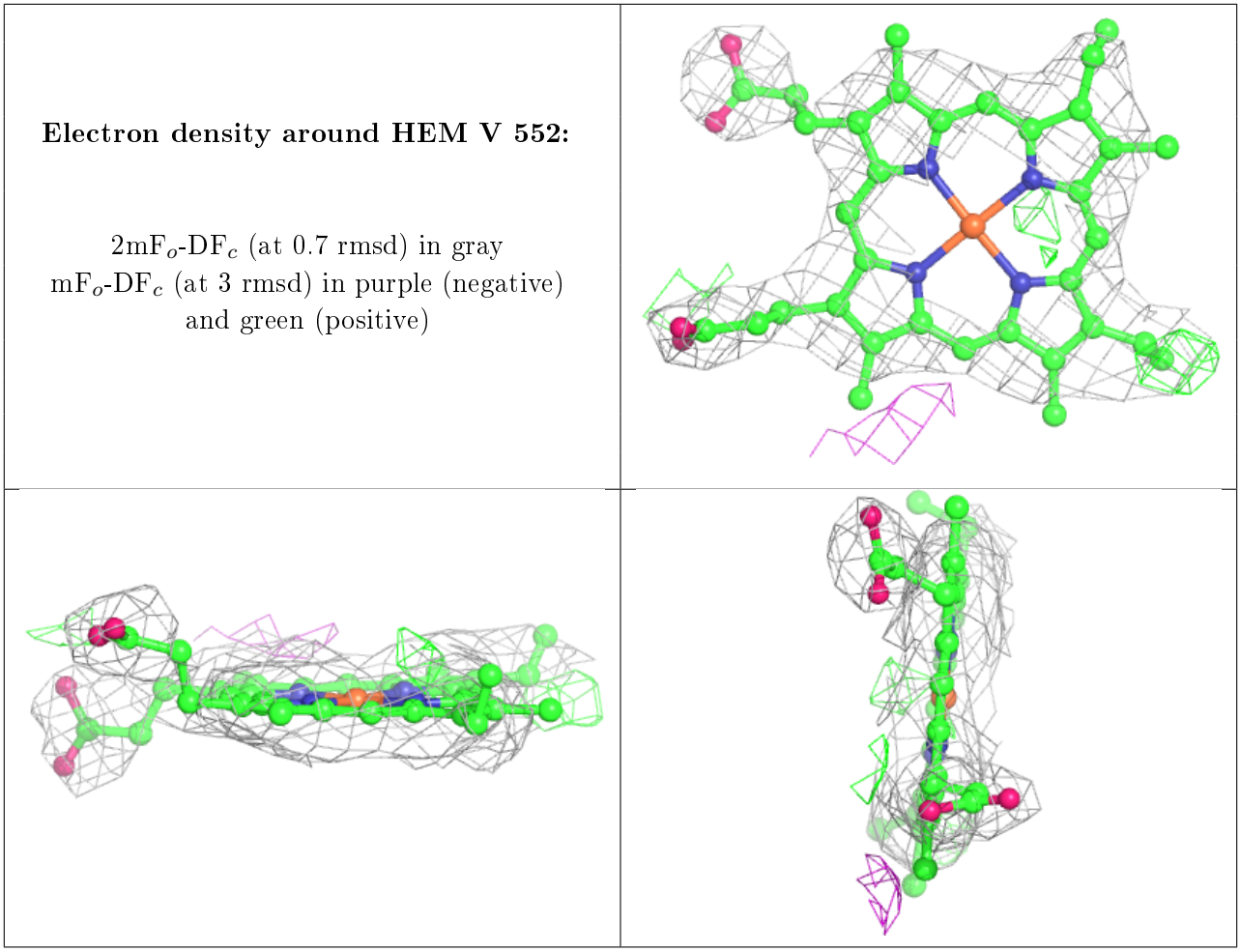
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEM V 552:

$2mF_o$-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.