wwPDB X-ray Structure Validation Summary Report (i)

Oct 8, 2023 – 07:30 PM EDT

PDB ID	:	6W1T
Title	:	RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 Angstrom resolution
Authors	:	Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovski, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on	:	2020-03-04
Resolution	:	2.01 Å(reported)

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

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

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

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

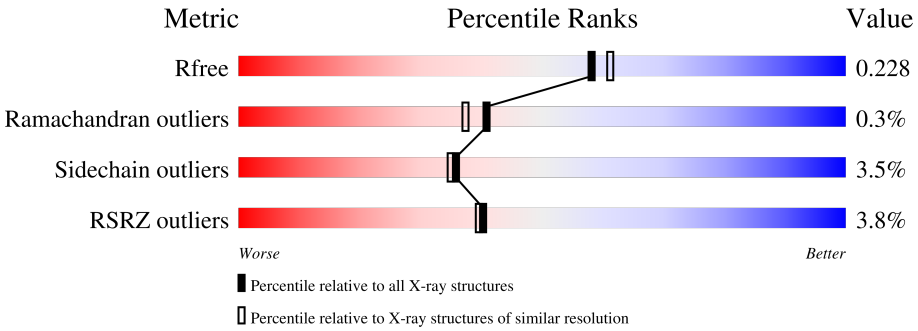
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	95%
1	a	344	93%
2	B	506	98%

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

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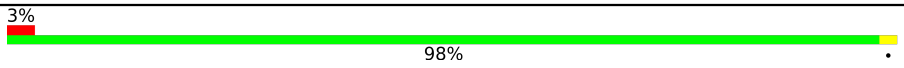
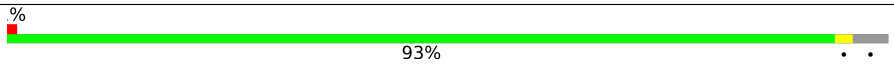
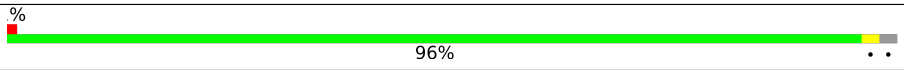
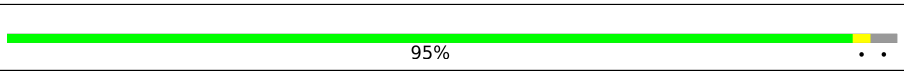
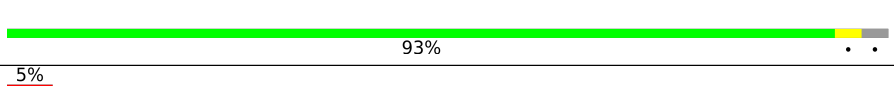
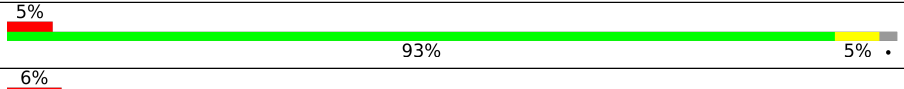
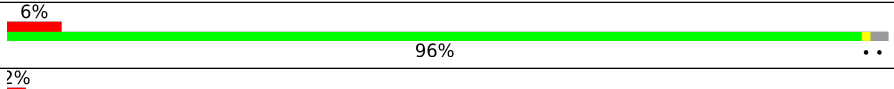
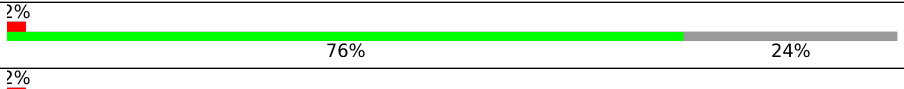
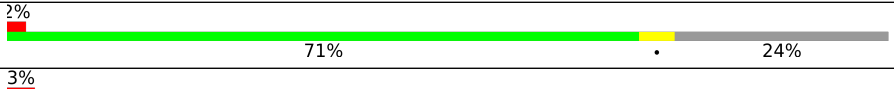
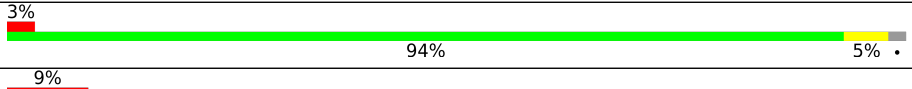
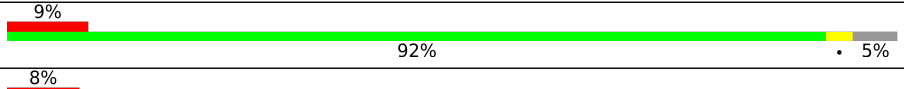
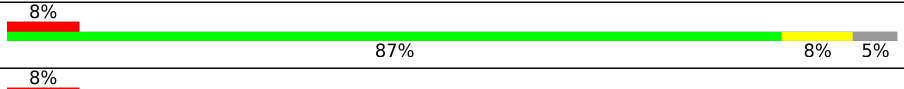
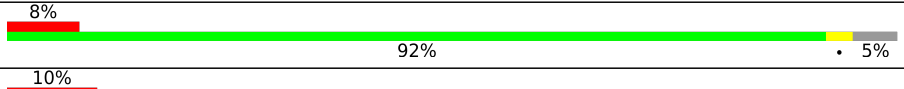
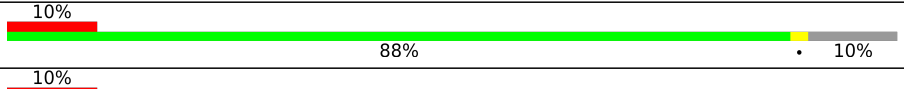
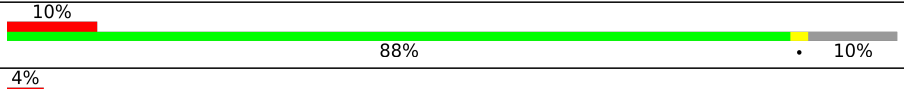
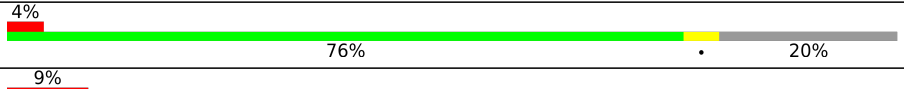
Mol	Chain	Length	Quality of chain
2	b	506	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
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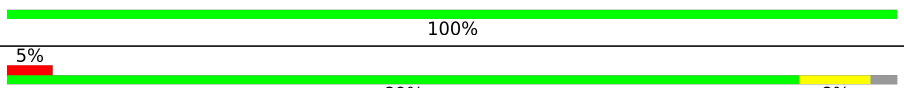
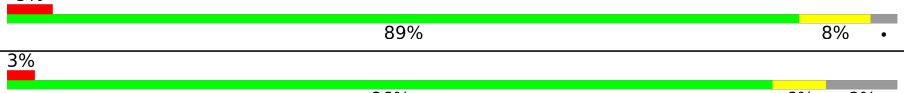
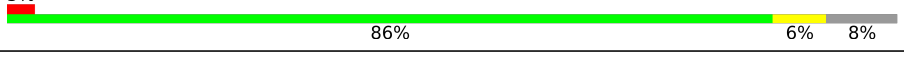
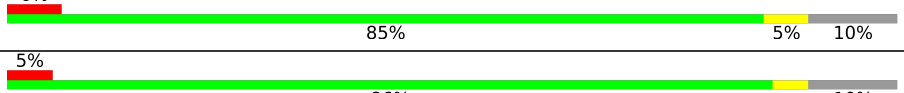
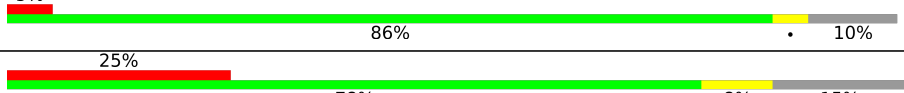
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	40	
14	r	40	

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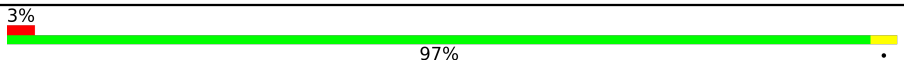
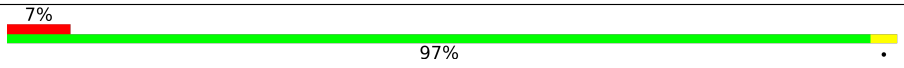
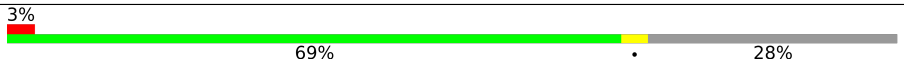
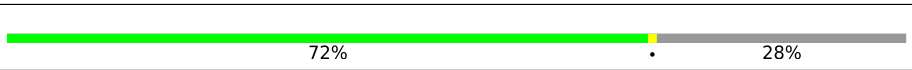
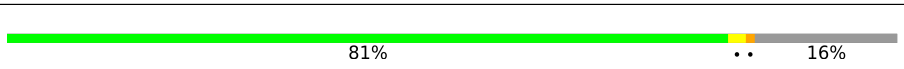
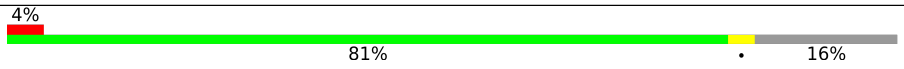
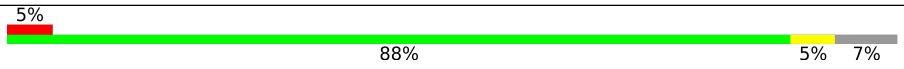
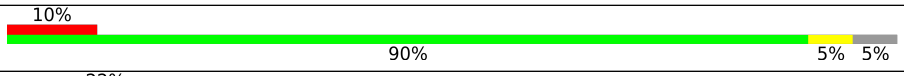
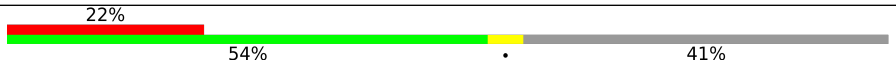
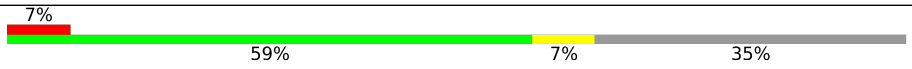
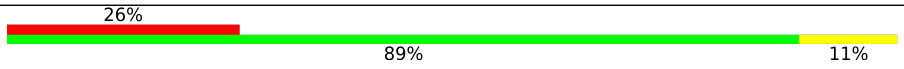
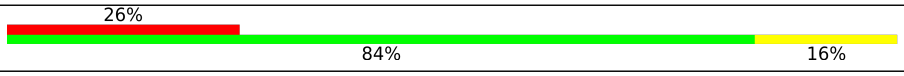
Mol	Chain	Length	Quality of chain
15	T	30	
15	t	30	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	z	62	

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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	501	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 105978 atoms, of which 52553 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			
6	f	34	Total	C	H	N	O	S	0	0	0
			556	187	281	45	42	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	S	0	0	0
			1042	341	532	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			
8	i	36	Total	C	H	N	O	S	0	0	0
			607	200	311	46	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0	0
			620	202	316	48	53	1			
11	l	36	Total	C	H	N	O		0	0	0
			600	197	304	47	52				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0	0
			525	171	269	37	47	1			
12	m	32	Total	C	H	N	O	S	0	0	0
			518	168	267	36	46	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3698	1168	1828	313	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0	0
			2132	675	1068	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2132	675	1068	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			
18	x	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

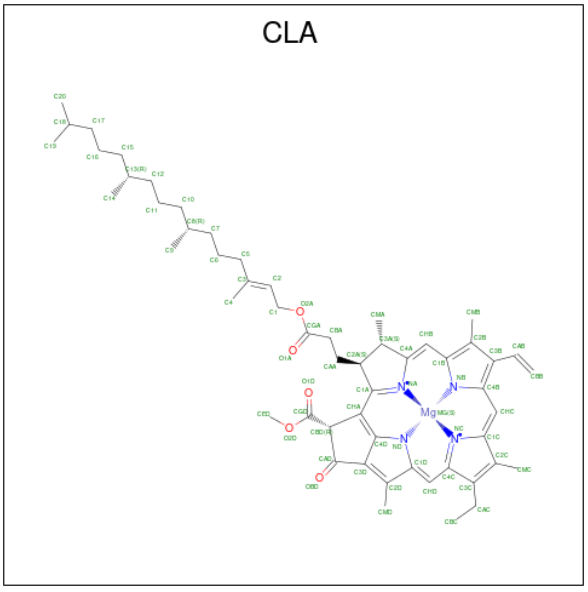
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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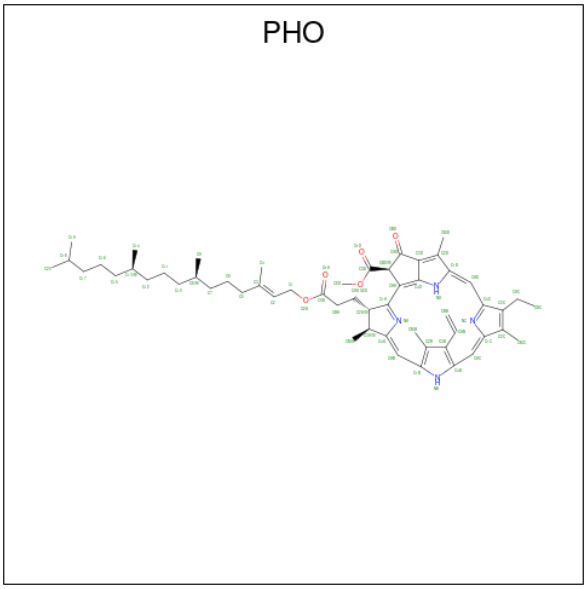
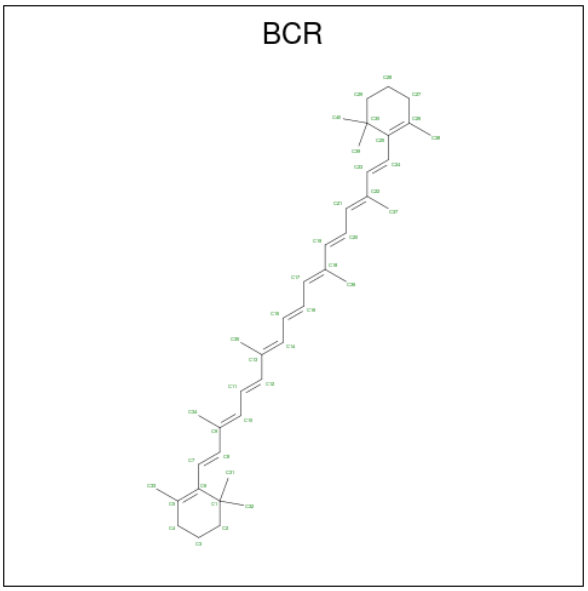
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- 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 H 96 40 56	0	0
24	B	1	Total C H 96 40 56	0	0
24	B	1	Total C H 96 40 56	0	0
24	B	1	Total C H 96 40 56	0	0
24	C	1	Total C H 96 40 56	0	0
24	C	1	Total C H 96 40 56	0	0
24	C	1	Total C H 96 40 56	0	0
24	D	1	Total C H 96 40 56	0	0
24	H	1	Total C H 96 40 56	0	0
24	T	1	Total C H 96 40 56	0	0
24	Y	1	Total C H 96 40 56	0	0
24	a	1	Total C H 96 40 56	0	0
24	b	1	Total C H 96 40 56	0	0
24	b	1	Total C H 96 40 56	0	0

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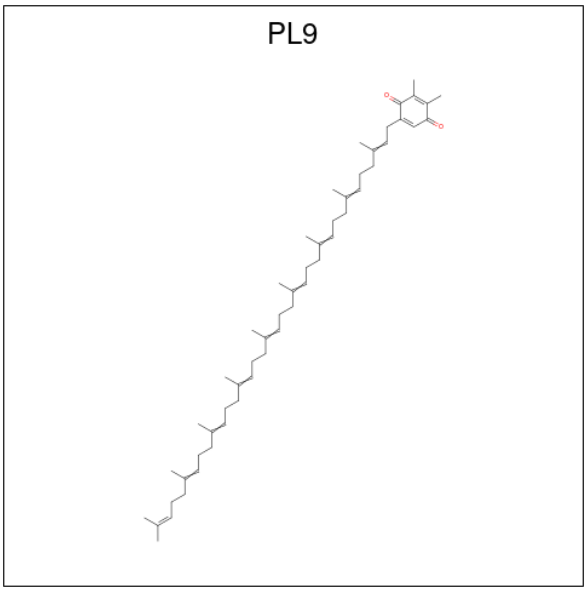
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C H 96 40 56	0	0
24	c	1	Total C H 96 40 56	0	0
24	c	1	Total C H 96 40 56	0	0
24	c	1	Total C H 96 40 56	0	0
24	d	1	Total C H 96 40 56	0	0
24	k	1	Total C H 96 40 56	0	0
24	t	1	Total C H 96 40 56	0	0
24	x	1	Total C H 96 40 56	0	0

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

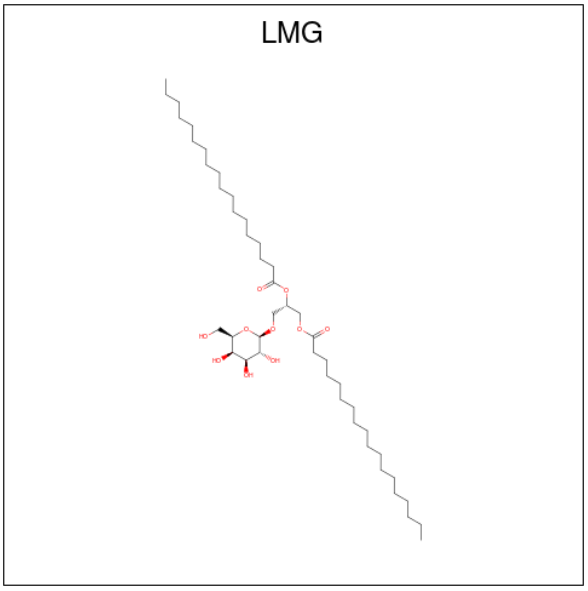
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	2	Total Cl 2 2	0	0
25	a	2	Total Cl 2 2	0	0

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



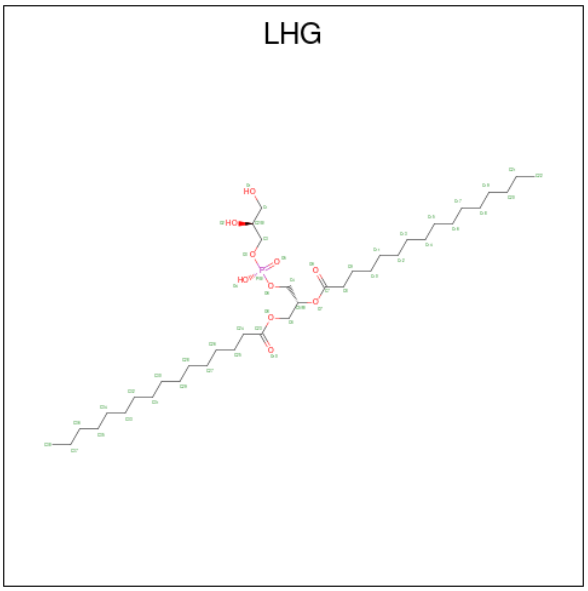
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



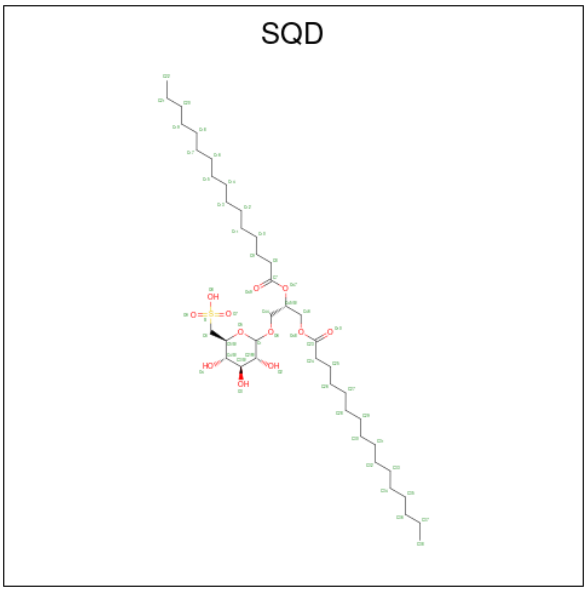
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			113	38	65	10		
27	C	1	Total	C	H	O	0	0
			113	38	65	10		
27	D	1	Total	C	H	O	0	0
			122	41	71	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			120	41	69	10		
27	a	1	Total	C	H	O	0	0
			138	45	83	10		
27	b	1	Total	C	H	O	0	0
			140	45	85	10		
27	c	1	Total	C	H	O	0	0
			78	27	41	10		
27	c	1	Total	C	H	O	0	0
			116	38	68	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			101	34	57	10		
27	m	1	Total	C	H	O	0	0
			120	41	69	10		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



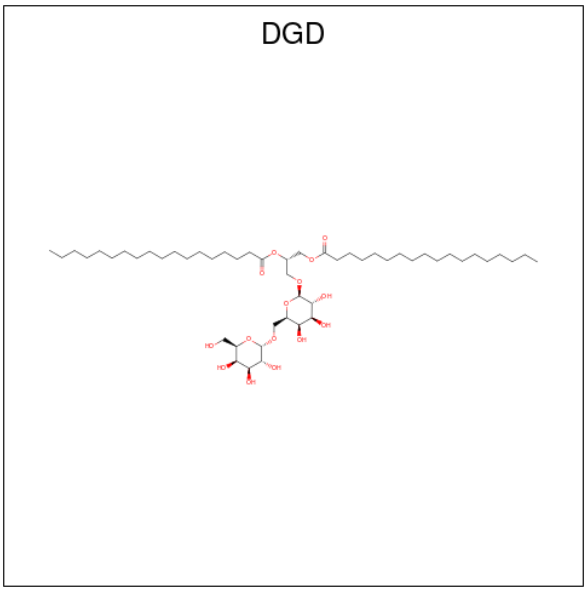
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	B	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	E	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	l	1	Total	C	H	O	P	0	0
			122	38	73	10	1		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



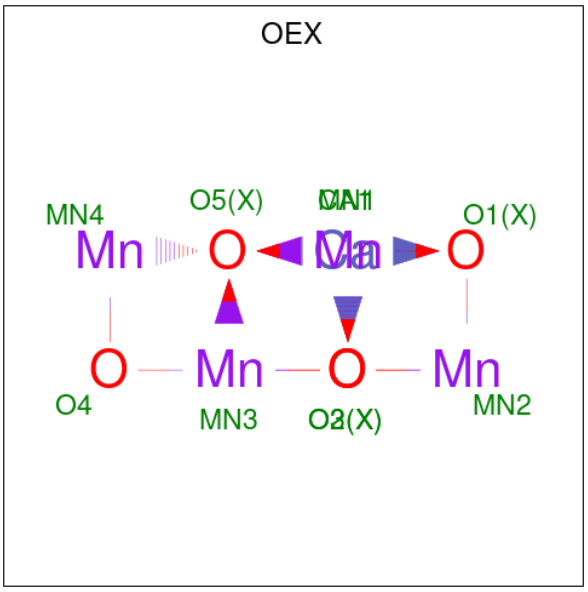
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C H O S 123 39 71 12 1	0	0
29	A	1	Total C H O 104 35 65 4	0	0
29	B	1	Total C H O S 131 41 77 12 1	0	0
29	D	1	Total C H O S 81 25 45 10 1	0	0
29	a	1	Total C H O S 131 41 77 12 1	0	0
29	a	1	Total C H O 92 31 56 5	0	0
29	b	1	Total C H O S 114 36 65 12 1	0	0
29	f	1	Total C H O S 89 28 48 12 1	0	0

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



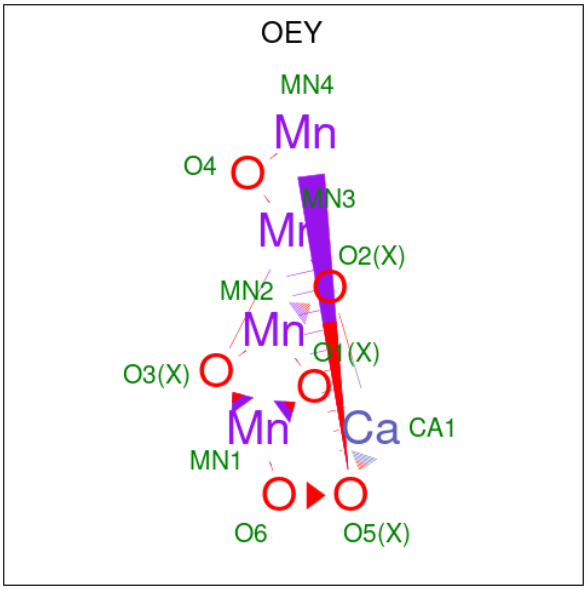
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			160	51	94	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	H	1	Total	C	H	O	0	0
			142	47	80	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	c	1	Total	C	H	O	0	0
			138	47	76	15		
30	c	1	Total	C	H	O	0	0
			142	47	80	15		
30	h	1	Total	C	H	O	0	0
			139	47	77	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



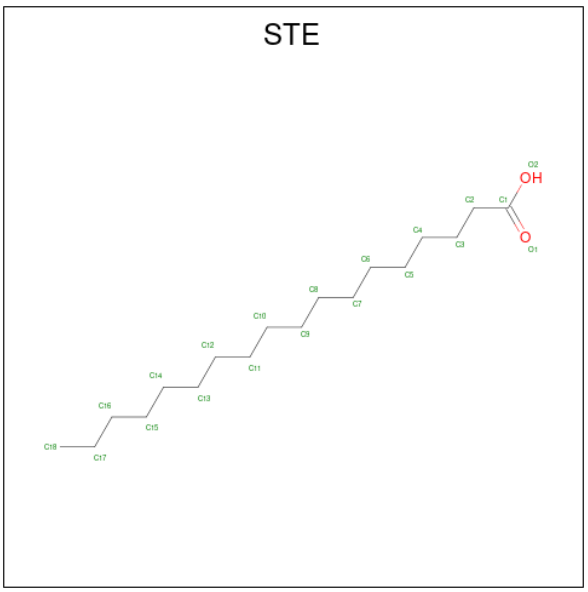
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: $CaMn_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
32	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 33 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C H O 43 15 26 2	0	0
33	B	1	Total C H O 28 10 16 2	0	0
33	B	1	Total C H 47 16 31	0	0
33	B	1	Total C H O 28 10 16 2	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	C	1	Total C H 47 16 31	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	D	1	Total C H O 55 18 35 2	0	0
33	H	1	Total C H 53 18 35	0	0
33	I	1	Total C H 41 15 26	0	0
33	J	1	Total C H O 28 10 16 2	0	0
33	M	1	Total C H O 37 13 22 2	0	0
33	M	1	Total C H 26 10 16	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	R	1	Total C H O 28 10 16 2	0	0
33	T	1	Total C H 44 15 29	0	0
33	Z	1	Total C H 20 8 12	0	0
33	a	1	Total C H 26 10 16	0	0
33	a	1	Total C H O 28 10 16 2	0	0
33	a	1	Total C H 41 15 26	0	0
33	b	1	Total C H 47 16 31	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H O 40 14 24 2	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total C H 26 10 16	0	0
33	b	1	Total C H 41 14 27	0	0
33	c	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 43 15 26 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	d	1	Total C H O 55 18 35 2	0	0
33	j	1	Total C H O 28 10 16 2	0	0
33	k	1	Total C H O 28 10 16 2	0	0
33	l	1	Total C H 53 18 35	0	0
33	m	1	Total C H O 28 10 16 2	0	0
33	t	1	Total C H O 34 12 20 2	0	0

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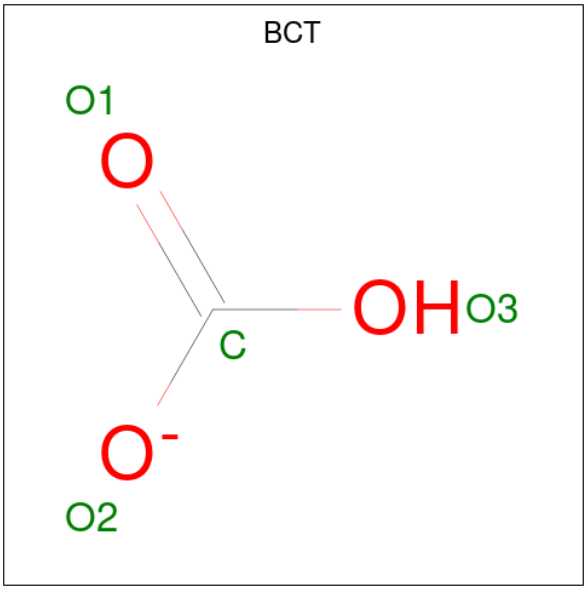
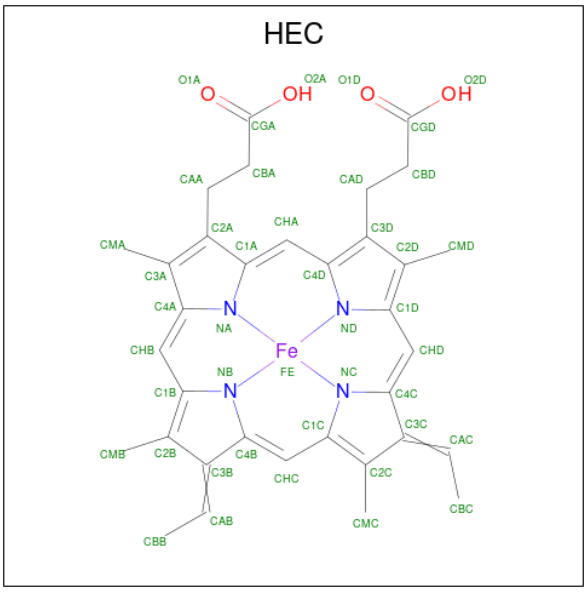
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	t	1	Total	C	H	O	0	0
			46	16	28	2		

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	f	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	146	Total	O	0	8
			146	146		
36	B	211	Total	O	0	0
			211	211		
36	C	185	Total	O	0	0
			185	185		
36	D	129	Total	O	0	0
			129	129		
36	E	34	Total	O	0	0
			34	34		
36	F	13	Total	O	0	0
			13	13		
36	H	33	Total	O	0	0
			33	33		
36	I	11	Total	O	0	0
			11	11		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	J	15	Total O 15 15	0	0
36	K	9	Total O 9 9	0	0
36	L	9	Total O 9 9	0	0
36	M	5	Total O 5 5	0	0
36	O	104	Total O 104 104	0	0
36	R	13	Total O 13 13	0	0
36	T	15	Total O 15 15	0	0
36	U	51	Total O 51 51	0	0
36	V	70	Total O 70 70	0	0
36	X	11	Total O 11 11	0	0
36	Y	2	Total O 2 2	0	0
36	Z	5	Total O 5 5	0	0
36	a	130	Total O 130 130	0	8
36	b	215	Total O 215 215	0	0
36	c	190	Total O 190 190	0	0
36	d	122	Total O 122 122	0	0
36	e	30	Total O 30 30	0	0
36	f	9	Total O 9 9	0	0
36	h	22	Total O 22 22	0	0
36	i	9	Total O 9 9	0	0
36	j	10	Total O 10 10	0	0

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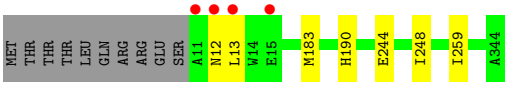
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	k	10	Total O 10 10	0	0
36	l	9	Total O 9 9	0	0
36	m	8	Total O 8 8	0	0
36	o	103	Total O 103 103	0	0
36	r	2	Total O 2 2	0	0
36	t	11	Total O 11 11	0	0
36	u	66	Total O 66 66	0	0
36	v	58	Total O 58 58	0	0
36	x	10	Total O 10 10	0	0
36	y	6	Total O 6 6	0	0
36	z	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

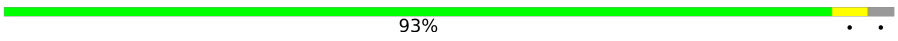
• Molecule 1: Photosystem II protein D1 1

Chain A:



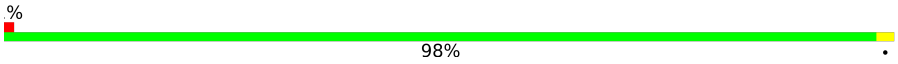
• Molecule 1: Photosystem II protein D1 1

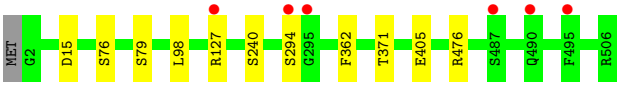
Chain a:



• Molecule 2: Photosystem II CP47 reaction center protein

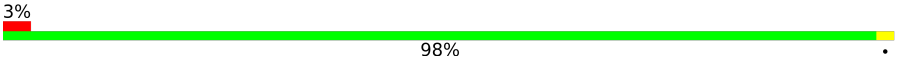
Chain B:

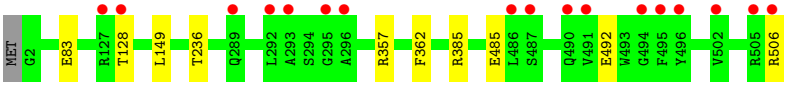




• Molecule 2: Photosystem II CP47 reaction center protein

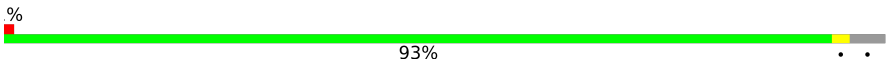
Chain b:

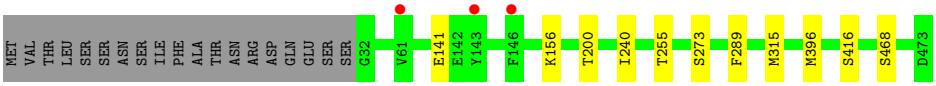




• Molecule 3: Photosystem II CP43 reaction center protein

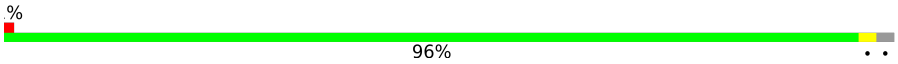
Chain C:





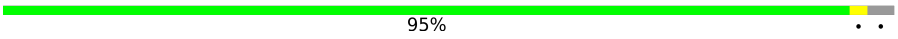
• Molecule 3: Photosystem II CP43 reaction center protein

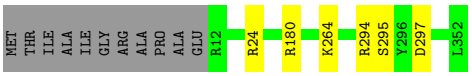
Chain c:



• Molecule 4: Photosystem II D2 protein

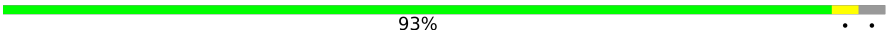
Chain D:

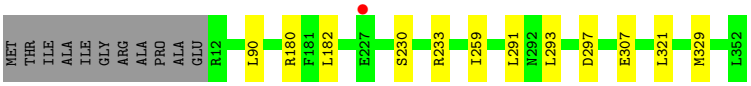




• Molecule 4: Photosystem II D2 protein

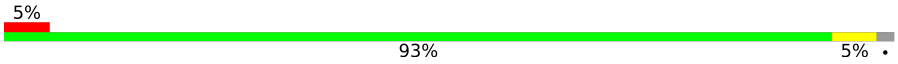
Chain d:





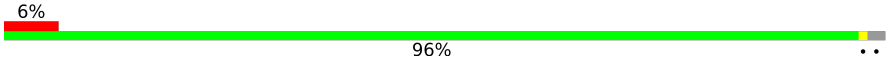
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



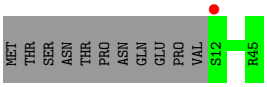
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



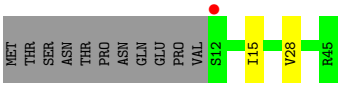
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



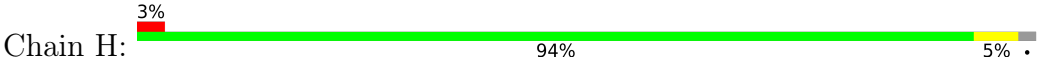
• Molecule 6: Cytochrome b559 subunit beta

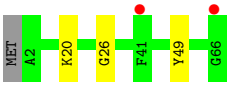
Chain f:



• Molecule 7: Photosystem II reaction center protein H

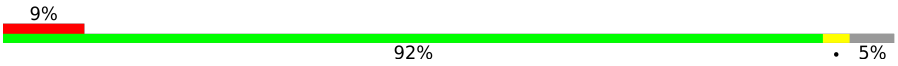
Chain H:

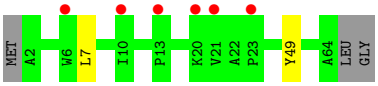




• Molecule 7: Photosystem II reaction center protein H

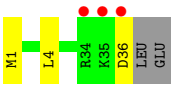
Chain h:





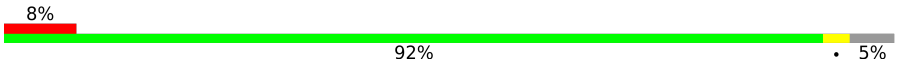
• Molecule 8: Photosystem II reaction center protein I

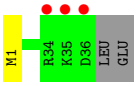
Chain I:



• Molecule 8: Photosystem II reaction center protein I

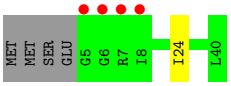
Chain i:





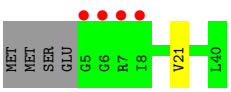
• Molecule 9: Photosystem II reaction center protein J

Chain J:



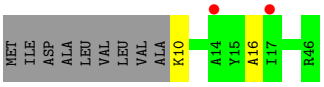
• Molecule 9: Photosystem II reaction center protein J

Chain j:



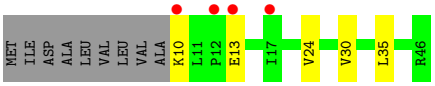
• Molecule 10: Photosystem II reaction center protein K

Chain K:



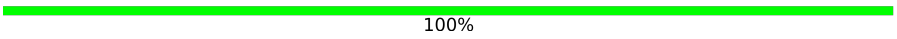
• Molecule 10: Photosystem II reaction center protein K

Chain k:



• Molecule 11: Photosystem II reaction center protein L

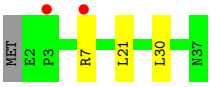
Chain L:



There are no outlier residues recorded for this chain.

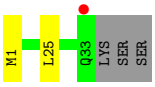
• Molecule 11: Photosystem II reaction center protein L

Chain l:



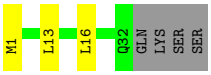
• Molecule 12: Photosystem II reaction center protein M

Chain M:



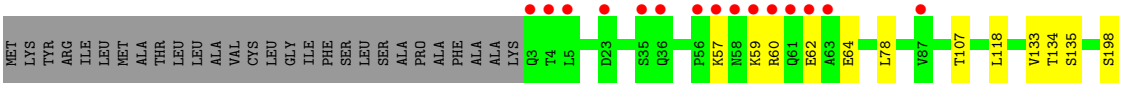
• Molecule 12: Photosystem II reaction center protein M

Chain m:



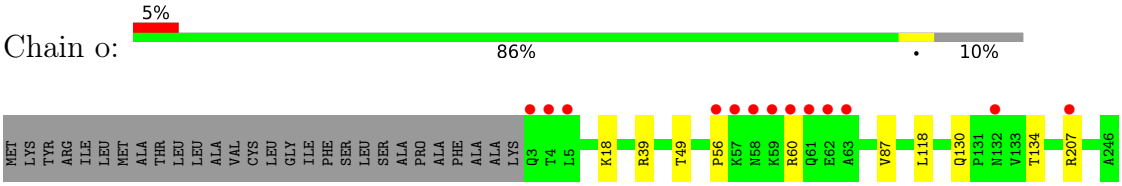
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



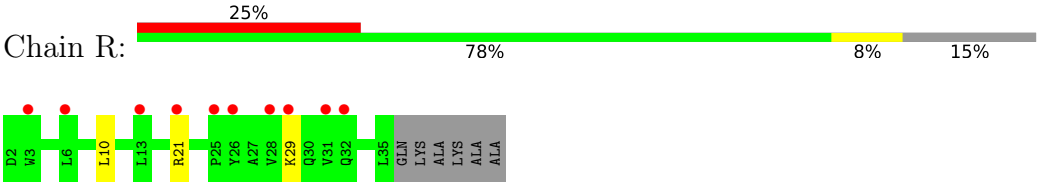
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



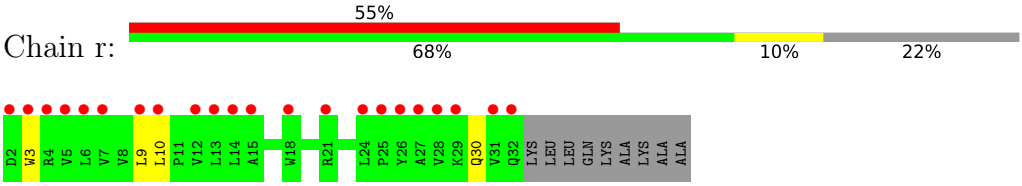
• Molecule 14: Photosystem II protein Y

Chain R:



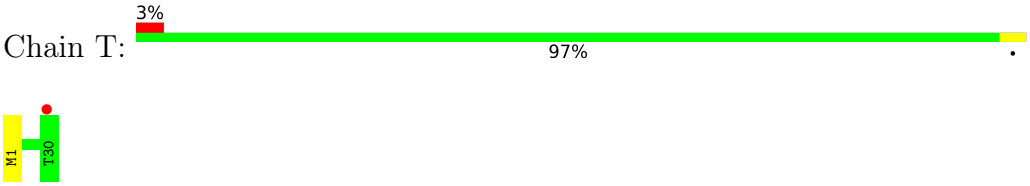
• Molecule 14: Photosystem II protein Y

Chain r:



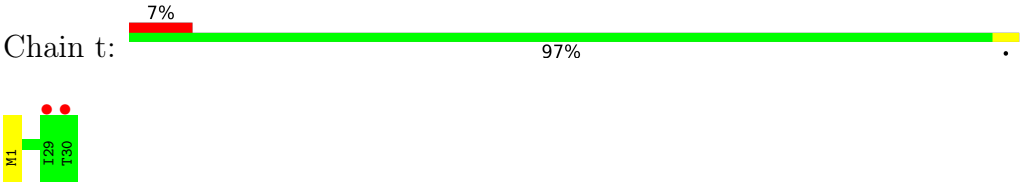
• Molecule 15: Photosystem II reaction center protein T

Chain T:



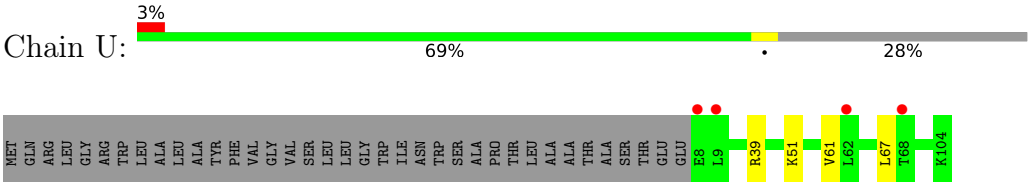
• Molecule 15: Photosystem II reaction center protein T

Chain t:



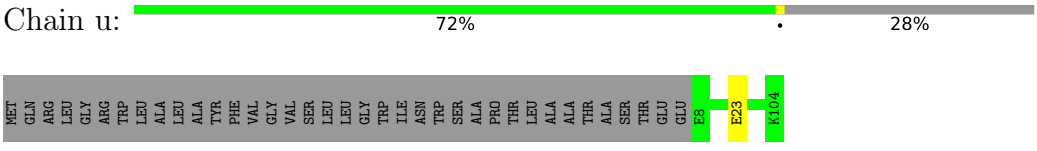
• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:



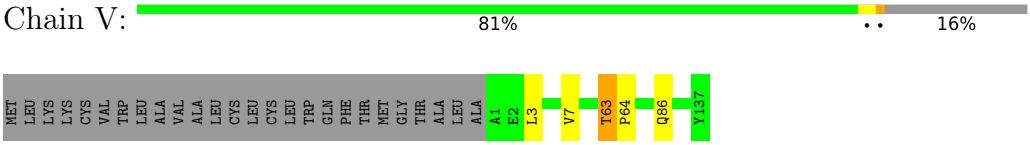
• Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:



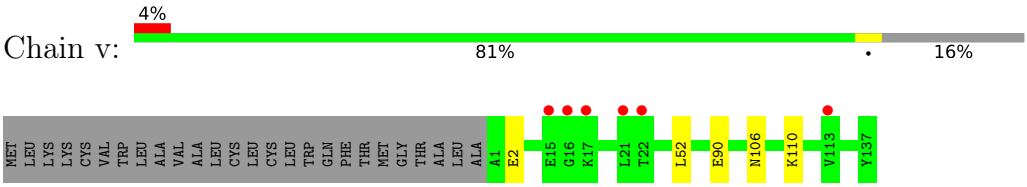
• Molecule 17: Cytochrome c-550

Chain V:



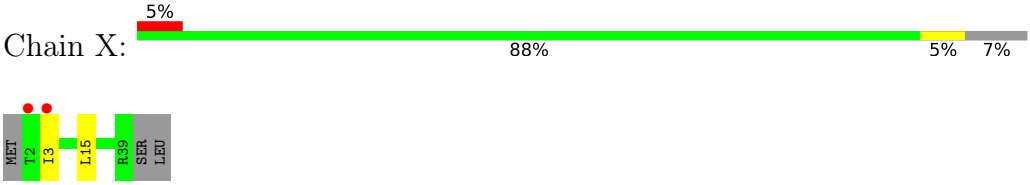
• Molecule 17: Cytochrome c-550

Chain v:



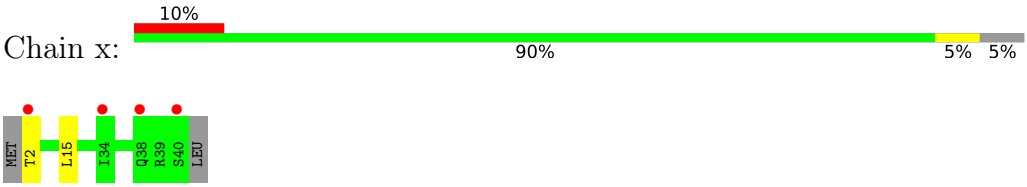
• Molecule 18: Photosystem II reaction center X protein

Chain X:



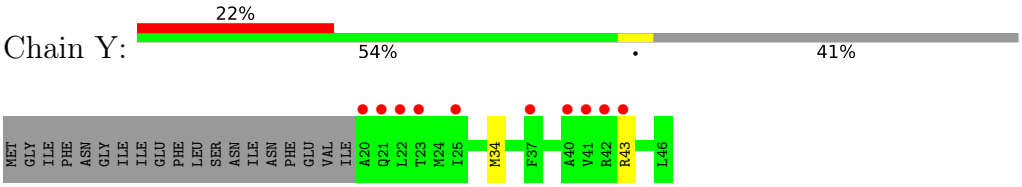
• Molecule 18: Photosystem II reaction center X protein

Chain x:



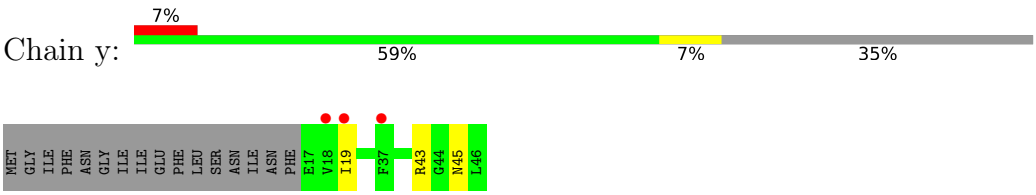
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



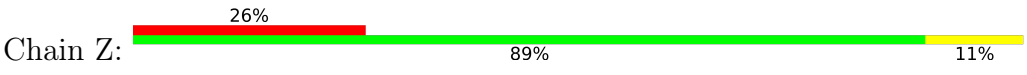
• Molecule 19: Photosystem II reaction center protein Ycf12

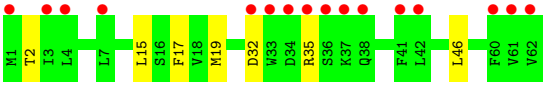
Chain y:



• Molecule 20: Photosystem II reaction center protein Z

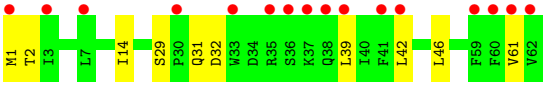
Chain Z:





• Molecule 20: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.04Å 221.92Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.59 – 2.01 33.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.59-2.01) 86.7 (33.59-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.175 , 0.228 0.175 , 0.228	Depositor DCC
R_{free} test set	4767 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	105978	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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, BCR, OEY, SQD, FME, FE2, PHO, CLA, OEX, PL9, STE, DGD, CL, HEC, BCT, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.62	0/3187	0.66	2/4342 (0.0%)
1	a	0.60	0/3184	0.82	11/4338 (0.3%)
2	B	0.64	0/4161	0.69	1/5669 (0.0%)
2	b	0.61	0/4118	0.68	1/5611 (0.0%)
3	C	0.62	1/3621 (0.0%)	0.66	1/4930 (0.0%)
3	c	0.59	0/3693	0.66	0/5026
4	D	0.67	0/2820	0.69	2/3840 (0.1%)
4	d	0.64	0/2829	0.70	1/3852 (0.0%)
5	E	0.57	0/688	0.62	0/940
5	e	0.51	0/683	0.62	0/932
6	F	0.54	0/284	0.58	0/387
6	f	0.53	0/284	0.60	0/387
7	H	0.63	0/523	0.68	0/713
7	h	0.58	0/511	0.68	0/697
8	I	0.61	0/293	0.68	0/396
8	i	0.66	0/293	0.63	0/396
9	J	0.49	0/263	0.63	0/356
9	j	0.53	0/263	0.63	0/356
10	K	0.50	0/303	0.65	0/416
10	k	0.54	0/303	0.64	0/416
11	L	0.60	0/311	0.65	0/422
11	l	0.66	0/303	0.69	0/412
12	M	0.63	0/249	0.67	0/341
12	m	0.62	0/244	0.76	0/334
13	O	0.61	0/1904	0.70	0/2585
13	o	0.61	0/1905	0.72	0/2583
14	R	0.47	0/277	0.56	0/380
14	r	0.36	0/246	0.51	0/339
15	T	0.71	0/257	0.63	0/349
15	t	0.75	0/255	0.63	0/346
16	U	0.55	0/785	0.67	0/1064
16	u	0.60	0/785	0.68	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	V	0.58	0/1085	0.70	1/1473 (0.1%)
17	v	0.55	0/1085	0.63	0/1473
18	X	0.51	0/284	0.60	0/384
18	x	0.44	0/289	0.55	0/391
19	Y	0.48	0/197	0.59	0/264
19	y	0.45	0/219	0.61	0/294
20	Z	0.45	0/490	0.58	0/669
20	z	0.41	0/488	0.52	0/666
All	All	0.60	1/43962 (0.0%)	0.68	20/59833 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
17	V	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	468	SER	C-N	-5.64	1.21	1.34

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	190[A]	HIS	O-C-N	-14.28	99.85	122.70
1	a	190[B]	HIS	O-C-N	-14.28	99.85	122.70
1	a	190[A]	HIS	CA-C-N	11.07	141.56	117.20
1	a	190[B]	HIS	CA-C-N	11.07	141.56	117.20
1	a	190[A]	HIS	C-N-CA	9.85	146.32	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
17	V	63	THR	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	41	37
1	a	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	41	37
2	B	508/506 (100%)	497 (98%)	10 (2%)	1 (0%)	47	44
2	b	503/506 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	47	44
3	c	459/461 (100%)	443 (96%)	15 (3%)	1 (0%)	47	44
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
7	H	63/66 (96%)	58 (92%)	4 (6%)	1 (2%)	9	4
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	0	1 (3%)	4	1
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	227 (93%)	12 (5%)	4 (2%)	9	4
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	34	30
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	27 (93%)	2 (7%)	0	100	100
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	16
17	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	3	1
20	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	1
All	All	5374/5686 (94%)	5216 (97%)	141 (3%)	17 (0%)	41	37

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	60	ARG
17	V	64	PRO
3	c	416	SER

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	320/280 (114%)	316 (99%)	4 (1%)	69 74
1	a	319/280 (114%)	310 (97%)	9 (3%)	43 44
2	B	408/404 (101%)	399 (98%)	9 (2%)	52 55
2	b	402/404 (100%)	393 (98%)	9 (2%)	52 55
3	C	353/362 (98%)	345 (98%)	8 (2%)	50 53
3	c	361/362 (100%)	353 (98%)	8 (2%)	52 55
4	D	277/283 (98%)	273 (99%)	4 (1%)	67 72
4	d	278/283 (98%)	267 (96%)	11 (4%)	31 29
5	E	72/73 (99%)	67 (93%)	5 (7%)	15 11
5	e	71/73 (97%)	70 (99%)	1 (1%)	67 72
6	F	28/39 (72%)	28 (100%)	0	100 100
6	f	28/39 (72%)	26 (93%)	2 (7%)	14 10
7	H	54/55 (98%)	52 (96%)	2 (4%)	34 32
7	h	53/55 (96%)	51 (96%)	2 (4%)	33 31
8	I	32/34 (94%)	30 (94%)	2 (6%)	18 13
8	i	32/34 (94%)	32 (100%)	0	100 100
9	J	24/28 (86%)	23 (96%)	1 (4%)	30 27
9	j	24/28 (86%)	23 (96%)	1 (4%)	30 27
10	K	30/37 (81%)	29 (97%)	1 (3%)	38 37
10	k	30/37 (81%)	25 (83%)	5 (17%)	2 1
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10 6
12	M	28/32 (88%)	27 (96%)	1 (4%)	35 34
12	m	28/32 (88%)	26 (93%)	2 (7%)	14 10
13	O	206/228 (90%)	197 (96%)	9 (4%)	28 25
13	o	207/228 (91%)	198 (96%)	9 (4%)	29 26
14	R	28/32 (88%)	25 (89%)	3 (11%)	6 3
14	r	23/32 (72%)	19 (83%)	4 (17%)	2 1
15	T	26/26 (100%)	26 (100%)	0	100 100
15	t	25/26 (96%)	25 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	U	84/112 (75%)	80 (95%)	4 (5%)	25 22
16	u	84/112 (75%)	83 (99%)	1 (1%)	71 76
17	V	117/138 (85%)	114 (97%)	3 (3%)	46 48
17	v	117/138 (85%)	112 (96%)	5 (4%)	29 26
18	X	31/34 (91%)	29 (94%)	2 (6%)	17 12
18	x	31/34 (91%)	29 (94%)	2 (6%)	17 12
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22 18
19	y	22/37 (60%)	20 (91%)	2 (9%)	9 5
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4 2
20	z	51/52 (98%)	43 (84%)	8 (16%)	2 1
All	All	4444/4642 (96%)	4294 (97%)	150 (3%)	36 36

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	l	21	LEU
20	z	14	ILE
13	o	18	LYS
14	r	10	LEU
14	R	29	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	179	GLN
20	z	31	GLN
3	c	378	ASN
20	z	58	ASN
14	r	30	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	0.98	1 (12%)	7,9,11	0.82	0
15	FME	T	1	15	8,9,10	1.02	1 (12%)	7,9,11	1.53	2 (28%)
8	FME	I	1	8	8,9,10	0.92	0	7,9,11	1.05	1 (14%)
12	FME	M	1	12	8,9,10	1.08	1 (12%)	7,9,11	0.82	0
15	FME	t	1	15	8,9,10	1.53	1 (12%)	7,9,11	0.45	0
8	FME	i	1	8	8,9,10	1.13	1 (12%)	7,9,11	1.14	1 (14%)

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
12	FME	m	1	12	-	1/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.60	1.41	1.46
8	i	1	FME	CA-N	-2.48	1.42	1.46
15	T	1	FME	CA-N	-2.27	1.43	1.46
12	M	1	FME	CA-N	-2.11	1.43	1.46
12	m	1	FME	CA-N	-2.08	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	1	FME	O1-CN-N	-2.57	118.51	125.27
8	i	1	FME	CA-N-CN	-2.13	119.54	122.82
8	I	1	FME	C-CA-N	2.02	113.37	109.73
15	T	1	FME	C-CA-N	2.01	113.35	109.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	b	607	36	65,73,73	1.40	10 (15%)	76,113,113	1.29	6 (7%)
22	CLA	b	613	-	65,73,73	1.43	8 (12%)	76,113,113	1.37	9 (11%)
24	BCR	t	101	-	41,41,41	1.07	4 (9%)	56,56,56	1.42	11 (19%)
27	LMG	c	522	-	48,48,55	1.05	5 (10%)	56,56,63	1.28	4 (7%)
22	CLA	D	404	-	65,73,73	1.51	9 (13%)	76,113,113	1.25	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	608	-	65,73,73	1.42	7 (10%)	76,113,113	1.37	10 (13%)
22	CLA	d	403	-	65,73,73	1.69	9 (13%)	76,113,113	1.48	12 (15%)
22	CLA	D	403	36	65,73,73	1.52	9 (13%)	76,113,113	1.37	8 (10%)
22	CLA	c	504	36	60,68,73	1.61	8 (13%)	70,107,113	1.50	11 (15%)
27	LMG	a	416	-	55,55,55	1.05	2 (3%)	63,63,63	1.37	7 (11%)
22	CLA	b	601	36	65,73,73	1.55	9 (13%)	76,113,113	1.40	7 (9%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
24	BCR	d	406	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	6 (10%)
29	SQD	A	414	-	38,38,54	1.02	4 (10%)	40,40,65	1.60	4 (10%)
22	CLA	B	612	-	65,73,73	1.65	6 (9%)	76,113,113	1.70	11 (14%)
33	STE	D	412	-	19,19,19	0.53	0	19,19,19	1.35	2 (10%)
29	SQD	b	620	-	48,49,54	0.98	2 (4%)	57,60,65	1.97	14 (24%)
22	CLA	B	604	-	65,73,73	1.47	9 (13%)	76,113,113	1.65	8 (10%)
24	BCR	B	617	-	41,41,41	1.10	4 (9%)	56,56,56	1.30	12 (21%)
22	CLA	C	503	-	65,73,73	1.63	7 (10%)	76,113,113	1.87	13 (17%)
24	BCR	b	617	-	41,41,41	1.08	3 (7%)	56,56,56	1.48	9 (16%)
27	LMG	A	411	-	48,48,55	1.09	4 (8%)	56,56,63	1.33	7 (12%)
33	STE	m	102	-	11,11,19	0.76	0	11,11,19	1.24	1 (9%)
23	PHO	a	403	-	51,69,69	1.05	5 (9%)	47,99,99	1.29	5 (10%)
33	STE	b	627	-	13,13,19	0.51	0	12,12,19	0.46	0
31	OEX	A	416[A]	1,3,36	0,15,15	-	-	-		
22	CLA	c	502	-	65,73,73	1.43	6 (9%)	76,113,113	1.42	9 (11%)
24	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.36	9 (16%)
27	LMG	c	520	-	37,37,55	1.23	5 (13%)	45,45,63	1.34	8 (17%)
24	BCR	C	516	-	41,41,41	1.15	3 (7%)	56,56,56	1.20	4 (7%)
24	BCR	a	405	-	41,41,41	0.97	3 (7%)	56,56,56	1.27	8 (14%)
27	LMG	D	410	-	31,31,55	1.11	3 (9%)	33,33,63	1.10	2 (6%)
33	STE	b	621	-	15,15,19	0.40	0	14,14,19	0.80	0
22	CLA	A	406	-	54,62,73	1.68	8 (14%)	62,99,113	1.51	10 (16%)
22	CLA	b	611	-	65,73,73	1.22	7 (10%)	76,113,113	1.48	12 (15%)
22	CLA	c	507	36	65,73,73	1.38	8 (12%)	76,113,113	1.60	12 (15%)
22	CLA	B	606	-	65,73,73	1.72	12 (18%)	76,113,113	1.43	10 (13%)
23	PHO	A	404	-	51,69,69	1.10	5 (9%)	47,99,99	1.34	7 (14%)
33	STE	d	412	-	19,19,19	0.79	0	19,19,19	1.17	2 (10%)
28	LHG	e	101	-	41,41,48	0.94	3 (7%)	44,47,54	1.30	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	512	-	65,73,73	1.43	11 (16%)	76,113,113	1.48	11 (14%)
22	CLA	b	605	-	65,73,73	1.47	6 (9%)	76,113,113	1.59	12 (15%)
32	OEY	A	417[B]	1,3,36	0,16,16	-	-	-		
24	BCR	c	516	-	41,41,41	1.08	3 (7%)	56,56,56	1.15	3 (5%)
22	CLA	B	602	-	65,73,73	1.70	7 (10%)	76,113,113	1.29	10 (13%)
22	CLA	C	505	-	65,73,73	1.57	8 (12%)	76,113,113	1.40	5 (6%)
22	CLA	B	610	36	65,73,73	1.77	10 (15%)	76,113,113	1.54	12 (15%)
22	CLA	C	511	3	65,73,73	1.65	9 (13%)	76,113,113	1.44	7 (9%)
22	CLA	d	405	-	65,73,73	1.60	11 (16%)	76,113,113	1.31	10 (13%)
24	BCR	C	515	-	41,41,41	1.16	4 (9%)	56,56,56	1.33	9 (16%)
22	CLA	B	609	-	65,73,73	1.71	9 (13%)	76,113,113	1.51	13 (17%)
30	DGD	A	415	-	67,67,67	1.39	11 (16%)	81,81,81	1.34	11 (13%)
33	STE	C	522	-	15,15,19	0.46	0	14,14,19	0.65	0
33	STE	C	523	-	11,11,19	0.61	0	11,11,19	1.44	2 (18%)
30	DGD	h	101	-	63,63,67	1.18	7 (11%)	77,77,81	1.36	8 (10%)
30	DGD	c	518	-	63,63,67	1.25	10 (15%)	77,77,81	1.38	10 (12%)
28	LHG	l	101	-	48,48,48	0.84	1 (2%)	51,54,54	1.29	7 (13%)
33	STE	j	101	-	11,11,19	0.95	1 (9%)	11,11,19	1.12	2 (18%)
22	CLA	d	401	36	65,73,73	1.66	10 (15%)	76,113,113	1.56	15 (19%)
22	CLA	B	615	-	65,73,73	1.54	11 (16%)	76,113,113	1.41	11 (14%)
33	STE	t	103	-	17,17,19	0.61	0	17,17,19	1.12	1 (5%)
24	BCR	T	101	-	41,41,41	1.04	3 (7%)	56,56,56	1.42	6 (10%)
22	CLA	c	508	-	64,72,73	1.59	8 (12%)	74,111,113	1.51	13 (17%)
33	STE	B	626	-	11,11,19	0.96	0	11,11,19	0.85	0
33	STE	l	102	-	17,17,19	0.37	0	16,16,19	0.91	0
22	CLA	B	605	-	65,73,73	1.24	4 (6%)	76,113,113	1.49	10 (13%)
28	LHG	a	410	-	48,48,48	0.89	2 (4%)	51,54,54	1.47	8 (15%)
28	LHG	B	622	-	48,48,48	0.89	3 (6%)	51,54,54	1.27	5 (9%)
22	CLA	C	507	36	65,73,73	1.39	7 (10%)	76,113,113	1.65	12 (15%)
29	SQD	B	623	-	53,54,54	0.97	4 (7%)	62,65,65	1.88	14 (22%)
22	CLA	B	603	-	65,73,73	1.56	10 (15%)	76,113,113	1.73	13 (17%)
33	STE	C	521	-	11,11,19	0.77	0	11,11,19	1.22	2 (18%)
22	CLA	C	504	36	59,67,73	1.33	7 (11%)	68,105,113	1.45	11 (16%)
24	BCR	Y	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.36	8 (14%)
24	BCR	c	514	-	41,41,41	1.15	2 (4%)	56,56,56	1.33	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PL9	A	410	-	55,55,55	1.25	6 (10%)	68,69,69	1.46	11 (16%)
27	LMG	d	410	-	44,44,55	1.11	3 (6%)	52,52,63	1.29	7 (13%)
29	SQD	D	408	-	35,36,54	1.00	4 (11%)	42,45,65	2.21	10 (23%)
22	CLA	B	611	-	65,73,73	1.56	7 (10%)	76,113,113	1.75	11 (14%)
33	STE	a	413	-	9,9,19	0.52	0	8,8,19	0.52	0
27	LMG	C	520	-	48,48,55	0.86	3 (6%)	56,56,63	1.36	8 (14%)
24	BCR	c	515	-	41,41,41	1.21	3 (7%)	56,56,56	1.45	12 (21%)
22	CLA	b	602	-	65,73,73	1.26	8 (12%)	76,113,113	1.61	13 (17%)
22	CLA	B	601	36	65,73,73	1.67	10 (15%)	76,113,113	1.49	7 (9%)
28	LHG	D	409	-	48,48,48	1.09	3 (6%)	51,54,54	1.24	6 (11%)
30	DGD	C	518	-	63,63,67	1.20	8 (12%)	77,77,81	1.35	10 (12%)
33	STE	k	102	-	11,11,19	0.80	0	11,11,19	1.12	1 (9%)
33	STE	R	101	-	11,11,19	0.95	0	11,11,19	0.93	0
35	HEC	v	201	17	32,50,50	2.23	3 (9%)	24,82,82	1.99	9 (37%)
22	CLA	a	402	-	65,73,73	1.57	9 (13%)	76,113,113	1.48	8 (10%)
22	CLA	b	606	-	65,73,73	1.83	12 (18%)	76,113,113	1.65	9 (11%)
22	CLA	a	404	-	65,73,73	1.75	7 (10%)	76,113,113	1.46	13 (17%)
24	BCR	k	101	-	41,41,41	1.05	4 (9%)	56,56,56	1.08	3 (5%)
35	HEC	V	201	17	32,50,50	2.02	3 (9%)	24,82,82	1.82	5 (20%)
22	CLA	C	502	-	65,73,73	1.56	10 (15%)	76,113,113	1.41	12 (15%)
24	BCR	A	407	-	41,41,41	1.13	4 (9%)	56,56,56	1.47	11 (19%)
33	STE	B	620	-	16,16,19	0.75	0	16,16,19	1.01	0
24	BCR	x	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	8 (14%)
27	LMG	M	101	-	51,51,55	1.01	4 (7%)	59,59,63	1.55	9 (15%)
26	PL9	D	406	-	55,55,55	1.70	7 (12%)	68,69,69	1.76	18 (26%)
22	CLA	C	508	-	65,73,73	1.70	11 (16%)	76,113,113	1.68	11 (14%)
22	CLA	b	612	-	65,73,73	1.76	9 (13%)	76,113,113	1.54	13 (17%)
34	BCT	a	408	21	2,3,3	1.28	0	2,3,3	3.54	2 (100%)
22	CLA	c	501	-	65,73,73	1.40	7 (10%)	76,113,113	1.52	10 (13%)
28	LHG	A	412	-	46,46,48	1.15	5 (10%)	49,52,54	1.37	7 (14%)
28	LHG	B	621	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	2 (3%)
22	CLA	b	603	-	65,73,73	1.74	10 (15%)	76,113,113	1.52	12 (15%)
30	DGD	C	519	-	63,63,67	1.21	7 (11%)	77,77,81	1.33	7 (9%)
33	STE	b	625	-	19,19,19	0.71	0	19,19,19	0.82	0
33	STE	b	626	-	9,9,19	0.48	0	8,8,19	0.55	0
22	CLA	c	503	-	65,73,73	1.51	9 (13%)	76,113,113	1.39	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PHO	A	405	-	51,69,69	1.07	7 (13%)	47,99,99	1.24	6 (12%)
22	CLA	c	505	-	65,73,73	1.63	10 (15%)	76,113,113	1.41	9 (11%)
24	BCR	b	619	-	41,41,41	1.02	2 (4%)	56,56,56	1.27	7 (12%)
30	DGD	c	519	-	63,63,67	1.11	4 (6%)	77,77,81	1.38	7 (9%)
33	STE	M	103	-	9,9,19	0.42	0	8,8,19	0.81	0
27	LMG	m	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.48	8 (13%)
22	CLA	b	610	36	65,73,73	1.62	12 (18%)	76,113,113	1.56	13 (17%)
22	CLA	D	402	-	65,73,73	1.39	8 (12%)	76,113,113	1.43	12 (15%)
33	STE	b	624	-	15,15,19	0.80	0	15,15,19	0.99	1 (6%)
22	CLA	b	604	-	65,73,73	1.46	7 (10%)	76,113,113	1.64	18 (23%)
22	CLA	b	609	-	65,73,73	1.62	10 (15%)	76,113,113	1.64	12 (15%)
22	CLA	c	509	-	65,73,73	1.48	7 (10%)	76,113,113	1.58	10 (13%)
33	STE	B	625	-	15,15,19	0.45	0	14,14,19	0.62	0
33	STE	H	103	-	17,17,19	0.49	0	16,16,19	0.69	0
35	HEC	F	101	6,5	32,50,50	2.20	5 (15%)	24,82,82	2.51	6 (25%)
22	CLA	C	510	-	65,73,73	1.49	9 (13%)	76,113,113	1.47	8 (10%)
22	CLA	b	615	-	65,73,73	1.78	9 (13%)	76,113,113	1.67	12 (15%)
22	CLA	C	509	-	65,73,73	1.47	9 (13%)	76,113,113	1.58	11 (14%)
28	LHG	d	409	-	38,38,48	1.02	2 (5%)	41,44,54	1.16	4 (9%)
33	STE	Z	101	-	7,7,19	0.45	0	6,6,19	0.54	0
28	LHG	E	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.24	5 (9%)
22	CLA	b	614	-	65,73,73	1.55	8 (12%)	76,113,113	1.59	11 (14%)
24	BCR	b	618	-	41,41,41	1.17	2 (4%)	56,56,56	1.29	8 (14%)
33	STE	M	102	-	14,14,19	0.59	0	14,14,19	1.17	0
33	STE	T	102	-	14,14,19	0.46	0	13,13,19	0.65	0
22	CLA	C	506	-	65,73,73	1.80	11 (16%)	76,113,113	1.27	9 (11%)
29	SQD	a	411	-	53,54,54	1.03	5 (9%)	62,65,65	1.85	11 (17%)
24	BCR	D	405	-	41,41,41	1.18	3 (7%)	56,56,56	1.37	9 (16%)
33	STE	t	102	-	13,13,19	0.70	0	13,13,19	1.35	2 (15%)
22	CLA	B	614	-	65,73,73	1.55	7 (10%)	76,113,113	1.33	11 (14%)
26	PL9	a	409	-	55,55,55	1.09	5 (9%)	68,69,69	1.67	13 (19%)
33	STE	c	521	-	19,19,19	0.65	0	19,19,19	0.94	0
33	STE	a	415	-	14,14,19	0.39	0	13,13,19	0.73	0
34	BCT	D	401	21	2,3,3	0.94	0	2,3,3	3.60	2 (100%)
29	SQD	a	412	-	35,35,54	1.08	2 (5%)	37,37,65	1.62	5 (13%)
27	LMG	c	523	-	49,49,55	0.85	1 (2%)	57,57,63	1.29	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	607	36	65,73,73	1.34	8 (12%)	76,113,113	1.37	9 (11%)
22	CLA	c	512	-	65,73,73	1.35	8 (12%)	76,113,113	1.38	11 (14%)
22	CLA	A	403	36	65,73,73	1.58	8 (12%)	76,113,113	1.40	10 (13%)
28	LHG	d	408	-	48,48,48	0.95	2 (4%)	51,54,54	1.18	4 (7%)
33	STE	a	414	-	11,11,19	0.86	0	11,11,19	1.09	1 (9%)
22	CLA	B	608	-	65,73,73	1.27	7 (10%)	76,113,113	1.40	12 (15%)
27	LMG	b	623	-	55,55,55	0.99	3 (5%)	63,63,63	1.49	9 (14%)
35	HEC	f	101	6,5	32,50,50	2.34	3 (9%)	24,82,82	2.16	5 (20%)
31	OEX	a	417[A]	1,3,36	0,15,15	-	-	-		
30	DGD	c	517	-	63,63,67	1.20	10 (15%)	77,77,81	1.42	15 (19%)
22	CLA	c	510	-	65,73,73	1.73	9 (13%)	76,113,113	1.45	12 (15%)
33	STE	J	101	-	11,11,19	0.64	0	11,11,19	1.37	2 (18%)
22	CLA	c	513	-	65,73,73	1.50	9 (13%)	76,113,113	1.34	8 (10%)
27	LMG	D	411	-	26,26,55	0.66	0	26,26,63	1.25	1 (3%)
33	STE	d	413	-	19,19,19	0.53	0	19,19,19	1.01	0
22	CLA	c	506	-	65,73,73	1.58	10 (15%)	76,113,113	1.48	11 (14%)
22	CLA	d	404	36	65,73,73	1.84	8 (12%)	76,113,113	1.61	9 (11%)
33	STE	d	411	-	16,16,19	0.62	0	16,16,19	1.43	3 (18%)
33	STE	b	622	-	19,19,19	0.60	0	19,19,19	1.01	0
29	SQD	f	102	-	40,41,54	1.09	4 (10%)	49,52,65	2.11	10 (20%)
23	PHO	d	402	-	51,69,69	1.04	4 (7%)	47,99,99	1.43	5 (10%)
32	OEY	a	418[B]	1,3,36	0,16,16	-	-	-		
24	BCR	B	619	-	41,41,41	1.14	2 (4%)	56,56,56	1.34	5 (8%)
22	CLA	C	501	-	65,73,73	1.58	6 (9%)	76,113,113	1.44	7 (9%)
22	CLA	B	613	-	65,73,73	1.65	10 (15%)	76,113,113	1.14	8 (10%)
29	SQD	A	413	-	51,52,54	1.08	7 (13%)	60,63,65	2.05	13 (21%)
22	CLA	A	402	-	65,73,73	1.62	8 (12%)	76,113,113	1.34	9 (11%)
22	CLA	c	511	3	65,73,73	1.69	9 (13%)	76,113,113	1.39	9 (11%)
24	BCR	C	514	-	41,41,41	1.13	3 (7%)	56,56,56	1.39	12 (21%)
30	DGD	C	517	-	63,63,67	1.29	10 (15%)	77,77,81	1.42	11 (14%)
22	CLA	C	513	-	65,73,73	1.39	8 (12%)	76,113,113	1.50	8 (10%)
27	LMG	D	407	-	51,51,55	0.98	5 (9%)	59,59,63	1.25	4 (6%)
33	STE	B	624	-	11,11,19	0.81	0	11,11,19	1.32	1 (9%)
33	STE	I	101	-	14,14,19	0.54	0	13,13,19	0.53	0
26	PL9	d	407	-	55,55,55	1.57	10 (18%)	68,69,69	1.89	20 (29%)
22	CLA	b	616	-	60,68,73	1.43	10 (16%)	70,107,113	1.54	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	616	-	60,68,73	1.64	9 (15%)	70,107,113	1.70	9 (12%)
30	DGD	H	102	-	63,63,67	1.41	13 (20%)	77,77,81	1.42	10 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	607	36	1/1/20/20	13/37/115/115	-
22	CLA	b	613	-	1/1/20/20	10/37/115/115	-
24	BCR	t	101	-	-	6/29/63/63	0/2/2/2
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
22	CLA	d	403	-	1/1/20/20	7/37/115/115	-
22	CLA	D	404	-	-	10/37/115/115	-
22	CLA	b	608	-	-	1/37/115/115	-
22	CLA	D	403	36	-	7/37/115/115	-
22	CLA	c	504	36	1/1/19/20	8/31/109/115	-
27	LMG	a	416	-	-	30/50/70/70	0/1/1/1
22	CLA	b	601	36	1/1/20/20	13/37/115/115	-
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
29	SQD	A	414	-	-	21/39/39/69	-
22	CLA	B	612	-	1/1/20/20	6/37/115/115	-
33	STE	D	412	-	-	9/17/17/17	-
29	SQD	b	620	-	-	20/44/64/69	0/1/1/1
22	CLA	B	604	-	1/1/20/20	10/37/115/115	-
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
22	CLA	C	503	-	1/1/20/20	5/37/115/115	-
24	BCR	b	617	-	-	7/29/63/63	0/2/2/2
27	LMG	A	411	-	-	21/43/63/70	0/1/1/1
33	STE	m	102	-	-	4/9/9/17	-
23	PHO	a	403	-	-	2/37/103/103	0/5/6/6
33	STE	b	627	-	-	5/11/11/17	-
22	CLA	c	502	-	-	5/37/115/115	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	c	520	-	-	10/31/51/70	0/1/1/1
24	BCR	C	516	-	-	10/29/63/63	0/2/2/2
24	BCR	a	405	-	-	1/29/63/63	0/2/2/2
27	LMG	D	410	-	-	15/33/33/70	-
33	STE	b	621	-	-	8/13/13/17	-
22	CLA	A	406	-	1/1/17/20	3/24/102/115	-
22	CLA	b	611	-	1/1/20/20	6/37/115/115	-
22	CLA	c	507	36	1/1/20/20	6/37/115/115	-
22	CLA	B	606	-	1/1/20/20	9/37/115/115	-
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
33	STE	d	412	-	-	8/17/17/17	-
28	LHG	e	101	-	-	31/46/46/53	-
22	CLA	C	512	-	1/1/20/20	13/37/115/115	-
22	CLA	b	605	-	1/1/20/20	4/37/115/115	-
24	BCR	c	516	-	-	3/29/63/63	0/2/2/2
22	CLA	B	602	-	1/1/20/20	5/37/115/115	-
22	CLA	C	505	-	1/1/20/20	11/37/115/115	-
22	CLA	B	610	36	1/1/20/20	6/37/115/115	-
22	CLA	C	511	3	1/1/20/20	4/37/115/115	-
22	CLA	d	405	-	1/1/20/20	12/37/115/115	-
24	BCR	C	515	-	-	6/29/63/63	0/2/2/2
22	CLA	B	609	-	-	6/37/115/115	-
30	DGD	A	415	-	-	20/55/95/95	0/2/2/2
33	STE	C	522	-	-	5/13/13/17	-
33	STE	C	523	-	-	3/9/9/17	-
30	DGD	h	101	-	-	19/51/91/95	0/2/2/2
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
28	LHG	l	101	-	-	15/53/53/53	-
33	STE	j	101	-	-	3/9/9/17	-
22	CLA	d	401	36	-	13/37/115/115	-
22	CLA	B	615	-	1/1/20/20	9/37/115/115	-
33	STE	t	103	-	-	8/15/15/17	-
24	BCR	T	101	-	-	7/29/63/63	0/2/2/2
22	CLA	c	508	-	-	11/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	B	626	-	-	5/9/9/17	-
33	STE	l	102	-	-	9/15/15/17	-
22	CLA	B	605	-	1/1/20/20	9/37/115/115	-
28	LHG	a	410	-	-	23/53/53/53	-
28	LHG	B	622	-	-	18/53/53/53	-
22	CLA	C	507	36	1/1/20/20	10/37/115/115	-
29	SQD	B	623	-	-	24/49/69/69	0/1/1/1
22	CLA	B	603	-	1/1/20/20	5/37/115/115	-
33	STE	C	521	-	-	7/9/9/17	-
22	CLA	C	504	36	1/1/18/20	6/30/108/115	-
24	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
24	BCR	c	514	-	-	15/29/63/63	0/2/2/2
26	PL9	A	410	-	-	24/53/73/73	0/1/1/1
27	LMG	d	410	-	-	10/39/59/70	0/1/1/1
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
22	CLA	B	611	-	1/1/20/20	9/37/115/115	-
33	STE	a	413	-	-	3/7/7/17	-
27	LMG	C	520	-	-	12/43/63/70	0/1/1/1
24	BCR	c	515	-	-	6/29/63/63	0/2/2/2
22	CLA	b	602	-	-	4/37/115/115	-
22	CLA	B	601	36	1/1/20/20	12/37/115/115	-
28	LHG	D	409	-	-	20/53/53/53	-
30	DGD	C	518	-	-	23/51/91/95	0/2/2/2
33	STE	k	102	-	-	6/9/9/17	-
33	STE	R	101	-	-	4/9/9/17	-
35	HEC	v	201	17	-	2/10/54/54	-
22	CLA	a	402	-	1/1/20/20	6/37/115/115	-
22	CLA	b	606	-	1/1/20/20	7/37/115/115	-
22	CLA	a	404	-	1/1/20/20	8/37/115/115	-
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
35	HEC	V	201	17	-	2/10/54/54	-
22	CLA	C	502	-	-	8/37/115/115	-
24	BCR	A	407	-	-	10/29/63/63	0/2/2/2
33	STE	B	620	-	-	5/14/14/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	x	101	-	-	5/29/63/63	0/2/2/2
27	LMG	M	101	-	-	22/46/66/70	0/1/1/1
26	PL9	D	406	-	-	10/53/73/73	0/1/1/1
22	CLA	C	508	-	-	11/37/115/115	-
22	CLA	b	612	-	1/1/20/20	4/37/115/115	-
22	CLA	c	501	-	1/1/20/20	2/37/115/115	-
28	LHG	A	412	-	-	19/51/51/53	-
28	LHG	B	621	-	-	25/53/53/53	-
22	CLA	b	603	-	1/1/20/20	6/37/115/115	-
30	DGD	C	519	-	-	11/51/91/95	0/2/2/2
33	STE	b	625	-	-	9/17/17/17	-
33	STE	b	626	-	-	4/7/7/17	-
22	CLA	c	503	-	1/1/20/20	7/37/115/115	-
23	PHO	A	405	-	-	2/37/103/103	0/5/6/6
22	CLA	c	505	-	1/1/20/20	10/37/115/115	-
24	BCR	b	619	-	-	0/29/63/63	0/2/2/2
30	DGD	c	519	-	-	13/51/91/95	0/2/2/2
33	STE	M	103	-	-	2/7/7/17	-
27	LMG	m	101	-	-	25/46/66/70	0/1/1/1
22	CLA	b	610	36	1/1/20/20	4/37/115/115	-
22	CLA	D	402	-	1/1/20/20	6/37/115/115	-
33	STE	b	624	-	-	7/13/13/17	-
22	CLA	b	604	-	1/1/20/20	9/37/115/115	-
22	CLA	b	609	-	1/1/20/20	10/37/115/115	-
22	CLA	c	509	-	1/1/20/20	9/37/115/115	-
33	STE	B	625	-	-	9/13/13/17	-
33	STE	H	103	-	-	10/15/15/17	-
35	HEC	F	101	6,5	-	2/10/54/54	-
22	CLA	C	510	-	1/1/20/20	9/37/115/115	-
22	CLA	b	615	-	1/1/20/20	7/37/115/115	-
22	CLA	C	509	-	1/1/20/20	12/37/115/115	-
28	LHG	d	409	-	-	14/43/43/53	-
33	STE	Z	101	-	-	2/5/5/17	-
28	LHG	E	101	-	-	23/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	614	-	1/1/20/20	14/37/115/115	-
24	BCR	b	618	-	-	6/29/63/63	0/2/2/2
33	STE	M	102	-	-	5/12/12/17	-
33	STE	T	102	-	-	11/12/12/17	-
22	CLA	C	506	-	1/1/20/20	8/37/115/115	-
29	SQD	a	411	-	-	22/49/69/69	0/1/1/1
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
33	STE	t	102	-	-	3/11/11/17	-
22	CLA	B	614	-	1/1/20/20	18/37/115/115	-
26	PL9	a	409	-	-	27/53/73/73	0/1/1/1
33	STE	c	521	-	-	7/17/17/17	-
33	STE	a	415	-	-	6/12/12/17	-
29	SQD	a	412	-	-	18/37/37/69	-
27	LMG	c	523	-	-	20/44/64/70	0/1/1/1
22	CLA	B	607	36	1/1/20/20	5/37/115/115	-
22	CLA	c	512	-	1/1/20/20	18/37/115/115	-
22	CLA	A	403	36	1/1/20/20	13/37/115/115	-
28	LHG	d	408	-	-	17/53/53/53	-
33	STE	a	414	-	-	3/9/9/17	-
22	CLA	B	608	-	-	1/37/115/115	-
27	LMG	b	623	-	-	22/50/70/70	0/1/1/1
35	HEC	f	101	6,5	-	3/10/54/54	-
30	DGD	c	517	-	-	27/51/91/95	0/2/2/2
22	CLA	c	510	-	1/1/20/20	11/37/115/115	-
33	STE	J	101	-	-	6/9/9/17	-
22	CLA	c	513	-	-	6/37/115/115	-
27	LMG	D	411	-	-	7/22/22/70	-
33	STE	d	413	-	-	8/17/17/17	-
22	CLA	c	506	-	1/1/20/20	17/37/115/115	-
22	CLA	d	404	36	1/1/20/20	4/37/115/115	-
33	STE	d	411	-	-	5/14/14/17	-
33	STE	b	622	-	-	8/17/17/17	-
29	SQD	f	102	-	-	11/36/56/69	0/1/1/1
23	PHO	d	402	-	-	0/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/20/20	3/37/115/115	-
22	CLA	B	613	-	1/1/20/20	11/37/115/115	-
29	SQD	A	413	-	-	16/47/67/69	0/1/1/1
22	CLA	A	402	-	1/1/20/20	5/37/115/115	-
22	CLA	c	511	3	1/1/20/20	11/37/115/115	-
24	BCR	C	514	-	-	11/29/63/63	0/2/2/2
30	DGD	C	517	-	-	25/51/91/95	0/2/2/2
22	CLA	C	513	-	-	9/37/115/115	-
27	LMG	D	407	-	-	15/46/66/70	0/1/1/1
33	STE	B	624	-	-	3/9/9/17	-
33	STE	I	101	-	-	3/12/12/17	-
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
22	CLA	b	616	-	1/1/19/20	7/31/109/115	-
22	CLA	B	616	-	1/1/19/20	7/31/109/115	-
30	DGD	H	102	-	-	16/51/91/95	0/2/2/2

The worst 5 of 905 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C4B-NB	9.29	1.43	1.35
22	b	606	CLA	MG-NA	9.01	2.27	2.06
22	b	603	CLA	C4B-NB	8.74	1.43	1.35
35	f	101	HEC	C2B-C3B	-8.44	1.31	1.40
22	B	602	CLA	C4B-NB	8.29	1.42	1.35

The worst 5 of 1338 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	503	CLA	C4A-NA-C1A	10.58	111.46	106.71
22	B	604	CLA	C4A-NA-C1A	9.47	110.96	106.71
22	B	611	CLA	C4A-NA-C1A	8.94	110.72	106.71
22	C	507	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	B	601	CLA	C4A-NA-C1A	8.84	110.68	106.71

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	406	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND

5 of 1761 torsion outliers are listed below:

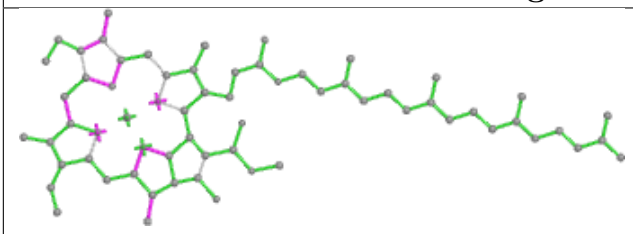
Mol	Chain	Res	Type	Atoms
22	A	406	CLA	C2-C3-C5-C6
22	A	406	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

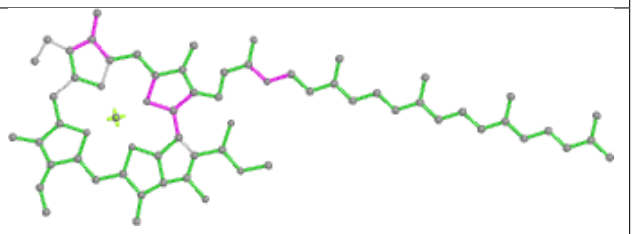
No monomer is involved in short contacts.

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

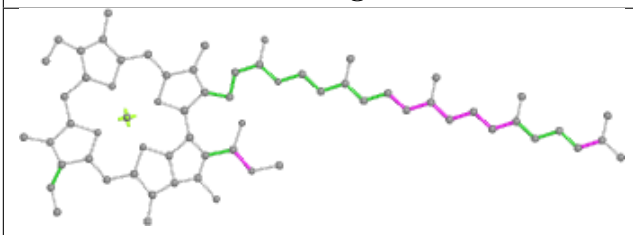
Ligand CLA b 607



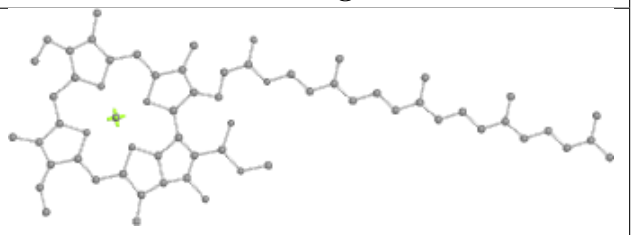
Bond lengths



Bond angles

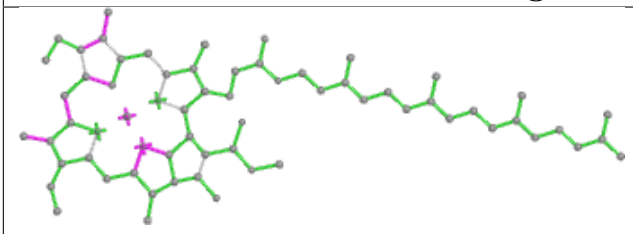


Torsions

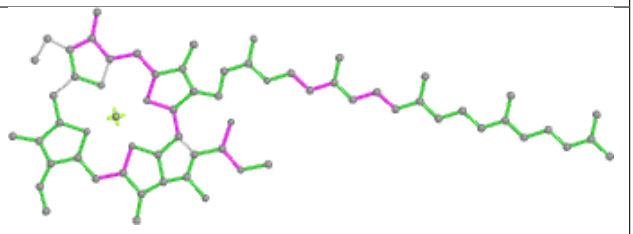


Rings

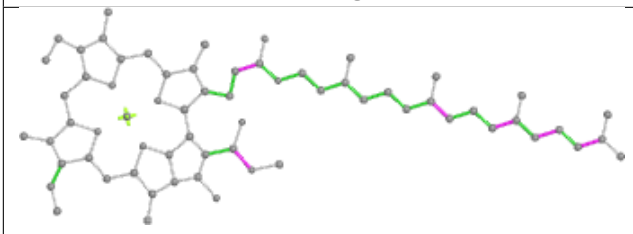
Ligand CLA b 613



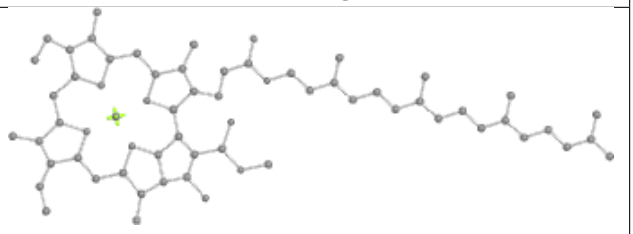
Bond lengths



Bond angles

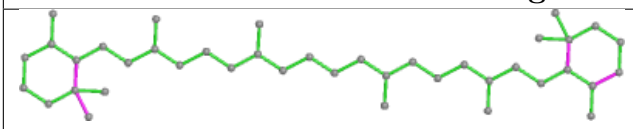


Torsions

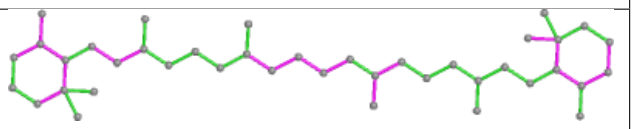


Rings

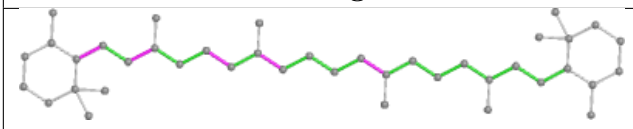
Ligand BCR t 101



Bond lengths



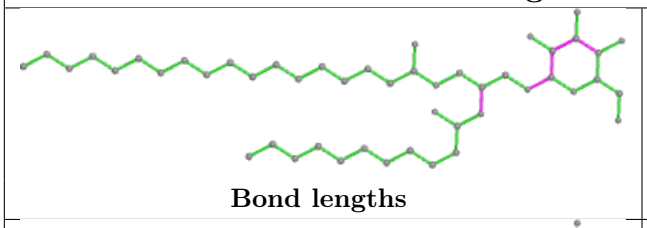
Bond angles

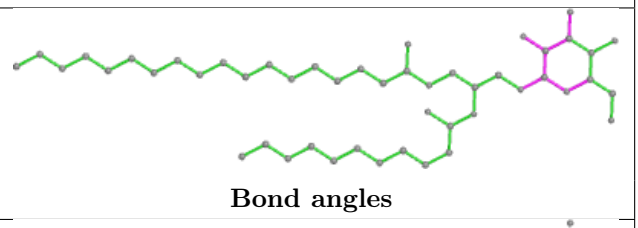


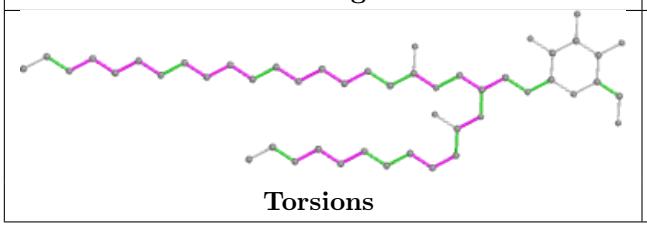
Torsions

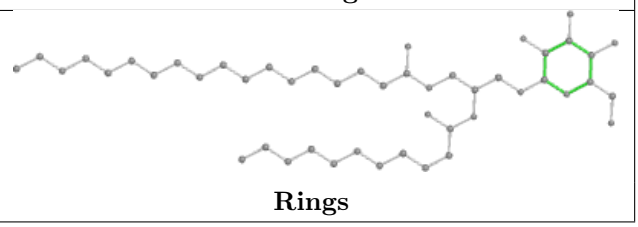
Rings

Ligand LMG c 522

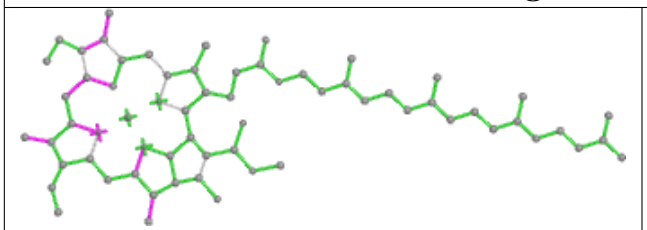

Bond lengths

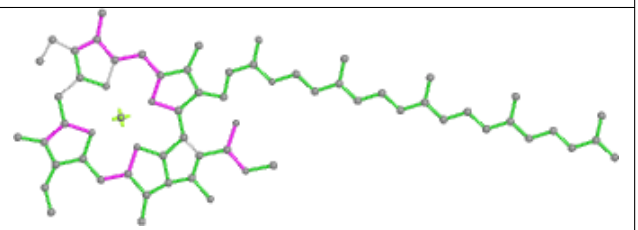

Bond angles


Torsions


Rings

Ligand CLA D 404


Bond lengths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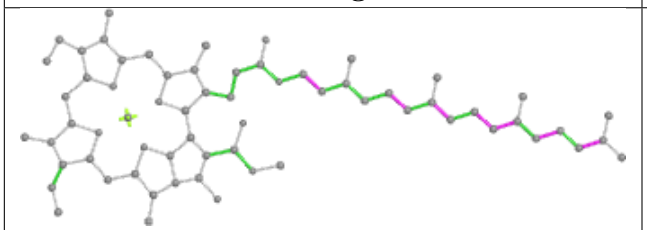
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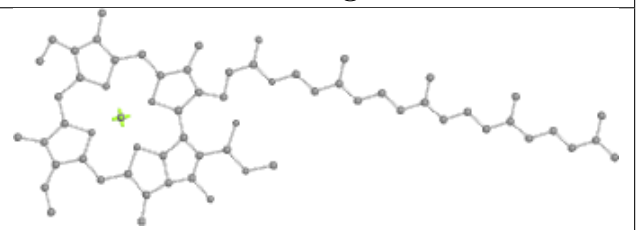
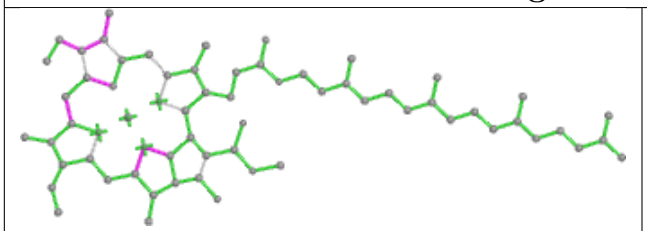

Rings

Ligand CLA b 608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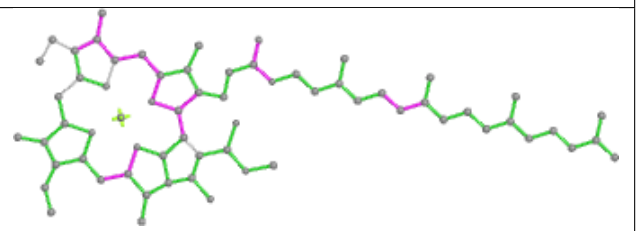
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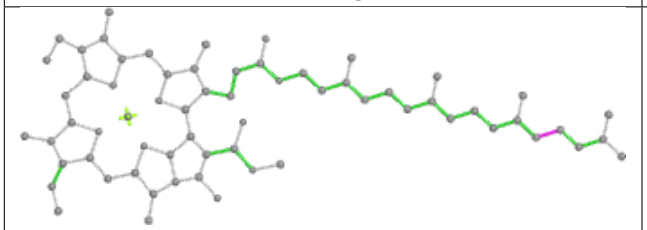
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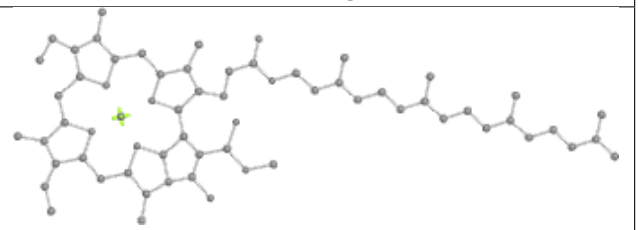
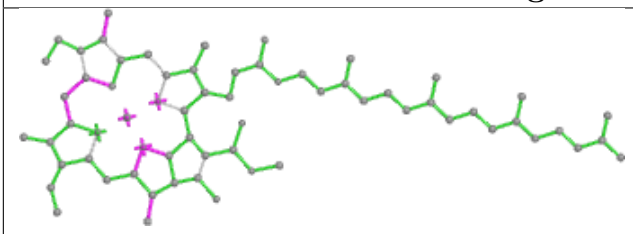

Rings

Ligand CLA d 403



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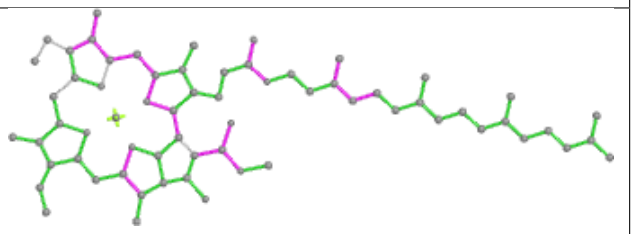
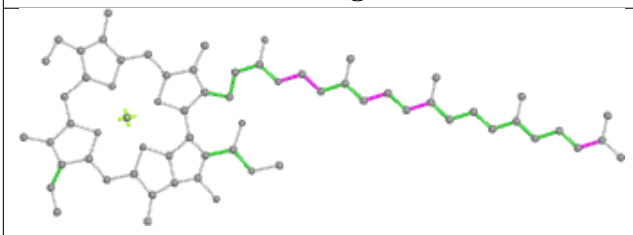


Bond angles



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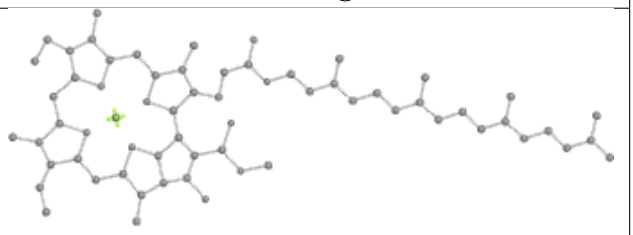
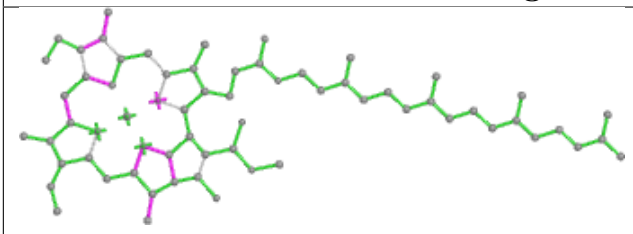


Rings

Ligand CLA D 403



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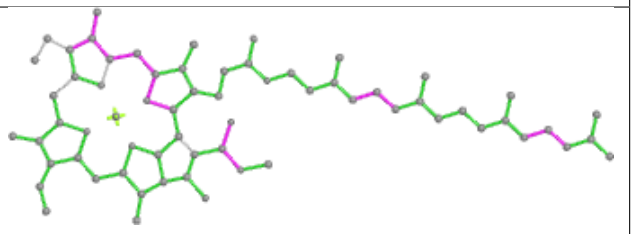
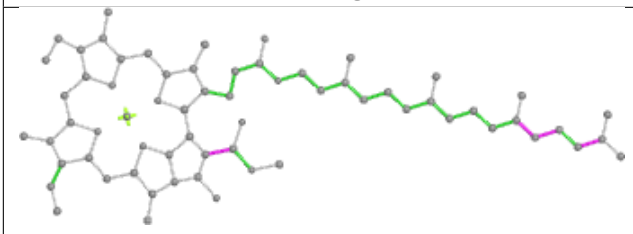


Bond angles



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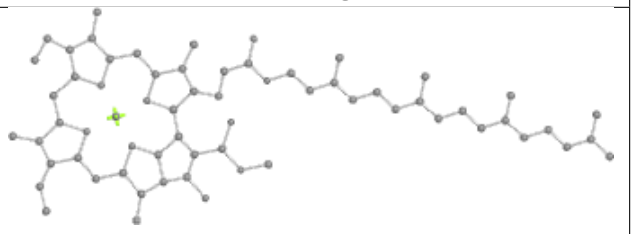
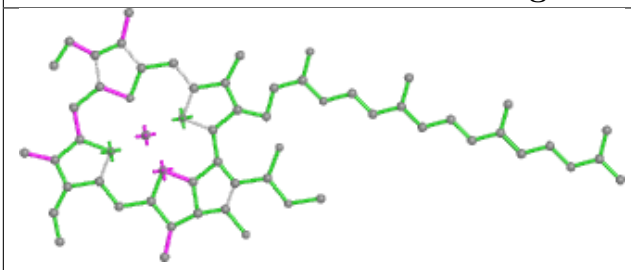


Rings

Ligand CLA c 504



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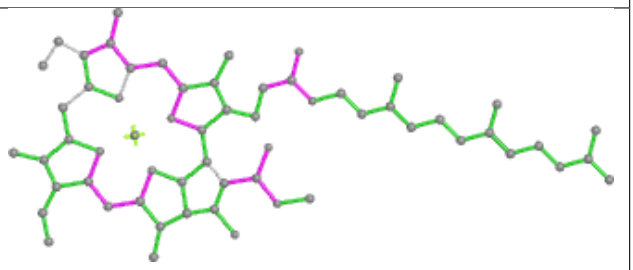
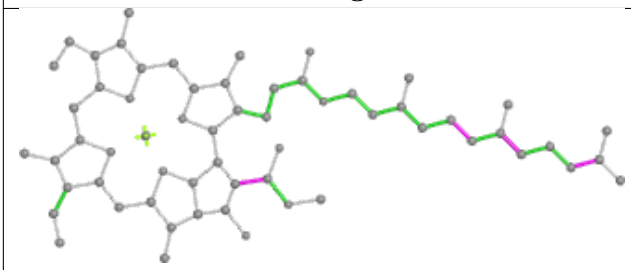


Bond angles



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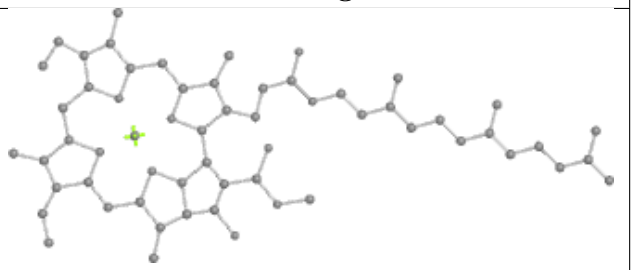
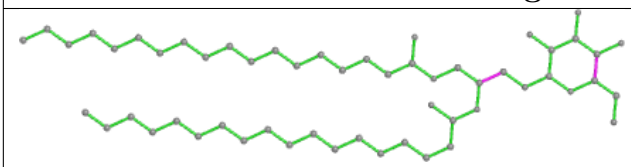


Rings

Ligand LMG a 416



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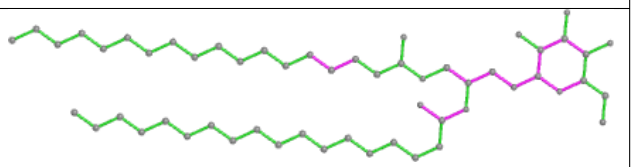
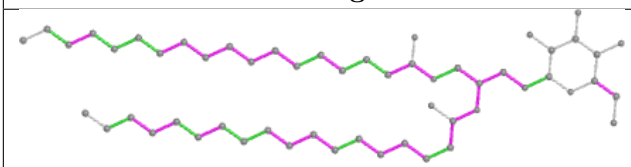


Bond angles



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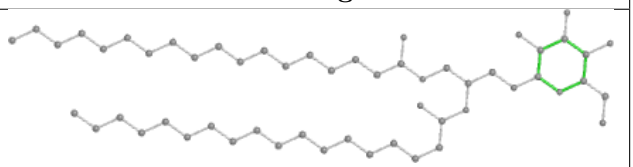
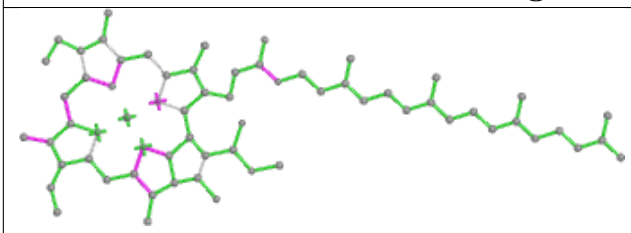


Rings

Ligand CLA b 601



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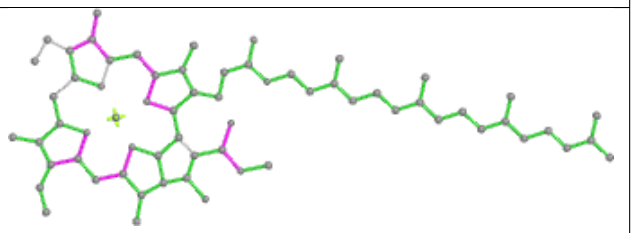
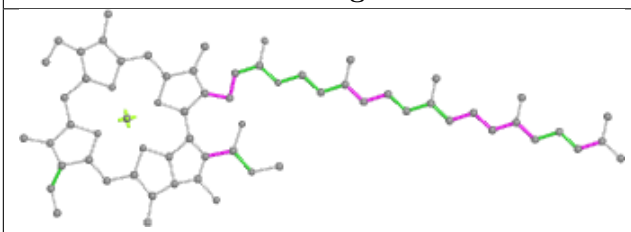


Bond angles



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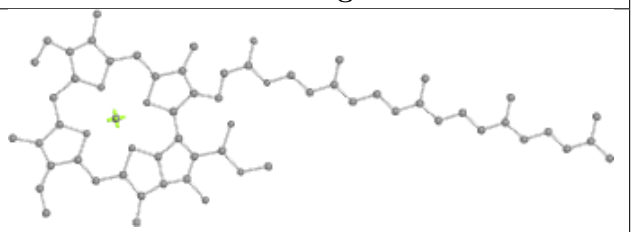
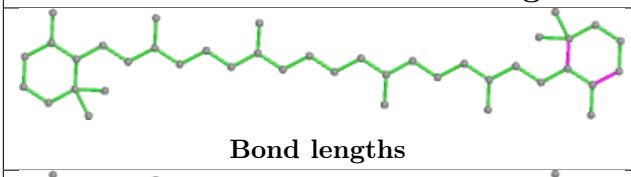
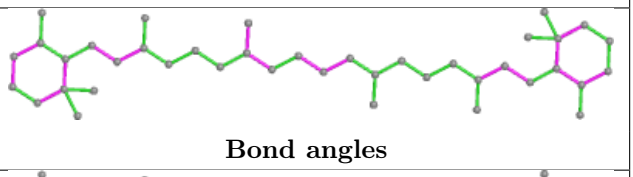


Rings

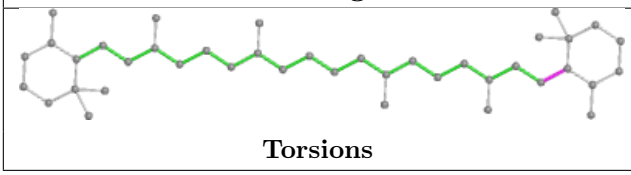
Ligand BCR B 618



Bond lengths



Bond angles



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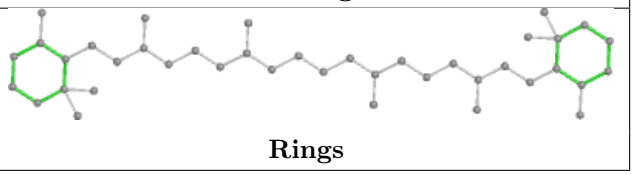
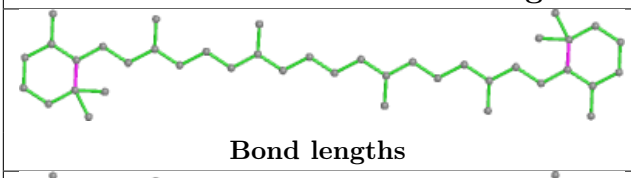


Rings

Ligand BCR d 406



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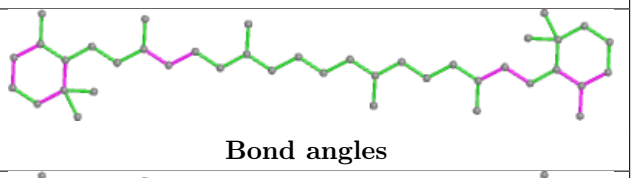
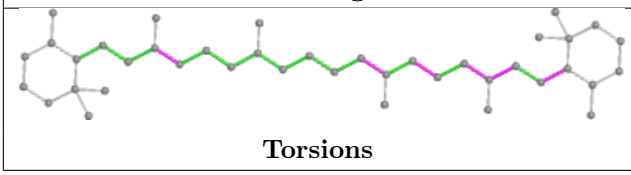


Bond angles



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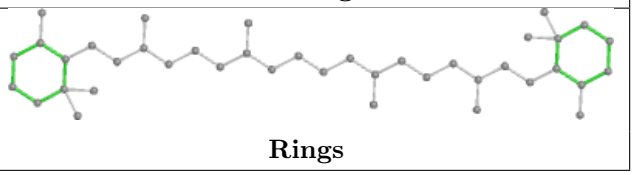
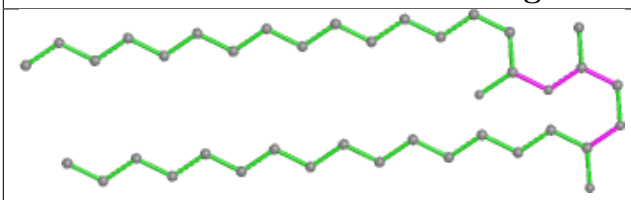


Rings

Ligand SQD A 414



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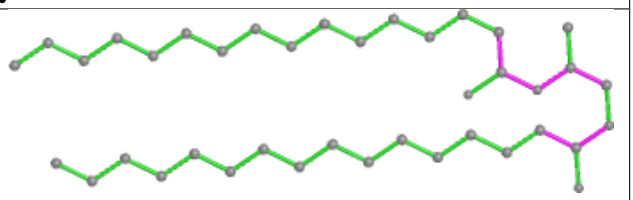
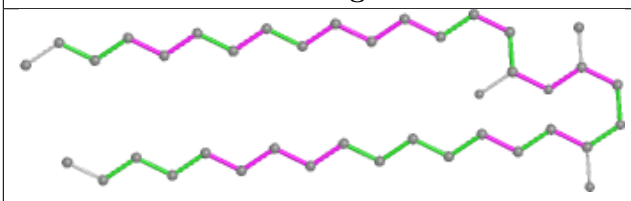
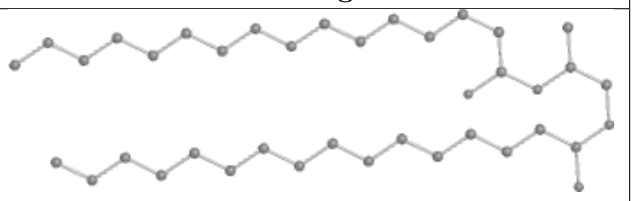


Bond angles

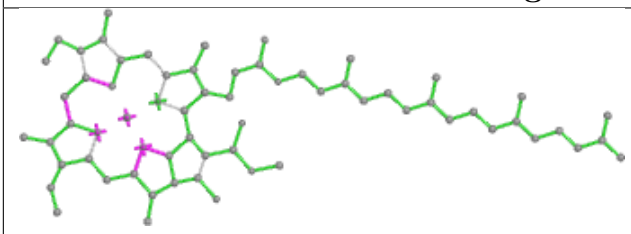


Torsions



Rings

Ligand CLA B 612



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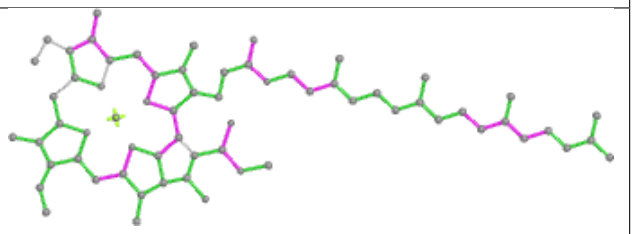
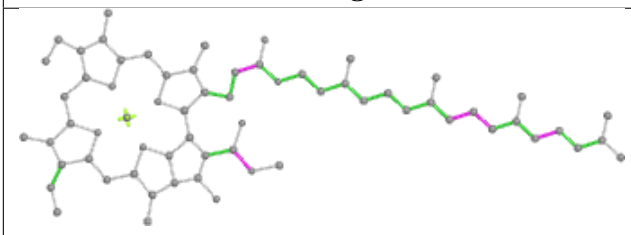


Bond angles



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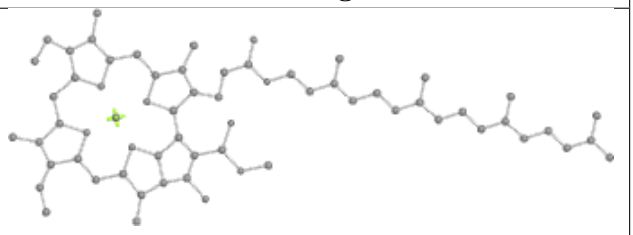
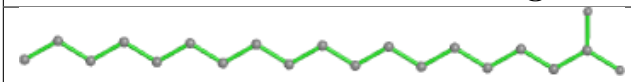


Rings

Ligand STE D 412



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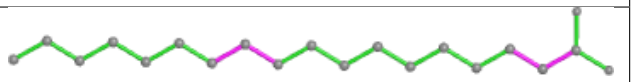
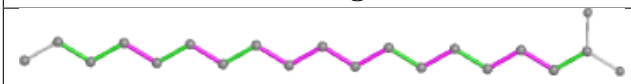


Bond angles



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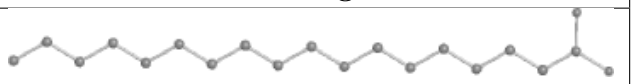
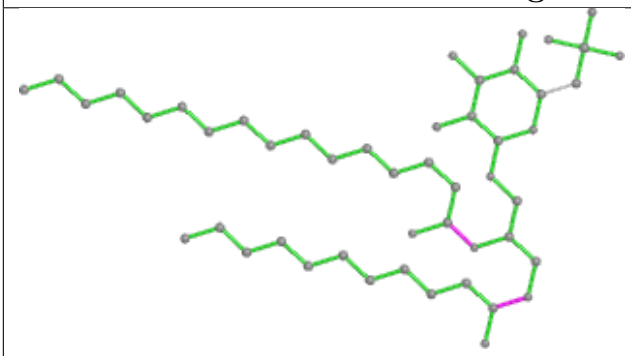
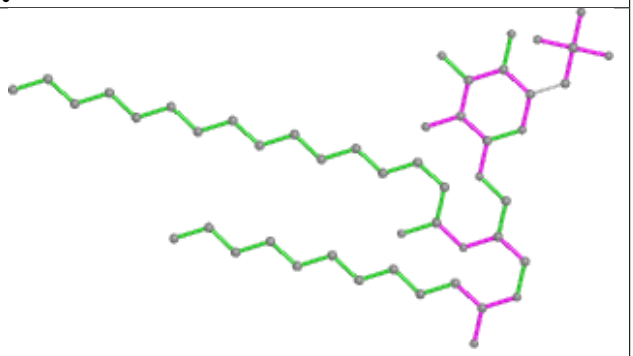


Rings

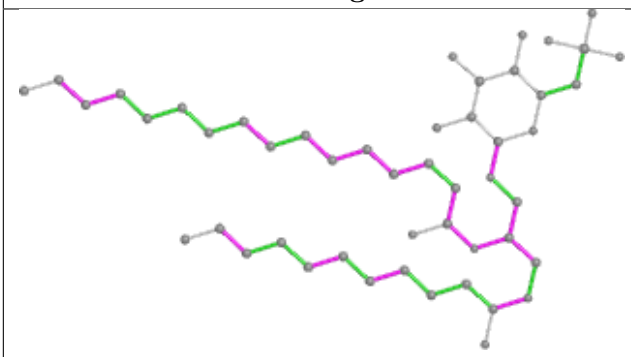
Ligand SQD b 620



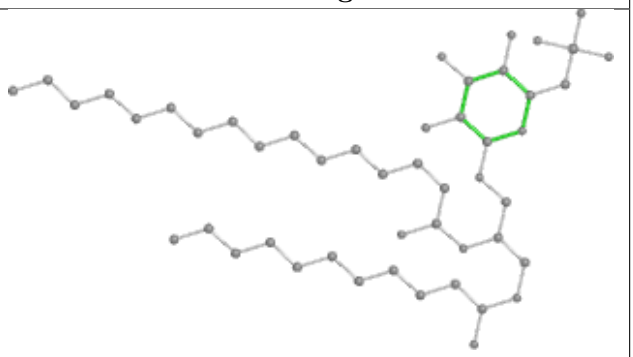
Bond lengths



Bond angles

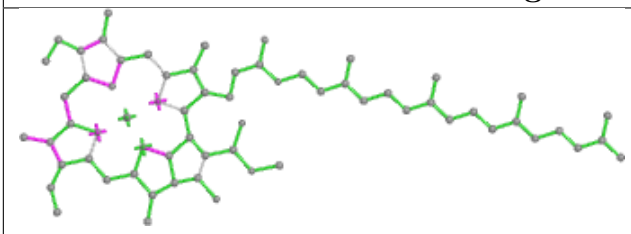


Torsions

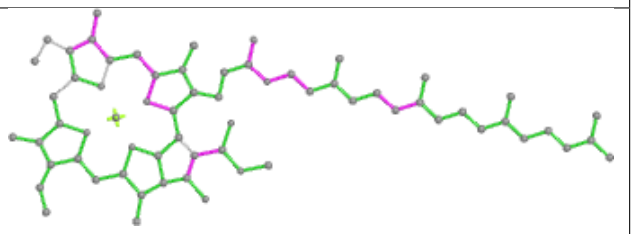


Rings

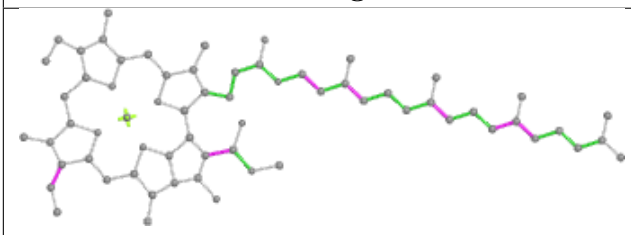
Ligand CLA B 604



Bond lengths



Bond angles



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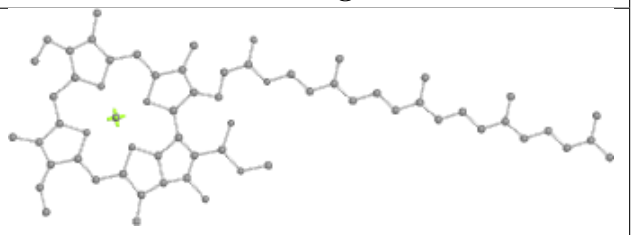
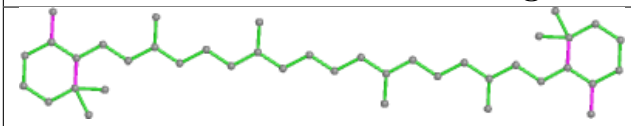
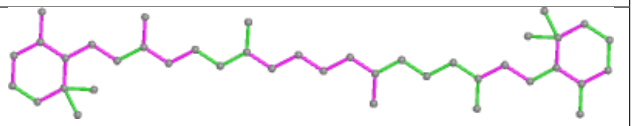


Rings

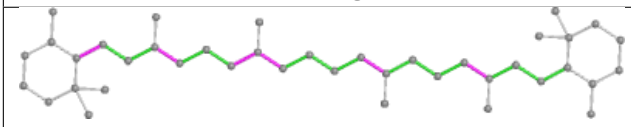
Ligand BCR B 617



Bond lengths



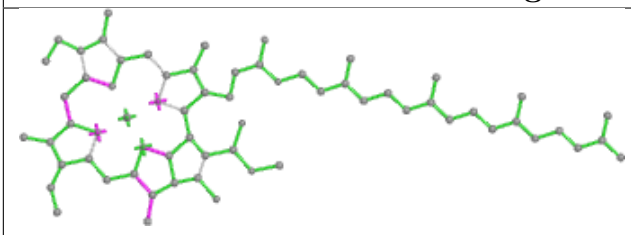
Bond angles



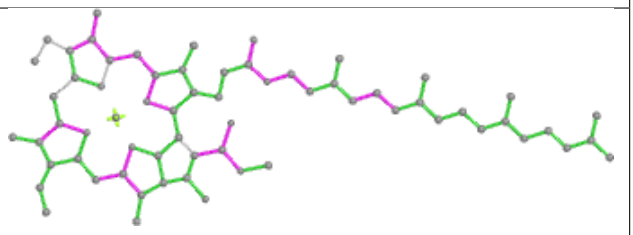
Torsions

Rings

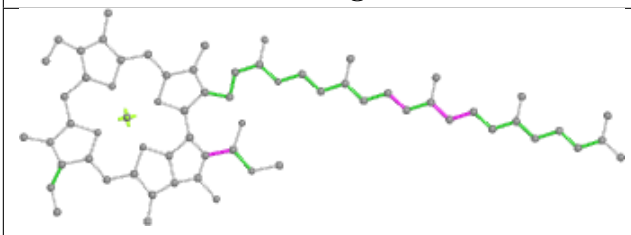
Ligand CLA C 503



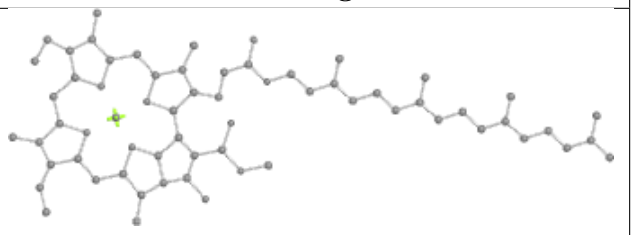
Bond lengths



Bond angles

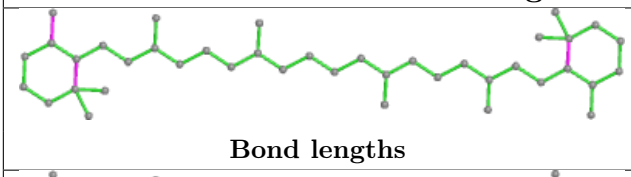


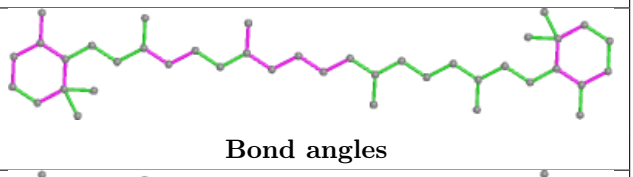
Torsions

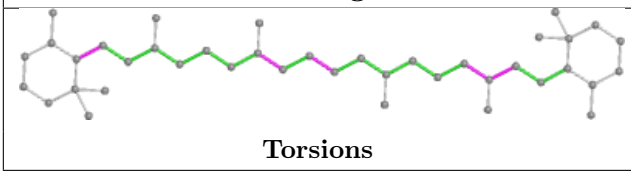


Rings

Ligand BCR b 617


Bond lengths


Bond angles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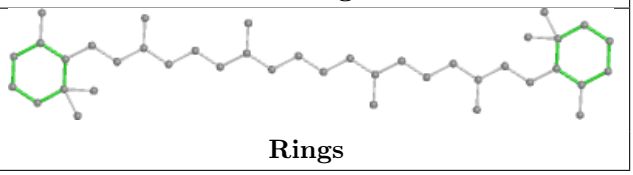
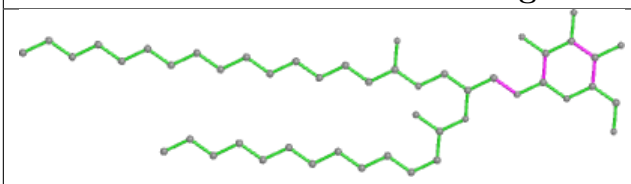
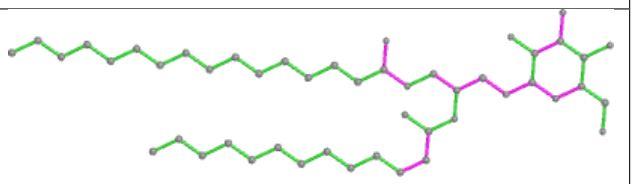
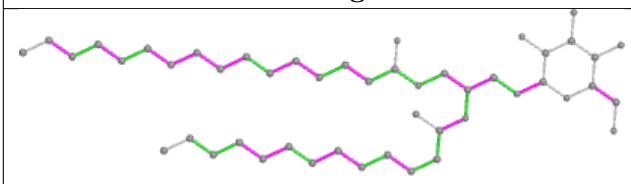
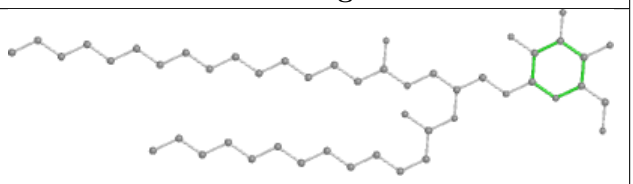

Rings

Ligand LMG A 411

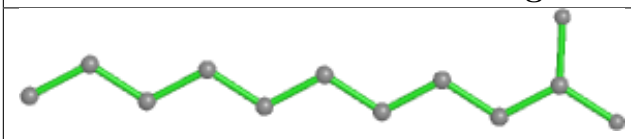

Bond lengths

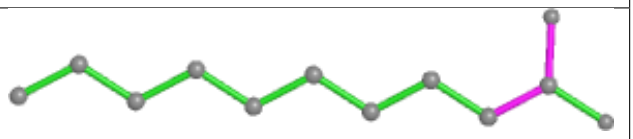

Bond angles

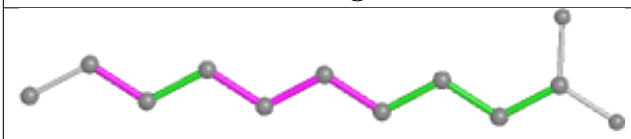

Torsions

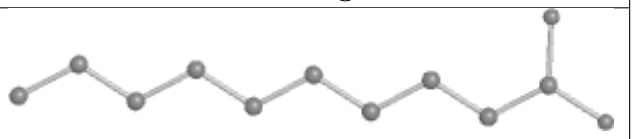

Rings

Ligand STE m 102

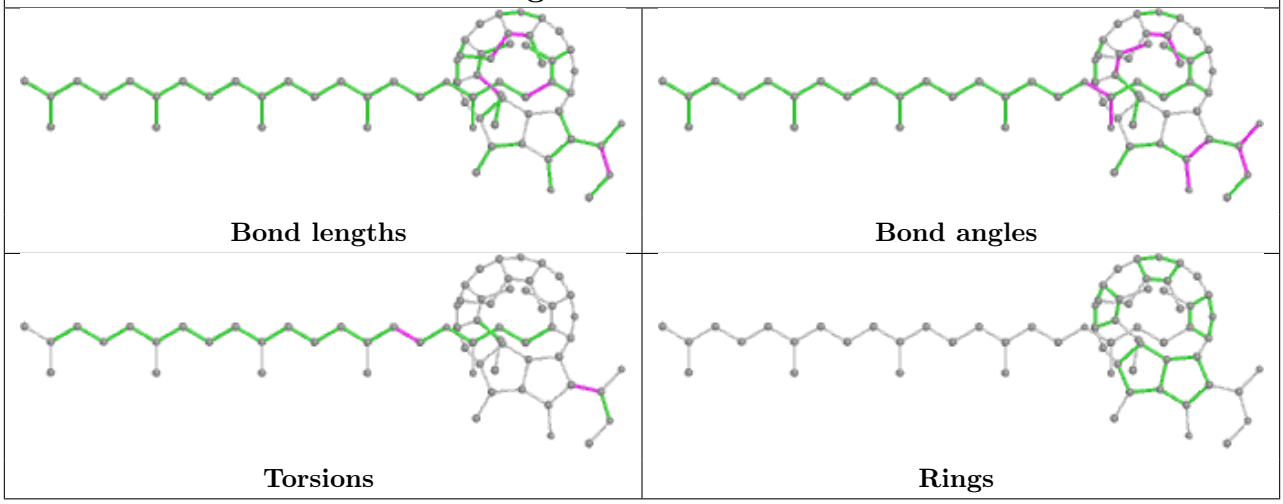

Bond lengths


Bond angles

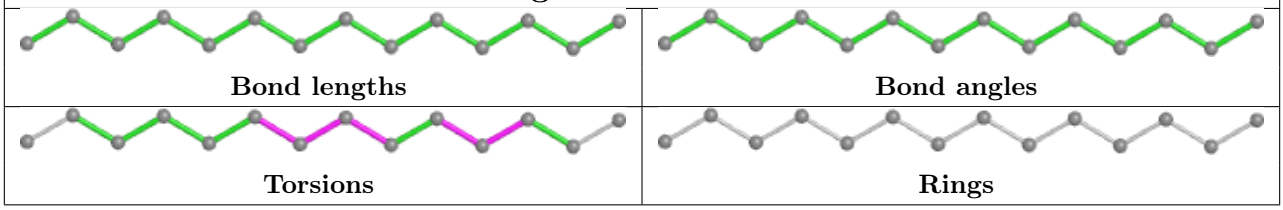

Torsions


Rings

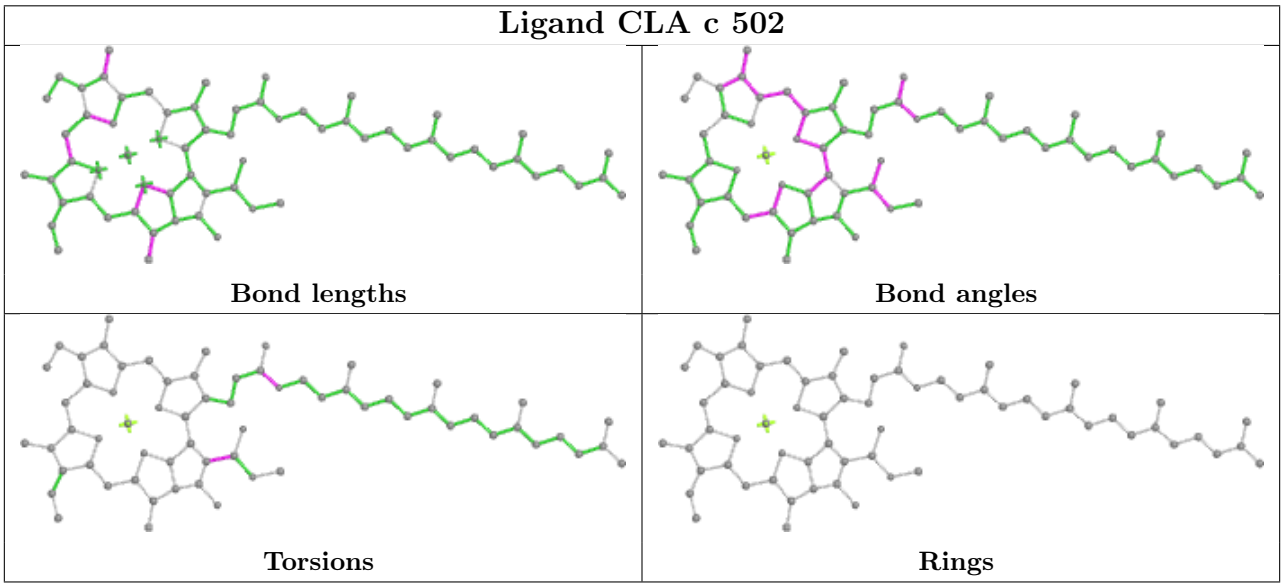
Ligand PHO a 403



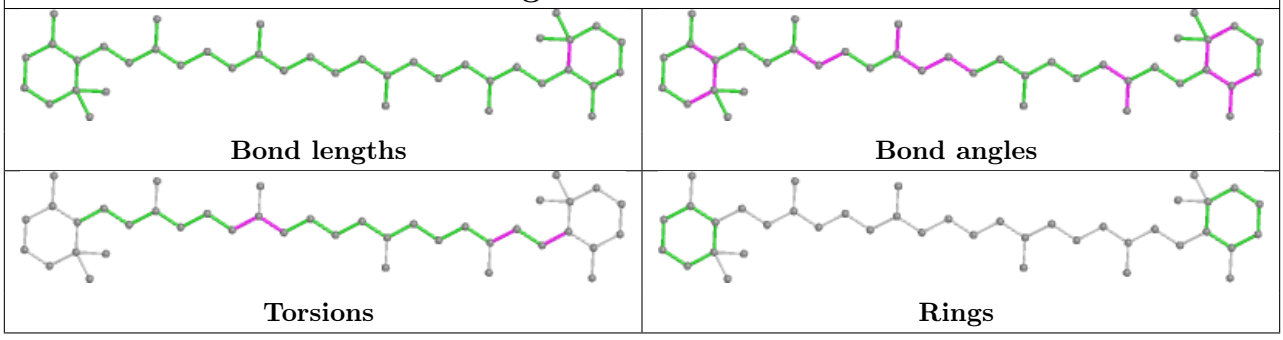
Ligand STE b 627



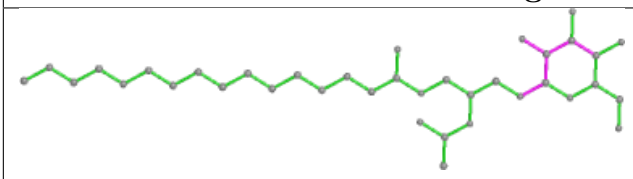
Ligand CLA c 502

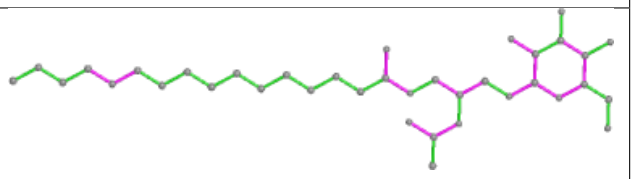


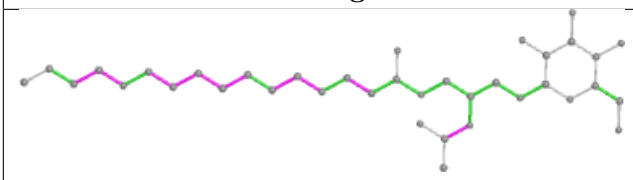
Ligand BCR H 101

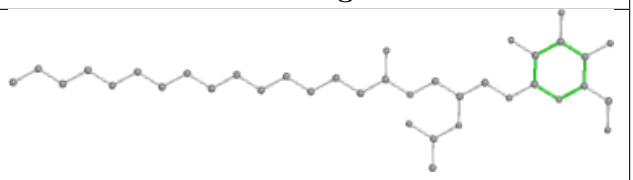


Ligand LMG c 520

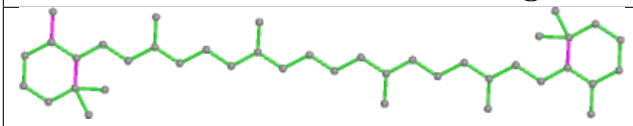

Bond lengths

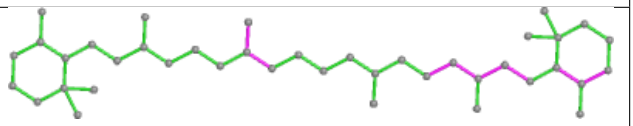

Bond angles

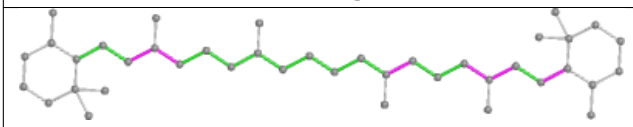

Torsions

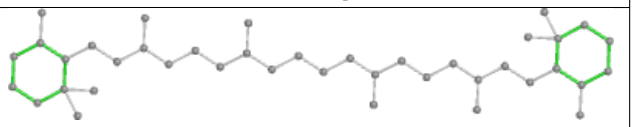

Rings

Ligand BCR C 516

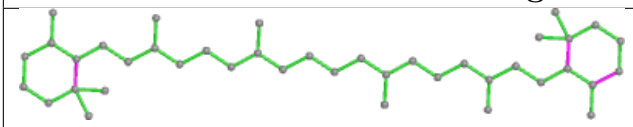

Bond lengths

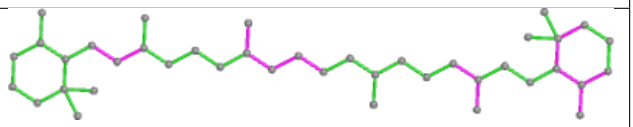

Bond angles

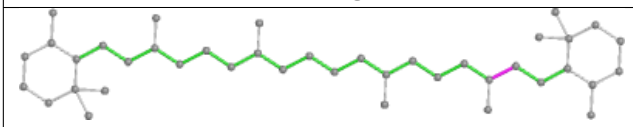

Torsions

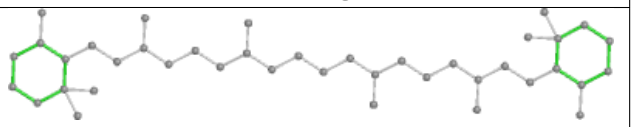

Rings

Ligand BCR a 405

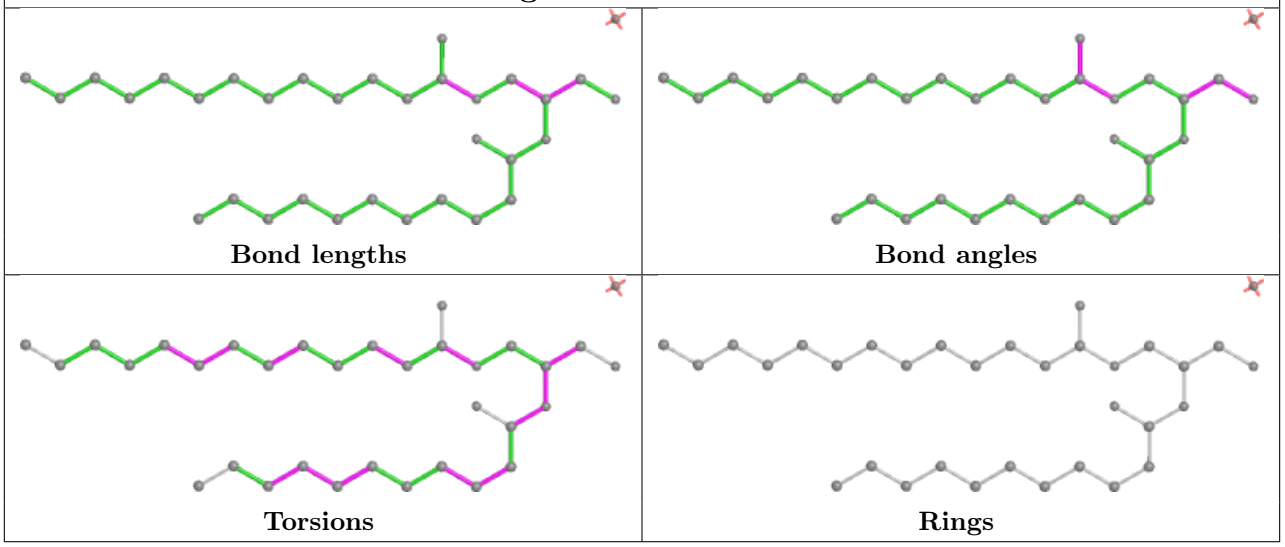

Bond lengths


Bond angles

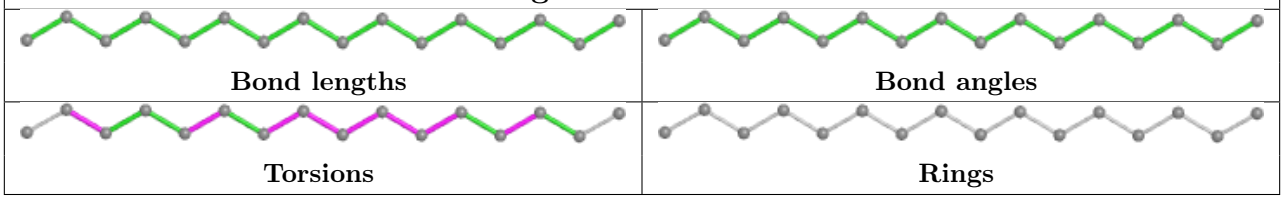

Torsions


Rings

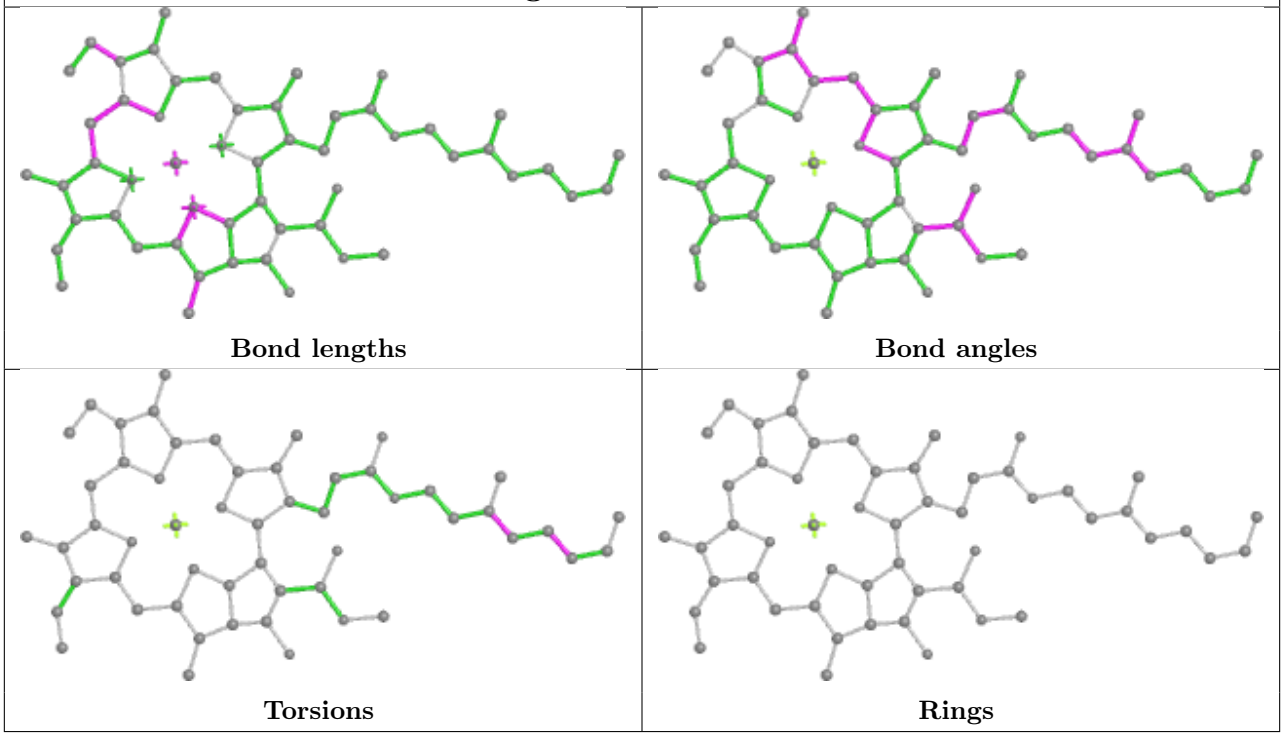
Ligand LMG D 410



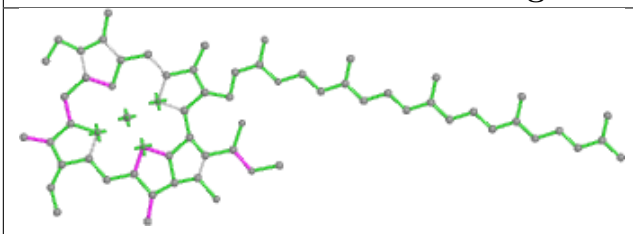
Ligand STE b 621



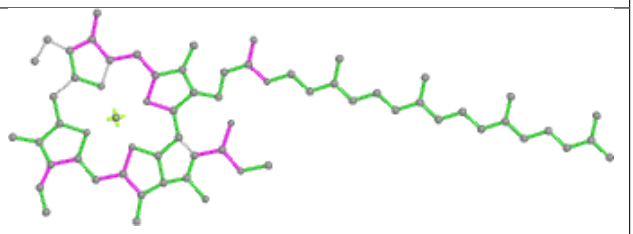
Ligand CLA A 406



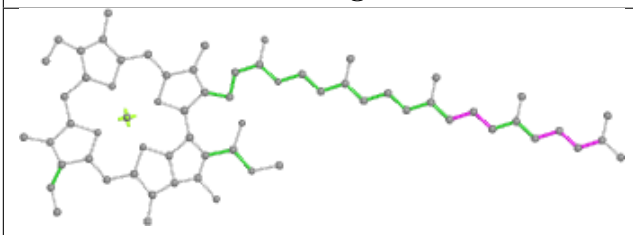
Ligand CLA b 611



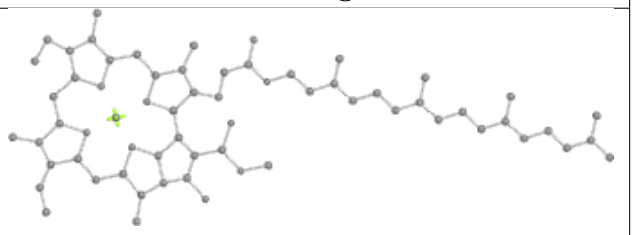
Bond lengths



Bond angles

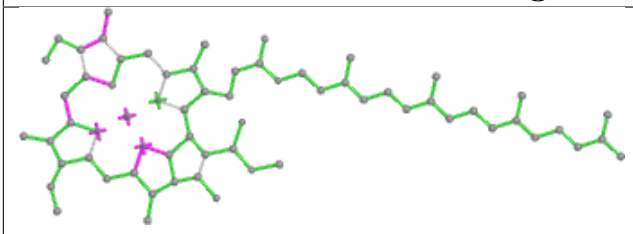


Torsions

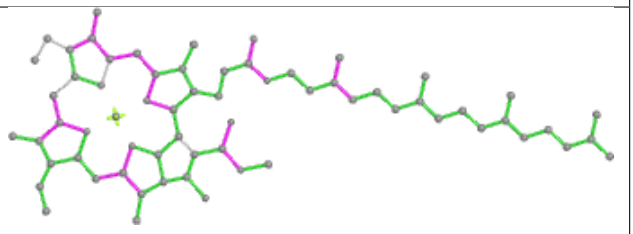


Rings

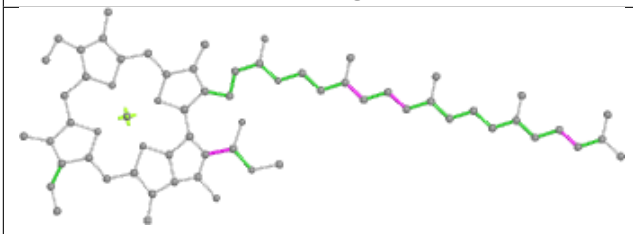
Ligand CLA c 507



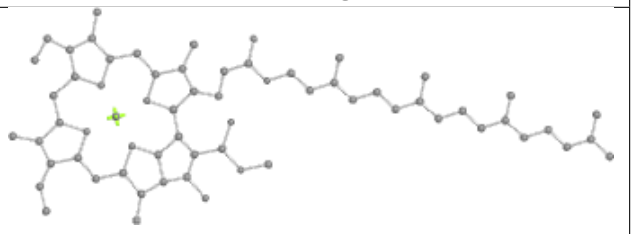
Bond lengths



Bond angles

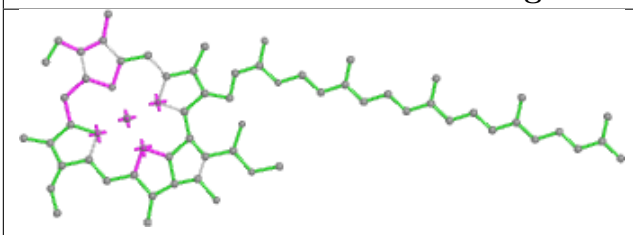


Torsions

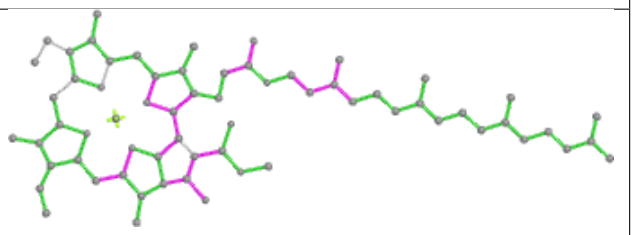


Rings

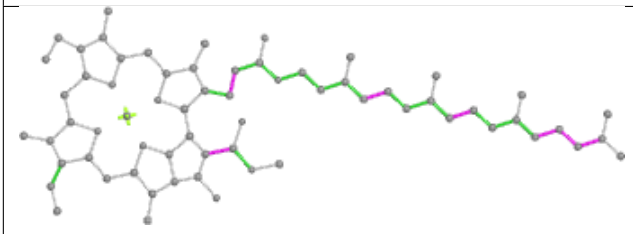
Ligand CLA B 606



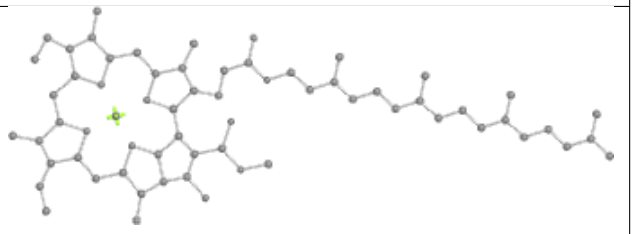
Bond lengths



Bond angles

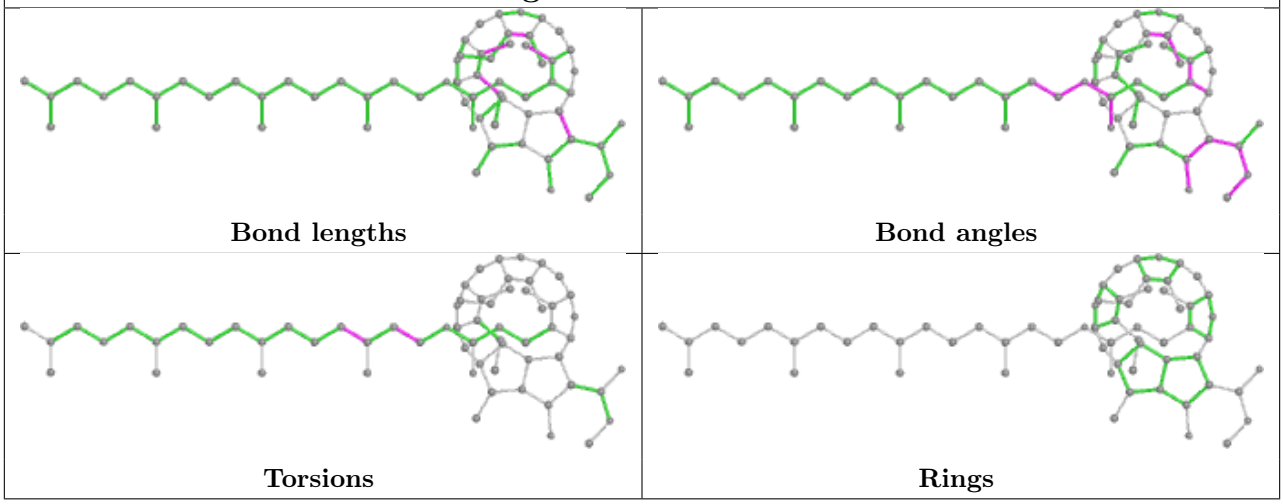


Torsions

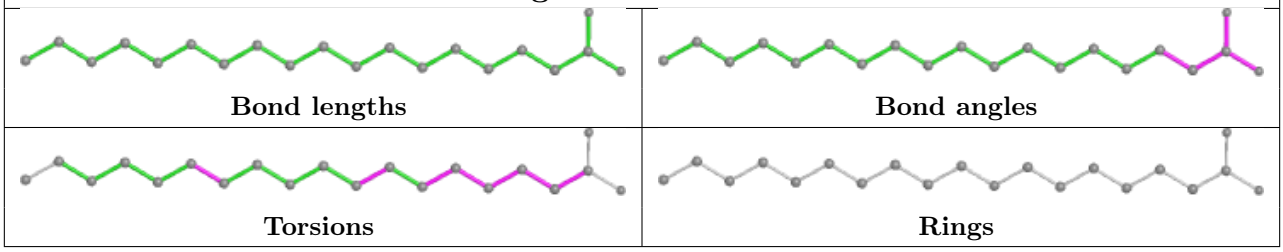


Rings

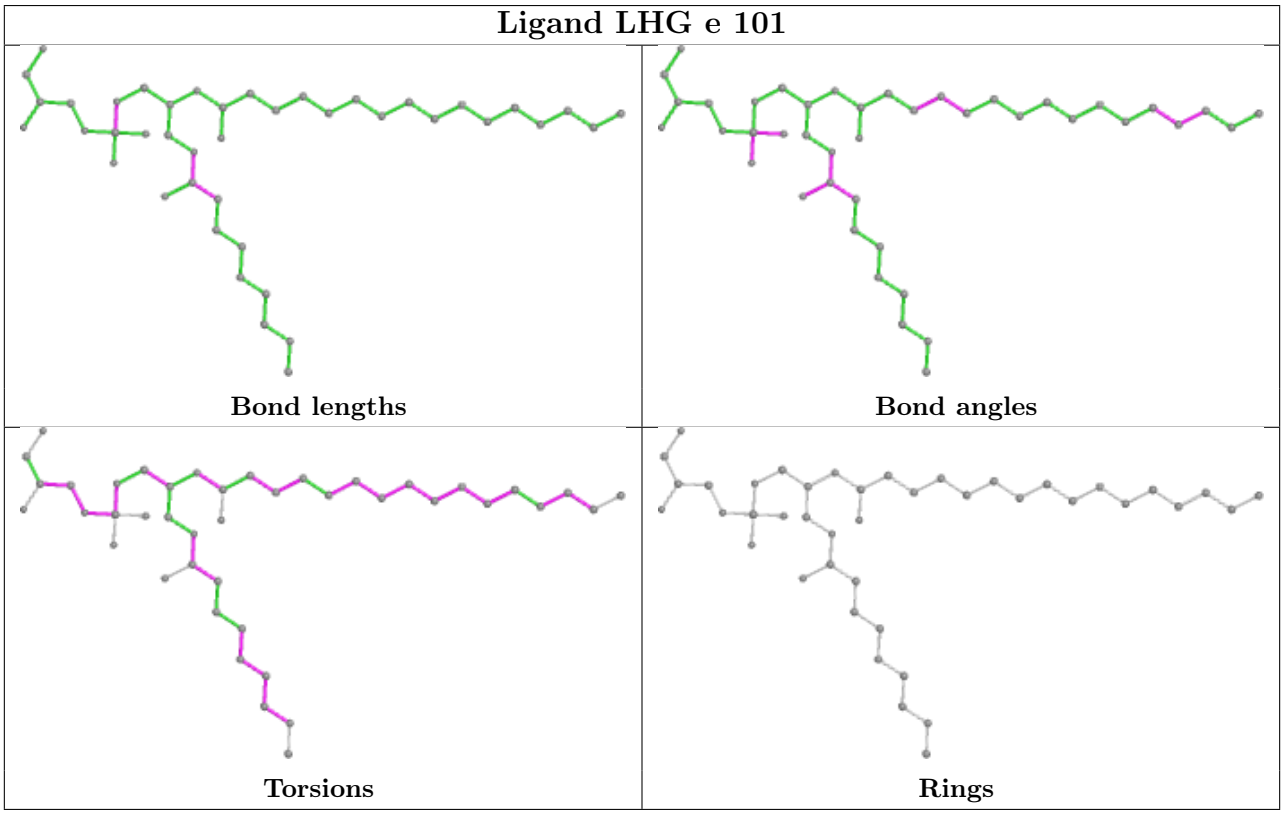
Ligand PHO A 404



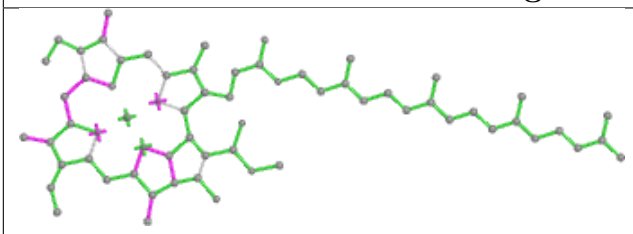
Ligand STE d 412



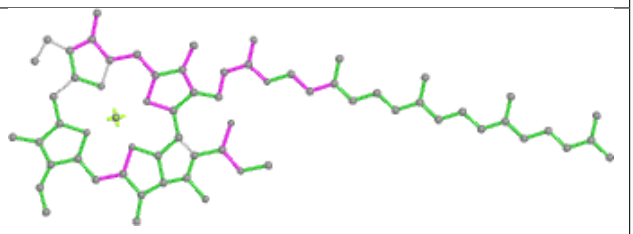
Ligand LHG e 101



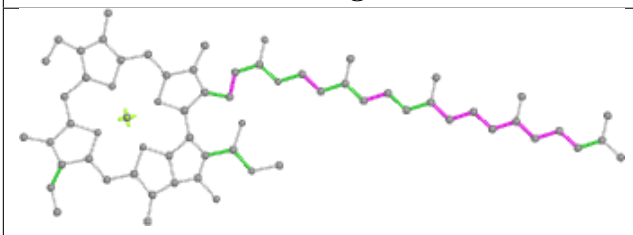
Ligand CLA C 512



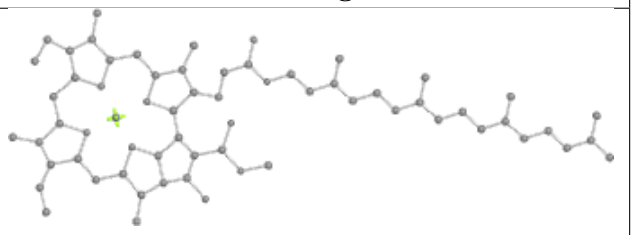
Bond lengths



Bond angles

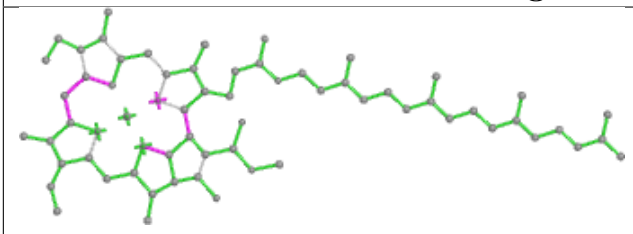


Torsions

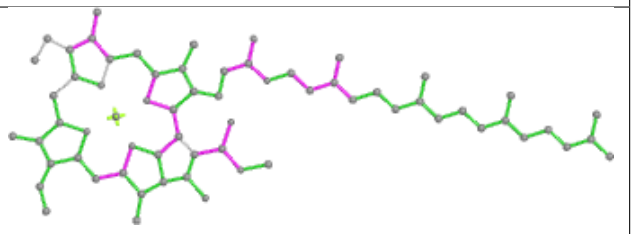


Rings

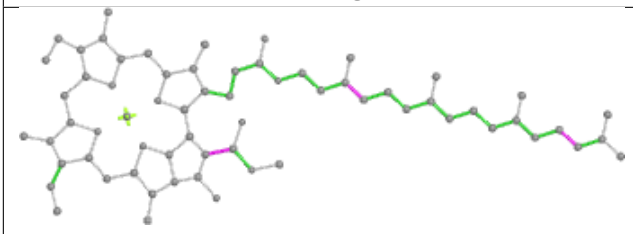
Ligand CLA b 605



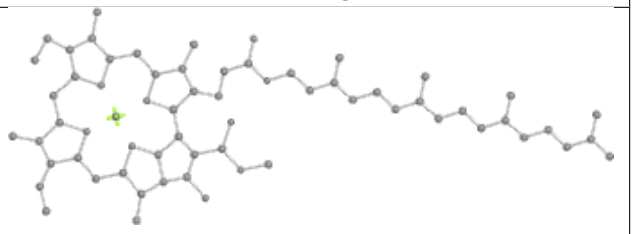
Bond lengths



Bond angles

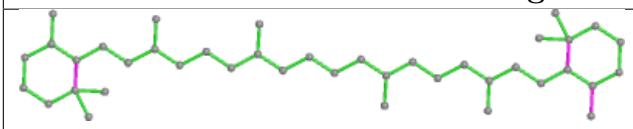


Torsions



Rings

Ligand BCR c 516



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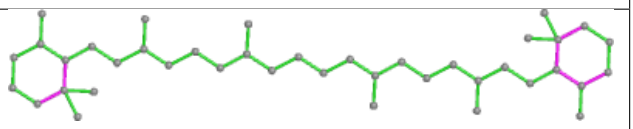
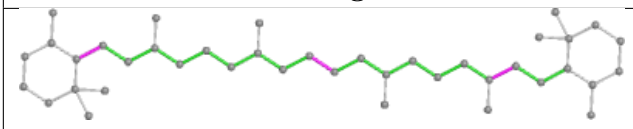


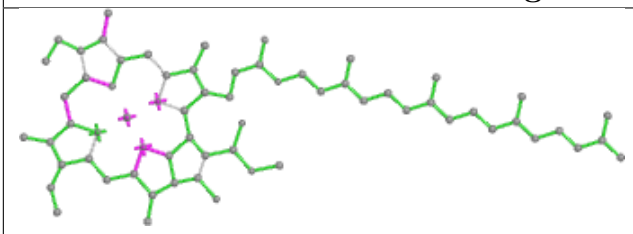
Bond angles



Torsions

Rings

Ligand CLA B 602



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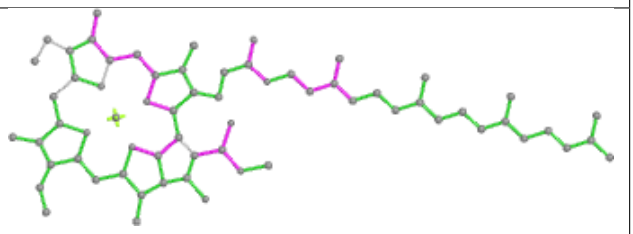
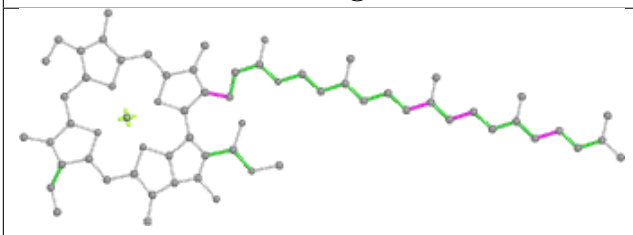
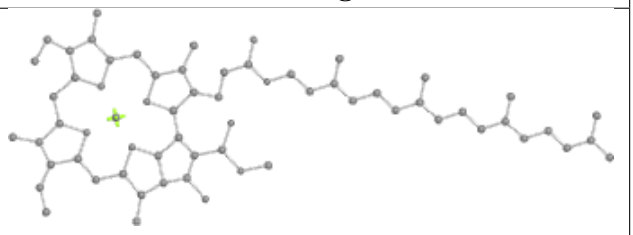


Bond angles

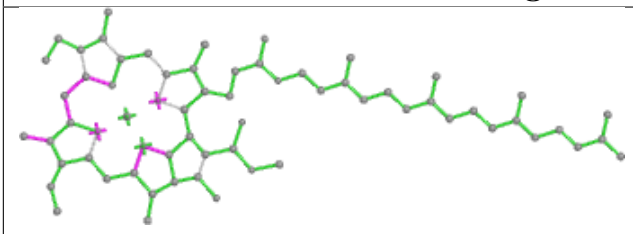


Torsions



Rings

Ligand CLA C 505



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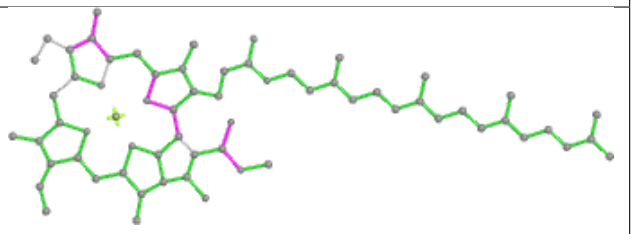
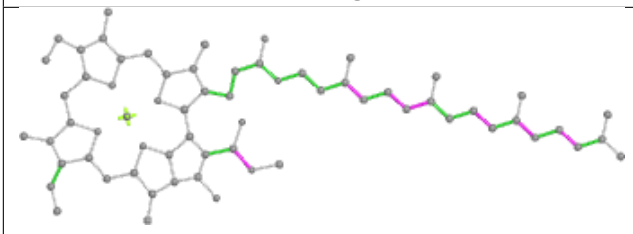
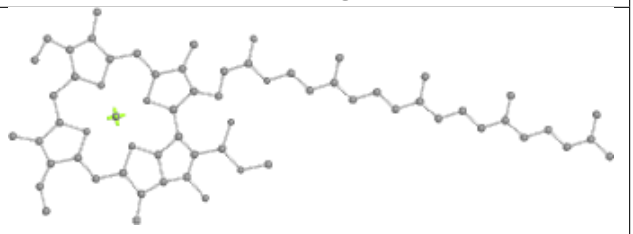


Bond angles

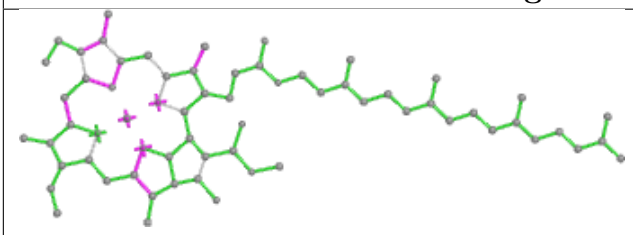


Torsions



Rings

Ligand CLA B 610



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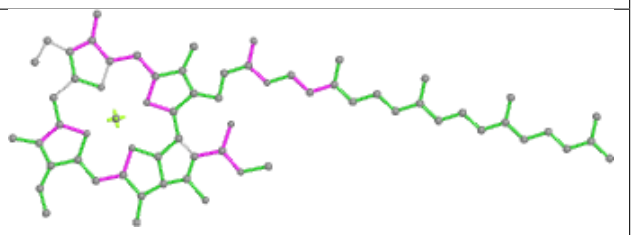
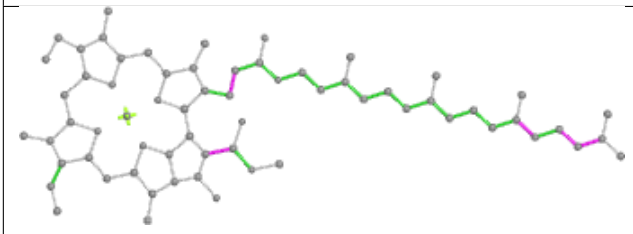
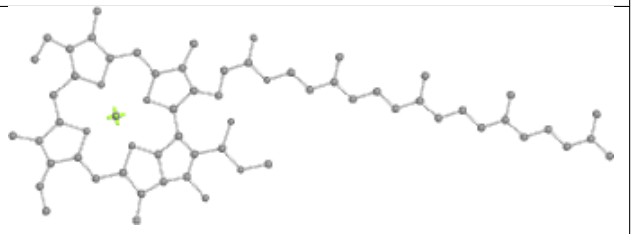


Bond angles

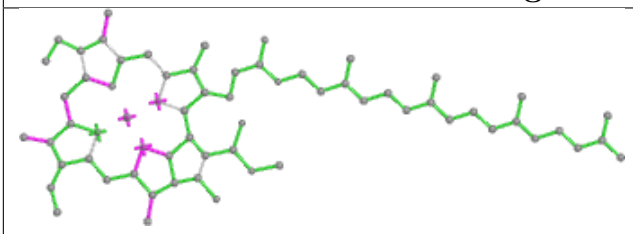


Torsions

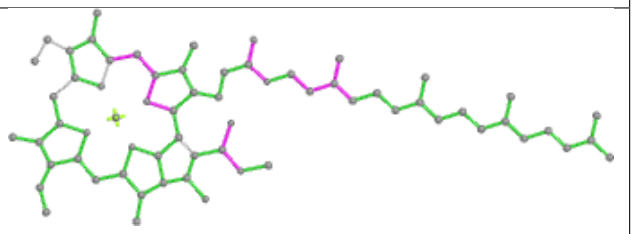


Rings

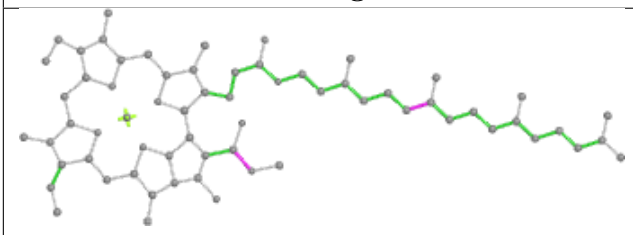
Ligand CLA C 511



Bond lengths



Bond angles



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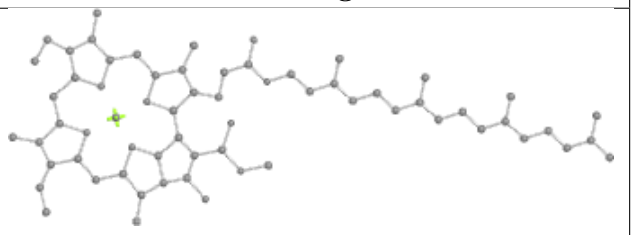
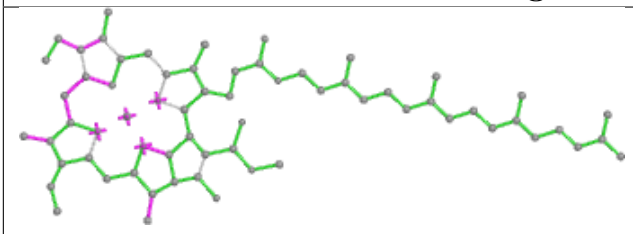
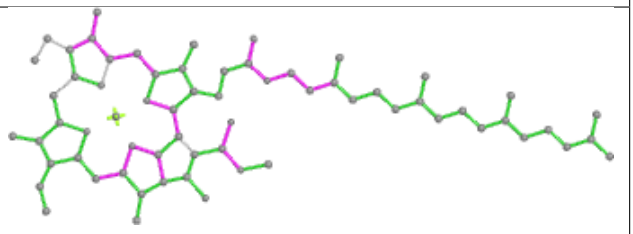


Rings

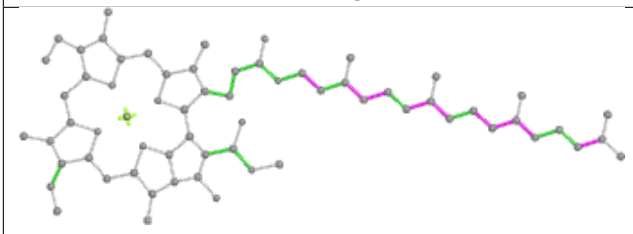
Ligand CLA d 405



Bond lengths



Bond angles



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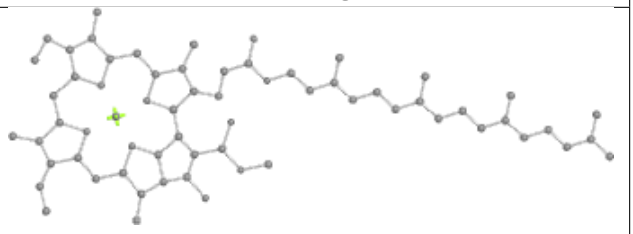
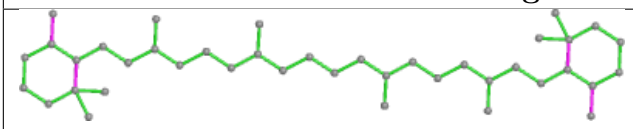


Rings

Ligand BCR C 515



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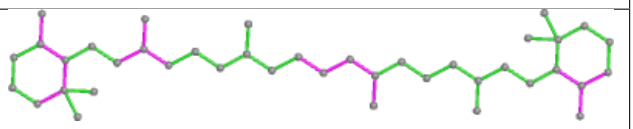
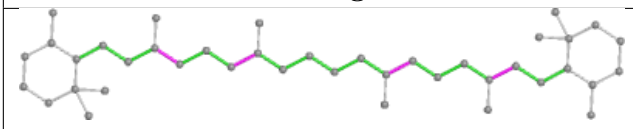


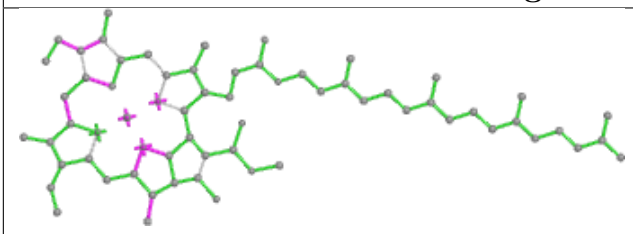
Bond angles



Torsions

Rings

Ligand CLA B 609



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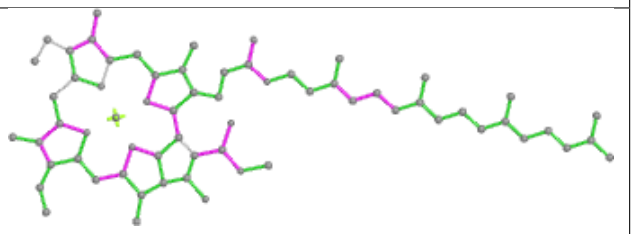
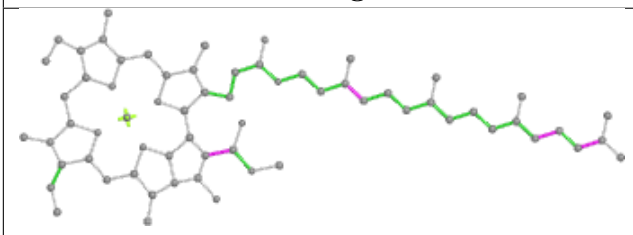
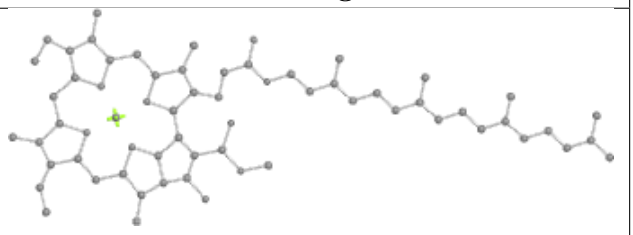


Bond angles

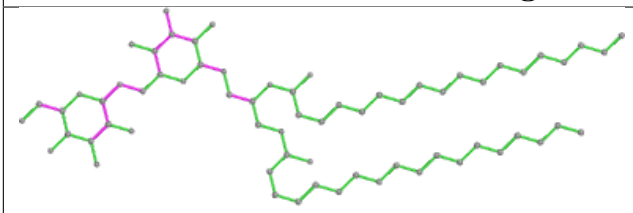


Torsions

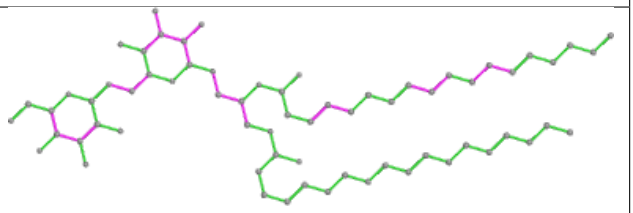


Rings

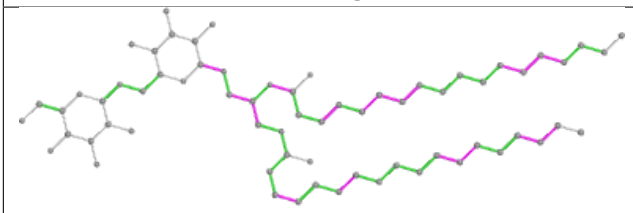
Ligand DGD A 415



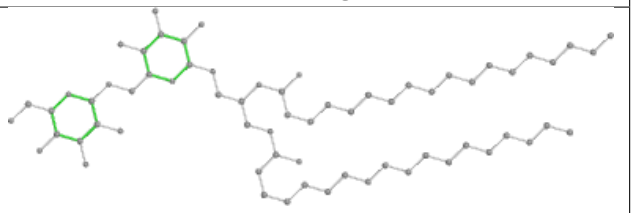
Bond lengths



Bond angles



Torsions

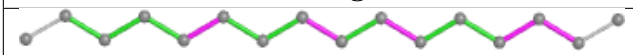


Rings

Ligand STE C 522

Bond lengths

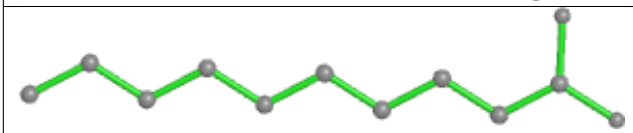
Bond angles



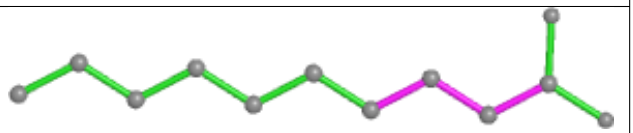
Torsions

Rings

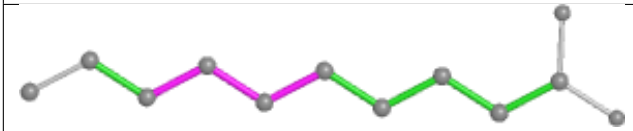
Ligand STE C 523



Bond lengths



Bond angles



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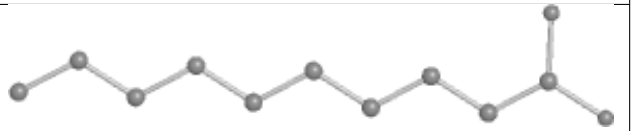
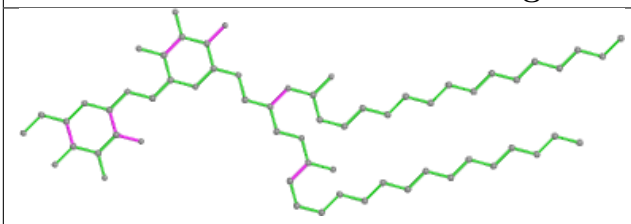


Rings

Ligand DGD h 101



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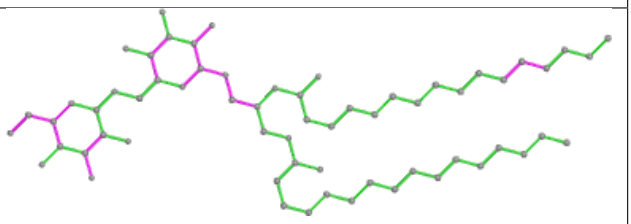
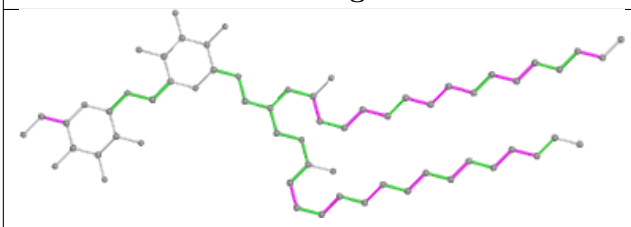


Bond angles



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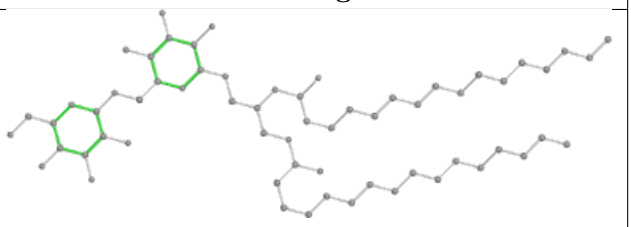
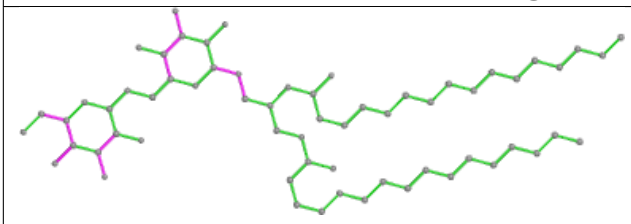
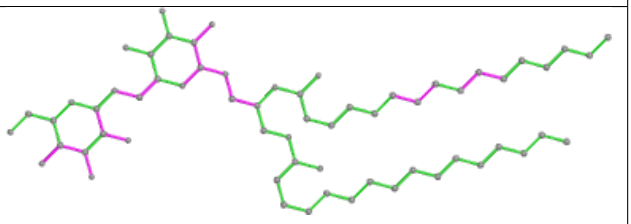


Rings

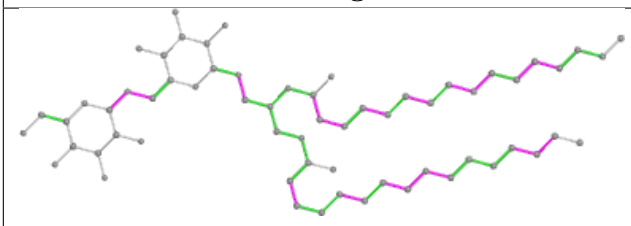
Ligand DGD c 518



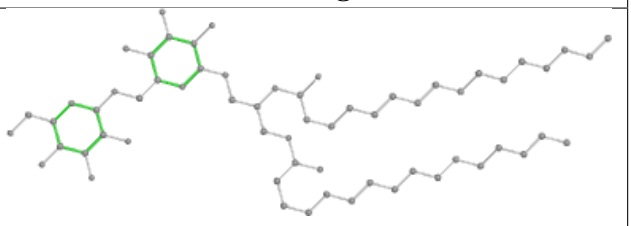
Bond lengths



Bond angles

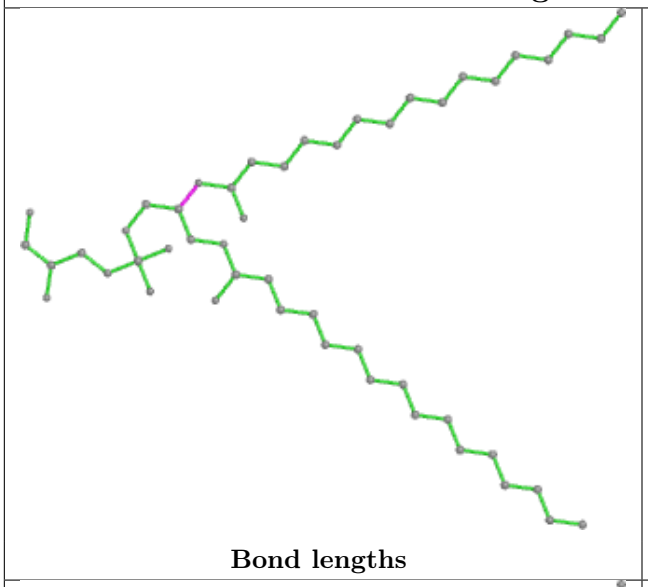


Torsions

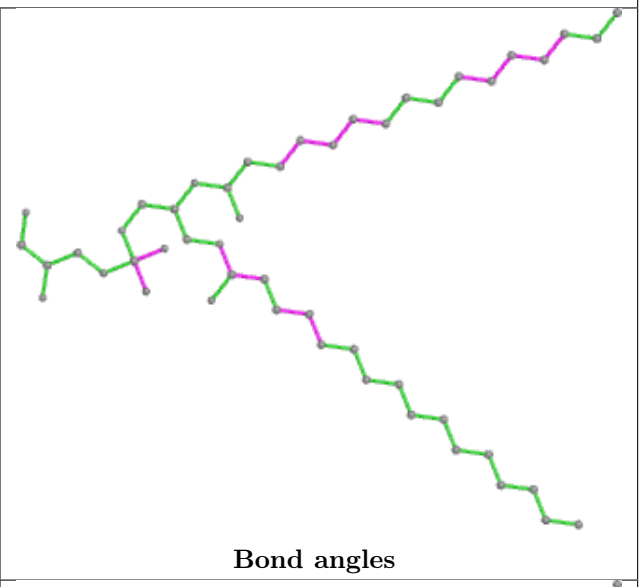


Rings

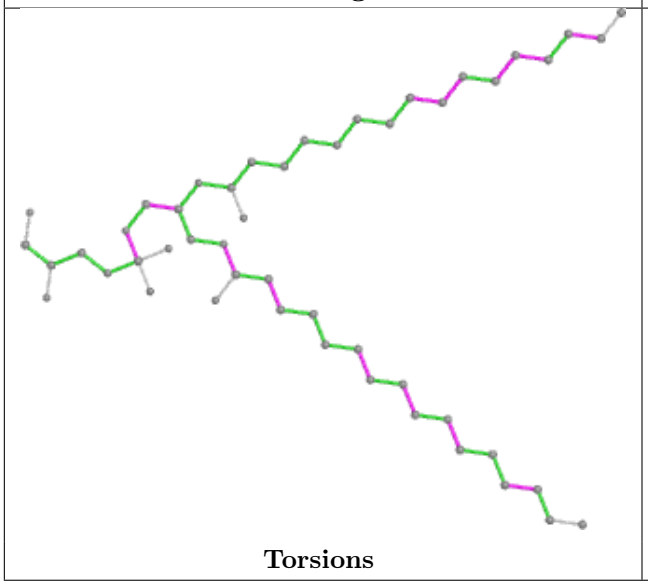
Ligand LHG l 101



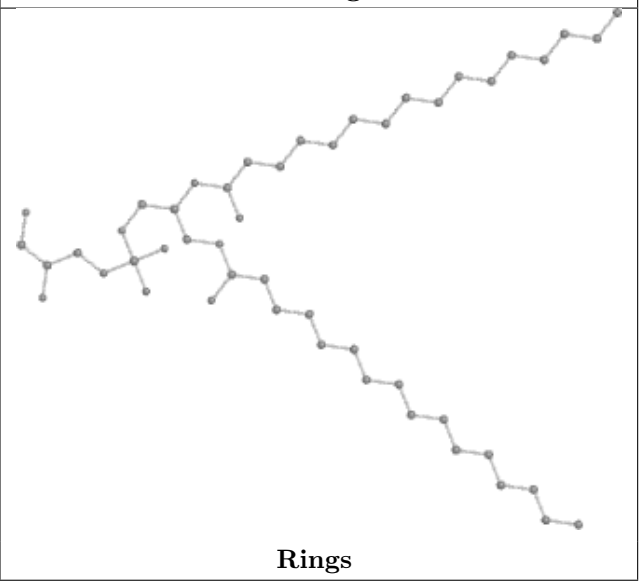
Bond lengths



Bond angles

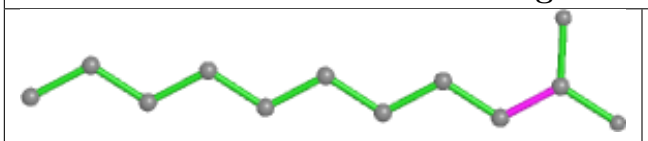


Torsions

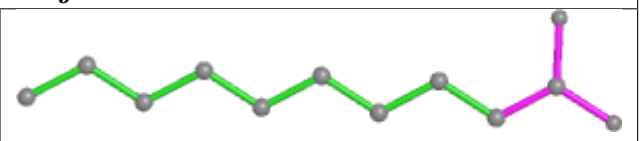


Rings

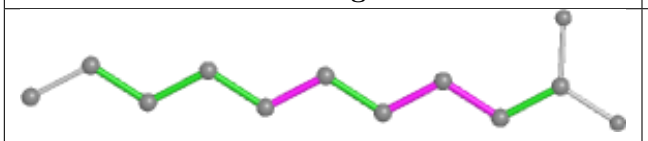
Ligand STE j 101



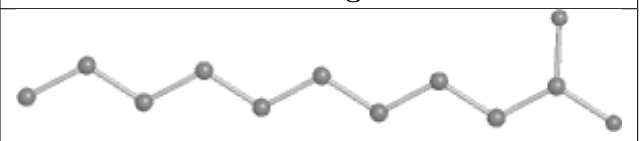
Bond lengths



Bond angles

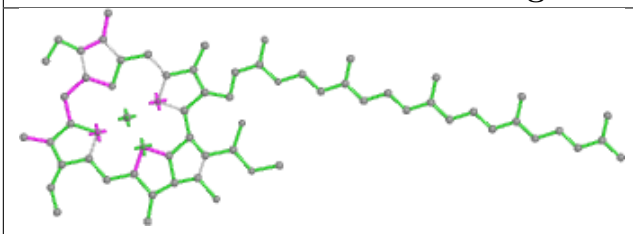


Torsions

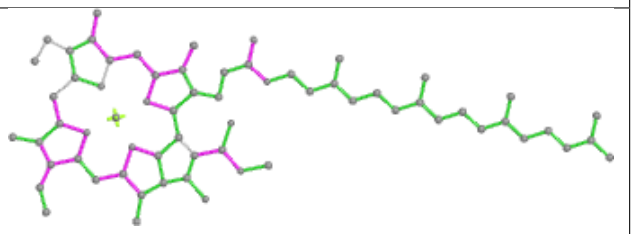


Rings

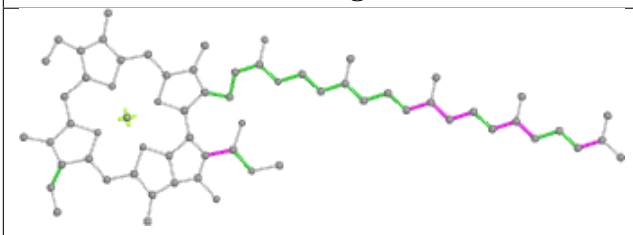
Ligand CLA d 401



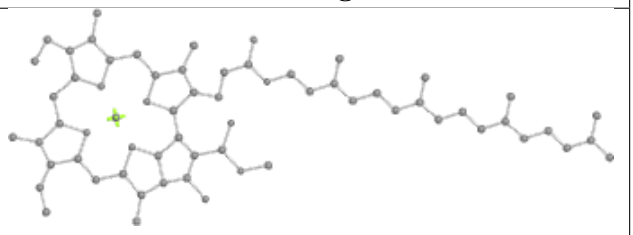
Bond lengths



Bond angles

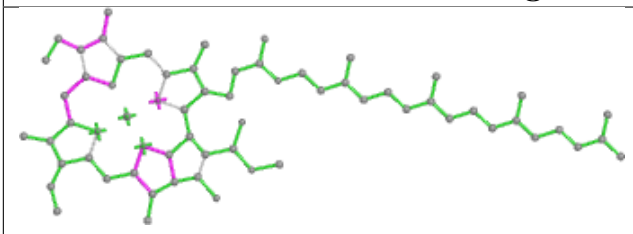


Torsions



Rings

Ligand CLA B 615



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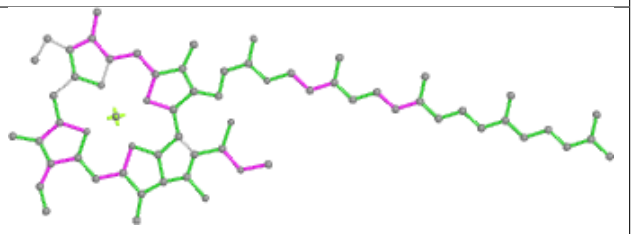
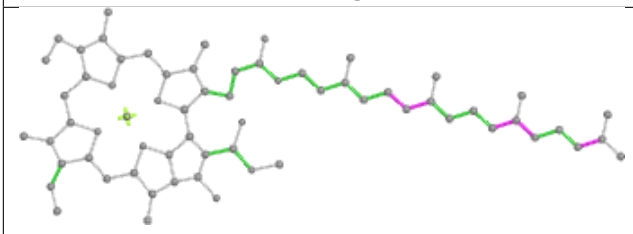
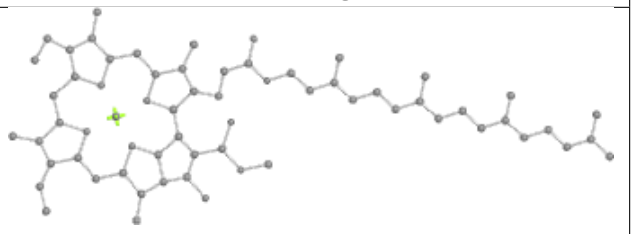


Bond angles

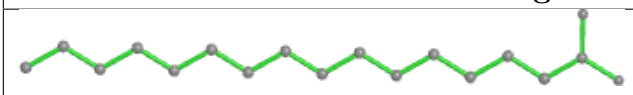


Torsions



Rings

Ligand STE t 103



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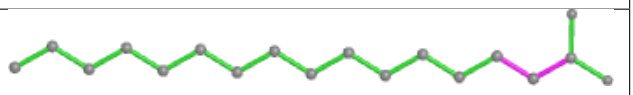
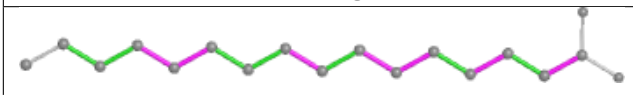
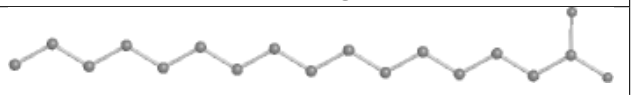


Bond angles

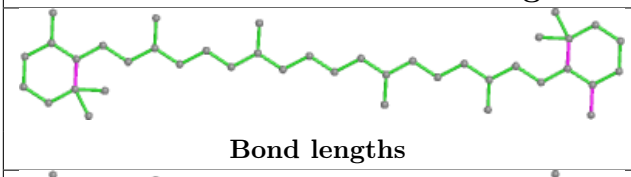


Torsions



Rings

Ligand BCR T 101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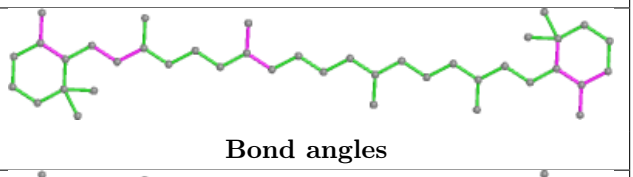
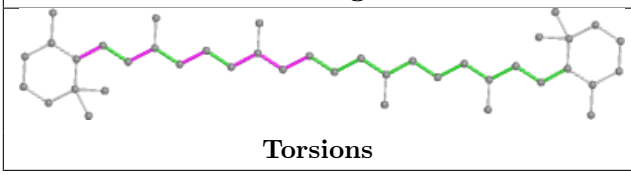

Bond angles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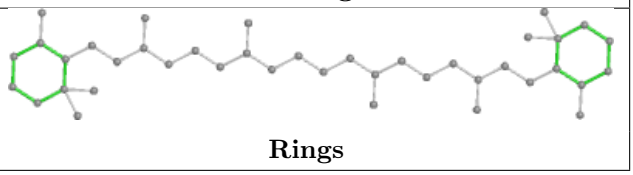
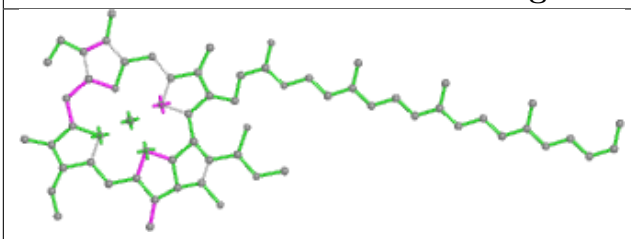
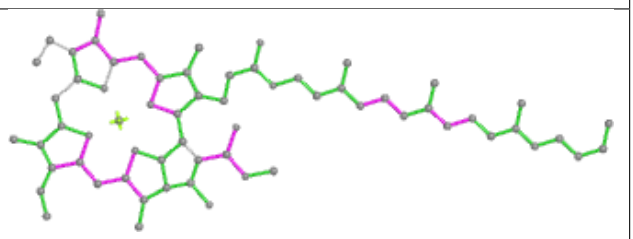
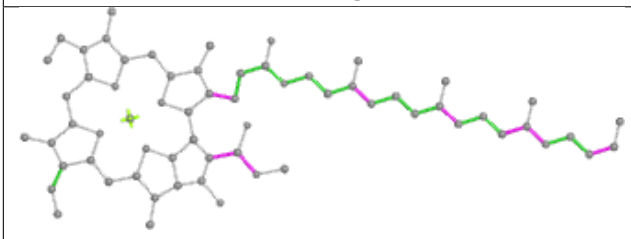

Rings

Ligand CLA c 508


Bond lengths


Bond angles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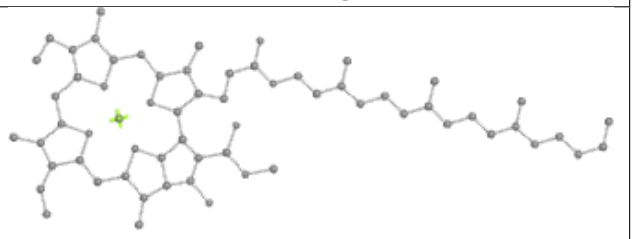
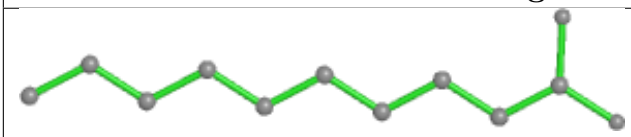

Rings

Ligand STE B 626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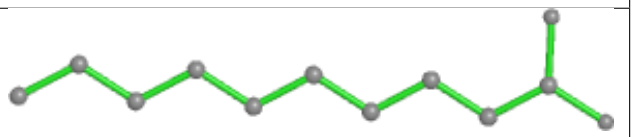
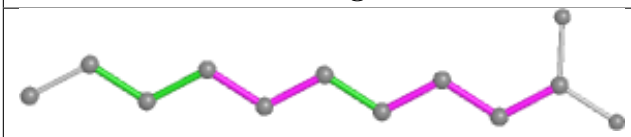

Bond angles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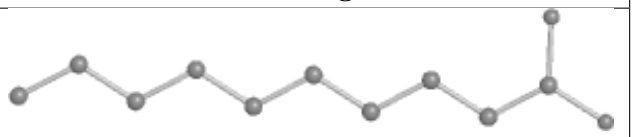
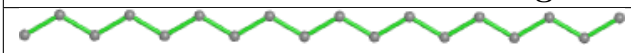

Rings

Ligand STE l 102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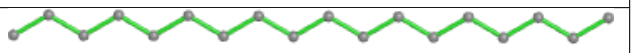
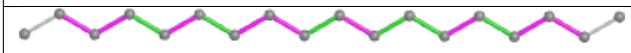

Bond angles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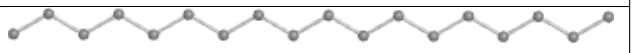
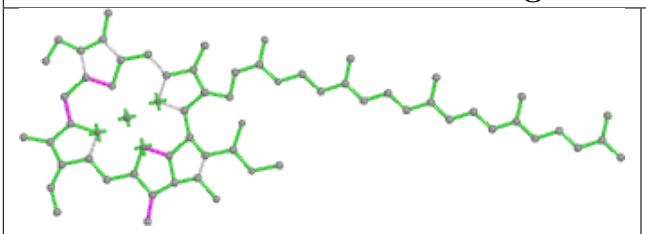
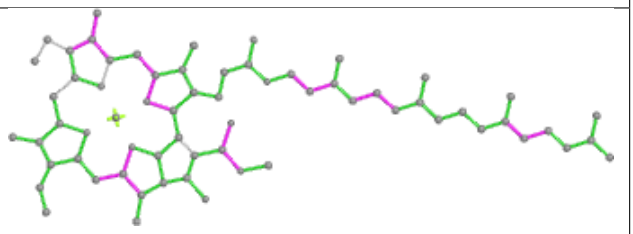

Rings

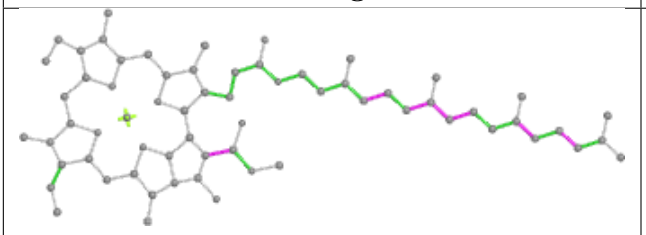
Ligand CLA B 605



Bond lengths



Bond angles



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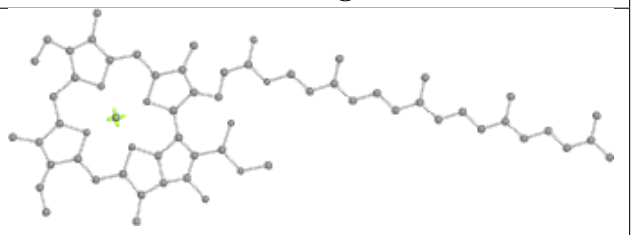
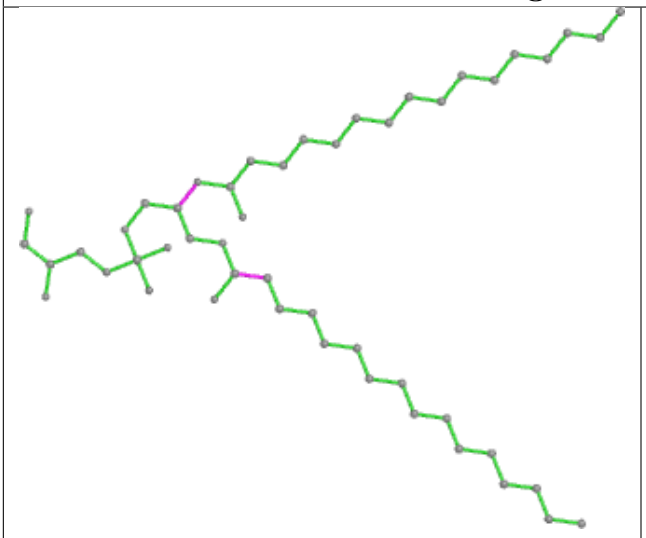
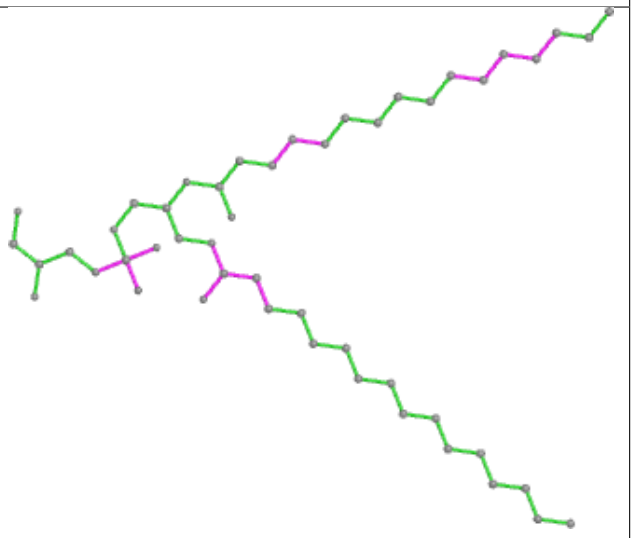


Rings

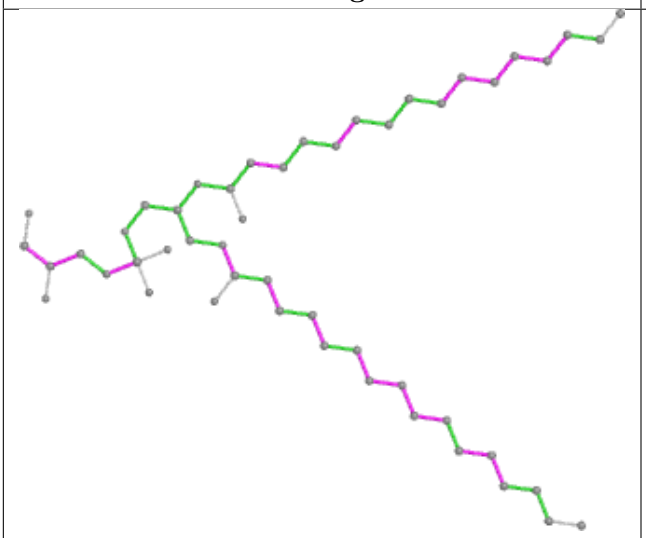
Ligand LHG a 410



Bond lengths



Bond angles



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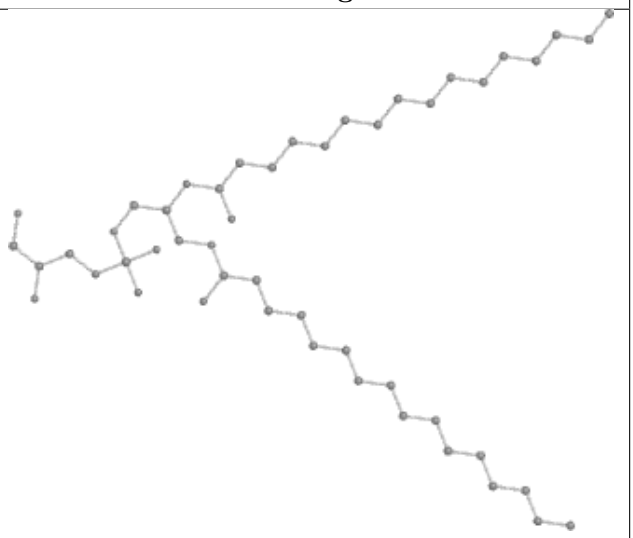
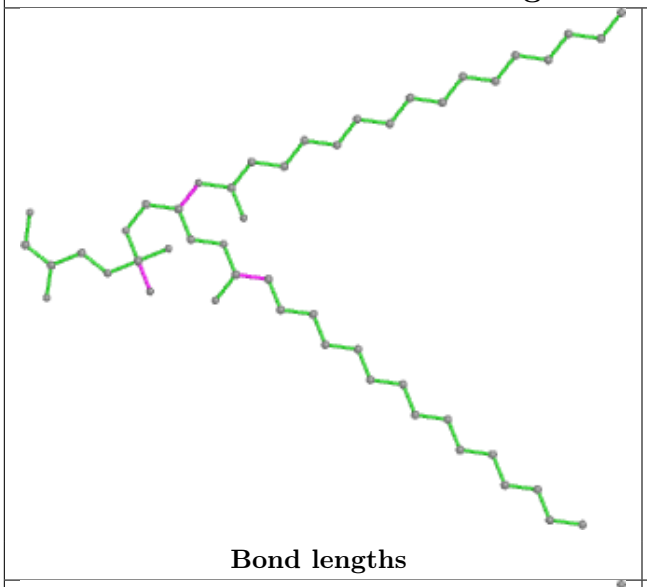


Rings

Ligand LHG B 622



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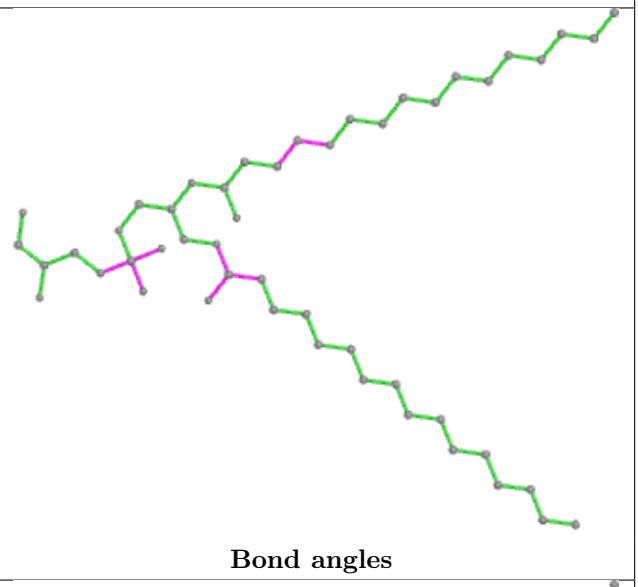
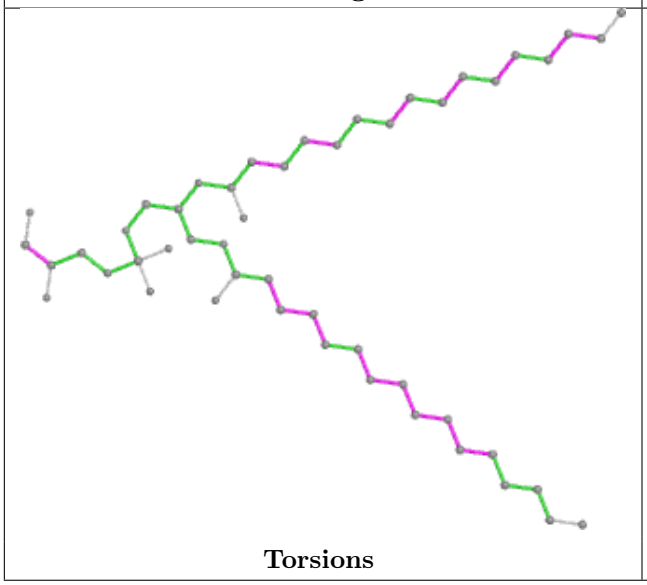


Bond angles



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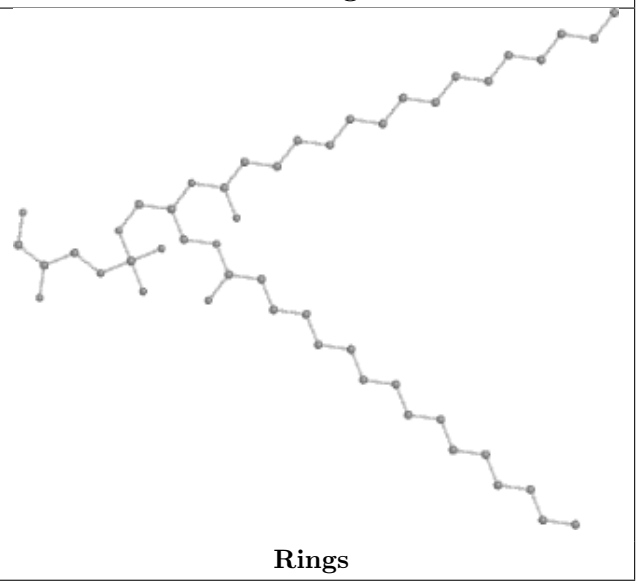
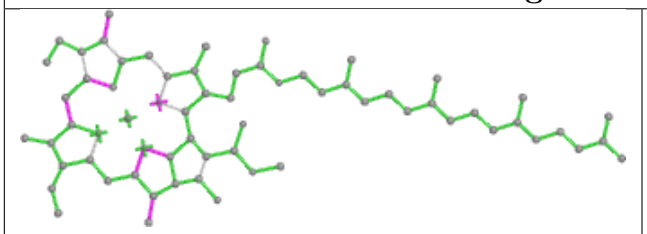


Rings

Ligand CLA C 507



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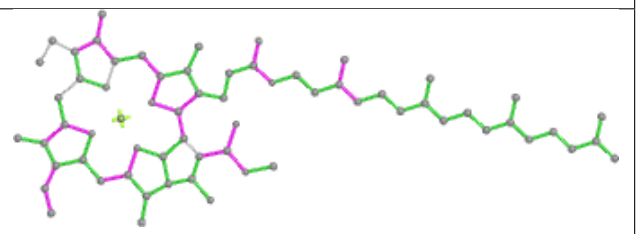
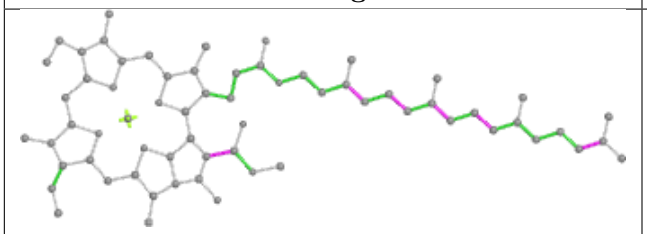


Bond angles



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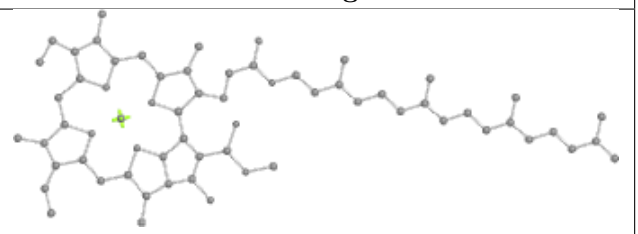
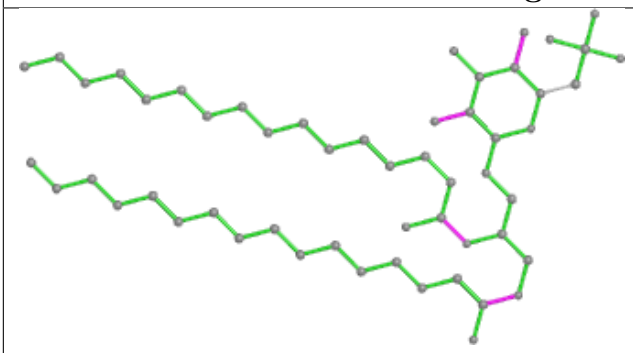
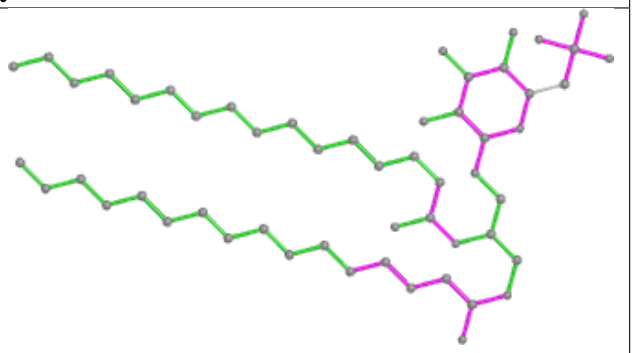


Rings

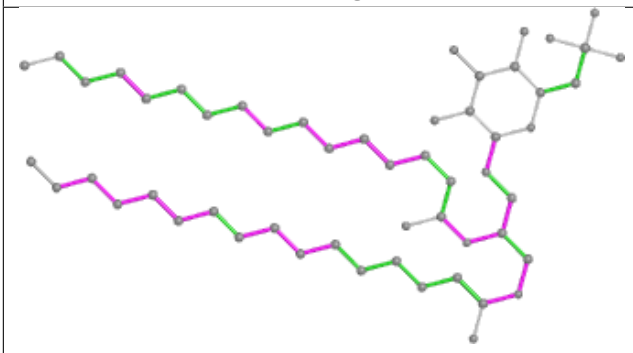
Ligand SQD B 623



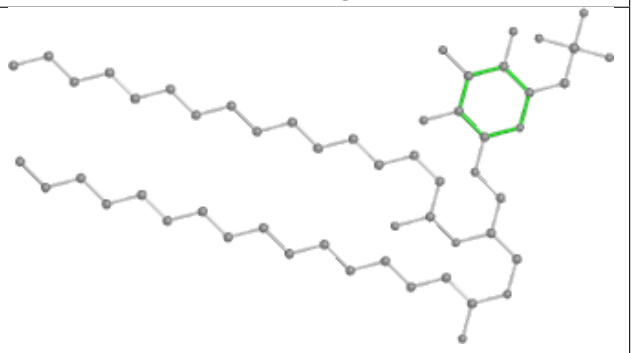
Bond lengths



Bond angles

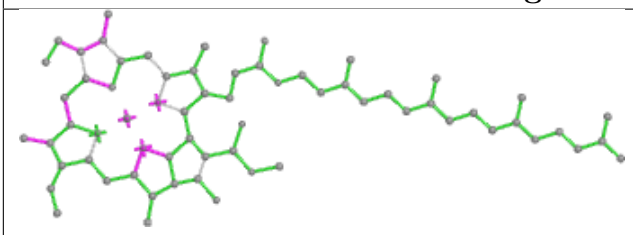


Torsions

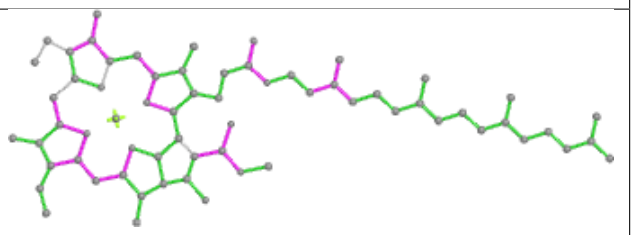


Rings

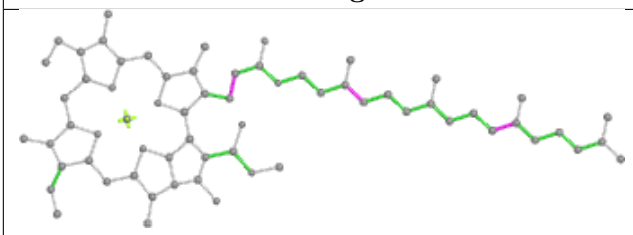
Ligand CLA B 603



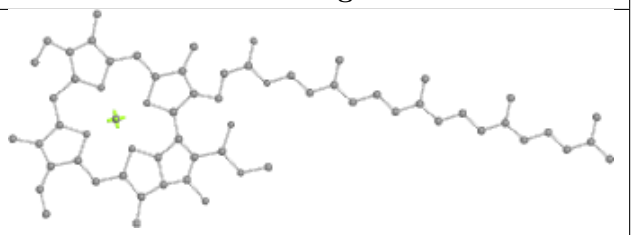
Bond lengths



Bond angles

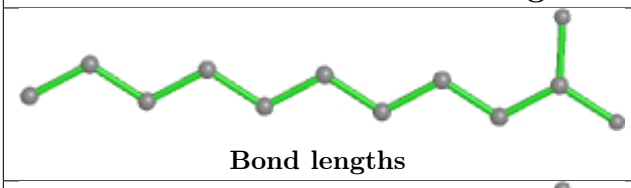


Torsions

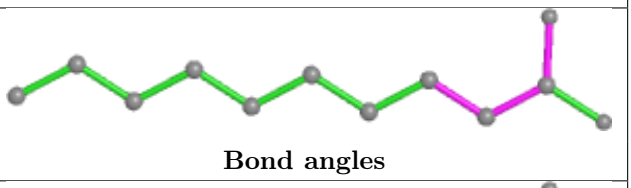


Rings

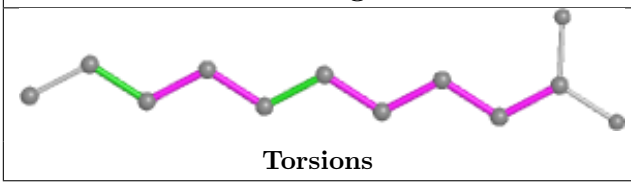
Ligand STE C 521



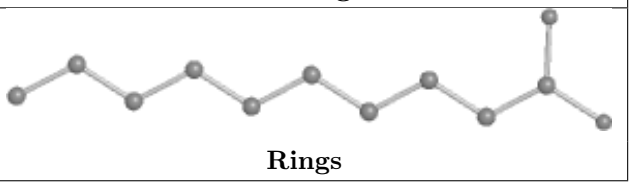
Bond lengths



Bond angles

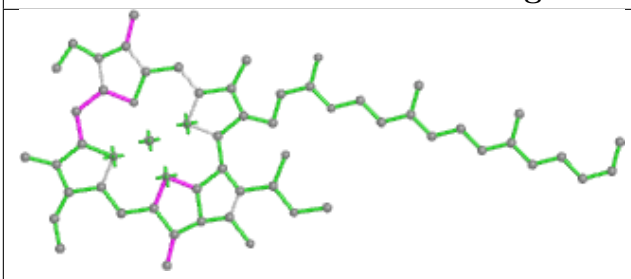


Torsions

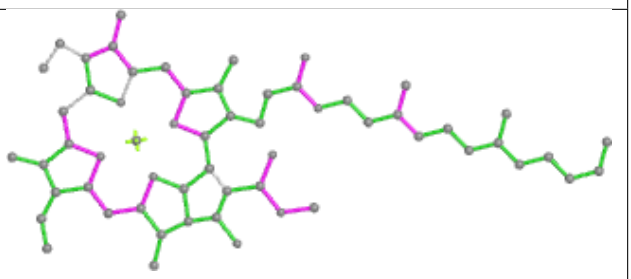


Rings

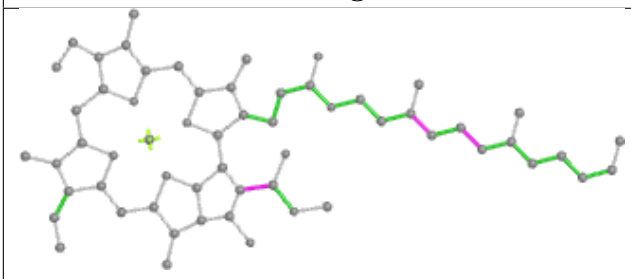
Ligand CLA C 504



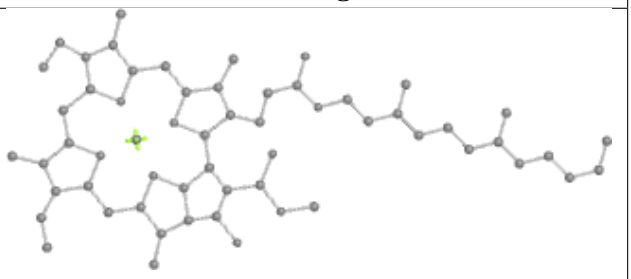
Bond lengths



Bond angles

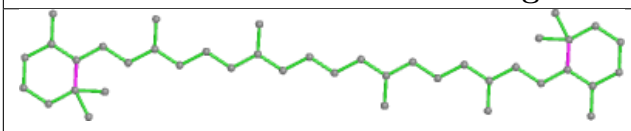


Torsions

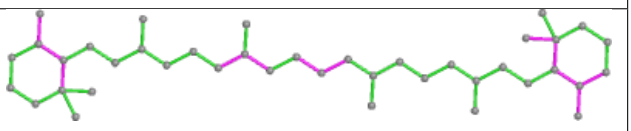


Rings

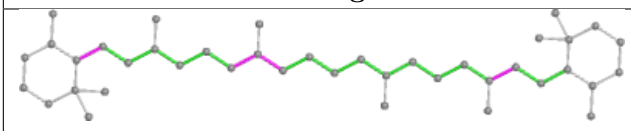
Ligand BCR Y 101



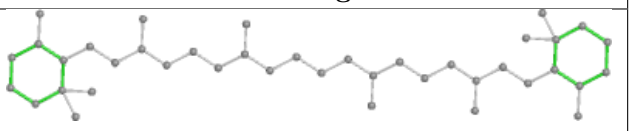
Bond lengths



Bond angles

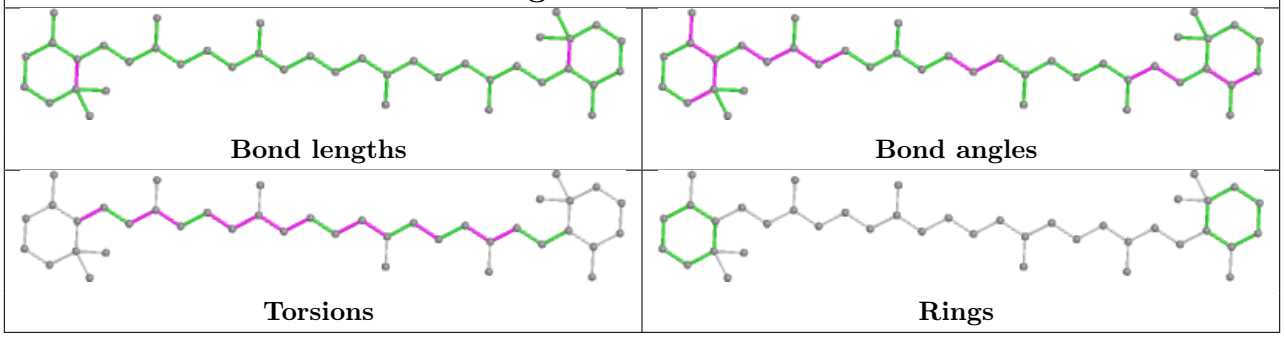


Torsions

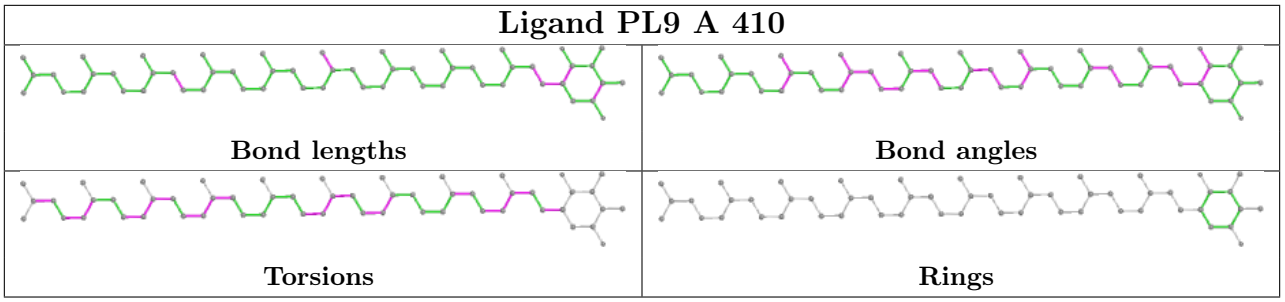


Rings

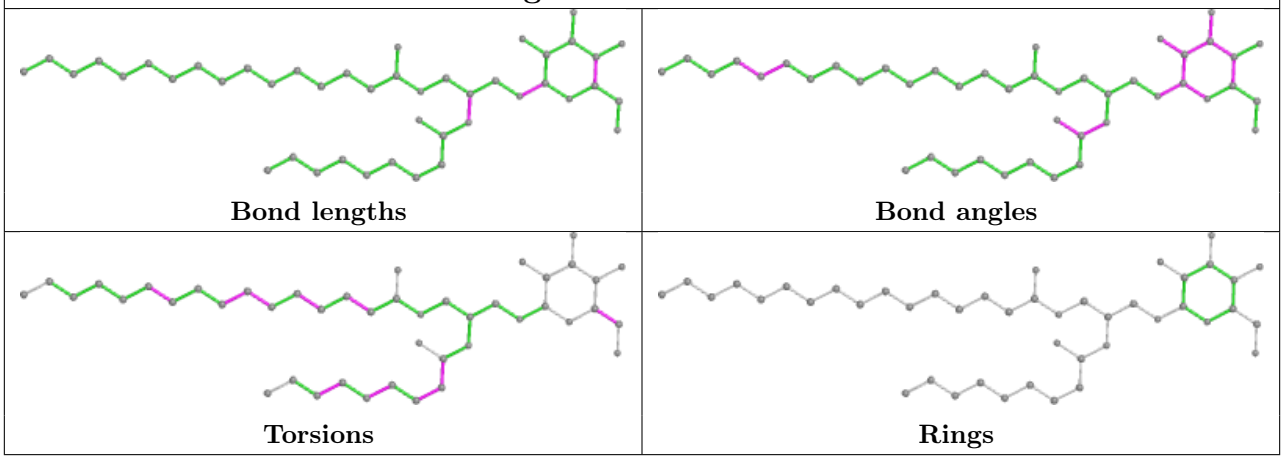
Ligand BCR c 514



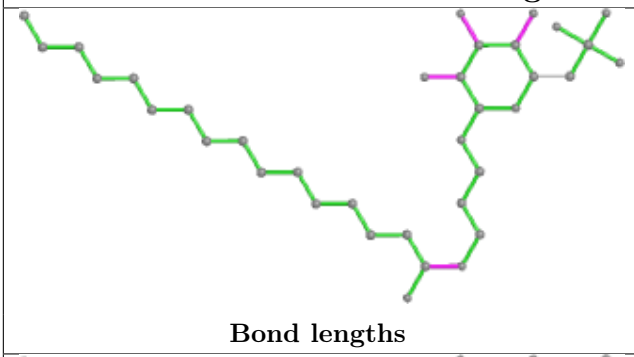
Ligand PL9 A 410



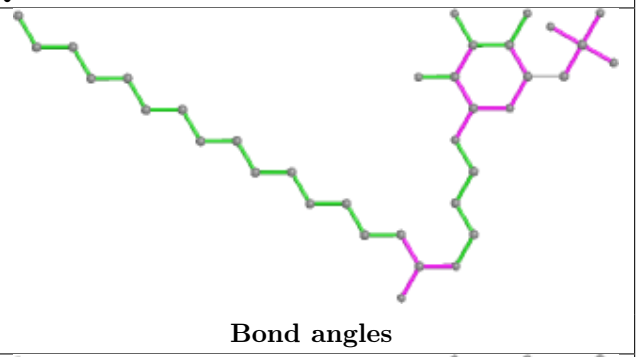
Ligand LMG d 410



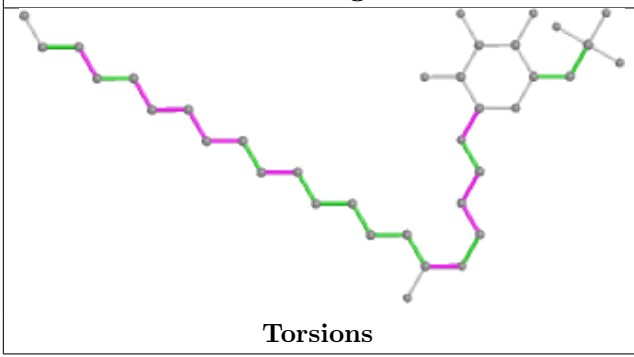
Ligand SQD D 408



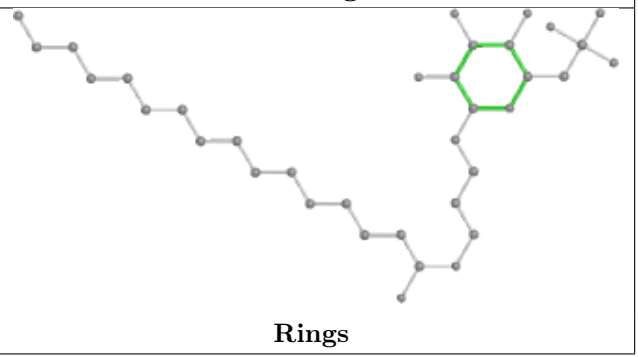
Bond lengths



Bond angles

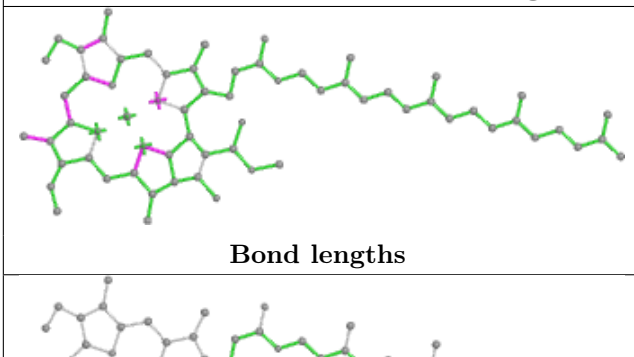


Torsions

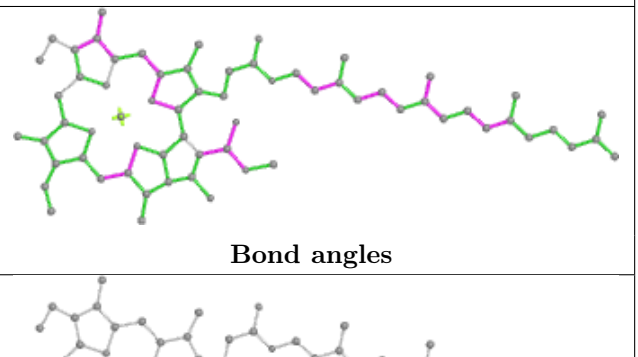


Rings

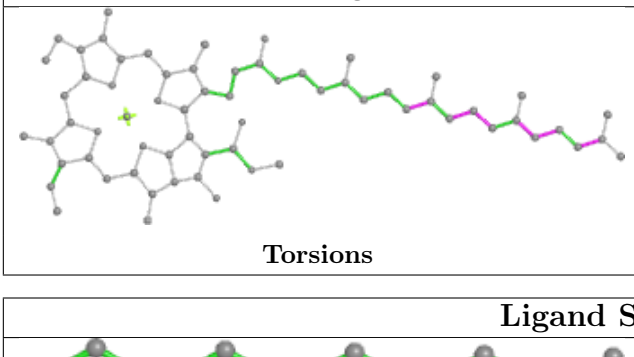
Ligand CLA B 611



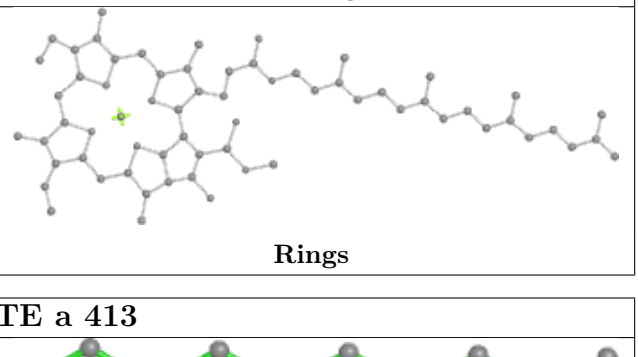
Bond lengths



Bond angles

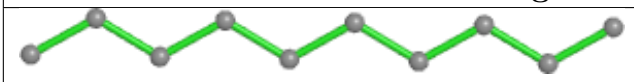


Torsions

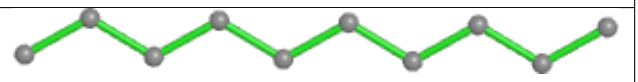


Rings

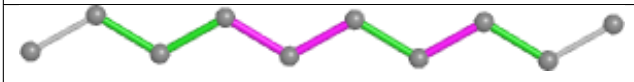
Ligand STE a 413



Bond lengths



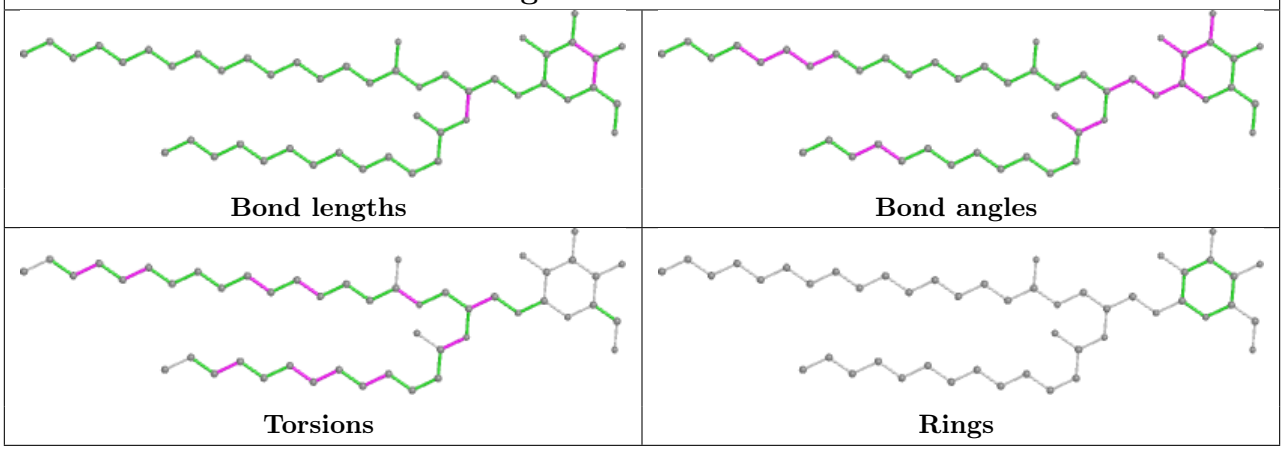
Bond angles



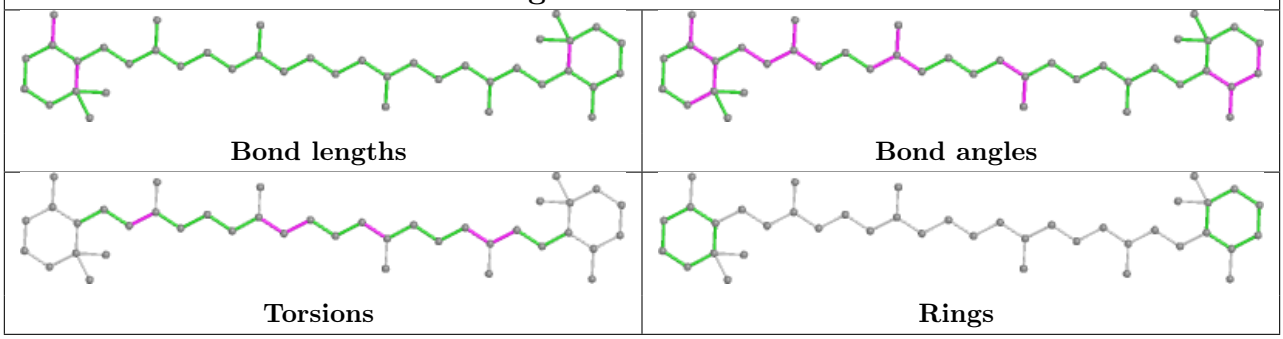
Torsions

Rings

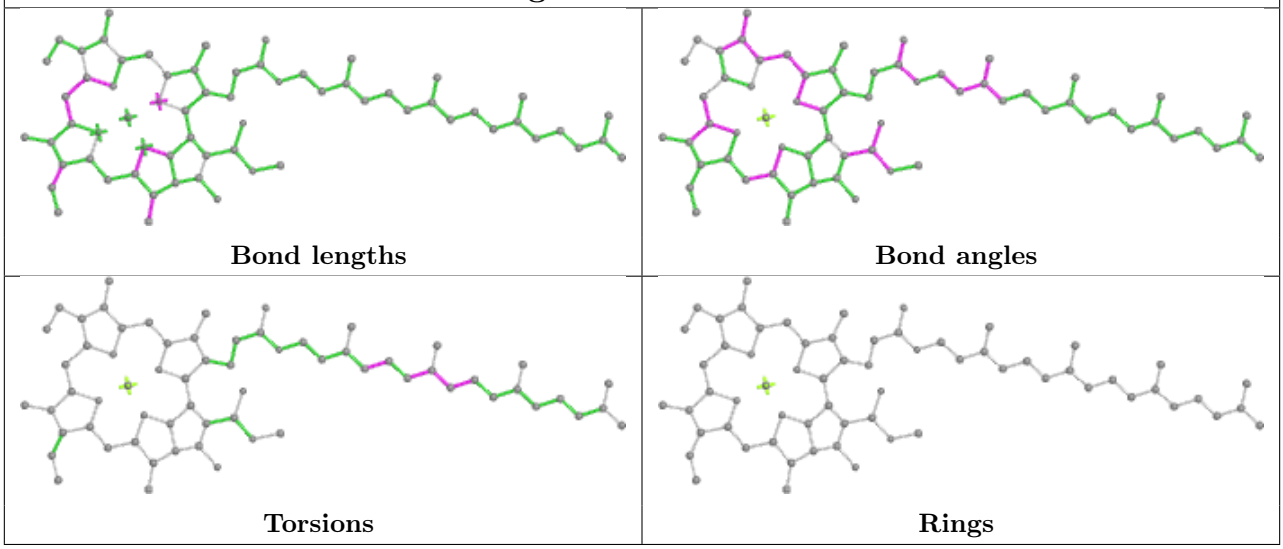
Ligand LMG C 520



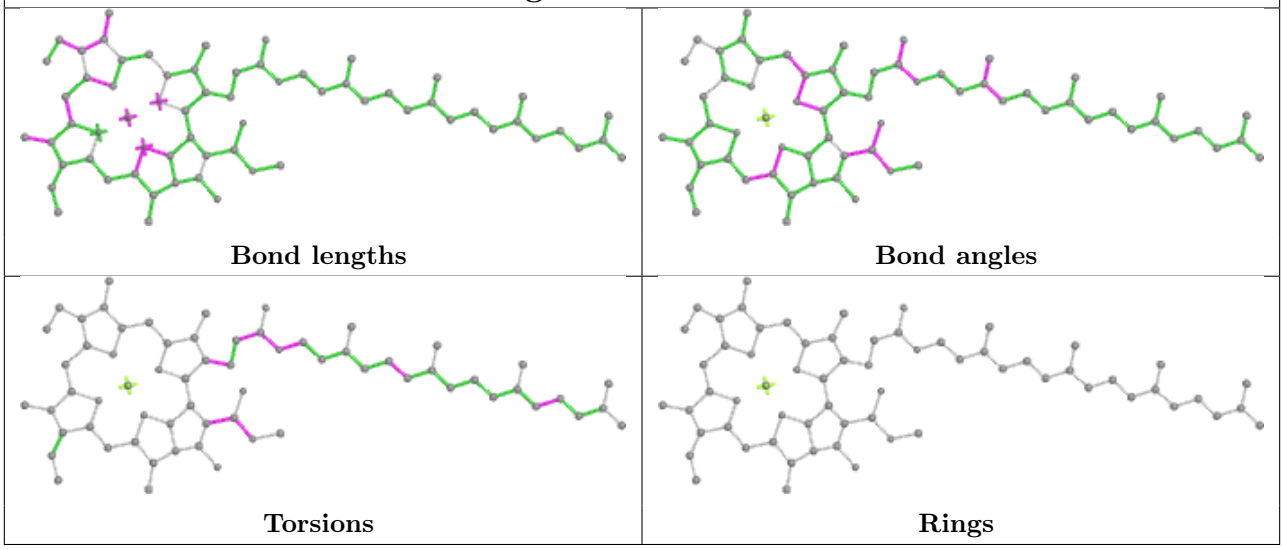
Ligand BCR c 515



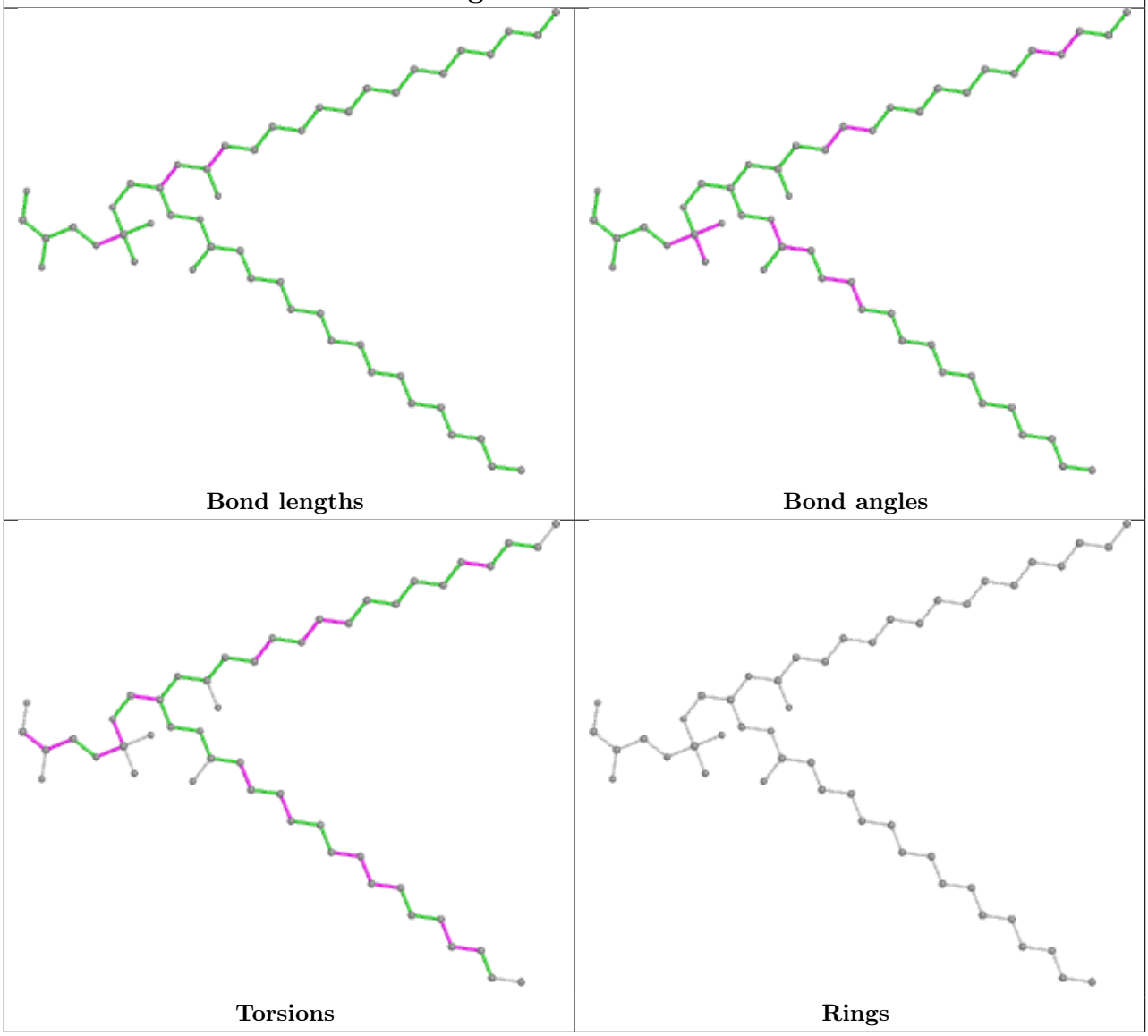
Ligand CLA b 602



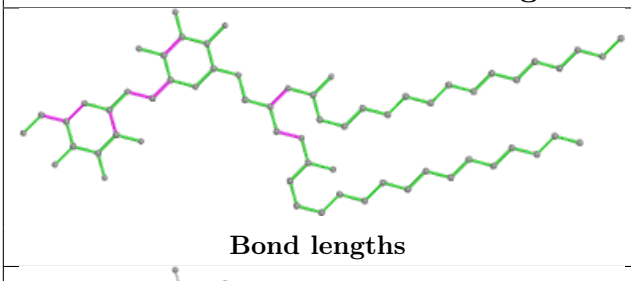
Ligand CLA B 601



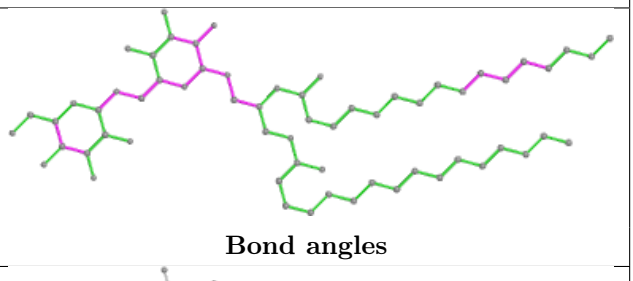
Ligand LHG D 409



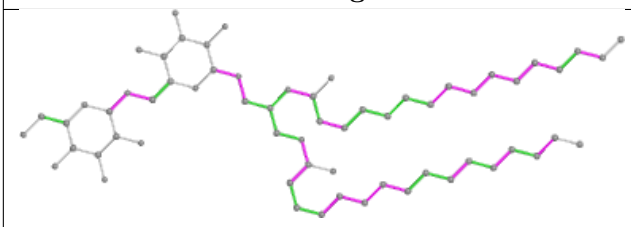
Ligand DGD C 518



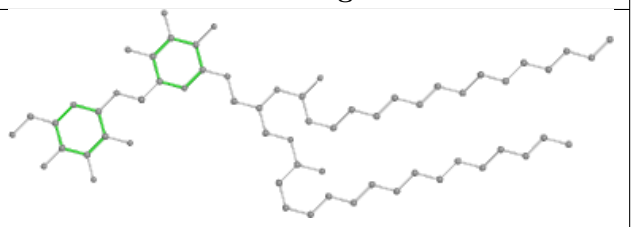
Bond lengths



Bond angles

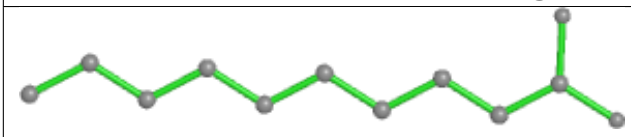


Torsions

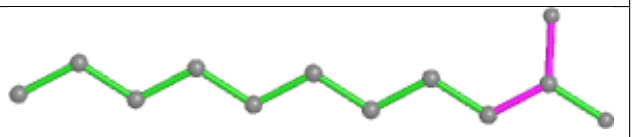


Rings

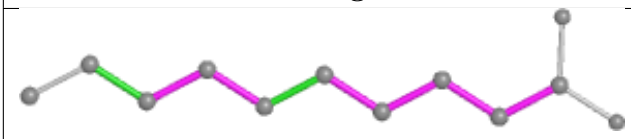
Ligand STE k 102



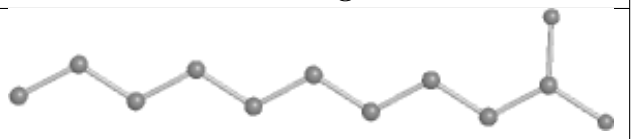
Bond lengths



Bond angles

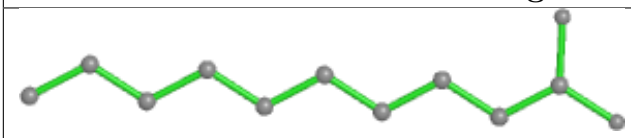


Torsions

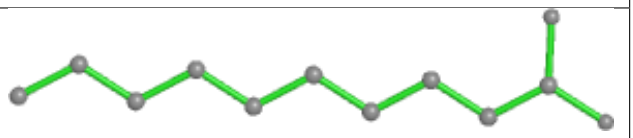


Rings

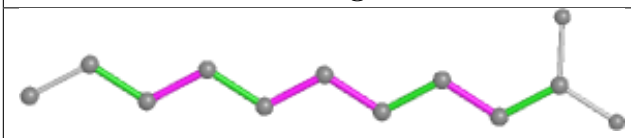
Ligand STE R 101



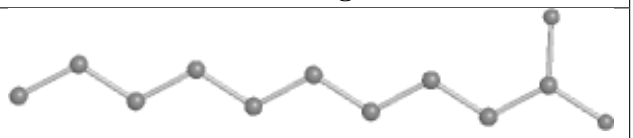
Bond lengths



Bond angles

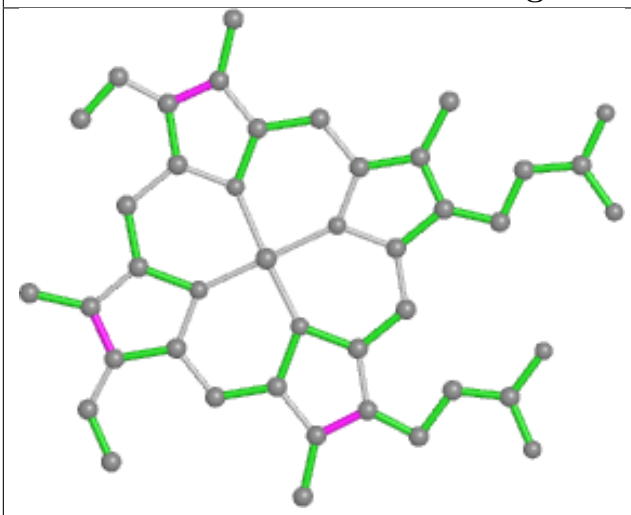


Torsions

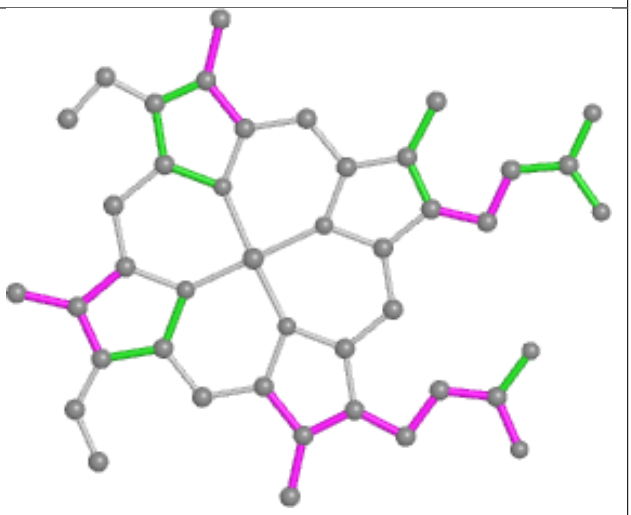


Rings

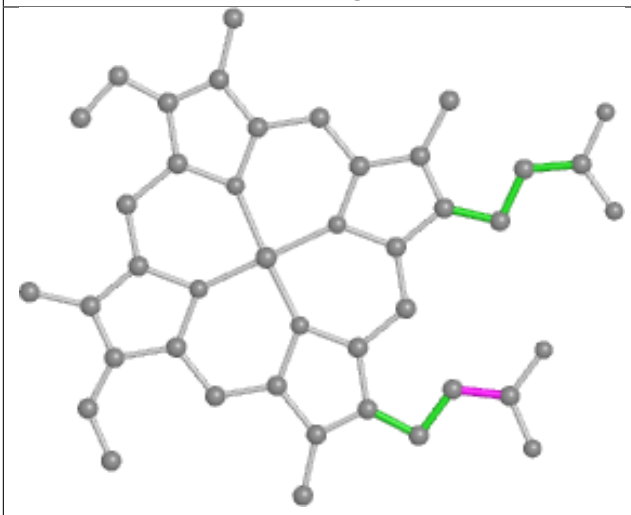
Ligand HEC v 201



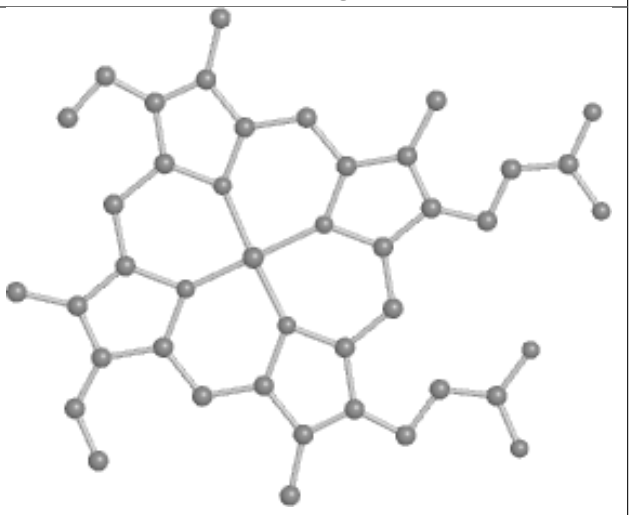
Bond lengths



Bond angles

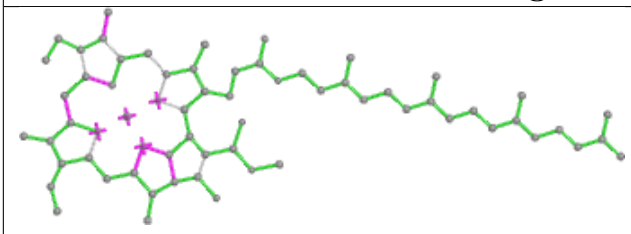


Torsions

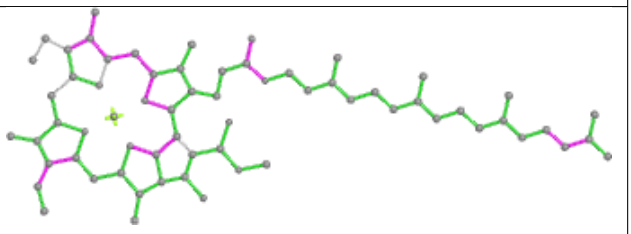


Rings

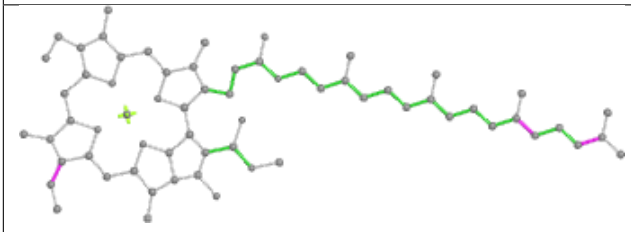
Ligand CLA a 402



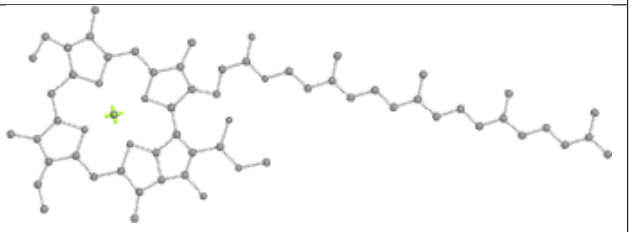
Bond lengths



Bond angles

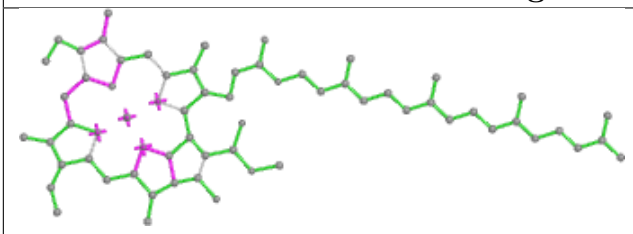


Torsions

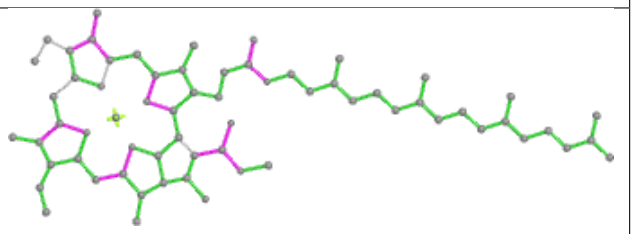


Rings

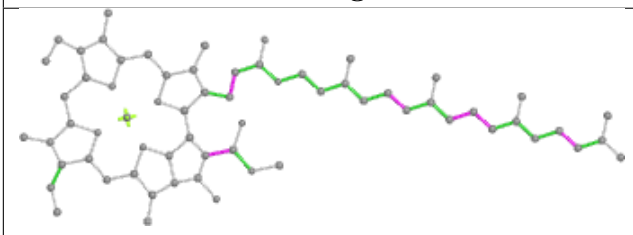
Ligand CLA b 606



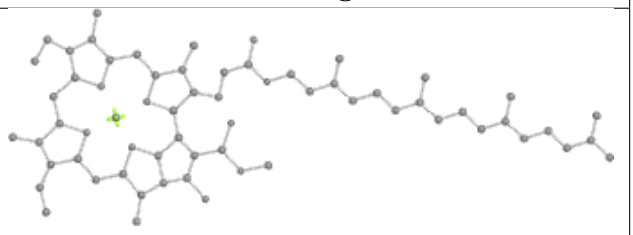
Bond lengths



Bond angles

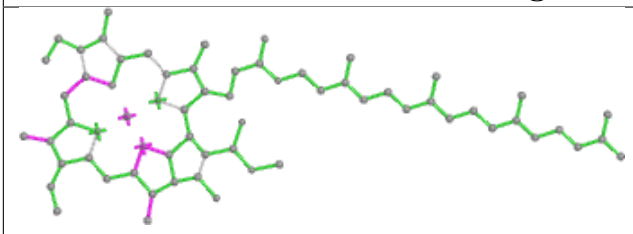


Torsions

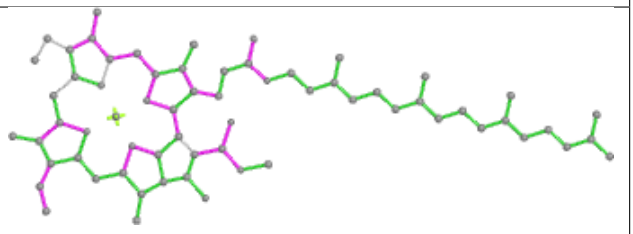


Rings

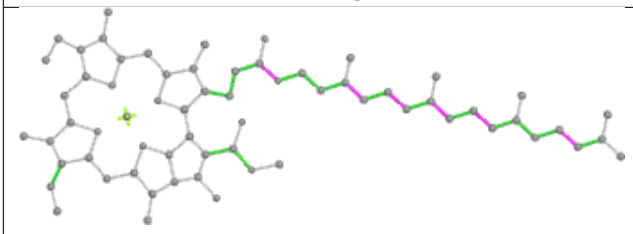
Ligand CLA a 404



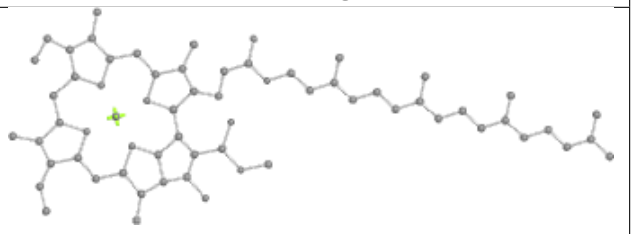
Bond lengths



Bond angles

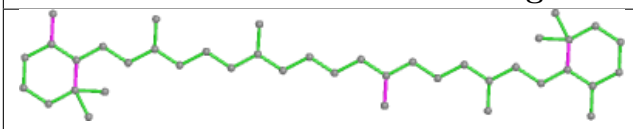


Torsions

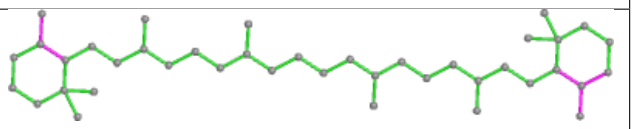


Rings

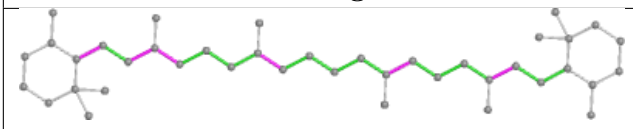
Ligand BCR k 101



Bond lengths



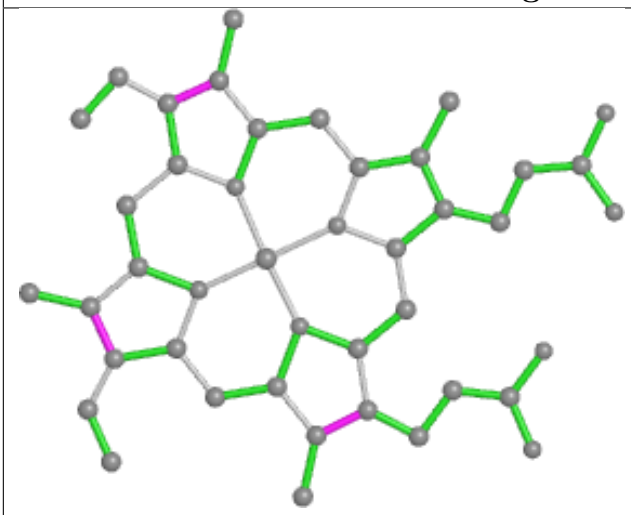
Bond angles



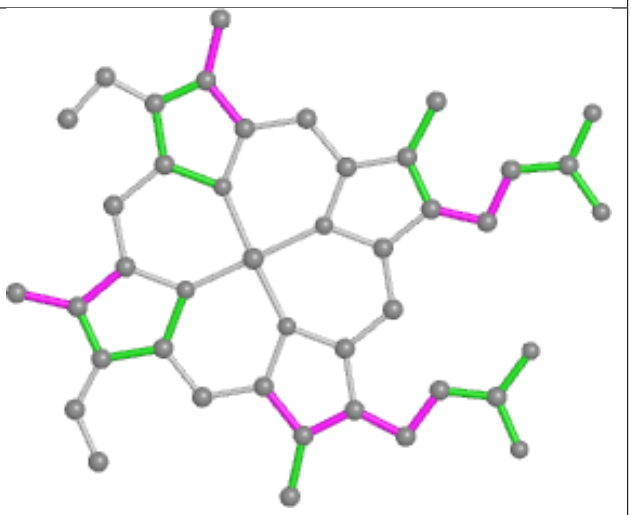
Torsions

Rings

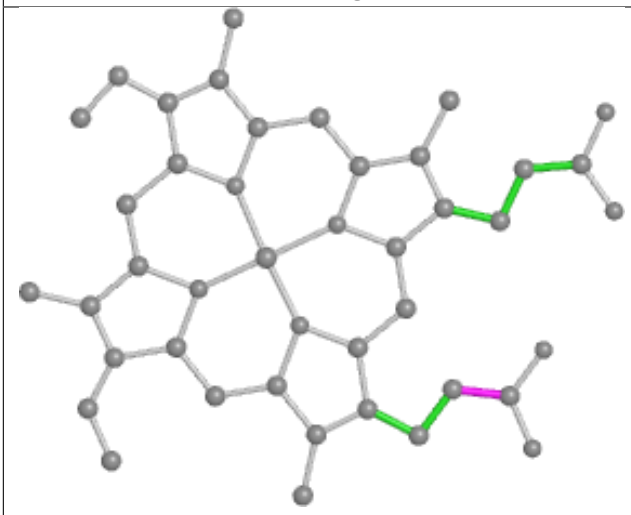
Ligand HEC V 201



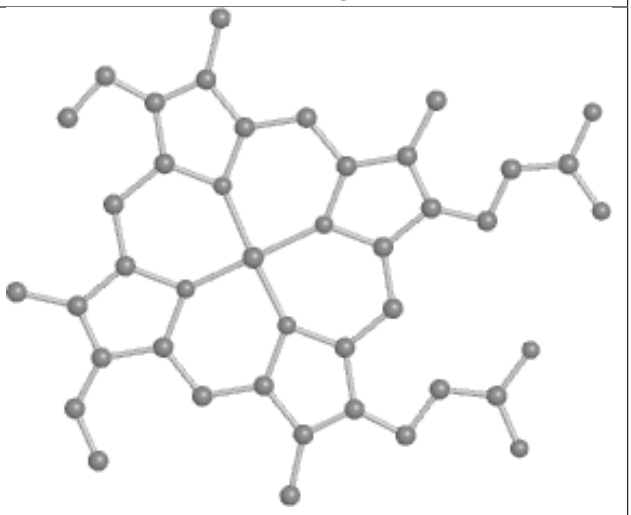
Bond lengths



Bond angles

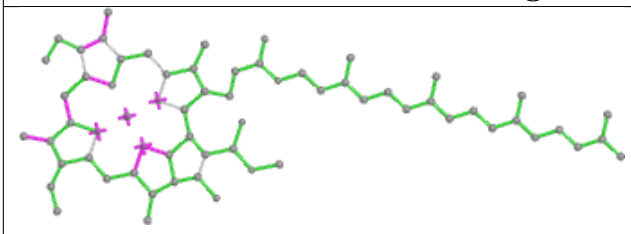


Torsions

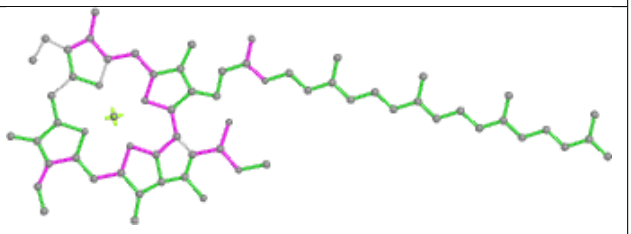


Rings

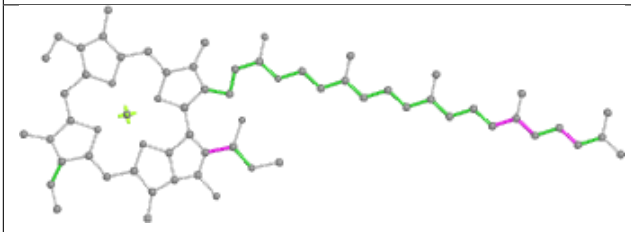
Ligand CLA C 502



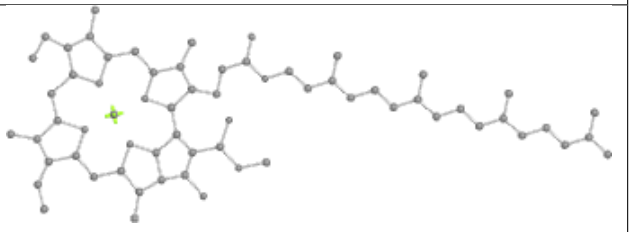
Bond lengths



Bond angles

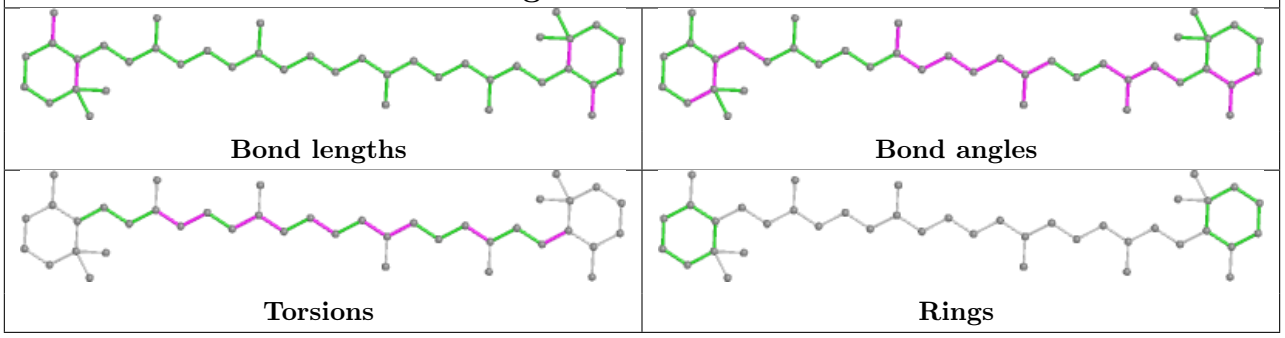


Torsions

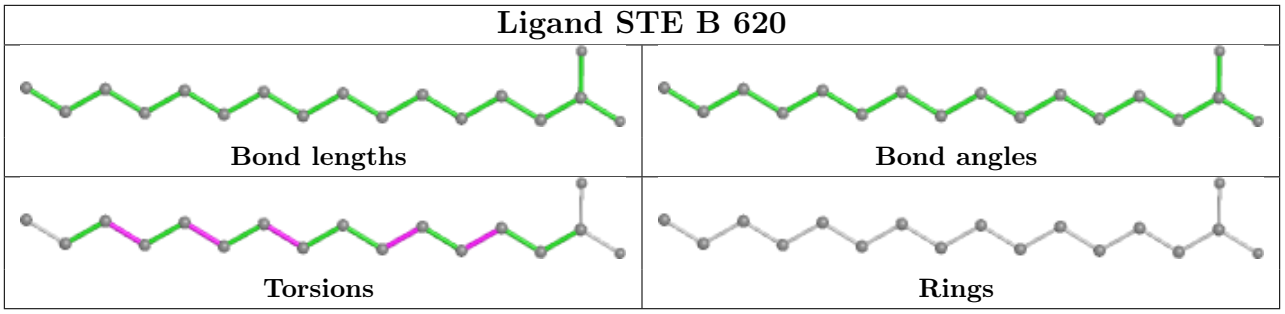


Rings

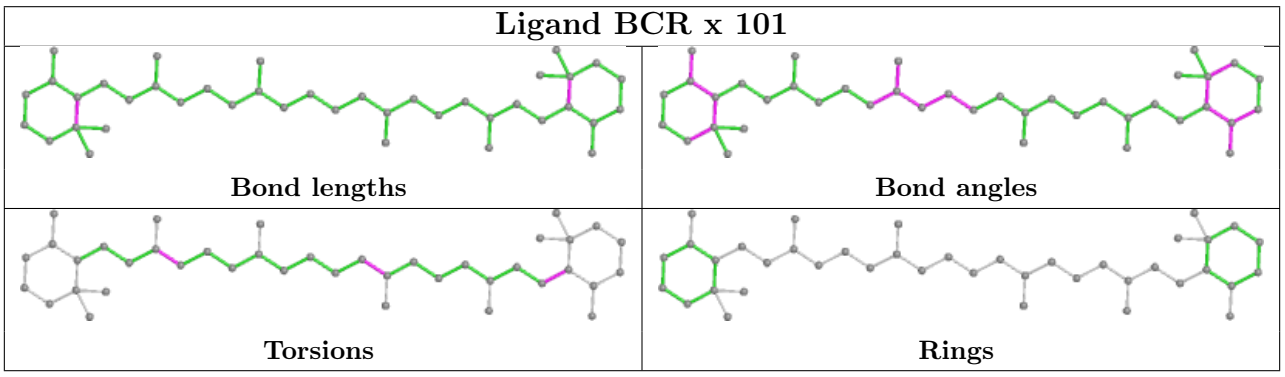
Ligand BCR A 407



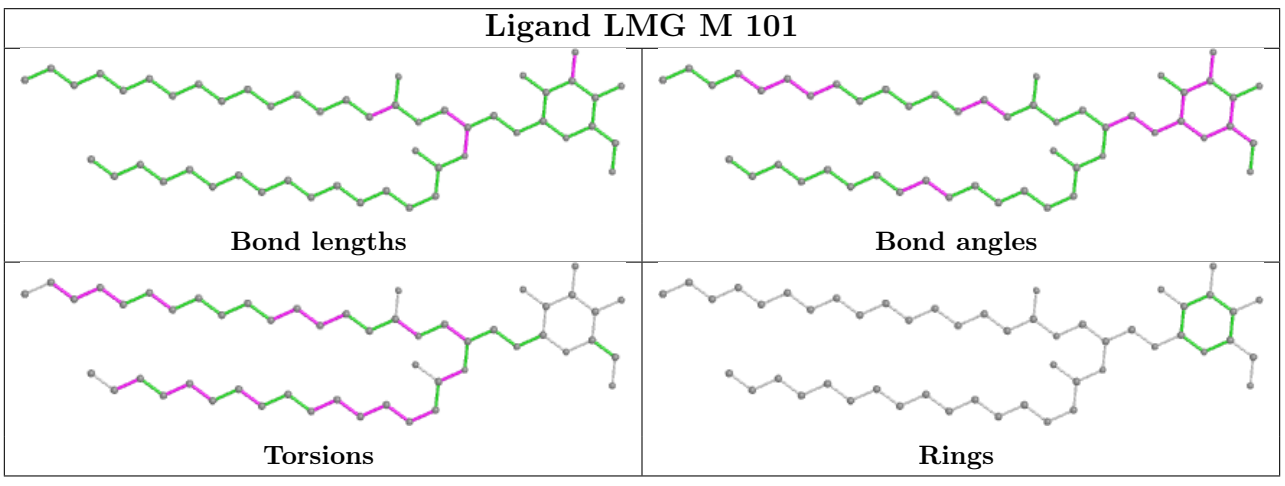
Ligand STE B 620



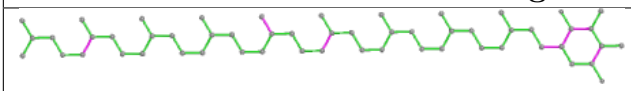
Ligand BCR x 101

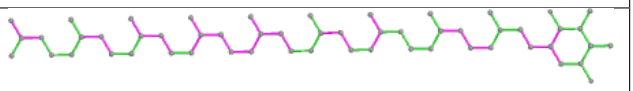


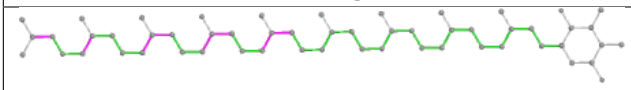
Ligand LMG M 101

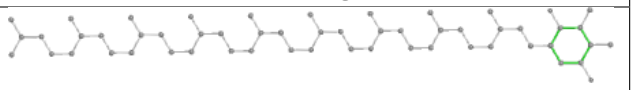


Ligand PL9 D 406

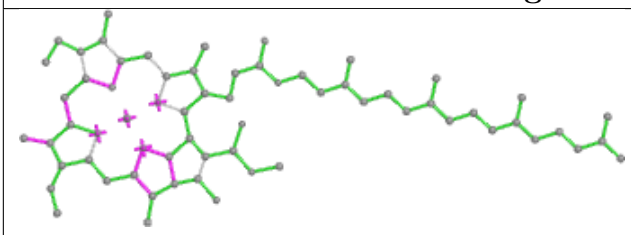

Bond lengths

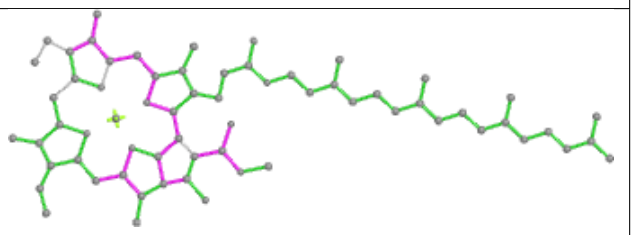

Bond angles

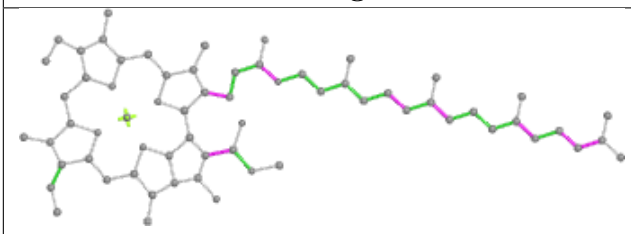

Torsions


Rings

Ligand CLA C 508


Bond lengths


Bond angles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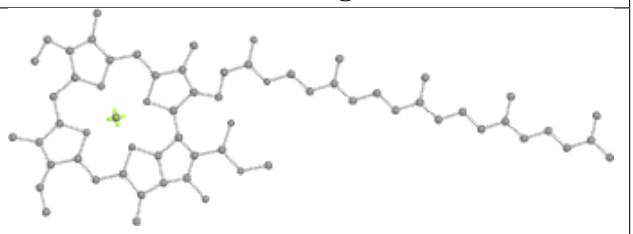
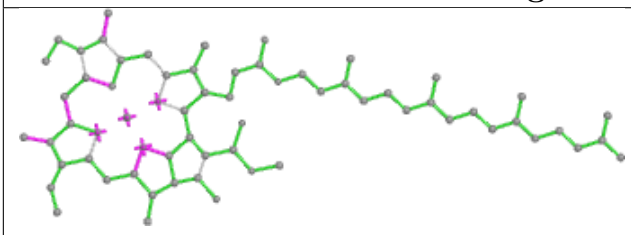

Rings

Ligand CLA b 612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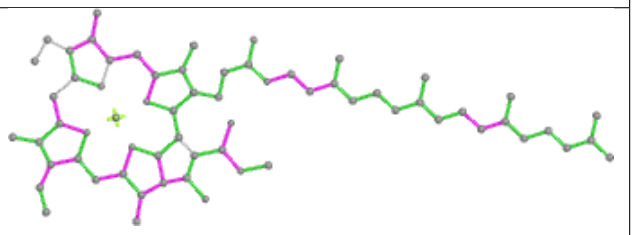
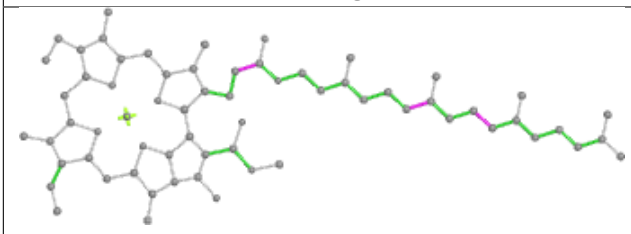
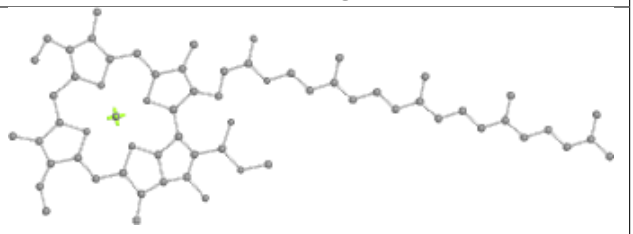
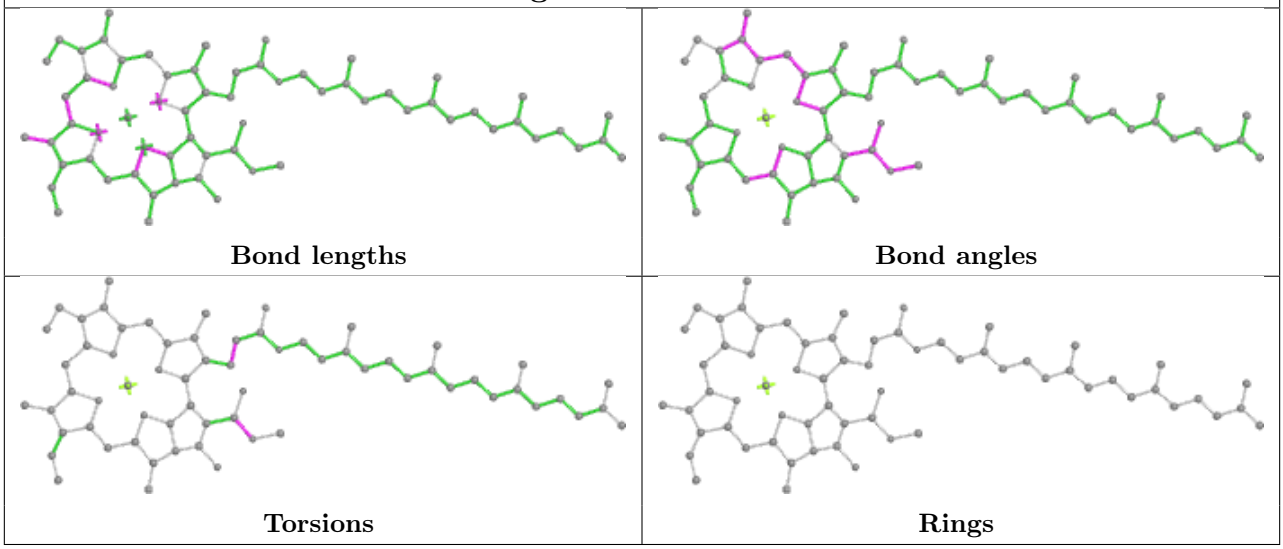

Bond angles

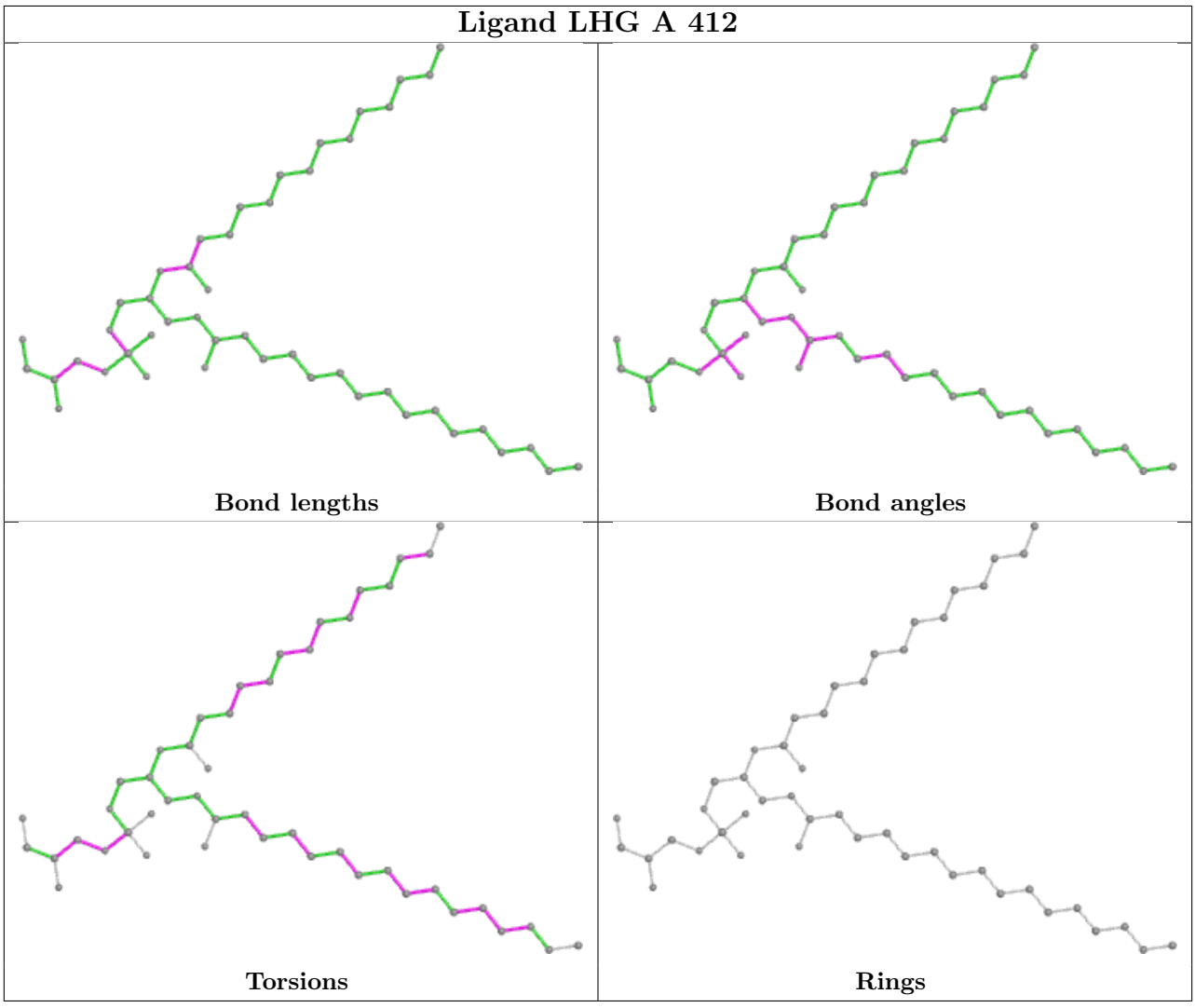

Torsions


Rings

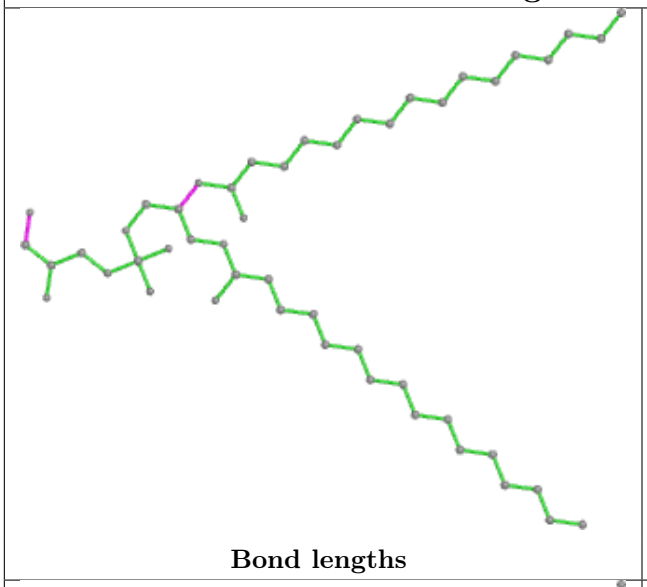
Ligand CLA c 501



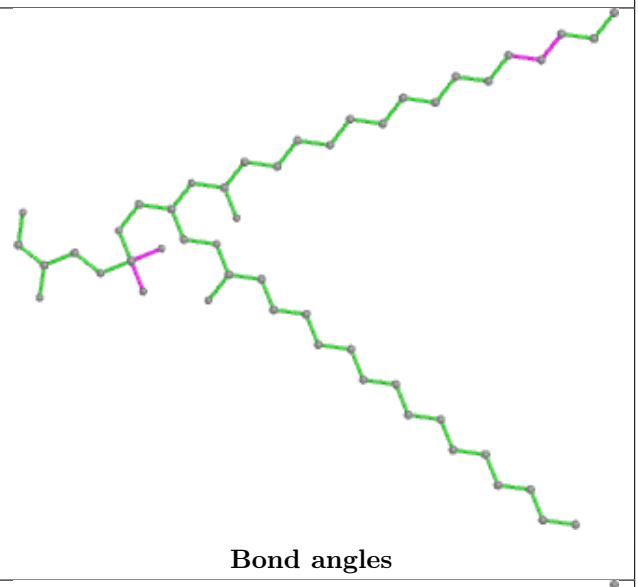
Ligand LHG A 412



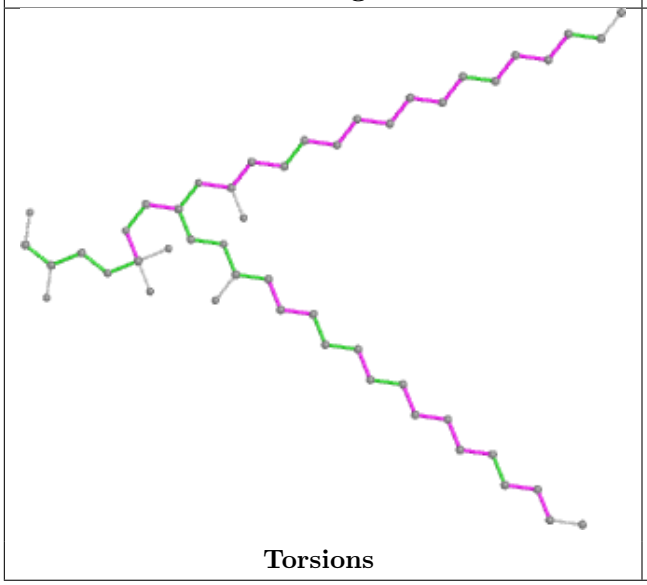
Ligand LHG B 621



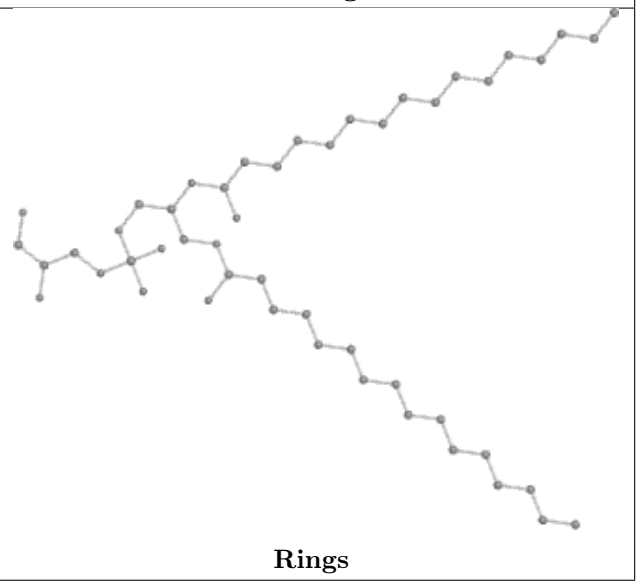
Bond lengths



Bond angles

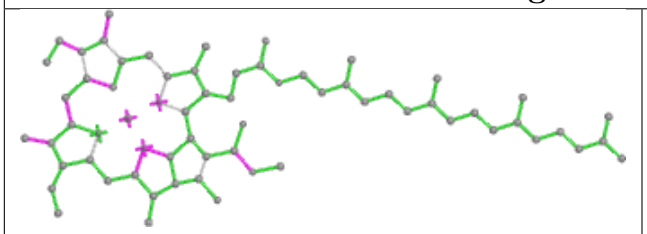


Torsions

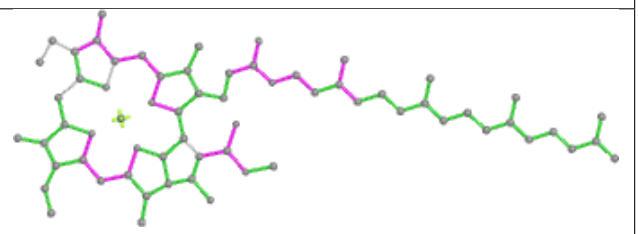


Rings

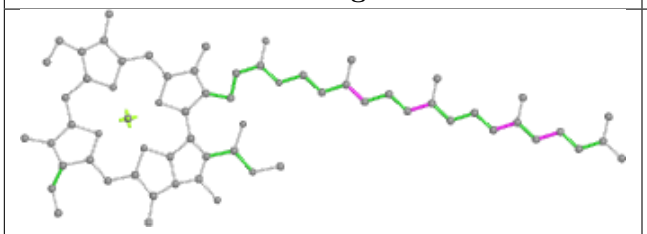
Ligand CLA b 603



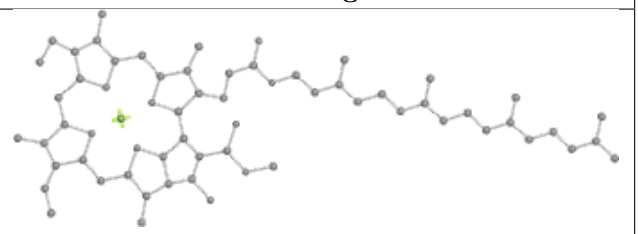
Bond lengths



Bond angles

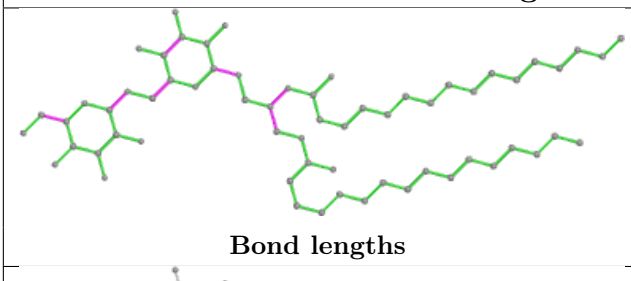


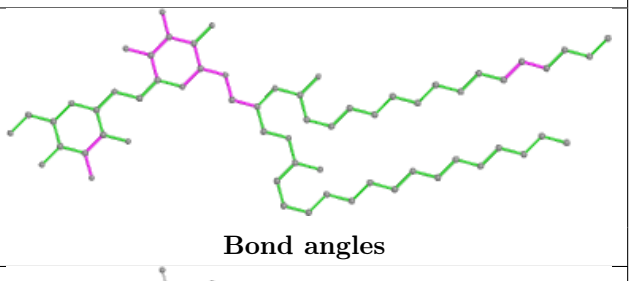
Torsions

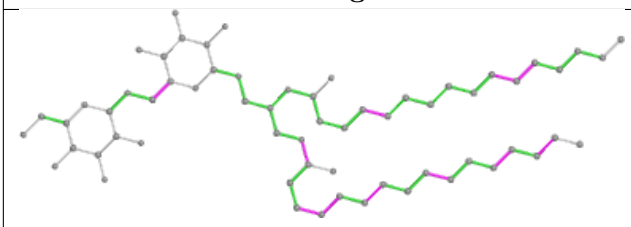


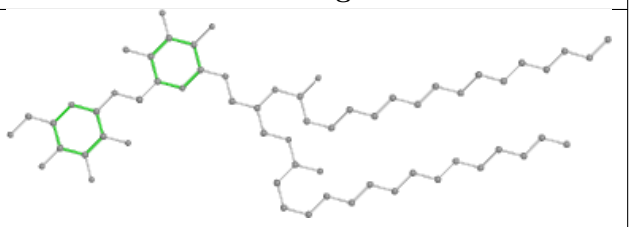
Rings

Ligand DGD C 519

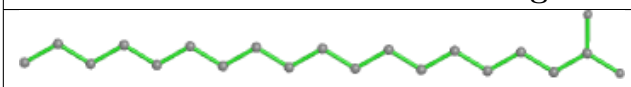

Bond lengths

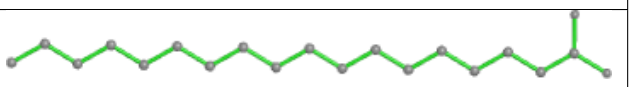

Bond angles

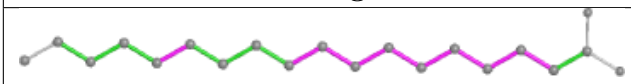

Torsions

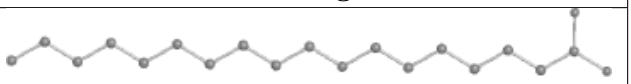

Rings

Ligand STE b 625


Bond lengths


Bond angles


Torsions

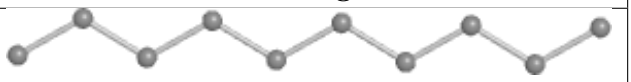

Rings

Ligand STE b 626

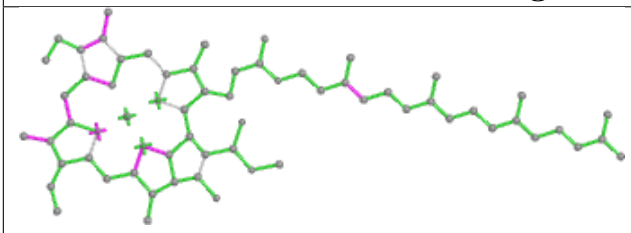

Bond lengths

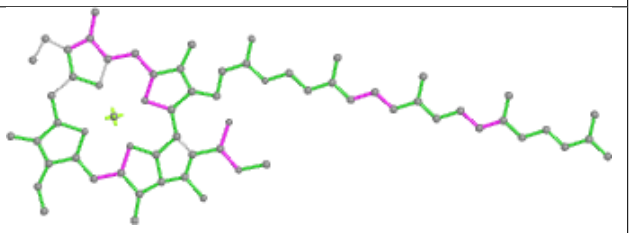

Bond angles

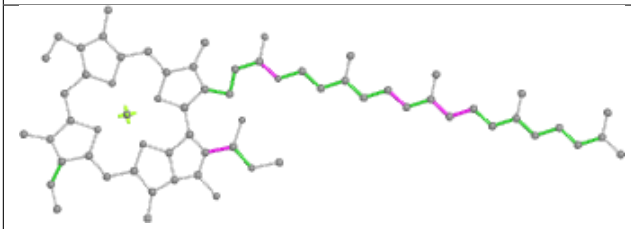

Torsions

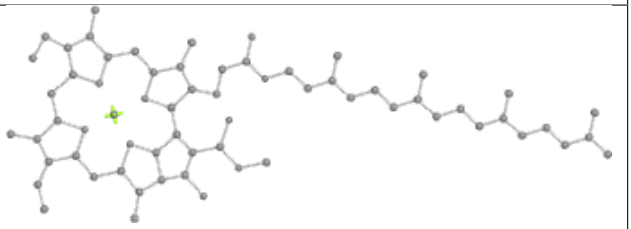

Rings

Ligand CLA c 503

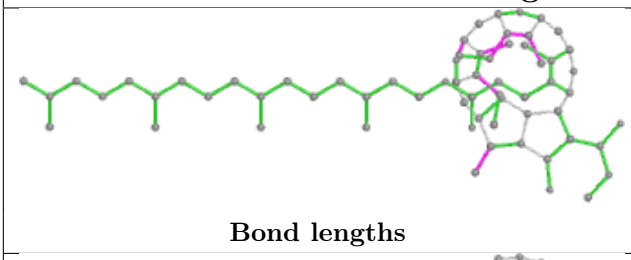

Bond lengths


Bond angles

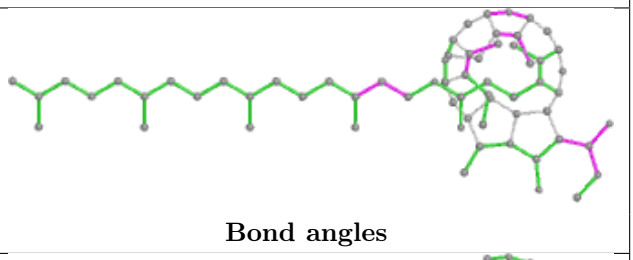

Torsions


Rings

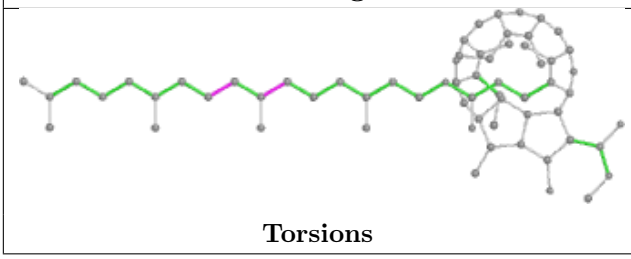
Ligand PHO A 405



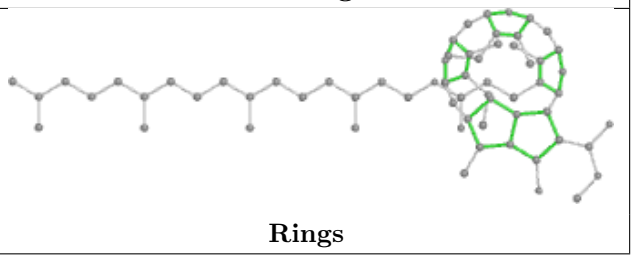
Bond lengths



Bond angles

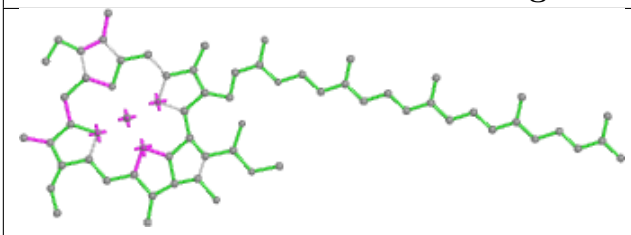


Torsions

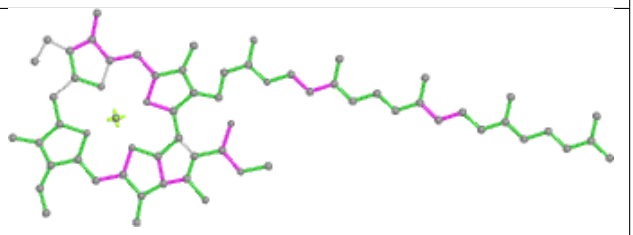


Rings

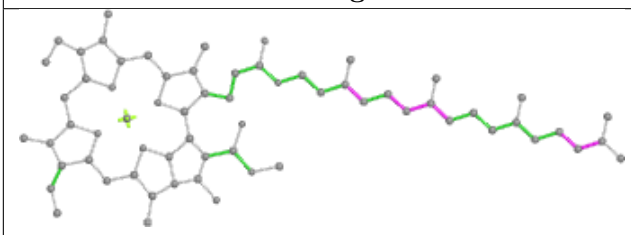
Ligand CLA c 505



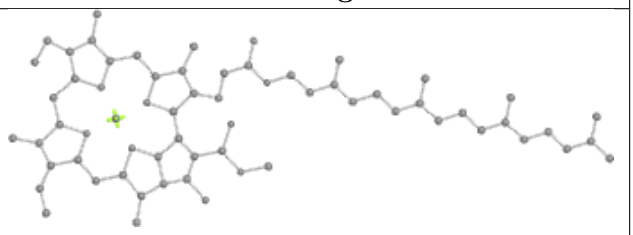
Bond lengths



Bond angles

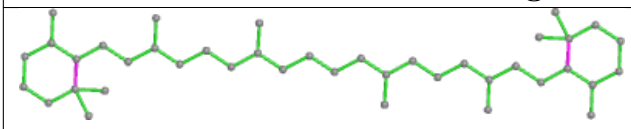


Torsions

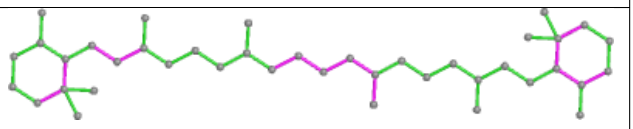


Rings

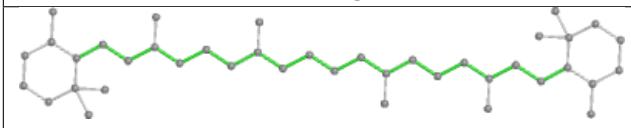
Ligand BCR b 619



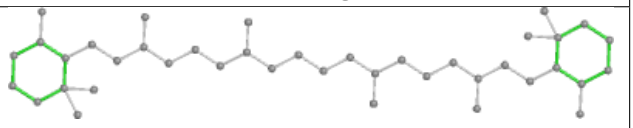
Bond lengths



Bond angles

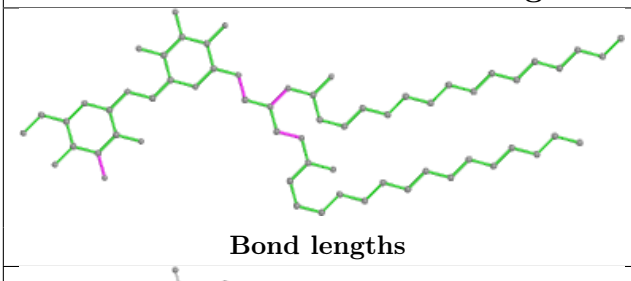


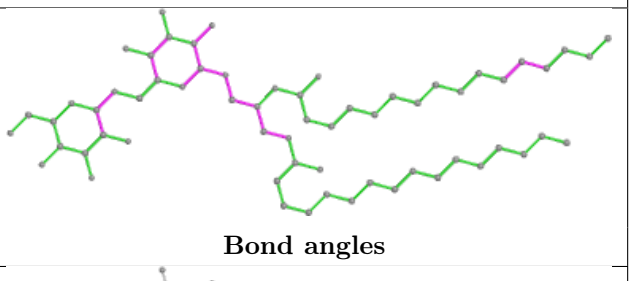
Torsions

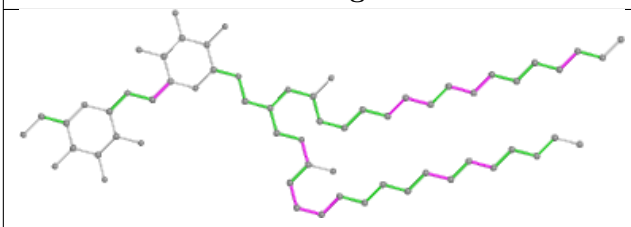


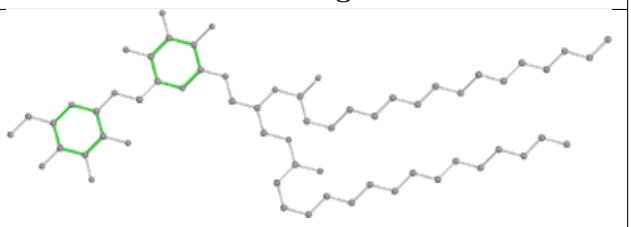
Rings

Ligand DGD c 519

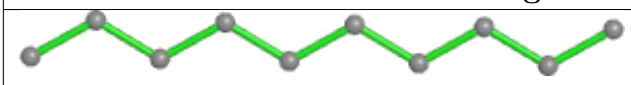

Bond lengths


Bond angles


Torsions


Rings

Ligand STE M 103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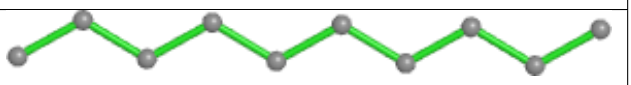
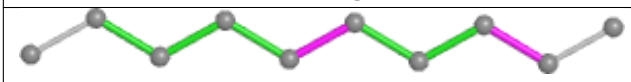
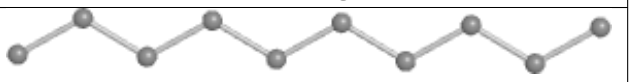
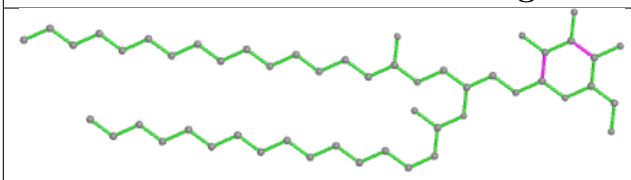

Bond angles


Torsions


Rings

Ligand LMG m 101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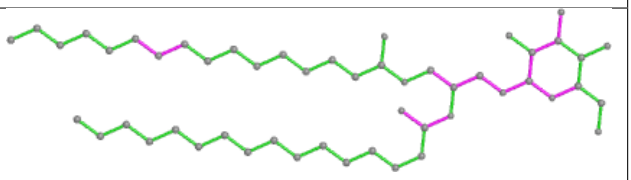
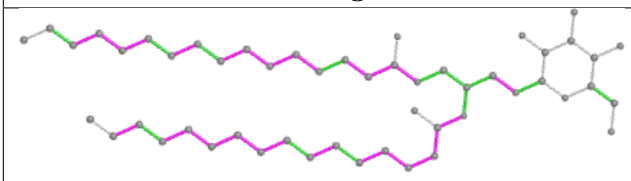

Bond angles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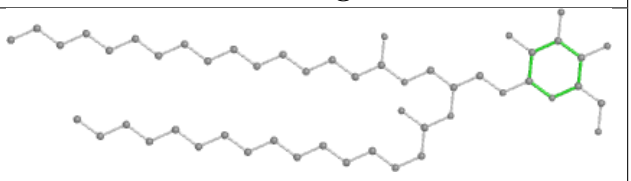
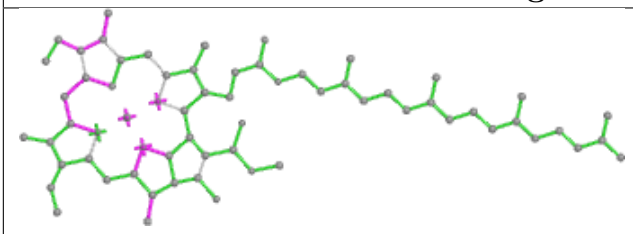

Rings

Ligand CLA b 610



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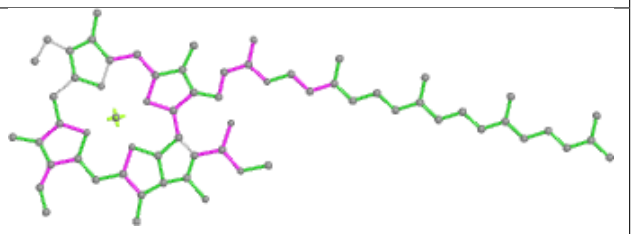
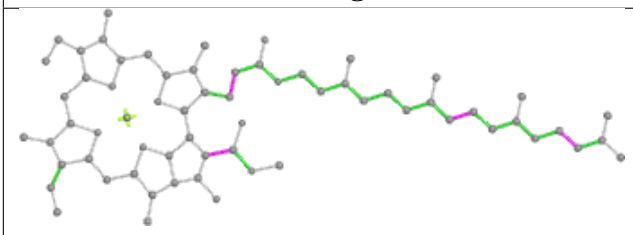


Bond angles



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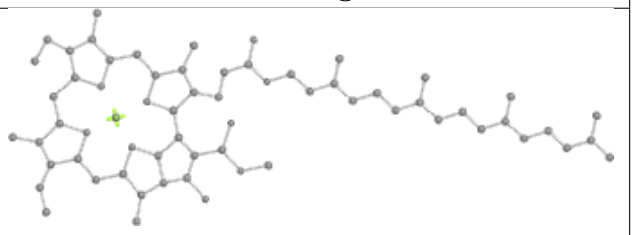
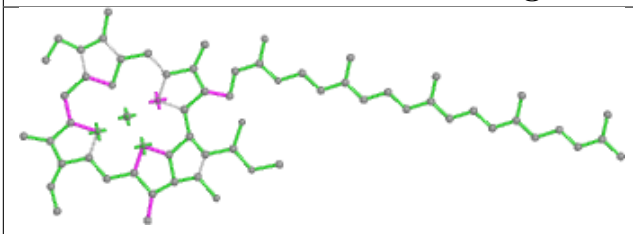


Rings

Ligand CLA D 402



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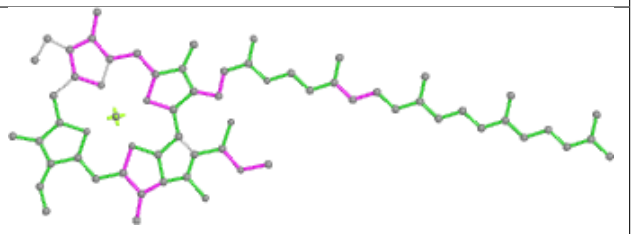
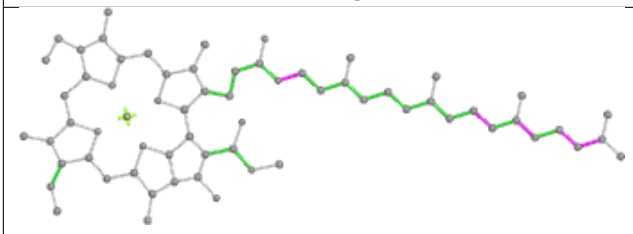


Bond angles



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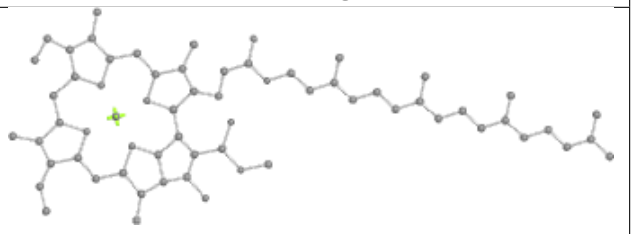
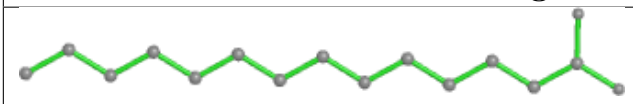


Rings

Ligand STE b 624



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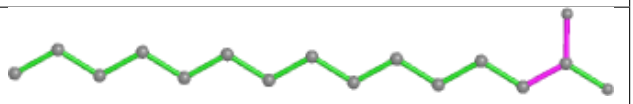
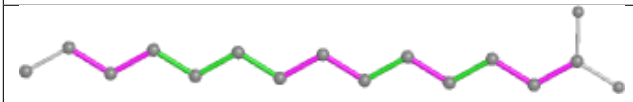


Bond angles



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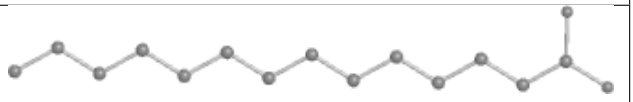
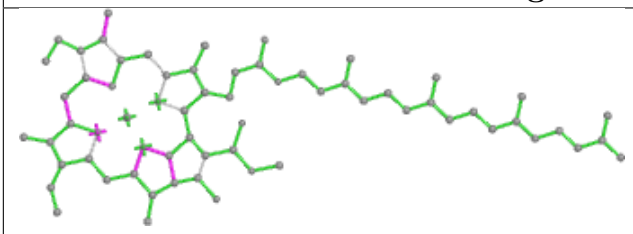


Rings

Ligand CLA b 604



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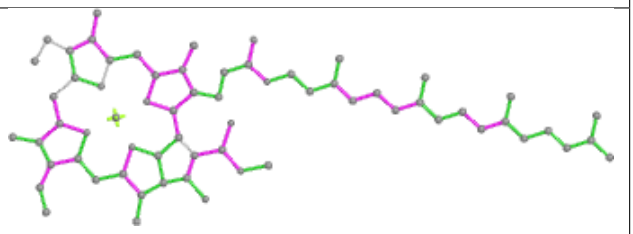
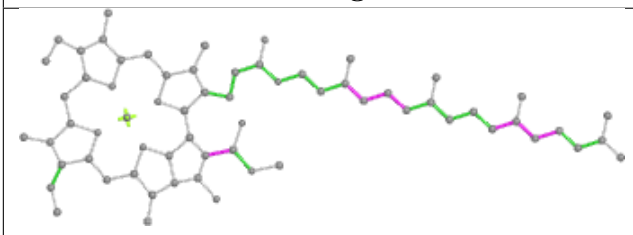


Bond angles



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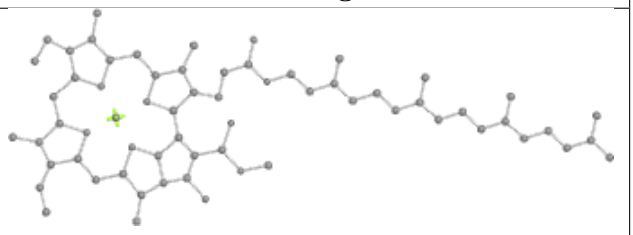
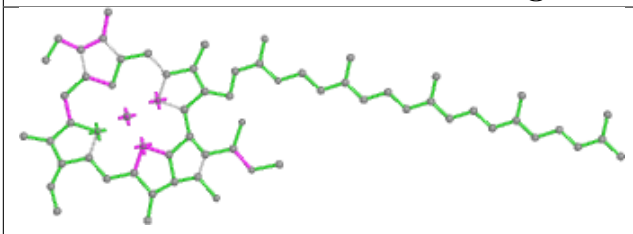


Rings

Ligand CLA b 609



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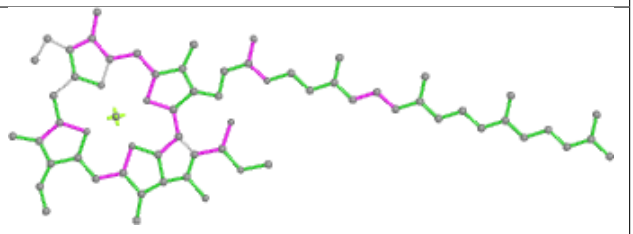
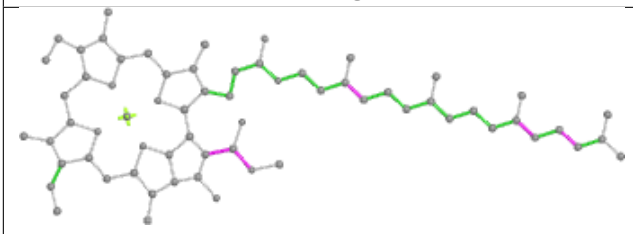


Bond angles



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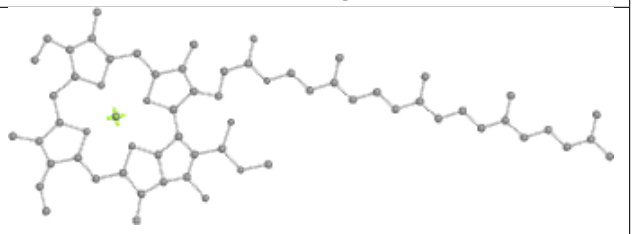
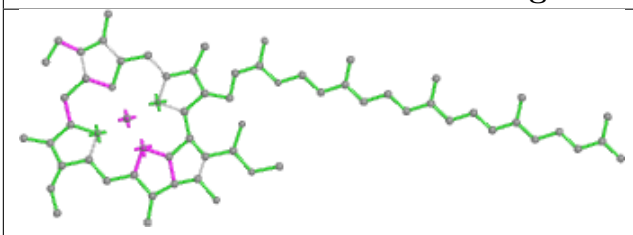


Rings

Ligand CLA c 509



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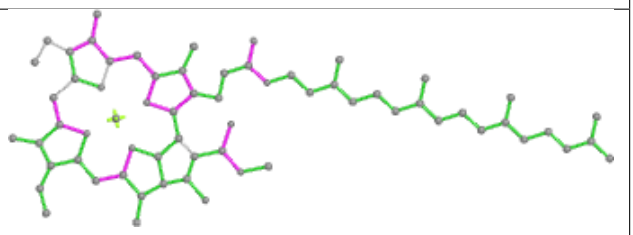
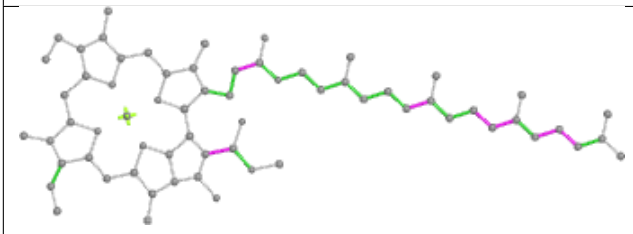


Bond angles



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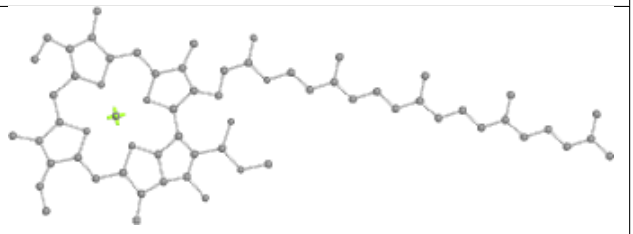
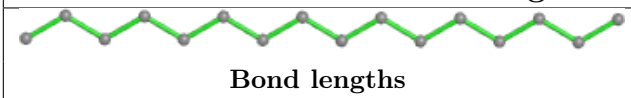


Rings

Ligand STE B 625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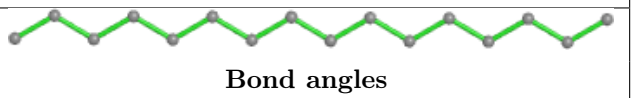
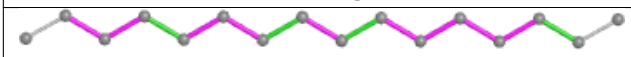

Bond angles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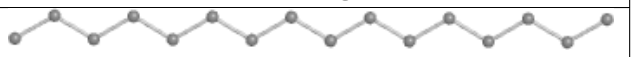
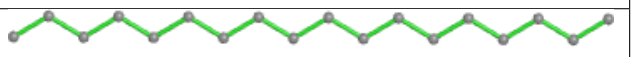
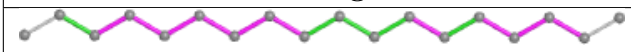

Rings

Ligand STE H 103


Bond lengths


Bond angles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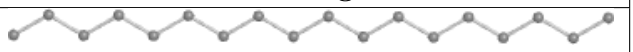
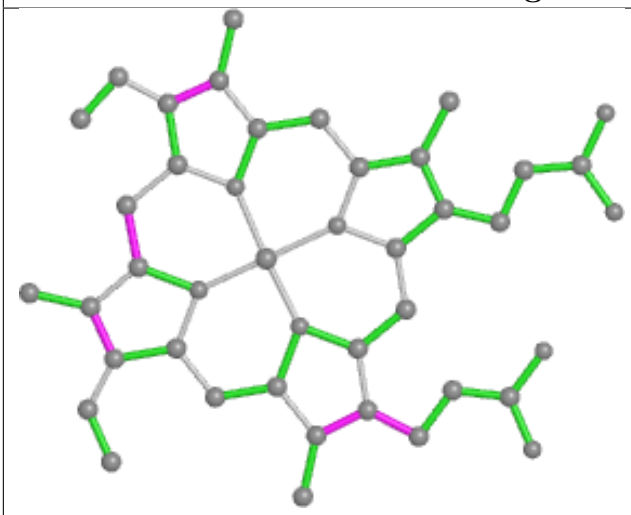
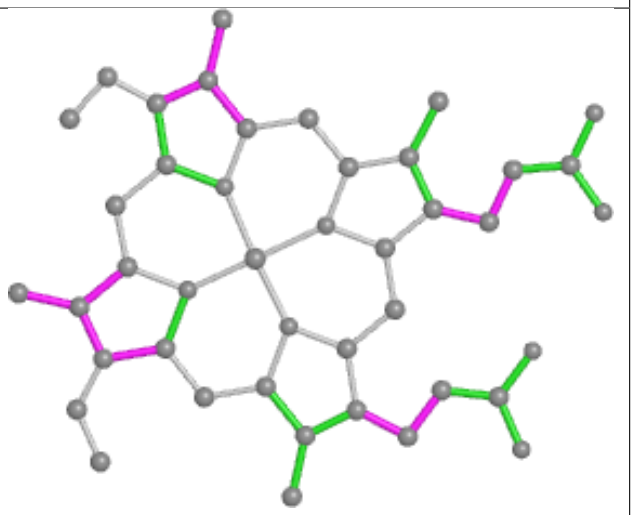
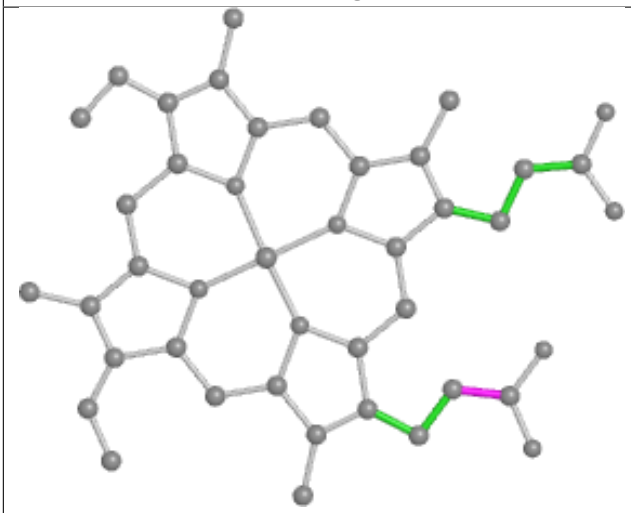

Rings

Ligand HEC F 101


Bond lengths


Bond angles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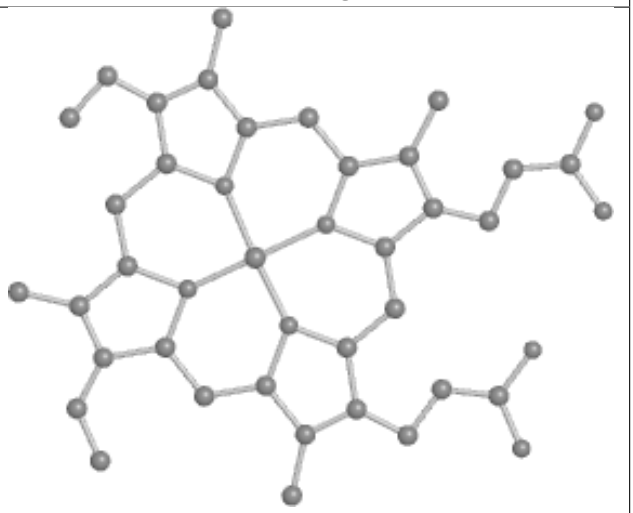
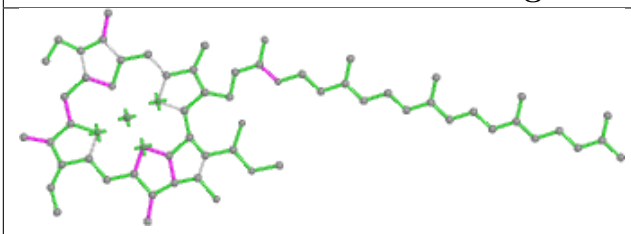
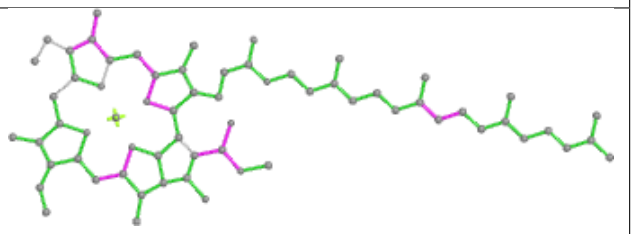

Rings

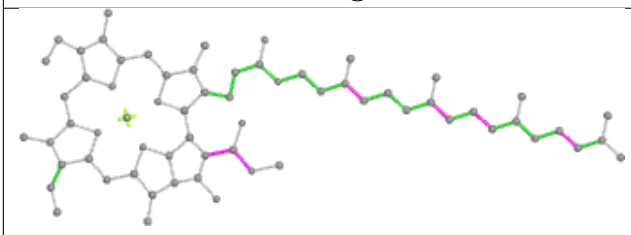
Ligand CLA C 510



Bond lengths



Bond angles



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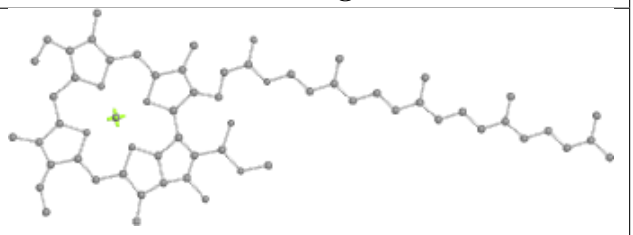
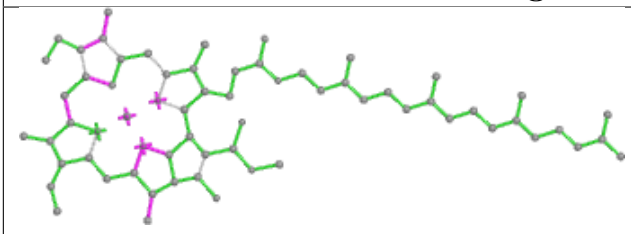
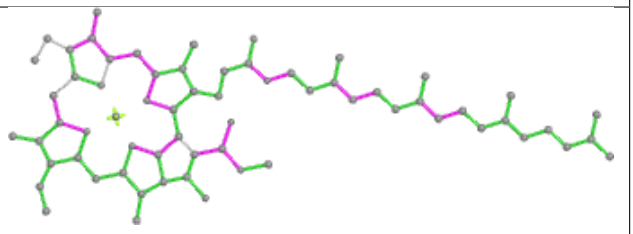


Rings

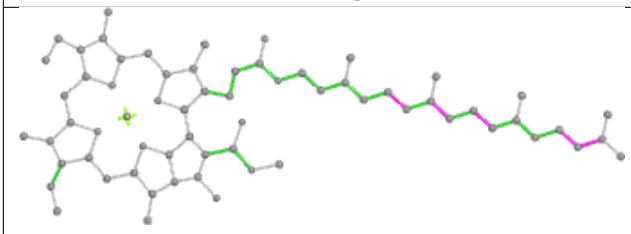
Ligand CLA b 615



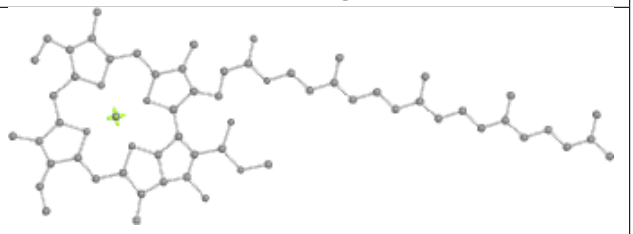
Bond lengths



Bond angles

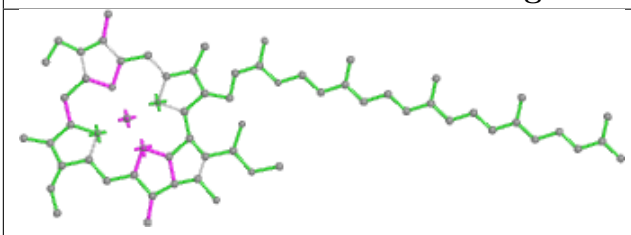


Torsions

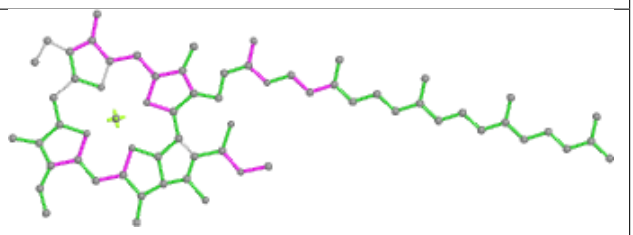


Rings

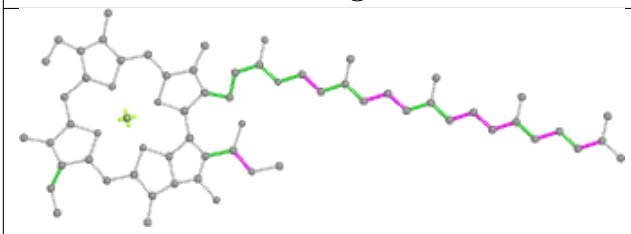
Ligand CLA C 509



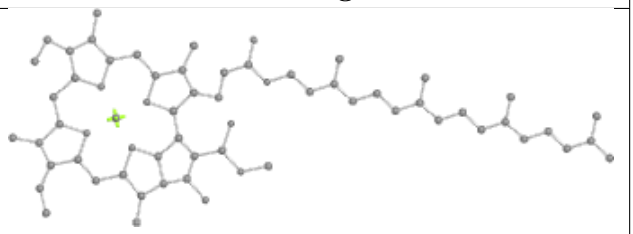
Bond lengths



Bond angles

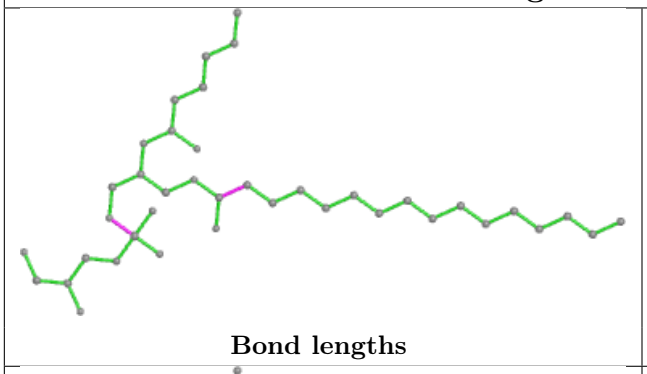


Torsions

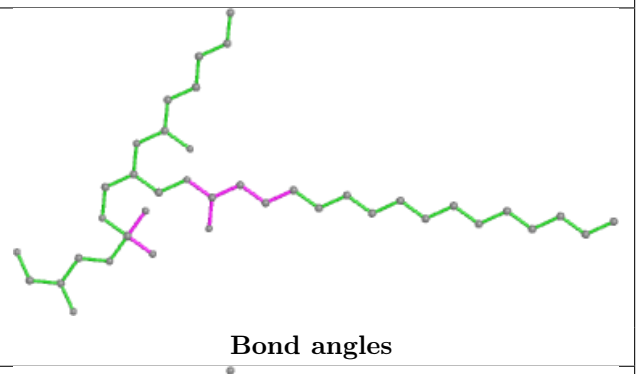


Rings

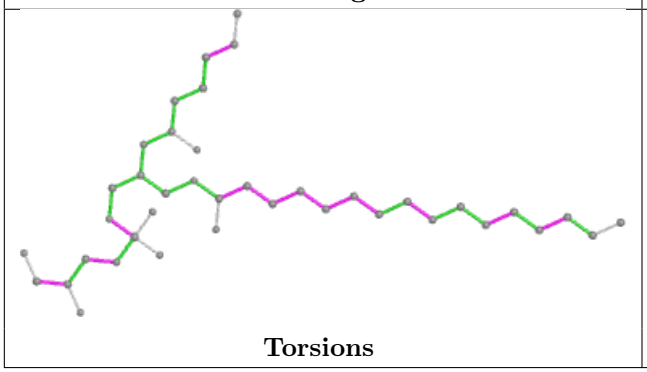
Ligand LHG d 409



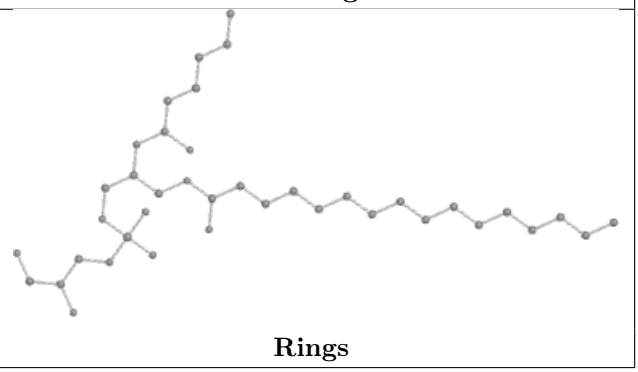
Bond lengths



Bond angles



Torsions

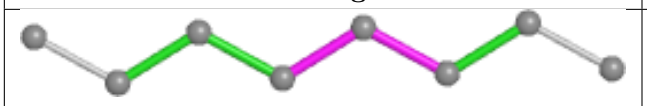


Rings

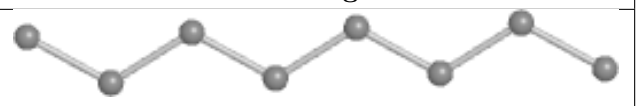
Ligand STE Z 101

Bond lengths

Bond angles

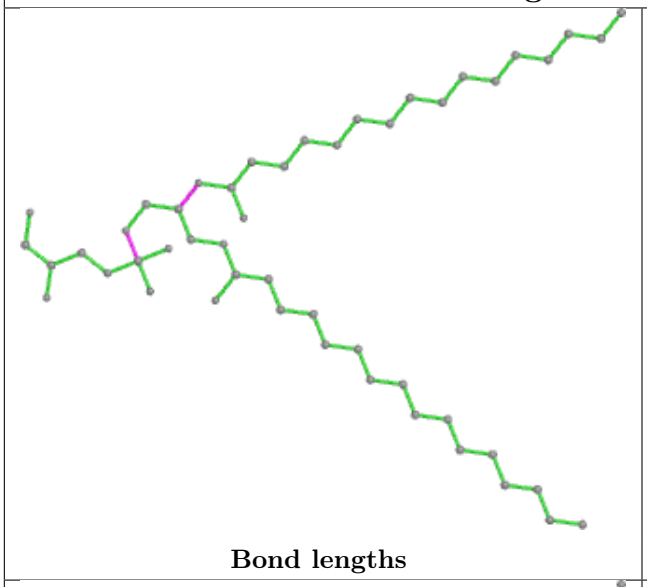


Torsions

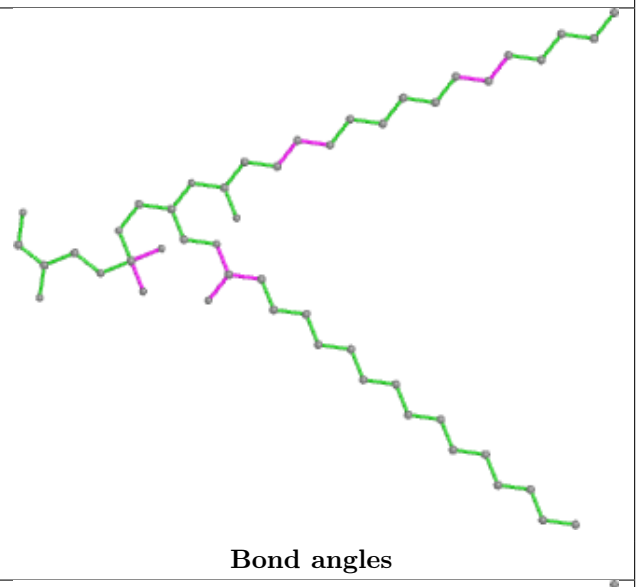


Rings

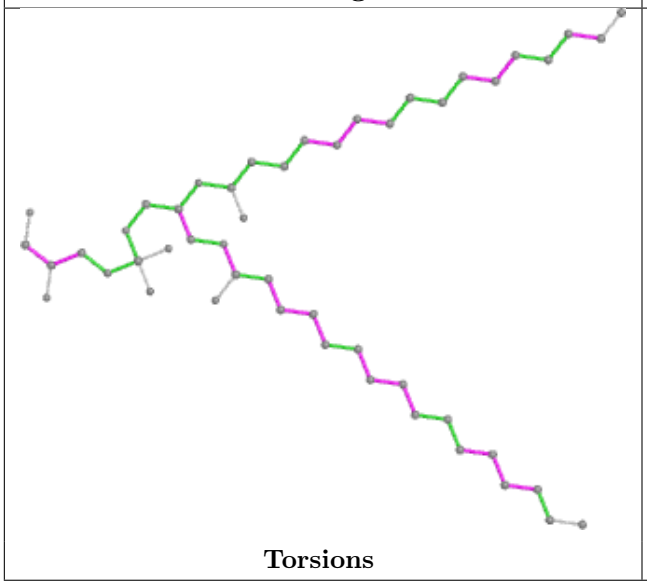
Ligand LHG E 101



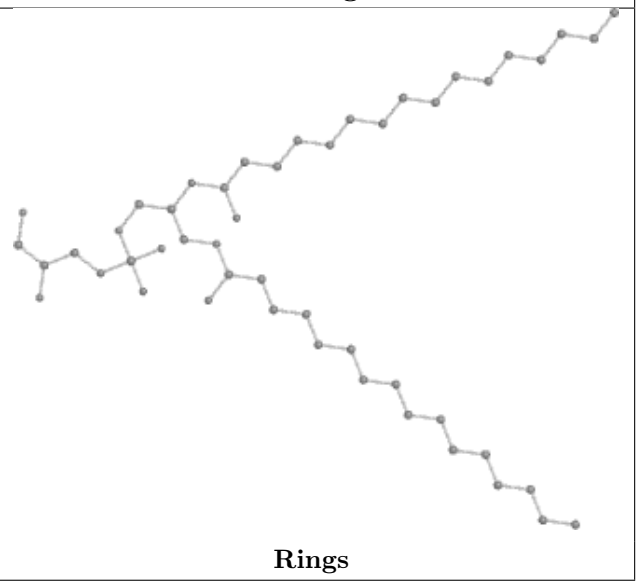
Bond lengths



Bond angles

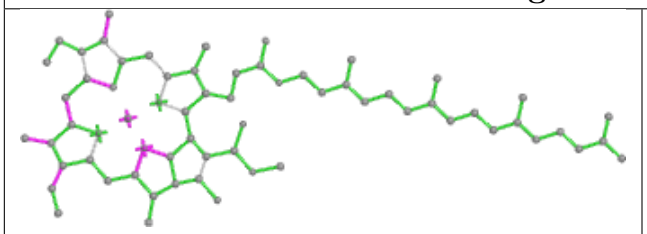


Torsions

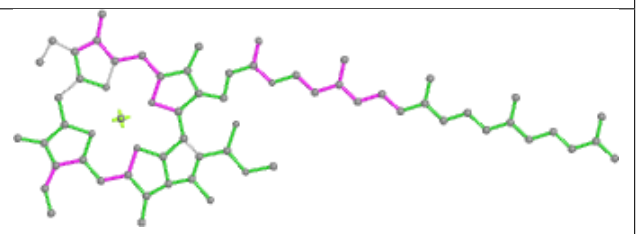


Rings

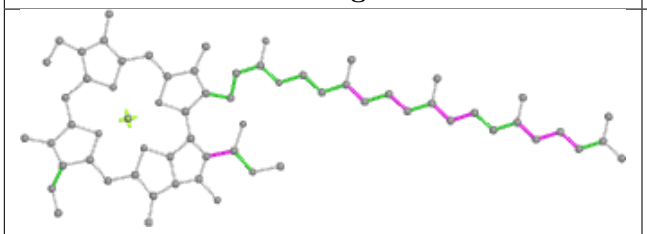
Ligand CLA b 614



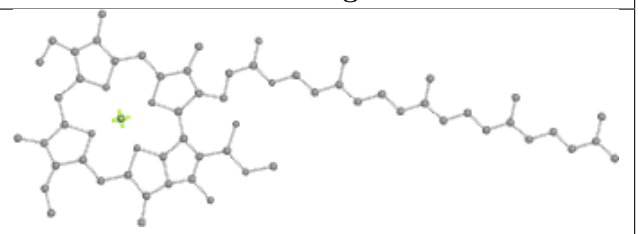
Bond lengths



Bond angles

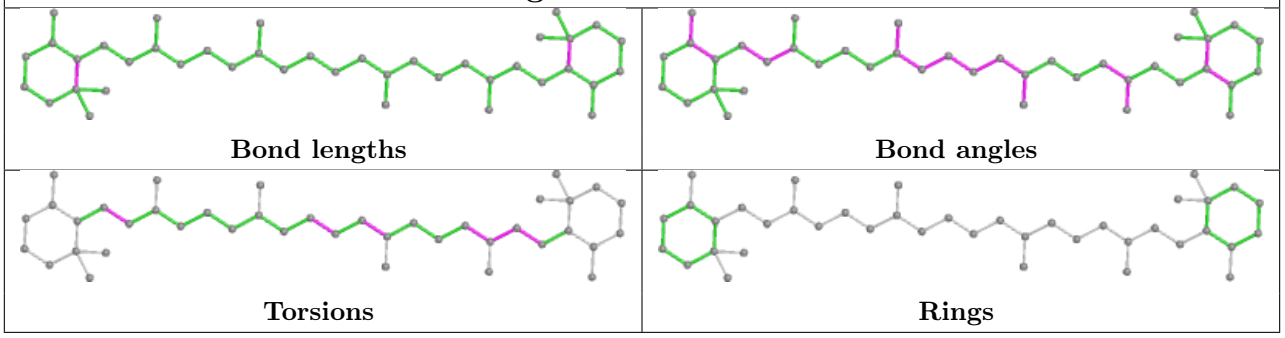


Torsions

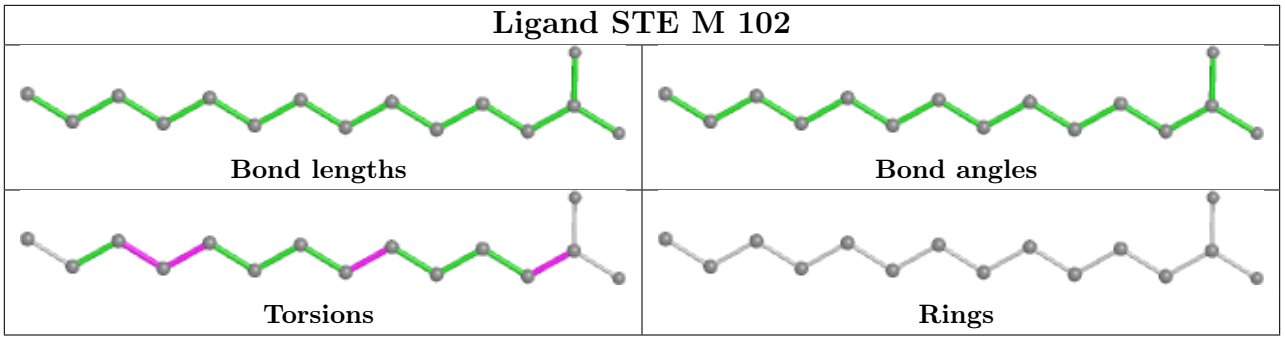


Rings

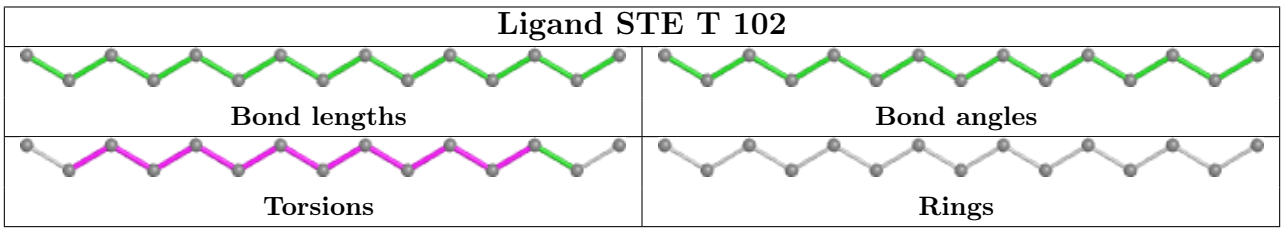
Ligand BCR b 618



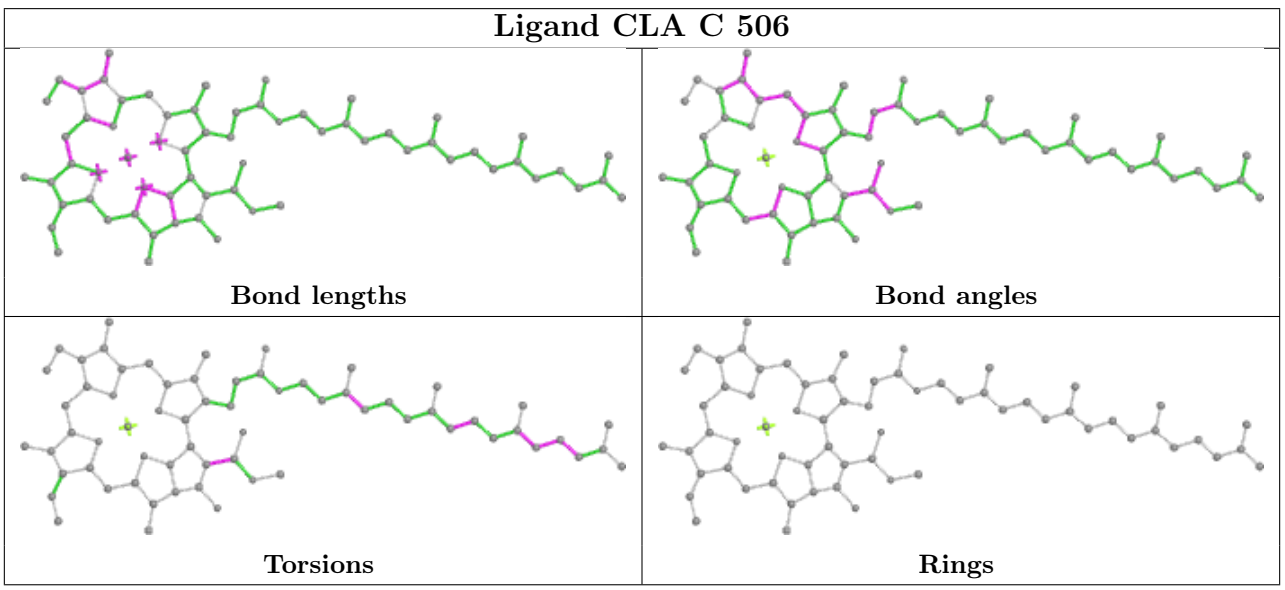
Ligand STE M 102



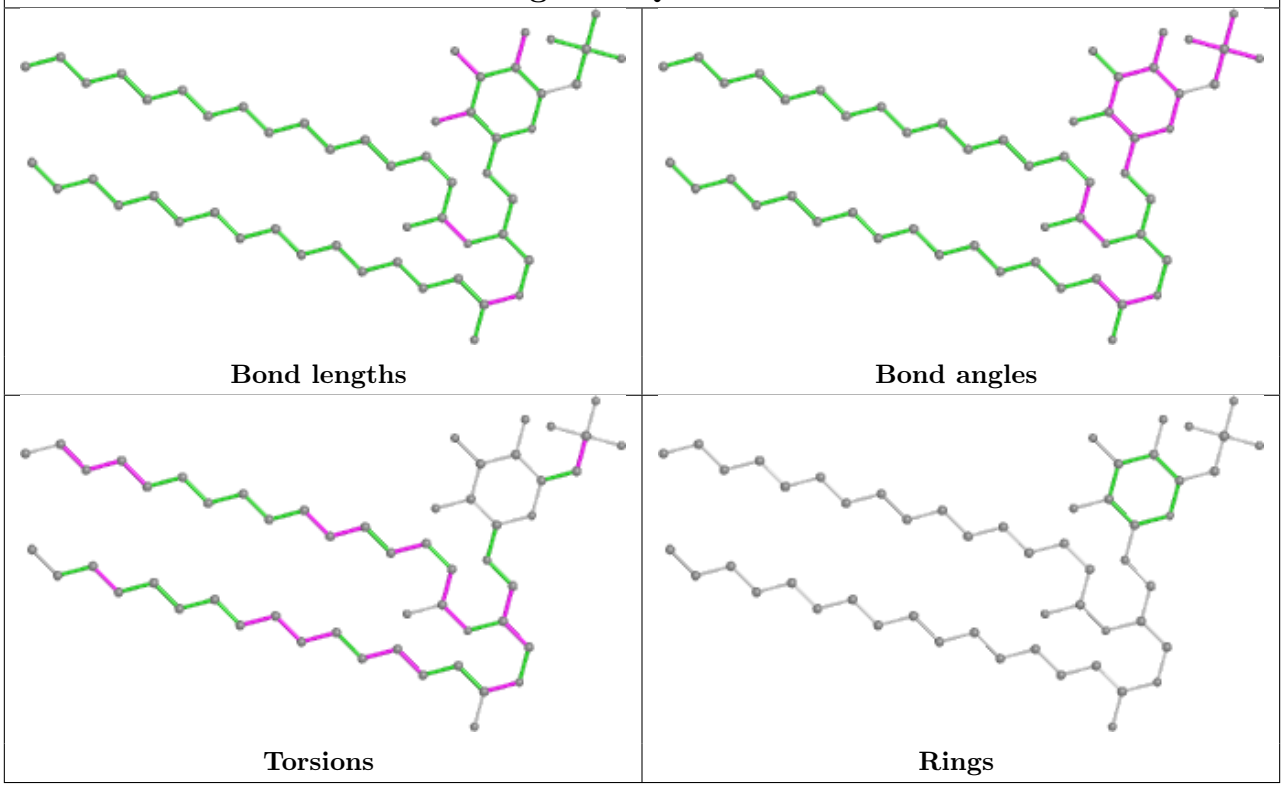
Ligand STE T 102



Ligand CLA C 506



Ligand SQD a 411



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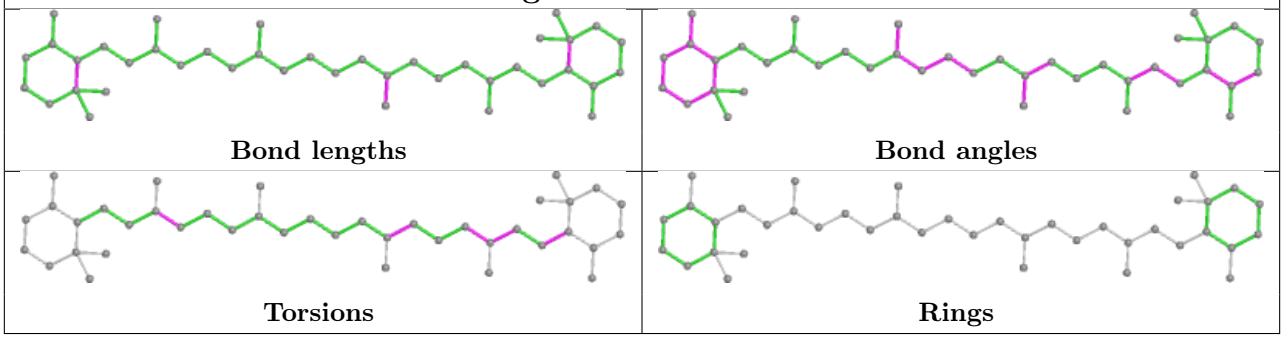

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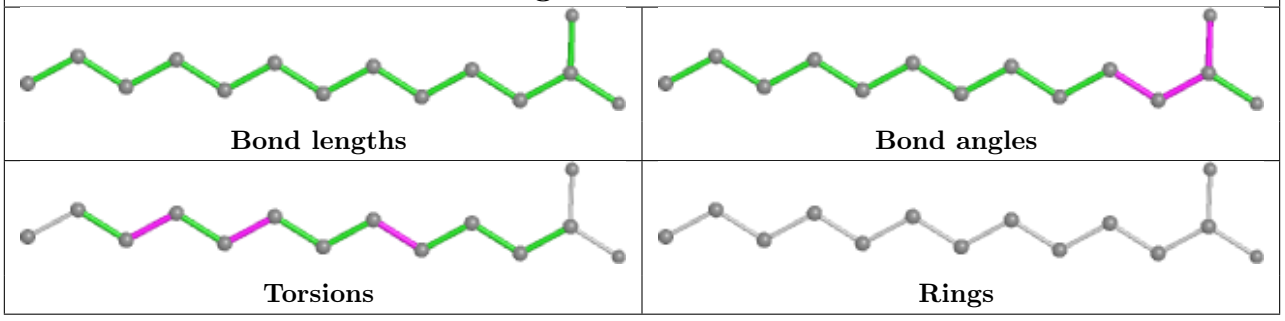
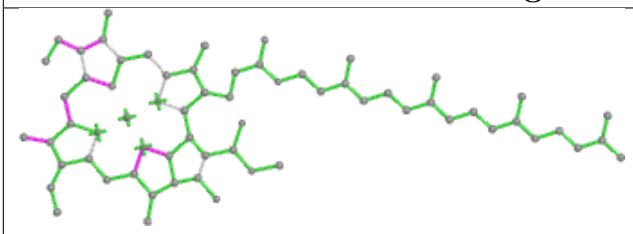
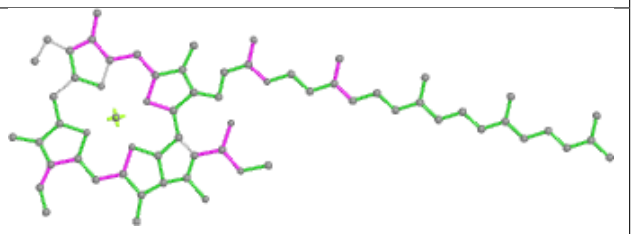
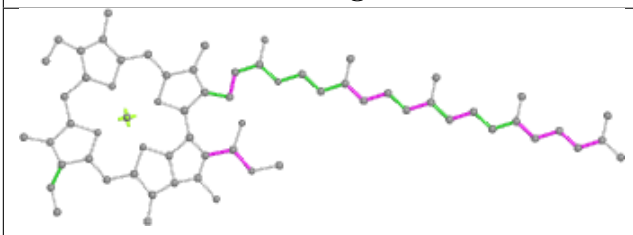
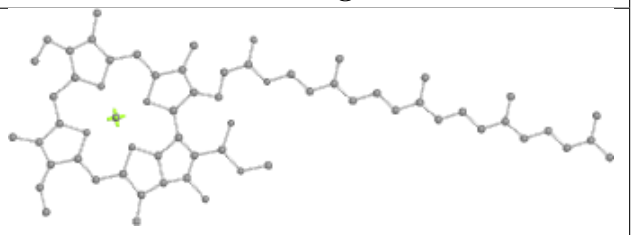


Ligand CLA B 614

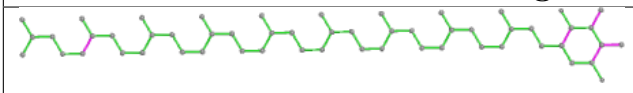

Bond lengths

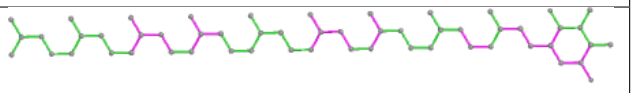

Bond angles

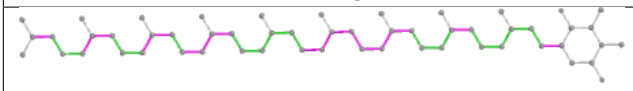

Torsions


Rings

Ligand PL9 a 409


Bond lengths


Bond angles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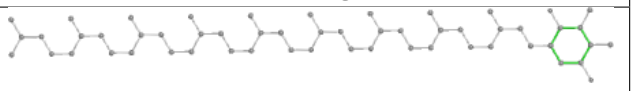
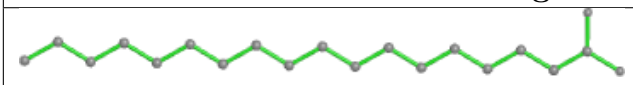
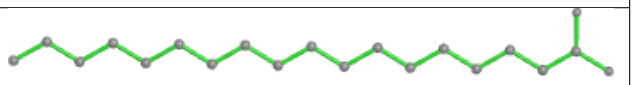
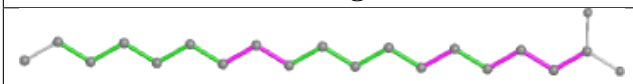
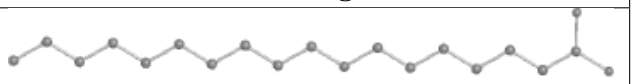

Rings

Ligand STE c 521


Bond lengths


Bond angles


Torsions


Rings

Ligand STE a 415

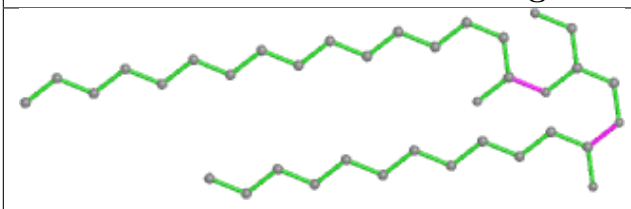

Bond lengths


Bond angles

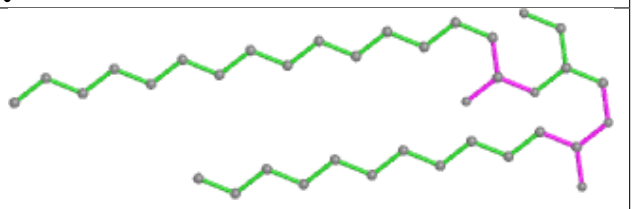

Torsions


Rings

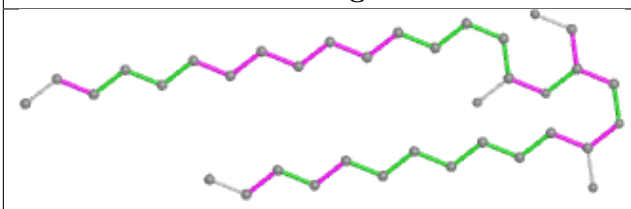
Ligand SQD a 412



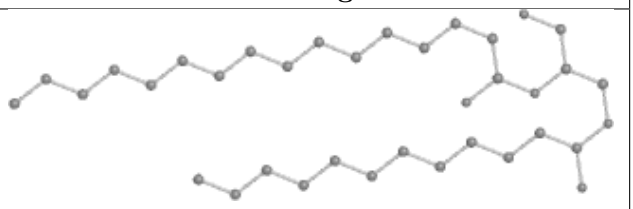
Bond lengths



Bond angles

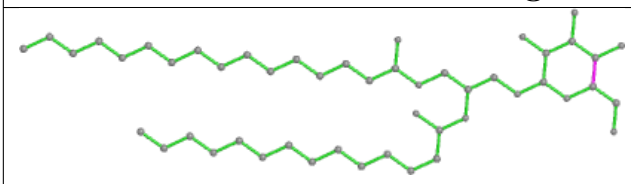


Torsions

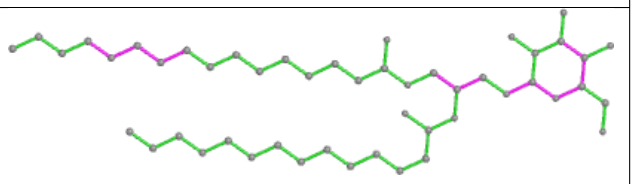


Rings

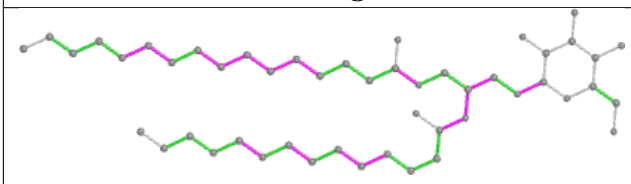
Ligand LMG c 523



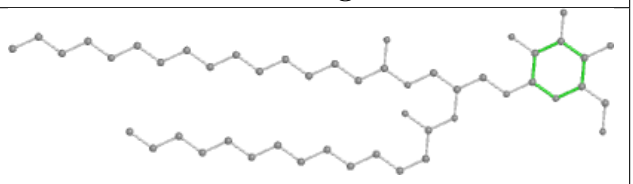
Bond lengths



Bond angles

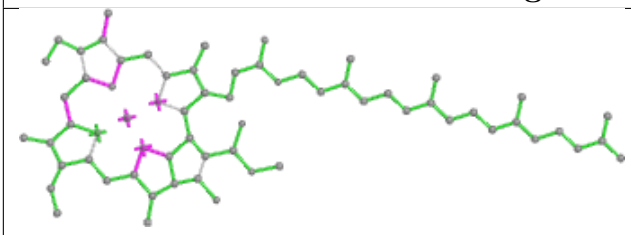


Torsions

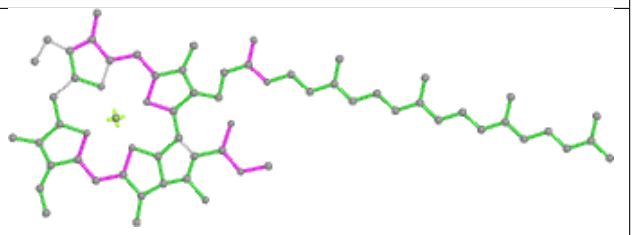


Rings

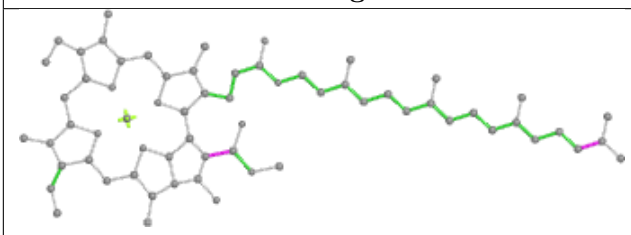
Ligand CLA B 607



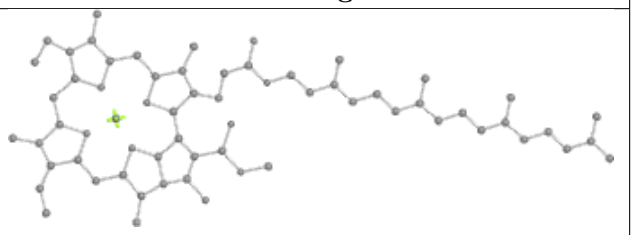
Bond lengths



Bond angles

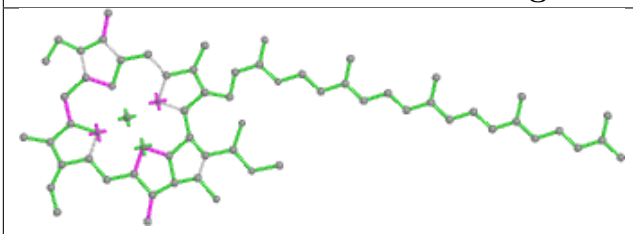


Torsions

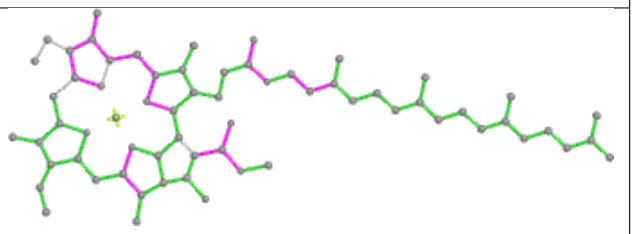


Rings

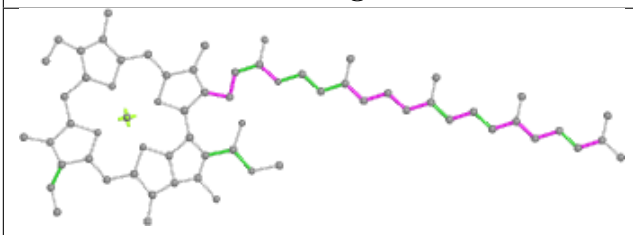
Ligand CLA c 512



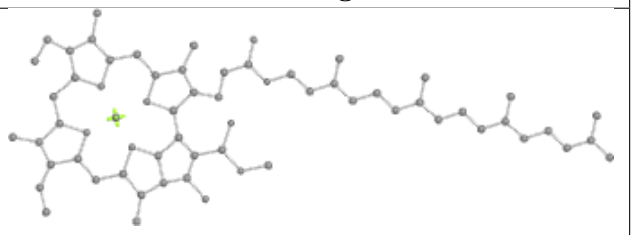
Bond lengths



Bond angles

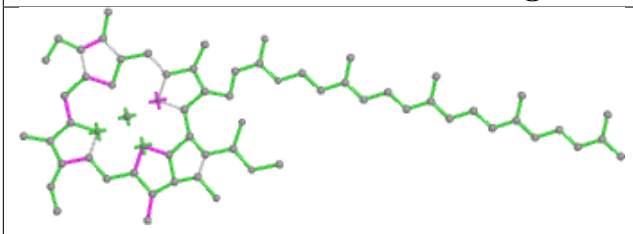


Torsions

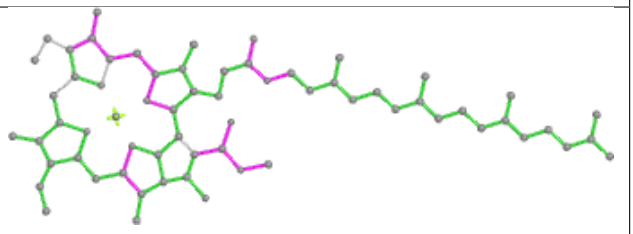


Rings

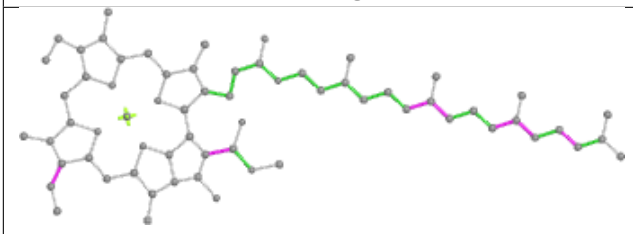
Ligand CLA A 403



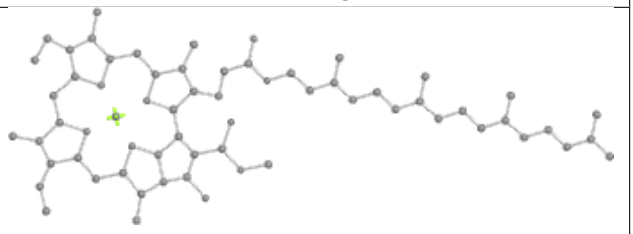
Bond lengths



Bond angles

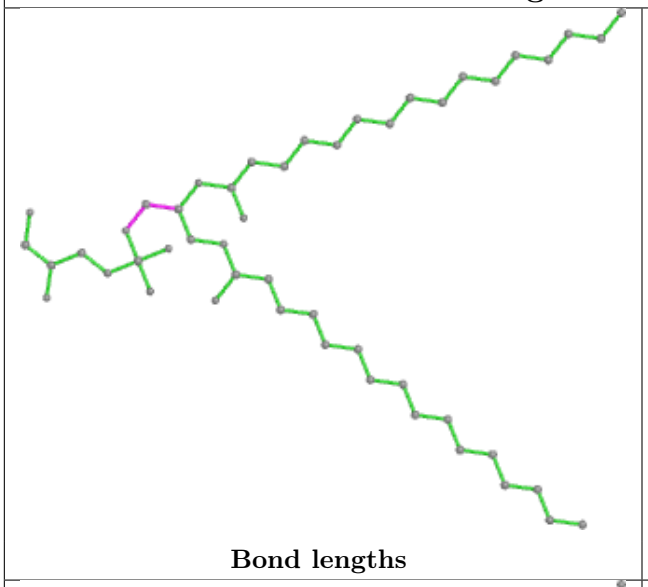


Torsions

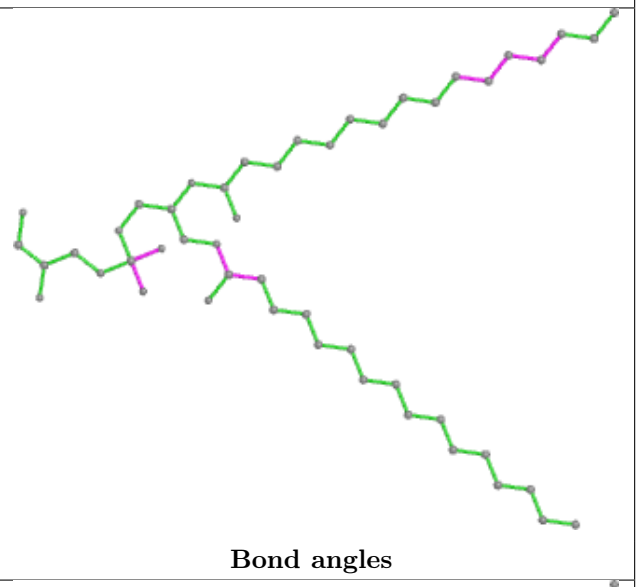


Rings

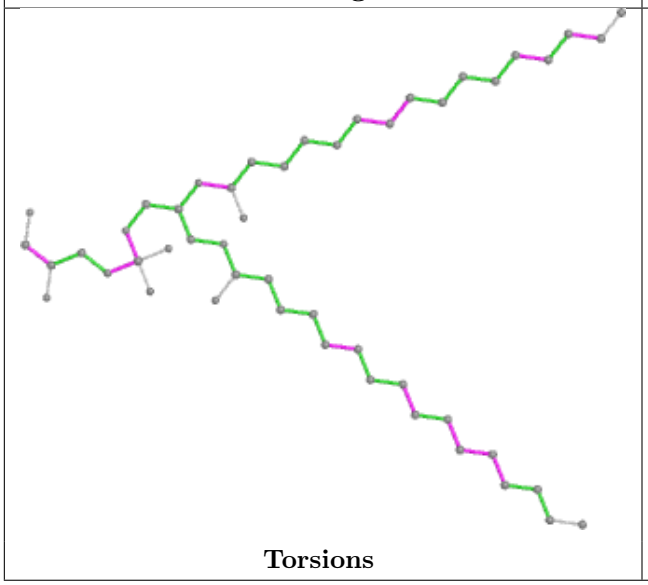
Ligand LHG d 408



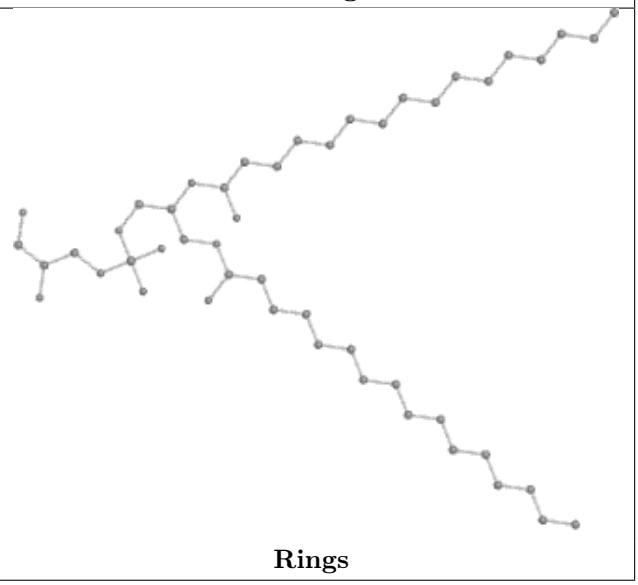
Bond lengths



Bond angles

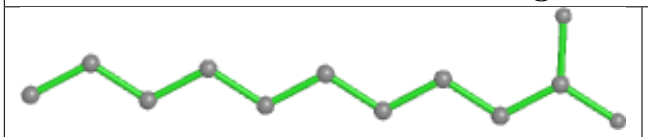


Torsions



Rings

Ligand STE a 414



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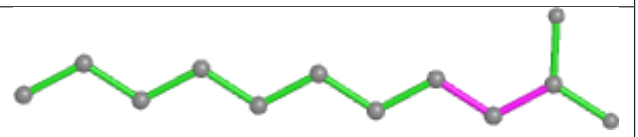
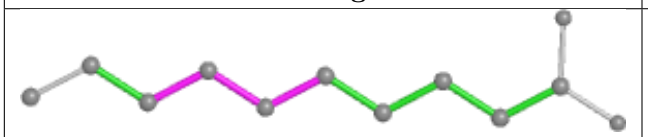
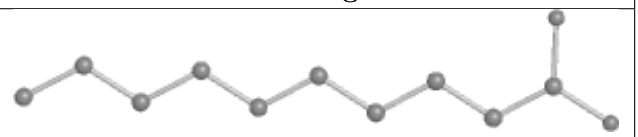


Bond angles

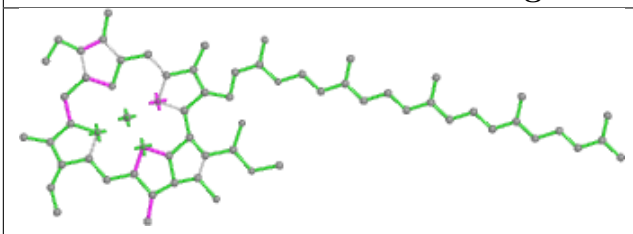


Torsions

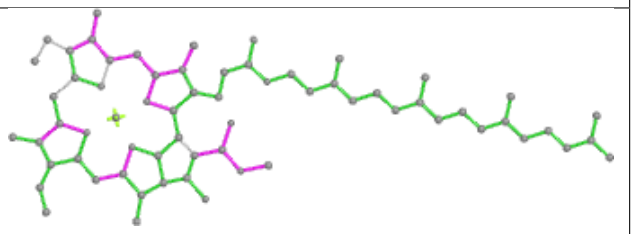


Rings

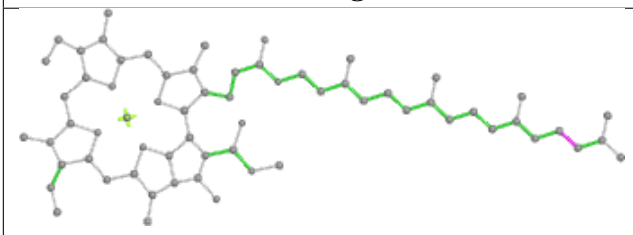
Ligand CLA B 608



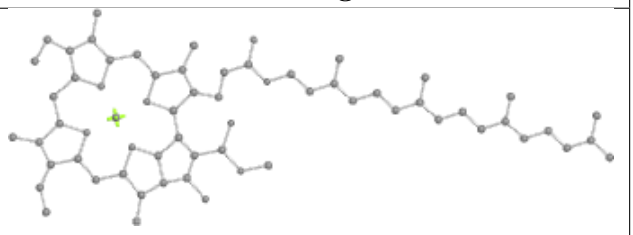
Bond lengths



Bond angles

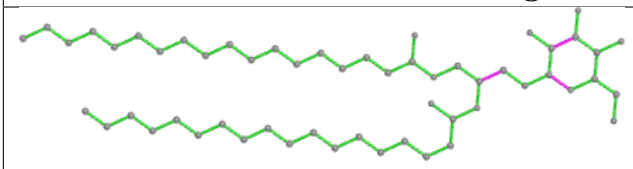


Torsions



Rings

Ligand LMG b 623



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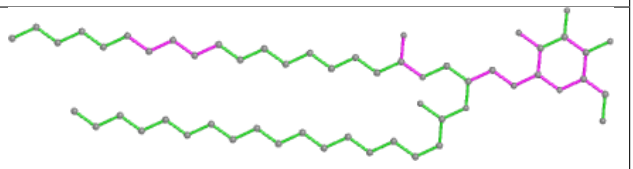
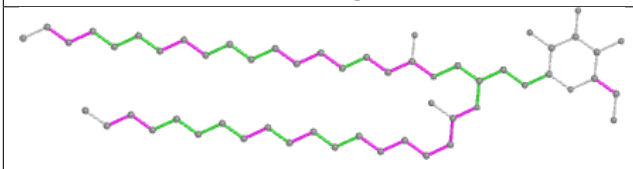
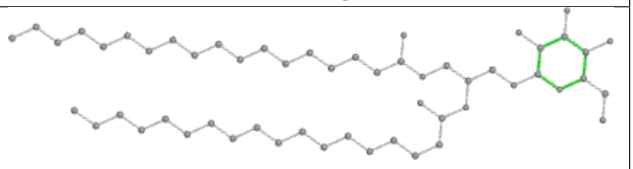


Bond angles

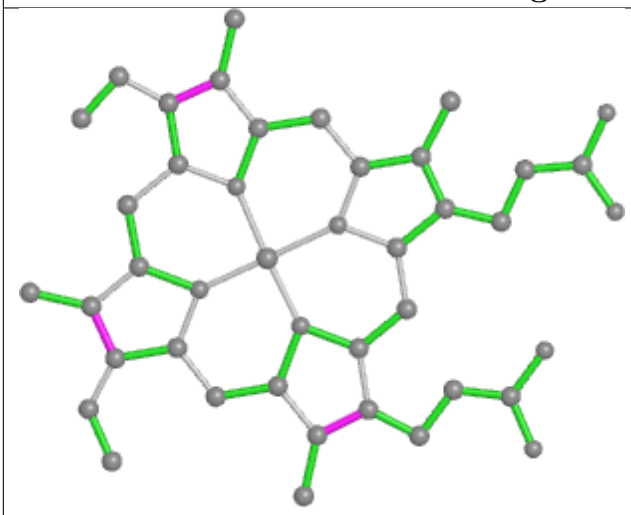


Torsions



Rings

Ligand HEC f 101



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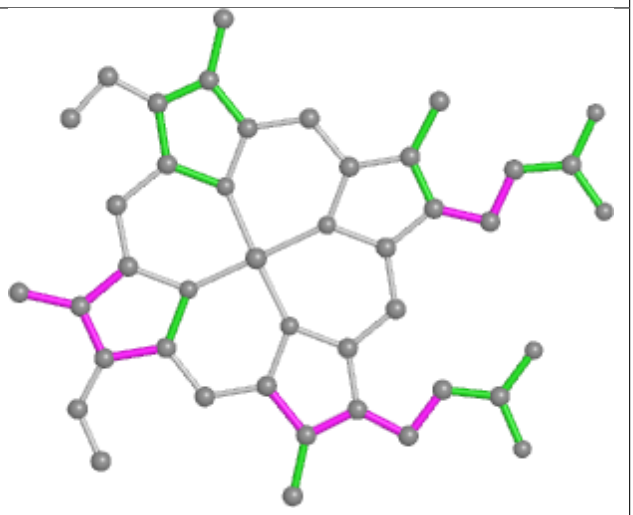
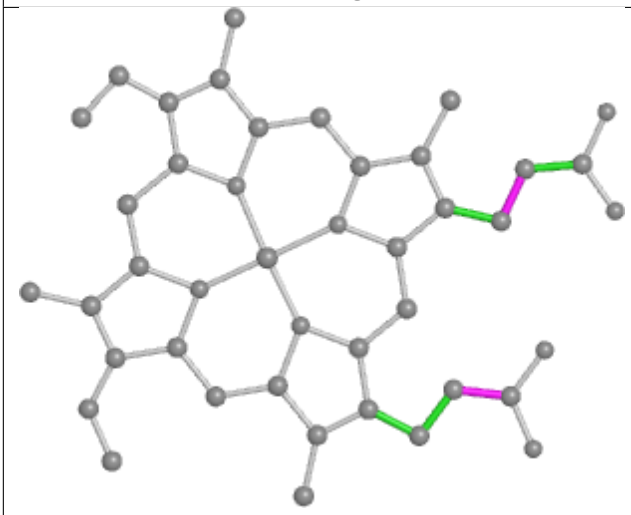
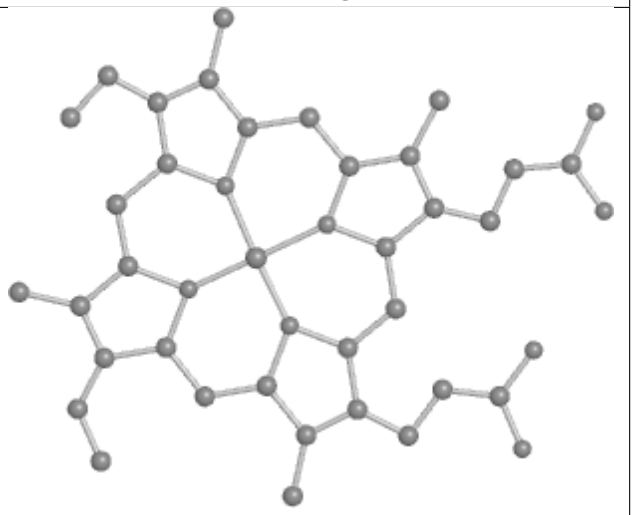


Bond angles

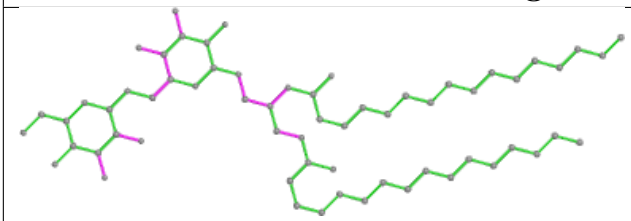


Torsions

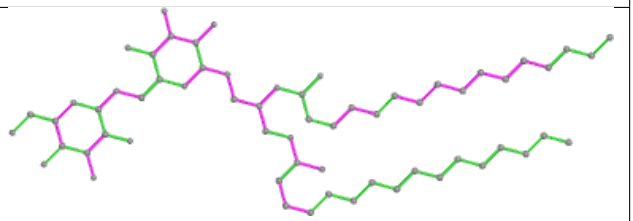


Rings

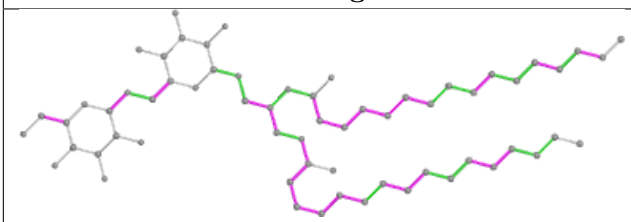
Ligand DGD c 517



Bond lengths



Bond angles



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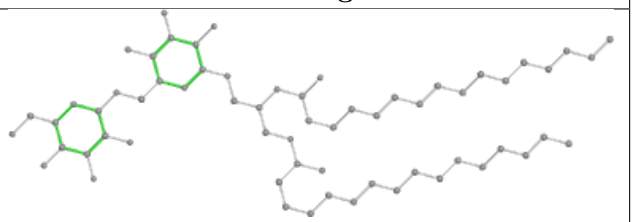
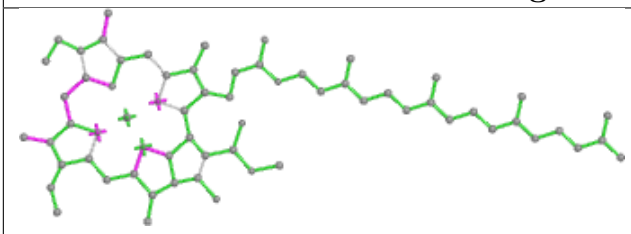
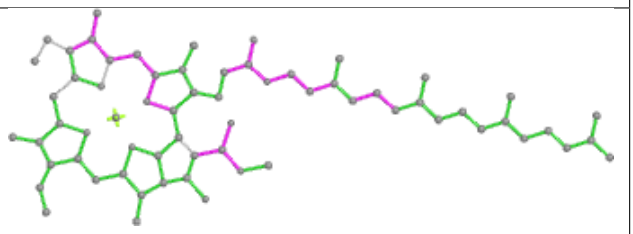


Rings

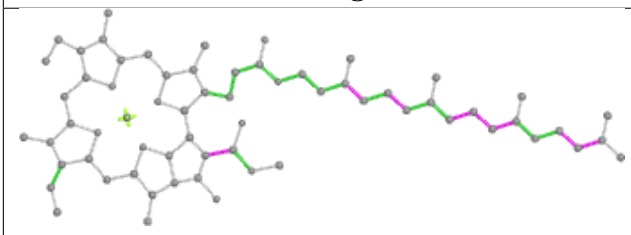
Ligand CLA c 510



Bond lengths



Bond angles



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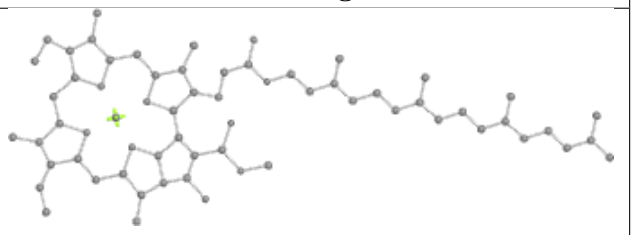
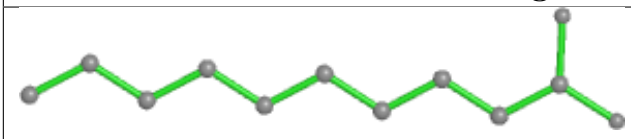
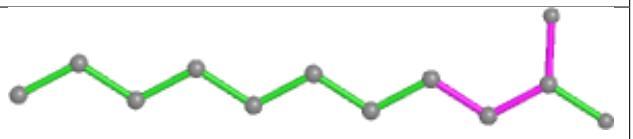


Rings

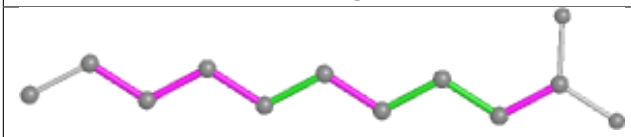
Ligand STE J 101



Bond lengths



Bond angles



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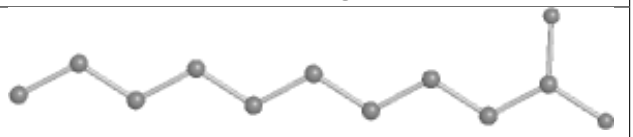
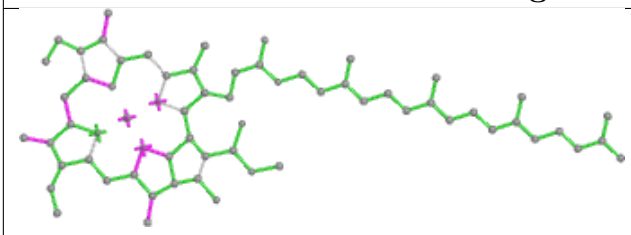
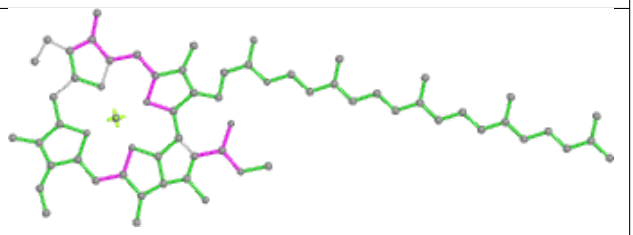


Rings

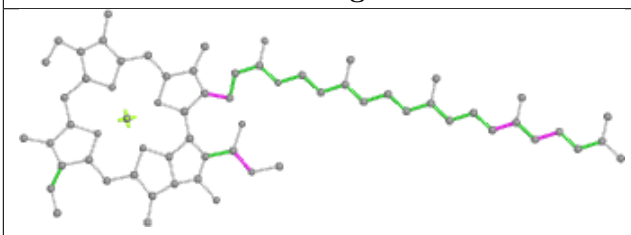
Ligand CLA c 513



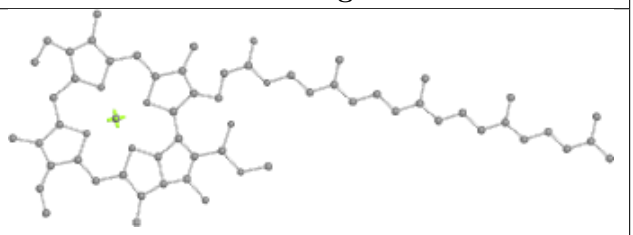
Bond lengths



Bond angles

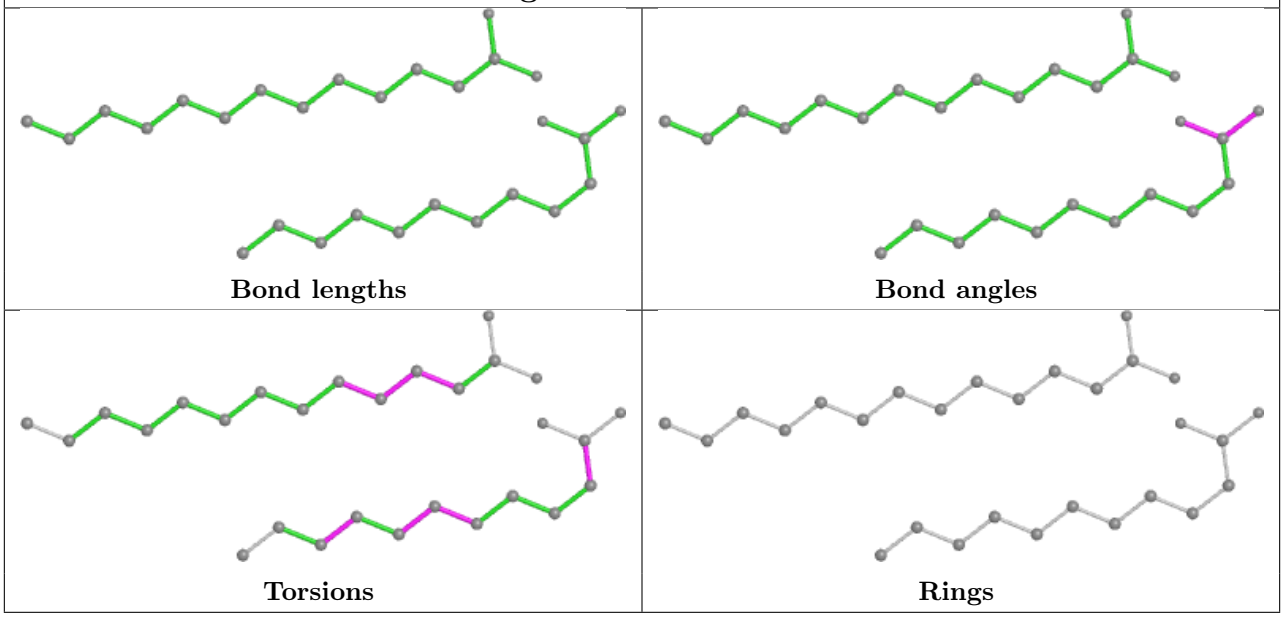


Torsions

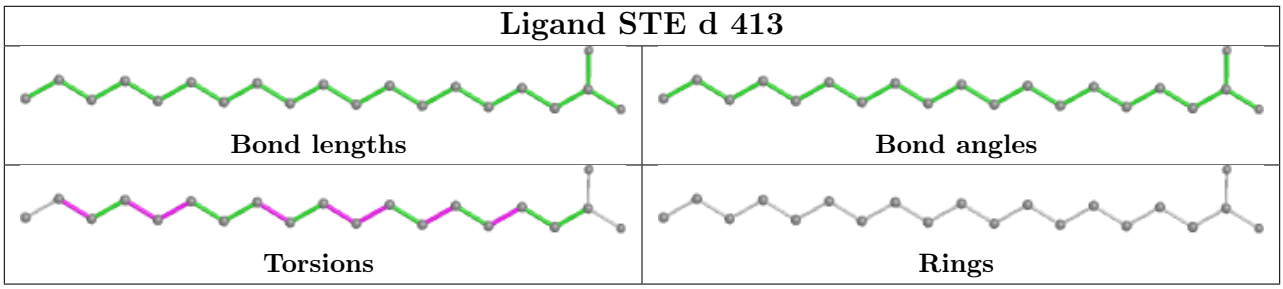


Rings

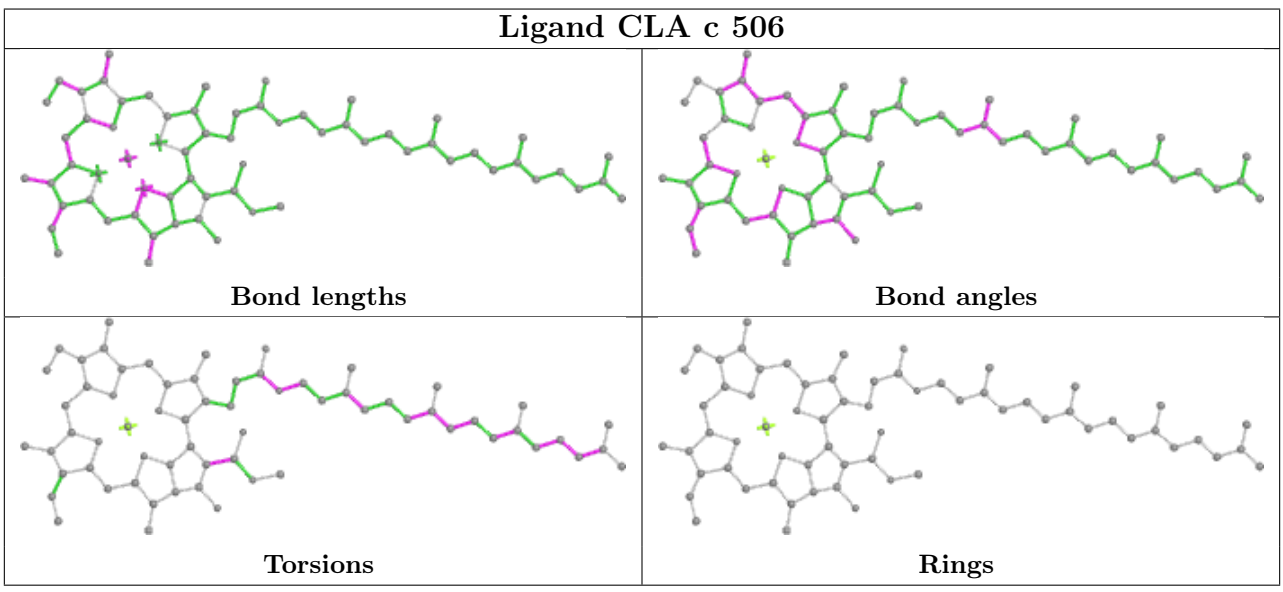
Ligand LMG D 411



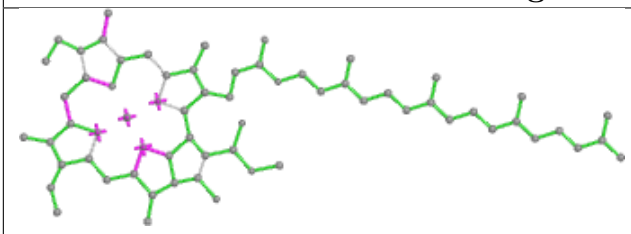
Ligand STE d 413



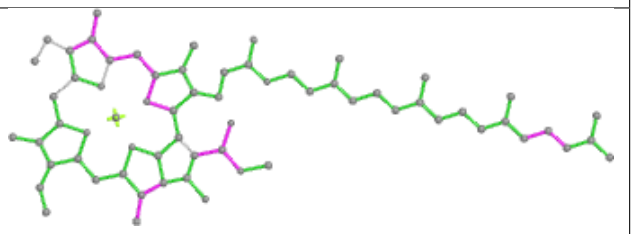
Ligand CLA c 506



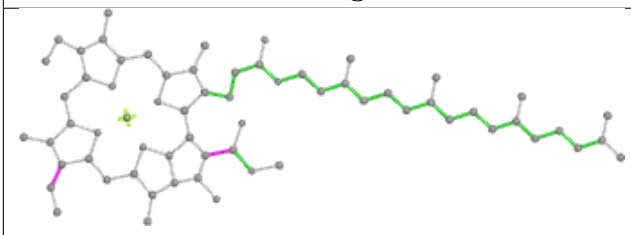
Ligand CLA d 404



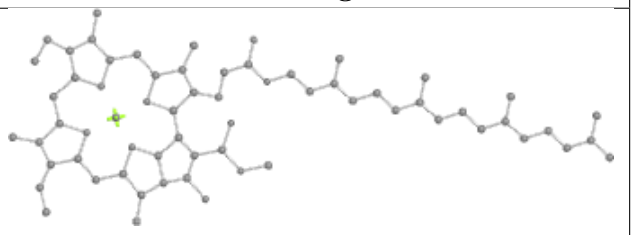
Bond lengths



Bond angles

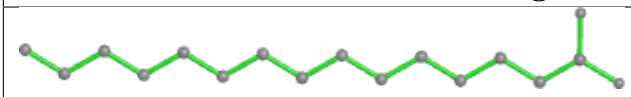


Torsions

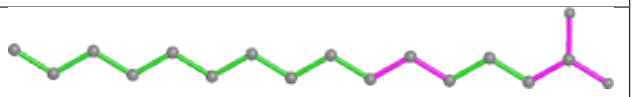


Rings

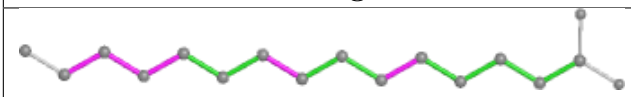
Ligand STE d 411



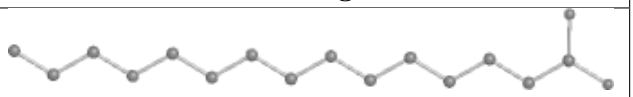
Bond lengths



Bond angles

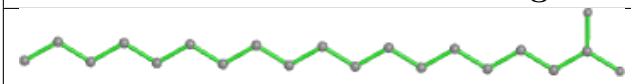


Torsions

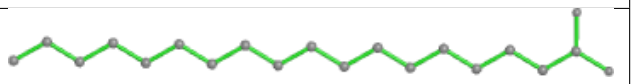


Rings

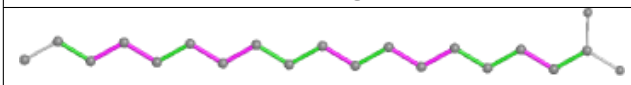
Ligand STE b 622



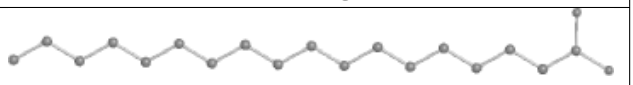
Bond lengths



Bond angles

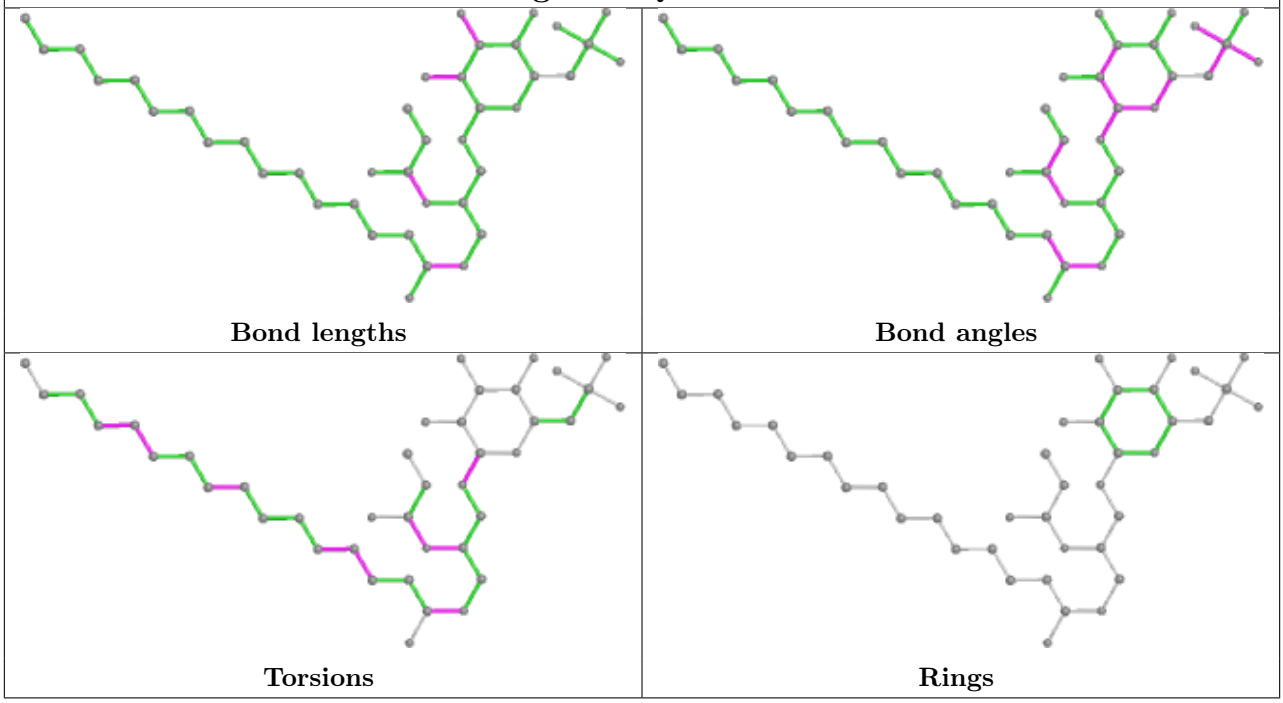


Torsions

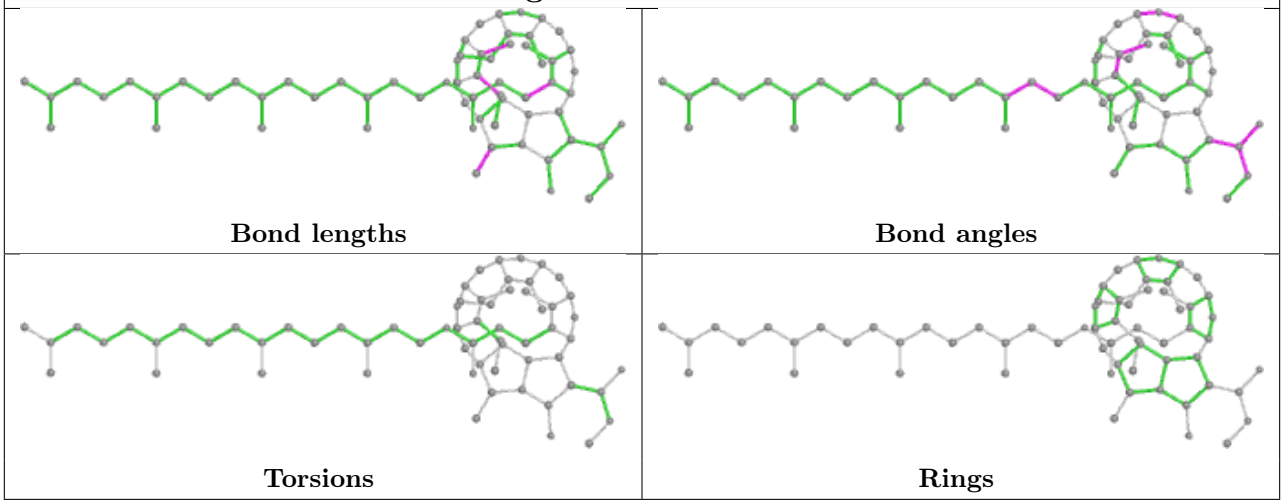


Rings

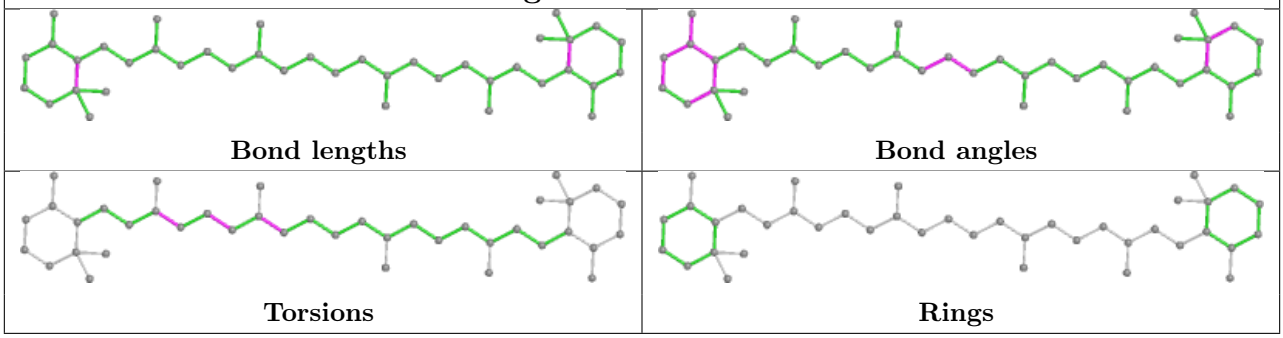
Ligand SQD f 102



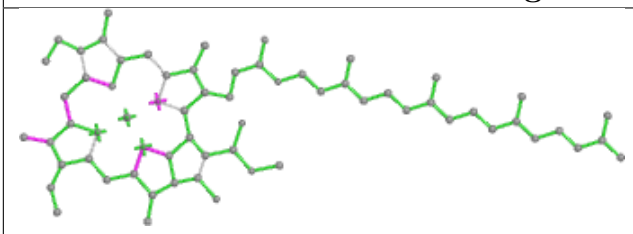
Ligand PHO d 402



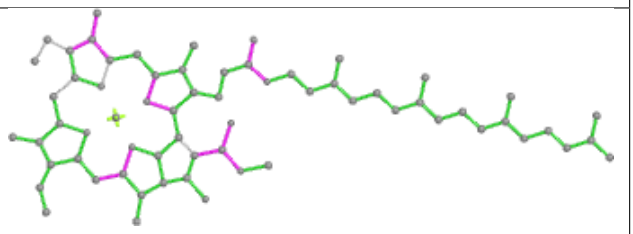
Ligand BCR B 619



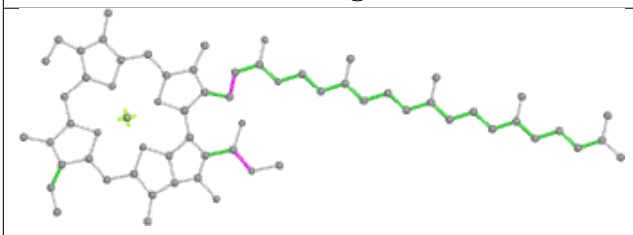
Ligand CLA C 501



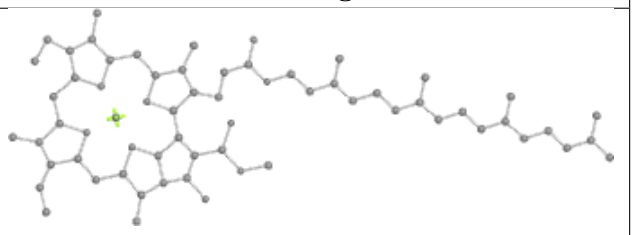
Bond lengths



Bond angles

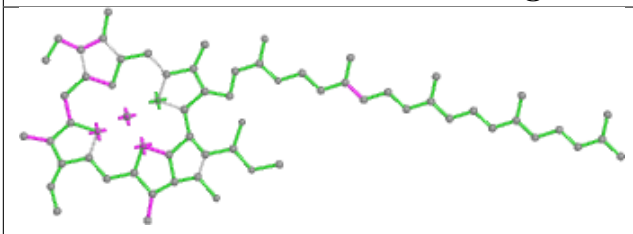


Torsions

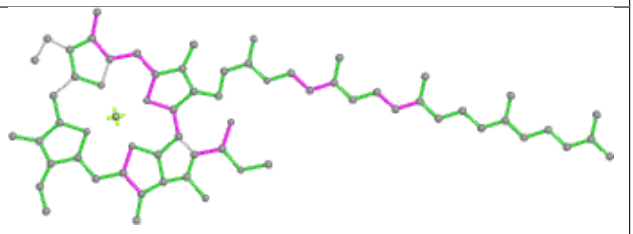


Rings

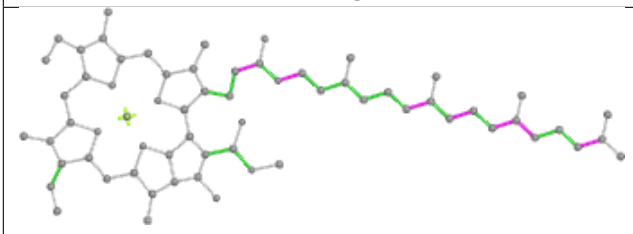
Ligand CLA B 613



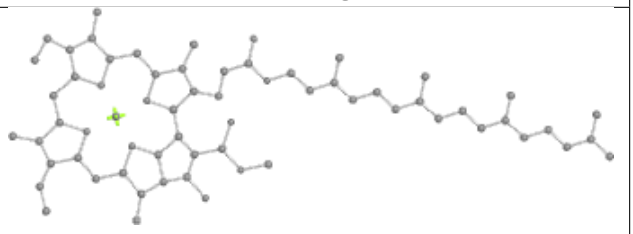
Bond lengths



Bond angles

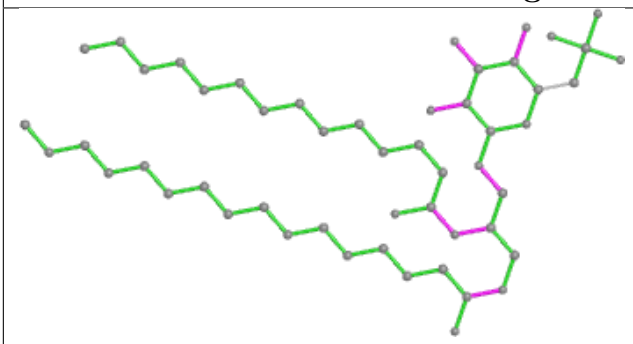


Torsions

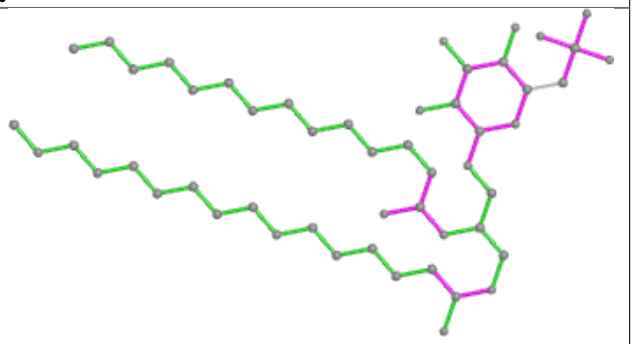


Rings

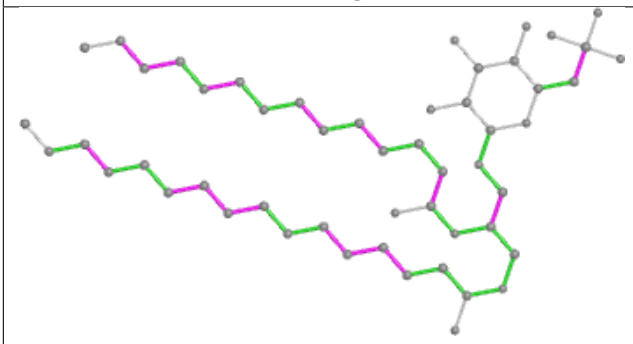
Ligand SQD A 413



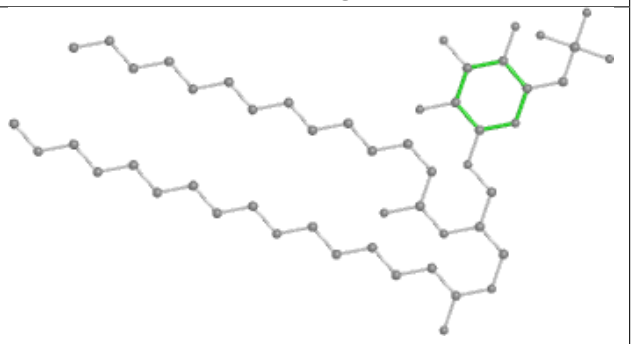
Bond lengths



Bond angles

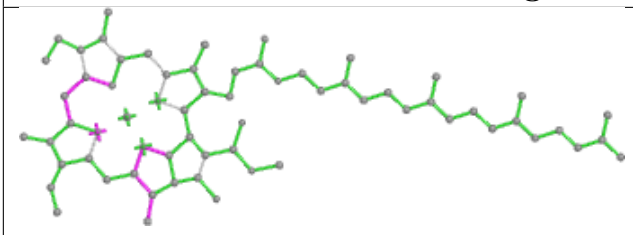


Torsions

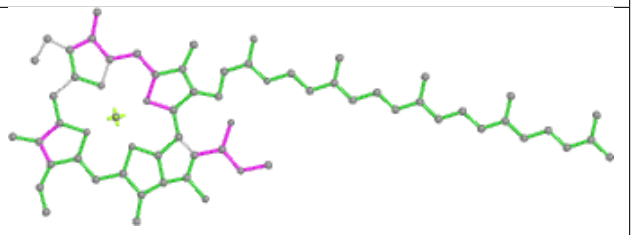


Rings

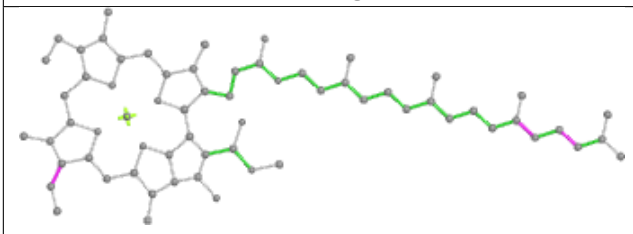
Ligand CLA A 402



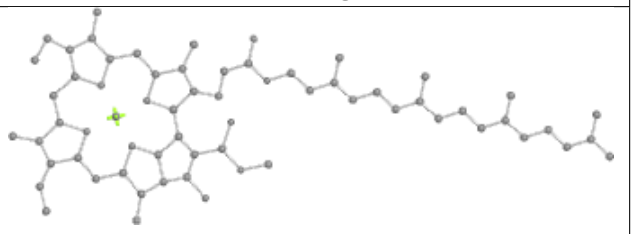
Bond lengths



Bond angles

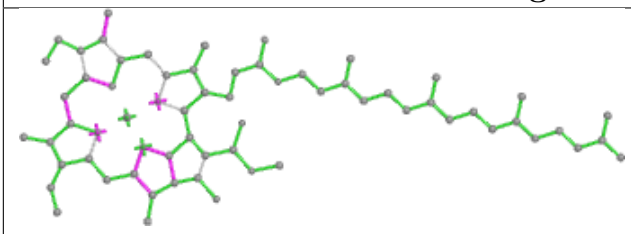


Torsions

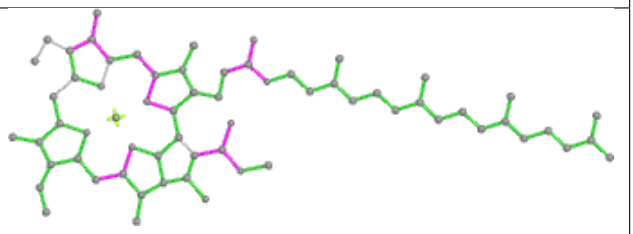


Rings

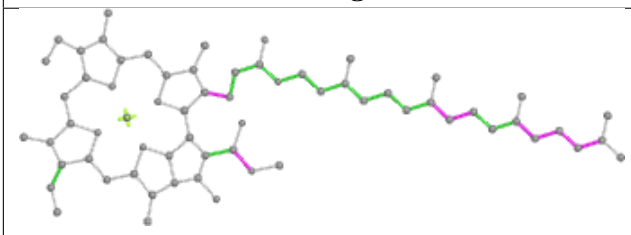
Ligand CLA c 511



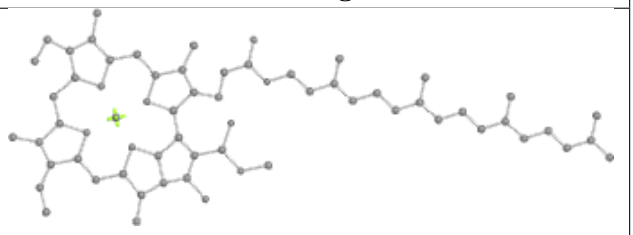
Bond lengths



Bond angles

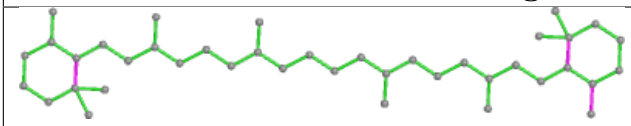


Torsions

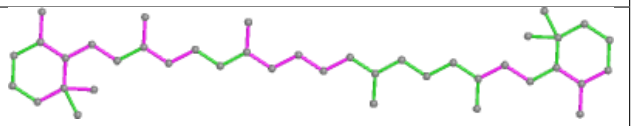


Rings

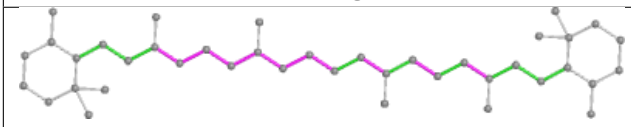
Ligand BCR C 514



Bond lengths



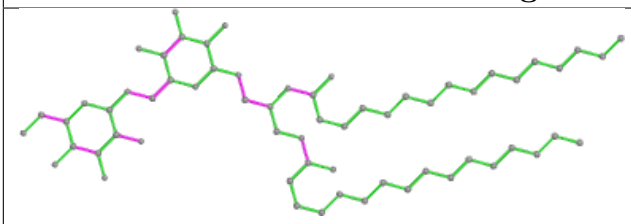
Bond angles



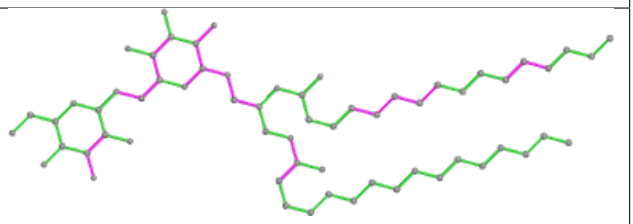
Torsions

Rings

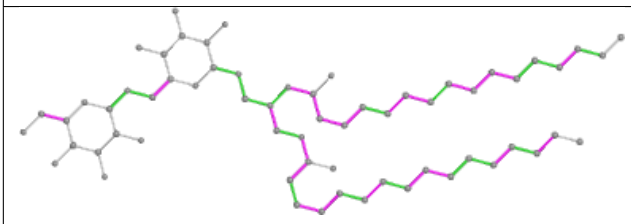
Ligand DGD C 517



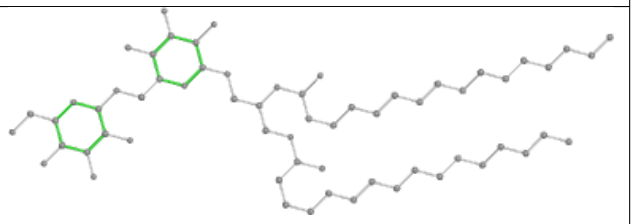
Bond lengths



Bond angles

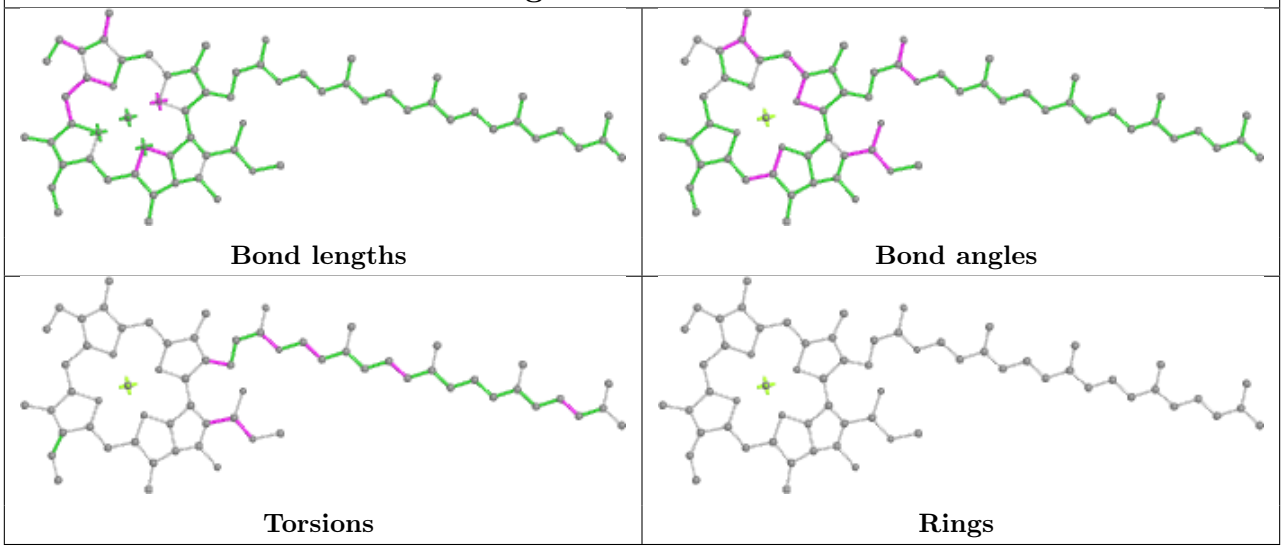


Torsions

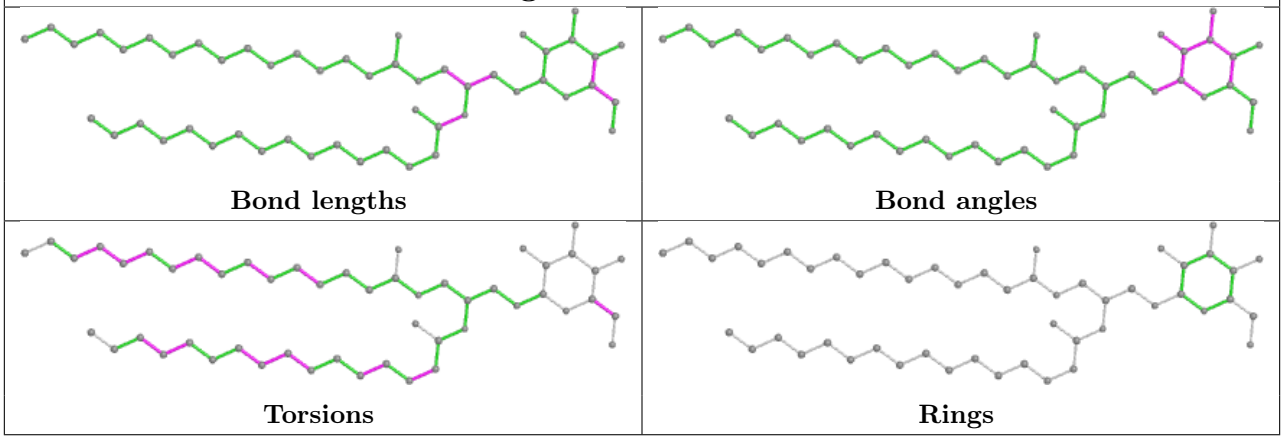


Rings

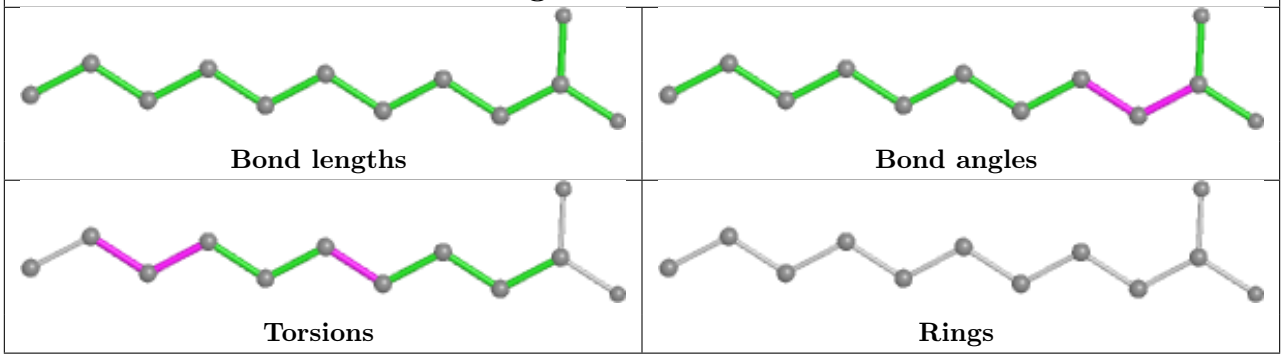
Ligand CLA C 513



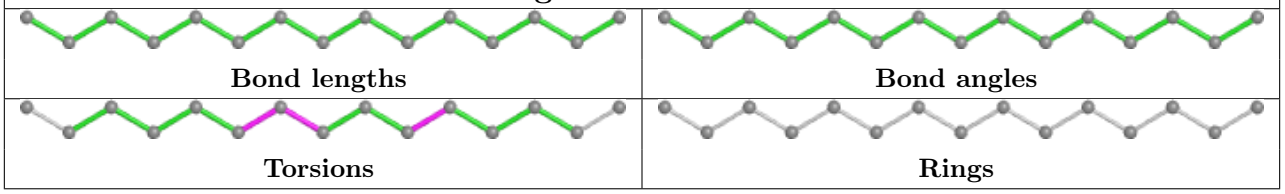
Ligand LMG D 407



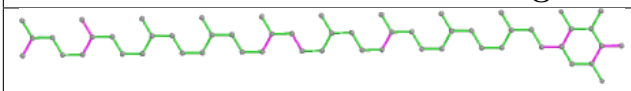
Ligand STE B 624



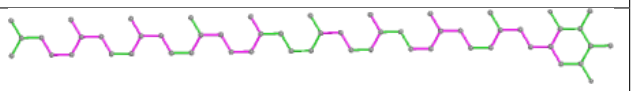
Ligand STE I 101



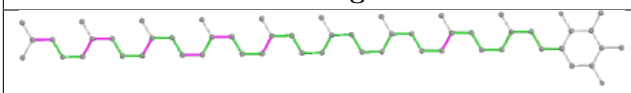
Ligand PL9 d 407



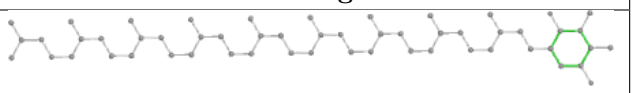
Bond lengths



Bond angles

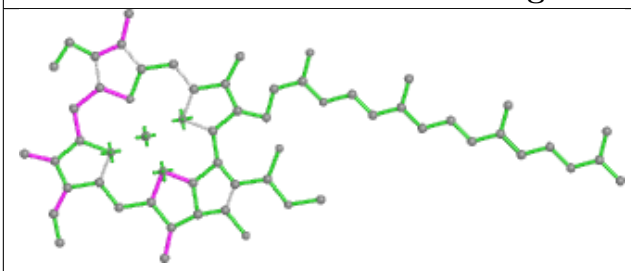


Torsions

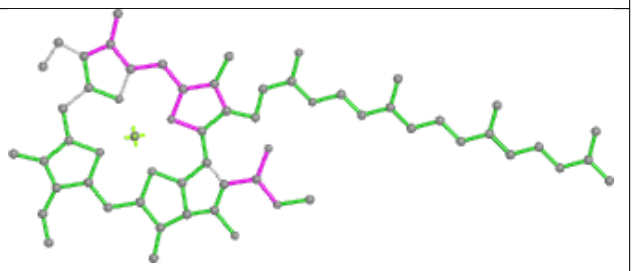


Rings

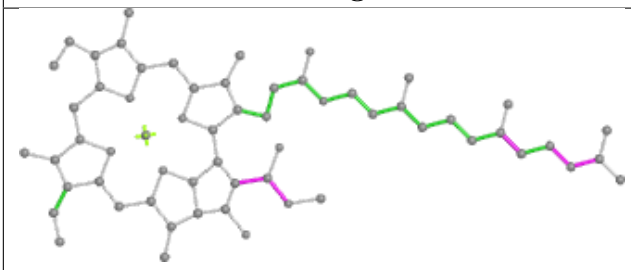
Ligand CLA b 616



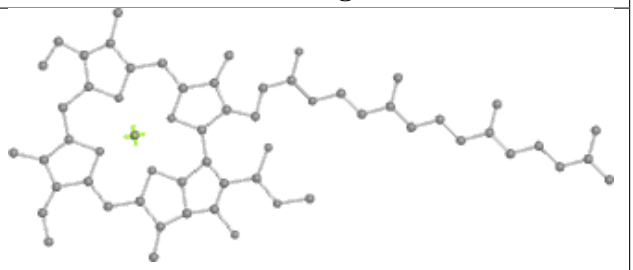
Bond lengths



Bond angles

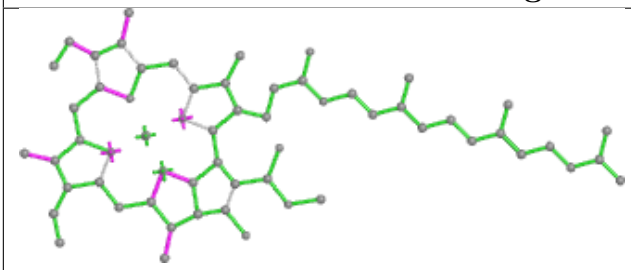


Torsions

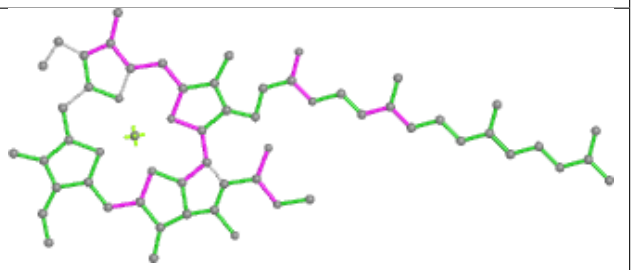


Rings

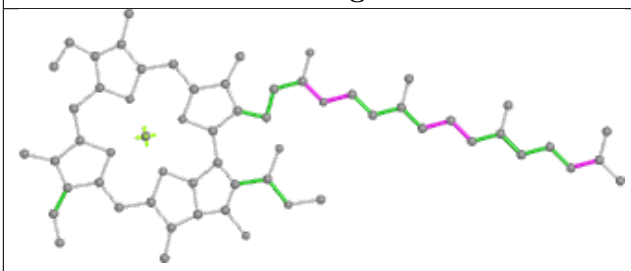
Ligand CLA B 616



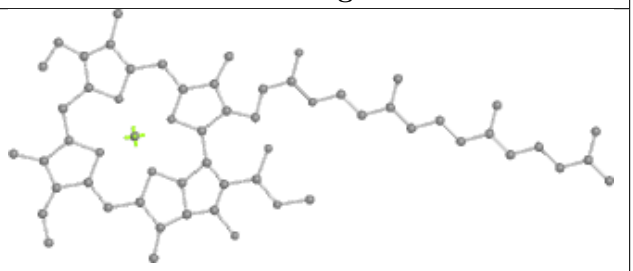
Bond lengths



Bond angles

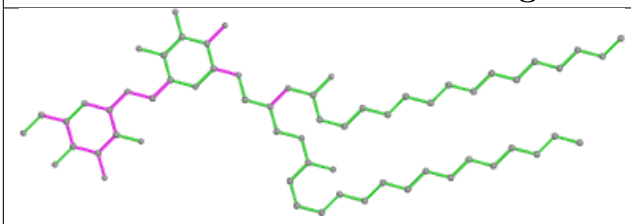


Torsions

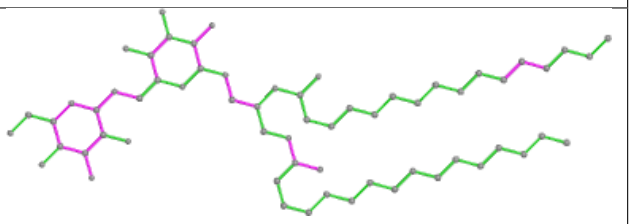


Rings

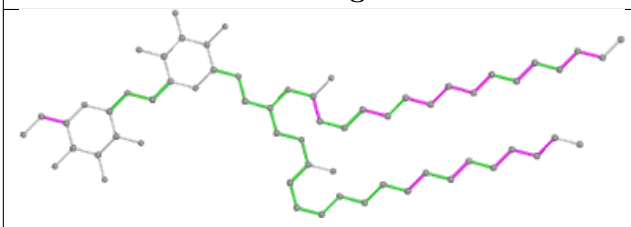
Ligand DGD H 102



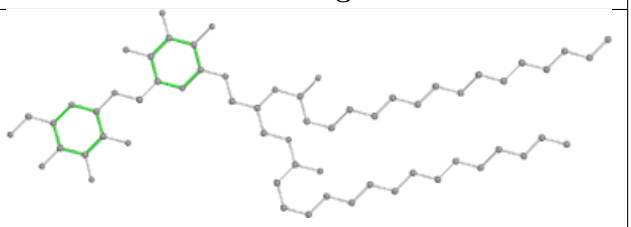
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.34	4 (1%) 79 78	19, 27, 44, 79	0
1	a	334/344 (97%)	-0.33	1 (0%) 94 93	22, 28, 51, 82	0
2	B	505/506 (99%)	-0.32	6 (1%) 79 78	22, 31, 57, 82	0
2	b	505/506 (99%)	-0.12	17 (3%) 45 44	22, 34, 66, 98	0
3	C	442/461 (95%)	-0.23	3 (0%) 87 87	23, 34, 49, 71	0
3	c	451/461 (97%)	-0.15	6 (1%) 77 76	23, 37, 59, 97	0
4	D	341/352 (96%)	-0.33	0 100 100	21, 28, 44, 76	0
4	d	341/352 (96%)	-0.23	1 (0%) 94 93	22, 31, 53, 75	0
5	E	82/84 (97%)	0.08	4 (4%) 29 28	32, 46, 68, 80	0
5	e	82/84 (97%)	0.31	5 (6%) 21 20	35, 53, 75, 81	0
6	F	34/45 (75%)	-0.38	1 (2%) 51 50	33, 39, 58, 80	0
6	f	34/45 (75%)	-0.13	1 (2%) 51 50	37, 44, 69, 85	0
7	H	65/66 (98%)	0.01	2 (3%) 49 48	30, 37, 56, 68	0
7	h	63/66 (95%)	0.36	6 (9%) 8 7	37, 46, 59, 66	0
8	I	35/38 (92%)	-0.11	3 (8%) 10 9	30, 36, 68, 82	0
8	i	35/38 (92%)	0.04	3 (8%) 10 9	28, 38, 70, 86	0
9	J	36/40 (90%)	0.13	4 (11%) 5 4	31, 46, 66, 87	0
9	j	36/40 (90%)	0.22	4 (11%) 5 4	35, 49, 88, 99	0
10	K	37/46 (80%)	0.14	2 (5%) 25 24	37, 47, 65, 71	0
10	k	37/46 (80%)	0.15	4 (10%) 5 5	44, 50, 63, 76	0
11	L	37/37 (100%)	-0.40	0 100 100	23, 27, 59, 65	0
11	l	36/37 (97%)	-0.14	2 (5%) 24 23	24, 28, 72, 83	0
12	M	32/36 (88%)	0.02	1 (3%) 49 48	24, 32, 60, 69	0
12	m	31/36 (86%)	-0.11	0 100 100	24, 32, 48, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	0.08	15 (6%) 21 20	24, 39, 78, 126	0
13	o	244/272 (89%)	-0.06	13 (5%) 26 25	25, 38, 76, 124	0
14	R	34/40 (85%)	1.52	10 (29%) 0 0	53, 64, 85, 97	0
14	r	31/40 (77%)	3.85	22 (70%) 0 0	66, 82, 100, 106	0
15	T	29/30 (96%)	-0.38	1 (3%) 45 44	25, 29, 60, 72	0
15	t	29/30 (96%)	-0.26	2 (6%) 16 16	25, 29, 76, 80	0
16	U	97/134 (72%)	-0.16	4 (4%) 37 36	30, 40, 66, 85	0
16	u	97/134 (72%)	-0.32	0 100 100	29, 37, 55, 82	0
17	V	137/163 (84%)	-0.38	0 100 100	28, 37, 54, 78	0
17	v	137/163 (84%)	-0.12	6 (4%) 34 33	30, 43, 64, 83	0
18	X	38/41 (92%)	0.12	2 (5%) 26 25	35, 45, 64, 73	0
18	x	39/41 (95%)	0.47	4 (10%) 6 6	44, 52, 78, 94	0
19	Y	27/46 (58%)	1.21	10 (37%) 0 0	48, 63, 88, 92	0
19	y	30/46 (65%)	0.58	3 (10%) 7 6	53, 64, 85, 91	0
20	Z	62/62 (100%)	1.01	16 (25%) 0 0	48, 61, 103, 118	0
20	z	62/62 (100%)	0.96	16 (25%) 0 0	53, 66, 102, 109	0
All	All	5302/5686 (93%)	-0.10	204 (3%) 40 39	19, 35, 69, 126	0

The worst 5 of 204 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	32	GLN	16.8
13	o	58	ASN	9.3
13	O	56	PRO	7.8
14	r	6	LEU	6.5
13	o	60	ARG	6.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	FME	t	1	10/11	0.93	0.10	32,45,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.95	0.15	40,51,73,84	0
8	FME	I	1	10/11	0.95	0.18	33,44,65,71	0
15	FME	T	1	10/11	0.96	0.08	27,46,65,65	0
8	FME	i	1	10/11	0.97	0.16	36,50,62,65	0
12	FME	m	1	10/11	0.97	0.15	34,45,71,80	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	STE	R	101	12/20	0.60	0.31	55,77,85,87	0
33	STE	H	103	18/20	0.69	0.32	51,74,87,90	0
33	STE	b	625	20/20	0.73	0.24	49,66,82,85	0
33	STE	a	414	12/20	0.75	0.24	35,62,69,75	0
27	LMG	a	416	55/55	0.80	0.18	37,63,101,136	0
33	STE	a	413	10/20	0.80	0.21	40,62,75,75	0
33	STE	a	415	15/20	0.81	0.19	39,68,86,93	0
33	STE	b	627	14/20	0.81	0.22	52,65,84,93	0
28	LHG	E	101	49/49	0.82	0.22	43,76,103,113	0
27	LMG	c	522	48/55	0.82	0.26	43,75,106,112	0
24	BCR	H	101	40/40	0.83	0.16	28,44,58,65	0
33	STE	k	102	12/20	0.83	0.18	43,65,78,83	0
33	STE	B	626	12/20	0.84	0.32	49,62,79,84	0
22	CLA	b	601	65/65	0.84	0.18	46,65,86,102	0
26	PL9	A	410	55/55	0.84	0.25	32,65,86,92	0
27	LMG	c	523	49/55	0.84	0.18	36,57,92,106	0
27	LMG	D	410	33/55	0.84	0.18	35,55,80,90	0
28	LHG	e	101	42/49	0.84	0.23	51,78,103,123	0
33	STE	b	624	16/20	0.84	0.15	42,62,79,80	0
29	SQD	a	412	36/54	0.84	0.17	31,63,87,91	0
33	STE	b	626	10/20	0.84	0.23	39,53,59,69	0
30	DGD	A	415	66/66	0.84	0.17	42,64,85,88	0
33	STE	B	625	16/20	0.84	0.26	43,62,82,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	STE	m	102	12/20	0.84	0.20	49,62,82,84	0
33	STE	d	413	20/20	0.85	0.18	38,68,92,97	0
27	LMG	b	623	55/55	0.86	0.29	49,71,96,103	0
33	STE	c	521	20/20	0.86	0.20	37,59,72,75	0
29	SQD	A	414	39/54	0.86	0.19	40,64,96,106	0
22	CLA	C	512	65/65	0.86	0.17	32,52,84,94	0
33	STE	l	102	18/20	0.86	0.15	36,48,82,86	0
33	STE	C	523	12/20	0.86	0.12	36,48,55,59	0
33	STE	t	102	14/20	0.86	0.14	34,50,66,67	0
33	STE	j	101	12/20	0.87	0.14	45,57,71,73	0
24	BCR	Y	101	40/40	0.87	0.13	32,48,64,68	0
24	BCR	x	101	40/40	0.87	0.14	34,49,67,71	0
22	CLA	C	513	65/65	0.87	0.19	38,62,94,108	0
26	PL9	a	409	55/55	0.87	0.18	34,68,87,99	0
33	STE	t	103	18/20	0.87	0.14	44,57,78,85	0
33	STE	d	411	17/20	0.88	0.16	39,56,68,71	0
24	BCR	d	406	40/40	0.88	0.14	35,52,96,100	0
33	STE	b	621	16/20	0.88	0.18	29,47,69,70	0
33	STE	B	620	17/20	0.88	0.19	33,52,69,70	0
29	SQD	B	623	54/54	0.88	0.15	37,61,86,98	0
33	STE	T	102	15/20	0.88	0.18	42,58,79,80	0
24	BCR	k	101	40/40	0.88	0.14	34,57,72,73	0
33	STE	C	522	16/20	0.88	0.12	34,51,75,83	0
33	STE	Z	101	8/20	0.89	0.16	37,55,66,66	0
33	STE	C	521	12/20	0.89	0.13	41,58,69,70	0
22	CLA	c	512	65/65	0.89	0.15	37,54,91,108	0
22	CLA	c	513	65/65	0.89	0.20	41,66,110,114	0
22	CLA	B	601	65/65	0.89	0.15	27,57,88,102	0
33	STE	J	101	12/20	0.89	0.15	46,57,67,69	0
33	STE	M	103	10/20	0.89	0.16	32,43,56,63	0
27	LMG	c	520	37/55	0.89	0.15	43,67,84,90	0
27	LMG	A	411	48/55	0.89	0.14	35,56,78,89	0
33	STE	d	412	20/20	0.90	0.22	36,54,71,77	0
33	STE	b	622	20/20	0.90	0.22	34,60,72,74	0
33	STE	B	624	12/20	0.90	0.10	31,47,59,67	0
33	STE	D	412	20/20	0.90	0.19	34,52,73,77	0
29	SQD	b	620	49/54	0.90	0.15	40,58,92,111	0
29	SQD	f	102	41/54	0.90	0.19	52,83,112,115	0
24	BCR	C	514	40/40	0.90	0.15	39,54,67,68	0
27	LMG	D	411	28/55	0.90	0.14	34,48,64,74	0
27	LMG	D	407	51/55	0.91	0.18	26,54,85,89	0
22	CLA	D	404	65/65	0.91	0.14	22,43,109,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	a	404	65/65	0.91	0.14	19,35,84,101	0
27	LMG	m	101	51/55	0.91	0.13	34,50,80,88	0
27	LMG	M	101	51/55	0.91	0.12	30,46,67,80	0
24	BCR	c	516	40/40	0.91	0.17	35,48,63,67	0
27	LMG	C	520	48/55	0.91	0.15	41,67,88,95	0
33	STE	I	101	15/20	0.91	0.14	38,55,77,81	0
22	CLA	d	405	65/65	0.92	0.14	26,48,89,100	0
22	CLA	c	508	64/65	0.92	0.15	28,42,82,101	0
24	BCR	D	405	40/40	0.92	0.12	26,42,77,91	0
22	CLA	b	615	65/65	0.92	0.14	26,38,61,66	0
22	CLA	c	502	65/65	0.92	0.14	28,39,58,65	0
24	BCR	c	514	40/40	0.92	0.14	44,57,70,72	0
22	CLA	c	510	65/65	0.93	0.15	26,45,59,77	0
22	CLA	b	606	65/65	0.93	0.13	26,39,76,82	0
24	BCR	b	619	40/40	0.93	0.12	27,47,63,72	0
30	DGD	C	518	62/66	0.93	0.13	27,49,99,122	0
30	DGD	c	519	62/66	0.93	0.14	26,52,87,92	0
22	CLA	C	511	65/65	0.93	0.12	27,48,66,69	0
22	CLA	B	616	60/65	0.93	0.14	23,36,91,109	0
24	BCR	B	618	40/40	0.93	0.10	24,36,49,50	0
24	BCR	B	619	40/40	0.93	0.11	24,41,59,71	0
22	CLA	c	507	65/65	0.93	0.14	26,42,60,70	0
29	SQD	D	408	36/54	0.93	0.16	42,67,91,95	0
29	SQD	a	411	54/54	0.93	0.16	39,62,89,99	0
22	CLA	C	502	65/65	0.93	0.14	25,39,52,58	0
22	CLA	B	606	65/65	0.94	0.11	20,34,67,72	0
22	CLA	b	616	60/65	0.94	0.13	26,40,82,91	0
24	BCR	C	515	40/40	0.94	0.11	26,39,52,64	0
22	CLA	B	615	65/65	0.94	0.11	24,35,63,75	0
22	CLA	c	506	65/65	0.94	0.12	29,45,94,103	0
30	DGD	C	519	62/66	0.94	0.13	24,47,77,91	0
30	DGD	H	102	62/66	0.94	0.10	26,43,57,60	0
30	DGD	c	518	62/66	0.94	0.12	29,51,95,99	0
22	CLA	B	602	65/65	0.94	0.15	22,35,55,61	0
30	DGD	h	101	62/66	0.94	0.12	32,46,57,68	0
24	BCR	b	618	40/40	0.94	0.10	27,38,52,52	0
22	CLA	B	604	65/65	0.94	0.12	20,32,74,85	0
22	CLA	c	509	65/65	0.94	0.18	32,45,61,69	0
22	CLA	C	505	65/65	0.94	0.15	23,38,71,87	0
27	LMG	d	410	44/55	0.94	0.14	30,49,84,89	0
22	CLA	c	511	65/65	0.94	0.13	30,50,70,75	0
22	CLA	C	506	65/65	0.94	0.12	26,41,85,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	602	65/65	0.94	0.15	25,40,64,71	0
22	CLA	d	401	65/65	0.94	0.13	24,37,86,97	0
26	PL9	D	406	55/55	0.94	0.12	18,33,46,50	0
22	CLA	C	507	65/65	0.94	0.14	24,39,57,59	0
22	CLA	b	609	65/65	0.94	0.14	28,42,65,68	0
22	CLA	b	613	65/65	0.95	0.14	16,33,71,82	0
22	CLA	b	614	65/65	0.95	0.12	23,37,75,82	0
24	BCR	C	516	40/40	0.95	0.15	33,48,64,65	0
22	CLA	C	510	65/65	0.95	0.12	26,42,63,69	0
22	CLA	A	403	65/65	0.95	0.13	22,33,88,98	0
24	BCR	T	101	40/40	0.95	0.09	23,36,52,54	0
22	CLA	A	406	54/65	0.95	0.11	17,32,63,66	0
33	STE	M	102	15/20	0.95	0.11	35,45,62,62	0
28	LHG	A	412	47/49	0.95	0.13	26,49,84,100	0
24	BCR	a	405	40/40	0.95	0.09	23,33,43,46	0
28	LHG	d	409	39/49	0.95	0.12	30,45,75,83	0
24	BCR	b	617	40/40	0.95	0.12	28,40,50,53	0
22	CLA	c	503	65/65	0.95	0.14	27,42,53,57	0
22	CLA	c	504	60/65	0.95	0.12	29,44,81,89	0
22	CLA	c	505	65/65	0.95	0.17	23,40,71,74	0
24	BCR	c	515	40/40	0.95	0.10	28,41,58,63	0
22	CLA	B	609	65/65	0.95	0.13	24,36,56,65	0
22	CLA	C	504	59/65	0.95	0.11	27,40,82,87	0
22	CLA	B	610	65/65	0.95	0.14	20,32,40,47	0
24	BCR	t	101	40/40	0.95	0.10	24,36,51,57	0
30	DGD	C	517	62/66	0.95	0.12	22,42,80,92	0
22	CLA	B	613	65/65	0.95	0.13	17,31,70,80	0
22	CLA	B	614	65/65	0.95	0.15	19,37,81,90	0
22	CLA	b	604	65/65	0.95	0.12	17,37,86,98	0
22	CLA	C	508	65/65	0.95	0.12	24,38,99,119	0
22	CLA	b	608	65/65	0.95	0.14	23,41,63,71	0
22	CLA	C	509	65/65	0.95	0.17	25,42,62,65	0
22	CLA	b	610	65/65	0.95	0.19	22,35,51,53	0
24	BCR	B	617	40/40	0.95	0.11	25,38,57,65	0
22	CLA	b	611	65/65	0.95	0.13	21,32,55,60	0
22	CLA	b	612	65/65	0.95	0.16	20,33,47,54	0
29	SQD	A	413	52/54	0.96	0.15	34,58,103,107	0
23	PHO	a	403	64/64	0.96	0.12	19,29,37,48	0
23	PHO	d	402	64/64	0.96	0.10	25,35,45,52	0
24	BCR	A	407	40/40	0.96	0.09	19,33,41,42	0
22	CLA	c	501	65/65	0.96	0.13	28,38,50,55	0
22	CLA	b	603	65/65	0.96	0.14	21,35,71,79	0

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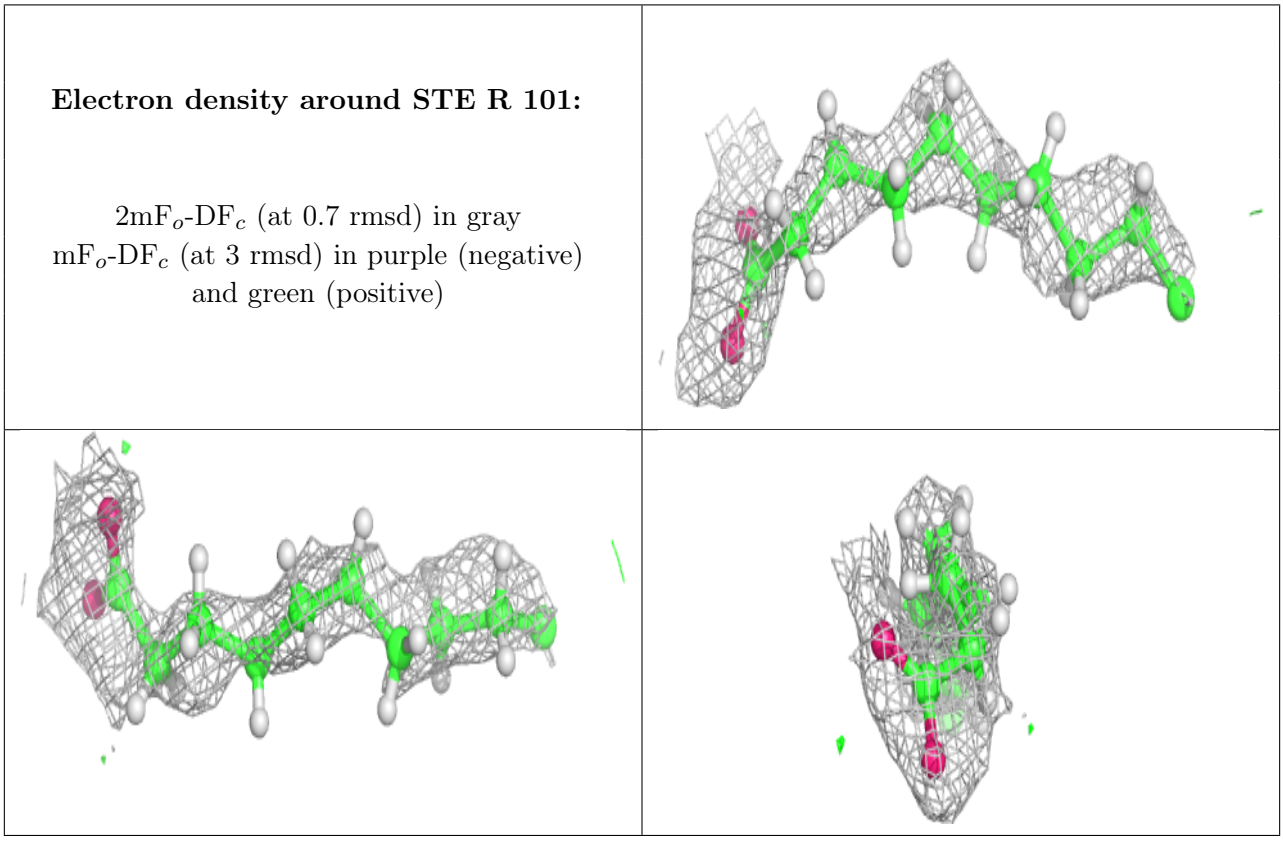
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	PL9	d	407	55/55	0.96	0.11	18,34,43,47	0
22	CLA	B	611	65/65	0.96	0.14	19,30,46,51	0
22	CLA	b	605	65/65	0.96	0.12	20,34,50,55	0
22	CLA	C	503	65/65	0.96	0.13	26,39,47,50	0
22	CLA	b	607	65/65	0.96	0.12	19,35,69,74	0
22	CLA	B	612	65/65	0.96	0.15	17,31,49,54	0
22	CLA	B	603	65/65	0.96	0.15	18,31,65,69	0
30	DGD	c	517	62/66	0.96	0.10	20,42,74,76	0
22	CLA	D	402	65/65	0.96	0.11	15,28,52,62	0
22	CLA	D	403	65/65	0.96	0.10	18,27,44,55	0
22	CLA	B	607	65/65	0.96	0.11	16,31,62,74	0
22	CLA	a	402	65/65	0.96	0.10	17,28,49,59	0
22	CLA	A	402	65/65	0.96	0.10	16,26,45,55	0
22	CLA	B	605	65/65	0.96	0.13	20,31,46,48	0
22	CLA	d	403	65/65	0.96	0.10	18,31,53,65	0
22	CLA	d	404	65/65	0.96	0.11	19,28,45,54	0
22	CLA	C	501	65/65	0.96	0.14	21,35,47,53	0
28	LHG	a	410	49/49	0.96	0.13	28,48,77,84	0
23	PHO	A	404	64/64	0.96	0.10	17,27,36,43	0
23	PHO	A	405	64/64	0.96	0.11	21,30,38,40	0
35	HEC	F	101	43/43	0.96	0.11	31,45,59,61	0
28	LHG	l	101	49/49	0.97	0.09	27,42,52,59	0
22	CLA	B	608	65/65	0.97	0.12	17,32,54,58	0
28	LHG	B	621	49/49	0.97	0.11	25,39,58,66	0
28	LHG	d	408	49/49	0.97	0.09	25,40,51,57	0
28	LHG	B	622	49/49	0.97	0.10	29,43,69,78	0
28	LHG	D	409	49/49	0.97	0.10	22,39,51,55	0
35	HEC	f	101	43/43	0.97	0.12	36,52,70,71	0
34	BCT	D	401	4/4	0.98	0.19	29,31,31,37	0
34	BCT	a	408	4/4	0.98	0.23	27,33,39,46	0
32	OEY	A	417[B]	11/11	0.98	0.13	18,21,25,25	11
35	HEC	V	201	43/43	0.98	0.12	22,31,40,41	0
31	OEX	A	416[A]	10/10	0.98	0.13	28,31,34,36	10
35	HEC	v	201	43/43	0.98	0.13	25,36,44,46	0
32	OEY	a	418[B]	11/11	0.99	0.10	16,21,24,25	11
25	CL	A	409	1/1	0.99	0.04	27,27,27,27	0
25	CL	a	406	1/1	0.99	0.05	26,26,26,26	0
21	FE2	a	401	1/1	0.99	0.06	29,29,29,29	0
31	OEX	a	417[A]	10/10	0.99	0.10	25,31,35,35	10
25	CL	A	408	1/1	0.99	0.06	28,28,28,28	0
25	CL	a	407	1/1	1.00	0.02	26,26,26,26	0
21	FE2	A	401	1/1	1.00	0.12	29,29,29,29	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.

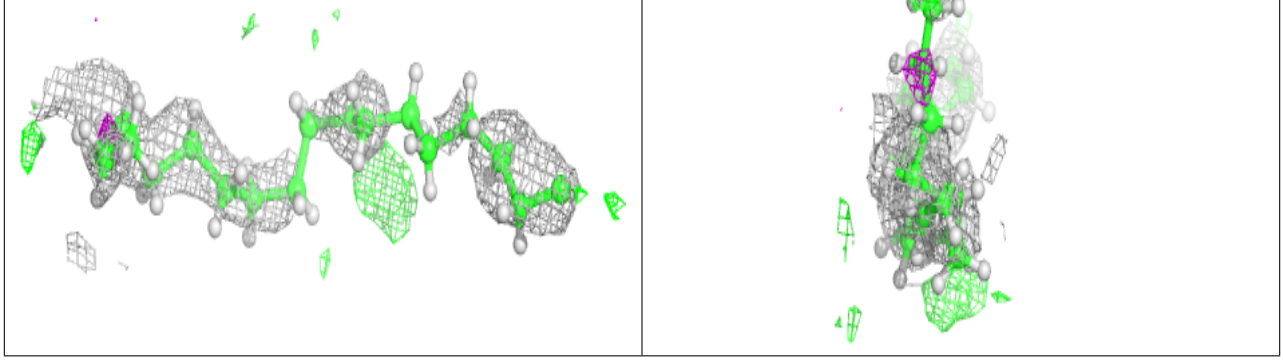
Electron density around STE R 101:

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



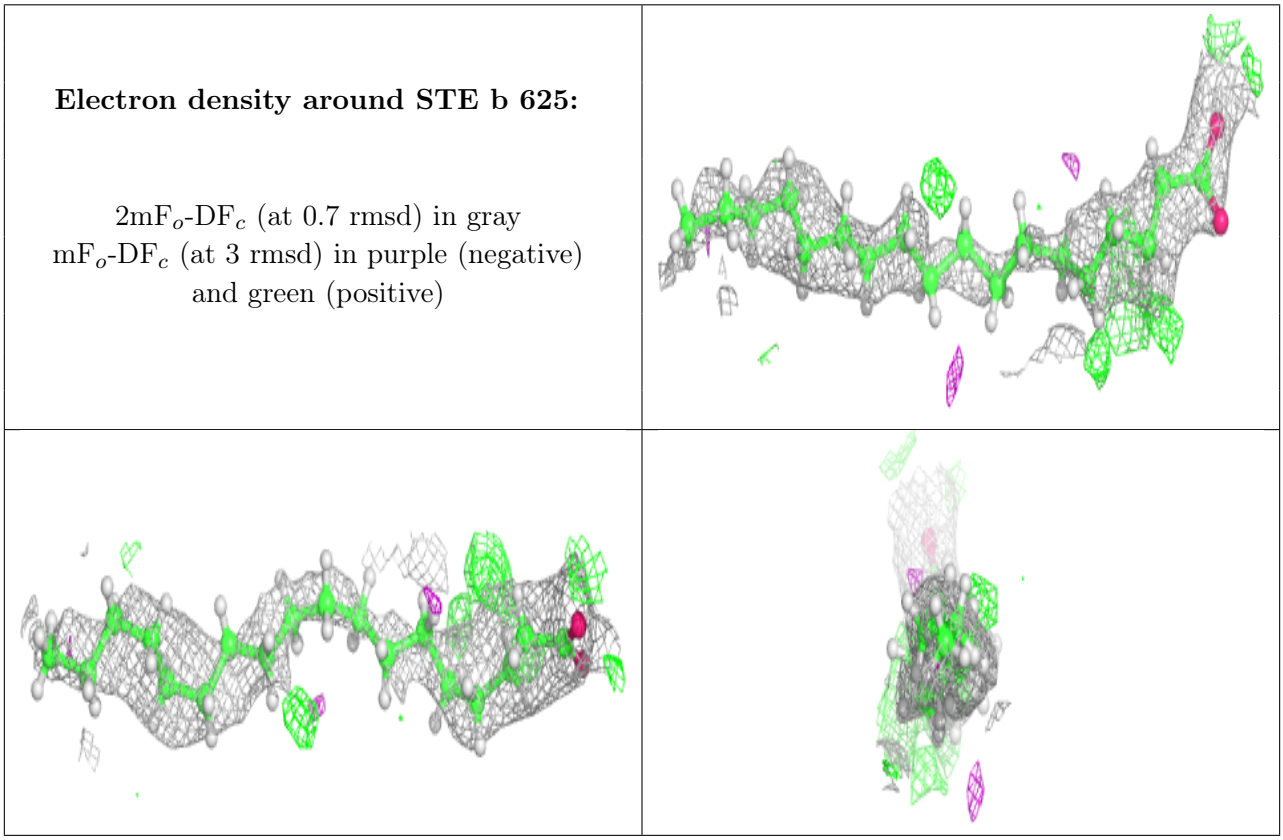
Electron density around STE H 103:

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



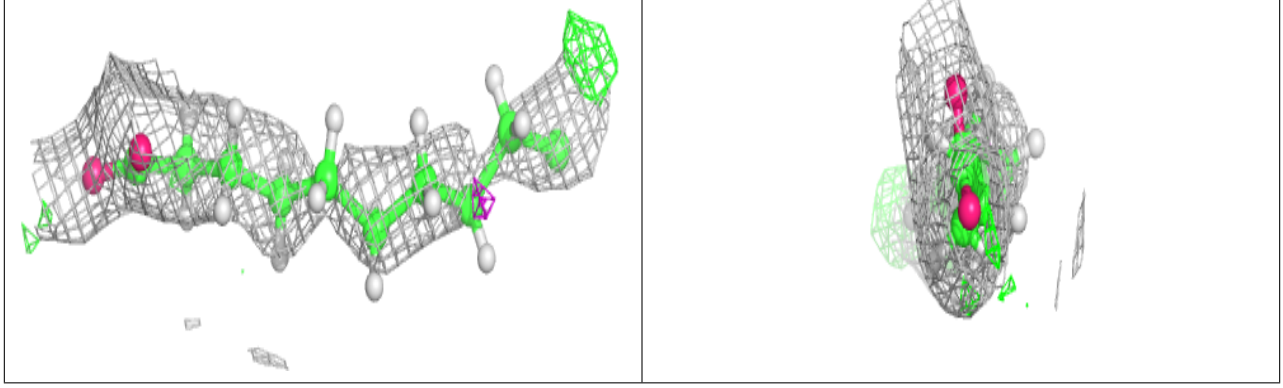
Electron density around STE b 625:

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



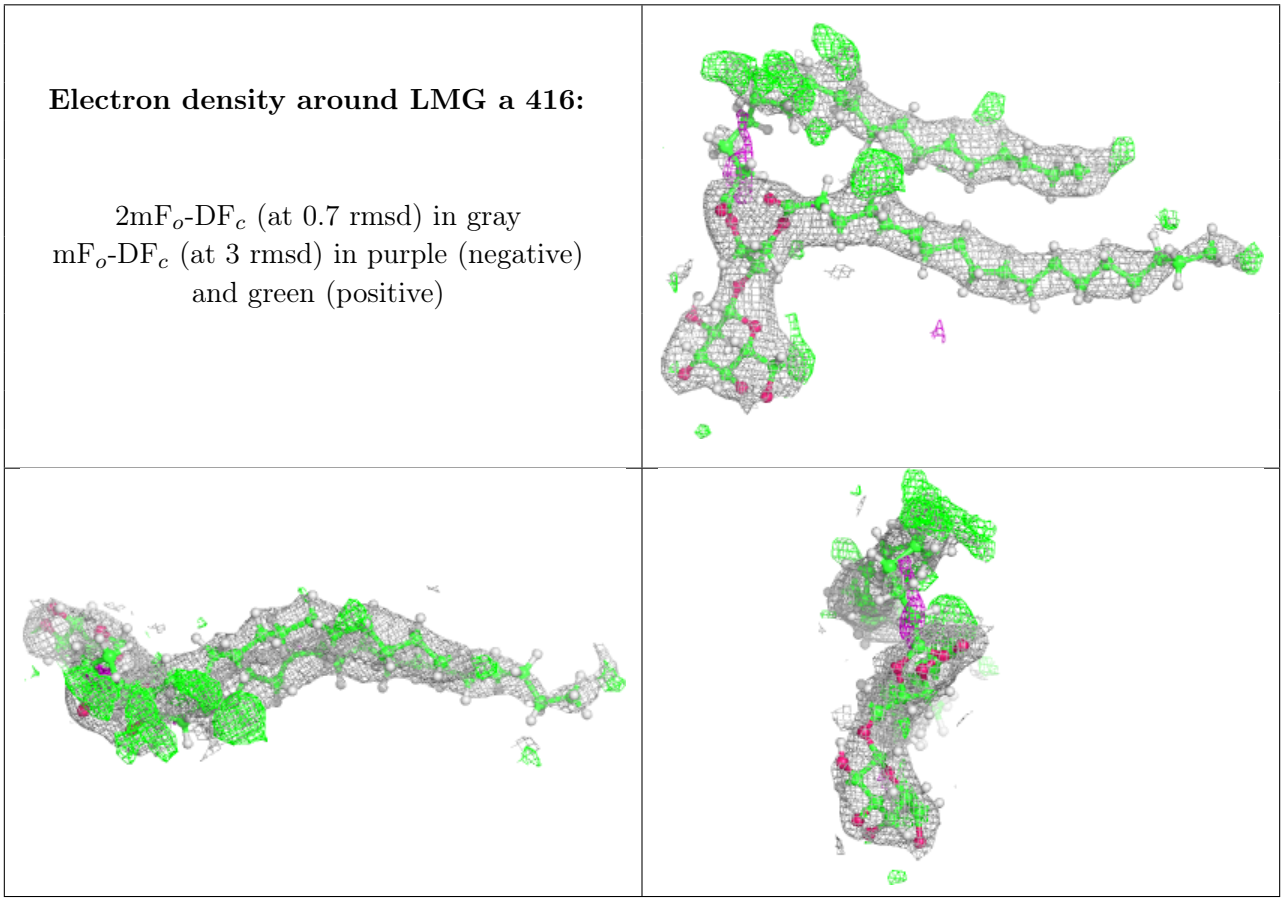
Electron density around STE a 414:

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



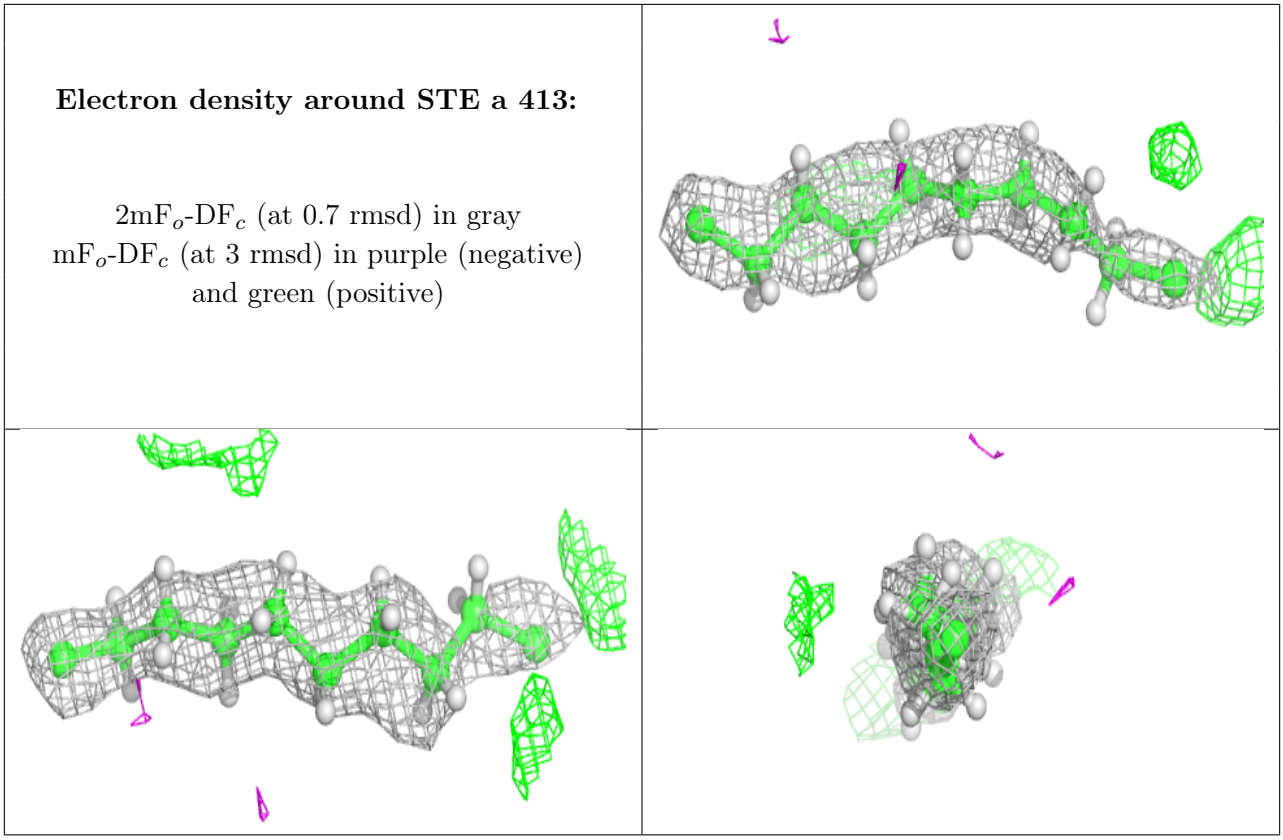
Electron density around LMG a 416:

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



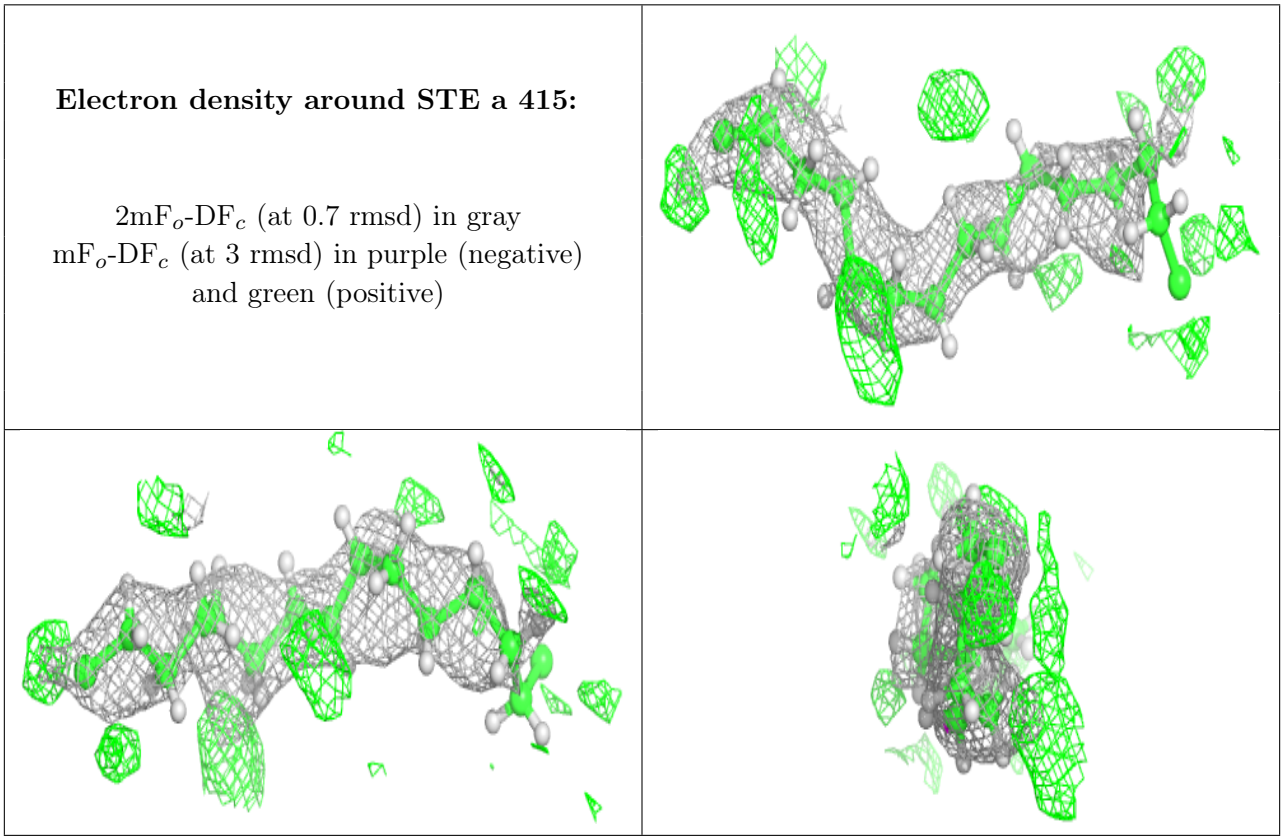
Electron density around STE a 413:

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



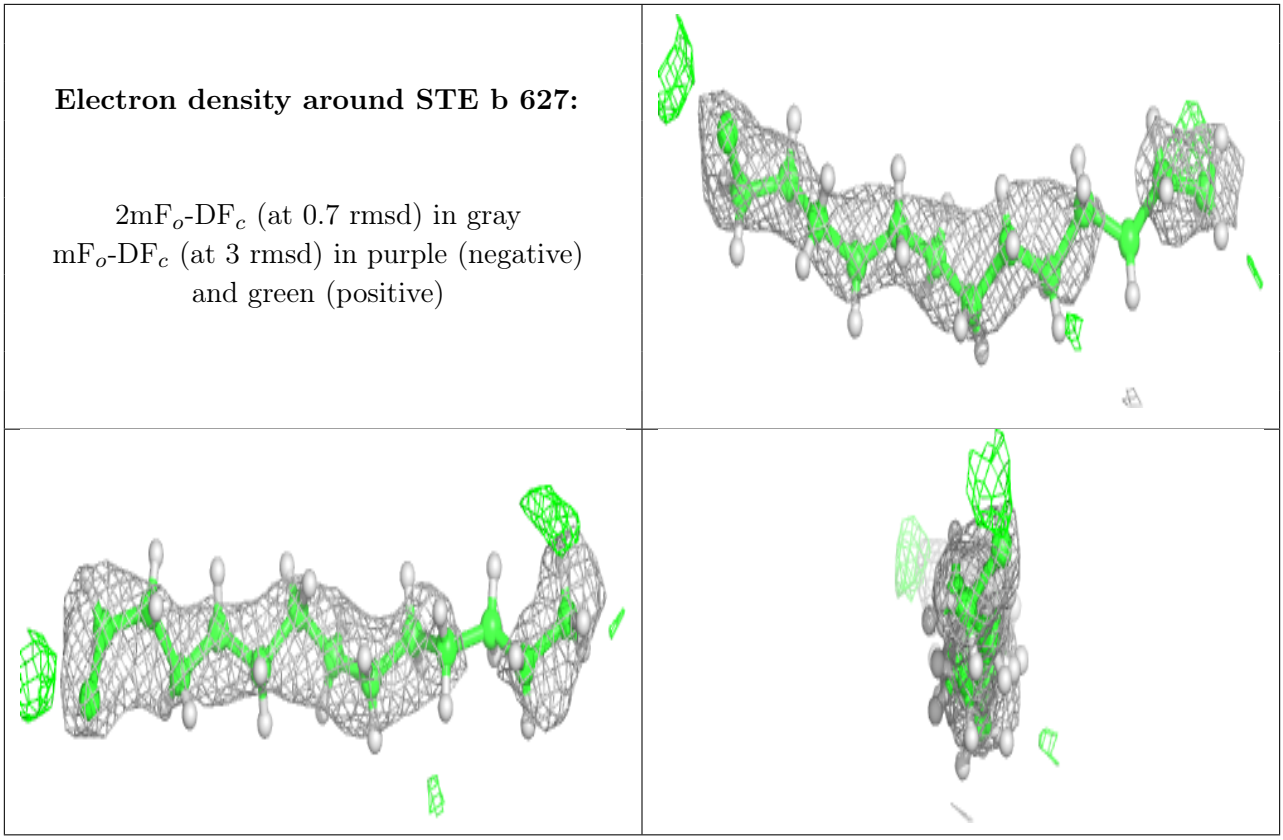
Electron density around STE a 415:

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



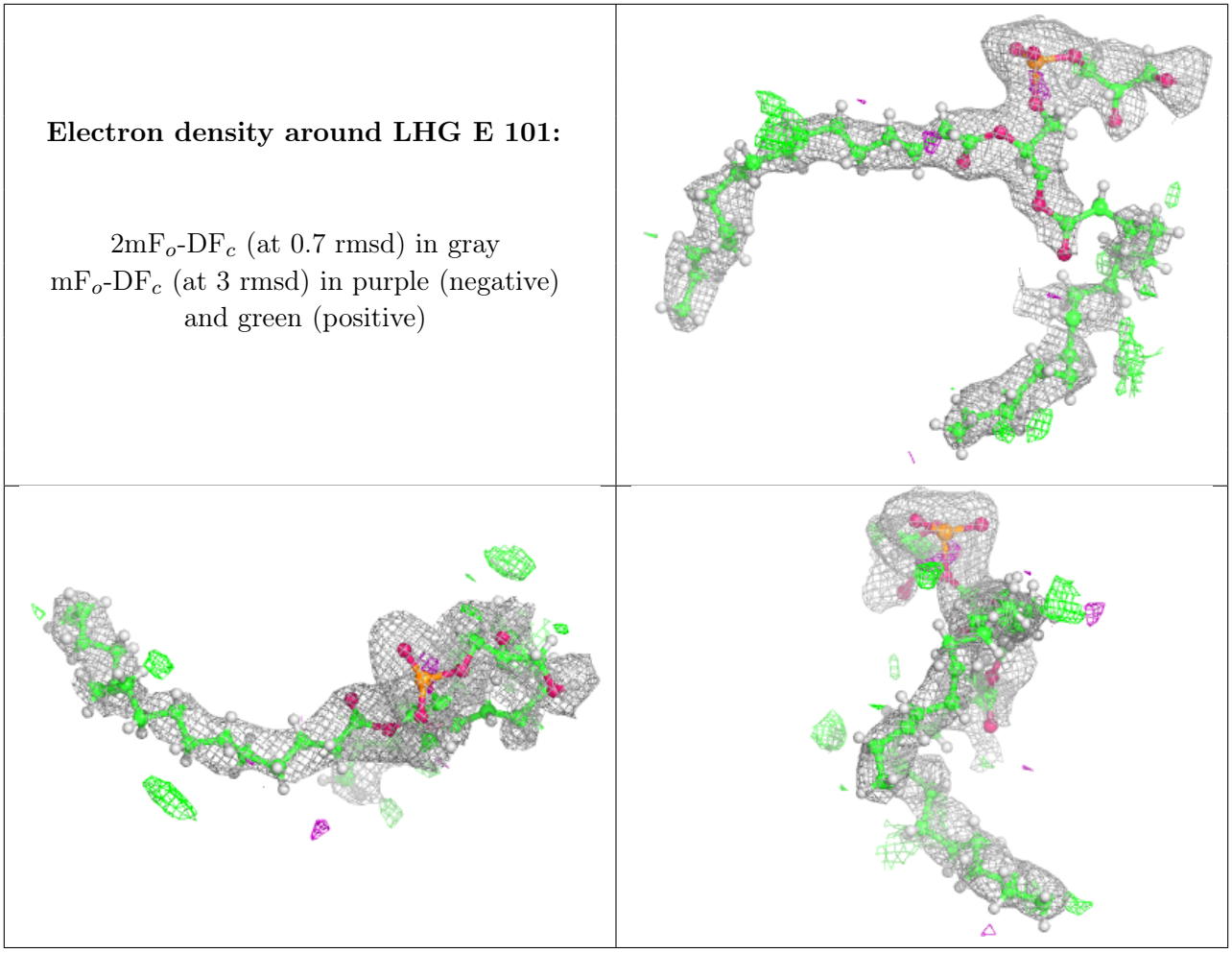
Electron density around STE b 627:

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



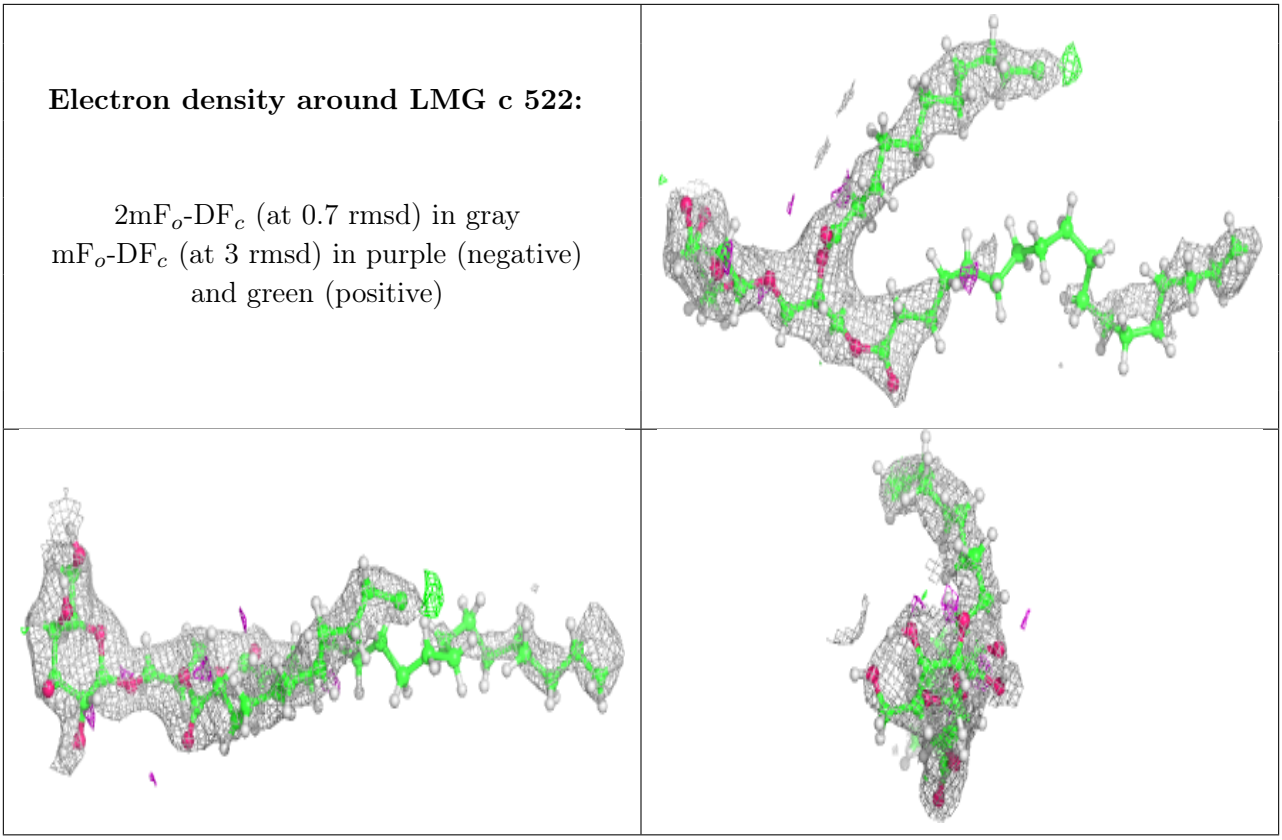
Electron density around LHG E 101:

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



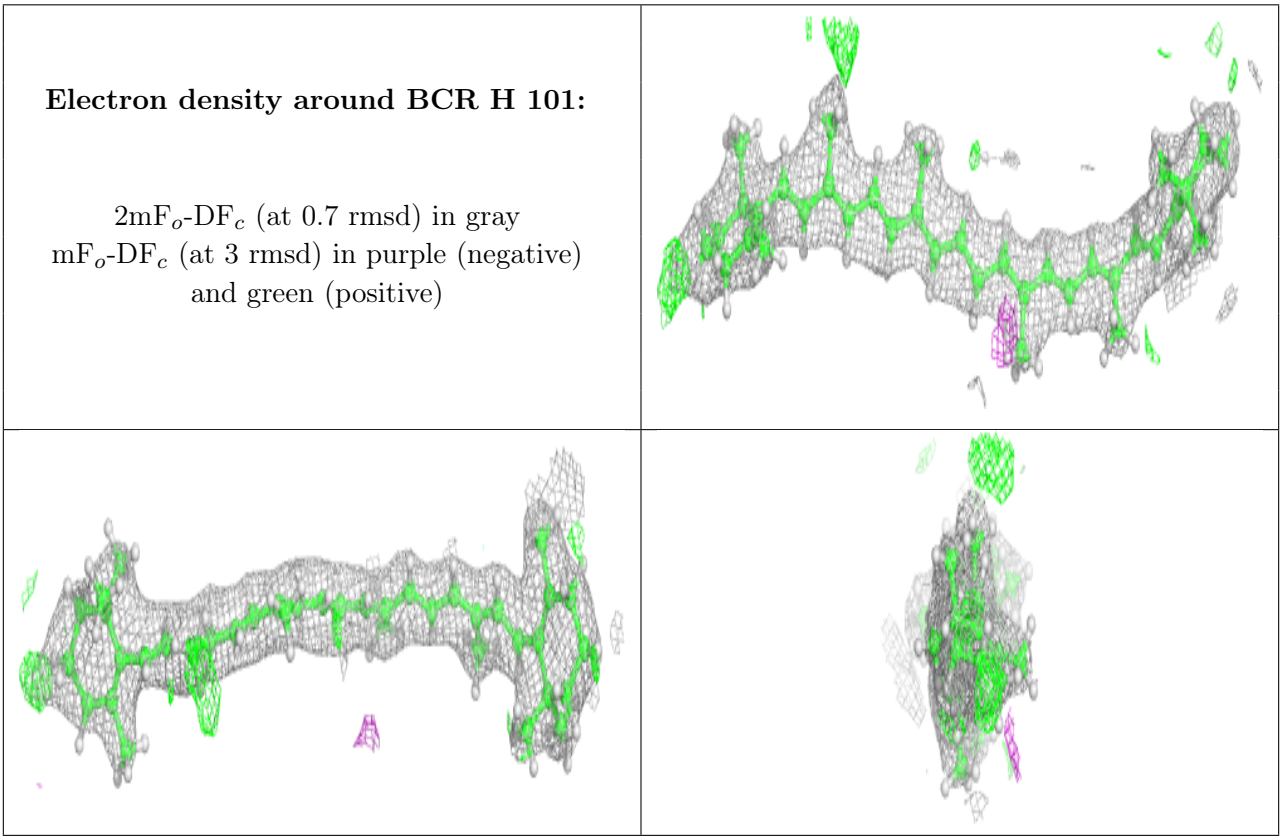
Electron density around LMG c 522:

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



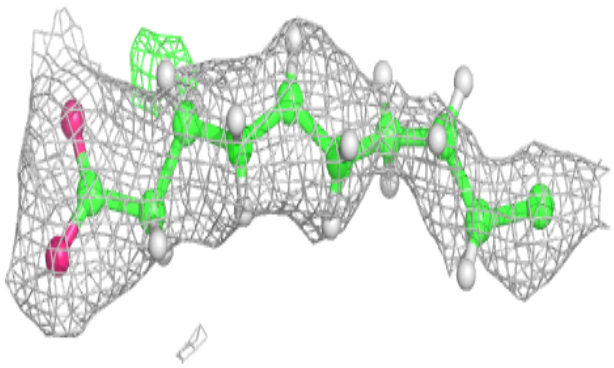
Electron density around BCR H 101:

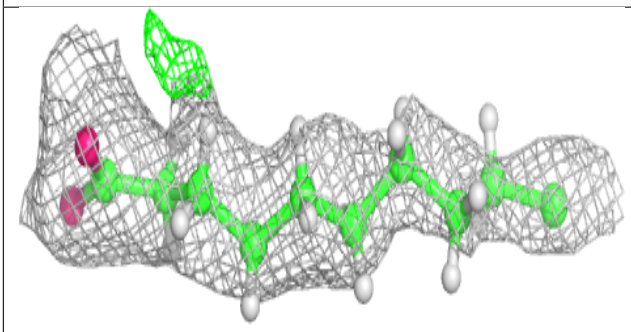
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

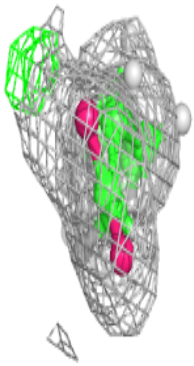


Electron density around STE k 102:

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

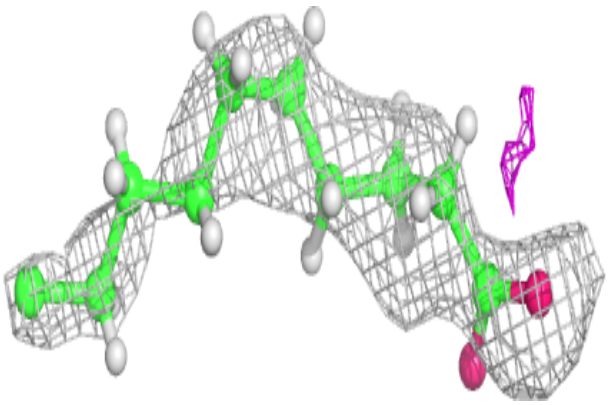


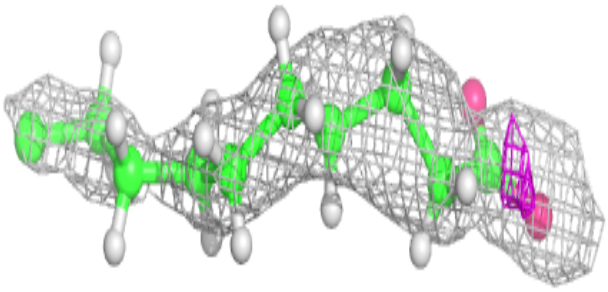


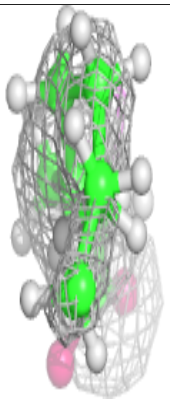


Electron density around STE B 626:

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

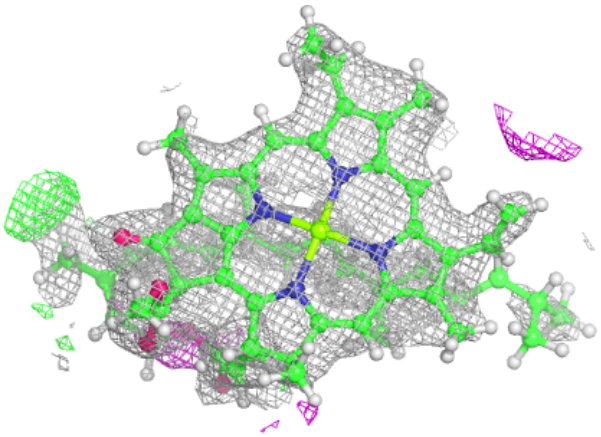


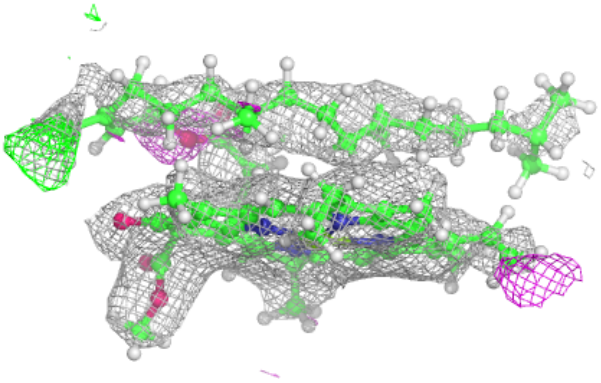


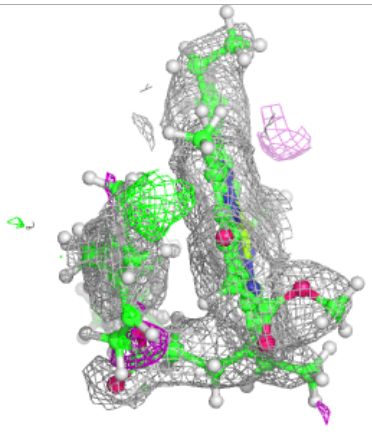


Electron density around CLA b 601:

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

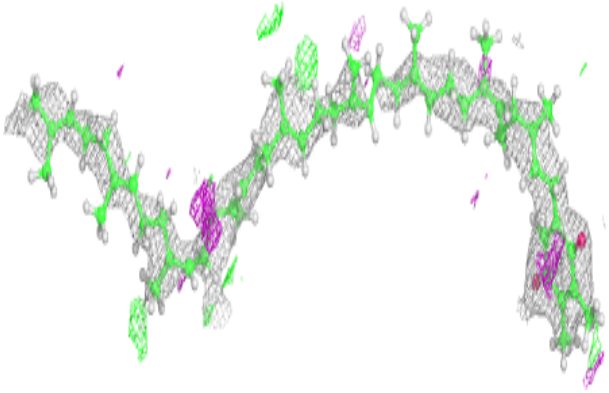


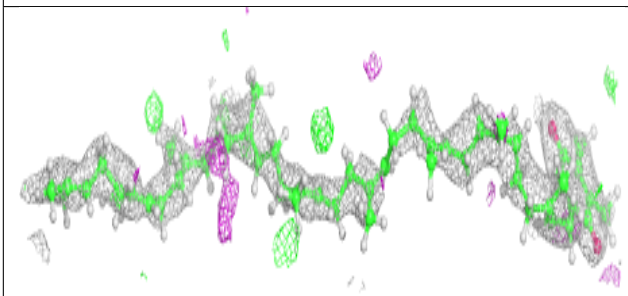


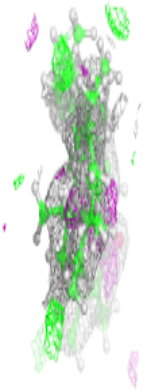


Electron density around PL9 A 410:

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

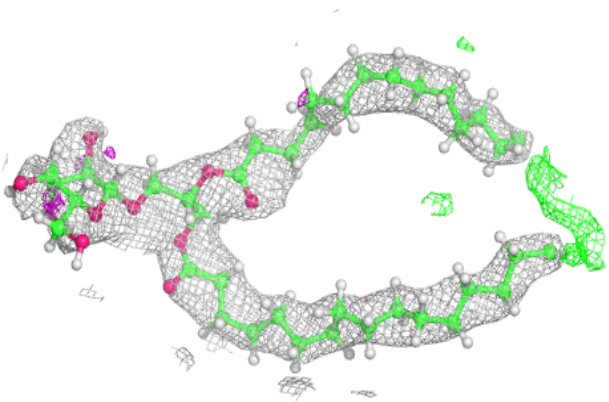


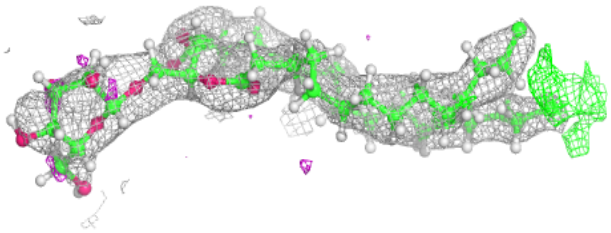


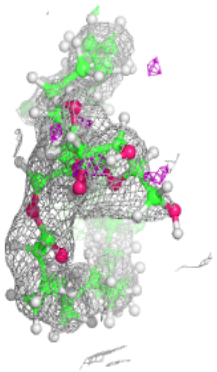


Electron density around LMG c 523:

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

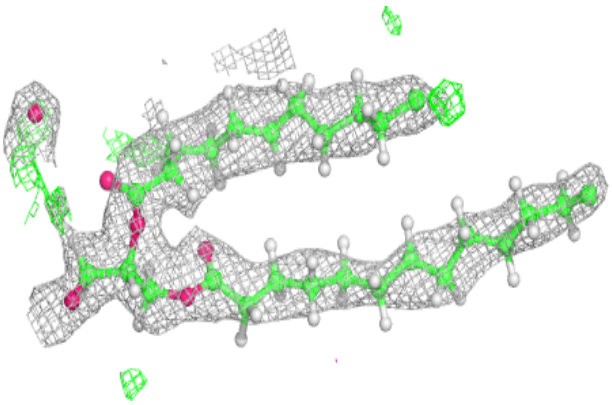


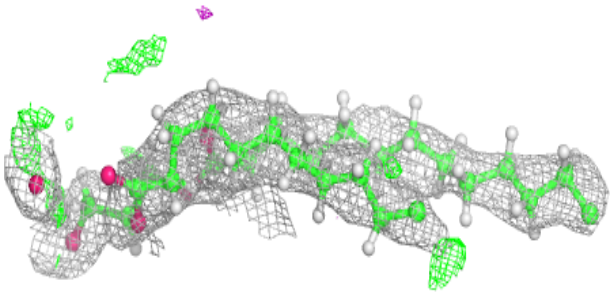


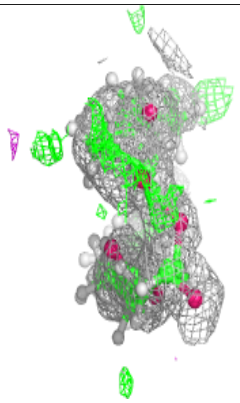


Electron density around LMG D 410:

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

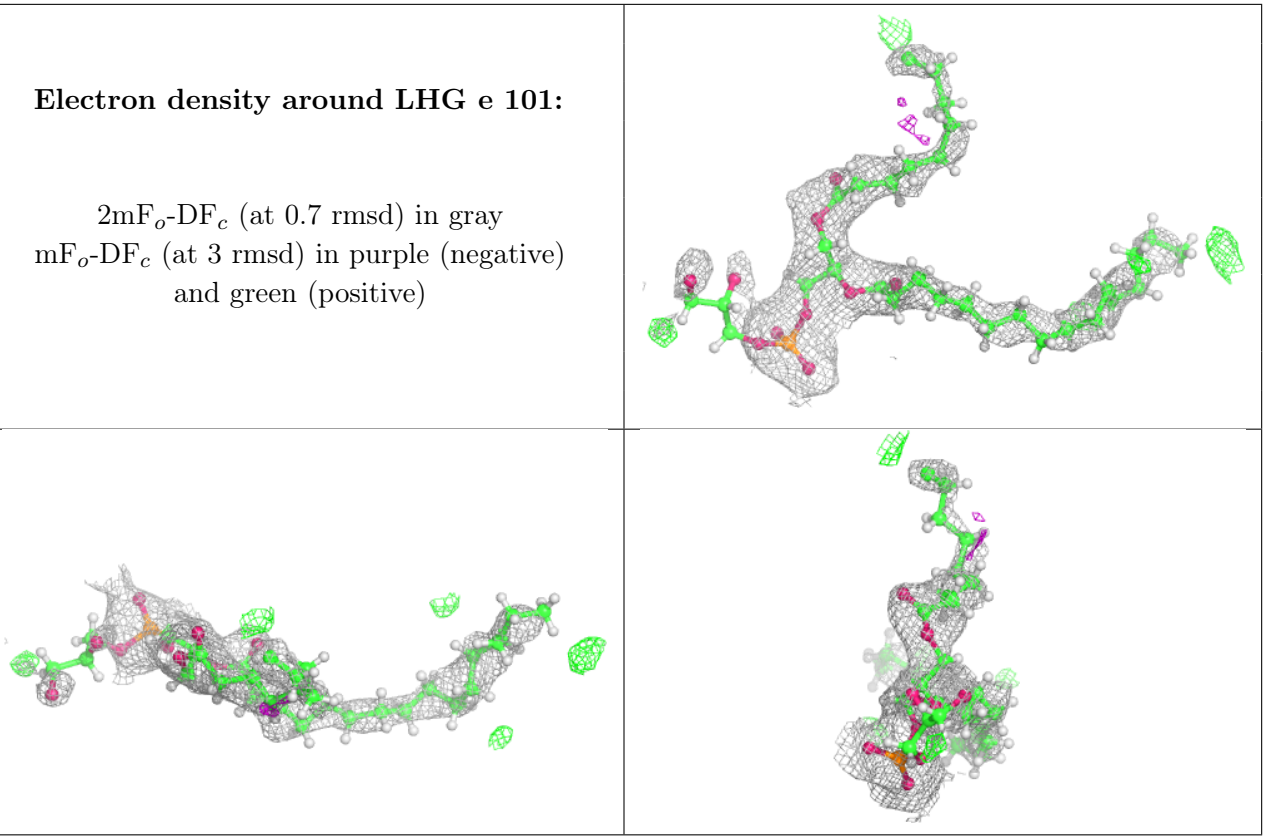






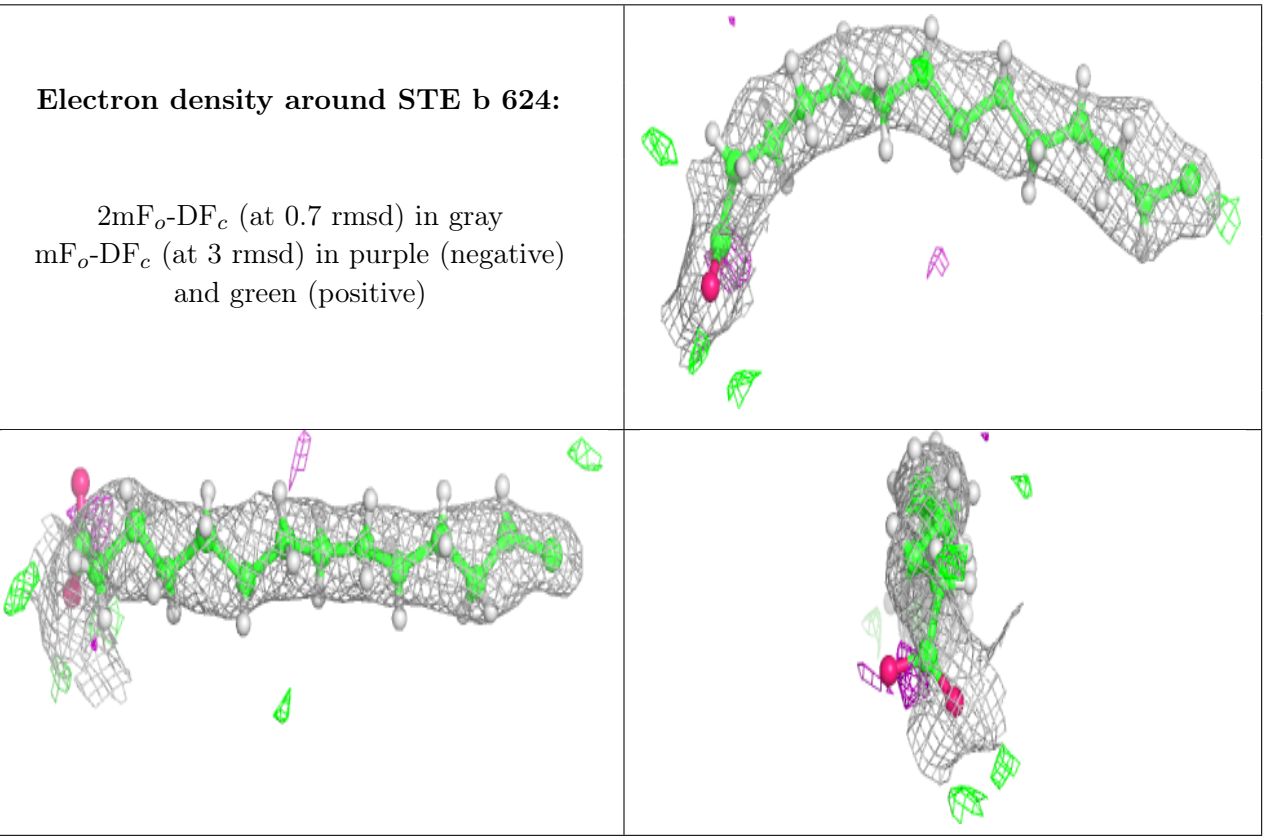
Electron density around LHG e 101:

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



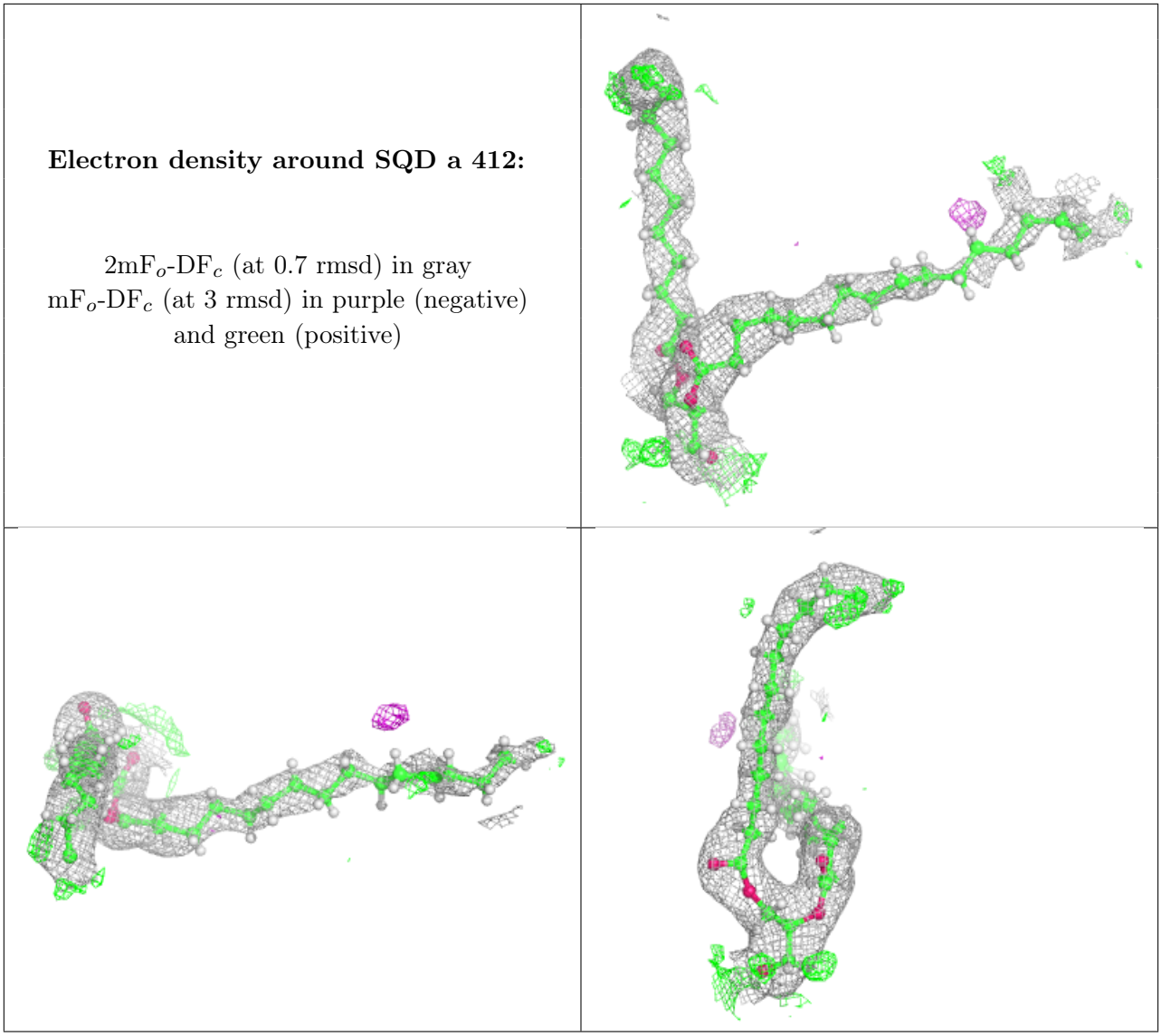
Electron density around STE b 624:

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



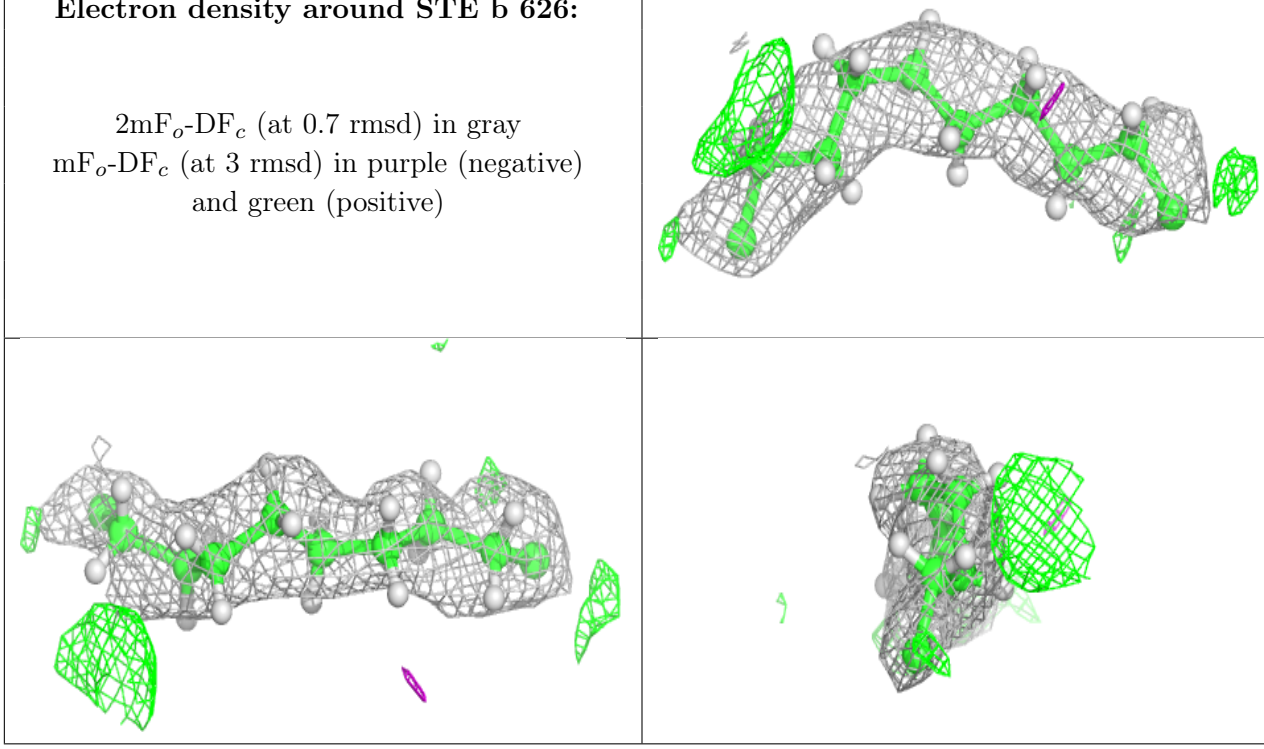
Electron density around SQD a 412:

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



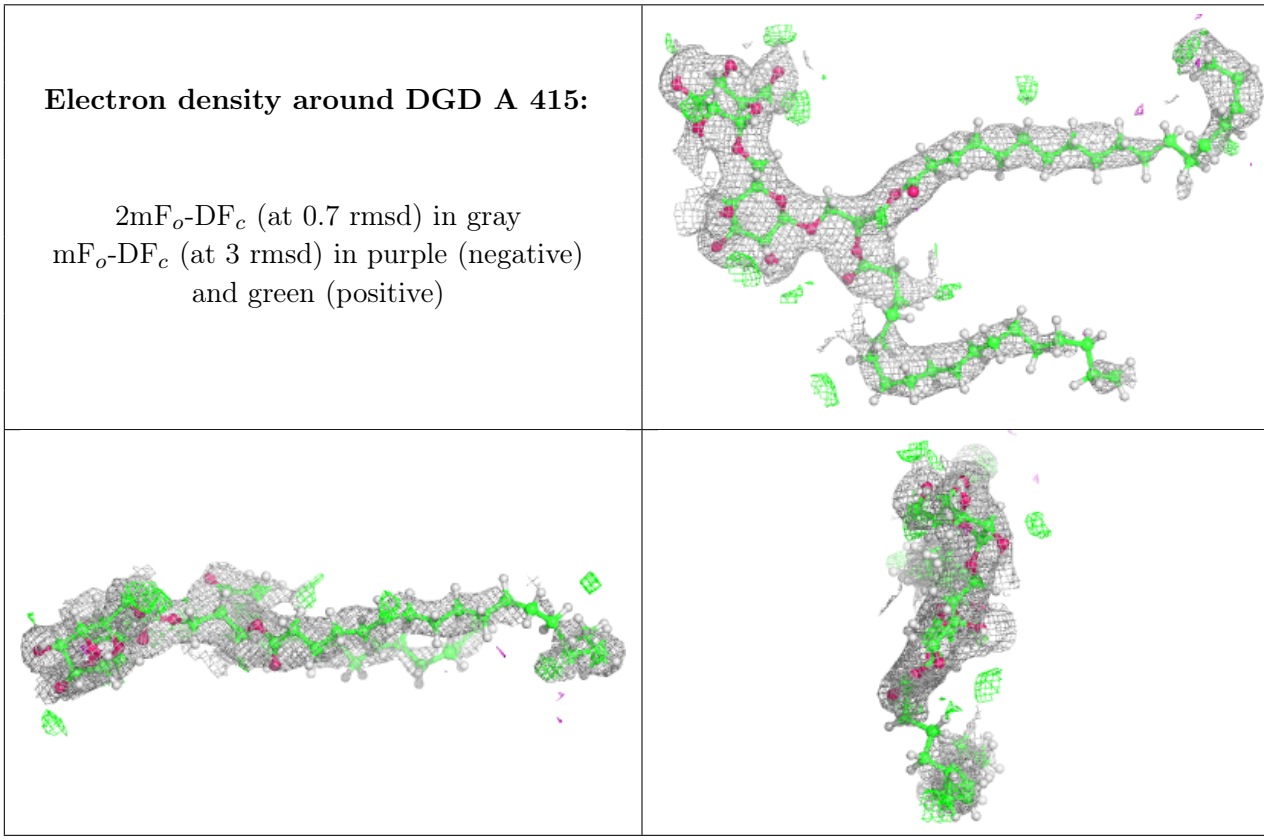
Electron density around STE b 626:

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



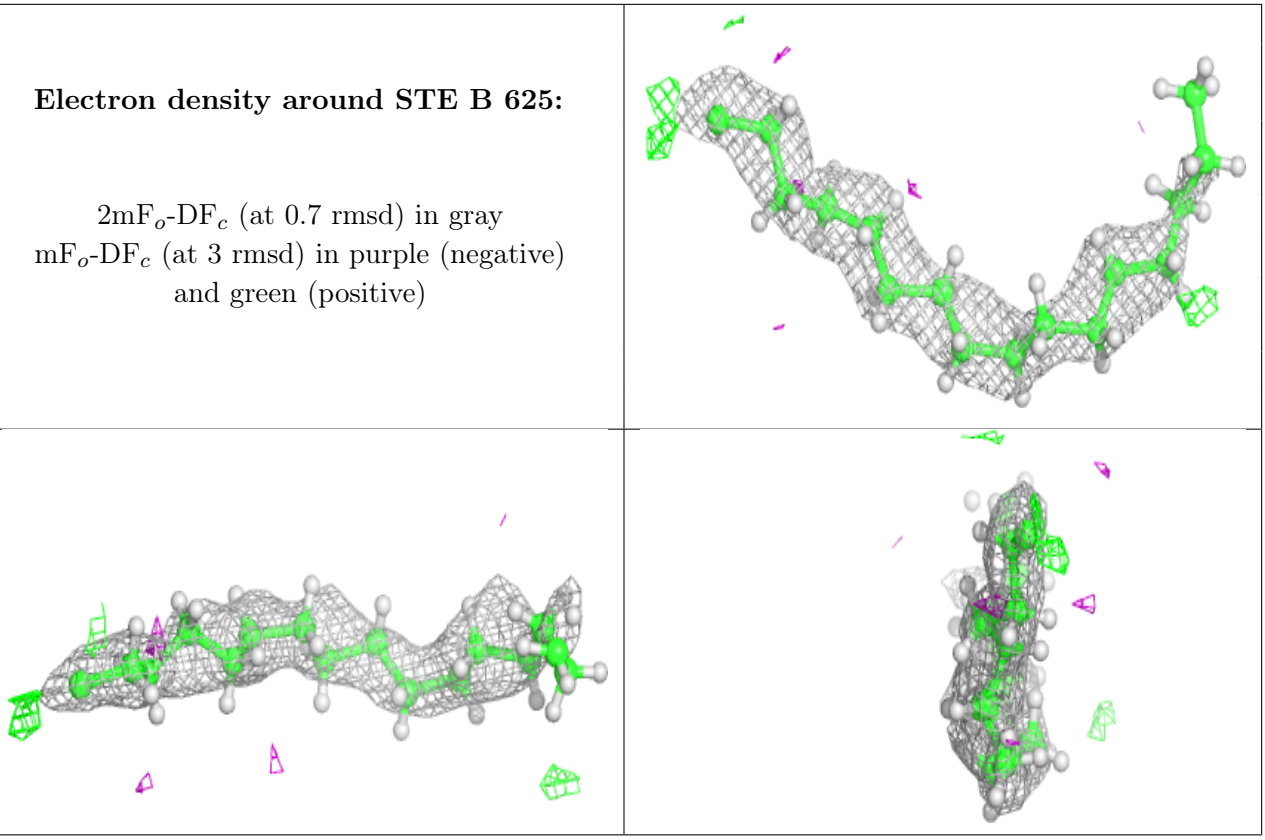
Electron density around DGD A 415:

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



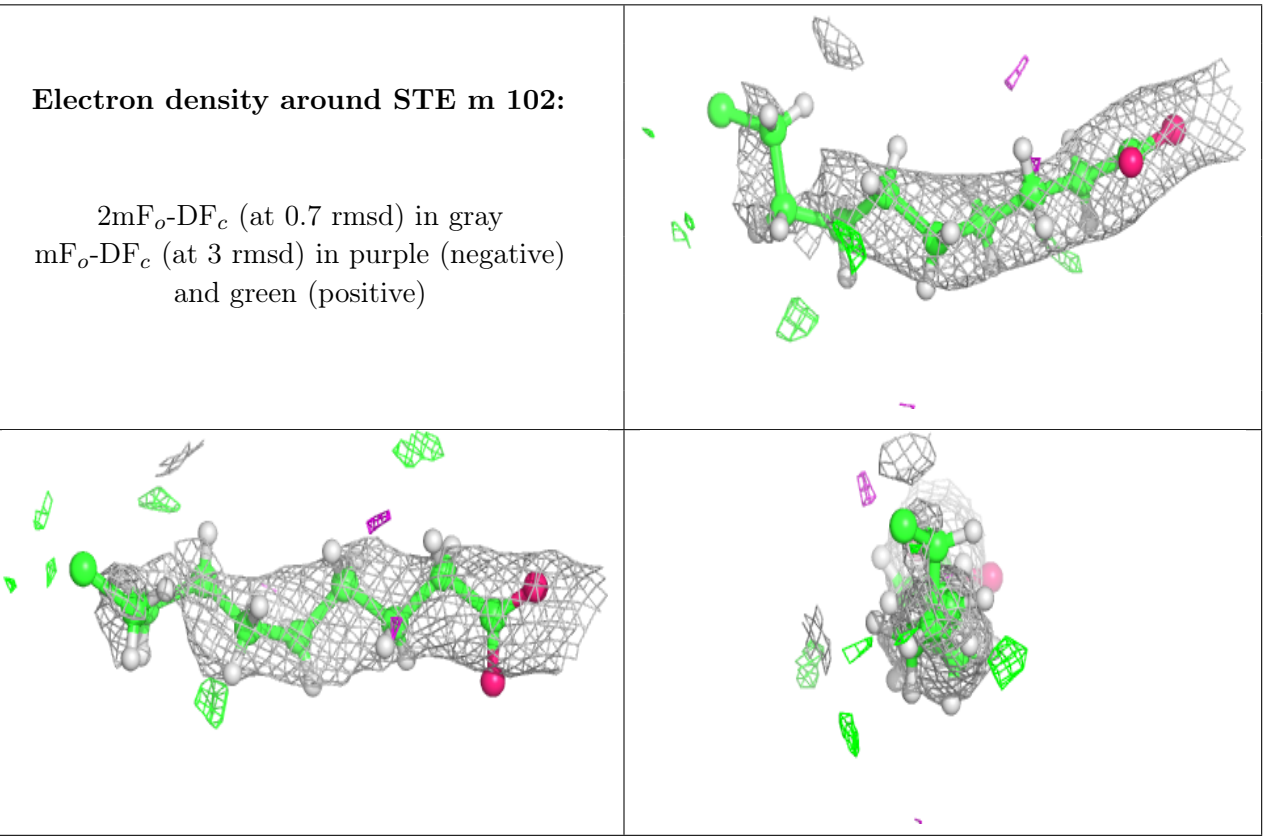
Electron density around STE B 625:

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



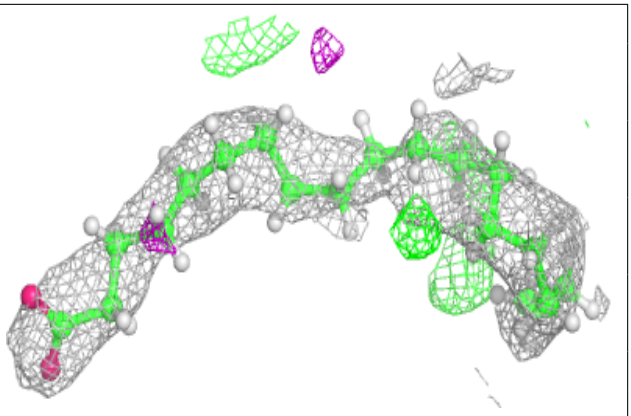
Electron density around STE m 102:

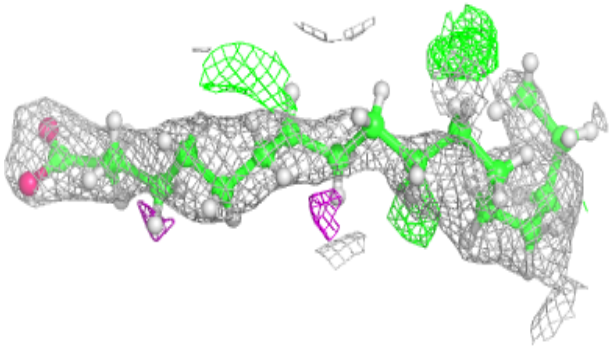
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

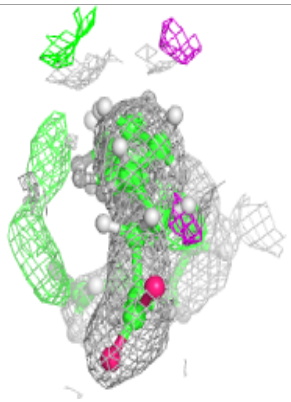


Electron density around STE d 413:

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

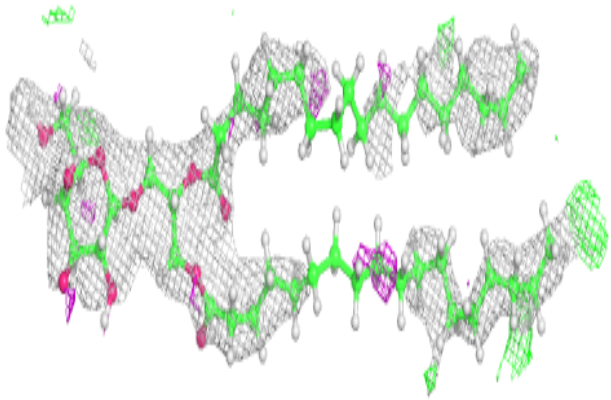


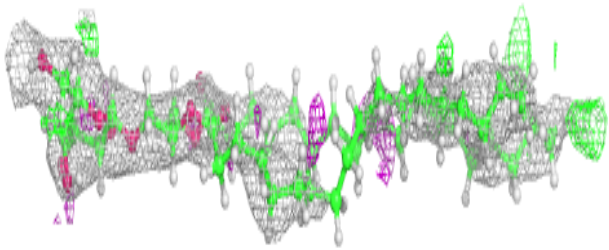


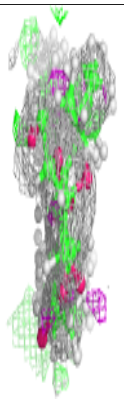


Electron density around LMG b 623:

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

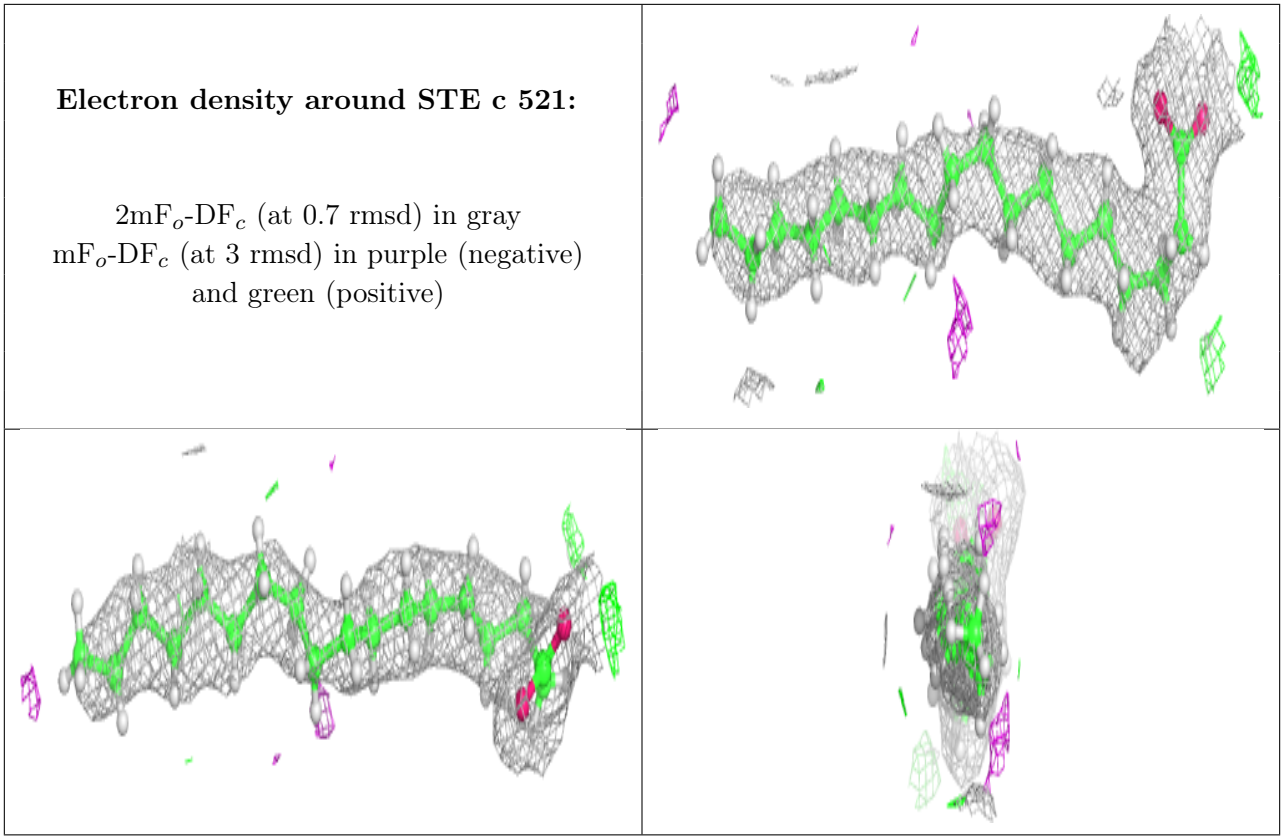






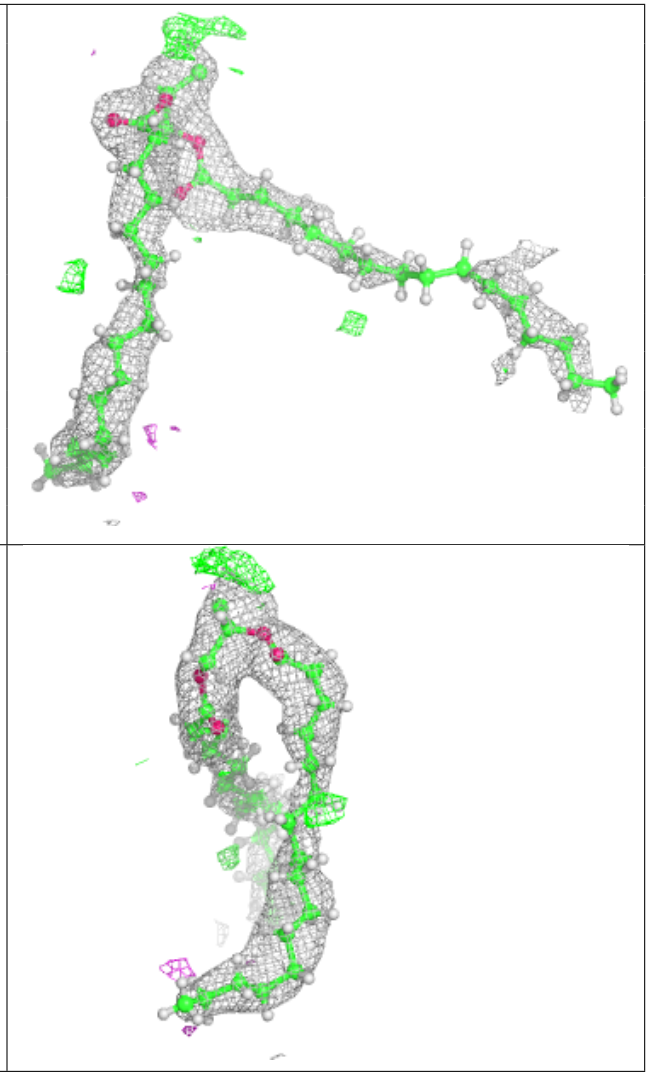
Electron density around STE c 521:

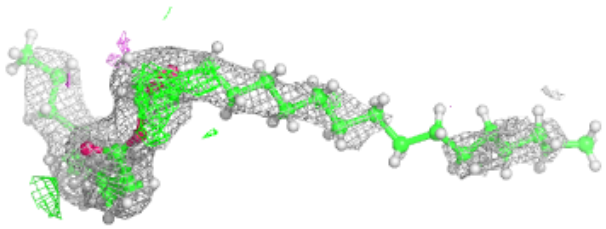
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD A 414:

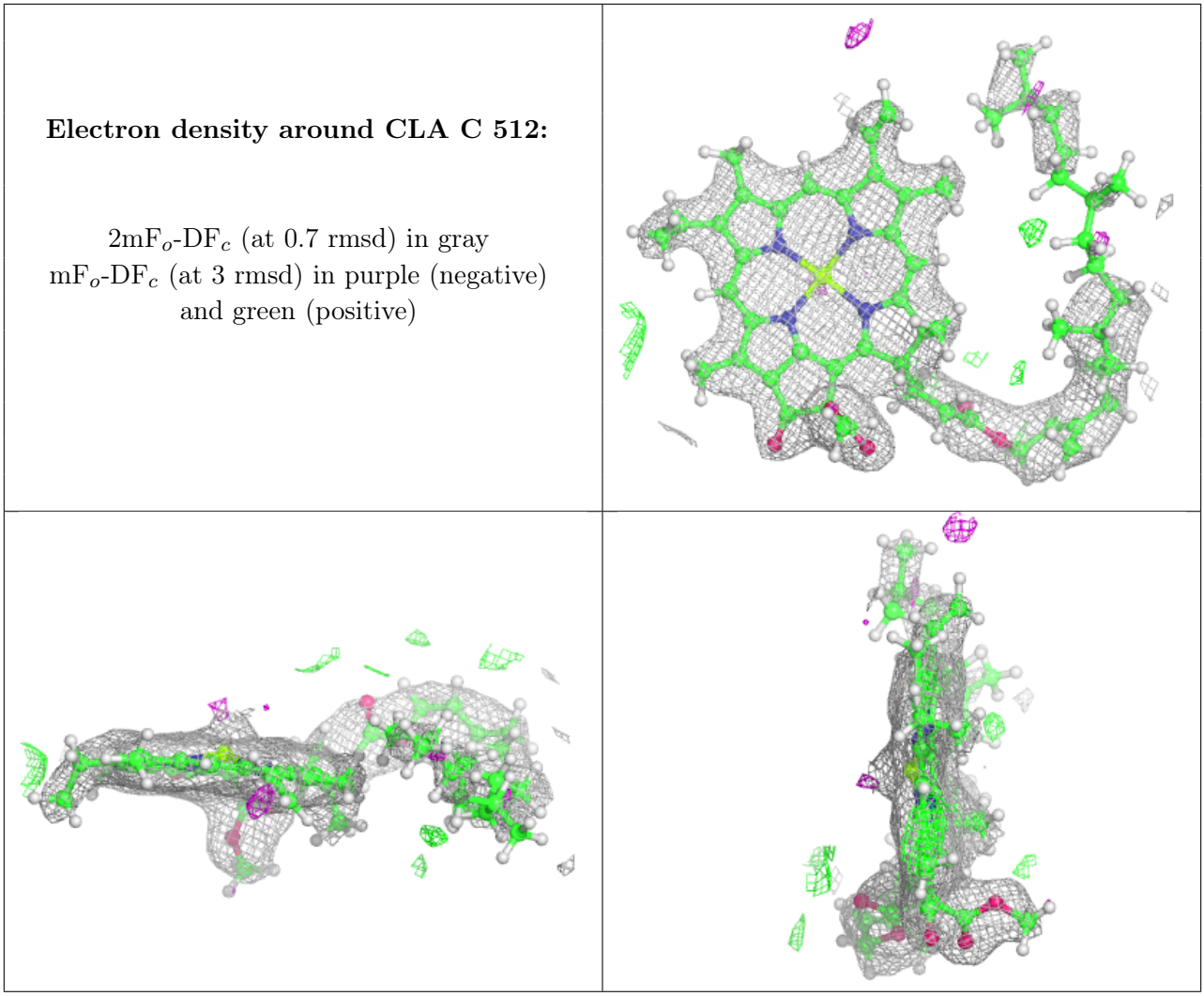
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





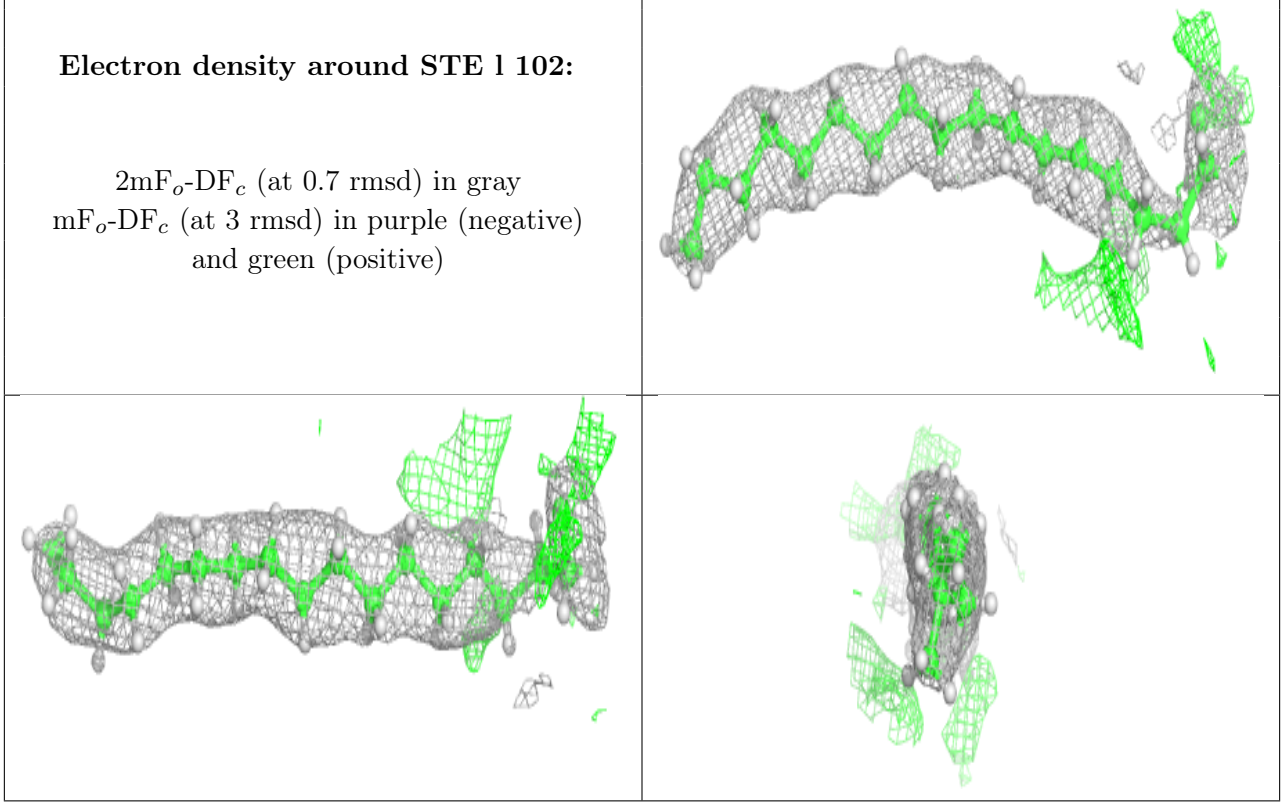
Electron density around CLA C 512:

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



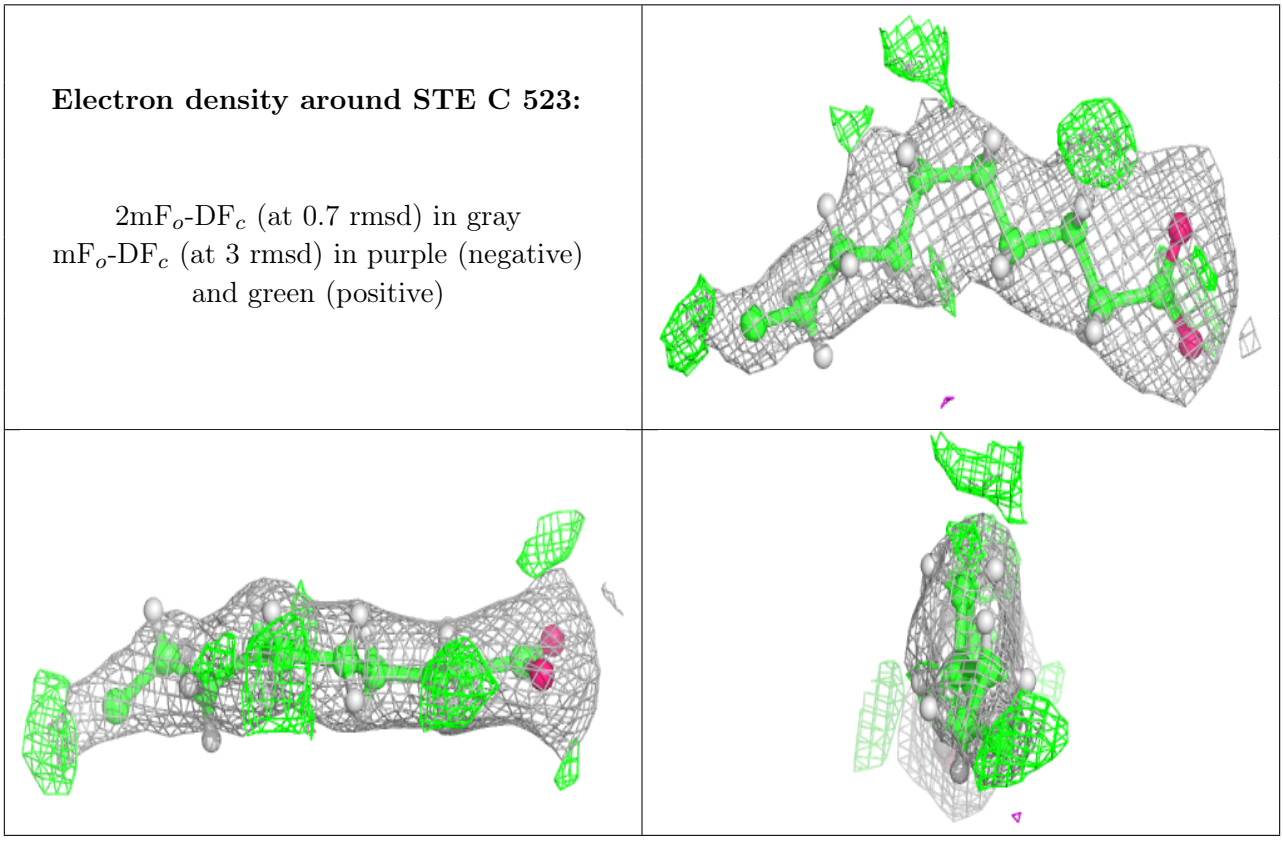
Electron density around STE l 102:

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



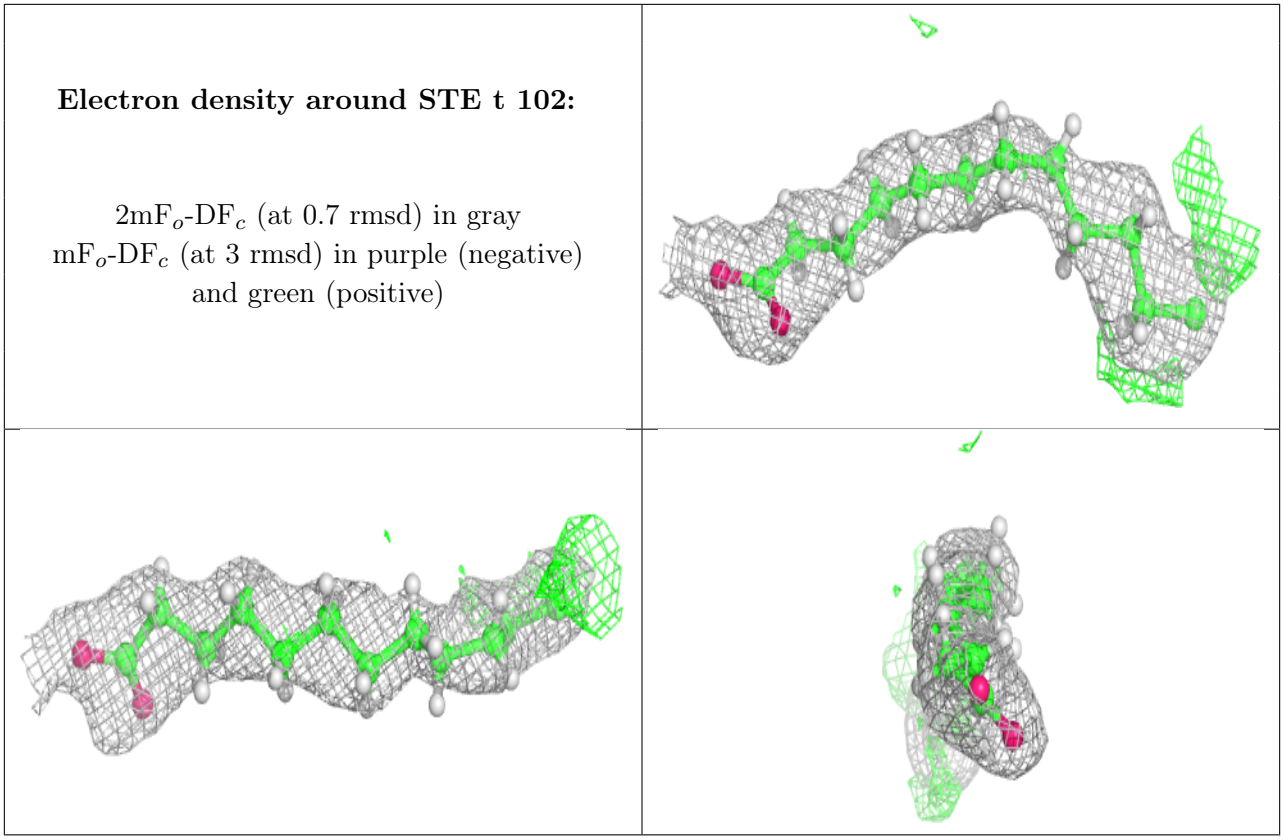
Electron density around STE C 523:

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



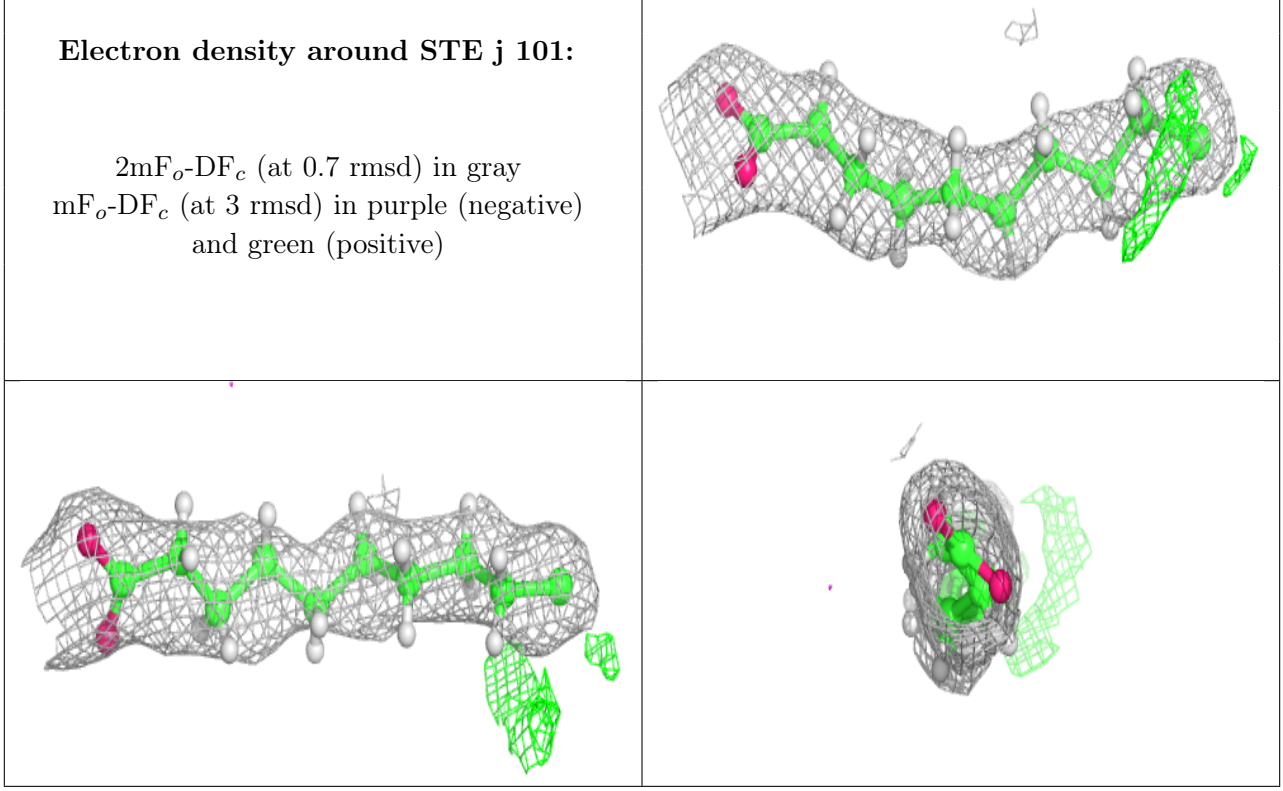
Electron density around STE t 102:

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



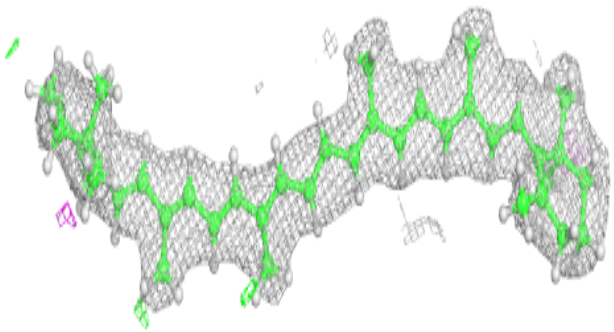
Electron density around STE j 101:

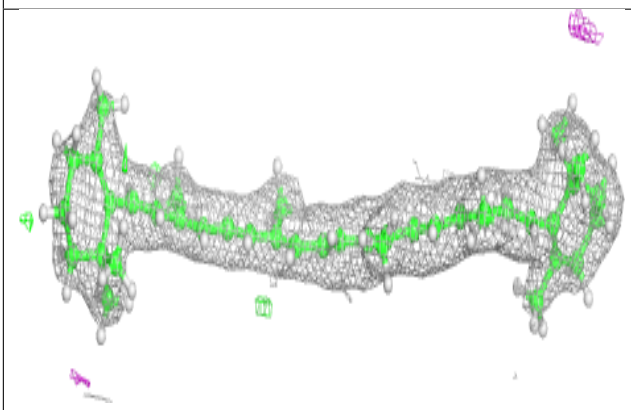
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

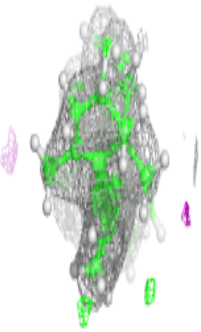


Electron density around BCR Y 101:

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

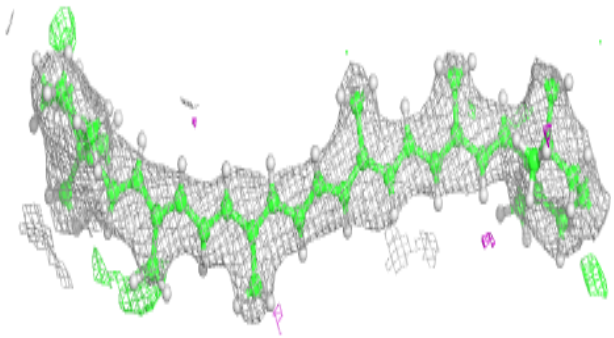


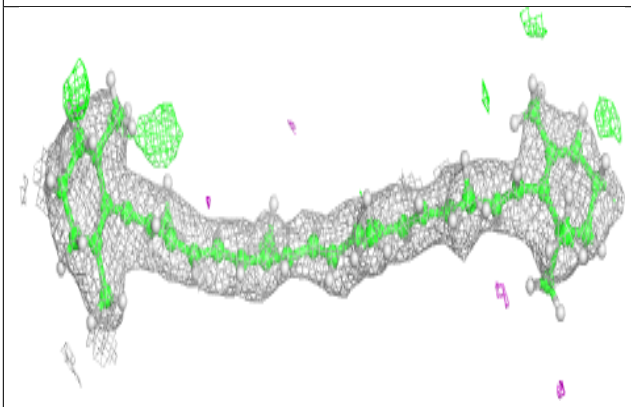


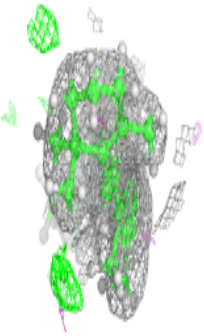


Electron density around BCR x 101:

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

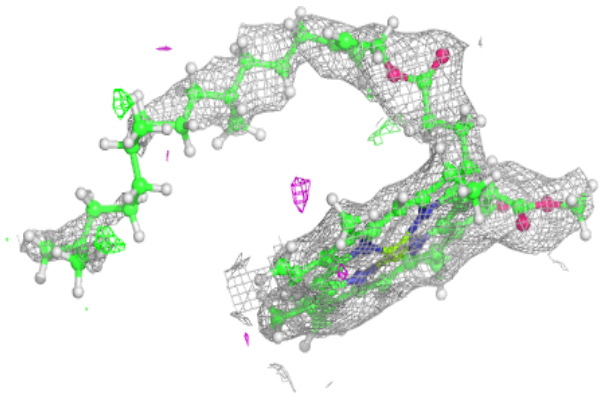


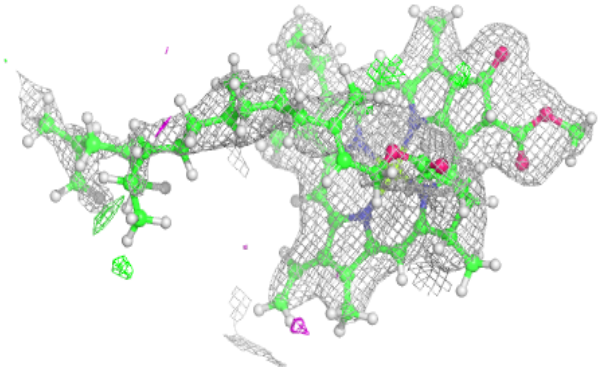


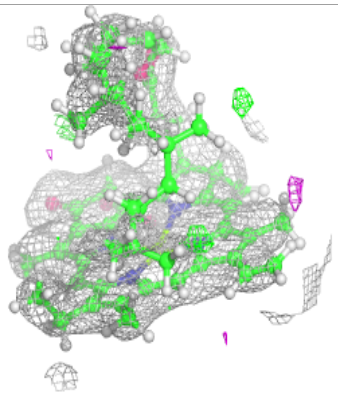


Electron density around CLA C 513:

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

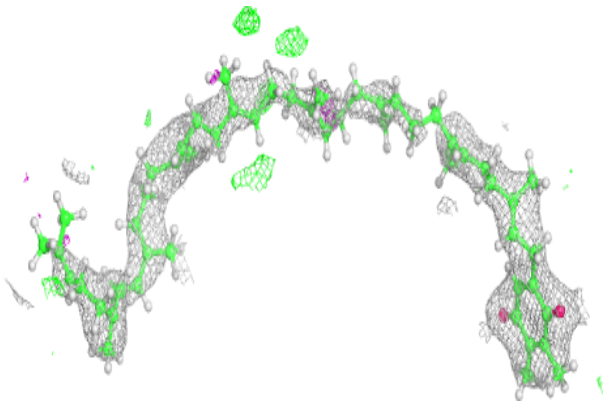


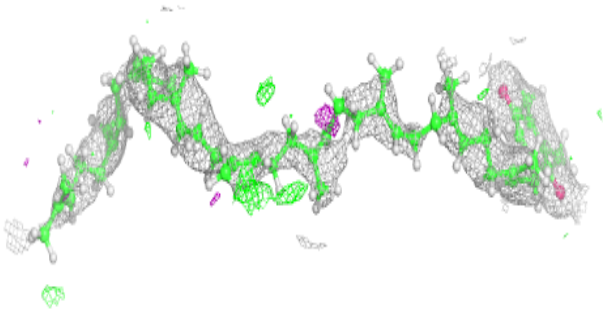


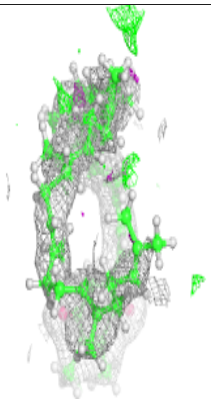


Electron density around PL9 a 409:

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

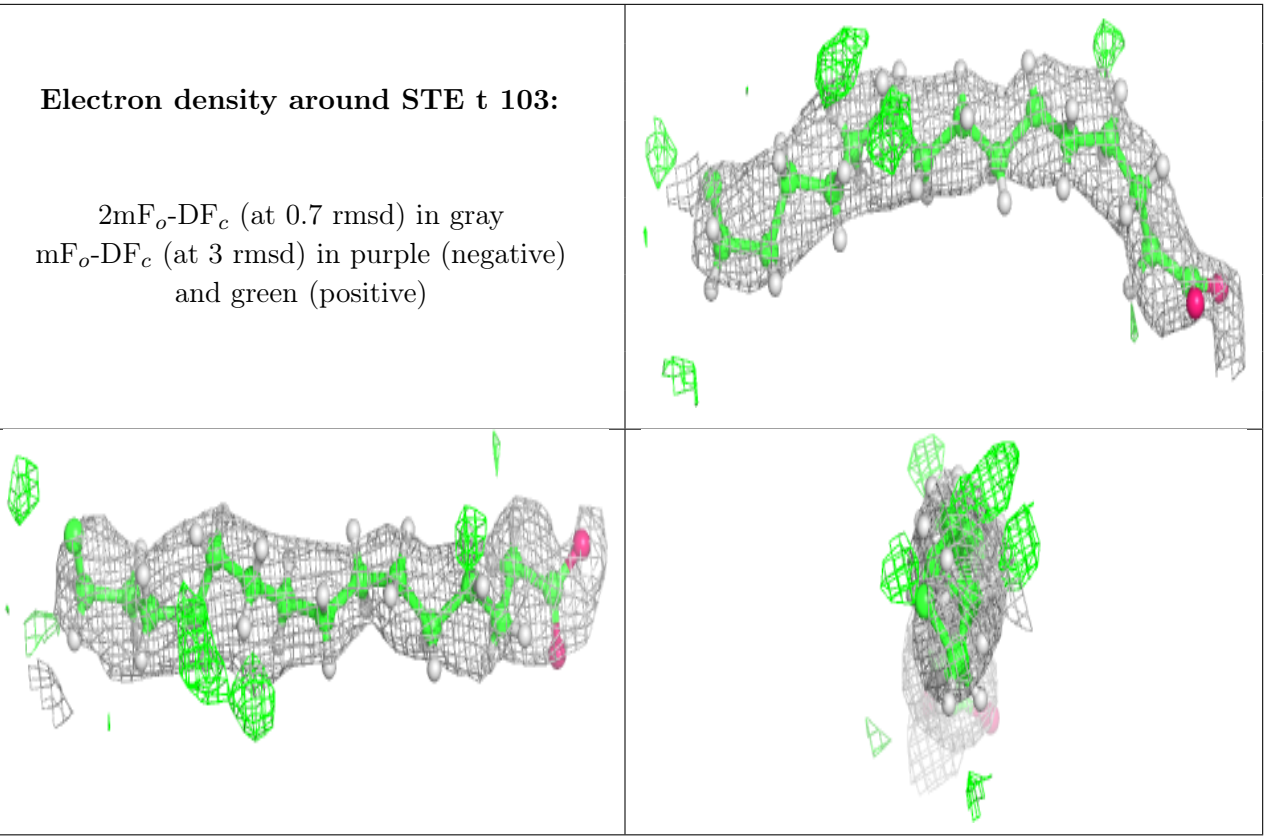






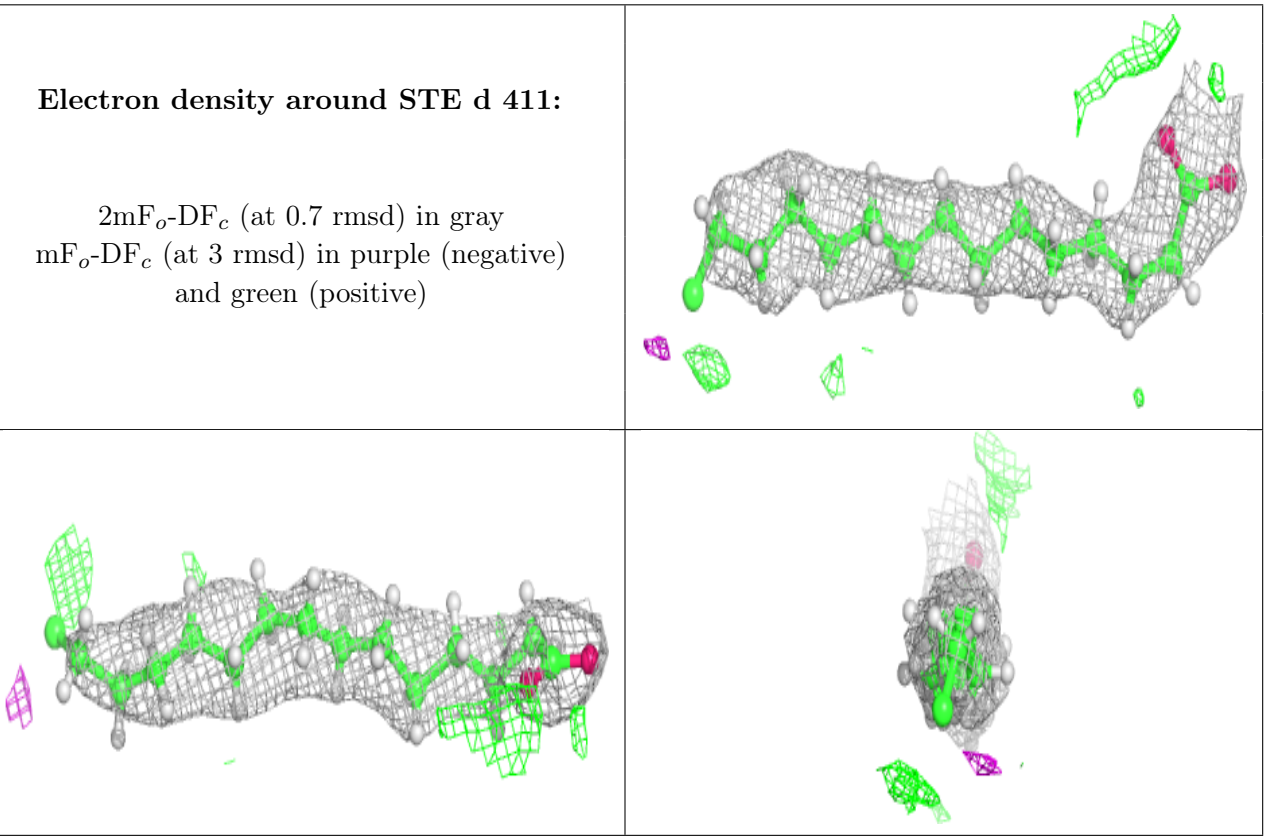
Electron density around STE t 103:

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



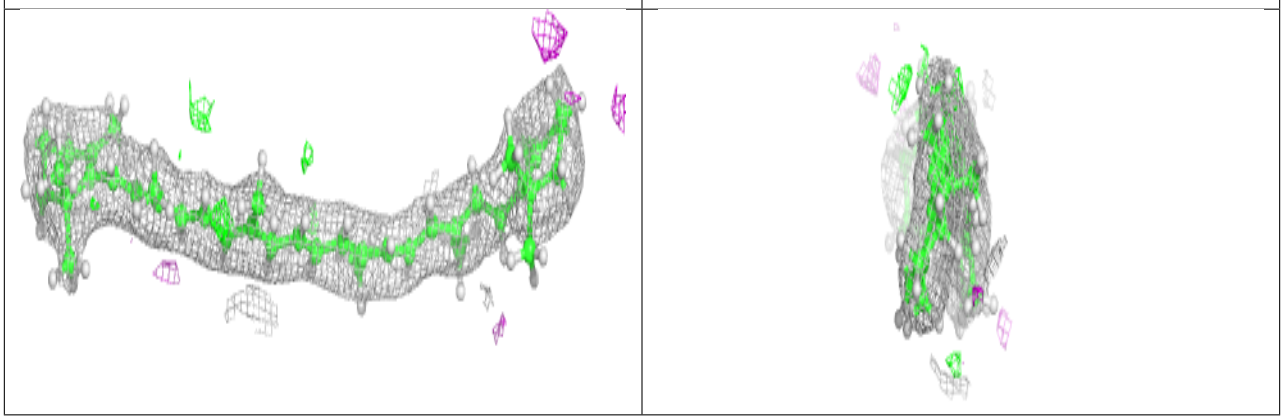
Electron density around STE d 411:

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



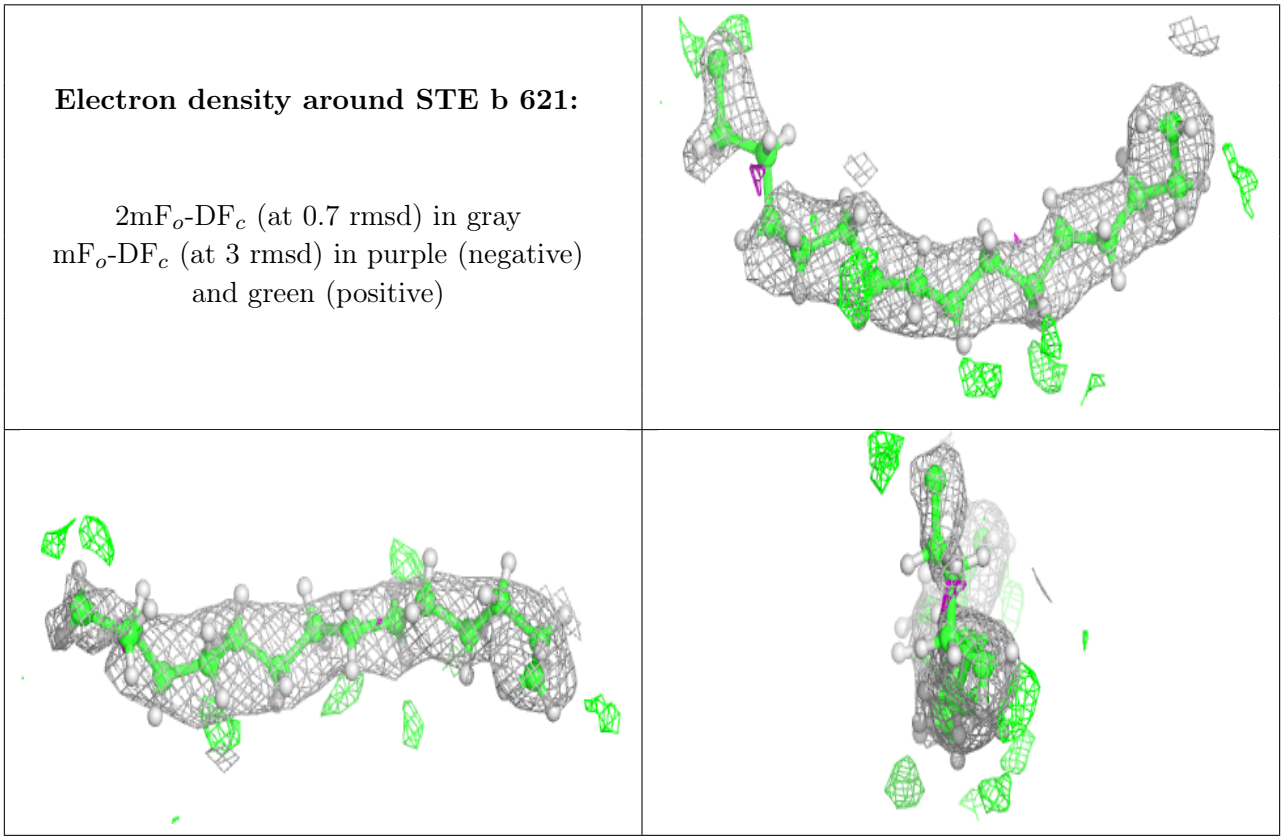
Electron density around BCR d 406:

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



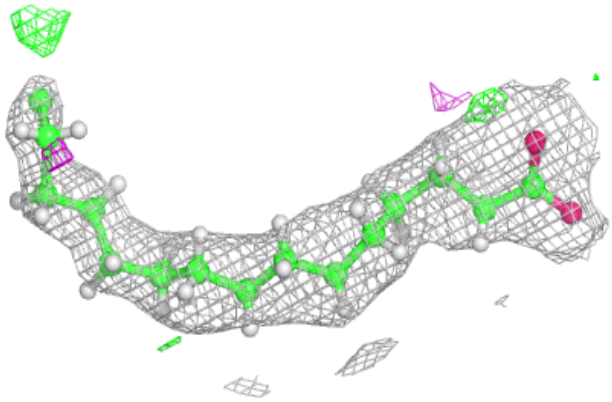
Electron density around STE b 621:

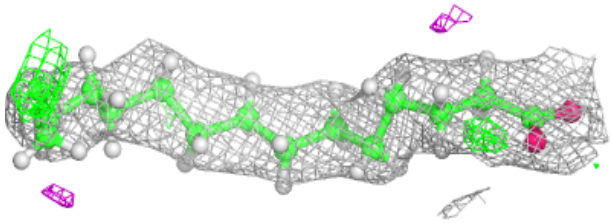
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

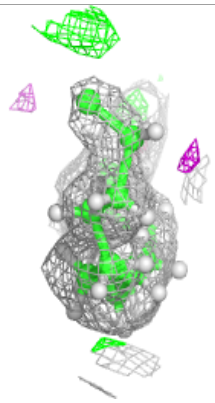


Electron density around STE B 620:

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

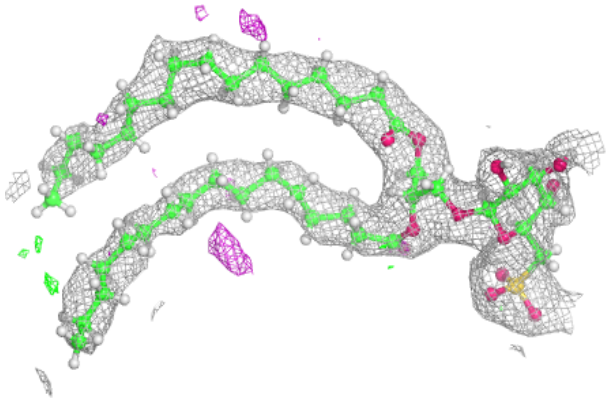


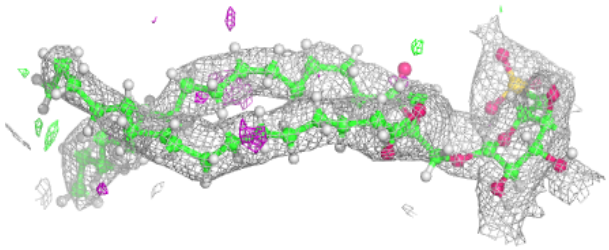


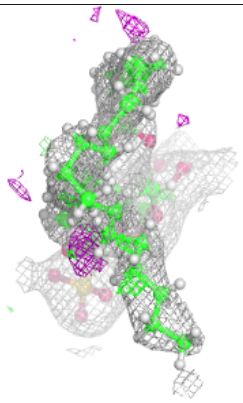


Electron density around SQD B 623:

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

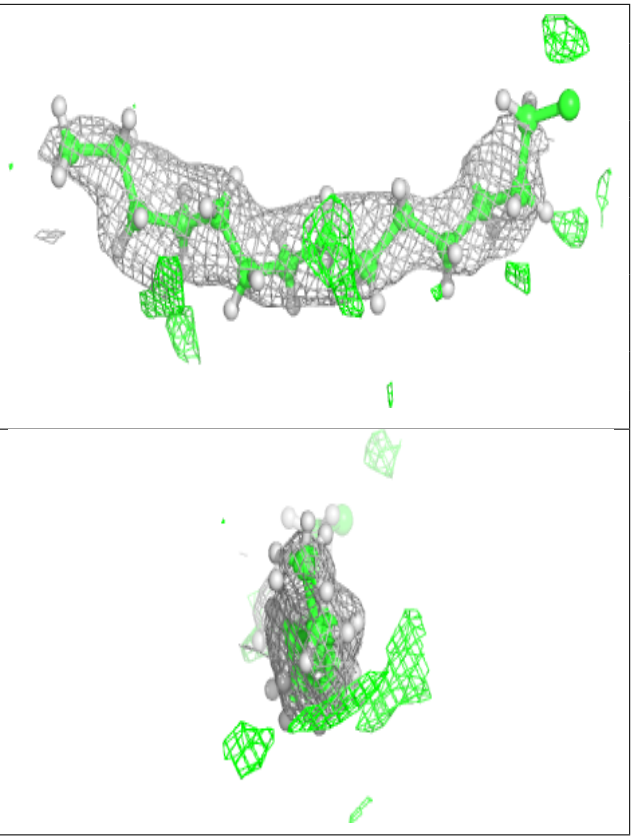






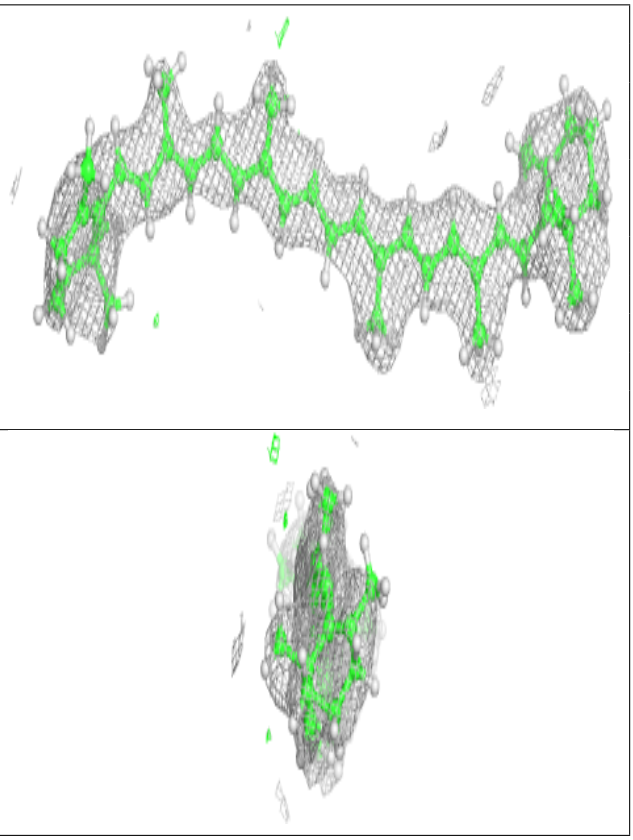
Electron density around STE T 102:

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



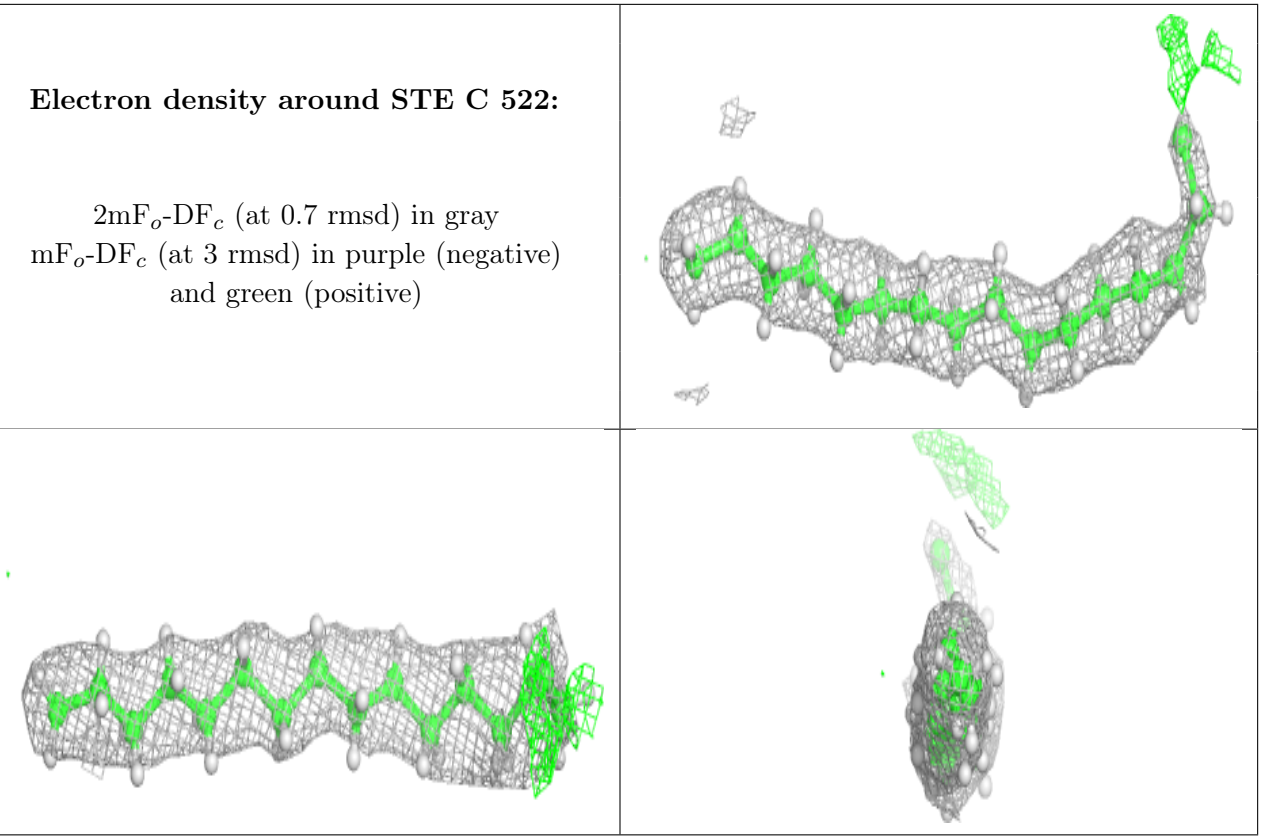
Electron density around BCR k 101:

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



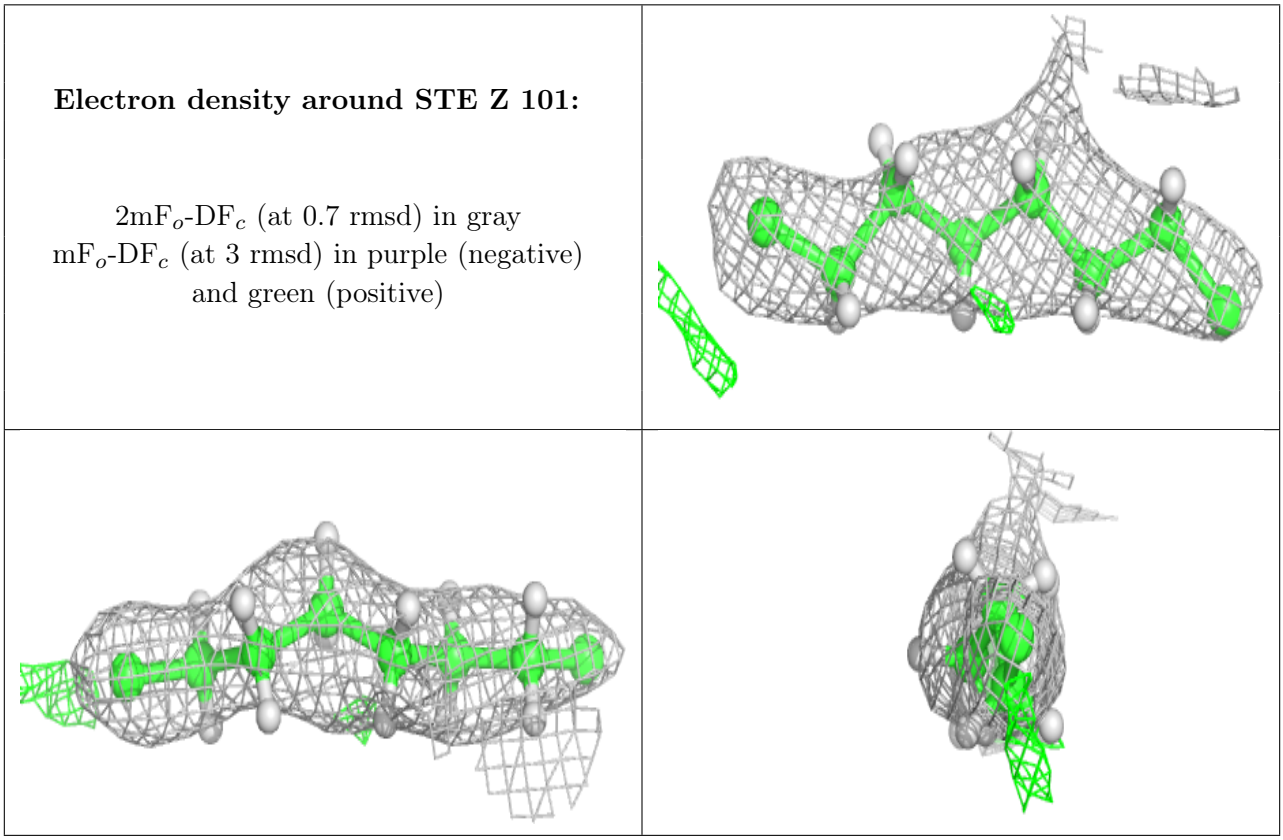
Electron density around STE C 522:

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



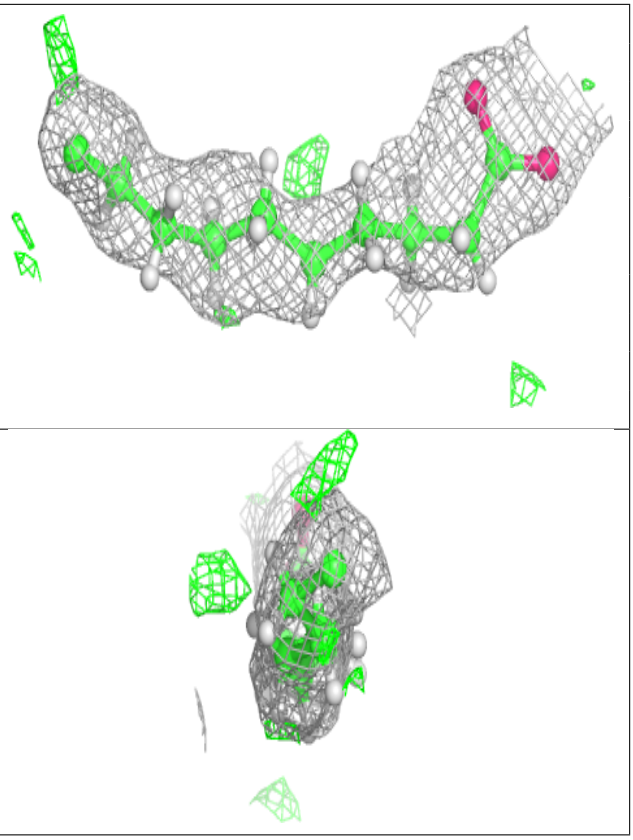
Electron density around STE Z 101:

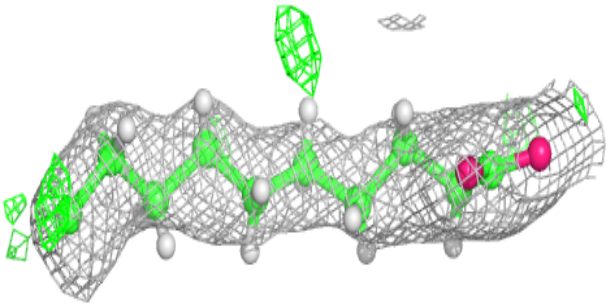
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around STE C 521:

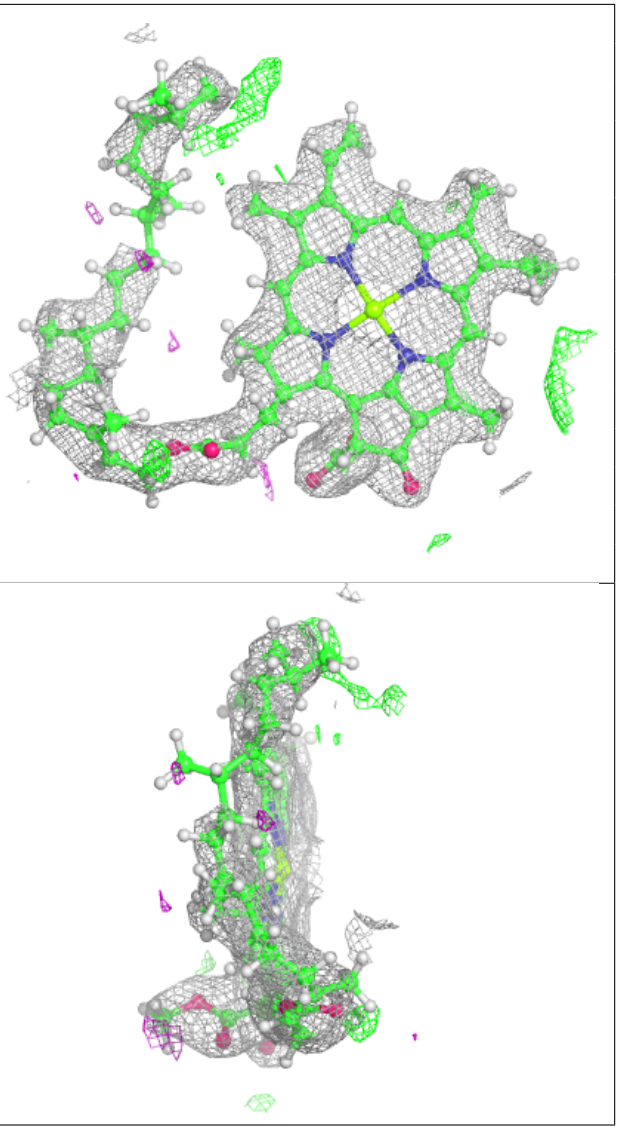
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

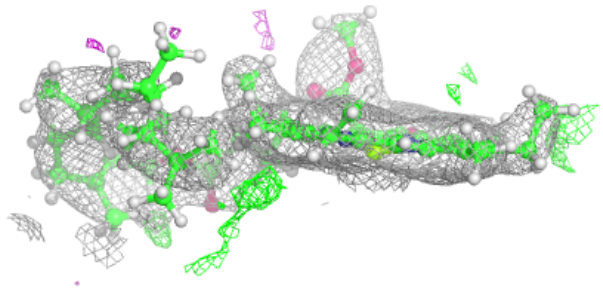




Electron density around CLA c 512:

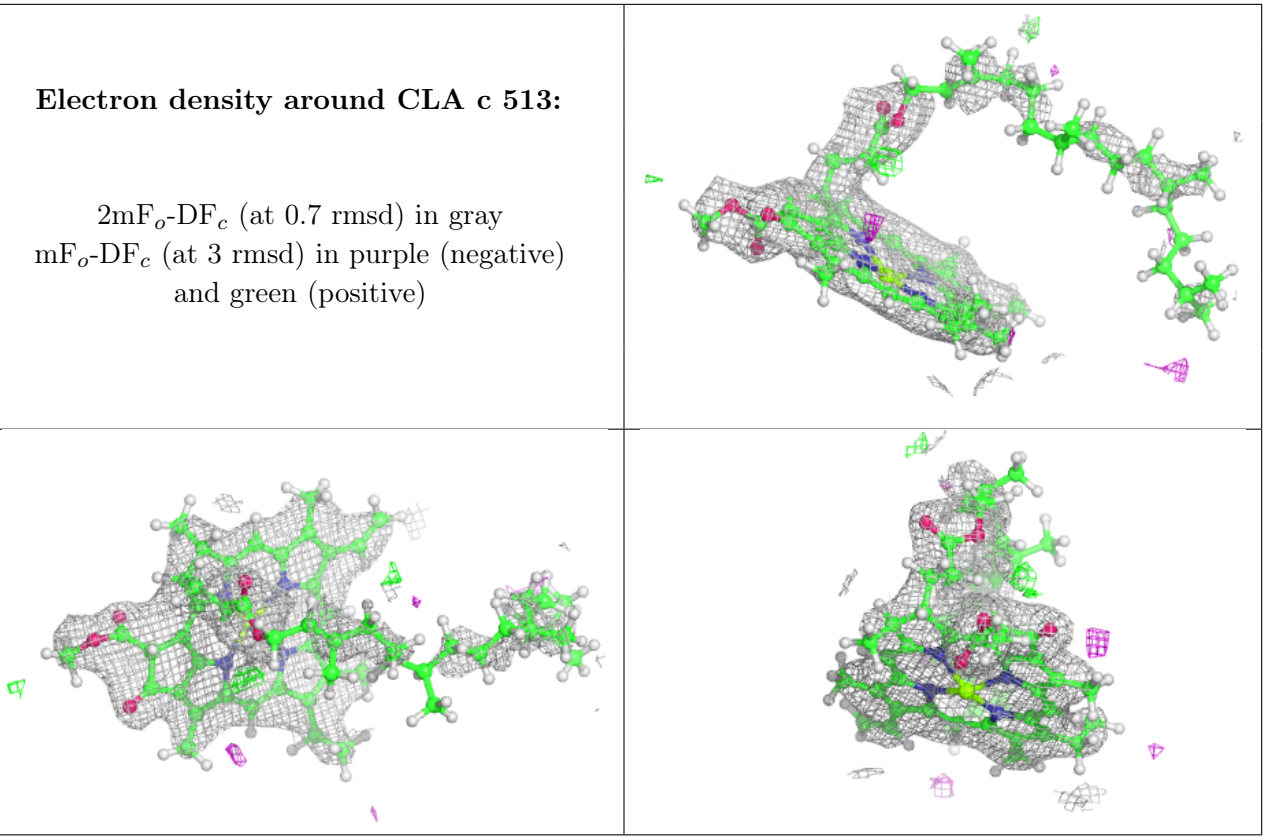
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





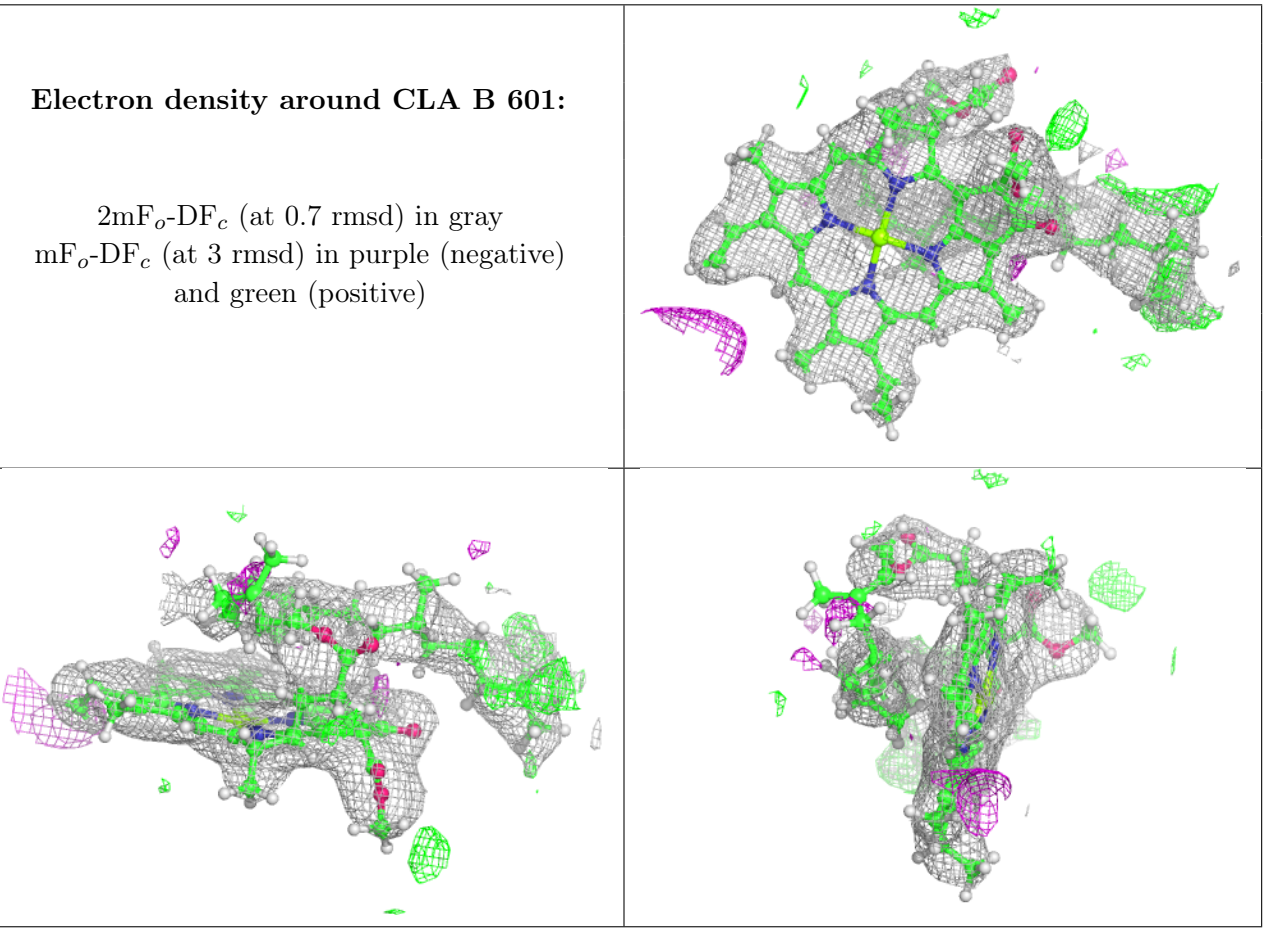
Electron density around CLA c 513:

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



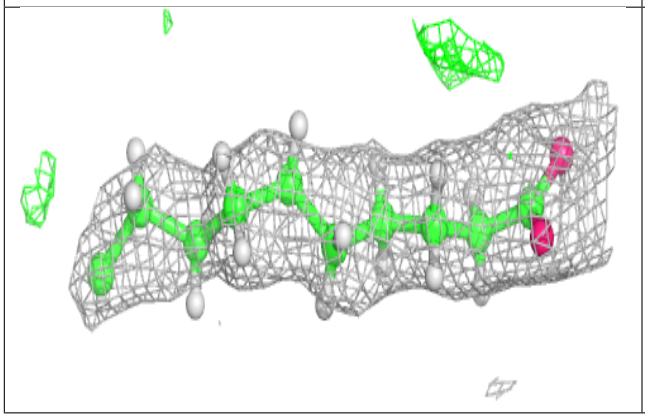
Electron density around CLA B 601:

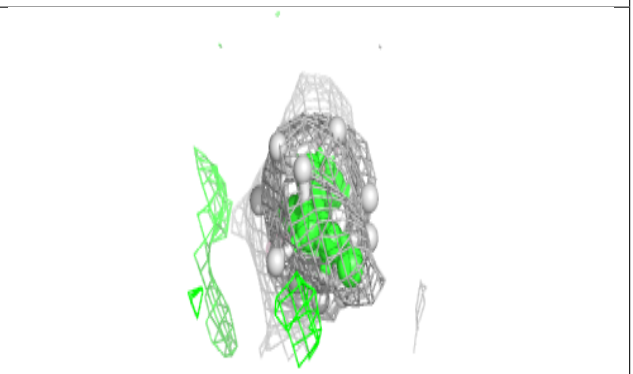
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around STE J 101:

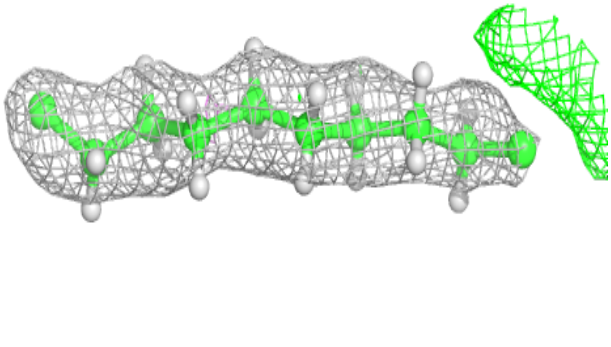
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

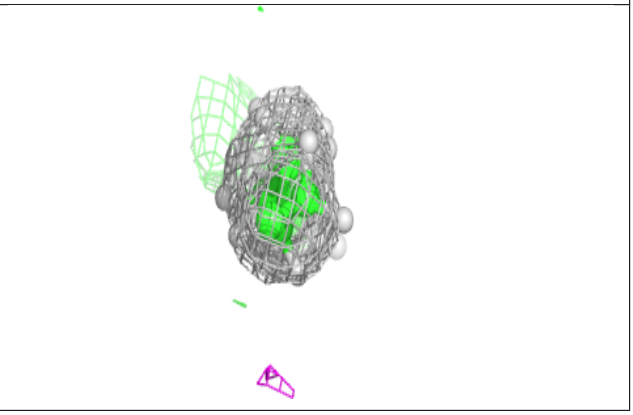




Electron density around STE M 103:

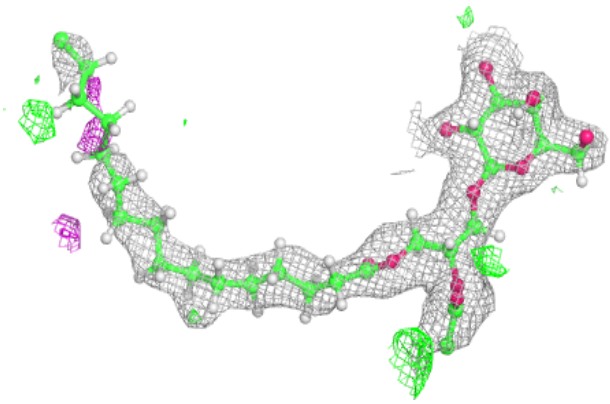
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

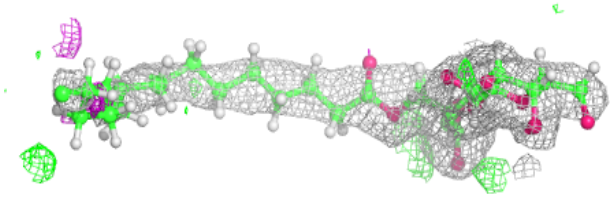


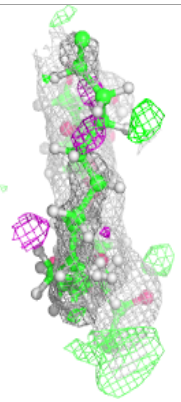


Electron density around LMG c 520:

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

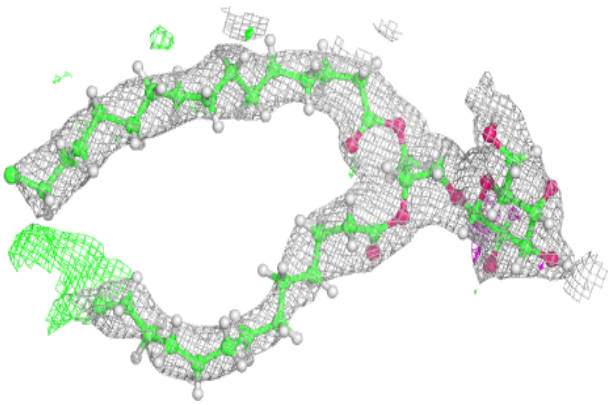


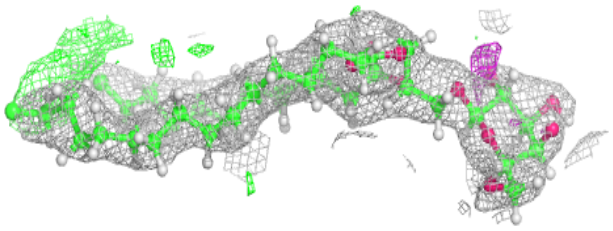


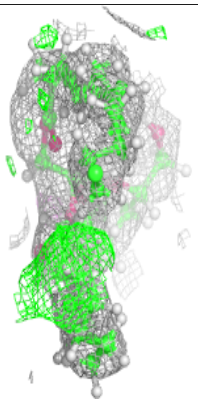


Electron density around LMG A 411:

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

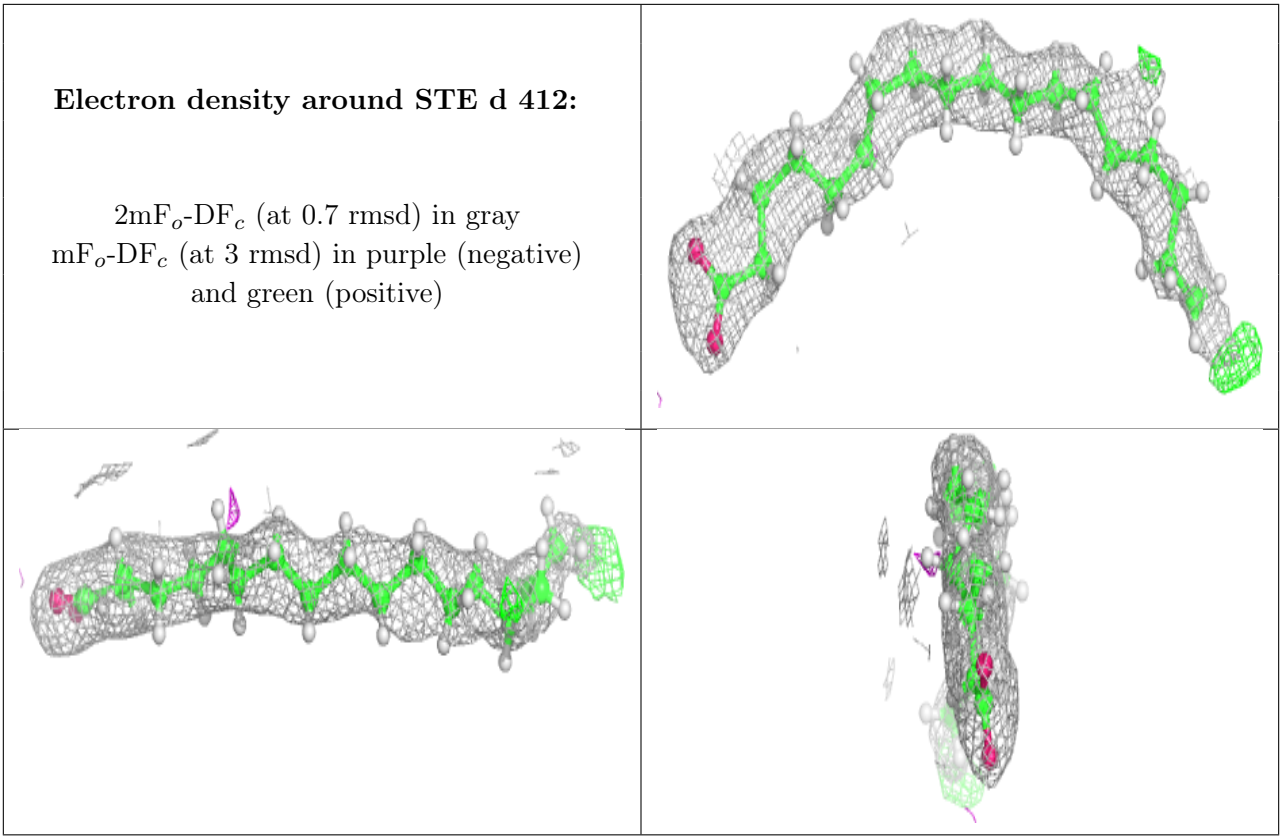






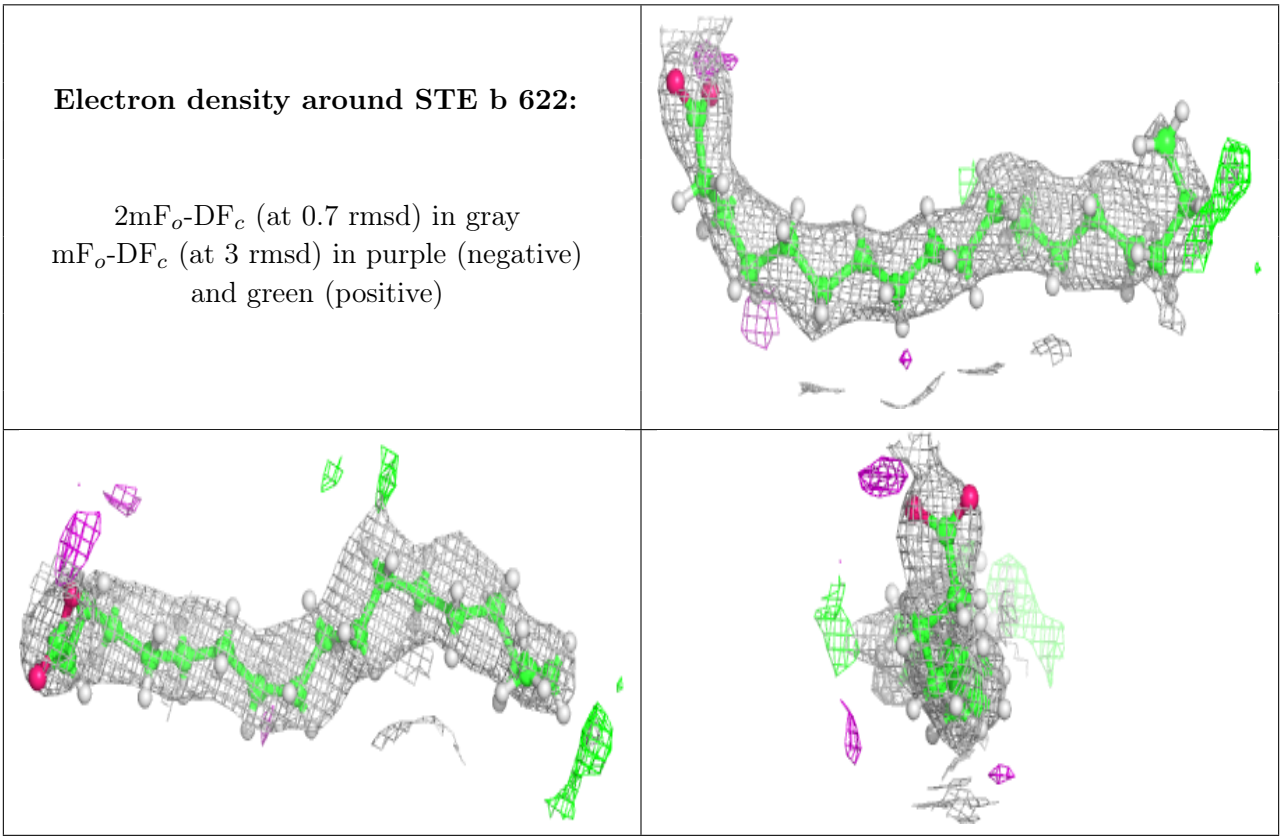
Electron density around STE d 412:

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



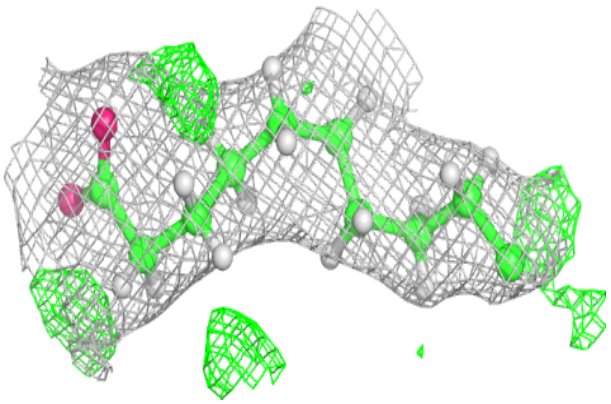
Electron density around STE b 622:

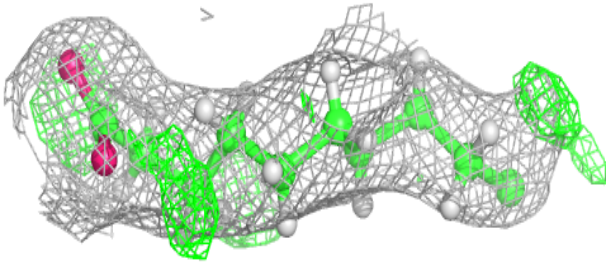
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

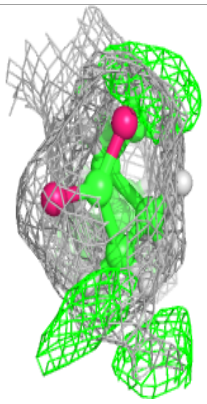


Electron density around STE B 624:

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

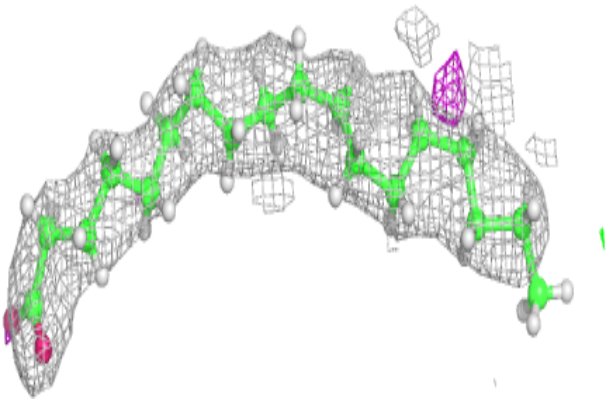


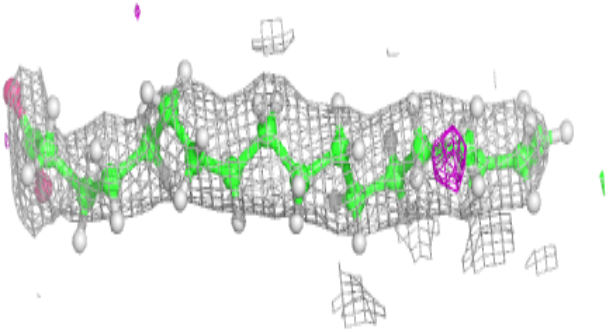


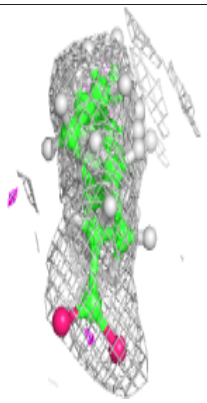


Electron density around STE D 412:

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

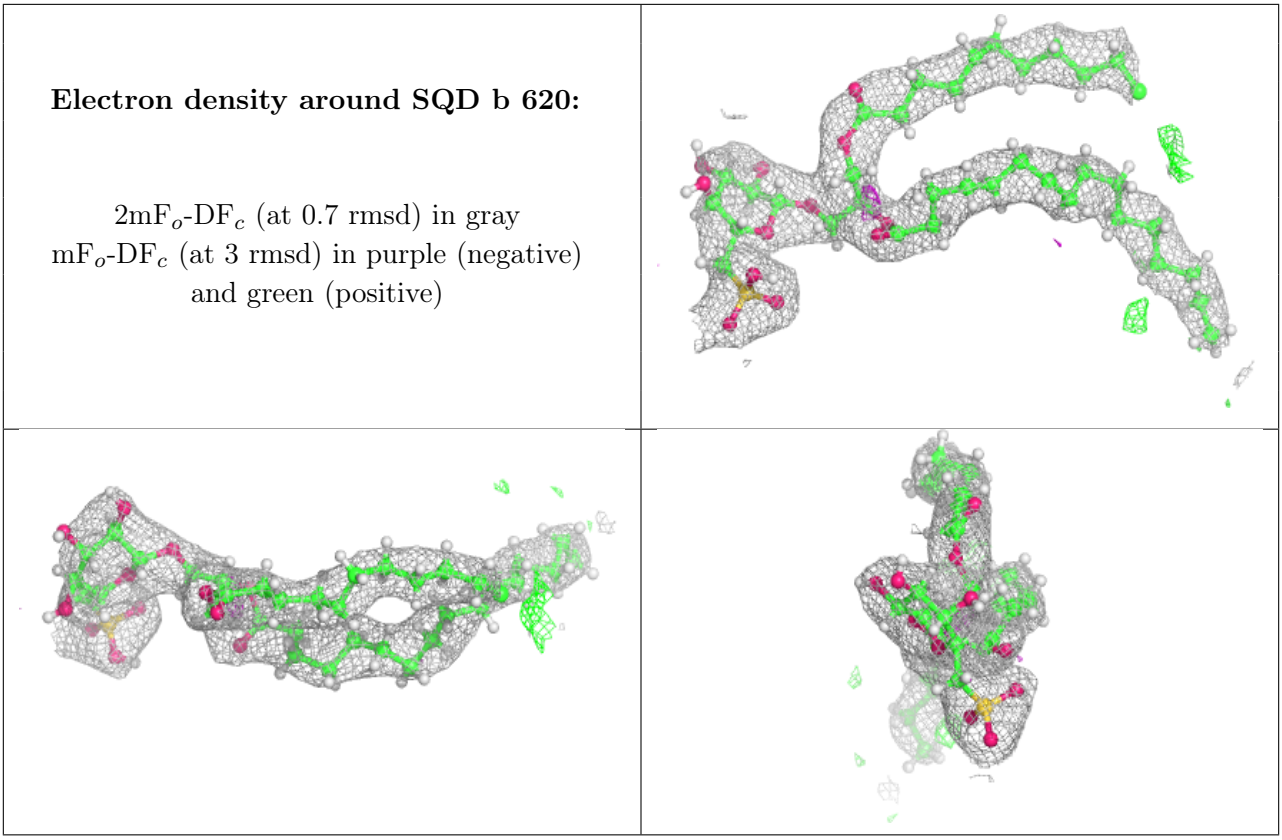






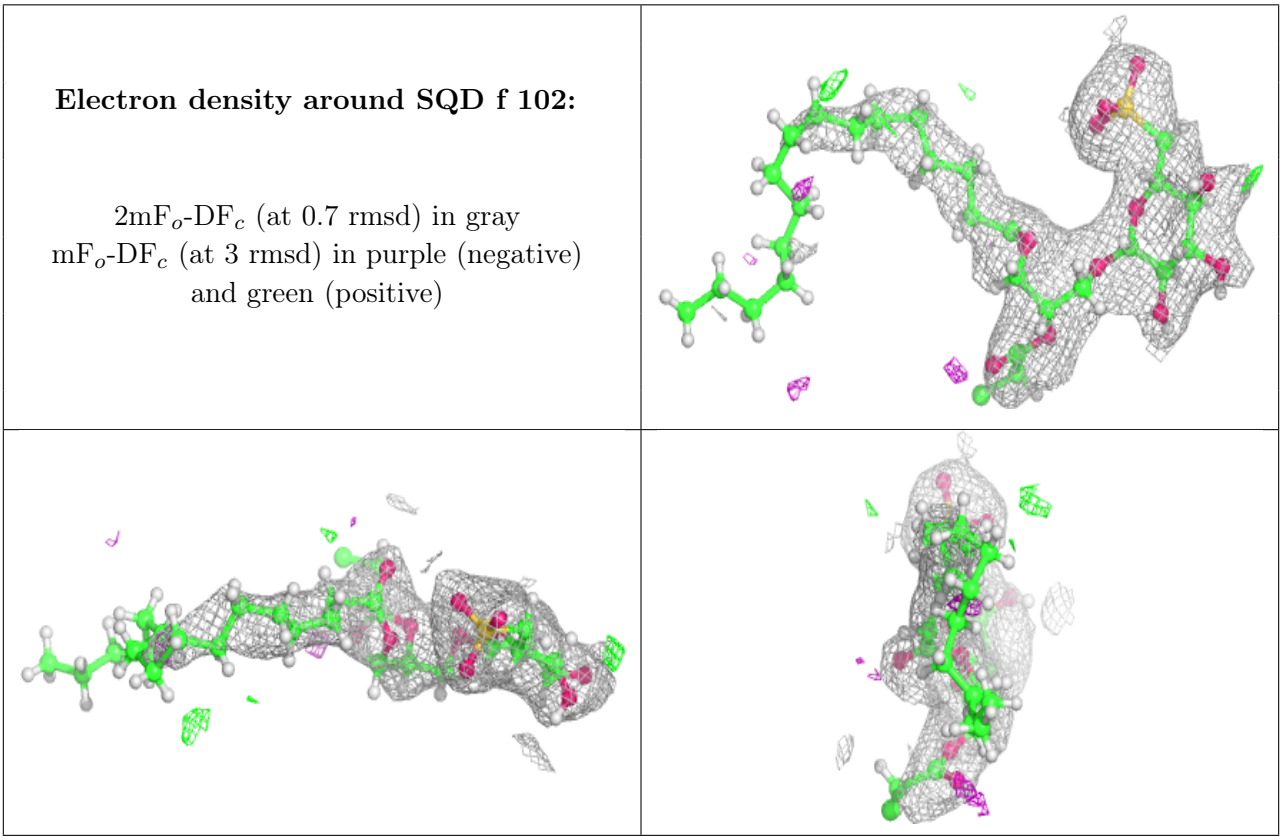
Electron density around SQD b 620:

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



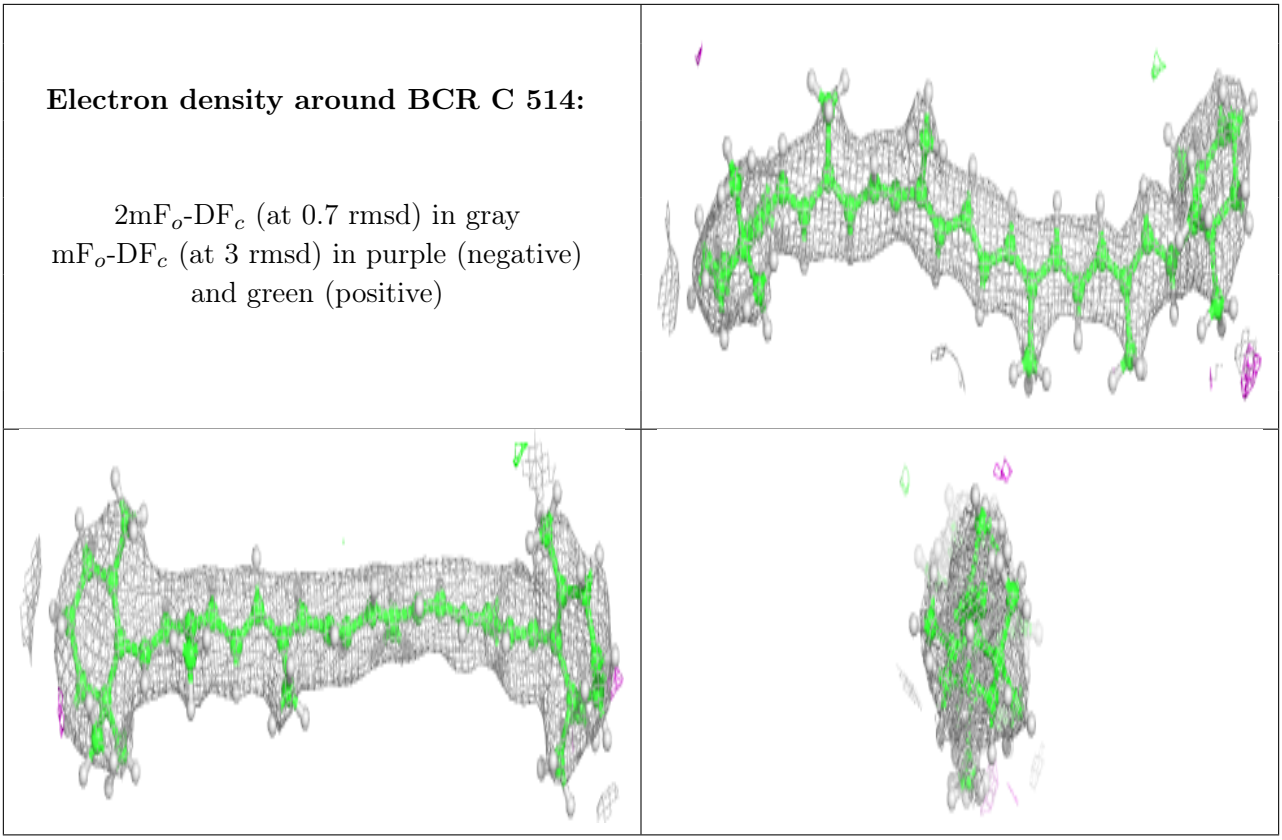
Electron density around SQD f 102:

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



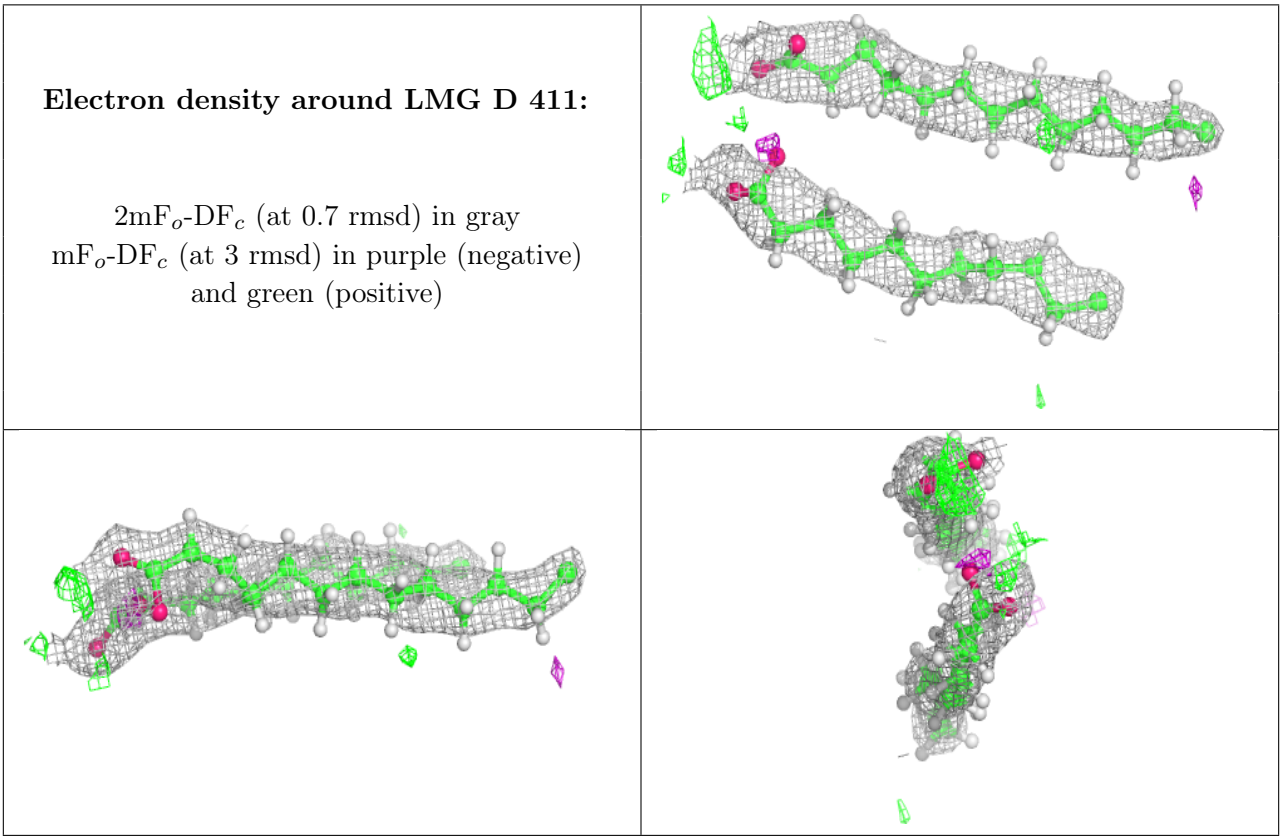
Electron density around BCR C 514:

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



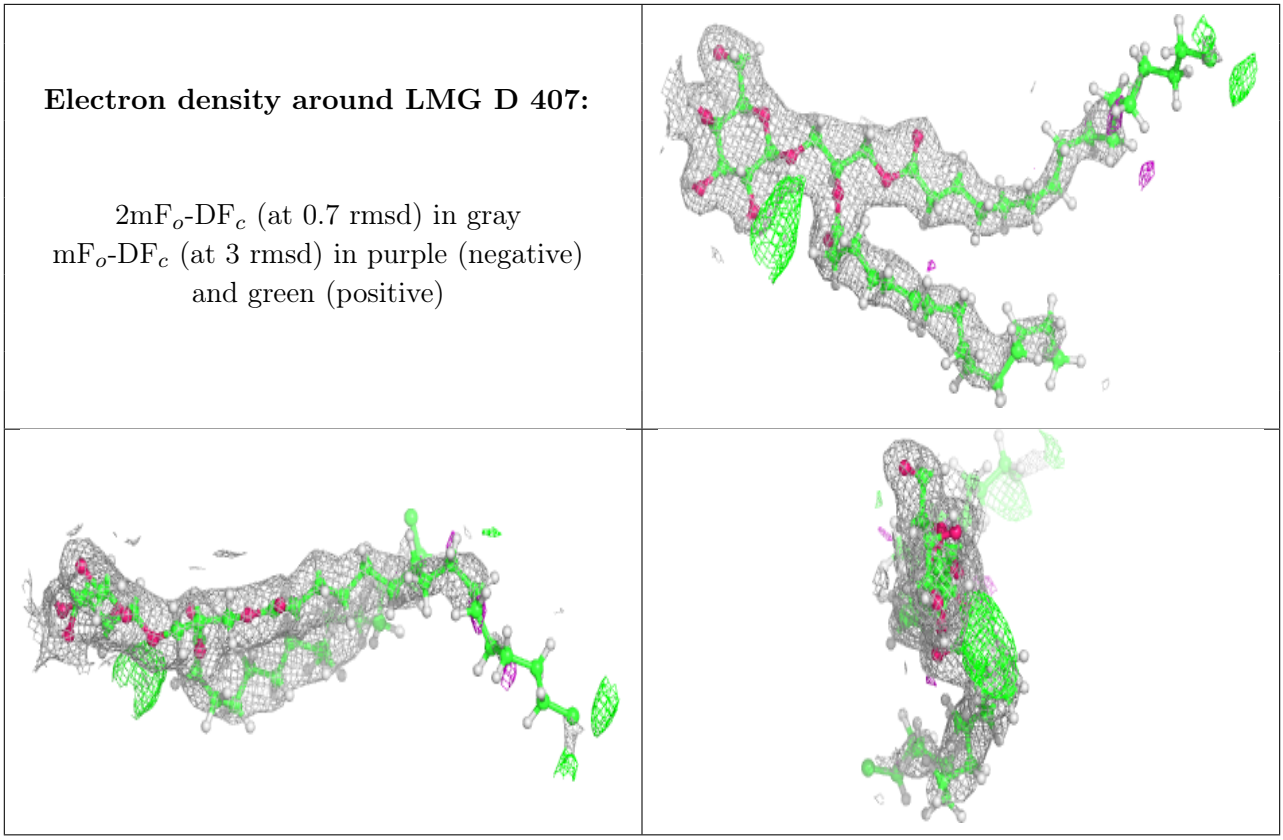
Electron density around LMG D 411:

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



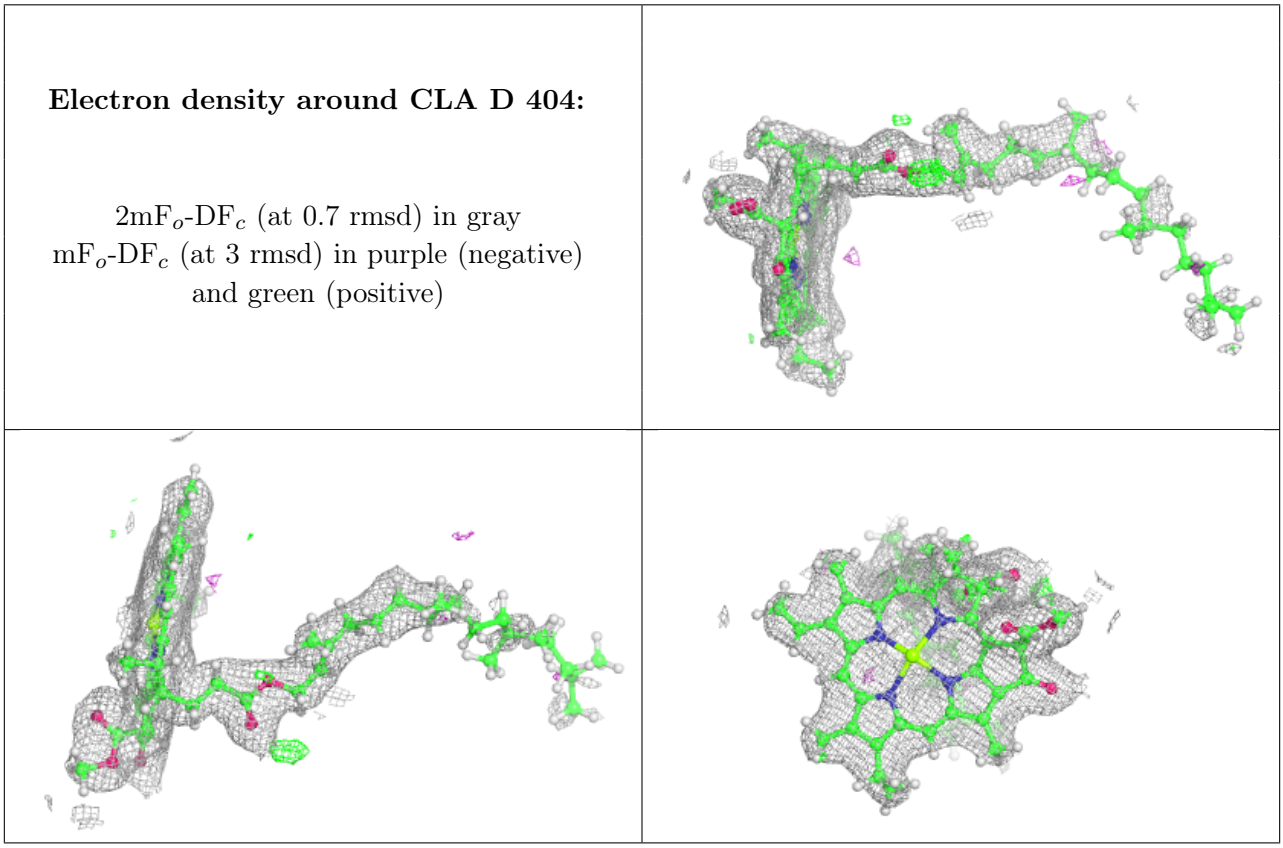
Electron density around LMG D 407:

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



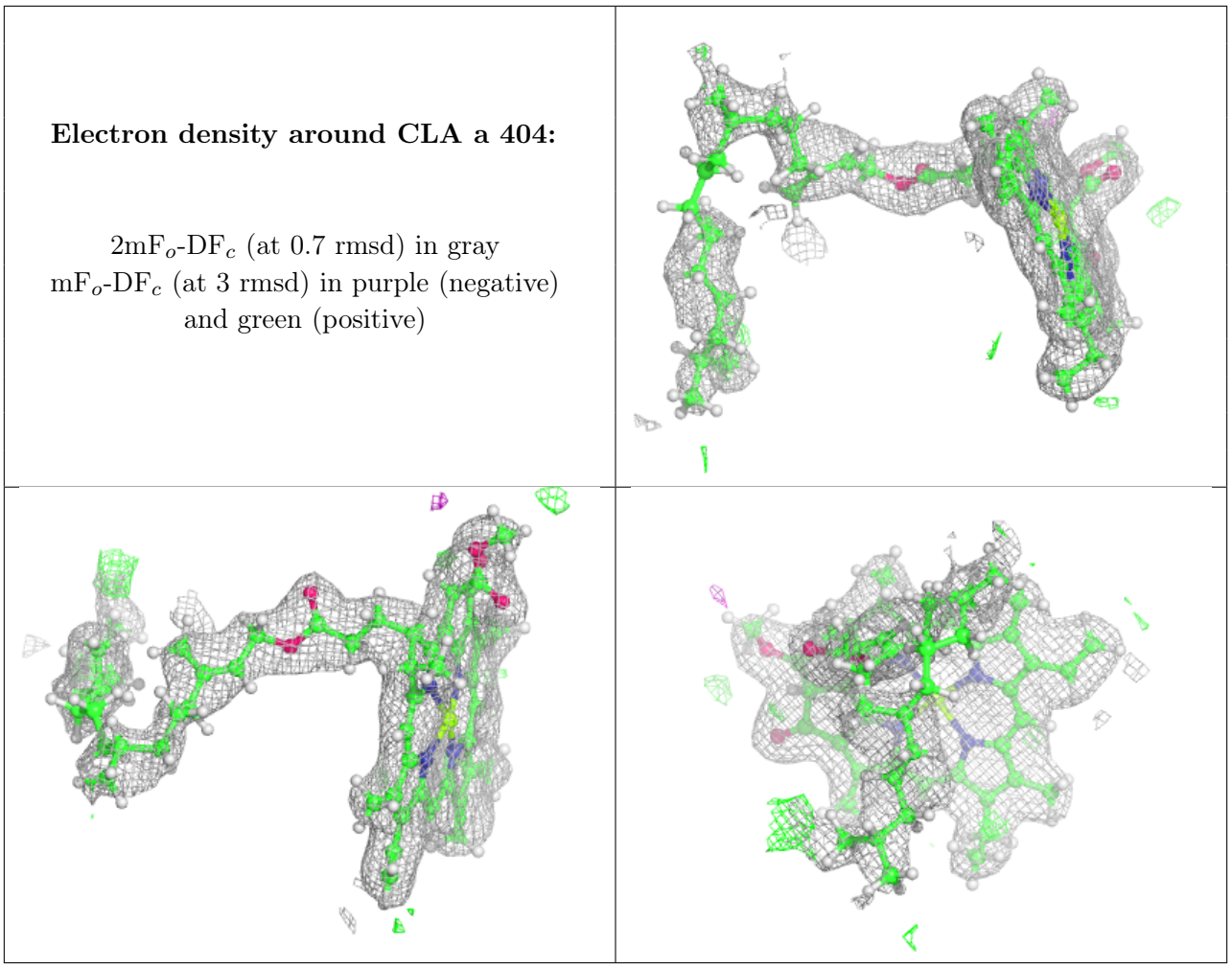
Electron density around CLA D 404:

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



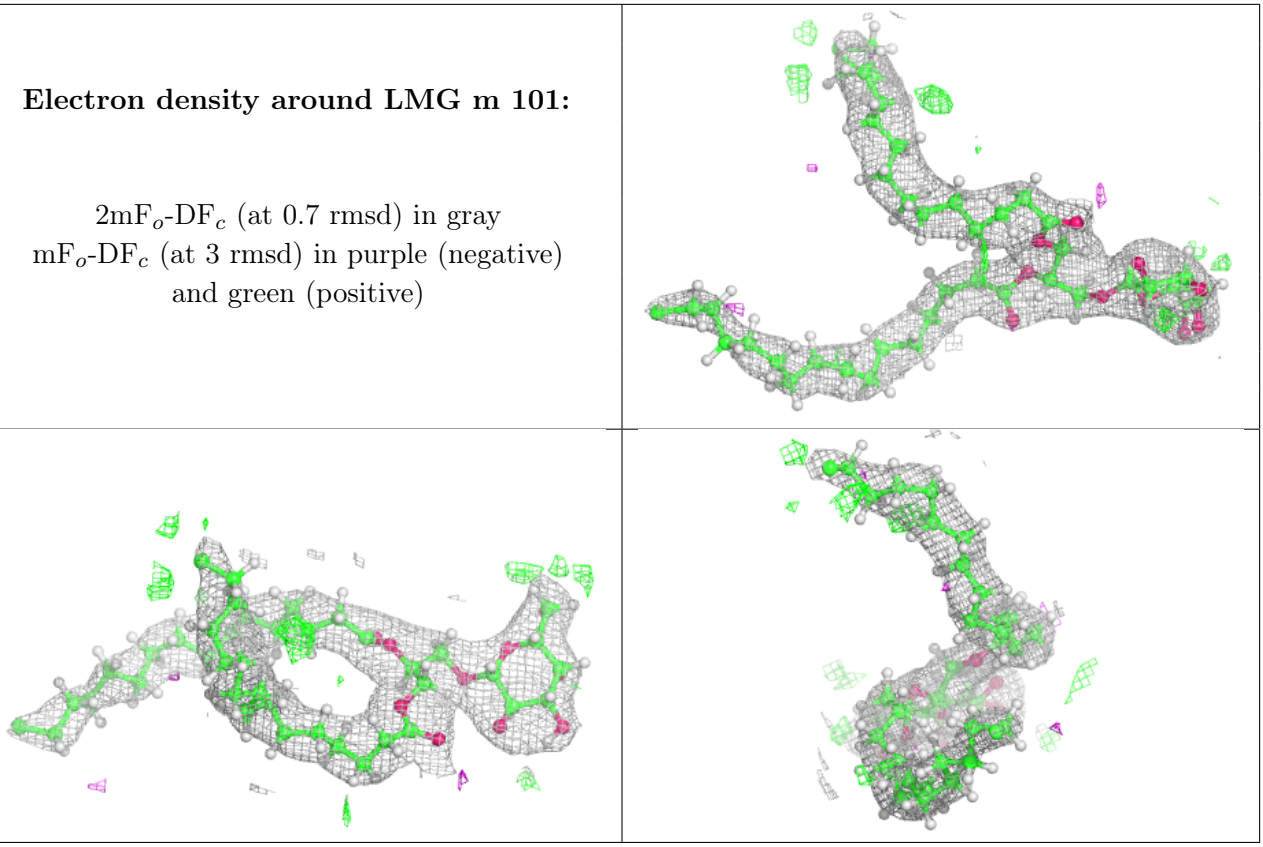
Electron density around CLA a 404:

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



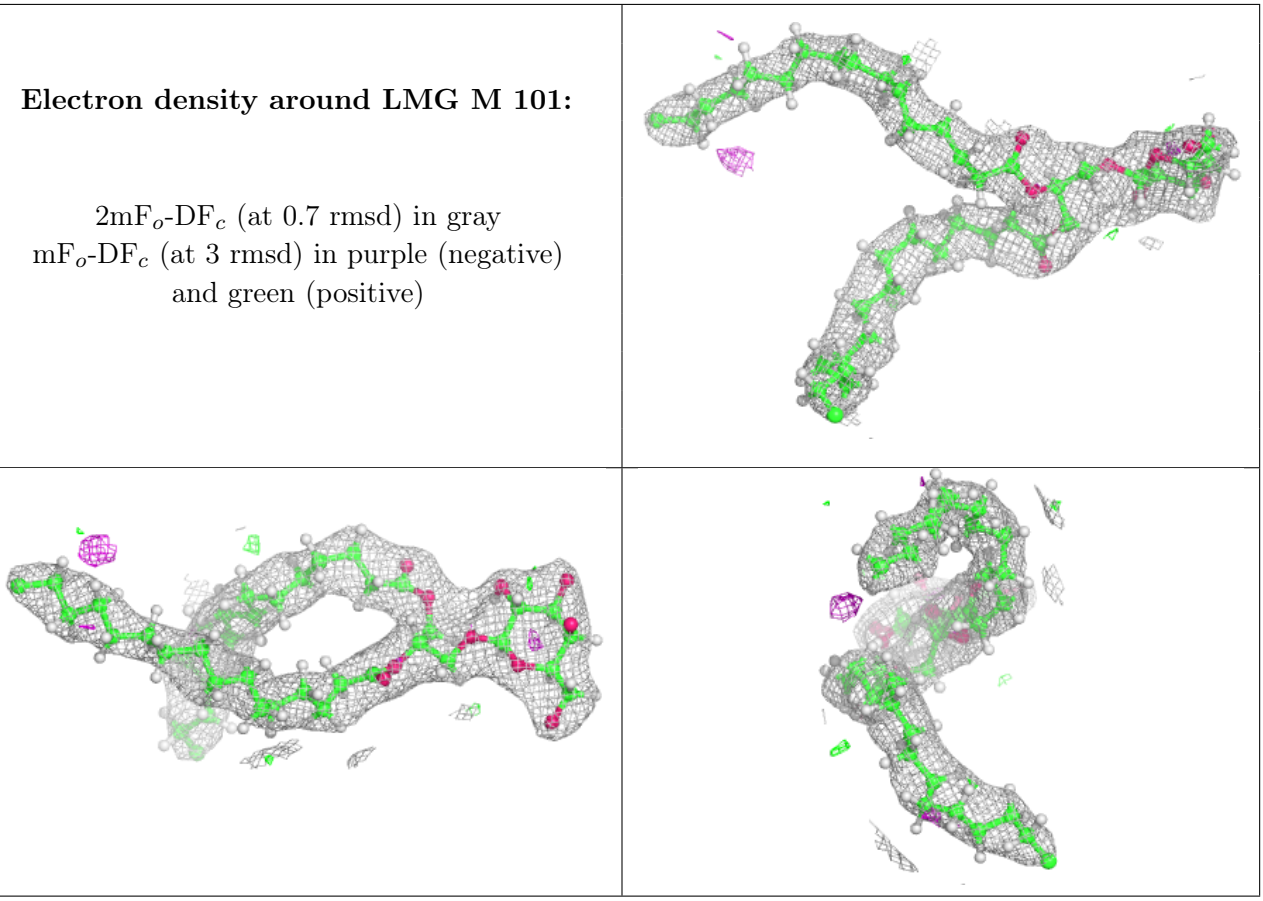
Electron density around LMG m 101:

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



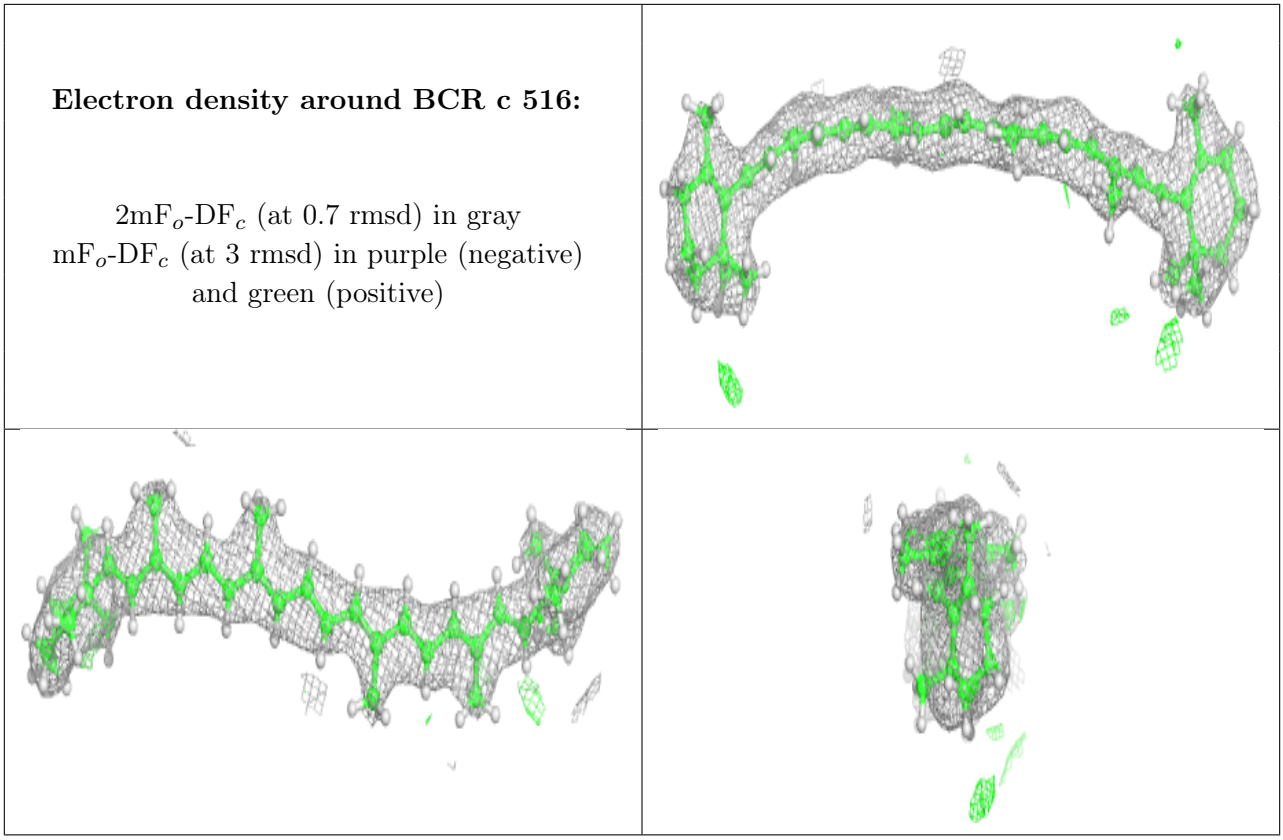
Electron density around LMG M 101:

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



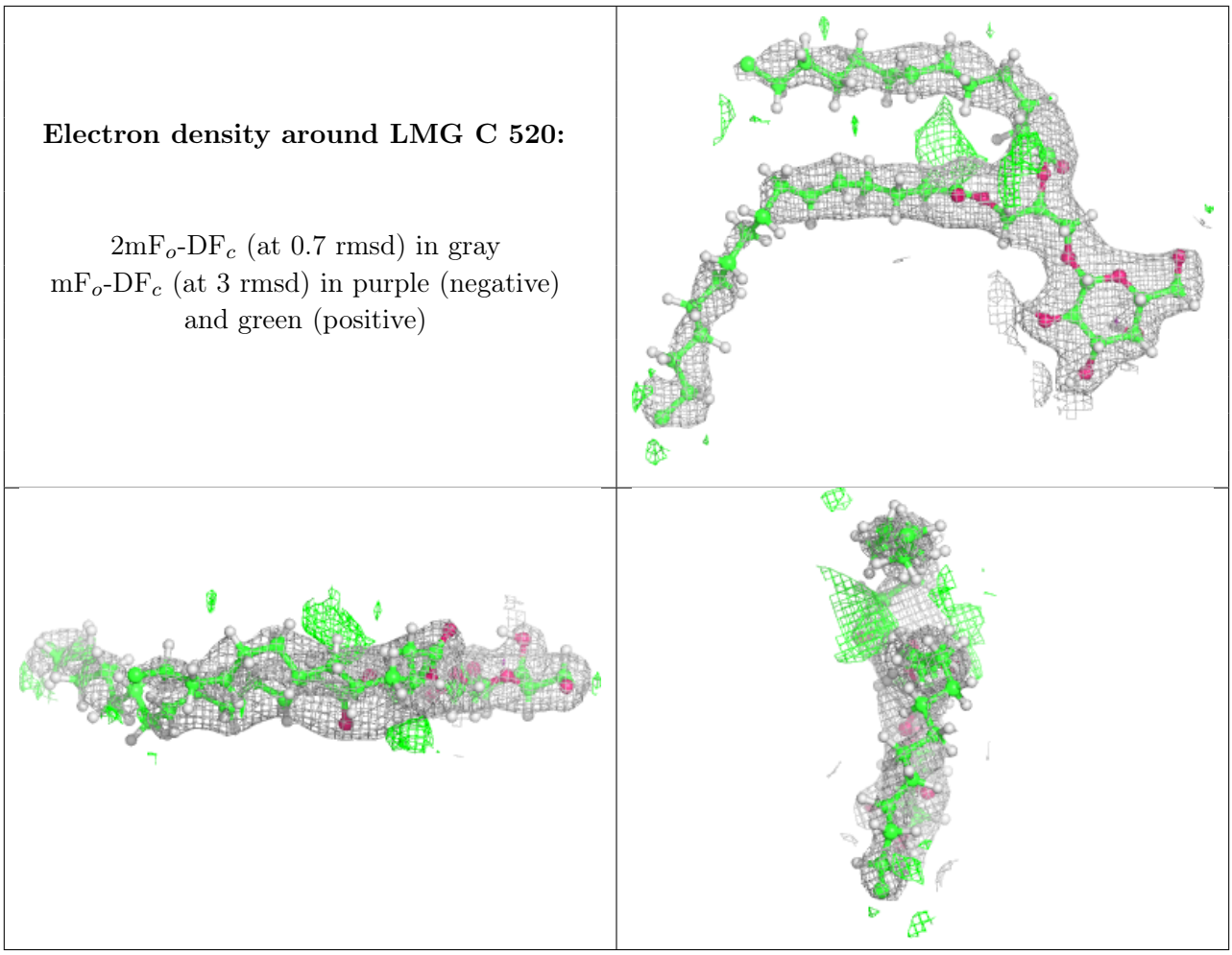
Electron density around BCR c 516:

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



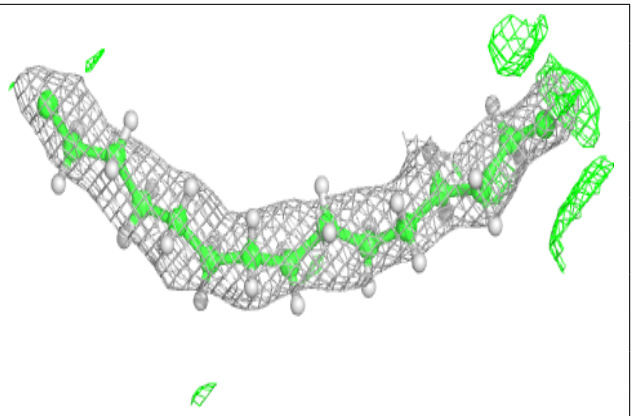
Electron density around LMG C 520:

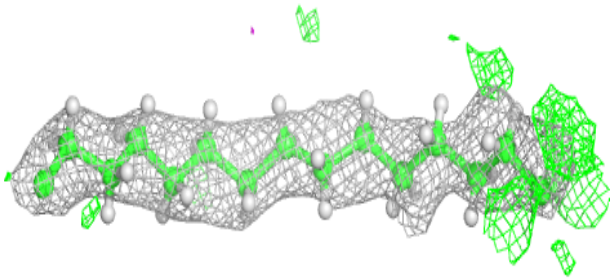
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

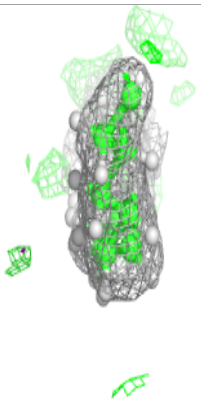


Electron density around STE I 101:

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

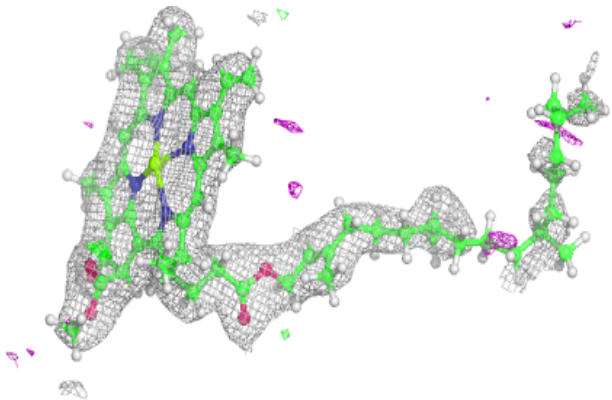


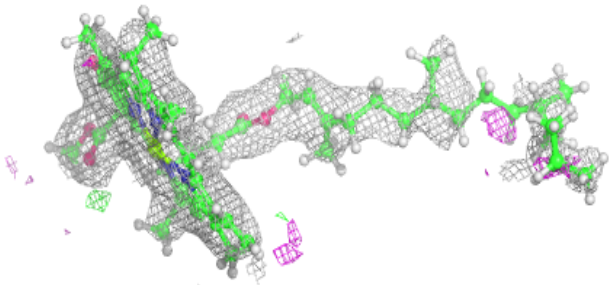


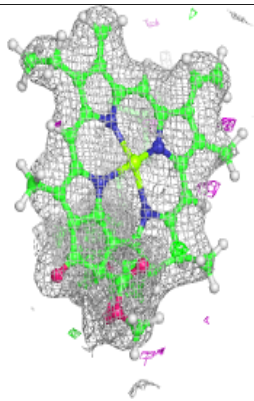


Electron density around CLA d 405:

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

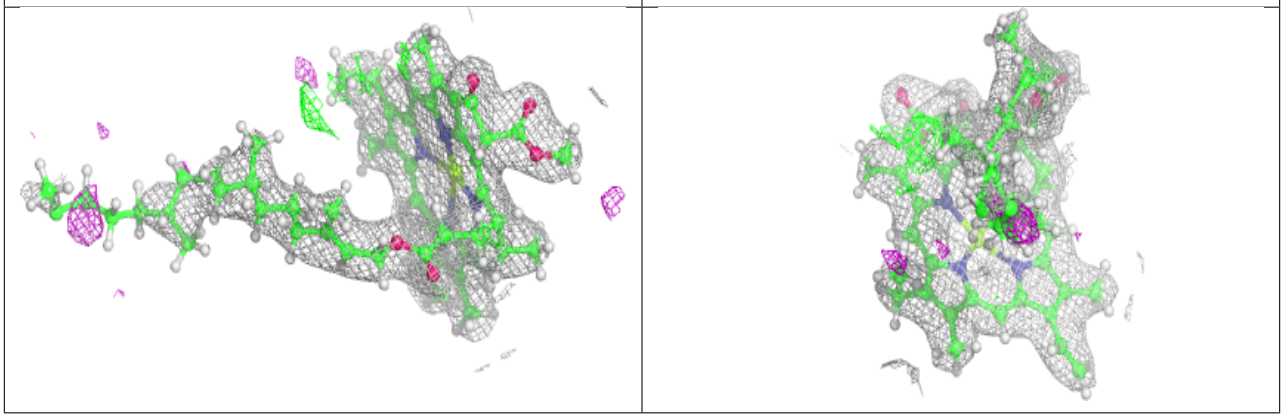






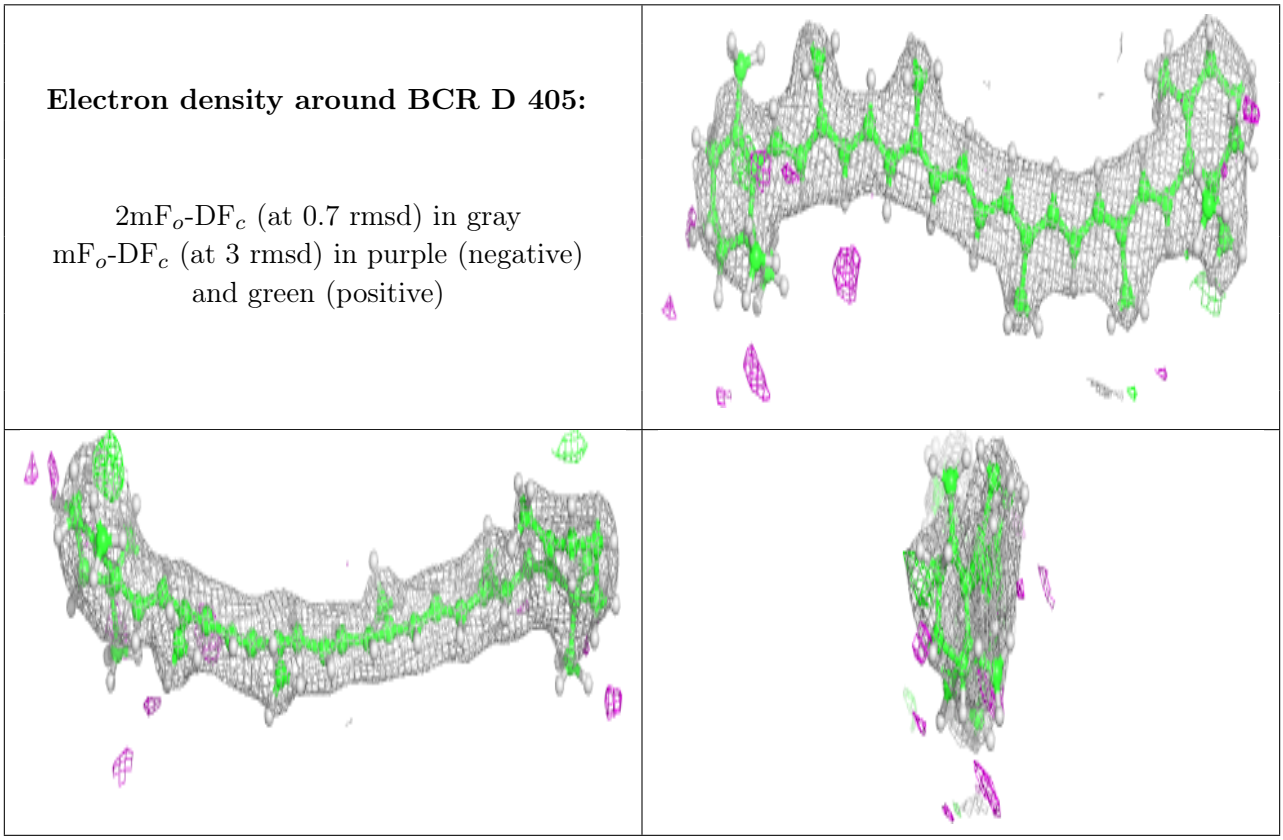
Electron density around CLA c 508:

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



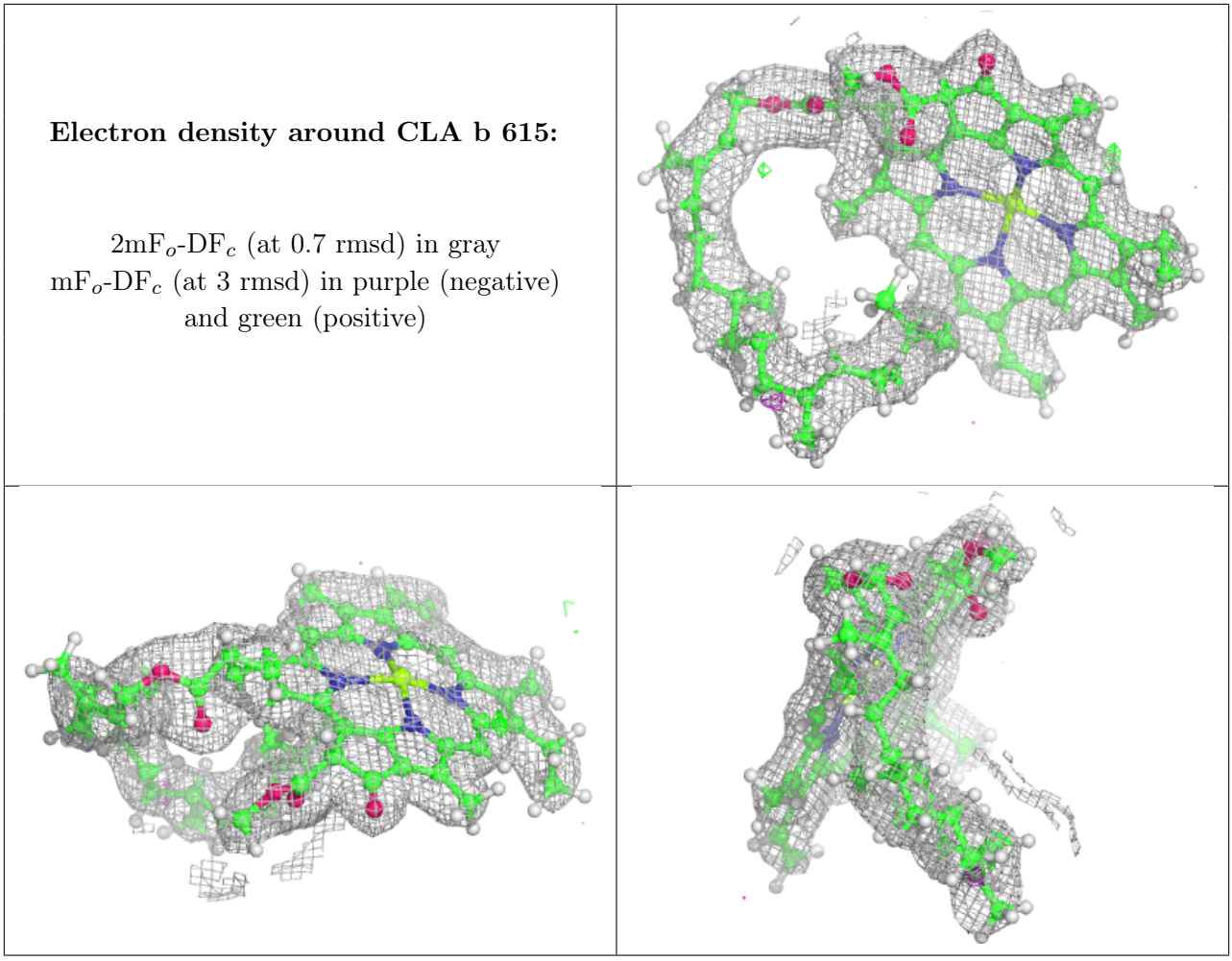
Electron density around BCR D 405:

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



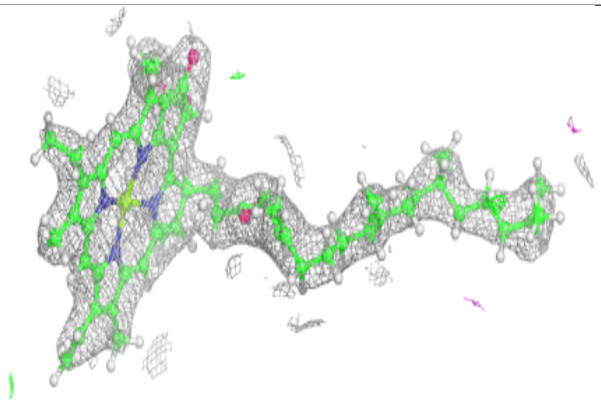
Electron density around CLA b 615:

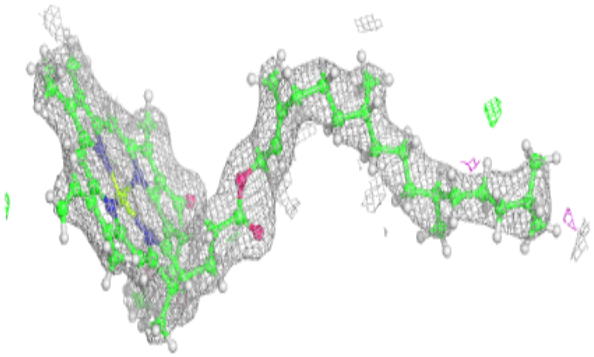
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

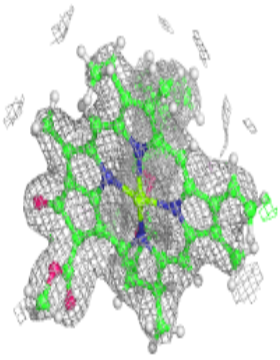


Electron density around CLA c 502:

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

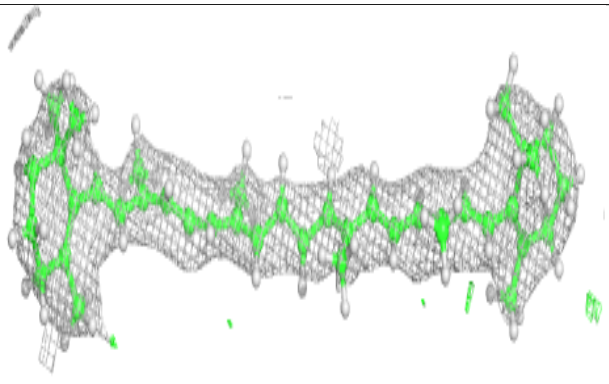


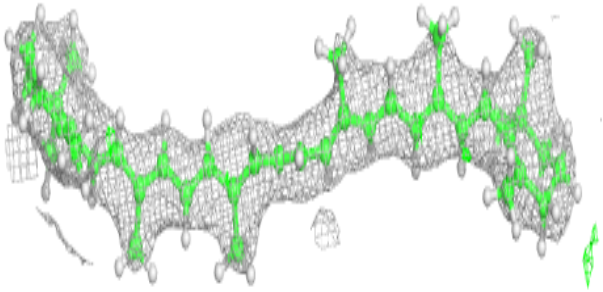


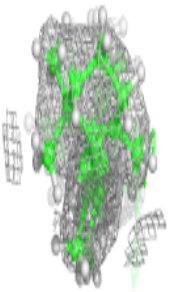


Electron density around BCR c 514:

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

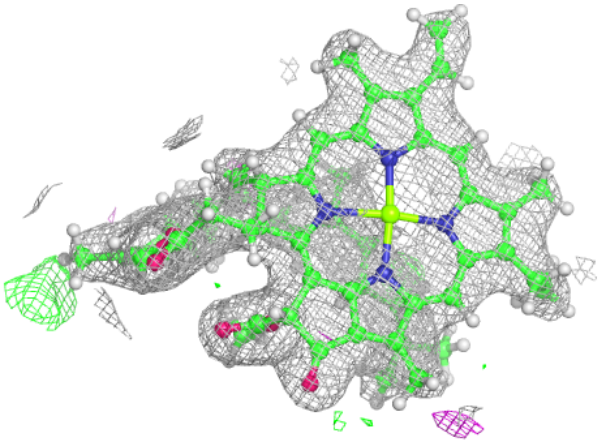


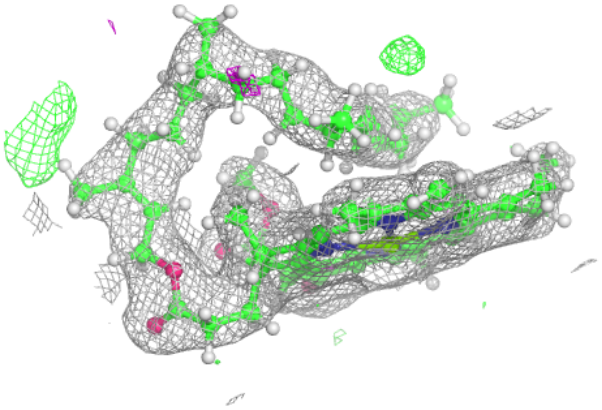




Electron density around CLA c 510:

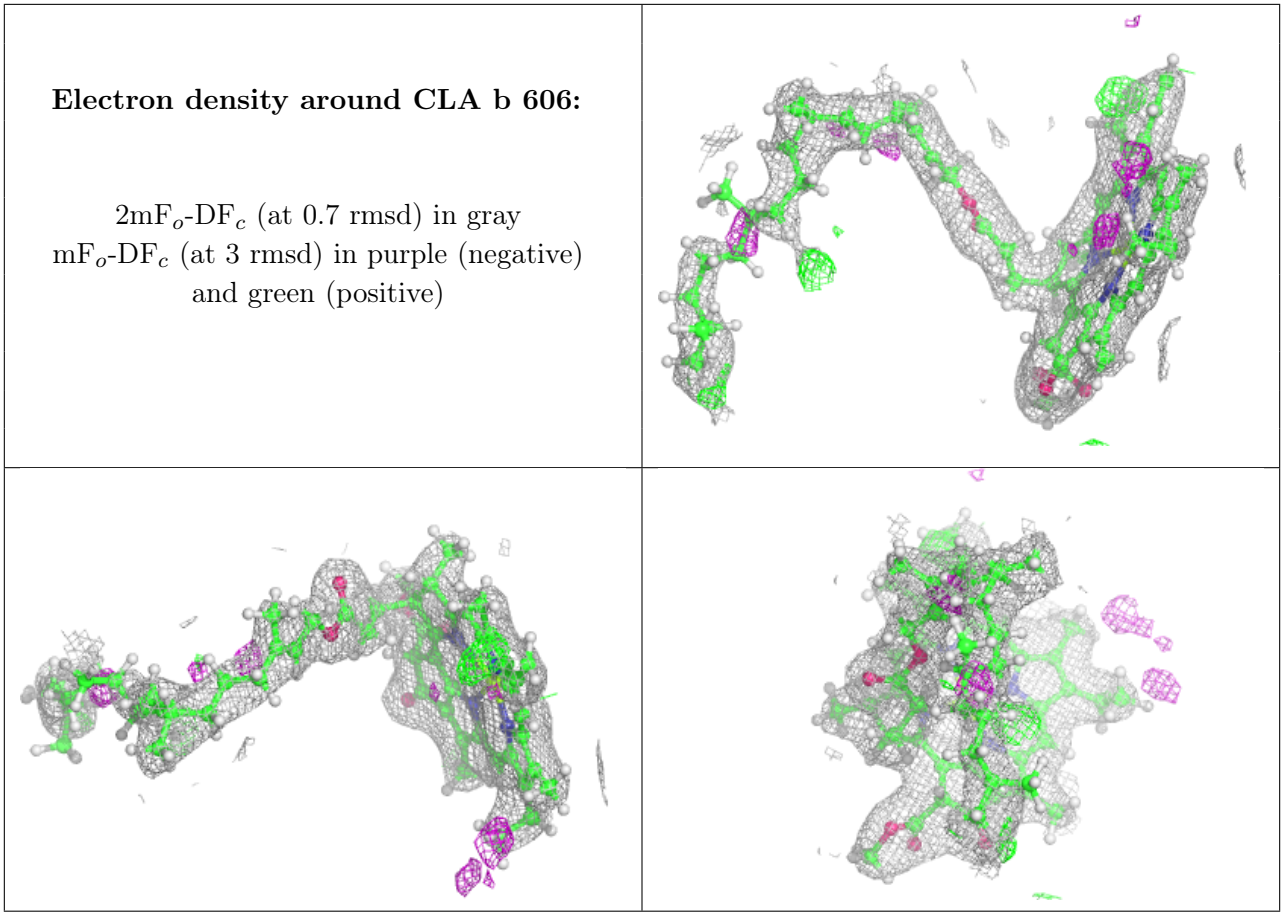
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





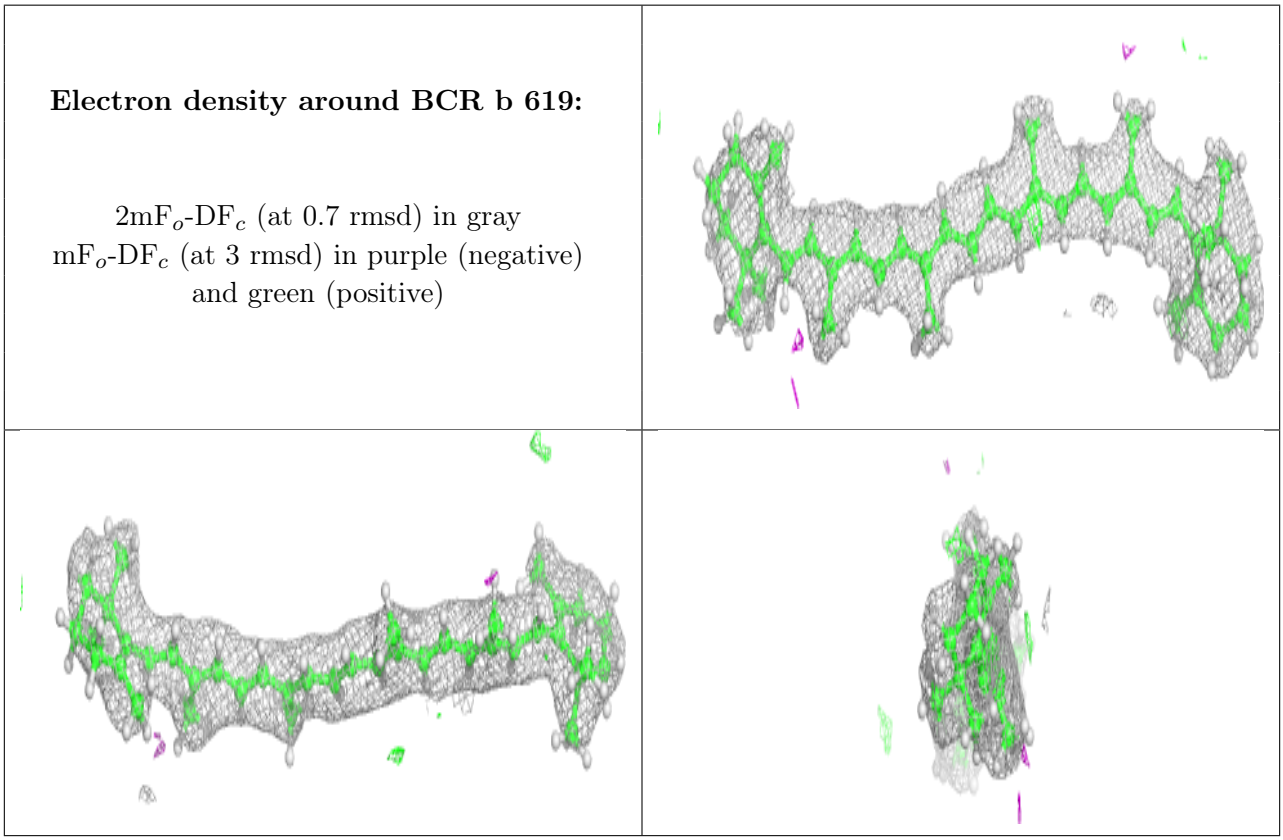
Electron density around CLA b 606:

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



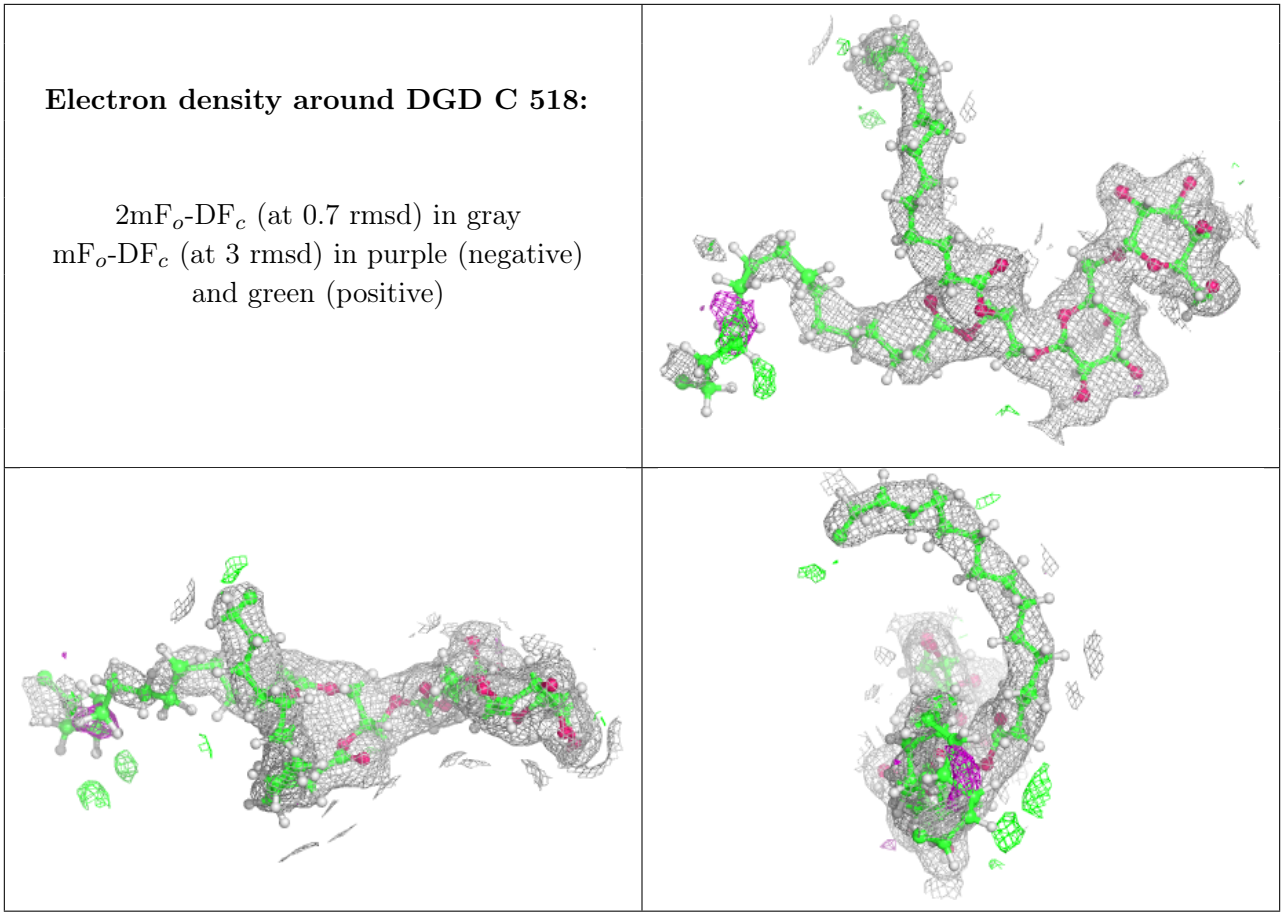
Electron density around BCR b 619:

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



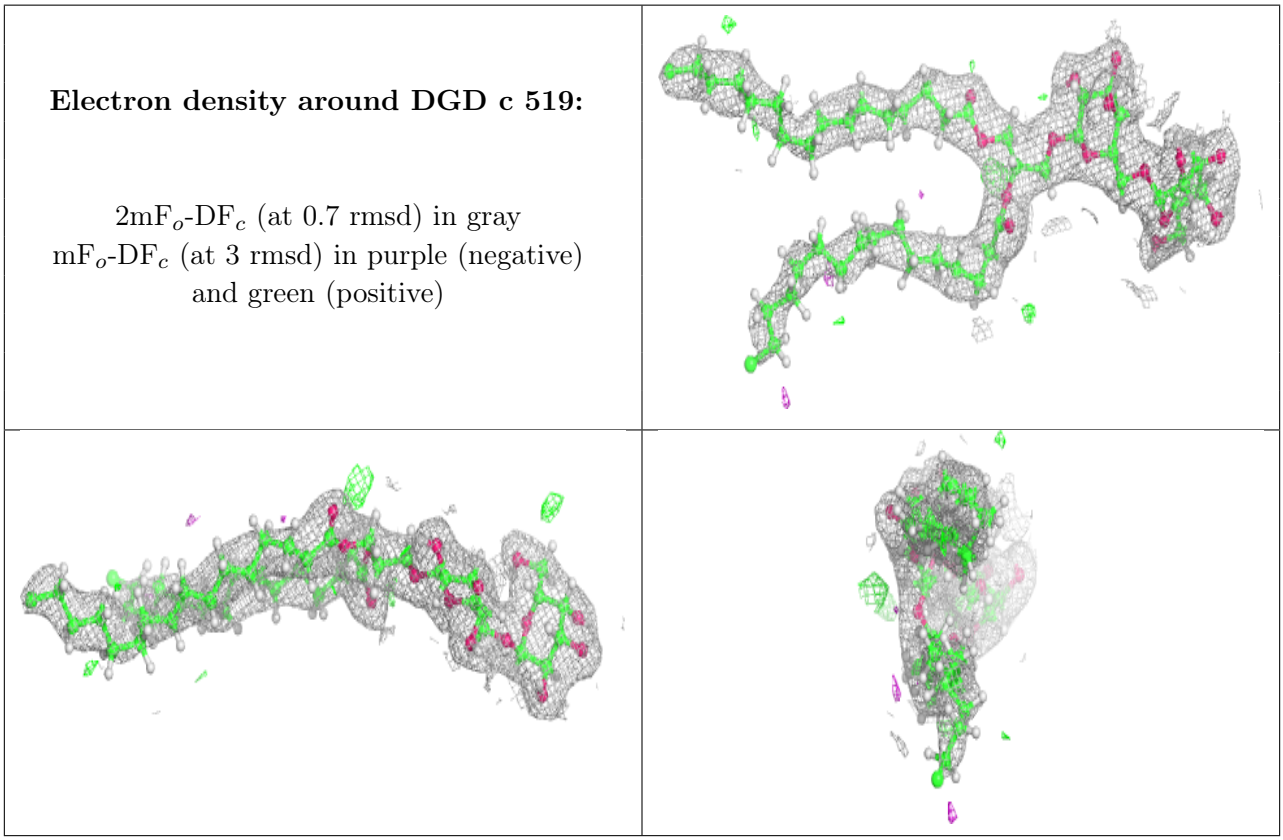
Electron density around DGD C 518:

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



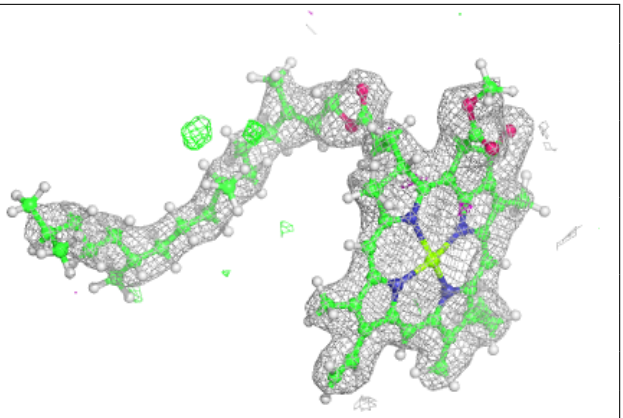
Electron density around DGD c 519:

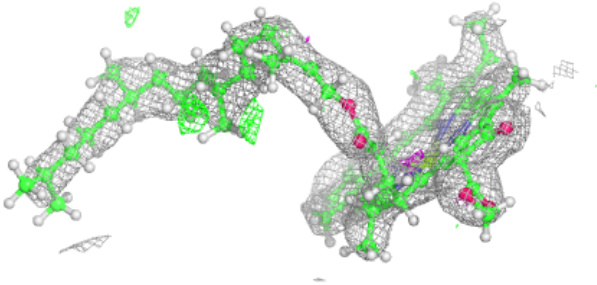
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

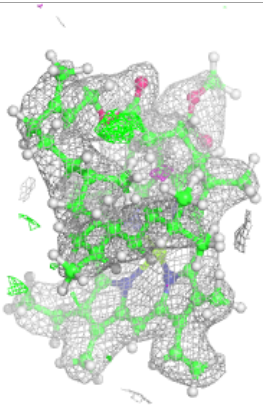


Electron density around CLA C 511:

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

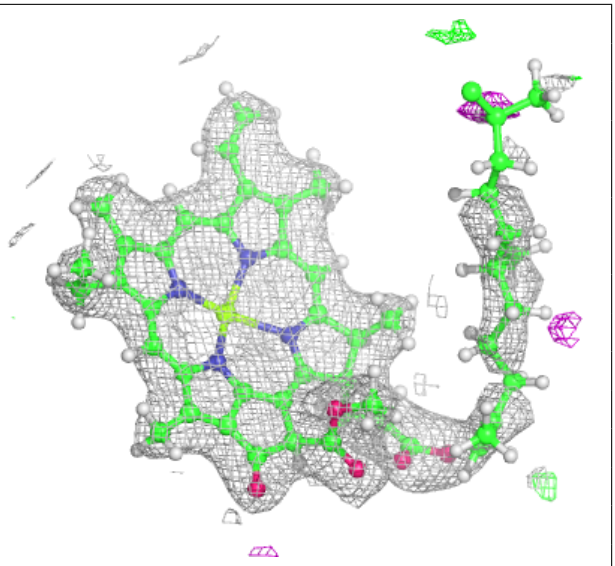


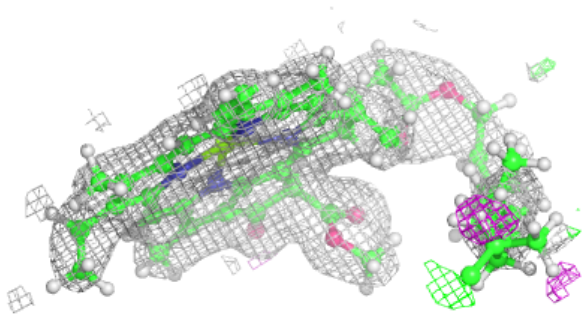


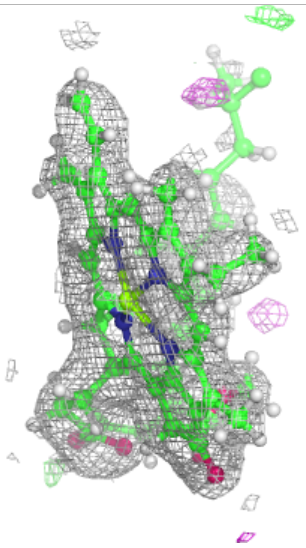


Electron density around CLA B 616:

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

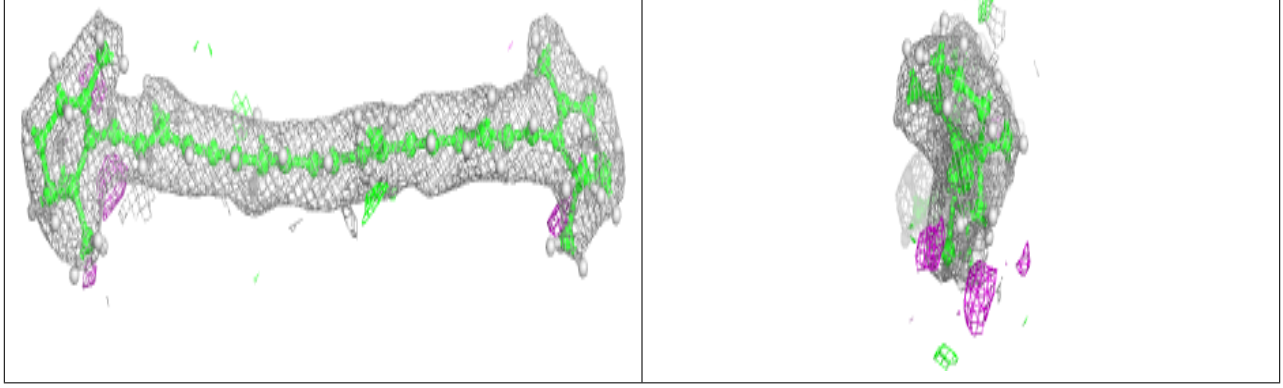






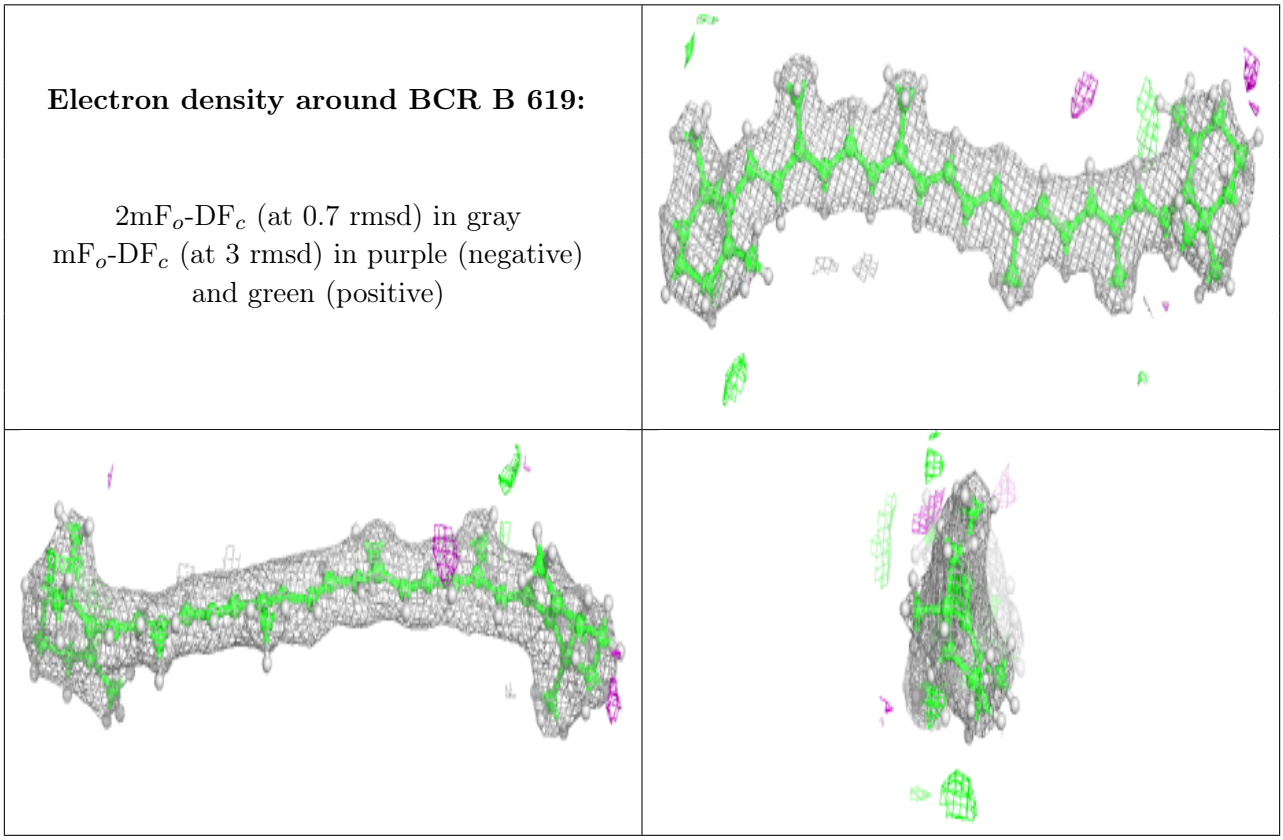
Electron density around BCR B 618:

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



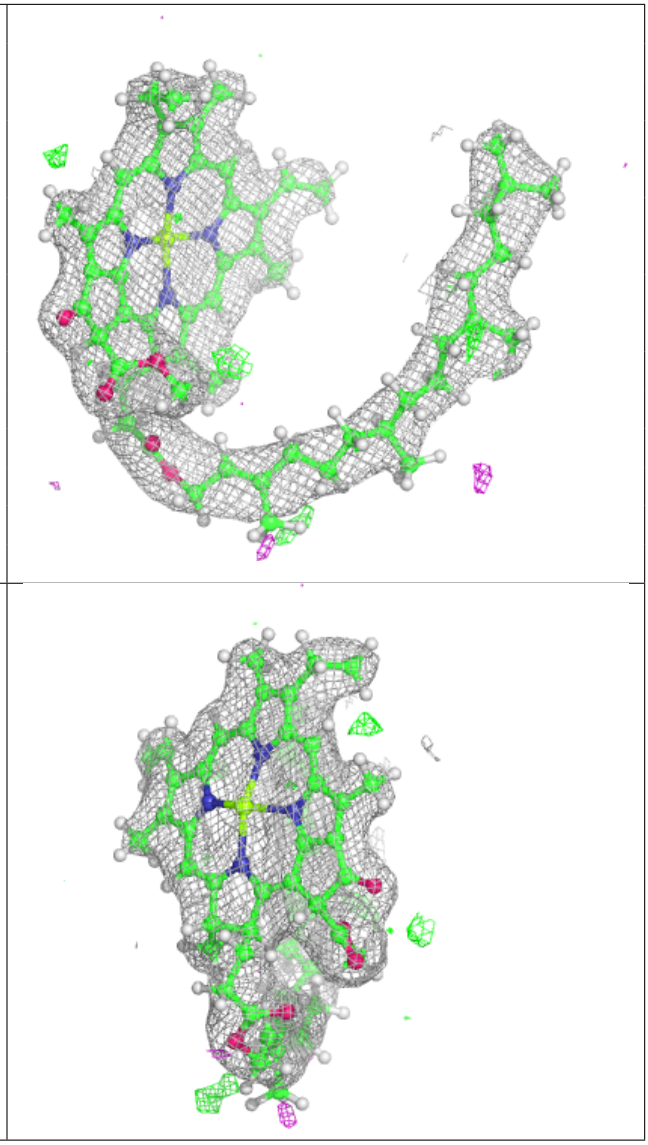
Electron density around BCR B 619:

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



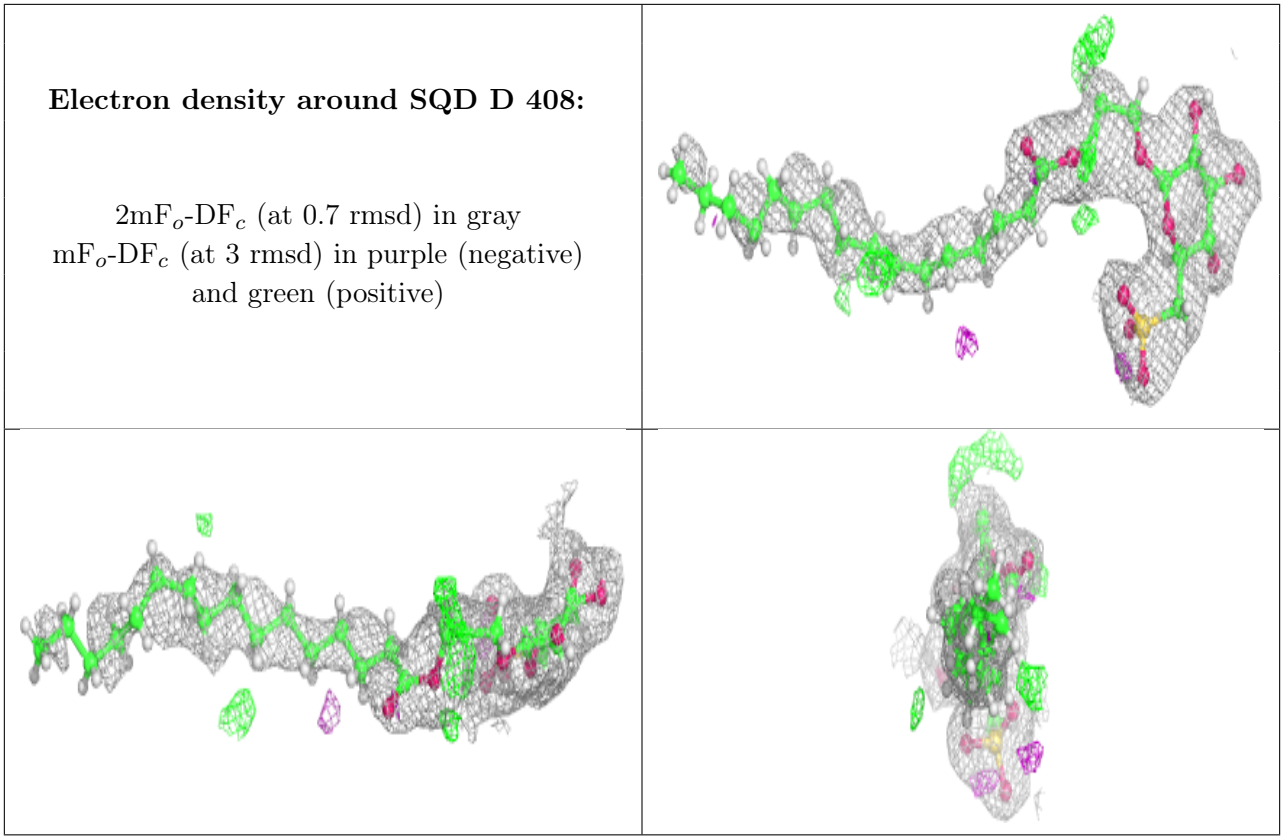
Electron density around CLA c 507:

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



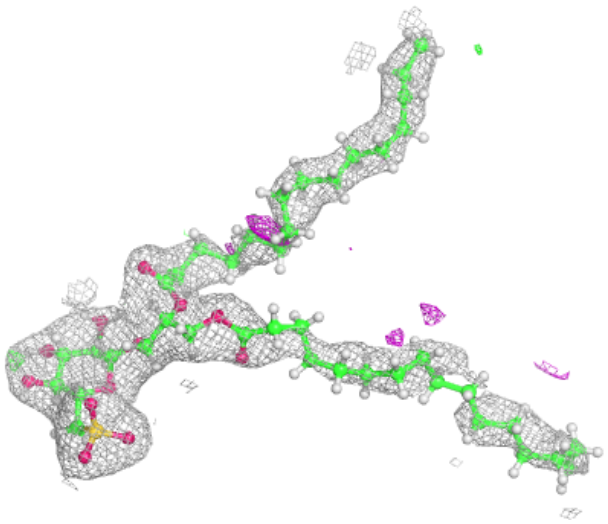
Electron density around SQD D 408:

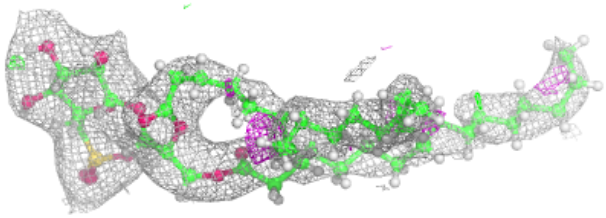
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD a 411:

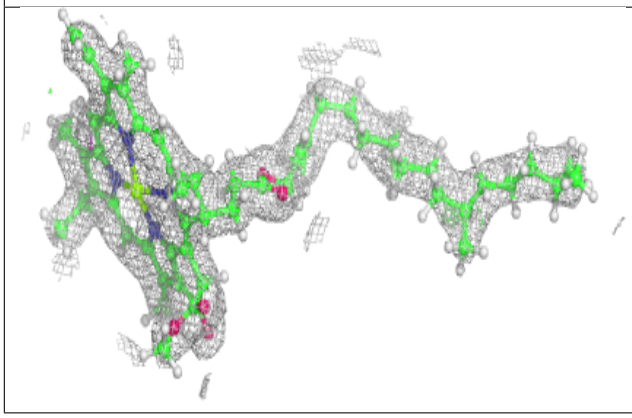
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

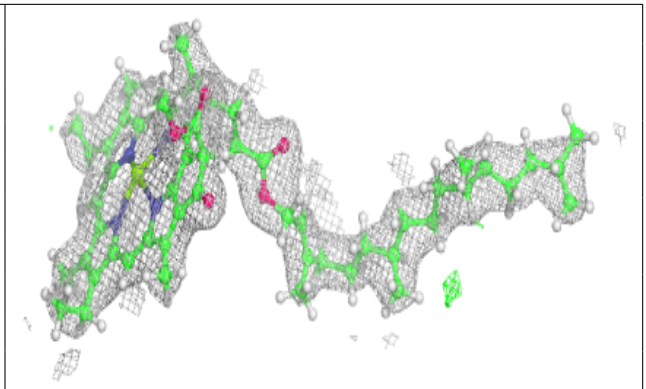


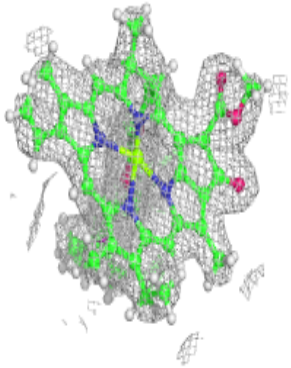


Electron density around CLA C 502:

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

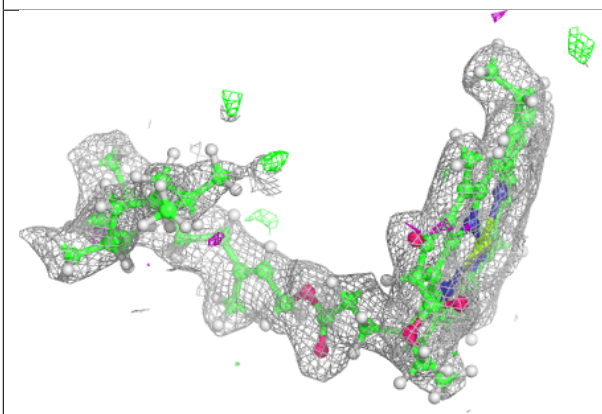


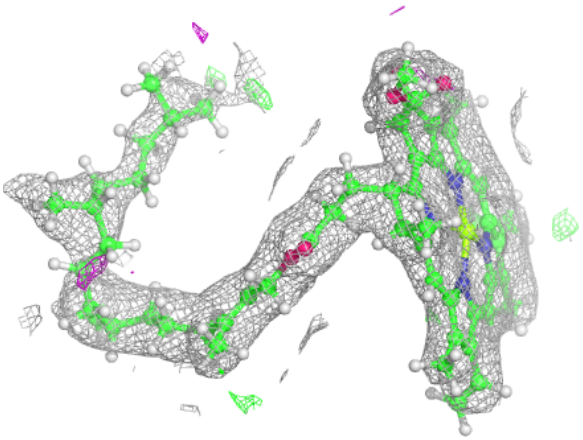


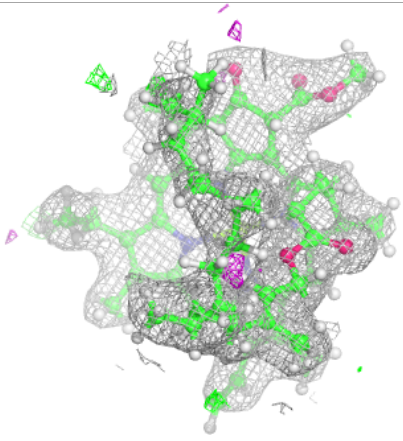


Electron density around CLA B 606:

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

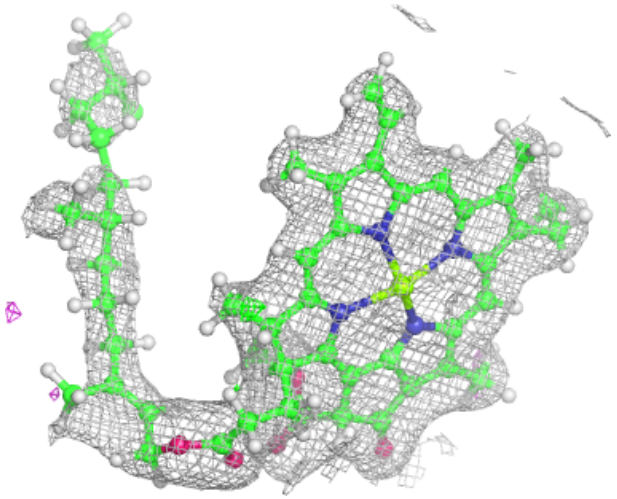


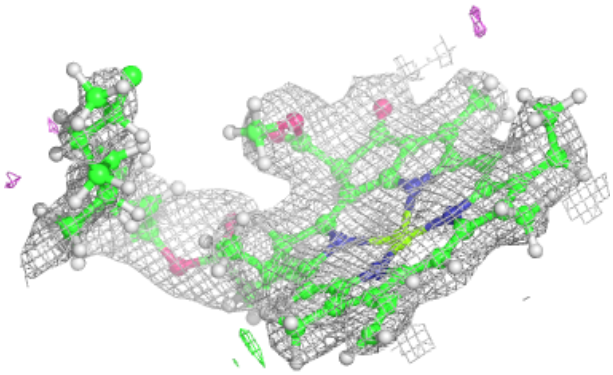


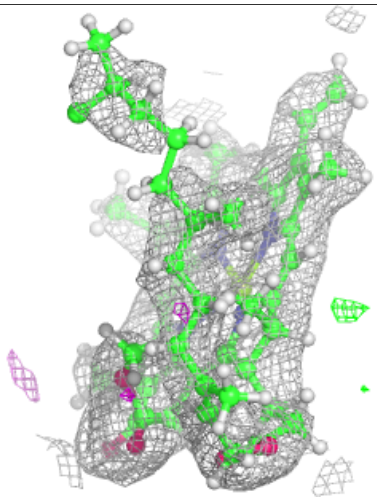


Electron density around CLA b 616:

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

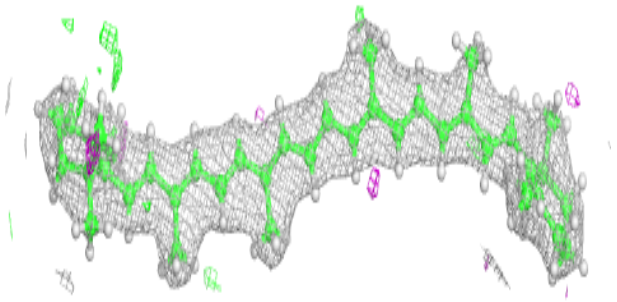


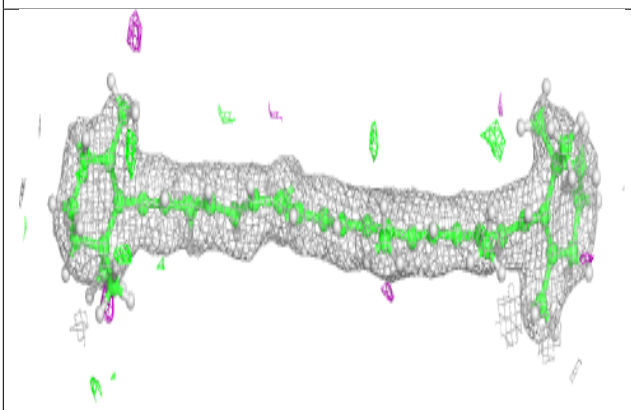


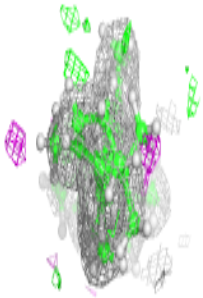


Electron density around BCR C 515:

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

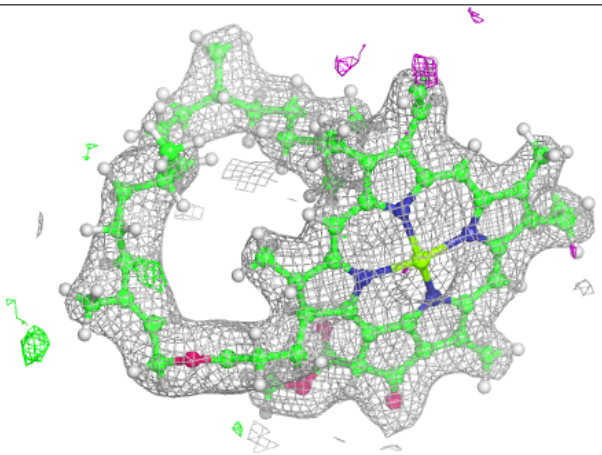


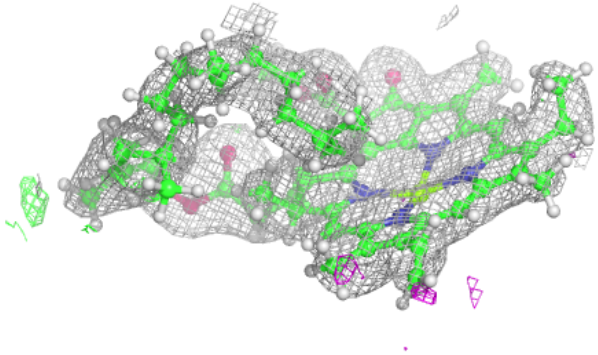


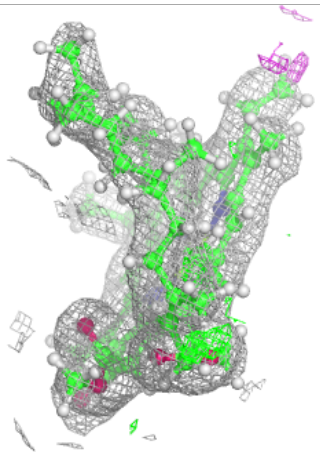


Electron density around CLA B 615:

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

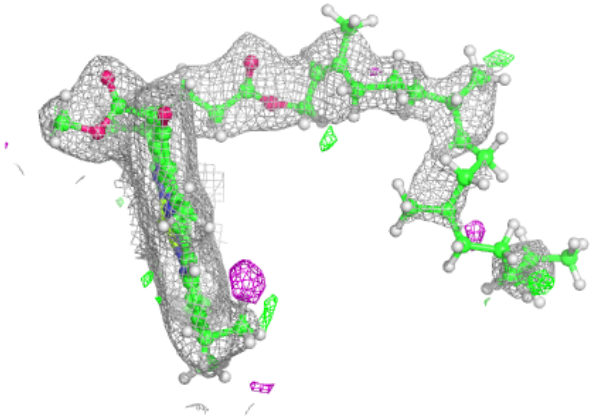


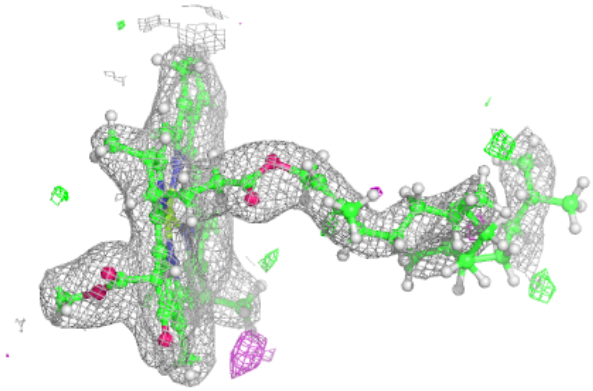


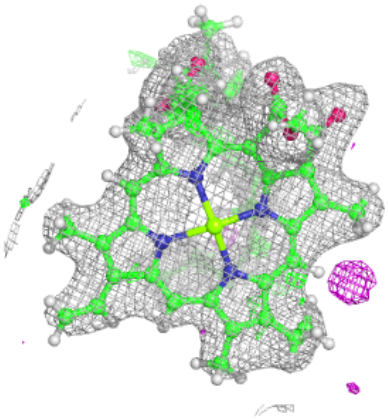


Electron density around CLA c 506:

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

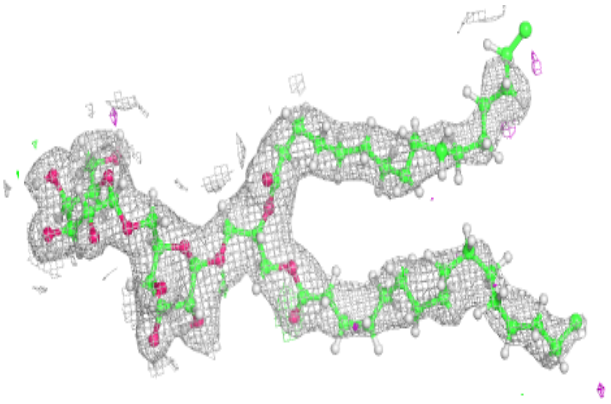


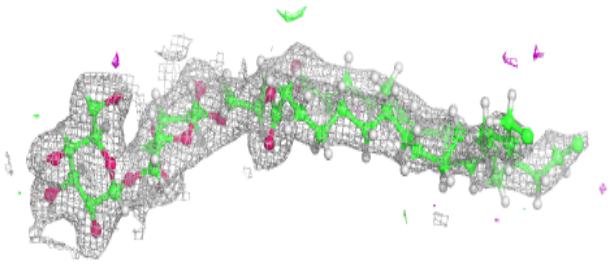


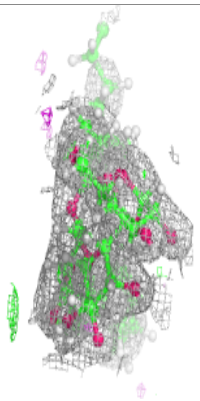


Electron density around DGD C 519:

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

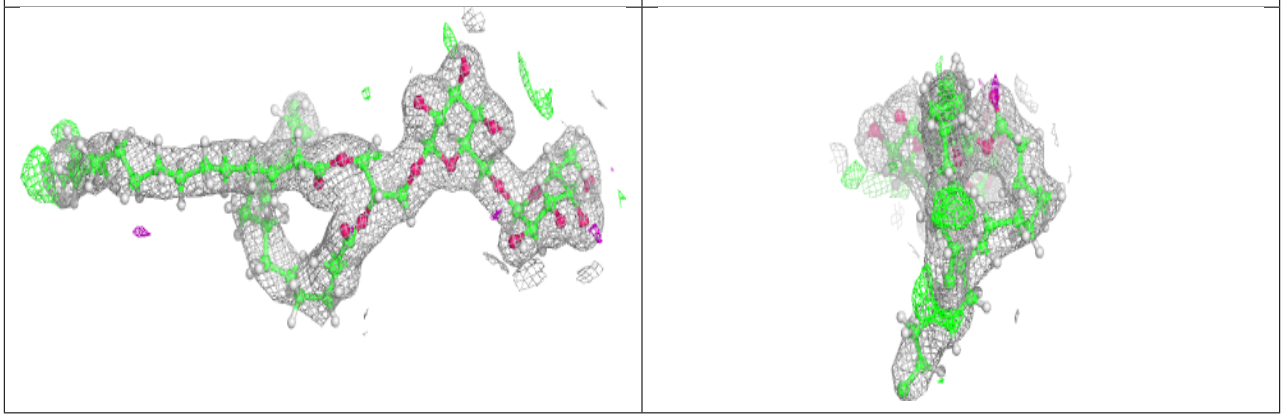






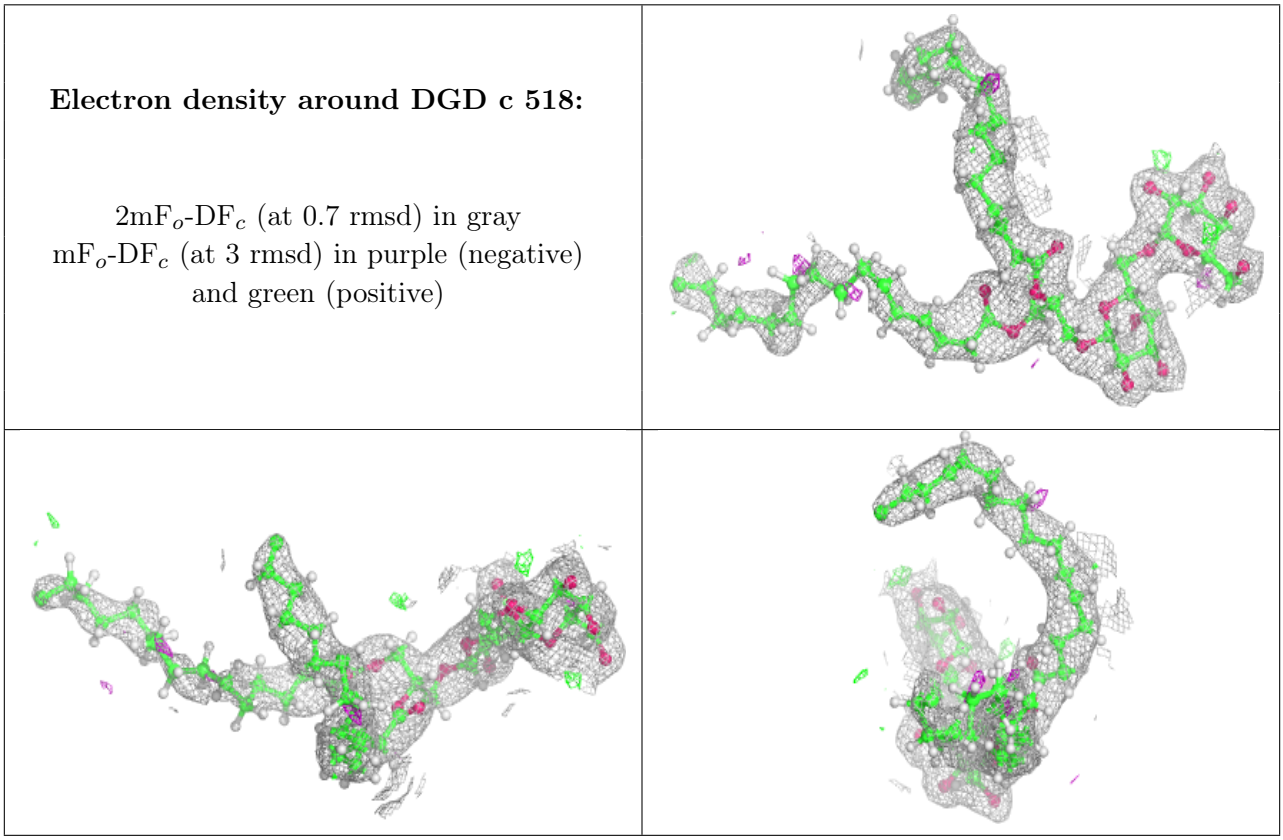
Electron density around DGD H 102:

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



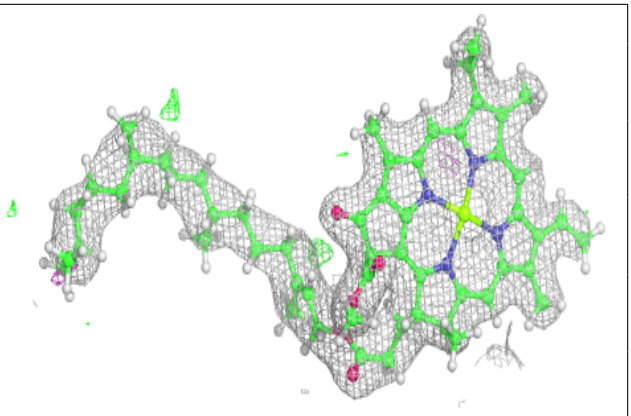
Electron density around DGD c 518:

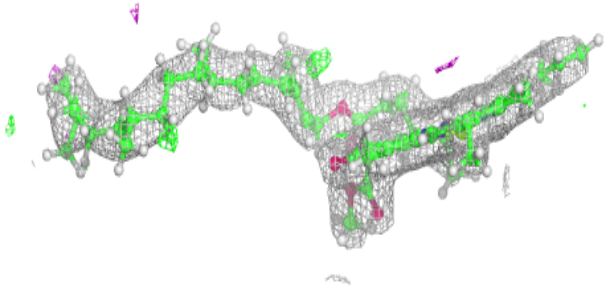
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

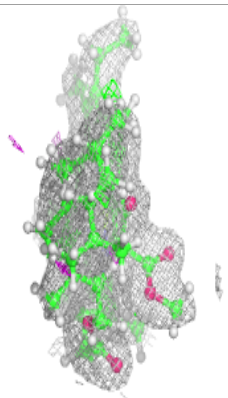


Electron density around CLA B 602:

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

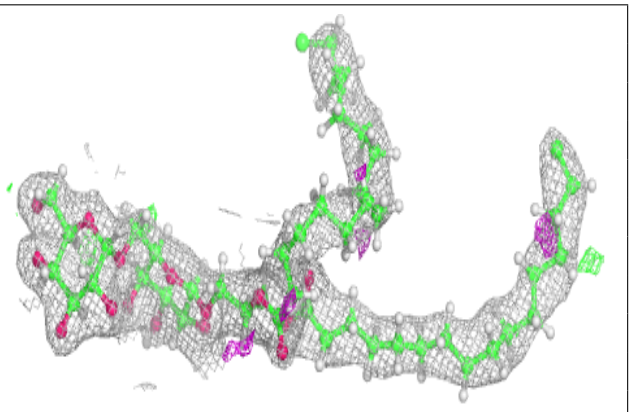


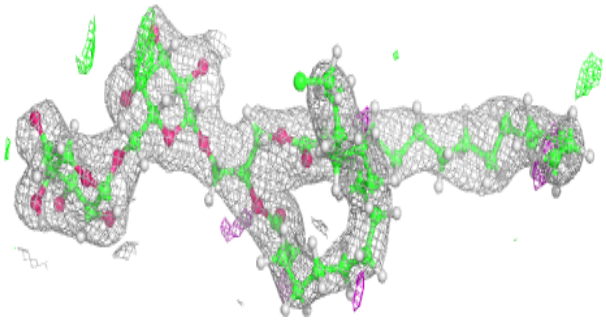


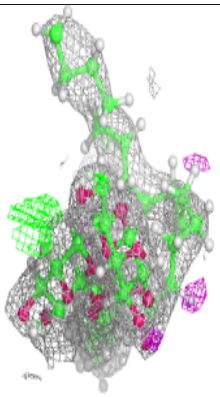


Electron density around DGD h 101:

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

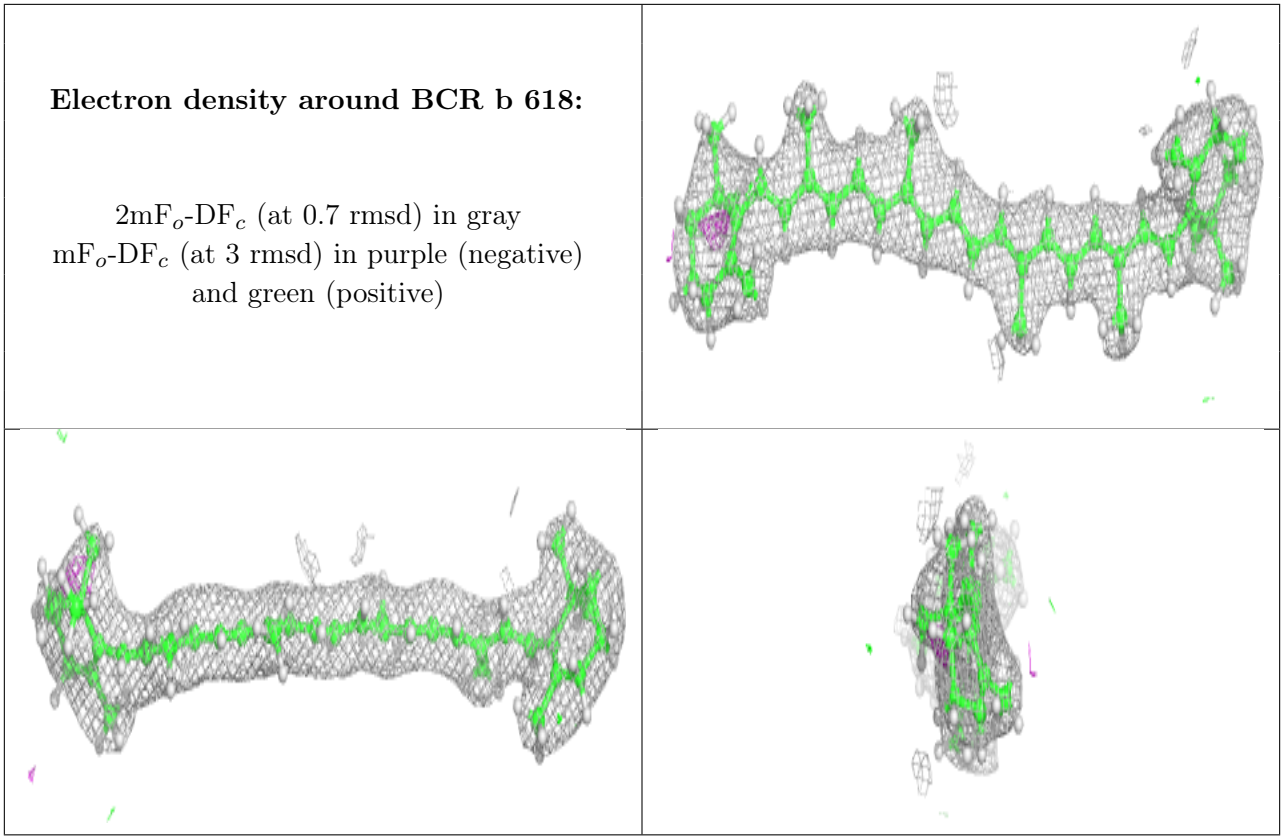






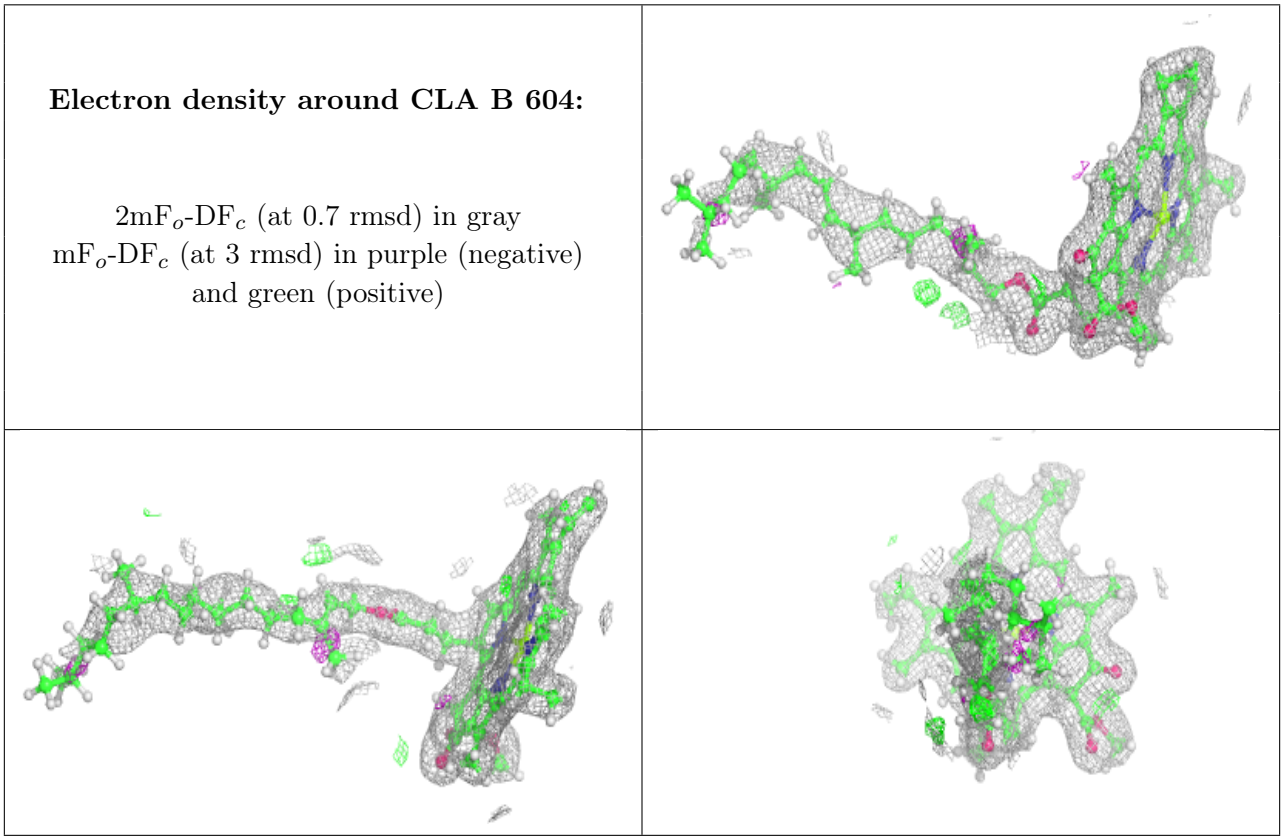
Electron density around BCR b 618:

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



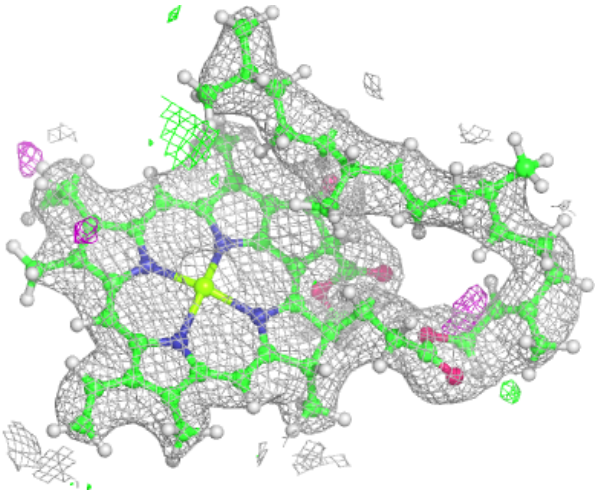
Electron density around CLA B 604:

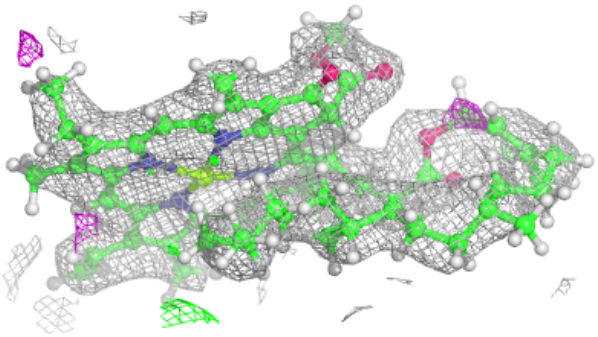
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

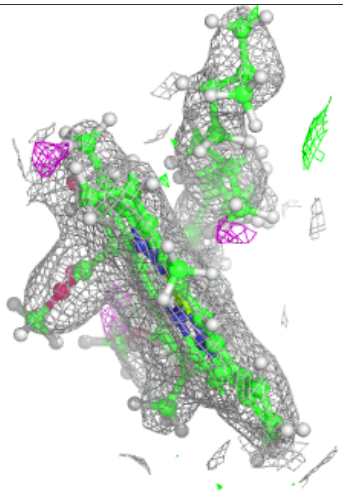


Electron density around CLA c 509:

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

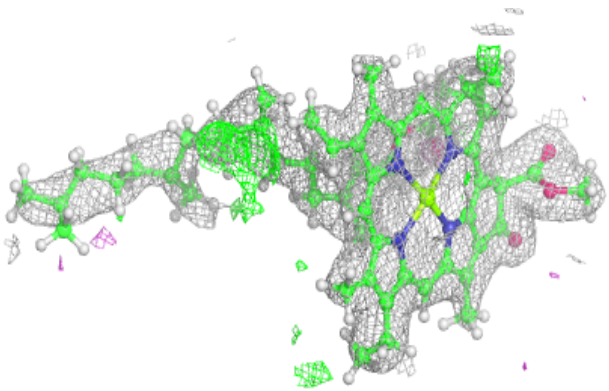


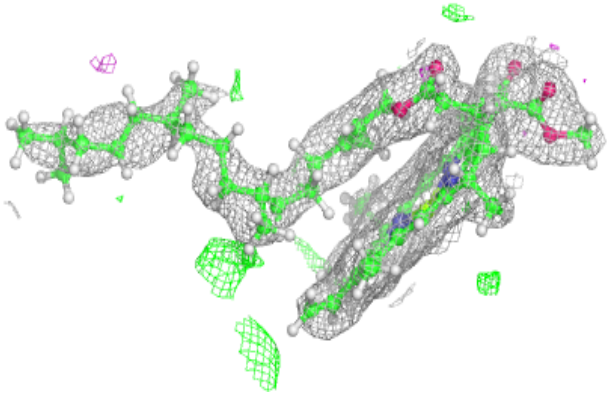


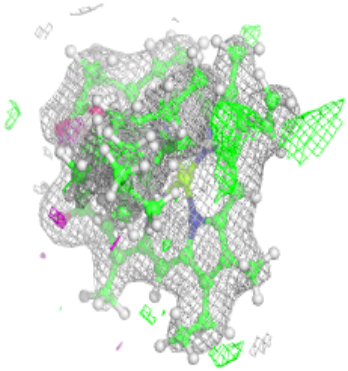


Electron density around CLA C 505:

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

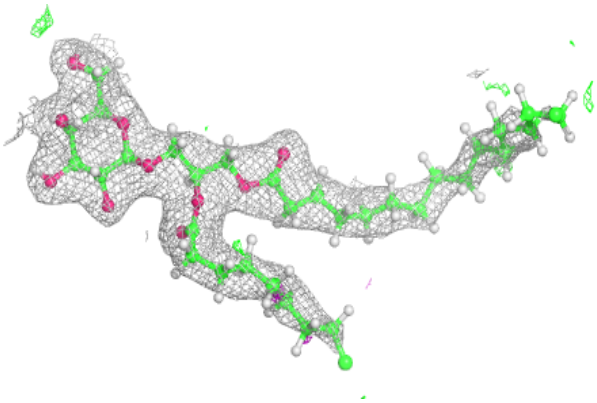


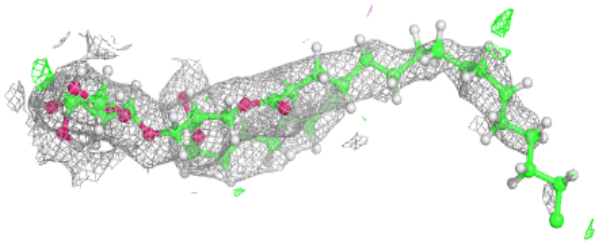


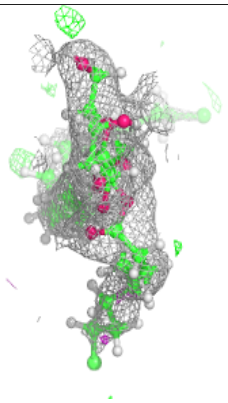


Electron density around LMG d 410:

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

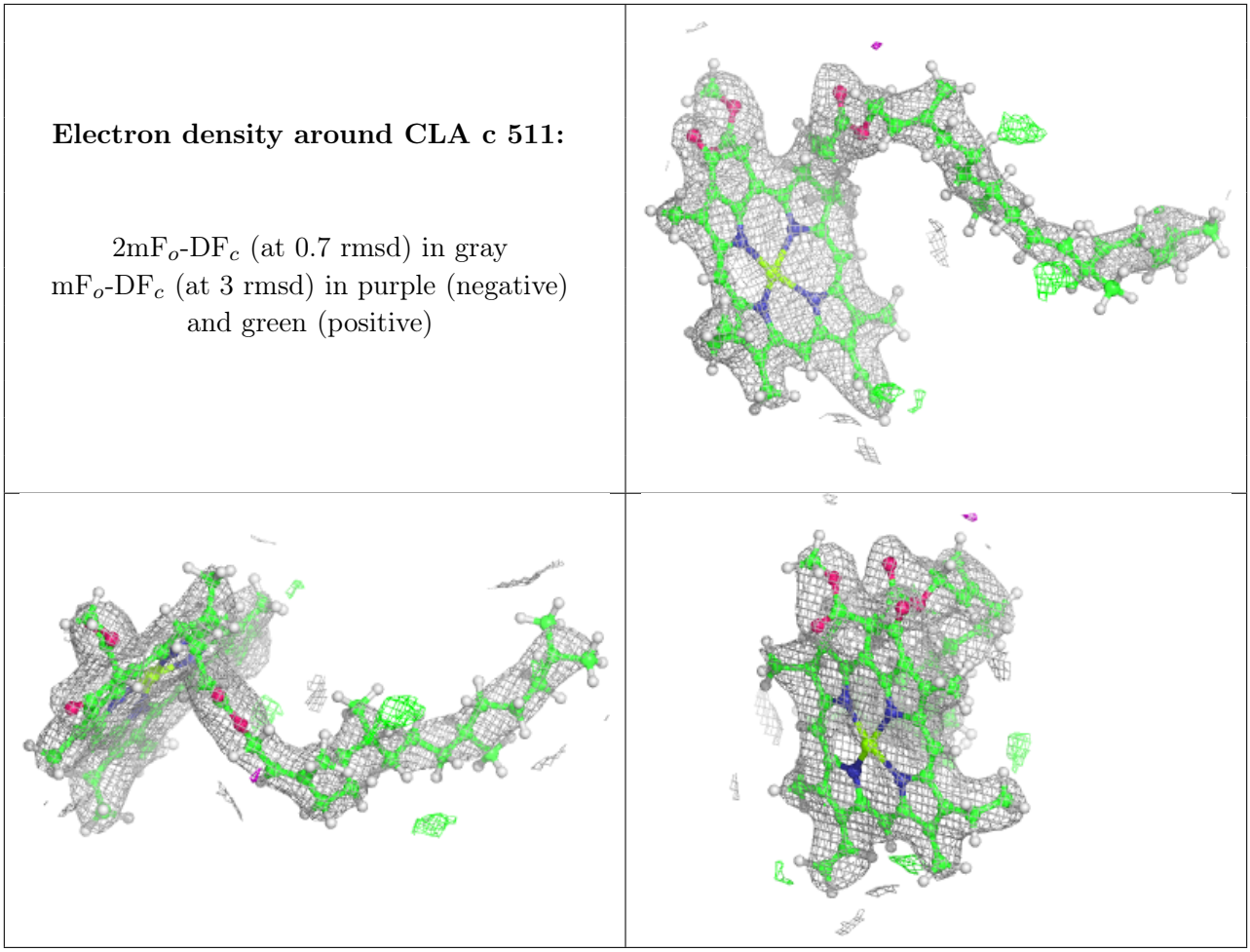






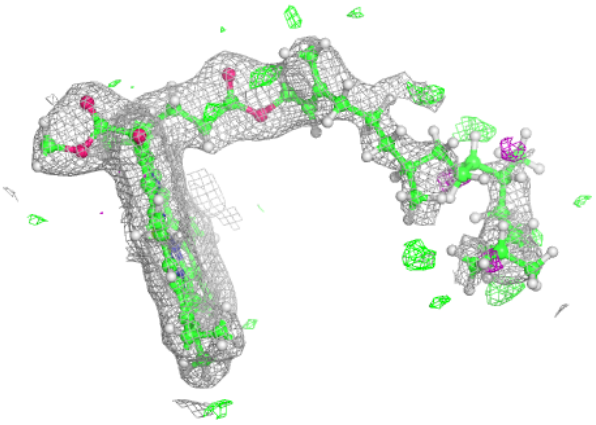
Electron density around CLA c 511:

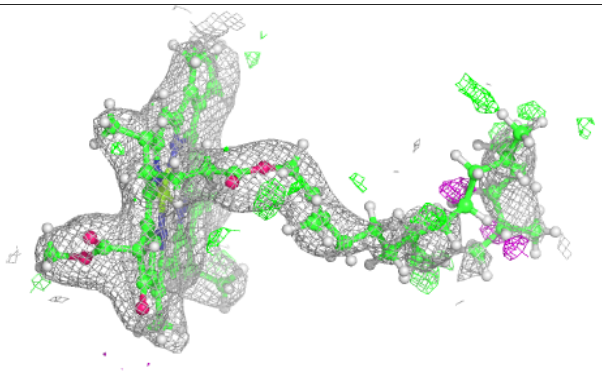
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

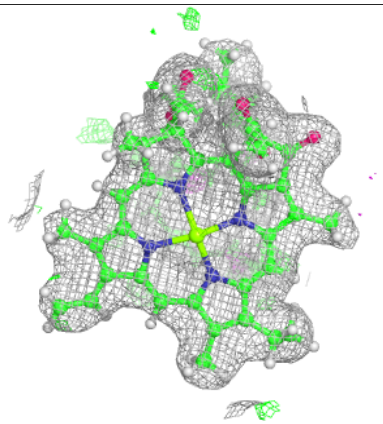


Electron density around CLA C 506:

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

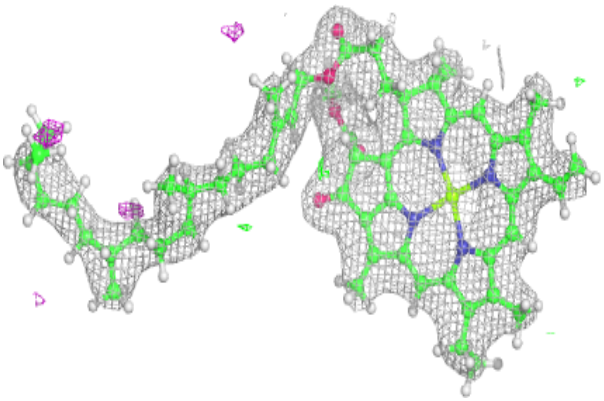


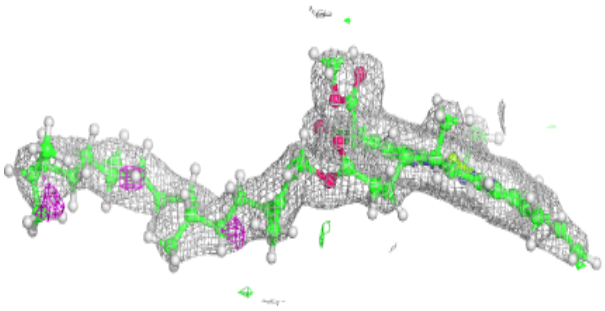


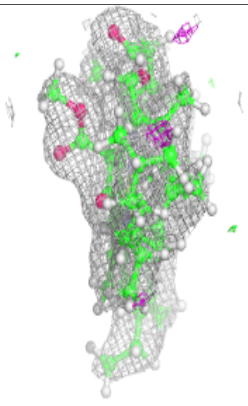


Electron density around CLA b 602:

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

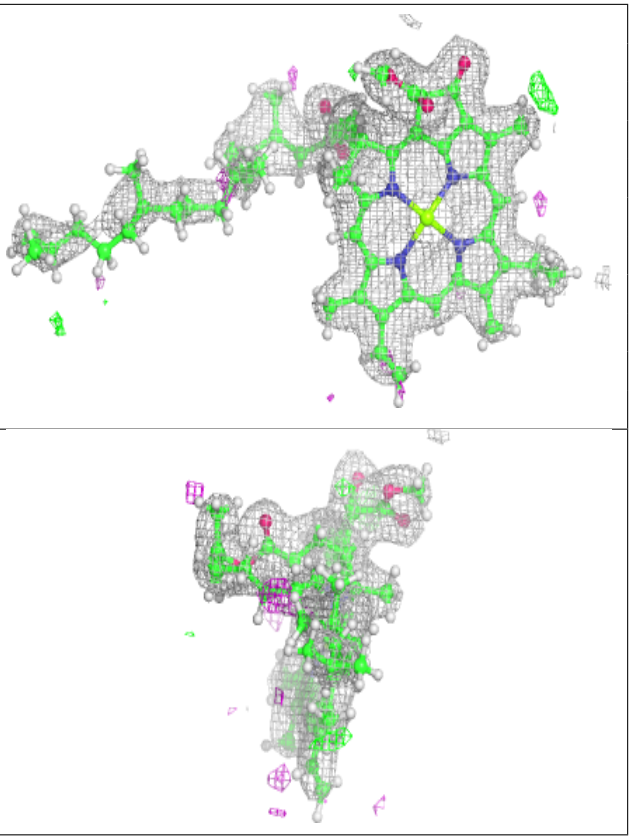






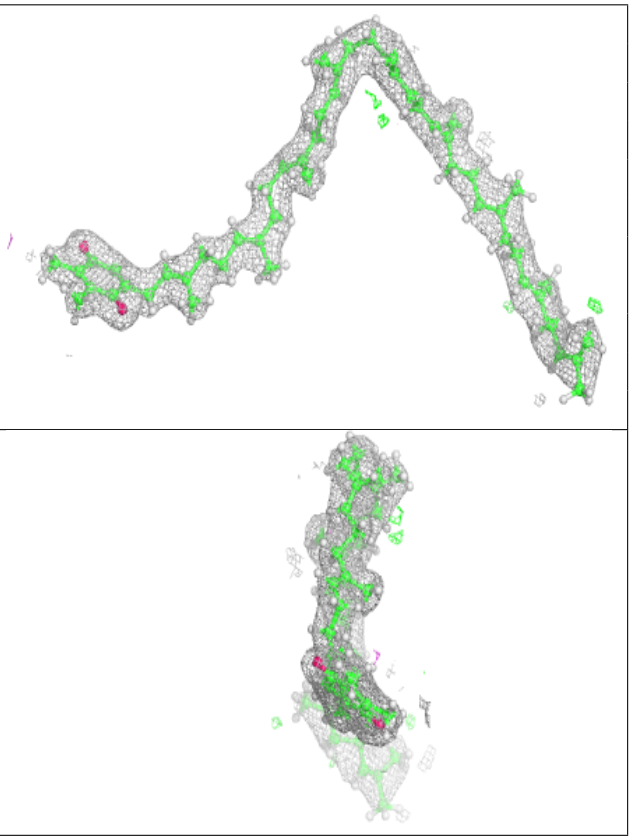
Electron density around CLA d 401:

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



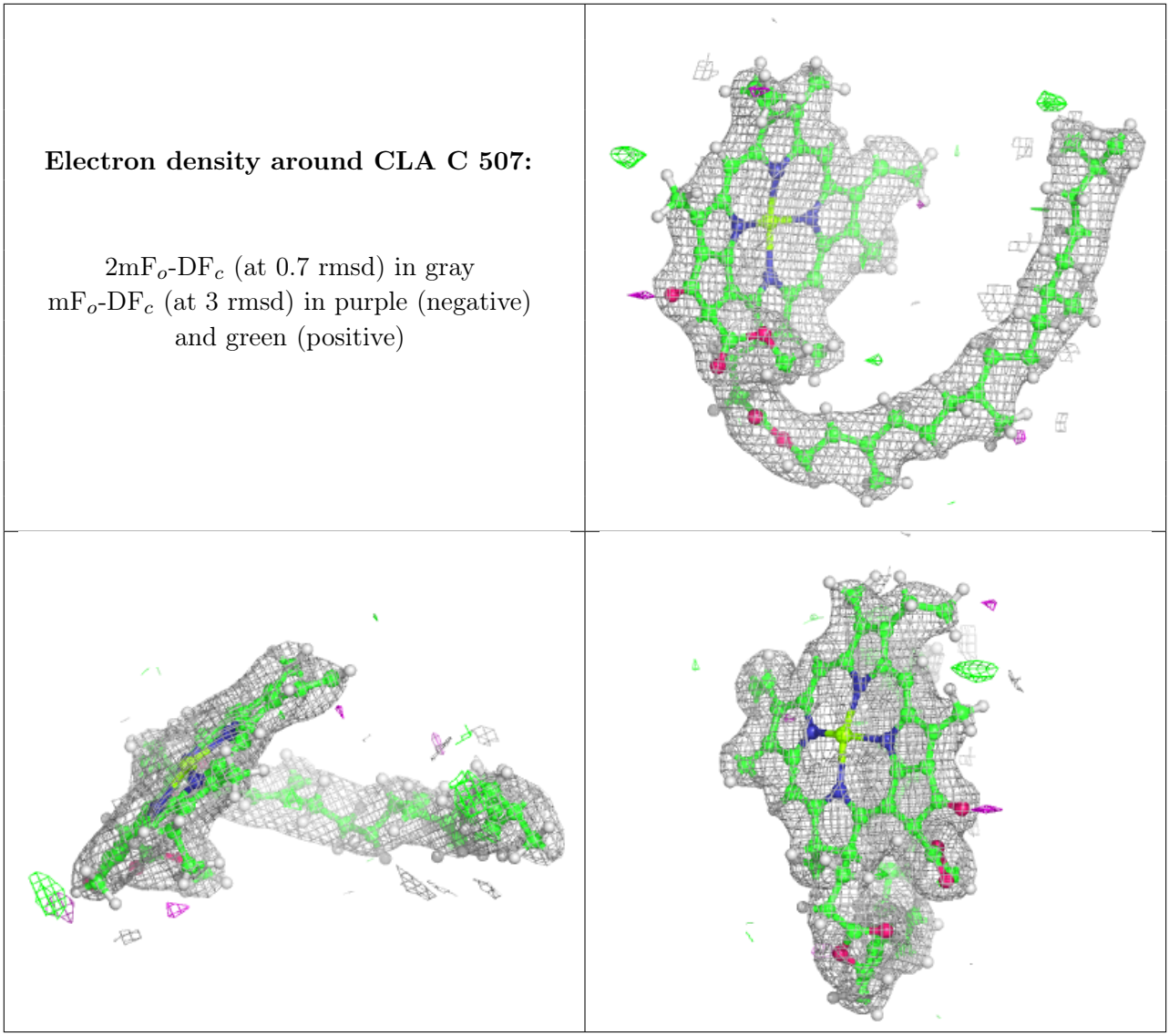
Electron density around PL9 D 406:

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



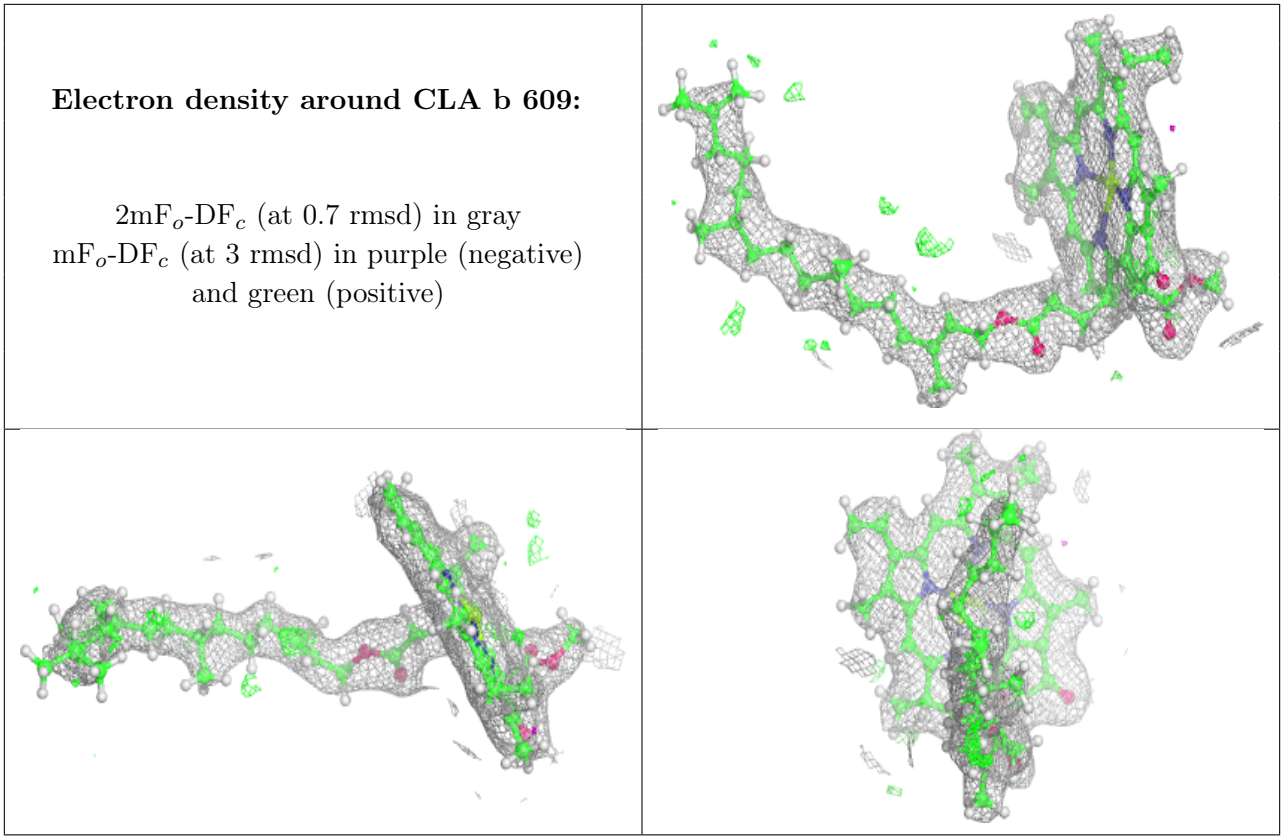
Electron density around CLA C 507:

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



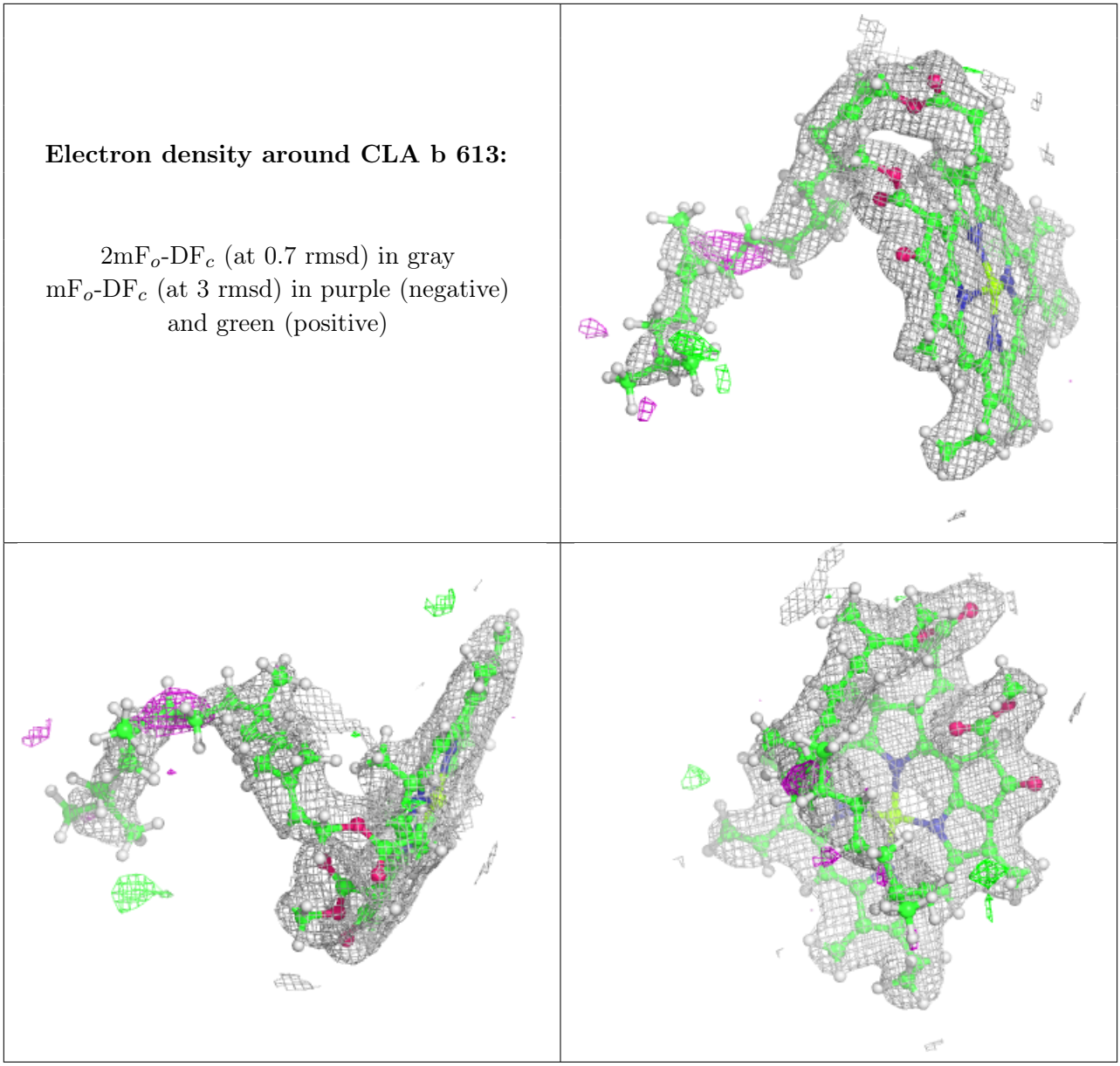
Electron density around CLA b 609:

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



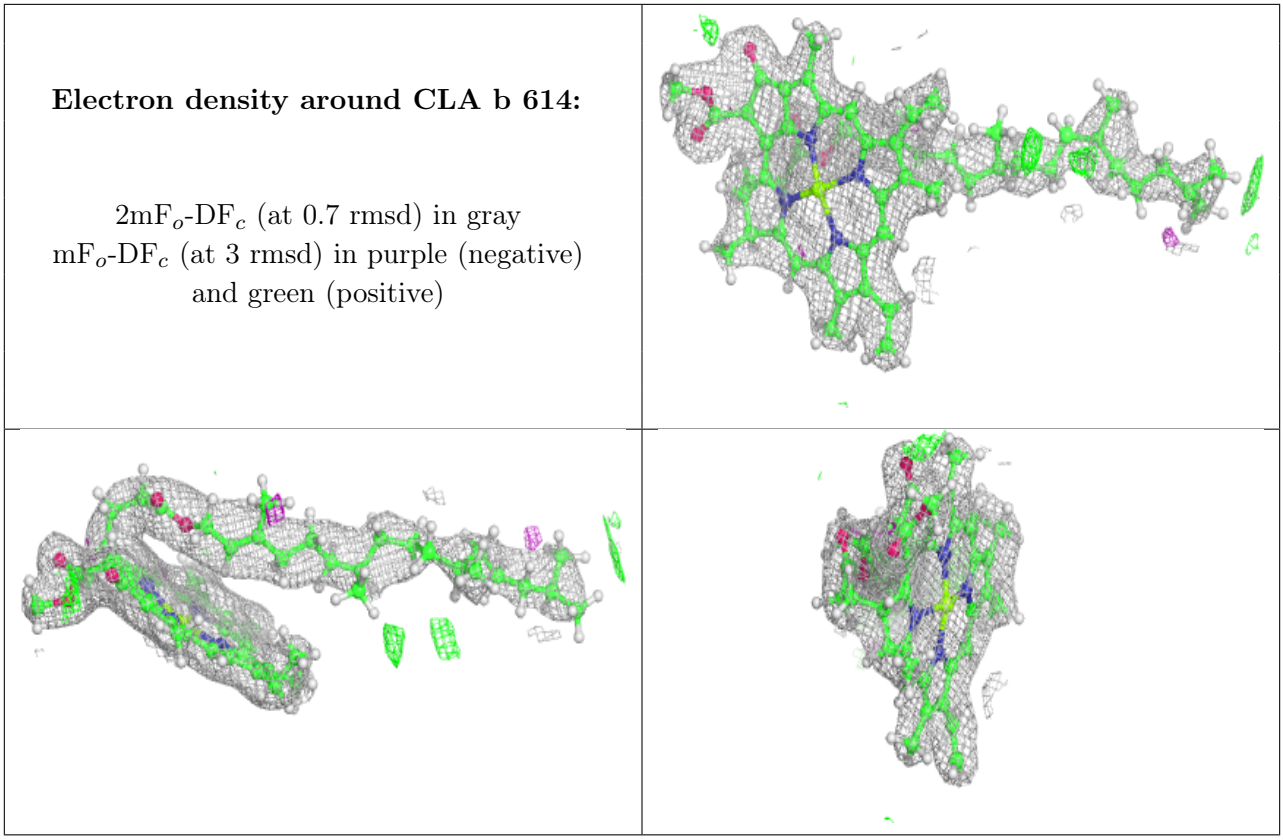
Electron density around CLA b 613:

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



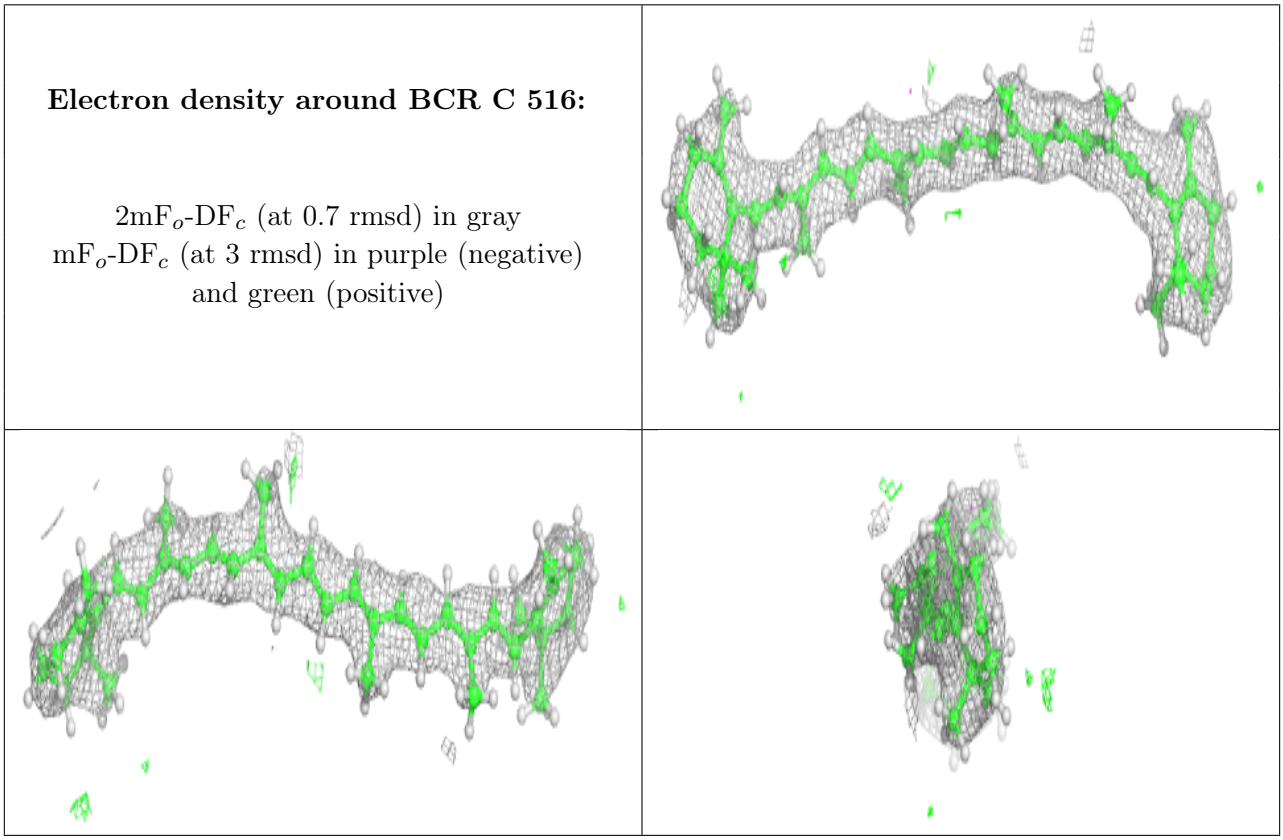
Electron density around CLA b 614:

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



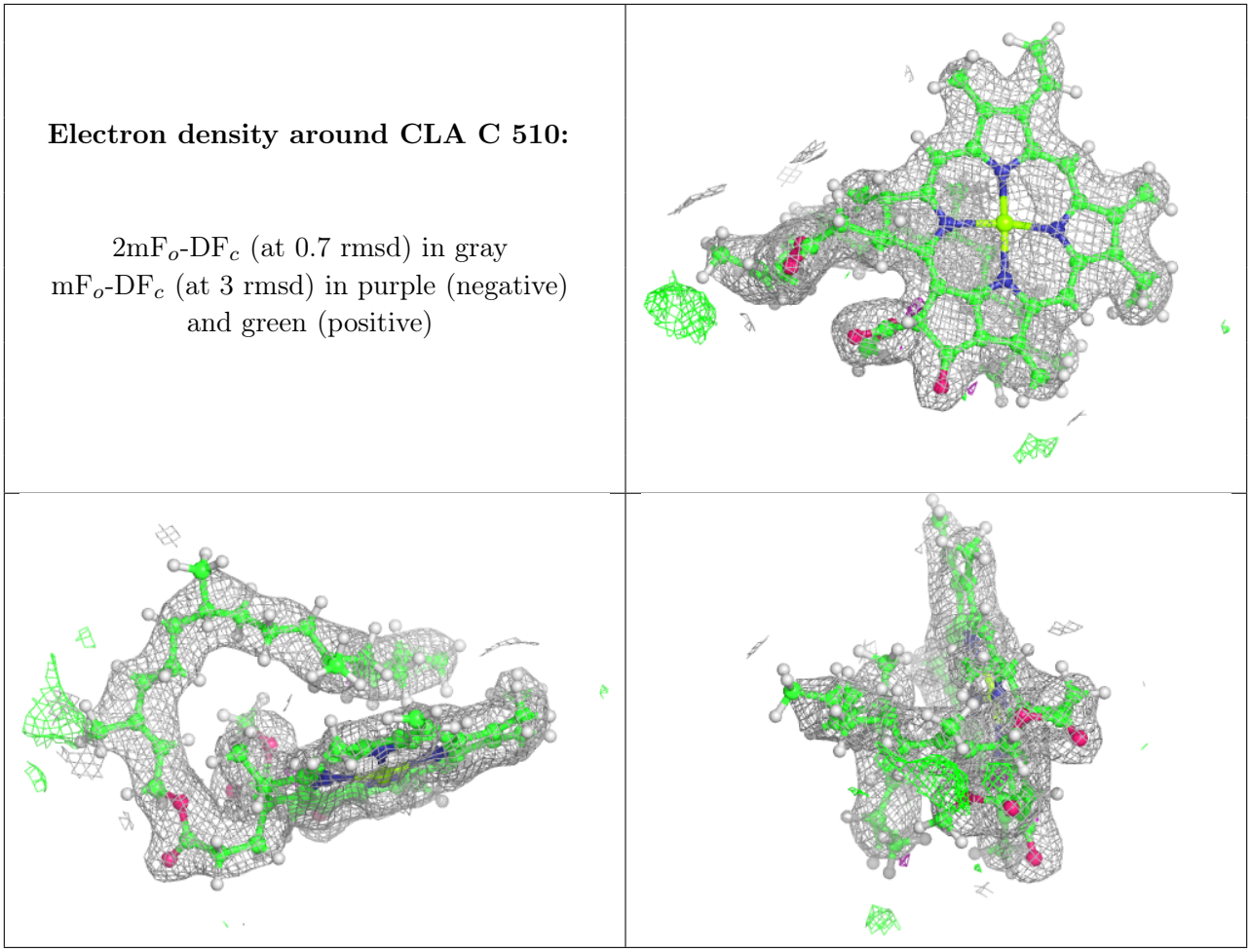
Electron density around BCR C 516:

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



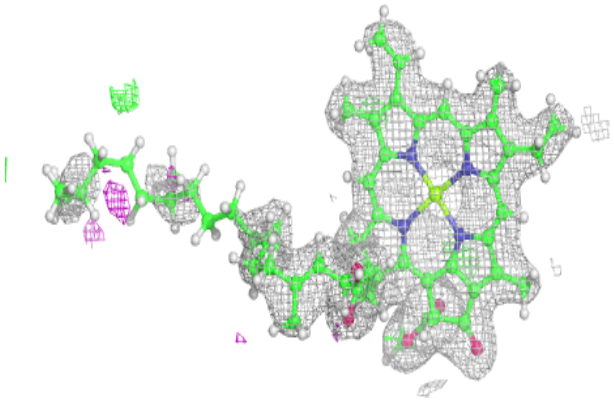
Electron density around CLA C 510:

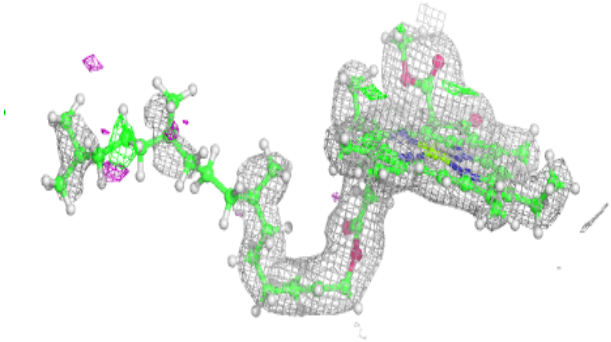
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

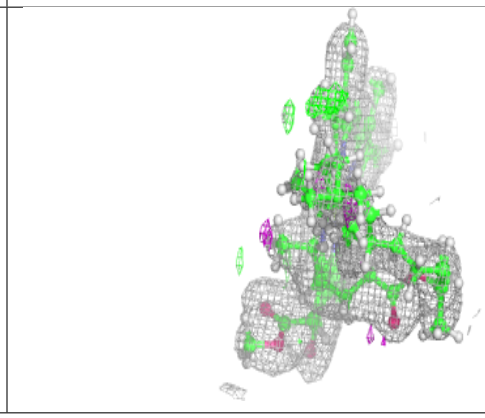


Electron density around CLA A 403:

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

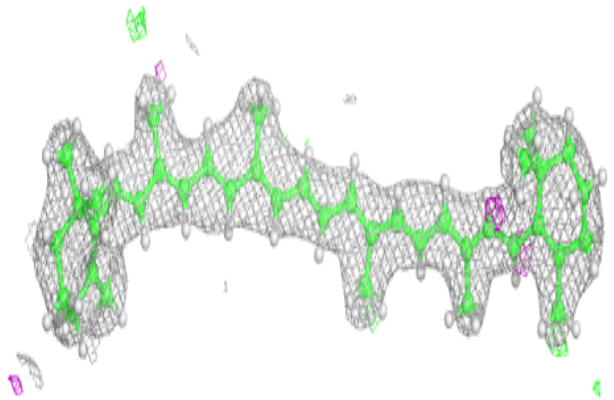


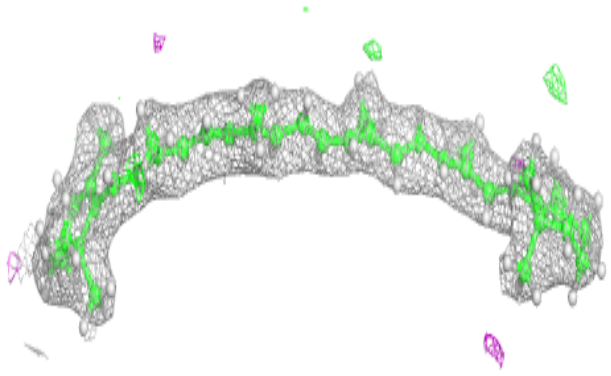


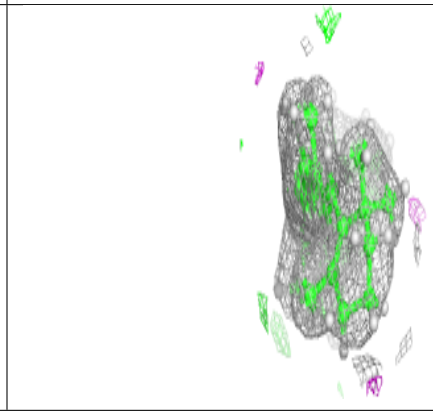


Electron density around BCR T 101:

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

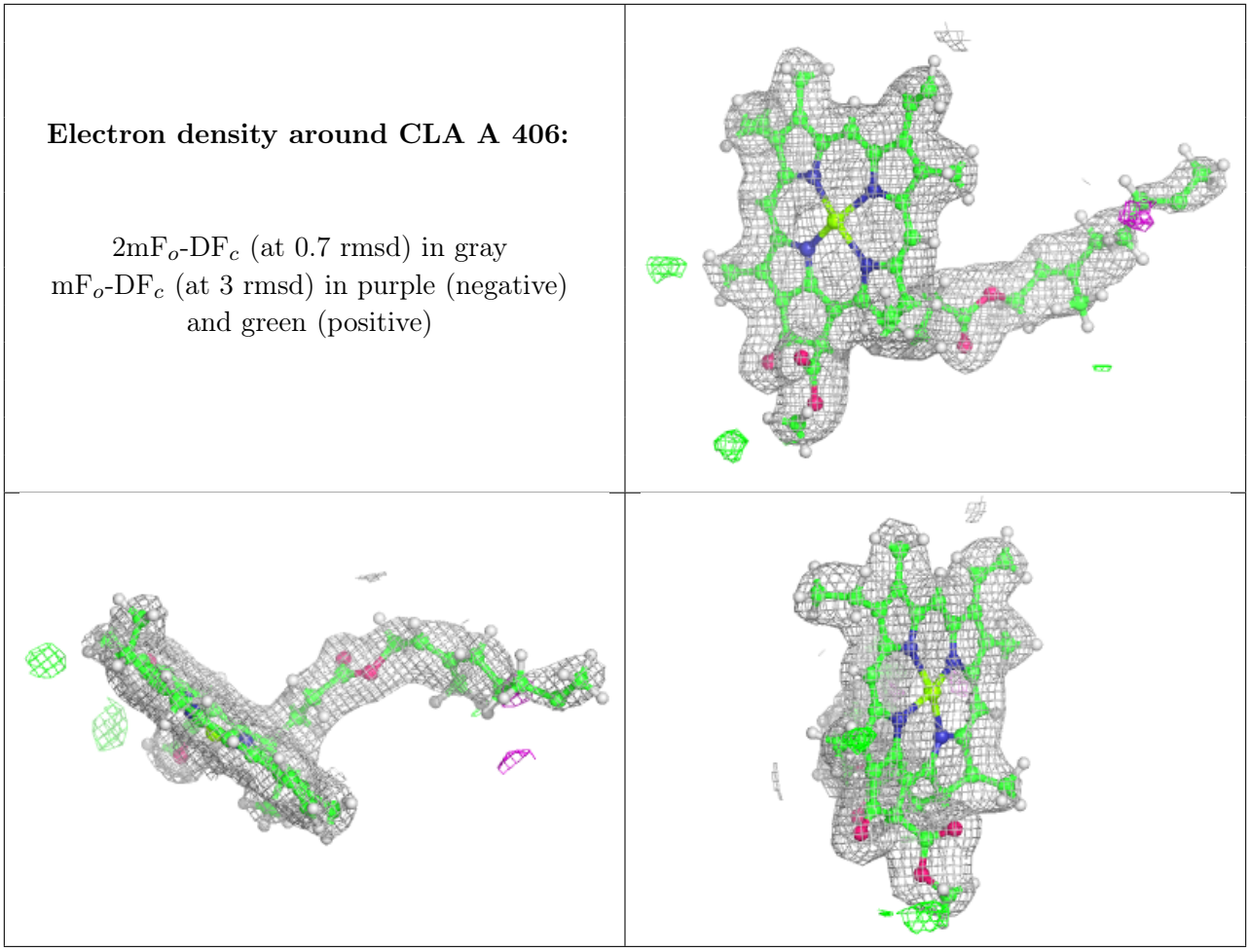






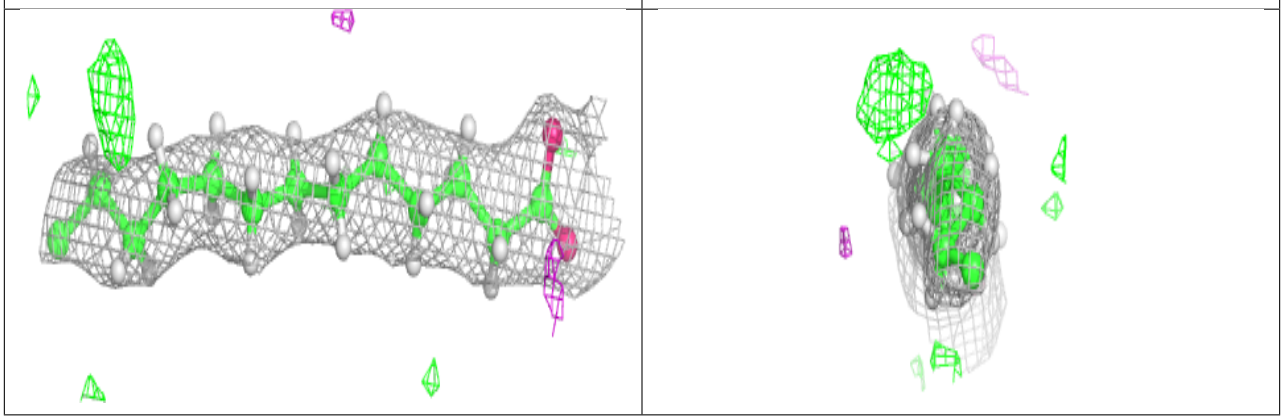
Electron density around CLA A 406:

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



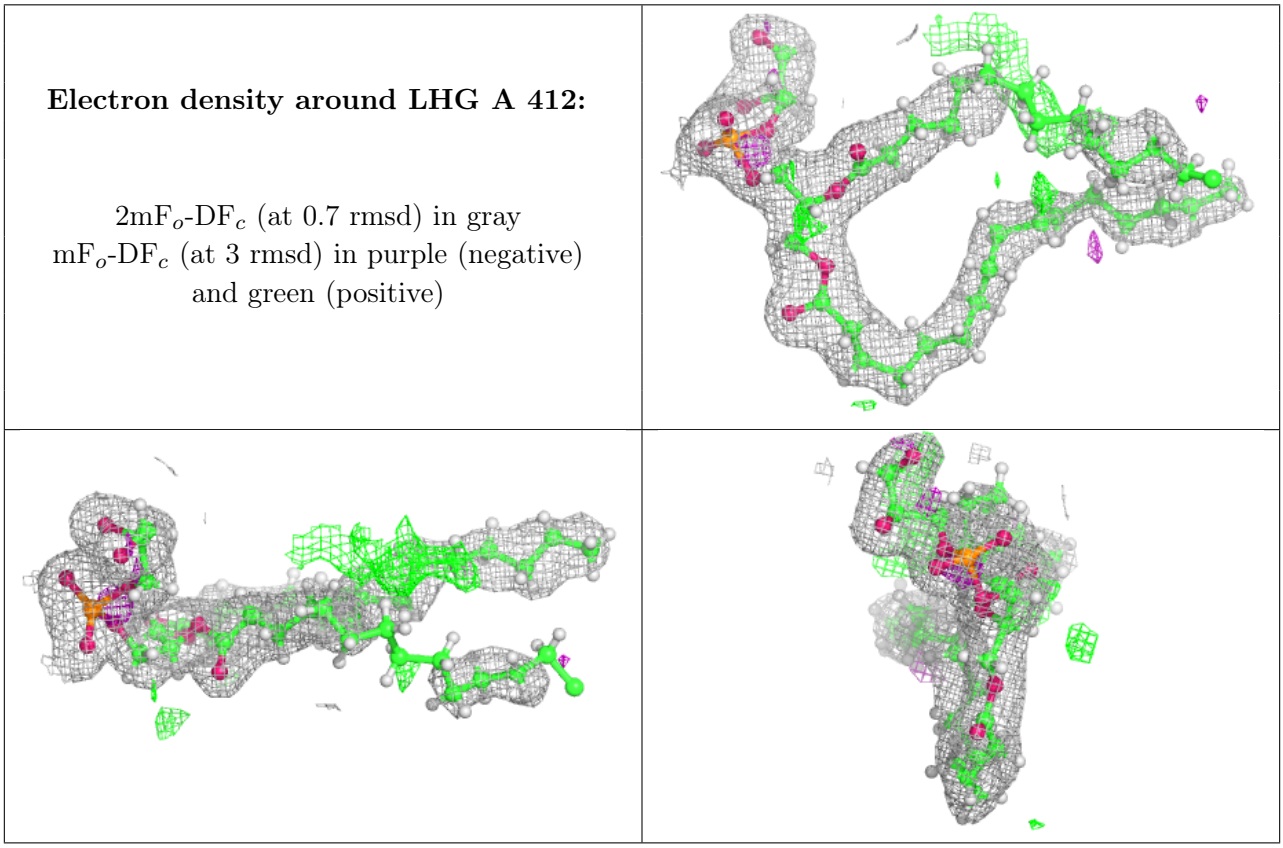
Electron density around STE M 102:

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



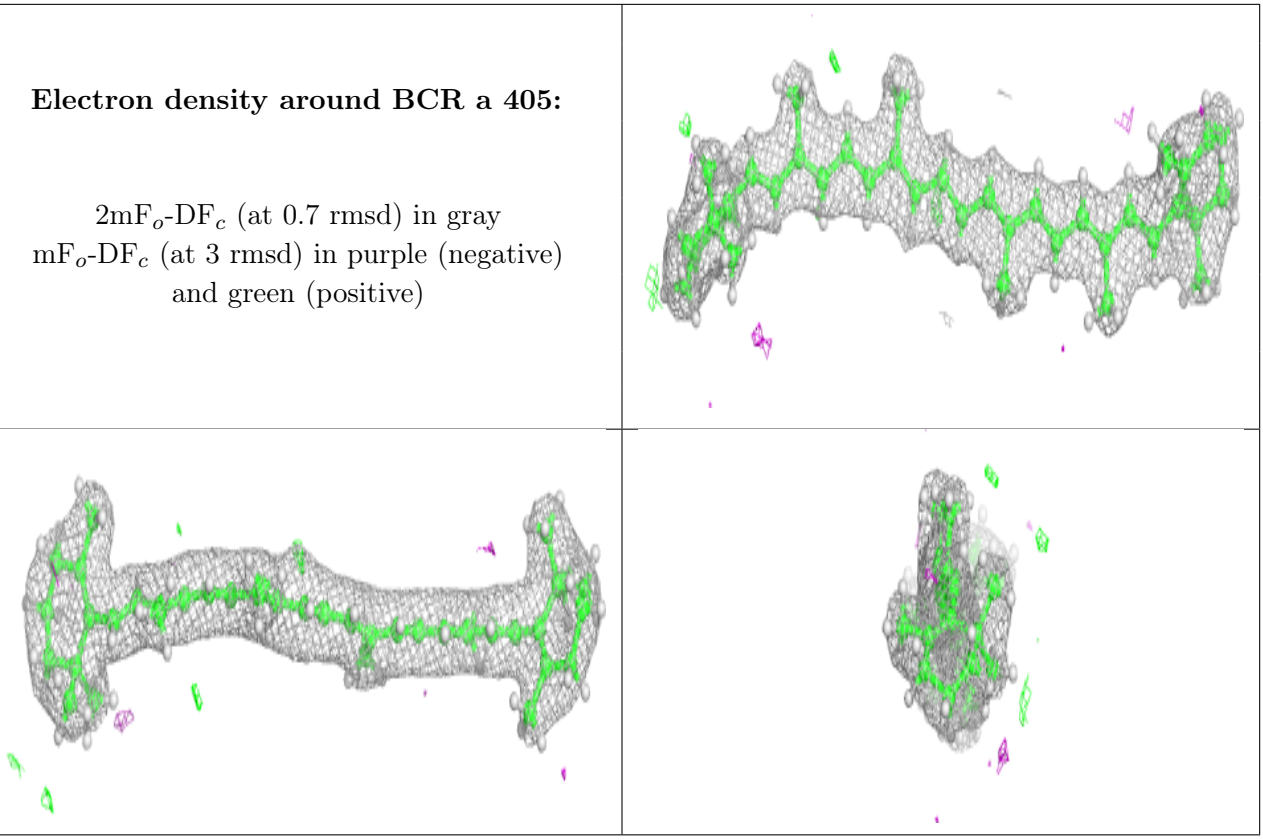
Electron density around LHG A 412:

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



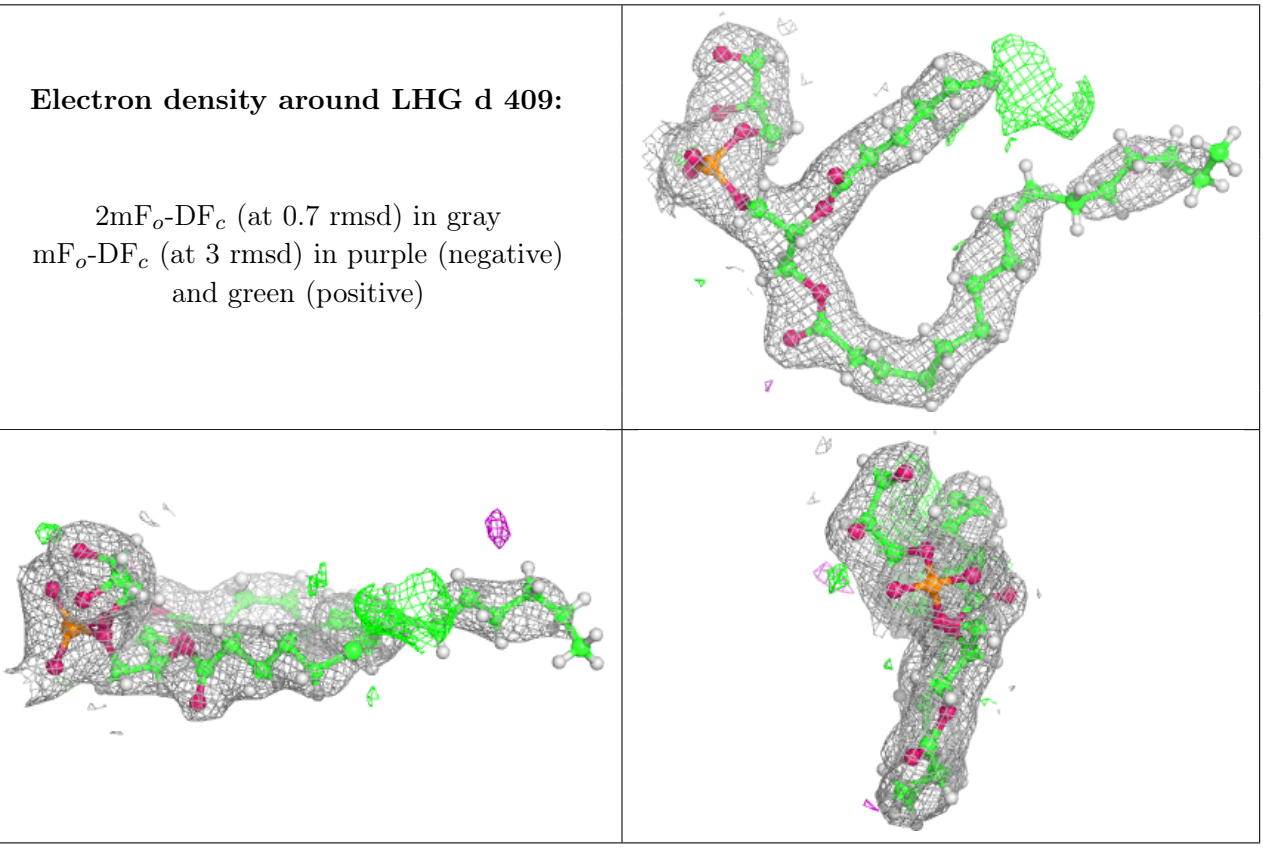
Electron density around BCR a 405:

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



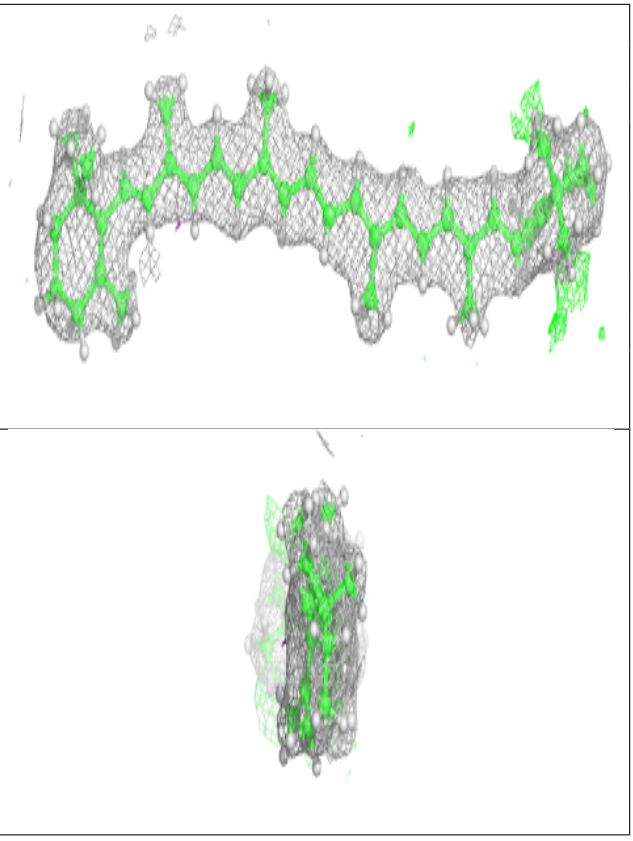
Electron density around LHG d 409:

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



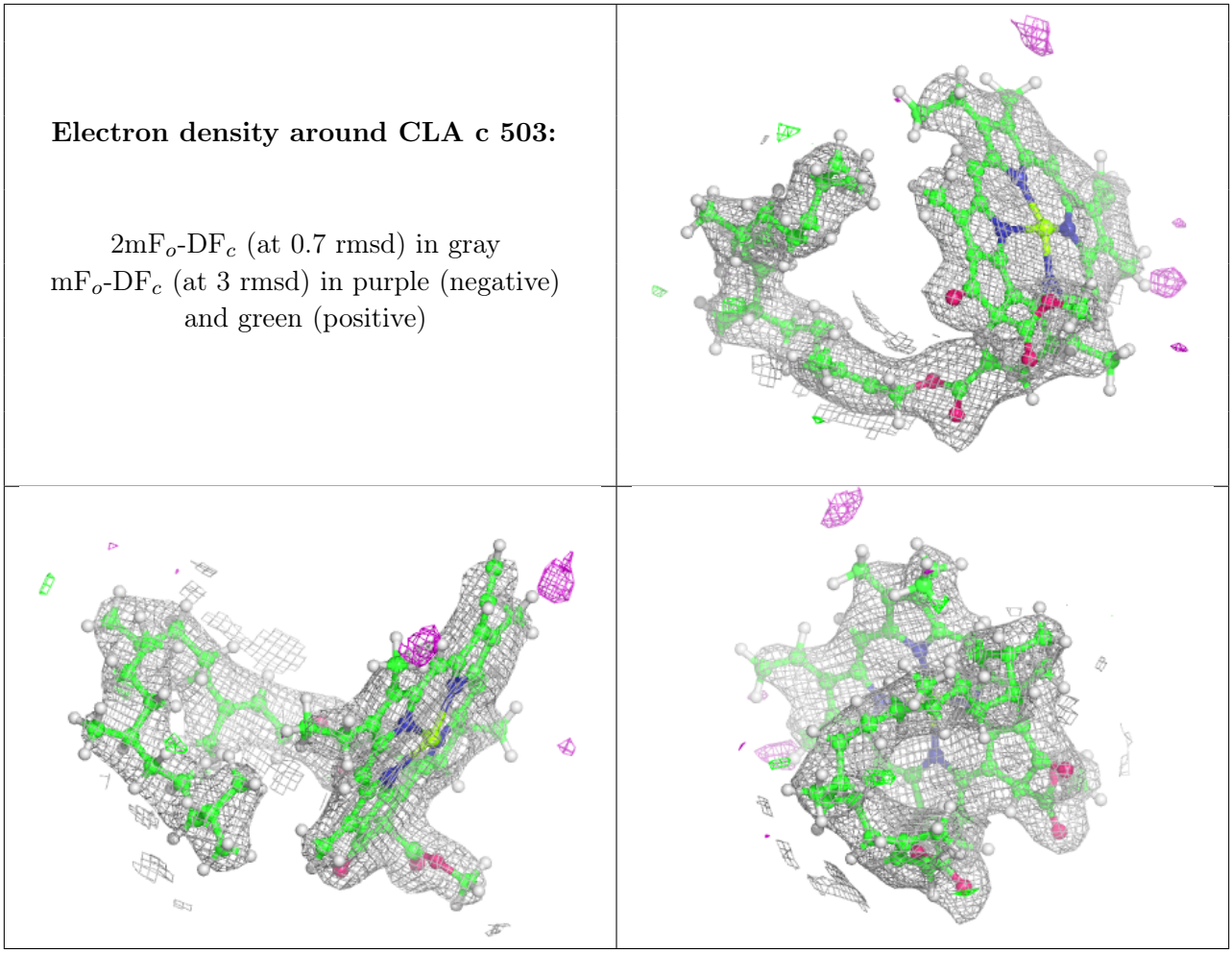
Electron density around BCR b 617:

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



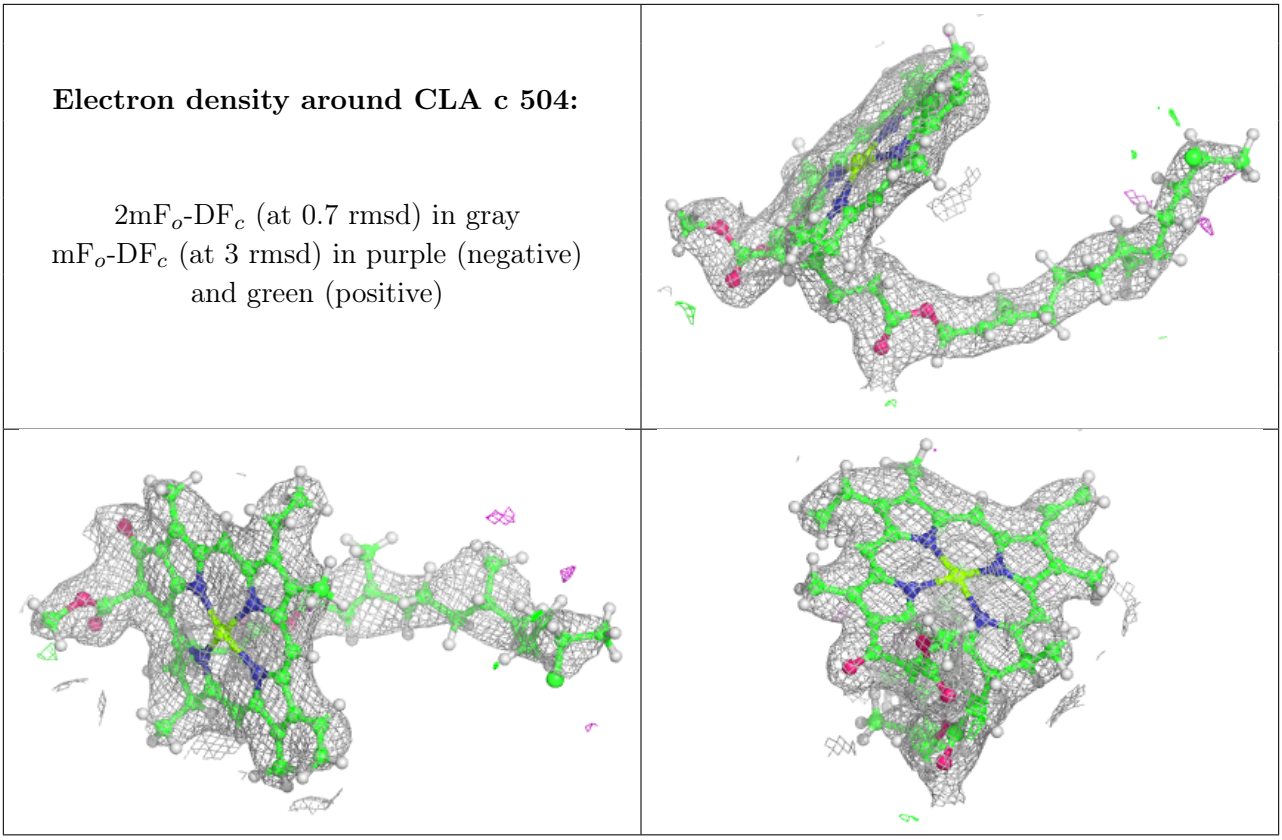
Electron density around CLA c 503:

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



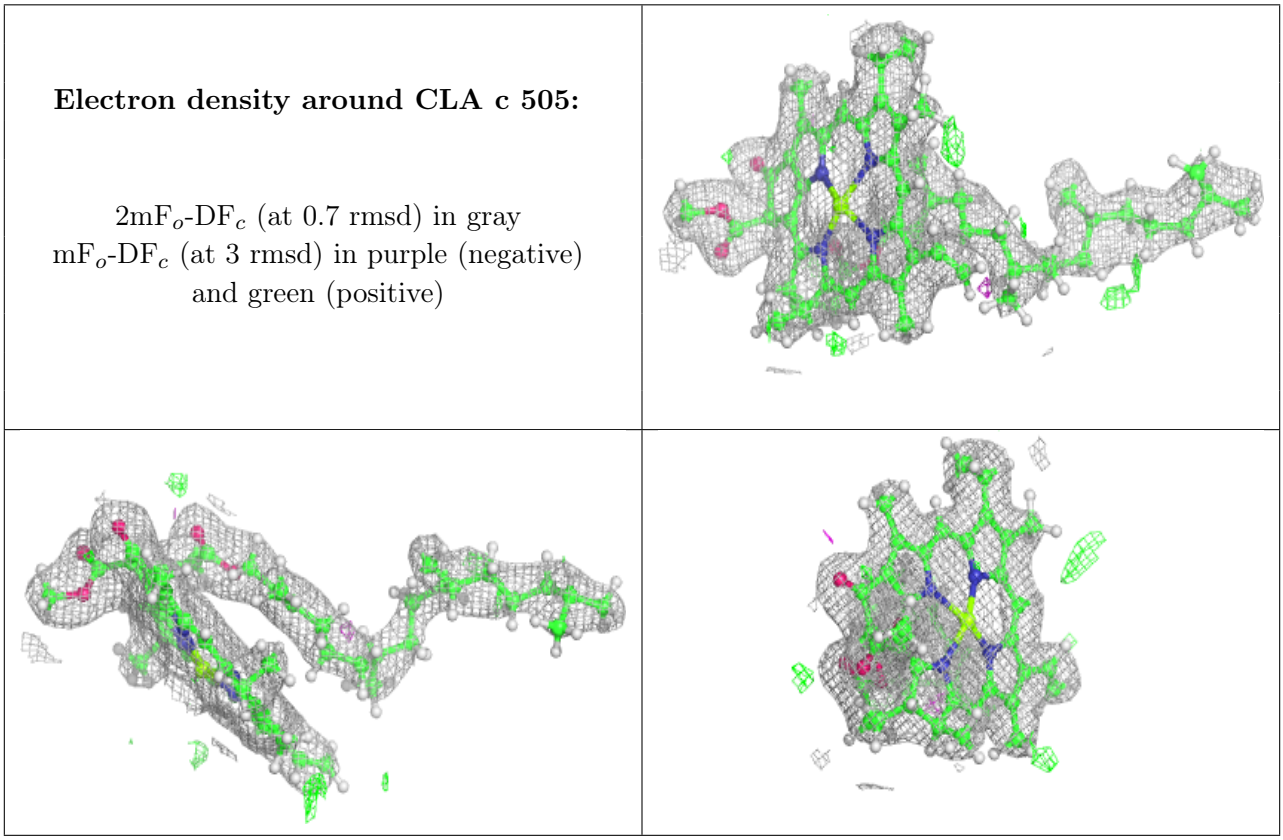
Electron density around CLA c 504:

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



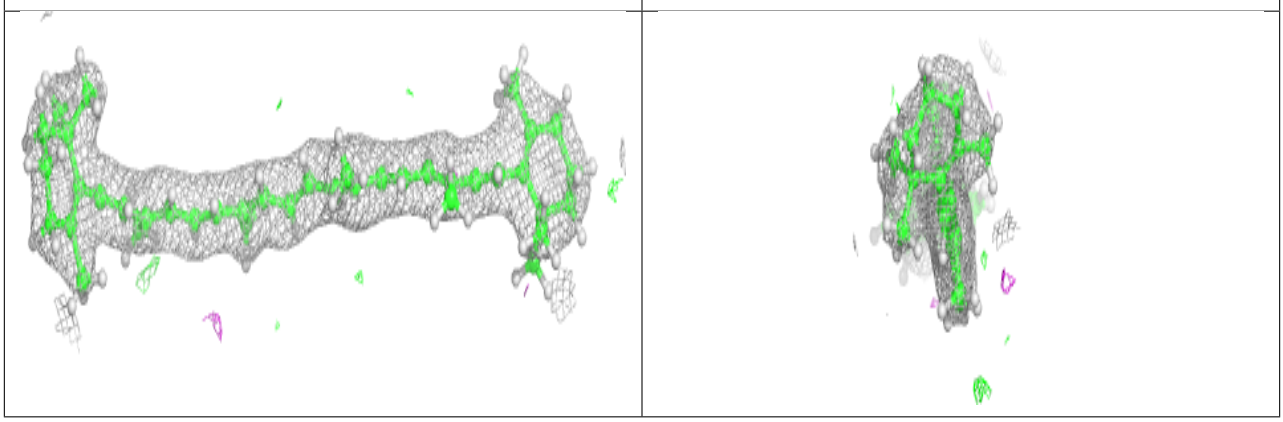
Electron density around CLA c 505:

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



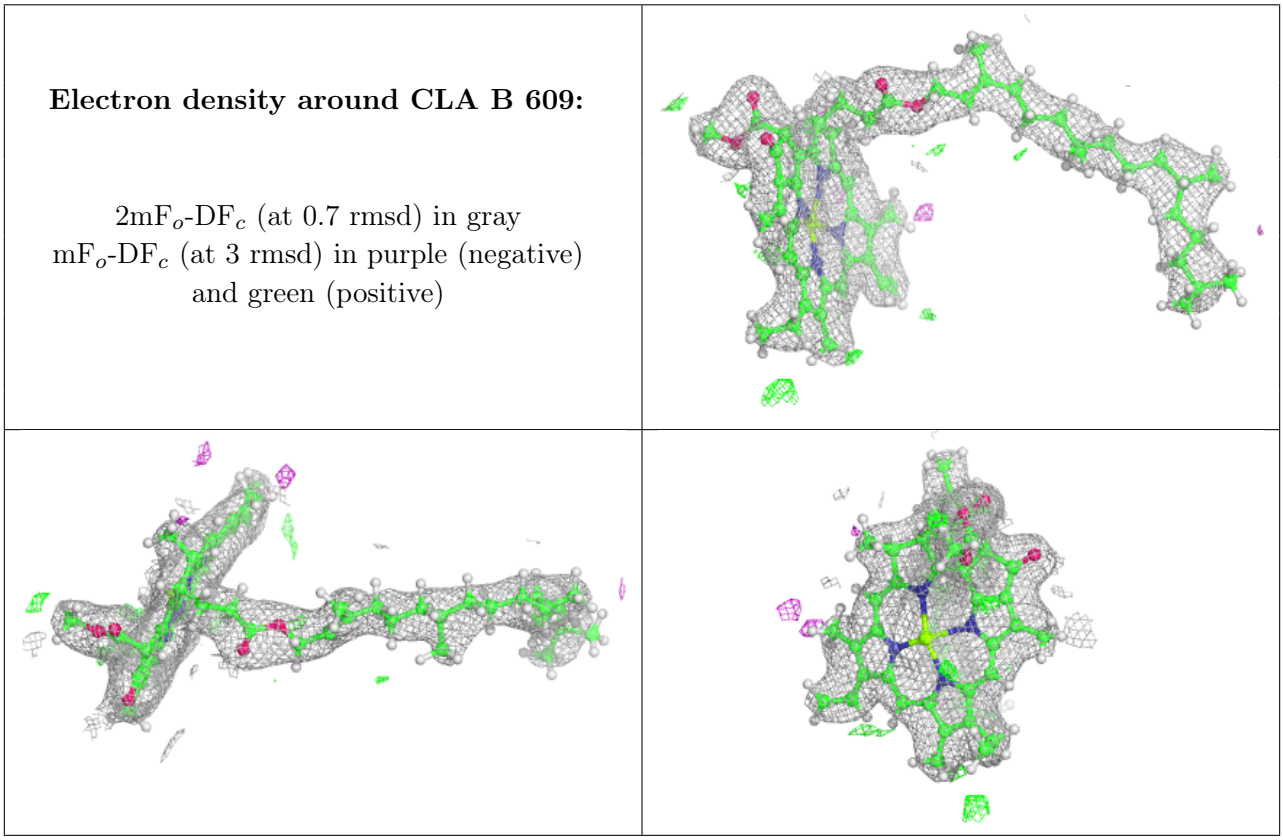
Electron density around BCR c 515:

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



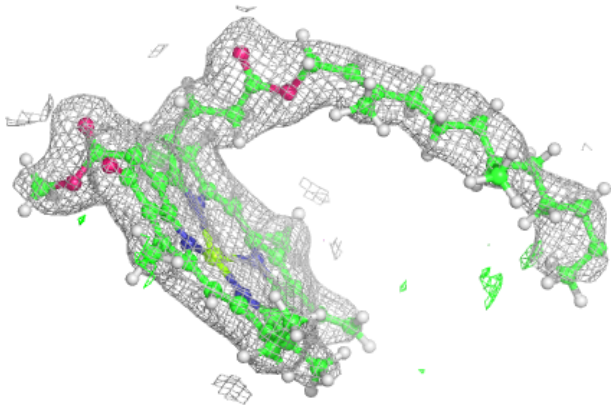
Electron density around CLA B 609:

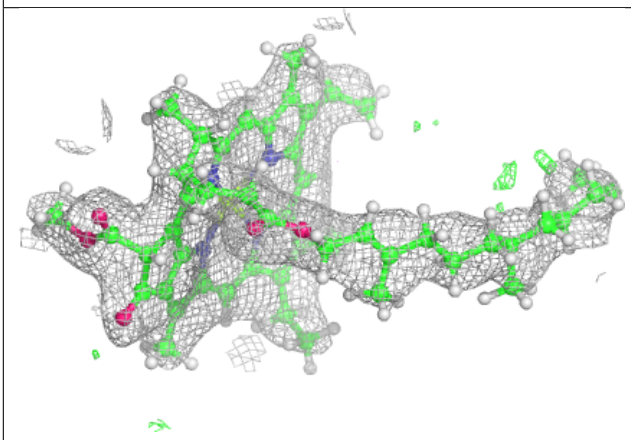
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

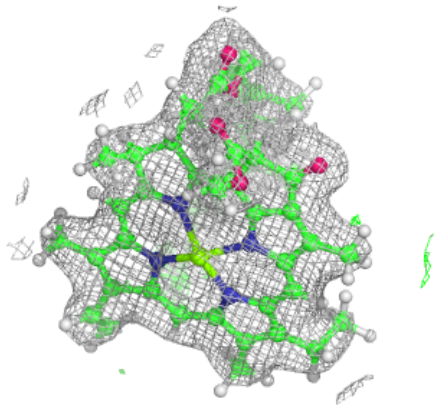


Electron density around CLA C 504:

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

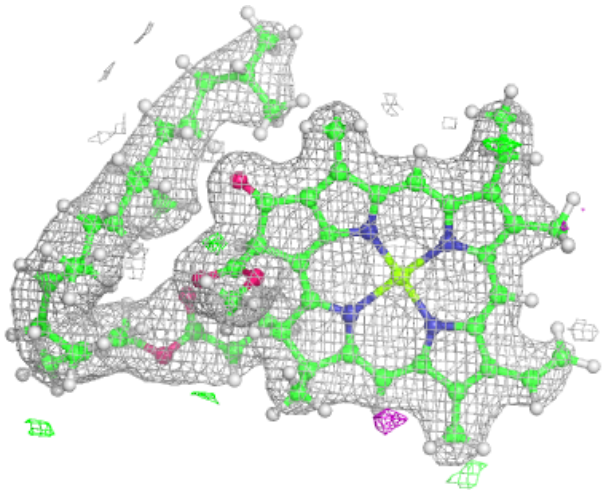


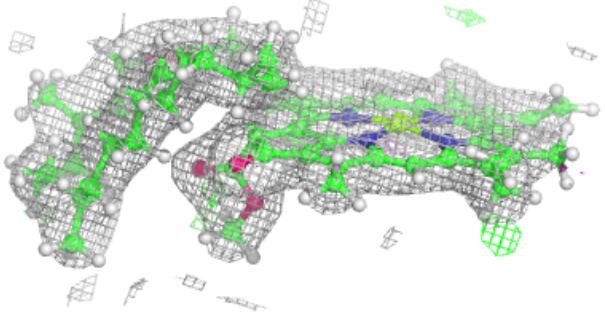




Electron density around CLA B 610:

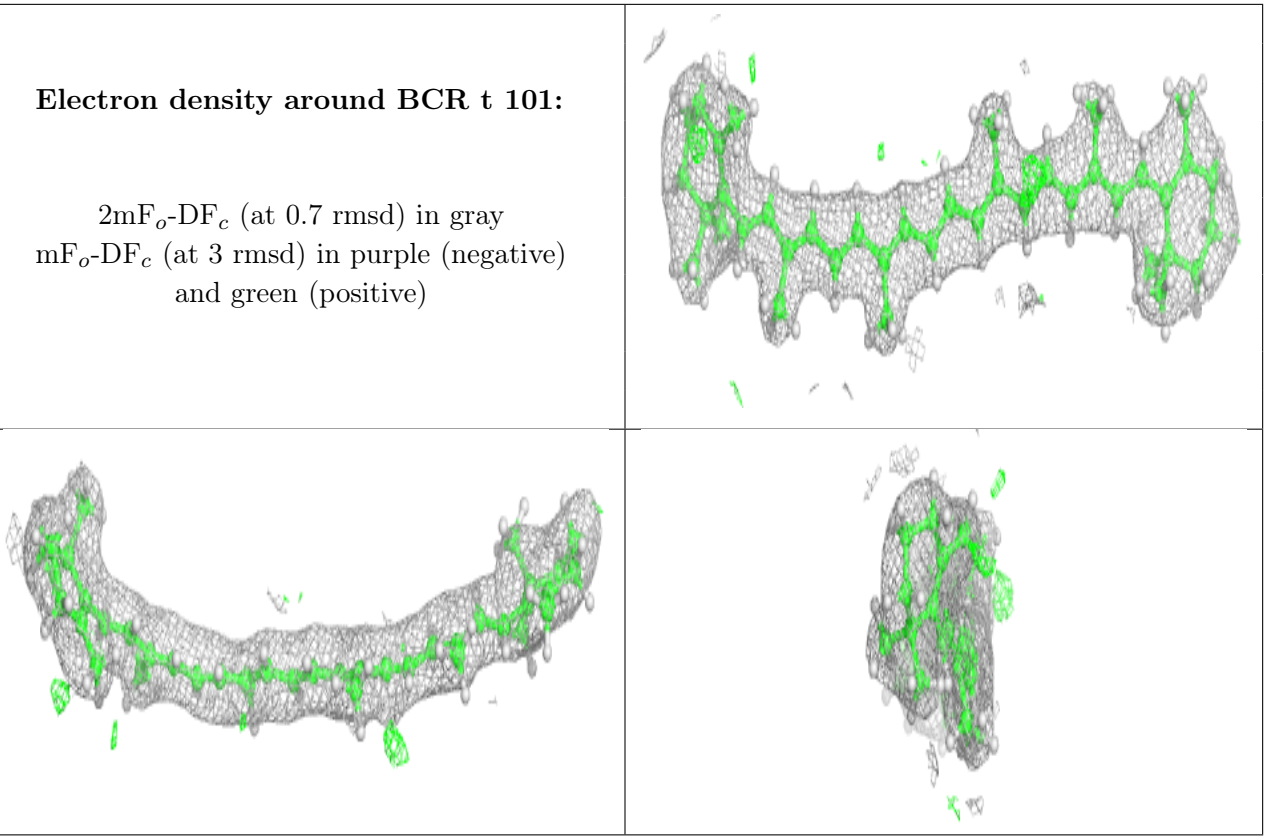
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





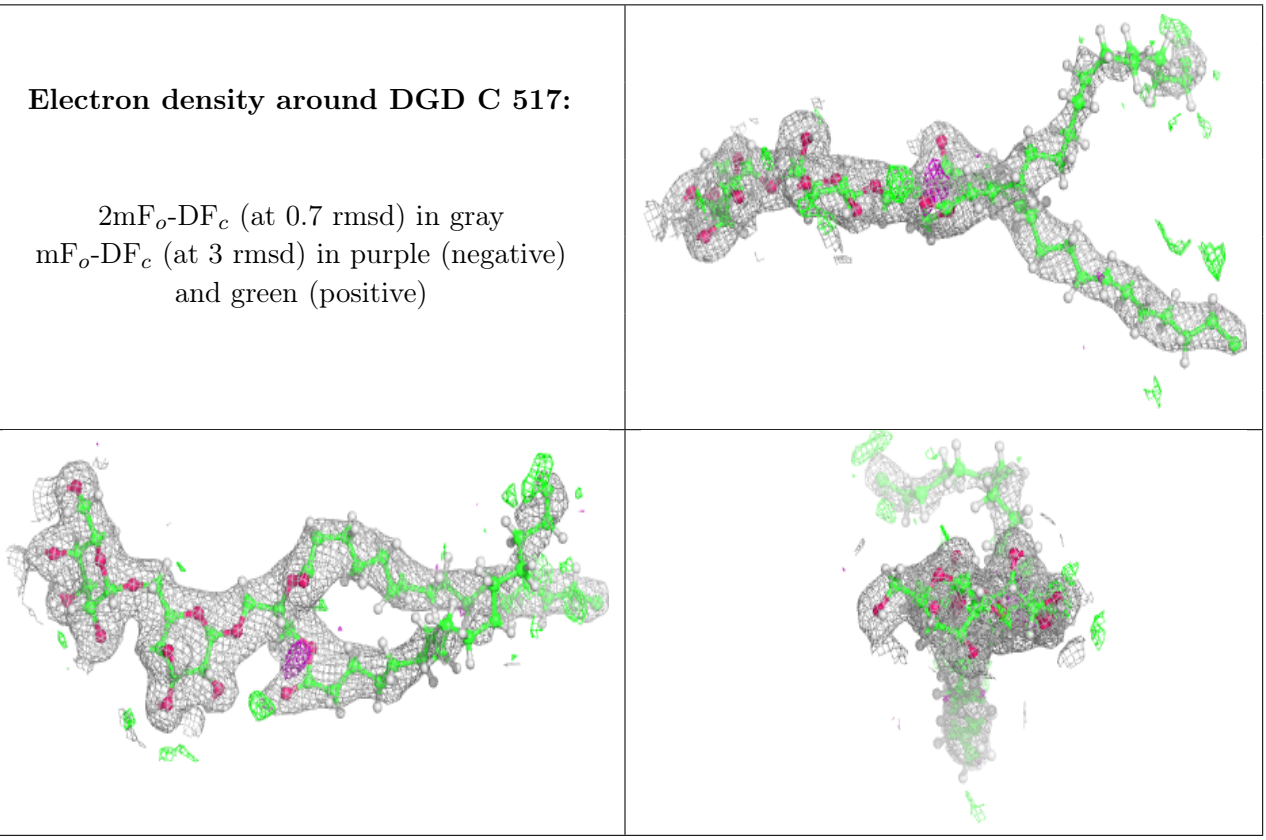
Electron density around BCR t 101:

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



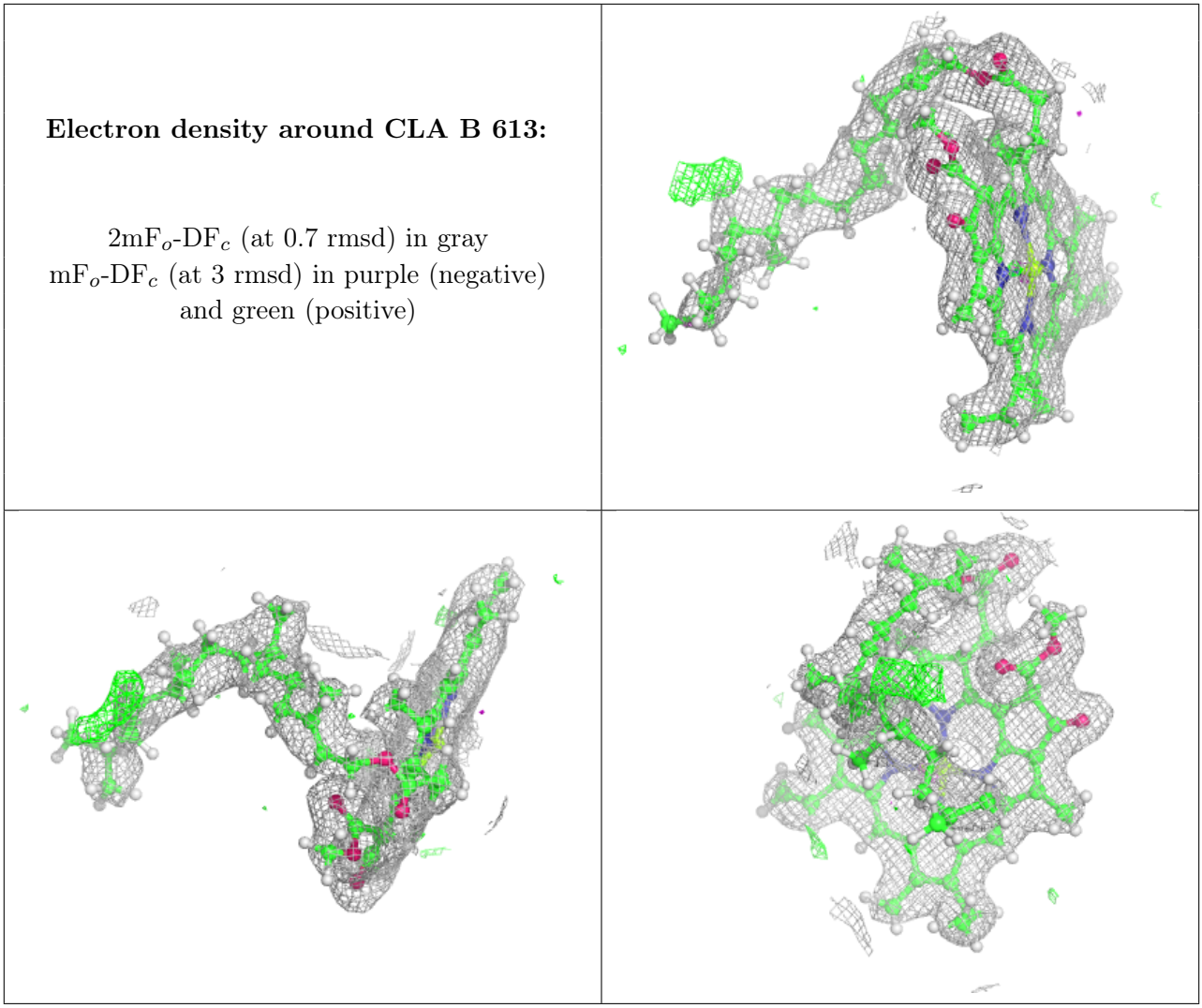
Electron density around DGD C 517:

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



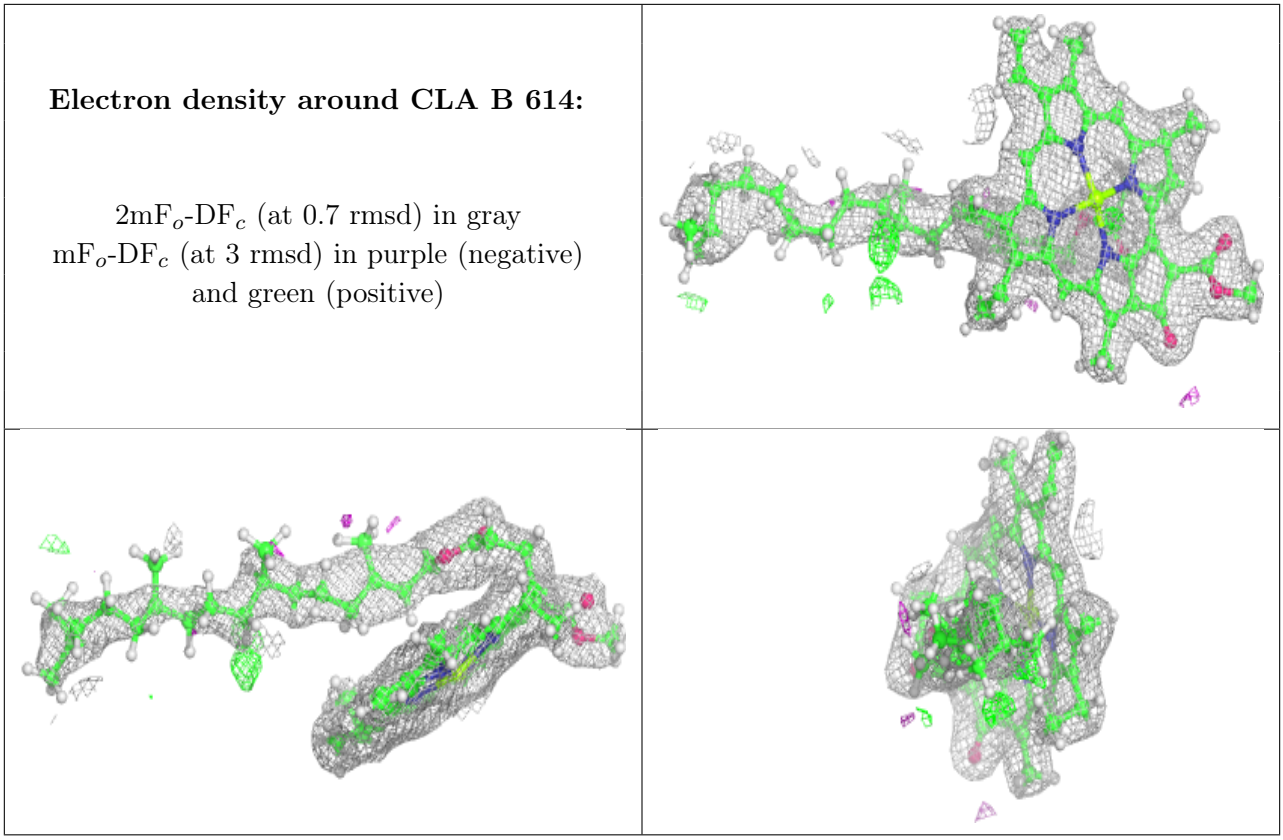
Electron density around CLA B 613:

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



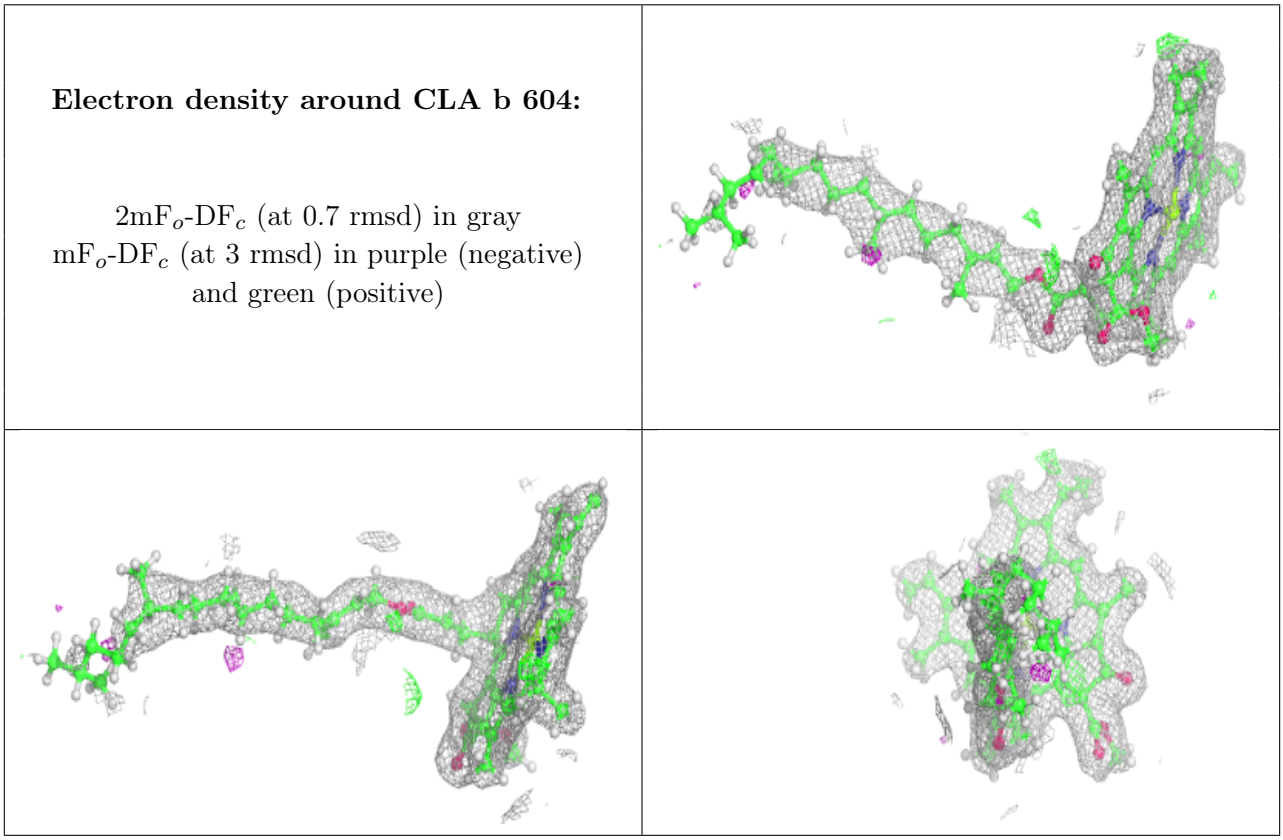
Electron density around CLA B 614:

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



Electron density around CLA b 604:

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

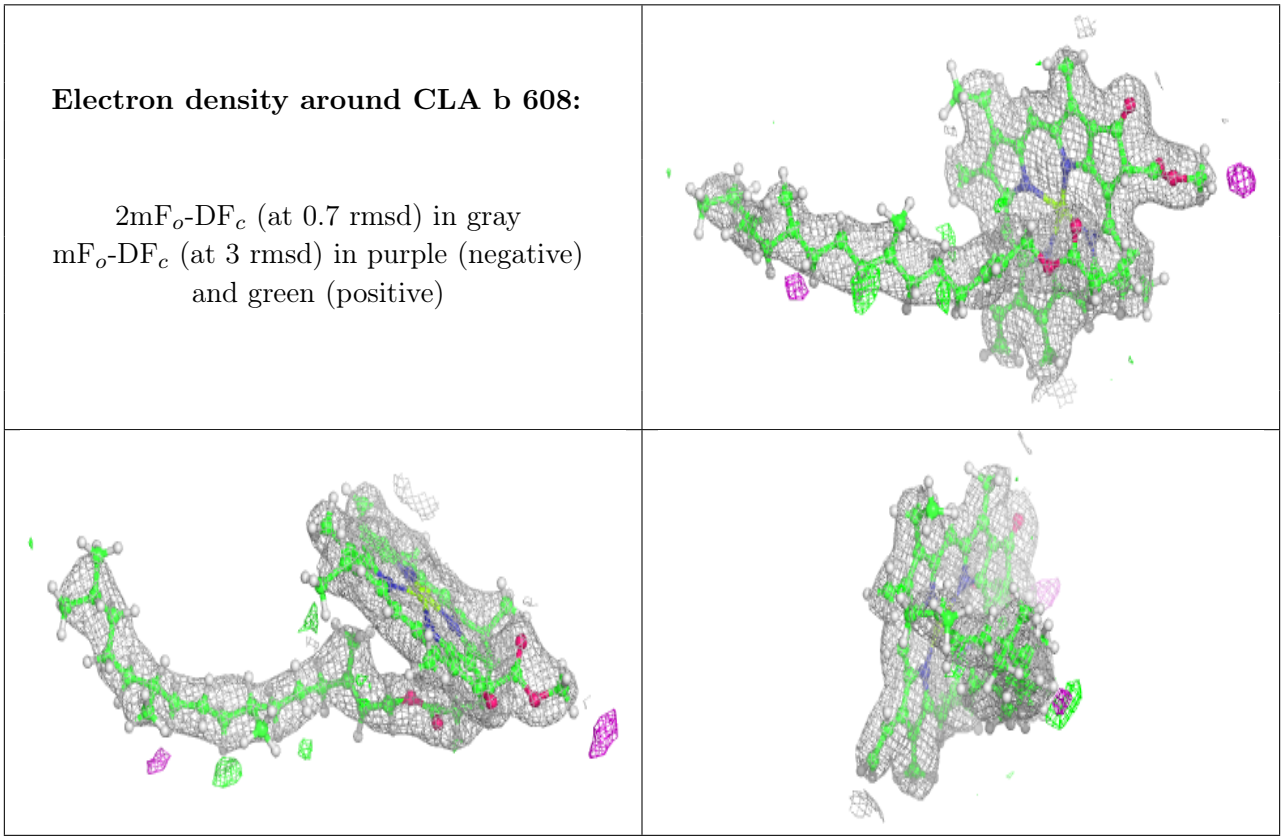


Electron density around CLA C 508:

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

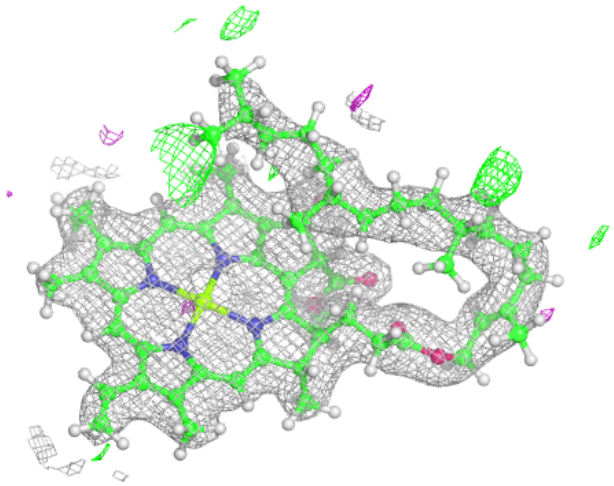
Electron density around CLA b 608:

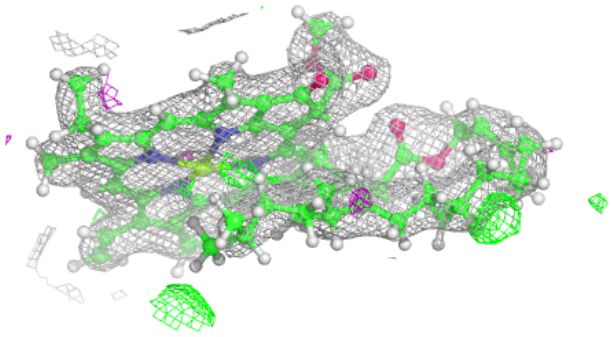
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

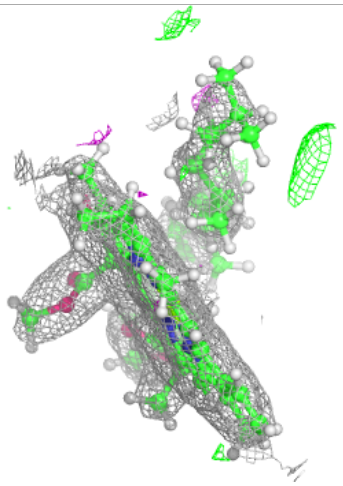


Electron density around CLA C 509:

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

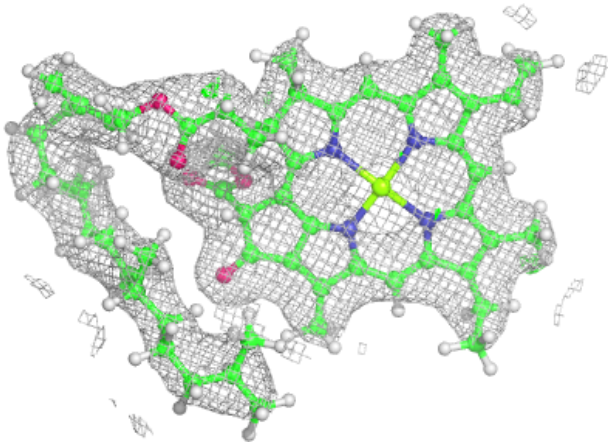


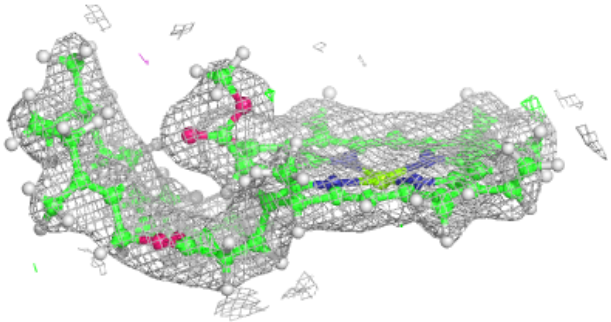


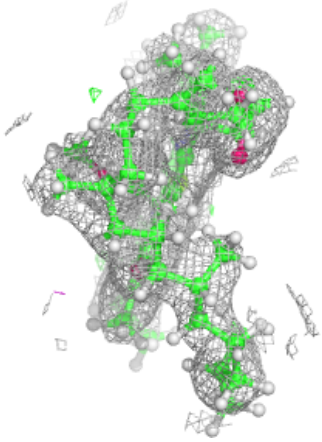


Electron density around CLA b 610:

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

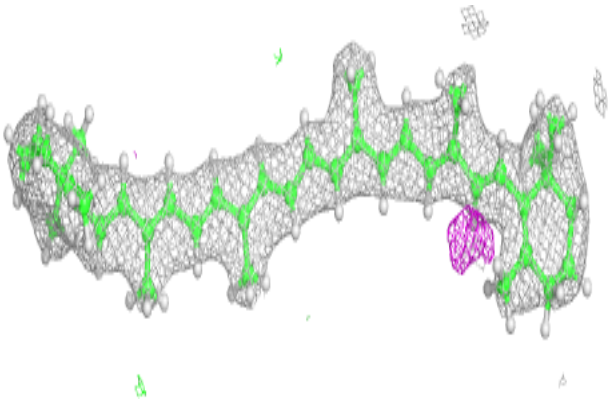


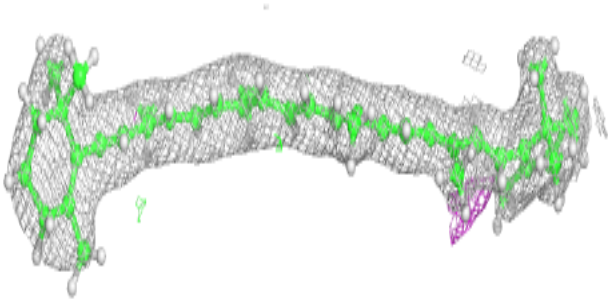


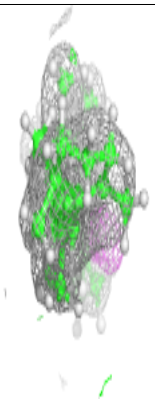


Electron density around BCR B 617:

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

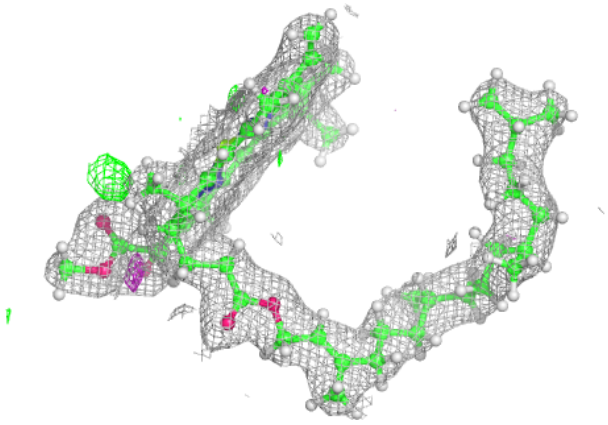


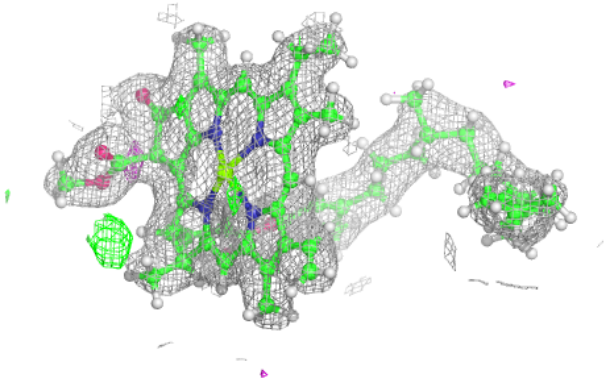


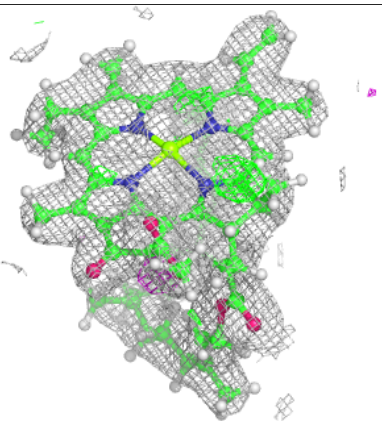


Electron density around CLA b 611:

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

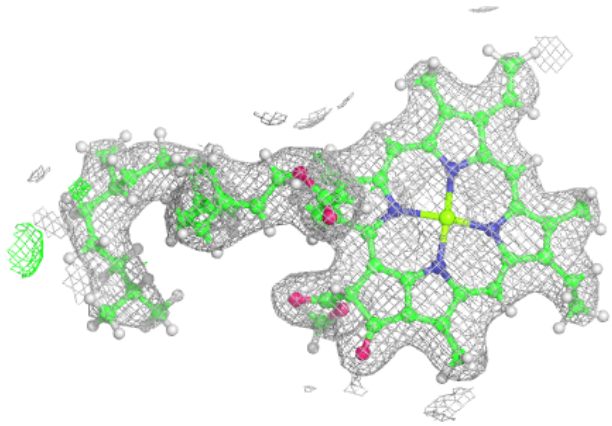


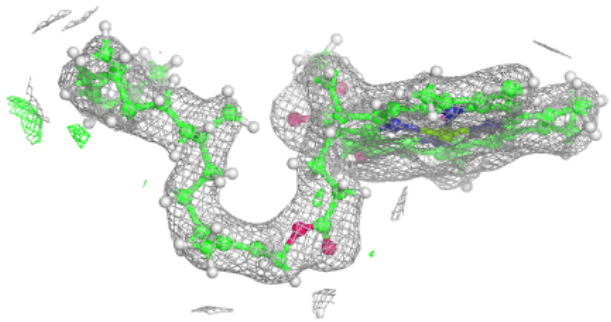


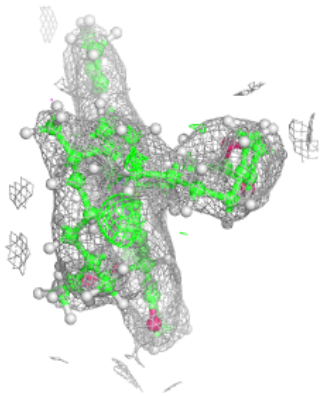


Electron density around CLA b 612:

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

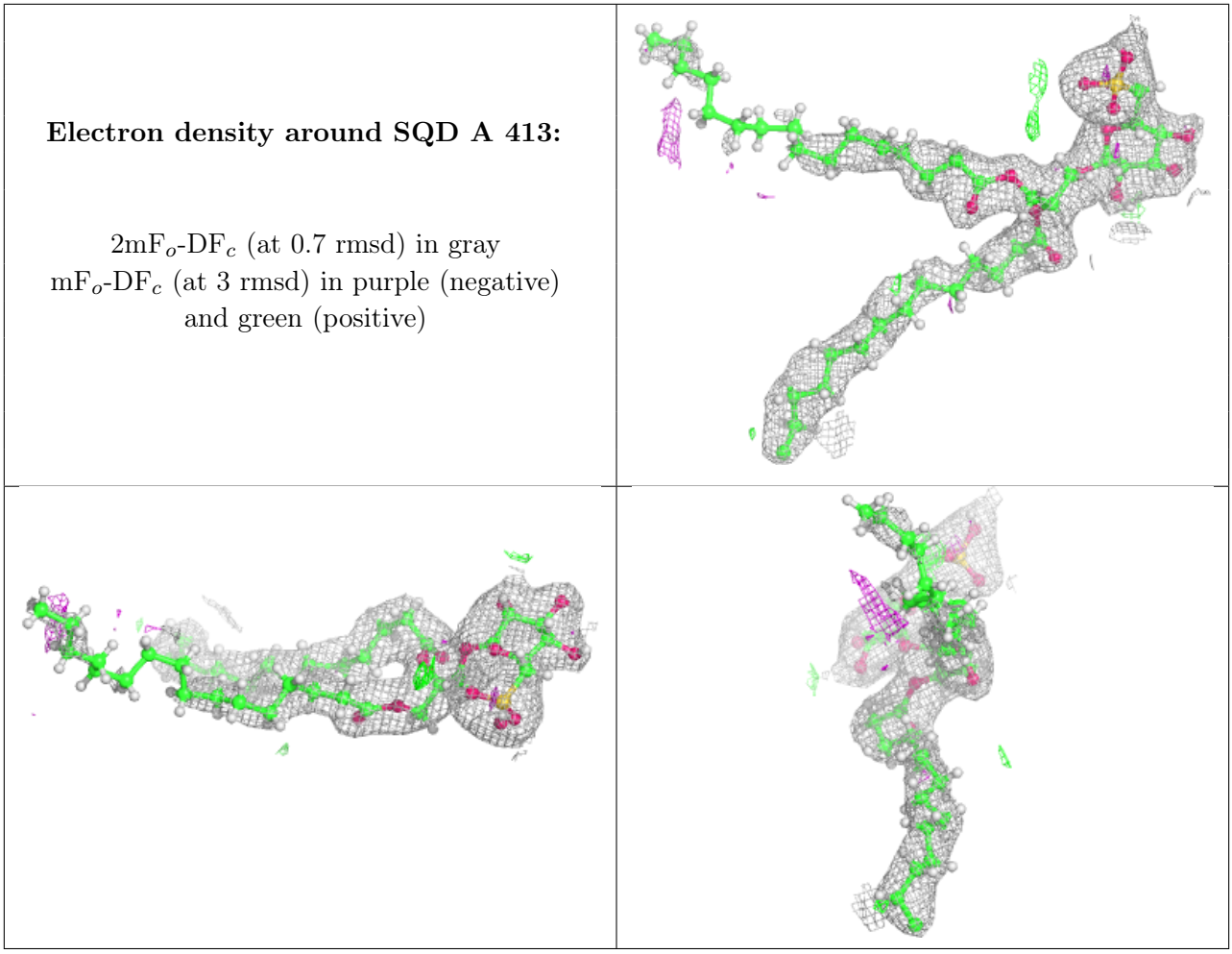






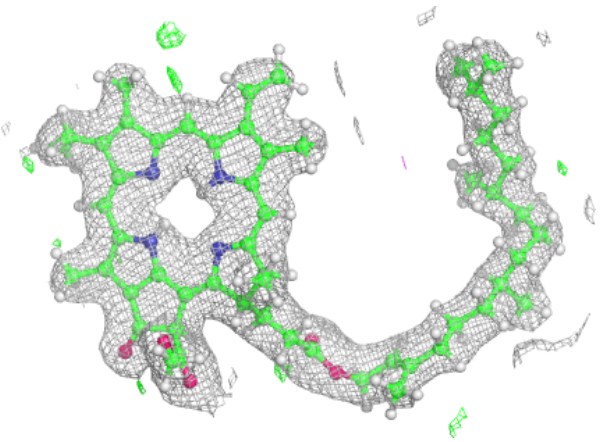
Electron density around SQD A 413:

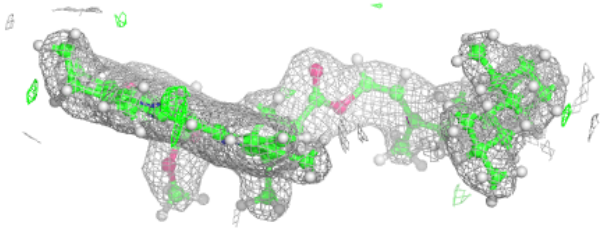
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

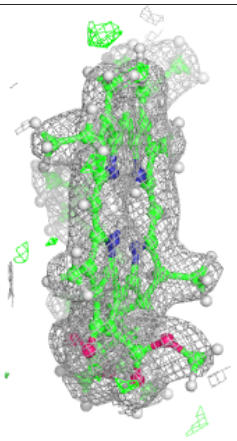


Electron density around PHO a 403:

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

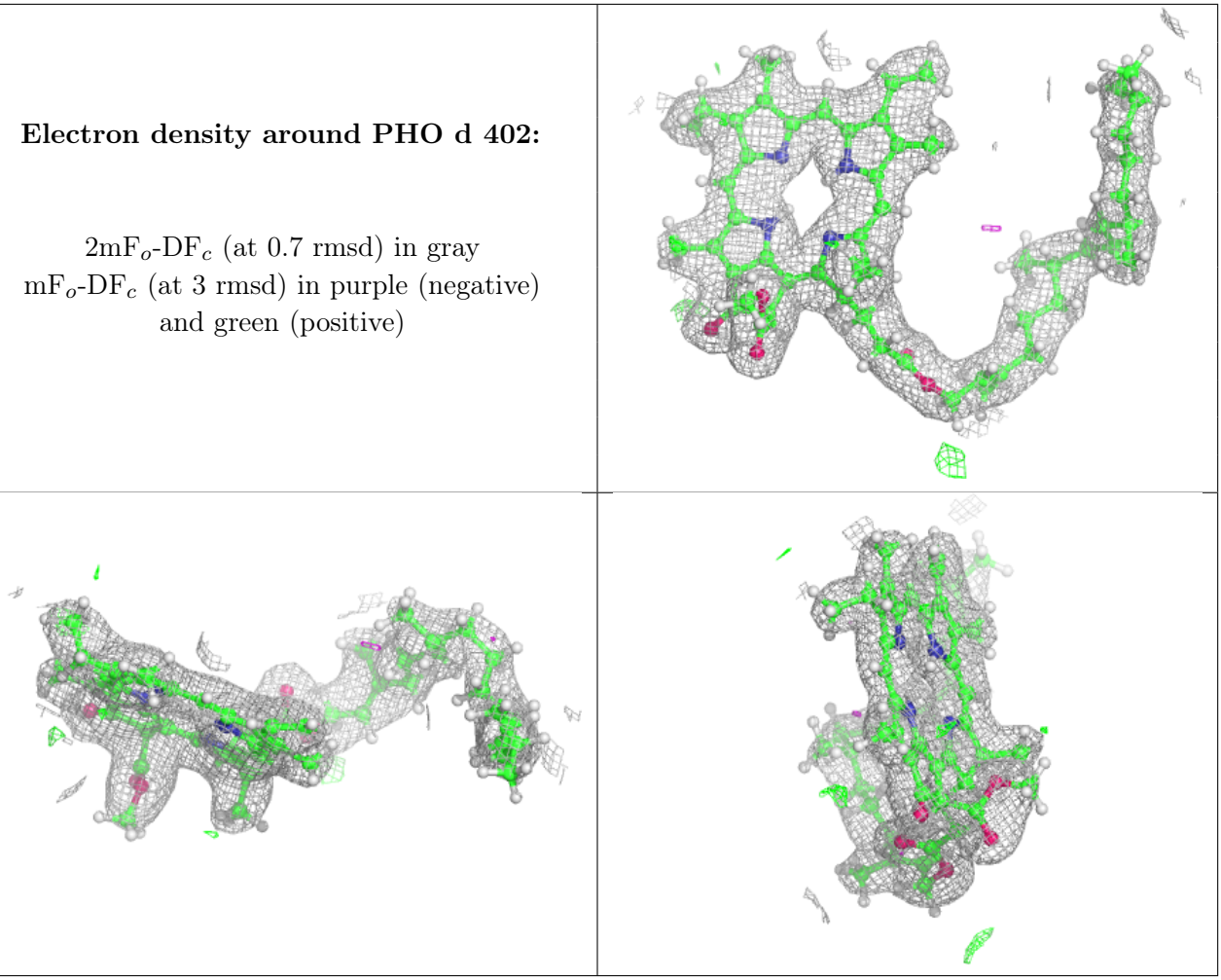






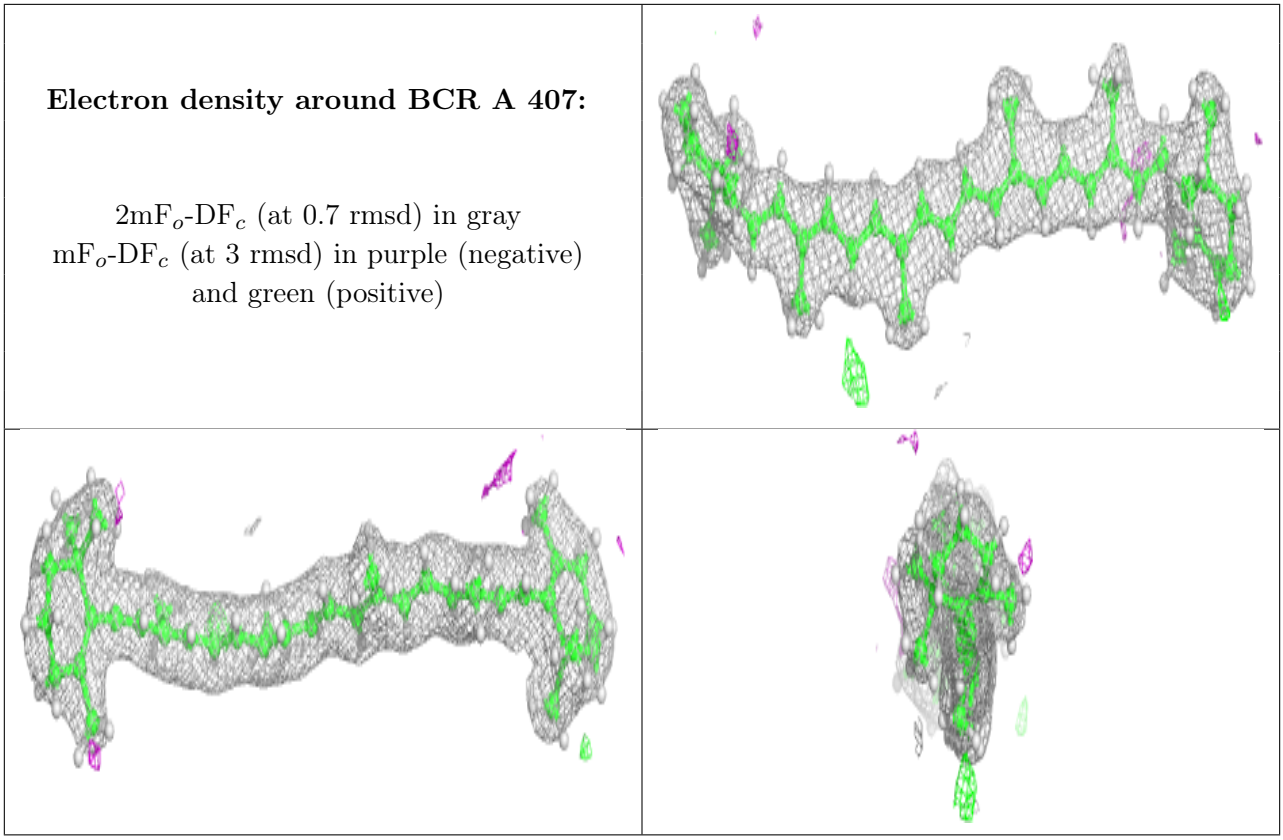
Electron density around PHO d 402:

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



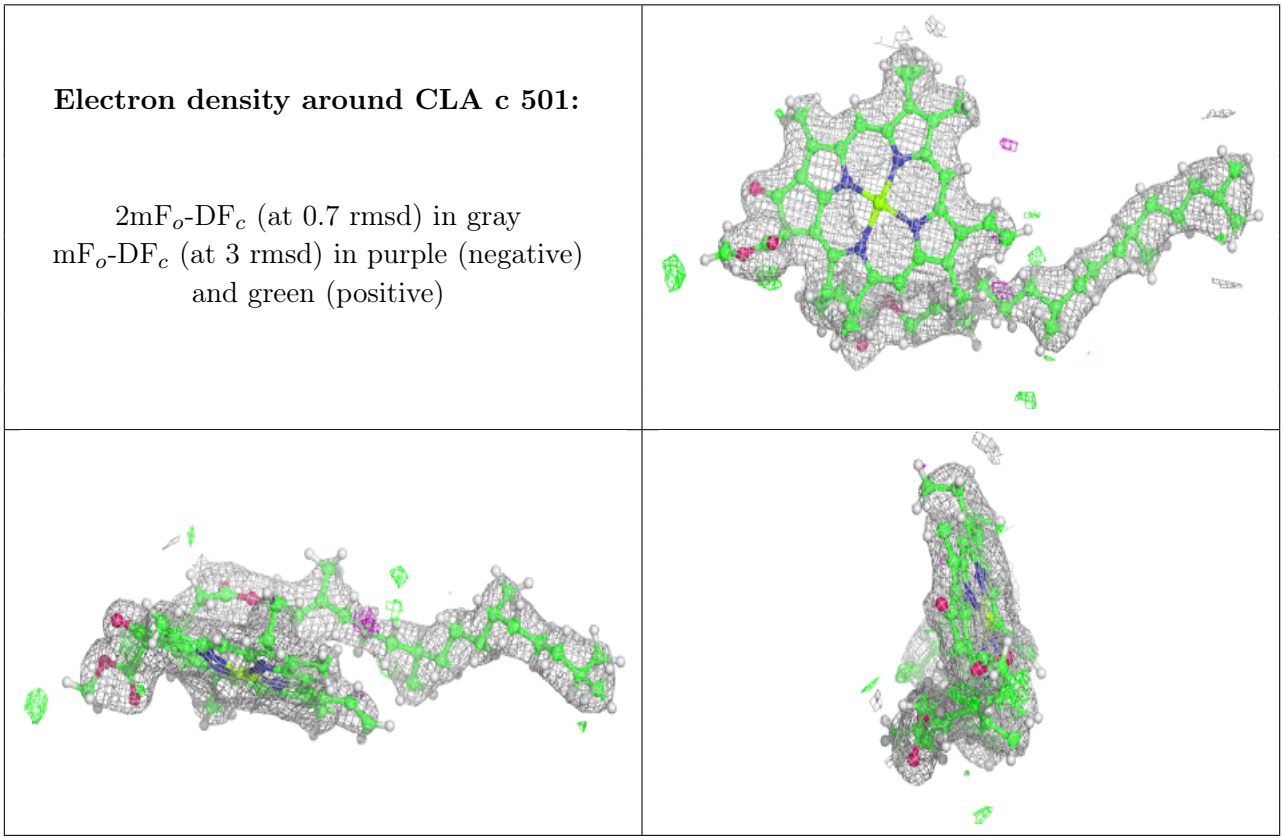
Electron density around BCR A 407:

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



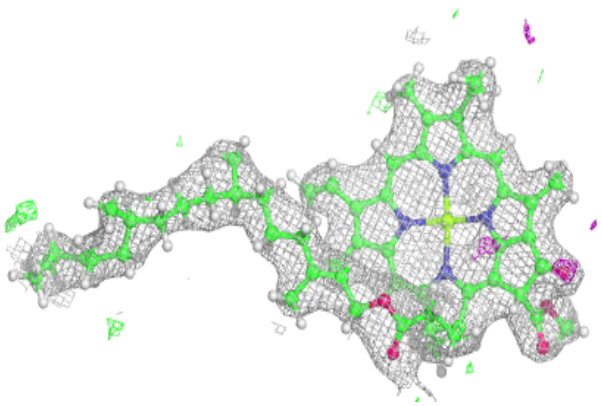
Electron density around CLA c 501:

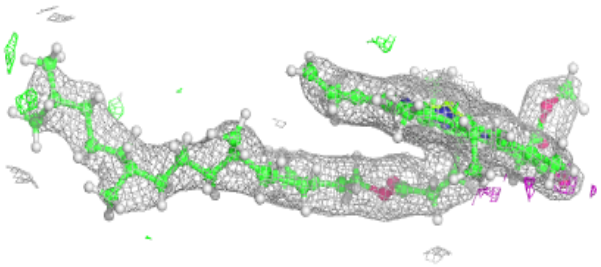
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

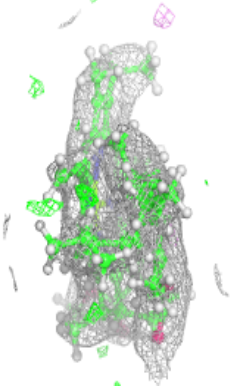


Electron density around CLA b 603:

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

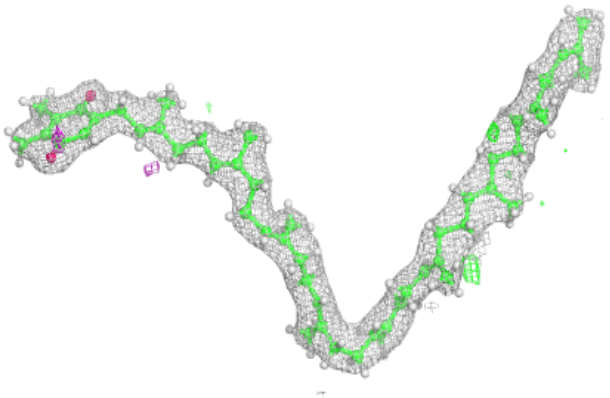


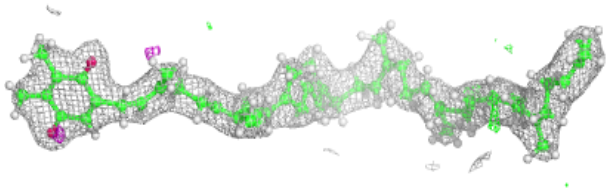


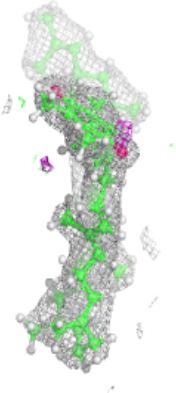


Electron density around PL9 d 407:

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

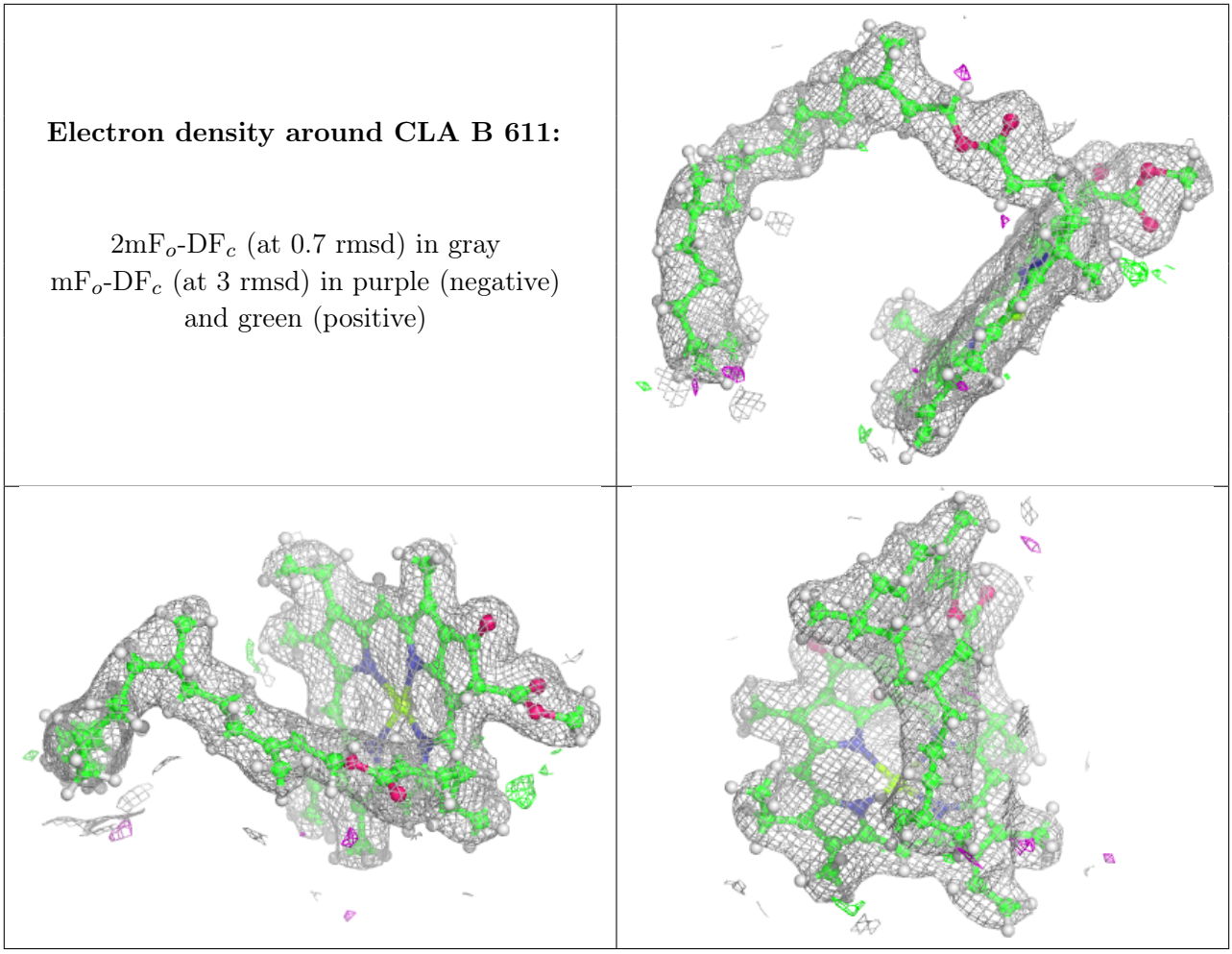






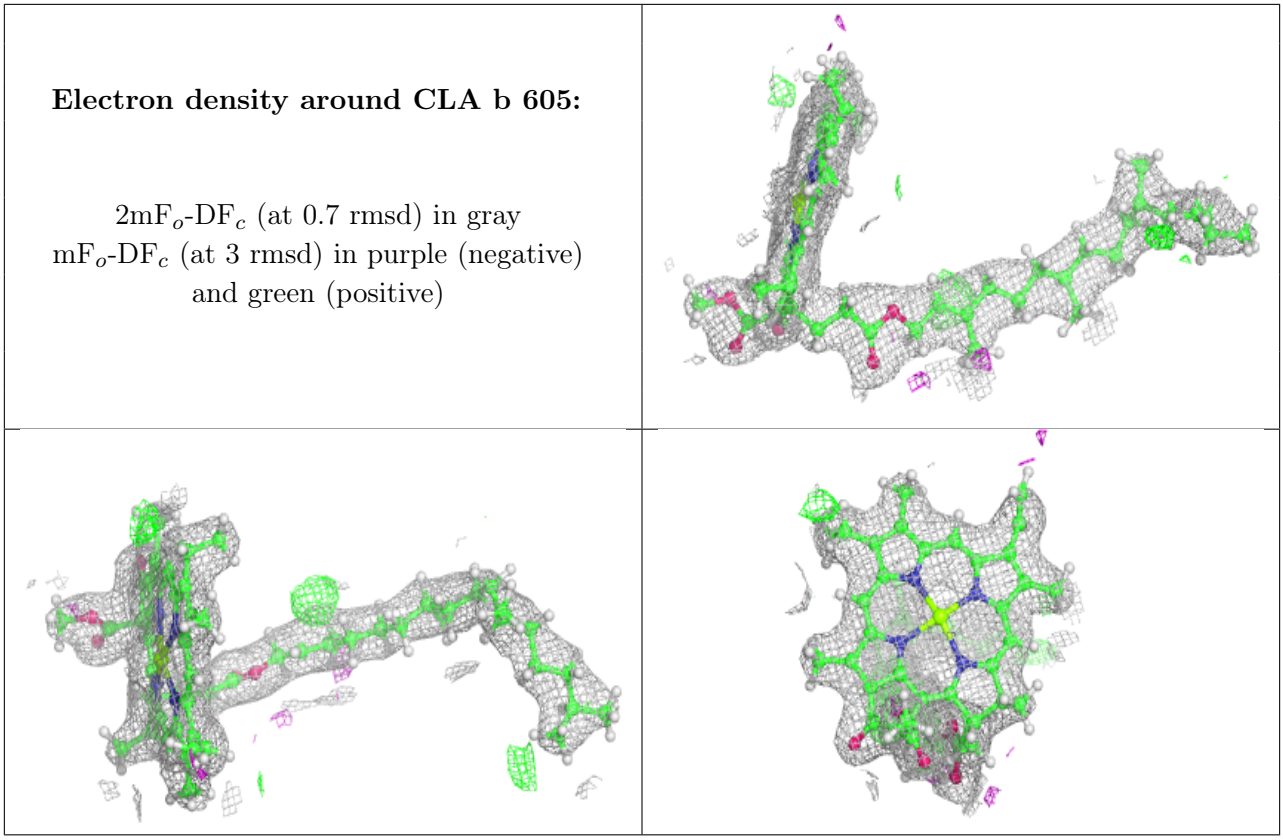
Electron density around CLA B 611:

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



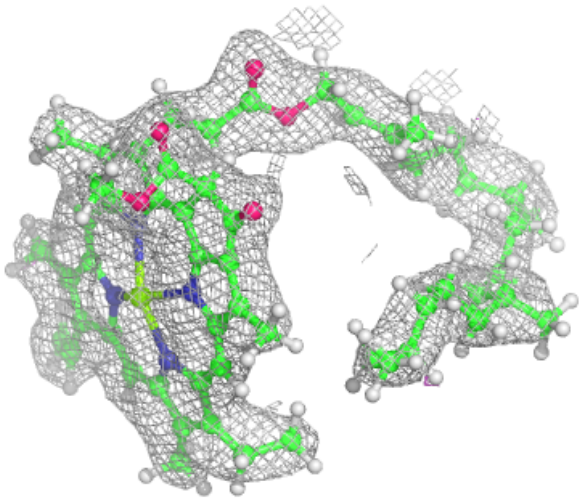
Electron density around CLA b 605:

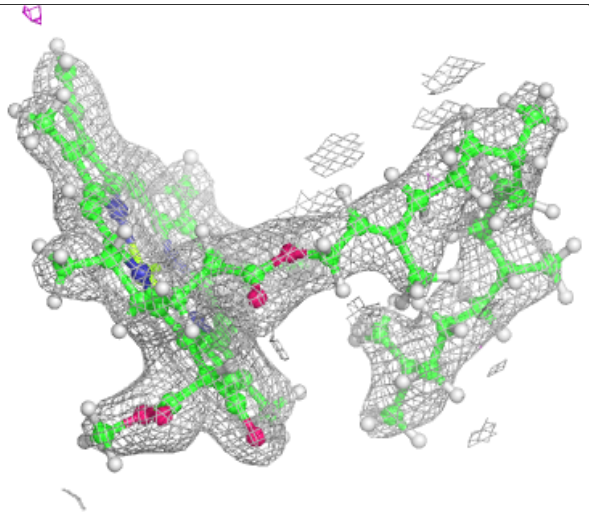
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

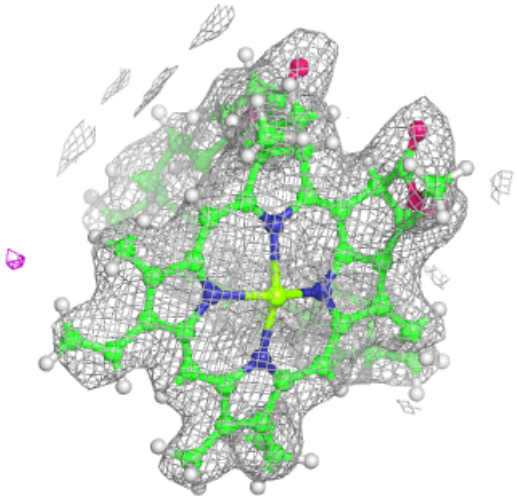


Electron density around CLA C 503:

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

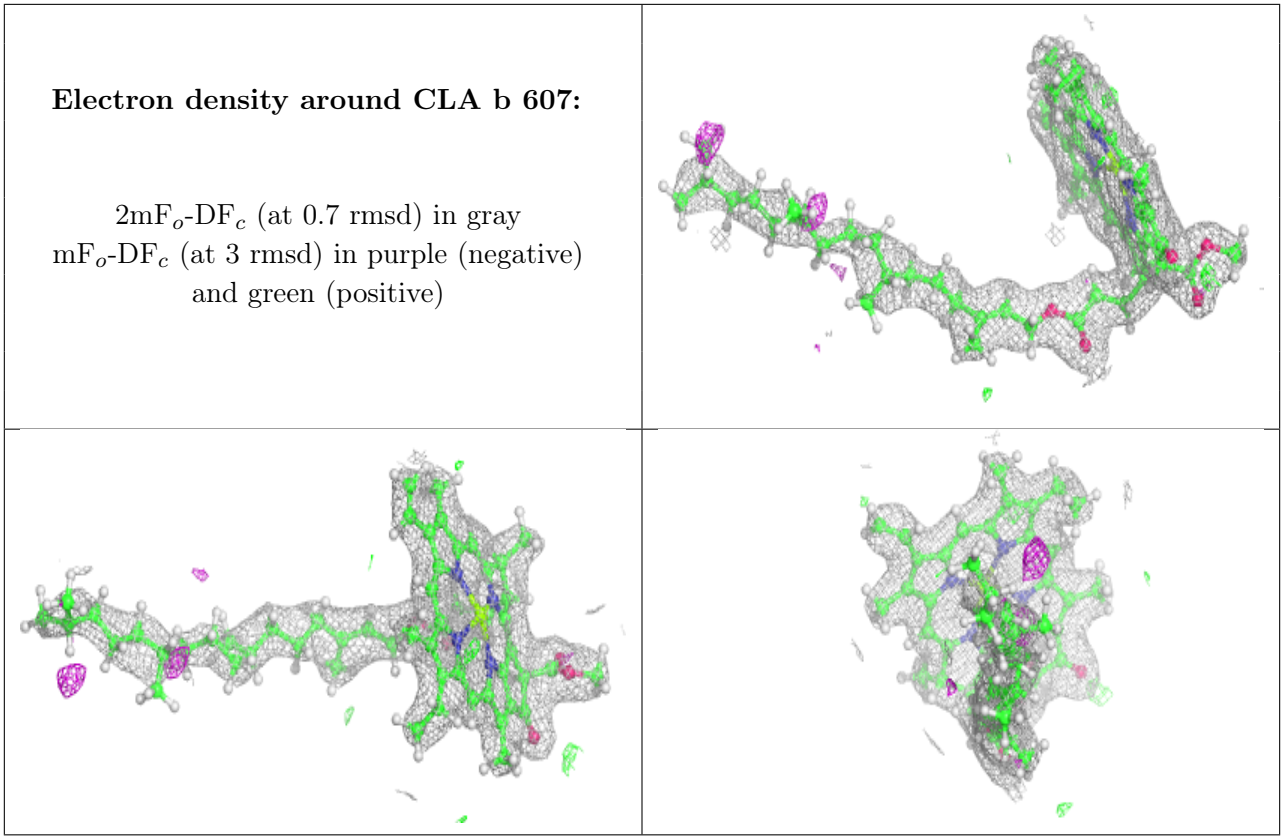






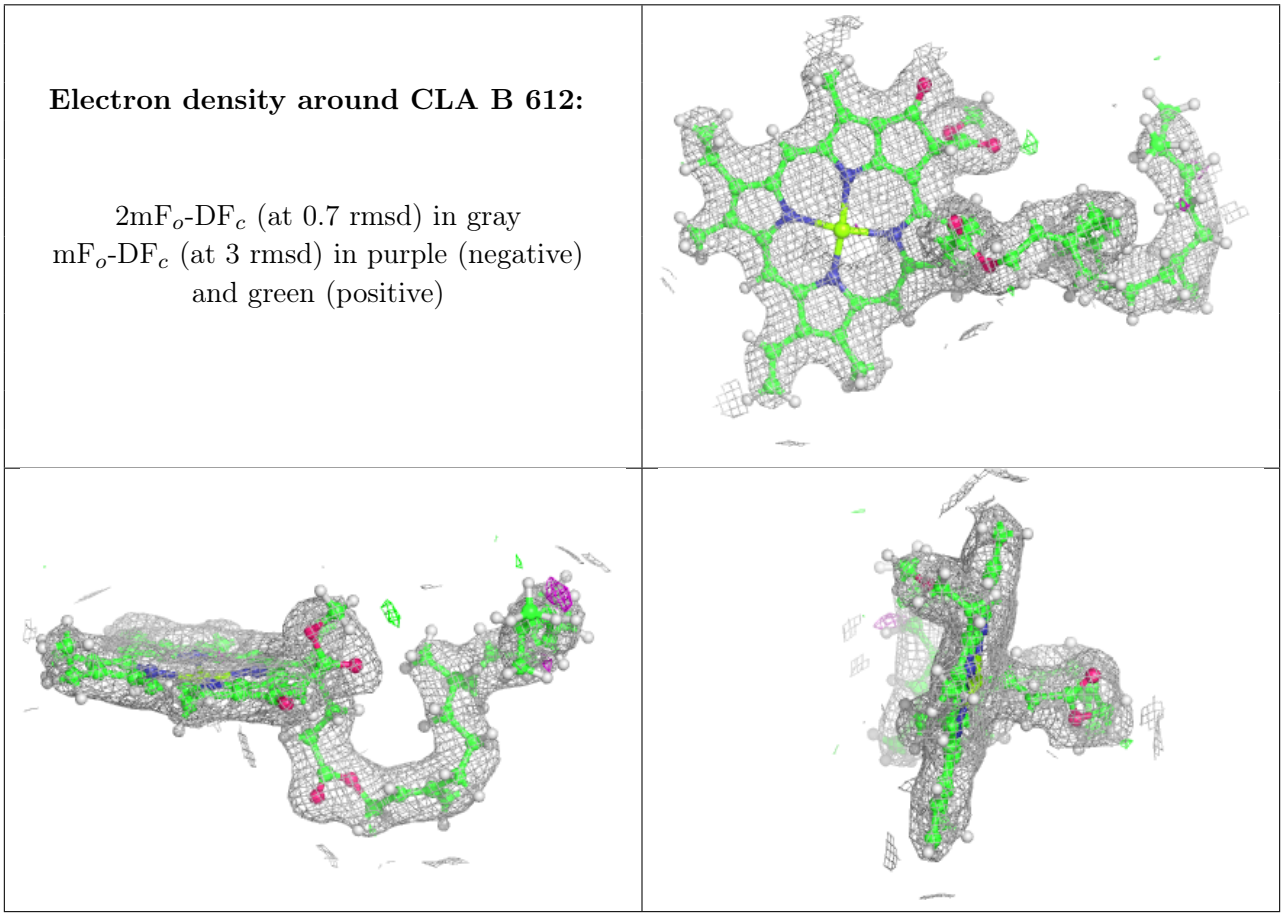
Electron density around CLA b 607:

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



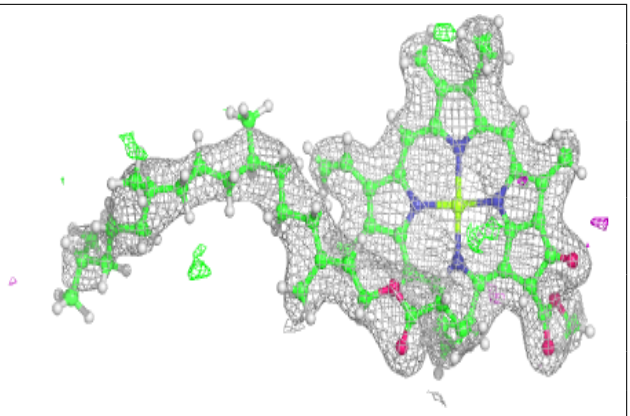
Electron density around CLA B 612:

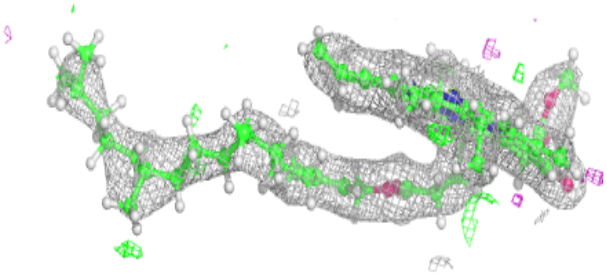
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

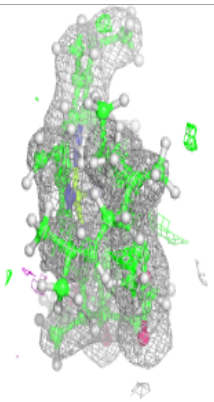


Electron density around CLA B 603:

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

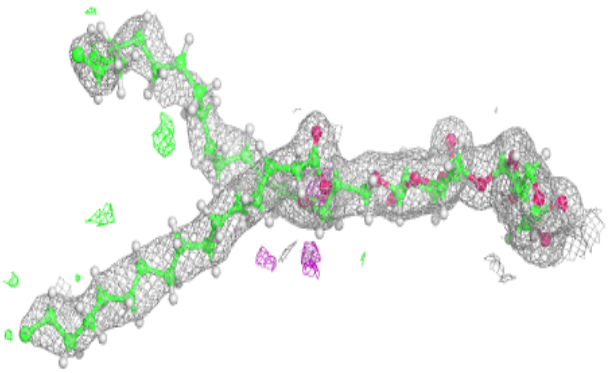


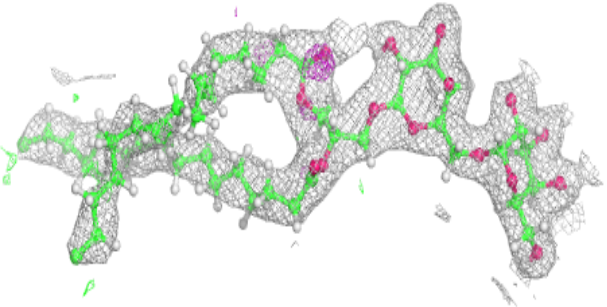


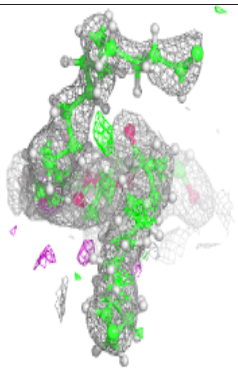


Electron density around DGD c 517:

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

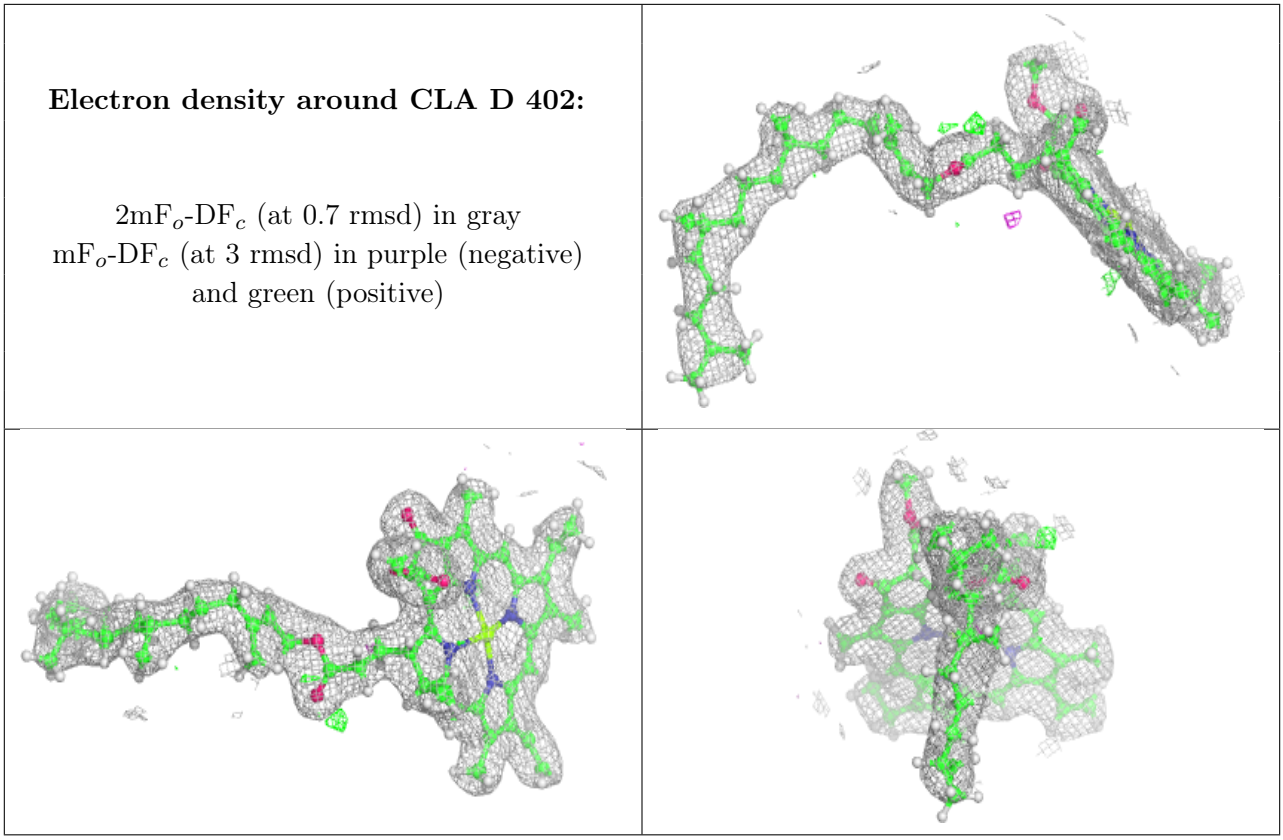






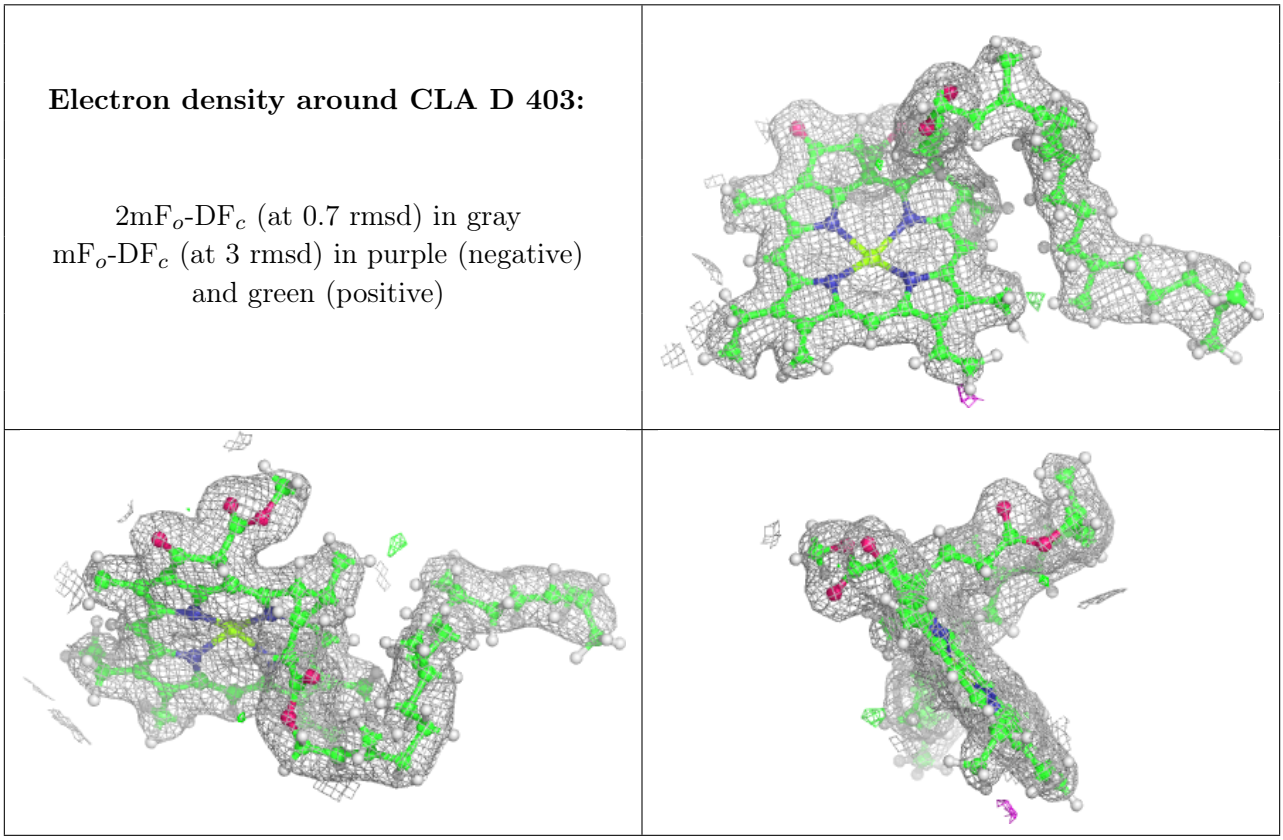
Electron density around CLA D 402:

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



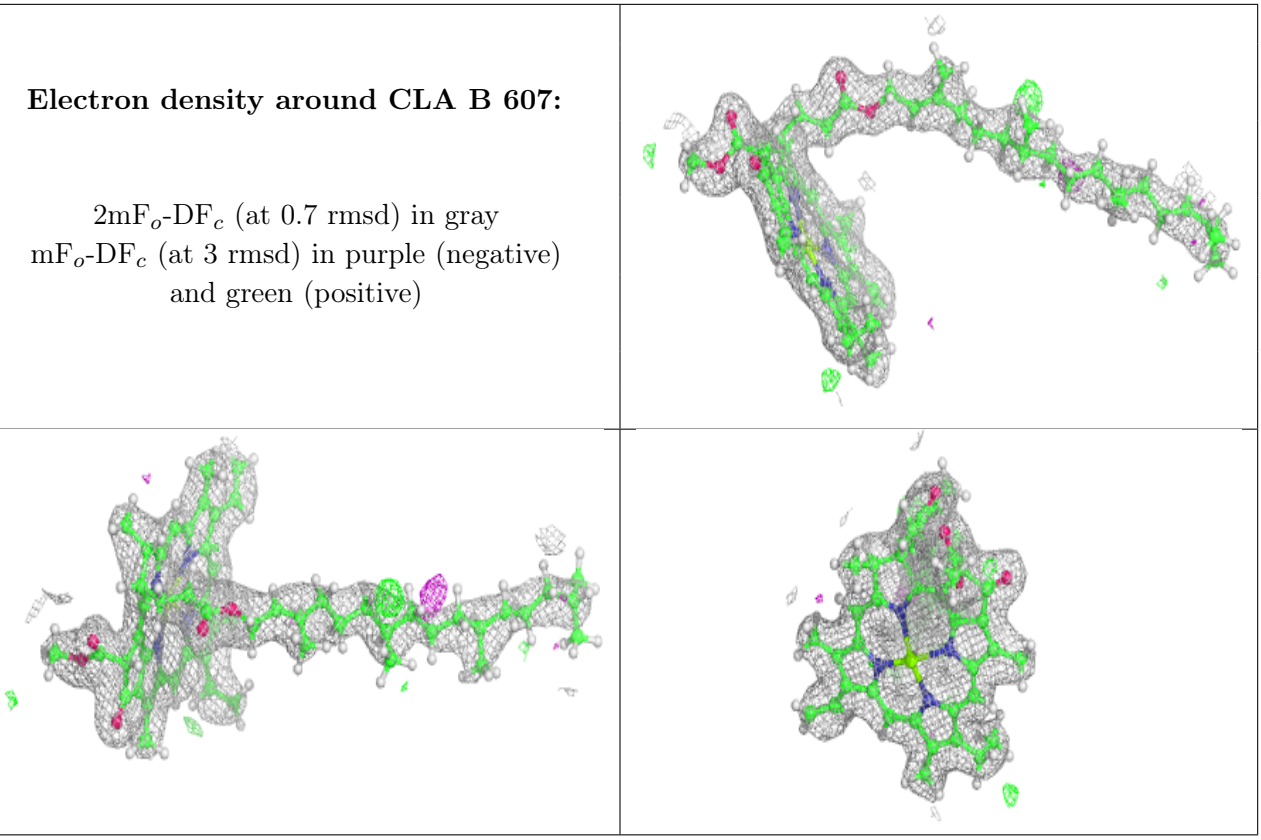
Electron density around CLA D 403:

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



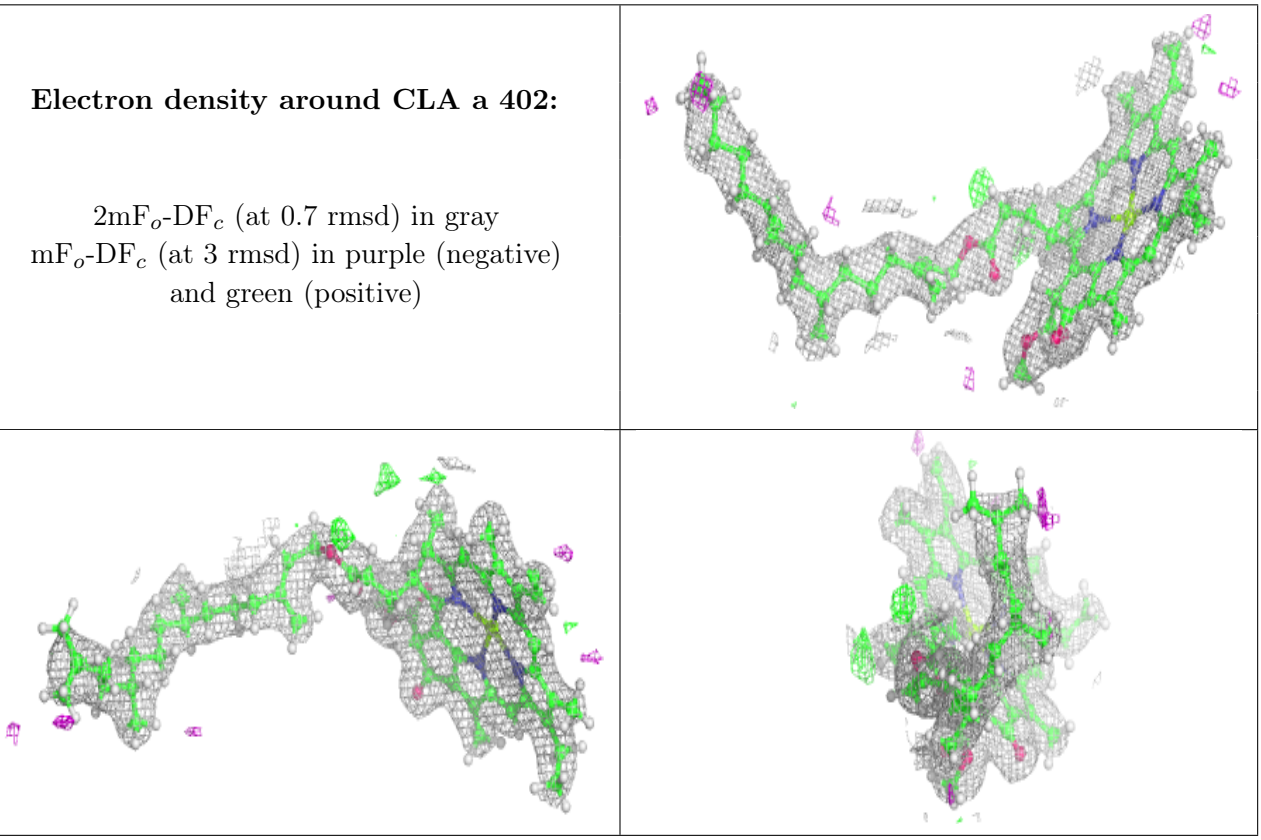
Electron density around CLA B 607:

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



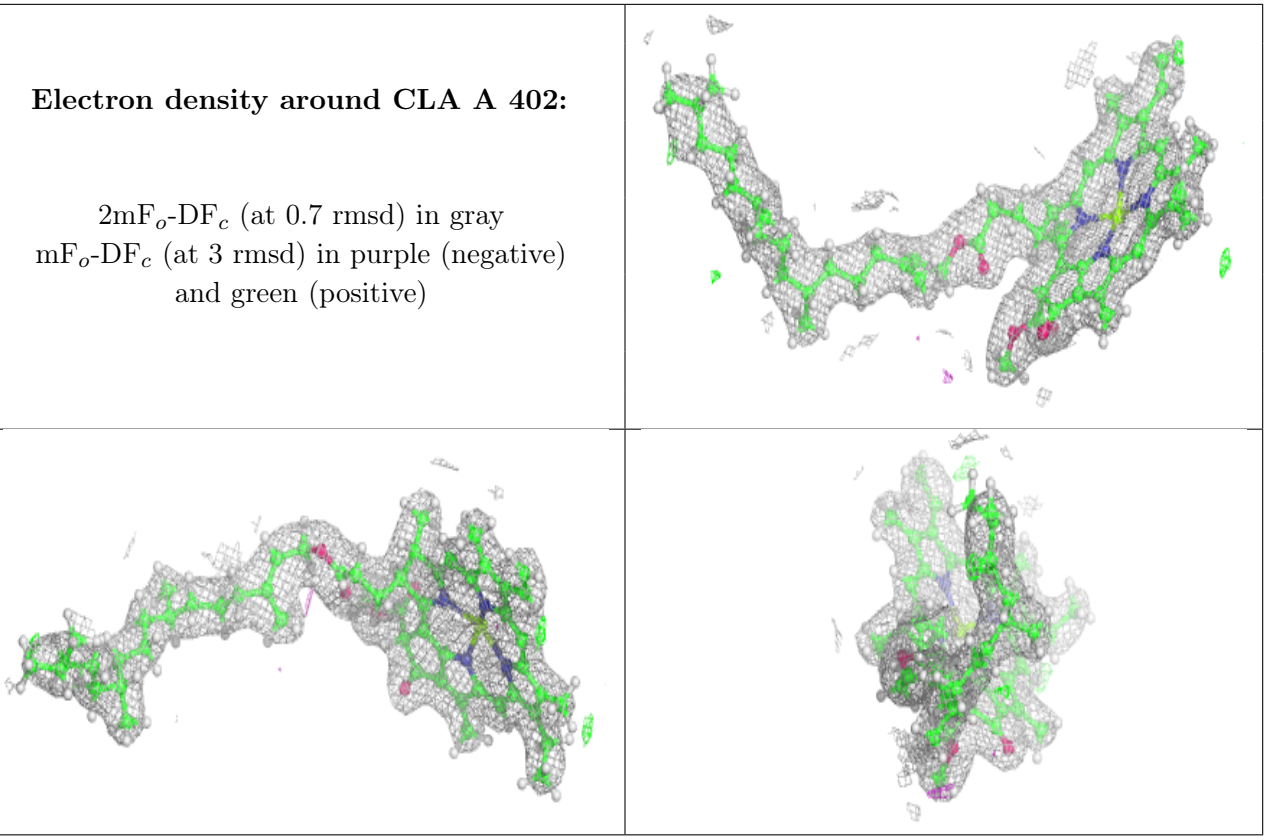
Electron density around CLA a 402:

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



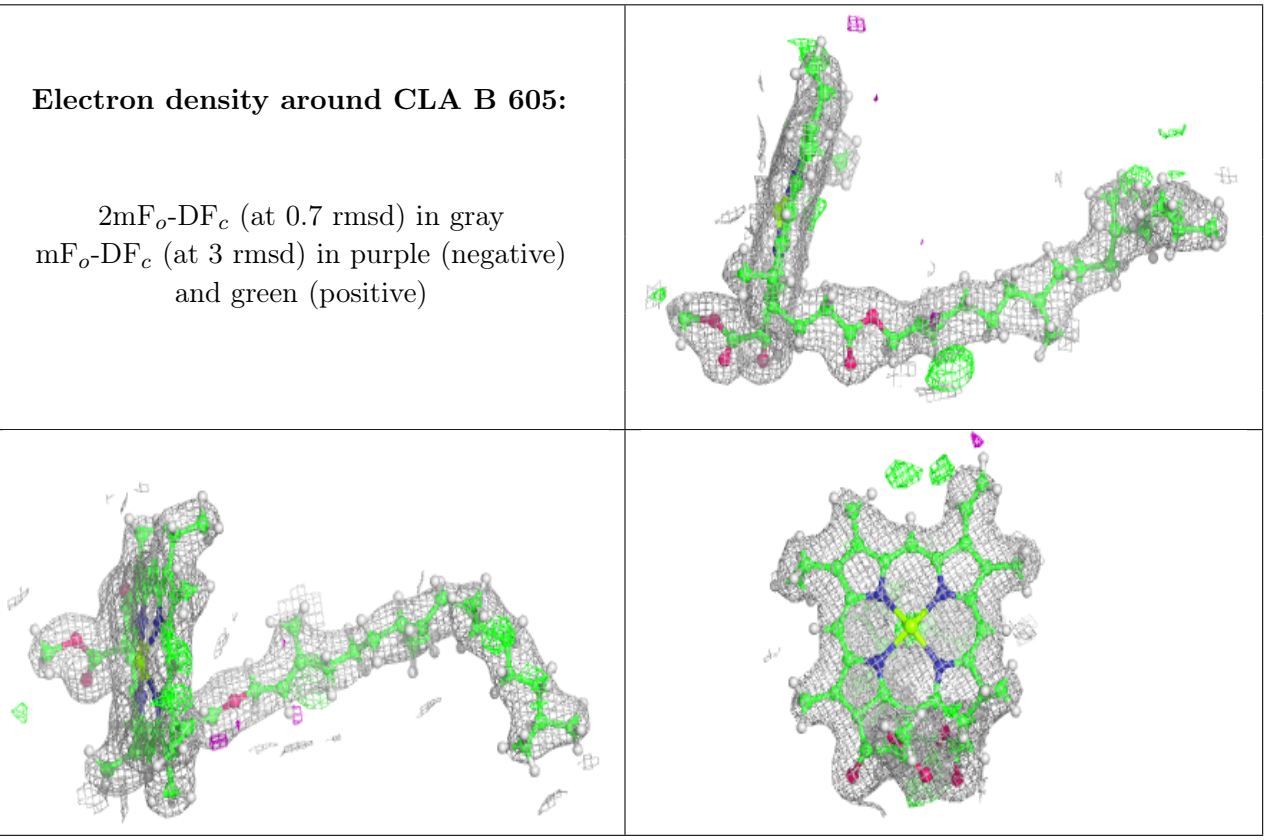
Electron density around CLA A 402:

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



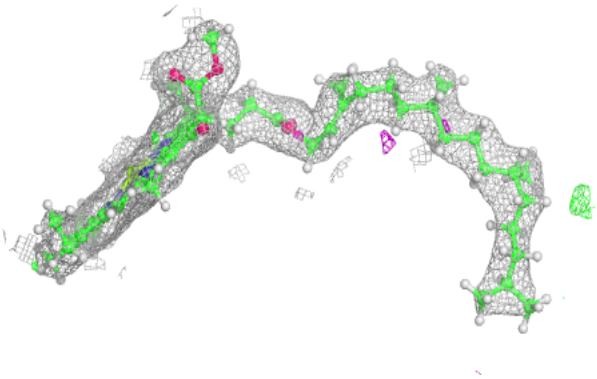
Electron density around CLA B 605:

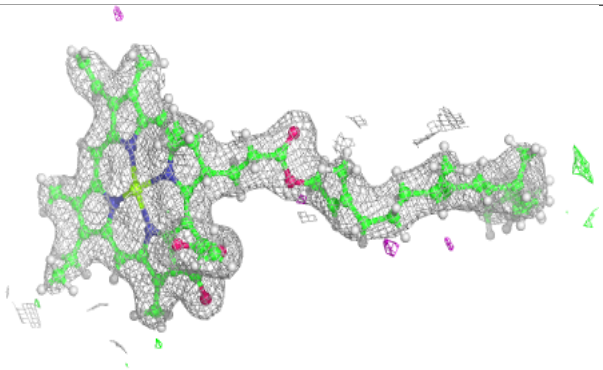
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

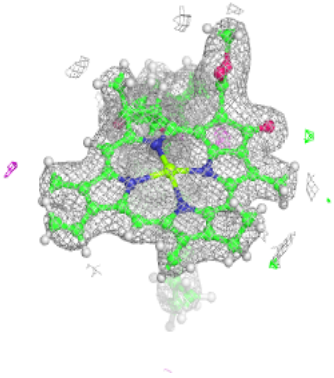


Electron density around CLA d 403:

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

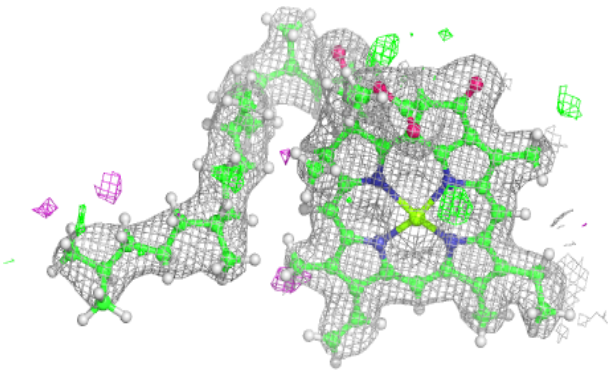


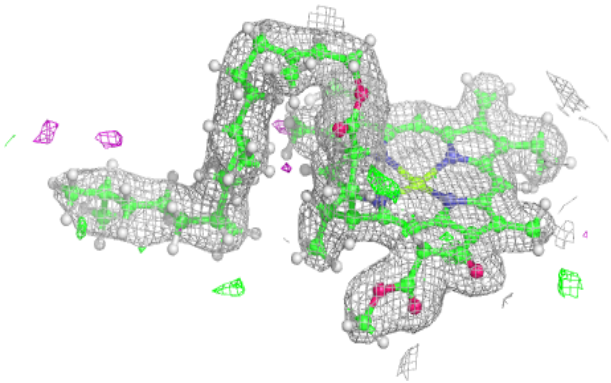


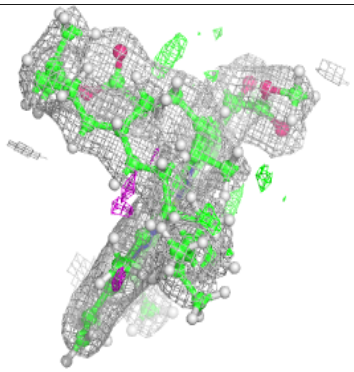


Electron density around CLA d 404:

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

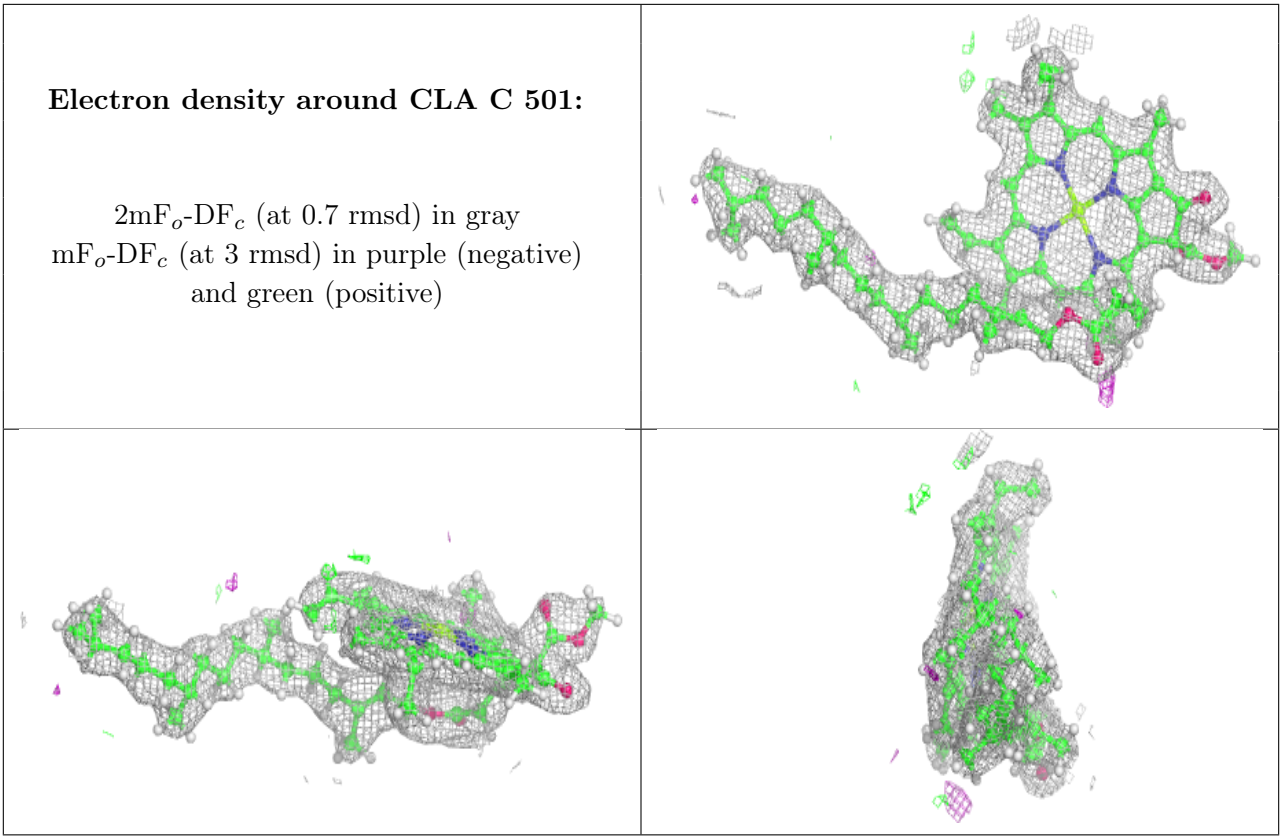






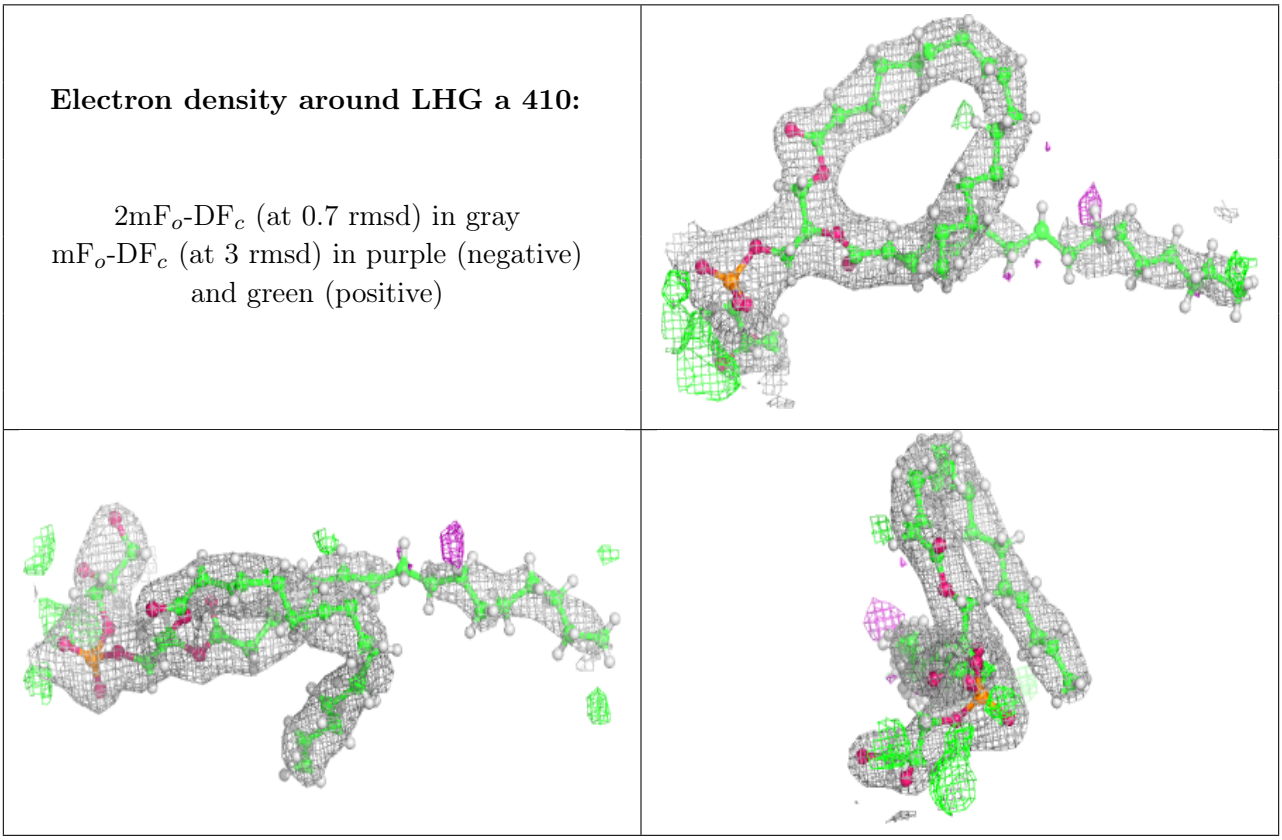
Electron density around CLA C 501:

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



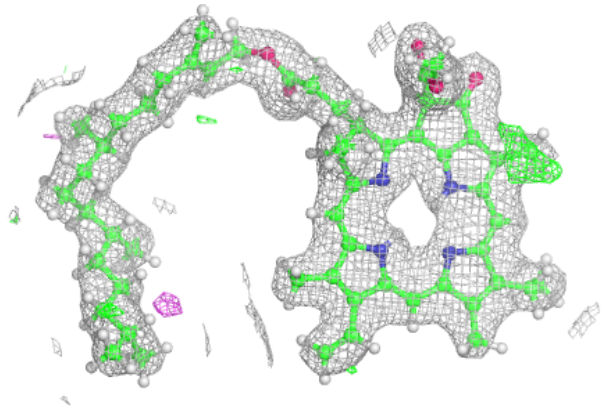
Electron density around LHG a 410:

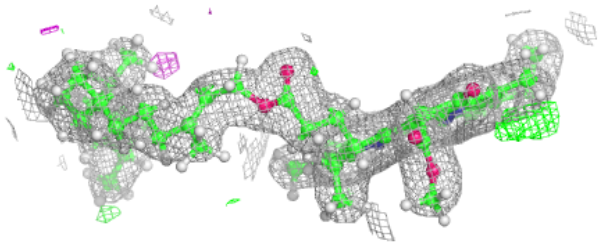
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

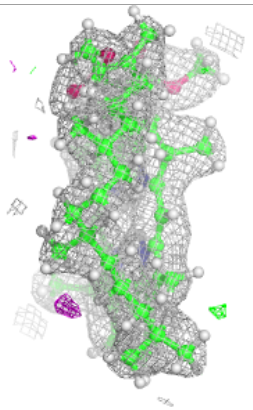


Electron density around PHO A 404:

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

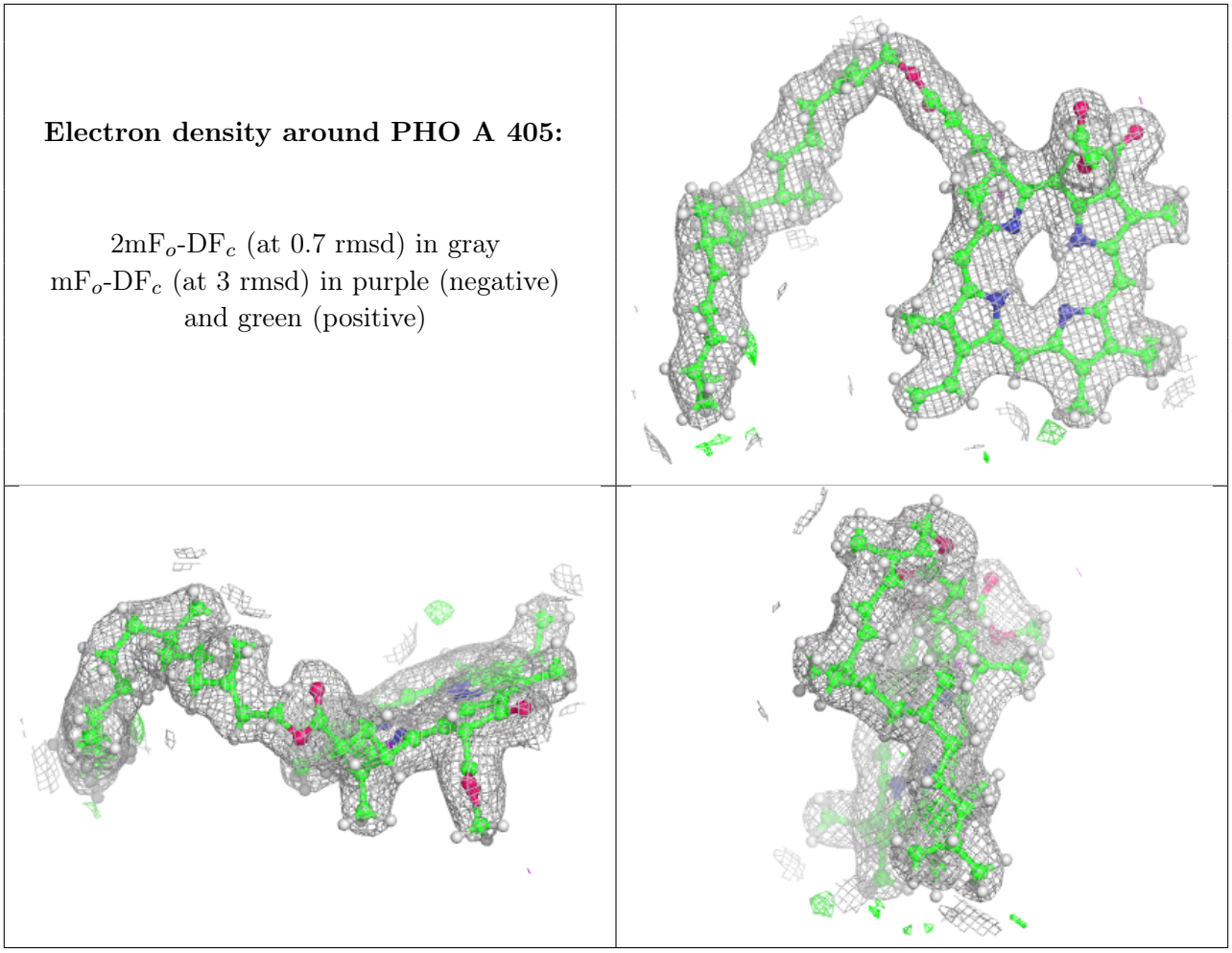






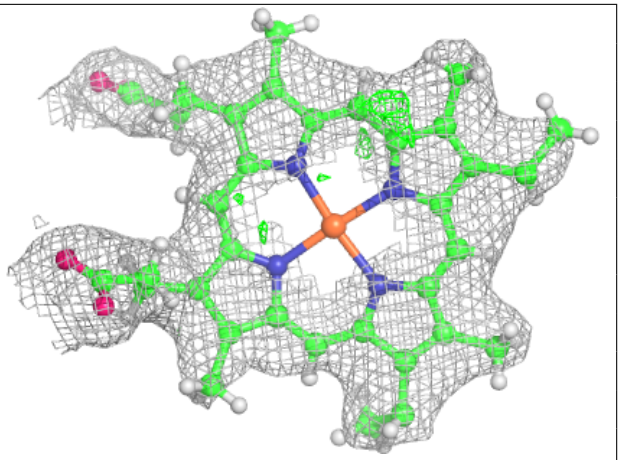
Electron density around PHO A 405:

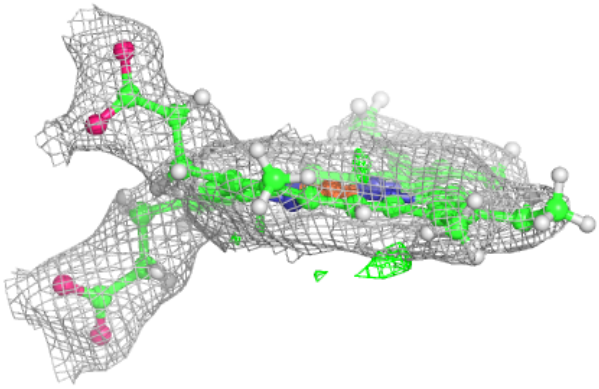
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

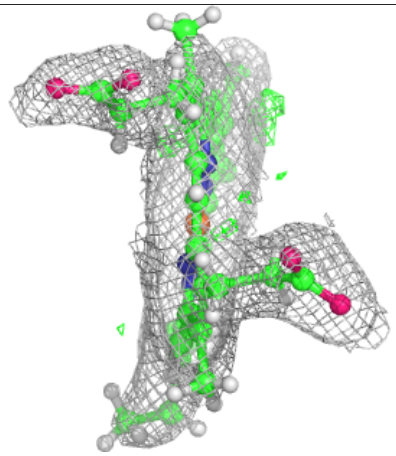


Electron density around HEC F 101:

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

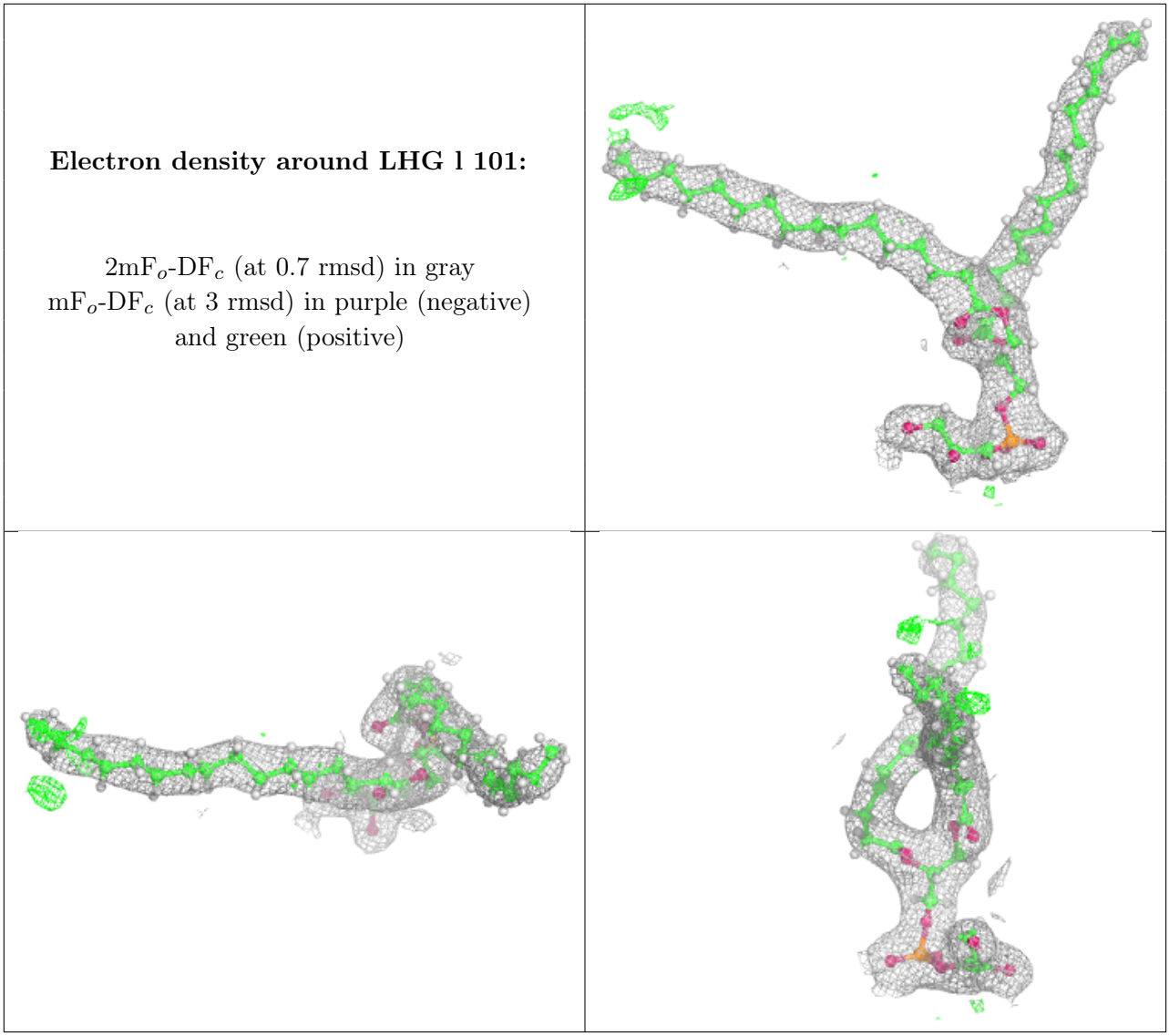






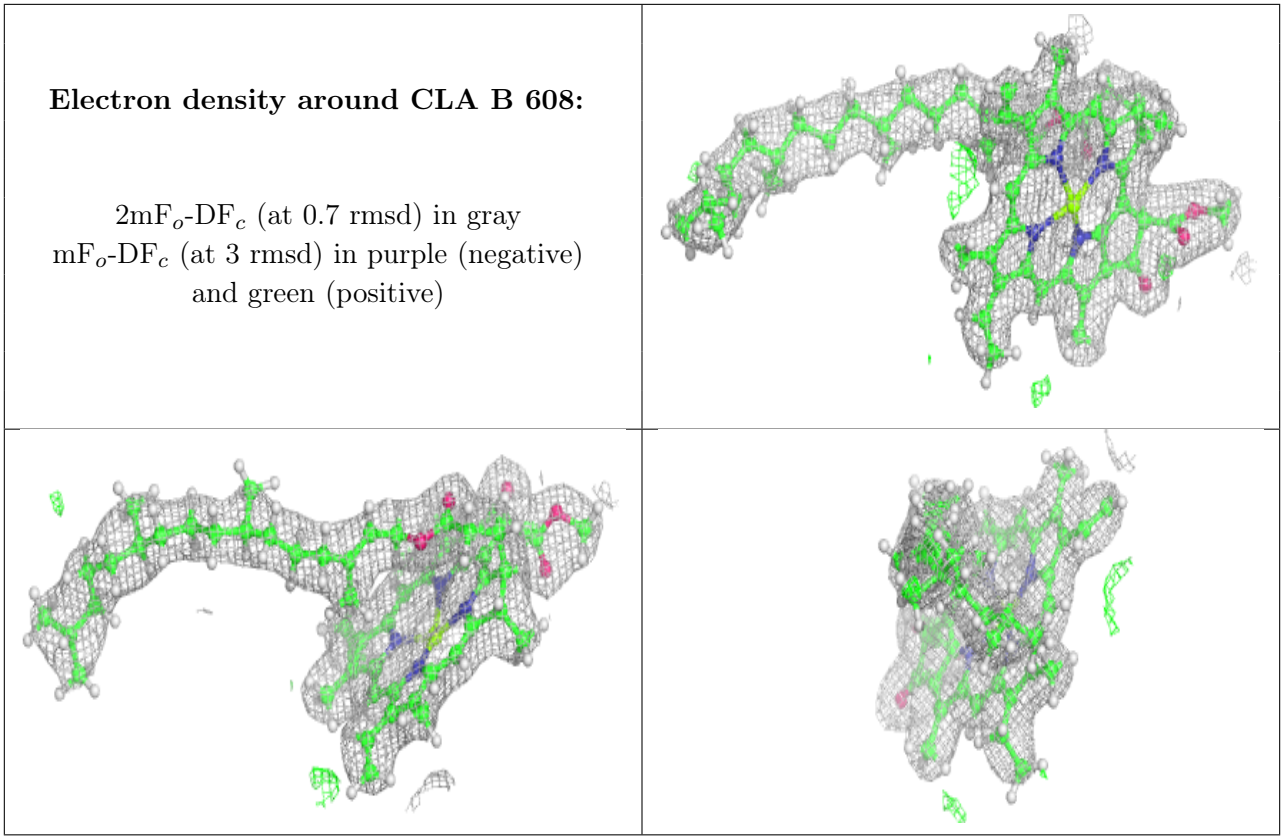
Electron density around LHG l 101:

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



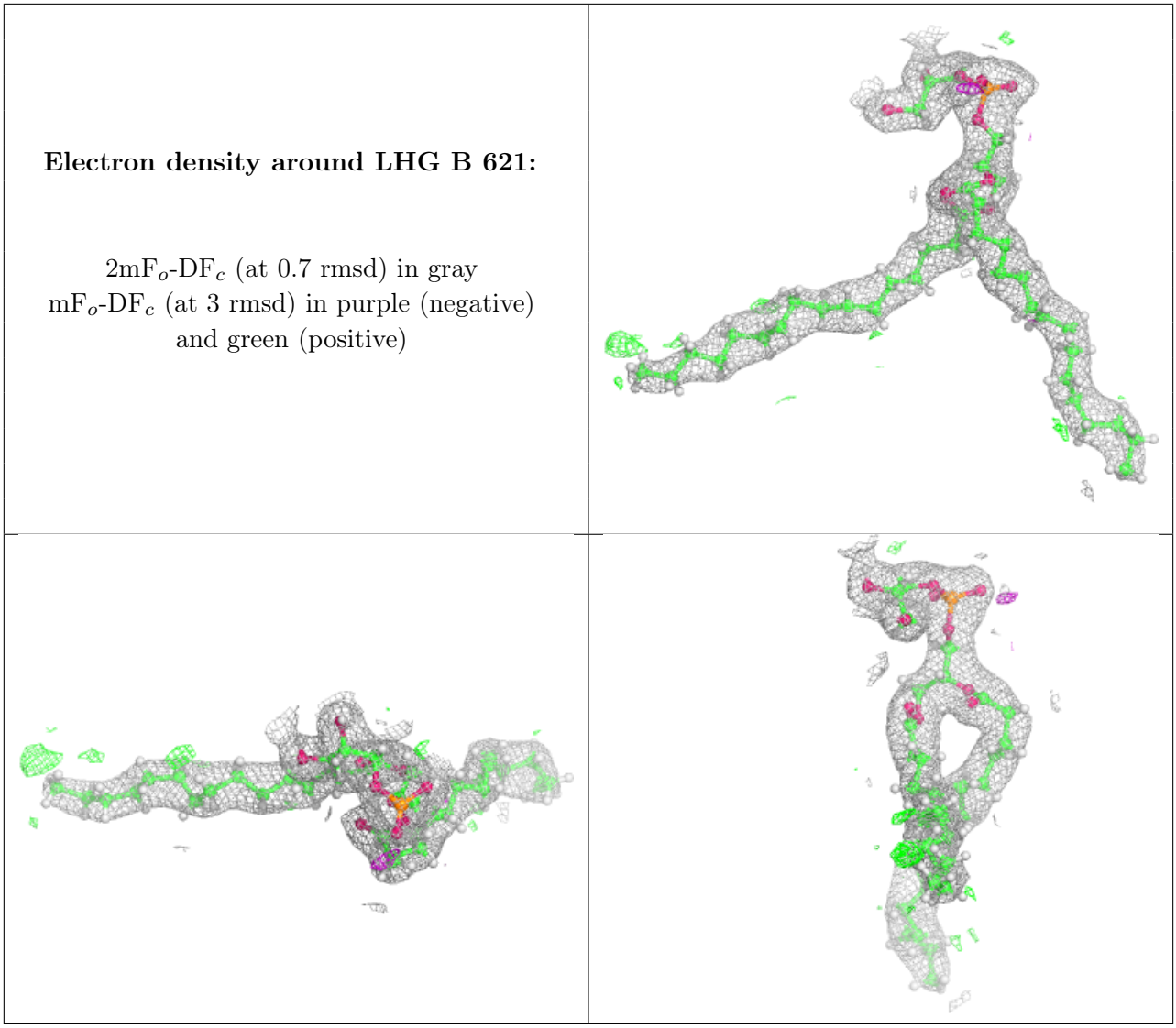
Electron density around CLA B 608:

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



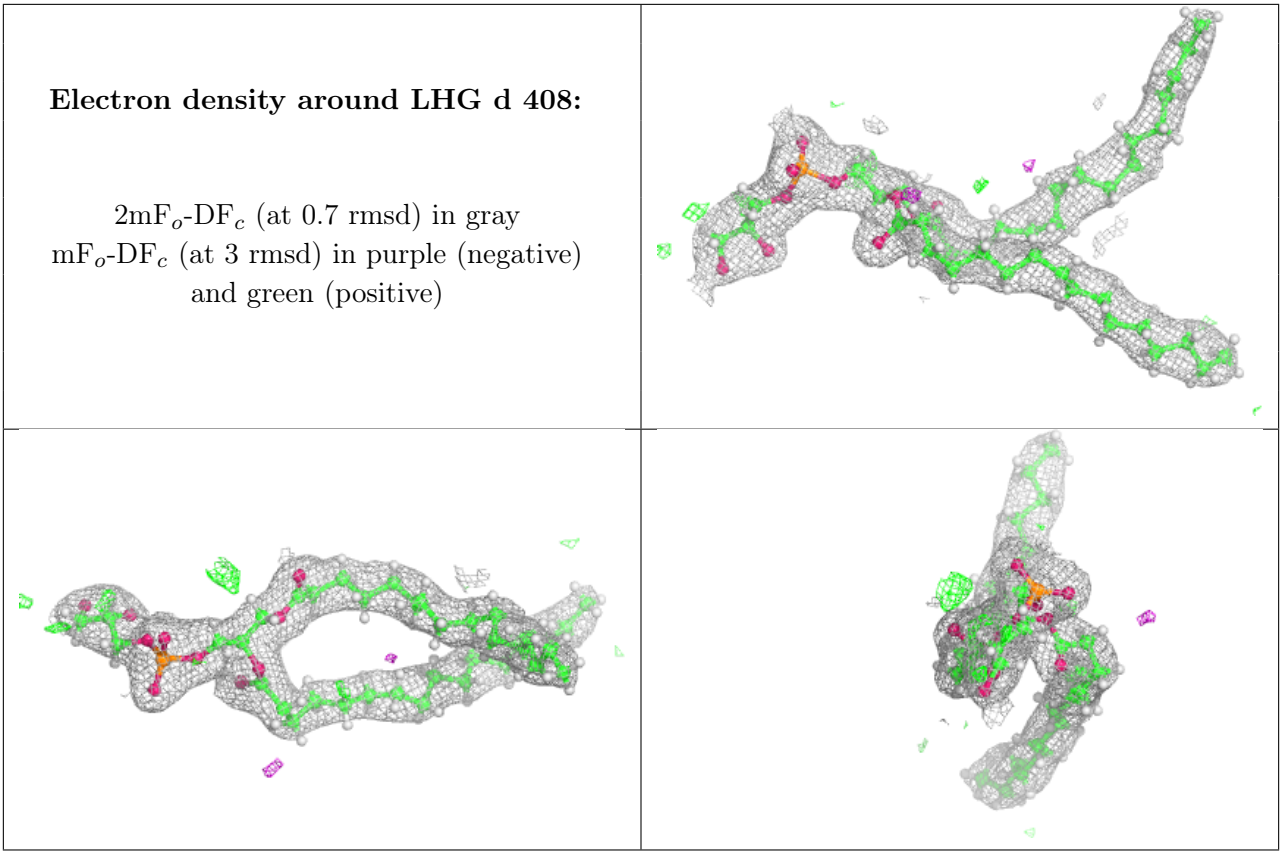
Electron density around LHG B 621:

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



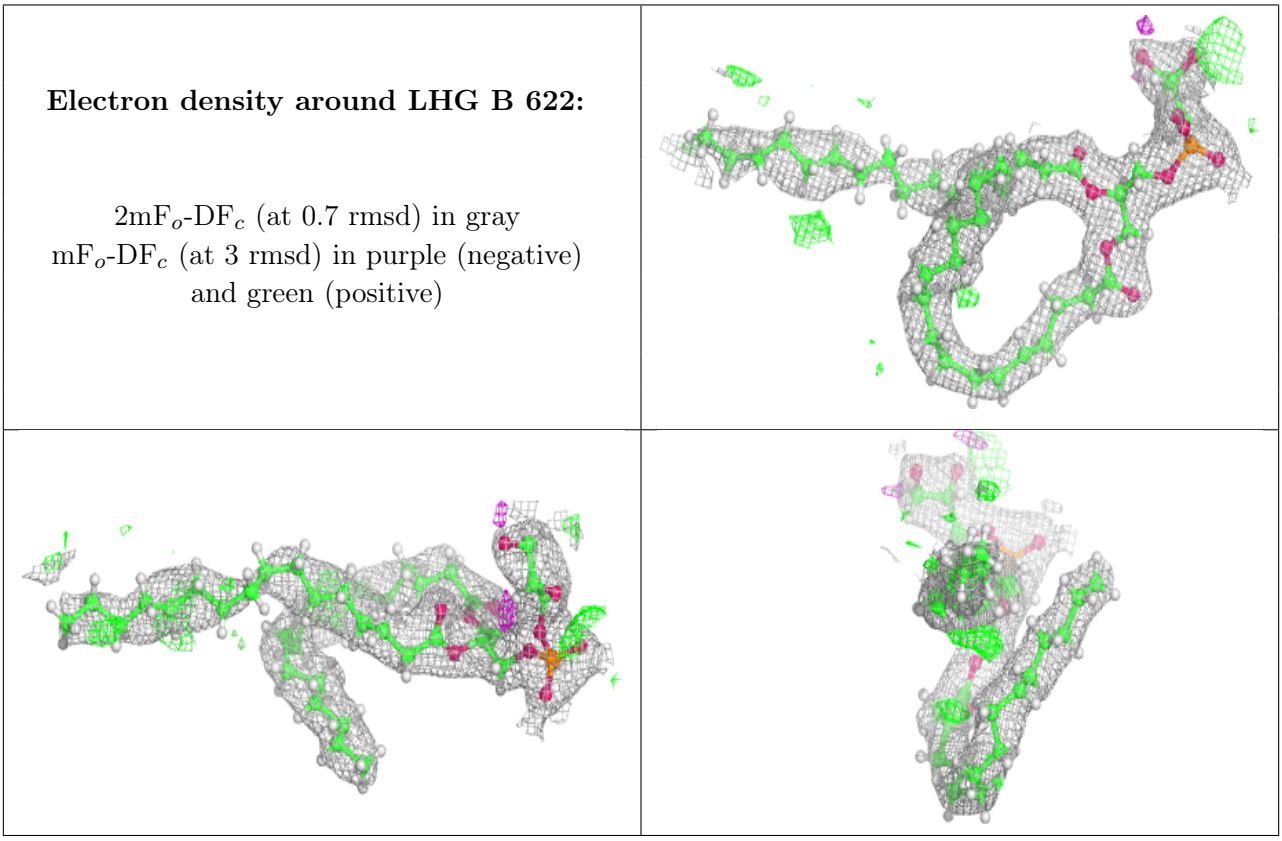
Electron density around LHG d 408:

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



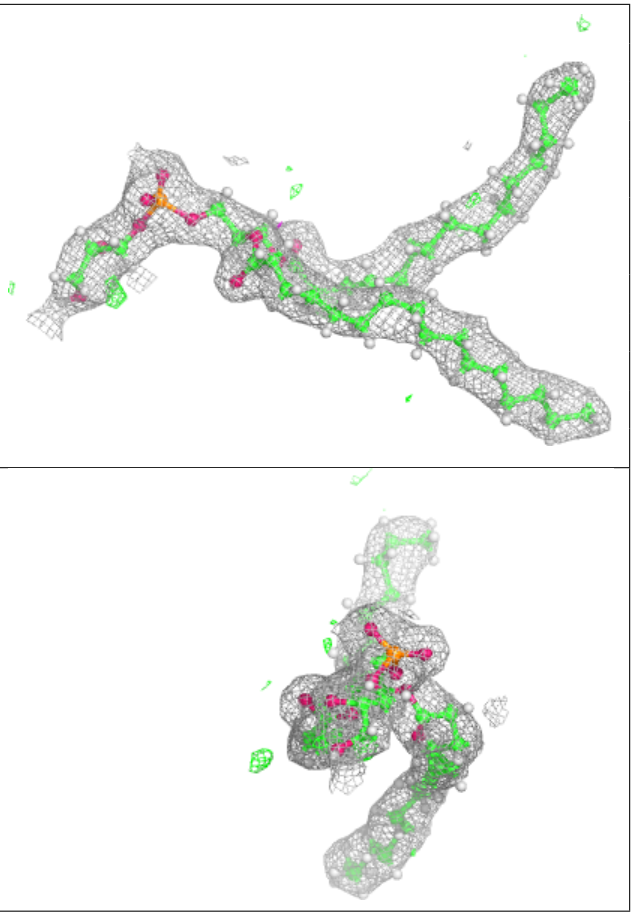
Electron density around LHG B 622:

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



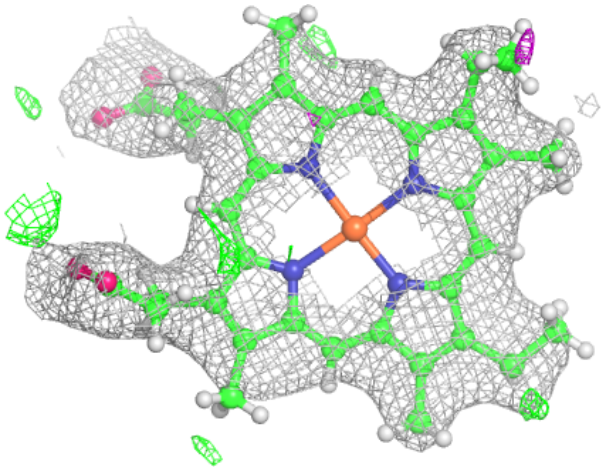
Electron density around LHG D 409:

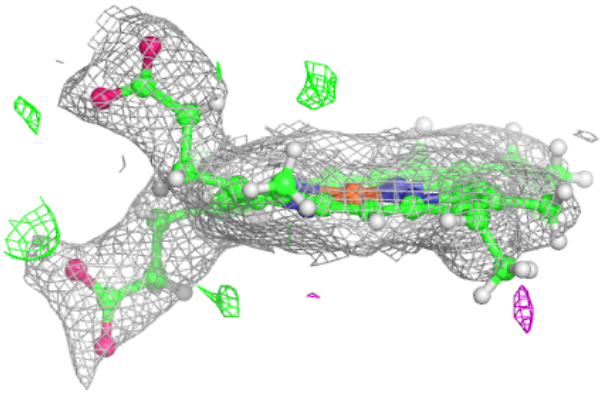
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

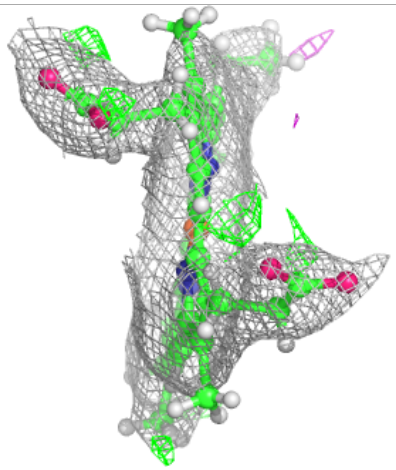


Electron density around HEC f 101:

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

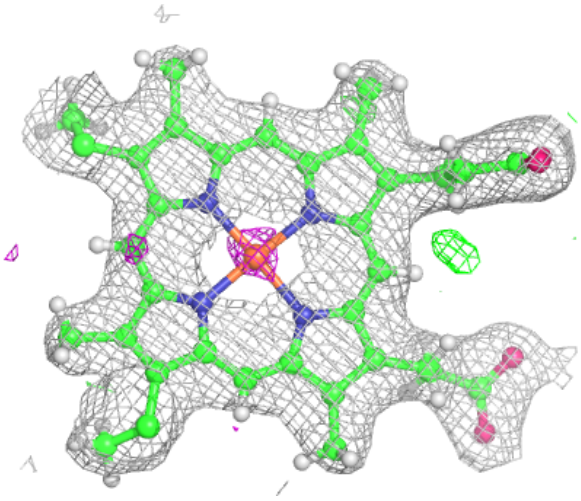


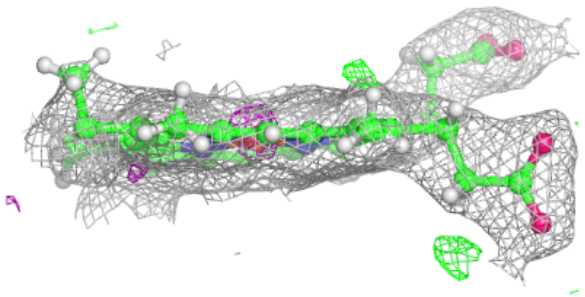


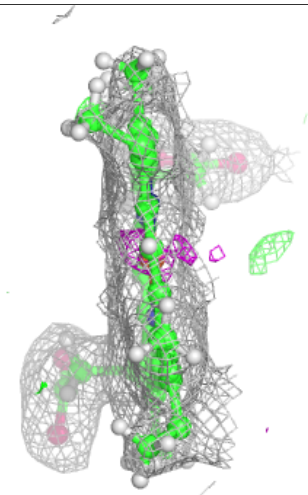


Electron density around HEC V 201:

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

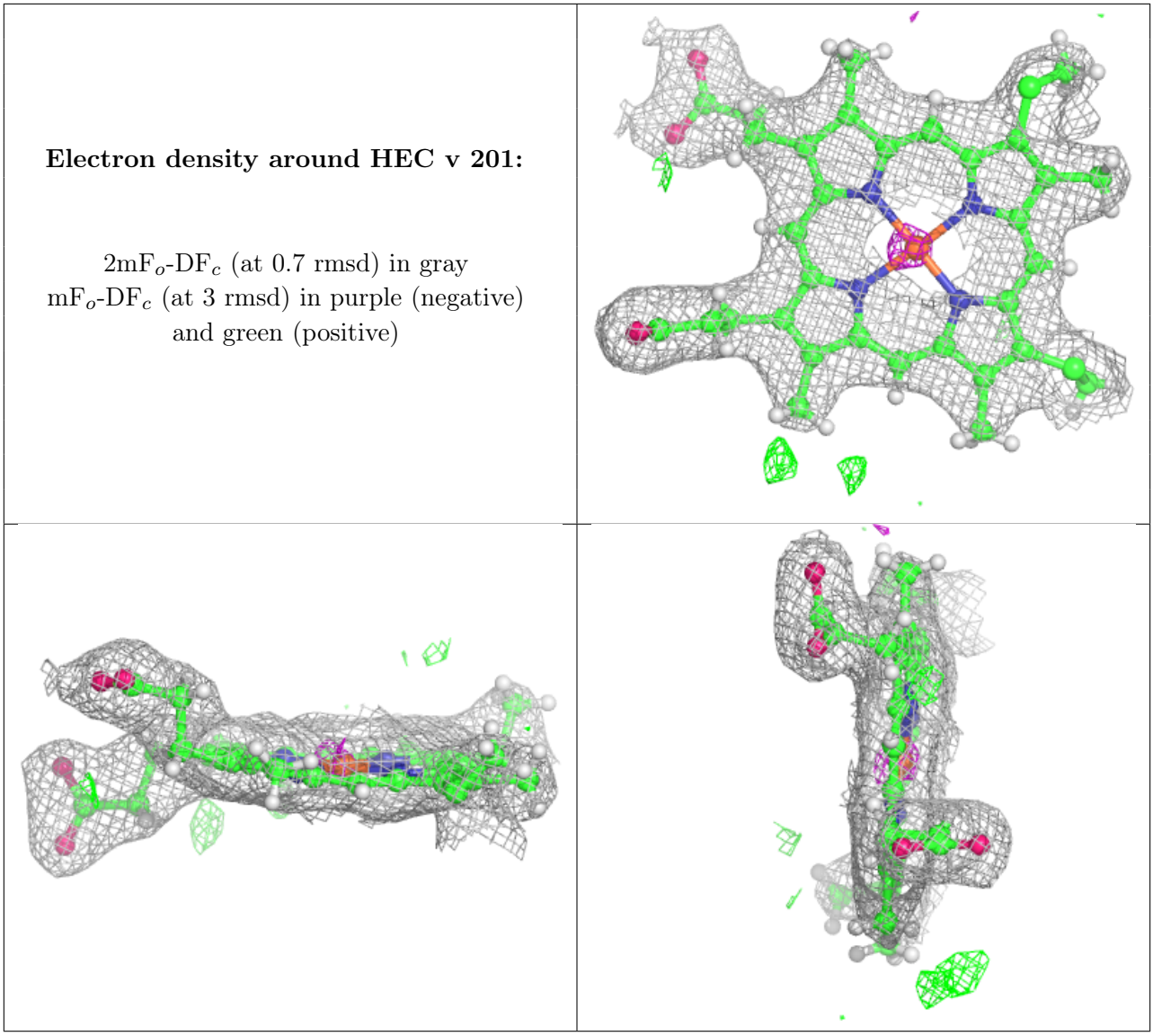






Electron density around HEC v 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.