Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 05:37 PM EDT

PDB ID	:	5TIS
Title	:	Room temperature XFEL structure of the native, doubly-illuminated photosystem II complex
Authors	:	Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Fuller, F.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Hussein, R.; Zhang, M.; Douthit, L.; Kubin, M.; de Lichtenberg, C.; Pham, L.V.; Nilsson, H.; Cheah, M.H.; Shevela, D.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Pastor, E.; Weninger, C.; Fransson, T.; Lassalle, L.; Braeuer, P.; Aller, P.; Docker, P.T.; Andi, B.; Orville, A.M.; Glownia, J.M.; Nelson, S.; Sikorski, M.; Zhu, D.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Watermann, D.G.; Evans, G.; Wernet, P.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on	:	2016-10-03
Resolution	:	2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

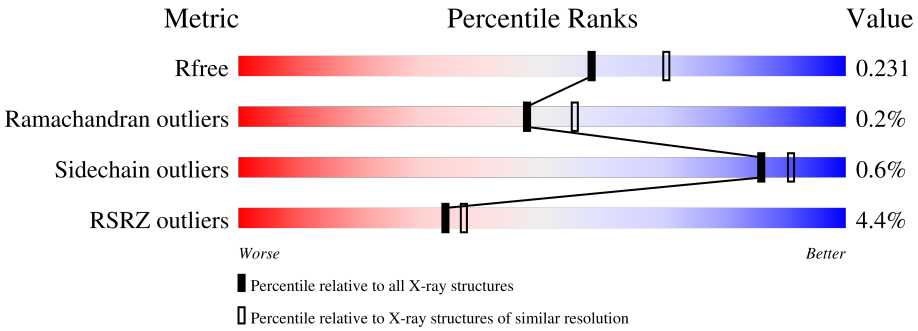
The following versions of software and data (see references (1)) were used in the production of this report:

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 2.25 Å.

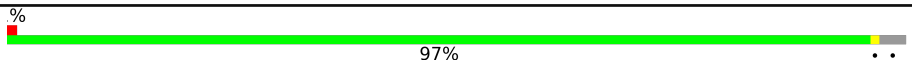
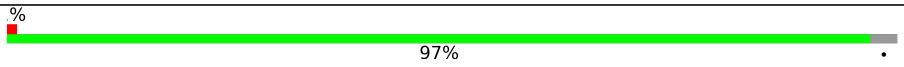
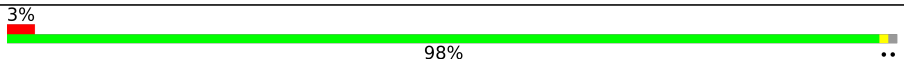
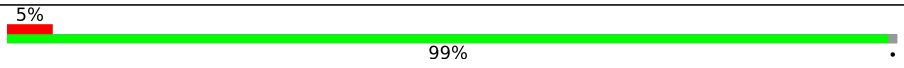
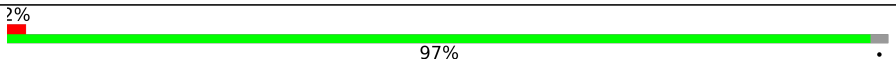
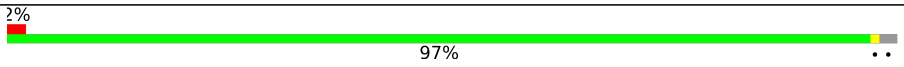
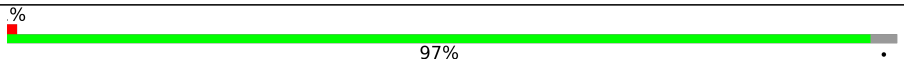
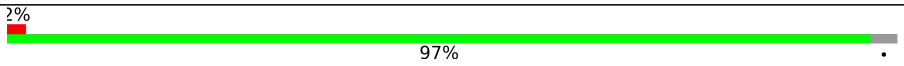
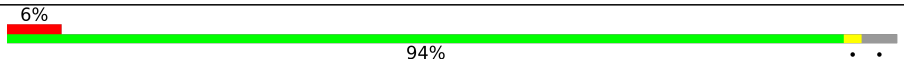
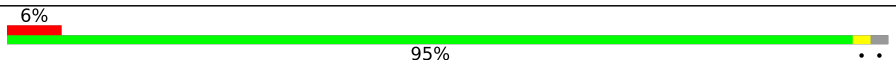
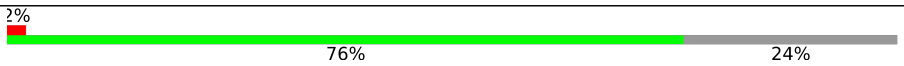
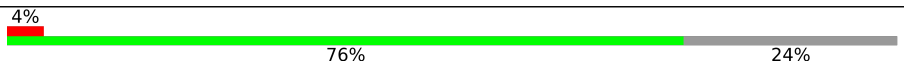
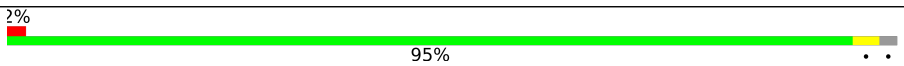
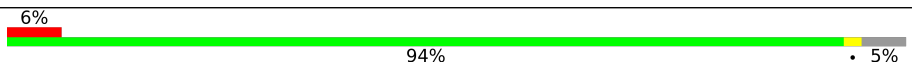
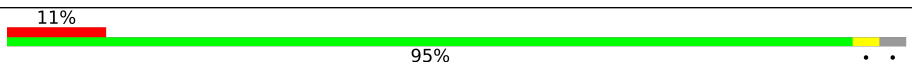
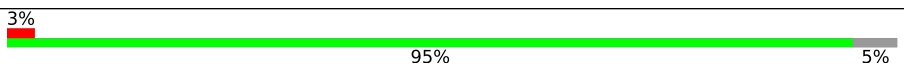
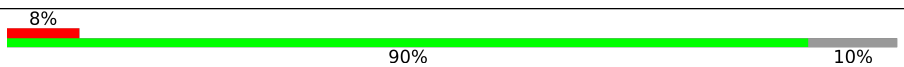
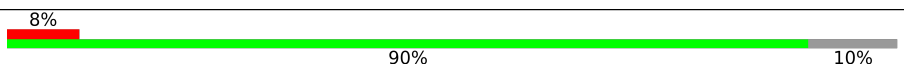
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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.

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)
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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
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	
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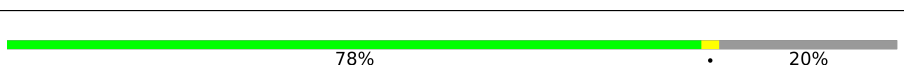
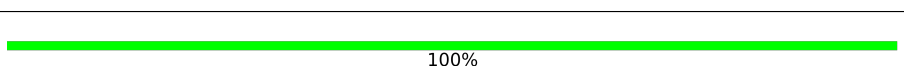
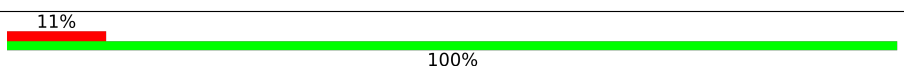
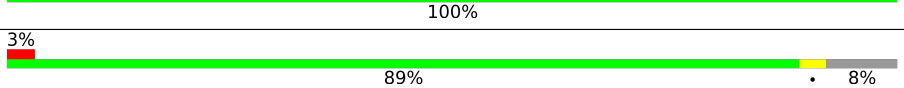
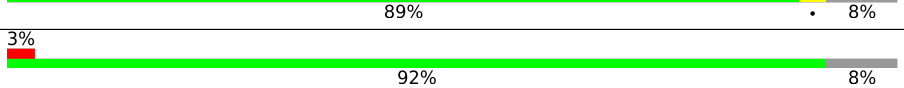
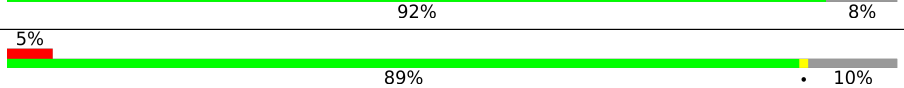
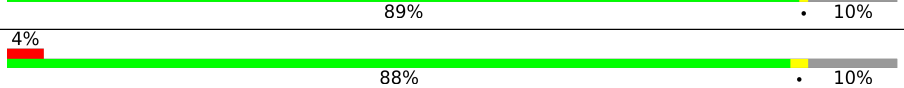
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	

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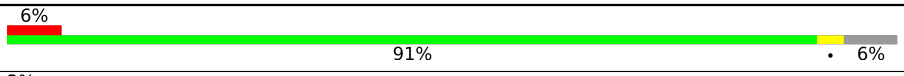
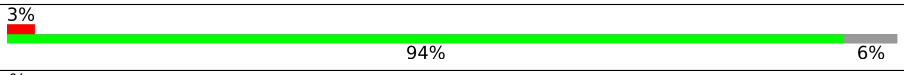
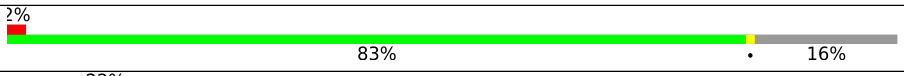
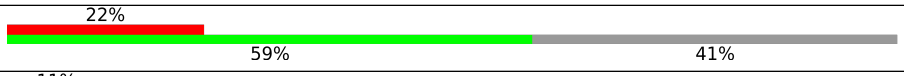
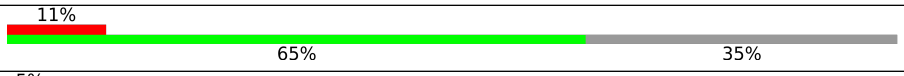
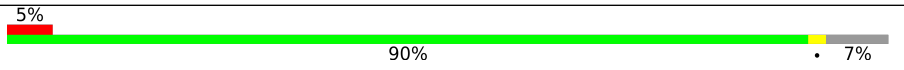
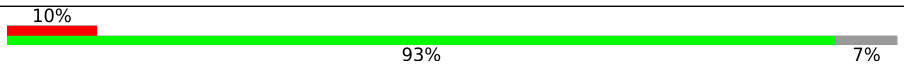
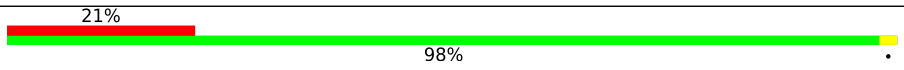
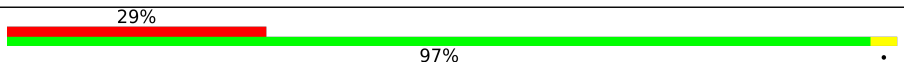
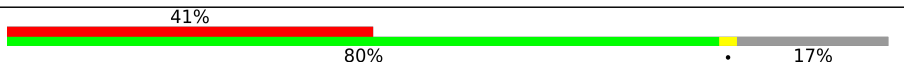
Mol	Chain	Length	Quality of chain
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	613	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	C	514	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	610	X	-	-	-
25	CLA	a	615	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606[A]	X	-	-	-
25	CLA	b	606[B]	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	402	X	-	-	-

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 51757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2625	1719	431	460	15			
1	a	334	Total	C	N	O	S	0	0	0
			2622	1717	431	459	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	5	0
			4005	2629	667	696	13			
2	b	504	Total	C	N	O	S	0	2	0
			3982	2613	665	691	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	1	0
			3494	2287	585	609	13			
3	c	451	Total	C	N	O	S	0	1	0
			3494	2286	587	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			
4	d	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 670	C 437	N 109	O 124	0	1	0
5	e	82	Total 671	C 438	N 108	O 125	0	1	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 510	C 341	N 82	O 85	S 2	0	0	0
7	h	63	Total 498	C 333	N 80	O 83	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	37	Total 304	C 206	N 47	O 50	S 1	0	0	0
8	i	36	Total 296	C 200	N 46	O 49	S 1	0	0	0

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total 269	C 178	N 39	O 51	S 1	0	1	0
12	m	33	Total 260	C 173	N 38	O 48	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total 1888	C 1179	N 320	O 385	S 4	0	2	0
13	o	244	Total 1888	C 1179	N 320	O 385	S 4	0	2	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1070	680	178	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0	0
			200	131	35	31	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
18	x	38	Total	C	N	O	0	1	0
			285	192	46	47			

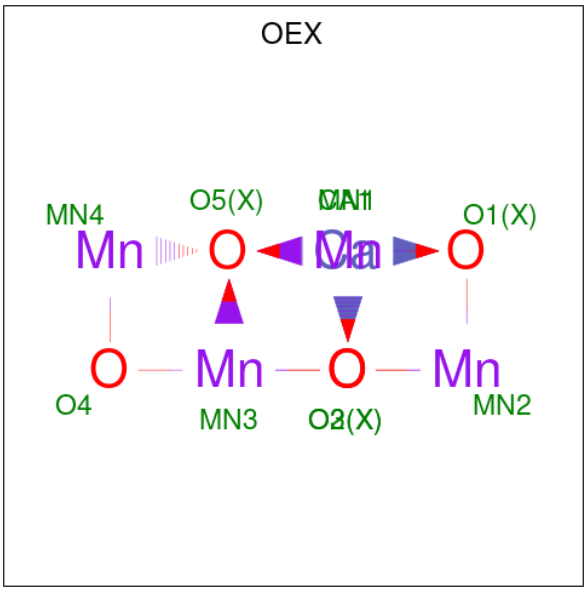
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			478	328	72	76	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			
20	r	34	Total	C	N	O	0	0	0
			270	183	47	40			

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



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

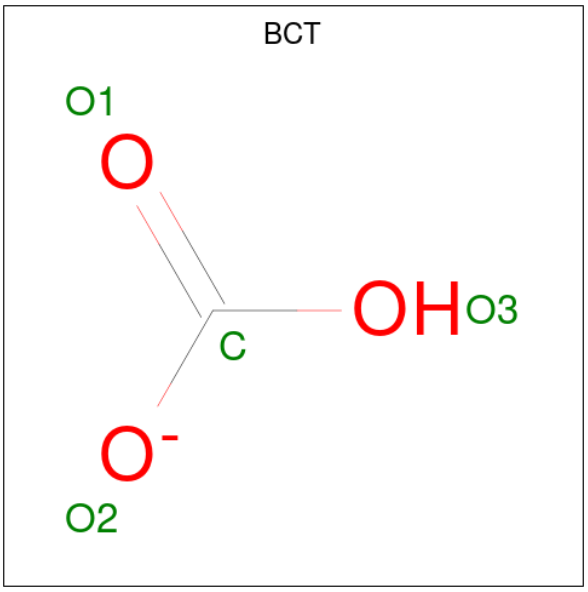
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

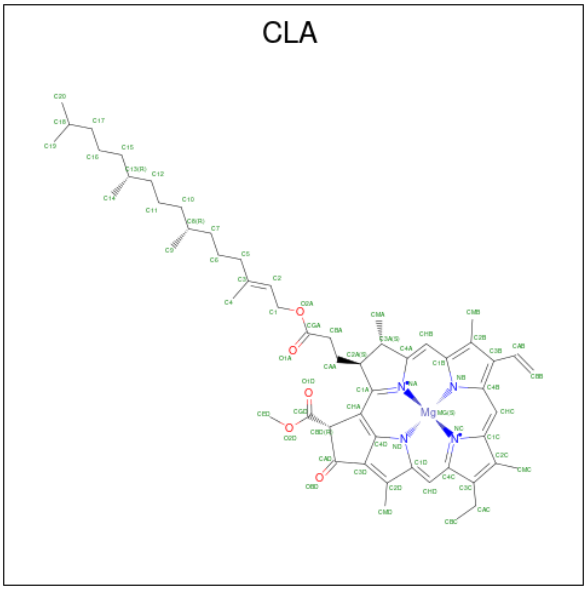
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	2	Total Cl 2 2	0	0
23	a	2	Total Cl 2 2	0	0

- Molecule 24 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
25	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	1
			129	110	1	8	10		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			64	54	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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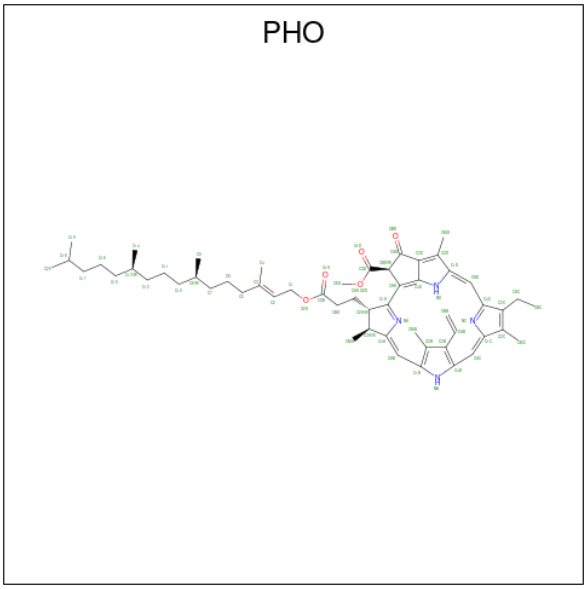
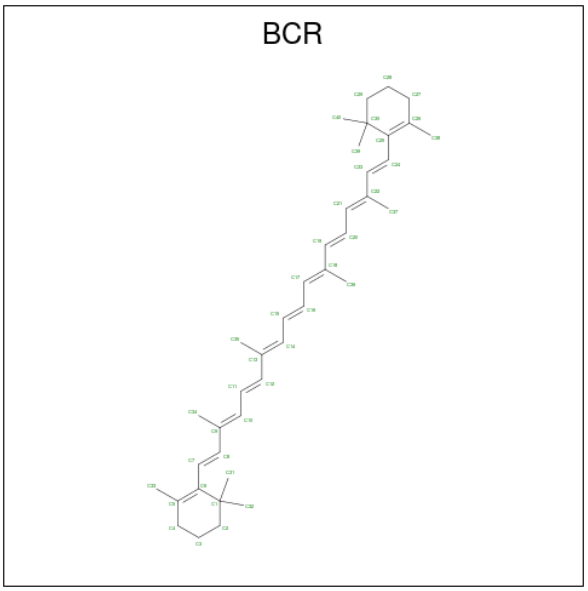
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	Y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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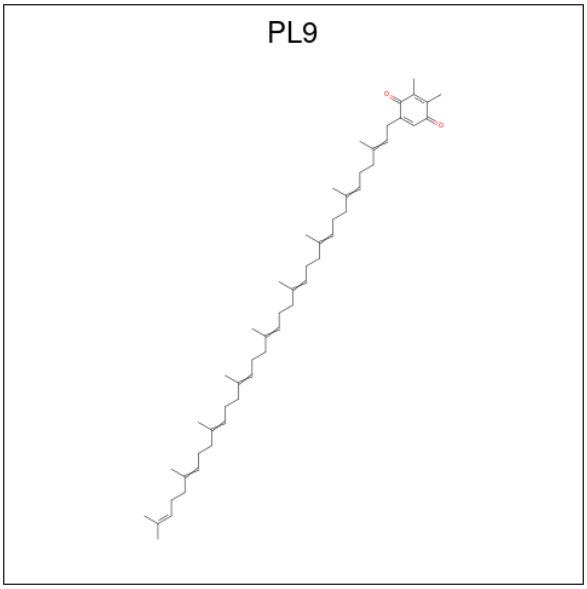
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



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

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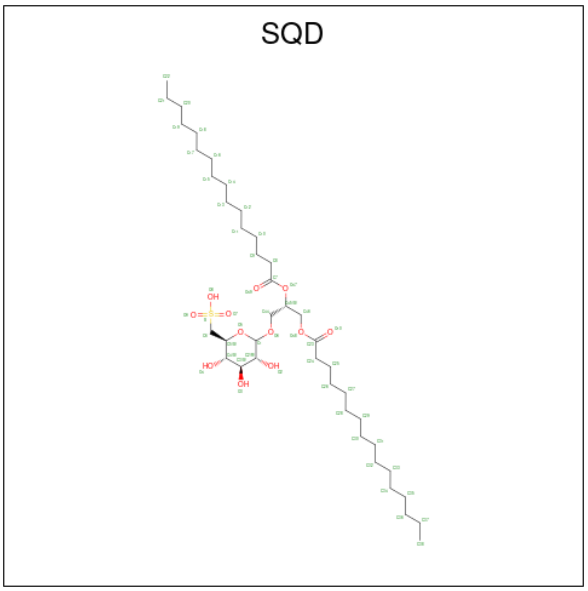
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	a	1	Total C O 55 53 2	0	0
28	d	1	Total C O 55 53 2	0	0

- 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 O S 52 39 12 1	0	0
29	A	1	Total C O S 54 41 12 1	0	0
29	B	1	Total C O S 54 41 12 1	0	0
29	B	1	Total C O S 54 41 12 1	0	0
29	D	1	Total C O S 43 30 12 1	0	0
29	D	1	Total C O S 47 34 12 1	0	0
29	L	1	Total C O S 49 36 12 1	0	0
29	a	1	Total C O S 54 41 12 1	0	0
29	b	1	Total C O 40 35 5	0	0

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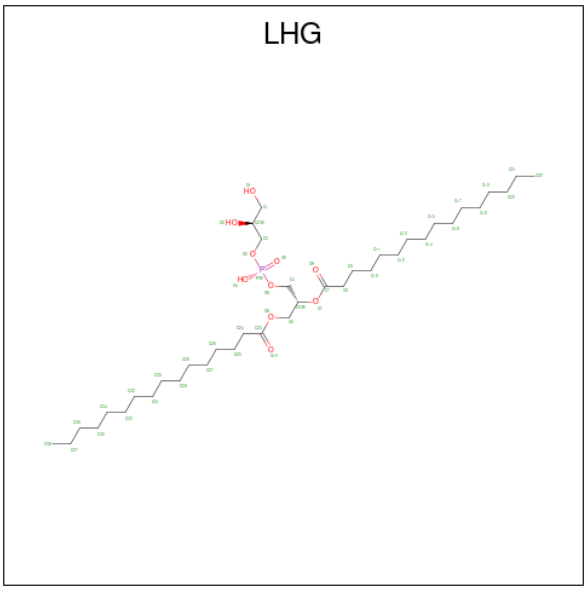
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).

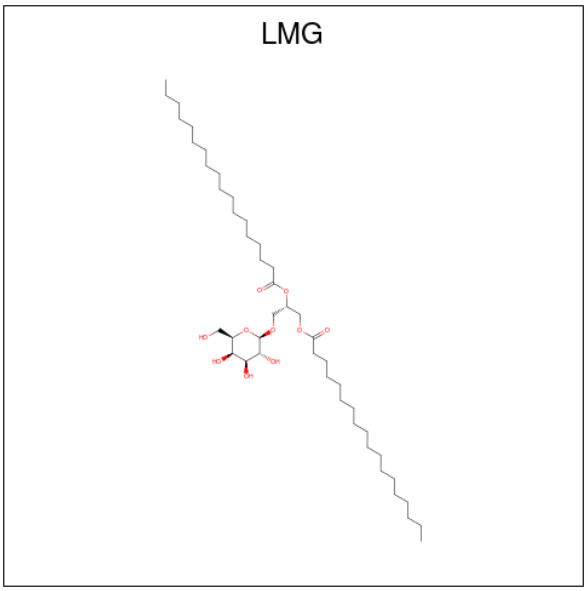


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			47	36	10	1		
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	B	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			39	28	10	1		
30	a	1	Total	C	O	P	0	0
			42	31	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

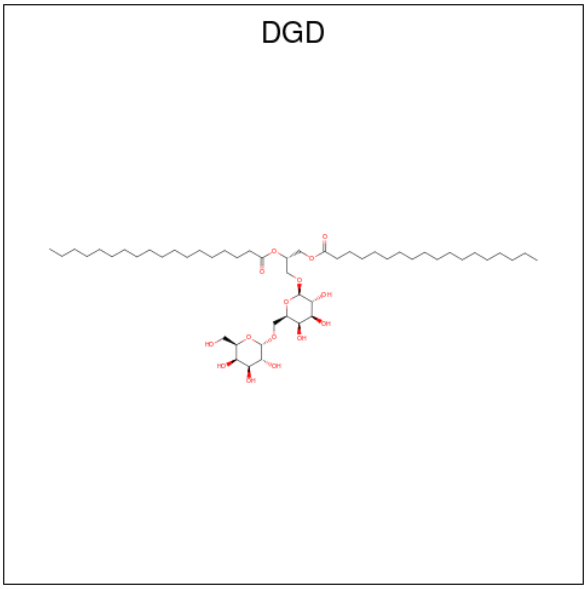
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	2	Total C O 29 27 2	0	0
31	B	2	Total C 26 26	0	0
31	C	2	Total C O 33 31 2	0	0
31	D	2	Total C 28 28	0	0
31	E	1	Total C O 12 10 2	0	0
31	H	1	Total C 7 7	0	0
31	I	2	Total C O 27 25 2	0	0
31	J	2	Total C O 23 21 2	0	0
31	M	2	Total C O 32 30 2	0	0
31	T	2	Total C 26 26	0	0
31	a	2	Total C O 29 27 2	0	0
31	b	2	Total C 28 28	0	0
31	c	3	Total C O 40 34 6	0	0
31	d	1	Total C 17 17	0	0
31	i	1	Total C O 20 18 2	0	0
31	j	2	Total C O 27 25 2	0	0
31	m	2	Total C O 25 23 2	0	0
31	t	1	Total C 18 18	0	0
31	x	1	Total C 16 16	0	0

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



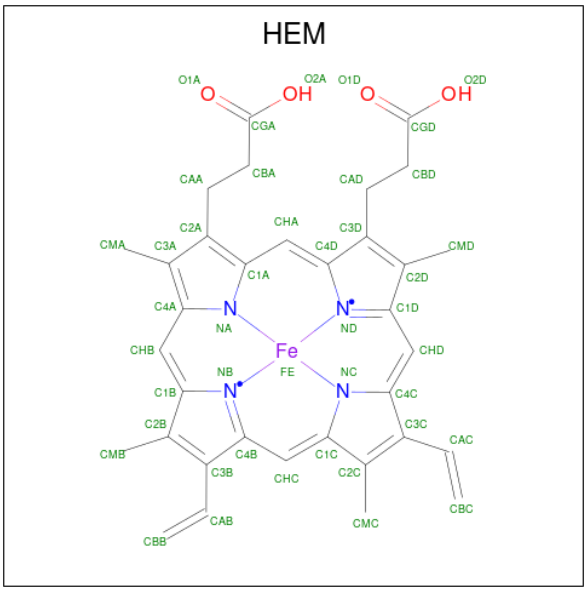
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			48	38	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	b	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			37	27	10		
32	c	1	Total	C	O	0	0
			34	24	10		
32	d	1	Total	C	O	0	0
			51	41	10		
32	d	1	Total	C	O	0	0
			38	36	2		
32	m	1	Total	C	O	0	0
			51	41	10		

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



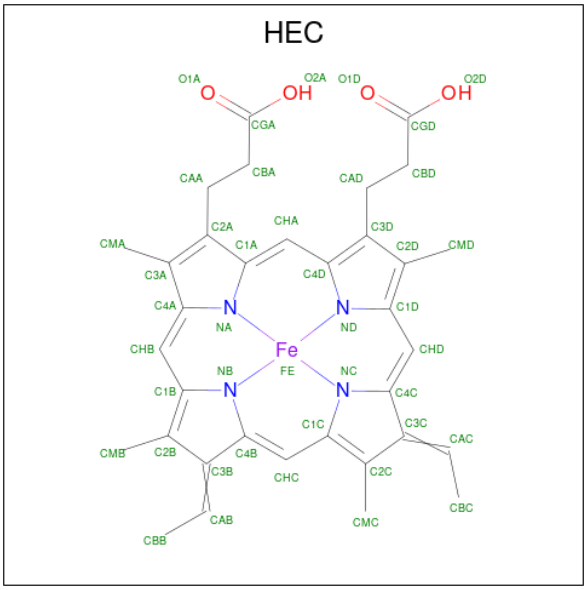
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	H	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	h	1	Total C O 62 47 15	0	0

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



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

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



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	86	Total O 86 86	0	0
36	B	109	Total O 109 109	0	0
36	C	95	Total O 95 95	0	0
36	D	82	Total O 82 82	0	0
36	E	14	Total O 14 14	0	0
36	F	3	Total O 3 3	0	0
36	H	11	Total O 11 11	0	0
36	I	3	Total O 3 3	0	0
36	J	5	Total O 5 5	0	0
36	K	2	Total O 2 2	0	0
36	L	3	Total O 3 3	0	0
36	M	5	Total O 5 5	0	0
36	O	72	Total O 72 72	0	0
36	T	9	Total O 9 9	0	0
36	U	22	Total O 22 22	0	0
36	V	42	Total O 42 42	0	0
36	X	5	Total O 5 5	0	0
36	Z	3	Total O 3 3	0	0
36	a	90	Total O 90 90	0	0
36	b	129	Total O 129 129	0	0
36	c	95	Total O 95 95	0	0

Continued on next page...

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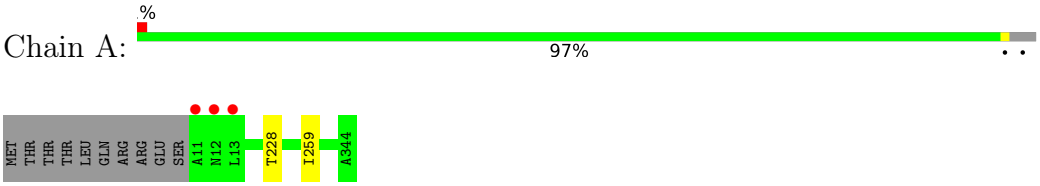
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	d	87	Total O 87 87	0	0
36	e	9	Total O 9 9	0	0
36	f	2	Total O 2 2	0	0
36	h	13	Total O 13 13	0	0
36	i	6	Total O 6 6	0	0
36	j	2	Total O 2 2	0	0
36	k	4	Total O 4 4	0	0
36	l	10	Total O 10 10	0	0
36	m	10	Total O 10 10	0	0
36	o	69	Total O 69 69	0	0
36	t	4	Total O 4 4	0	0
36	u	34	Total O 34 34	0	0
36	v	37	Total O 37 37	0	0
36	y	1	Total O 1 1	0	0
36	x	4	Total O 4 4	0	0
36	z	1	Total O 1 1	0	0
36	r	1	Total O 1 1	0	0

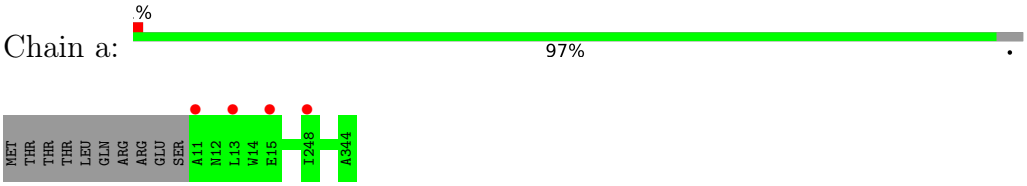
3 Residue-property plots

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.

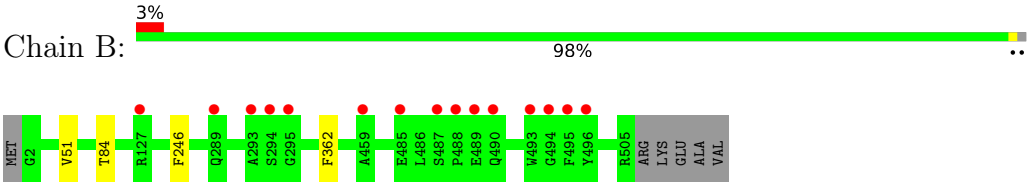
• Molecule 1: Photosystem II protein D1 1



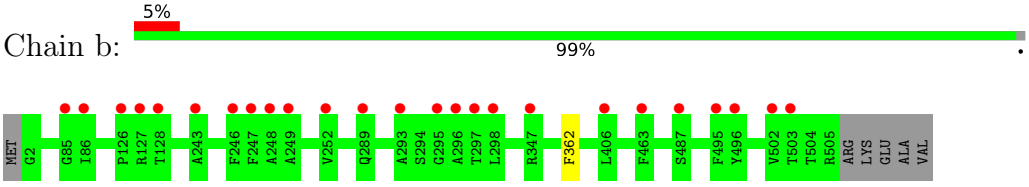
• Molecule 1: Photosystem II protein D1 1



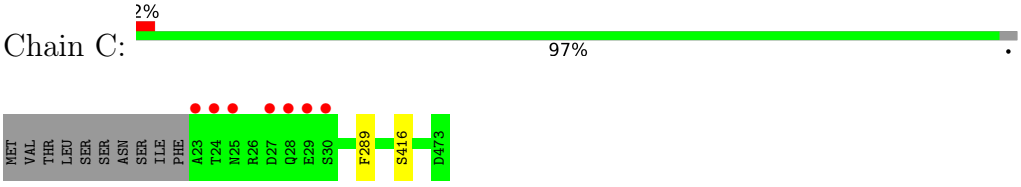
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

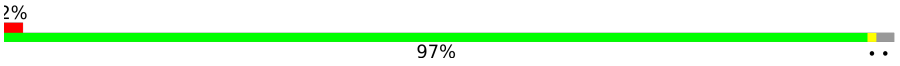


• Molecule 3: Photosystem II CP43 reaction center protein



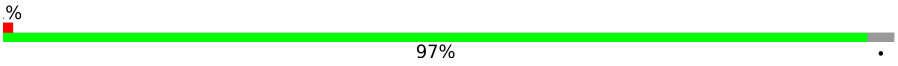
• Molecule 3: Photosystem II CP43 reaction center protein

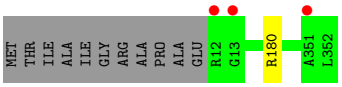
Chain c:



• Molecule 4: Photosystem II D2 protein

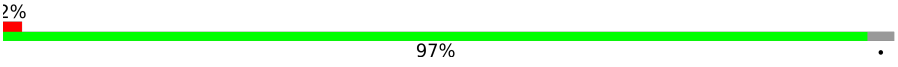
Chain D:

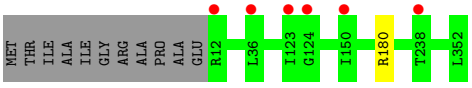




• Molecule 4: Photosystem II D2 protein

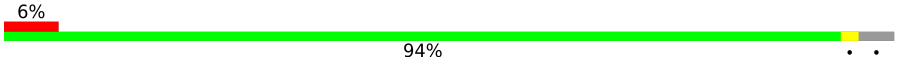
Chain d:

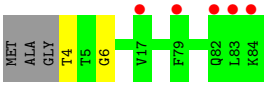




• Molecule 5: Cytochrome b559 subunit alpha

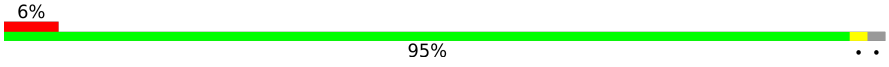
Chain E:

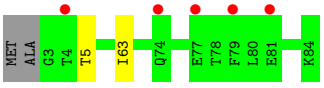




• Molecule 5: Cytochrome b559 subunit alpha

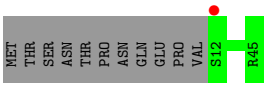
Chain e:





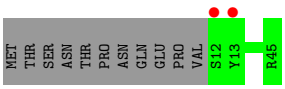
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



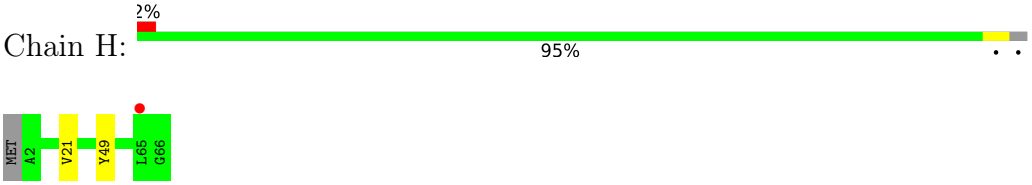
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



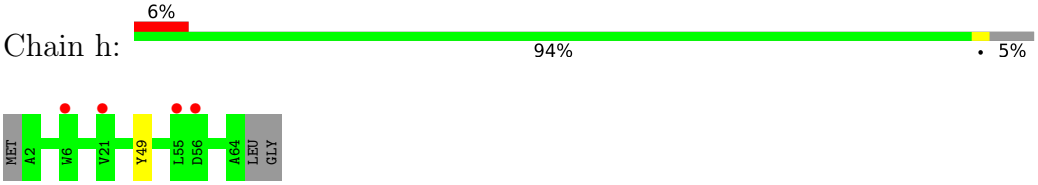
• Molecule 7: Photosystem II reaction center protein H

Chain H:



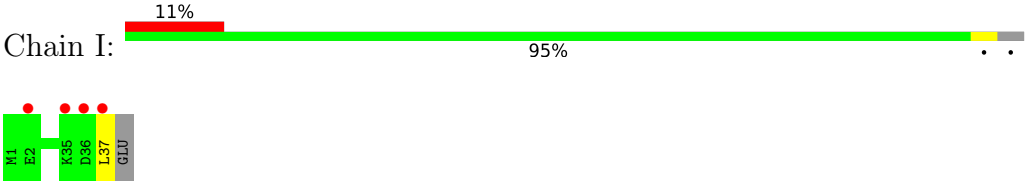
• Molecule 7: Photosystem II reaction center protein H

Chain h:



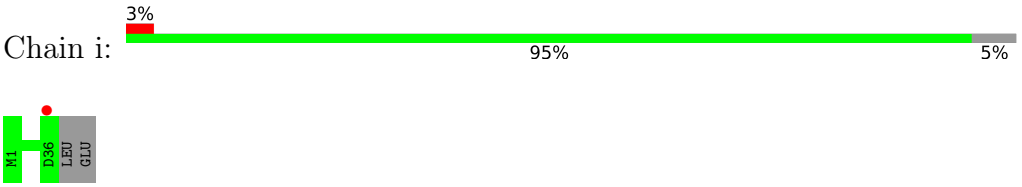
• Molecule 8: Photosystem II reaction center protein I

Chain I:



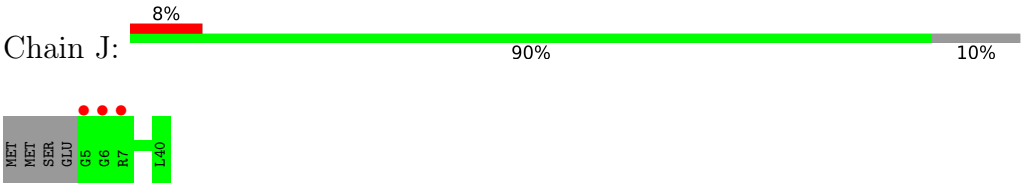
• Molecule 8: Photosystem II reaction center protein I

Chain i:



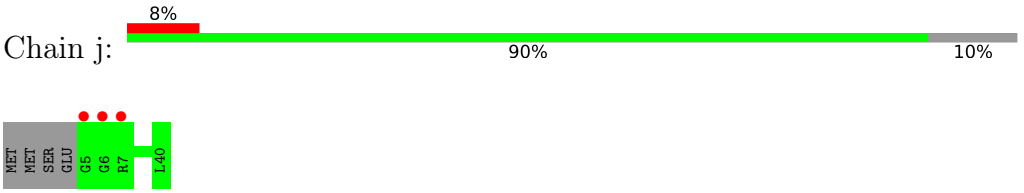
• Molecule 9: Photosystem II reaction center protein J

Chain J:



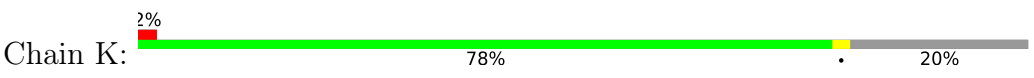
• Molecule 9: Photosystem II reaction center protein J

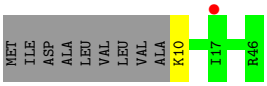
Chain j:



• Molecule 10: Photosystem II reaction center protein K

Chain K:



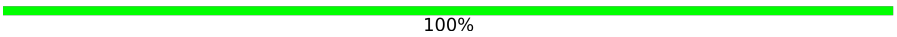


• Molecule 10: Photosystem II reaction center protein K

Chain k:

• Molecule 11: Photosystem II reaction center protein L

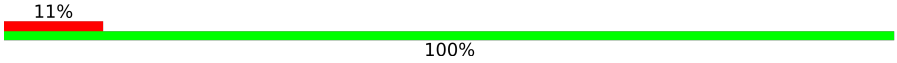
Chain L:

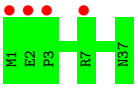


There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem II reaction center protein L

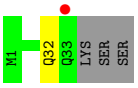
Chain l:





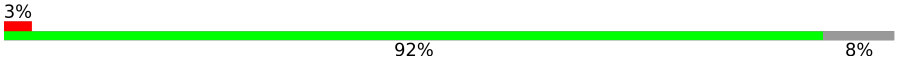
• Molecule 12: Photosystem II reaction center protein M

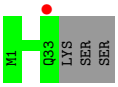
Chain M:



• Molecule 12: Photosystem II reaction center protein M

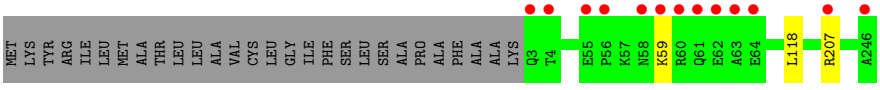
Chain m:





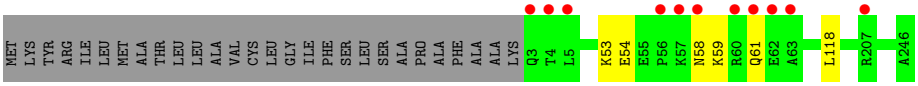
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

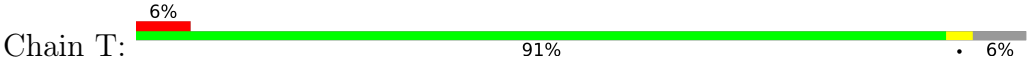


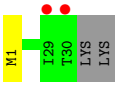
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

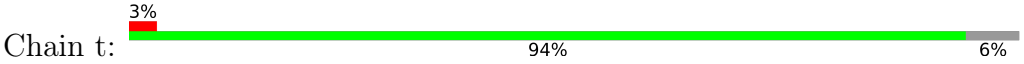


• Molecule 14: Photosystem II reaction center protein T

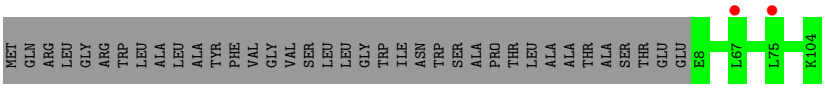




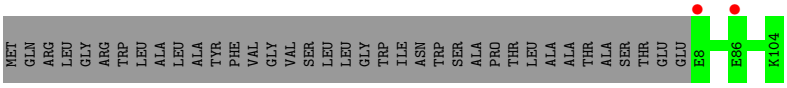
• Molecule 14: Photosystem II reaction center protein T



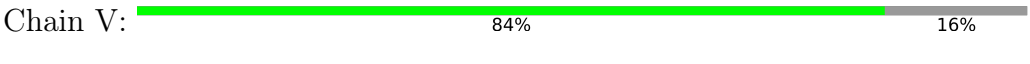
• Molecule 15: Photosystem II 12 kDa extrinsic protein

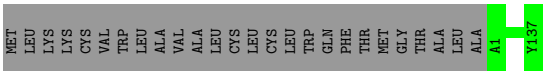


• Molecule 15: Photosystem II 12 kDa extrinsic protein

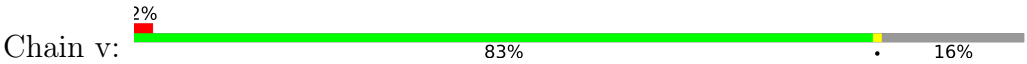


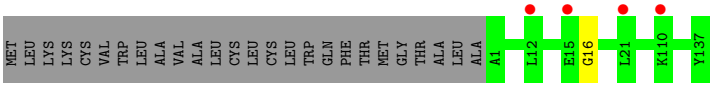
• Molecule 16: Cytochrome c-550





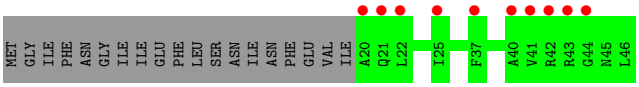
• Molecule 16: Cytochrome c-550





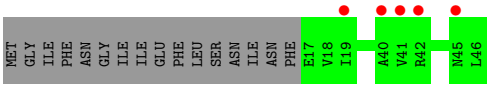
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



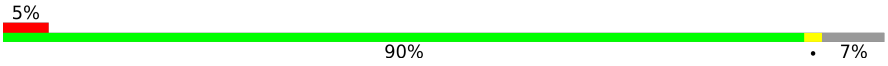
• Molecule 17: Photosystem II reaction center protein Ycf12

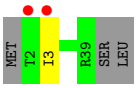
Chain y:



• Molecule 18: Photosystem II reaction center X protein

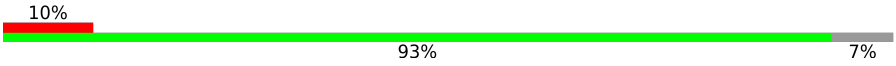
Chain X:

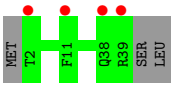




• Molecule 18: Photosystem II reaction center X protein

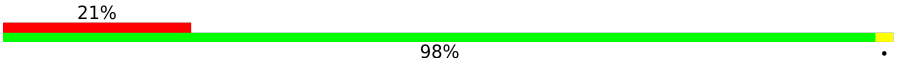
Chain x:

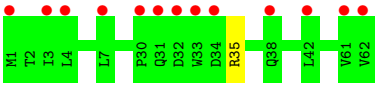




• Molecule 19: Photosystem II reaction center protein Z

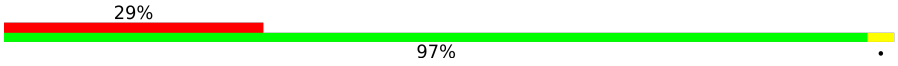
Chain Z:

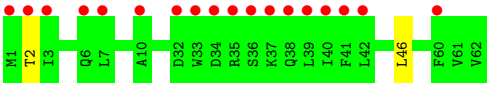




• Molecule 19: Photosystem II reaction center protein Z

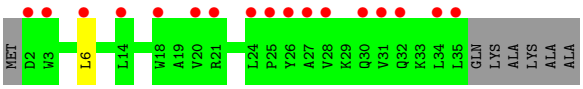
Chain z:



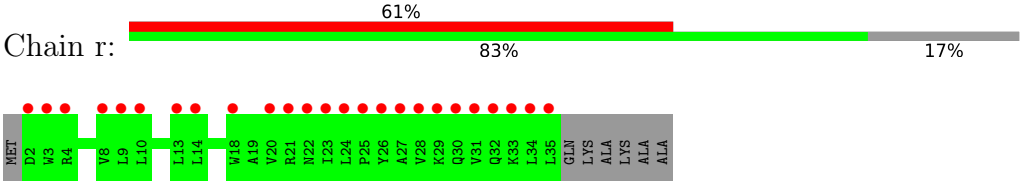


• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.87Å 223.14Å 310.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 2.25 44.28 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.28-2.25) 90.6 (44.28-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.78 (at 2.24Å)	Xtriage
Refinement program	PHENIX dev_2481	Depositor
R, R_{free}	0.193 , 0.231 0.193 , 0.231	Depositor DCC
R_{free} test set	3426 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	51757	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OEX, CLA, PL9, PHO, FME, BCT, HEC, DGD, LHG, FE2, UNL, CL, HEM, SQD, BCR, 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	0.25	0/2713	0.40	0/3700
1	a	0.25	0/2707	0.40	0/3692
2	B	0.25	0/4155	0.40	0/5661
2	b	0.25	0/4125	0.40	0/5621
3	C	0.25	0/3607	0.40	0/4911
3	c	0.25	0/3610	0.40	0/4914
4	D	0.26	0/2812	0.41	0/3832
4	d	0.25	0/2811	0.41	0/3830
5	E	0.23	0/689	0.37	0/940
5	e	0.30	1/693 (0.1%)	0.38	0/945
6	F	0.24	0/284	0.36	0/387
6	f	0.24	0/284	0.35	0/387
7	H	0.25	0/523	0.41	0/713
7	h	0.24	0/511	0.39	0/697
8	I	0.25	0/301	0.43	0/407
8	i	0.26	0/293	0.38	0/396
9	J	0.25	0/263	0.40	0/356
9	j	0.25	0/263	0.39	0/356
10	K	0.26	0/303	0.39	0/416
10	k	0.26	0/303	0.37	0/416
11	L	0.24	0/311	0.37	0/422
11	l	0.24	0/311	0.37	0/422
12	M	0.24	0/262	0.34	0/358
12	m	0.24	0/253	0.35	0/346
13	O	0.24	0/1925	0.46	0/2610
13	o	0.25	0/1925	0.47	0/2609
14	T	0.27	0/257	0.34	0/349
14	t	0.27	0/257	0.36	0/349
15	U	0.24	0/785	0.42	0/1064
15	u	0.24	0/785	0.42	0/1064
16	V	0.23	0/1085	0.41	0/1473
16	v	0.23	0/1094	0.40	0/1484

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.24	0/201	0.39	0/268
17	y	0.24	0/225	0.37	0/301
18	X	0.24	0/284	0.37	0/384
18	x	0.24	0/291	0.38	0/392
19	Z	0.24	0/490	0.35	0/669
19	z	0.24	0/489	0.36	0/669
20	R	0.22	0/279	0.40	0/383
20	r	0.22	0/276	0.36	0/379
All	All	0.25	1/43035 (0.0%)	0.40	0/58572

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	5.06	1.43	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	327 (98%)	5 (2%)	1 (0%)	41	46
1	a	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
2	B	507/510 (99%)	498 (98%)	9 (2%)	0	100	100
2	b	504/510 (99%)	491 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	450/461 (98%)	439 (98%)	10 (2%)	1 (0%)	47 55
3	c	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	47 55
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100 100
4	d	339/352 (96%)	328 (97%)	11 (3%)	0	100 100
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12 8
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100 100
6	F	32/45 (71%)	32 (100%)	0	0	100 100
6	f	32/45 (71%)	32 (100%)	0	0	100 100
7	H	63/66 (96%)	60 (95%)	3 (5%)	0	100 100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100 100
8	I	35/38 (92%)	32 (91%)	3 (9%)	0	100 100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100 100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100 100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100 100
10	K	35/46 (76%)	35 (100%)	0	0	100 100
10	k	35/46 (76%)	35 (100%)	0	0	100 100
11	L	35/37 (95%)	35 (100%)	0	0	100 100
11	l	35/37 (95%)	35 (100%)	0	0	100 100
12	M	32/36 (89%)	30 (94%)	1 (3%)	1 (3%)	4 1
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100 100
13	O	244/272 (90%)	235 (96%)	8 (3%)	1 (0%)	34 37
13	o	244/272 (90%)	229 (94%)	11 (4%)	4 (2%)	9 5
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100 100
14	t	28/32 (88%)	28 (100%)	0	0	100 100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100 100
15	u	95/134 (71%)	91 (96%)	4 (4%)	0	100 100
16	V	135/163 (83%)	130 (96%)	5 (4%)	0	100 100
16	v	136/163 (83%)	130 (96%)	5 (4%)	1 (1%)	22 21
17	Y	25/46 (54%)	25 (100%)	0	0	100 100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100 100
18	X	36/41 (88%)	34 (94%)	1 (3%)	1 (3%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100 100
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9 4
20	R	32/41 (78%)	32 (100%)	0	0	100 100
20	r	32/41 (78%)	31 (97%)	1 (3%)	0	100 100
All	All	5258/5700 (92%)	5108 (97%)	137 (3%)	13 (0%)	47 55

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	53	LYS
13	o	58	ASN
3	C	416	SER
3	c	416	SER
13	o	59	LYS
19	z	2	THR
13	o	54	GLU
13	O	59	LYS
5	E	6	GLY
12	M	32	GLN
18	X	3	ILE
16	v	16	GLY
1	A	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/280 (97%)	270 (100%)	1 (0%)	91 94
1	a	270/280 (96%)	270 (100%)	0	100 100
2	B	407/407 (100%)	403 (99%)	4 (1%)	76 84
2	b	403/407 (99%)	402 (100%)	1 (0%)	93 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	353/362 (98%)	352 (100%)	1 (0%)	92	95
3	c	353/362 (98%)	349 (99%)	4 (1%)	73	82
4	D	276/283 (98%)	275 (100%)	1 (0%)	91	94
4	d	276/283 (98%)	275 (100%)	1 (0%)	91	94
5	E	73/73 (100%)	72 (99%)	1 (1%)	67	76
5	e	73/73 (100%)	72 (99%)	1 (1%)	67	76
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	28 (100%)	0	100	100
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	40
7	h	53/55 (96%)	52 (98%)	1 (2%)	57	66
8	I	33/34 (97%)	32 (97%)	1 (3%)	41	50
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	29 (97%)	1 (3%)	38	46
10	k	30/37 (81%)	29 (97%)	1 (3%)	38	46
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	29/32 (91%)	29 (100%)	0	100	100
13	O	209/228 (92%)	207 (99%)	2 (1%)	76	84
13	o	209/228 (92%)	207 (99%)	2 (1%)	76	84
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	84 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	118/138 (86%)	118 (100%)	0	100	100
17	Y	20/37 (54%)	20 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	31/34 (91%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	x	31/34 (91%)	31 (100%)	0	100 100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57 66
19	z	52/52 (100%)	51 (98%)	1 (2%)	57 66
20	R	29/33 (88%)	28 (97%)	1 (3%)	37 45
20	r	28/33 (85%)	28 (100%)	0	100 100
All	All	4359/4654 (94%)	4331 (99%)	28 (1%)	86 91

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
2	B	51	VAL
2	B	84	THR
2	B	246	PHE
2	B	362	PHE
3	C	289	PHE
4	D	180	ARG
5	E	4	THR
7	H	21	VAL
7	H	49	TYR
8	I	37	LEU
10	K	10	LYS
13	O	118	LEU
13	O	207	ARG
19	Z	35	ARG
20	R	6	LEU
2	b	362	PHE
3	c	29	GLU
3	c	289	PHE
3	c	391[A]	ARG
3	c	391[B]	ARG
4	d	180	ARG
5	e	5	THR
7	h	49	TYR
10	k	19	ASP
13	o	61	GLN
13	o	118	LEU
19	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	HIS
2	B	285	ASN
2	B	490	GLN
5	E	82	GLN
12	M	32	GLN
13	O	3	GLN
13	O	82	GLN
15	U	63	ASN
16	V	86	GLN
19	Z	31	GLN
1	a	312	ASN
2	b	216	HIS
2	b	223	GLN
2	b	394	GLN
2	b	409	GLN
3	c	25	ASN
3	c	418	ASN
5	e	74	GLN
13	o	200	ASN
16	v	25	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.94	0	7,9,11	0.86	0
12	FME	M	1	12	8,9,10	0.93	0	7,9,11	0.90	0
14	FME	t	1	14	8,9,10	0.96	0	7,9,11	0.93	0
12	FME	m	1	12	8,9,10	0.94	0	7,9,11	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	FME	T	1	14	8,9,10	0.91	0	7,9,11	1.20	1 (14%)
8	FME	i	1	8	8,9,10	0.95	0	7,9,11	0.84	0

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	1	FME	C-CA-N	2.29	113.87	109.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

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 190 ligands modelled in this entry, 6 are monoatomic and 33 are unknown - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	CLA	A	607	36	65,73,73	1.47	5 (7%)	76,113,113	1.27	10 (13%)
25	CLA	A	606	-	65,73,73	1.45	6 (9%)	76,113,113	1.24	9 (11%)
25	CLA	B	607	36	65,73,73	1.46	5 (7%)	76,113,113	1.24	8 (10%)
26	PHO	a	609	-	51,69,69	0.98	3 (5%)	47,99,99	1.16	5 (10%)
25	CLA	C	502	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	8 (10%)
25	CLA	b	606[A]	-	65,73,73	1.46	5 (7%)	76,113,113	1.27	7 (9%)
25	CLA	c	502	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	7 (9%)
25	CLA	c	506	-	65,73,73	1.47	5 (7%)	76,113,113	1.29	7 (9%)
27	BCR	b	617	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
25	CLA	c	504	36	60,68,73	1.51	5 (8%)	70,107,113	1.34	8 (11%)
30	LHG	a	617	-	41,41,48	0.67	1 (2%)	44,47,54	1.32	6 (13%)
27	BCR	c	522	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	5 (8%)
25	CLA	c	508	-	64,72,73	1.47	5 (7%)	74,111,113	1.35	9 (12%)
27	BCR	c	515	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	5 (8%)
30	LHG	l	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.23	6 (11%)
32	LMG	a	614	-	51,51,55	0.73	0	59,59,63	1.33	7 (11%)
32	LMG	d	408	-	36,36,55	0.30	0	35,35,63	1.38	3 (8%)
25	CLA	c	510	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	7 (9%)
25	CLA	D	402	-	65,73,73	1.46	6 (9%)	76,113,113	1.27	7 (9%)
29	SQD	D	409	-	46,47,54	1.02	5 (10%)	55,58,65	1.58	9 (16%)
28	PL9	A	611	-	55,55,55	0.98	3 (5%)	68,69,69	1.51	12 (17%)
25	CLA	d	401	-	65,73,73	1.47	5 (7%)	76,113,113	1.25	8 (10%)
27	BCR	h	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	5 (8%)
27	BCR	C	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	6 (10%)
27	BCR	d	403	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	C	511	-	65,73,73	1.46	6 (9%)	76,113,113	1.32	8 (10%)
25	CLA	D	403	-	65,73,73	1.46	5 (7%)	76,113,113	1.38	10 (13%)
28	PL9	d	404	-	55,55,55	0.94	4 (7%)	68,69,69	1.49	10 (14%)
29	SQD	b	621	-	39,39,54	0.87	2 (5%)	41,41,65	1.14	2 (4%)
30	LHG	d	406	-	48,48,48	0.60	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	C	513	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	8 (10%)
25	CLA	b	611	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	10 (13%)
33	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.35	10 (12%)
25	CLA	b	616	-	47,55,73	1.71	6 (12%)	54,91,113	1.53	8 (14%)
32	LMG	D	407	-	51,51,55	0.72	0	59,59,63	1.31	5 (8%)
34	HEM	E	101	6,5	41,50,50	1.51	5 (12%)	45,82,82	1.31	6 (13%)
25	CLA	b	606[B]	-	65,73,73	1.47	5 (7%)	76,113,113	1.27	7 (9%)
21	OEX	A	601	1,3,36	0,15,15	-	-	-		
29	SQD	A	612	-	51,52,54	0.97	5 (9%)	60,63,65	1.50	9 (15%)
27	BCR	T	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	6 (10%)
29	SQD	A	616	-	53,54,54	0.95	5 (9%)	62,65,65	1.49	9 (14%)
25	CLA	B	602	-	65,73,73	1.46	5 (7%)	76,113,113	1.31	9 (11%)
25	CLA	C	504	-	65,73,73	1.47	5 (7%)	76,113,113	1.35	8 (10%)
25	CLA	a	610	-	65,73,73	1.47	5 (7%)	76,113,113	1.32	7 (9%)
25	CLA	b	608	-	65,73,73	1.46	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	C	505	36	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
30	LHG	B	623	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	C	506	-	65,73,73	1.46	6 (9%)	76,113,113	1.32	7 (9%)
32	LMG	C	520	-	48,48,55	0.76	0	56,56,63	1.32	6 (10%)
25	CLA	c	507	36	65,73,73	1.47	5 (7%)	76,113,113	1.36	8 (10%)
29	SQD	f	101	-	40,41,54	1.09	5 (12%)	49,52,65	1.58	9 (18%)
25	CLA	C	508	36	65,73,73	1.46	5 (7%)	76,113,113	1.38	8 (10%)
25	CLA	B	612	-	65,73,73	1.43	6 (9%)	76,113,113	1.37	9 (11%)
25	CLA	b	613	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	8 (10%)
33	DGD	C	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.38	10 (12%)
27	BCR	C	515	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	4 (7%)
25	CLA	B	605	-	65,73,73	1.45	6 (9%)	76,113,113	1.28	8 (10%)
25	CLA	b	612	-	65,73,73	1.45	6 (9%)	76,113,113	1.33	8 (10%)
33	DGD	c	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.37	7 (9%)
25	CLA	A	613	36	65,73,73	1.46	5 (7%)	76,113,113	1.25	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	613	-	65,73,73	1.45	5 (7%)	76,113,113	1.42	9 (11%)
27	BCR	K	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
25	CLA	c	509	-	65,73,73	1.44	5 (7%)	76,113,113	1.37	8 (10%)
25	CLA	b	605	-	65,73,73	1.47	6 (9%)	76,113,113	1.30	7 (9%)
25	CLA	B	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.24	9 (11%)
27	BCR	c	514	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	6 (10%)
25	CLA	B	615	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	b	614	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	9 (11%)
27	BCR	a	611	-	41,41,41	1.08	2 (4%)	56,56,56	1.15	5 (8%)
32	LMG	c	519	-	37,37,55	0.86	0	45,45,63	1.34	6 (13%)
27	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	5 (8%)
32	LMG	c	520	-	34,34,55	0.86	0	42,42,63	1.24	5 (11%)
25	CLA	b	607	36	65,73,73	1.45	6 (9%)	76,113,113	1.27	8 (10%)
30	LHG	d	405	-	48,48,48	0.61	1 (2%)	51,54,54	1.27	6 (11%)
25	CLA	C	512	3	65,73,73	1.46	5 (7%)	76,113,113	1.27	9 (11%)
25	CLA	B	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	8 (10%)
35	HEC	v	201	16	32,50,50	1.99	4 (12%)	24,82,82	1.75	5 (20%)
25	CLA	d	402	-	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	a	615	36	65,73,73	1.47	5 (7%)	76,113,113	1.26	7 (9%)
25	CLA	B	610	36	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
29	SQD	B	625	-	53,54,54	0.96	5 (9%)	62,65,65	1.49	8 (12%)
30	LHG	a	616	-	38,38,48	0.68	1 (2%)	41,44,54	1.16	3 (7%)
32	LMG	b	620	-	51,51,55	0.71	0	59,59,63	1.34	7 (11%)
33	DGD	C	517	-	63,63,67	0.83	0	77,77,81	1.35	9 (11%)
27	BCR	c	521	-	41,41,41	1.10	2 (4%)	56,56,56	1.14	5 (8%)
25	CLA	b	603	-	65,73,73	1.45	6 (9%)	76,113,113	1.27	8 (10%)
25	CLA	C	509	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	9 (11%)
25	CLA	B	604	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	9 (11%)
25	CLA	b	602	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	9 (11%)
25	CLA	C	514	-	65,73,73	1.45	5 (7%)	76,113,113	1.32	8 (10%)
27	BCR	B	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
34	HEM	e	101	6,5	41,50,50	1.53	4 (9%)	45,82,82	1.50	7 (15%)
33	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.41	10 (12%)
25	CLA	C	507	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	8 (10%)
25	CLA	c	503	-	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	9 (11%)
32	LMG	B	626	-	51,51,55	0.72	1 (1%)	59,59,63	1.30	5 (8%)
25	CLA	C	503	-	65,73,73	1.45	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	b	604	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	9 (11%)
32	LMG	B	621	-	51,51,55	0.72	0	59,59,63	1.32	6 (10%)
25	CLA	B	611	-	65,73,73	1.46	5 (7%)	76,113,113	1.34	10 (13%)
32	LMG	m	102	-	51,51,55	0.72	0	59,59,63	1.36	7 (11%)
25	CLA	B	601	36	65,73,73	1.46	5 (7%)	76,113,113	1.32	9 (11%)
33	DGD	c	518	-	63,63,67	0.84	1 (1%)	77,77,81	1.36	9 (11%)
25	CLA	C	510	-	65,73,73	1.44	5 (7%)	76,113,113	1.37	8 (10%)
25	CLA	b	615	-	65,73,73	1.47	6 (9%)	76,113,113	1.29	8 (10%)
33	DGD	h	102	-	63,63,67	0.88	0	77,77,81	1.35	8 (10%)
25	CLA	b	601	36	65,73,73	1.46	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	c	512	-	65,73,73	1.47	5 (7%)	76,113,113	1.36	9 (11%)
27	BCR	t	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
30	LHG	A	614	-	46,46,48	0.62	1 (2%)	49,52,54	1.24	5 (10%)
25	CLA	a	607	36	65,73,73	1.46	5 (7%)	76,113,113	1.26	9 (11%)
32	LMG	C	521	-	51,51,55	0.78	1 (1%)	59,59,63	1.35	6 (10%)
28	PL9	a	612	-	55,55,55	0.98	3 (5%)	68,69,69	1.53	12 (17%)
32	LMG	C	501	-	48,48,55	0.73	0	56,56,63	1.30	4 (7%)
29	SQD	D	408	-	42,43,54	1.06	5 (11%)	51,54,65	1.64	11 (21%)
25	CLA	b	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	8 (10%)
35	HEC	V	201	16	32,50,50	2.00	4 (12%)	24,82,82	1.74	5 (20%)
26	PHO	A	608	-	51,69,69	0.98	3 (5%)	47,99,99	1.12	5 (10%)
25	CLA	c	511	3	65,73,73	1.45	5 (7%)	76,113,113	1.28	9 (11%)
26	PHO	D	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.09	4 (8%)
25	CLA	A	609	-	54,62,73	1.60	5 (9%)	62,99,113	1.42	9 (14%)
27	BCR	B	617	-	41,41,41	1.06	2 (4%)	56,56,56	1.15	4 (7%)
27	BCR	D	404	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	5 (8%)
29	SQD	L	101	-	48,49,54	0.99	5 (10%)	57,60,65	1.58	10 (17%)
30	LHG	D	406	-	48,48,48	0.60	1 (2%)	51,54,54	1.25	6 (11%)
25	CLA	B	608	-	65,73,73	1.46	6 (9%)	76,113,113	1.28	7 (9%)
25	CLA	b	610	36	65,73,73	1.46	5 (7%)	76,113,113	1.31	9 (11%)
24	BCT	a	605	22	2,3,3	1.27	0	2,3,3	1.86	1 (50%)
25	CLA	B	606	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCT	A	605	22	2,3,3	1.27	0	2,3,3	1.87	1 (50%)
29	SQD	a	613	-	53,54,54	0.95	5 (9%)	62,65,65	1.48	9 (14%)
27	BCR	Y	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.13	4 (7%)
25	CLA	c	501	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	9 (11%)
27	BCR	H	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	4 (7%)
26	PHO	a	608	-	51,69,69	0.99	3 (5%)	47,99,99	1.15	6 (12%)
25	CLA	B	616	-	65,73,73	1.45	6 (9%)	76,113,113	1.37	8 (10%)
27	BCR	b	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	6 (10%)
30	LHG	L	102	-	48,48,48	0.62	1 (2%)	51,54,54	1.23	6 (11%)
32	LMG	B	620	-	51,51,55	0.72	0	59,59,63	1.34	6 (10%)
32	LMG	d	407	-	51,51,55	0.73	0	59,59,63	1.33	6 (10%)
25	CLA	a	606	-	65,73,73	1.43	5 (7%)	76,113,113	1.25	9 (11%)
27	BCR	A	610	-	41,41,41	1.08	2 (4%)	56,56,56	1.18	6 (10%)
25	CLA	c	505	-	65,73,73	1.46	6 (9%)	76,113,113	1.31	7 (9%)
21	OEX	a	601	1,3,36	0,15,15	-	-	-		
30	LHG	A	618	-	48,48,48	0.63	1 (2%)	51,54,54	1.25	6 (11%)
25	CLA	c	513	-	65,73,73	1.45	5 (7%)	76,113,113	1.30	7 (9%)
27	BCR	b	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	3 (5%)
28	PL9	D	405	-	55,55,55	0.94	2 (3%)	68,69,69	1.52	14 (20%)
25	CLA	B	603	-	65,73,73	1.45	6 (9%)	76,113,113	1.24	8 (10%)
29	SQD	B	624	-	53,54,54	0.95	5 (9%)	62,65,65	1.62	10 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	607	36	1/1/15/20	8/37/115/115	-
25	CLA	A	606	-	1/1/15/20	10/37/115/115	-
25	CLA	B	607	36	1/1/15/20	9/37/115/115	-
26	PHO	a	609	-	-	11/37/103/103	0/5/6/6
25	CLA	C	502	-	1/1/15/20	14/37/115/115	-
25	CLA	b	606[A]	-	1/1/15/20	13/37/115/115	-
25	CLA	c	502	-	1/1/15/20	11/37/115/115	-
25	CLA	c	506	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
25	CLA	c	504	36	1/1/14/20	4/31/109/115	-
30	LHG	a	617	-	-	19/46/46/53	-
27	BCR	c	522	-	-	4/29/63/63	0/2/2/2
25	CLA	c	508	-	1/1/14/20	9/36/114/115	-
27	BCR	c	515	-	-	3/29/63/63	0/2/2/2
30	LHG	l	101	-	-	20/53/53/53	-
32	LMG	a	614	-	-	18/46/66/70	0/1/1/1
32	LMG	d	408	-	-	18/32/32/70	-
25	CLA	c	510	-	1/1/15/20	14/37/115/115	-
25	CLA	D	402	-	1/1/15/20	5/37/115/115	-
29	SQD	D	409	-	-	19/42/62/69	0/1/1/1
28	PL9	A	611	-	-	13/53/73/73	0/1/1/1
25	CLA	d	401	-	1/1/15/20	7/37/115/115	-
27	BCR	h	101	-	-	6/29/63/63	0/2/2/2
27	BCR	C	516	-	-	4/29/63/63	0/2/2/2
27	BCR	d	403	-	-	6/29/63/63	0/2/2/2
25	CLA	C	511	-	1/1/15/20	10/37/115/115	-
25	CLA	D	403	-	1/1/15/20	9/37/115/115	-
28	PL9	d	404	-	-	9/53/73/73	0/1/1/1
29	SQD	b	621	-	-	9/41/41/69	-
30	LHG	d	406	-	-	24/53/53/53	-
25	CLA	C	513	-	1/1/15/20	14/37/115/115	-
25	CLA	b	611	-	1/1/15/20	8/37/115/115	-
33	DGD	H	102	-	-	11/51/91/95	0/2/2/2
25	CLA	b	616	-	1/1/11/20	3/16/94/115	-
32	LMG	D	407	-	-	14/46/66/70	0/1/1/1
34	HEM	E	101	6,5	-	2/12/54/54	-
25	CLA	b	606[B]	-	1/1/15/20	5/37/115/115	-
29	SQD	A	612	-	-	12/47/67/69	0/1/1/1
27	BCR	T	101	-	-	9/29/63/63	0/2/2/2
29	SQD	A	616	-	-	14/49/69/69	0/1/1/1
25	CLA	B	602	-	1/1/15/20	4/37/115/115	-
25	CLA	C	504	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	610	-	1/1/15/20	6/37/115/115	-
25	CLA	b	608	-	1/1/15/20	5/37/115/115	-
25	CLA	C	505	36	1/1/15/20	5/37/115/115	-
30	LHG	B	623	-	-	19/53/53/53	-
25	CLA	C	506	-	1/1/15/20	9/37/115/115	-
32	LMG	C	520	-	-	22/43/63/70	0/1/1/1
25	CLA	c	507	36	1/1/15/20	11/37/115/115	-
29	SQD	f	101	-	-	7/36/56/69	0/1/1/1
25	CLA	C	508	36	1/1/15/20	13/37/115/115	-
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
25	CLA	b	613	-	1/1/15/20	12/37/115/115	-
33	DGD	C	519	-	-	17/51/91/95	0/2/2/2
27	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	CLA	B	605	-	1/1/15/20	7/37/115/115	-
25	CLA	b	612	-	1/1/15/20	14/37/115/115	-
33	DGD	c	517	-	-	21/51/91/95	0/2/2/2
25	CLA	A	613	36	1/1/15/20	4/37/115/115	-
25	CLA	B	613	-	1/1/15/20	13/37/115/115	-
27	BCR	K	101	-	-	4/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	12/37/115/115	-
25	CLA	b	605	-	1/1/15/20	8/37/115/115	-
25	CLA	B	614	-	1/1/15/20	22/37/115/115	-
27	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CLA	B	615	-	1/1/15/20	5/37/115/115	-
25	CLA	b	614	-	1/1/15/20	20/37/115/115	-
27	BCR	a	611	-	-	4/29/63/63	0/2/2/2
32	LMG	c	519	-	-	13/31/51/70	0/1/1/1
27	BCR	B	619	-	-	5/29/63/63	0/2/2/2
32	LMG	c	520	-	-	18/29/49/70	0/1/1/1
25	CLA	b	607	36	1/1/15/20	12/37/115/115	-
30	LHG	d	405	-	-	23/53/53/53	-
25	CLA	C	512	3	1/1/15/20	9/37/115/115	-
25	CLA	B	609	-	1/1/15/20	11/37/115/115	-
35	HEC	v	201	16	-	2/10/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	402	-	1/1/15/20	7/37/115/115	-
25	CLA	a	615	36	1/1/15/20	10/37/115/115	-
25	CLA	B	610	36	1/1/15/20	6/37/115/115	-
29	SQD	B	625	-	-	24/49/69/69	0/1/1/1
30	LHG	a	616	-	-	18/43/43/53	-
32	LMG	b	620	-	-	19/46/66/70	0/1/1/1
33	DGD	C	517	-	-	24/51/91/95	0/2/2/2
27	BCR	c	521	-	-	7/29/63/63	0/2/2/2
25	CLA	b	603	-	1/1/15/20	13/37/115/115	-
25	CLA	C	509	-	1/1/15/20	10/37/115/115	-
25	CLA	B	604	-	1/1/15/20	7/37/115/115	-
25	CLA	b	602	-	1/1/15/20	9/37/115/115	-
25	CLA	C	514	-	1/1/15/20	13/37/115/115	-
27	BCR	B	618	-	-	6/29/63/63	0/2/2/2
34	HEM	e	101	6,5	-	3/12/54/54	-
33	DGD	c	516	-	-	19/51/91/95	0/2/2/2
25	CLA	C	507	-	1/1/15/20	12/37/115/115	-
25	CLA	c	503	-	1/1/15/20	13/37/115/115	-
33	DGD	C	518	-	-	22/51/91/95	0/2/2/2
32	LMG	B	626	-	-	25/46/66/70	0/1/1/1
25	CLA	C	503	-	1/1/15/20	8/37/115/115	-
25	CLA	b	604	-	1/1/15/20	11/37/115/115	-
32	LMG	B	621	-	-	21/46/66/70	0/1/1/1
25	CLA	B	611	-	1/1/15/20	9/37/115/115	-
32	LMG	m	102	-	-	23/46/66/70	0/1/1/1
25	CLA	B	601	36	1/1/15/20	21/37/115/115	-
33	DGD	c	518	-	-	15/51/91/95	0/2/2/2
25	CLA	C	510	-	1/1/15/20	5/37/115/115	-
25	CLA	b	615	-	1/1/15/20	3/37/115/115	-
33	DGD	h	102	-	-	15/51/91/95	0/2/2/2
25	CLA	b	601	36	1/1/15/20	14/37/115/115	-
25	CLA	c	512	-	1/1/15/20	12/37/115/115	-
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
30	LHG	A	614	-	-	16/51/51/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	607	36	1/1/15/20	9/37/115/115	-
32	LMG	C	521	-	-	21/46/66/70	0/1/1/1
28	PL9	a	612	-	-	3/53/73/73	0/1/1/1
32	LMG	C	501	-	-	23/43/63/70	0/1/1/1
29	SQD	D	408	-	-	9/38/58/69	0/1/1/1
25	CLA	b	609	-	1/1/15/20	11/37/115/115	-
35	HEC	V	201	16	-	2/10/54/54	-
26	PHO	A	608	-	-	5/37/103/103	0/5/6/6
25	CLA	c	511	3	1/1/15/20	11/37/115/115	-
26	PHO	D	401	-	-	5/37/103/103	0/5/6/6
25	CLA	A	609	-	1/1/12/20	4/24/102/115	-
27	BCR	B	617	-	-	4/29/63/63	0/2/2/2
27	BCR	D	404	-	-	4/29/63/63	0/2/2/2
29	SQD	L	101	-	-	21/44/64/69	0/1/1/1
30	LHG	D	406	-	-	18/53/53/53	-
25	CLA	B	608	-	1/1/15/20	10/37/115/115	-
25	CLA	b	610	36	1/1/15/20	10/37/115/115	-
25	CLA	B	606	-	1/1/15/20	16/37/115/115	-
29	SQD	a	613	-	-	22/49/69/69	0/1/1/1
27	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
25	CLA	c	501	-	1/1/15/20	4/37/115/115	-
27	BCR	H	101	-	-	5/29/63/63	0/2/2/2
26	PHO	a	608	-	-	7/37/103/103	0/5/6/6
25	CLA	B	616	-	1/1/15/20	12/37/115/115	-
27	BCR	b	618	-	-	10/29/63/63	0/2/2/2
30	LHG	L	102	-	-	19/53/53/53	-
32	LMG	B	620	-	-	17/46/66/70	0/1/1/1
32	LMG	d	407	-	-	18/46/66/70	0/1/1/1
25	CLA	a	606	-	1/1/15/20	3/37/115/115	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
25	CLA	c	505	-	1/1/15/20	15/37/115/115	-
30	LHG	A	618	-	-	21/53/53/53	-
25	CLA	c	513	-	1/1/15/20	10/37/115/115	-
27	BCR	b	619	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	D	405	-	-	9/53/73/73	0/1/1/1
25	CLA	B	603	-	1/1/15/20	9/37/115/115	-
29	SQD	B	624	-	-	26/49/69/69	0/1/1/1

All (532) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	609	CLA	C4B-NB	7.60	1.42	1.35
25	b	609	CLA	C4B-NB	7.52	1.41	1.35
25	B	614	CLA	C4B-NB	7.49	1.41	1.35
25	b	605	CLA	C4B-NB	7.46	1.41	1.35
25	b	606[B]	CLA	C4B-NB	7.44	1.41	1.35
25	B	610	CLA	C4B-NB	7.44	1.41	1.35
25	a	610	CLA	C4B-NB	7.44	1.41	1.35
25	c	507	CLA	C4B-NB	7.44	1.41	1.35
25	C	505	CLA	C4B-NB	7.43	1.41	1.35
25	b	614	CLA	C4B-NB	7.43	1.41	1.35
25	b	604	CLA	C4B-NB	7.42	1.41	1.35
25	b	606[A]	CLA	C4B-NB	7.42	1.41	1.35
25	C	506	CLA	C4B-NB	7.42	1.41	1.35
25	d	401	CLA	C4B-NB	7.42	1.41	1.35
25	d	402	CLA	C4B-NB	7.42	1.41	1.35
25	b	608	CLA	C4B-NB	7.41	1.41	1.35
25	c	505	CLA	C4B-NB	7.40	1.41	1.35
25	C	513	CLA	C4B-NB	7.39	1.41	1.35
25	C	508	CLA	C4B-NB	7.39	1.41	1.35
25	B	615	CLA	C4B-NB	7.39	1.41	1.35
25	C	504	CLA	C4B-NB	7.39	1.41	1.35
25	B	608	CLA	C4B-NB	7.37	1.41	1.35
25	b	613	CLA	C4B-NB	7.37	1.41	1.35
25	A	609	CLA	C4B-NB	7.36	1.41	1.35
25	c	504	CLA	C4B-NB	7.36	1.41	1.35
25	b	611	CLA	C4B-NB	7.36	1.41	1.35
25	B	602	CLA	C4B-NB	7.36	1.41	1.35
25	B	605	CLA	C4B-NB	7.36	1.41	1.35
25	b	615	CLA	C4B-NB	7.35	1.41	1.35
25	B	611	CLA	C4B-NB	7.35	1.41	1.35
25	b	602	CLA	C4B-NB	7.35	1.41	1.35
25	A	607	CLA	C4B-NB	7.35	1.41	1.35
25	c	502	CLA	C4B-NB	7.35	1.41	1.35
25	c	506	CLA	C4B-NB	7.35	1.41	1.35
25	C	514	CLA	C4B-NB	7.34	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	607	CLA	C4B-NB	7.34	1.41	1.35
25	B	604	CLA	C4B-NB	7.34	1.41	1.35
25	c	501	CLA	C4B-NB	7.34	1.41	1.35
25	c	512	CLA	C4B-NB	7.34	1.41	1.35
25	A	613	CLA	C4B-NB	7.33	1.41	1.35
25	B	601	CLA	C4B-NB	7.33	1.41	1.35
25	C	509	CLA	C4B-NB	7.32	1.41	1.35
25	B	607	CLA	C4B-NB	7.32	1.41	1.35
25	B	606	CLA	C4B-NB	7.31	1.41	1.35
25	D	402	CLA	C4B-NB	7.31	1.41	1.35
25	C	512	CLA	C4B-NB	7.30	1.41	1.35
25	b	603	CLA	C4B-NB	7.30	1.41	1.35
25	b	610	CLA	C4B-NB	7.30	1.41	1.35
25	a	615	CLA	C4B-NB	7.30	1.41	1.35
25	B	603	CLA	C4B-NB	7.29	1.41	1.35
25	c	508	CLA	C4B-NB	7.29	1.41	1.35
25	c	503	CLA	C4B-NB	7.29	1.41	1.35
25	b	601	CLA	C4B-NB	7.28	1.41	1.35
25	C	507	CLA	C4B-NB	7.28	1.41	1.35
25	b	616	CLA	C4B-NB	7.28	1.41	1.35
25	D	403	CLA	C4B-NB	7.28	1.41	1.35
25	A	606	CLA	C4B-NB	7.28	1.41	1.35
25	b	612	CLA	C4B-NB	7.27	1.41	1.35
25	C	511	CLA	C4B-NB	7.27	1.41	1.35
25	c	510	CLA	C4B-NB	7.27	1.41	1.35
25	c	511	CLA	C4B-NB	7.27	1.41	1.35
25	c	513	CLA	C4B-NB	7.26	1.41	1.35
25	C	502	CLA	C4B-NB	7.24	1.41	1.35
25	B	613	CLA	C4B-NB	7.18	1.41	1.35
25	B	612	CLA	C4B-NB	7.17	1.41	1.35
25	a	607	CLA	C4B-NB	7.16	1.41	1.35
25	c	509	CLA	C4B-NB	7.16	1.41	1.35
25	B	616	CLA	C4B-NB	7.16	1.41	1.35
25	C	510	CLA	C4B-NB	7.13	1.41	1.35
25	C	503	CLA	C4B-NB	7.02	1.41	1.35
25	a	606	CLA	C4B-NB	6.96	1.41	1.35
35	v	201	HEC	C2B-C3B	-5.25	1.35	1.40
35	V	201	HEC	C2B-C3B	-5.24	1.35	1.40
35	V	201	HEC	C3C-C2C	-5.23	1.35	1.40
35	v	201	HEC	C3C-C2C	-5.07	1.35	1.40
34	e	101	HEM	C3C-C2C	-4.63	1.33	1.40
34	E	101	HEM	C3C-C2C	-4.62	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	V	201	HEC	CBB-CAB	-4.07	1.34	1.49
35	v	201	HEC	CBB-CAB	-4.06	1.34	1.49
35	v	201	HEC	CBC-CAC	-4.05	1.34	1.49
35	V	201	HEC	CBC-CAC	-4.04	1.34	1.49
25	b	604	CLA	C1D-ND	3.82	1.42	1.37
25	C	502	CLA	C1D-ND	3.82	1.42	1.37
25	B	607	CLA	C1D-ND	3.81	1.42	1.37
25	B	615	CLA	C1D-ND	3.81	1.42	1.37
25	B	616	CLA	C1D-ND	3.81	1.42	1.37
25	D	403	CLA	C1D-ND	3.80	1.42	1.37
25	c	510	CLA	C1D-ND	3.77	1.42	1.37
25	a	606	CLA	C1D-ND	3.77	1.42	1.37
25	b	601	CLA	C1D-ND	3.76	1.42	1.37
25	C	512	CLA	C1D-ND	3.75	1.42	1.37
25	B	613	CLA	C1D-ND	3.75	1.42	1.37
25	c	512	CLA	C1D-ND	3.75	1.42	1.37
25	b	609	CLA	C1D-ND	3.75	1.42	1.37
25	C	508	CLA	C1D-ND	3.74	1.42	1.37
25	a	615	CLA	C1D-ND	3.74	1.42	1.37
25	B	609	CLA	C1D-ND	3.73	1.42	1.37
25	C	503	CLA	C1D-ND	3.73	1.42	1.37
25	b	602	CLA	C1D-ND	3.73	1.42	1.37
25	c	509	CLA	C1D-ND	3.72	1.42	1.37
25	b	615	CLA	C1D-ND	3.72	1.42	1.37
25	A	607	CLA	C1D-ND	3.72	1.42	1.37
25	C	507	CLA	C1D-ND	3.71	1.42	1.37
25	A	606	CLA	C1D-ND	3.71	1.42	1.37
25	C	509	CLA	C1D-ND	3.71	1.42	1.37
25	B	606	CLA	C1D-ND	3.71	1.42	1.37
25	c	508	CLA	C1D-ND	3.70	1.42	1.37
25	C	505	CLA	C1D-ND	3.70	1.42	1.37
25	b	616	CLA	C1D-ND	3.70	1.42	1.37
25	B	601	CLA	C1D-ND	3.70	1.42	1.37
25	a	610	CLA	C1D-ND	3.70	1.42	1.37
34	e	101	HEM	C3C-CAC	3.70	1.55	1.47
25	c	513	CLA	C1D-ND	3.69	1.42	1.37
25	A	609	CLA	C1D-ND	3.69	1.42	1.37
25	c	503	CLA	C1D-ND	3.69	1.42	1.37
25	B	610	CLA	C1D-ND	3.69	1.42	1.37
34	E	101	HEM	C3C-CAC	3.68	1.55	1.47
25	b	613	CLA	C1D-ND	3.68	1.42	1.37
25	c	501	CLA	C1D-ND	3.68	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C1D-ND	3.68	1.42	1.37
25	b	607	CLA	C1D-ND	3.67	1.42	1.37
25	B	602	CLA	C1D-ND	3.67	1.42	1.37
25	C	504	CLA	C1D-ND	3.67	1.42	1.37
25	B	604	CLA	C1D-ND	3.67	1.42	1.37
25	B	608	CLA	C1D-ND	3.67	1.42	1.37
25	C	511	CLA	C1D-ND	3.66	1.42	1.37
25	C	510	CLA	C1D-ND	3.65	1.42	1.37
25	b	606[A]	CLA	C1D-ND	3.65	1.42	1.37
25	b	610	CLA	C1D-ND	3.65	1.42	1.37
25	a	607	CLA	C1D-ND	3.65	1.42	1.37
25	c	506	CLA	C1D-ND	3.65	1.42	1.37
25	C	514	CLA	C1D-ND	3.64	1.42	1.37
25	d	401	CLA	C1D-ND	3.64	1.42	1.37
25	D	402	CLA	C1D-ND	3.64	1.42	1.37
25	c	511	CLA	C1D-ND	3.64	1.42	1.37
25	b	612	CLA	C1D-ND	3.63	1.42	1.37
25	C	513	CLA	C1D-ND	3.62	1.42	1.37
25	A	613	CLA	C1D-ND	3.62	1.42	1.37
25	b	606[B]	CLA	C1D-ND	3.62	1.42	1.37
25	b	611	CLA	C1D-ND	3.62	1.42	1.37
25	d	402	CLA	C1D-ND	3.61	1.42	1.37
25	c	502	CLA	C1D-ND	3.60	1.42	1.37
25	b	614	CLA	C1D-ND	3.57	1.42	1.37
25	b	605	CLA	C1D-ND	3.57	1.42	1.37
25	B	614	CLA	C1D-ND	3.56	1.42	1.37
25	c	504	CLA	C1D-ND	3.56	1.42	1.37
25	c	505	CLA	C1D-ND	3.56	1.42	1.37
25	B	603	CLA	C1D-ND	3.55	1.42	1.37
25	C	506	CLA	C1D-ND	3.54	1.42	1.37
25	b	603	CLA	C1D-ND	3.53	1.42	1.37
25	B	611	CLA	C1D-ND	3.53	1.42	1.37
28	a	612	PL9	C7-C3	-3.52	1.47	1.51
25	B	605	CLA	C1D-ND	3.45	1.42	1.37
25	b	608	CLA	C1D-ND	3.45	1.42	1.37
25	B	612	CLA	C1D-ND	3.45	1.42	1.37
27	d	403	BCR	C1-C6	-3.44	1.49	1.53
27	Y	101	BCR	C1-C6	-3.43	1.49	1.53
27	C	516	BCR	C1-C6	-3.42	1.49	1.53
27	c	522	BCR	C1-C6	-3.41	1.49	1.53
27	t	101	BCR	C1-C6	-3.39	1.49	1.53
27	c	515	BCR	C1-C6	-3.39	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	617	BCR	C1-C6	-3.37	1.49	1.53
28	A	611	PL9	C7-C3	-3.36	1.47	1.51
27	c	521	BCR	C1-C6	-3.36	1.49	1.53
27	K	101	BCR	C1-C6	-3.35	1.49	1.53
27	B	618	BCR	C1-C6	-3.35	1.49	1.53
25	b	608	CLA	CHC-C1C	3.34	1.43	1.35
27	b	618	BCR	C1-C6	-3.31	1.49	1.53
25	c	513	CLA	CHC-C1C	3.30	1.43	1.35
25	A	609	CLA	C4D-ND	-3.29	1.33	1.37
25	C	511	CLA	CHC-C1C	3.29	1.43	1.35
25	c	505	CLA	CHC-C1C	3.28	1.43	1.35
25	d	402	CLA	CHC-C1C	3.28	1.43	1.35
25	B	614	CLA	CHC-C1C	3.27	1.43	1.35
25	C	505	CLA	CHC-C1C	3.27	1.43	1.35
25	c	512	CLA	CHC-C1C	3.27	1.43	1.35
25	c	511	CLA	CHC-C1C	3.27	1.43	1.35
25	b	604	CLA	CHC-C1C	3.26	1.43	1.35
25	d	402	CLA	C4D-ND	-3.26	1.33	1.37
25	a	615	CLA	CHC-C1C	3.26	1.43	1.35
25	b	605	CLA	CHC-C1C	3.25	1.43	1.35
27	h	101	BCR	C1-C6	-3.25	1.49	1.53
25	a	607	CLA	CHC-C1C	3.25	1.43	1.35
25	C	506	CLA	CHC-C1C	3.25	1.43	1.35
25	a	607	CLA	C4D-ND	-3.24	1.33	1.37
25	A	607	CLA	CHC-C1C	3.24	1.43	1.35
25	b	602	CLA	CHC-C1C	3.24	1.43	1.35
27	A	610	BCR	C1-C6	-3.24	1.49	1.53
25	B	602	CLA	CHC-C1C	3.24	1.43	1.35
25	C	504	CLA	CHC-C1C	3.23	1.43	1.35
25	A	613	CLA	CHC-C1C	3.23	1.43	1.35
25	b	614	CLA	CHC-C1C	3.23	1.43	1.35
25	a	606	CLA	CHC-C1C	3.23	1.43	1.35
25	B	605	CLA	CHC-C1C	3.23	1.43	1.35
25	D	402	CLA	C4D-ND	-3.23	1.33	1.37
25	b	613	CLA	CHC-C1C	3.22	1.43	1.35
25	B	607	CLA	CHC-C1C	3.22	1.43	1.35
25	c	508	CLA	C4D-ND	-3.22	1.33	1.37
25	B	610	CLA	CHC-C1C	3.22	1.43	1.35
25	B	612	CLA	CHC-C1C	3.21	1.43	1.35
25	B	601	CLA	CHC-C1C	3.21	1.43	1.35
25	b	606[A]	CLA	CHC-C1C	3.21	1.43	1.35
25	c	508	CLA	CHC-C1C	3.21	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	603	CLA	CHC-C1C	3.21	1.43	1.35
25	C	513	CLA	CHC-C1C	3.21	1.43	1.35
27	a	611	BCR	C1-C6	-3.21	1.49	1.53
25	b	606[B]	CLA	CHC-C1C	3.21	1.43	1.35
25	A	606	CLA	CHC-C1C	3.21	1.43	1.35
25	C	514	CLA	CHC-C1C	3.20	1.43	1.35
25	b	616	CLA	CHC-C1C	3.20	1.43	1.35
25	c	509	CLA	CHC-C1C	3.20	1.43	1.35
25	C	507	CLA	CHC-C1C	3.20	1.43	1.35
25	b	610	CLA	C4D-ND	-3.20	1.33	1.37
27	Y	101	BCR	C30-C25	-3.20	1.49	1.53
25	C	512	CLA	CHC-C1C	3.19	1.43	1.35
25	B	603	CLA	CHC-C1C	3.19	1.43	1.35
25	B	605	CLA	C4D-ND	-3.19	1.33	1.37
25	a	610	CLA	CHC-C1C	3.19	1.43	1.35
25	A	613	CLA	C4D-ND	-3.19	1.33	1.37
25	D	403	CLA	CHC-C1C	3.19	1.43	1.35
25	c	501	CLA	CHC-C1C	3.19	1.43	1.35
27	H	101	BCR	C30-C25	-3.18	1.49	1.53
25	B	616	CLA	CHC-C1C	3.18	1.43	1.35
25	B	606	CLA	CHC-C1C	3.18	1.43	1.35
25	a	615	CLA	C4D-ND	-3.18	1.33	1.37
25	C	503	CLA	C4D-ND	-3.18	1.33	1.37
25	b	601	CLA	CHC-C1C	3.18	1.43	1.35
29	b	621	SQD	O48-C23	3.18	1.42	1.33
25	c	504	CLA	CHC-C1C	3.18	1.43	1.35
25	C	502	CLA	CHC-C1C	3.18	1.43	1.35
25	B	610	CLA	C4D-ND	-3.18	1.33	1.37
25	d	401	CLA	CHC-C1C	3.17	1.43	1.35
25	c	502	CLA	CHC-C1C	3.17	1.43	1.35
25	B	611	CLA	CHC-C1C	3.17	1.43	1.35
25	C	510	CLA	CHC-C1C	3.17	1.43	1.35
25	c	510	CLA	CHC-C1C	3.17	1.43	1.35
25	c	506	CLA	CHC-C1C	3.17	1.43	1.35
25	D	402	CLA	CHC-C1C	3.16	1.43	1.35
25	B	608	CLA	CHC-C1C	3.16	1.43	1.35
25	b	609	CLA	CHC-C1C	3.16	1.43	1.35
25	B	615	CLA	CHC-C1C	3.16	1.43	1.35
25	C	509	CLA	CHC-C1C	3.16	1.43	1.35
25	C	508	CLA	CHC-C1C	3.15	1.43	1.35
25	C	509	CLA	C4D-ND	-3.15	1.33	1.37
29	A	616	SQD	O48-C23	3.15	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	506	CLA	C4D-ND	-3.15	1.33	1.37
25	b	607	CLA	CHC-C1C	3.15	1.43	1.35
25	C	503	CLA	CHC-C1C	3.15	1.43	1.35
29	B	625	SQD	O48-C23	3.15	1.42	1.33
25	b	610	CLA	CHC-C1C	3.15	1.43	1.35
25	D	403	CLA	C4D-ND	-3.14	1.33	1.37
29	f	101	SQD	O48-C23	3.14	1.42	1.33
25	A	609	CLA	CHC-C1C	3.14	1.43	1.35
29	D	408	SQD	O48-C23	3.14	1.42	1.33
25	c	503	CLA	C4D-ND	-3.14	1.33	1.37
29	L	101	SQD	O48-C23	3.14	1.42	1.33
25	b	608	CLA	C4D-ND	-3.14	1.33	1.37
25	b	611	CLA	CHC-C1C	3.14	1.43	1.35
29	D	409	SQD	O48-C23	3.13	1.42	1.33
25	B	614	CLA	C4D-ND	-3.13	1.33	1.37
25	b	605	CLA	C4D-ND	-3.13	1.33	1.37
25	b	612	CLA	CHC-C1C	3.13	1.43	1.35
25	c	503	CLA	CHC-C1C	3.12	1.43	1.35
25	C	502	CLA	C4D-ND	-3.12	1.33	1.37
25	B	603	CLA	C4D-ND	-3.12	1.33	1.37
25	B	604	CLA	CHC-C1C	3.12	1.43	1.35
25	B	613	CLA	CHC-C1C	3.11	1.42	1.35
25	B	612	CLA	C4D-ND	-3.11	1.33	1.37
25	A	607	CLA	C4D-ND	-3.11	1.33	1.37
25	c	502	CLA	C4D-ND	-3.11	1.33	1.37
25	b	614	CLA	C4D-ND	-3.11	1.33	1.37
29	A	612	SQD	O48-C23	3.11	1.42	1.33
25	c	501	CLA	C4D-ND	-3.11	1.33	1.37
25	c	511	CLA	C4D-ND	-3.10	1.33	1.37
25	b	615	CLA	CHC-C1C	3.10	1.42	1.35
25	C	511	CLA	C4D-ND	-3.10	1.33	1.37
27	t	101	BCR	C30-C25	-3.10	1.49	1.53
27	c	514	BCR	C30-C25	-3.10	1.49	1.53
25	c	509	CLA	C4D-ND	-3.10	1.33	1.37
25	b	603	CLA	C4D-ND	-3.09	1.33	1.37
25	c	507	CLA	CHC-C1C	3.09	1.42	1.35
29	a	613	SQD	O48-C23	3.09	1.42	1.33
25	b	612	CLA	C4D-ND	-3.09	1.33	1.37
25	C	510	CLA	C4D-ND	-3.08	1.33	1.37
25	B	609	CLA	CHC-C1C	3.08	1.42	1.35
25	B	608	CLA	C4D-ND	-3.08	1.33	1.37
25	C	514	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	609	CLA	C4D-ND	-3.08	1.33	1.37
25	b	616	CLA	C4D-ND	-3.08	1.33	1.37
25	a	606	CLA	C4D-ND	-3.08	1.33	1.37
25	d	401	CLA	C4D-ND	-3.07	1.33	1.37
25	b	609	CLA	C4D-ND	-3.07	1.33	1.37
27	C	515	BCR	C1-C6	-3.06	1.49	1.53
27	b	619	BCR	C1-C6	-3.06	1.49	1.53
25	c	513	CLA	C4D-ND	-3.06	1.33	1.37
25	C	504	CLA	C4D-ND	-3.06	1.33	1.37
27	D	404	BCR	C30-C25	-3.06	1.49	1.53
25	c	504	CLA	C4D-ND	-3.06	1.33	1.37
28	D	405	PL9	C7-C3	-3.05	1.48	1.51
27	H	101	BCR	C1-C6	-3.05	1.49	1.53
25	b	607	CLA	C4D-ND	-3.05	1.33	1.37
25	C	505	CLA	C4D-ND	-3.05	1.33	1.37
25	C	513	CLA	C4D-ND	-3.05	1.33	1.37
29	B	624	SQD	O48-C23	3.04	1.42	1.33
25	b	601	CLA	C4D-ND	-3.04	1.33	1.37
25	B	616	CLA	C4D-ND	-3.04	1.33	1.37
25	b	615	CLA	C4D-ND	-3.04	1.33	1.37
25	C	512	CLA	C4D-ND	-3.04	1.33	1.37
25	c	507	CLA	C4D-ND	-3.04	1.33	1.37
27	D	404	BCR	C1-C6	-3.03	1.49	1.53
25	c	510	CLA	C4D-ND	-3.03	1.33	1.37
25	B	611	CLA	C4D-ND	-3.03	1.33	1.37
25	c	512	CLA	C4D-ND	-3.03	1.33	1.37
25	b	602	CLA	C4D-ND	-3.03	1.33	1.37
25	b	606[B]	CLA	C4D-ND	-3.03	1.33	1.37
25	b	611	CLA	C4D-ND	-3.02	1.33	1.37
27	T	101	BCR	C30-C25	-3.02	1.49	1.53
27	b	617	BCR	C30-C25	-3.02	1.49	1.53
27	c	521	BCR	C30-C25	-3.02	1.49	1.53
25	B	615	CLA	C4D-ND	-3.02	1.33	1.37
25	b	613	CLA	C4D-ND	-3.02	1.33	1.37
27	b	618	BCR	C30-C25	-3.01	1.49	1.53
27	C	515	BCR	C30-C25	-3.01	1.49	1.53
25	B	613	CLA	C4D-ND	-3.01	1.33	1.37
25	B	607	CLA	C4D-ND	-3.01	1.33	1.37
25	b	606[A]	CLA	C4D-ND	-3.01	1.33	1.37
27	c	515	BCR	C30-C25	-3.00	1.49	1.53
25	A	606	CLA	C4D-ND	-3.00	1.33	1.37
27	c	514	BCR	C1-C6	-3.00	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	E	101	HEM	CAB-C3B	3.00	1.55	1.47
27	a	611	BCR	C30-C25	-2.99	1.49	1.53
27	A	610	BCR	C30-C25	-2.99	1.49	1.53
25	B	606	CLA	C4D-ND	-2.99	1.33	1.37
25	C	506	CLA	C4D-ND	-2.98	1.33	1.37
25	a	610	CLA	C4D-ND	-2.98	1.33	1.37
25	B	601	CLA	C4D-ND	-2.97	1.33	1.37
25	C	508	CLA	C4D-ND	-2.97	1.33	1.37
25	C	507	CLA	C4D-ND	-2.97	1.33	1.37
27	B	617	BCR	C1-C6	-2.97	1.49	1.53
25	B	602	CLA	C4D-ND	-2.95	1.33	1.37
27	B	619	BCR	C1-C6	-2.95	1.49	1.53
27	B	617	BCR	C30-C25	-2.95	1.49	1.53
25	c	505	CLA	C4D-ND	-2.94	1.33	1.37
27	T	101	BCR	C1-C6	-2.91	1.49	1.53
29	b	621	SQD	O47-C7	2.91	1.42	1.34
25	B	604	CLA	C4D-ND	-2.90	1.33	1.37
29	B	624	SQD	O47-C7	2.90	1.42	1.34
29	D	408	SQD	O47-C7	2.90	1.42	1.34
29	D	409	SQD	O47-C7	2.89	1.42	1.34
29	B	625	SQD	O47-C7	2.89	1.42	1.34
29	A	616	SQD	O47-C7	2.89	1.42	1.34
27	C	516	BCR	C30-C25	-2.89	1.49	1.53
25	b	604	CLA	C4D-ND	-2.87	1.33	1.37
27	B	618	BCR	C30-C25	-2.87	1.49	1.53
27	h	101	BCR	C30-C25	-2.84	1.49	1.53
27	B	619	BCR	C30-C25	-2.84	1.49	1.53
29	f	101	SQD	O47-C7	2.84	1.42	1.34
27	c	522	BCR	C30-C25	-2.83	1.49	1.53
34	e	101	HEM	CAB-C3B	2.83	1.55	1.47
29	L	101	SQD	O47-C7	2.83	1.42	1.34
27	b	619	BCR	C30-C25	-2.82	1.49	1.53
27	K	101	BCR	C30-C25	-2.82	1.49	1.53
29	A	612	SQD	O47-C7	2.78	1.42	1.34
29	a	613	SQD	O47-C7	2.78	1.42	1.34
27	d	403	BCR	C30-C25	-2.75	1.50	1.53
28	d	404	PL9	C3-C4	-2.72	1.45	1.49
26	a	608	PHO	CAC-C3C	-2.63	1.47	1.52
28	D	405	PL9	C3-C4	-2.56	1.45	1.49
26	a	609	PHO	CAC-C3C	-2.55	1.47	1.52
28	a	612	PL9	C3-C4	-2.52	1.45	1.49
26	D	401	PHO	CAC-C3C	-2.50	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	CAC-C3C	-2.50	1.47	1.52
25	B	611	CLA	CMB-C2B	-2.49	1.46	1.51
28	A	611	PL9	C3-C4	-2.48	1.45	1.49
25	b	611	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	604	CLA	CMB-C2B	-2.46	1.46	1.51
32	C	521	LMG	C1-C2	2.46	1.59	1.52
25	c	506	CLA	CMB-C2B	-2.46	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	615	CLA	CMB-C2B	-2.44	1.46	1.51
28	d	404	PL9	C7-C3	-2.44	1.48	1.51
25	A	607	CLA	CMB-C2B	-2.42	1.46	1.51
25	d	402	CLA	CMB-C2B	-2.42	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.42	1.46	1.51
25	a	607	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	504	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.41	1.46	1.51
25	A	609	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	609	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	601	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	606[B]	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	508	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	604	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	606[A]	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	603	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.40	1.46	1.51
25	d	401	CLA	CMB-C2B	-2.40	1.46	1.51
25	A	613	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.39	1.46	1.51
30	L	102	LHG	O7-C5	-2.38	1.40	1.46
25	a	615	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	608	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.38	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	601	CLA	CMB-C2B	-2.38	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	CMB-C2B	-2.37	1.46	1.51
25	C	504	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.37	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.37	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.37	1.46	1.51
25	C	502	CLA	CMB-C2B	-2.36	1.46	1.51
25	B	613	CLA	CMB-C2B	-2.36	1.46	1.51
25	b	613	CLA	CMB-C2B	-2.36	1.46	1.51
25	C	507	CLA	CMB-C2B	-2.36	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.36	1.46	1.51
25	C	514	CLA	CMB-C2B	-2.35	1.46	1.51
25	b	614	CLA	CMB-C2B	-2.35	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.35	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.35	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.35	1.46	1.51
25	B	608	CLA	CMB-C2B	-2.35	1.46	1.51
25	D	402	CLA	CMB-C2B	-2.34	1.46	1.51
25	c	501	CLA	CMB-C2B	-2.34	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.34	1.46	1.51
25	b	602	CLA	CMB-C2B	-2.34	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.34	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.34	1.46	1.51
25	b	605	CLA	CMB-C2B	-2.34	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.33	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.33	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.33	1.46	1.51
25	a	610	CLA	CMB-C2B	-2.32	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.32	1.46	1.51
28	d	404	PL9	C6-C1	-2.32	1.44	1.48
25	B	605	CLA	CMB-C2B	-2.31	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.31	1.46	1.51
25	A	606	CLA	CMB-C2B	-2.30	1.46	1.51
33	C	519	DGD	O1G-C1G	-2.30	1.39	1.45
25	a	606	CLA	CMB-C2B	-2.28	1.46	1.51
25	B	612	CLA	CMB-C2B	-2.26	1.46	1.51
34	e	101	HEM	FE-NB	2.24	2.08	1.96
33	c	516	DGD	O1G-C1G	-2.20	1.40	1.45
29	f	101	SQD	O2-C2	-2.19	1.37	1.43
33	C	518	DGD	O1G-C1G	-2.18	1.40	1.45
29	A	612	SQD	O2-C2	-2.18	1.37	1.43
29	D	408	SQD	O2-C2	-2.18	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	613	SQD	O2-C2	-2.17	1.37	1.43
29	L	101	SQD	O2-C2	-2.17	1.37	1.43
29	B	625	SQD	O2-C2	-2.15	1.37	1.43
25	C	506	CLA	CMD-C2D	-2.14	1.46	1.50
33	c	516	DGD	O2G-C2G	-2.14	1.41	1.46
30	A	614	LHG	P-O6	2.13	1.67	1.59
30	d	405	LHG	O7-C5	-2.12	1.41	1.46
33	C	519	DGD	O2G-C2G	-2.12	1.41	1.46
30	l	101	LHG	O7-C5	-2.11	1.41	1.46
29	B	624	SQD	O2-C2	-2.11	1.38	1.43
29	A	616	SQD	O2-C2	-2.10	1.38	1.43
29	D	409	SQD	O2-C2	-2.10	1.38	1.43
25	C	511	CLA	CMD-C2D	-2.10	1.46	1.50
30	A	618	LHG	P-O6	2.09	1.67	1.59
30	a	616	LHG	P-O6	2.09	1.67	1.59
33	c	517	DGD	O2G-C2G	-2.09	1.41	1.46
34	E	101	HEM	FE-NB	2.08	2.07	1.96
30	a	617	LHG	O7-C5	-2.07	1.41	1.46
28	A	611	PL9	C53-C6	-2.07	1.46	1.50
29	f	101	SQD	O3-C3	-2.07	1.38	1.43
25	c	505	CLA	CMD-C2D	-2.07	1.46	1.50
26	D	401	PHO	CMC-C2C	-2.06	1.46	1.51
26	a	609	PHO	CMC-C2C	-2.06	1.46	1.51
29	f	101	SQD	O4-C4	-2.06	1.38	1.43
25	c	510	CLA	CMD-C2D	-2.06	1.46	1.50
30	B	623	LHG	O7-C5	-2.05	1.41	1.46
29	D	409	SQD	O3-C3	-2.05	1.38	1.43
26	A	608	PHO	CMC-C2C	-2.05	1.46	1.51
29	B	625	SQD	O4-C4	-2.05	1.38	1.43
25	B	605	CLA	CMD-C2D	-2.05	1.46	1.50
33	c	518	DGD	O2G-C2G	-2.05	1.41	1.46
25	B	604	CLA	CMD-C2D	-2.05	1.46	1.50
33	H	102	DGD	O1G-C1G	-2.05	1.40	1.45
28	a	612	PL9	C53-C6	-2.05	1.46	1.50
29	B	624	SQD	O4-C4	-2.05	1.38	1.43
29	D	408	SQD	O4-C4	-2.04	1.38	1.43
29	D	409	SQD	O4-C4	-2.04	1.38	1.43
29	A	616	SQD	O4-C4	-2.04	1.38	1.43
29	A	612	SQD	O3-C3	-2.03	1.38	1.43
28	d	404	PL9	C53-C6	-2.03	1.46	1.50
25	c	503	CLA	CMD-C2D	-2.03	1.46	1.50
29	B	625	SQD	O3-C3	-2.03	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	609	PHO	CMD-C2D	-2.03	1.46	1.51
29	A	616	SQD	O3-C3	-2.03	1.38	1.43
26	A	608	PHO	CMD-C2D	-2.03	1.46	1.51
25	B	606	CLA	CMD-C2D	-2.03	1.46	1.50
29	A	612	SQD	O4-C4	-2.03	1.38	1.43
29	a	613	SQD	O4-C4	-2.03	1.38	1.43
29	D	408	SQD	O3-C3	-2.03	1.38	1.43
25	C	513	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	612	CLA	CMD-C2D	-2.02	1.46	1.50
30	d	406	LHG	O7-C5	-2.02	1.41	1.46
32	B	626	LMG	C7-C8	2.02	1.56	1.50
29	L	101	SQD	O3-C3	-2.02	1.38	1.43
29	a	613	SQD	O3-C3	-2.02	1.38	1.43
29	B	624	SQD	O3-C3	-2.02	1.38	1.43
26	a	608	PHO	CMD-C2D	-2.02	1.46	1.51
33	C	518	DGD	O2G-C2G	-2.02	1.41	1.46
26	D	401	PHO	CMD-C2D	-2.02	1.46	1.51
33	c	517	DGD	O1G-C1G	-2.02	1.40	1.45
25	b	616	CLA	CMC-C2C	-2.02	1.46	1.50
25	b	605	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	502	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	603	CLA	CMD-C2D	-2.01	1.46	1.50
26	a	608	PHO	CMC-C2C	-2.01	1.46	1.51
25	b	615	CLA	CMD-C2D	-2.01	1.46	1.50
34	E	101	HEM	CMB-C2B	2.01	1.55	1.50
25	A	606	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	607	CLA	CMD-C2D	-2.01	1.46	1.50
25	B	608	CLA	CMD-C2D	-2.01	1.46	1.50
29	L	101	SQD	O4-C4	-2.01	1.38	1.43
30	D	406	LHG	O7-C5	-2.00	1.41	1.46
25	B	603	CLA	CMD-C2D	-2.00	1.46	1.50
25	B	616	CLA	CMC-C2C	-2.00	1.46	1.50
25	D	402	CLA	CMD-C2D	-2.00	1.46	1.50
25	B	612	CLA	CMD-C2D	-2.00	1.46	1.50
33	H	102	DGD	O2G-C2G	-2.00	1.41	1.46

All (1076) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	604	CLA	C4A-NA-C1A	6.83	109.78	106.71
25	B	604	CLA	C4A-NA-C1A	6.41	109.59	106.71
25	c	503	CLA	C4A-NA-C1A	6.39	109.58	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	508	CLA	C4A-NA-C1A	6.32	109.55	106.71
25	c	507	CLA	C4A-NA-C1A	6.31	109.54	106.71
25	b	615	CLA	C4A-NA-C1A	6.18	109.48	106.71
25	c	509	CLA	C4A-NA-C1A	6.17	109.48	106.71
25	C	504	CLA	C4A-NA-C1A	6.15	109.47	106.71
25	c	512	CLA	C4A-NA-C1A	6.05	109.43	106.71
25	B	609	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	B	615	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	B	606	CLA	C4A-NA-C1A	5.95	109.38	106.71
25	C	510	CLA	C4A-NA-C1A	5.87	109.35	106.71
25	b	613	CLA	C4A-NA-C1A	5.84	109.33	106.71
25	c	510	CLA	C4A-NA-C1A	5.84	109.33	106.71
25	C	507	CLA	C4A-NA-C1A	5.79	109.31	106.71
25	B	613	CLA	C4A-NA-C1A	5.78	109.30	106.71
25	B	616	CLA	C4A-NA-C1A	5.77	109.30	106.71
25	C	513	CLA	C4A-NA-C1A	5.76	109.30	106.71
25	C	506	CLA	C4A-NA-C1A	5.70	109.27	106.71
25	B	612	CLA	C4A-NA-C1A	5.69	109.27	106.71
25	b	616	CLA	C4A-NA-C1A	5.69	109.27	106.71
25	C	503	CLA	C4A-NA-C1A	5.67	109.26	106.71
25	c	502	CLA	C4A-NA-C1A	5.67	109.25	106.71
25	b	609	CLA	C4A-NA-C1A	5.66	109.25	106.71
25	B	601	CLA	C4A-NA-C1A	5.65	109.25	106.71
25	b	612	CLA	C4A-NA-C1A	5.63	109.24	106.71
25	c	501	CLA	C4A-NA-C1A	5.57	109.21	106.71
25	C	502	CLA	C4A-NA-C1A	5.51	109.18	106.71
25	C	511	CLA	C4A-NA-C1A	5.49	109.17	106.71
25	b	614	CLA	C4A-NA-C1A	5.45	109.16	106.71
25	B	611	CLA	C4A-NA-C1A	5.42	109.14	106.71
25	b	611	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	c	504	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	a	610	CLA	C4A-NA-C1A	5.41	109.14	106.71
28	a	612	PL9	C7-C3-C4	5.40	121.27	116.88
25	b	610	CLA	C4A-NA-C1A	5.39	109.13	106.71
25	c	505	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	b	601	CLA	C4A-NA-C1A	5.34	109.11	106.71
25	d	402	CLA	C4A-NA-C1A	5.32	109.10	106.71
25	C	509	CLA	C4A-NA-C1A	5.28	109.08	106.71
25	c	506	CLA	C4A-NA-C1A	5.27	109.07	106.71
25	B	605	CLA	C4A-NA-C1A	5.24	109.06	106.71
25	C	514	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	b	605	CLA	C4A-NA-C1A	5.20	109.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	608	CLA	C4A-NA-C1A	5.15	109.02	106.71
28	D	405	PL9	C7-C3-C4	5.15	121.06	116.88
25	d	401	CLA	C4A-NA-C1A	5.15	109.02	106.71
25	b	606[B]	CLA	C4A-NA-C1A	5.14	109.02	106.71
28	A	611	PL9	C7-C3-C4	5.13	121.04	116.88
25	b	606[A]	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	D	403	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	A	609	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	c	508	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	b	602	CLA	C4A-NA-C1A	5.04	108.97	106.71
28	d	404	PL9	C7-C3-C4	4.98	120.93	116.88
25	B	610	CLA	C4A-NA-C1A	4.97	108.94	106.71
25	D	402	CLA	C4A-NA-C1A	4.96	108.94	106.71
25	B	602	CLA	C4A-NA-C1A	4.78	108.85	106.71
25	C	505	CLA	C4A-NA-C1A	4.77	108.85	106.71
25	c	513	CLA	C4A-NA-C1A	4.68	108.81	106.71
25	B	603	CLA	C4A-NA-C1A	4.55	108.75	106.71
33	c	516	DGD	O3G-C3G-C2G	-4.52	100.00	110.90
33	C	518	DGD	O3G-C3G-C2G	-4.46	100.15	110.90
25	b	603	CLA	C4A-NA-C1A	4.44	108.70	106.71
25	b	607	CLA	C4A-NA-C1A	4.42	108.69	106.71
25	b	608	CLA	C4A-NA-C1A	4.36	108.67	106.71
25	a	607	CLA	C4A-NA-C1A	4.35	108.66	106.71
25	C	512	CLA	C4A-NA-C1A	4.35	108.66	106.71
33	c	517	DGD	O3G-C3G-C2G	-4.29	100.55	110.90
29	D	409	SQD	O9-S-C6	4.28	112.03	106.94
25	B	613	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
29	D	408	SQD	O9-S-C6	4.22	111.95	106.94
30	d	405	LHG	O4-P-O5	4.21	133.07	112.24
30	d	406	LHG	O4-P-O5	4.20	132.99	112.24
25	a	615	CLA	C4A-NA-C1A	4.19	108.59	106.71
30	a	617	LHG	O4-P-O5	4.19	132.95	112.24
29	L	101	SQD	O7-S-C6	4.18	111.91	106.94
30	L	102	LHG	O4-P-O5	4.18	132.90	112.24
25	c	511	CLA	C4A-NA-C1A	4.17	108.58	106.71
30	B	623	LHG	O4-P-O5	4.16	132.82	112.24
29	D	409	SQD	O7-S-C6	4.16	111.89	106.94
30	A	614	LHG	O4-P-O5	4.16	132.79	112.24
30	A	618	LHG	O4-P-O5	4.16	132.79	112.24
30	l	101	LHG	O4-P-O5	4.15	132.76	112.24
30	D	406	LHG	O4-P-O5	4.15	132.75	112.24
30	a	616	LHG	O4-P-O5	4.14	132.71	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	613	CLA	C4A-NA-C1A	4.13	108.56	106.71
25	A	607	CLA	C4A-NA-C1A	4.12	108.56	106.71
25	D	403	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
29	A	612	SQD	O7-S-C6	4.05	111.75	106.94
33	C	519	DGD	O3G-C3G-C2G	-4.02	101.21	110.90
25	A	606	CLA	C4A-NA-C1A	4.00	108.50	106.71
25	B	607	CLA	C4A-NA-C1A	4.00	108.50	106.71
25	C	510	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
25	a	606	CLA	C4A-NA-C1A	3.97	108.49	106.71
29	b	621	SQD	O47-C7-C8	3.96	120.04	111.50
25	b	613	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
25	c	509	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
29	A	612	SQD	O47-C7-C8	3.93	119.97	111.50
33	c	518	DGD	O3G-C3G-C2G	-3.91	101.46	110.90
25	b	611	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
29	B	625	SQD	O7-S-C6	3.89	111.57	106.94
25	c	508	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
25	B	612	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
29	a	613	SQD	O7-S-C6	3.88	111.55	106.94
29	B	624	SQD	O6-C1-C2	3.87	114.34	108.30
29	A	616	SQD	O7-S-C6	3.85	111.52	106.94
33	H	102	DGD	O3G-C3G-C2G	-3.85	101.62	110.90
25	B	607	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
29	B	624	SQD	O9-S-C6	3.81	111.47	106.94
25	b	603	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
25	B	611	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
29	D	408	SQD	O7-S-C6	3.79	111.44	106.94
25	A	606	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
29	f	101	SQD	O9-S-C6	3.78	111.44	106.94
25	b	612	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
29	A	612	SQD	O9-S-C6	3.77	111.42	106.94
33	h	102	DGD	O3G-C3G-C2G	-3.77	101.81	110.90
29	B	625	SQD	O47-C7-C8	3.76	119.61	111.50
29	A	616	SQD	O9-S-C6	3.75	111.40	106.94
35	v	201	HEC	CMC-C2C-C1C	-3.75	122.69	128.46
25	c	510	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
25	C	509	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
25	C	506	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	A	616	SQD	O47-C7-C8	3.71	119.49	111.50
25	A	609	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
33	C	517	DGD	O3G-C3G-C2G	-3.70	101.96	110.90
29	D	408	SQD	O9-S-O7	-3.70	101.13	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	511	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
29	B	625	SQD	O9-S-O7	-3.70	101.15	113.95
29	L	101	SQD	O9-S-O7	-3.70	101.16	113.95
28	a	612	PL9	C7-C3-C2	-3.69	118.45	123.30
29	B	624	SQD	O9-S-O7	-3.67	101.24	113.95
29	A	616	SQD	O9-S-O7	-3.67	101.25	113.95
25	B	614	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
25	b	602	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
29	D	409	SQD	O9-S-O7	-3.65	101.32	113.95
25	B	602	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
29	a	613	SQD	O9-S-O7	-3.64	101.34	113.95
25	C	514	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	a	606	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
25	b	608	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
29	f	101	SQD	O9-S-O7	-3.61	101.45	113.95
25	b	614	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
25	c	505	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
25	c	511	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
35	V	201	HEC	CMB-C2B-C1B	-3.60	122.93	128.46
25	C	508	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
29	A	612	SQD	O9-S-O7	-3.60	101.50	113.95
29	B	624	SQD	C44-O6-C1	3.60	120.77	113.74
25	c	513	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
32	C	521	LMG	O6-C1-O1	-3.59	101.47	109.97
25	C	507	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
25	B	614	CLA	C4A-NA-C1A	3.57	108.31	106.71
25	C	512	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
29	B	624	SQD	O47-C7-C8	3.56	119.18	111.50
29	B	625	SQD	O9-S-C6	3.56	111.17	106.94
29	A	612	SQD	O6-C1-C2	3.56	113.86	108.30
25	a	610	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
25	B	605	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
35	v	201	HEC	CMB-C2B-C1B	-3.54	123.03	128.46
25	B	613	CLA	CMB-C2B-C3B	3.54	131.29	124.68
25	C	505	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	B	608	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
25	b	607	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
25	b	616	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
25	c	506	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
29	L	101	SQD	O47-C7-C8	3.50	119.05	111.50
29	L	101	SQD	O9-S-C6	3.50	111.10	106.94
29	f	101	SQD	O7-S-C6	3.50	111.09	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	613	SQD	O9-S-C6	3.49	111.09	106.94
25	D	403	CLA	CMB-C2B-C3B	3.49	131.20	124.68
25	c	501	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
25	D	402	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
29	D	408	SQD	O47-C7-C8	3.47	118.97	111.50
29	D	409	SQD	O47-C7-C8	3.46	118.97	111.50
25	B	610	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
35	V	201	HEC	CMC-C2C-C1C	-3.45	123.16	128.46
25	b	609	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
28	A	611	PL9	C7-C3-C2	-3.43	118.78	123.30
25	B	616	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	A	607	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
25	B	603	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
25	B	601	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	d	402	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	C	510	CLA	CMB-C2B-C3B	3.39	131.03	124.68
28	D	405	PL9	C7-C3-C2	-3.39	118.85	123.30
29	a	613	SQD	O47-C7-C8	3.38	118.79	111.50
25	c	504	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
29	D	408	SQD	O6-C1-C2	3.38	113.58	108.30
25	B	612	CLA	CMB-C2B-C3B	3.38	131.00	124.68
29	L	101	SQD	O5-C5-C4	3.37	115.81	109.69
29	a	613	SQD	O6-C1-C2	3.36	113.55	108.30
29	B	624	SQD	O7-S-C6	3.36	110.93	106.94
25	C	504	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
25	b	606[A]	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	c	509	CLA	CMB-C2B-C3B	3.34	130.92	124.68
25	b	613	CLA	CMB-C2B-C3B	3.33	130.91	124.68
25	C	502	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
25	c	502	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
25	b	606[B]	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
27	b	618	BCR	C15-C14-C13	-3.31	122.58	127.31
25	C	513	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	a	607	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	b	610	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	b	601	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
25	A	613	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
25	B	604	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
33	c	517	DGD	O6D-C1D-O3G	-3.25	102.27	109.97
25	B	609	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
25	c	507	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
25	c	503	CLA	CMB-C2B-C1B	-3.25	123.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	615	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
26	a	609	PHO	CMB-C2B-C3B	3.24	130.74	124.68
25	c	508	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	C	503	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
28	d	404	PL9	C7-C3-C2	-3.21	119.07	123.30
32	c	520	LMG	O6-C1-O1	-3.20	102.39	109.97
25	c	512	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
25	B	607	CLA	CMB-C2B-C3B	3.20	130.67	124.68
25	b	606[B]	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
33	C	519	DGD	O6D-C1D-O3G	-3.19	102.43	109.97
25	B	606	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
33	c	518	DGD	O6D-C1D-O3G	-3.18	102.44	109.97
25	b	603	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	A	606	CLA	CMB-C2B-C3B	3.18	130.62	124.68
29	B	624	SQD	O8-S-C6	3.17	110.80	105.74
25	b	612	CLA	CMB-C2B-C3B	3.16	130.58	124.68
25	C	506	CLA	CMB-C2B-C3B	3.15	130.57	124.68
29	D	408	SQD	O5-C5-C4	3.15	115.41	109.69
25	b	605	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
28	D	405	PL9	C40-C39-C41	3.14	120.56	115.27
25	C	513	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	b	611	CLA	CMB-C2B-C3B	3.13	130.54	124.68
25	d	401	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
25	C	511	CLA	CMB-C2B-C3B	3.13	130.53	124.68
33	C	518	DGD	O6D-C1D-O3G	-3.13	102.56	109.97
25	C	509	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	B	602	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
33	C	517	DGD	O6D-C1D-O3G	-3.12	102.59	109.97
25	c	510	CLA	CMB-C2B-C3B	3.11	130.50	124.68
26	a	608	PHO	CMB-C2B-C3B	3.11	130.49	124.68
25	C	514	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
25	c	508	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
25	b	606[A]	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
33	c	516	DGD	O6D-C1D-O3G	-3.09	102.65	109.97
27	b	618	BCR	C15-C16-C17	-3.08	117.16	123.47
25	a	610	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	b	604	CLA	CMB-C2B-C1B	-3.08	123.74	128.46
29	a	613	SQD	O8-S-C6	3.07	110.64	105.74
25	c	513	CLA	CMB-C2B-C3B	3.07	130.43	124.68
25	b	602	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	B	615	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
25	b	602	CLA	CMB-C2B-C3B	3.07	130.43	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	501	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
25	B	602	CLA	CMB-C2B-C3B	3.07	130.42	124.68
29	B	624	SQD	O5-C5-C4	3.07	115.27	109.69
25	A	609	CLA	CMB-C2B-C3B	3.06	130.41	124.68
25	C	502	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
29	D	409	SQD	C1-O5-C5	3.06	119.69	113.69
25	c	505	CLA	CMB-C2B-C3B	3.06	130.40	124.68
25	a	606	CLA	CMB-C2B-C3B	3.05	130.39	124.68
25	c	505	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
25	C	509	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
29	f	101	SQD	O5-C5-C4	3.04	115.22	109.69
29	f	101	SQD	O8-S-C6	3.04	110.58	105.74
25	C	508	CLA	CMB-C2B-C3B	3.03	130.36	124.68
25	b	614	CLA	CMB-C2B-C3B	3.03	130.35	124.68
25	b	608	CLA	CMB-C2B-C3B	3.03	130.34	124.68
28	a	612	PL9	C40-C39-C41	3.03	120.36	115.27
25	C	514	CLA	CMB-C2B-C3B	3.02	130.33	124.68
26	D	401	PHO	CMB-C2B-C3B	3.02	130.33	124.68
25	b	603	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	a	615	CLA	CHD-C1D-ND	-3.02	121.68	124.45
25	c	511	CLA	CMB-C2B-C3B	3.02	130.32	124.68
25	B	614	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	D	403	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	C	508	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
34	e	101	HEM	C4B-CHC-C1C	3.01	126.54	122.56
25	A	609	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
29	f	101	SQD	O47-C7-C8	3.01	119.19	110.80
25	a	610	CLA	CMB-C2B-C3B	3.00	130.30	124.68
25	B	614	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	b	604	CLA	CHB-C4A-NA	3.00	128.66	124.51
25	C	507	CLA	CMB-C2B-C3B	2.99	130.28	124.68
29	L	101	SQD	O6-C1-C2	2.99	112.97	108.30
25	A	606	CLA	CHB-C4A-NA	2.98	128.64	124.51
25	B	605	CLA	CMB-C2B-C3B	2.98	130.26	124.68
25	B	601	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	B	611	CLA	CMB-C2B-C3B	2.98	130.25	124.68
29	B	625	SQD	C44-O6-C1	2.98	119.55	113.74
25	B	616	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
33	H	102	DGD	O6D-C1D-O3G	-2.97	102.94	109.97
25	b	607	CLA	CMB-C2B-C3B	2.96	130.21	124.68
25	A	607	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
26	A	608	PHO	CMB-C2B-C3B	2.95	130.20	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	507	CLA	CHB-C4A-NA	2.94	128.58	124.51
29	f	101	SQD	O6-C1-C2	2.94	112.90	108.30
25	c	507	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	d	402	CLA	CHB-C4A-NA	2.94	128.58	124.51
25	C	512	CLA	CMB-C2B-C3B	2.94	130.18	124.68
25	b	611	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
25	b	607	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	B	616	CLA	CMB-C2B-C3B	2.94	130.17	124.68
28	A	611	PL9	C40-C39-C41	2.93	120.20	115.27
35	v	201	HEC	CMC-C2C-C3C	2.93	129.27	125.82
25	b	612	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	c	512	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	b	605	CLA	CHD-C1D-ND	-2.93	121.76	124.45
25	a	606	CLA	CHB-C4A-NA	2.92	128.56	124.51
25	b	616	CLA	CMB-C2B-C3B	2.92	130.15	124.68
25	b	601	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
25	d	402	CLA	CHD-C1D-ND	-2.92	121.77	124.45
25	c	513	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
30	a	616	LHG	O8-C23-C24	2.92	121.06	111.91
25	A	613	CLA	CHB-C4A-NA	2.91	128.54	124.51
25	b	608	CLA	CHD-C1D-ND	-2.91	121.78	124.45
29	a	613	SQD	O5-C5-C4	2.91	114.98	109.69
26	a	609	PHO	O2D-CGD-O1D	-2.91	118.15	123.84
25	B	608	CLA	CMB-C2B-C3B	2.91	130.12	124.68
34	e	101	HEM	C1B-NB-C4B	2.91	108.08	105.07
25	a	607	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
25	A	613	CLA	CHD-C1D-ND	-2.91	121.78	124.45
25	c	512	CLA	CHB-C4A-NA	2.90	128.53	124.51
25	C	505	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	C	508	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	a	610	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	a	615	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
25	B	611	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	c	504	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
27	C	516	BCR	C15-C16-C17	-2.89	117.55	123.47
25	b	607	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	D	402	CLA	CMB-C2B-C3B	2.89	130.09	124.68
25	C	506	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	b	608	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	a	609	PHO	O1D-CGD-CBD	2.89	129.55	124.74
29	L	101	SQD	O8-S-C6	2.89	110.34	105.74
27	c	515	BCR	C15-C16-C17	-2.88	117.57	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	c	506	CLA	CMB-C2B-C3B	2.88	130.07	124.68
25	C	507	CLA	CHB-C4A-NA	2.88	128.50	124.51
25	B	612	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	c	510	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	C	505	CLA	CMB-C2B-C3B	2.88	130.06	124.68
25	d	401	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	C	503	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	B	604	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	b	602	CLA	CHD-C1D-ND	-2.87	121.81	124.45
34	E	101	HEM	C4B-CHC-C1C	2.87	126.34	122.56
25	A	609	CLA	CHB-C4A-NA	2.87	128.48	124.51
25	B	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
32	C	501	LMG	O6-C1-O1	-2.86	103.20	109.97
25	C	507	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	b	609	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	b	615	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
25	A	607	CLA	CMB-C2B-C3B	2.86	130.03	124.68
27	t	101	BCR	C33-C5-C6	-2.86	121.32	124.53
29	D	409	SQD	C44-O6-C1	2.86	119.32	113.74
25	b	610	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	B	603	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	D	403	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	B	603	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	c	501	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	b	604	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
33	h	102	DGD	O6D-C1D-O3G	-2.85	103.23	109.97
25	A	613	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	B	615	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	C	505	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	b	616	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	C	505	CLA	CHD-C1D-ND	-2.83	121.85	124.45
25	a	607	CLA	CHB-C4A-NA	2.83	128.43	124.51
25	c	504	CLA	CHB-C4A-NA	2.83	128.43	124.51
25	c	513	CLA	CHB-C4A-NA	2.83	128.43	124.51
27	h	101	BCR	C24-C23-C22	-2.83	121.96	126.23
25	A	607	CLA	CHD-C1D-ND	-2.83	121.85	124.45
25	a	615	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	B	612	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	c	511	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	C	512	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	B	610	CLA	CMB-C2B-C3B	2.82	129.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	402	CLA	CMB-C2B-C3B	2.82	129.95	124.68
25	B	605	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
28	d	404	PL9	C40-C39-C41	2.81	120.00	115.27
35	V	201	HEC	CMB-C2B-C3B	2.81	129.13	125.82
29	A	612	SQD	O5-C5-C4	2.81	114.80	109.69
25	c	504	CLA	CMB-C2B-C3B	2.81	129.93	124.68
25	B	615	CLA	CHB-C4A-NA	2.81	128.39	124.51
25	B	601	CLA	CMB-C2B-C3B	2.81	129.93	124.68
25	c	509	CLA	CHB-C4A-NA	2.81	128.39	124.51
29	B	624	SQD	C1-O5-C5	2.80	119.19	113.69
26	A	608	PHO	O1D-CGD-CBD	2.80	129.41	124.74
25	b	605	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	B	608	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	b	613	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	C	510	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	b	602	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	b	608	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	b	614	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	B	610	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	C	504	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	a	607	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	b	615	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	C	502	CLA	CMB-C2B-C3B	2.78	129.89	124.68
25	c	502	CLA	CMB-C2B-C3B	2.78	129.89	124.68
25	b	603	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	C	509	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	C	513	CLA	CHB-C4A-NA	2.77	128.35	124.51
26	D	401	PHO	O2D-CGD-O1D	-2.77	118.41	123.84
25	c	507	CLA	CMB-C2B-C3B	2.77	129.87	124.68
32	m	102	LMG	O6-C1-O1	-2.77	103.41	109.97
29	B	625	SQD	O8-S-C6	2.77	110.16	105.74
25	B	604	CLA	CHB-C4A-NA	2.77	128.34	124.51
33	C	519	DGD	CDB-CCB-CBB	-2.77	100.37	114.42
29	D	408	SQD	O8-S-C6	2.77	110.15	105.74
29	A	616	SQD	O8-S-C6	2.77	110.15	105.74
25	B	614	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	C	503	CLA	CMB-C2B-C3B	2.76	129.84	124.68
33	C	517	DGD	CDB-CCB-CBB	-2.76	100.43	114.42
25	C	513	CLA	CMB-C2B-C3B	2.76	129.84	124.68
25	B	608	CLA	CHB-C4A-NA	2.76	128.32	124.51
25	B	602	CLA	CHB-C4A-NA	2.75	128.32	124.51
34	e	101	HEM	C4D-ND-C1D	2.75	107.92	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	504	CLA	CMB-C2B-C3B	2.75	129.83	124.68
25	C	512	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	C	510	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	c	502	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
25	b	616	CLA	CHD-C1D-ND	-2.75	121.93	124.45
25	C	514	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	c	501	CLA	CHD-C1D-ND	-2.75	121.93	124.45
25	B	610	CLA	CHD-C1D-ND	-2.74	121.94	124.45
32	b	620	LMG	O6-C1-O1	-2.74	103.49	109.97
25	b	610	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
25	b	601	CLA	CMB-C2B-C3B	2.74	129.80	124.68
32	B	620	LMG	O6-C1-O1	-2.73	103.50	109.97
25	c	506	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	b	614	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
29	A	612	SQD	O8-S-C6	2.73	110.09	105.74
33	C	518	DGD	CDB-CCB-CBB	-2.73	100.55	114.42
25	b	616	CLA	CHB-C4A-NA	2.73	128.29	124.51
33	h	102	DGD	CDB-CCB-CBB	-2.73	100.57	114.42
25	b	606[A]	CLA	CMB-C2B-C3B	2.73	129.78	124.68
32	C	520	LMG	O6-C1-O1	-2.73	103.52	109.97
25	B	616	CLA	CHB-C4A-NA	2.72	128.28	124.51
25	c	503	CLA	CHB-C4A-NA	2.72	128.28	124.51
25	B	606	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	B	606	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	C	511	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
32	B	626	LMG	O6-C1-O1	-2.71	103.55	109.97
30	D	406	LHG	O8-C23-C24	2.71	120.42	111.91
35	v	201	HEC	CMB-C2B-C3B	2.71	129.01	125.82
25	c	508	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	B	613	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
33	c	517	DGD	CDB-CCB-CBB	-2.71	100.67	114.42
34	e	101	HEM	C3B-C2B-C1B	2.71	108.49	106.49
25	d	402	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
25	a	615	CLA	CMB-C2B-C3B	2.70	129.74	124.68
25	b	610	CLA	CMB-C2B-C3B	2.70	129.73	124.68
34	e	101	HEM	C4C-CHD-C1D	2.70	126.12	122.56
33	H	102	DGD	CDB-CCB-CBB	-2.70	100.73	114.42
25	D	402	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
25	c	503	CLA	CMB-C2B-C3B	2.70	129.72	124.68
25	b	606[B]	CLA	CMB-C2B-C3B	2.69	129.72	124.68
27	b	617	BCR	C33-C5-C6	-2.69	121.50	124.53
25	c	503	CLA	O2D-CGD-O1D	-2.69	118.58	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	512	CLA	CMB-C2B-C3B	2.69	129.71	124.68
25	D	403	CLA	CHD-C1D-ND	-2.69	121.98	124.45
34	e	101	HEM	CBA-CAA-C2A	-2.68	108.04	112.62
25	B	601	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	B	607	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	A	613	CLA	CMB-C2B-C3B	2.68	129.70	124.68
27	t	101	BCR	C15-C16-C17	-2.68	117.98	123.47
25	b	601	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	C	502	CLA	CHB-C4A-NA	2.68	128.21	124.51
25	C	511	CLA	CHB-C4A-NA	2.68	128.21	124.51
25	c	505	CLA	CHB-C4A-NA	2.68	128.21	124.51
25	c	511	CLA	CHD-C1D-ND	-2.68	122.00	124.45
33	c	516	DGD	CDB-CCB-CBB	-2.67	100.85	114.42
25	b	615	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	B	603	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	b	606[A]	CLA	CHB-C4A-NA	2.67	128.21	124.51
32	B	621	LMG	O6-C1-O1	-2.67	103.65	109.97
25	C	504	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	b	611	CLA	CHB-C4A-NA	2.67	128.20	124.51
25	B	613	CLA	CHB-C4A-NA	2.67	128.20	124.51
34	E	101	HEM	C4D-ND-C1D	2.67	107.83	105.07
25	B	609	CLA	CMB-C2B-C3B	2.67	129.67	124.68
30	d	406	LHG	O8-C23-C24	2.66	120.26	111.91
25	B	611	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	d	401	CLA	CMB-C2B-C3B	2.66	129.66	124.68
32	c	519	LMG	O6-C1-O1	-2.66	103.67	109.97
25	B	609	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
25	b	609	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
25	c	506	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	b	617	BCR	C15-C16-C17	-2.65	118.04	123.47
25	B	604	CLA	C1-C2-C3	-2.65	121.45	126.04
28	A	611	PL9	C7-C8-C9	-2.65	122.38	126.79
27	H	101	BCR	C27-C26-C25	2.65	126.58	122.73
25	b	606[B]	CLA	CHB-C4A-NA	2.65	128.17	124.51
32	d	407	LMG	O6-C1-O1	-2.65	103.70	109.97
25	b	613	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	b	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
25	b	601	CLA	CHD-C1D-ND	-2.64	122.03	124.45
25	C	514	CLA	CHD-C1D-ND	-2.64	122.03	124.45
25	c	508	CLA	CHD-C1D-ND	-2.64	122.03	124.45
29	A	616	SQD	C44-O6-C1	2.64	118.89	113.74
30	l	101	LHG	O8-C23-C24	2.63	120.17	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	617	BCR	C15-C14-C13	-2.63	123.55	127.31
25	C	504	CLA	CHD-C1D-ND	-2.63	122.04	124.45
28	A	611	PL9	C22-C23-C24	-2.63	121.33	127.66
29	D	409	SQD	O8-S-C6	2.63	109.92	105.74
25	C	509	CLA	CHD-C1D-ND	-2.62	122.04	124.45
25	B	605	CLA	CHD-C1D-ND	-2.62	122.04	124.45
27	c	521	BCR	C33-C5-C6	-2.62	121.58	124.53
25	a	607	CLA	CHD-C1D-ND	-2.62	122.04	124.45
28	D	405	PL9	C7-C8-C9	-2.62	122.43	126.79
25	B	606	CLA	CMB-C2B-C3B	2.62	129.58	124.68
25	b	605	CLA	CMB-C2B-C3B	2.62	129.57	124.68
26	a	608	PHO	O2D-CGD-O1D	-2.62	118.72	123.84
27	Y	101	BCR	C33-C5-C6	-2.61	121.60	124.53
30	B	623	LHG	C11-C10-C9	-2.61	101.19	114.42
25	c	504	CLA	CHD-C1D-ND	-2.61	122.06	124.45
25	A	607	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	c	502	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	b	605	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	B	603	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
25	D	402	CLA	CHD-C1D-ND	-2.60	122.06	124.45
27	K	101	BCR	C15-C16-C17	-2.60	118.15	123.47
25	a	606	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
30	A	614	LHG	O8-C23-C24	2.59	120.05	111.91
25	B	605	CLA	CHB-C4A-NA	2.59	128.10	124.51
27	T	101	BCR	C15-C16-C17	-2.59	118.17	123.47
27	t	101	BCR	C15-C14-C13	-2.59	123.62	127.31
25	B	604	CLA	CMB-C2B-C3B	2.58	129.51	124.68
29	D	408	SQD	O48-C23-C24	2.58	120.02	111.91
27	T	101	BCR	C15-C14-C13	-2.58	123.62	127.31
28	d	404	PL9	C27-C28-C29	-2.58	121.45	127.66
25	C	510	CLA	CHD-C1D-ND	-2.57	122.09	124.45
25	C	503	CLA	CHB-C4A-NA	2.57	128.07	124.51
25	c	506	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
25	c	510	CLA	CHB-C4A-NA	2.57	128.06	124.51
26	a	608	PHO	O1D-CGD-CBD	2.57	129.02	124.74
25	A	609	CLA	CHD-C1D-ND	-2.57	122.10	124.45
25	B	606	CLA	CHD-C1D-ND	-2.57	122.10	124.45
30	d	405	LHG	C11-C10-C9	-2.56	101.40	114.42
25	C	511	CLA	CHD-C1D-ND	-2.56	122.10	124.45
27	h	101	BCR	C11-C10-C9	-2.56	123.65	127.31
30	A	618	LHG	O8-C23-C24	2.56	119.95	111.91
25	B	602	CLA	CHD-C1D-ND	-2.56	122.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	404	PL9	C7-C8-C9	-2.56	122.53	126.79
25	b	612	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	D	402	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	b	611	CLA	CHD-C1D-ND	-2.55	122.11	124.45
27	b	618	BCR	C27-C26-C25	2.55	126.44	122.73
33	c	518	DGD	CDB-CCB-CBB	-2.55	101.48	114.42
25	B	609	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	B	609	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
25	c	509	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
30	a	617	LHG	C20-C19-C18	-2.55	101.50	114.42
25	D	402	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
33	c	517	DGD	O5D-C6D-C5D	-2.54	104.34	109.05
26	A	608	PHO	O2D-CGD-O1D	-2.54	118.86	123.84
25	c	501	CLA	CHB-C4A-NA	2.54	128.03	124.51
35	V	201	HEC	CBA-CAA-C2A	-2.54	108.32	112.60
25	d	401	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	B	615	CLA	CMB-C2B-C3B	2.54	129.42	124.68
28	a	612	PL9	C20-C19-C21	2.54	119.54	115.27
25	c	512	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	L	101	SQD	C44-O6-C1	2.54	118.69	113.74
30	a	617	LHG	O8-C23-C24	2.54	119.86	111.91
25	c	505	CLA	CHD-C1D-ND	-2.53	122.13	124.45
30	d	405	LHG	O8-C23-C24	2.53	119.85	111.91
27	B	618	BCR	C15-C14-C13	-2.53	123.70	127.31
29	f	101	SQD	C44-O6-C1	2.53	118.68	113.74
25	b	609	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
25	b	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	d	403	BCR	C33-C5-C6	-2.52	121.69	124.53
25	B	607	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
27	Y	101	BCR	C27-C26-C25	2.52	126.39	122.73
33	c	516	DGD	O5D-C6D-C5D	-2.52	104.39	109.05
25	b	609	CLA	CHD-C1D-ND	-2.52	122.14	124.45
25	C	512	CLA	CHD-C1D-ND	-2.52	122.14	124.45
30	L	102	LHG	O8-C23-C24	2.52	119.80	111.91
35	V	201	HEC	CMC-C2C-C3C	2.51	128.78	125.82
25	B	610	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
25	D	403	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
30	B	623	LHG	O8-C23-C24	2.51	119.77	111.91
27	c	515	BCR	C27-C26-C25	2.50	126.37	122.73
27	c	514	BCR	C15-C16-C17	-2.50	118.35	123.47
27	b	617	BCR	C27-C26-C25	2.50	126.36	122.73
25	A	606	CLA	CHD-C1D-ND	-2.50	122.16	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	503	CLA	CHD-C1D-ND	-2.50	122.16	124.45
25	B	611	CLA	CHB-C4A-NA	2.50	127.96	124.51
29	B	625	SQD	O48-C23-C24	2.49	119.73	111.91
25	B	608	CLA	CHD-C1D-ND	-2.49	122.16	124.45
25	c	506	CLA	CHD-C1D-ND	-2.49	122.16	124.45
27	t	101	BCR	C27-C26-C25	2.48	126.34	122.73
25	d	401	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
28	D	405	PL9	C20-C19-C21	2.48	119.45	115.27
32	c	519	LMG	C38-C37-C36	-2.48	101.83	114.42
27	h	101	BCR	C33-C5-C6	-2.48	121.74	124.53
27	A	610	BCR	C27-C26-C25	2.48	126.33	122.73
27	c	514	BCR	C27-C26-C25	2.48	126.33	122.73
24	A	605	BCT	O2-C-O1	-2.48	113.12	119.55
32	D	407	LMG	O6-C1-O1	-2.48	104.11	109.97
29	D	409	SQD	O5-C5-C4	2.48	114.19	109.69
29	A	612	SQD	O48-C23-C24	2.47	119.67	111.91
33	c	516	DGD	C3G-C2G-C1G	-2.47	105.94	111.79
30	d	405	LHG	C20-C19-C18	-2.47	101.88	114.42
29	a	613	SQD	O48-C23-C24	2.47	119.66	111.91
24	a	605	BCT	O2-C-O1	-2.47	113.14	119.55
25	B	609	CLA	CHD-C1D-ND	-2.47	122.19	124.45
32	m	102	LMG	C40-C39-C38	-2.47	101.90	114.42
25	c	502	CLA	CHD-C1D-ND	-2.47	122.19	124.45
27	C	515	BCR	C27-C26-C25	2.46	126.31	122.73
27	c	522	BCR	C33-C5-C6	-2.46	121.76	124.53
25	b	604	CLA	CMB-C2B-C3B	2.46	129.29	124.68
25	b	606[A]	CLA	CHD-C1D-ND	-2.46	122.19	124.45
25	c	513	CLA	CHD-C1D-ND	-2.46	122.19	124.45
27	K	101	BCR	C33-C5-C6	-2.46	121.76	124.53
25	B	602	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
29	L	101	SQD	O48-C23-C24	2.46	119.63	111.91
30	A	618	LHG	C11-C10-C9	-2.46	101.95	114.42
30	l	101	LHG	C11-C10-C9	-2.46	101.95	114.42
27	T	101	BCR	C27-C26-C25	2.46	126.30	122.73
29	A	616	SQD	O5-C5-C4	2.46	114.15	109.69
25	d	401	CLA	CHD-C1D-ND	-2.45	122.20	124.45
25	b	608	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
33	C	517	DGD	O5D-C6D-C5D	-2.45	104.51	109.05
25	C	508	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	b	607	CLA	CHD-C1D-ND	-2.45	122.20	124.45
25	B	612	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	b	610	CLA	CHD-C1D-ND	-2.45	122.20	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	522	BCR	C24-C23-C22	-2.45	122.54	126.23
25	A	609	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
33	C	518	DGD	O5D-C6D-C5D	-2.44	104.52	109.05
27	a	611	BCR	C27-C26-C25	2.44	126.28	122.73
25	b	607	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
29	B	625	SQD	O5-C5-C4	2.44	114.13	109.69
27	B	618	BCR	C15-C16-C17	-2.44	118.47	123.47
30	D	406	LHG	C20-C19-C18	-2.44	102.04	114.42
30	A	614	LHG	C11-C10-C9	-2.44	102.05	114.42
25	b	602	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
25	C	502	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	c	507	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
28	a	612	PL9	C27-C28-C29	-2.44	121.80	127.66
26	D	401	PHO	O1D-CGD-CBD	2.43	128.79	124.74
30	L	102	LHG	C11-C10-C9	-2.43	102.07	114.42
25	b	606[B]	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	B	614	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
25	B	613	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	B	611	CLA	C1-C2-C3	-2.43	121.84	126.04
25	b	603	CLA	CHD-C1D-ND	-2.43	122.22	124.45
32	b	620	LMG	C40-C39-C38	-2.42	102.12	114.42
25	C	506	CLA	CHB-C4A-NA	2.42	127.86	124.51
32	C	520	LMG	C40-C39-C38	-2.42	102.12	114.42
32	B	620	LMG	C40-C39-C38	-2.42	102.13	114.42
27	b	619	BCR	C27-C26-C25	2.42	126.25	122.73
27	B	617	BCR	C15-C16-C17	-2.42	118.52	123.47
28	A	611	PL9	C27-C28-C29	-2.42	121.83	127.66
25	d	402	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
25	B	608	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
25	B	614	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
32	d	408	LMG	C40-C39-C38	-2.42	102.15	114.42
25	C	513	CLA	CHD-C1D-ND	-2.42	122.23	124.45
32	b	620	LMG	O1-C1-C2	-2.42	104.53	108.30
27	C	516	BCR	C11-C10-C9	-2.42	123.86	127.31
32	B	620	LMG	O1-C7-C8	-2.42	105.07	110.90
32	c	519	LMG	C40-C39-C38	-2.41	102.17	114.42
28	a	612	PL9	C22-C23-C24	-2.41	121.85	127.66
27	C	516	BCR	C15-C14-C13	-2.41	123.87	127.31
32	C	501	LMG	C40-C39-C38	-2.41	102.18	114.42
25	b	614	CLA	CHD-C1D-ND	-2.41	122.24	124.45
27	C	515	BCR	C15-C16-C17	-2.41	118.54	123.47
25	B	601	CLA	CHD-C1D-ND	-2.41	122.24	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	521	BCR	C27-C26-C25	2.41	126.23	122.73
32	C	521	LMG	C40-C39-C38	-2.41	102.20	114.42
25	b	616	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
25	c	505	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
27	C	516	BCR	C33-C5-C6	-2.41	121.83	124.53
27	K	101	BCR	C27-C26-C25	2.41	126.22	122.73
25	B	616	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	a	610	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	b	610	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	B	612	CLA	CHD-C1D-ND	-2.40	122.25	124.45
25	B	607	CLA	CHD-C1D-ND	-2.39	122.25	124.45
27	c	522	BCR	C15-C16-C17	-2.39	118.57	123.47
25	b	615	CLA	CMB-C2B-C3B	2.39	129.15	124.68
25	c	508	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
30	B	623	LHG	C20-C19-C18	-2.39	102.29	114.42
29	D	409	SQD	O48-C23-C24	2.39	119.41	111.91
27	B	618	BCR	C27-C26-C25	2.39	126.20	122.73
27	c	515	BCR	C33-C5-C6	-2.39	121.85	124.53
25	B	607	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
29	f	101	SQD	O48-C23-C24	2.39	119.40	111.91
25	A	606	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
25	c	513	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
27	B	617	BCR	C27-C26-C25	2.38	126.19	122.73
25	B	612	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
28	D	405	PL9	C27-C28-C29	-2.38	121.92	127.66
25	b	614	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
32	B	626	LMG	C38-C37-C36	-2.38	102.33	114.42
25	C	510	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
25	a	606	CLA	CHD-C1D-ND	-2.38	122.27	124.45
32	a	614	LMG	C40-C39-C38	-2.38	102.35	114.42
27	c	514	BCR	C15-C14-C13	-2.38	123.92	127.31
25	b	601	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	c	509	CLA	CHD-C1D-ND	-2.38	122.27	124.45
25	C	503	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	C	509	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
27	C	516	BCR	C7-C8-C9	-2.38	122.64	126.23
28	d	404	PL9	C20-C19-C21	2.38	119.27	115.27
32	D	407	LMG	C40-C39-C38	-2.38	102.37	114.42
32	d	407	LMG	C40-C39-C38	-2.37	102.37	114.42
25	C	503	CLA	CHD-C1D-ND	-2.37	122.27	124.45
25	c	504	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	A	607	CLA	C1B-CHB-C4A	-2.37	125.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	406	LHG	C11-C10-C9	-2.37	102.39	114.42
32	a	614	LMG	O1-C7-C8	-2.37	105.18	110.90
25	A	613	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	C	507	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
25	b	606[B]	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
32	B	626	LMG	C40-C39-C38	-2.37	102.39	114.42
32	m	102	LMG	C38-C37-C36	-2.37	102.40	114.42
30	l	101	LHG	C20-C19-C18	-2.37	102.40	114.42
33	C	519	DGD	C1D-C2D-C3D	-2.37	105.07	110.00
32	C	521	LMG	C38-C37-C36	-2.37	102.41	114.42
25	B	616	CLA	CHD-C1D-ND	-2.37	122.28	124.45
29	b	621	SQD	O48-C23-C24	2.37	119.33	111.91
27	D	404	BCR	C27-C26-C25	2.36	126.16	122.73
27	A	610	BCR	C33-C5-C6	-2.36	121.87	124.53
25	a	607	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
27	A	610	BCR	C11-C10-C9	-2.36	123.94	127.31
33	H	102	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
27	B	618	BCR	C33-C5-C6	-2.36	121.88	124.53
30	d	406	LHG	C20-C19-C18	-2.36	102.46	114.42
25	c	502	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
32	C	520	LMG	C38-C37-C36	-2.36	102.47	114.42
25	C	511	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	h	101	BCR	C27-C26-C25	2.35	126.15	122.73
25	b	606[A]	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
25	c	509	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
30	L	102	LHG	C20-C19-C18	-2.35	102.49	114.42
27	d	403	BCR	C28-C27-C26	-2.35	109.88	114.08
33	C	519	DGD	O5D-C6D-C5D	-2.35	104.70	109.05
25	a	606	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	B	605	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
32	a	614	LMG	C38-C37-C36	-2.34	102.53	114.42
25	C	513	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
32	b	620	LMG	C38-C37-C36	-2.34	102.55	114.42
25	b	611	CLA	C1-C2-C3	-2.34	122.00	126.04
32	d	408	LMG	C38-C37-C36	-2.34	102.56	114.42
25	C	507	CLA	CHD-C1D-ND	-2.34	122.31	124.45
30	D	406	LHG	C11-C10-C9	-2.33	102.57	114.42
30	a	617	LHG	C11-C10-C9	-2.33	102.57	114.42
25	C	508	CLA	CHD-C1D-ND	-2.33	122.31	124.45
32	d	407	LMG	C38-C37-C36	-2.33	102.58	114.42
32	C	501	LMG	C38-C37-C36	-2.33	102.59	114.42
32	B	621	LMG	C40-C39-C38	-2.33	102.59	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	m	102	LMG	O1-C7-C8	-2.33	105.28	110.90
25	C	505	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	A	618	LHG	C20-C19-C18	-2.33	102.61	114.42
25	c	511	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
32	b	620	LMG	O1-C7-C8	-2.32	105.29	110.90
25	b	605	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
27	B	619	BCR	C27-C26-C25	2.32	126.11	122.73
28	d	404	PL9	C22-C23-C24	-2.32	122.07	127.66
25	c	510	CLA	CHD-C1D-ND	-2.32	122.32	124.45
27	c	522	BCR	C27-C26-C25	2.32	126.10	122.73
34	E	101	HEM	C1B-NB-C4B	2.32	107.47	105.07
27	b	618	BCR	C33-C5-C6	-2.32	121.93	124.53
25	b	604	CLA	CHD-C1D-ND	-2.32	122.33	124.45
29	A	616	SQD	O48-C23-C24	2.31	119.17	111.91
27	C	516	BCR	C27-C26-C25	2.31	126.09	122.73
25	B	614	CLA	CHD-C1D-ND	-2.31	122.33	124.45
27	K	101	BCR	C15-C14-C13	-2.31	124.01	127.31
27	C	515	BCR	C15-C14-C13	-2.31	124.01	127.31
25	b	611	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
25	a	615	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
33	c	517	DGD	CBB-CAB-C9B	-2.31	102.70	114.42
32	B	621	LMG	C38-C37-C36	-2.31	102.71	114.42
27	c	514	BCR	C24-C23-C22	-2.31	122.75	126.23
25	A	606	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
25	c	507	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
25	B	616	CLA	C1-C2-C3	-2.30	122.06	126.04
25	C	502	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	a	611	BCR	C33-C5-C6	-2.30	121.94	124.53
27	D	404	BCR	C15-C16-C17	-2.30	118.76	123.47
25	B	604	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	C	506	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
25	b	613	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
28	a	612	PL9	C7-C8-C9	-2.29	122.97	126.79
33	h	102	DGD	C1D-C2D-C3D	-2.29	105.22	110.00
25	B	603	CLA	CHD-C1D-ND	-2.29	122.35	124.45
27	B	619	BCR	C24-C23-C22	-2.29	122.77	126.23
32	a	614	LMG	O3-C3-C2	-2.29	105.05	110.35
29	A	612	SQD	C44-O6-C1	2.29	118.21	113.74
25	c	509	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
27	b	617	BCR	C11-C10-C9	-2.29	124.04	127.31
29	D	408	SQD	C3-C4-C5	2.29	114.32	110.24
30	d	405	LHG	C18-C17-C16	-2.28	102.83	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	403	BCR	C11-C10-C9	-2.28	124.05	127.31
25	B	601	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
27	Y	101	BCR	C15-C16-C17	-2.28	118.80	123.47
33	C	519	DGD	C3G-C2G-C1G	-2.28	106.40	111.79
26	A	608	PHO	CMC-C2C-C3C	2.28	129.24	124.94
25	B	606	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
25	B	611	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
25	A	606	CLA	C1-C2-C3	-2.28	122.11	126.04
27	c	515	BCR	C15-C14-C13	-2.28	124.06	127.31
32	d	407	LMG	O2-C2-C1	-2.27	104.52	110.05
25	c	510	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
25	c	507	CLA	CHD-C1D-ND	-2.27	122.36	124.45
32	B	620	LMG	C38-C37-C36	-2.27	102.90	114.42
29	L	101	SQD	C3-C4-C5	2.27	114.28	110.24
33	c	517	DGD	C3G-C2G-C1G	-2.26	106.43	111.79
25	B	615	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
25	c	512	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
32	b	620	LMG	O3-C3-C2	-2.26	105.12	110.35
26	a	609	PHO	C1-C2-C3	-2.26	122.13	126.04
27	B	617	BCR	C15-C14-C13	-2.26	124.09	127.31
28	D	405	PL9	C22-C23-C24	-2.26	122.22	127.66
25	c	503	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
25	D	403	CLA	C1-C2-C3	-2.25	122.15	126.04
33	h	102	DGD	C3G-C2G-C1G	-2.25	106.47	111.79
25	b	612	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
25	A	609	CLA	O2D-CGD-CBD	2.25	115.26	111.27
25	C	514	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
25	C	504	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
25	B	610	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
27	b	619	BCR	C15-C16-C17	-2.24	118.88	123.47
27	T	101	BCR	C33-C5-C6	-2.24	122.01	124.53
32	C	521	LMG	O3-C3-C2	-2.24	105.16	110.35
28	d	404	PL9	C36-C34-C33	-2.24	116.58	121.12
27	T	101	BCR	C2-C1-C6	2.24	113.93	110.48
32	C	520	LMG	O3-C3-C2	-2.24	105.17	110.35
27	B	617	BCR	C33-C5-C6	-2.24	122.01	124.53
27	K	101	BCR	C24-C23-C22	-2.24	122.85	126.23
27	a	611	BCR	C11-C10-C9	-2.24	124.12	127.31
32	c	519	LMG	O3-C3-C2	-2.24	105.18	110.35
27	b	618	BCR	C35-C13-C14	-2.23	119.79	122.92
27	D	404	BCR	C7-C8-C9	-2.23	122.86	126.23
30	B	623	LHG	C27-C26-C25	-2.23	103.09	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	407	LMG	C38-C37-C36	-2.23	103.10	114.42
28	D	405	PL9	C37-C38-C39	-2.23	122.29	127.66
25	B	613	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
25	b	603	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	D	401	PHO	CMC-C2C-C3C	2.23	129.14	124.94
32	m	102	LMG	O3-C3-C2	-2.23	105.20	110.35
25	c	508	CLA	O2D-CGD-CBD	2.22	115.22	111.27
30	A	614	LHG	C18-C17-C16	-2.22	103.14	114.42
25	A	607	CLA	O2D-CGD-CBD	2.22	115.22	111.27
27	c	514	BCR	C33-C5-C6	-2.22	122.03	124.53
28	D	405	PL9	C36-C34-C33	-2.22	116.62	121.12
28	D	405	PL9	C12-C13-C14	-2.22	122.31	127.66
27	h	101	BCR	C15-C14-C13	-2.22	124.14	127.31
30	L	102	LHG	C27-C26-C25	-2.22	103.16	114.42
27	B	619	BCR	C2-C1-C6	2.22	113.89	110.48
25	b	615	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
25	c	511	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
25	B	601	CLA	C1-C2-C3	-2.21	122.22	126.04
25	B	611	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
27	B	618	BCR	C11-C10-C9	-2.21	124.15	127.31
25	B	602	CLA	O2D-CGD-CBD	2.21	115.20	111.27
30	L	102	LHG	C18-C17-C16	-2.21	103.21	114.42
25	a	610	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	D	403	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
32	B	626	LMG	O3-C3-C2	-2.21	105.25	110.35
30	l	101	LHG	C18-C17-C16	-2.20	103.23	114.42
32	d	407	LMG	O1-C7-C8	-2.20	105.58	110.90
30	A	618	LHG	C18-C17-C16	-2.20	103.24	114.42
28	a	612	PL9	O2-C1-C6	2.20	124.40	120.59
25	b	604	CLA	C1-C2-C3	-2.20	122.23	126.04
25	b	612	CLA	CHD-C1D-ND	-2.20	122.43	124.45
32	B	621	LMG	O3-C3-C2	-2.20	105.26	110.35
32	c	520	LMG	O3-C3-C2	-2.20	105.27	110.35
25	C	512	CLA	C1-C2-C3	-2.20	122.24	126.04
27	c	521	BCR	C15-C16-C17	-2.20	118.97	123.47
27	t	101	BCR	C11-C10-C9	-2.20	124.18	127.31
33	C	517	DGD	C3G-C2G-C1G	-2.19	106.60	111.79
25	B	609	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
33	c	516	DGD	O3G-C1D-C2D	-2.19	104.88	108.30
35	v	201	HEC	CBA-CAA-C2A	-2.19	108.92	112.60
30	D	406	LHG	C27-C26-C25	-2.19	103.32	114.42
25	B	613	CLA	O2A-CGA-O1A	-2.19	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	617	LHG	C27-C26-C25	-2.19	103.33	114.42
26	a	608	PHO	CMC-C2C-C3C	2.19	129.06	124.94
25	C	512	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
33	H	102	DGD	CBB-CAB-C9B	-2.18	103.34	114.42
27	a	611	BCR	C15-C14-C13	-2.18	124.19	127.31
25	b	613	CLA	CHD-C1D-ND	-2.18	122.45	124.45
30	d	405	LHG	C27-C26-C25	-2.18	103.35	114.42
33	c	516	DGD	CBB-CAB-C9B	-2.18	103.35	114.42
30	A	618	LHG	C27-C26-C25	-2.18	103.36	114.42
25	B	615	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
30	l	101	LHG	C27-C26-C25	-2.18	103.36	114.42
30	a	617	LHG	C18-C17-C16	-2.18	103.36	114.42
28	A	611	PL9	C32-C33-C34	-2.18	122.42	127.66
33	c	518	DGD	C3G-C2G-C1G	-2.18	106.64	111.79
25	b	610	CLA	C1-C2-C3	-2.18	122.28	126.04
32	d	408	LMG	C42-C41-C40	-2.18	103.37	114.42
27	b	619	BCR	C33-C5-C6	-2.17	122.09	124.53
27	d	403	BCR	C29-C30-C25	2.17	113.83	110.48
34	e	101	HEM	CHC-C4B-C3B	2.17	127.89	124.57
30	D	406	LHG	C18-C17-C16	-2.17	103.42	114.42
32	b	620	LMG	O2-C2-C1	-2.17	104.78	110.05
30	d	406	LHG	C18-C17-C16	-2.17	103.42	114.42
27	H	101	BCR	C7-C8-C9	-2.17	122.96	126.23
25	A	609	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
27	B	619	BCR	C15-C16-C17	-2.16	119.04	123.47
27	c	521	BCR	C24-C23-C22	-2.16	122.97	126.23
30	A	614	LHG	C27-C26-C25	-2.16	103.45	114.42
25	a	606	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
27	C	515	BCR	C33-C5-C6	-2.16	122.10	124.53
25	C	507	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
25	B	604	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
33	h	102	DGD	CBB-CAB-C9B	-2.16	103.46	114.42
25	B	613	CLA	C1-C2-C3	-2.16	122.31	126.04
25	B	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
25	B	615	CLA	CHD-C1D-ND	-2.16	122.47	124.45
33	C	519	DGD	CBB-CAB-C9B	-2.16	103.47	114.42
32	a	614	LMG	O6-C1-O1	-2.16	104.87	109.97
25	c	501	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
33	C	519	DGD	O3E-C3E-C2E	-2.16	105.37	110.35
28	D	405	PL9	C31-C32-C33	-2.15	104.81	111.88
32	C	521	LMG	C3-C4-C5	-2.15	106.40	110.24
32	d	407	LMG	O3-C3-C2	-2.15	105.38	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	521	LMG	O2-C2-C3	-2.15	105.38	110.35
25	B	603	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
32	m	102	LMG	O2-C2-C1	-2.15	104.83	110.05
34	E	101	HEM	CBA-CAA-C2A	-2.15	108.95	112.62
25	C	509	CLA	O2D-CGD-CBD	2.15	115.08	111.27
32	m	102	LMG	O1-C1-C2	-2.15	104.95	108.30
28	A	611	PL9	O1-C4-C3	-2.15	118.36	120.72
25	C	512	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
27	a	611	BCR	C7-C8-C9	-2.15	122.99	126.23
28	d	404	PL9	C37-C38-C39	-2.15	122.49	127.66
25	A	613	CLA	O2D-CGD-CBD	2.14	115.08	111.27
32	C	520	LMG	O1-C7-C8	-2.14	105.72	110.90
25	b	604	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
26	a	608	PHO	O2A-CGA-O1A	-2.14	118.18	123.59
29	a	613	SQD	C44-O6-C1	2.14	117.92	113.74
29	A	616	SQD	O6-C1-C2	2.14	111.65	108.30
30	B	623	LHG	C18-C17-C16	-2.14	103.56	114.42
32	D	407	LMG	O2-C2-C1	-2.14	104.85	110.05
33	h	102	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
33	C	517	DGD	CBB-CAB-C9B	-2.13	103.59	114.42
33	C	518	DGD	C3G-C2G-C1G	-2.13	106.74	111.79
25	d	401	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
32	c	519	LMG	O1-C7-C8	-2.13	105.75	110.90
25	A	607	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
27	A	610	BCR	C15-C16-C17	-2.13	119.11	123.47
33	c	518	DGD	CBB-CAB-C9B	-2.13	103.61	114.42
28	a	612	PL9	O2-C1-C2	-2.13	116.90	121.78
25	b	613	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
32	B	620	LMG	O3-C3-C2	-2.13	105.43	110.35
32	B	621	LMG	O2-C2-C1	-2.12	104.88	110.05
25	C	506	CLA	CHD-C1D-ND	-2.12	122.50	124.45
28	d	404	PL9	O1-C4-C3	-2.12	118.38	120.72
27	A	610	BCR	C15-C14-C13	-2.12	124.28	127.31
33	c	518	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
34	E	101	HEM	C4C-CHD-C1D	2.12	125.35	122.56
32	c	519	LMG	O2-C2-C1	-2.12	104.90	110.05
28	D	405	PL9	O2-C1-C6	2.12	124.26	120.59
33	C	518	DGD	CBB-CAB-C9B	-2.12	103.68	114.42
25	B	607	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	C	513	CLA	C1-C2-C3	-2.12	122.39	126.04
29	B	624	SQD	O48-C23-C24	2.11	118.54	111.91
33	c	518	DGD	O5D-C6D-C5D	-2.11	105.14	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	508	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
30	a	616	LHG	C27-C26-C25	-2.11	103.72	114.42
26	A	608	PHO	C1-C2-C3	-2.11	122.39	126.04
26	a	609	PHO	CMC-C2C-C3C	2.11	128.92	124.94
33	H	102	DGD	CAB-C9B-C8B	-2.11	103.72	114.42
27	A	610	BCR	C24-C23-C22	-2.11	123.05	126.23
25	C	510	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
33	C	517	DGD	CAB-C9B-C8B	-2.10	103.75	114.42
32	B	621	LMG	O1-C7-C8	-2.10	105.83	110.90
25	C	509	CLA	C1-C2-C3	-2.10	122.41	126.04
28	a	612	PL9	C32-C33-C34	-2.10	122.61	127.66
25	C	508	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	C	501	LMG	O3-C3-C2	-2.09	105.51	110.35
25	b	614	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
32	C	520	LMG	O2-C2-C1	-2.09	104.96	110.05
28	a	612	PL9	C37-C38-C39	-2.09	122.62	127.66
33	c	517	DGD	C5B-C4B-C3B	-2.09	103.80	114.42
25	a	607	CLA	C2D-C1D-ND	-2.09	108.56	110.10
27	B	619	BCR	C33-C5-C6	-2.09	122.18	124.53
25	b	602	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
27	c	522	BCR	C15-C14-C13	-2.09	124.33	127.31
25	b	607	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	a	608	PHO	C1-C2-C3	-2.09	122.43	126.04
28	A	611	PL9	O2-C1-C2	-2.09	116.99	121.78
25	B	606	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
28	A	611	PL9	O2-C1-C6	2.09	124.21	120.59
25	c	512	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	b	616	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
25	c	504	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
32	a	614	LMG	O2-C2-C1	-2.08	104.99	110.05
32	a	614	LMG	O1-C1-C2	-2.08	105.06	108.30
28	a	612	PL9	O1-C4-C3	-2.08	118.43	120.72
25	c	511	CLA	C1-C2-C3	-2.08	122.45	126.04
25	A	607	CLA	C2D-C1D-ND	-2.07	108.58	110.10
32	c	520	LMG	C3-C4-C5	-2.07	106.54	110.24
33	c	518	DGD	C1D-C2D-C3D	-2.07	105.68	110.00
33	c	516	DGD	C4E-C3E-C2E	-2.07	107.21	110.82
25	b	612	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
27	c	521	BCR	C15-C14-C13	-2.07	124.36	127.31
33	H	102	DGD	C1D-C2D-C3D	-2.07	105.69	110.00
25	A	606	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	D	405	PL9	O1-C4-C3	-2.07	118.44	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	501	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
28	A	611	PL9	C12-C13-C14	-2.07	122.69	127.66
33	C	518	DGD	O3E-C3E-C2E	-2.06	105.58	110.35
33	c	516	DGD	CAB-C9B-C8B	-2.06	103.96	114.42
25	C	502	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
33	C	518	DGD	O2G-C1B-O1B	-2.06	118.72	123.70
28	D	405	PL9	O2-C1-C2	-2.06	117.06	121.78
32	B	626	LMG	O7-C10-O9	-2.06	118.72	123.70
27	c	514	BCR	C11-C10-C9	-2.06	124.38	127.31
33	C	519	DGD	CAB-C9B-C8B	-2.06	103.99	114.42
25	B	611	CLA	O2D-CGD-CBD	2.06	114.92	111.27
28	A	611	PL9	C37-C38-C39	-2.05	122.72	127.66
25	C	505	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	C	503	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	b	610	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	b	608	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	b	602	CLA	C1-C2-C3	-2.05	122.50	126.04
27	H	101	BCR	C16-C15-C14	-2.05	119.28	123.47
25	c	512	CLA	C1-C2-C3	-2.05	122.51	126.04
30	d	406	LHG	C27-C26-C25	-2.04	104.05	114.42
25	B	602	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	b	611	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
33	H	102	DGD	C4E-C3E-C2E	-2.04	107.26	110.82
25	D	403	CLA	O2D-CGD-CBD	2.04	114.89	111.27
25	C	514	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	B	612	CLA	C1-C2-C3	-2.04	122.52	126.04
25	C	504	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
32	B	620	LMG	O2-C2-C1	-2.04	105.10	110.05
25	b	604	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
33	C	519	DGD	C5B-C4B-C3B	-2.04	104.08	114.42
34	E	101	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
25	b	614	CLA	C1-C2-C3	-2.03	122.53	126.04
25	B	605	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
32	c	520	LMG	C6-C5-C4	-2.03	108.24	113.00
27	D	404	BCR	C33-C5-C6	-2.03	122.25	124.53
33	C	518	DGD	CAB-C9B-C8B	-2.03	104.12	114.42
33	c	516	DGD	C5B-C4B-C3B	-2.03	104.12	114.42
25	b	609	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	c	501	CLA	O2D-CGD-CBD	2.03	114.87	111.27
32	D	407	LMG	O3-C3-C2	-2.03	105.66	110.35
33	C	517	DGD	C5B-C4B-C3B	-2.02	104.15	114.42
33	c	518	DGD	C5B-C4B-C3B	-2.02	104.16	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	611	CLA	O2D-CGD-CBD	2.02	114.86	111.27
27	T	101	BCR	C3-C4-C5	-2.02	110.47	114.08
33	h	102	DGD	O3E-C3E-C2E	-2.02	105.68	110.35
27	D	404	BCR	C11-C10-C9	-2.02	124.43	127.31
25	B	614	CLA	C1-C2-C3	-2.02	122.56	126.04
25	B	601	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
27	b	618	BCR	C24-C23-C22	-2.02	123.19	126.23
27	t	101	BCR	C7-C8-C9	-2.02	123.19	126.23
33	C	517	DGD	O6E-C5E-C4E	2.01	113.35	109.69
33	H	102	DGD	C5B-C4B-C3B	-2.01	104.20	114.42
25	C	511	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	b	615	CLA	CHD-C1D-ND	-2.01	122.61	124.45
25	a	607	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
27	c	515	BCR	C11-C10-C9	-2.01	124.44	127.31
29	D	408	SQD	C44-O6-C1	2.01	117.66	113.74
32	c	520	LMG	O7-C10-O9	-2.01	118.86	123.70
25	d	402	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	D	408	SQD	C4-C3-C2	2.00	114.32	110.82
33	H	102	DGD	C3D-C4D-C5D	-2.00	106.66	110.24
27	Y	101	BCR	C15-C14-C13	-2.00	124.45	127.31
25	b	615	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
27	H	101	BCR	C33-C5-C6	-2.00	122.28	124.53
25	a	606	CLA	O1D-CGD-CBD	2.00	128.58	124.48

All (71) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	613	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND

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Mol	Chain	Res	Type	Atom
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	511	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	C	514	CLA	ND
25	D	402	CLA	ND
25	D	403	CLA	ND
25	a	606	CLA	ND
25	a	607	CLA	ND
25	a	610	CLA	ND
25	a	615	CLA	ND
25	b	601	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606[A]	CLA	ND
25	b	606[B]	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND

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Mol	Chain	Res	Type	Atom
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	401	CLA	ND
25	d	402	CLA	ND

All (1663) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	613	CLA	CHA-CBD-CGD-O1D
25	A	613	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	608	CLA	C6-C7-C8-C9
25	B	614	CLA	CBA-CGA-O2A-C1
25	B	614	CLA	O1A-CGA-O2A-C1
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CBD-CGD-O2D-CED
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	C	510	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	CHA-CBD-CGD-O1D
25	a	607	CLA	CHA-CBD-CGD-O2D
25	a	615	CLA	CHA-CBD-CGD-O1D
25	a	615	CLA	CHA-CBD-CGD-O2D
25	b	601	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	C4-C3-C5-C6
25	b	614	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	C1A-C2A-CAA-CBA
25	c	506	CLA	C3A-C2A-CAA-CBA
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C15
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C3A-C2A-CAA-CBA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	d	402	CLA	C1A-C2A-CAA-CBA
27	B	618	BCR	C7-C8-C9-C34
27	B	619	BCR	C11-C12-C13-C35
27	H	101	BCR	C21-C22-C23-C24
27	H	101	BCR	C37-C22-C23-C24
27	T	101	BCR	C6-C7-C8-C9
27	Y	101	BCR	C7-C8-C9-C34
27	b	617	BCR	C1-C6-C7-C8
27	b	618	BCR	C11-C10-C9-C8
27	b	618	BCR	C11-C10-C9-C34
27	b	618	BCR	C9-C10-C11-C12
27	b	618	BCR	C10-C11-C12-C13
27	b	619	BCR	C7-C8-C9-C34
27	c	521	BCR	C7-C8-C9-C10
27	c	521	BCR	C7-C8-C9-C34
27	d	403	BCR	C7-C8-C9-C34
27	h	101	BCR	C1-C6-C7-C8
28	A	611	PL9	C9-C11-C12-C13
28	A	611	PL9	C17-C18-C19-C20
28	A	611	PL9	C17-C18-C19-C21
28	A	611	PL9	C39-C41-C42-C43
28	D	405	PL9	C38-C39-C41-C42
28	D	405	PL9	C39-C41-C42-C43
28	a	612	PL9	C42-C43-C44-C45
28	a	612	PL9	C42-C43-C44-C46
29	A	612	SQD	C5-C6-S-O7
29	A	616	SQD	O47-C45-C46-O48
29	A	616	SQD	O5-C5-C6-S
29	B	624	SQD	O5-C1-O6-C44
29	B	624	SQD	O6-C44-C45-O47
29	B	624	SQD	C8-C7-O47-C45
29	B	624	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
29	B	625	SQD	C2-C1-O6-C44
29	B	625	SQD	C44-C45-O47-C7
29	B	625	SQD	C8-C7-O47-C45
29	B	625	SQD	C5-C6-S-O9
29	D	409	SQD	C8-C7-O47-C45
29	D	409	SQD	C24-C23-O48-C46
29	D	409	SQD	C5-C6-S-O9
29	L	101	SQD	O5-C1-O6-C44
30	A	618	LHG	O1-C1-C2-C3
30	D	406	LHG	C1-C2-C3-O3
30	D	406	LHG	C3-O3-P-O4
30	D	406	LHG	C4-O6-P-O4
30	a	616	LHG	O1-C1-C2-C3
30	d	405	LHG	O1-C1-C2-C3
30	d	406	LHG	C3-O3-P-O4
30	d	406	LHG	C4-O6-P-O3
30	l	101	LHG	C4-O6-P-O5
32	B	620	LMG	C2-C1-O1-C7
32	B	620	LMG	O6-C1-O1-C7
32	B	626	LMG	C2-C1-O1-C7
32	B	626	LMG	O6-C1-O1-C7
32	B	626	LMG	C8-C7-O1-C1
32	B	626	LMG	C7-C8-O7-C10
32	B	626	LMG	C11-C10-O7-C8
32	C	520	LMG	C2-C1-O1-C7
32	C	520	LMG	O6-C1-O1-C7
32	C	521	LMG	O6-C1-O1-C7
32	C	521	LMG	O7-C8-C9-O8
32	a	614	LMG	O6-C1-O1-C7
32	c	520	LMG	C2-C1-O1-C7
32	c	520	LMG	O6-C1-O1-C7
32	c	520	LMG	O7-C8-C9-O8
32	c	520	LMG	C7-C8-O7-C10
33	C	518	DGD	O1G-C1G-C2G-O2G
25	B	601	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
29	B	624	SQD	O10-C23-O48-C46
29	D	409	SQD	O10-C23-O48-C46
25	b	609	CLA	CBD-CGD-O2D-CED
29	A	616	SQD	O10-C23-O48-C46
29	b	621	SQD	O10-C23-O48-C46
32	B	626	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	C	507	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	O1D-CGD-O2D-CED
25	C	510	CLA	O1D-CGD-O2D-CED
29	B	625	SQD	O49-C7-O47-C45
32	c	520	LMG	O9-C10-O7-C8
30	a	617	LHG	O10-C23-O8-C6
25	B	608	CLA	C3-C5-C6-C7
25	C	502	CLA	C3-C5-C6-C7
26	a	609	PHO	C3-C5-C6-C7
25	C	514	CLA	CBA-CGA-O2A-C1
29	b	621	SQD	C24-C23-O48-C46
32	B	626	LMG	C29-C28-O8-C9
25	b	614	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
32	B	626	LMG	O6-C5-C6-O5
25	b	605	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
28	D	405	PL9	C40-C39-C41-C42
25	b	604	CLA	C2-C3-C5-C6
25	c	506	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	606[A]	CLA	C2A-CAA-CBA-CGA
25	b	606[B]	CLA	C2A-CAA-CBA-CGA
30	A	618	LHG	C32-C33-C34-C35
25	c	510	CLA	C3-C5-C6-C7
25	B	616	CLA	CBA-CGA-O2A-C1
30	a	617	LHG	C24-C23-O8-C6
32	c	520	LMG	C29-C28-O8-C9
32	c	519	LMG	O6-C5-C6-O5
25	B	601	CLA	O1D-CGD-O2D-CED
29	B	624	SQD	O49-C7-O47-C45
32	B	626	LMG	O9-C10-O7-C8
28	D	405	PL9	C42-C43-C44-C46
25	C	514	CLA	O1A-CGA-O2A-C1
25	a	607	CLA	O1A-CGA-O2A-C1
25	b	616	CLA	O1A-CGA-O2A-C1
32	c	520	LMG	O10-C28-O8-C9
25	B	614	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	CBD-CGD-O2D-CED
30	d	406	LHG	O2-C2-C3-O3
25	B	614	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C3-C5-C6-C7
25	a	607	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
25	b	616	CLA	CBA-CGA-O2A-C1
29	A	616	SQD	C24-C23-O48-C46
32	C	521	LMG	O6-C5-C6-O5
32	c	519	LMG	C4-C5-C6-O5
32	b	620	LMG	C11-C10-O7-C8
25	B	616	CLA	O1A-CGA-O2A-C1
32	b	620	LMG	O6-C5-C6-O5
25	c	513	CLA	O1D-CGD-O2D-CED
30	A	618	LHG	C23-C24-C25-C26
29	L	101	SQD	O10-C23-O48-C46
25	B	614	CLA	C4-C3-C5-C6
32	B	626	LMG	C4-C5-C6-O5
25	B	614	CLA	C2-C3-C5-C6
32	a	614	LMG	O6-C5-C6-O5
32	c	520	LMG	O6-C5-C6-O5
33	h	102	DGD	O6E-C5E-C6E-O5E
25	b	613	CLA	O1A-CGA-O2A-C1
32	C	520	LMG	C4-C5-C6-O5
28	D	405	PL9	C42-C43-C44-C45
30	d	406	LHG	C1-C2-C3-O3
32	a	614	LMG	C4-C5-C6-O5
25	B	604	CLA	O1A-CGA-O2A-C1
25	B	604	CLA	CBA-CGA-O2A-C1
25	C	508	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
29	L	101	SQD	C24-C23-O48-C46
33	h	102	DGD	C4E-C5E-C6E-O5E
32	c	520	LMG	C4-C5-C6-O5
30	l	101	LHG	C28-C29-C30-C31
25	b	614	CLA	C5-C6-C7-C8
25	c	510	CLA	C5-C6-C7-C8
30	D	406	LHG	O2-C2-C3-O3
30	d	405	LHG	O2-C2-C3-O3
30	d	405	LHG	C23-C24-C25-C26
29	D	409	SQD	C2-C1-O6-C44
25	b	605	CLA	C2-C3-C5-C6
25	c	506	CLA	C2-C3-C5-C6
25	B	609	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B	614	CLA	C11-C10-C8-C9
25	B	616	CLA	C6-C7-C8-C9
25	C	508	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C12-C13-C14
25	b	606[A]	CLA	C11-C10-C8-C9
25	b	606[B]	CLA	C11-C12-C13-C14
25	b	610	CLA	C14-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C9
25	c	505	CLA	C11-C10-C8-C9
25	c	506	CLA	C6-C7-C8-C9
25	c	511	CLA	C11-C12-C13-C14
25	B	614	CLA	C15-C16-C17-C18
27	A	610	BCR	C7-C8-C9-C34
27	T	101	BCR	C7-C8-C9-C34
27	T	101	BCR	C7-C8-C9-C10
27	t	101	BCR	C7-C8-C9-C10
32	C	520	LMG	O6-C5-C6-O5
32	B	621	LMG	C11-C10-O7-C8
29	A	612	SQD	C7-C8-C9-C10
30	l	101	LHG	C23-C24-C25-C26
25	B	604	CLA	C15-C16-C17-C18
25	B	614	CLA	C8-C10-C11-C12
25	B	614	CLA	C13-C15-C16-C17
25	a	607	CLA	C13-C15-C16-C17
25	b	612	CLA	C13-C15-C16-C17
25	C	504	CLA	C8-C10-C11-C12
25	C	509	CLA	C10-C11-C12-C13
25	C	509	CLA	C15-C16-C17-C18
25	D	403	CLA	C13-C15-C16-C17
25	a	610	CLA	C5-C6-C7-C8
25	b	602	CLA	C15-C16-C17-C18
25	c	502	CLA	C8-C10-C11-C12
25	c	505	CLA	C10-C11-C12-C13
26	a	609	PHO	C10-C11-C12-C13
30	A	614	LHG	C7-C8-C9-C10
30	a	616	LHG	C23-C24-C25-C26
25	B	608	CLA	C5-C6-C7-C8
25	B	608	CLA	C8-C10-C11-C12
25	C	504	CLA	C13-C15-C16-C17
25	b	609	CLA	C8-C10-C11-C12
25	b	613	CLA	C8-C10-C11-C12
25	d	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	A	612	SQD	C12-C13-C14-C15
25	b	609	CLA	O1D-CGD-O2D-CED
28	A	611	PL9	C12-C13-C14-C15
30	L	102	LHG	C23-C24-C25-C26
30	d	406	LHG	C23-C24-C25-C26
32	b	620	LMG	C28-C29-C30-C31
33	C	518	DGD	C1B-C2B-C3B-C4B
25	C	504	CLA	CBD-CGD-O2D-CED
25	A	606	CLA	C10-C11-C12-C13
25	B	601	CLA	C5-C6-C7-C8
25	B	608	CLA	C13-C15-C16-C17
25	b	602	CLA	C10-C11-C12-C13
25	c	502	CLA	C10-C11-C12-C13
25	c	512	CLA	C13-C15-C16-C17
25	a	607	CLA	C2-C1-O2A-CGA
25	B	615	CLA	C5-C6-C7-C8
30	B	623	LHG	C23-C24-C25-C26
32	B	620	LMG	C28-C29-C30-C31
25	c	503	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	C15-C16-C17-C18
25	B	614	CLA	C5-C6-C7-C8
26	a	608	PHO	C15-C16-C17-C18
25	A	607	CLA	C12-C13-C15-C16
25	B	610	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	a	615	CLA	C11-C12-C13-C15
25	c	505	CLA	C11-C10-C8-C7
25	d	401	CLA	C12-C13-C15-C16
25	b	604	CLA	C3-C5-C6-C7
25	C	508	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
25	B	609	CLA	C5-C6-C7-C8
25	C	513	CLA	C5-C6-C7-C8
30	d	405	LHG	C29-C30-C31-C32
25	c	512	CLA	O1A-CGA-O2A-C1
32	C	521	LMG	C4-C5-C6-O5
29	B	625	SQD	O5-C1-O6-C44
29	D	409	SQD	O5-C1-O6-C44
25	C	514	CLA	C5-C6-C7-C8
25	b	609	CLA	C10-C11-C12-C13
28	d	404	PL9	C39-C41-C42-C43
30	B	623	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	C	519	DGD	C1A-C2A-C3A-C4A
27	H	101	BCR	C18-C19-C20-C21
30	a	617	LHG	O2-C2-C3-O3
25	C	504	CLA	C15-C16-C17-C18
25	b	606[A]	CLA	C8-C10-C11-C12
25	b	611	CLA	C10-C11-C12-C13
25	C	513	CLA	CBA-CGA-O2A-C1
25	A	606	CLA	C5-C6-C7-C8
25	B	616	CLA	C13-C15-C16-C17
25	b	614	CLA	C10-C11-C12-C13
25	c	512	CLA	O1D-CGD-O2D-CED
32	c	520	LMG	C11-C10-O7-C8
25	b	602	CLA	C8-C10-C11-C12
25	c	506	CLA	C5-C6-C7-C8
30	D	406	LHG	C3-O3-P-O6
30	L	102	LHG	C4-O6-P-O3
30	d	405	LHG	C3-O3-P-O6
30	d	406	LHG	C3-O3-P-O6
25	B	611	CLA	C13-C15-C16-C17
25	B	615	CLA	C15-C16-C17-C18
30	a	617	LHG	C23-C24-C25-C26
25	b	614	CLA	O1D-CGD-O2D-CED
30	a	617	LHG	C1-C2-C3-O3
33	C	519	DGD	O6E-C5E-C6E-O5E
25	A	606	CLA	C4-C3-C5-C6
25	C	505	CLA	C8-C10-C11-C12
25	b	602	CLA	C13-C15-C16-C17
25	d	401	CLA	C16-C17-C18-C19
25	A	606	CLA	C3-C5-C6-C7
32	B	621	LMG	C10-C11-C12-C13
29	a	613	SQD	C12-C13-C14-C15
32	b	620	LMG	C18-C19-C20-C21
32	c	519	LMG	C38-C39-C40-C41
32	m	102	LMG	C18-C19-C20-C21
33	C	518	DGD	C9B-CAB-CBB-CCB
33	c	516	DGD	C4B-C5B-C6B-C7B
32	m	102	LMG	C11-C10-O7-C8
25	B	601	CLA	C13-C15-C16-C17
27	Y	101	BCR	C20-C21-C22-C37
27	t	101	BCR	C20-C21-C22-C37
29	B	624	SQD	C13-C14-C15-C16
29	L	101	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	b	621	SQD	C12-C13-C14-C15
30	L	102	LHG	C16-C17-C18-C19
30	d	405	LHG	C11-C12-C13-C14
30	l	101	LHG	C30-C31-C32-C33
32	B	620	LMG	C38-C39-C40-C41
32	a	614	LMG	C32-C33-C34-C35
32	b	620	LMG	C38-C39-C40-C41
32	d	408	LMG	C32-C33-C34-C35
32	m	102	LMG	C32-C33-C34-C35
33	c	517	DGD	C4A-C5A-C6A-C7A
25	c	506	CLA	O1D-CGD-O2D-CED
25	a	615	CLA	C16-C17-C18-C20
30	A	614	LHG	C10-C11-C12-C13
32	B	621	LMG	C17-C18-C19-C20
32	D	407	LMG	C38-C39-C40-C41
32	b	620	LMG	C20-C21-C22-C23
32	c	519	LMG	C30-C31-C32-C33
32	d	407	LMG	C38-C39-C40-C41
32	C	501	LMG	C4-C5-C6-O5
29	D	409	SQD	C29-C30-C31-C32
29	b	621	SQD	C16-C17-C18-C19
30	l	101	LHG	C24-C25-C26-C27
32	B	621	LMG	C33-C34-C35-C36
32	B	626	LMG	C17-C18-C19-C20
33	C	518	DGD	C4A-C5A-C6A-C7A
30	D	406	LHG	C29-C30-C31-C32
30	D	406	LHG	C32-C33-C34-C35
32	B	621	LMG	C37-C38-C39-C40
32	C	521	LMG	C34-C35-C36-C37
32	a	614	LMG	C30-C31-C32-C33
32	m	102	LMG	C33-C34-C35-C36
33	c	518	DGD	C6B-C7B-C8B-C9B
33	c	518	DGD	C8B-C9B-CAB-CBB
30	B	623	LHG	C32-C33-C34-C35
30	D	406	LHG	C25-C26-C27-C28
30	d	406	LHG	C24-C25-C26-C27
32	C	501	LMG	C17-C18-C19-C20
32	C	521	LMG	C37-C38-C39-C40
25	B	609	CLA	C3-C5-C6-C7
30	A	614	LHG	C23-C24-C25-C26
30	D	406	LHG	C23-C24-C25-C26
32	C	520	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
32	C	521	LMG	C28-C29-C30-C31
27	c	521	BCR	C20-C21-C22-C23
29	B	624	SQD	C2-C1-O6-C44
29	D	408	SQD	C2-C1-O6-C44
32	a	614	LMG	C2-C1-O1-C7
33	C	518	DGD	C2E-C1E-O5D-C6D
33	c	517	DGD	C2E-C1E-O5D-C6D
30	a	617	LHG	C15-C16-C17-C18
32	B	621	LMG	C18-C19-C20-C21
32	B	621	LMG	C31-C32-C33-C34
32	B	626	LMG	C16-C17-C18-C19
32	a	614	LMG	C11-C12-C13-C14
32	d	408	LMG	C37-C38-C39-C40
33	C	519	DGD	C7A-C8A-C9A-CAA
33	c	517	DGD	C6B-C7B-C8B-C9B
25	B	606	CLA	C8-C10-C11-C12
25	b	602	CLA	C16-C17-C18-C20
25	b	610	CLA	C4-C3-C5-C6
28	A	611	PL9	C40-C39-C41-C42
30	A	618	LHG	C9-C10-C11-C12
30	D	406	LHG	C27-C28-C29-C30
30	a	616	LHG	C25-C26-C27-C28
30	a	617	LHG	C24-C25-C26-C27
30	d	405	LHG	C32-C33-C34-C35
30	l	101	LHG	C25-C26-C27-C28
32	C	501	LMG	C33-C34-C35-C36
32	C	520	LMG	C17-C18-C19-C20
32	c	519	LMG	C32-C33-C34-C35
33	C	519	DGD	C6A-C7A-C8A-C9A
33	c	518	DGD	C4A-C5A-C6A-C7A
25	B	603	CLA	C6-C7-C8-C9
25	B	606	CLA	C14-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C14
25	C	503	CLA	C11-C12-C13-C14
25	C	512	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	605	CLA	C11-C12-C13-C14
25	b	608	CLA	C14-C13-C15-C16
25	b	612	CLA	C14-C13-C15-C16
25	c	503	CLA	C6-C7-C8-C9
29	B	625	SQD	C24-C25-C26-C27
29	D	409	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
32	C	501	LMG	C38-C39-C40-C41
32	C	520	LMG	C12-C13-C14-C15
32	b	620	LMG	C17-C18-C19-C20
32	d	407	LMG	C32-C33-C34-C35
32	d	408	LMG	C17-C18-C19-C20
32	d	408	LMG	C33-C34-C35-C36
33	C	517	DGD	C6A-C7A-C8A-C9A
33	C	517	DGD	C4B-C5B-C6B-C7B
33	C	517	DGD	C5B-C6B-C7B-C8B
33	C	519	DGD	C2A-C3A-C4A-C5A
33	H	102	DGD	CBA-CCA-CDA-CEA
25	c	506	CLA	C10-C11-C12-C13
25	B	614	CLA	C2A-CAA-CBA-CGA
27	h	101	BCR	C7-C8-C9-C34
27	t	101	BCR	C7-C8-C9-C34
29	a	613	SQD	C9-C10-C11-C12
30	l	101	LHG	C32-C33-C34-C35
32	B	621	LMG	C32-C33-C34-C35
32	d	407	LMG	C18-C19-C20-C21
30	A	614	LHG	O1-C1-C2-C3
30	a	617	LHG	O1-C1-C2-C3
27	B	617	BCR	C21-C22-C23-C24
29	D	409	SQD	O49-C7-O47-C45
33	C	518	DGD	C2B-C1B-O2G-C2G
30	a	616	LHG	C11-C10-C9-C8
32	B	620	LMG	C32-C33-C34-C35
32	B	621	LMG	C19-C20-C21-C22
32	B	626	LMG	C29-C30-C31-C32
32	C	521	LMG	C16-C17-C18-C19
32	D	407	LMG	C17-C18-C19-C20
32	b	620	LMG	C19-C20-C21-C22
32	c	519	LMG	C28-C29-C30-C31
32	c	520	LMG	C28-C29-C30-C31
33	c	518	DGD	C1A-C2A-C3A-C4A
25	C	502	CLA	O1D-CGD-O2D-CED
29	B	625	SQD	C31-C32-C33-C34
29	L	101	SQD	C11-C10-C9-C8
30	A	614	LHG	C25-C26-C27-C28
30	A	614	LHG	C32-C33-C34-C35
30	a	616	LHG	C27-C28-C29-C30
30	d	405	LHG	C28-C29-C30-C31
32	C	501	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
32	C	520	LMG	C15-C16-C17-C18
32	C	520	LMG	C30-C31-C32-C33
32	D	407	LMG	C16-C17-C18-C19
32	D	407	LMG	C39-C40-C41-C42
32	b	620	LMG	C32-C33-C34-C35
32	b	620	LMG	C37-C38-C39-C40
32	d	408	LMG	C16-C17-C18-C19
33	C	519	DGD	CCA-CDA-CEA-CFA
33	c	516	DGD	C5B-C6B-C7B-C8B
33	c	518	DGD	C4B-C5B-C6B-C7B
33	h	102	DGD	C8A-C9A-CAA-CBA
25	C	514	CLA	C16-C17-C18-C20
25	a	615	CLA	C16-C17-C18-C19
33	C	518	DGD	O6E-C1E-O5D-C6D
33	c	517	DGD	O6E-C1E-O5D-C6D
25	B	605	CLA	C5-C6-C7-C8
25	b	606[A]	CLA	C10-C11-C12-C13
25	b	606[A]	CLA	C15-C16-C17-C18
25	c	507	CLA	C15-C16-C17-C18
29	b	621	SQD	C25-C26-C27-C28
32	d	407	LMG	C33-C34-C35-C36
33	C	518	DGD	C4B-C5B-C6B-C7B
33	C	519	DGD	C5B-C6B-C7B-C8B
25	b	613	CLA	CBD-CGD-O2D-CED
29	A	616	SQD	C9-C10-C11-C12
30	d	406	LHG	C32-C33-C34-C35
32	D	407	LMG	C18-C19-C20-C21
32	a	614	LMG	C18-C19-C20-C21
32	d	408	LMG	C31-C32-C33-C34
32	m	102	LMG	C31-C32-C33-C34
33	h	102	DGD	C6A-C7A-C8A-C9A
32	B	621	LMG	C28-C29-C30-C31
32	B	626	LMG	C10-C11-C12-C13
25	B	616	CLA	C5-C6-C7-C8
29	B	624	SQD	C14-C15-C16-C17
29	B	625	SQD	C12-C13-C14-C15
30	B	623	LHG	C10-C11-C12-C13
32	C	501	LMG	C31-C32-C33-C34
33	H	102	DGD	C5A-C6A-C7A-C8A
32	B	621	LMG	O6-C5-C6-O5
32	m	102	LMG	O6-C5-C6-O5
29	L	101	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	B	626	LMG	C37-C38-C39-C40
32	d	408	LMG	C19-C20-C21-C22
33	c	516	DGD	C6B-C7B-C8B-C9B
25	B	614	CLA	O1D-CGD-O2D-CED
25	C	512	CLA	C3A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	c	511	CLA	C3A-C2A-CAA-CBA
25	B	615	CLA	C13-C15-C16-C17
30	D	406	LHG	C31-C32-C33-C34
32	B	626	LMG	C30-C31-C32-C33
32	C	521	LMG	C17-C18-C19-C20
32	a	614	LMG	C15-C16-C17-C18
32	d	408	LMG	C18-C19-C20-C21
33	H	102	DGD	C2B-C3B-C4B-C5B
25	C	513	CLA	O1A-CGA-O2A-C1
25	C	514	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C19
30	B	623	LHG	C29-C30-C31-C32
30	a	616	LHG	C33-C34-C35-C36
32	c	520	LMG	C11-C12-C13-C14
32	d	408	LMG	C41-C42-C43-C44
33	C	518	DGD	C8A-C9A-CAA-CBA
25	b	605	CLA	CBD-CGD-O2D-CED
32	B	626	LMG	C18-C19-C20-C21
32	D	407	LMG	C34-C35-C36-C37
25	C	514	CLA	C3-C5-C6-C7
29	B	624	SQD	C23-C24-C25-C26
32	d	408	LMG	C15-C16-C17-C18
33	C	517	DGD	C5A-C6A-C7A-C8A
33	h	102	DGD	CCA-CDA-CEA-CFA
26	D	401	PHO	C4-C3-C5-C6
25	c	505	CLA	CBA-CGA-O2A-C1
25	A	606	CLA	C2-C3-C5-C6
28	A	611	PL9	C28-C29-C31-C32
28	A	611	PL9	C38-C39-C41-C42
28	d	404	PL9	C28-C29-C31-C32
32	a	614	LMG	C11-C10-O7-C8
29	A	612	SQD	C9-C10-C11-C12
29	D	409	SQD	C9-C10-C11-C12
30	A	618	LHG	C27-C28-C29-C30
33	C	519	DGD	C4B-C5B-C6B-C7B
30	d	405	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
29	B	625	SQD	C14-C15-C16-C17
29	f	101	SQD	C30-C31-C32-C33
30	A	618	LHG	C30-C31-C32-C33
32	C	520	LMG	C34-C35-C36-C37
30	l	101	LHG	C33-C34-C35-C36
32	C	520	LMG	C31-C32-C33-C34
30	a	617	LHG	C14-C15-C16-C17
25	B	615	CLA	C3-C5-C6-C7
29	L	101	SQD	C16-C17-C18-C19
29	a	613	SQD	C18-C19-C20-C21
30	A	618	LHG	C28-C29-C30-C31
25	B	606	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
29	a	613	SQD	C14-C15-C16-C17
30	a	616	LHG	C29-C30-C31-C32
32	m	102	LMG	C34-C35-C36-C37
33	c	517	DGD	C5A-C6A-C7A-C8A
33	c	517	DGD	C6A-C7A-C8A-C9A
32	B	621	LMG	O9-C10-O7-C8
28	d	404	PL9	C32-C33-C34-C36
29	B	624	SQD	C27-C28-C29-C30
30	L	102	LHG	C27-C28-C29-C30
30	L	102	LHG	C32-C33-C34-C35
30	d	406	LHG	C15-C16-C17-C18
33	C	517	DGD	C4A-C5A-C6A-C7A
25	c	503	CLA	C5-C6-C7-C8
30	L	102	LHG	C31-C32-C33-C34
32	C	521	LMG	C29-C30-C31-C32
32	d	408	LMG	C23-C24-C25-C26
29	L	101	SQD	C23-C24-C25-C26
27	Y	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	b	617	BCR	C5-C6-C7-C8
27	c	521	BCR	C1-C6-C7-C8
27	c	521	BCR	C5-C6-C7-C8
27	c	522	BCR	C1-C6-C7-C8
27	h	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
33	C	517	DGD	O6E-C5E-C6E-O5E
30	A	618	LHG	C29-C30-C31-C32
30	a	617	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	c	516	DGD	C5A-C6A-C7A-C8A
33	c	518	DGD	C5A-C6A-C7A-C8A
33	h	102	DGD	C7A-C8A-C9A-CAA
33	h	102	DGD	CAB-CBB-CCB-CDB
25	b	614	CLA	CBA-CGA-O2A-C1
25	C	506	CLA	C15-C16-C17-C18
25	b	607	CLA	C13-C15-C16-C17
30	a	616	LHG	C28-C29-C30-C31
32	C	521	LMG	C18-C19-C20-C21
33	C	518	DGD	C5A-C6A-C7A-C8A
32	B	626	LMG	C14-C15-C16-C17
28	d	404	PL9	C47-C48-C49-C50
25	c	509	CLA	C5-C6-C7-C8
32	D	407	LMG	C32-C33-C34-C35
32	d	407	LMG	C36-C37-C38-C39
25	C	514	CLA	C4-C3-C5-C6
25	A	606	CLA	C6-C7-C8-C10
25	B	603	CLA	C6-C7-C8-C10
25	B	606	CLA	C12-C13-C15-C16
25	C	502	CLA	C12-C13-C15-C16
25	C	503	CLA	C11-C12-C13-C15
25	C	506	CLA	C6-C7-C8-C10
25	C	512	CLA	C6-C7-C8-C10
25	C	513	CLA	C11-C12-C13-C15
25	b	604	CLA	C11-C12-C13-C15
25	b	605	CLA	C11-C12-C13-C15
25	b	606[B]	CLA	C11-C12-C13-C15
25	b	608	CLA	C12-C13-C15-C16
25	b	610	CLA	C2-C3-C5-C6
25	b	612	CLA	C12-C13-C15-C16
25	b	614	CLA	C6-C7-C8-C10
25	c	503	CLA	C6-C7-C8-C10
25	c	505	CLA	C6-C7-C8-C10
25	c	511	CLA	C11-C12-C13-C15
26	D	401	PHO	C2-C3-C5-C6
25	c	505	CLA	O1A-CGA-O2A-C1
30	A	618	LHG	C12-C13-C14-C15
32	b	620	LMG	C33-C34-C35-C36
25	b	614	CLA	C13-C15-C16-C17
25	C	511	CLA	C16-C17-C18-C20
25	b	603	CLA	O1D-CGD-O2D-CED
32	b	620	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
32	m	102	LMG	C10-C11-C12-C13
25	B	607	CLA	CBA-CGA-O2A-C1
25	D	403	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	CBA-CGA-O2A-C1
25	A	613	CLA	C13-C15-C16-C17
25	b	606[A]	CLA	C13-C15-C16-C17
29	b	621	SQD	C9-C10-C11-C12
32	c	519	LMG	C31-C32-C33-C34
29	B	625	SQD	C23-C24-C25-C26
32	d	407	LMG	C28-C29-C30-C31
32	m	102	LMG	C19-C20-C21-C22
33	C	519	DGD	C4A-C5A-C6A-C7A
33	c	516	DGD	C6A-C7A-C8A-C9A
30	A	614	LHG	C29-C30-C31-C32
33	H	102	DGD	C5B-C6B-C7B-C8B
33	c	516	DGD	CCA-CDA-CEA-CFA
29	D	408	SQD	O5-C1-O6-C44
30	A	614	LHG	C11-C10-C9-C8
30	d	405	LHG	C12-C13-C14-C15
29	f	101	SQD	C8-C7-O47-C45
32	B	620	LMG	C11-C10-O7-C8
27	T	101	BCR	C18-C19-C20-C21
30	B	623	LHG	C34-C35-C36-C37
30	L	102	LHG	C10-C11-C12-C13
33	H	102	DGD	C7B-C8B-C9B-CAB
34	e	101	HEM	C4B-C3B-CAB-CBB
29	f	101	SQD	C2-C1-O6-C44
32	C	521	LMG	C2-C1-O1-C7
29	L	101	SQD	O47-C45-C46-O48
32	a	614	LMG	O1-C7-C8-O7
30	L	102	LHG	C24-C25-C26-C27
33	c	516	DGD	C3B-C4B-C5B-C6B
25	b	614	CLA	O1A-CGA-O2A-C1
25	C	502	CLA	C16-C17-C18-C20
25	d	401	CLA	C16-C17-C18-C20
33	c	516	DGD	C7B-C8B-C9B-CAB
25	b	611	CLA	C15-C16-C17-C18
25	b	607	CLA	C4-C3-C5-C6
28	d	404	PL9	C30-C29-C31-C32
32	B	626	LMG	C28-C29-C30-C31
28	a	612	PL9	C4-C3-C7-C8
29	a	613	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C14-C13-C15-C16
25	B	616	CLA	C14-C13-C15-C16
25	C	502	CLA	C14-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	511	CLA	C11-C10-C8-C9
25	a	615	CLA	C11-C12-C13-C14
25	b	615	CLA	C11-C10-C8-C9
25	c	505	CLA	C6-C7-C8-C9
25	C	514	CLA	CBD-CGD-O2D-CED
32	D	407	LMG	C36-C37-C38-C39
33	C	517	DGD	C7A-C8A-C9A-CAA
25	b	610	CLA	C2A-CAA-CBA-CGA
33	c	518	DGD	C7B-C8B-C9B-CAB
27	b	619	BCR	C37-C22-C23-C24
25	b	607	CLA	C5-C6-C7-C8
32	b	620	LMG	C39-C40-C41-C42
27	b	618	BCR	C11-C12-C13-C14
27	h	101	BCR	C7-C8-C9-C10
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	607	CLA	C1A-C2A-CAA-CBA
25	B	614	CLA	C1A-C2A-CAA-CBA
25	a	610	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C16-C17-C18-C20
26	D	401	PHO	C16-C17-C18-C20
33	c	516	DGD	O1B-C1B-O2G-C2G
30	l	101	LHG	C9-C10-C11-C12
33	C	517	DGD	CCA-CDA-CEA-CFA
25	B	601	CLA	C8-C10-C11-C12
25	c	505	CLA	C8-C10-C11-C12
30	D	406	LHG	C4-O6-P-O3
32	B	621	LMG	C38-C39-C40-C41
30	d	406	LHG	O6-C4-C5-C6
30	l	101	LHG	O6-C4-C5-C6
29	a	613	SQD	C11-C12-C13-C14
33	h	102	DGD	C5B-C6B-C7B-C8B
25	c	510	CLA	C15-C16-C17-C18
25	B	612	CLA	C16-C17-C18-C20
25	C	511	CLA	C16-C17-C18-C19
33	C	518	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	B	621	LMG	C16-C17-C18-C19
32	d	408	LMG	C40-C41-C42-C43
32	m	102	LMG	C38-C39-C40-C41
30	L	102	LHG	C11-C12-C13-C14
28	A	611	PL9	C30-C29-C31-C32
28	D	405	PL9	C30-C29-C31-C32
30	L	102	LHG	C25-C26-C27-C28
32	a	614	LMG	C38-C39-C40-C41
32	d	407	LMG	C16-C17-C18-C19
29	a	613	SQD	C8-C7-O47-C45
25	D	403	CLA	O1A-CGA-O2A-C1
32	C	521	LMG	C32-C33-C34-C35
25	C	502	CLA	C16-C17-C18-C19
32	C	501	LMG	O6-C5-C6-O5
33	c	516	DGD	O6E-C5E-C6E-O5E
29	D	409	SQD	O6-C44-C45-C46
30	A	618	LHG	C4-C5-C6-O8
30	a	617	LHG	C4-C5-C6-O8
32	C	520	LMG	C7-C8-C9-O8
32	C	521	LMG	C30-C31-C32-C33
32	a	614	LMG	O1-C7-C8-C9
32	c	520	LMG	C7-C8-C9-O8
33	C	518	DGD	O1G-C1G-C2G-C3G
32	d	407	LMG	O6-C5-C6-O5
33	C	518	DGD	C5D-C6D-O5D-C1E
33	c	517	DGD	C5D-C6D-O5D-C1E
30	A	614	LHG	C30-C31-C32-C33
33	C	518	DGD	O6E-C5E-C6E-O5E
30	d	406	LHG	C11-C10-C9-C8
32	d	408	LMG	C38-C39-C40-C41
33	h	102	DGD	C9A-CAA-CBA-CCA
32	d	407	LMG	C17-C18-C19-C20
25	B	603	CLA	C15-C16-C17-C18
25	C	507	CLA	C15-C16-C17-C18
29	B	624	SQD	C12-C13-C14-C15
30	d	406	LHG	C16-C17-C18-C19
30	A	618	LHG	O1-C1-C2-O2
33	c	517	DGD	C2A-C3A-C4A-C5A
25	C	505	CLA	C13-C15-C16-C17
32	D	407	LMG	C37-C38-C39-C40
33	c	518	DGD	CCA-CDA-CEA-CFA
25	C	502	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C10-C11-C12-C13
32	D	407	LMG	O6-C5-C6-O5
25	c	505	CLA	C4-C3-C5-C6
30	B	623	LHG	C28-C29-C30-C31
32	C	521	LMG	C33-C34-C35-C36
25	c	501	CLA	CBD-CGD-O2D-CED
25	B	608	CLA	C15-C16-C17-C18
32	B	626	LMG	C32-C33-C34-C35
25	B	607	CLA	O1A-CGA-O2A-C1
30	B	623	LHG	C30-C31-C32-C33
32	B	621	LMG	C34-C35-C36-C37
32	d	407	LMG	C34-C35-C36-C37
33	C	519	DGD	C5A-C6A-C7A-C8A
25	c	509	CLA	C3-C5-C6-C7
29	a	613	SQD	C31-C32-C33-C34
32	B	620	LMG	C12-C13-C14-C15
32	m	102	LMG	C37-C38-C39-C40
33	c	516	DGD	CAB-CBB-CCB-CDB
29	A	616	SQD	C12-C13-C14-C15
30	d	406	LHG	C33-C34-C35-C36
25	A	609	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1
25	c	507	CLA	O1A-CGA-O2A-C1
25	b	608	CLA	C16-C17-C18-C19
33	c	517	DGD	C4B-C5B-C6B-C7B
29	L	101	SQD	C24-C25-C26-C27
25	C	504	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
29	B	625	SQD	C11-C10-C9-C8
32	d	407	LMG	C13-C14-C15-C16
25	B	606	CLA	C10-C11-C12-C13
33	C	517	DGD	O2G-C2G-C3G-O3G
30	B	623	LHG	C16-C17-C18-C19
30	l	101	LHG	C14-C15-C16-C17
32	d	408	LMG	C39-C40-C41-C42
25	C	505	CLA	CBD-CGD-O2D-CED
32	C	501	LMG	C12-C13-C14-C15
32	C	520	LMG	C33-C34-C35-C36
33	c	517	DGD	CDA-CEA-CFA-CGA
30	d	406	LHG	C31-C32-C33-C34
32	m	102	LMG	C29-C30-C31-C32
25	A	607	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C11-C10-C8-C7
25	B	603	CLA	C12-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C10
25	B	608	CLA	C12-C13-C15-C16
25	B	609	CLA	C11-C12-C13-C15
25	B	616	CLA	C12-C13-C15-C16
25	C	507	CLA	C12-C13-C15-C16
25	C	508	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C12-C13-C15
25	C	511	CLA	C6-C7-C8-C10
25	C	511	CLA	C11-C10-C8-C7
25	D	403	CLA	C12-C13-C15-C16
25	a	610	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	b	603	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C12-C13-C15
26	a	608	PHO	C12-C13-C15-C16
30	A	618	LHG	C11-C12-C13-C14
25	A	607	CLA	C6-C7-C8-C9
25	B	601	CLA	C11-C12-C13-C14
25	B	603	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C14
25	B	614	CLA	C6-C7-C8-C9
25	C	503	CLA	C6-C7-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	507	CLA	C14-C13-C15-C16
25	C	508	CLA	C6-C7-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	C	511	CLA	C6-C7-C8-C9
25	a	610	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	602	CLA	C14-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C9
25	b	603	CLA	C11-C12-C13-C14
25	b	603	CLA	C14-C13-C15-C16
25	b	604	CLA	C14-C13-C15-C16
25	b	611	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	c	504	CLA	C11-C10-C8-C9
25	c	505	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C12-C13-C14
25	c	508	CLA	C11-C10-C8-C9
25	c	508	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C10-C8-C9
25	c	513	CLA	C11-C10-C8-C9
25	c	513	CLA	C14-C13-C15-C16
25	d	401	CLA	C14-C13-C15-C16
26	a	608	PHO	C14-C13-C15-C16
26	a	609	PHO	C11-C10-C8-C9
33	c	516	DGD	O6D-C5D-C6D-O5D
30	D	406	LHG	C30-C31-C32-C33
25	C	502	CLA	C2A-CAA-CBA-CGA
29	B	624	SQD	C10-C11-C12-C13
29	B	624	SQD	C24-C25-C26-C27
32	c	520	LMG	C30-C31-C32-C33
27	d	403	BCR	C7-C8-C9-C10
25	c	511	CLA	C8-C10-C11-C12
29	a	613	SQD	C35-C36-C37-C38
30	l	101	LHG	C17-C18-C19-C20
33	C	517	DGD	O6D-C5D-C6D-O5D
27	H	101	BCR	C22-C23-C24-C25
32	C	521	LMG	C14-C15-C16-C17
25	b	606[A]	CLA	C16-C17-C18-C20
25	B	612	CLA	C10-C11-C12-C13
30	a	617	LHG	O6-C4-C5-C6
32	B	621	LMG	C14-C15-C16-C17
33	c	516	DGD	C2B-C3B-C4B-C5B
25	B	613	CLA	C8-C10-C11-C12
25	C	508	CLA	C13-C15-C16-C17
29	L	101	SQD	C25-C26-C27-C28
30	B	623	LHG	C14-C15-C16-C17
30	a	617	LHG	C28-C29-C30-C31
25	c	506	CLA	C15-C16-C17-C18
32	d	407	LMG	C30-C31-C32-C33
33	c	516	DGD	C4D-C5D-C6D-O5D
30	A	618	LHG	C11-C10-C9-C8
25	c	506	CLA	C8-C10-C11-C12
30	a	616	LHG	C7-C8-C9-C10
32	b	620	LMG	C29-C30-C31-C32
25	b	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	B	601	CLA	C3A-C2A-CAA-CBA
25	C	513	CLA	C3A-C2A-CAA-CBA
25	D	402	CLA	C3A-C2A-CAA-CBA
25	c	507	CLA	C3A-C2A-CAA-CBA
25	d	402	CLA	C3A-C2A-CAA-CBA
25	B	613	CLA	C15-C16-C17-C18
32	C	501	LMG	C18-C19-C20-C21
29	B	624	SQD	C16-C17-C18-C19
29	a	613	SQD	C10-C11-C12-C13
33	c	517	DGD	C4E-C5E-C6E-O5E
25	B	611	CLA	C15-C16-C17-C18
29	B	624	SQD	C28-C29-C30-C31
25	a	607	CLA	C15-C16-C17-C18
29	B	624	SQD	O6-C44-C45-C46
29	B	625	SQD	C44-C45-C46-O48
29	L	101	SQD	C44-C45-C46-O48
32	B	626	LMG	O1-C7-C8-C9
32	C	521	LMG	C7-C8-C9-O8
32	a	614	LMG	C7-C8-C9-O8
33	C	517	DGD	C1G-C2G-C3G-O3G
32	m	102	LMG	O9-C10-O7-C8
30	d	405	LHG	C26-C27-C28-C29
30	d	405	LHG	C27-C28-C29-C30
32	C	520	LMG	C32-C33-C34-C35
28	A	611	PL9	C22-C23-C24-C26
32	B	620	LMG	C16-C17-C18-C19
30	D	406	LHG	C9-C10-C11-C12
33	c	517	DGD	C5B-C6B-C7B-C8B
25	b	603	CLA	C4-C3-C5-C6
33	C	517	DGD	C4D-C5D-C6D-O5D
29	A	612	SQD	C31-C32-C33-C34
28	A	611	PL9	C16-C17-C18-C19
25	C	514	CLA	C8-C10-C11-C12
32	C	521	LMG	C35-C36-C37-C38
25	b	605	CLA	O1D-CGD-O2D-CED
30	a	616	LHG	O1-C1-C2-O2
30	L	102	LHG	C12-C13-C14-C15
30	L	102	LHG	O6-C4-C5-O7
30	d	406	LHG	O6-C4-C5-O7
33	H	102	DGD	C8A-C9A-CAA-CBA
25	A	609	CLA	O1A-CGA-O2A-C1
25	B	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C8-C10-C11-C12
25	c	509	CLA	C10-C11-C12-C13
32	c	519	LMG	C34-C35-C36-C37
33	c	518	DGD	C9B-CAB-CBB-CCB
29	D	409	SQD	O6-C44-C45-O47
32	B	620	LMG	O1-C7-C8-O7
32	B	626	LMG	O1-C7-C8-O7
32	C	501	LMG	O7-C8-C9-O8
32	C	520	LMG	O7-C8-C9-O8
33	c	517	DGD	O1G-C1G-C2G-O2G
25	B	601	CLA	CBA-CGA-O2A-C1
30	l	101	LHG	C10-C11-C12-C13
25	B	606	CLA	C16-C17-C18-C20
32	d	408	LMG	C42-C43-C44-C45
28	d	404	PL9	C34-C36-C37-C38
30	D	406	LHG	C26-C27-C28-C29
30	a	616	LHG	C30-C31-C32-C33
32	B	620	LMG	C37-C38-C39-C40
32	C	521	LMG	C39-C40-C41-C42
29	a	613	SQD	C16-C17-C18-C19
33	c	516	DGD	C8B-C9B-CAB-CBB
25	B	606	CLA	C11-C10-C8-C9
25	B	607	CLA	C6-C7-C8-C9
25	B	607	CLA	C14-C13-C15-C16
25	B	608	CLA	C11-C12-C13-C14
25	D	403	CLA	C6-C7-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	b	604	CLA	C6-C7-C8-C9
25	b	606[B]	CLA	C14-C13-C15-C16
25	b	611	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	511	CLA	C6-C7-C8-C9
29	A	612	SQD	C10-C11-C12-C13
32	a	614	LMG	C34-C35-C36-C37
33	c	517	DGD	O6E-C5E-C6E-O5E
33	C	517	DGD	C3B-C4B-C5B-C6B
25	B	615	CLA	C10-C11-C12-C13
30	d	405	LHG	C2-C3-O3-P
33	h	102	DGD	C4B-C5B-C6B-C7B
25	B	612	CLA	C16-C17-C18-C19
25	b	606[A]	CLA	C16-C17-C18-C19
26	D	401	PHO	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	A	610	BCR	C1-C6-C7-C8
27	A	610	BCR	C5-C6-C7-C8
27	B	617	BCR	C5-C6-C7-C8
27	B	618	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	C	516	BCR	C5-C6-C7-C8
27	K	101	BCR	C1-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C26
27	K	101	BCR	C23-C24-C25-C30
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	a	611	BCR	C5-C6-C7-C8
27	b	618	BCR	C1-C6-C7-C8
27	b	618	BCR	C5-C6-C7-C8
27	b	618	BCR	C23-C24-C25-C26
27	b	618	BCR	C23-C24-C25-C30
27	c	515	BCR	C1-C6-C7-C8
27	c	515	BCR	C5-C6-C7-C8
27	c	522	BCR	C5-C6-C7-C8
27	c	522	BCR	C23-C24-C25-C26
27	d	403	BCR	C1-C6-C7-C8
27	d	403	BCR	C5-C6-C7-C8
27	h	101	BCR	C23-C24-C25-C26
27	h	101	BCR	C23-C24-C25-C30
29	A	612	SQD	C14-C15-C16-C17
25	B	601	CLA	CAA-CBA-CGA-O2A
25	c	507	CLA	O1D-CGD-O2D-CED
27	t	101	BCR	C21-C22-C23-C24
25	B	602	CLA	C8-C10-C11-C12
32	a	614	LMG	O9-C10-O7-C8
29	A	612	SQD	C16-C17-C18-C19
25	c	510	CLA	C8-C10-C11-C12
30	A	618	LHG	O6-C4-C5-C6
30	L	102	LHG	O6-C4-C5-C6
32	B	620	LMG	C19-C20-C21-C22
25	B	601	CLA	C11-C12-C13-C15
25	B	605	CLA	C11-C12-C13-C15
25	B	606	CLA	C11-C10-C8-C7
25	B	607	CLA	C12-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	C	514	CLA	C11-C10-C8-C7
25	D	403	CLA	C6-C7-C8-C10
25	b	603	CLA	C11-C12-C13-C15
25	b	603	CLA	C12-C13-C15-C16
25	b	604	CLA	C6-C7-C8-C10
25	b	606[A]	CLA	C11-C10-C8-C7
25	b	606[B]	CLA	C12-C13-C15-C16
25	b	610	CLA	C11-C12-C13-C15
25	c	506	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C10-C8-C7
25	c	508	CLA	C11-C10-C8-C7
25	c	509	CLA	C6-C7-C8-C10
25	c	510	CLA	C11-C12-C13-C15
25	c	511	CLA	C11-C10-C8-C7
25	c	513	CLA	C11-C10-C8-C7
25	c	513	CLA	C12-C13-C15-C16
26	a	609	PHO	C11-C10-C8-C7
32	b	620	LMG	C4-C5-C6-O5
27	T	101	BCR	C20-C21-C22-C37
27	b	619	BCR	C20-C21-C22-C37
25	C	511	CLA	C8-C10-C11-C12
30	B	623	LHG	C24-C23-O8-C6
29	L	101	SQD	C28-C29-C30-C31
25	c	513	CLA	C8-C10-C11-C12
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	c	512	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	C3-C5-C6-C7
32	C	520	LMG	O9-C10-O7-C8
30	D	406	LHG	C11-C10-C9-C8
32	C	520	LMG	C37-C38-C39-C40
32	m	102	LMG	C39-C40-C41-C42
25	A	613	CLA	C15-C16-C17-C18
25	b	612	CLA	C15-C16-C17-C18
29	L	101	SQD	C17-C18-C19-C20
30	l	101	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	b	601	CLA	C15-C16-C17-C18
25	c	505	CLA	C2-C3-C5-C6
29	D	408	SQD	C7-C8-C9-C10
29	A	616	SQD	C44-C45-C46-O48
29	B	625	SQD	O6-C44-C45-C46
29	D	408	SQD	C44-C45-C46-O48
29	L	101	SQD	O6-C44-C45-C46
32	B	620	LMG	O1-C7-C8-C9
25	b	612	CLA	CBD-CGD-O2D-CED
30	A	618	LHG	O6-C4-C5-O7
30	a	617	LHG	O6-C4-C5-O7
25	C	506	CLA	CBA-CGA-O2A-C1
25	B	606	CLA	C16-C17-C18-C19
32	B	620	LMG	C33-C34-C35-C36
33	C	517	DGD	O1B-C1B-O2G-C2G
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	607	CLA	CHA-CBD-CGD-O2D
25	C	503	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	b	601	CLA	CHA-CBD-CGD-O1D
25	b	601	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	CHA-CBD-CGD-O2D
25	b	610	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	O1A-CGA-O2A-C1
32	C	501	LMG	C16-C17-C18-C19
25	C	503	CLA	C13-C15-C16-C17
33	H	102	DGD	C4B-C5B-C6B-C7B
29	B	624	SQD	O47-C45-C46-O48
29	B	625	SQD	O6-C44-C45-O47
29	L	101	SQD	O6-C44-C45-O47
32	a	614	LMG	O7-C8-C9-O8
33	c	516	DGD	O1A-C1A-O1G-C1G
29	A	616	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	d	408	LMG	C14-C15-C16-C17
30	d	406	LHG	O1-C1-C2-O2
25	C	507	CLA	C3-C5-C6-C7
25	c	505	CLA	C3-C5-C6-C7
33	c	518	DGD	CCB-CDB-CEB-CFB
25	C	514	CLA	C2-C3-C5-C6
28	A	611	PL9	C4-C3-C7-C8
25	B	605	CLA	C14-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C14
29	A	612	SQD	C5-C6-S-O8
29	B	625	SQD	C5-C6-S-O8
32	B	621	LMG	C20-C21-C22-C23
25	C	514	CLA	O1D-CGD-O2D-CED
33	C	518	DGD	C2A-C3A-C4A-C5A
33	C	519	DGD	CAB-CBB-CCB-CDB
27	b	618	BCR	C11-C12-C13-C35
32	D	407	LMG	C30-C31-C32-C33
25	C	504	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	D	402	CLA	C1A-C2A-CAA-CBA
25	b	607	CLA	C1A-C2A-CAA-CBA
29	b	621	SQD	C31-C32-C33-C34
25	C	513	CLA	C2-C1-O2A-CGA
25	B	606	CLA	O1D-CGD-O2D-CED
30	B	623	LHG	C3-O3-P-O6
33	C	518	DGD	C5B-C6B-C7B-C8B
26	a	609	PHO	C4-C3-C5-C6
25	b	607	CLA	C2-C3-C5-C6
33	C	518	DGD	CCA-CDA-CEA-CFA
30	B	623	LHG	C3-O3-P-O4
30	B	623	LHG	C4-O6-P-O5
30	L	102	LHG	C4-O6-P-O5
30	d	405	LHG	C3-O3-P-O5
30	d	406	LHG	C3-O3-P-O5
30	d	406	LHG	C4-O6-P-O5
25	c	512	CLA	C16-C17-C18-C20
33	c	517	DGD	O6D-C1D-O3G-C3G
29	B	625	SQD	C24-C23-O48-C46
25	B	613	CLA	CBD-CGD-O2D-CED
33	c	517	DGD	C1A-C2A-C3A-C4A
25	b	612	CLA	C16-C17-C18-C20
25	B	607	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C	503	CLA	CAD-CBD-CGD-O1D
25	C	507	CLA	CAD-CBD-CGD-O1D
25	b	601	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
29	B	625	SQD	O47-C7-C8-C9
30	a	616	LHG	C34-C35-C36-C37
32	d	408	LMG	C34-C35-C36-C37
32	C	501	LMG	O10-C28-O8-C9
29	D	408	SQD	C24-C25-C26-C27
25	C	505	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C10-C8-C7
25	C	513	CLA	C12-C13-C15-C16
25	a	606	CLA	C11-C12-C13-C15
25	a	607	CLA	C12-C13-C15-C16
25	b	609	CLA	C11-C10-C8-C7
25	b	610	CLA	C12-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C15
25	c	502	CLA	C12-C13-C15-C16
25	c	503	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C12-C13-C15
25	c	509	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
28	D	405	PL9	C13-C14-C16-C17
30	l	101	LHG	O6-C4-C5-O7
29	D	409	SQD	C31-C32-C33-C34
33	H	102	DGD	O2G-C1B-C2B-C3B
29	B	625	SQD	C25-C26-C27-C28
32	D	407	LMG	C33-C34-C35-C36
25	B	613	CLA	C13-C15-C16-C17
25	C	509	CLA	C8-C10-C11-C12
30	a	617	LHG	C8-C7-O7-C5
30	A	618	LHG	C24-C25-C26-C27
25	C	506	CLA	O1A-CGA-O2A-C1
25	A	607	CLA	C16-C17-C18-C20
29	B	624	SQD	C44-C45-C46-O48
30	d	406	LHG	C28-C29-C30-C31
32	C	501	LMG	C7-C8-C9-O8
29	D	408	SQD	O47-C45-C46-O48
29	a	613	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	L	101	SQD	C11-C12-C13-C14
29	f	101	SQD	C25-C26-C27-C28
25	c	501	CLA	O1D-CGD-O2D-CED
29	f	101	SQD	C24-C23-O48-C46
30	d	406	LHG	C17-C18-C19-C20
32	d	407	LMG	C14-C15-C16-C17
25	c	511	CLA	CAA-CBA-CGA-O2A
32	C	501	LMG	C11-C12-C13-C14
32	d	407	LMG	C21-C22-C23-C24
33	c	517	DGD	C8A-C9A-CAA-CBA
25	c	509	CLA	C8-C10-C11-C12
25	B	601	CLA	C14-C13-C15-C16
25	B	610	CLA	C14-C13-C15-C16
25	C	508	CLA	C11-C12-C13-C14
25	C	514	CLA	C11-C10-C8-C9
25	b	609	CLA	C6-C7-C8-C9
25	b	610	CLA	C11-C12-C13-C14
25	c	509	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C12-C13-C14
33	C	519	DGD	O1A-C1A-O1G-C1G
25	c	508	CLA	C16-C17-C18-C19
29	B	624	SQD	C17-C18-C19-C20
25	b	612	CLA	O1D-CGD-O2D-CED
25	d	402	CLA	C13-C15-C16-C17
32	c	520	LMG	C10-C11-C12-C13
30	L	102	LHG	C29-C30-C31-C32
32	C	501	LMG	C13-C14-C15-C16
32	c	519	LMG	C37-C38-C39-C40
32	c	520	LMG	C15-C16-C17-C18
33	C	518	DGD	C3B-C4B-C5B-C6B
30	a	617	LHG	C11-C12-C13-C14
25	c	509	CLA	CAA-CBA-CGA-O2A
25	c	512	CLA	C16-C17-C18-C19
30	B	623	LHG	C31-C32-C33-C34
29	f	101	SQD	C24-C25-C26-C27
30	a	616	LHG	C26-C27-C28-C29
25	b	601	CLA	C8-C10-C11-C12
33	C	518	DGD	CBA-CCA-CDA-CEA
30	d	405	LHG	C1-C2-C3-O3
25	c	501	CLA	C2A-CAA-CBA-CGA
33	c	516	DGD	C4A-C5A-C6A-C7A
25	B	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	A	606	CLA	C2-C1-O2A-CGA
25	b	610	CLA	C3-C5-C6-C7
30	A	614	LHG	C28-C29-C30-C31
33	h	102	DGD	C3A-C4A-C5A-C6A
32	C	520	LMG	C38-C39-C40-C41
32	C	501	LMG	C37-C38-C39-C40
27	A	610	BCR	C23-C24-C25-C26
27	A	610	BCR	C23-C24-C25-C30
27	B	617	BCR	C1-C6-C7-C8
27	B	618	BCR	C1-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C30
27	B	619	BCR	C23-C24-C25-C26
27	B	619	BCR	C23-C24-C25-C30
27	C	515	BCR	C23-C24-C25-C30
27	C	516	BCR	C1-C6-C7-C8
27	C	516	BCR	C23-C24-C25-C30
27	D	404	BCR	C23-C24-C25-C30
27	K	101	BCR	C5-C6-C7-C8
27	a	611	BCR	C1-C6-C7-C8
27	a	611	BCR	C23-C24-C25-C30
27	b	619	BCR	C23-C24-C25-C26
27	b	619	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
27	c	514	BCR	C5-C6-C7-C8
27	c	521	BCR	C23-C24-C25-C26
27	c	521	BCR	C23-C24-C25-C30
27	c	522	BCR	C23-C24-C25-C30
25	B	605	CLA	C13-C15-C16-C17
32	C	501	LMG	C35-C36-C37-C38
33	C	517	DGD	C2B-C3B-C4B-C5B
25	c	510	CLA	C16-C17-C18-C20
29	f	101	SQD	O5-C1-O6-C44
32	b	620	LMG	O6-C1-O1-C7
25	b	601	CLA	C2A-CAA-CBA-CGA
27	H	101	BCR	C11-C10-C9-C8
30	A	618	LHG	O7-C5-C6-O8
30	a	617	LHG	O7-C5-C6-O8
32	C	520	LMG	O1-C7-C8-O7
30	l	101	LHG	C4-O6-P-O3
29	a	613	SQD	C23-C24-C25-C26
30	A	614	LHG	C12-C13-C14-C15
26	a	609	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	a	609	PHO	CHA-CBD-CGD-O2D
32	C	501	LMG	C14-C15-C16-C17
30	a	616	LHG	C4-C5-C6-O8
25	B	601	CLA	C12-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C15
25	b	602	CLA	C12-C13-C15-C16
25	b	611	CLA	C6-C7-C8-C10
25	b	611	CLA	C12-C13-C15-C16
25	B	601	CLA	C11-C10-C8-C9
25	B	608	CLA	C14-C13-C15-C16
25	b	614	CLA	C11-C10-C8-C9
25	b	614	CLA	C11-C12-C13-C14
25	c	506	CLA	C11-C10-C8-C9
25	c	510	CLA	C6-C7-C8-C9
25	B	611	CLA	C16-C17-C18-C19
25	B	614	CLA	C16-C17-C18-C20
25	B	610	CLA	CBA-CGA-O2A-C1
29	B	624	SQD	C9-C10-C11-C12
30	A	614	LHG	C24-C25-C26-C27
30	L	102	LHG	C9-C10-C11-C12
27	B	619	BCR	C37-C22-C23-C24
25	B	603	CLA	C16-C17-C18-C20
30	A	614	LHG	C2-C3-O3-P
25	C	508	CLA	C15-C16-C17-C18
25	C	509	CLA	C13-C15-C16-C17
30	l	101	LHG	C27-C28-C29-C30
32	C	501	LMG	C8-C9-O8-C28
25	b	603	CLA	C2-C3-C5-C6
30	d	405	LHG	C24-C23-O8-C6
30	B	623	LHG	C17-C18-C19-C20
30	d	406	LHG	C9-C10-C11-C12
25	B	605	CLA	C15-C16-C17-C18
32	c	519	LMG	C40-C41-C42-C43
33	c	518	DGD	C5B-C6B-C7B-C8B
25	A	607	CLA	C16-C17-C18-C19
33	C	517	DGD	CDA-CEA-CFA-CGA
25	c	511	CLA	C5-C6-C7-C8
26	A	608	PHO	C15-C16-C17-C18
25	C	512	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	O1A-CGA-O2A-C1
25	b	606[A]	CLA	C3-C5-C6-C7
28	d	404	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
30	d	405	LHG	C14-C15-C16-C17
33	h	102	DGD	CBA-CCA-CDA-CEA
25	B	604	CLA	C8-C10-C11-C12
29	B	625	SQD	C11-C12-C13-C14
32	m	102	LMG	O8-C28-C29-C30
32	C	501	LMG	C36-C37-C38-C39
25	B	603	CLA	C2A-CAA-CBA-CGA
25	b	614	CLA	C2A-CAA-CBA-CGA
32	C	501	LMG	C34-C35-C36-C37
33	h	102	DGD	C3B-C4B-C5B-C6B
30	A	614	LHG	C24-C23-O8-C6
32	B	626	LMG	O7-C10-C11-C12
32	m	102	LMG	C30-C31-C32-C33
25	b	613	CLA	C16-C17-C18-C20
25	B	609	CLA	CBD-CGD-O2D-CED
30	A	618	LHG	C24-C23-O8-C6
30	d	406	LHG	C29-C30-C31-C32
29	B	625	SQD	C28-C29-C30-C31
25	b	615	CLA	C6-C7-C8-C9
25	c	502	CLA	C14-C13-C15-C16
25	B	601	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C19
25	c	503	CLA	CBA-CGA-O2A-C1
27	B	617	BCR	C20-C21-C22-C37
32	C	520	LMG	O1-C7-C8-C9
33	C	517	DGD	O1G-C1G-C2G-C3G
25	B	601	CLA	C2A-CAA-CBA-CGA
32	B	621	LMG	C15-C16-C17-C18
33	H	102	DGD	C4A-C5A-C6A-C7A
25	B	611	CLA	C16-C17-C18-C20
26	a	608	PHO	C16-C17-C18-C19
29	a	613	SQD	C24-C23-O48-C46
32	m	102	LMG	C4-C5-C6-O5
32	m	102	LMG	O6-C1-O1-C7
33	c	516	DGD	O6E-C1E-O5D-C6D
33	c	518	DGD	O6D-C1D-O3G-C3G
28	A	611	PL9	C14-C16-C17-C18
29	a	613	SQD	C32-C33-C34-C35
29	a	613	SQD	C11-C10-C9-C8
25	C	506	CLA	C10-C11-C12-C13
25	b	601	CLA	C10-C11-C12-C13
25	c	507	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	CBA-CGA-O2A-C1
33	C	519	DGD	CDA-CEA-CFA-CGA
25	A	606	CLA	C11-C12-C13-C15
25	B	611	CLA	C12-C13-C15-C16
25	C	506	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	a	615	CLA	C12-C13-C15-C16
25	c	502	CLA	C11-C10-C8-C7
25	d	402	CLA	C12-C13-C15-C16
26	a	609	PHO	C11-C12-C13-C15
32	b	620	LMG	C34-C35-C36-C37
25	c	505	CLA	C2A-CAA-CBA-CGA
30	A	614	LHG	C15-C16-C17-C18
32	C	501	LMG	C11-C10-O7-C8
30	B	623	LHG	C11-C12-C13-C14
32	B	620	LMG	C30-C31-C32-C33
33	c	518	DGD	C6A-C7A-C8A-C9A
25	c	503	CLA	O1A-CGA-O2A-C1
29	a	613	SQD	C7-C8-C9-C10
32	m	102	LMG	C14-C15-C16-C17
30	a	616	LHG	O7-C5-C6-O8
32	C	521	LMG	C29-C28-O8-C9
29	a	613	SQD	C30-C31-C32-C33
29	a	613	SQD	C34-C35-C36-C37
25	C	508	CLA	C16-C17-C18-C19
29	a	613	SQD	O5-C1-O6-C44
25	b	601	CLA	O1A-CGA-O2A-C1
25	B	609	CLA	O1D-CGD-O2D-CED
25	a	606	CLA	C2-C1-O2A-CGA
32	B	626	LMG	C19-C20-C21-C22
29	D	408	SQD	C23-C24-C25-C26
25	B	613	CLA	C11-C12-C13-C14
25	B	613	CLA	C14-C13-C15-C16
25	C	502	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C12-C13-C14
25	b	611	CLA	C11-C12-C13-C14
25	b	607	CLA	CBA-CGA-O2A-C1
25	c	502	CLA	O1A-CGA-O2A-C1
29	B	624	SQD	C26-C27-C28-C29
32	a	614	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
26	a	609	PHO	C16-C17-C18-C20
27	B	619	BCR	C1-C6-C7-C8
27	C	515	BCR	C1-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C26
27	C	516	BCR	C23-C24-C25-C26
27	T	101	BCR	C23-C24-C25-C30
27	Y	101	BCR	C23-C24-C25-C30
27	a	611	BCR	C23-C24-C25-C26
27	b	619	BCR	C1-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C30
27	c	515	BCR	C23-C24-C25-C30
27	d	403	BCR	C23-C24-C25-C30
33	C	517	DGD	O1G-C1A-C2A-C3A
25	b	604	CLA	C13-C15-C16-C17
30	L	102	LHG	C17-C18-C19-C20
30	a	617	LHG	C11-C10-C9-C8
27	b	617	BCR	C21-C22-C23-C24
25	C	513	CLA	O1D-CGD-O2D-CED
25	A	609	CLA	C5-C6-C7-C8
28	d	404	PL9	C13-C14-C16-C17
35	V	201	HEC	CAD-CBD-CGD-O2D
35	v	201	HEC	CAD-CBD-CGD-O2D
29	D	409	SQD	C12-C13-C14-C15
25	A	606	CLA	C13-C15-C16-C17
33	C	517	DGD	C5D-C6D-O5D-C1E
32	C	520	LMG	C11-C12-C13-C14
25	c	504	CLA	C11-C12-C13-C14
33	h	102	DGD	O2G-C1B-C2B-C3B
25	b	607	CLA	C3-C5-C6-C7
30	L	102	LHG	C28-C29-C30-C31
32	d	407	LMG	C35-C36-C37-C38
25	b	614	CLA	C4-C3-C5-C6
33	H	102	DGD	C4E-C5E-C6E-O5E
25	B	606	CLA	C6-C7-C8-C10
25	B	609	CLA	C2-C3-C5-C6
25	C	502	CLA	C6-C7-C8-C10
32	b	620	LMG	C16-C17-C18-C19
33	C	517	DGD	CBA-CCA-CDA-CEA
33	c	517	DGD	C2D-C1D-O3G-C3G
25	b	607	CLA	C16-C17-C18-C20
30	a	616	LHG	C2-C3-O3-P
33	C	517	DGD	O1G-C1G-C2G-O2G

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Mol	Chain	Res	Type	Atoms
25	b	607	CLA	O1A-CGA-O2A-C1
29	L	101	SQD	C12-C13-C14-C15
25	B	604	CLA	C3-C5-C6-C7
25	C	511	CLA	CAA-CBA-CGA-O2A
33	C	517	DGD	C6B-C7B-C8B-C9B
32	C	521	LMG	C19-C20-C21-C22
25	c	502	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	C10-C11-C12-C13
25	B	611	CLA	C2-C3-C5-C6
26	a	609	PHO	C2-C3-C5-C6
33	C	519	DGD	C4E-C5E-C6E-O5E
25	D	402	CLA	CAA-CBA-CGA-O2A
25	B	601	CLA	C6-C7-C8-C9
25	B	606	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	a	607	CLA	C14-C13-C15-C16
25	b	609	CLA	C11-C10-C8-C9
25	c	503	CLA	C11-C10-C8-C9
25	d	402	CLA	C14-C13-C15-C16
33	c	518	DGD	O1A-C1A-O1G-C1G
25	A	609	CLA	C6-C7-C8-C9
25	b	609	CLA	C3A-C2A-CAA-CBA
25	b	612	CLA	C3A-C2A-CAA-CBA
33	c	517	DGD	O2G-C1B-C2B-C3B
32	d	407	LMG	C19-C20-C21-C22
25	B	603	CLA	CAD-CBD-CGD-O2D
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	C	511	CLA	CAD-CBD-CGD-O2D
25	b	603	CLA	CAD-CBD-CGD-O2D
25	b	612	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	C2A-CAA-CBA-CGA
32	B	620	LMG	O9-C10-O7-C8
25	D	402	CLA	C2-C1-O2A-CGA
32	b	620	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	A	616	SQD	C23-C24-C25-C26
25	b	606[A]	CLA	CBD-CGD-O2D-CED
35	V	201	HEC	CAD-CBD-CGD-O1D
33	C	518	DGD	O6D-C1D-O3G-C3G
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	612	CLA	CAA-CBA-CGA-O2A
29	L	101	SQD	O47-C7-C8-C9
29	b	621	SQD	C24-C25-C26-C27
27	T	101	BCR	C21-C22-C23-C24
27	Y	101	BCR	C7-C8-C9-C10
29	B	625	SQD	C13-C14-C15-C16
35	v	201	HEC	CAD-CBD-CGD-O1D
30	d	405	LHG	C25-C26-C27-C28
33	C	519	DGD	C9B-CAB-CBB-CCB
33	C	518	DGD	C6B-C7B-C8B-C9B
26	D	401	PHO	O2A-C1-C2-C3
26	a	608	PHO	O2A-C1-C2-C3
30	d	406	LHG	C19-C20-C21-C22
33	C	519	DGD	C7B-C8B-C9B-CAB
29	A	612	SQD	O47-C7-C8-C9
29	B	624	SQD	O47-C7-C8-C9
33	C	517	DGD	O1A-C1A-C2A-C3A
34	e	101	HEM	CAA-CBA-CGA-O2A
25	B	616	CLA	C16-C17-C18-C20
25	b	613	CLA	C16-C17-C18-C19
29	L	101	SQD	O49-C7-O47-C45
25	A	607	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	609	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O1D
25	C	510	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	CHA-CBD-CGD-O1D
25	C	512	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	606[A]	CLA	CHA-CBD-CGD-O1D
25	b	606[A]	CLA	CHA-CBD-CGD-O2D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	c	510	CLA	CHA-CBD-CGD-O1D
25	B	609	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	l	101	LHG	O7-C7-C8-C9
32	c	520	LMG	O7-C10-C11-C12
32	c	520	LMG	O8-C28-C29-C30
25	C	513	CLA	CBD-CGD-O2D-CED
27	Y	101	BCR	C20-C21-C22-C23
29	A	616	SQD	O47-C7-C8-C9
32	B	621	LMG	O1-C7-C8-O7
32	c	519	LMG	O7-C8-C9-O8
25	c	512	CLA	C15-C16-C17-C18
25	C	512	CLA	O1D-CGD-O2D-CED
25	d	401	CLA	CAA-CBA-CGA-O2A
30	L	102	LHG	O7-C7-C8-C9
32	m	102	LMG	C35-C36-C37-C38
26	A	608	PHO	CHA-CBD-CGD-O1D
26	A	608	PHO	CHA-CBD-CGD-O2D
29	A	616	SQD	C17-C18-C19-C20
25	C	507	CLA	C4-C3-C5-C6
29	b	621	SQD	C14-C15-C16-C17
25	b	613	CLA	C12-C13-C15-C16
33	H	102	DGD	C3B-C4B-C5B-C6B
25	B	606	CLA	C6-C7-C8-C9
25	B	613	CLA	C6-C7-C8-C9
25	a	606	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	c	502	CLA	C11-C10-C8-C9
29	A	616	SQD	O49-C7-C8-C9
25	b	614	CLA	C15-C16-C17-C18
29	B	625	SQD	C9-C10-C11-C12
29	D	409	SQD	C4-C5-C6-S
29	D	409	SQD	C5-C6-S-O8
25	C	503	CLA	C16-C17-C18-C20
26	A	608	PHO	C16-C17-C18-C20
29	D	409	SQD	C10-C11-C12-C13
33	h	102	DGD	C2B-C3B-C4B-C5B
28	d	404	PL9	C11-C12-C13-C14
29	A	612	SQD	C35-C36-C37-C38
25	c	510	CLA	CAA-CBA-CGA-O2A
32	B	620	LMG	O7-C10-C11-C12
27	D	404	BCR	C7-C8-C9-C34
25	b	612	CLA	CAA-CBA-CGA-O1A
29	A	616	SQD	O10-C23-C24-C25
26	a	608	PHO	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	d	405	LHG	C34-C35-C36-C37
30	d	406	LHG	O1-C1-C2-C3
33	c	517	DGD	O1A-C1A-O1G-C1G
30	B	623	LHG	C12-C13-C14-C15
25	B	601	CLA	CAA-CBA-CGA-O1A
27	b	619	BCR	C7-C8-C9-C10
33	C	519	DGD	C6B-C7B-C8B-C9B
25	b	612	CLA	CBA-CGA-O2A-C1
30	A	618	LHG	C34-C35-C36-C37
25	B	612	CLA	C1A-C2A-CAA-CBA
25	b	609	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	d	401	CLA	C1A-C2A-CAA-CBA
32	B	626	LMG	C13-C14-C15-C16
25	B	601	CLA	C16-C17-C18-C20
25	d	402	CLA	C16-C17-C18-C19
25	B	612	CLA	CAA-CBA-CGA-O1A
32	C	520	LMG	C36-C37-C38-C39
25	D	403	CLA	C2-C1-O2A-CGA
30	A	614	LHG	C31-C32-C33-C34
25	B	611	CLA	C8-C10-C11-C12
25	C	504	CLA	C10-C11-C12-C13
25	c	503	CLA	C15-C16-C17-C18
25	C	511	CLA	CAA-CBA-CGA-O1A
29	a	613	SQD	O49-C7-C8-C9
32	m	102	LMG	O9-C10-C11-C12
30	D	406	LHG	C33-C34-C35-C36
32	d	407	LMG	C12-C13-C14-C15
32	c	519	LMG	O1-C7-C8-C9
32	m	102	LMG	O1-C7-C8-C9
33	c	517	DGD	O1G-C1G-C2G-C3G
25	b	608	CLA	C2A-CAA-CBA-CGA
30	a	617	LHG	C16-C17-C18-C19
25	a	610	CLA	C16-C17-C18-C20
30	d	405	LHG	C33-C34-C35-C36
25	b	612	CLA	O1A-CGA-O2A-C1
28	D	405	PL9	C15-C14-C16-C17
30	a	616	LHG	O8-C23-C24-C25
25	D	402	CLA	CAA-CBA-CGA-O1A
25	d	401	CLA	CAA-CBA-CGA-O1A
29	A	612	SQD	O49-C7-C8-C9
32	d	407	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	E	101	HEM	CAD-CBD-CGD-O2D
30	D	406	LHG	C4-O6-P-O5
33	C	518	DGD	C6A-C7A-C8A-C9A
30	A	618	LHG	O10-C23-C24-C25
30	l	101	LHG	O9-C7-C8-C9
32	B	621	LMG	O9-C10-C11-C12
34	e	101	HEM	CAA-CBA-CGA-O1A
25	B	616	CLA	C3-C5-C6-C7
27	C	515	BCR	C5-C6-C7-C8
27	D	404	BCR	C23-C24-C25-C26
27	Y	101	BCR	C23-C24-C25-C26
27	b	619	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	d	403	BCR	C23-C24-C25-C26
27	t	101	BCR	C23-C24-C25-C30
30	l	101	LHG	C11-C12-C13-C14
25	b	603	CLA	C8-C10-C11-C12
25	c	510	CLA	CAA-CBA-CGA-O1A
25	B	613	CLA	CAA-CBA-CGA-O2A
32	C	501	LMG	O8-C28-C29-C30
32	D	407	LMG	O7-C10-C11-C12
32	d	408	LMG	C30-C31-C32-C33
30	d	405	LHG	O10-C23-C24-C25
25	B	611	CLA	C4-C3-C5-C6
25	B	604	CLA	C2C-C3C-CAC-CBC
29	B	625	SQD	C16-C17-C18-C19
33	c	516	DGD	C9A-CAA-CBA-CCA
25	B	609	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	b	602	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
29	B	624	SQD	O5-C5-C6-S
29	D	409	SQD	O5-C5-C6-S
29	L	101	SQD	O5-C5-C6-S
29	B	624	SQD	C29-C30-C31-C32
25	B	609	CLA	C14-C13-C15-C16
25	a	610	CLA	C14-C13-C15-C16
25	a	615	CLA	C14-C13-C15-C16
25	b	613	CLA	C14-C13-C15-C16
26	a	609	PHO	C11-C12-C13-C14
29	D	408	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	d	405	LHG	O8-C23-C24-C25
32	D	407	LMG	C31-C32-C33-C34
25	b	604	CLA	CBD-CGD-O2D-CED
30	A	618	LHG	O8-C23-C24-C25
25	B	603	CLA	C13-C15-C16-C17
25	b	613	CLA	C10-C11-C12-C13
34	E	101	HEM	CAD-CBD-CGD-O1D
30	B	623	LHG	O10-C23-C24-C25
33	c	518	DGD	O1B-C1B-C2B-C3B
30	d	405	LHG	C15-C16-C17-C18
25	B	602	CLA	C11-C12-C13-C15
25	B	613	CLA	C6-C7-C8-C10
25	b	611	CLA	C11-C12-C13-C15
25	b	614	CLA	C11-C10-C8-C7
25	c	508	CLA	C12-C13-C15-C16
25	c	511	CLA	C12-C13-C15-C16
29	a	613	SQD	O47-C7-C8-C9
32	B	621	LMG	O7-C10-C11-C12
32	m	102	LMG	O7-C10-C11-C12
25	a	615	CLA	C2C-C3C-CAC-CBC
25	A	606	CLA	C8-C10-C11-C12
27	B	618	BCR	C7-C8-C9-C10
27	D	404	BCR	C21-C22-C23-C24
32	B	620	LMG	O10-C28-C29-C30
25	b	603	CLA	C16-C17-C18-C20
32	c	519	LMG	O6-C1-O1-C7
33	C	517	DGD	O6E-C1E-O5D-C6D
25	B	612	CLA	C13-C15-C16-C17
25	B	616	CLA	C8-C10-C11-C12
25	b	609	CLA	C15-C16-C17-C18
28	D	405	PL9	C44-C46-C47-C48
29	D	408	SQD	C8-C7-O47-C45
29	D	409	SQD	O47-C7-C8-C9
30	a	616	LHG	C35-C36-C37-C38
29	B	624	SQD	O49-C7-C8-C9
25	C	508	CLA	C16-C17-C18-C20
25	a	615	CLA	C4C-C3C-CAC-CBC
25	D	403	CLA	C5-C6-C7-C8
25	c	503	CLA	C8-C10-C11-C12
26	a	608	PHO	C8-C10-C11-C12
29	A	616	SQD	C7-C8-C9-C10
25	C	512	CLA	CAA-CBA-CGA-O2A

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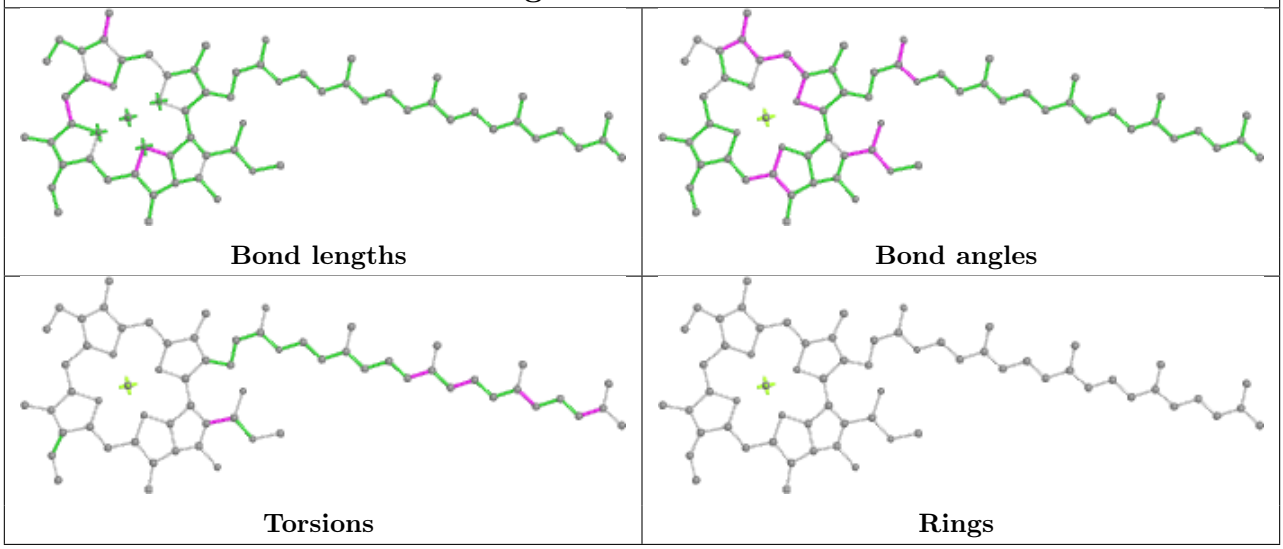
Mol	Chain	Res	Type	Atoms
25	c	501	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

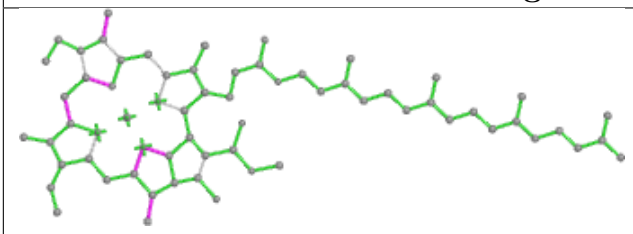
No monomer is involved in short contacts.

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.

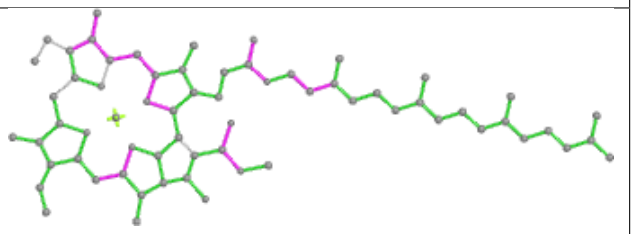
Ligand CLA A 607



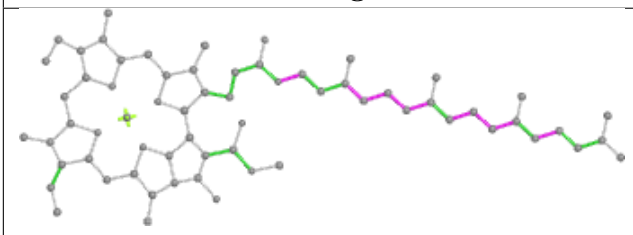
Ligand CLA A 606



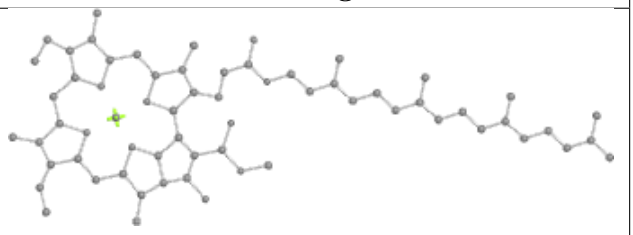
Bond lengths



Bond angles

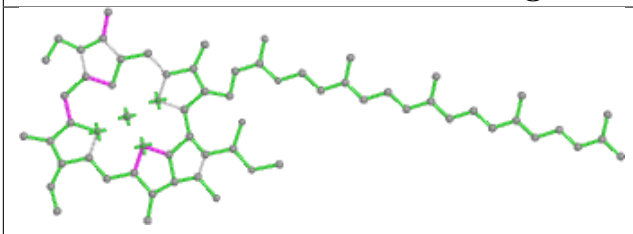


Torsions

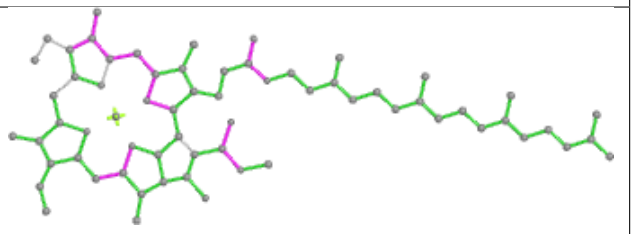


Rings

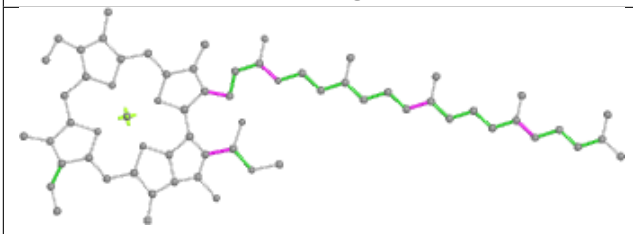
Ligand CLA B 607



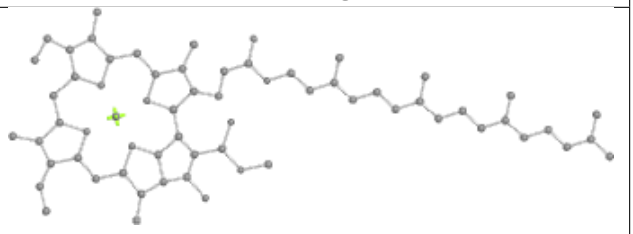
Bond lengths



Bond angles

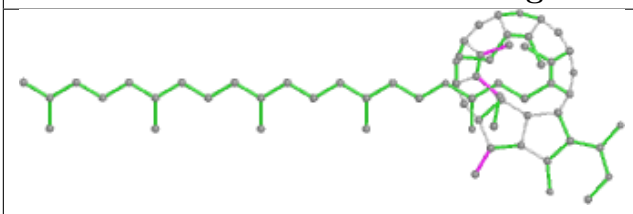


Torsions

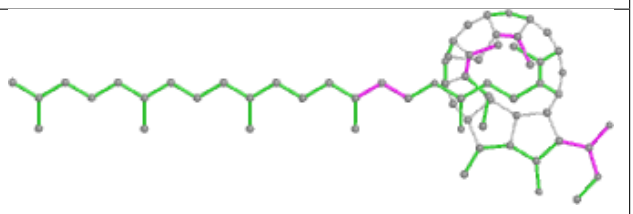


Rings

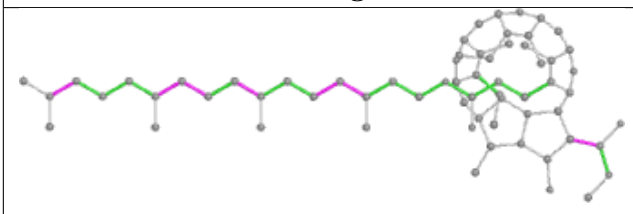
Ligand PHO a 609



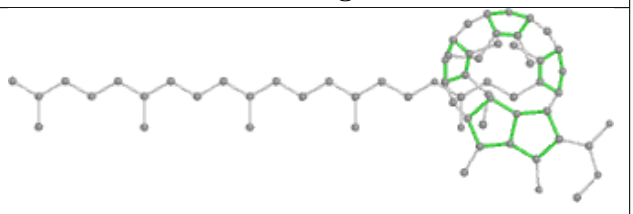
Bond lengths



Bond angles

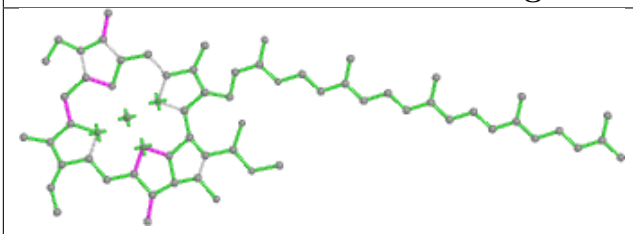


Torsions

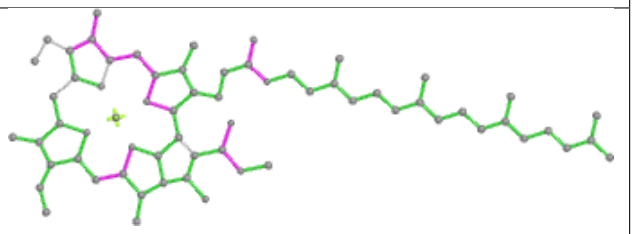


Rings

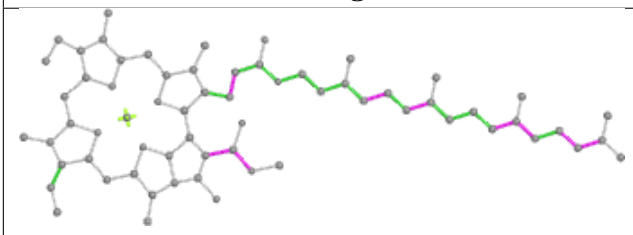
Ligand CLA C 502



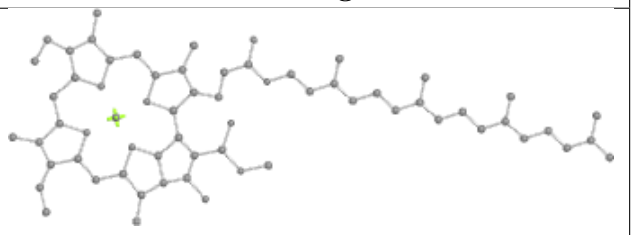
Bond lengths



Bond angles

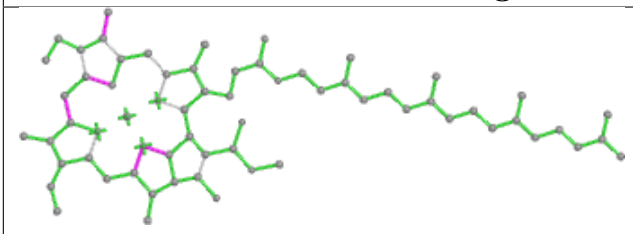


Torsions



Rings

Ligand CLA b 606 (A)



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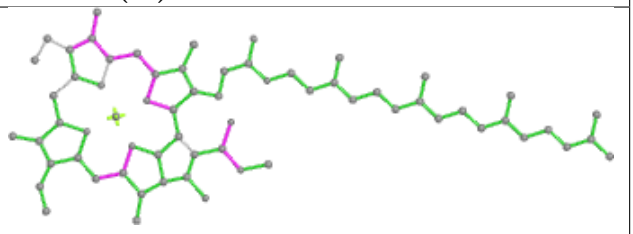

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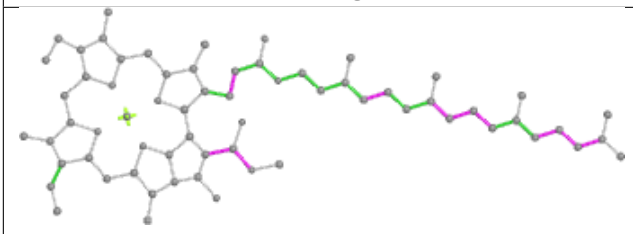

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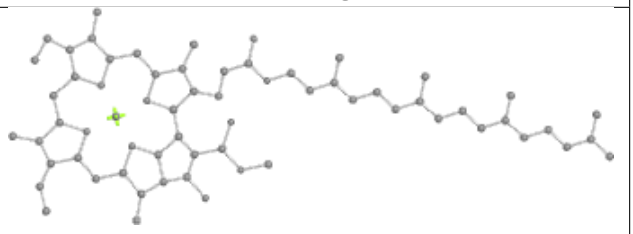
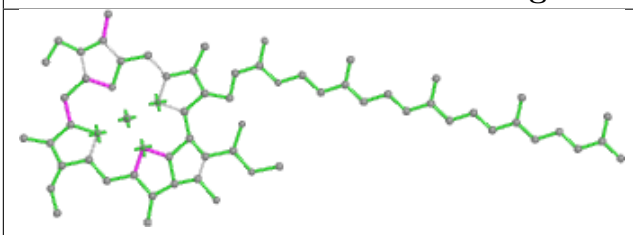


Rings

Ligand CLA c 502



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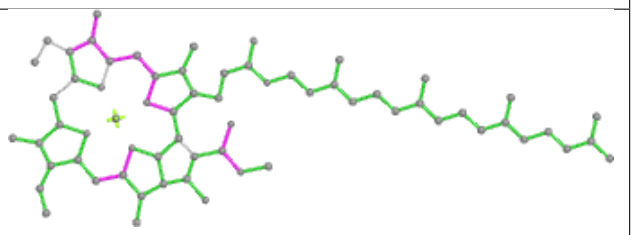
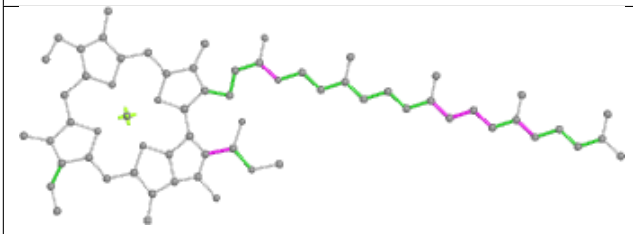


Bond angles



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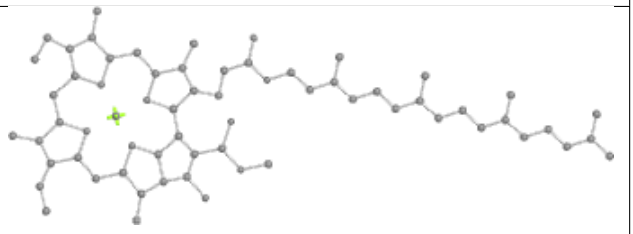
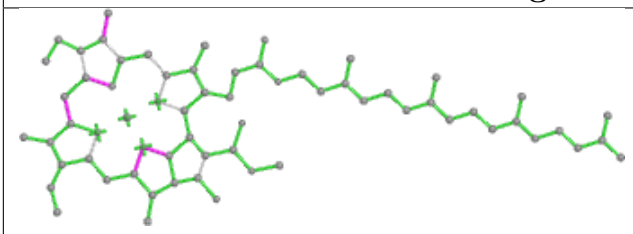


Rings

Ligand CLA c 506



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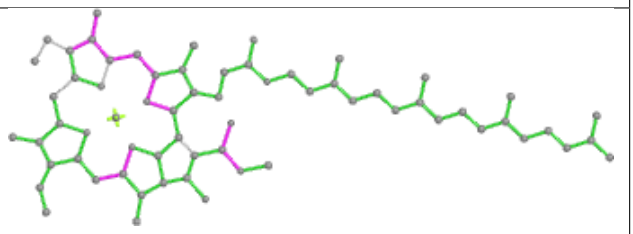
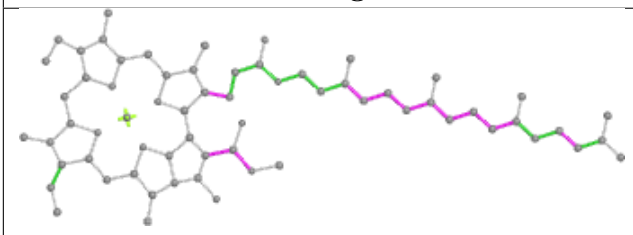


Bond angles



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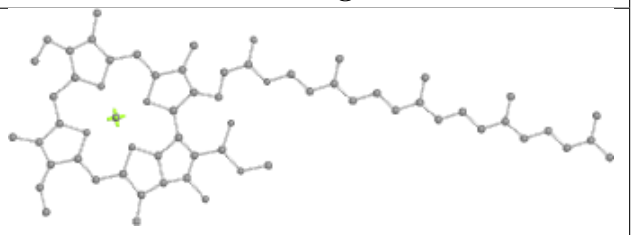
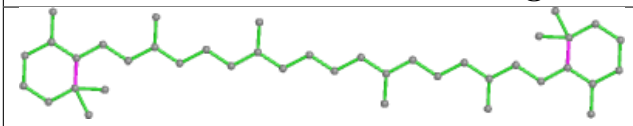
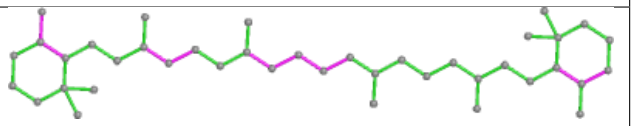


Rings

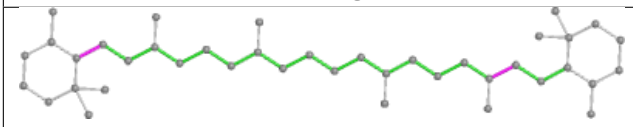
Ligand BCR b 617



Bond lengths



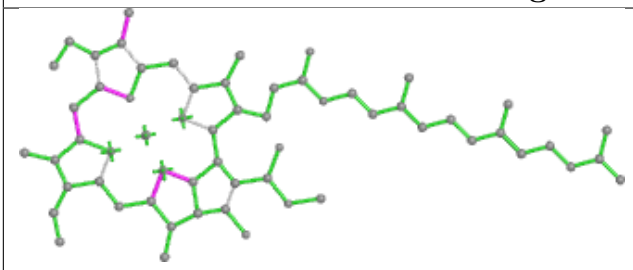
Bond angles



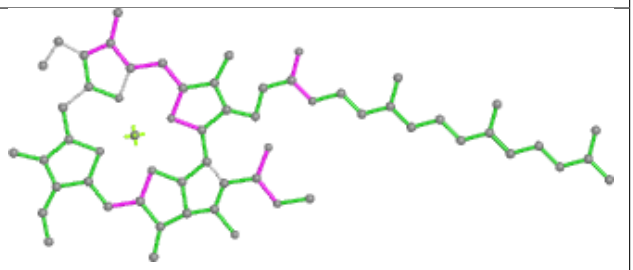
Torsions

Rings

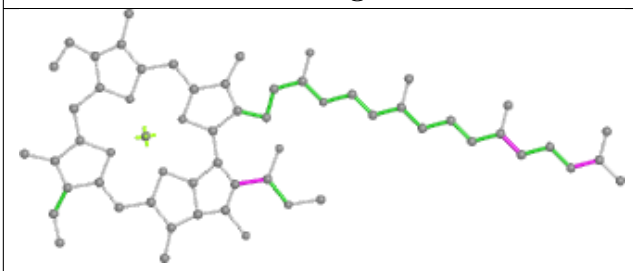
Ligand CLA c 504



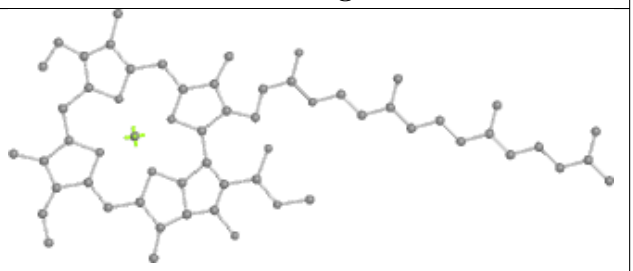
Bond lengths



Bond angles

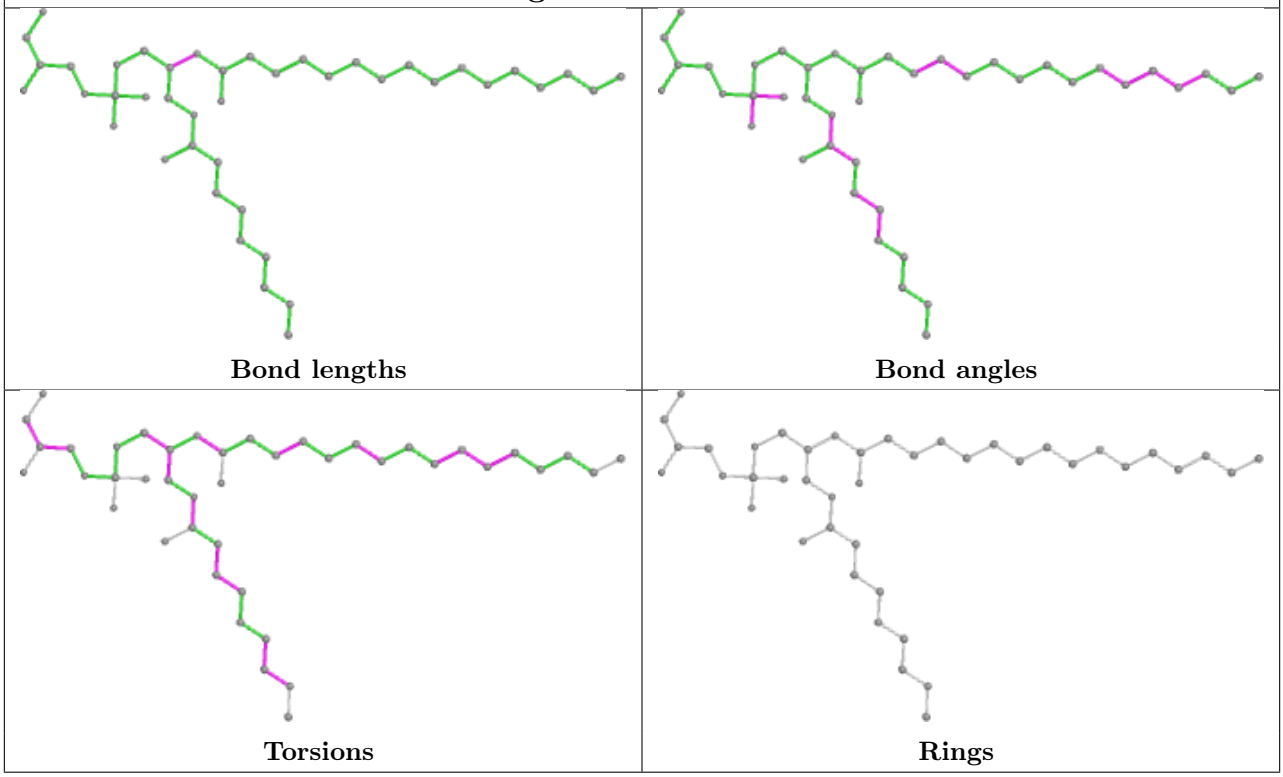


Torsions

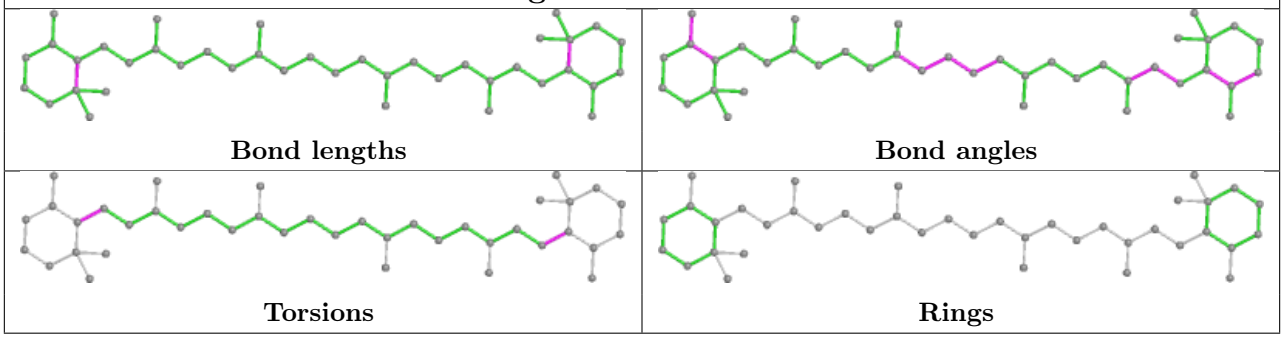


Rings

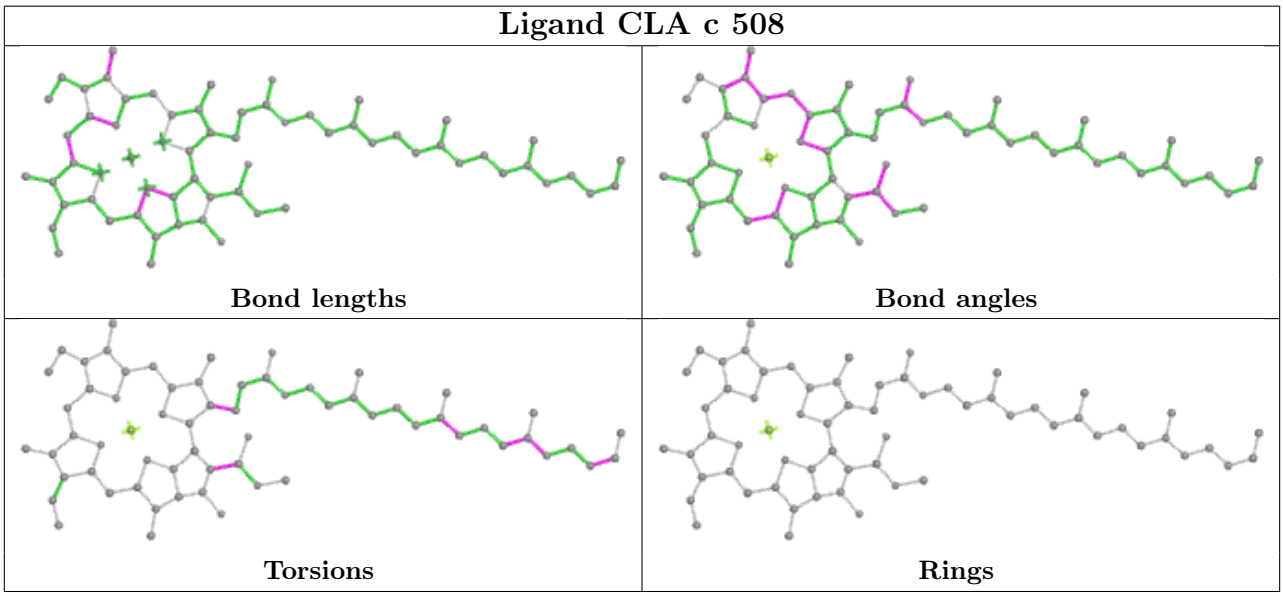
Ligand LHG a 617



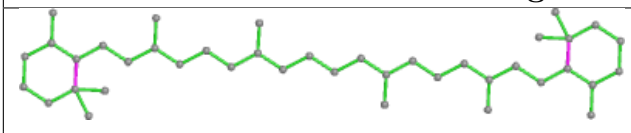
Ligand BCR c 522



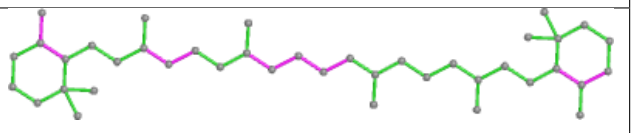
Ligand CLA c 508



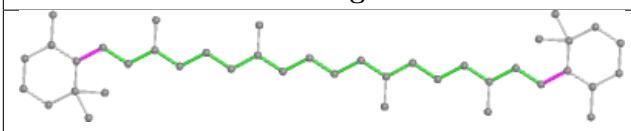
Ligand BCR c 515



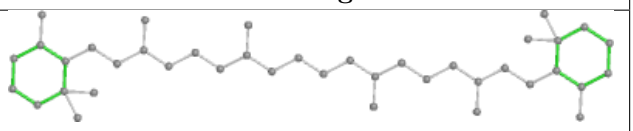
Bond lengths



Bond angles

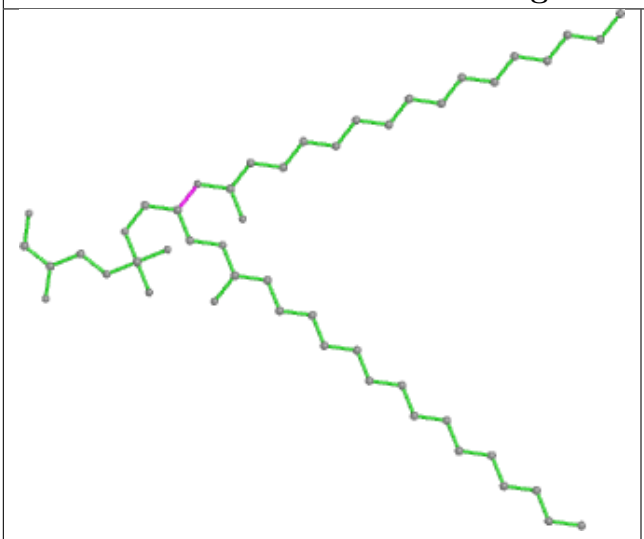


Torsions

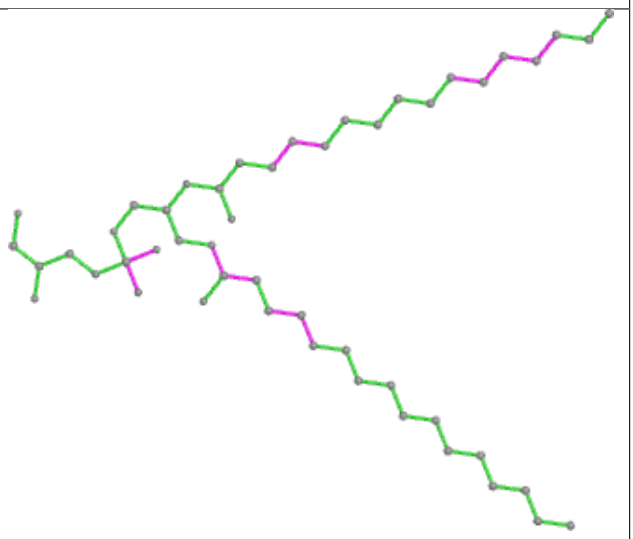


Rings

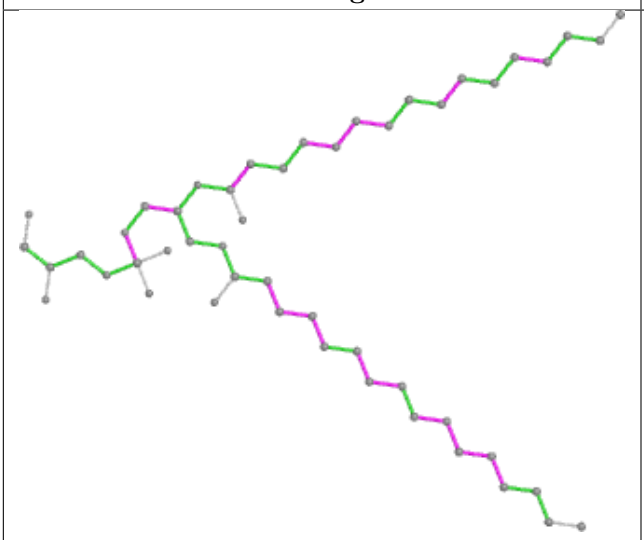
Ligand LHG l 101



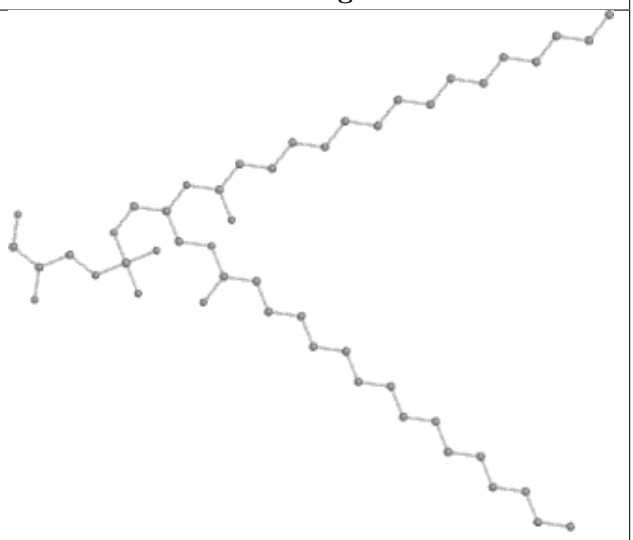
Bond lengths



Bond angles

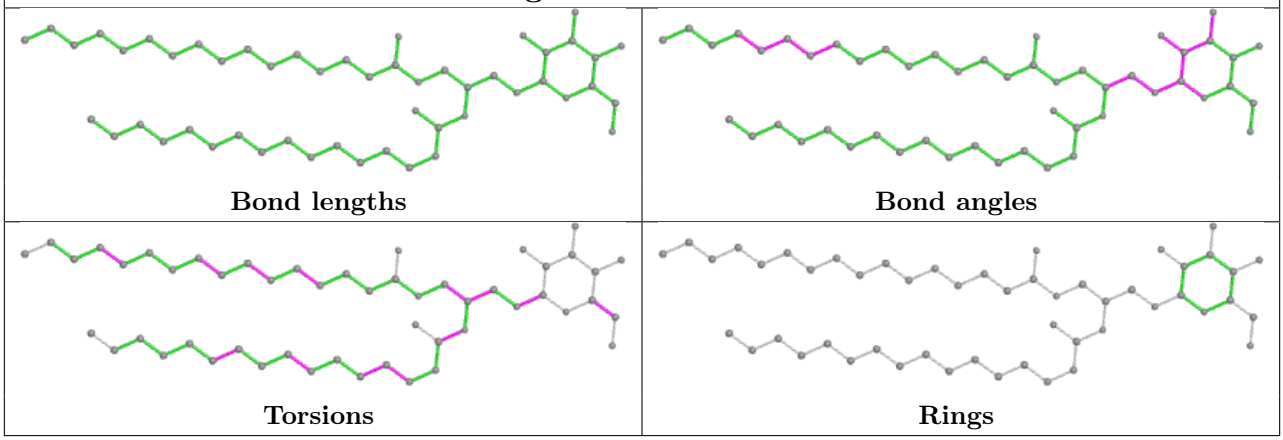


Torsions

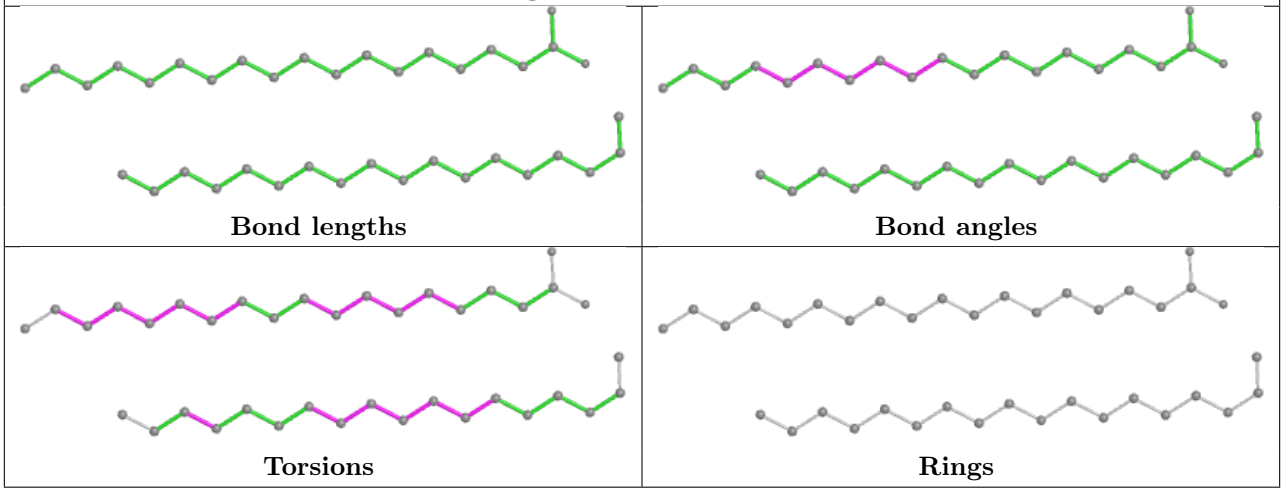


Rings

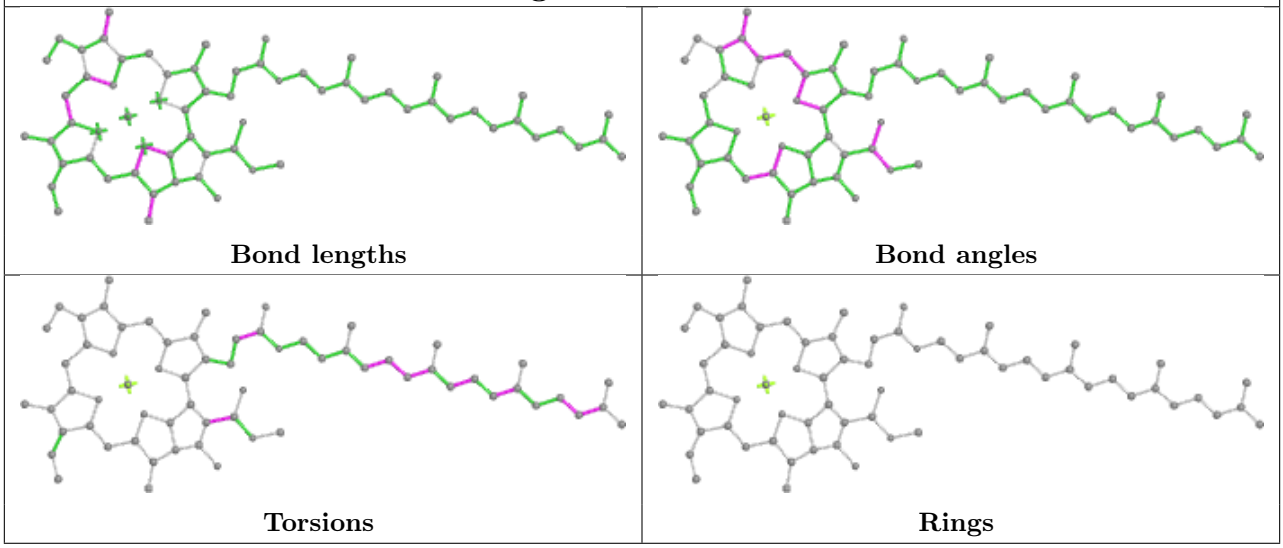
Ligand LMG a 614



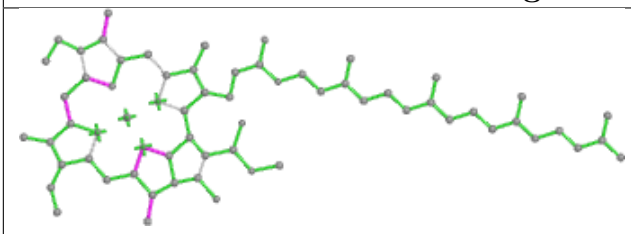
Ligand LMG d 408



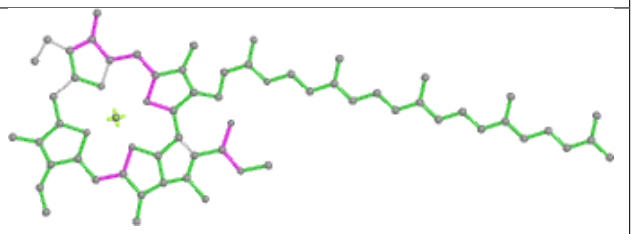
Ligand CLA c 510



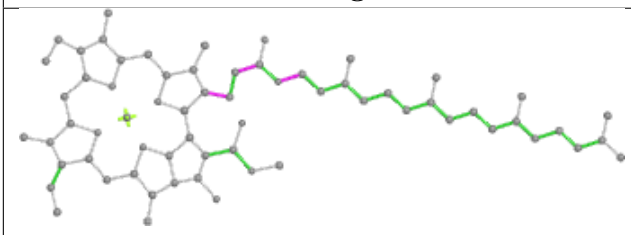
Ligand CLA D 402



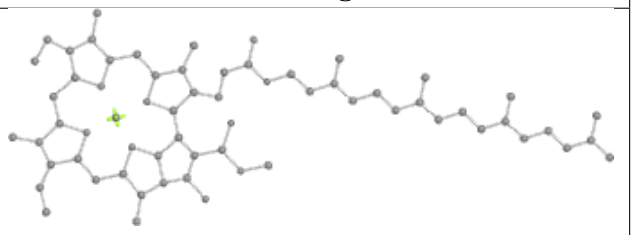
Bond lengths



Bond angles

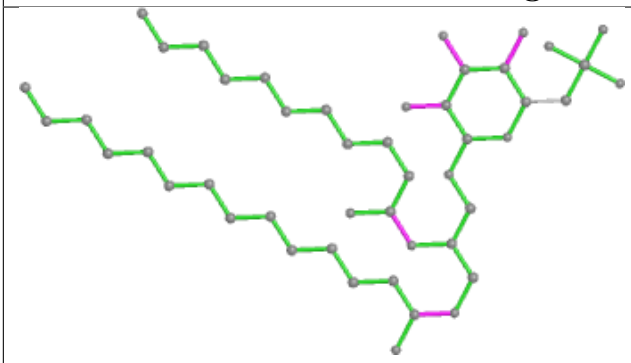


Torsions

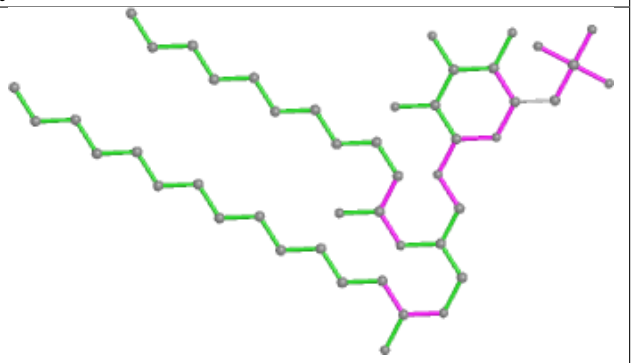


Rings

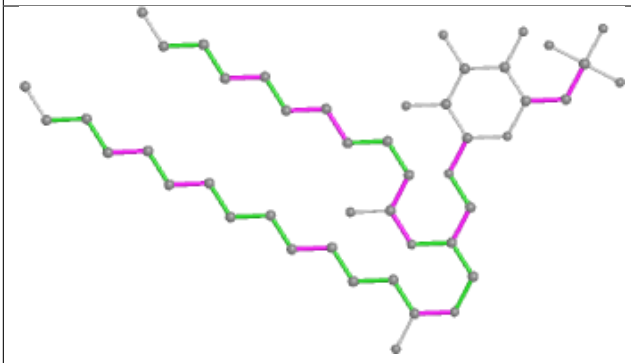
Ligand SQD D 409



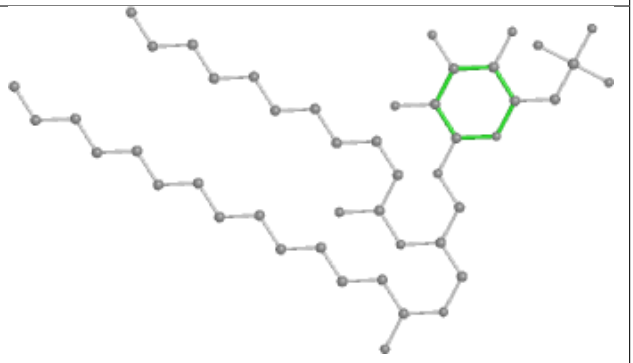
Bond lengths



Bond angles

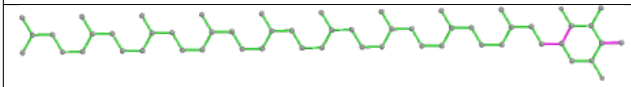


Torsions

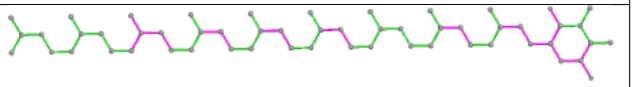


Rings

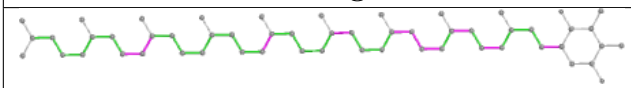
Ligand PL9 A 611



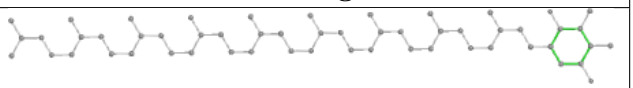
Bond lengths



Bond angles

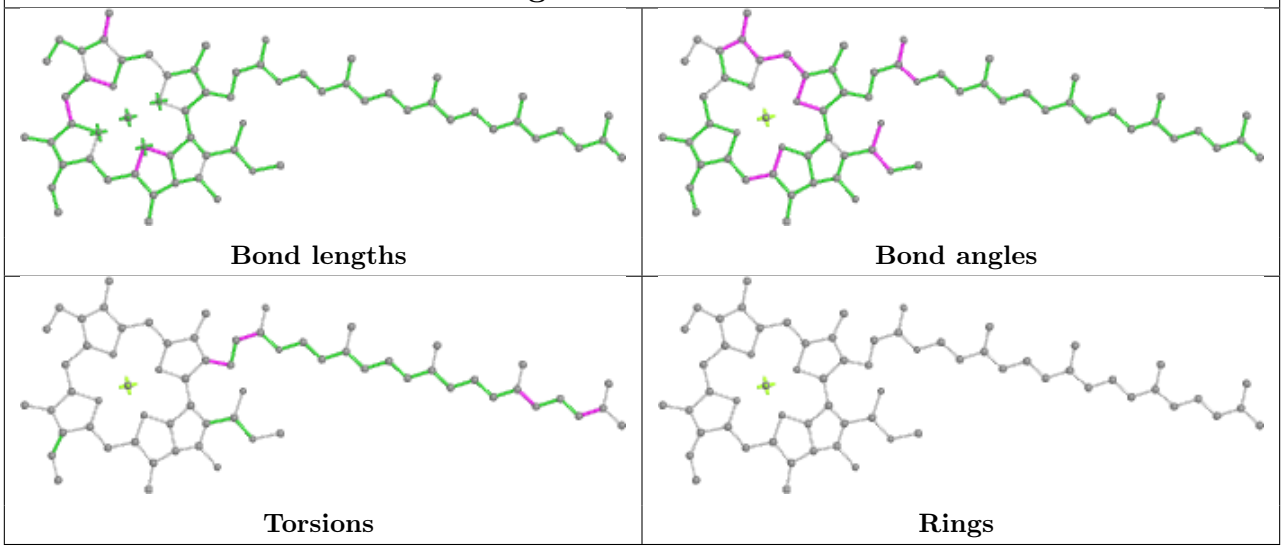


Torsions

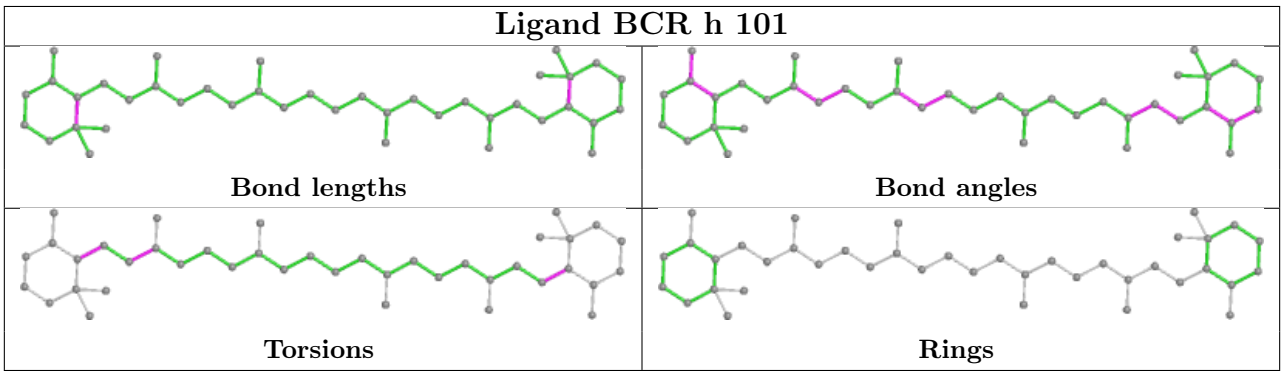


Rings

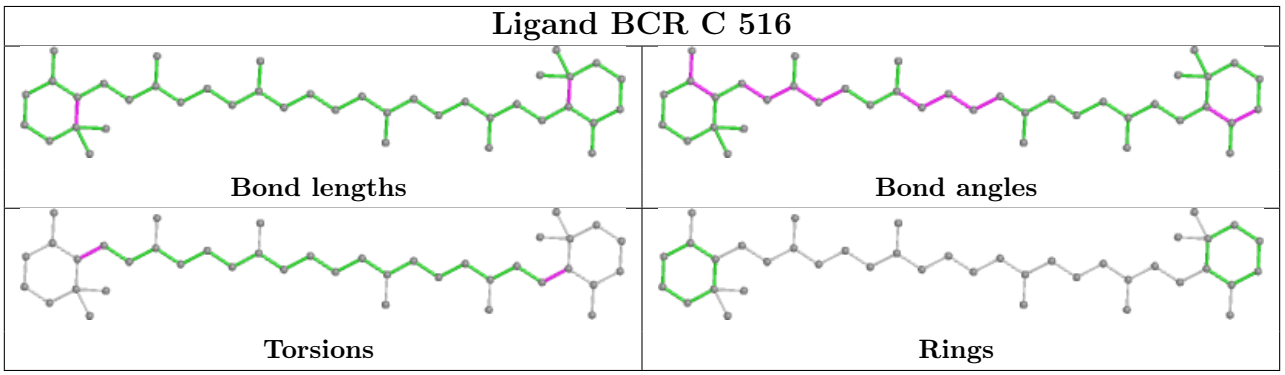
Ligand CLA d 401



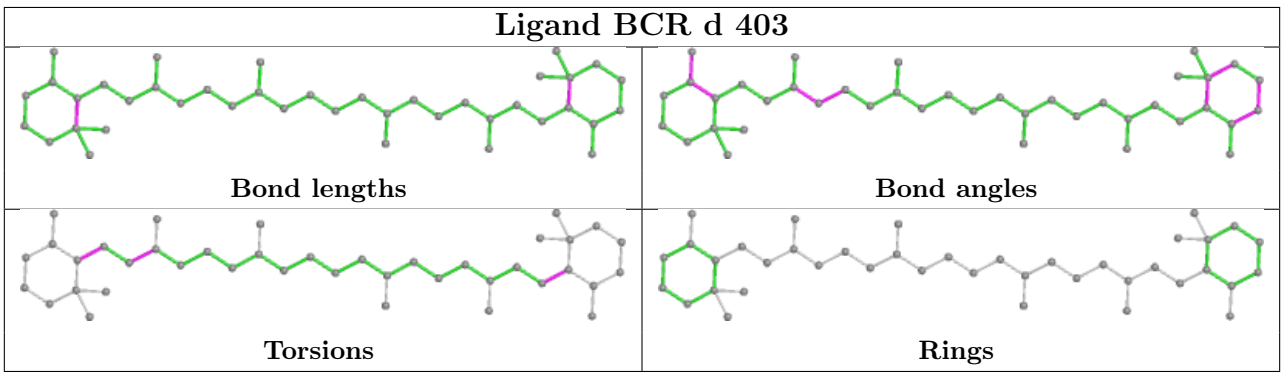
Ligand BCR h 101



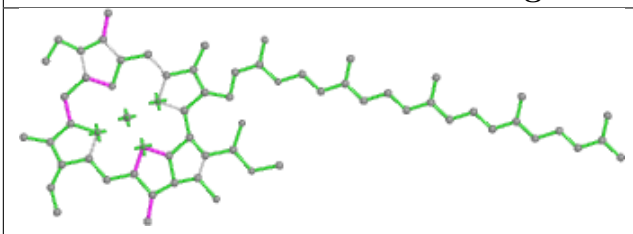
Ligand BCR C 516



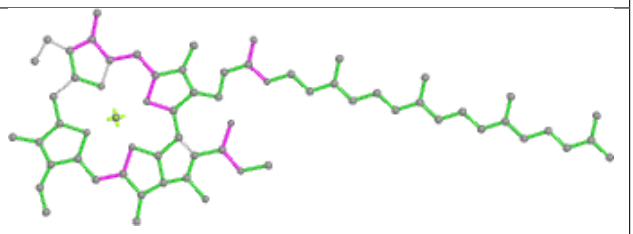
Ligand BCR d 403



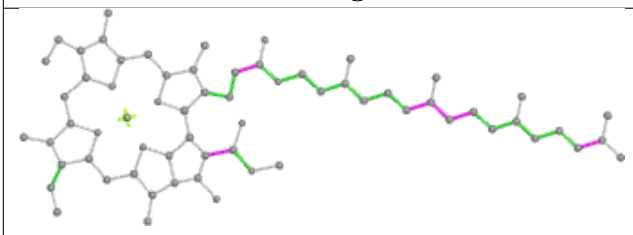
Ligand CLA C 511



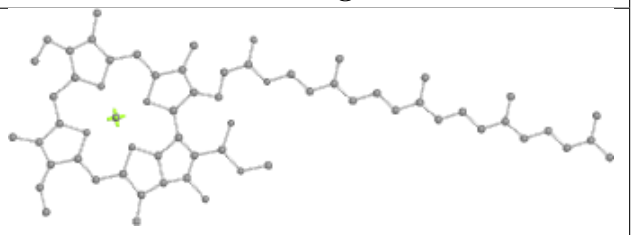
Bond lengths



Bond angles

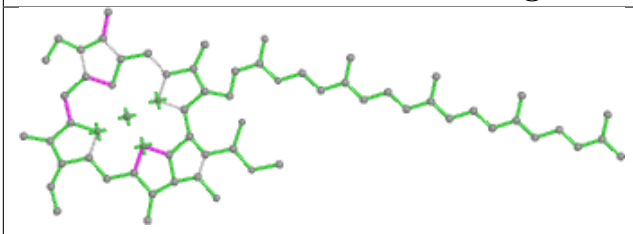


Torsions

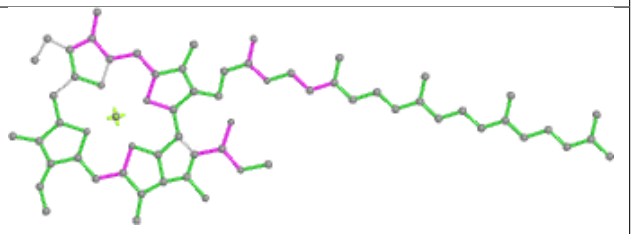


Rings

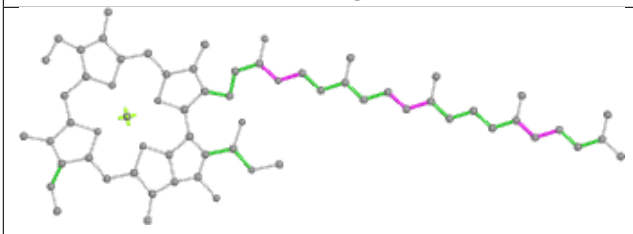
Ligand CLA D 403



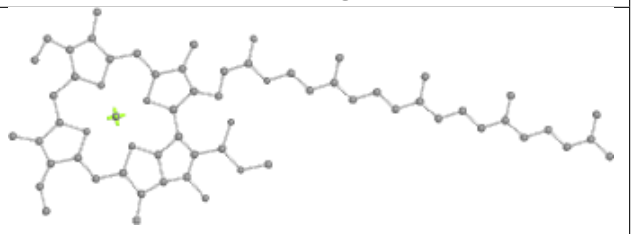
Bond lengths



Bond angles

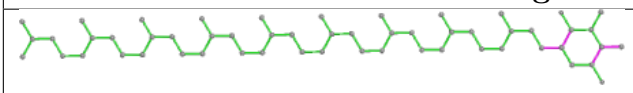


Torsions

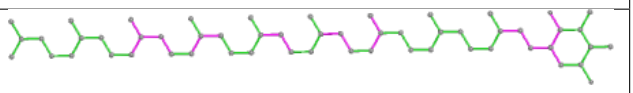


Rings

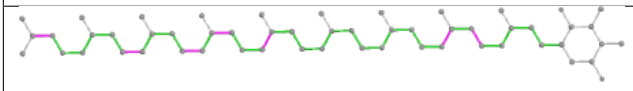
Ligand PL9 d 404



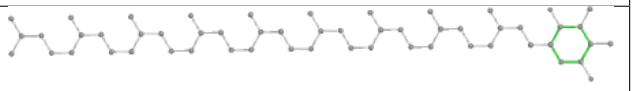
Bond lengths



Bond angles

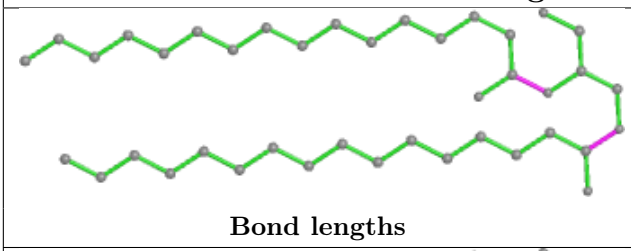


Torsions

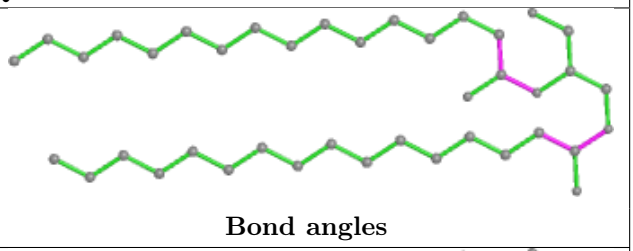


Rings

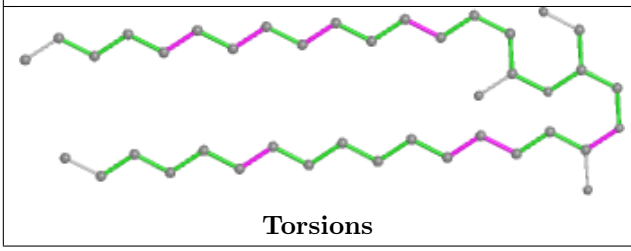
Ligand SQD b 621



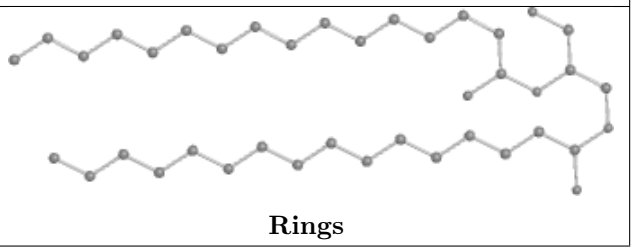
Bond lengths



Bond angles

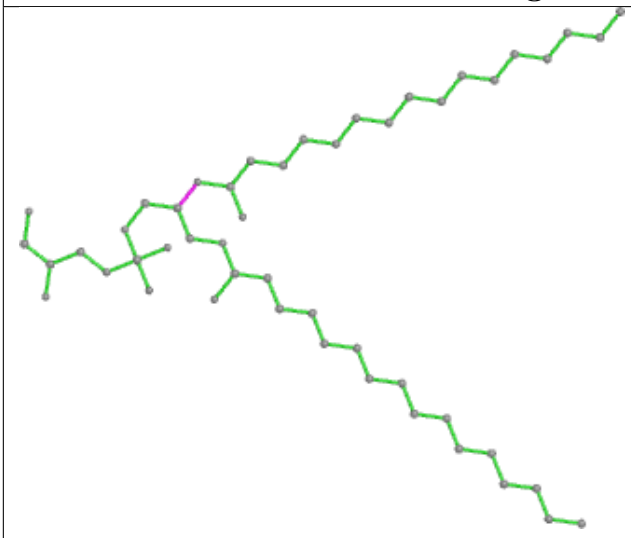


Torsions

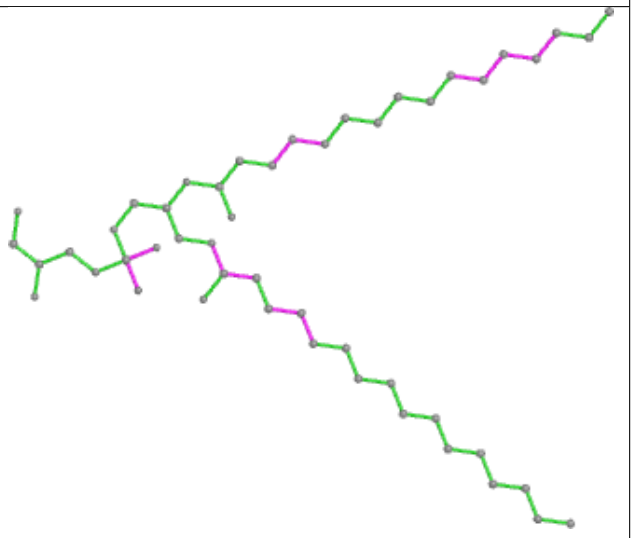


Rings

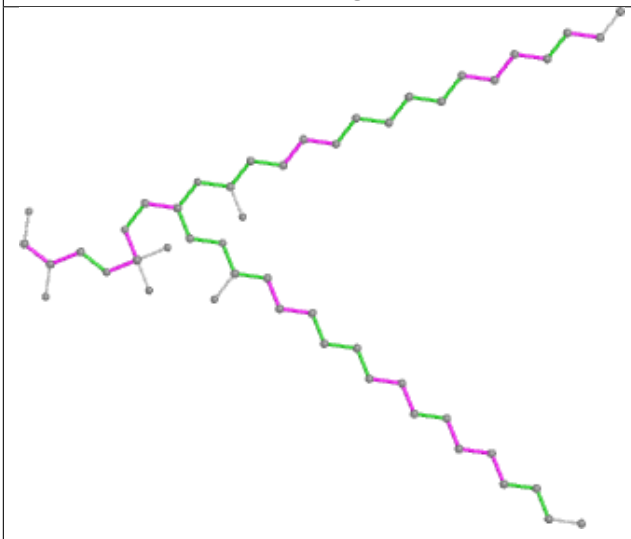
Ligand LHG d 406



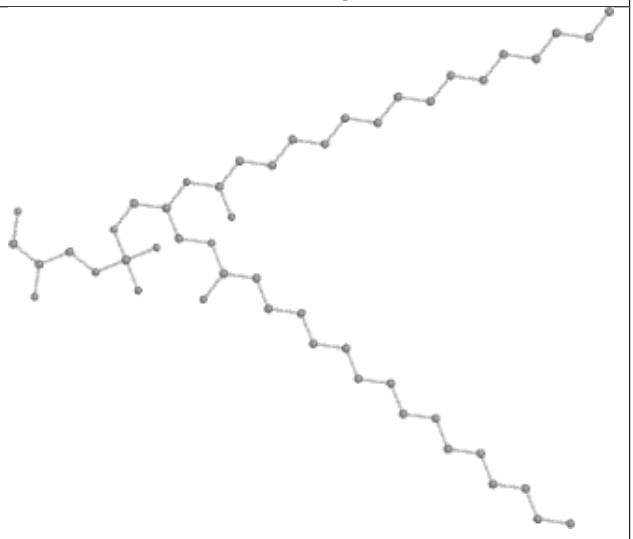
Bond lengths



Bond angles

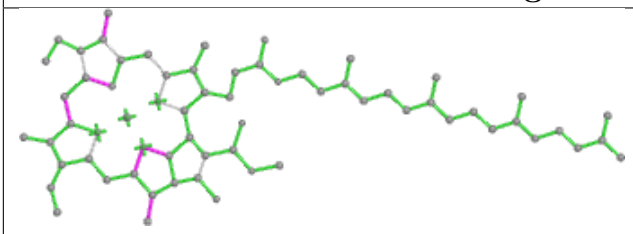


Torsions

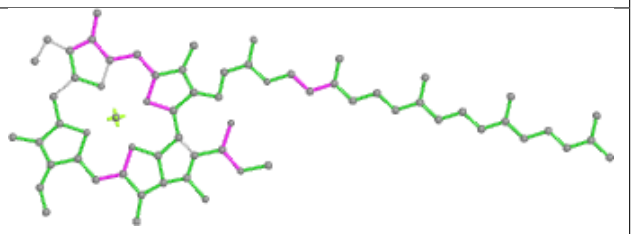


Rings

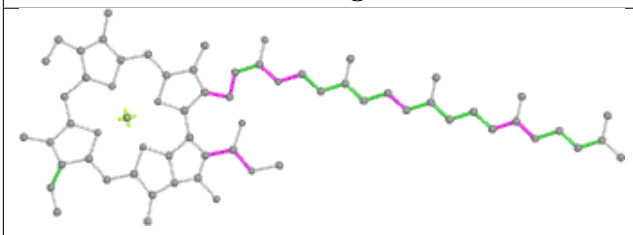
Ligand CLA C 513



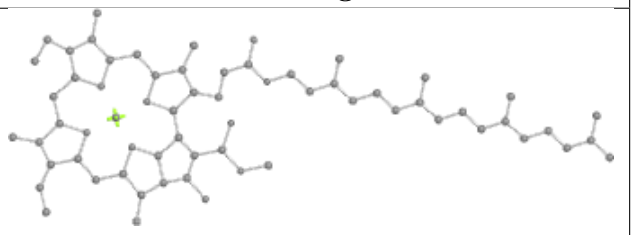
Bond lengths



Bond angles

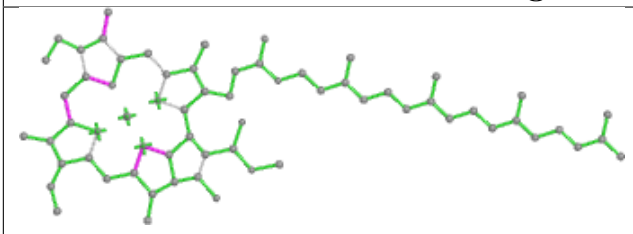


Torsions

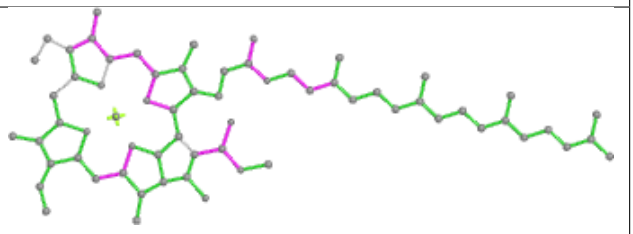


Rings

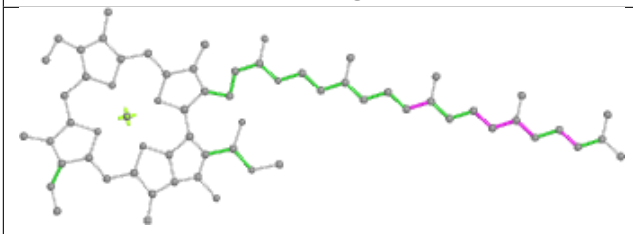
Ligand CLA b 611



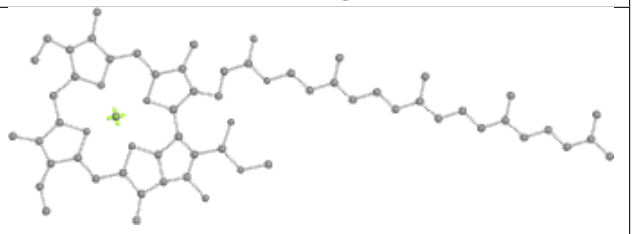
Bond lengths



Bond angles

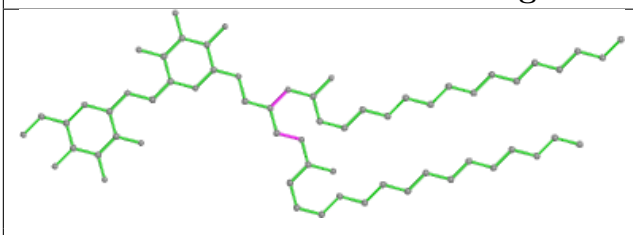


Torsions



Rings

Ligand DGD H 102



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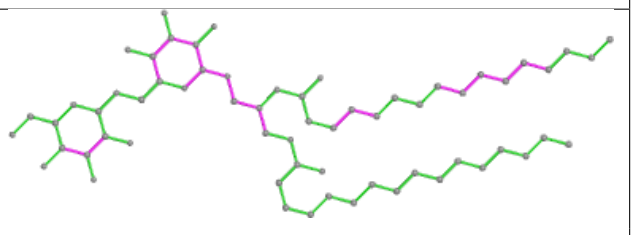
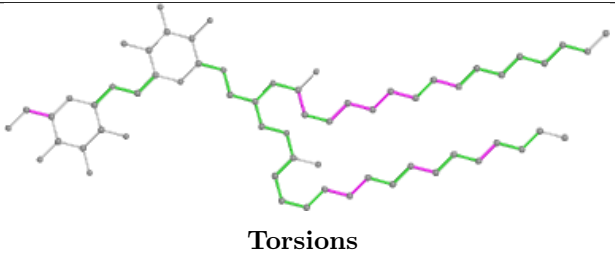
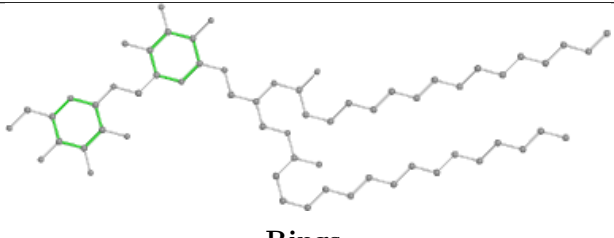


Bond angles

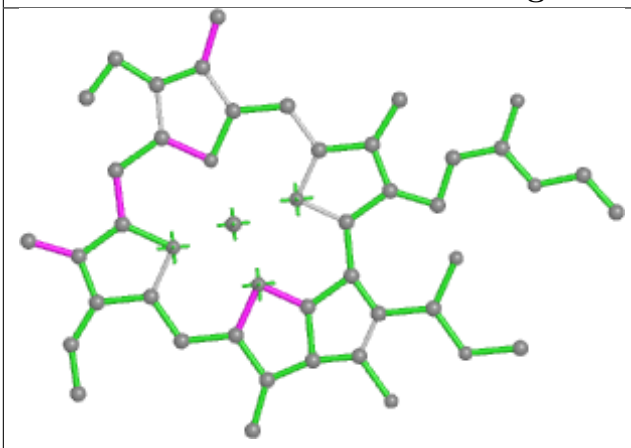


Torsions



Rings

Ligand CLA b 616



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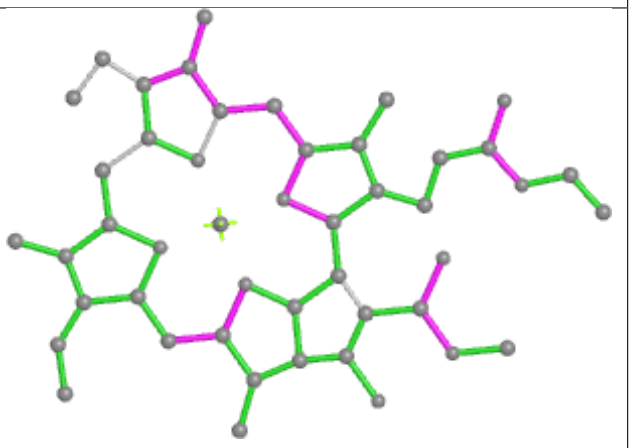
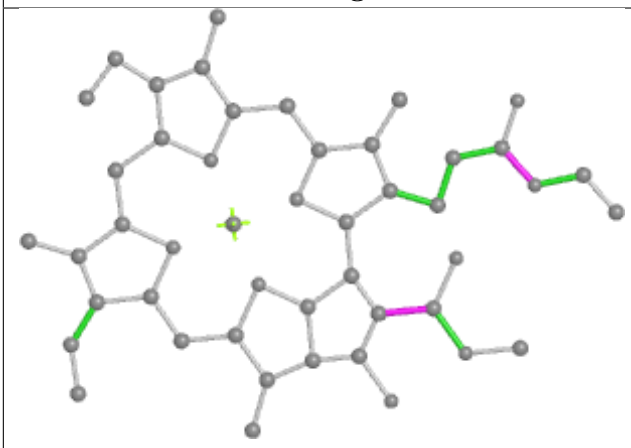
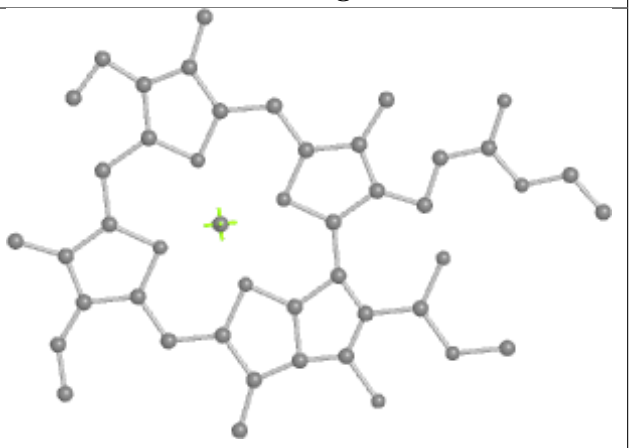


Bond angles

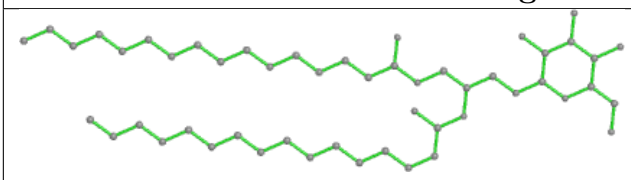


Torsions

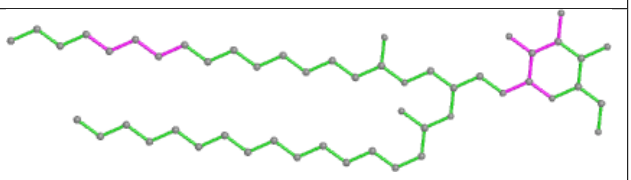


Rings

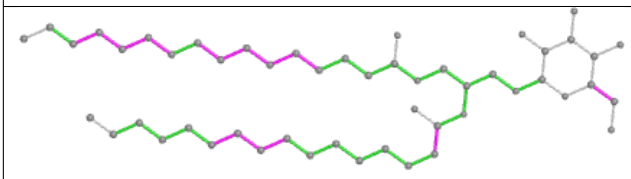
Ligand LMG D 407



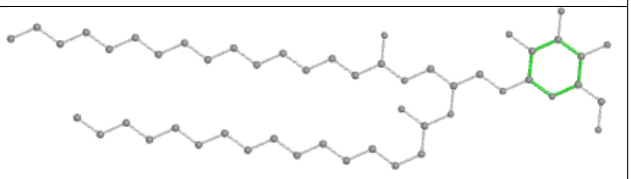
Bond lengths



Bond angles

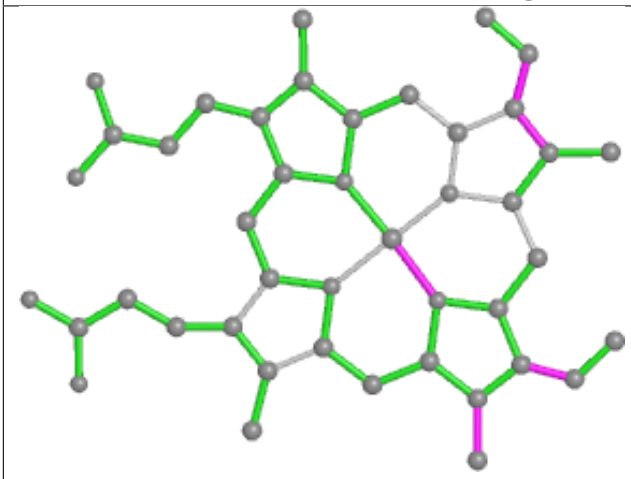


Torsions



Rings

Ligand HEM E 101



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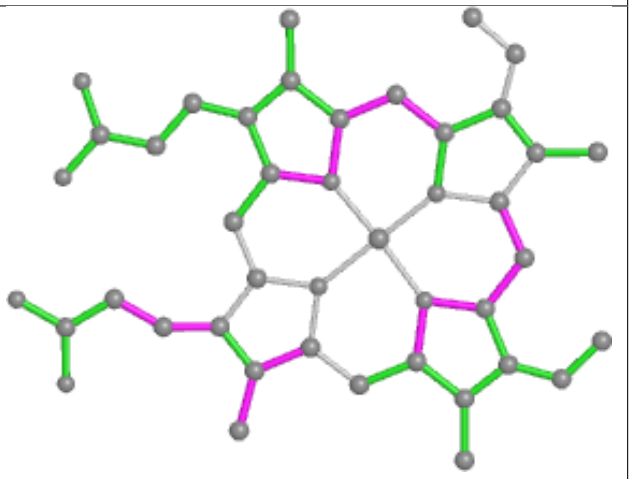
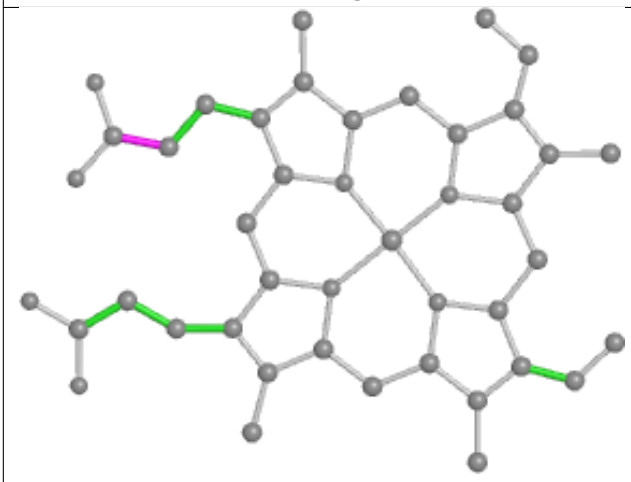


Bond angles



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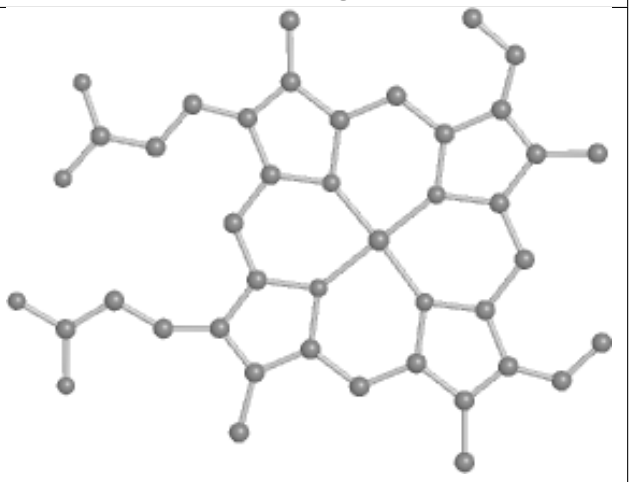
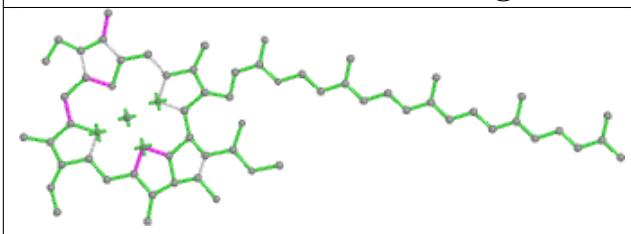


Rings

Ligand CLA b 606 (B)



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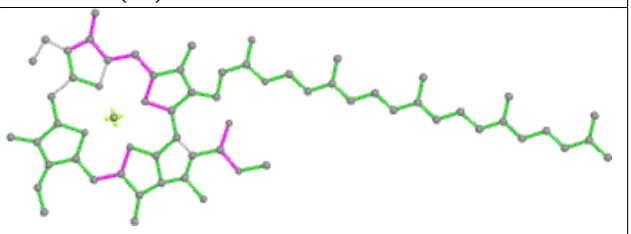
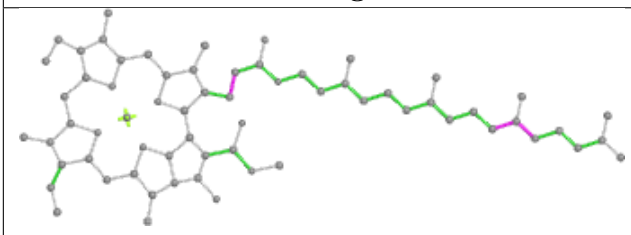


Bond angles



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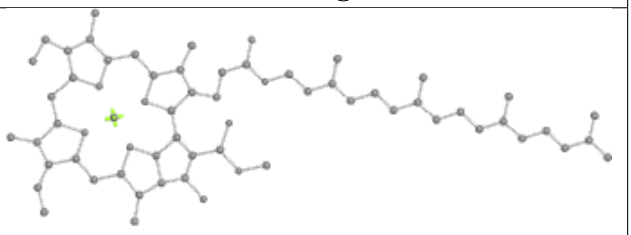
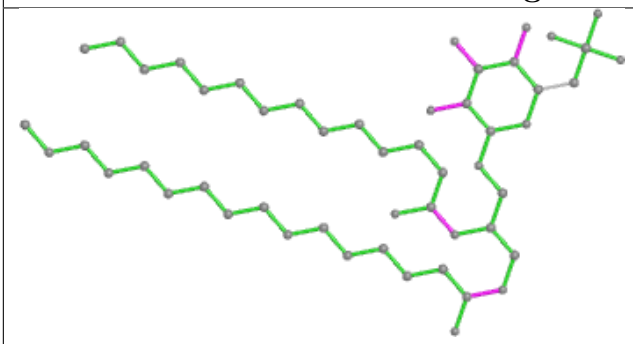
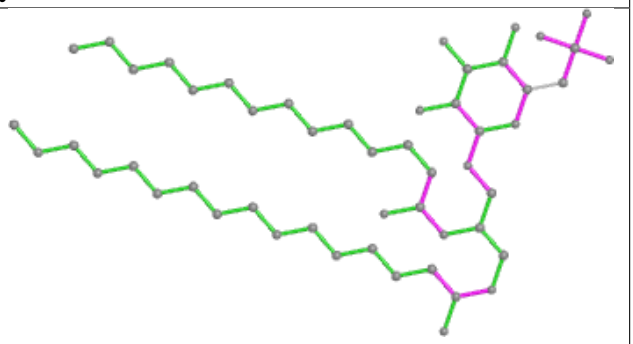


Rings

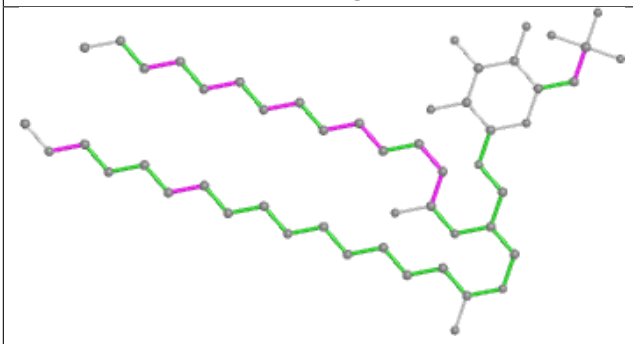
Ligand SQD A 612



Bond lengths



Bond angles



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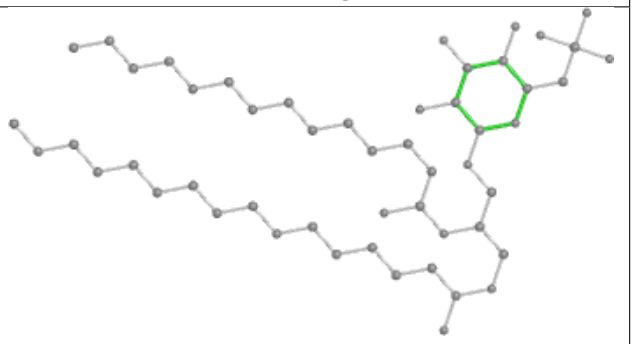
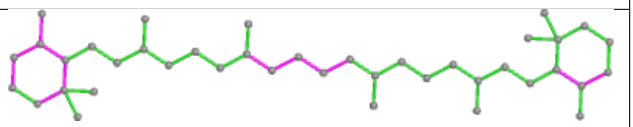


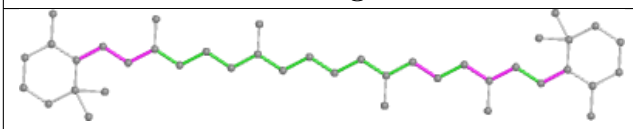
Rings

Ligand BCR T 101

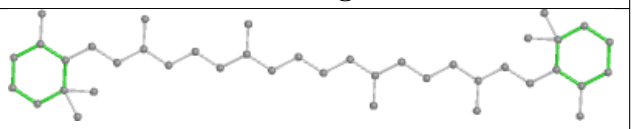
Bond lengths



Bond angles

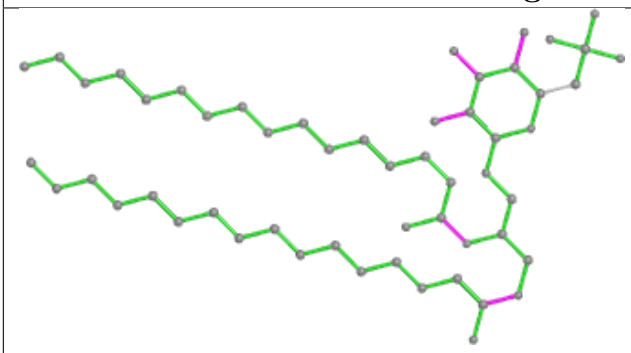


Torsions



Rings

Ligand SQD A 616



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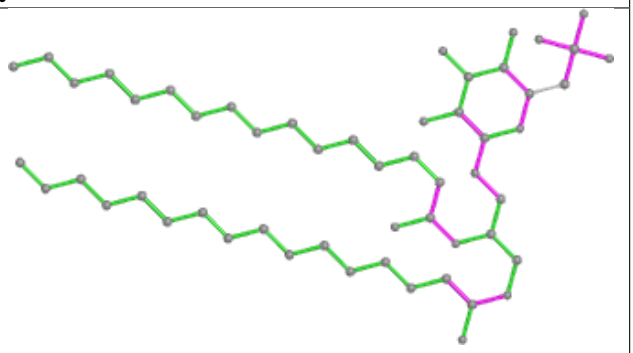
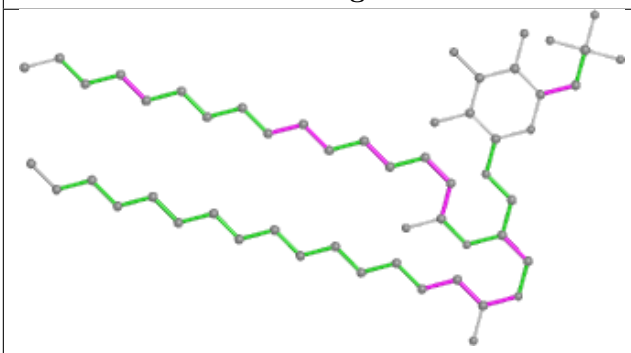
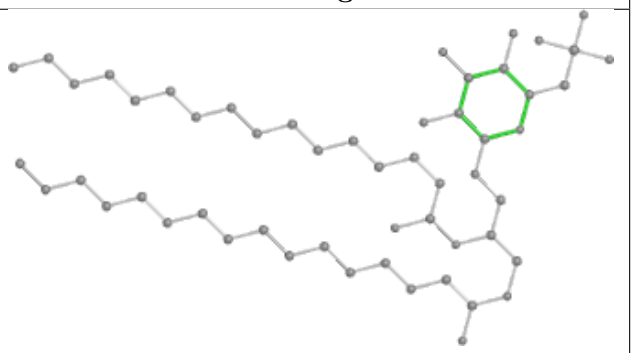


Bond angles

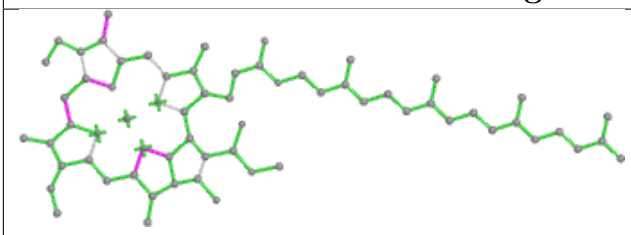


Torsions

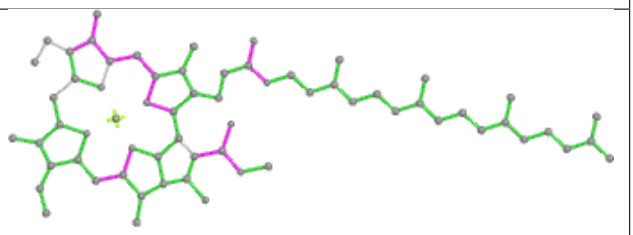


Rings

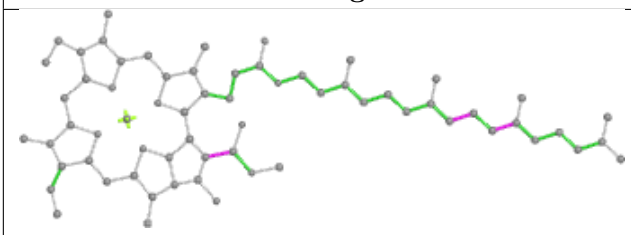
Ligand CLA B 602



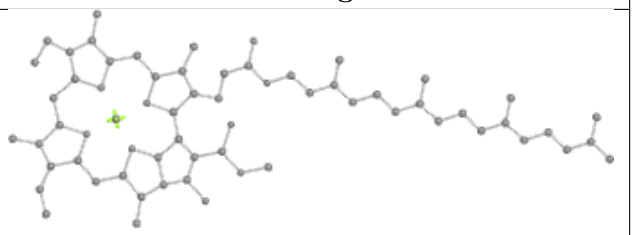
Bond lengths



Bond angles

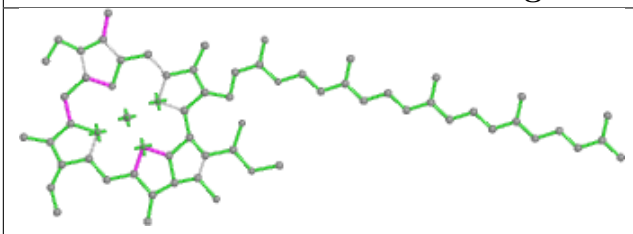


Torsions



Rings

Ligand CLA C 504



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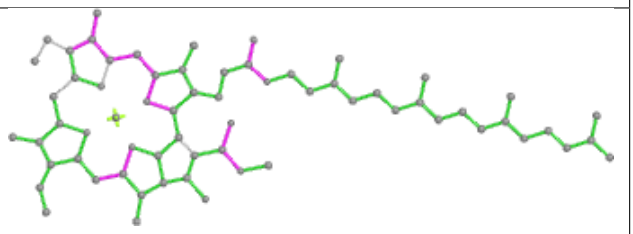
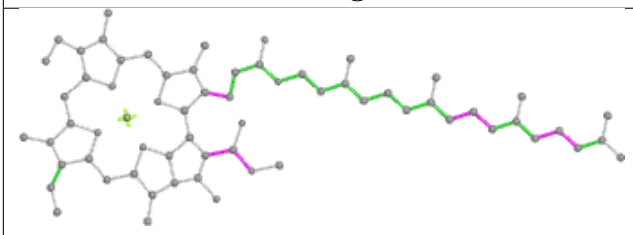
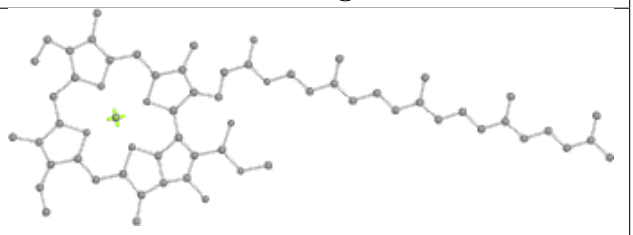


Bond angles

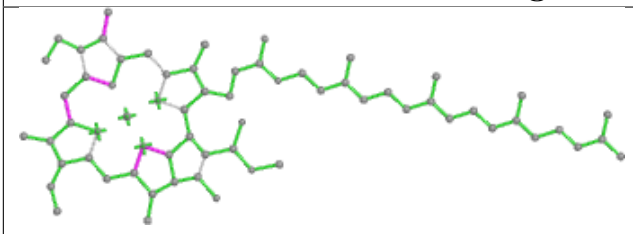


Torsions



Rings

Ligand CLA a 610



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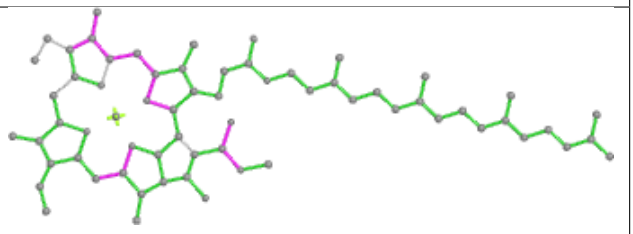
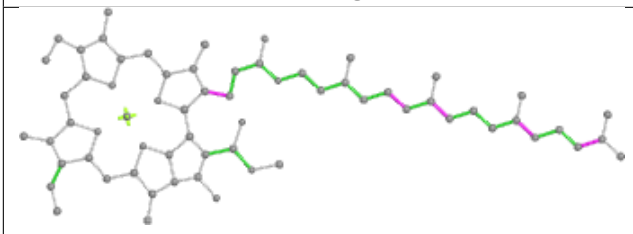
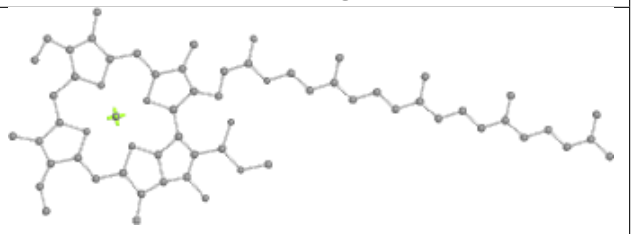


Bond angles

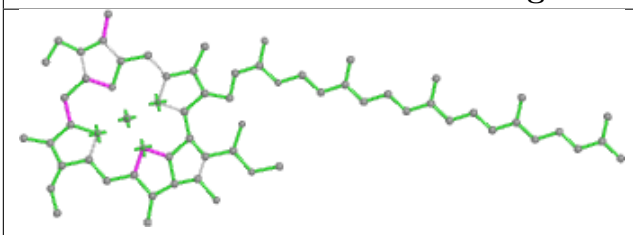


Torsions

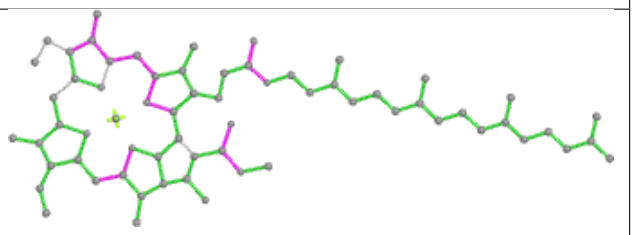


Rings

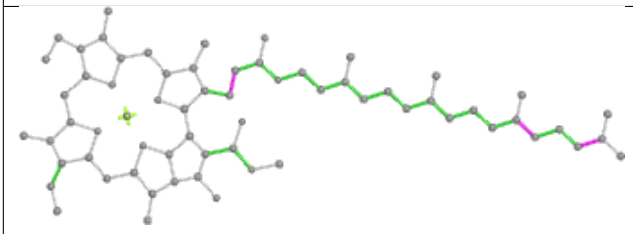
Ligand CLA b 608



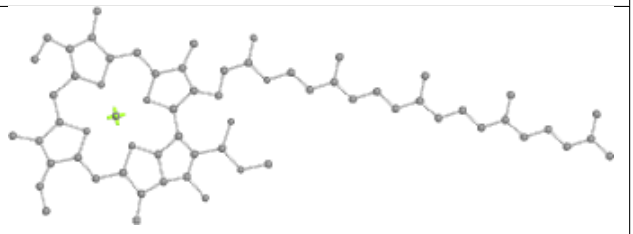
Bond lengths



Bond angles

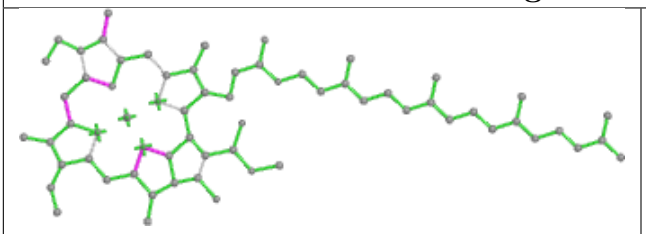


Torsions

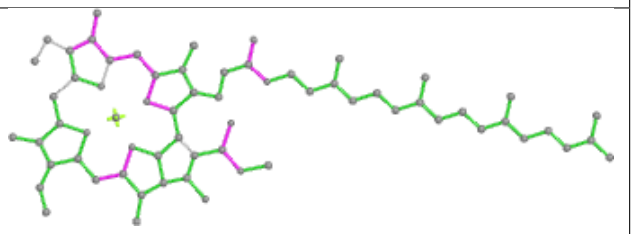


Rings

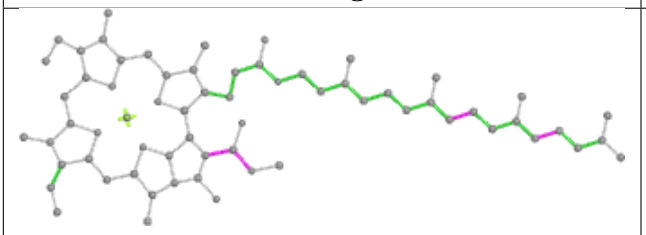
Ligand CLA C 505



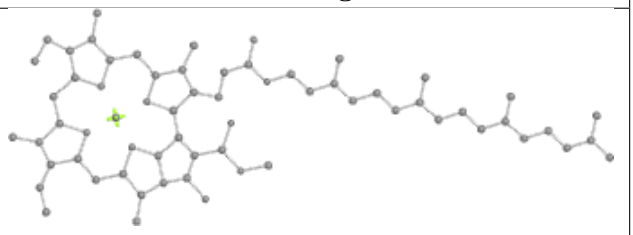
Bond lengths



Bond angles

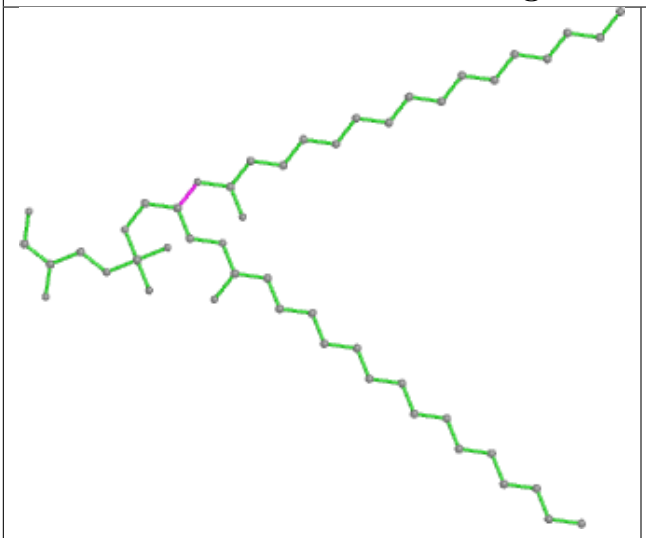


Torsions

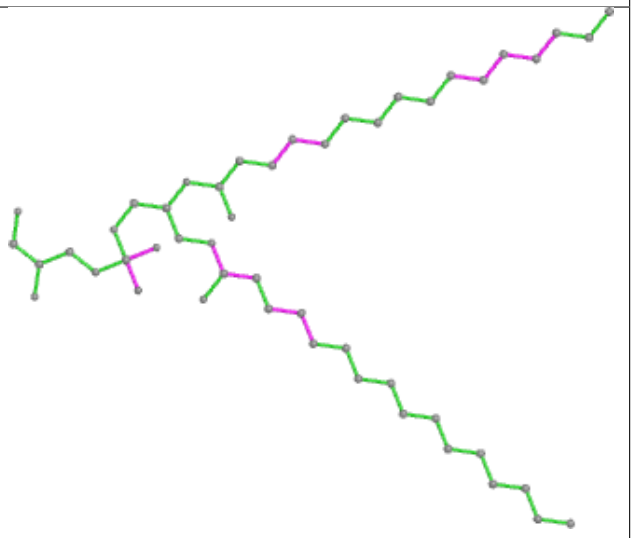


Rings

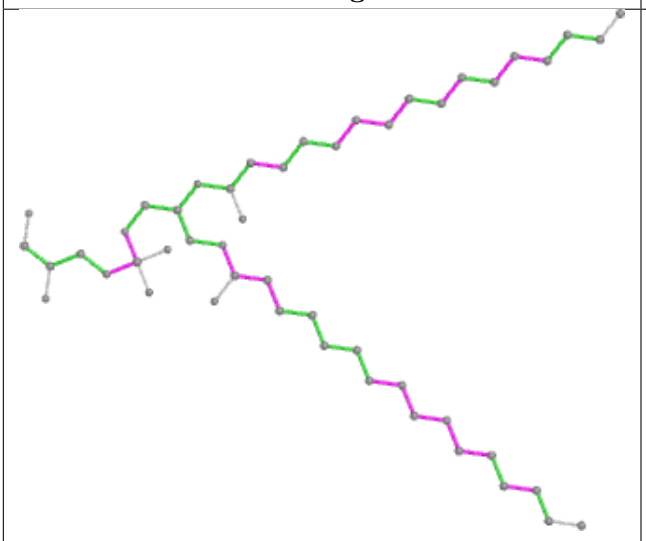
Ligand LHG B 623



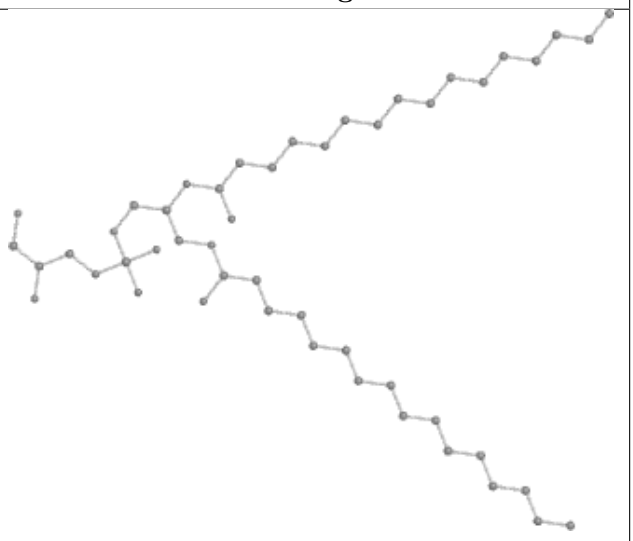
Bond lengths



Bond angles

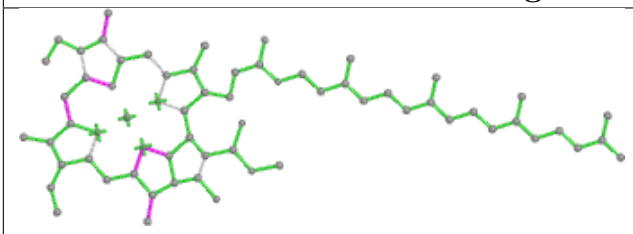


Torsions

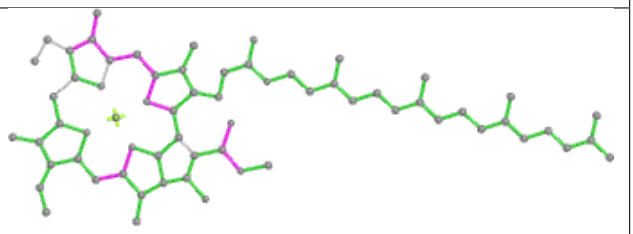


Rings

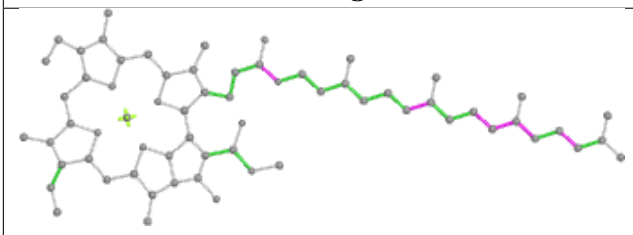
Ligand CLA C 506



Bond lengths



Bond angles



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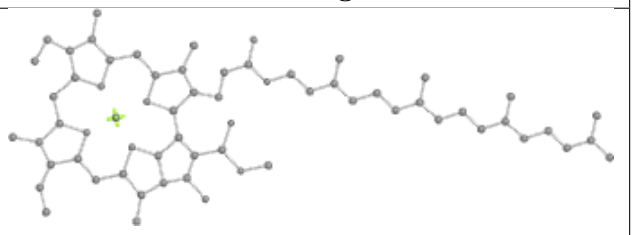
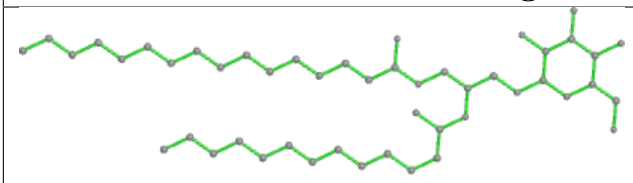


Rings

Ligand LMG C 520



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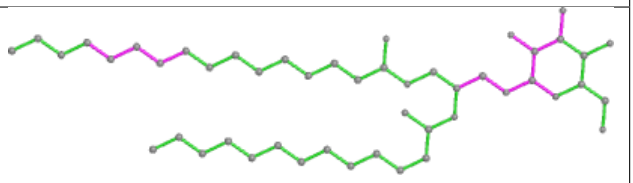

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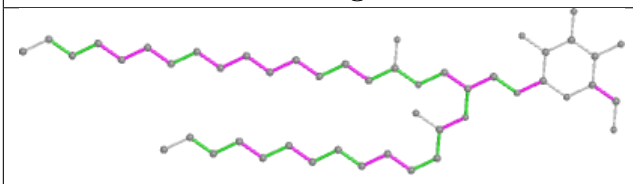

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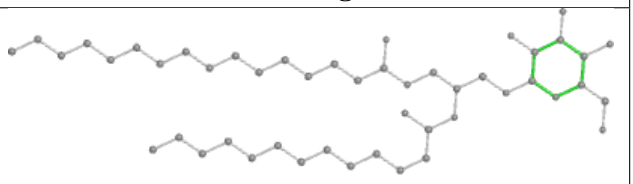
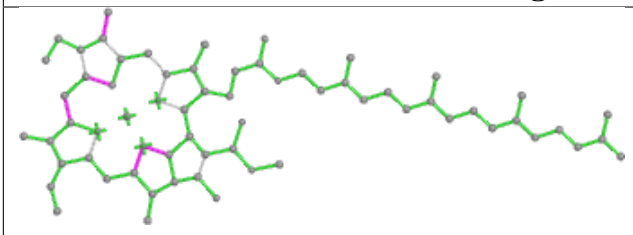


Rings

Ligand CLA c 507



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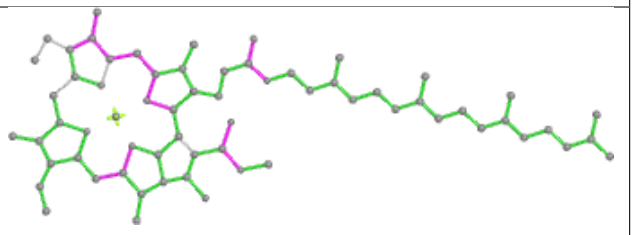
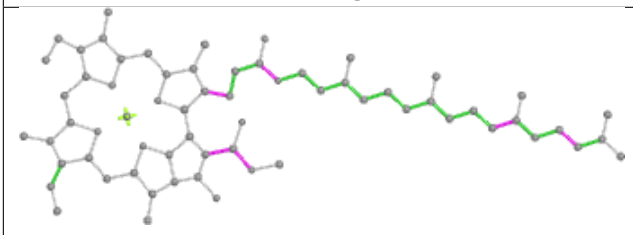


Bond angles



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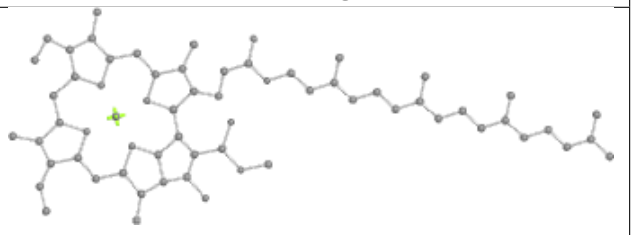
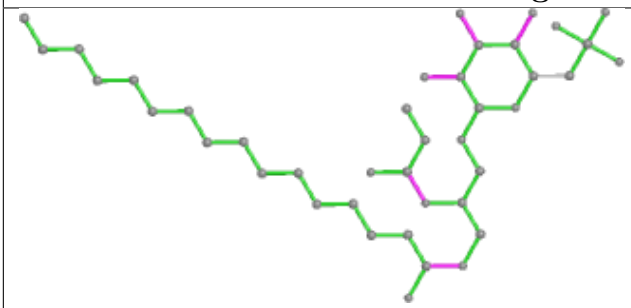


Rings

Ligand SQD f 101



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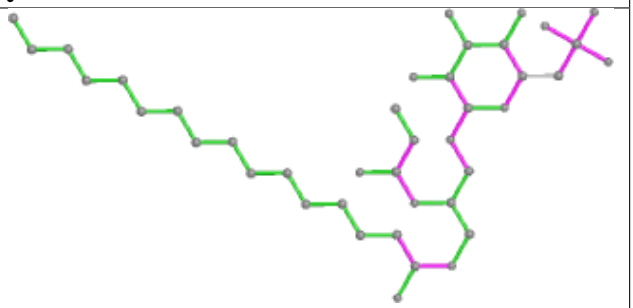
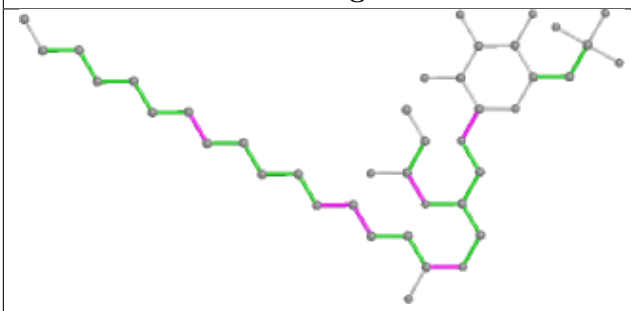


Bond angles



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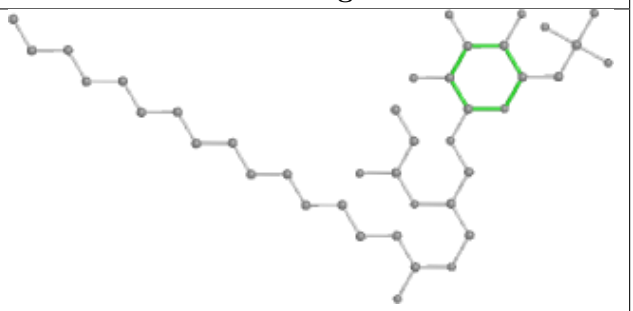
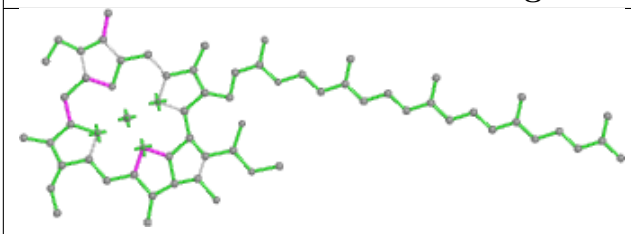


Rings

Ligand CLA C 508



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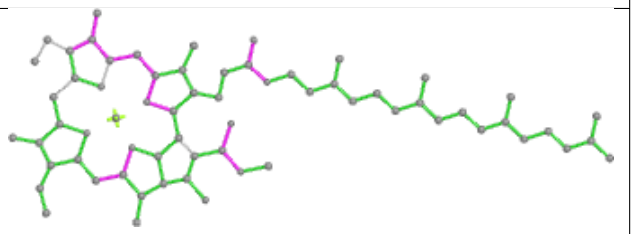
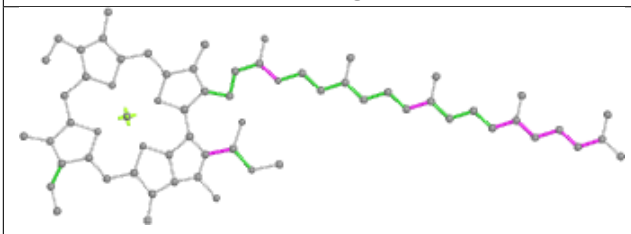


Bond angles



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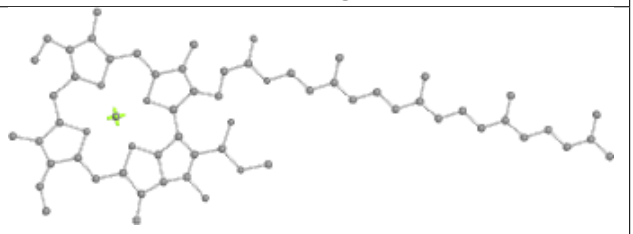
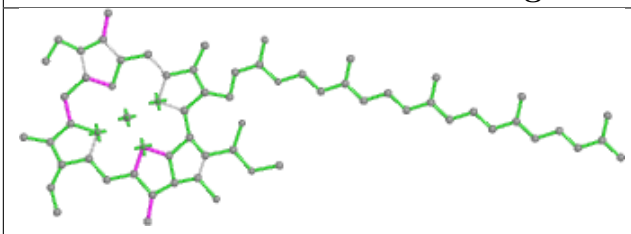


Rings

Ligand CLA B 612



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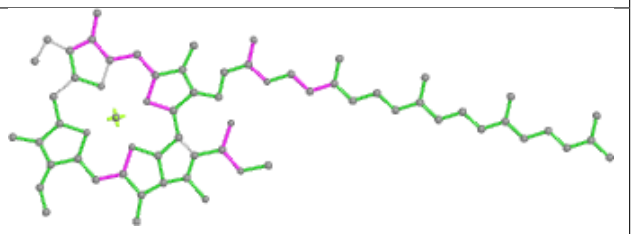
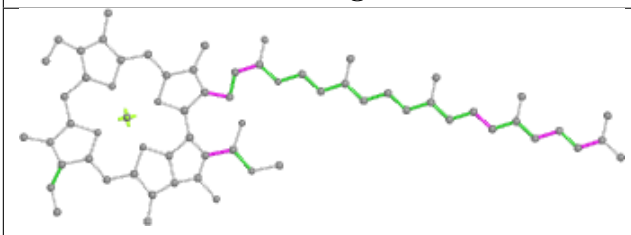


Bond angles



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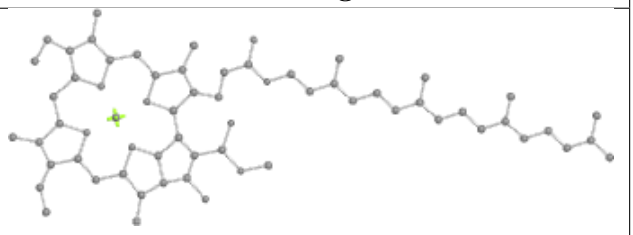
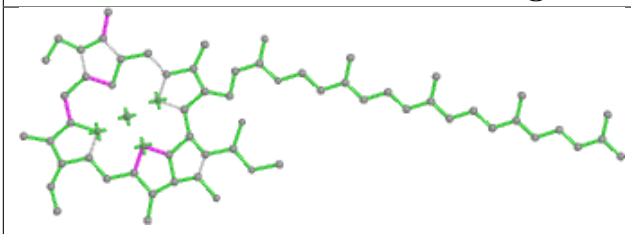


Rings

Ligand CLA b 613



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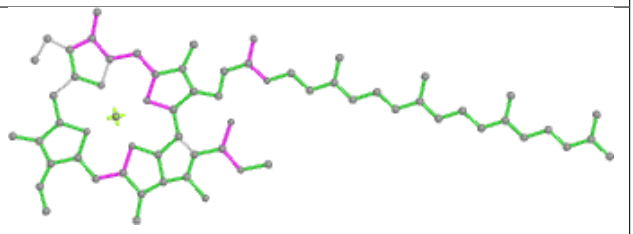
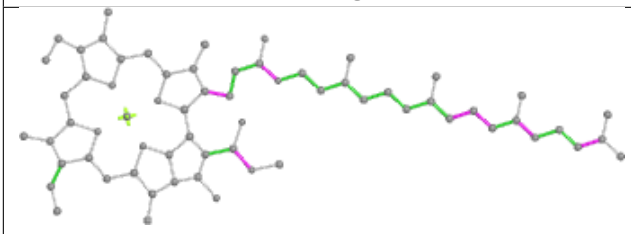


Bond angles



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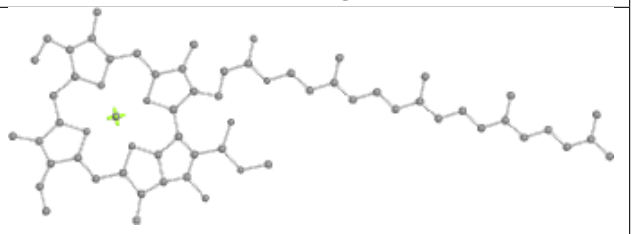
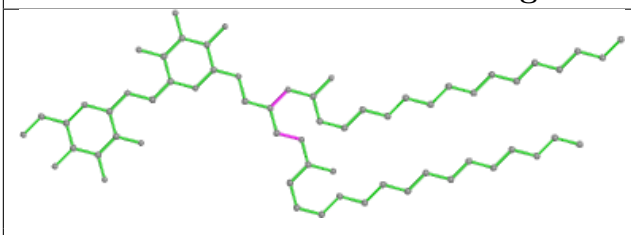
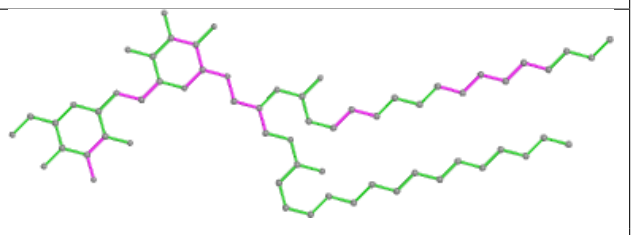


Rings

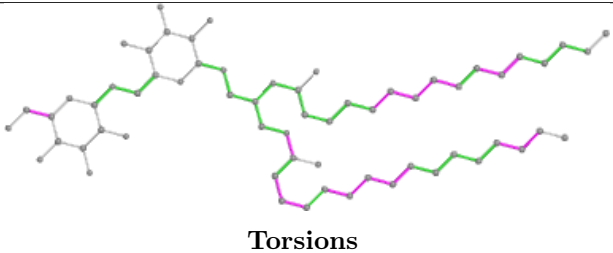
Ligand DGD C 519



Bond lengths



Bond angles



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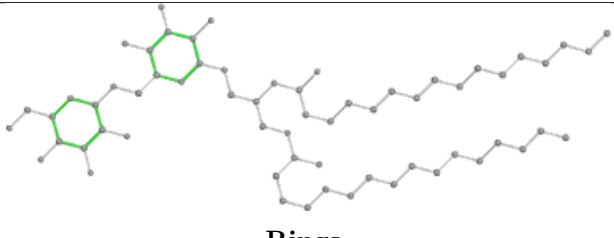
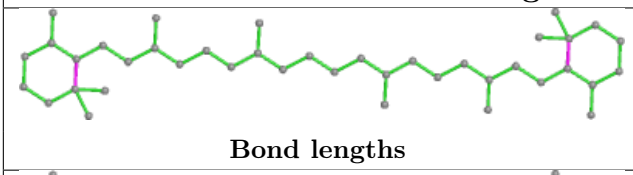


Rings

Ligand BCR C 515



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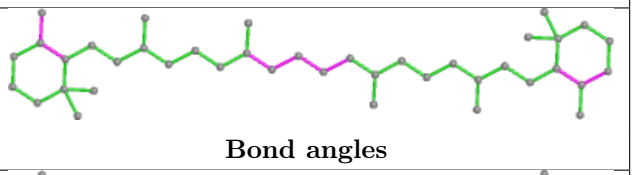
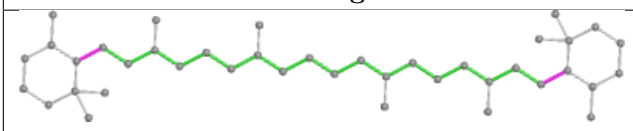


Bond angles



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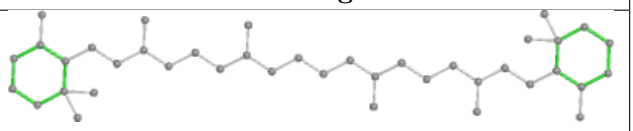
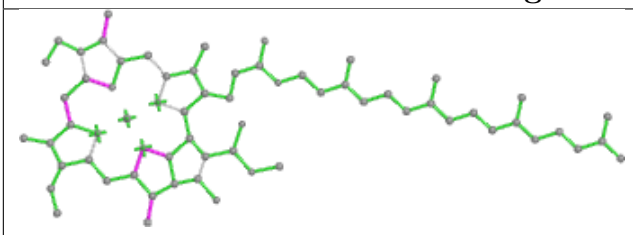
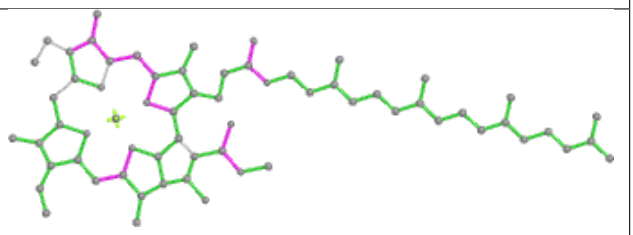


Rings

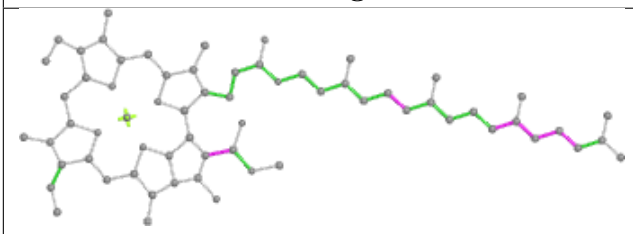
Ligand CLA B 605



Bond lengths



Bond angles



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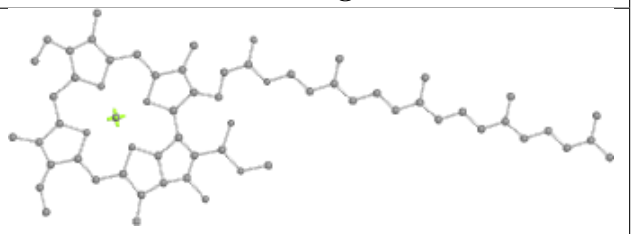
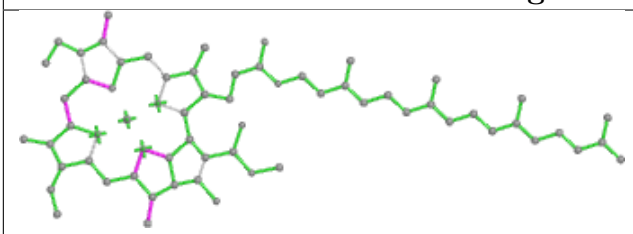


Rings

Ligand CLA b 612



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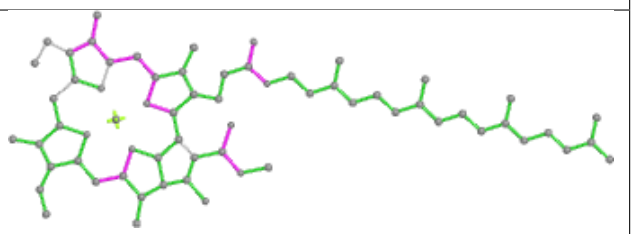
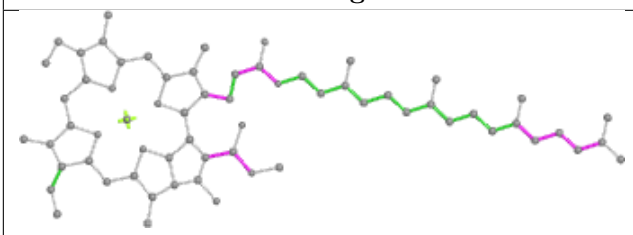


Bond angles



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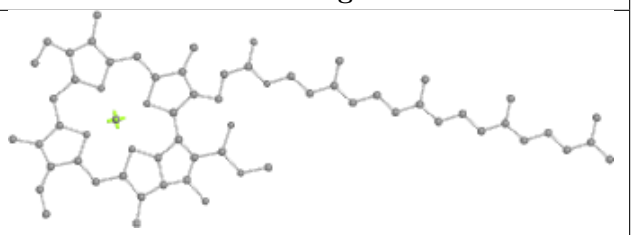
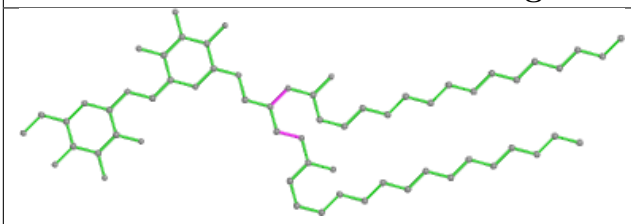


Rings

Ligand DGD c 517



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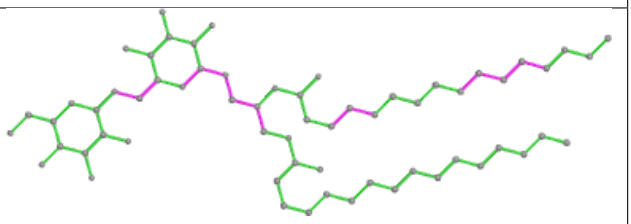
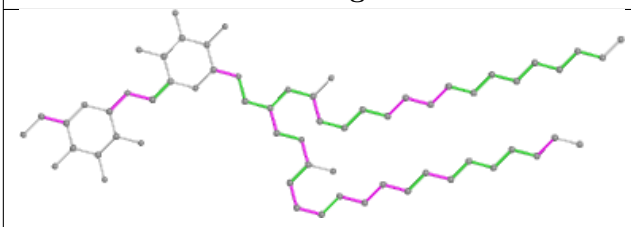


Bond angles



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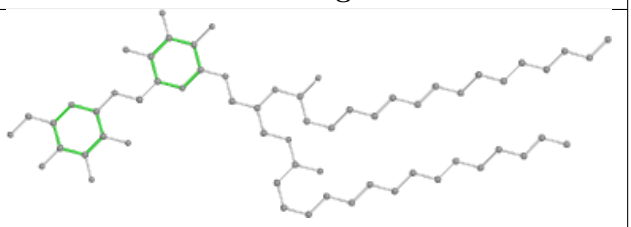
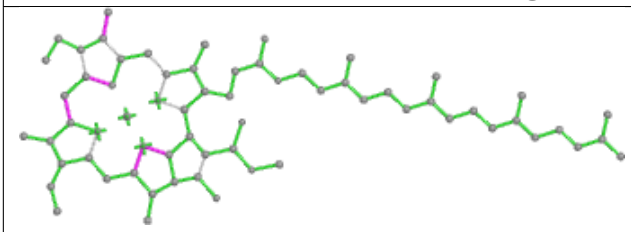
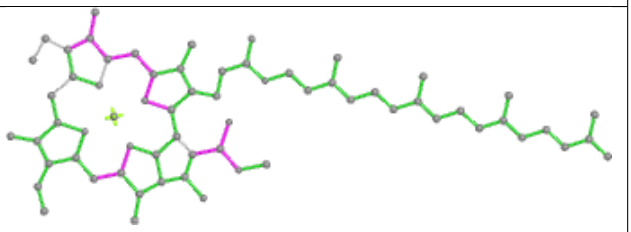


Rings

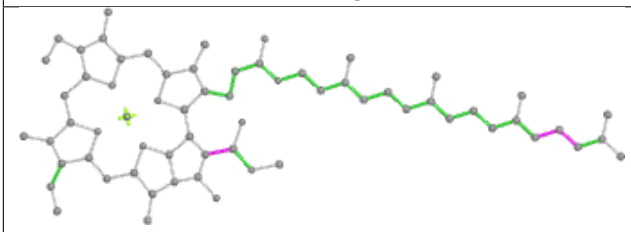
Ligand CLA A 613



Bond lengths



Bond angles



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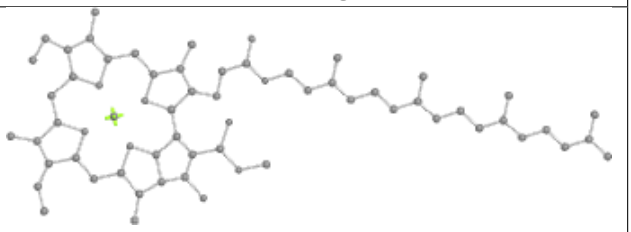
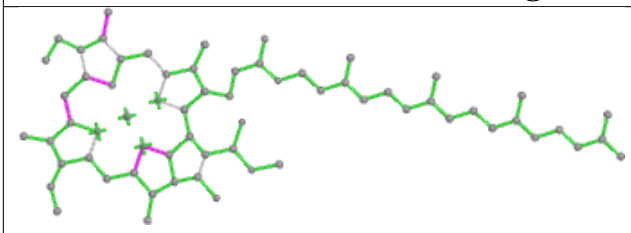


Rings

Ligand CLA B 613



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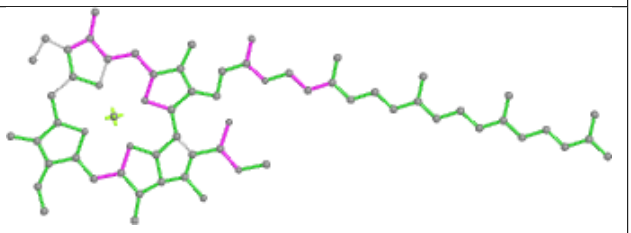
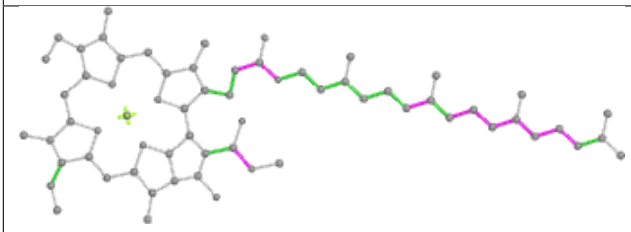


Bond angles



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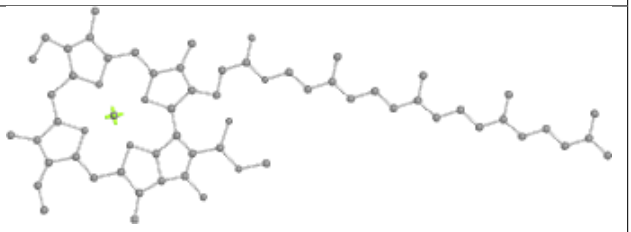
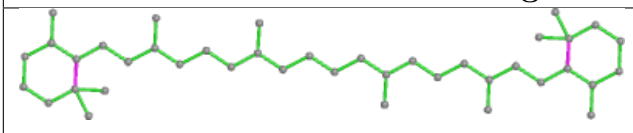
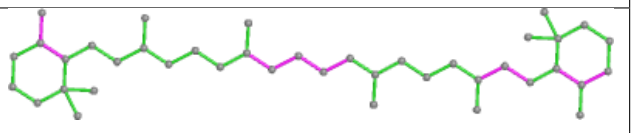


Rings

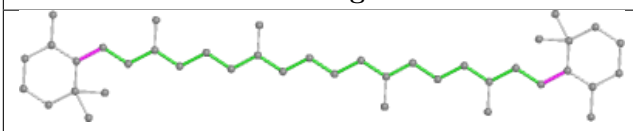
Ligand BCR K 101



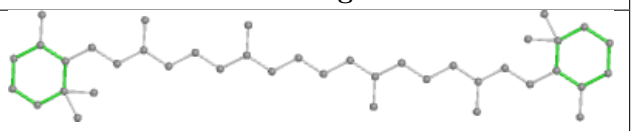
Bond lengths



Bond angles

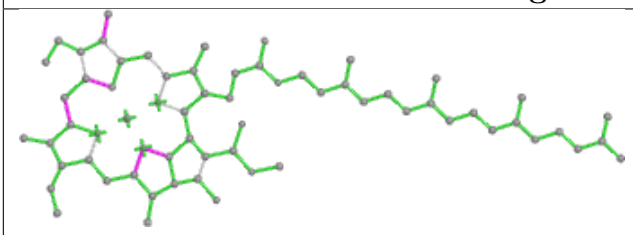


Torsions

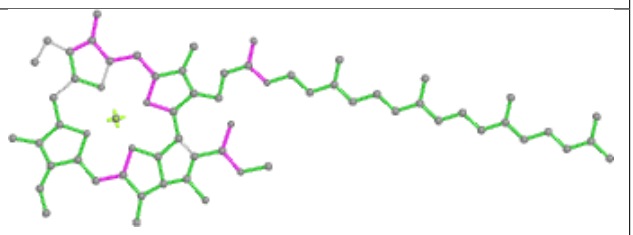


Rings

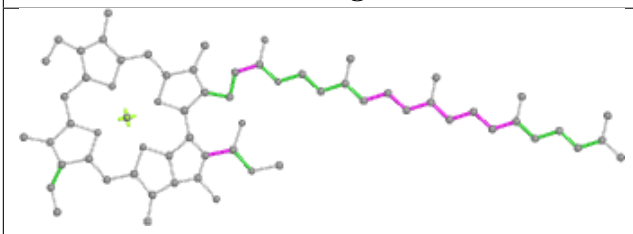
Ligand CLA c 509



Bond lengths



Bond angles



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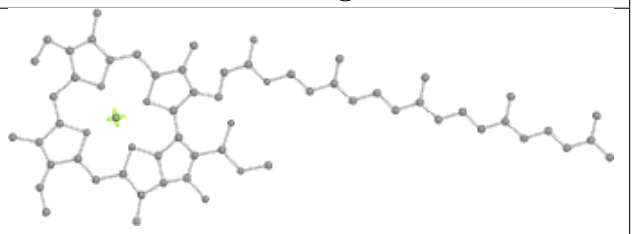
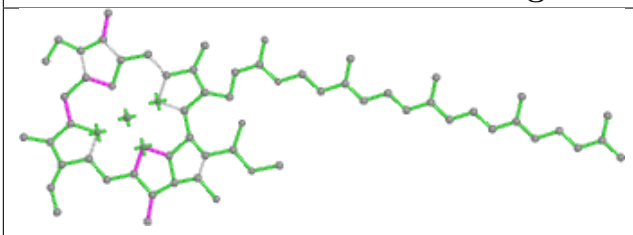
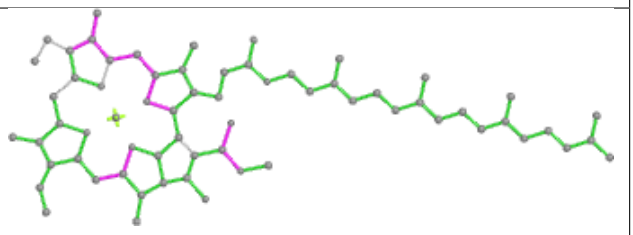


Rings

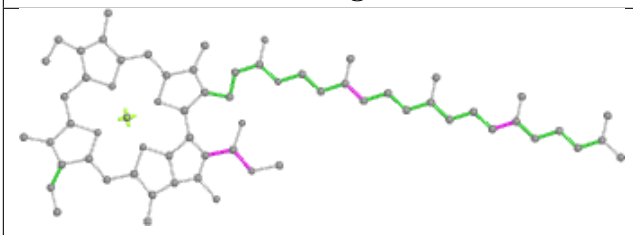
Ligand CLA b 605



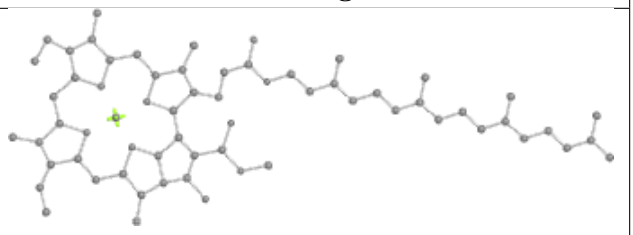
Bond lengths



Bond angles

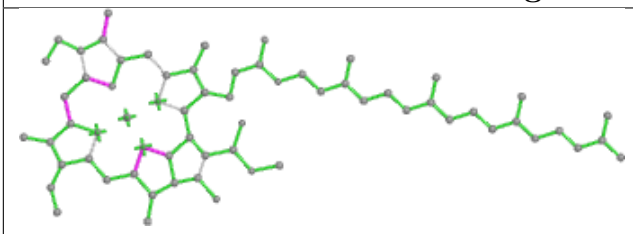


Torsions

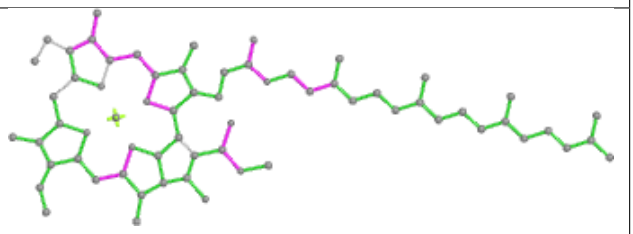


Rings

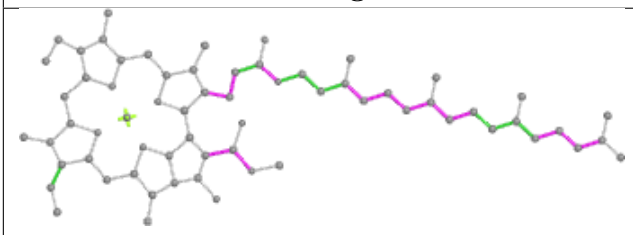
Ligand CLA B 614



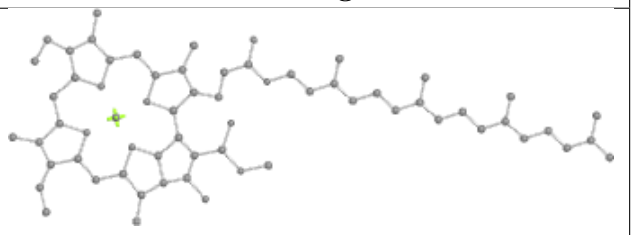
Bond lengths



Bond angles

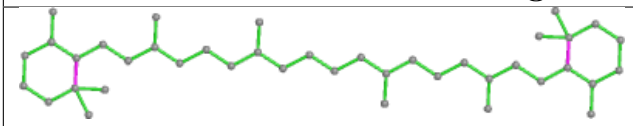


Torsions

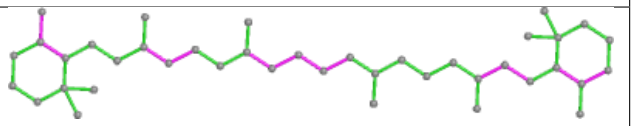


Rings

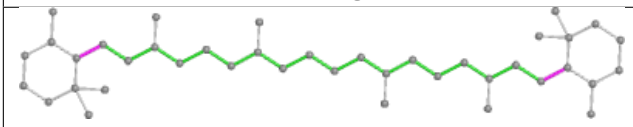
Ligand BCR c 514



Bond lengths



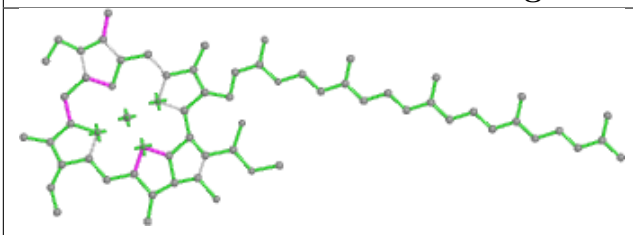
Bond angles



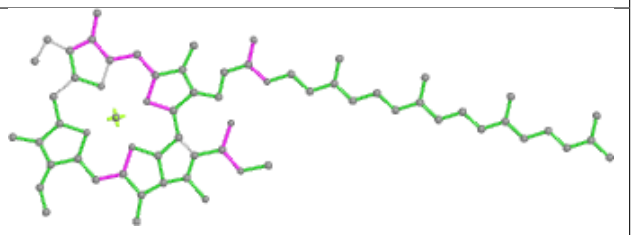
Torsions

Rings

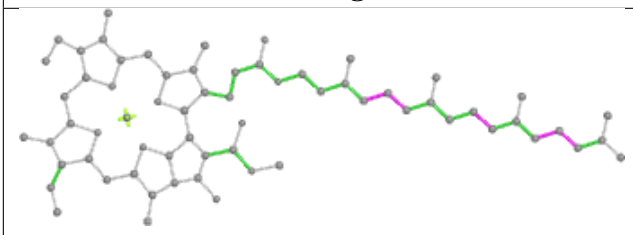
Ligand CLA B 615



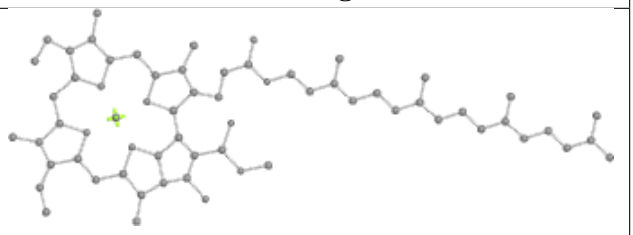
Bond lengths



Bond angles

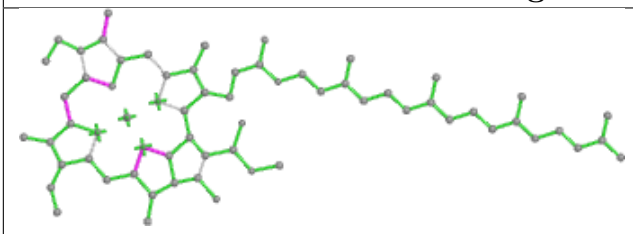


Torsions

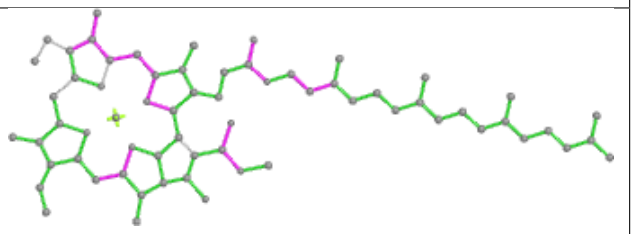


Rings

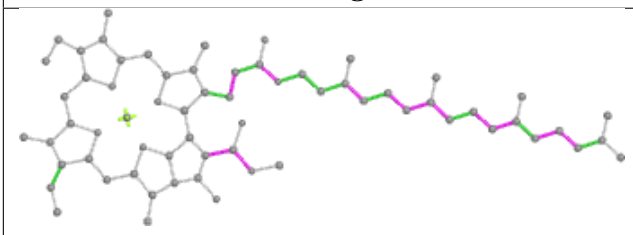
Ligand CLA b 614



Bond lengths



Bond angles



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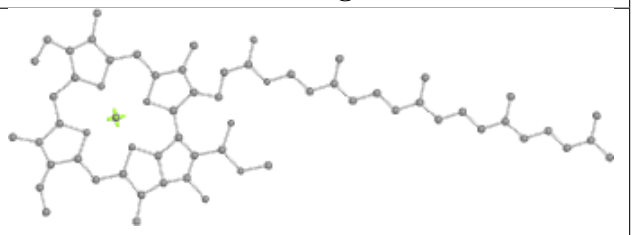
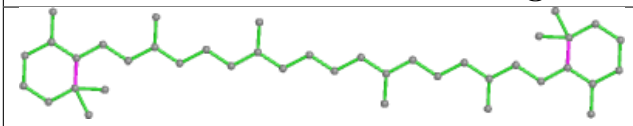
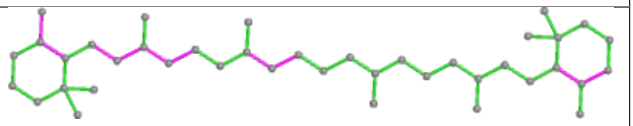


Rings

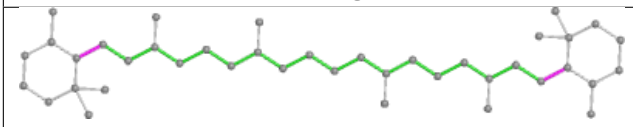
Ligand BCR a 611



Bond lengths



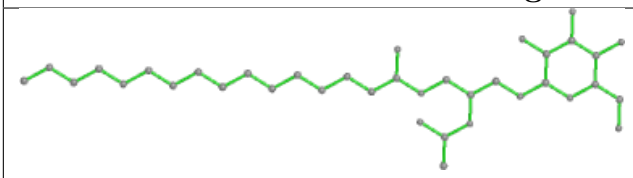
Bond angles



Torsions

Rings

Ligand LMG c 519



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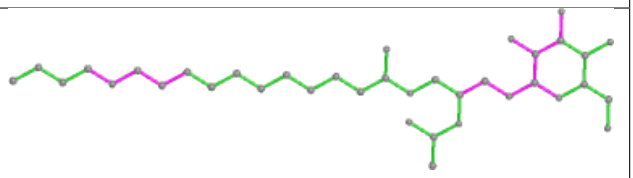
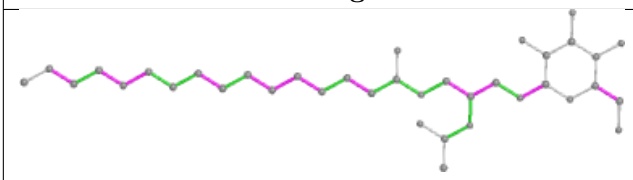
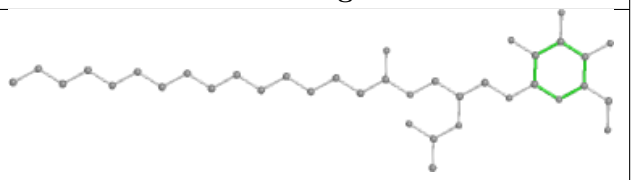


Bond angles

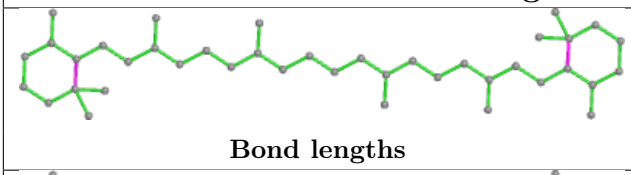


Torsions



Rings

Ligand BCR B 619



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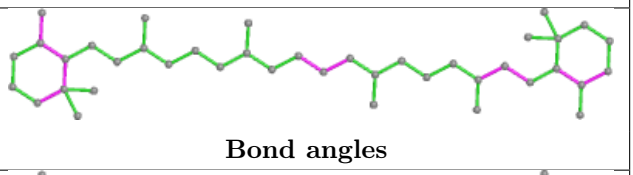
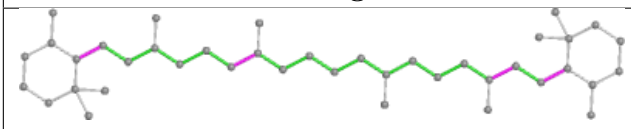
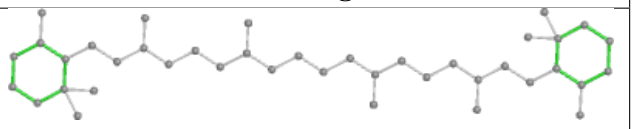


Bond angles

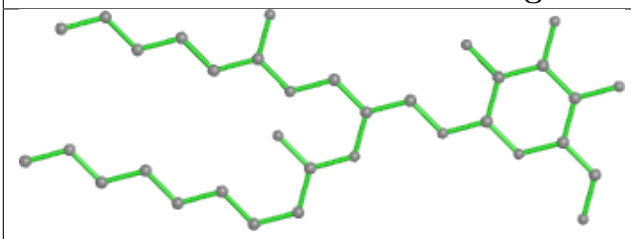


Torsions



Rings

Ligand LMG c 520



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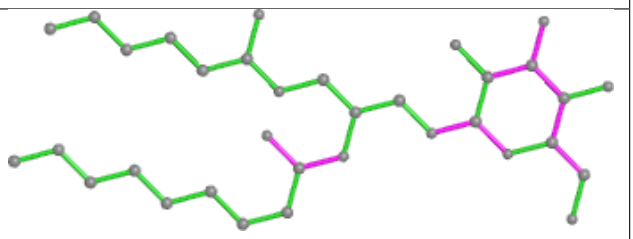
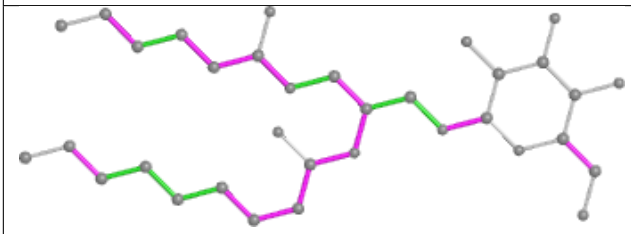
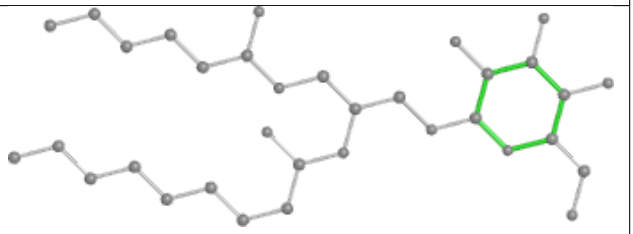


Bond angles

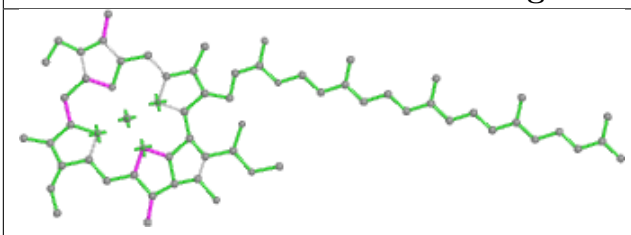


Torsions



Rings

Ligand CLA b 607



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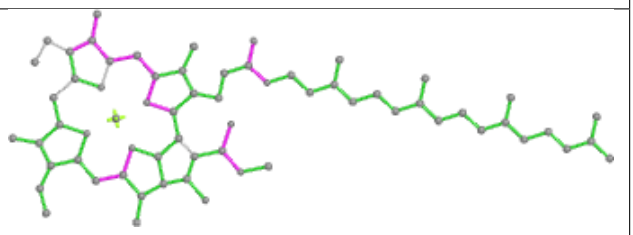
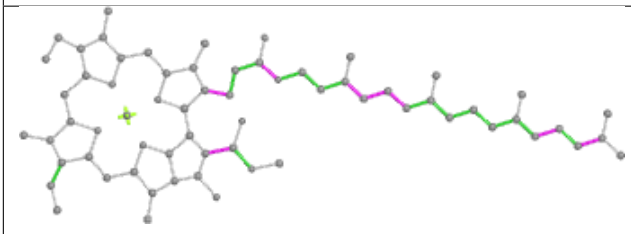
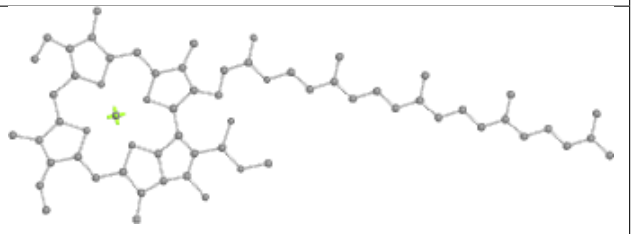


Bond angles

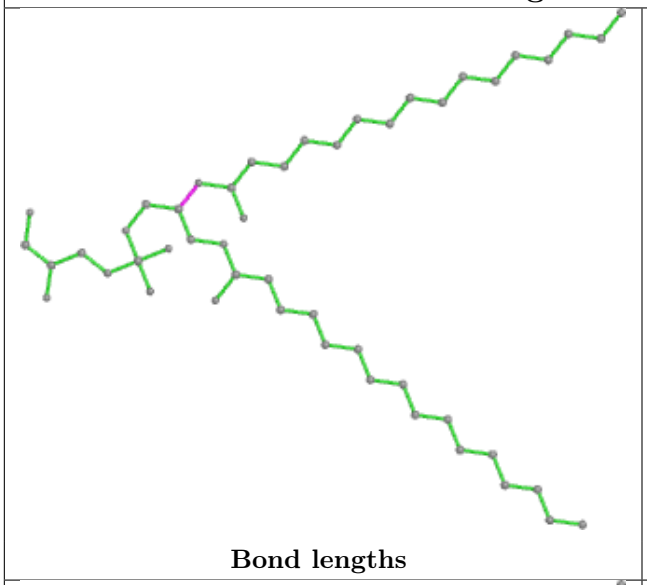


Torsions

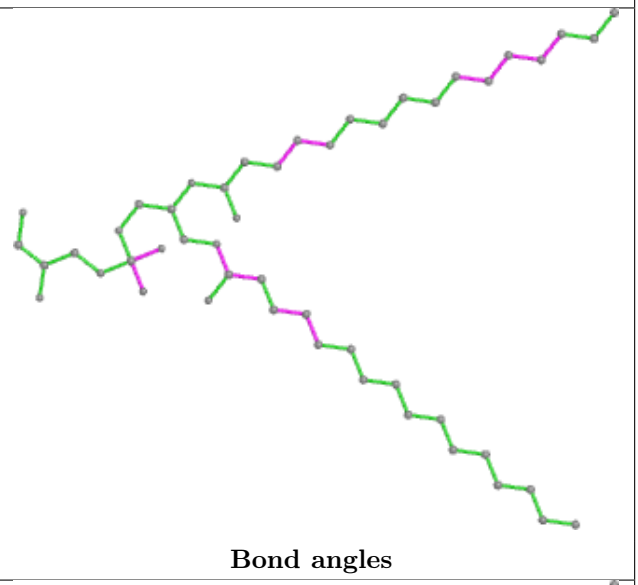


Rings

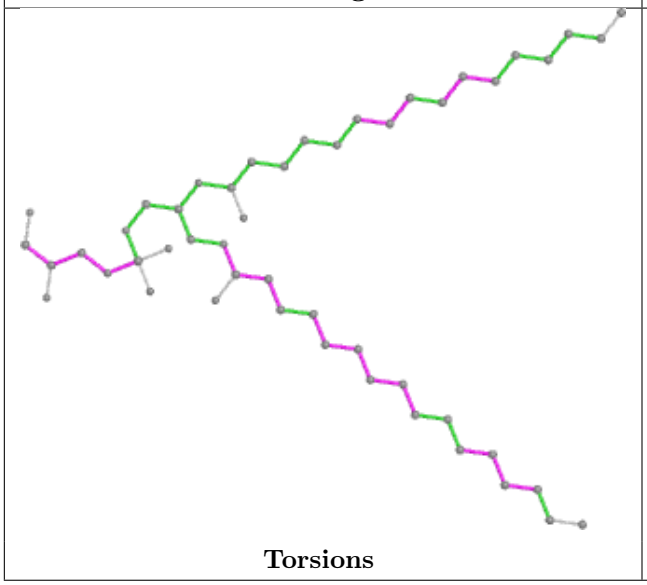
Ligand LHG d 405



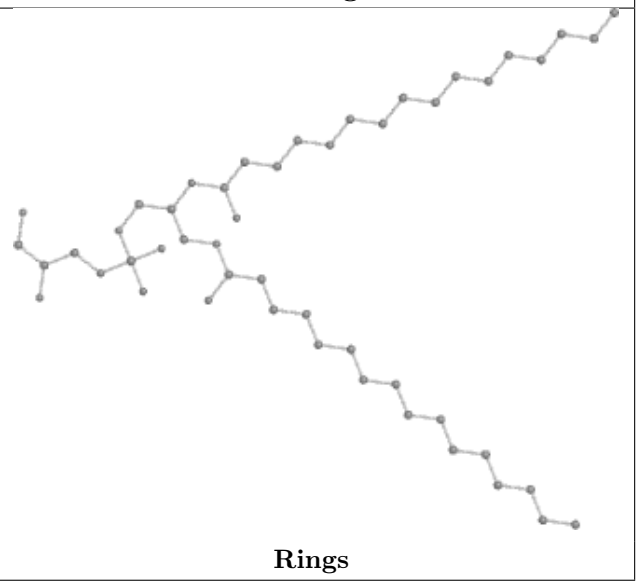
Bond lengths



Bond angles

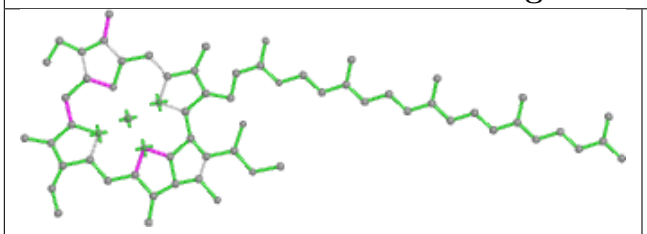


Torsions



Rings

Ligand CLA C 512



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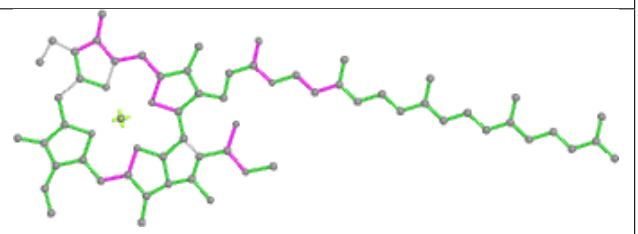
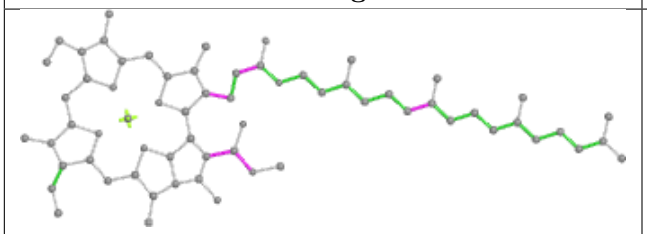
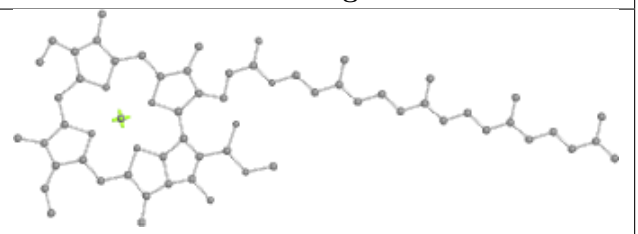


Bond angles

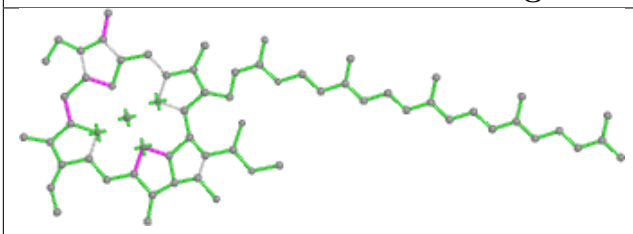


Torsions

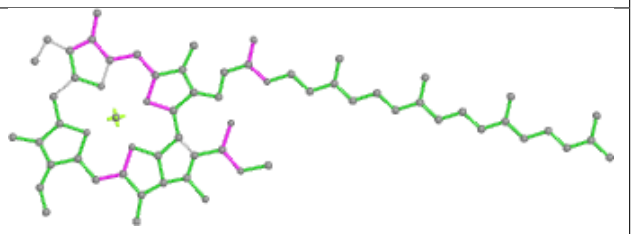


Rings

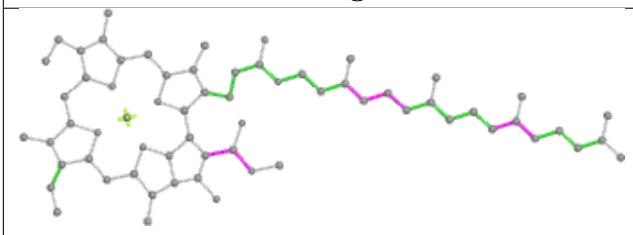
Ligand CLA B 609



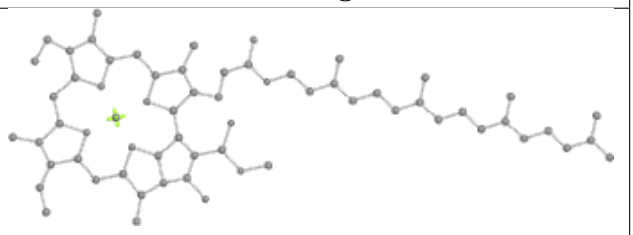
Bond lengths



Bond angles

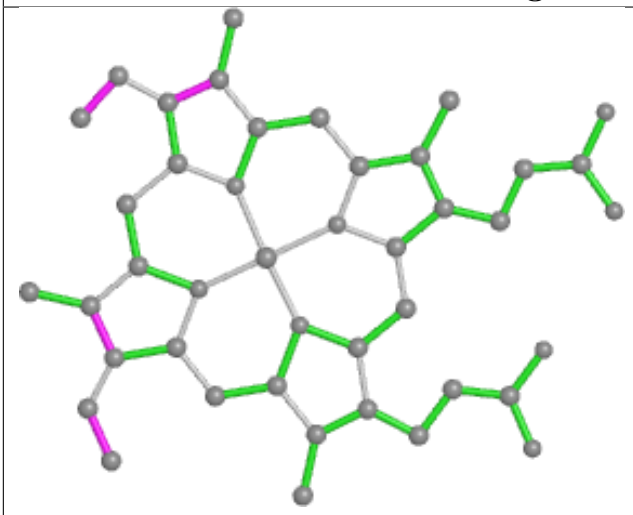


Torsions

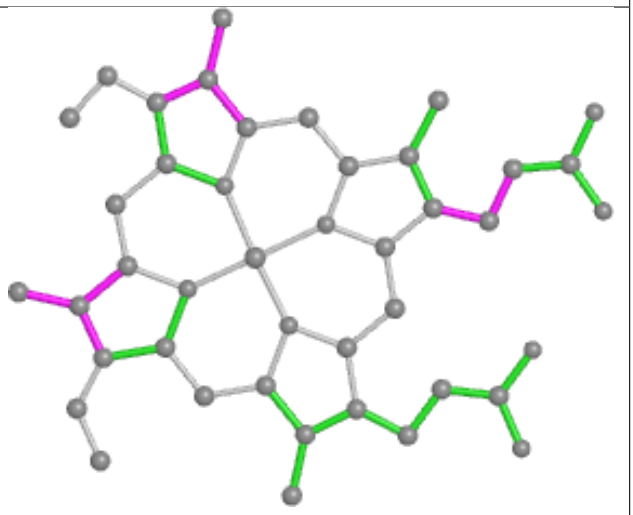


Rings

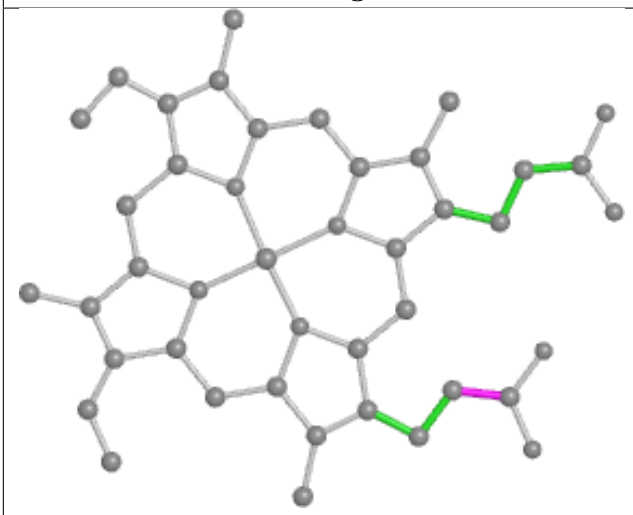
Ligand HEC v 201



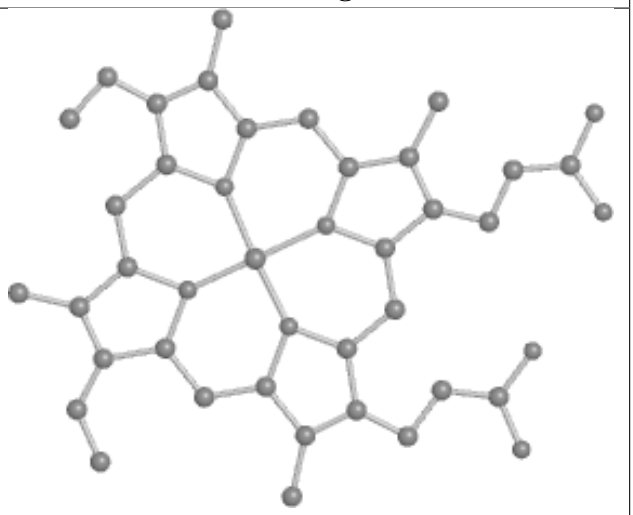
Bond lengths



Bond angles

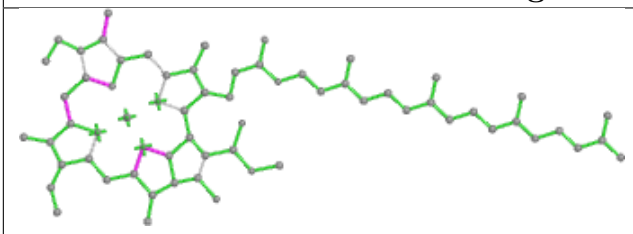


Torsions

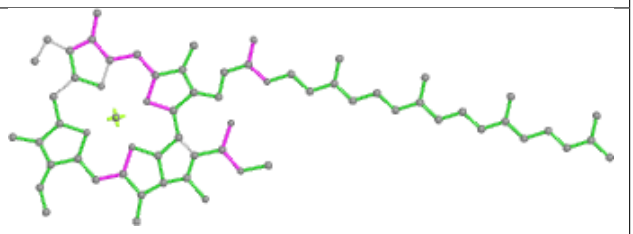


Rings

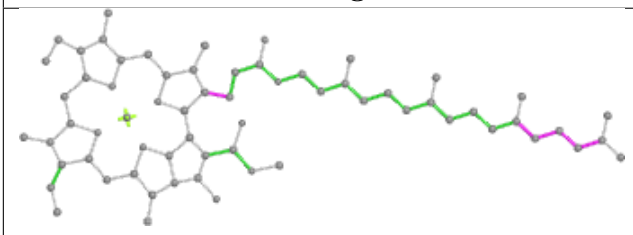
Ligand CLA d 402



Bond lengths



Bond angles



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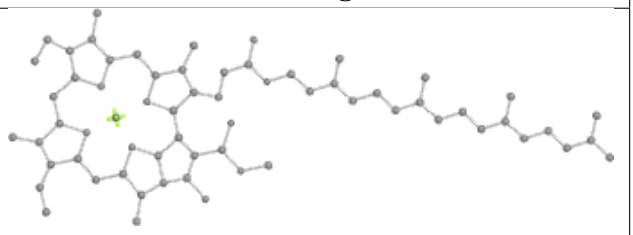
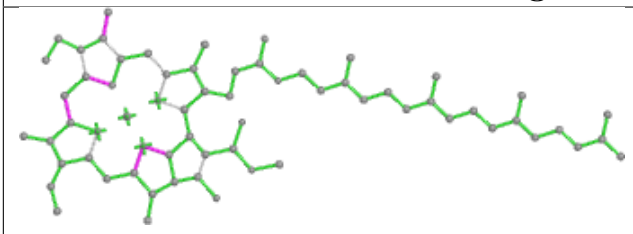
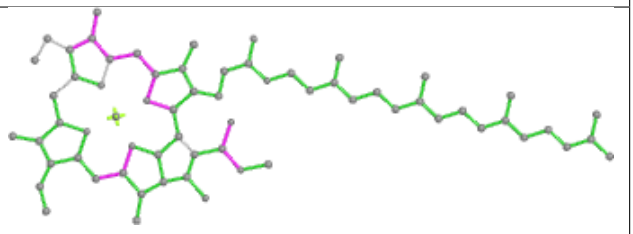


Rings

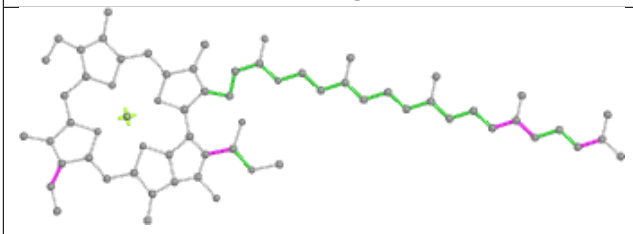
Ligand CLA a 615



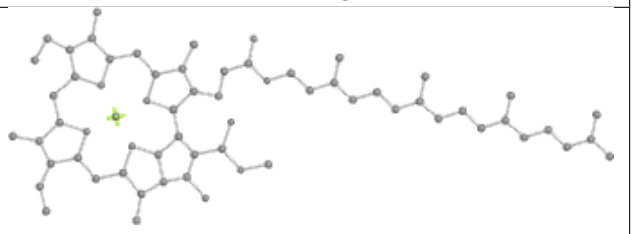
Bond lengths



Bond angles

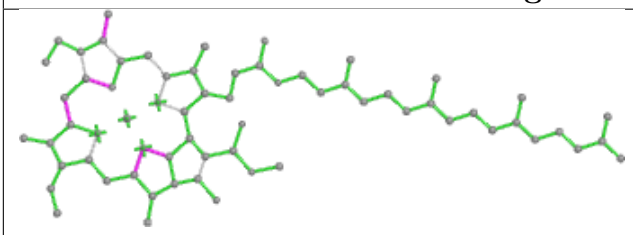


Torsions



Rings

Ligand CLA B 610



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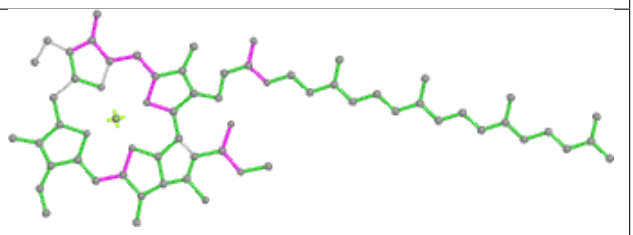
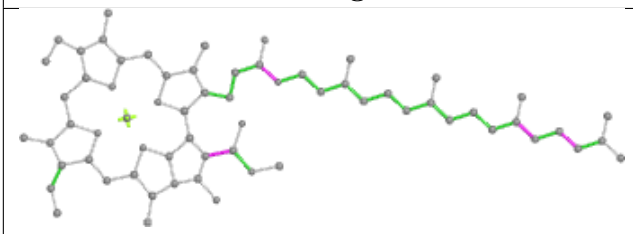


Bond angles



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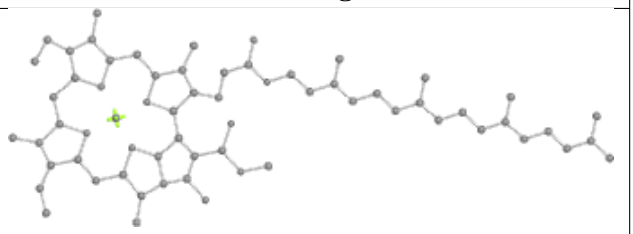
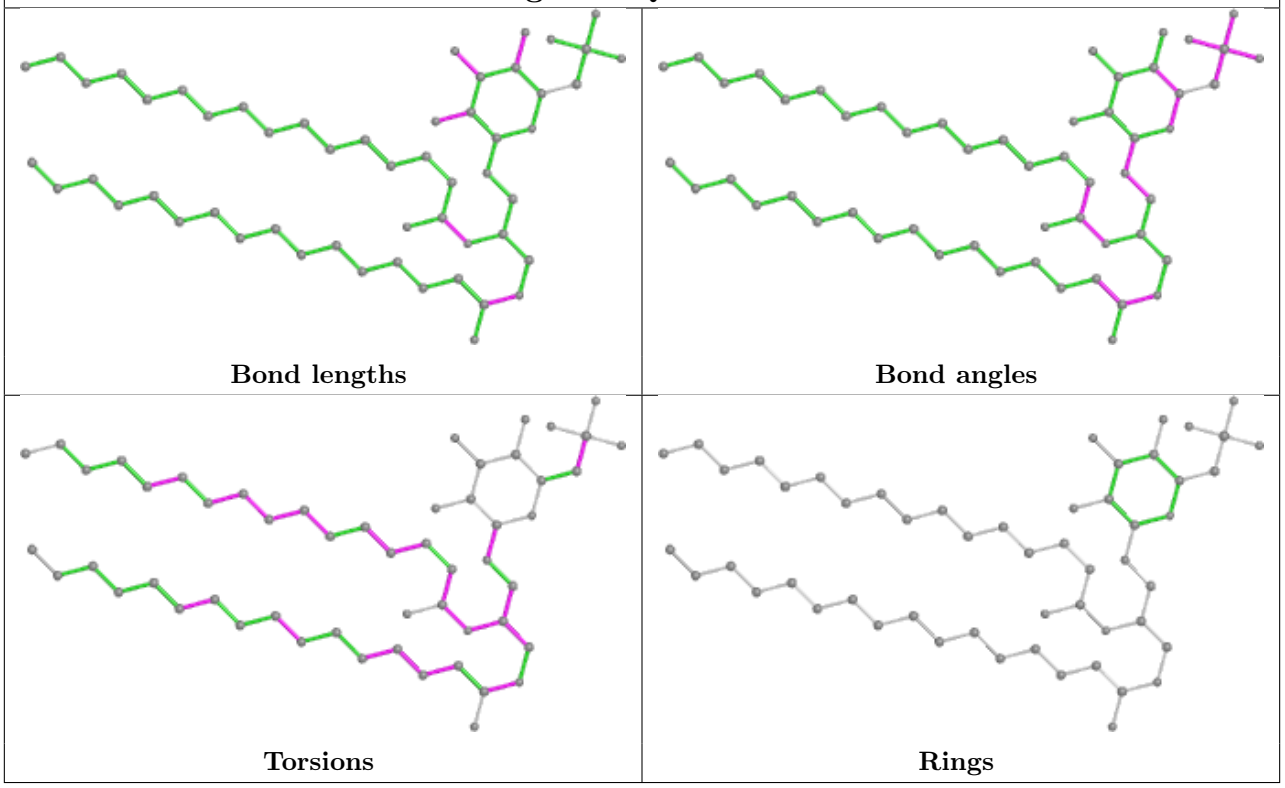
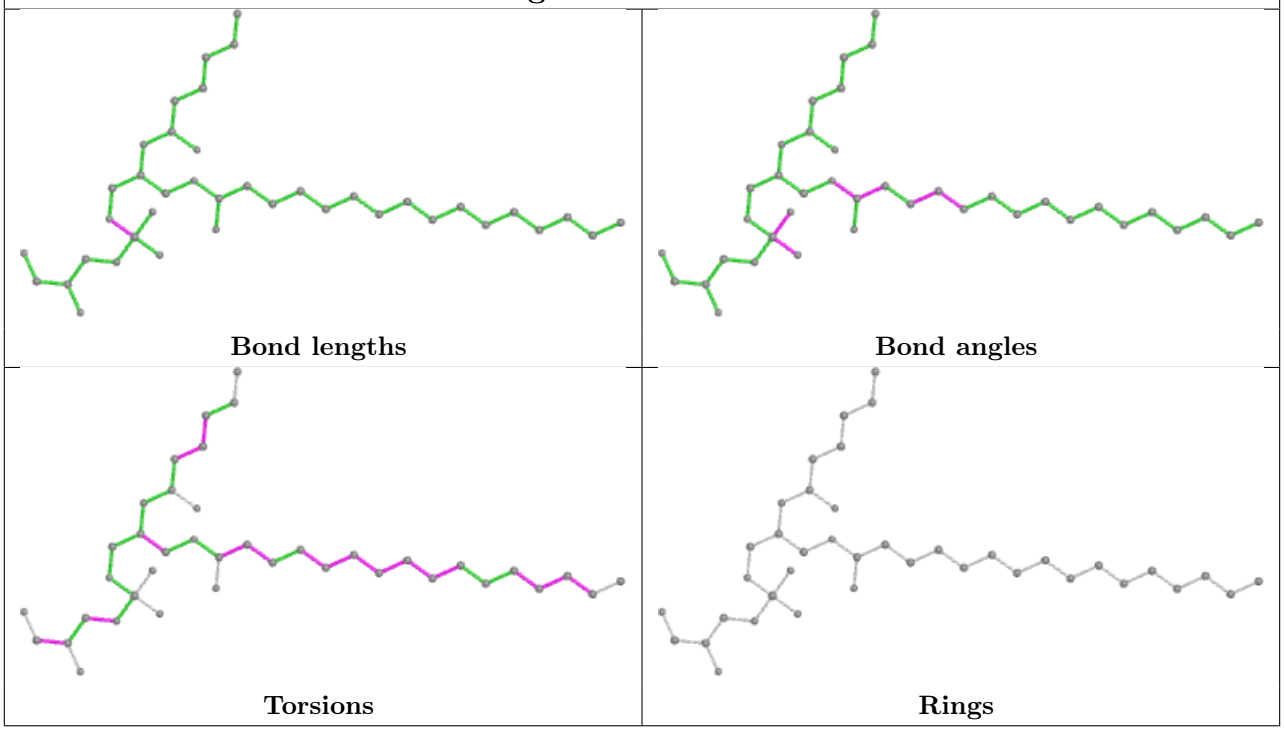


Rings

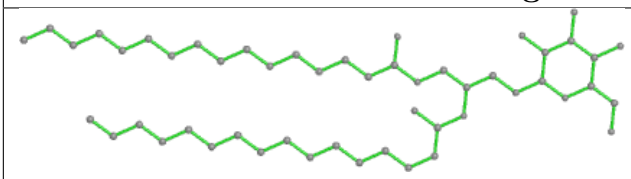
Ligand SQD B 625



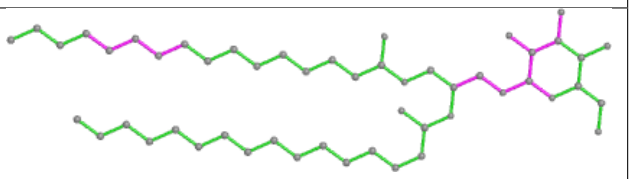
Ligand LHG a 616



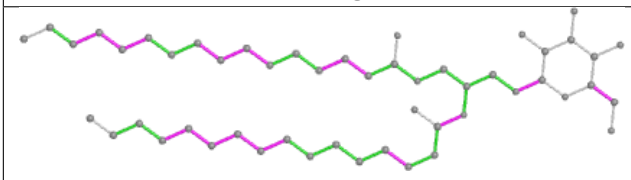
Ligand LMG b 620



Bond lengths



Bond angles



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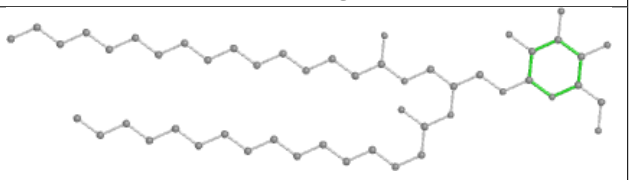
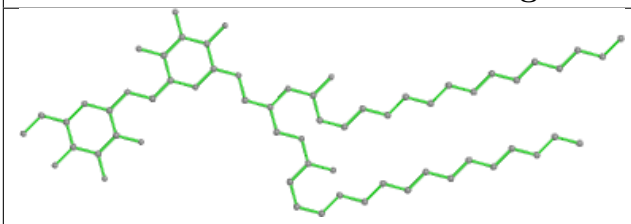


Rings

Ligand DGD C 517



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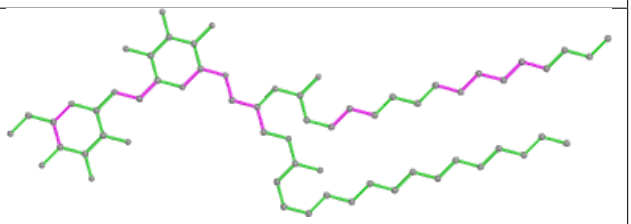
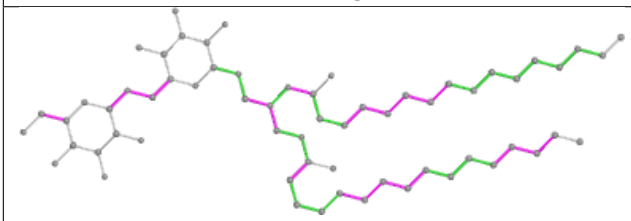


Bond angles



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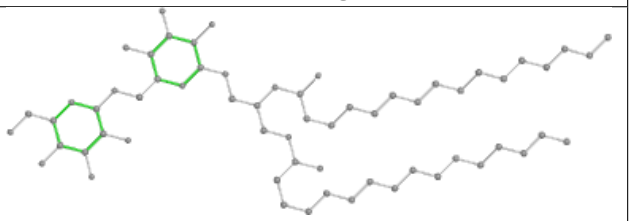
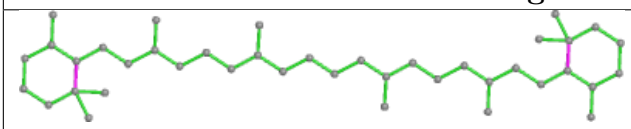
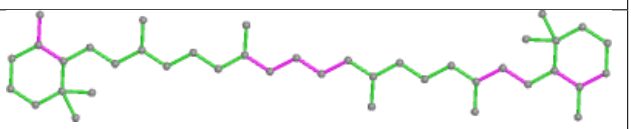


Rings

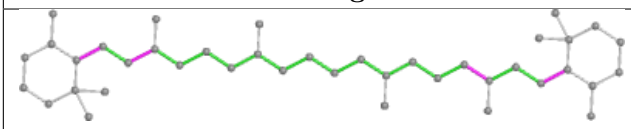
Ligand BCR c 521



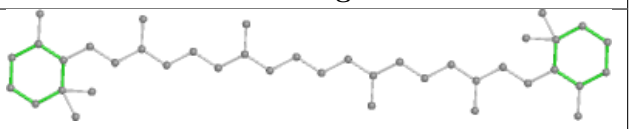
Bond lengths



Bond angles

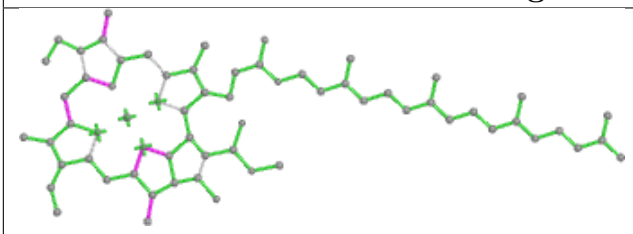


Torsions

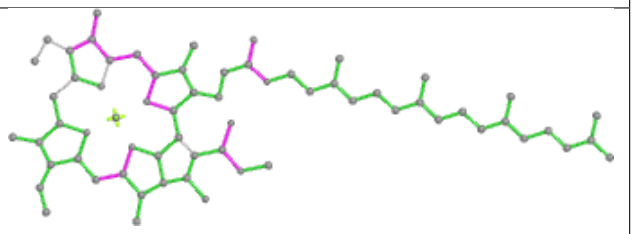


Rings

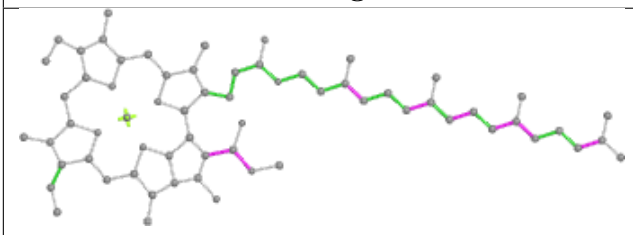
Ligand CLA b 603



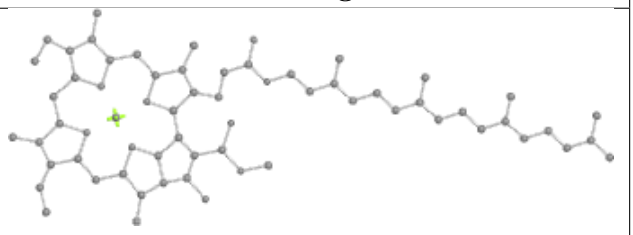
Bond lengths



Bond angles

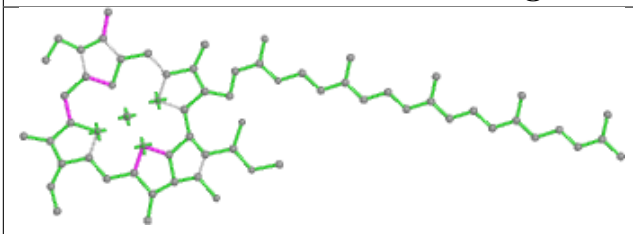


Torsions



Rings

Ligand CLA C 509



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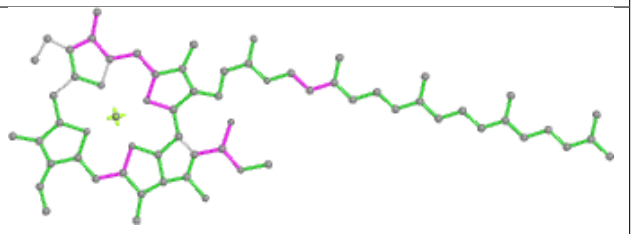
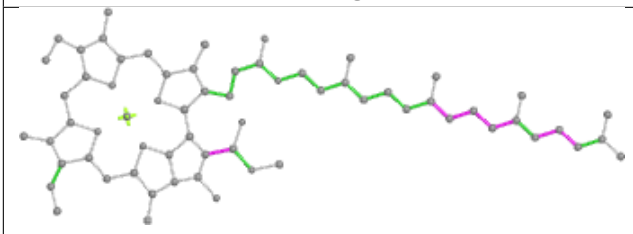
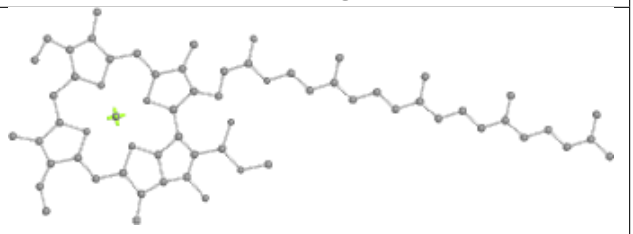


Bond angles

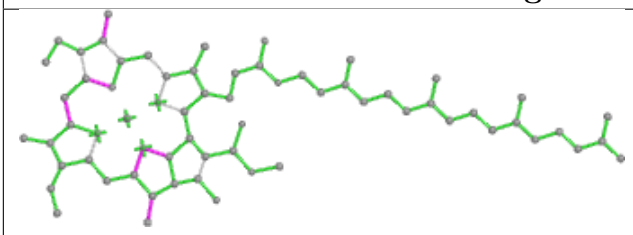


Torsions



Rings

Ligand CLA B 604



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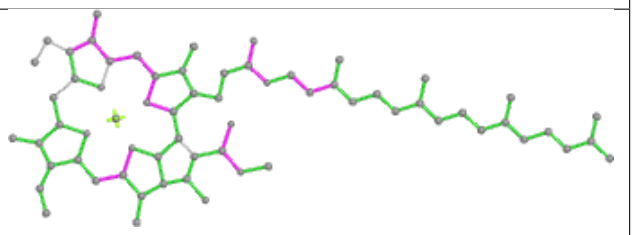

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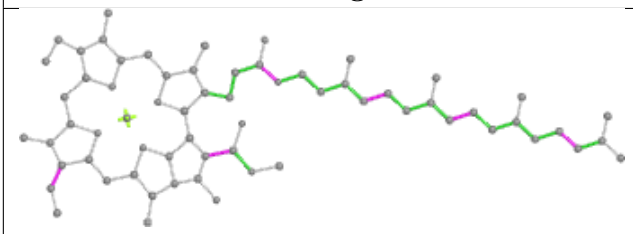

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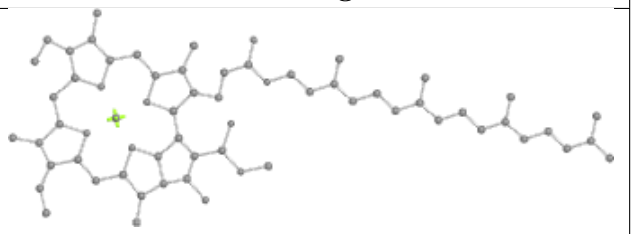
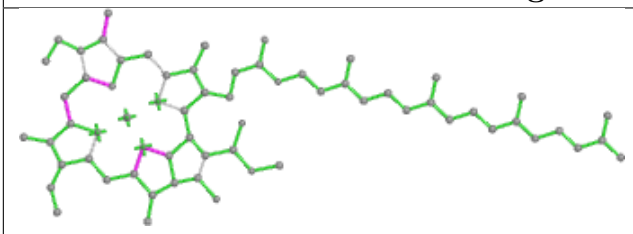


Rings

Ligand CLA b 602



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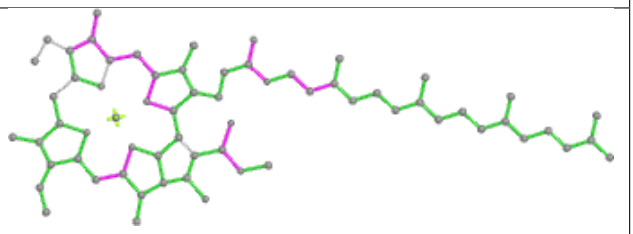
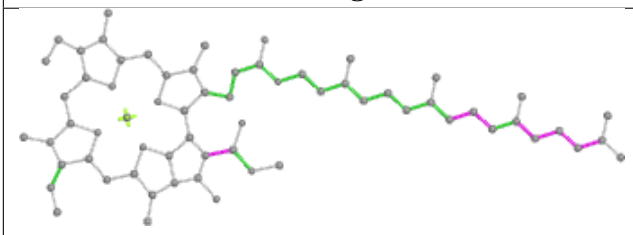


Bond angles



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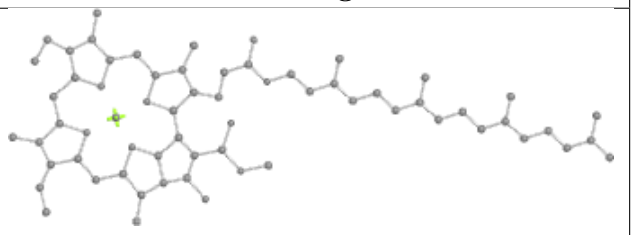
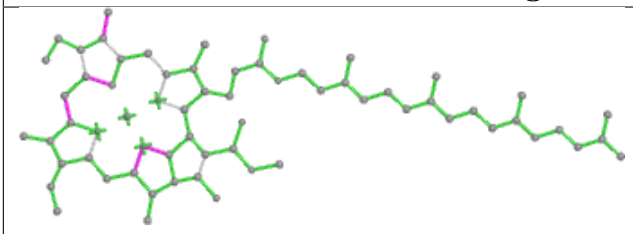
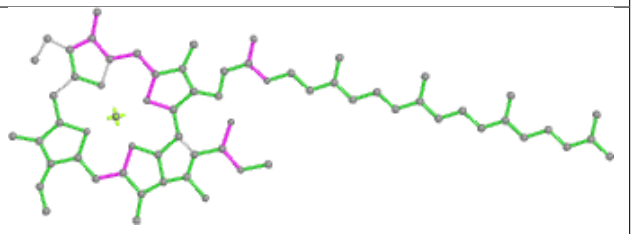


Rings

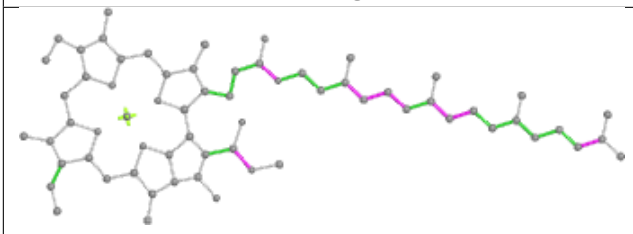
Ligand CLA C 514



Bond lengths



Bond angles



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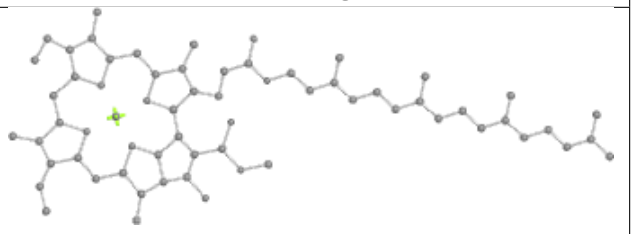
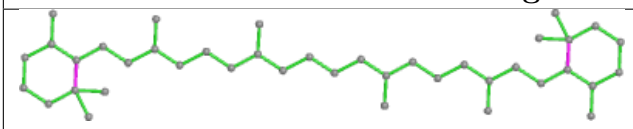


Rings

Ligand BCR B 618



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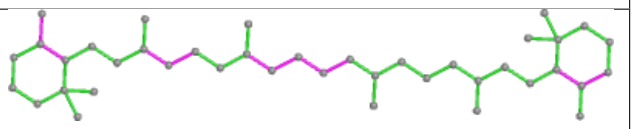
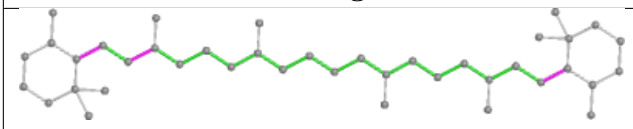


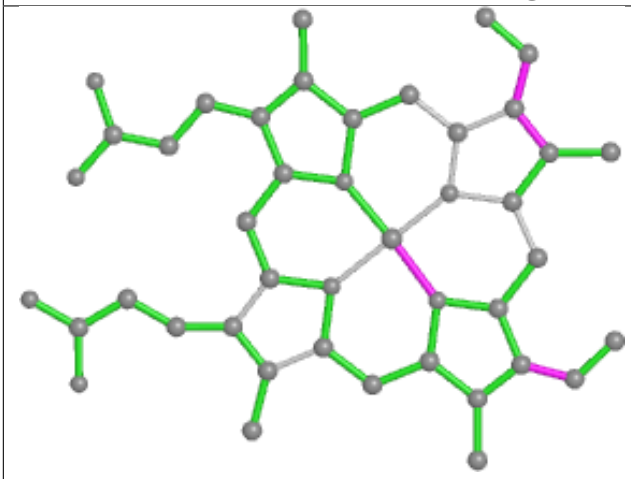
Bond angles



Torsions

Rings

Ligand HEM e 101



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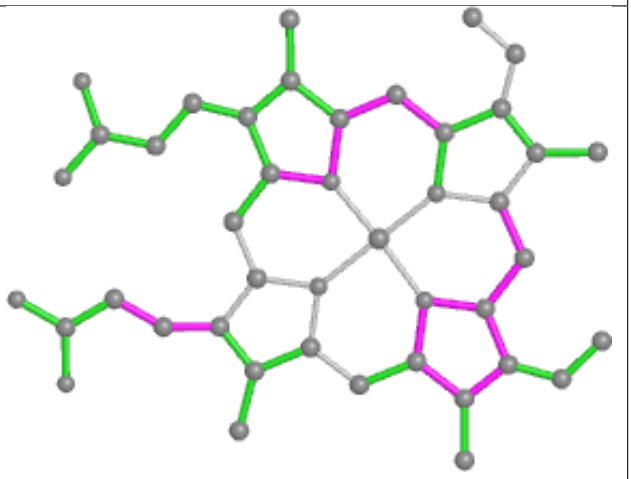
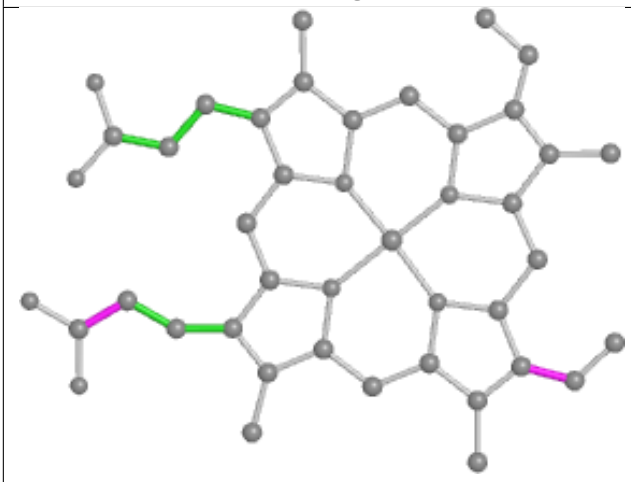
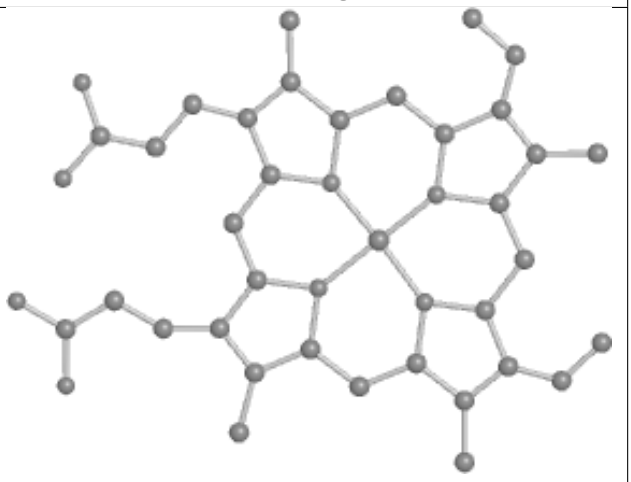


Bond angles

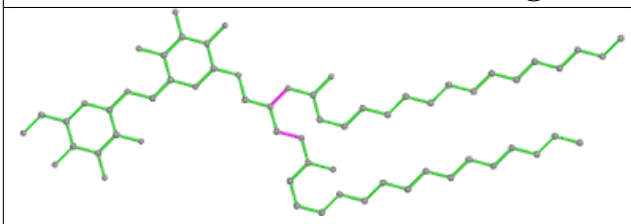


Torsions

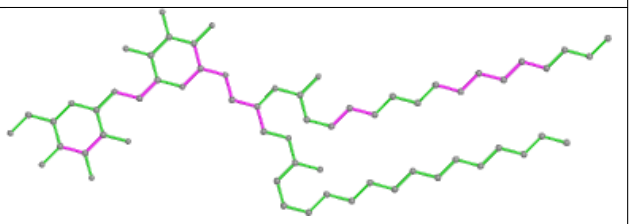


Rings

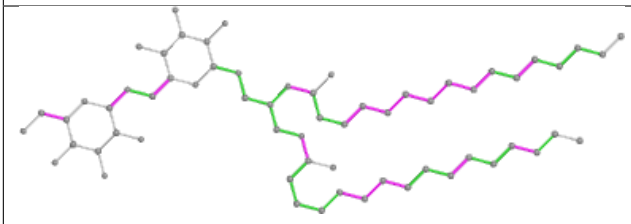
Ligand DGD c 516



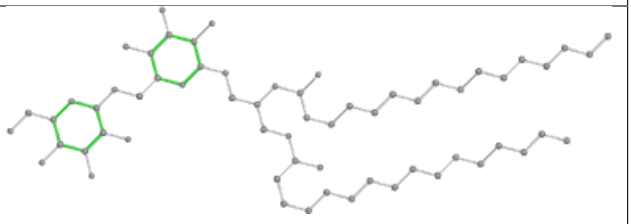
Bond lengths



Bond angles

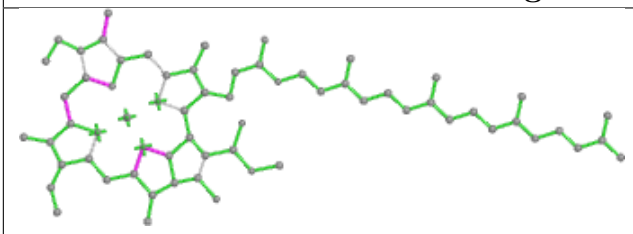


Torsions

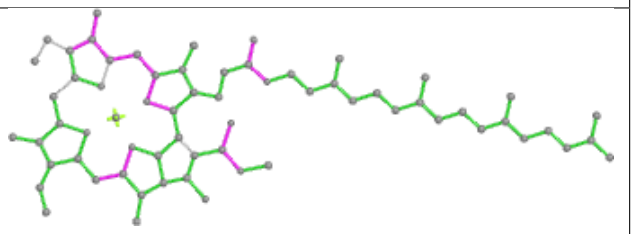


Rings

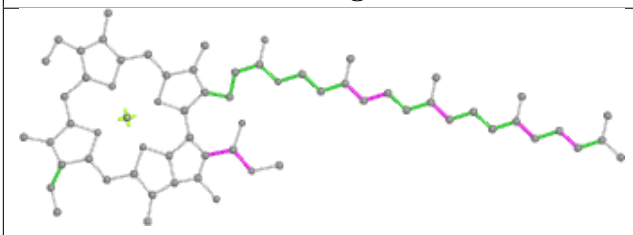
Ligand CLA C 507



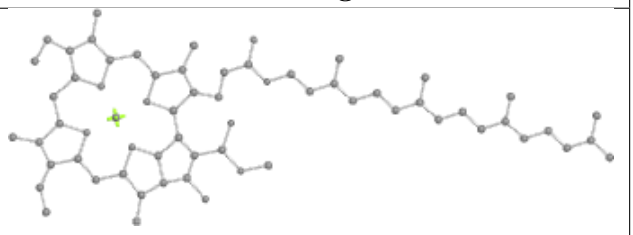
Bond lengths



Bond angles

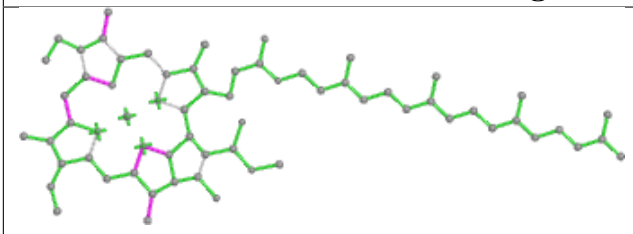


Torsions

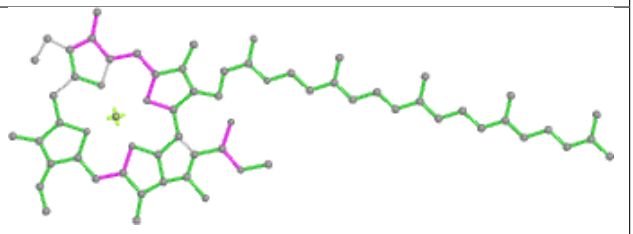


Rings

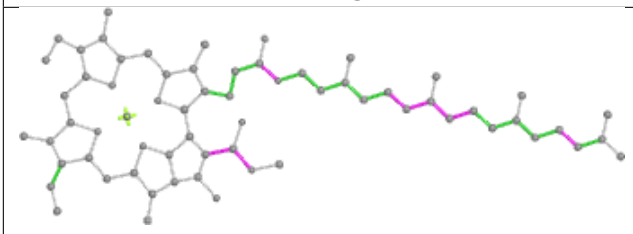
Ligand CLA c 503



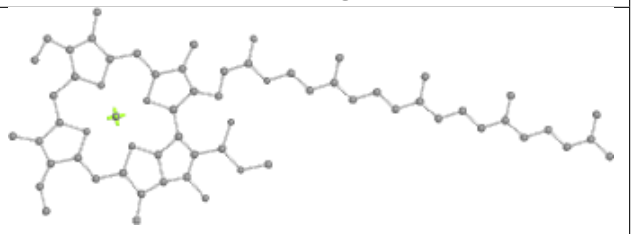
Bond lengths



Bond angles

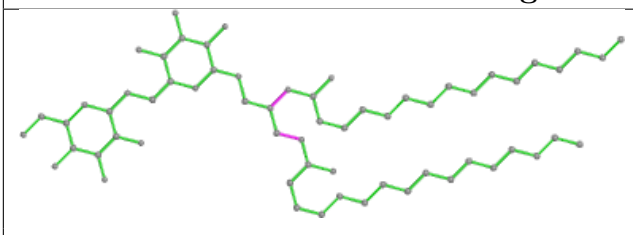


Torsions

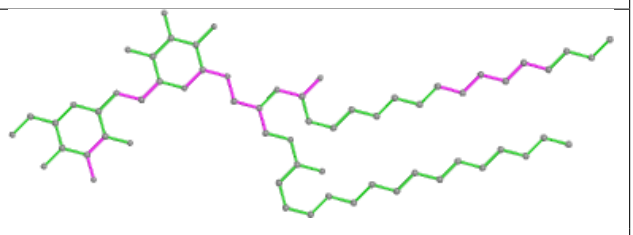


Rings

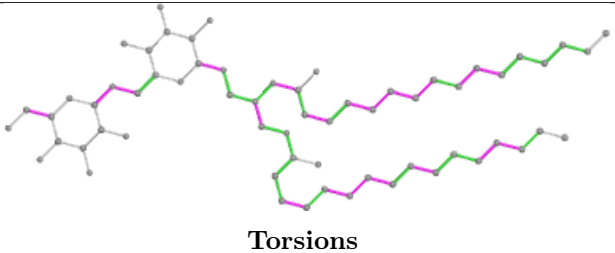
Ligand DGD C 518



Bond lengths



Bond angles



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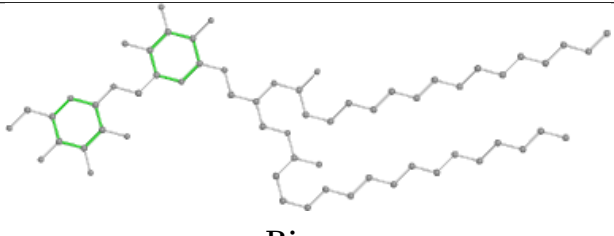
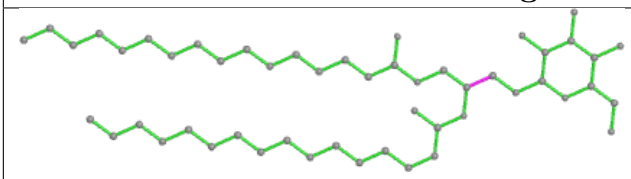
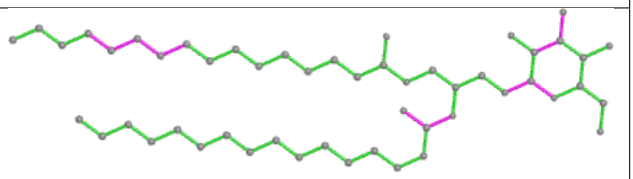


Rings

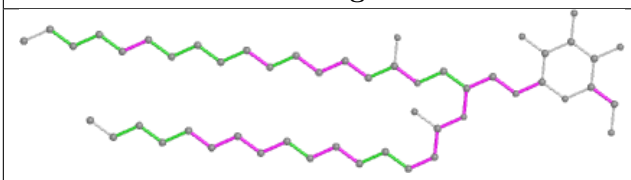
Ligand LMG B 626



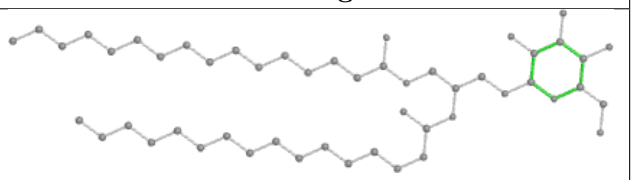
Bond lengths



Bond angles

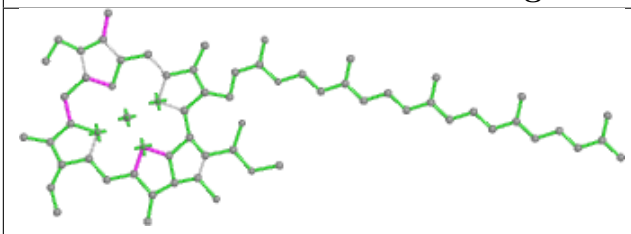


Torsions

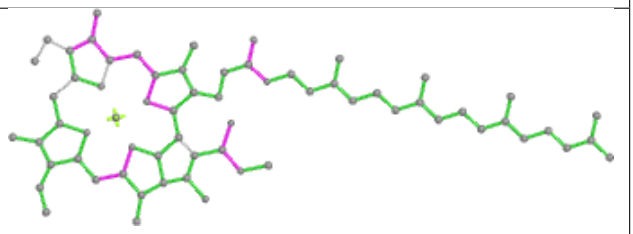


Rings

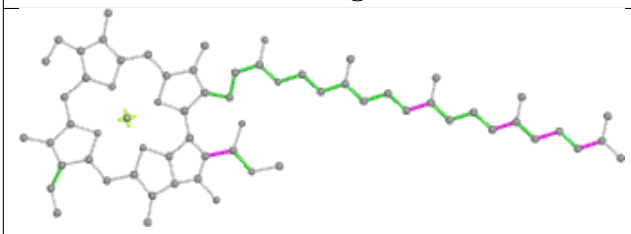
Ligand CLA C 503



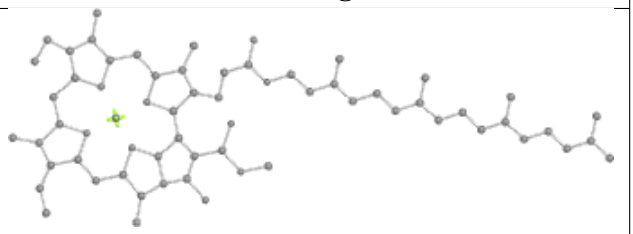
Bond lengths



Bond angles

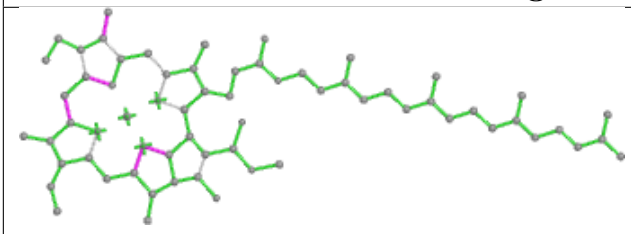


Torsions

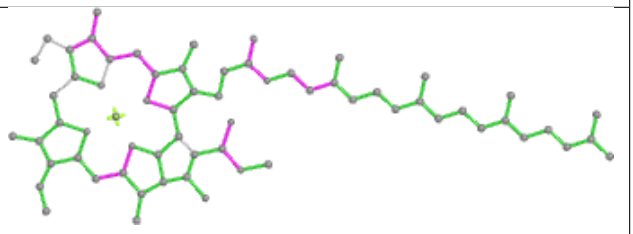


Rings

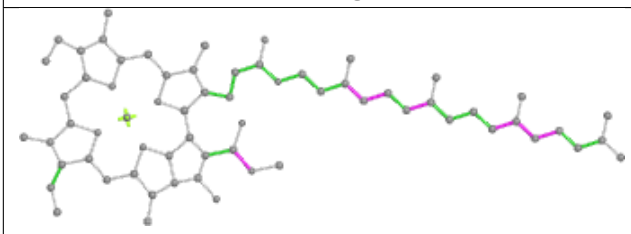
Ligand CLA b 604



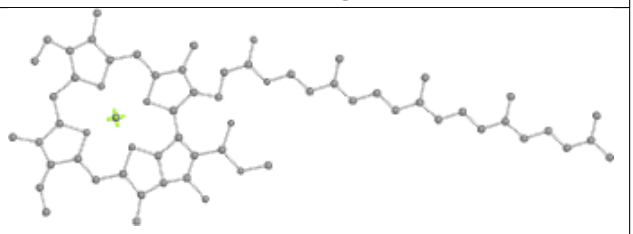
Bond lengths



Bond angles

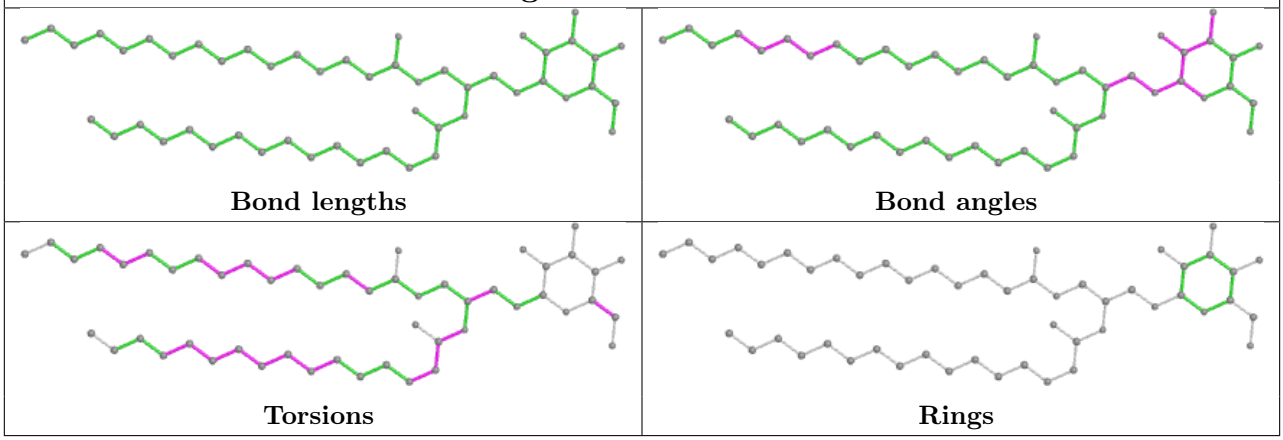


Torsions

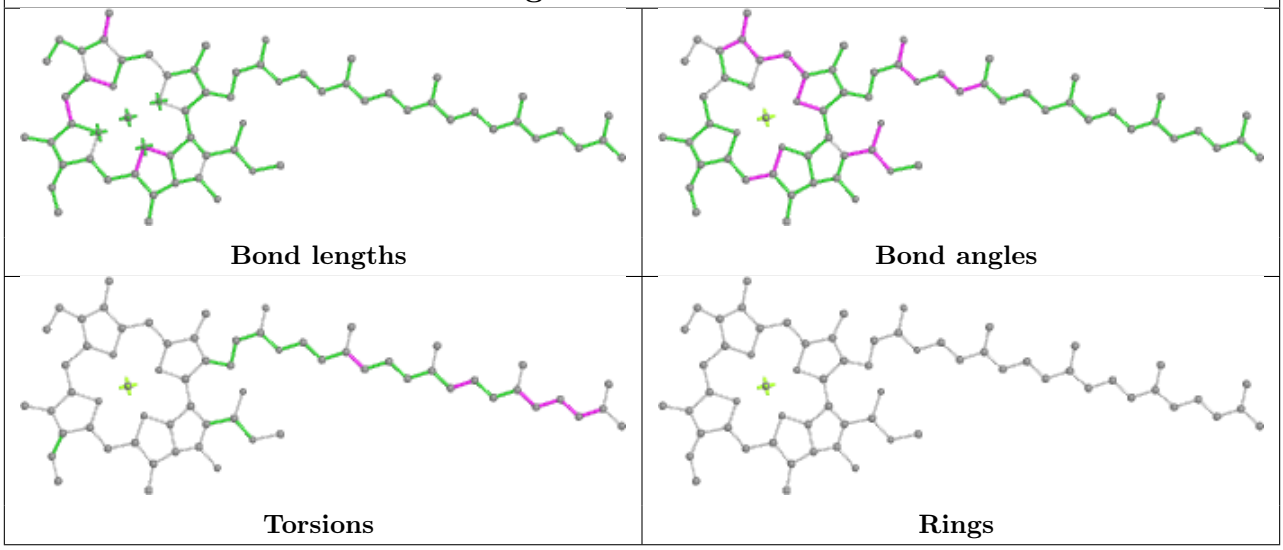


Rings

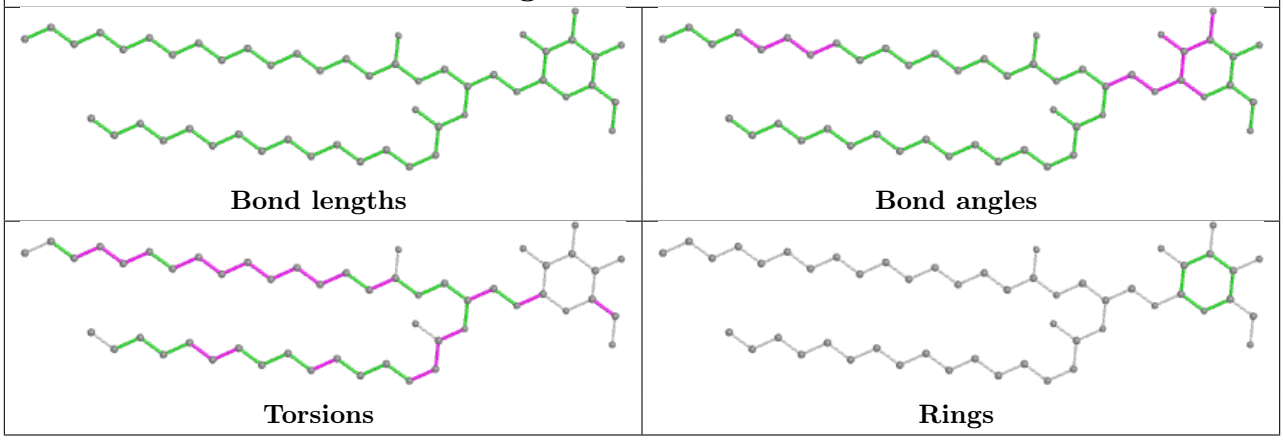
Ligand LMG B 621



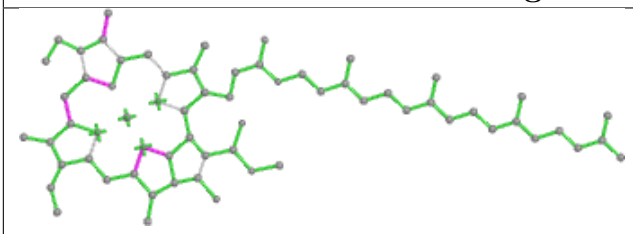
Ligand CLA B 611



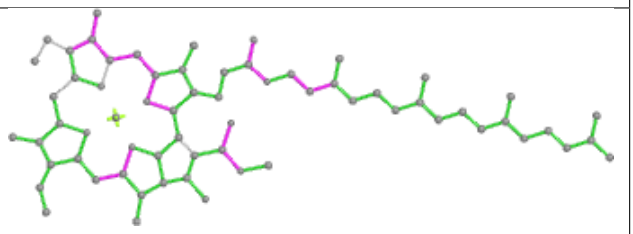
Ligand LMG m 102



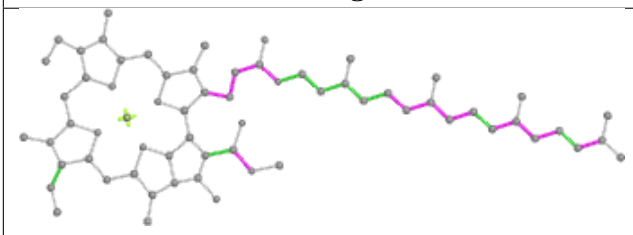
Ligand CLA B 601



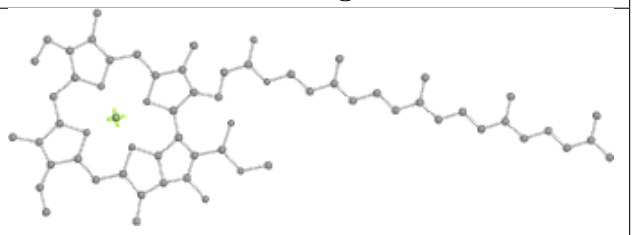
Bond lengths



Bond angles

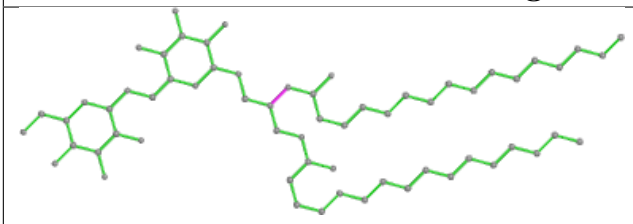


Torsions

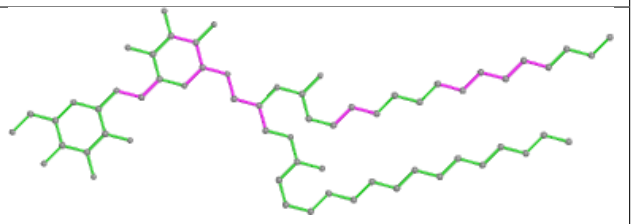


Rings

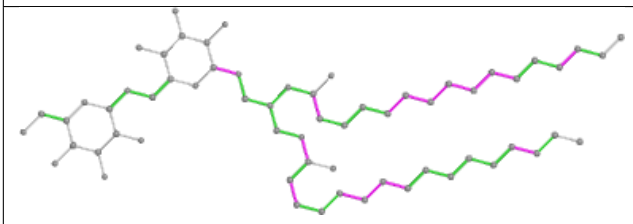
Ligand DGD c 518



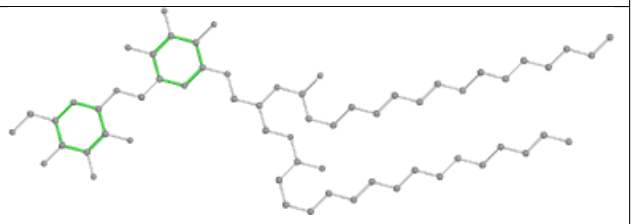
Bond lengths



Bond angles

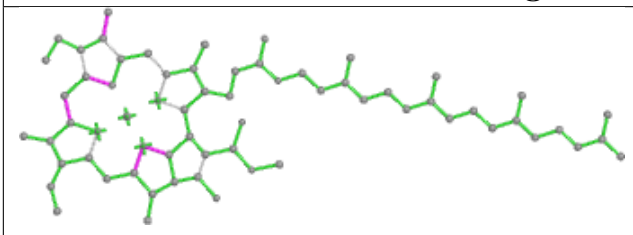


Torsions

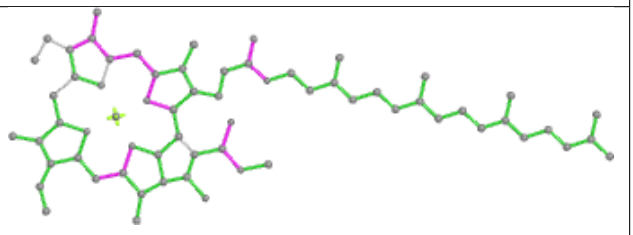


Rings

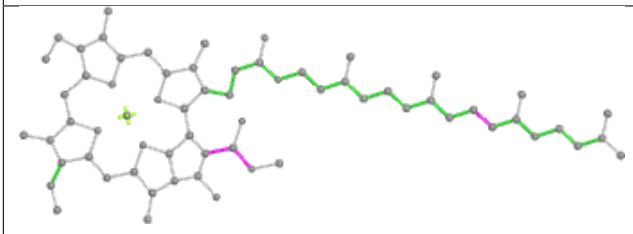
Ligand CLA C 510



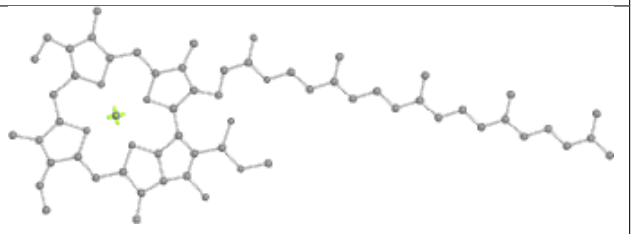
Bond lengths



Bond angles

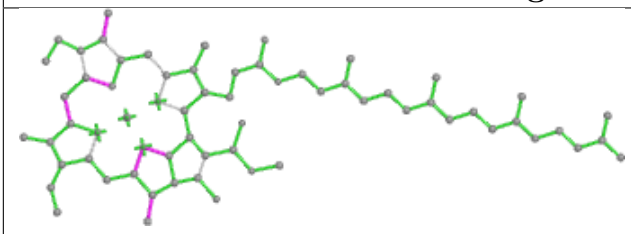


Torsions

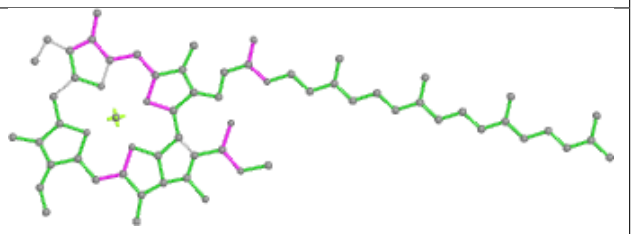


Rings

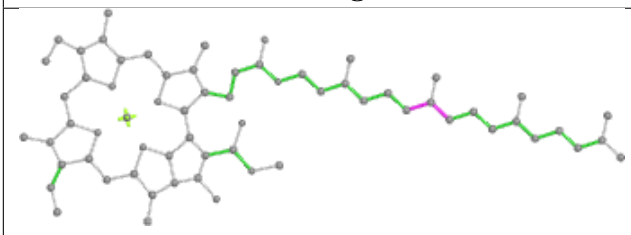
Ligand CLA b 615



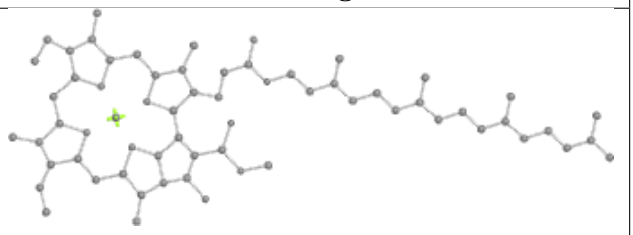
Bond lengths



Bond angles

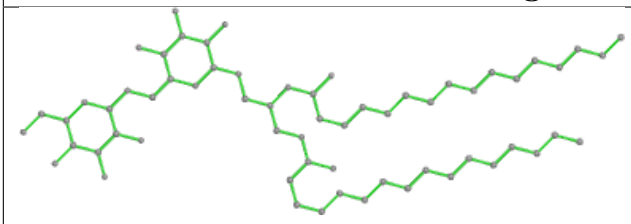


Torsions

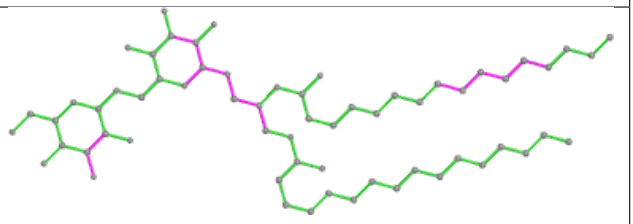


Rings

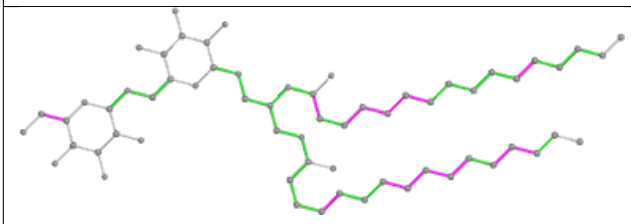
Ligand DGD h 102



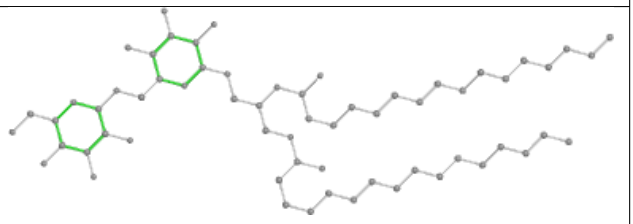
Bond lengths



Bond angles

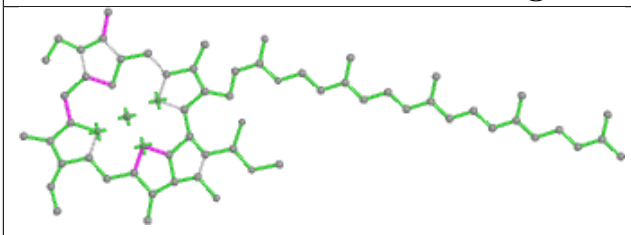


Torsions

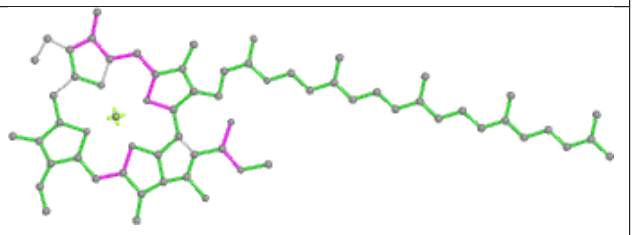


Rings

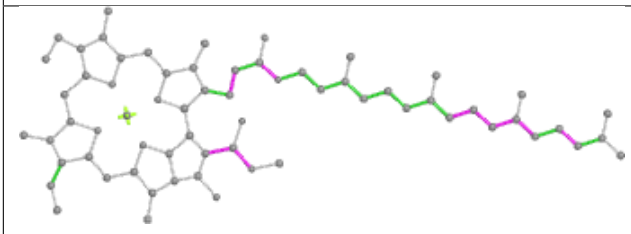
Ligand CLA b 601



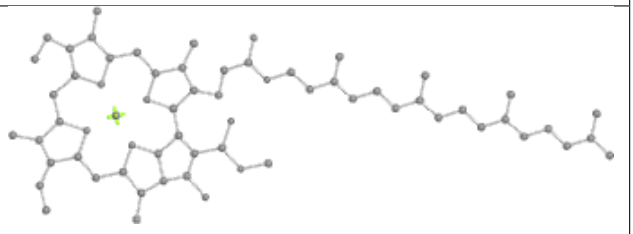
Bond lengths



Bond angles

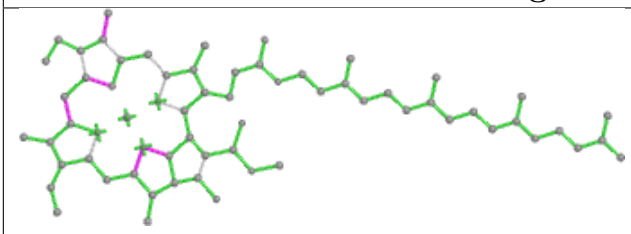


Torsions

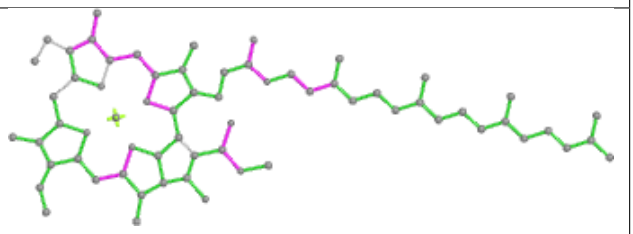


Rings

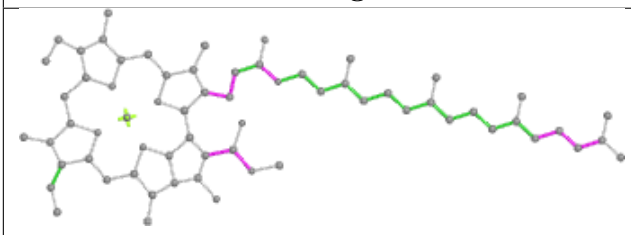
Ligand CLA c 512



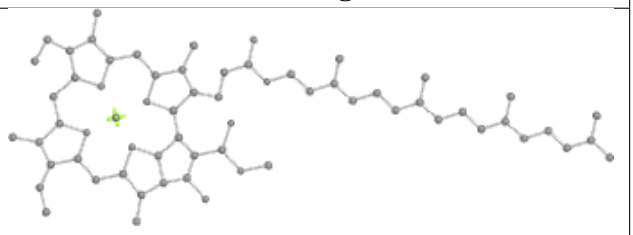
Bond lengths



Bond angles

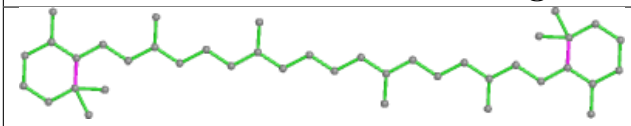


Torsions

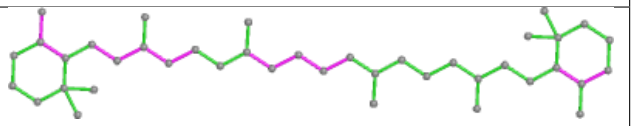


Rings

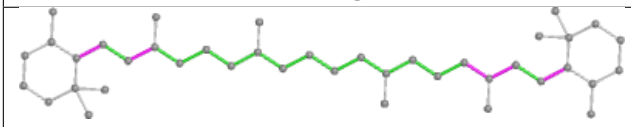
Ligand BCR t 101



Bond lengths



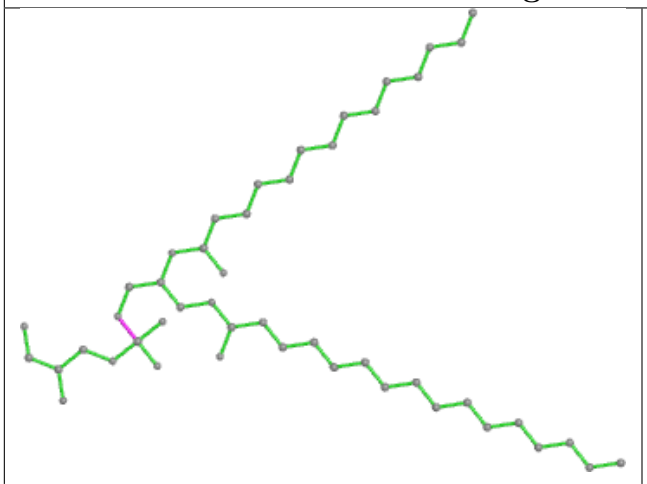
Bond angles



Torsions

Rings

Ligand LHG A 614



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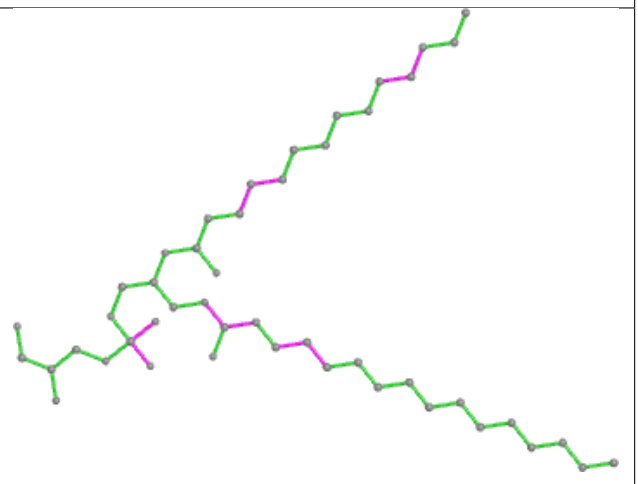

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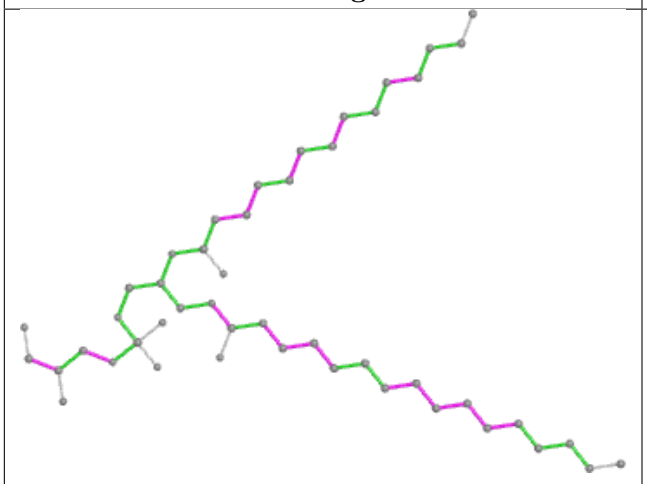
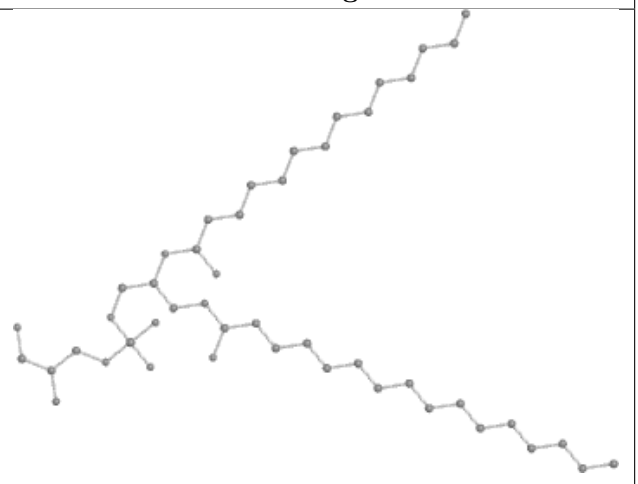
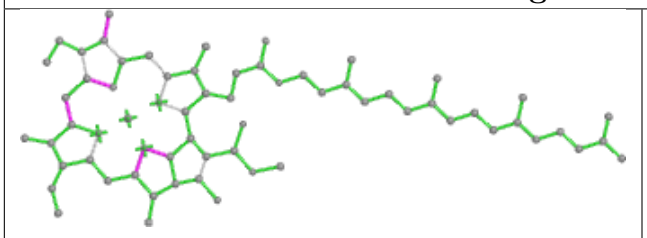


Torsions



Rings

Ligand CLA a 607



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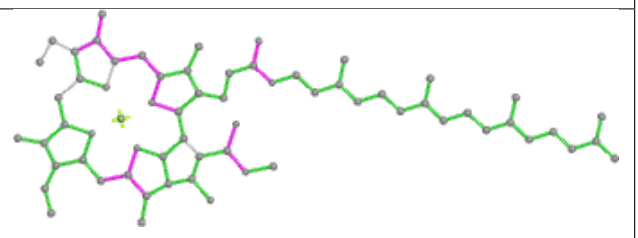
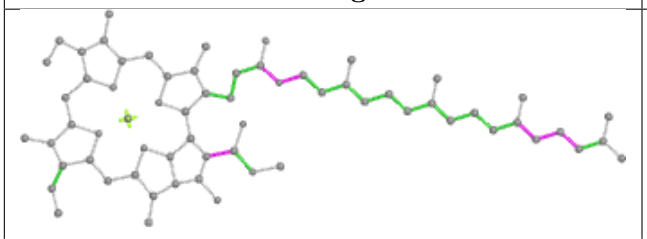


Bond angles



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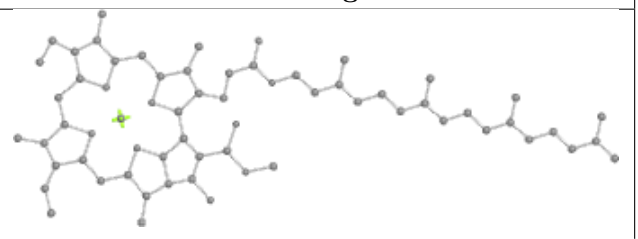
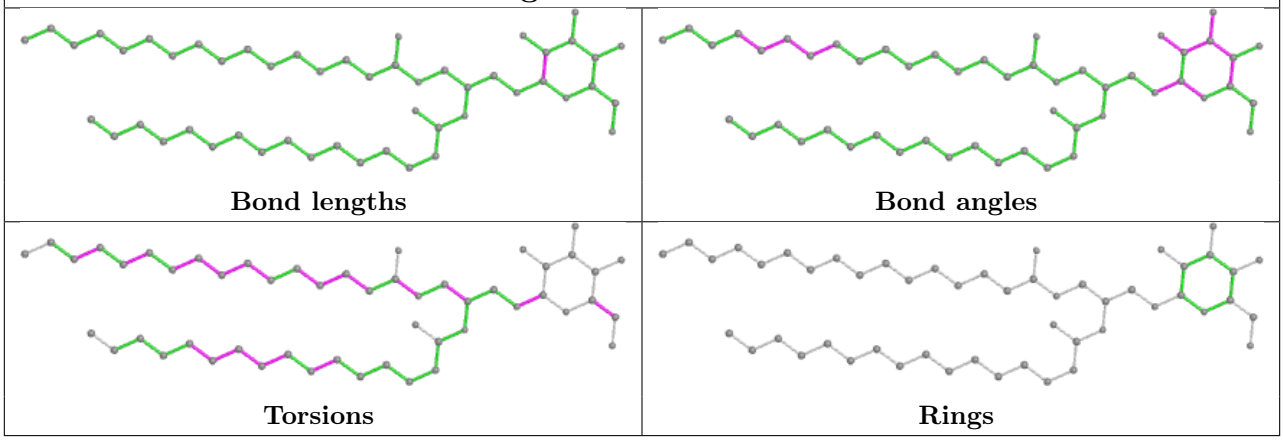


Rings

Ligand LMG C 521



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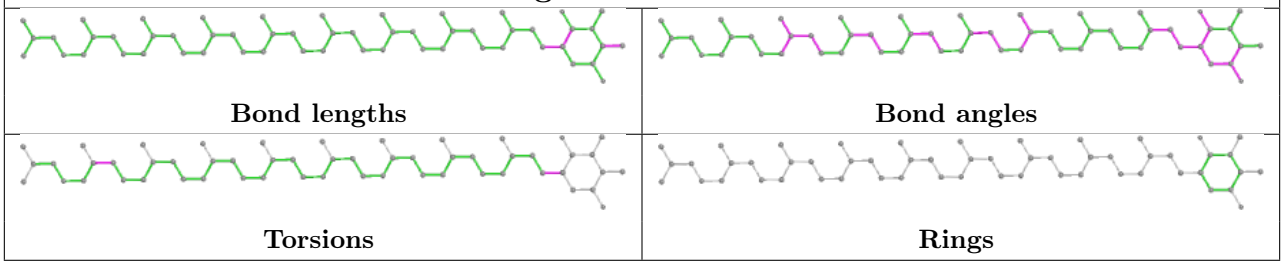

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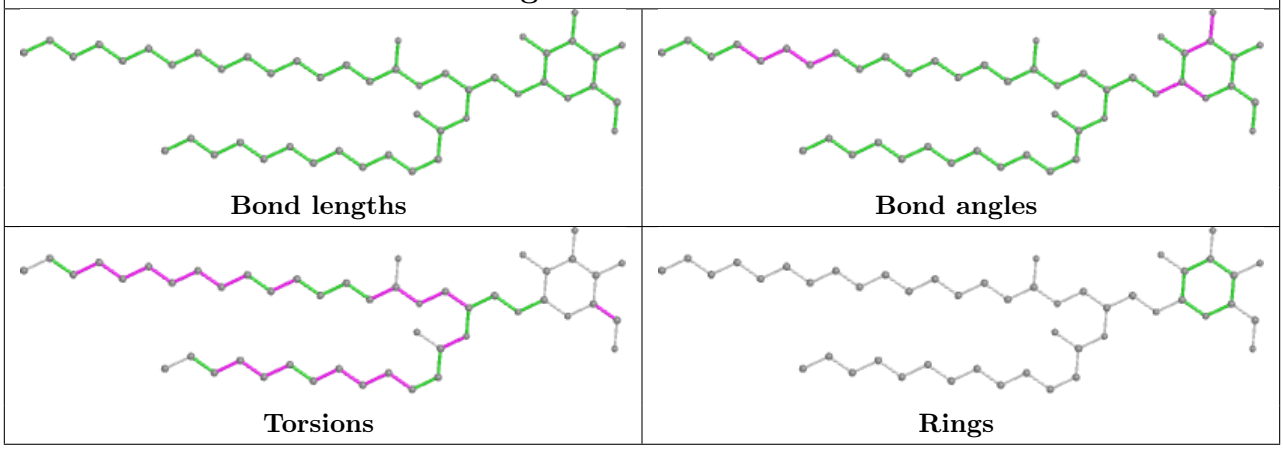
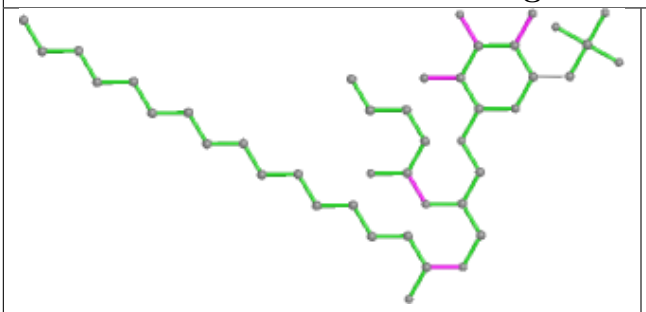
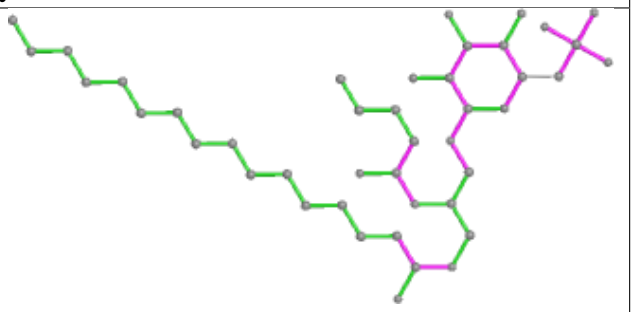


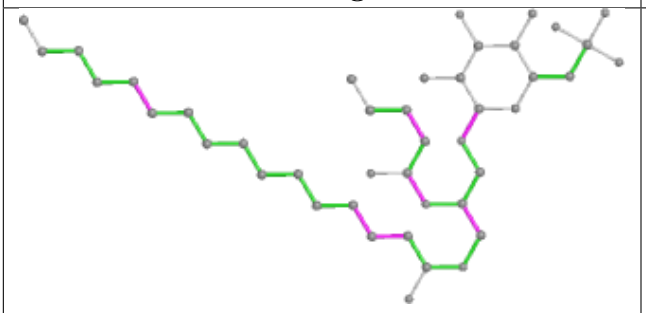
Ligand SQD D 408



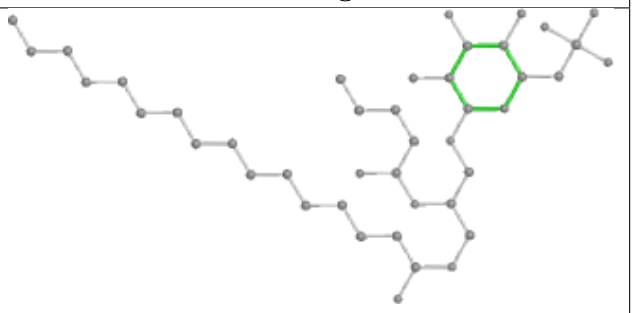
Bond lengths



Bond angles

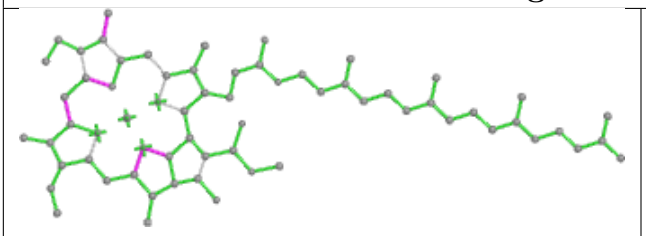


Torsions



Rings

Ligand CLA b 609



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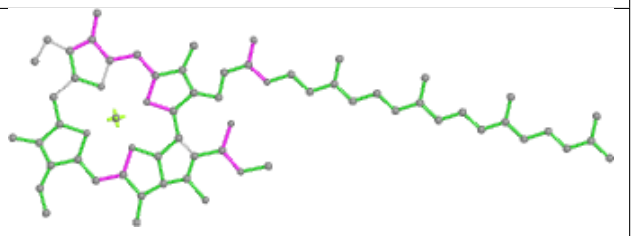
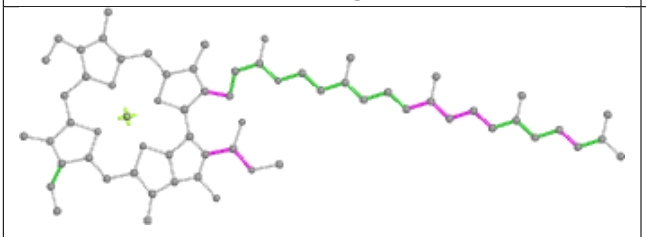


Bond angles



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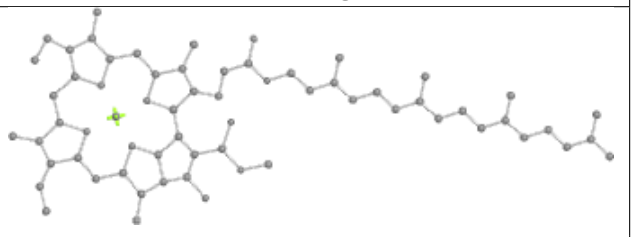
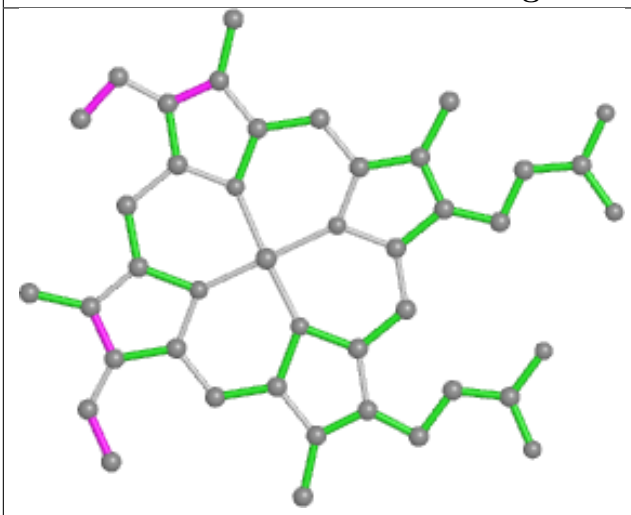


Rings

Ligand HEC V 201



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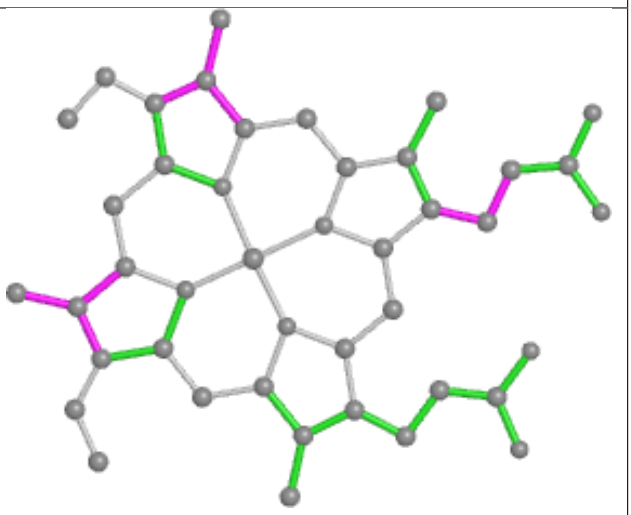
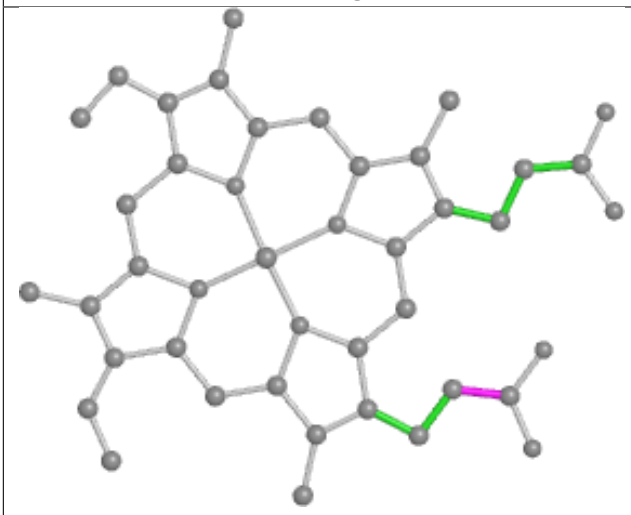


Bond angles



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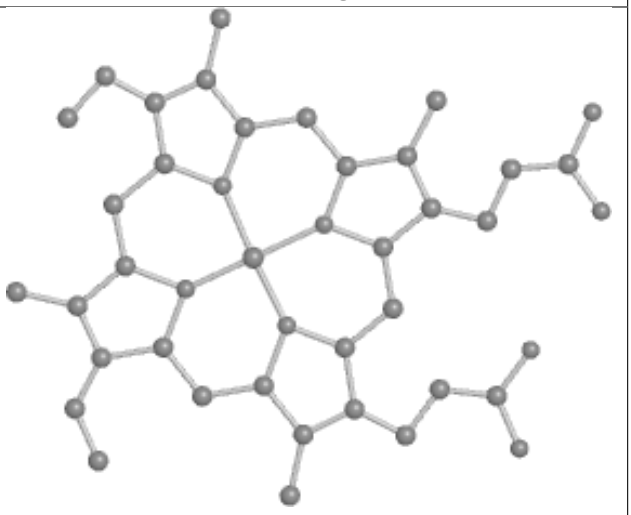
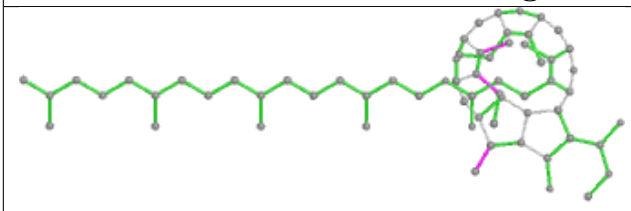


Rings

Ligand PHO A 608



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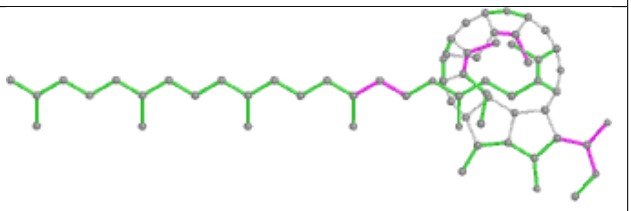
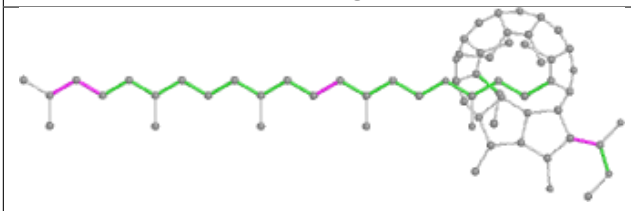


Bond angles



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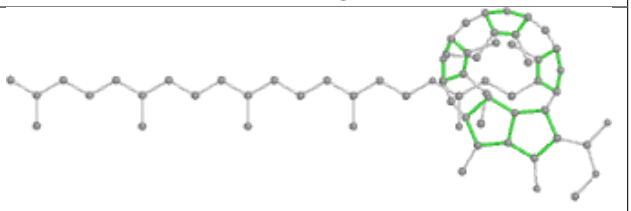
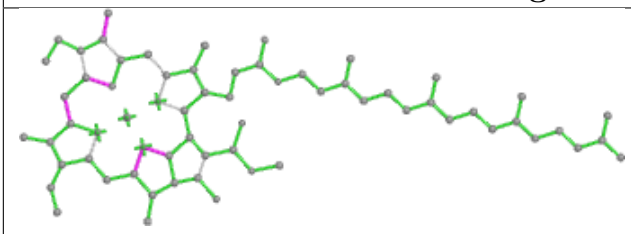


Rings

Ligand CLA c 511



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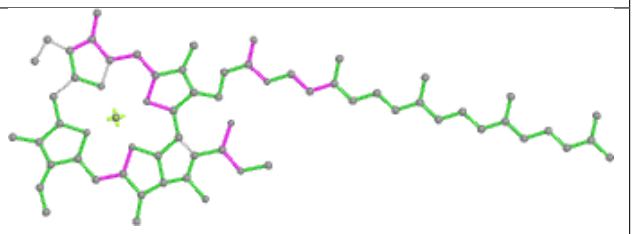
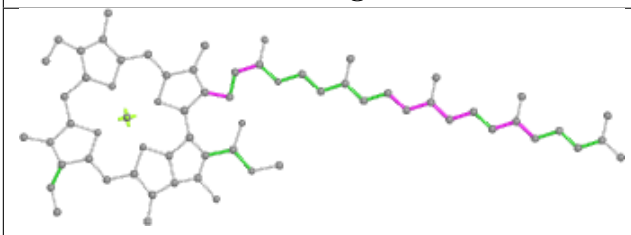


Bond angles



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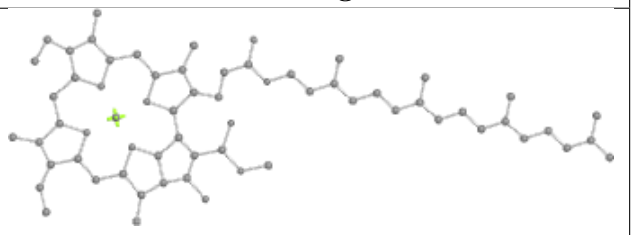
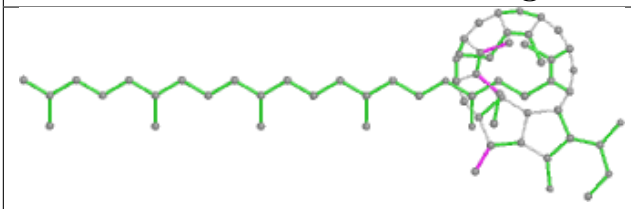


Rings

Ligand PHO D 401



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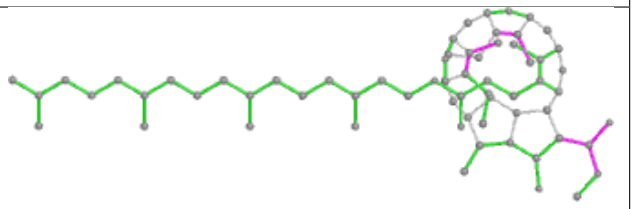
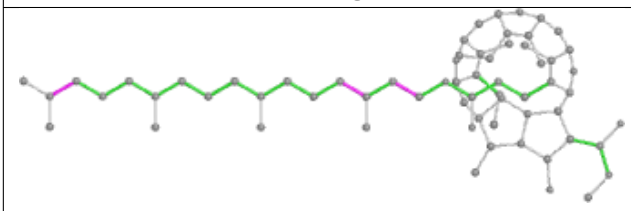


Bond angles



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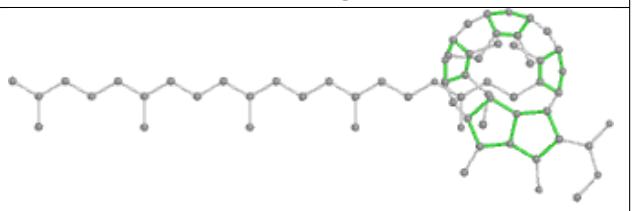
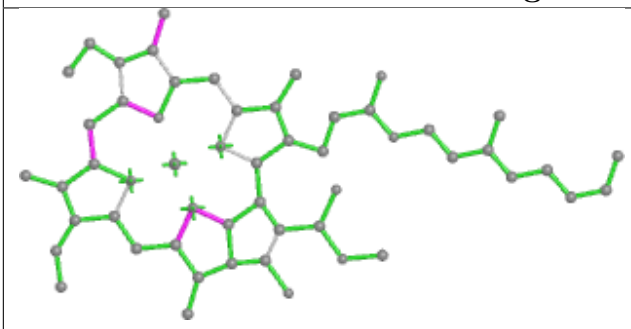


Rings

Ligand CLA A 609



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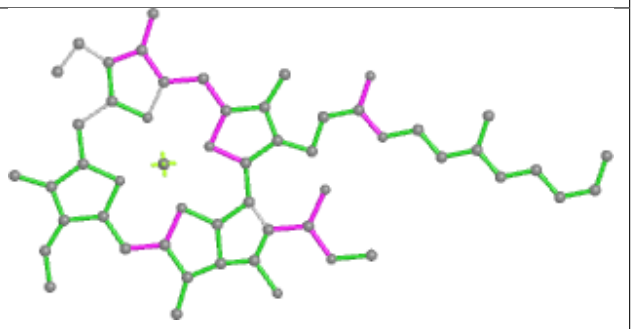

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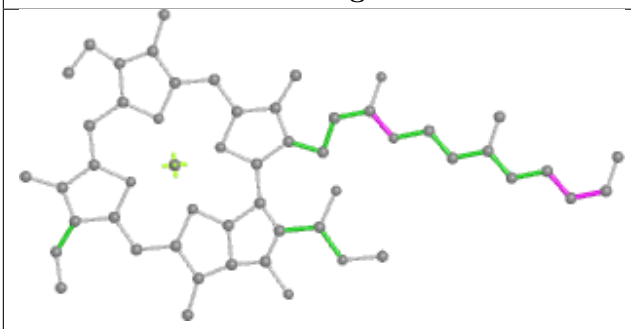

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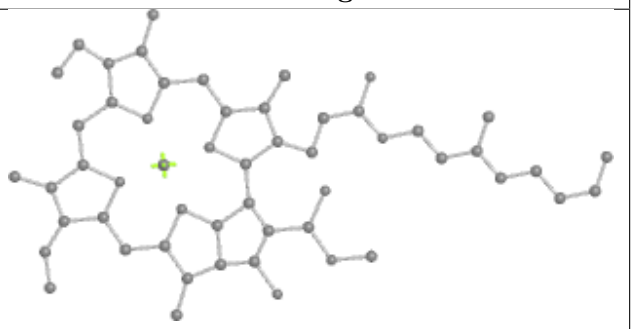
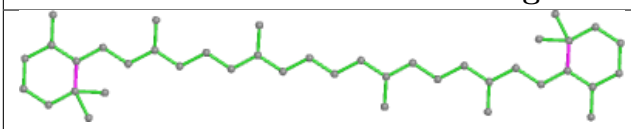


Rings

Ligand BCR B 617



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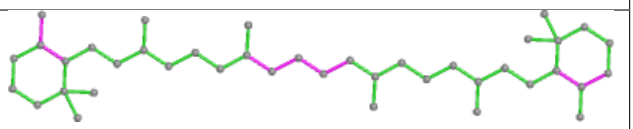
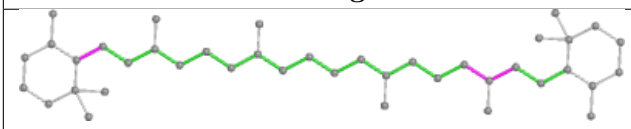


Bond angles



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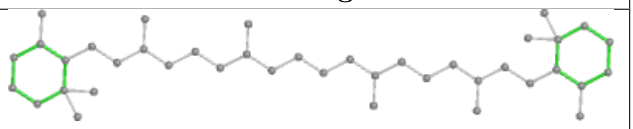
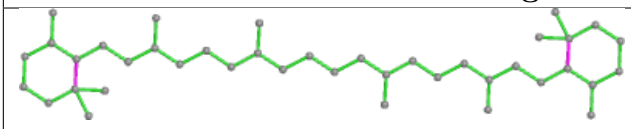


Rings

Ligand BCR D 404



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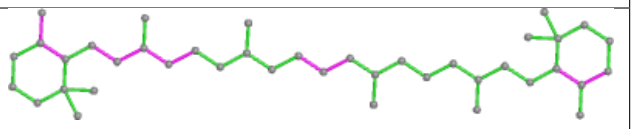
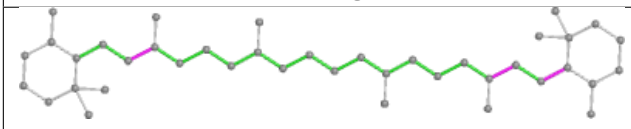


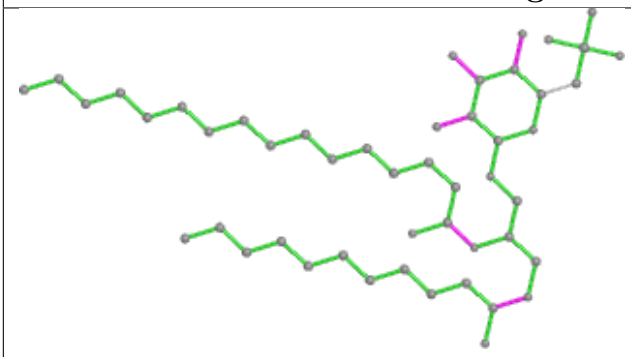
Bond angles



Torsions

Rings

Ligand SQD L 101



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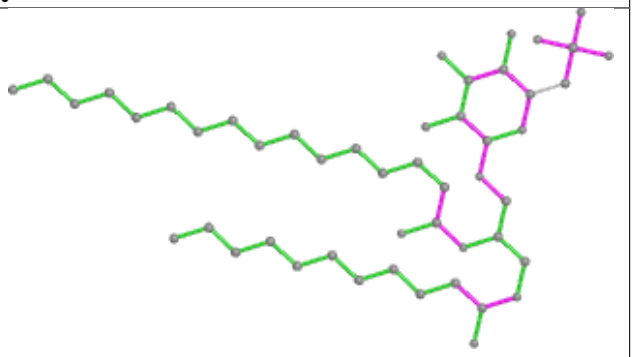
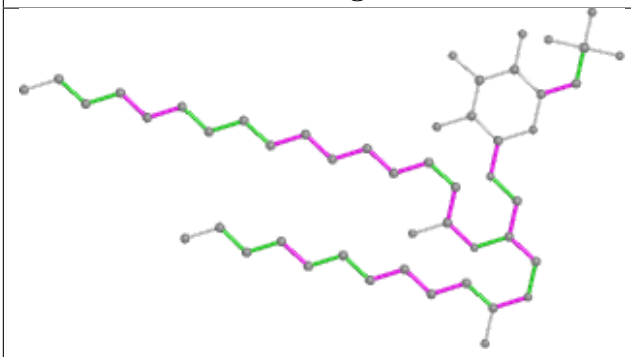
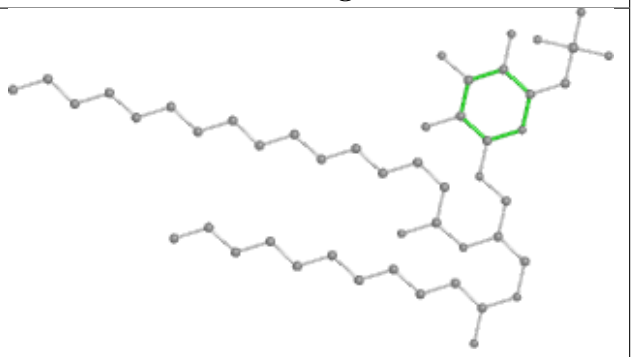


Bond angles

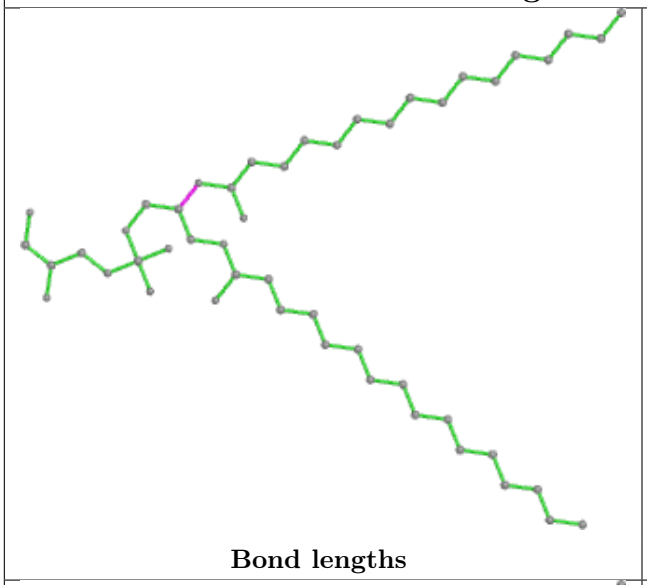


Torsions



Rings

Ligand LHG D 406



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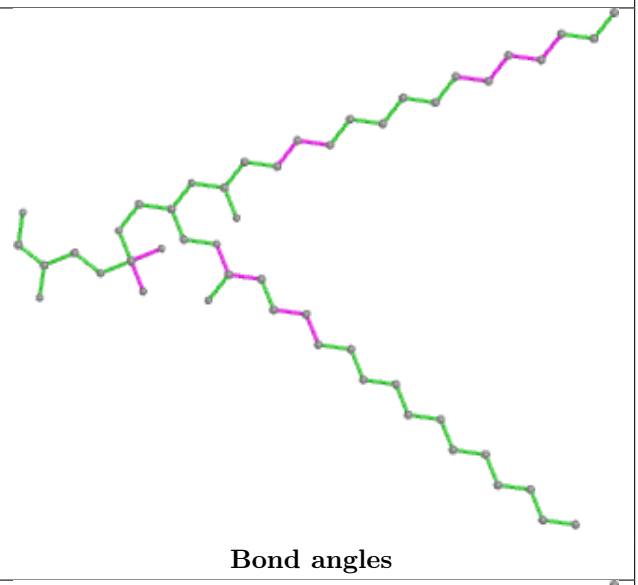
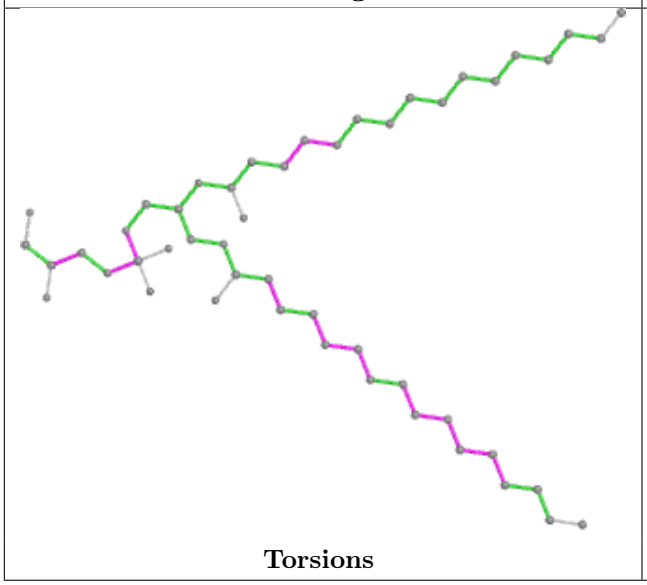


Bond angles



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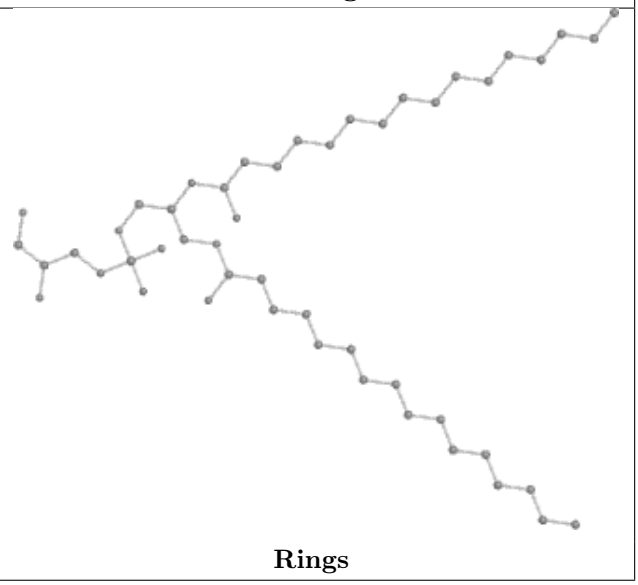
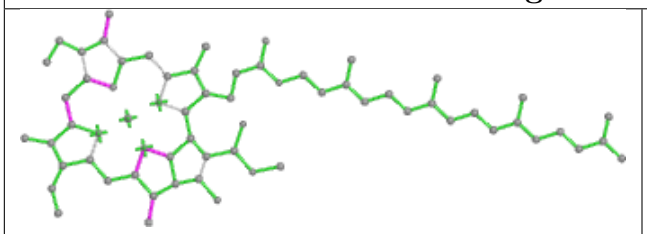
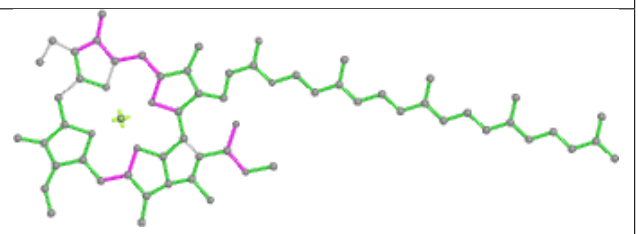


Rings

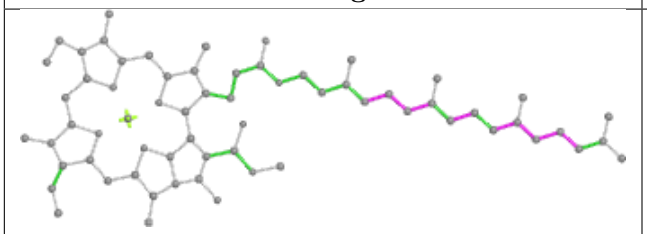
Ligand CLA B 608



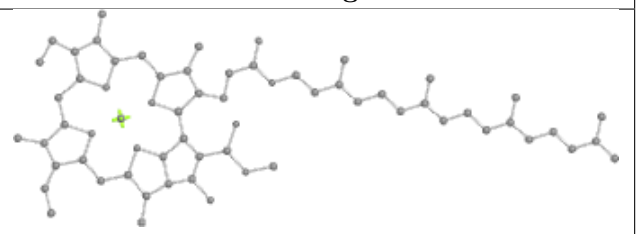
Bond lengths



Bond angles

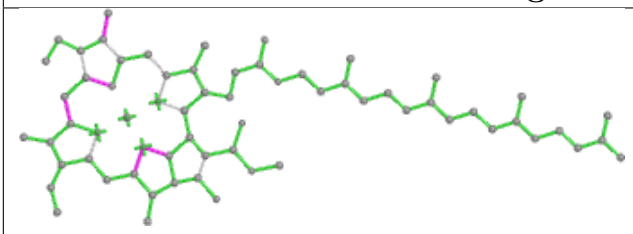


Torsions

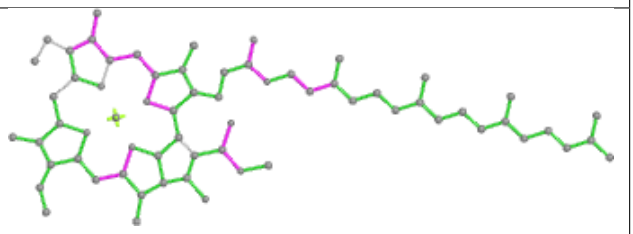


Rings

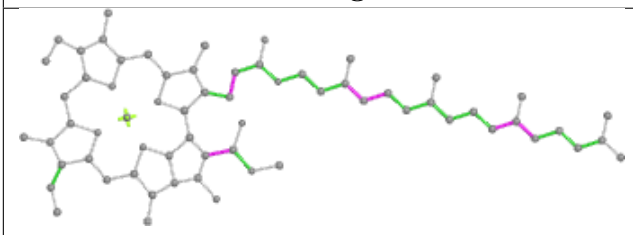
Ligand CLA b 610



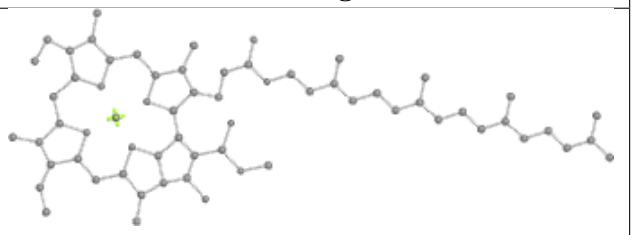
Bond lengths



Bond angles

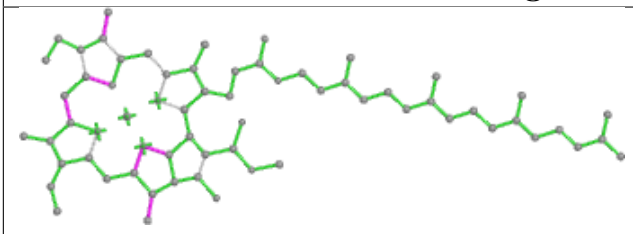


Torsions

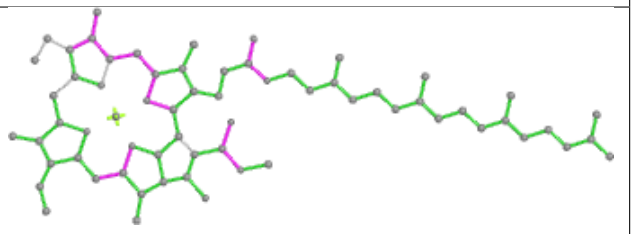


Rings

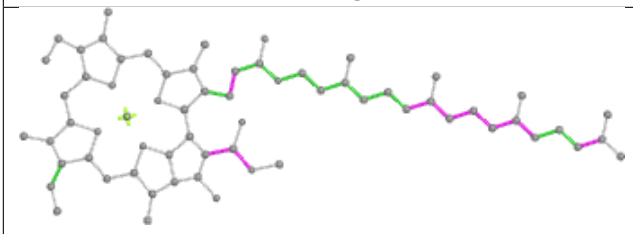
Ligand CLA B 606



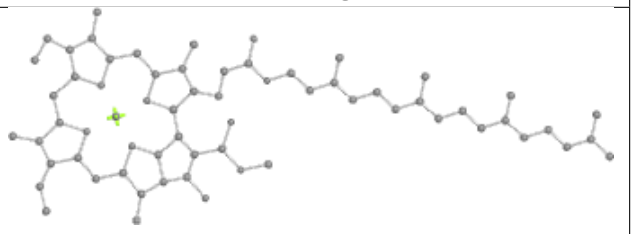
Bond lengths



Bond angles

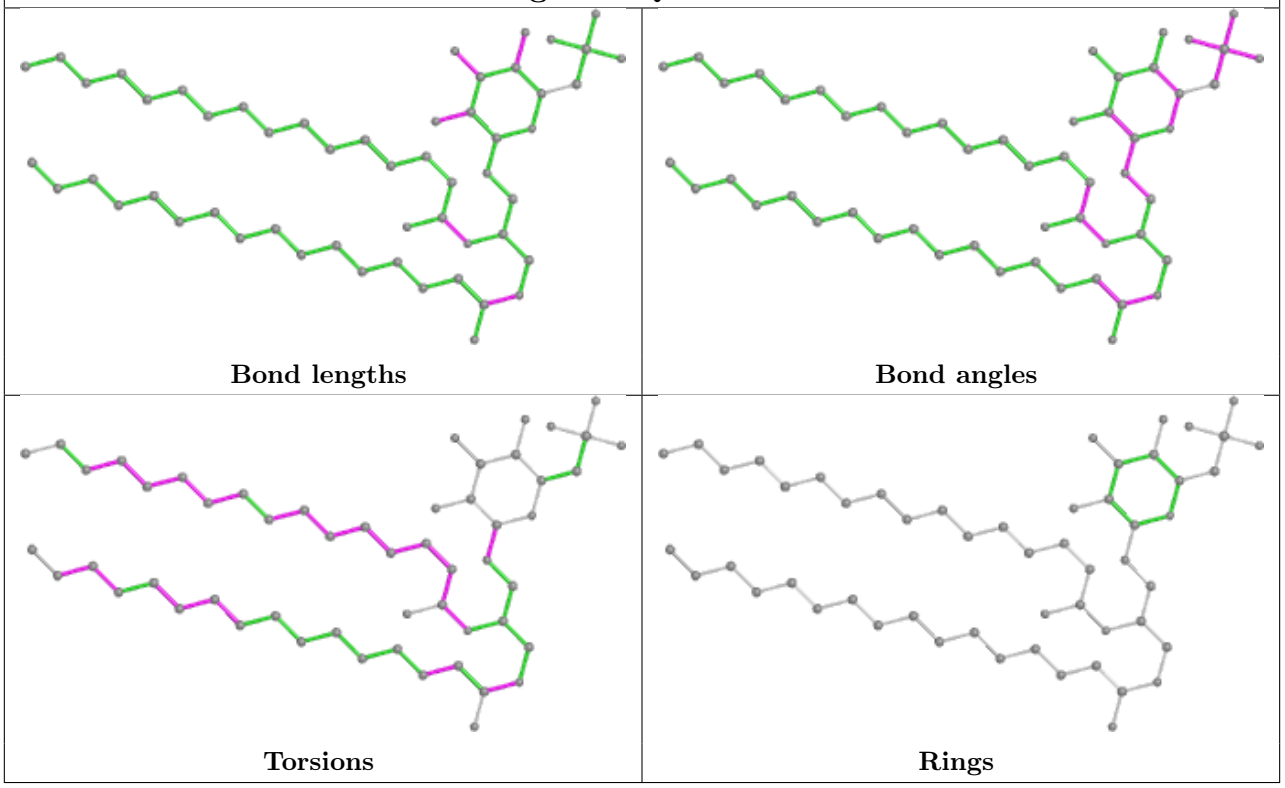


Torsions

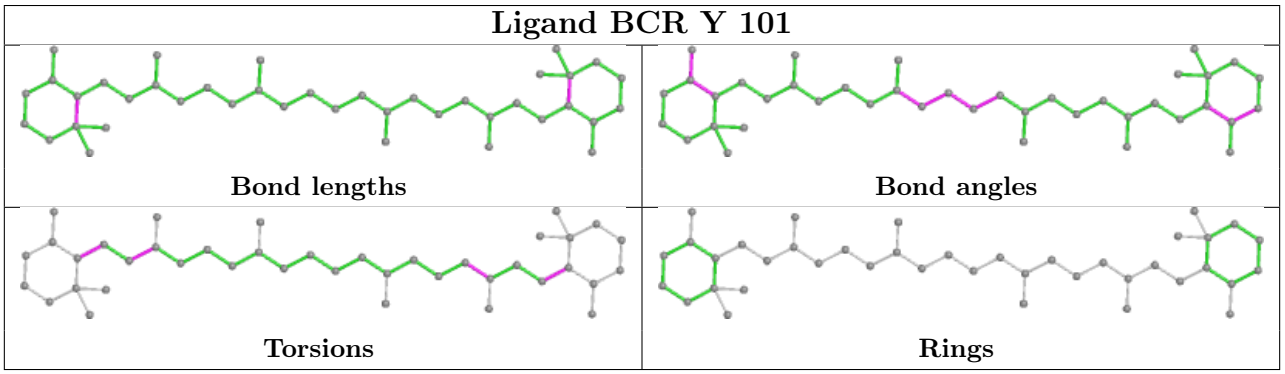


Rings

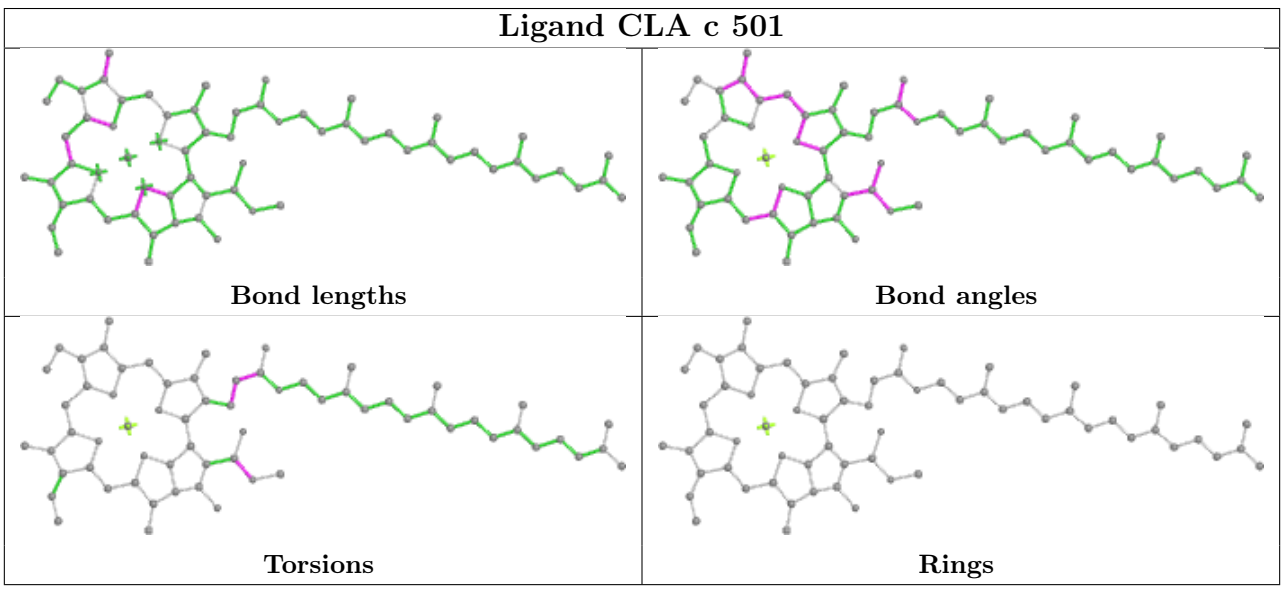
Ligand SQD a 613



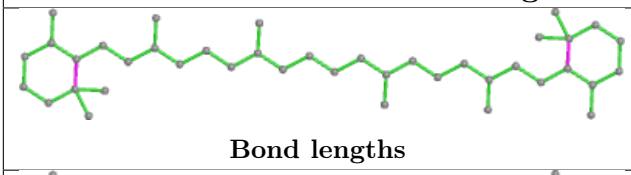
Ligand BCR Y 101



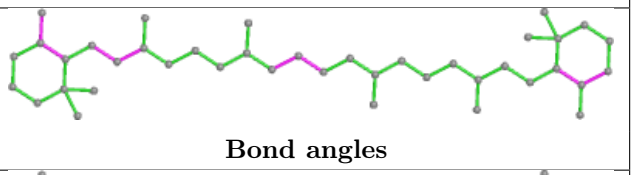
Ligand CLA c 501



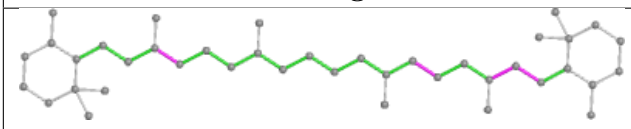
Ligand BCR H 101



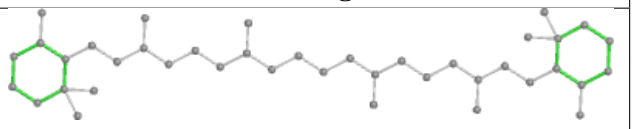
Bond lengths



Bond angles

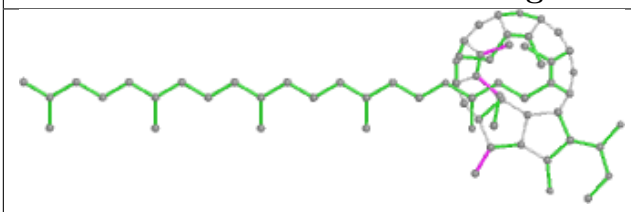


Torsions

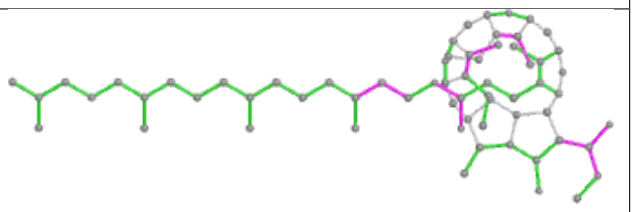


Rings

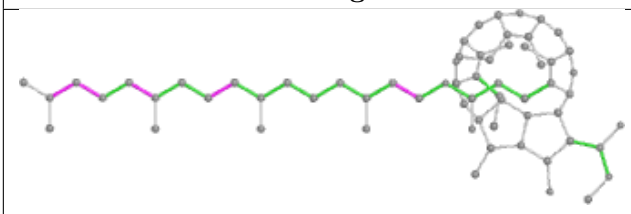
Ligand PHO a 608



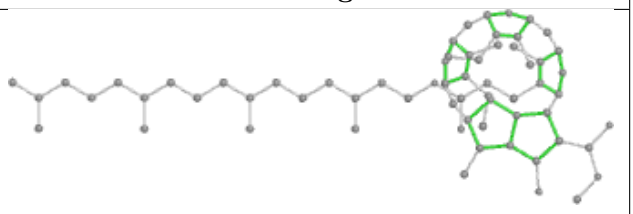
Bond lengths



Bond angles

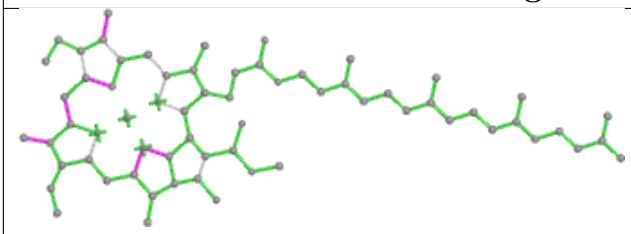


Torsions

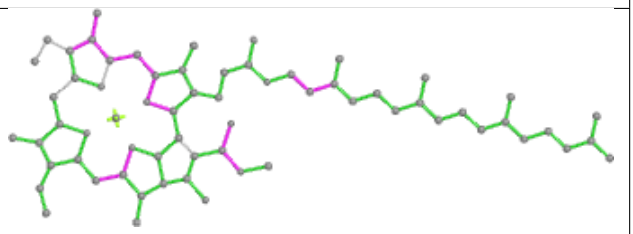


Rings

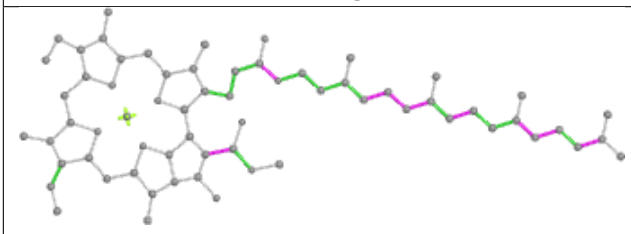
Ligand CLA B 616



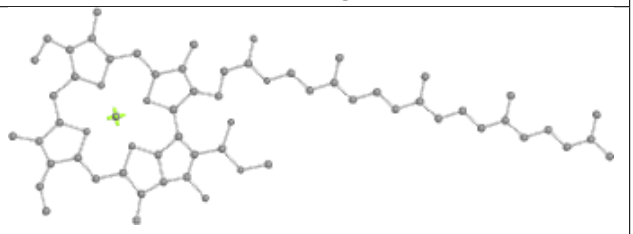
Bond lengths



Bond angles

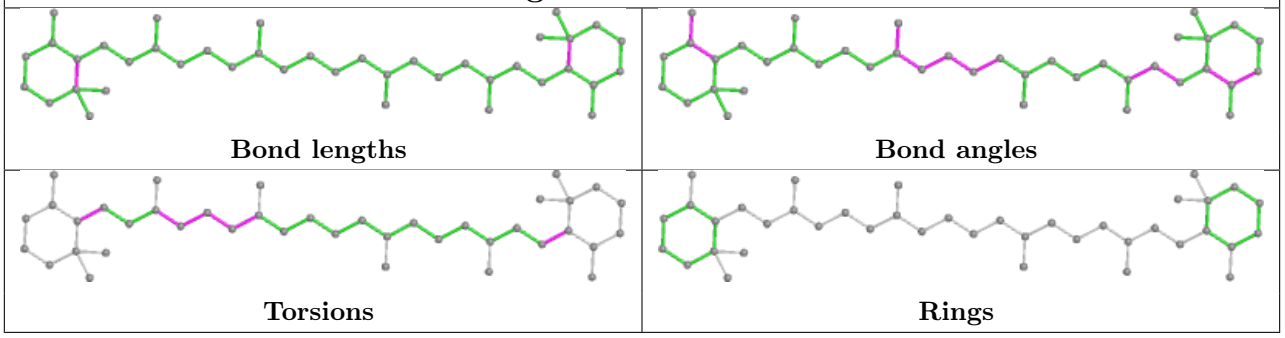


Torsions

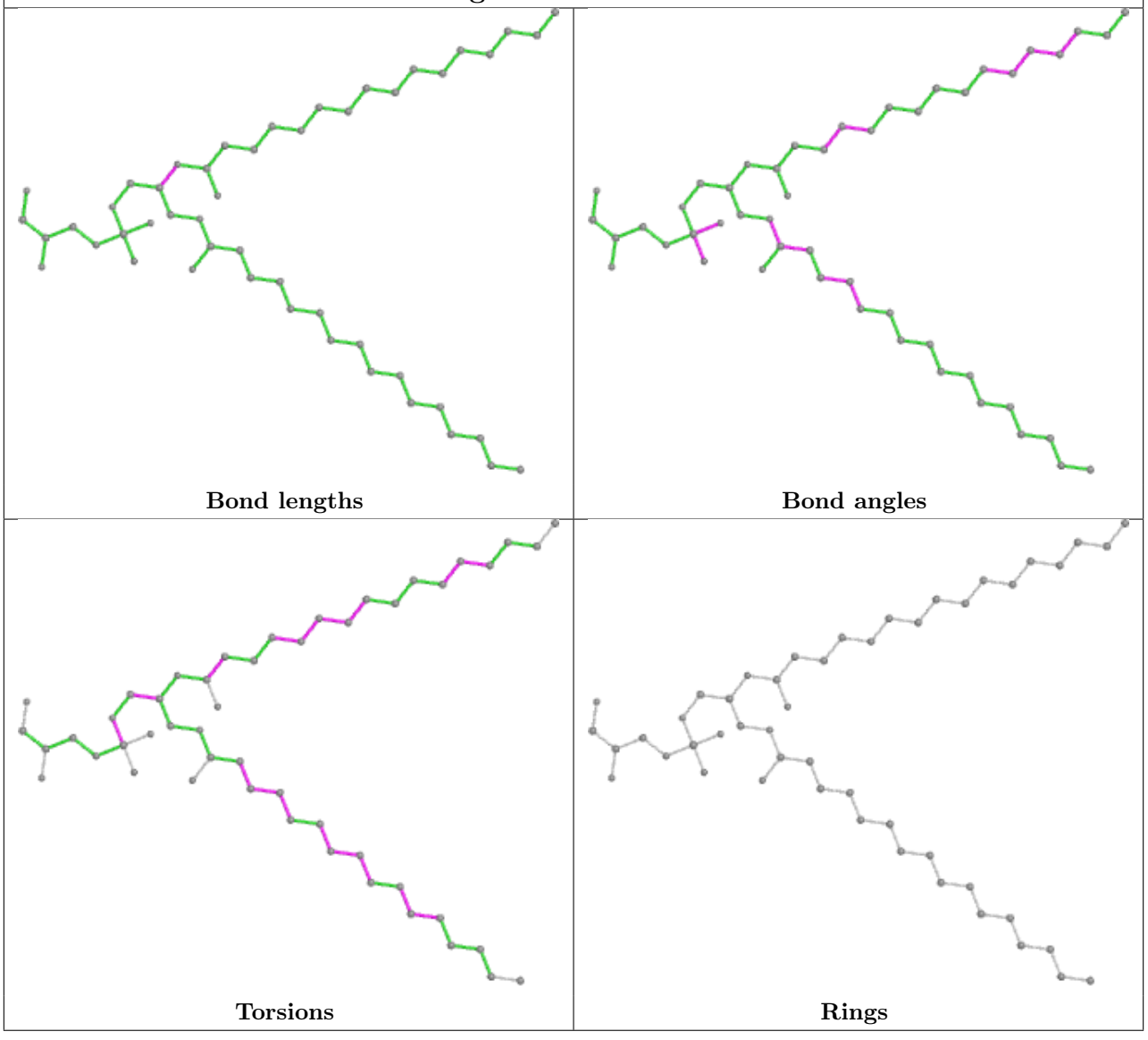


Rings

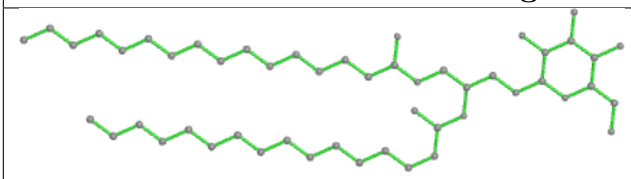
Ligand BCR b 618



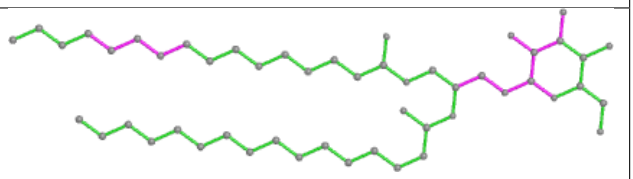
Ligand LHG L 102



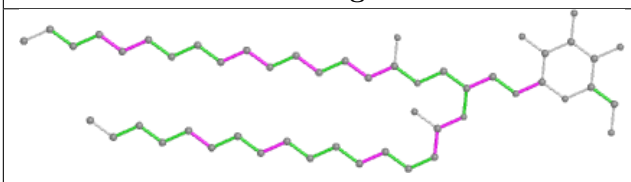
Ligand LMG B 620



Bond lengths



Bond angles



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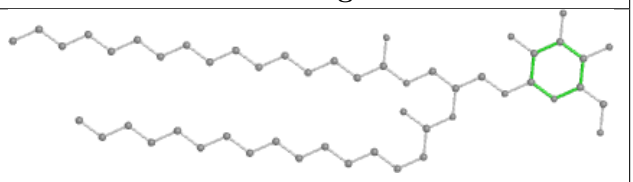
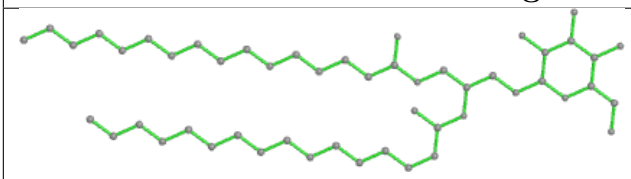
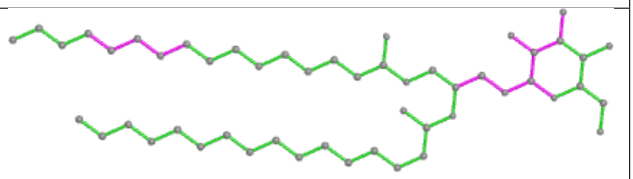


Rings

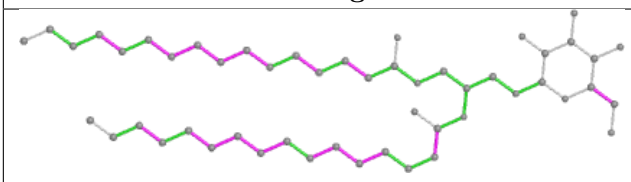
Ligand LMG d 407



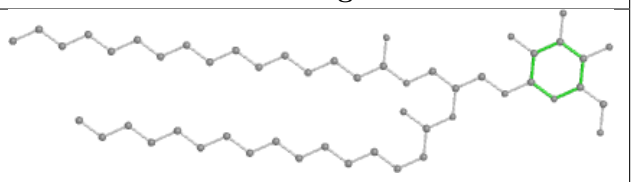
Bond lengths



Bond angles

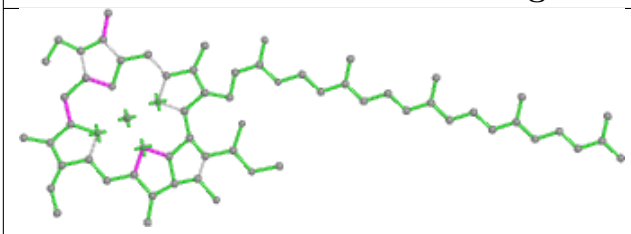


Torsions

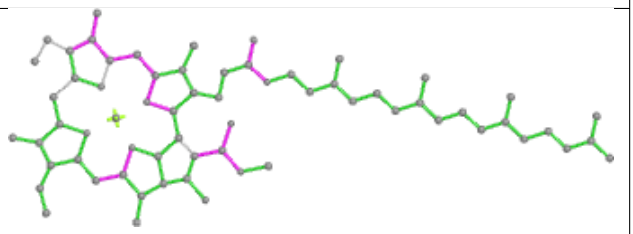


Rings

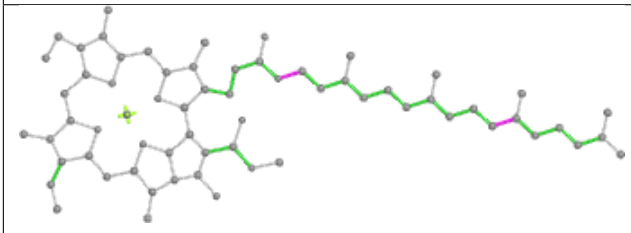
Ligand CLA a 606



Bond lengths



Bond angles



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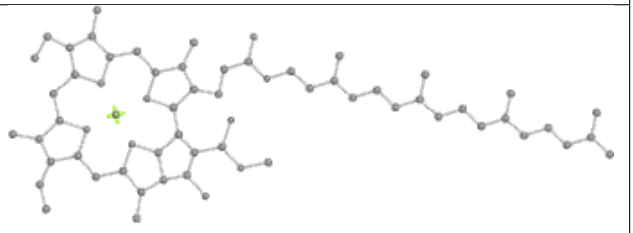
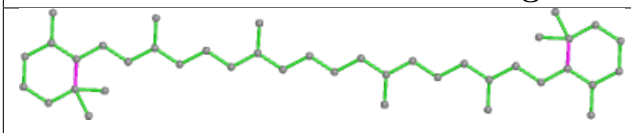
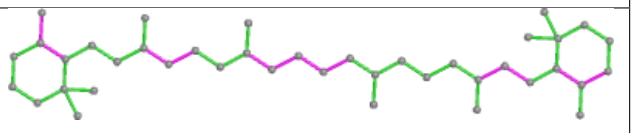


Rings

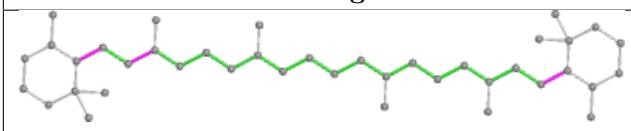
Ligand BCR A 610



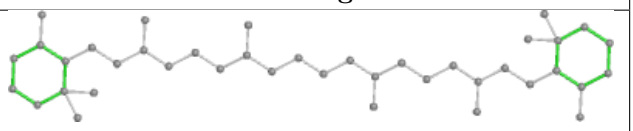
Bond lengths



Bond angles

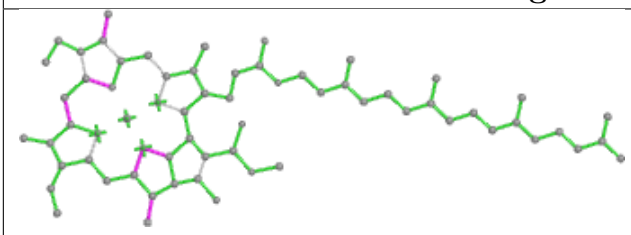


Torsions



Rings

Ligand CLA c 505



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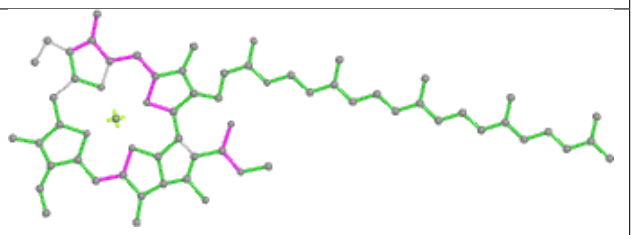
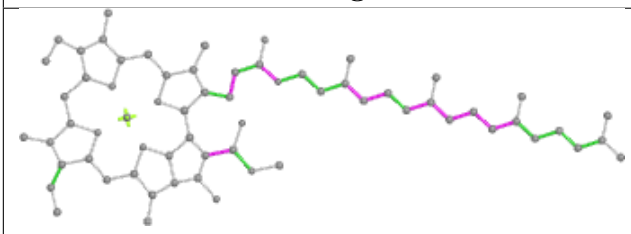
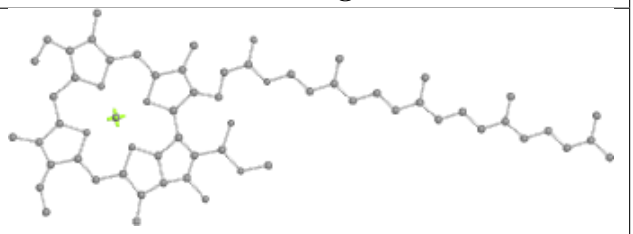


Bond angles

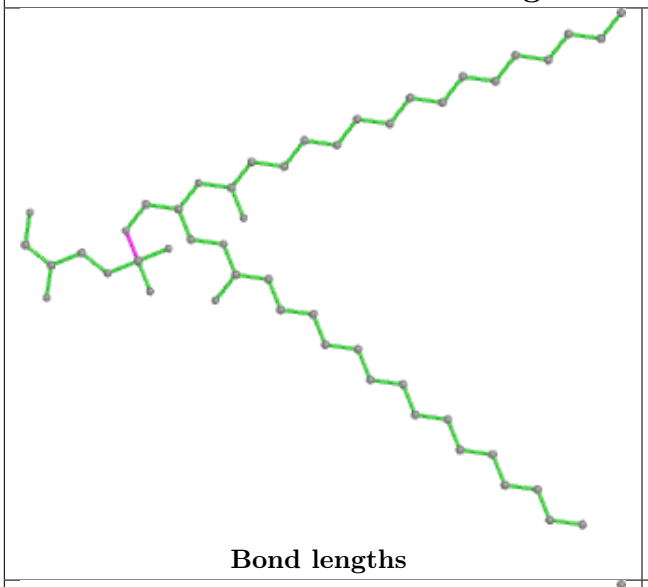


Torsions

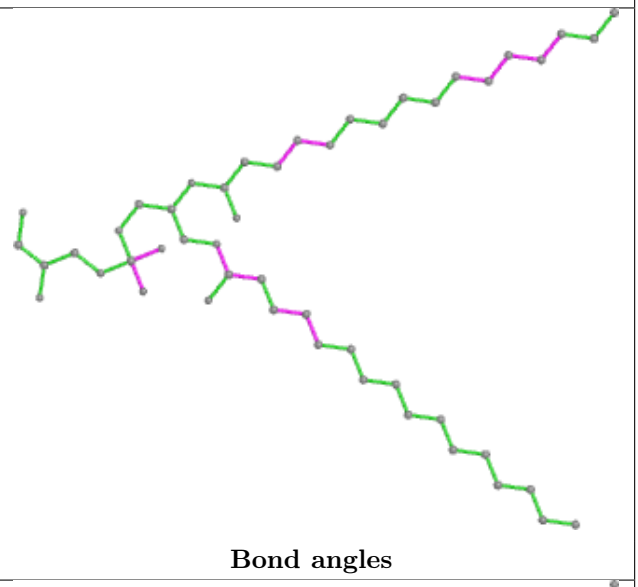


Rings

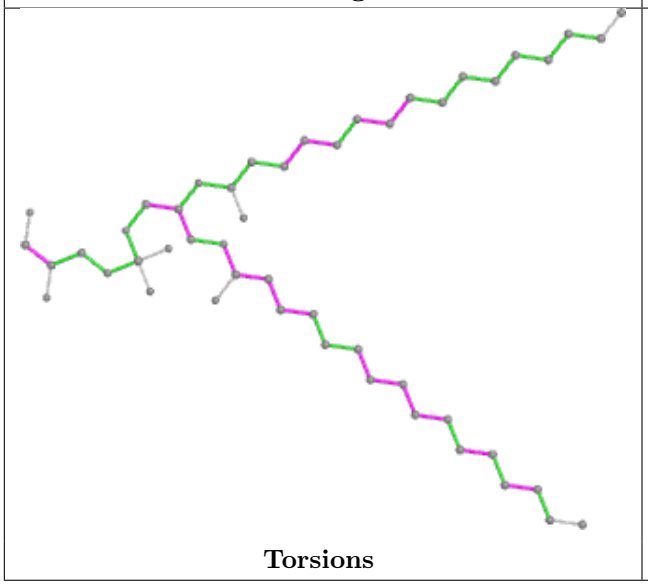
Ligand LHG A 618



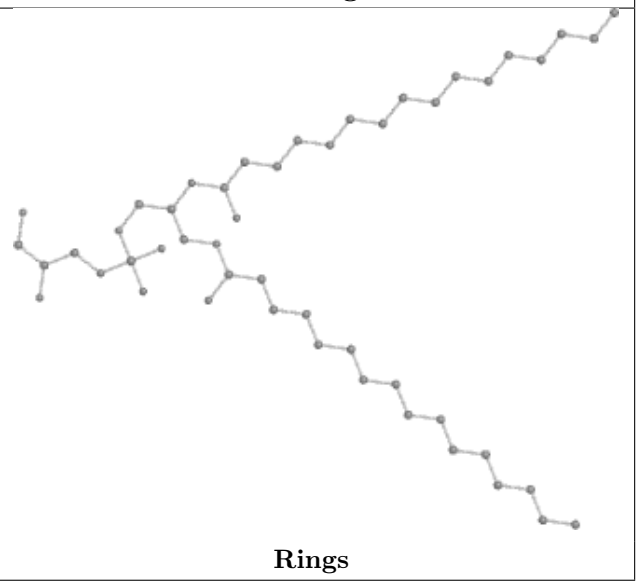
Bond lengths



Bond angles

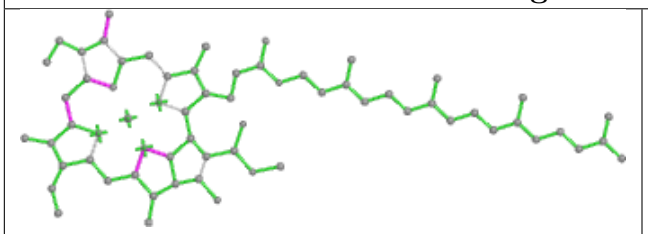


Torsions

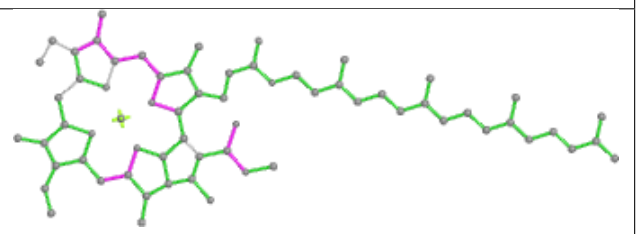


Rings

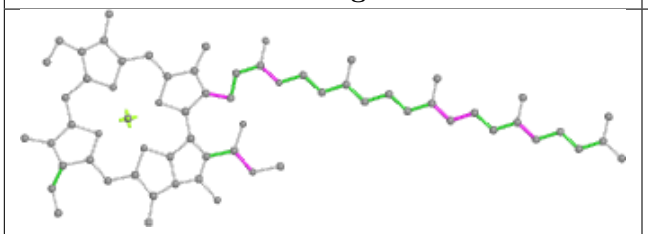
Ligand CLA c 513



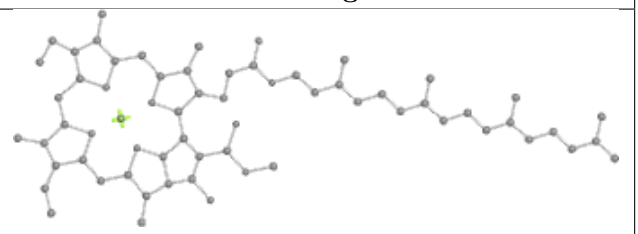
Bond lengths



Bond angles

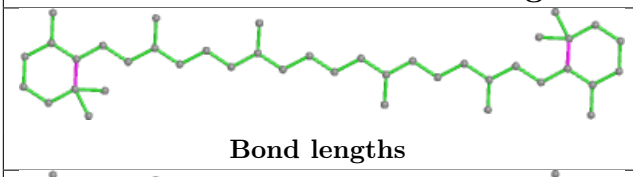


Torsions

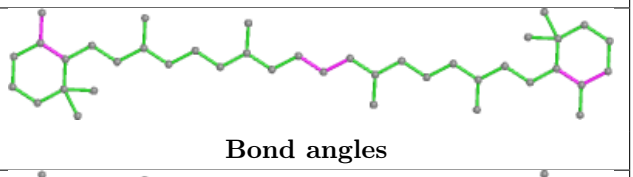


Rings

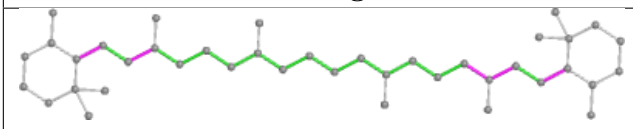
Ligand BCR b 619



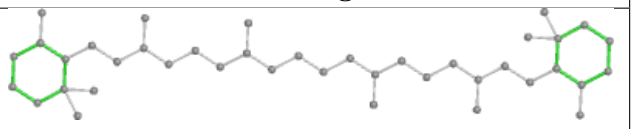
Bond lengths



Bond angles

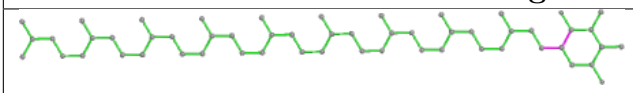


Torsions

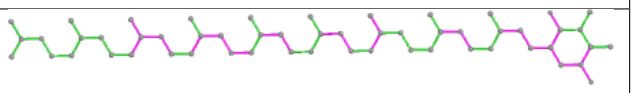


Rings

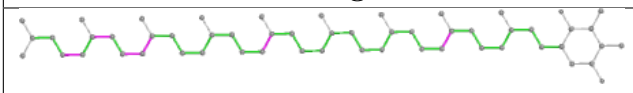
Ligand PL9 D 405



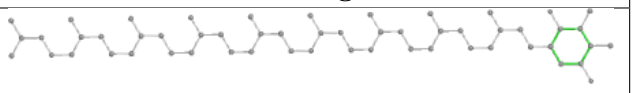
Bond lengths



Bond angles

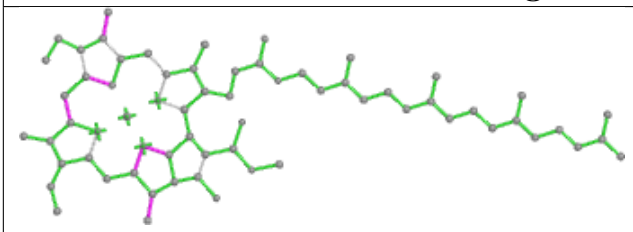


Torsions

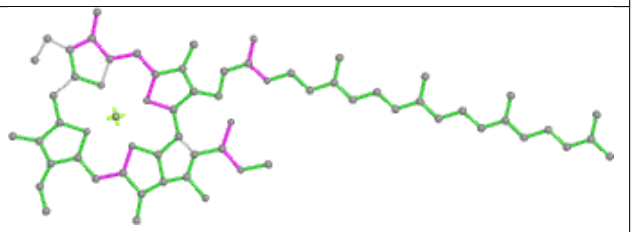


Rings

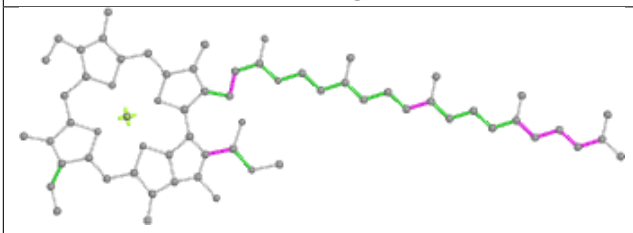
Ligand CLA B 603



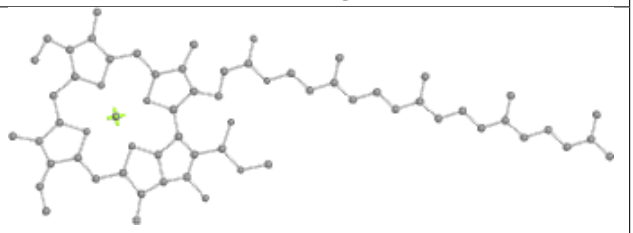
Bond lengths



Bond angles

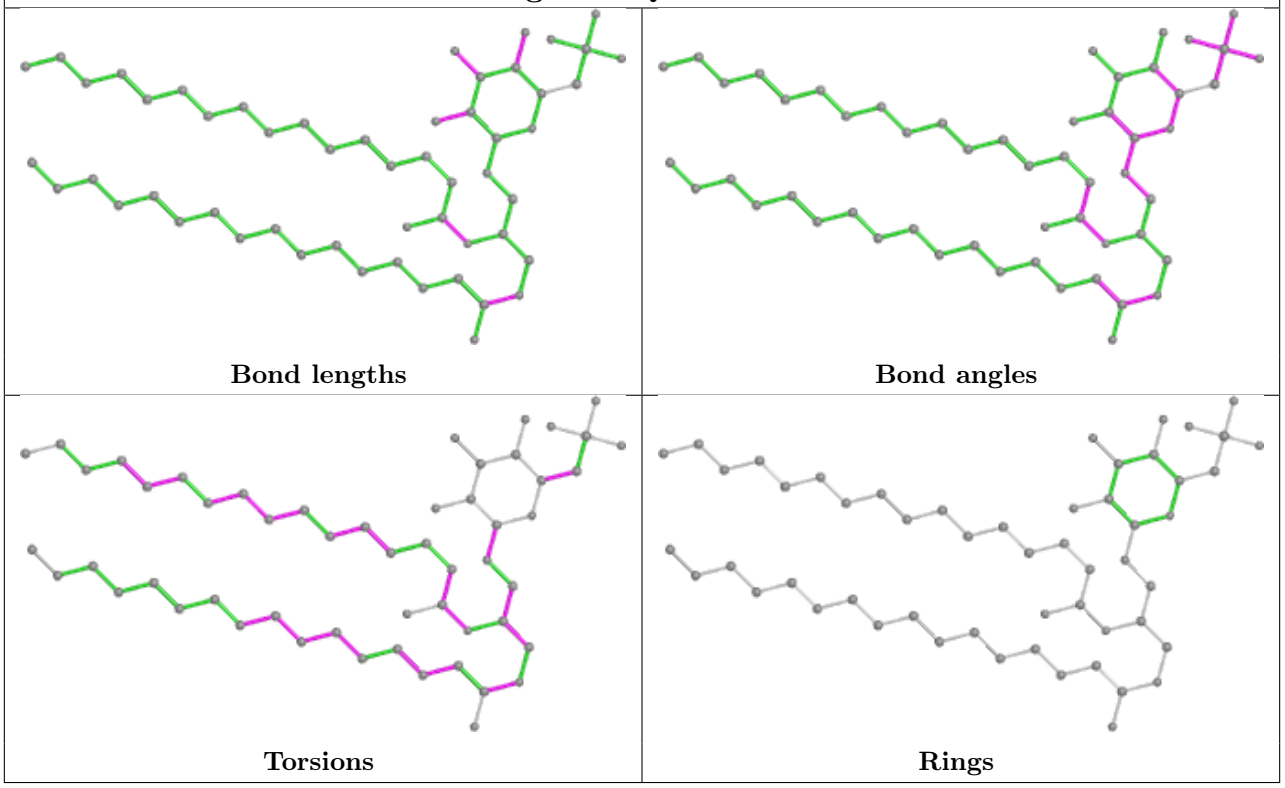


Torsions



Rings

Ligand SQD B 624



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.36	3 (0%) 84 85	28, 34, 52, 81	0
1	a	334/344 (97%)	-0.21	4 (1%) 79 81	28, 36, 63, 83	0
2	B	504/510 (98%)	-0.30	15 (2%) 50 53	28, 38, 65, 97	0
2	b	504/510 (98%)	-0.10	25 (4%) 28 31	29, 41, 76, 102	0
3	C	451/461 (97%)	-0.20	7 (1%) 72 74	30, 41, 61, 101	0
3	c	451/461 (97%)	-0.15	7 (1%) 72 74	31, 44, 65, 97	0
4	D	341/352 (96%)	-0.34	3 (0%) 84 85	28, 35, 52, 92	0
4	d	341/352 (96%)	-0.18	6 (1%) 68 71	28, 39, 61, 98	0
5	E	81/84 (96%)	0.12	5 (6%) 20 22	37, 55, 75, 97	0
5	e	82/84 (97%)	0.53	5 (6%) 21 23	42, 61, 83, 99	0
6	F	34/45 (75%)	-0.45	1 (2%) 51 55	41, 48, 70, 82	0
6	f	34/45 (75%)	-0.08	2 (5%) 22 24	44, 55, 83, 91	0
7	H	65/66 (98%)	-0.32	1 (1%) 73 75	36, 44, 61, 93	0
7	h	63/66 (95%)	0.14	4 (6%) 20 22	42, 51, 66, 70	0
8	I	36/38 (94%)	0.39	4 (11%) 5 5	36, 44, 78, 90	0
8	i	35/38 (92%)	-0.22	1 (2%) 51 55	36, 45, 72, 94	0
9	J	36/40 (90%)	-0.18	3 (8%) 11 12	39, 54, 81, 88	0
9	j	36/40 (90%)	0.15	3 (8%) 11 12	41, 57, 87, 96	0
10	K	37/46 (80%)	-0.03	1 (2%) 54 57	47, 56, 76, 83	0
10	k	37/46 (80%)	-0.21	0 100 100	52, 58, 74, 89	0
11	L	37/37 (100%)	-0.16	0 100 100	31, 34, 67, 72	0
11	l	37/37 (100%)	-0.17	4 (10%) 5 5	30, 37, 80, 104	0
12	M	32/36 (88%)	-0.36	1 (3%) 49 52	34, 39, 69, 93	0
12	m	32/36 (88%)	-0.46	1 (3%) 49 52	34, 40, 60, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.12	13 (5%) 26 29	28, 46, 84, 131	0
13	o	244/272 (89%)	-0.06	11 (4%) 33 36	30, 46, 85, 133	0
14	T	29/32 (90%)	0.30	2 (6%) 16 18	33, 37, 58, 84	0
14	t	29/32 (90%)	-0.12	1 (3%) 45 47	32, 37, 71, 88	0
15	U	97/134 (72%)	0.11	2 (2%) 63 66	36, 47, 74, 103	0
15	u	97/134 (72%)	-0.24	2 (2%) 63 66	34, 44, 62, 102	0
16	V	137/163 (84%)	-0.43	0 100 100	35, 44, 60, 85	0
16	v	137/163 (84%)	0.08	4 (2%) 51 55	37, 50, 71, 92	0
17	Y	27/46 (58%)	1.63	10 (37%) 0 0	57, 75, 102, 112	0
17	y	30/46 (65%)	0.42	5 (16%) 1 1	59, 74, 88, 97	0
18	X	38/41 (92%)	0.00	2 (5%) 26 29	43, 51, 76, 83	0
18	x	38/41 (92%)	0.51	4 (10%) 6 6	48, 60, 81, 100	0
19	Z	62/62 (100%)	1.15	13 (20%) 1 1	57, 72, 113, 123	0
19	z	62/62 (100%)	1.48	18 (29%) 0 0	59, 74, 111, 124	0
20	R	34/41 (82%)	1.79	17 (50%) 0 0	64, 76, 94, 102	0
20	r	34/41 (82%)	3.50	25 (73%) 0 0	75, 91, 109, 110	0
All	All	5313/5700 (93%)	-0.08	235 (4%) 34 37	28, 42, 78, 133	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	30	PRO	11.2
8	I	37	LEU	10.7
13	o	61	GLN	9.8
2	b	127	ARG	8.7
20	r	35	LEU	8.0
19	z	33	TRP	7.8
19	z	34	ASP	7.1
19	Z	62	VAL	7.1
20	r	26	TYR	6.9
3	c	23	ALA	6.9
17	Y	20	ALA	6.6
3	C	23	ALA	6.5
3	C	24	THR	6.5
20	r	25	PRO	6.5
17	Y	22	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
13	o	3	GLN	6.3
19	z	3	ILE	6.3
2	b	128	THR	6.3
13	O	60	ARG	6.2
13	O	62	GLU	6.0
19	Z	32	ASP	6.0
17	Y	40	ALA	6.0
19	z	36	SER	5.8
20	r	9	LEU	5.7
13	O	61	GLN	5.5
18	x	38	GLN	5.5
13	o	60	ARG	5.5
14	T	29	ILE	5.5
4	D	12	ARG	5.4
6	f	12	SER	5.3
20	r	28	VAL	5.3
20	r	23	ILE	5.3
19	z	1	MET	5.2
1	A	13	LEU	5.2
5	e	4	THR	5.0
20	r	27	ALA	5.0
11	l	1	MET	5.0
2	b	85	GLY	5.0
5	e	79	PHE	4.9
13	O	56	PRO	4.8
20	r	13	LEU	4.8
20	r	34	LEU	4.8
3	C	29	GLU	4.7
8	I	36	ASP	4.7
18	X	2	THR	4.7
13	o	62	GLU	4.7
8	i	36	ASP	4.6
19	Z	42	LEU	4.6
20	r	31	VAL	4.6
20	R	35	LEU	4.5
1	a	11	ALA	4.5
12	m	33	GLN	4.5
20	r	20	VAL	4.5
13	o	56	PRO	4.4
19	Z	33	TRP	4.4
13	O	4	THR	4.4
20	r	10	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
9	J	5	GLY	4.3
13	O	3	GLN	4.3
20	r	29	LYS	4.3
2	b	86	ILE	4.2
20	r	18	TRP	4.2
2	b	487	SER	4.2
20	R	27	ALA	4.2
20	R	3	TRP	4.0
17	Y	42	ARG	4.0
9	j	7	ARG	3.9
20	r	14	LEU	3.9
20	R	6	LEU	3.9
13	o	57	LYS	3.9
20	r	2	ASP	3.7
9	j	6	GLY	3.7
3	c	143	TYR	3.7
2	B	494	GLY	3.7
5	E	84	LYS	3.7
20	r	24	LEU	3.7
20	r	30	GLN	3.7
13	o	58	ASN	3.6
4	d	12	ARG	3.6
2	b	495	PHE	3.6
9	J	6	GLY	3.6
2	b	298	LEU	3.5
5	e	74	GLN	3.5
19	Z	1	MET	3.5
13	O	63	ALA	3.5
17	Y	41	VAL	3.5
20	r	32	GLN	3.5
12	M	33	GLN	3.5
2	B	295	GLY	3.4
3	c	24	THR	3.4
19	z	39	LEU	3.4
2	B	289	GLN	3.3
13	o	5	LEU	3.3
20	r	21	ARG	3.3
6	F	12	SER	3.3
11	l	2	GLU	3.3
5	e	81[A]	GLU	3.3
2	B	488	PRO	3.2
20	r	33	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	b	503	THR	3.2
19	Z	34	ASP	3.2
20	R	21	ARG	3.2
17	Y	21	GLN	3.2
4	d	238	THR	3.1
1	a	13	LEU	3.1
20	R	28	VAL	3.1
20	R	18	TRP	3.1
14	T	30	THR	3.0
5	E	79	PHE	3.0
19	z	35	ARG	3.0
13	O	246	ALA	3.0
19	z	10	ALA	3.0
2	B	489	GLU	3.0
16	v	12	LEU	3.0
16	v	21	LEU	3.0
9	j	5	GLY	3.0
13	O	59	LYS	3.0
2	B	293	ALA	2.9
8	I	2	GLU	2.9
1	a	15	GLU	2.9
7	h	21	VAL	2.9
2	b	289	GLN	2.9
2	B	487	SER	2.9
17	y	40	ALA	2.9
1	A	11	ALA	2.8
2	B	490	GLN	2.8
2	B	496	TYR	2.8
7	h	55	LEU	2.8
4	D	13	GLY	2.8
11	l	3	PRO	2.8
7	h	56	ASP	2.8
19	z	40	ILE	2.8
19	z	41	PHE	2.8
19	z	60	PHE	2.8
3	c	29	GLU	2.8
20	R	20	VAL	2.7
6	f	13	TYR	2.7
19	z	42	LEU	2.7
13	o	207	ARG	2.7
2	b	295	GLY	2.7
19	Z	38	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	294	SER	2.7
19	z	32	ASP	2.7
3	C	27	ASP	2.7
2	B	127	ARG	2.6
15	u	86	GLU	2.6
19	z	7	LEU	2.6
20	r	3	TRP	2.6
2	b	496	TYR	2.6
15	u	8	GLU	2.6
13	o	63	ALA	2.6
13	O	55	GLU	2.6
2	b	126	PRO	2.6
3	C	25	ASN	2.6
20	r	22	ASN	2.6
7	h	6	TRP	2.5
3	C	30	SER	2.5
2	B	493	TRP	2.5
17	Y	37	PHE	2.5
20	R	26	TYR	2.5
20	R	2	ASP	2.5
15	U	75	LEU	2.5
19	Z	31	GLN	2.5
13	o	4	THR	2.4
19	z	37	LYS	2.4
18	x	39	ARG	2.4
19	Z	4	LEU	2.4
3	c	191	PRO	2.4
3	C	28	GLN	2.4
19	Z	7	LEU	2.4
2	b	293	ALA	2.4
13	O	207	ARG	2.4
2	b	463	PHE	2.4
4	d	123	ILE	2.4
1	A	12	ASN	2.4
20	R	25	PRO	2.3
17	y	45	ASN	2.3
4	d	150	ILE	2.3
16	v	15	GLU	2.3
7	H	65	LEU	2.3
17	Y	43	ARG	2.3
17	y	42	ARG	2.3
2	b	243	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	d	124	GLY	2.2
17	Y	44	GLY	2.2
3	c	279	LEU	2.2
2	b	247	PHE	2.2
15	U	67	LEU	2.2
2	b	252	VAL	2.2
2	b	248	ALA	2.2
2	b	249	ALA	2.2
2	b	297	THR	2.2
17	Y	25	ILE	2.2
17	y	19	ILE	2.2
18	X	3	ILE	2.2
11	l	7	ARG	2.2
19	Z	61	VAL	2.2
13	O	58	ASN	2.2
17	y	41	VAL	2.2
9	J	7	ARG	2.2
20	r	4	ARG	2.2
20	R	24	LEU	2.2
20	R	30	GLN	2.2
20	R	32	GLN	2.2
2	B	485	GLU	2.1
4	d	36	LEU	2.1
20	R	14	LEU	2.1
2	b	246	PHE	2.1
5	E	82	GLN	2.1
19	z	6	GLN	2.1
2	b	406	LEU	2.1
13	O	64	GLU	2.1
5	E	17	VAL	2.1
20	R	31	VAL	2.1
5	e	77	GLU	2.1
10	K	17	ILE	2.1
2	b	296	ALA	2.1
5	E	83	LEU	2.1
19	z	38	GLN	2.1
2	B	495	PHE	2.1
8	I	35	LYS	2.1
18	x	11	PHE	2.1
1	a	248	ILE	2.0
19	Z	3	ILE	2.0
14	t	30	THR	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	351	ALA	2.0
2	b	347	ARG	2.0
16	v	110	LYS	2.0
20	R	34	LEU	2.0
19	z	2	THR	2.0
2	B	459	ALA	2.0
2	b	502	VAL	2.0
20	r	8	VAL	2.0
3	c	262	ARG	2.0
18	x	2	THR	2.0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	i	1	10/11	0.93	0.18	45,53,58,58	0
12	FME	M	1	10/11	0.94	0.14	41,53,62,63	0
14	FME	T	1	10/11	0.95	0.10	32,40,59,74	0
8	FME	I	1	10/11	0.96	0.17	45,49,54,55	0
12	FME	m	1	10/11	0.96	0.14	39,51,70,77	0
14	FME	t	1	10/11	0.96	0.10	31,38,58,64	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, 95^{th} 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
31	UNL	E	102	12/-	0.49	0.26	63,85,93,95	0
31	UNL	J	102	12/-	0.62	0.39	61,79,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LMG	B	626	51/55	0.62	0.31	55,76,89,91	0
31	UNL	A	617	20/-	0.65	0.23	58,66,76,77	0
31	UNL	j	802	12/-	0.66	0.21	62,72,86,89	0
31	UNL	D	410	18/-	0.66	0.20	41,53,74,74	0
31	UNL	C	523	16/-	0.68	0.22	55,71,94,101	0
32	LMG	d	408	38/55	0.69	0.27	58,68,101,106	0
31	UNL	I	102	20/-	0.73	0.22	46,64,81,84	0
29	SQD	D	409	47/54	0.74	0.21	41,59,109,125	0
29	SQD	B	625	54/54	0.74	0.26	52,72,92,105	0
29	SQD	b	621	40/54	0.75	0.20	48,58,68,70	0
28	PL9	a	612	55/55	0.77	0.28	51,67,89,96	0
31	UNL	J	101	11/-	0.77	0.23	48,61,68,68	0
31	UNL	a	619	12/-	0.78	0.26	60,65,71,76	0
31	UNL	c	525	12/-	0.79	0.25	50,62,73,73	0
32	LMG	C	501	48/55	0.79	0.20	46,61,76,89	0
31	UNL	x	101	16/-	0.79	0.22	41,51,65,68	0
28	PL9	A	611	55/55	0.80	0.27	42,60,82,88	55
30	LHG	A	618	49/49	0.80	0.27	56,90,112,115	0
29	SQD	A	616	54/54	0.80	0.21	50,70,96,103	0
31	UNL	a	618	17/-	0.80	0.16	46,57,71,72	0
31	UNL	I	101	7/-	0.80	0.19	53,57,64,65	0
31	UNL	c	523	8/-	0.80	0.15	49,59,77,84	0
29	SQD	B	624	54/54	0.81	0.20	43,62,96,106	0
31	UNL	c	524	20/-	0.81	0.18	45,67,82,83	0
31	UNL	M	102	17/-	0.81	0.21	52,61,73,74	0
32	LMG	C	520	48/55	0.81	0.19	47,69,88,95	0
31	UNL	b	622	17/-	0.81	0.19	47,53,63,65	0
27	BCR	h	101	40/40	0.82	0.17	40,48,64,68	0
32	LMG	C	521	51/55	0.82	0.27	45,65,116,118	0
31	UNL	C	522	17/-	0.82	0.21	42,56,67,75	0
32	LMG	b	620	51/55	0.83	0.27	55,72,98,110	0
30	LHG	a	617	42/49	0.83	0.30	67,88,102,111	0
31	UNL	b	623	11/-	0.84	0.18	59,66,68,71	0
32	LMG	a	614	51/55	0.84	0.19	41,60,74,80	0
29	SQD	L	101	49/54	0.84	0.18	41,66,96,109	0
32	LMG	B	620	51/55	0.84	0.18	32,57,73,77	0
31	UNL	B	627	15/-	0.85	0.19	48,55,65,68	0
31	UNL	m	101	9/-	0.85	0.18	51,53,61,62	0
31	UNL	m	103	16/-	0.85	0.16	39,51,73,76	0
31	UNL	t	102	18/-	0.86	0.18	43,56,65,66	0
31	UNL	D	411	10/-	0.86	0.20	49,55,72,79	0
31	UNL	T	103	12/-	0.87	0.13	42,54,59,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	BCR	H	101	40/40	0.87	0.14	36,50,64,65	0
31	UNL	d	409	17/-	0.87	0.28	51,58,67,70	0
32	LMG	c	520	34/55	0.87	0.26	58,66,78,88	0
25	CLA	b	601	65/65	0.87	0.21	40,61,83,94	0
31	UNL	M	101	15/-	0.88	0.14	42,52,63,75	0
32	LMG	B	621	51/55	0.88	0.23	54,71,102,110	0
31	UNL	i	101	20/-	0.88	0.23	51,59,77,79	0
32	LMG	c	519	37/55	0.88	0.15	48,67,76,77	0
31	UNL	j	801	15/-	0.88	0.18	50,60,77,77	0
31	UNL	B	622	11/-	0.88	0.15	41,47,60,61	0
25	CLA	d	402	65/65	0.89	0.17	36,43,83,90	0
31	UNL	H	103	7/-	0.89	0.15	48,53,60,61	0
29	SQD	a	613	54/54	0.89	0.14	40,62,72,76	0
25	CLA	C	513	65/65	0.89	0.17	41,54,81,86	0
27	BCR	d	403	40/40	0.89	0.15	41,54,79,82	0
25	CLA	C	508	65/65	0.89	0.18	30,42,59,78	0
25	CLA	c	512	65/65	0.89	0.15	45,57,89,94	0
32	LMG	m	102	51/55	0.89	0.16	43,56,69,77	0
33	DGD	h	102	62/66	0.89	0.21	38,51,60,64	0
31	UNL	T	102	14/-	0.90	0.16	36,53,63,67	0
29	SQD	f	101	41/54	0.90	0.20	59,84,105,109	0
25	CLA	c	513	65/65	0.90	0.18	48,63,86,90	0
27	BCR	T	101	40/40	0.91	0.17	35,46,57,68	0
27	BCR	Y	101	40/40	0.91	0.12	43,51,62,68	0
27	BCR	b	617	40/40	0.91	0.14	33,44,52,52	0
27	BCR	b	618	40/40	0.91	0.17	33,44,56,59	0
27	BCR	c	521	40/40	0.91	0.12	49,59,72,73	0
31	UNL	A	615	9/-	0.91	0.17	41,52,68,70	0
27	BCR	c	522	40/40	0.91	0.14	42,54,63,69	0
25	CLA	a	610	65/65	0.91	0.15	24,32,77,81	0
25	CLA	C	504	65/65	0.91	0.17	36,44,50,59	0
25	CLA	b	609	65/65	0.91	0.14	35,46,60,66	0
25	CLA	c	506	65/65	0.91	0.15	33,48,82,95	0
25	CLA	B	601	65/65	0.91	0.15	39,54,81,87	0
25	CLA	B	609	65/65	0.91	0.12	28,39,58,69	0
25	CLA	C	514	65/65	0.91	0.23	49,60,136,139	0
29	SQD	D	408	43/54	0.91	0.22	54,76,105,108	0
27	BCR	D	404	40/40	0.91	0.16	31,44,82,86	0
33	DGD	H	102	62/66	0.91	0.16	39,47,63,65	0
25	CLA	D	403	65/65	0.91	0.19	31,37,89,99	0
25	CLA	c	507	65/65	0.92	0.14	36,46,62,72	0
27	BCR	C	515	40/40	0.92	0.13	44,53,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	c	510	65/65	0.92	0.16	36,46,61,72	0
27	BCR	c	514	40/40	0.92	0.13	49,58,62,64	0
29	SQD	A	612	52/54	0.92	0.16	48,63,85,91	0
25	CLA	B	606	65/65	0.92	0.13	28,37,63,74	0
33	DGD	c	517	62/66	0.92	0.13	39,52,81,86	0
25	CLA	b	602	65/65	0.92	0.17	33,41,59,66	0
25	CLA	B	604	65/65	0.93	0.16	27,33,72,81	0
25	CLA	C	510	65/65	0.93	0.17	32,42,66,70	0
30	LHG	d	405	49/49	0.93	0.15	43,53,68,72	0
25	CLA	C	512	65/65	0.93	0.13	39,52,67,71	0
25	CLA	b	606[A]	65/65	0.93	0.15	37,43,52,55	64
27	BCR	B	619	40/40	0.93	0.10	34,45,56,58	0
25	CLA	b	606[B]	65/65	0.93	0.15	37,43,52,58	64
27	BCR	C	516	40/40	0.93	0.14	34,44,55,57	0
25	CLA	C	503	65/65	0.93	0.19	28,39,53,65	0
25	CLA	b	615	65/65	0.93	0.11	33,44,62,69	0
27	BCR	K	101	40/40	0.93	0.14	37,52,63,66	0
25	CLA	c	502	65/65	0.93	0.18	31,41,55,63	0
25	CLA	c	503	65/65	0.93	0.15	36,45,50,57	0
25	CLA	A	606	65/65	0.93	0.12	23,32,50,59	0
33	DGD	C	518	62/66	0.93	0.15	40,50,89,97	0
25	CLA	C	507	65/65	0.93	0.12	34,46,77,89	0
27	BCR	b	619	40/40	0.93	0.10	32,48,60,61	0
25	CLA	c	509	65/65	0.93	0.15	37,45,61,64	0
25	CLA	c	501	65/65	0.94	0.15	29,38,53,56	0
25	CLA	C	506	65/65	0.94	0.12	27,40,65,70	0
25	CLA	a	606	65/65	0.94	0.12	26,33,42,58	0
30	LHG	B	623	49/49	0.94	0.17	36,47,63,70	0
30	LHG	D	406	49/49	0.94	0.18	32,40,56,74	0
30	LHG	a	616	39/49	0.94	0.13	39,48,66,71	0
27	BCR	a	611	40/40	0.94	0.11	26,37,49,54	0
25	CLA	c	505	65/65	0.94	0.12	32,41,69,76	0
30	LHG	l	101	49/49	0.94	0.12	37,49,62,76	0
25	CLA	B	611	65/65	0.94	0.15	25,34,48,52	0
25	CLA	B	614	65/65	0.94	0.13	25,37,75,81	0
25	CLA	C	509	65/65	0.94	0.12	31,41,86,89	0
27	BCR	c	515	40/40	0.94	0.12	30,46,51,63	0
25	CLA	b	604	65/65	0.94	0.18	25,35,69,82	0
25	CLA	c	511	65/65	0.94	0.12	40,54,66,73	0
25	CLA	B	616	65/65	0.94	0.15	29,39,96,102	0
25	CLA	C	502	65/65	0.94	0.17	31,37,50,59	0
27	BCR	t	101	40/40	0.94	0.15	33,43,53,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	B	607	65/65	0.94	0.16	27,36,63,71	0
32	LMG	D	407	51/55	0.94	0.14	32,52,72,82	0
26	PHO	a	608	64/64	0.94	0.14	28,34,42,49	0
28	PL9	d	404	55/55	0.94	0.14	27,39,50,54	0
26	PHO	a	609	64/64	0.94	0.17	34,40,49,52	0
27	BCR	B	617	40/40	0.94	0.13	29,45,53,57	0
32	LMG	d	407	51/55	0.94	0.15	38,58,88,93	0
27	BCR	B	618	40/40	0.94	0.16	30,44,55,60	0
25	CLA	b	610	65/65	0.94	0.15	31,40,51,66	0
25	CLA	b	611	65/65	0.94	0.12	29,36,55,66	0
33	DGD	C	519	62/66	0.94	0.12	33,50,79,84	0
25	CLA	b	614	65/65	0.94	0.13	31,39,75,79	0
25	CLA	A	607	65/65	0.94	0.16	25,35,123,129	0
33	DGD	c	518	62/66	0.94	0.12	34,48,73,77	0
25	CLA	b	616	47/65	0.94	0.09	31,42,53,57	0
25	CLA	b	613	65/65	0.95	0.18	29,38,74,89	0
27	BCR	A	610	40/40	0.95	0.09	31,37,41,41	0
28	PL9	D	405	55/55	0.95	0.13	25,35,47,49	0
25	CLA	B	608	65/65	0.95	0.18	30,38,57,60	0
25	CLA	a	607	65/65	0.95	0.12	28,43,84,90	0
25	CLA	B	615	65/65	0.95	0.11	28,40,58,66	0
25	CLA	a	615	65/65	0.95	0.13	24,34,52,62	0
24	BCT	a	605	4/4	0.95	0.14	37,45,46,53	2
25	CLA	B	610	65/65	0.95	0.13	26,37,47,55	0
25	CLA	c	504	60/65	0.95	0.12	34,47,69,77	0
25	CLA	C	511	65/65	0.95	0.18	30,43,58,70	0
25	CLA	b	605	65/65	0.95	0.14	25,37,46,52	0
25	CLA	A	613	65/65	0.95	0.13	25,33,44,53	0
25	CLA	c	508	64/65	0.95	0.11	36,45,82,87	0
25	CLA	B	612	65/65	0.95	0.15	25,33,42,45	0
30	LHG	A	614	47/49	0.95	0.13	33,44,73,76	0
25	CLA	b	607	65/65	0.95	0.12	29,37,62,68	0
25	CLA	b	608	65/65	0.95	0.22	32,41,56,60	0
25	CLA	C	505	65/65	0.95	0.17	34,42,80,85	0
30	LHG	L	102	49/49	0.95	0.15	35,42,50,58	0
33	DGD	C	517	62/66	0.95	0.16	29,42,72,81	0
25	CLA	D	402	65/65	0.95	0.12	21,31,54,78	0
25	CLA	d	401	65/65	0.95	0.12	25,34,55,69	0
25	CLA	B	613	65/65	0.95	0.20	26,33,63,76	0
33	DGD	c	516	62/66	0.95	0.17	28,44,67,72	0
30	LHG	d	406	49/49	0.95	0.17	31,44,55,64	0
26	PHO	A	608	64/64	0.95	0.15	29,37,43,46	0

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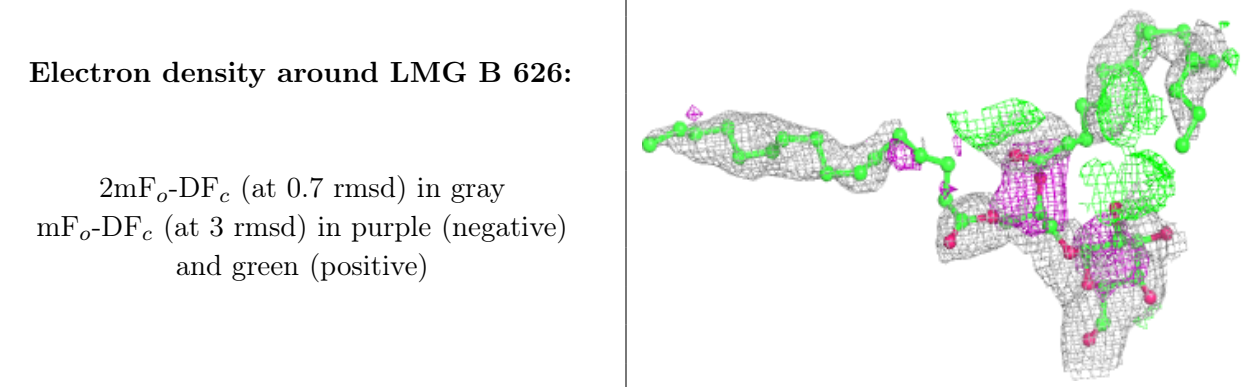
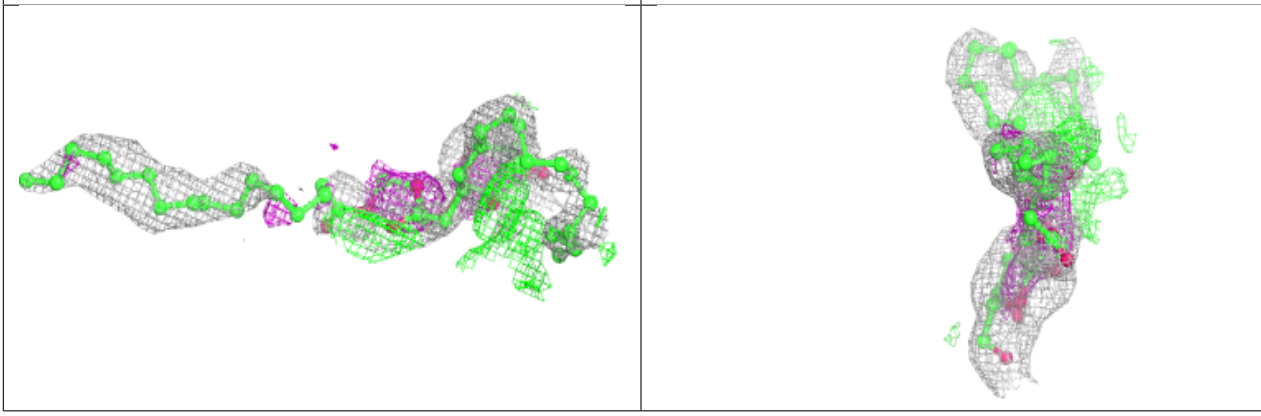
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	b	612	65/65	0.95	0.14	26,38,49,56	0
34	HEM	e	101	43/43	0.95	0.13	47,58,73,80	0
25	CLA	A	609	54/65	0.96	0.12	25,32,72,78	0
25	CLA	B	605	65/65	0.96	0.14	26,33,48,53	0
25	CLA	b	603	65/65	0.96	0.16	29,38,57,62	0
26	PHO	D	401	64/64	0.96	0.14	23,33,38,44	0
25	CLA	B	602	65/65	0.96	0.12	26,36,57,66	0
34	HEM	E	101	43/43	0.96	0.11	43,49,57,65	0
25	CLA	B	603	65/65	0.96	0.15	25,36,56,63	0
35	HEC	V	201	43/43	0.97	0.09	29,36,44,46	0
35	HEC	v	201	43/43	0.97	0.12	31,40,47,54	0
24	BCT	A	605	4/4	0.98	0.07	42,43,44,53	0
23	CL	a	603	1/1	0.98	0.07	33,33,33,33	0
21	OEX	a	601	10/10	0.99	0.11	28,32,35,42	0
22	FE2	A	602	1/1	0.99	0.04	36,36,36,36	0
22	FE2	a	602	1/1	0.99	0.05	43,43,43,43	0
23	CL	A	603	1/1	0.99	0.06	32,32,32,32	0
23	CL	A	604	1/1	0.99	0.13	33,33,33,33	0
21	OEX	A	601	10/10	0.99	0.11	32,34,40,41	1
23	CL	a	604	1/1	0.99	0.08	35,35,35,35	0

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

Electron density around LMG B 626:

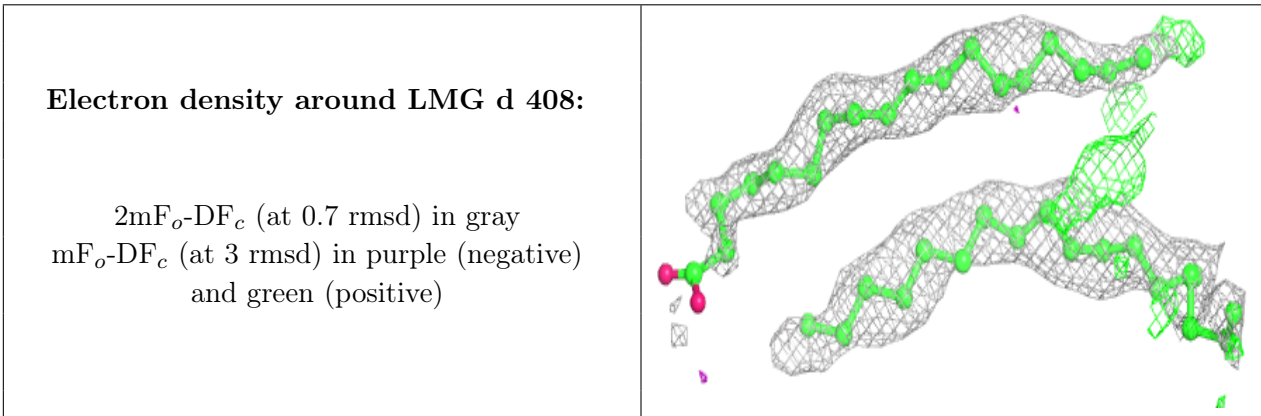
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

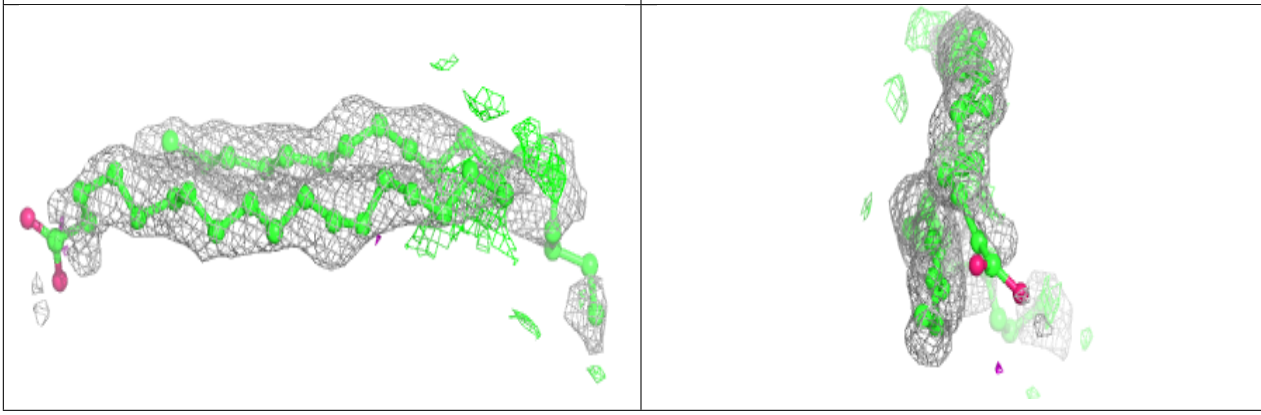




Electron density around LMG d 408:

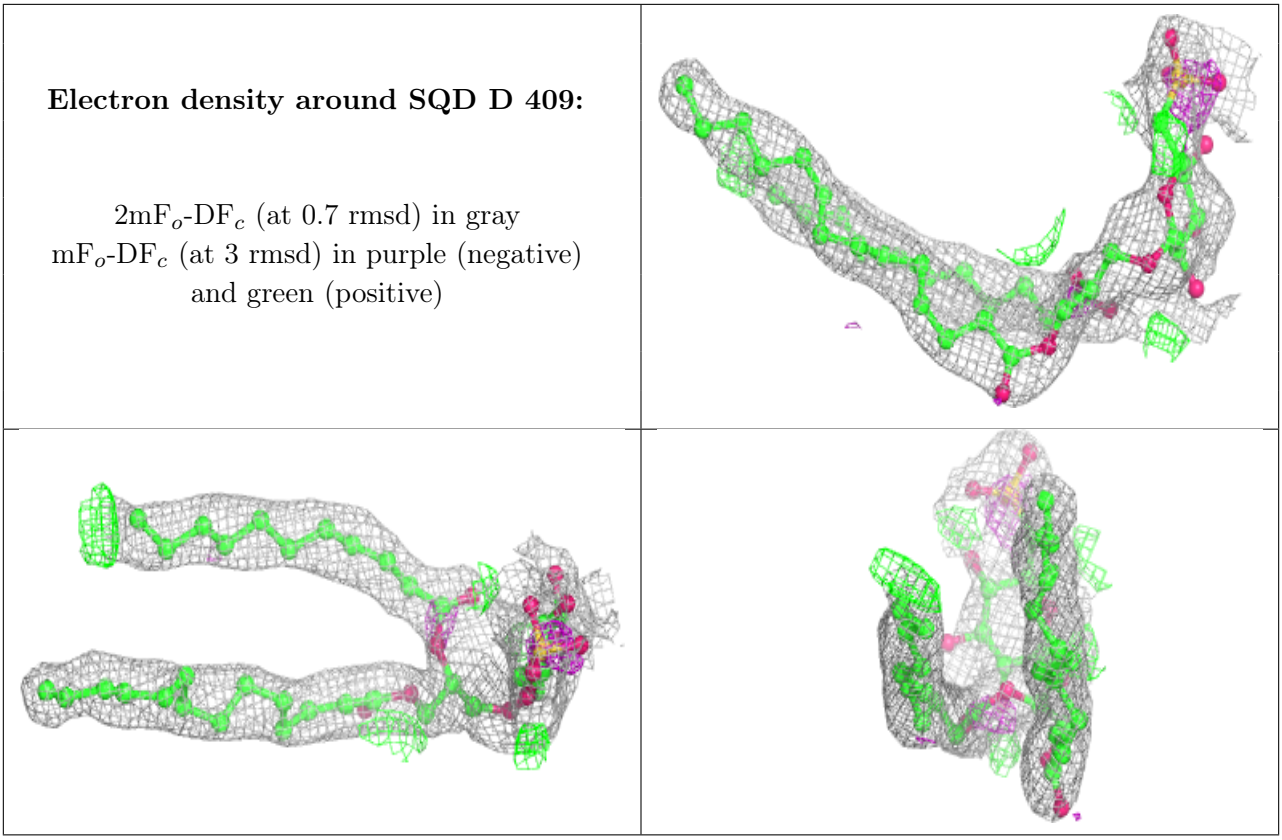
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





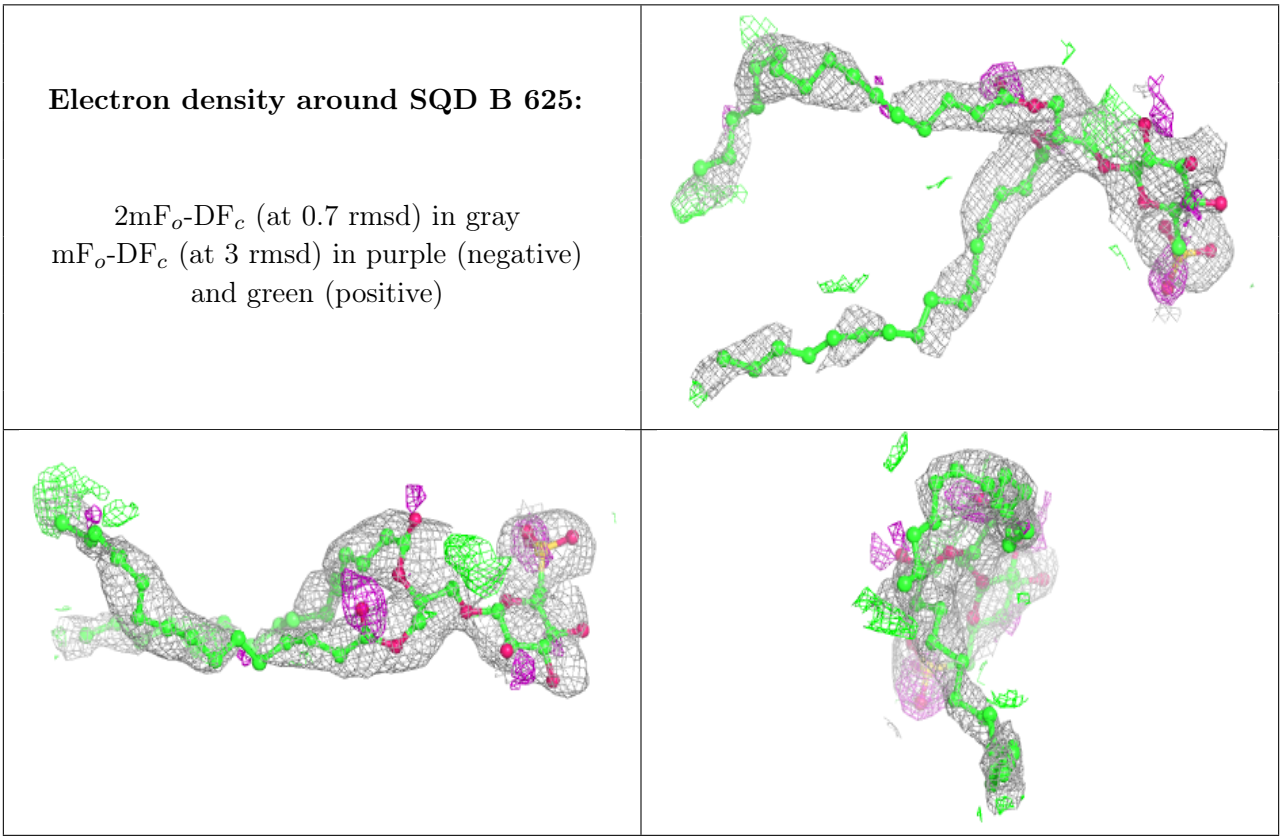
Electron density around SQD D 409:

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



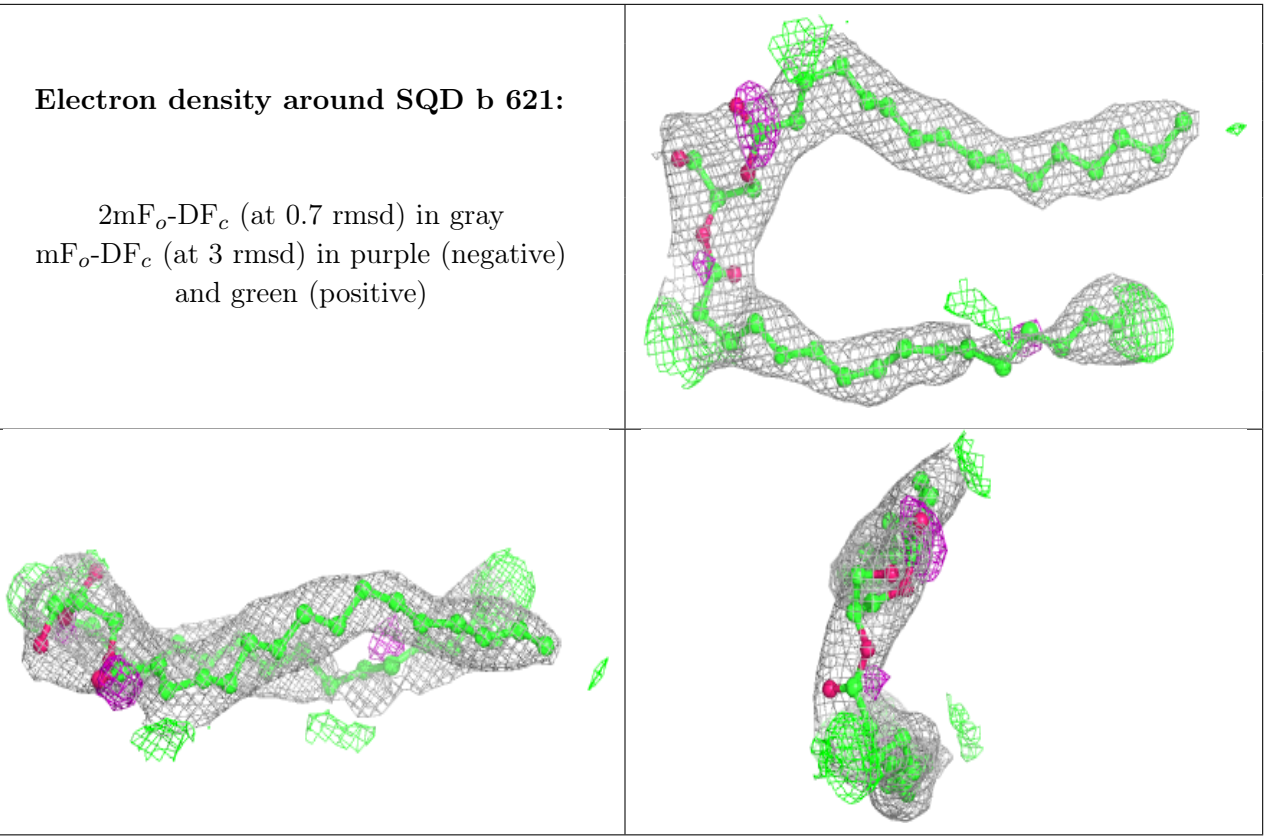
Electron density around SQD B 625:

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



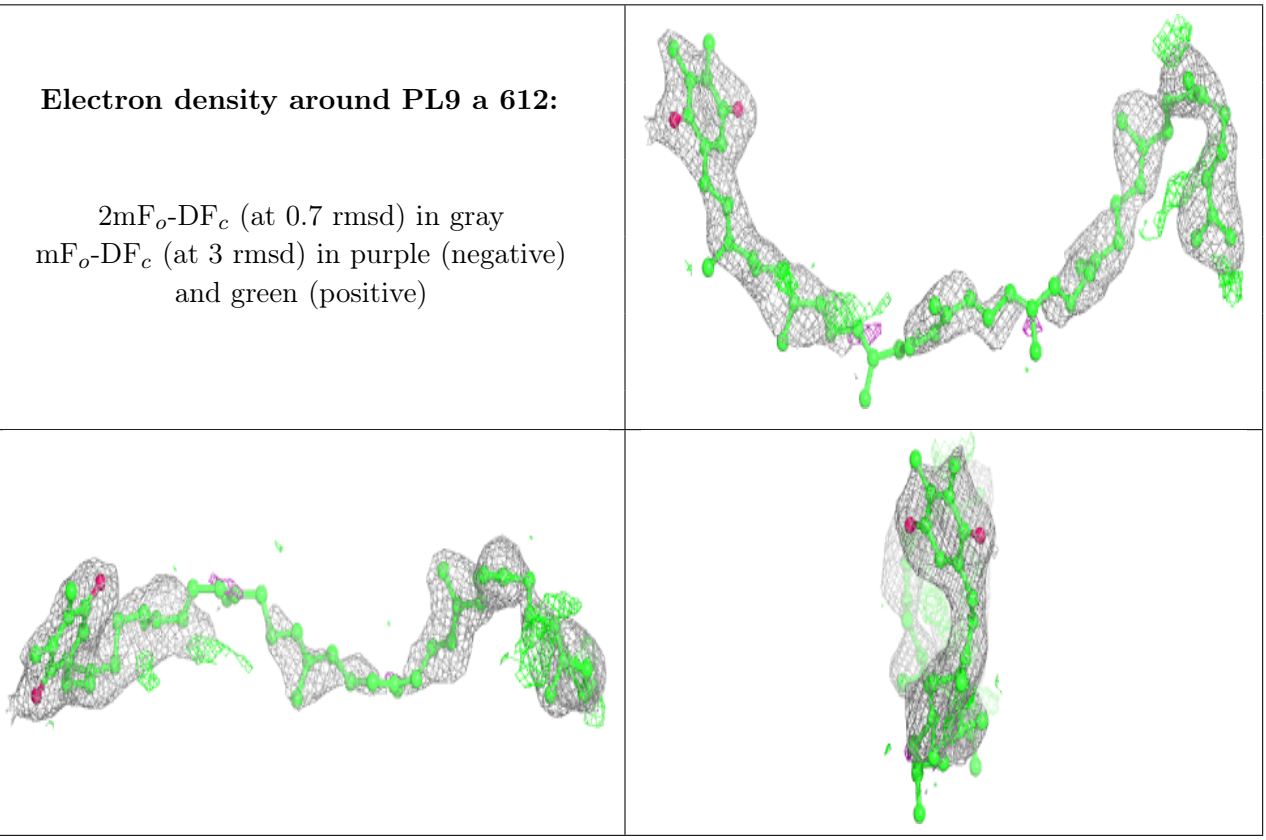
Electron density around SQD b 621:

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



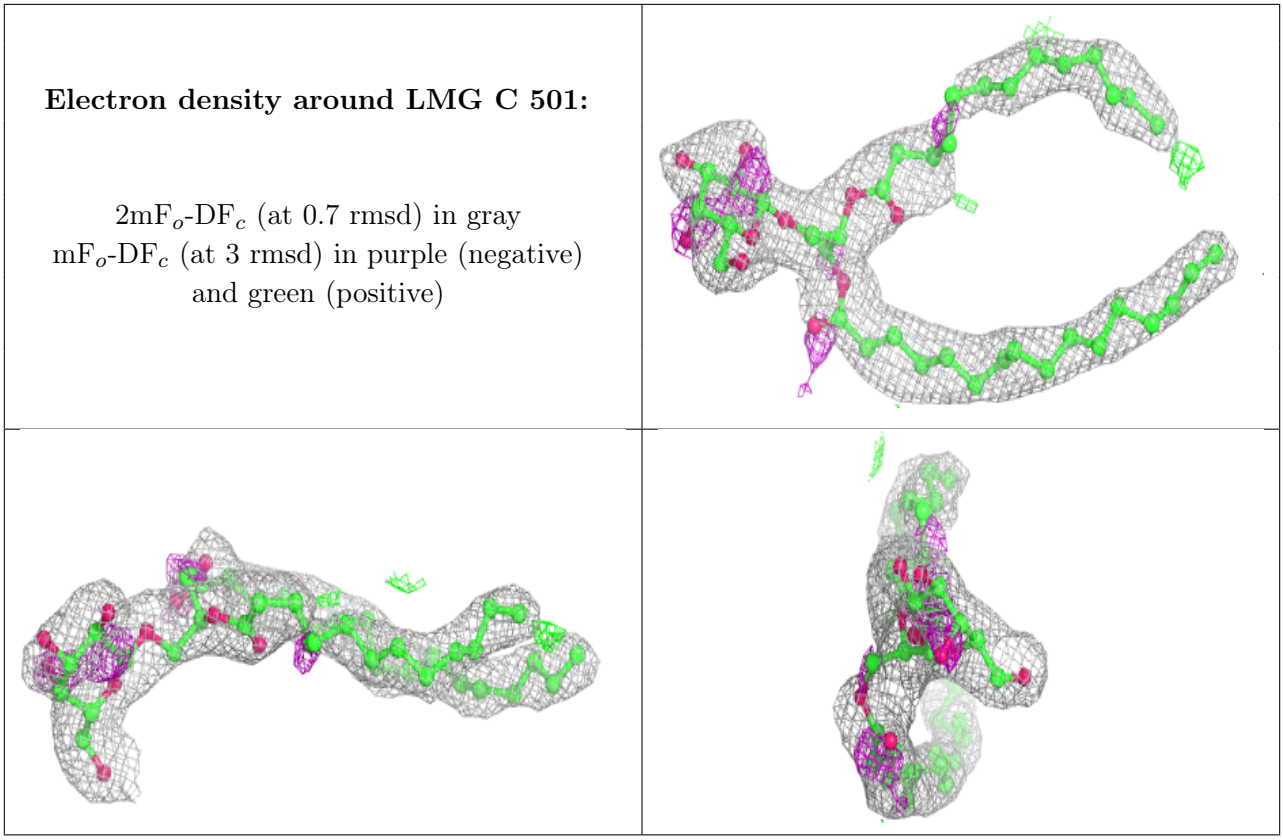
Electron density around PL9 a 612:

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



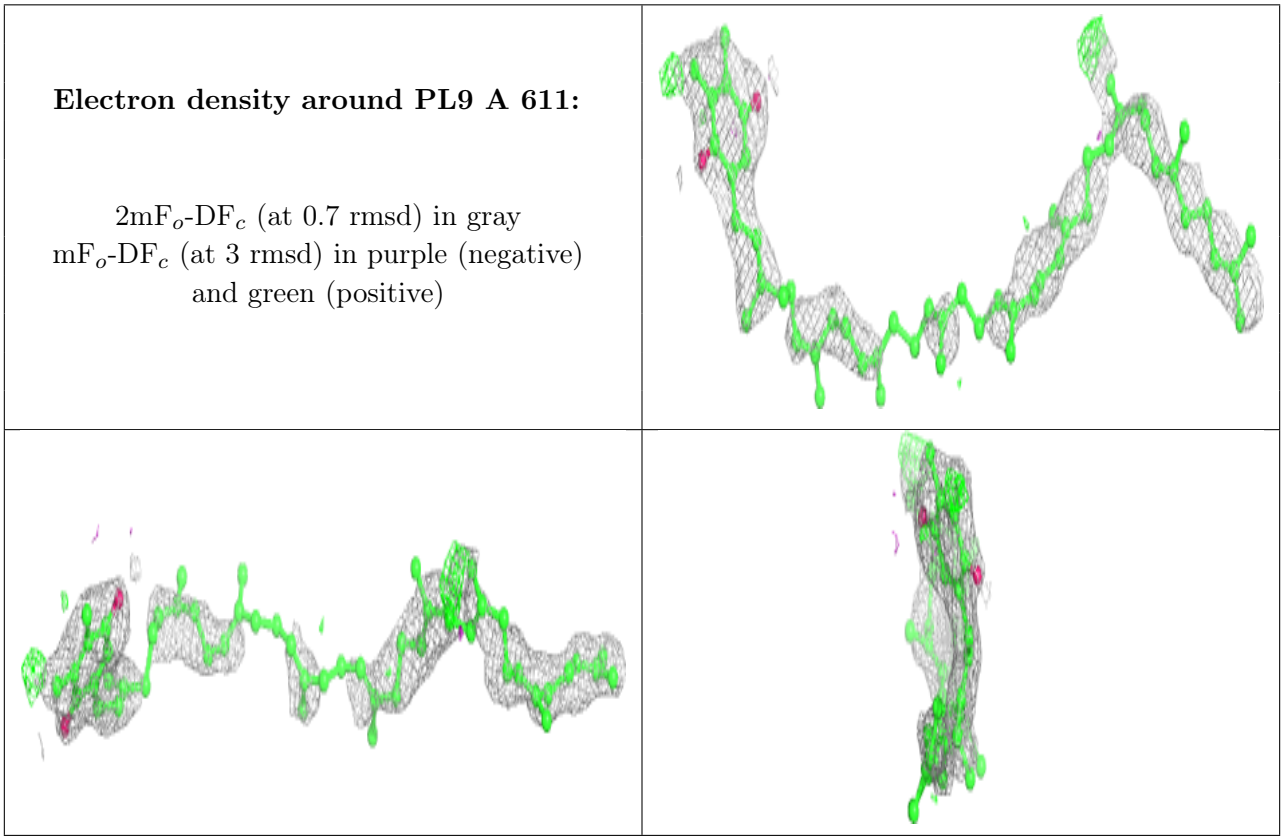
Electron density around LMG C 501:

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



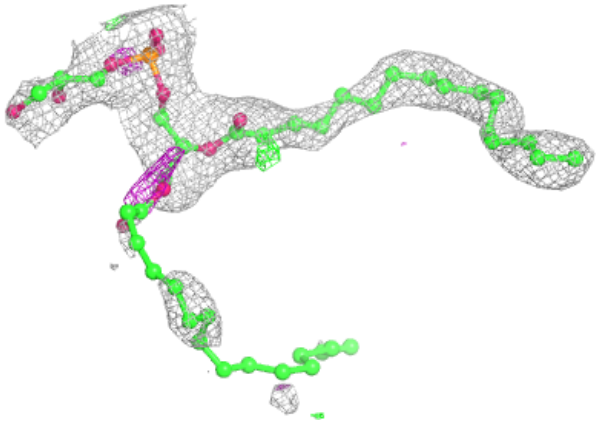
Electron density around PL9 A 611:

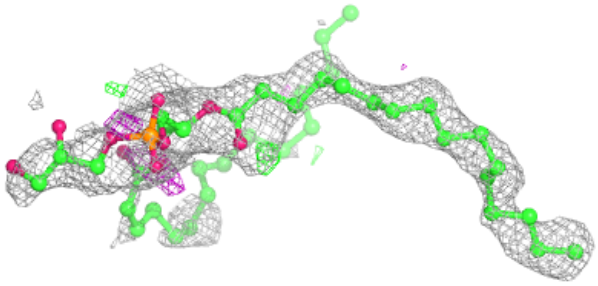
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

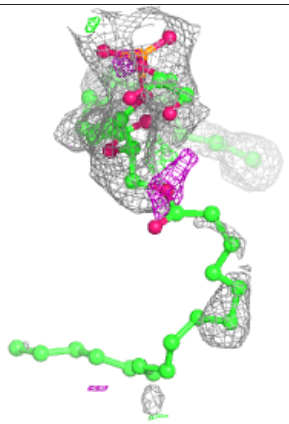


Electron density around LHG A 618:

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

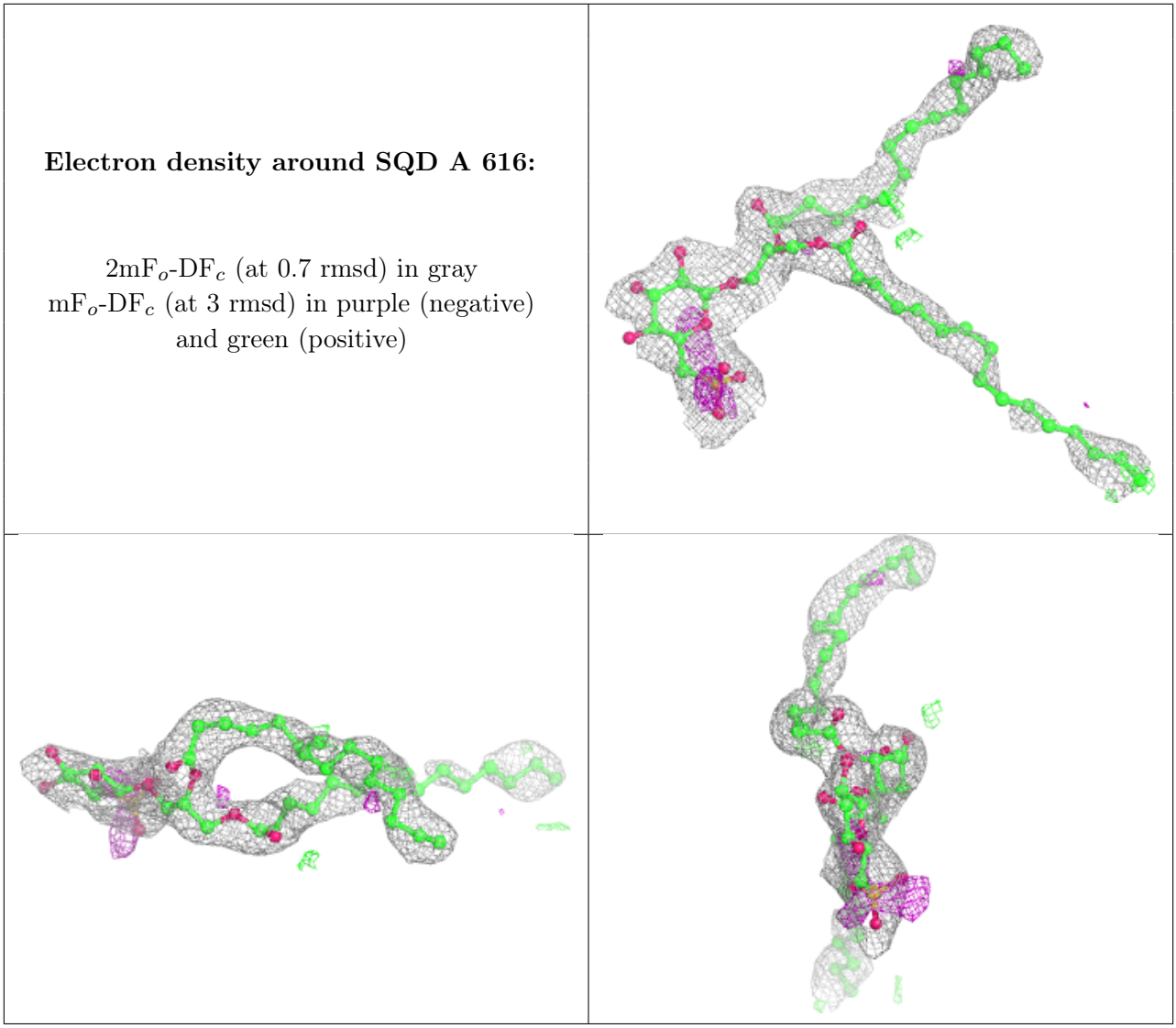






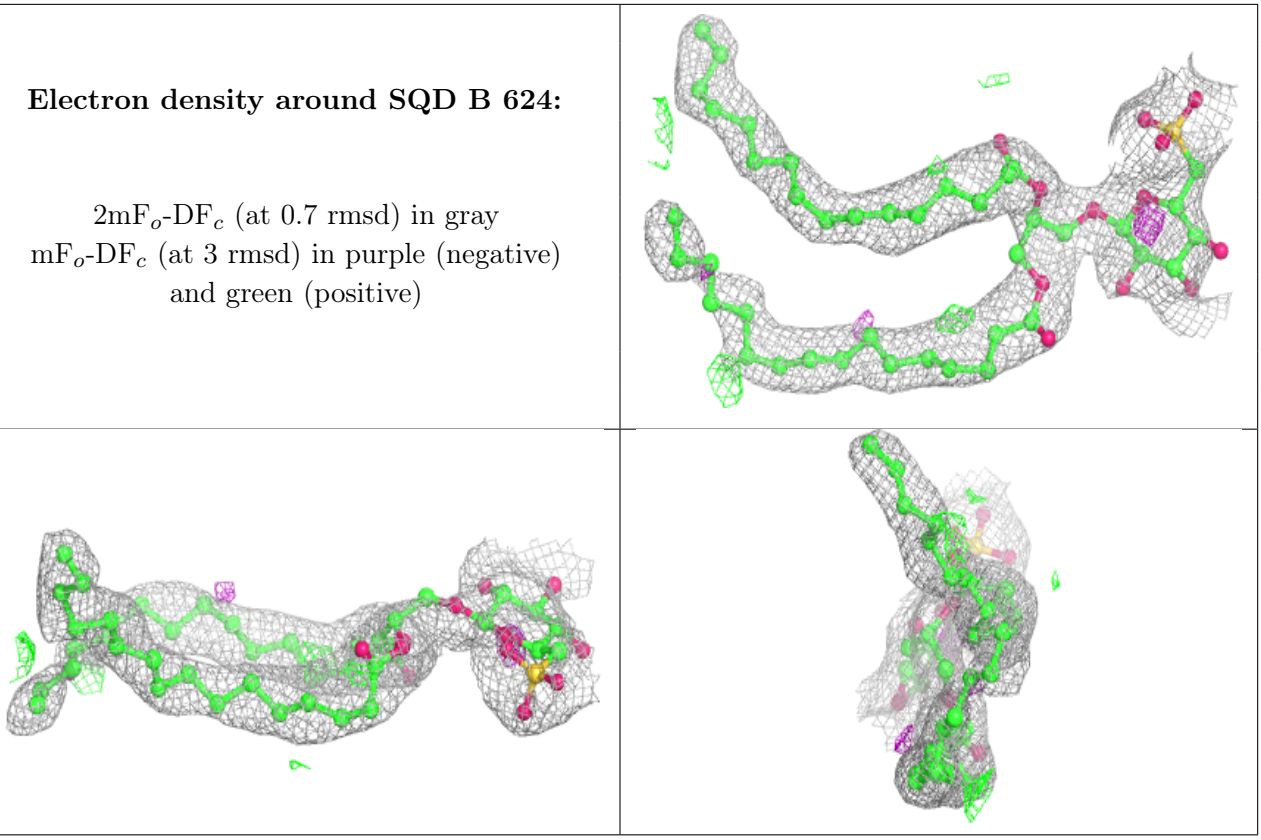
Electron density around SQD A 616:

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



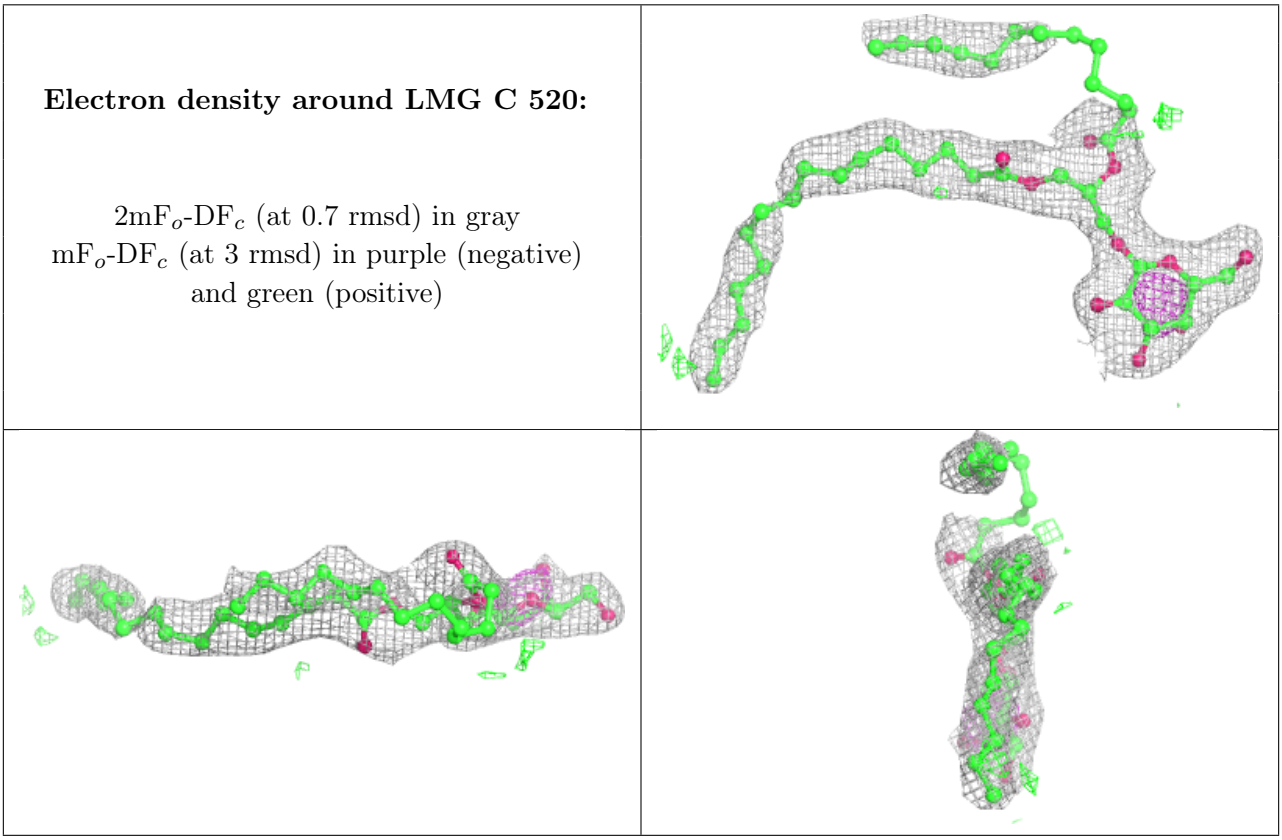
Electron density around SQD B 624:

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



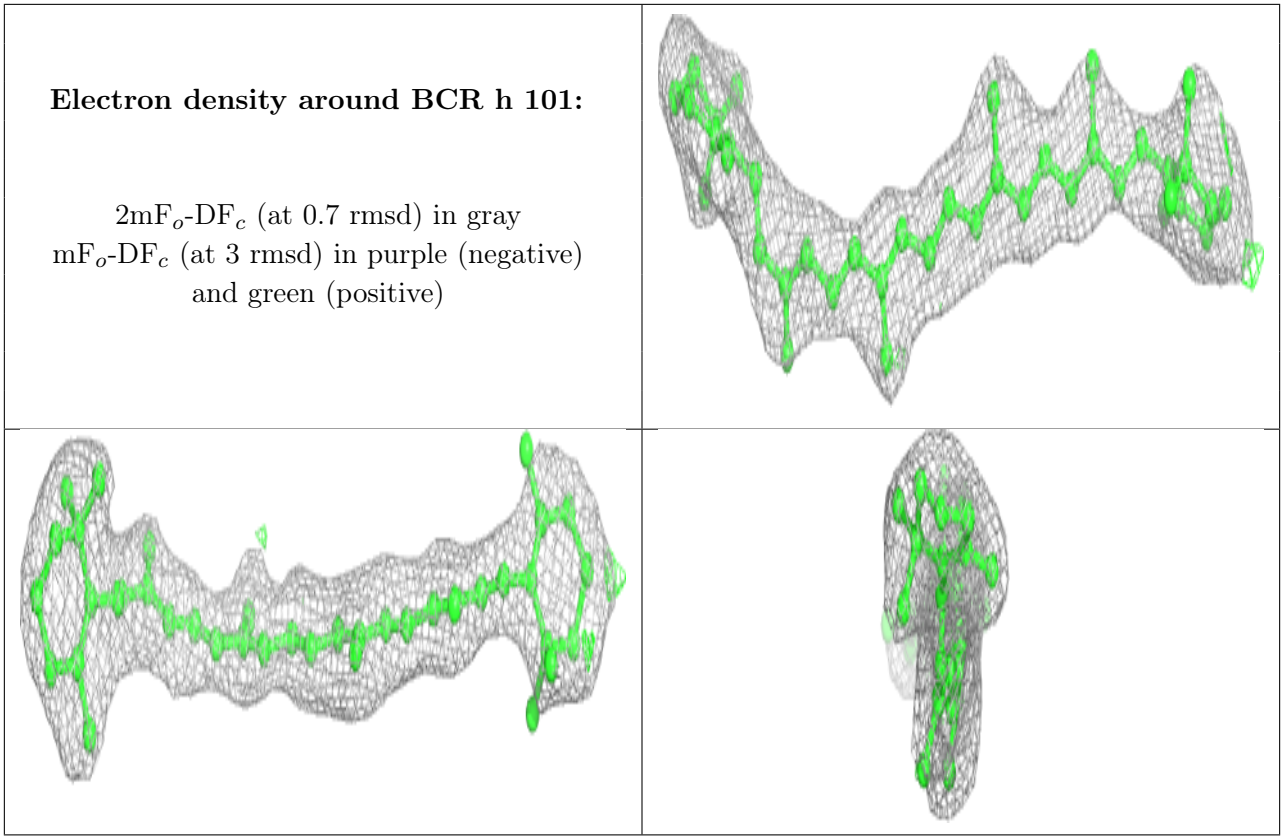
Electron density around LMG C 520:

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



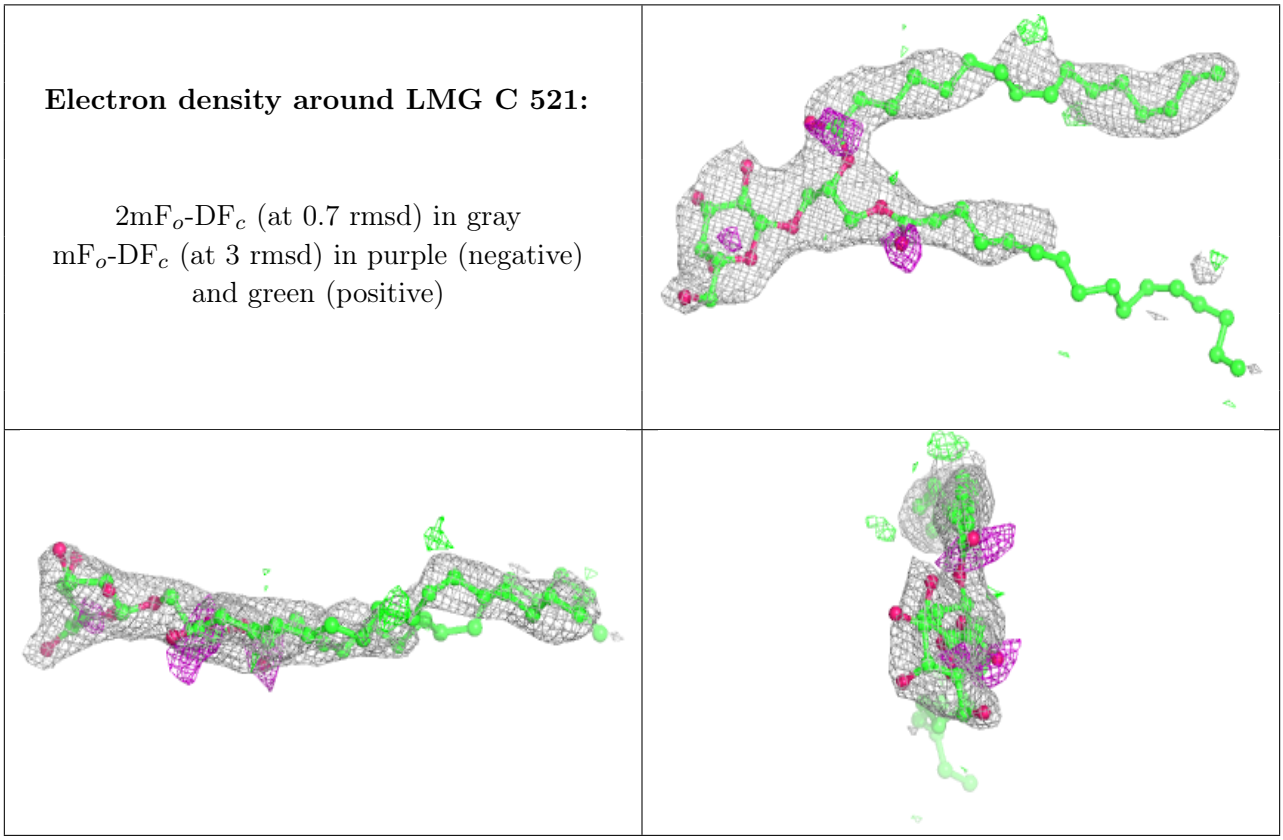
Electron density around BCR h 101:

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



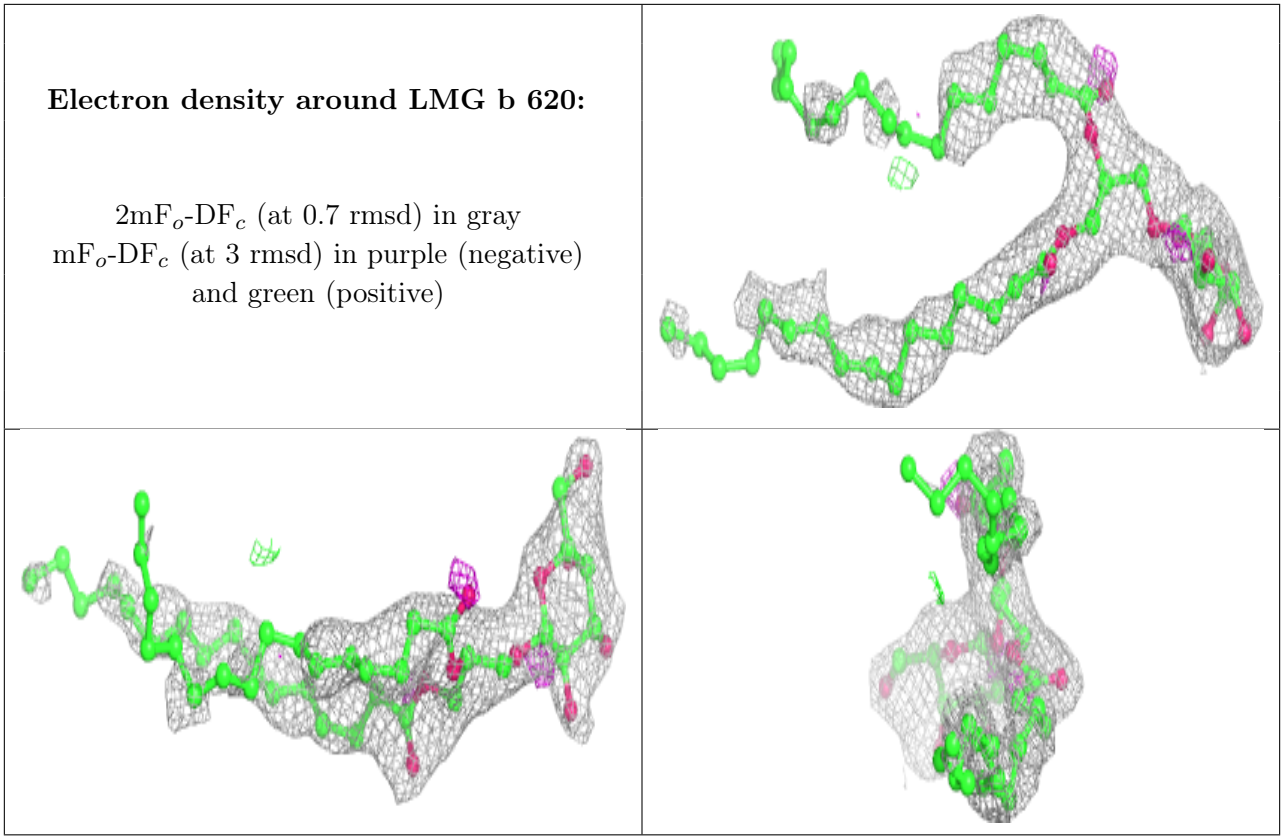
Electron density around LMG C 521:

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



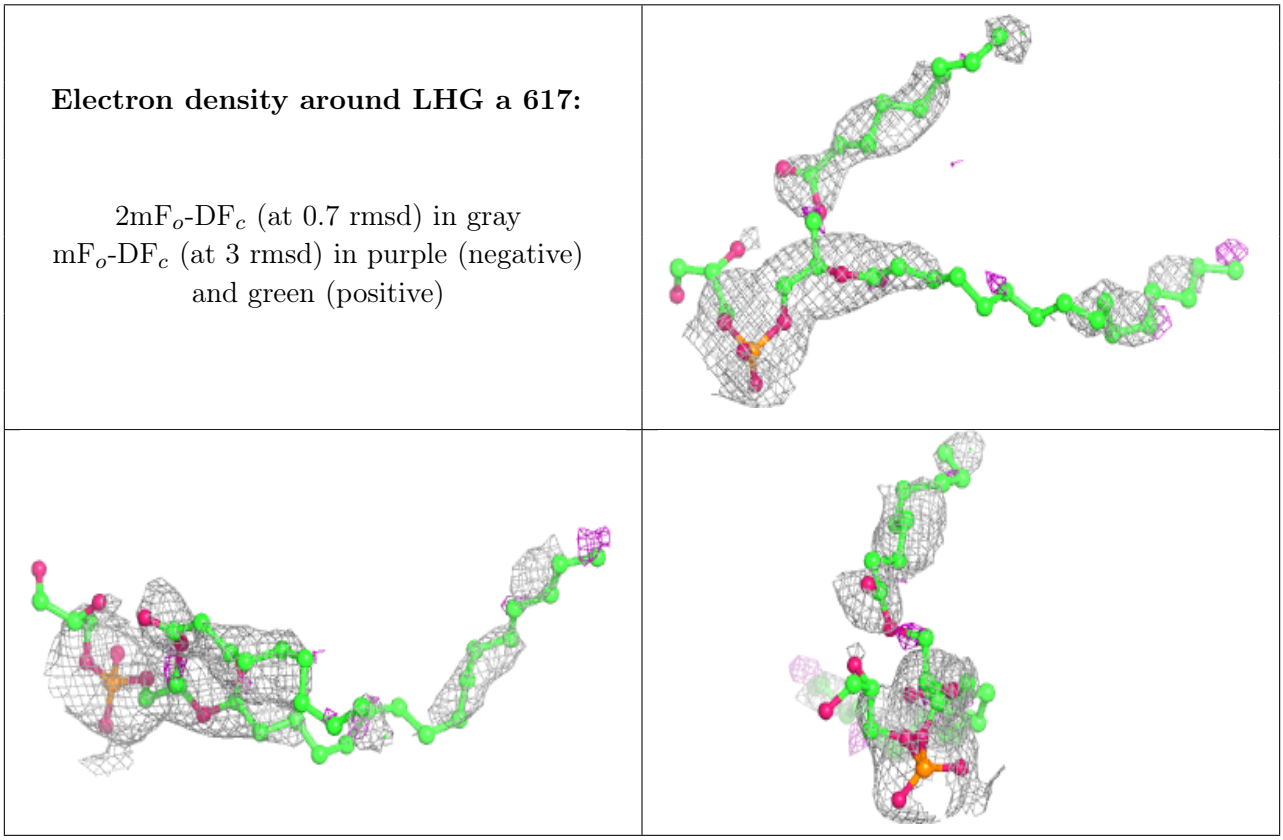
Electron density around LMG b 620:

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



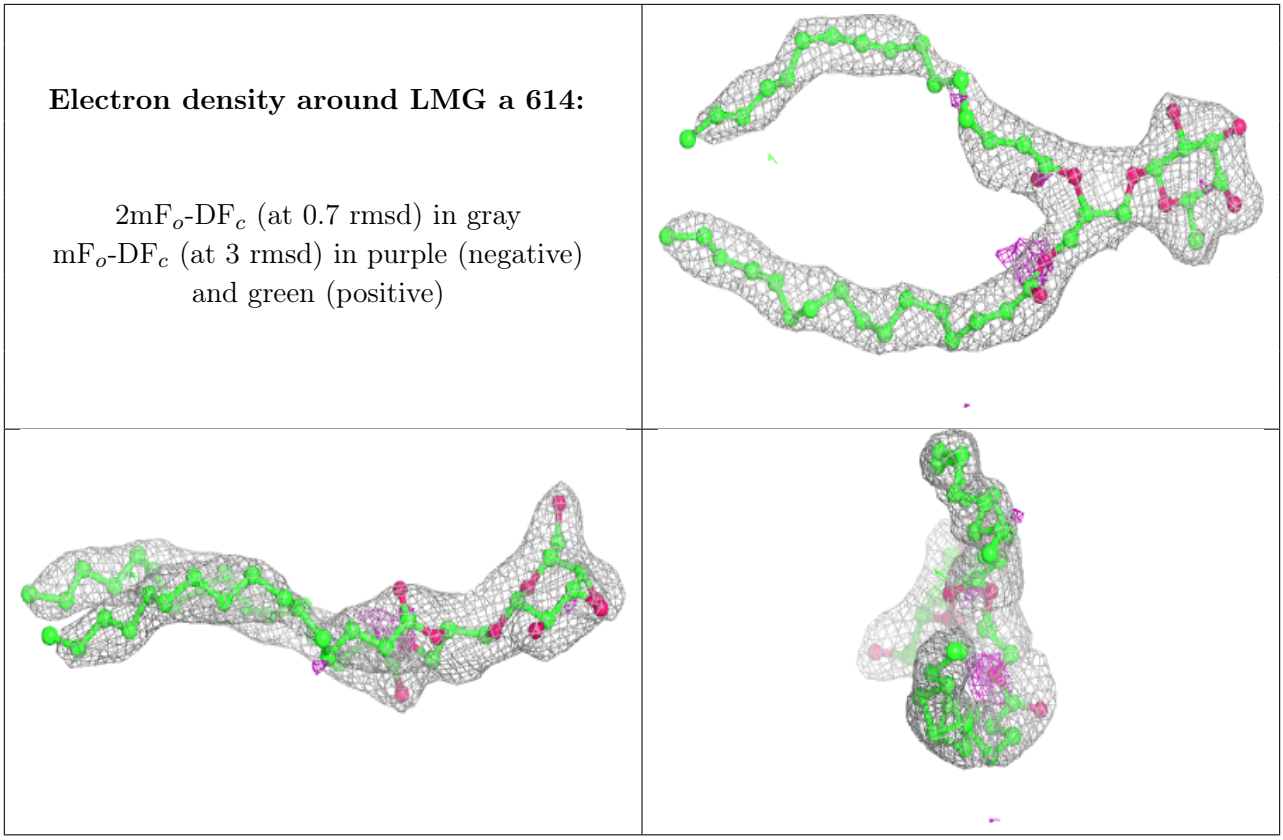
Electron density around LHG a 617:

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



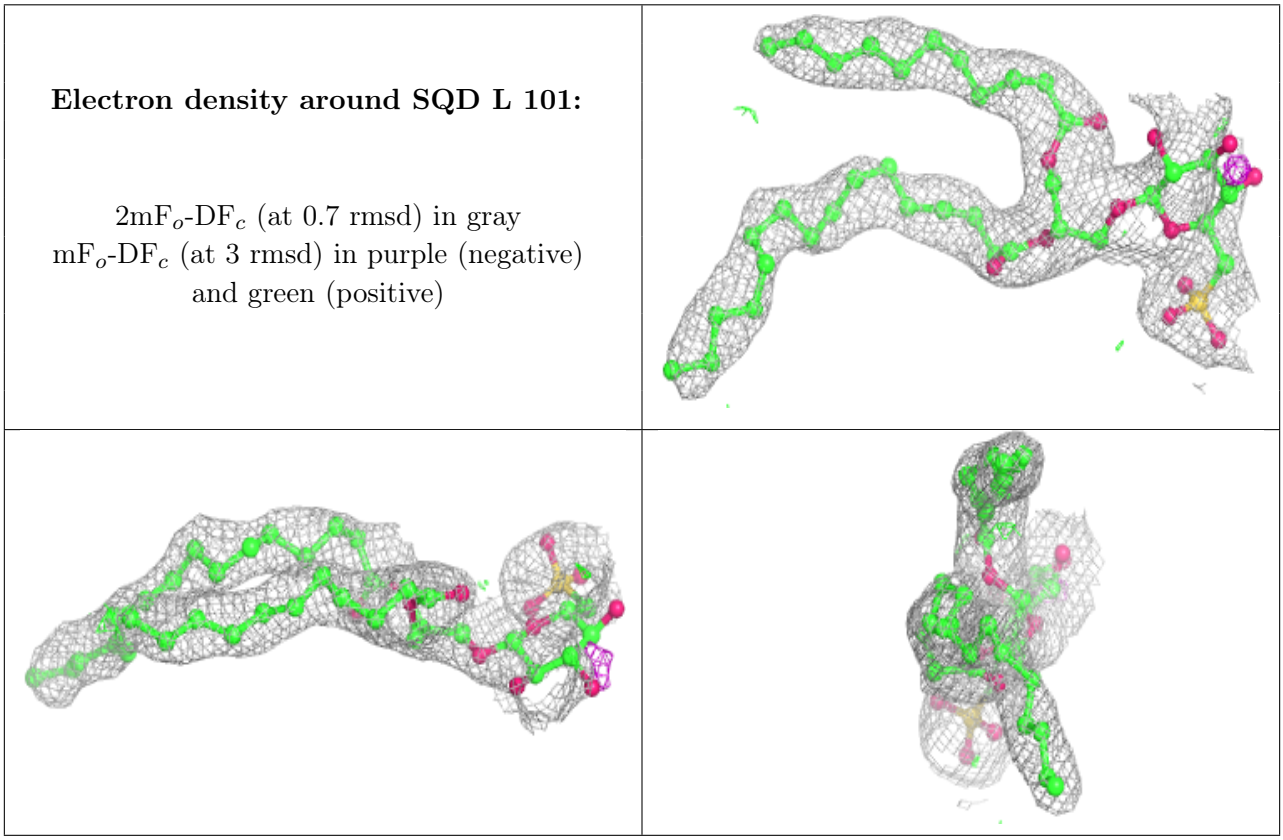
Electron density around LMG a 614:

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



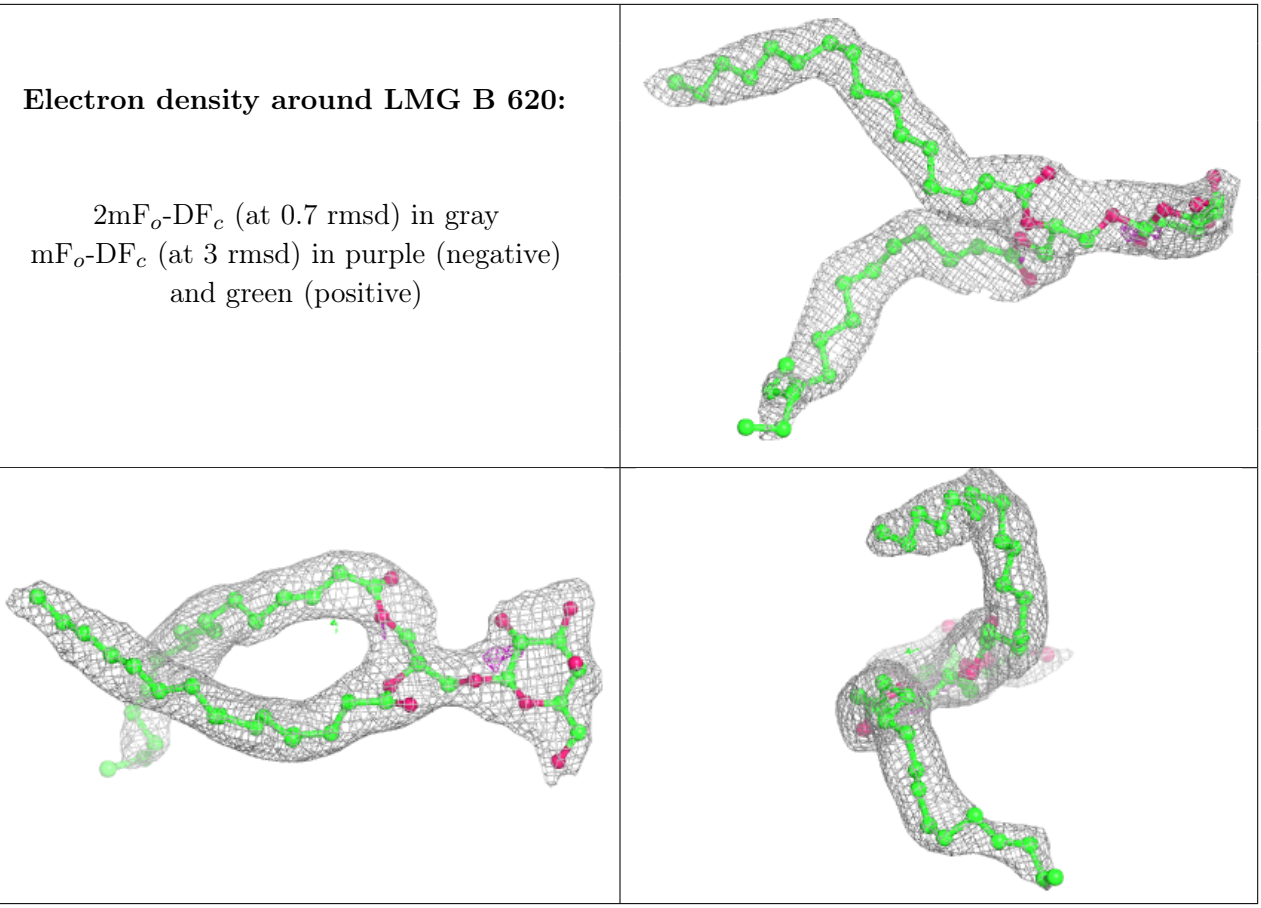
Electron density around SQD L 101:

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



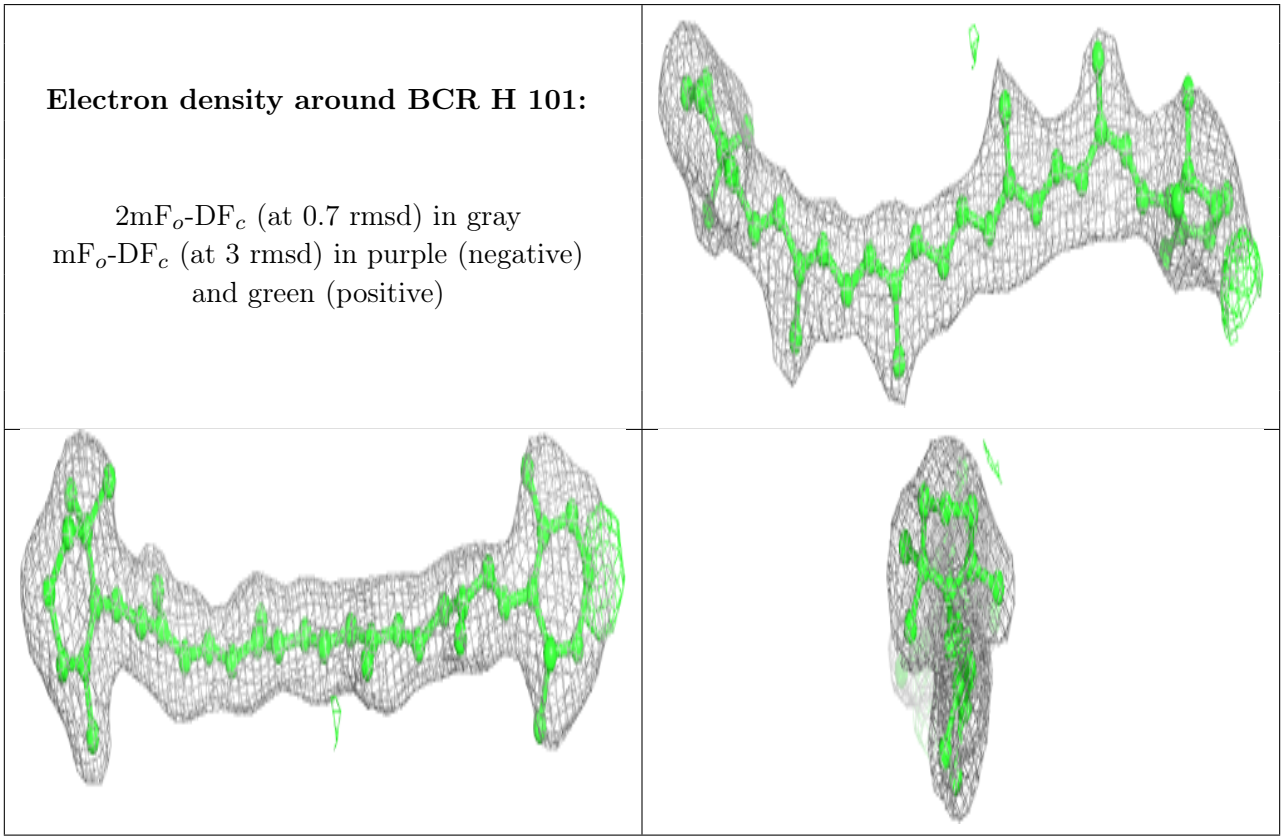
Electron density around LMG B 620:

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



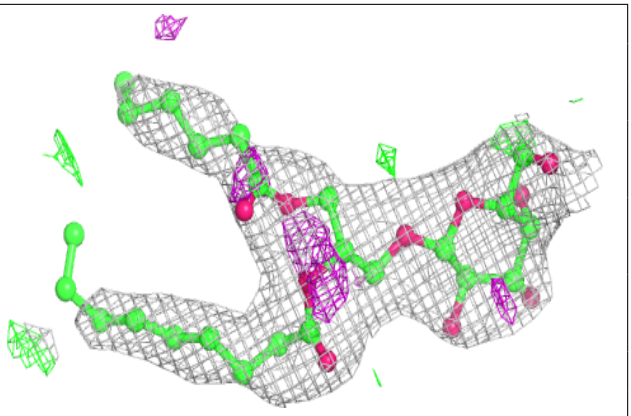
Electron density around BCR H 101:

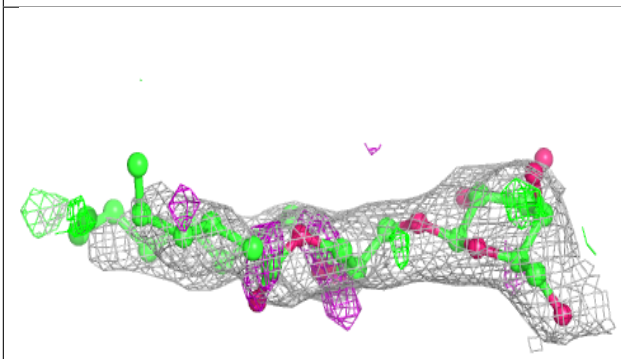
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

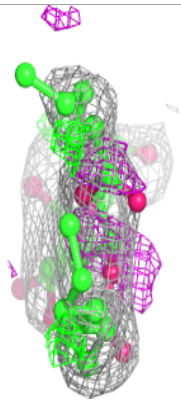


Electron density around LMG c 520:

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

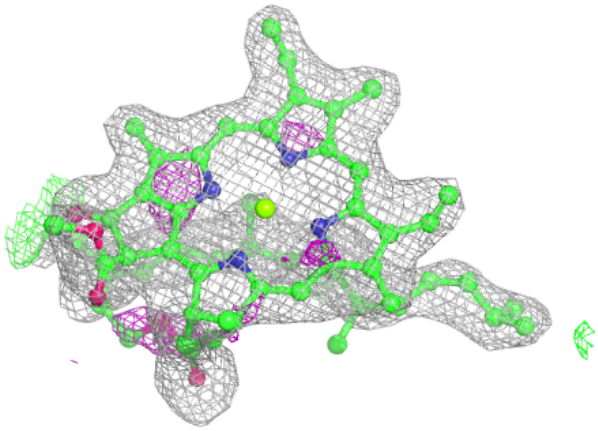


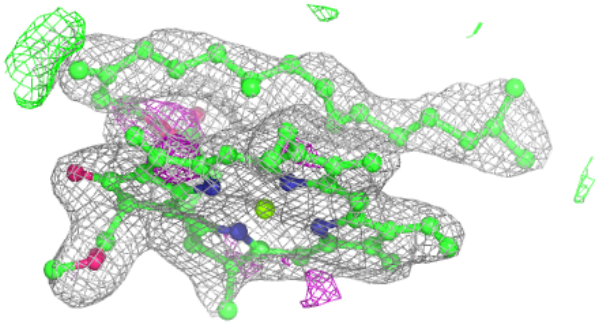


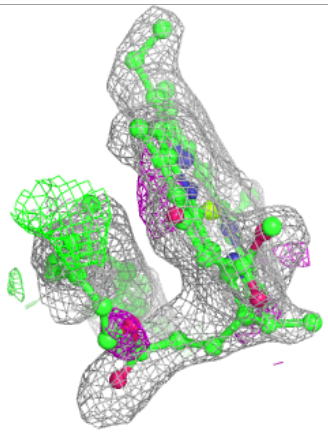


Electron density around CLA b 601:

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

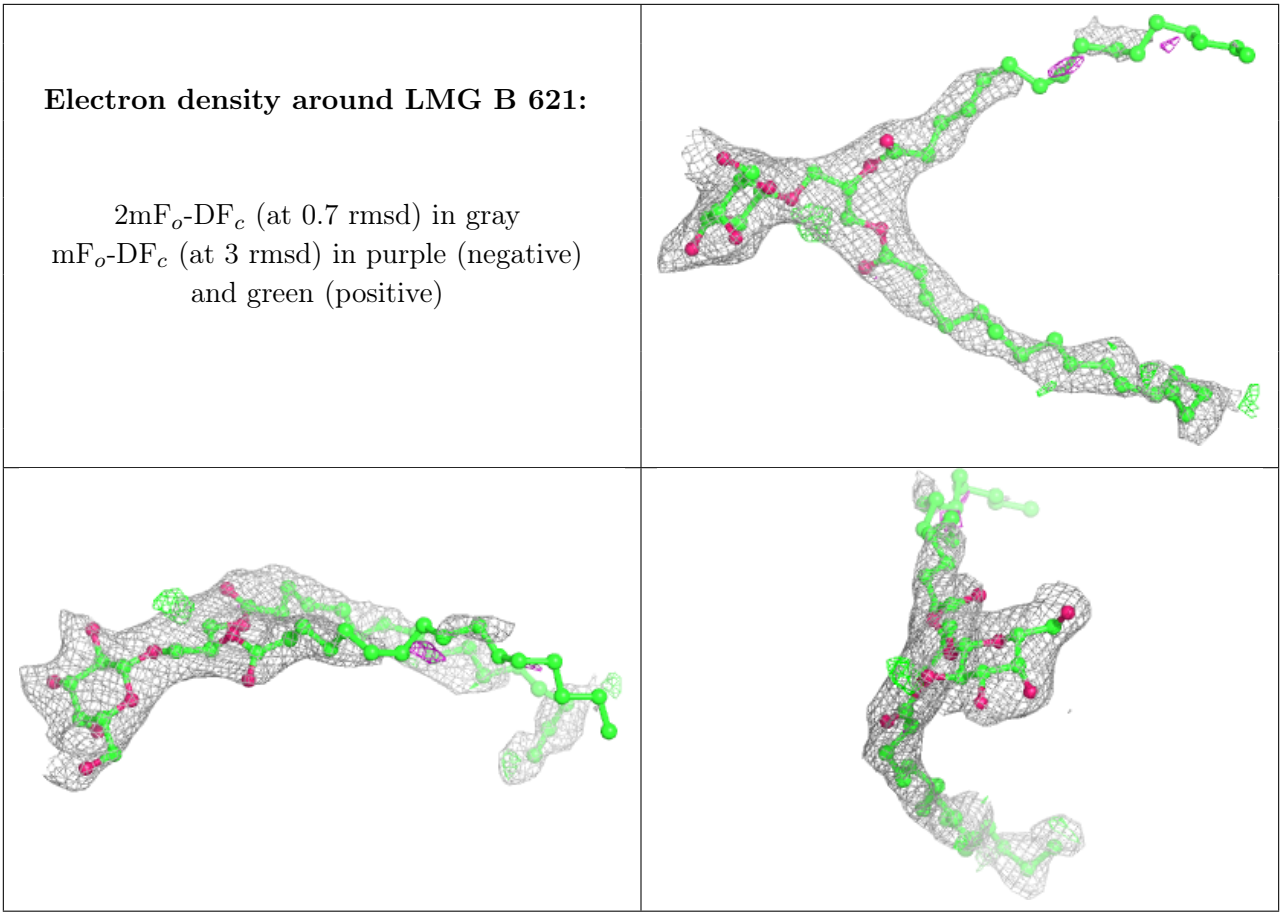






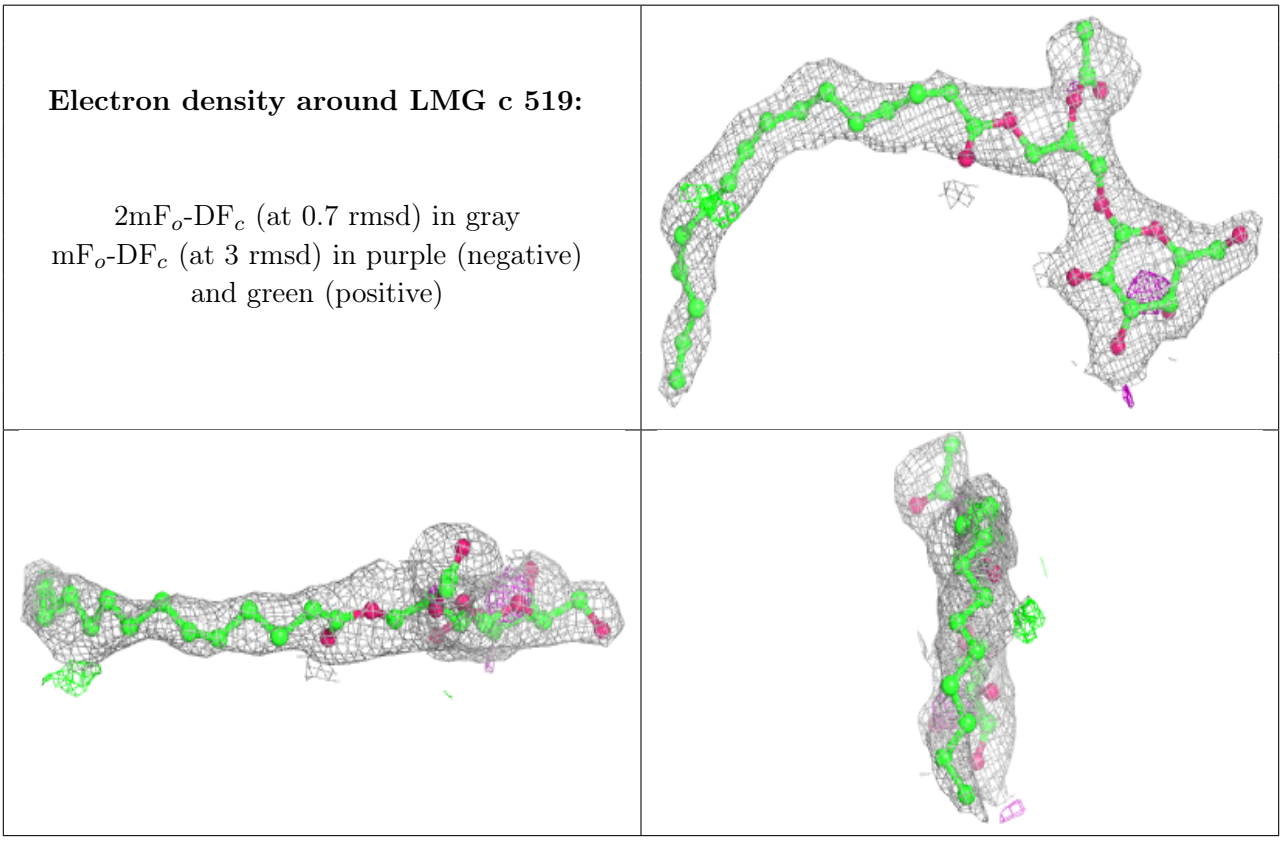
Electron density around LMG B 621:

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



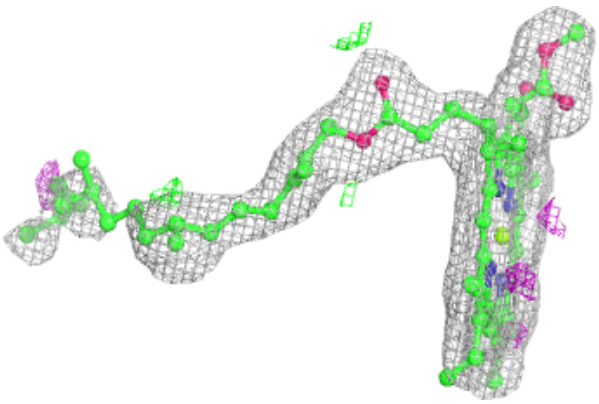
Electron density around LMG c 519:

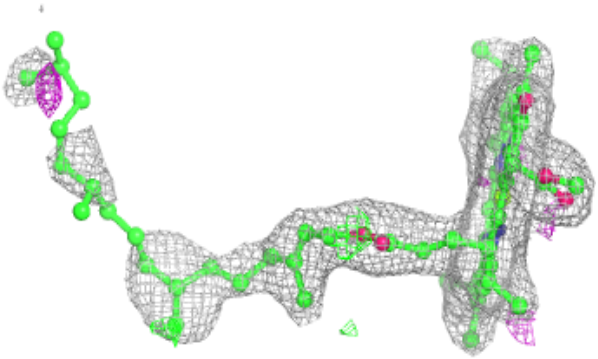
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

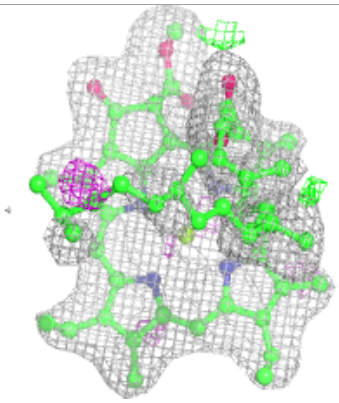


Electron density around CLA d 402:

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

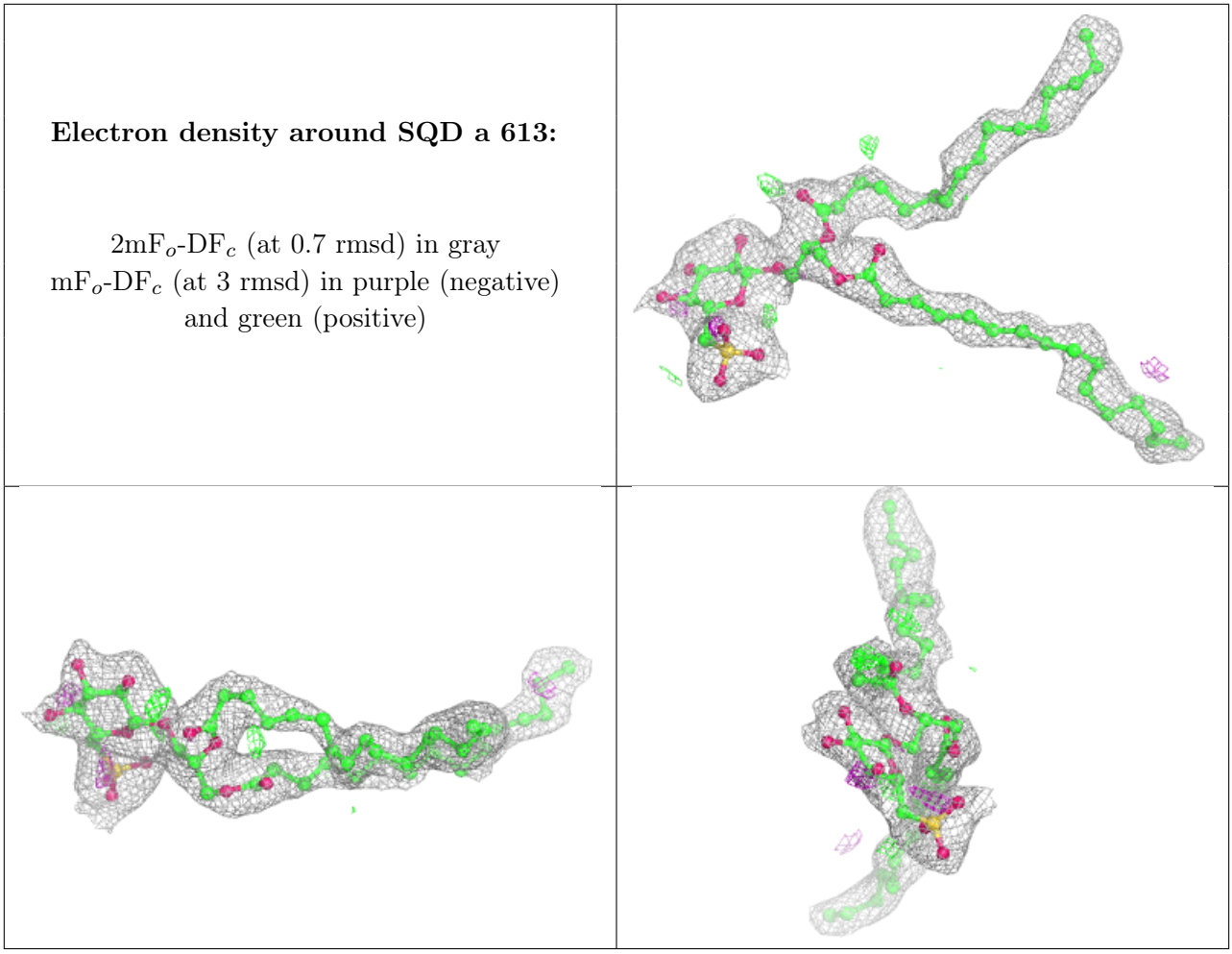






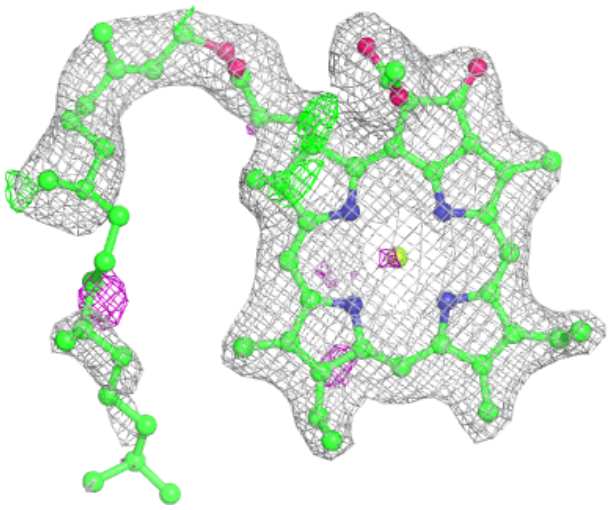
Electron density around SQD a 613:

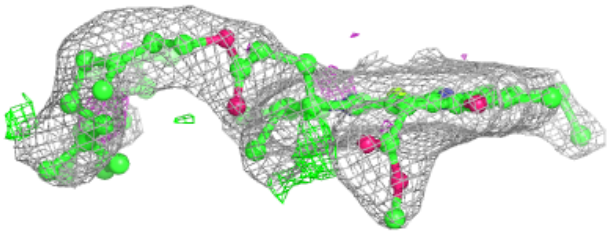
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

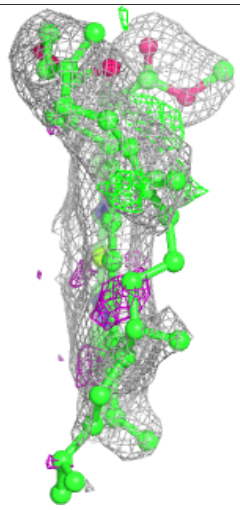


Electron density around CLA C 513:

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

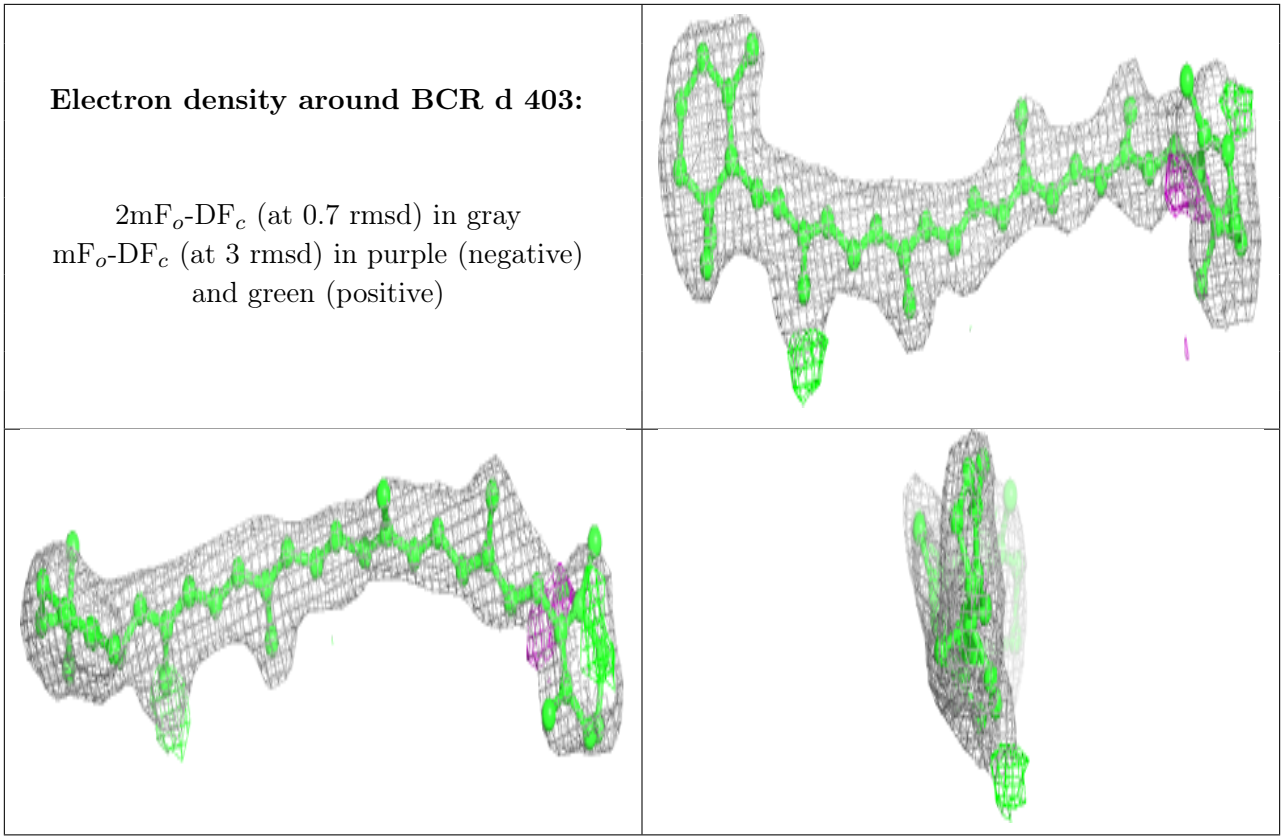






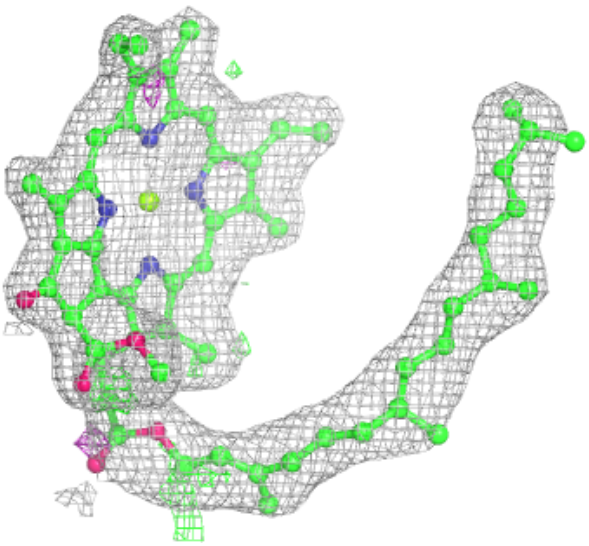
Electron density around BCR d 403:

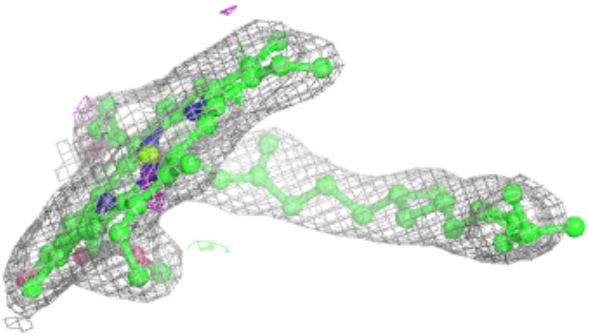
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

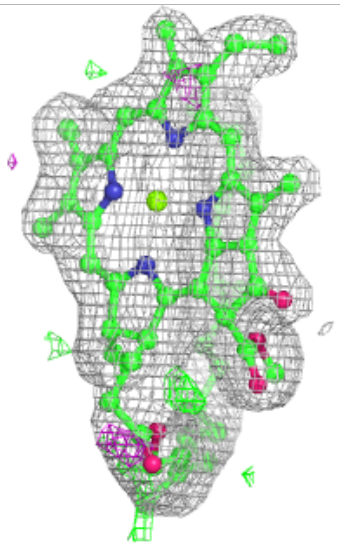


Electron density around CLA C 508:

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

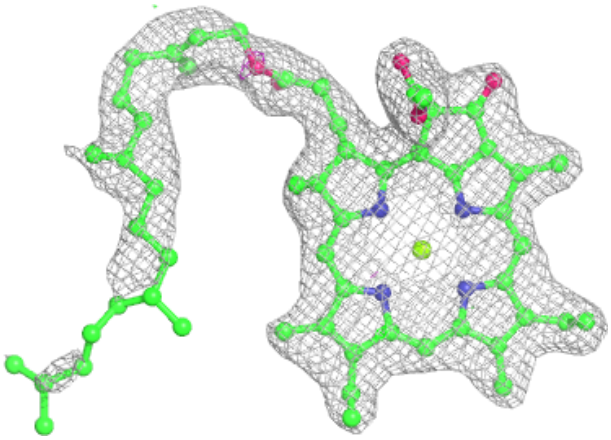


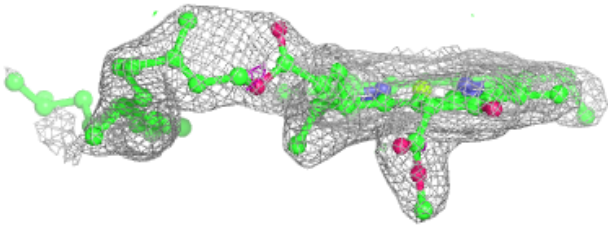


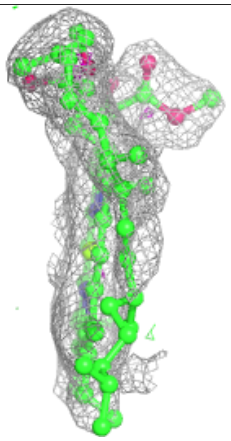


Electron density around CLA c 512:

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

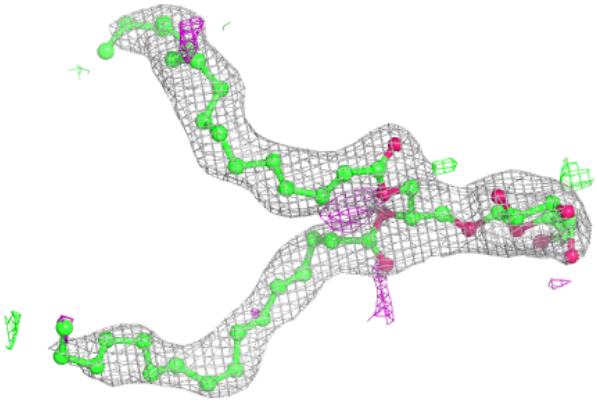


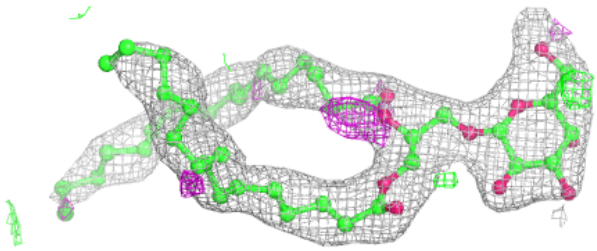


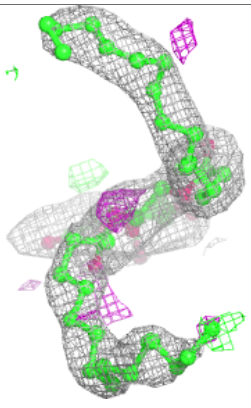


Electron density around LMG m 102:

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

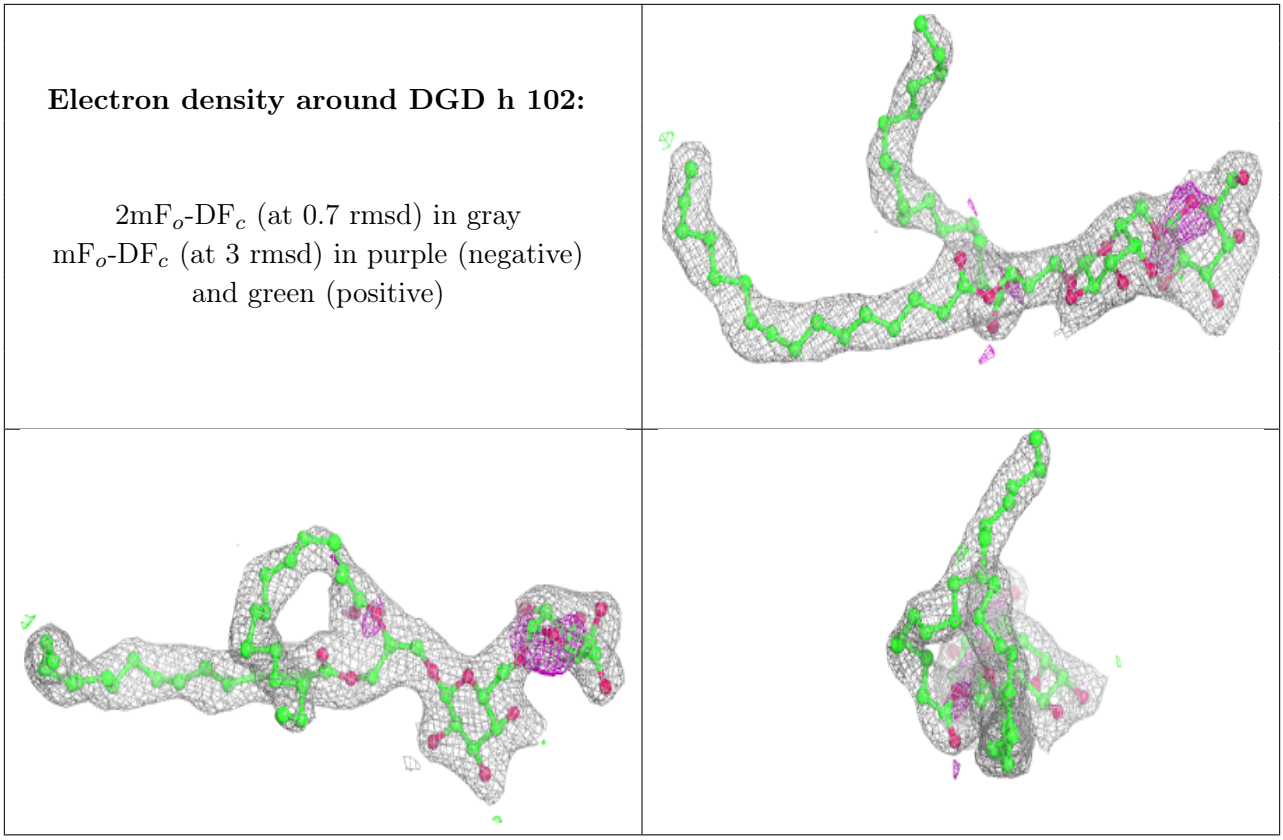






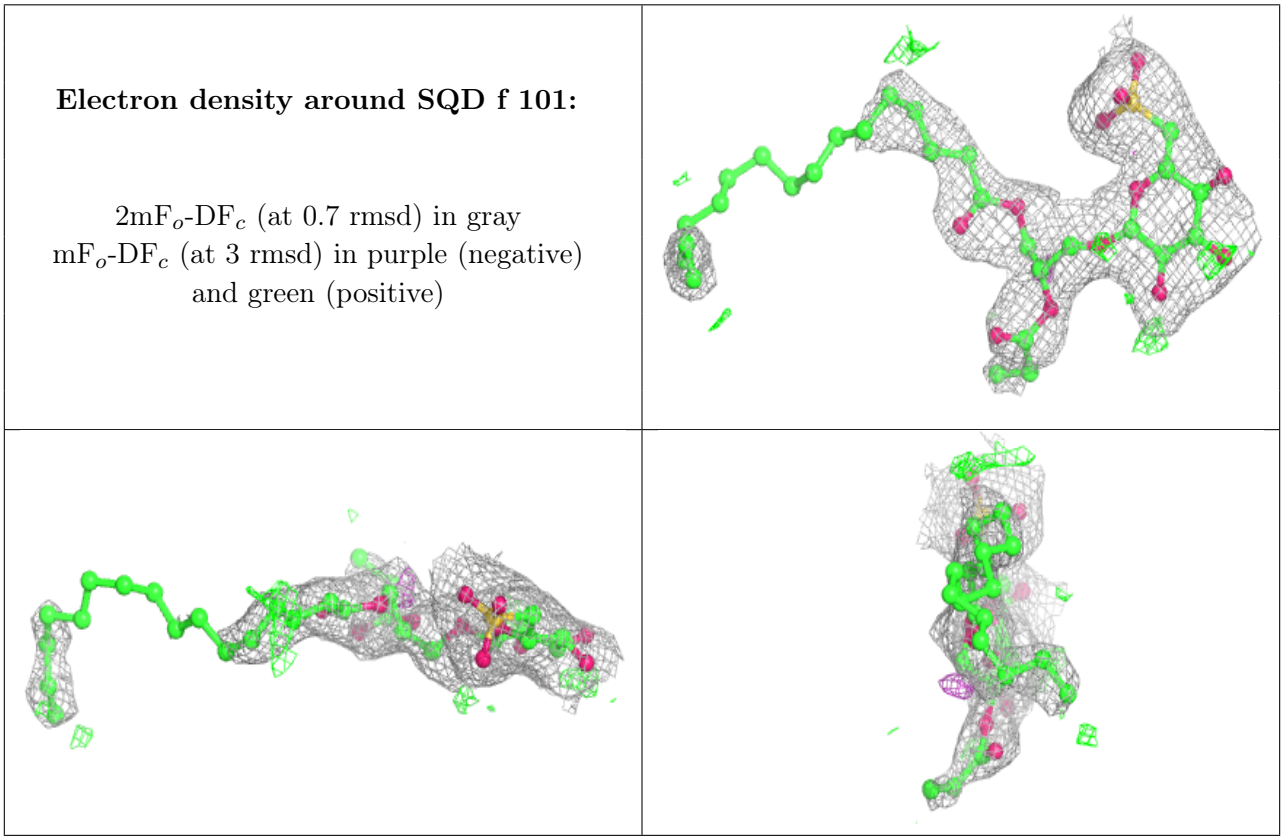
Electron density around DGD h 102:

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



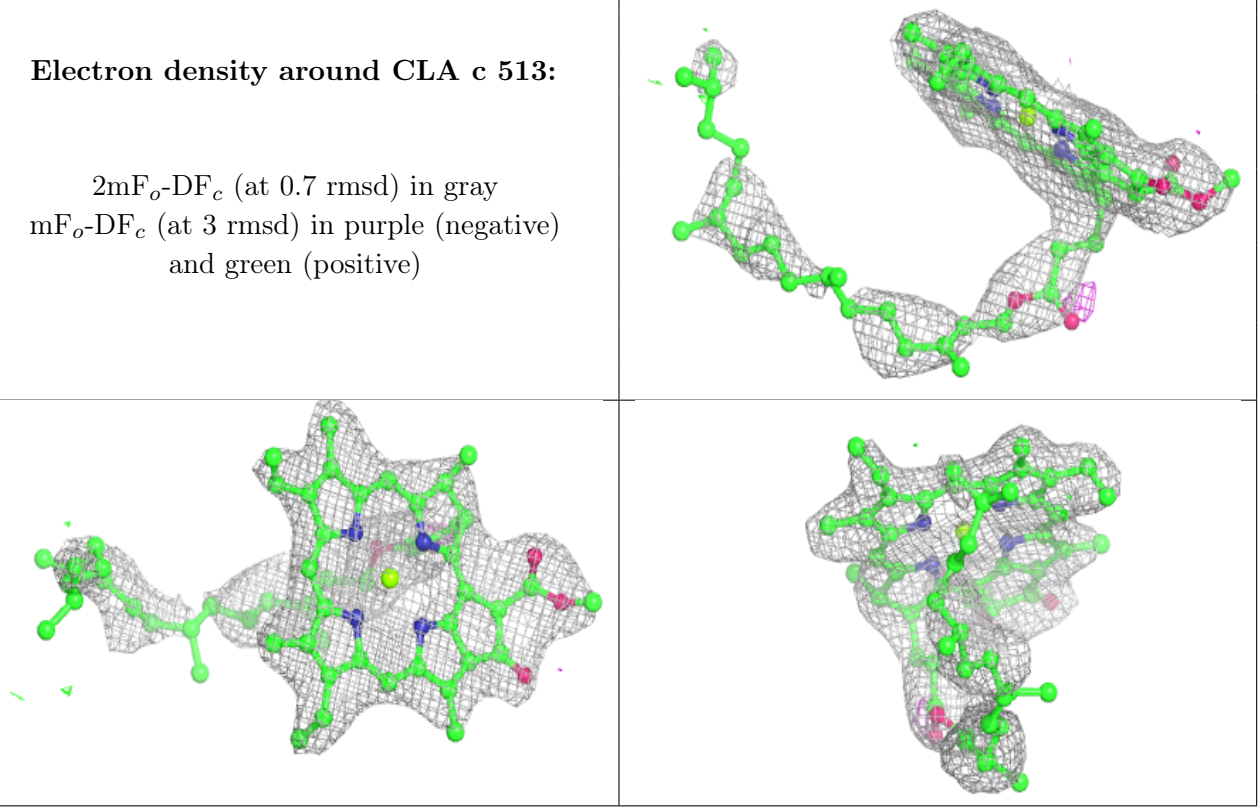
Electron density around SQD f 101:

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



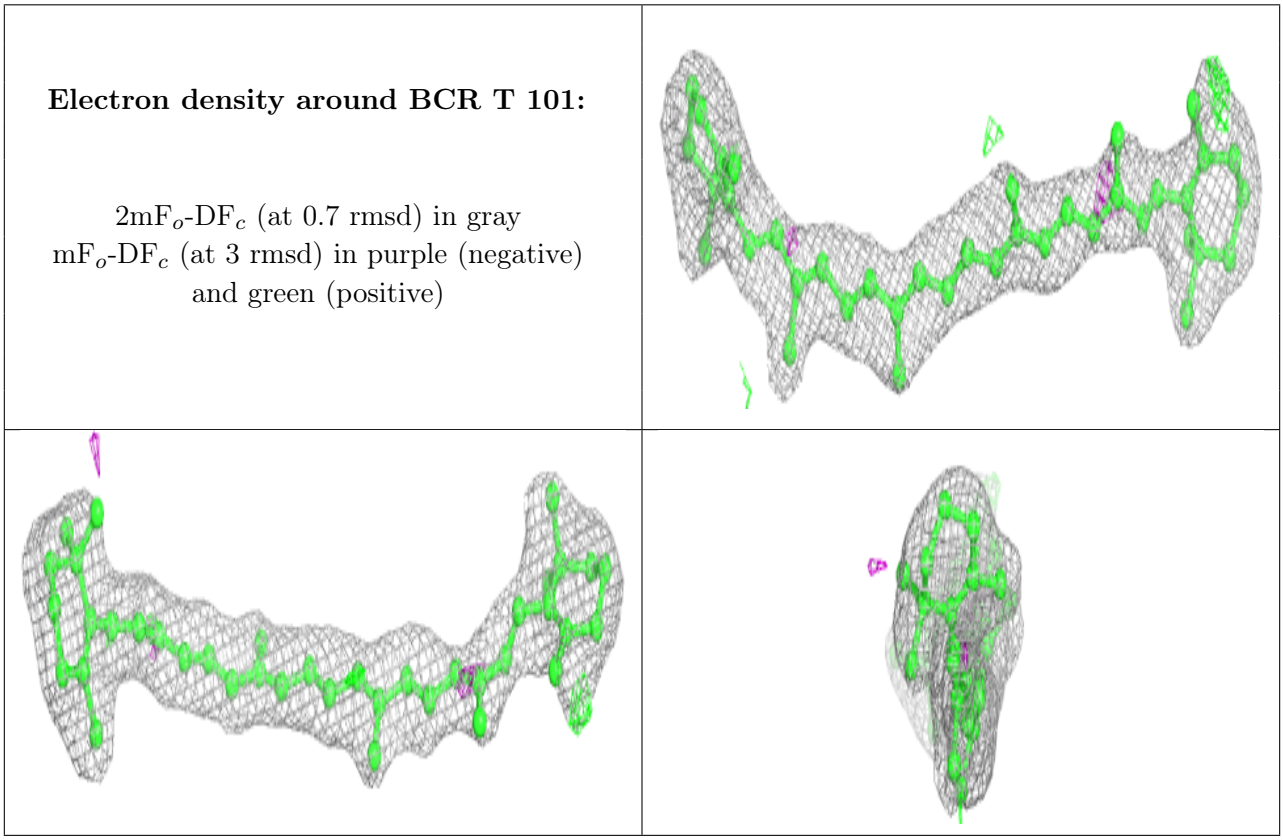
Electron density around CLA c 513:

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



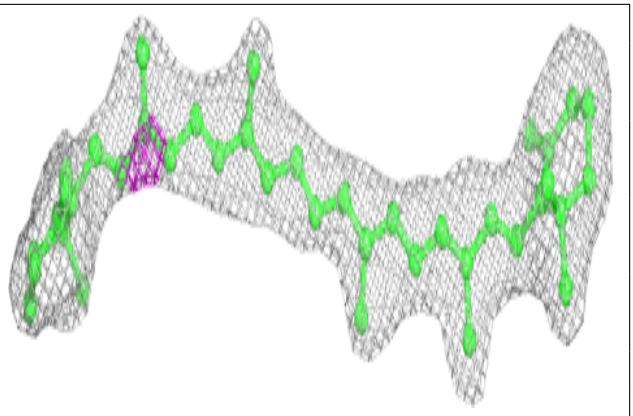
Electron density around BCR T 101:

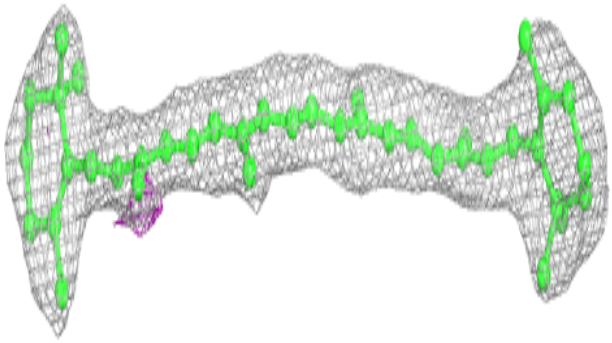
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

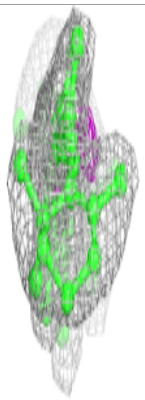


Electron density around BCR Y 101:

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

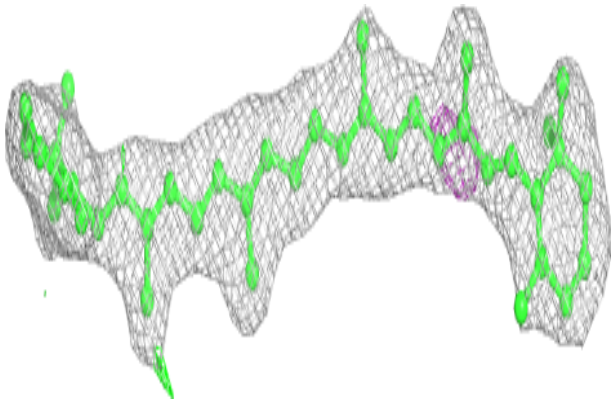


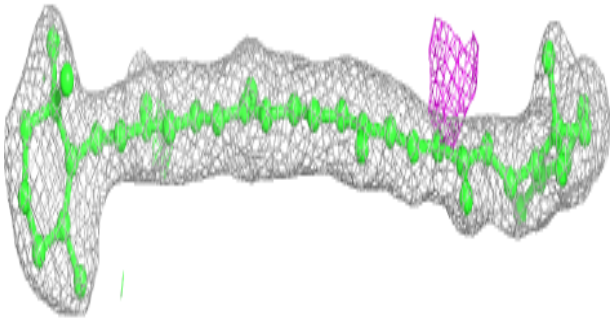


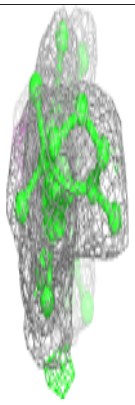


Electron density around BCR b 617:

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

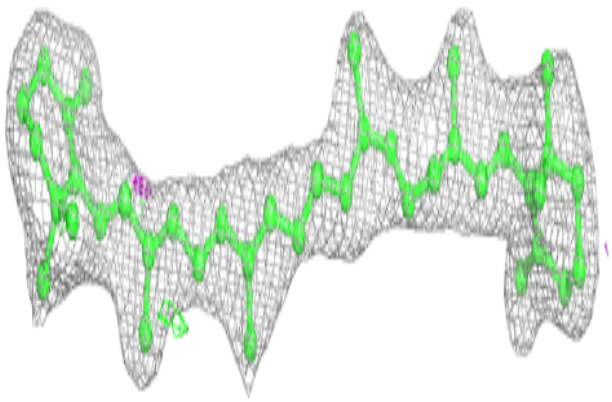


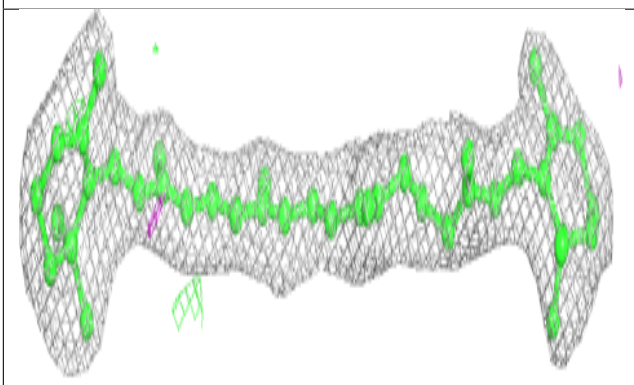


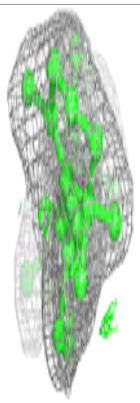


Electron density around BCR b 618:

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

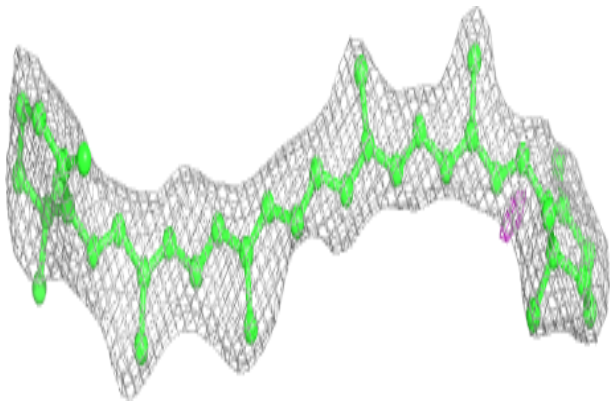


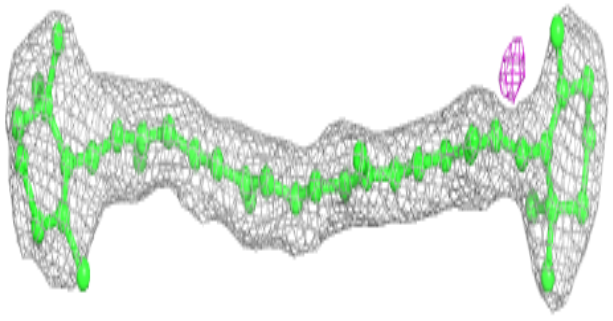


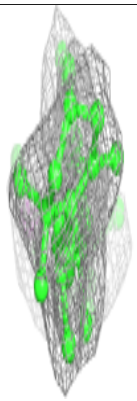


Electron density around BCR c 521:

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

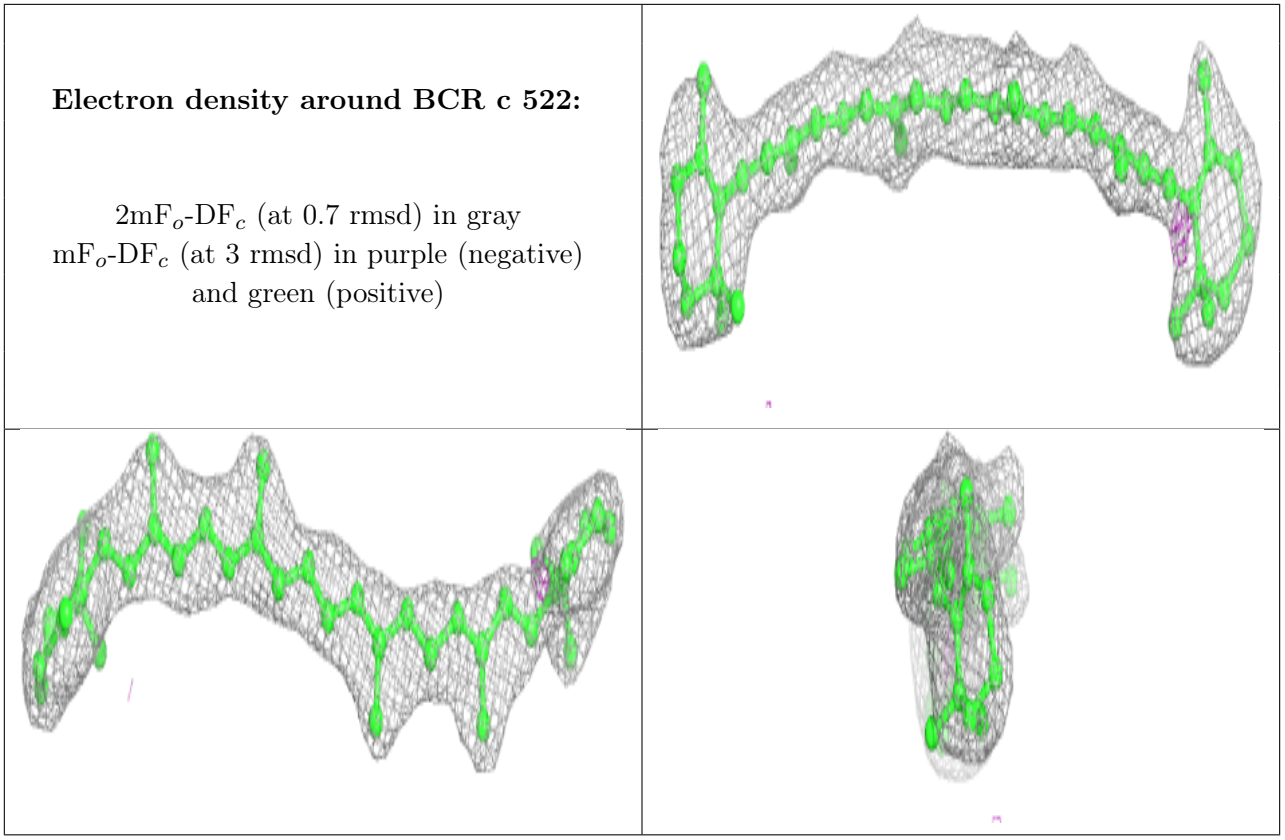






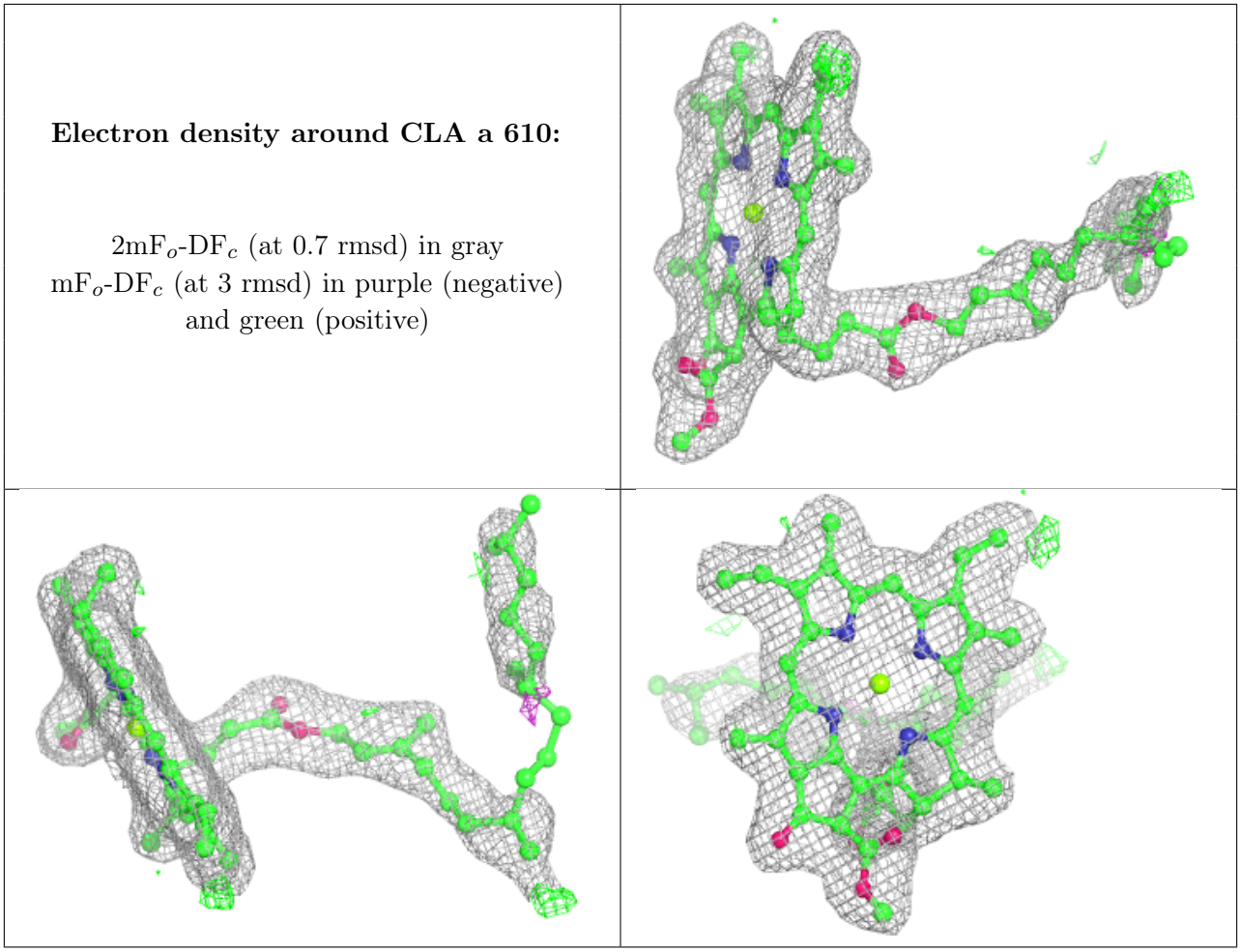
Electron density around BCR c 522:

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



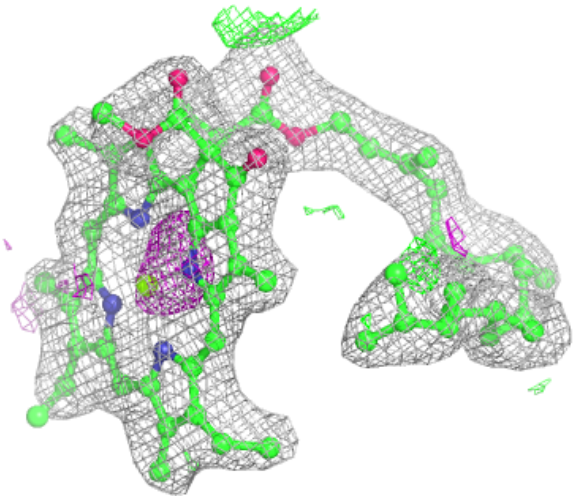
Electron density around CLA a 610:

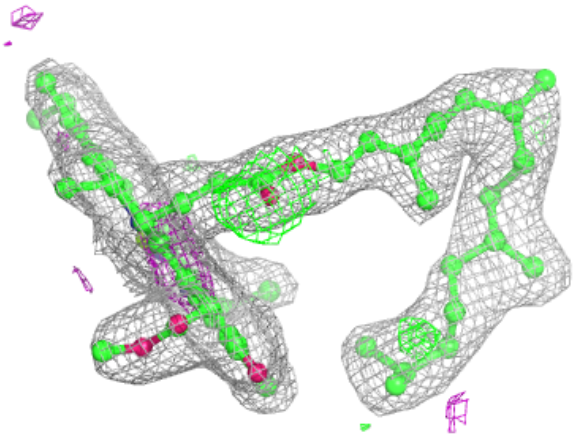
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

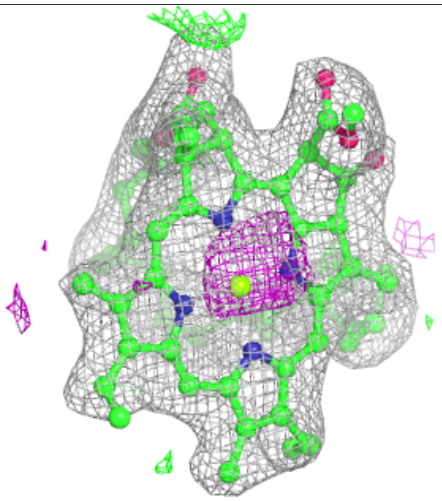


Electron density around CLA C 504:

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

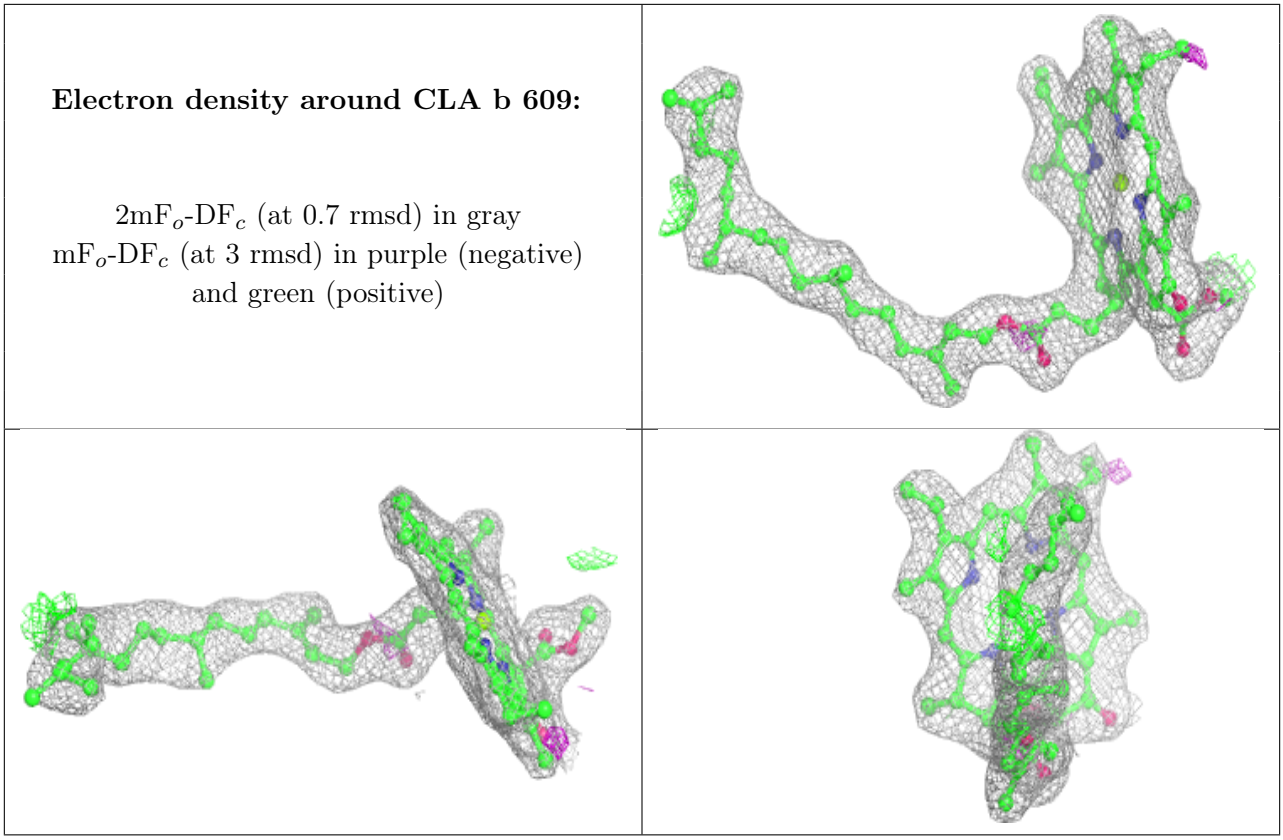






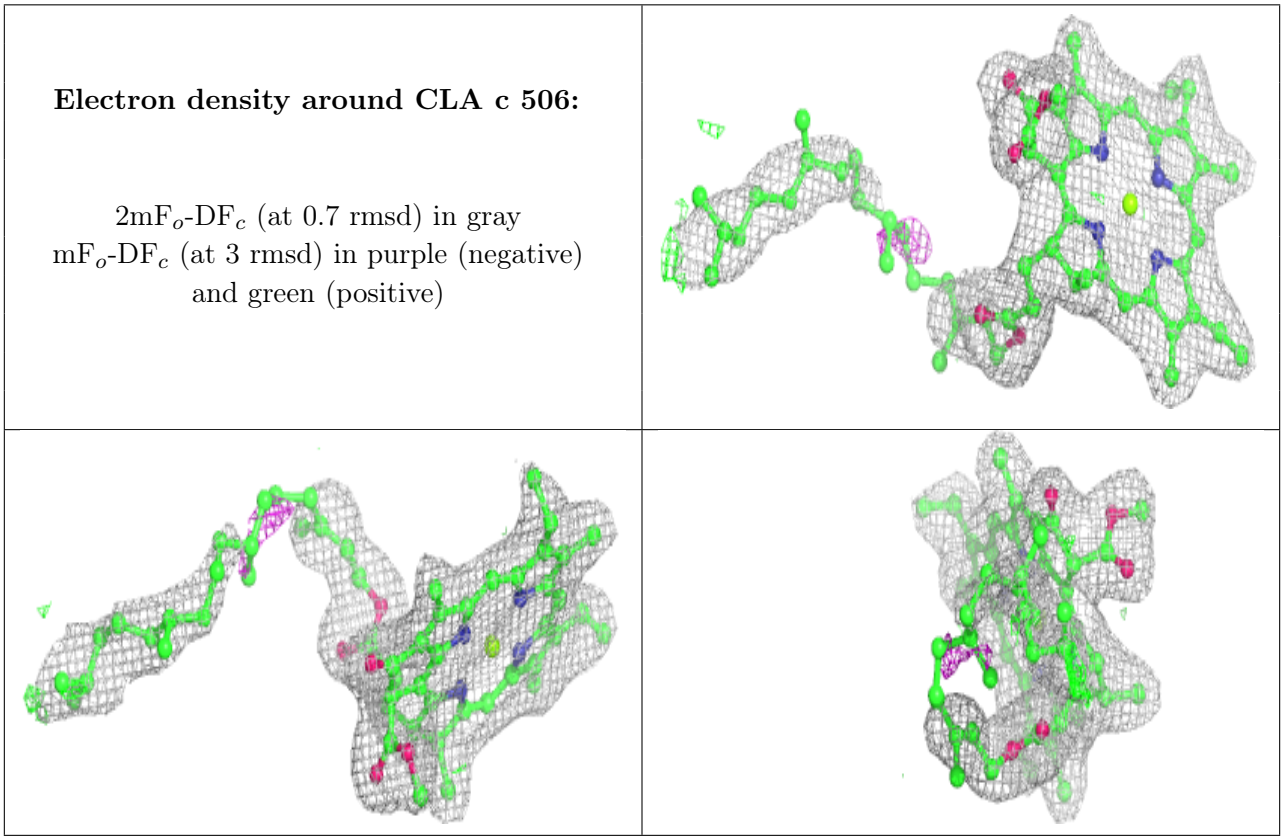
Electron density around CLA b 609:

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



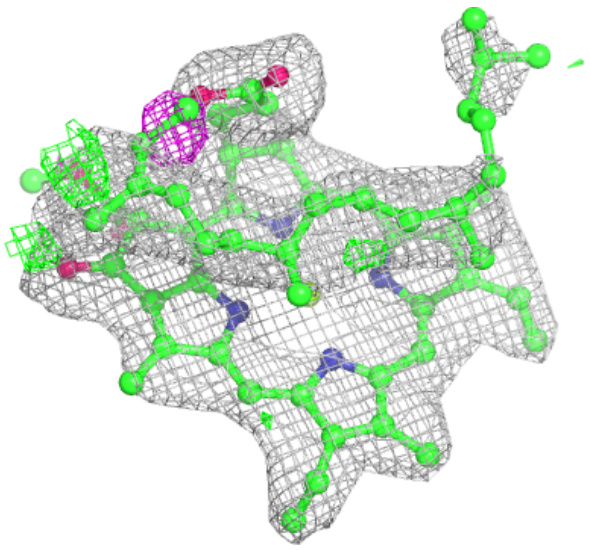
Electron density around CLA c 506:

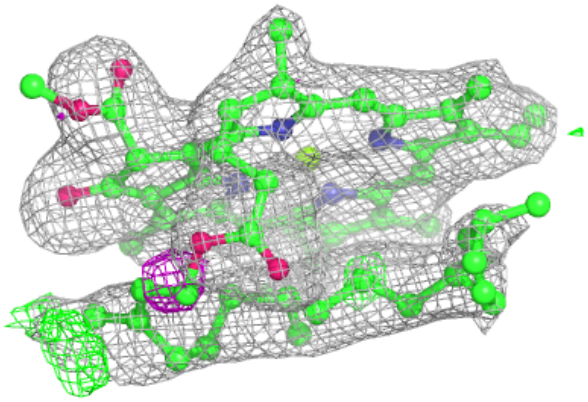
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

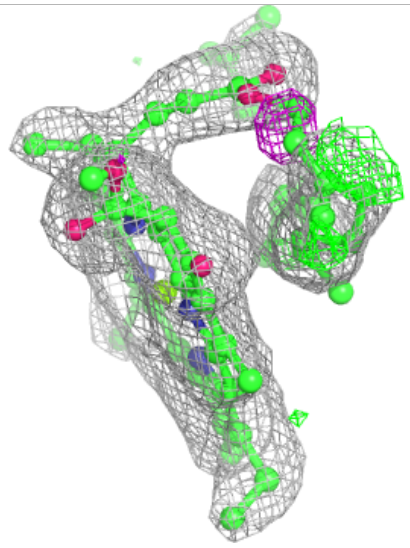


Electron density around CLA B 601:

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

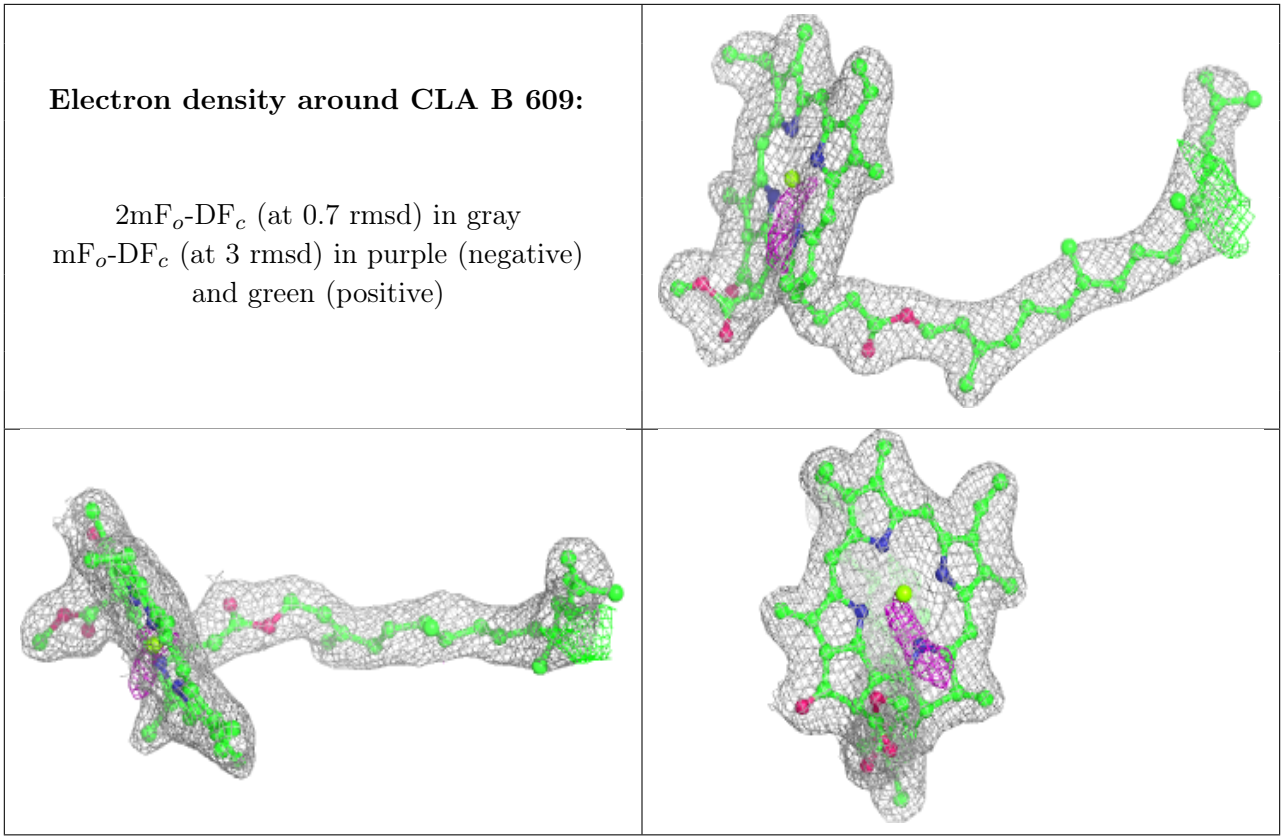






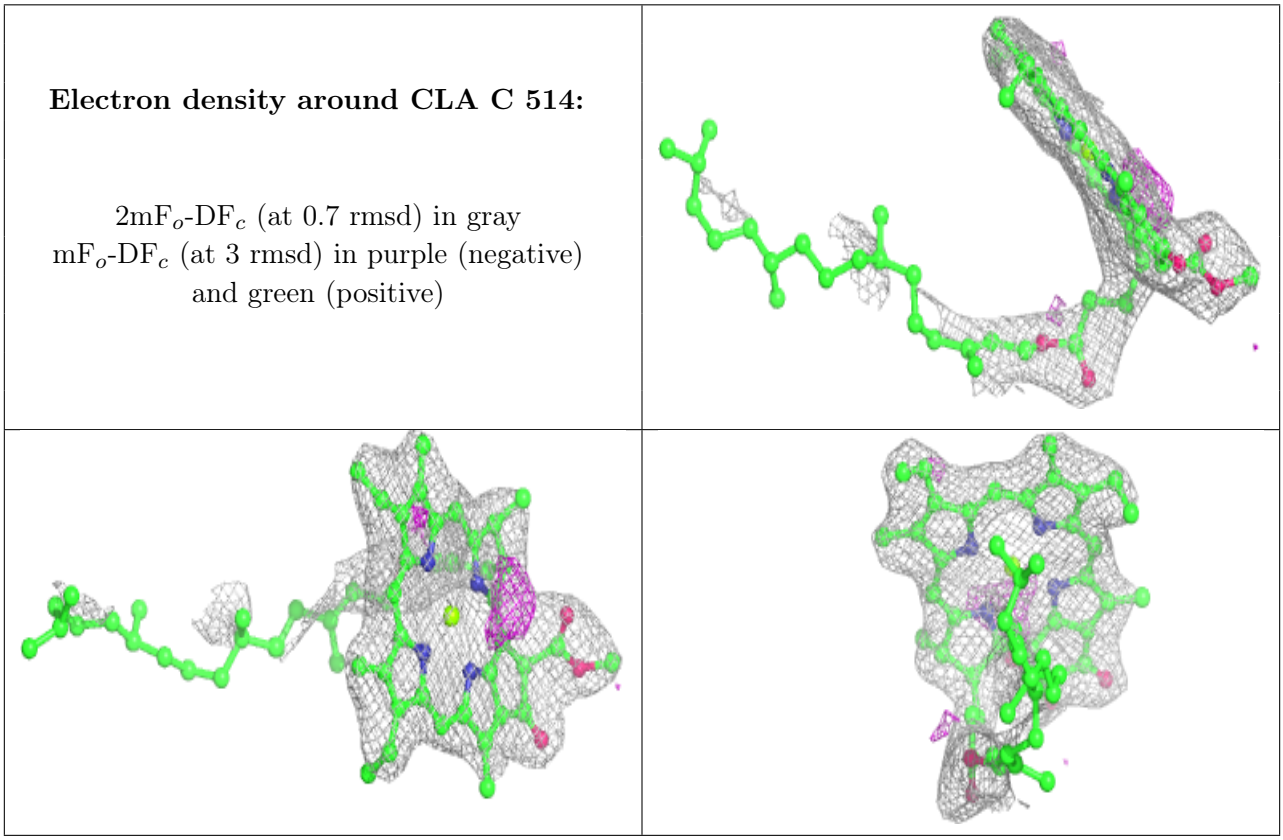
Electron density around CLA B 609:

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



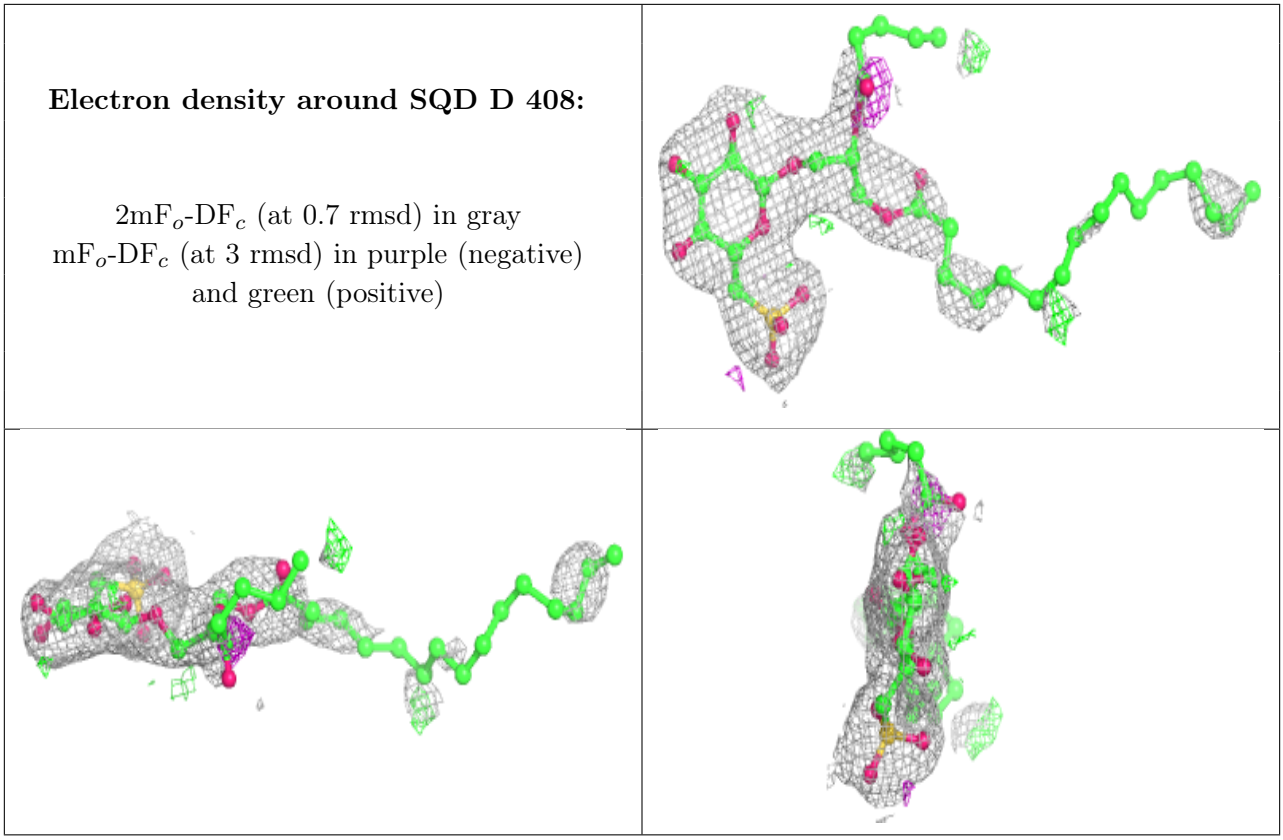
Electron density around CLA C 514:

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



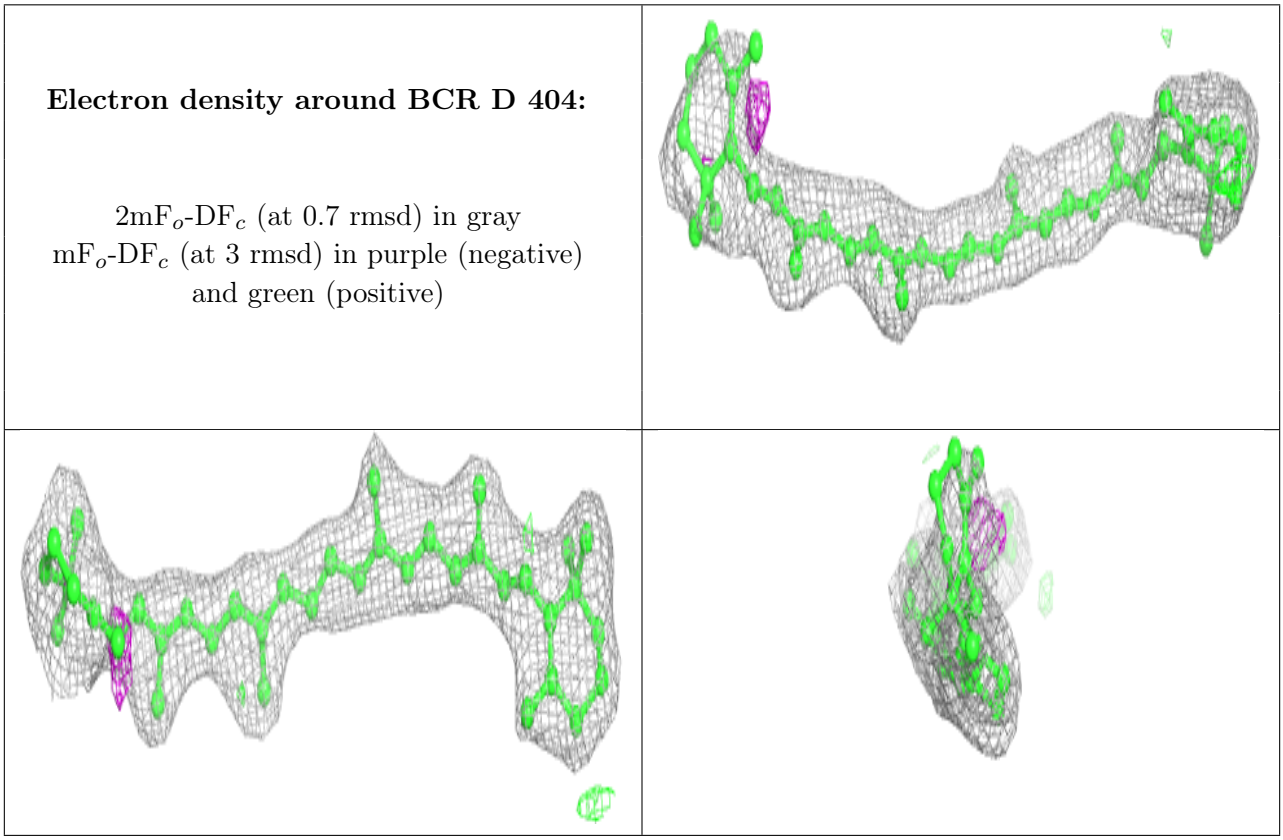
Electron density around SQD D 408:

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



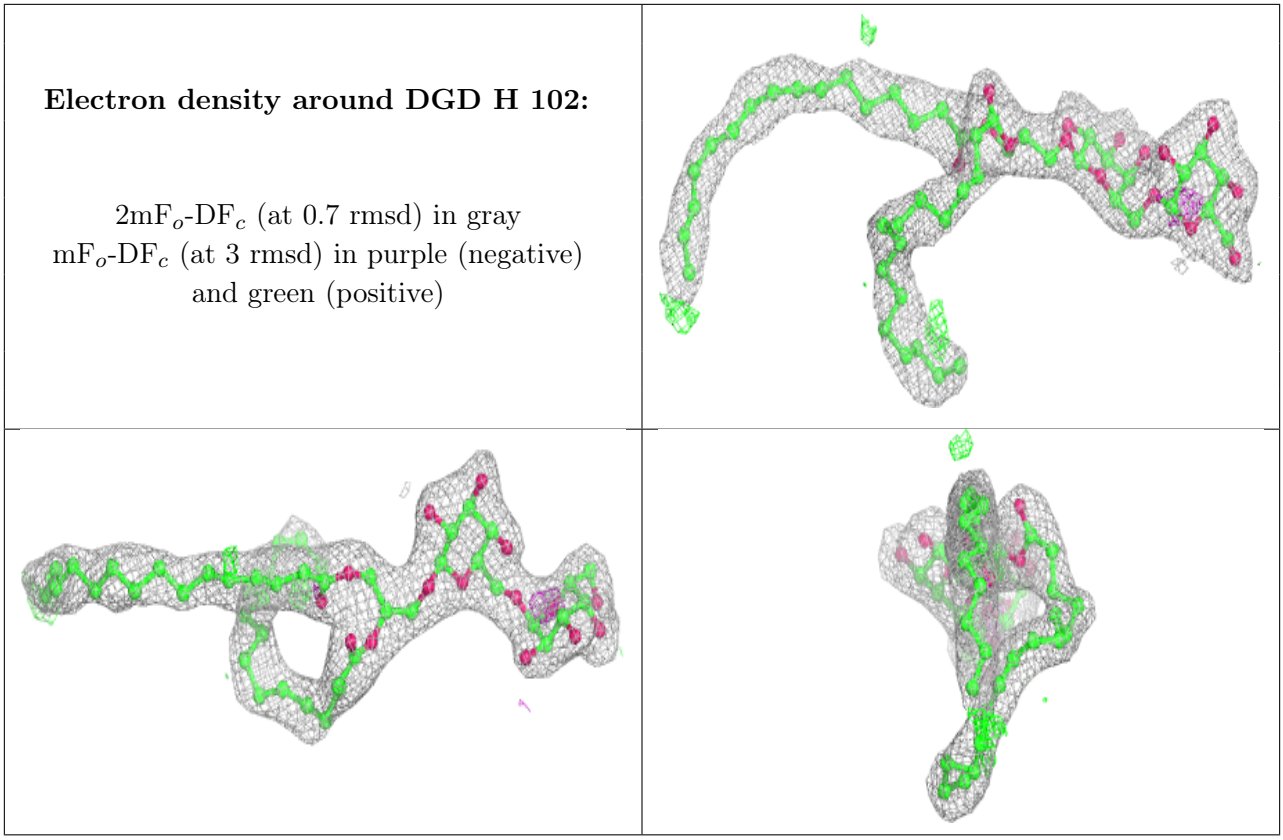
Electron density around BCR D 404:

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



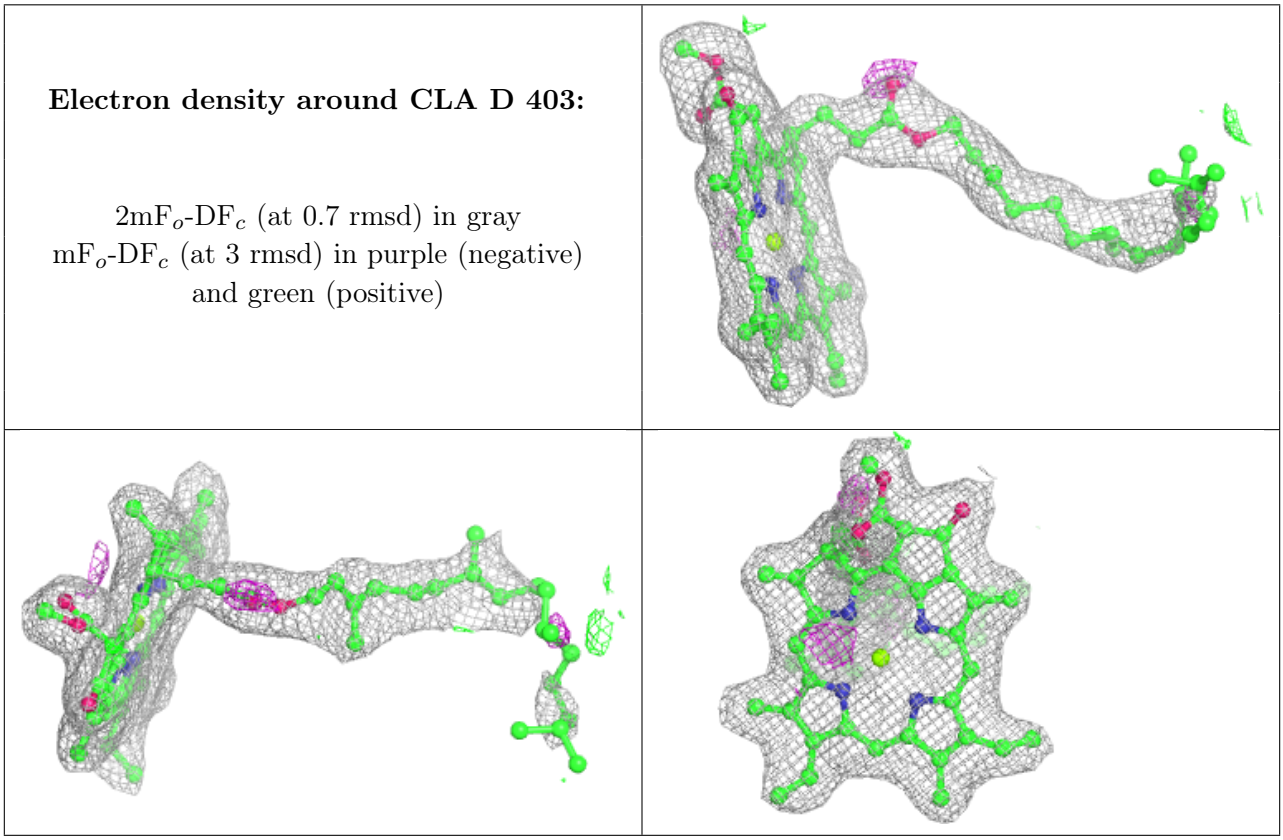
Electron density around DGD H 102:

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



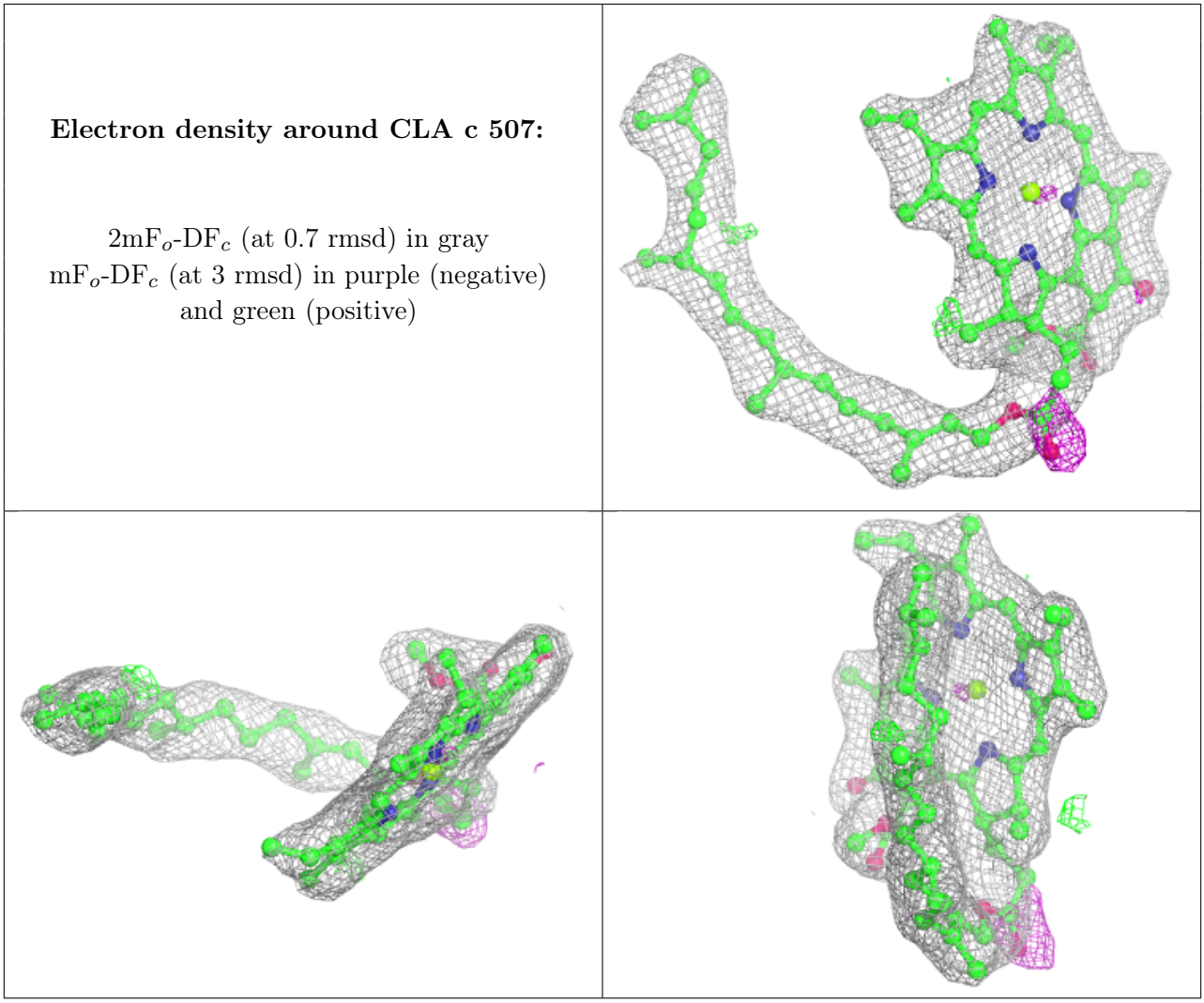
Electron density around CLA D 403:

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



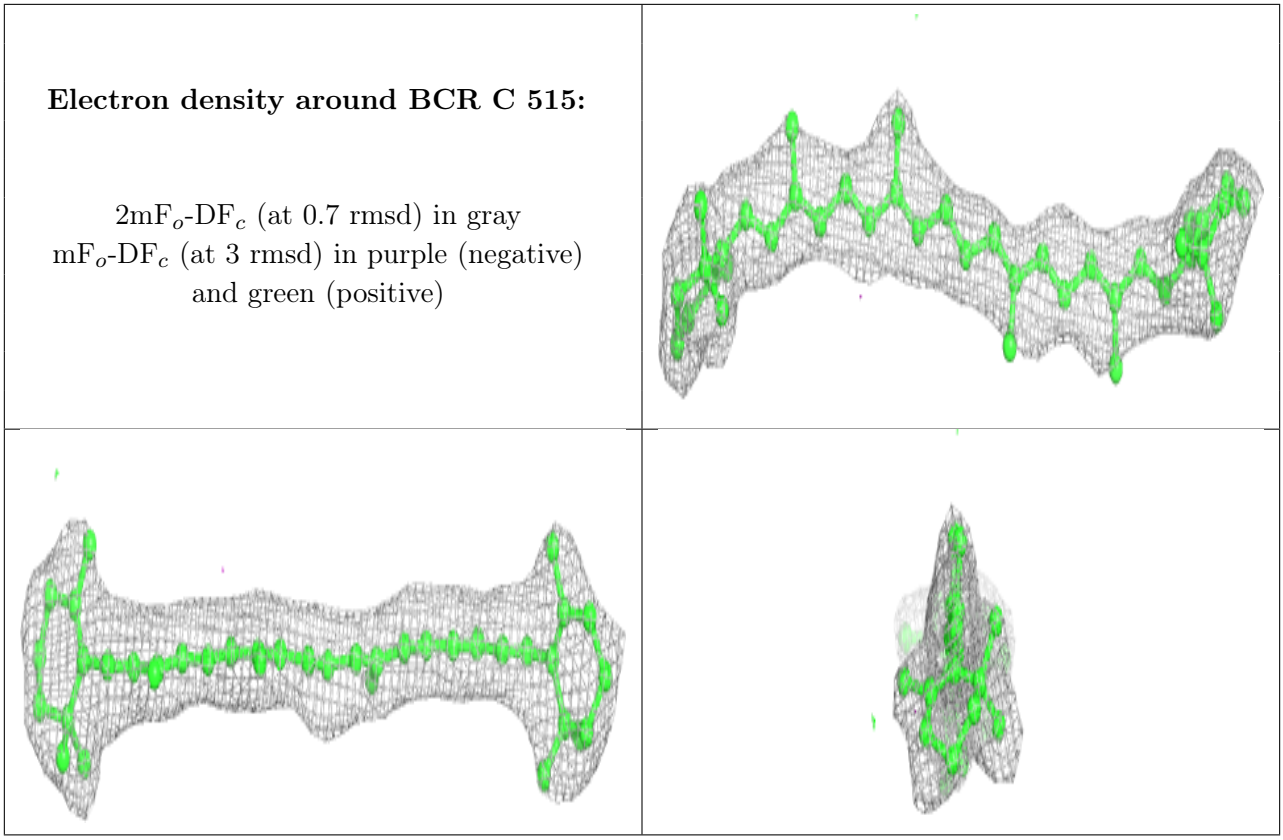
Electron density around CLA c 507:

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



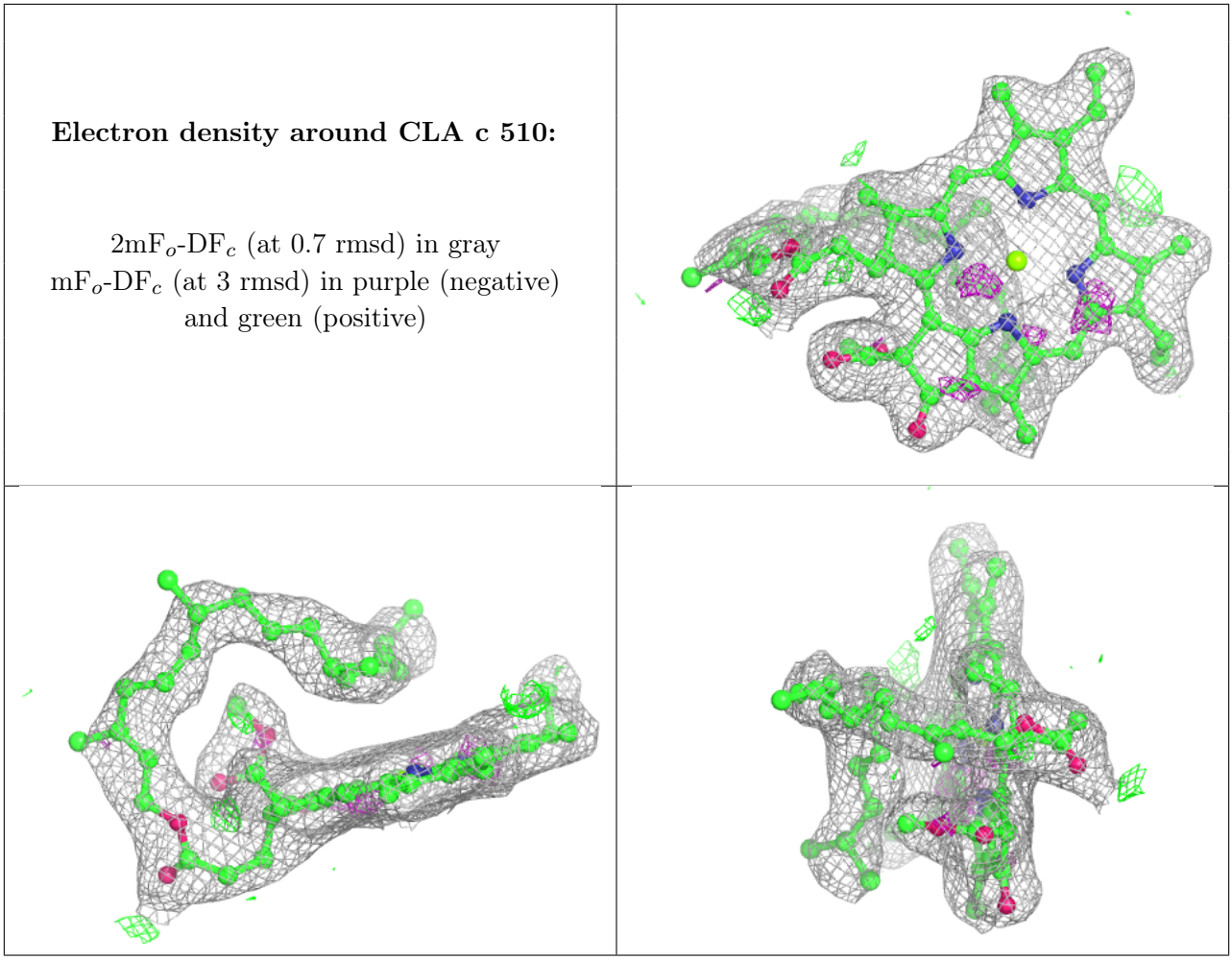
Electron density around BCR C 515:

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



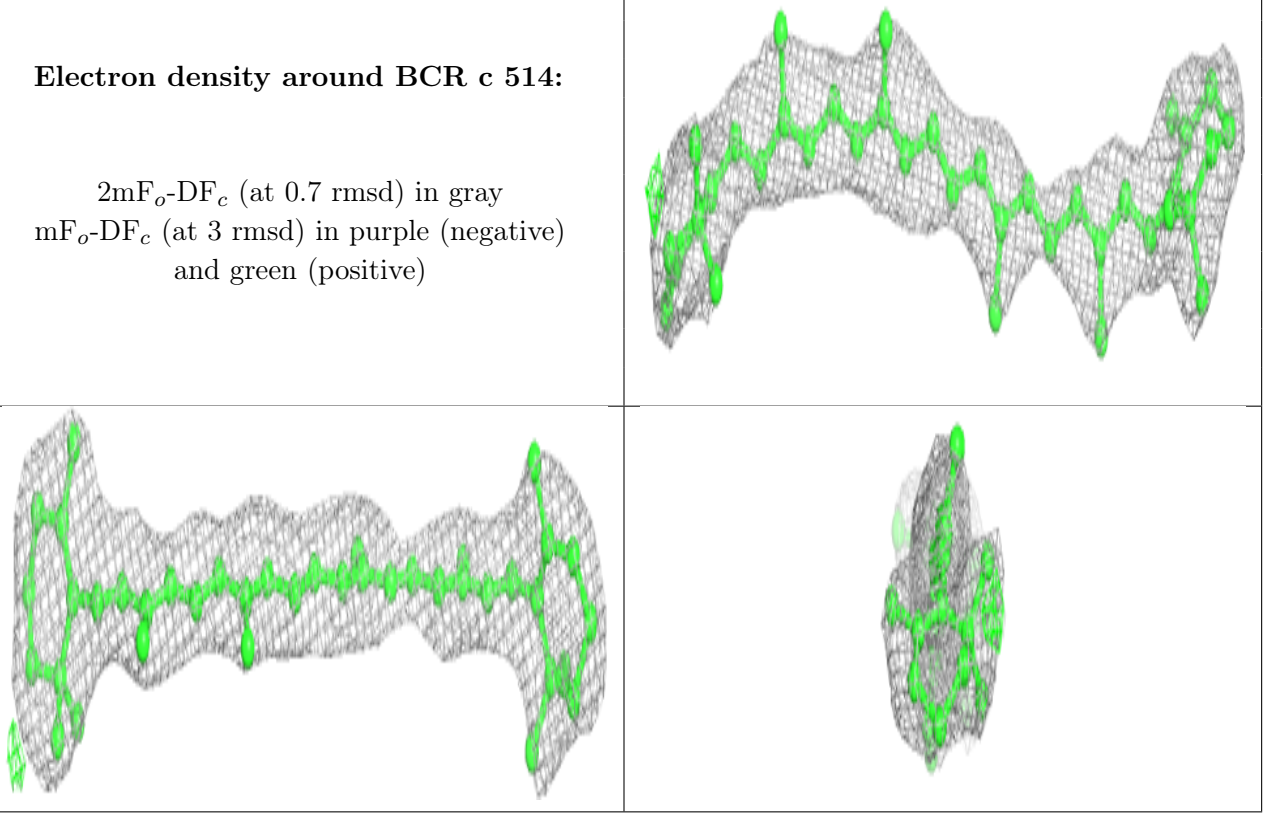
Electron density around CLA c 510:

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



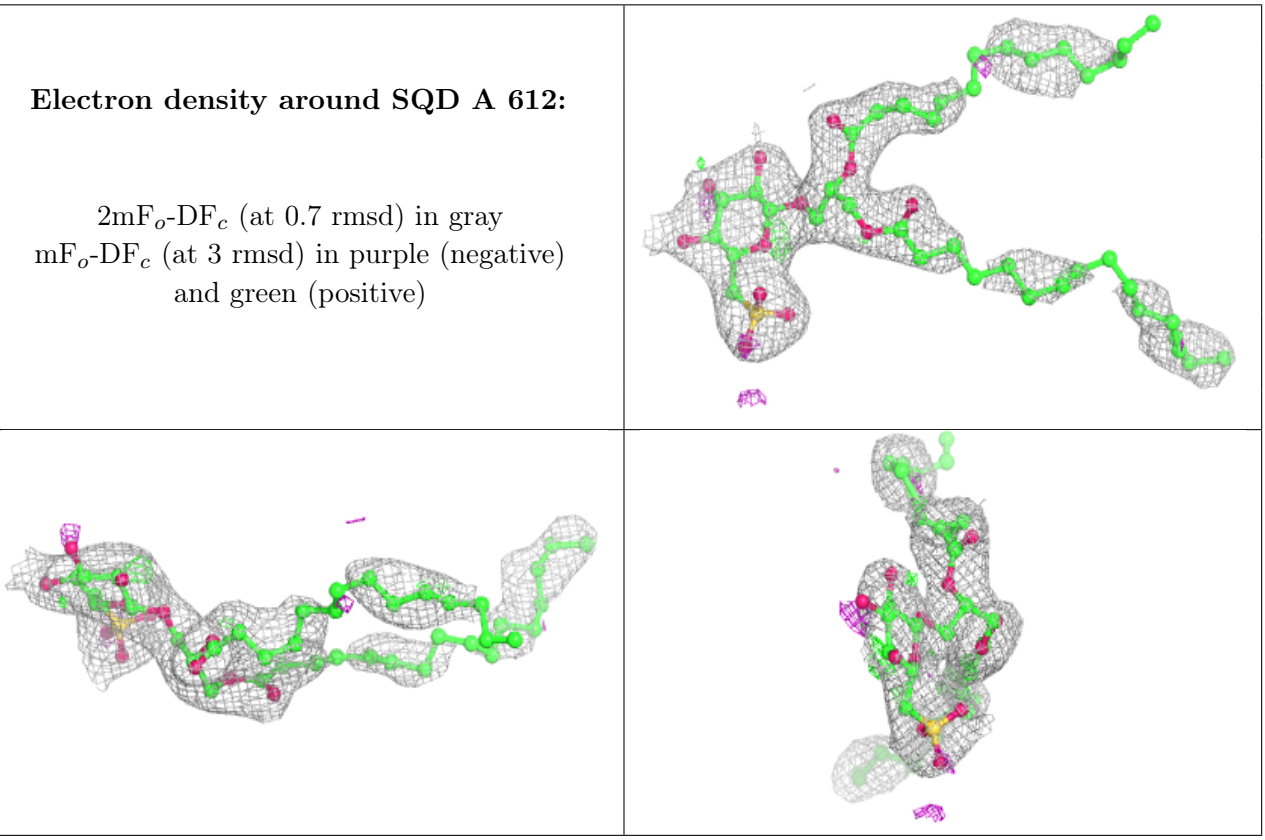
Electron density around BCR c 514:

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



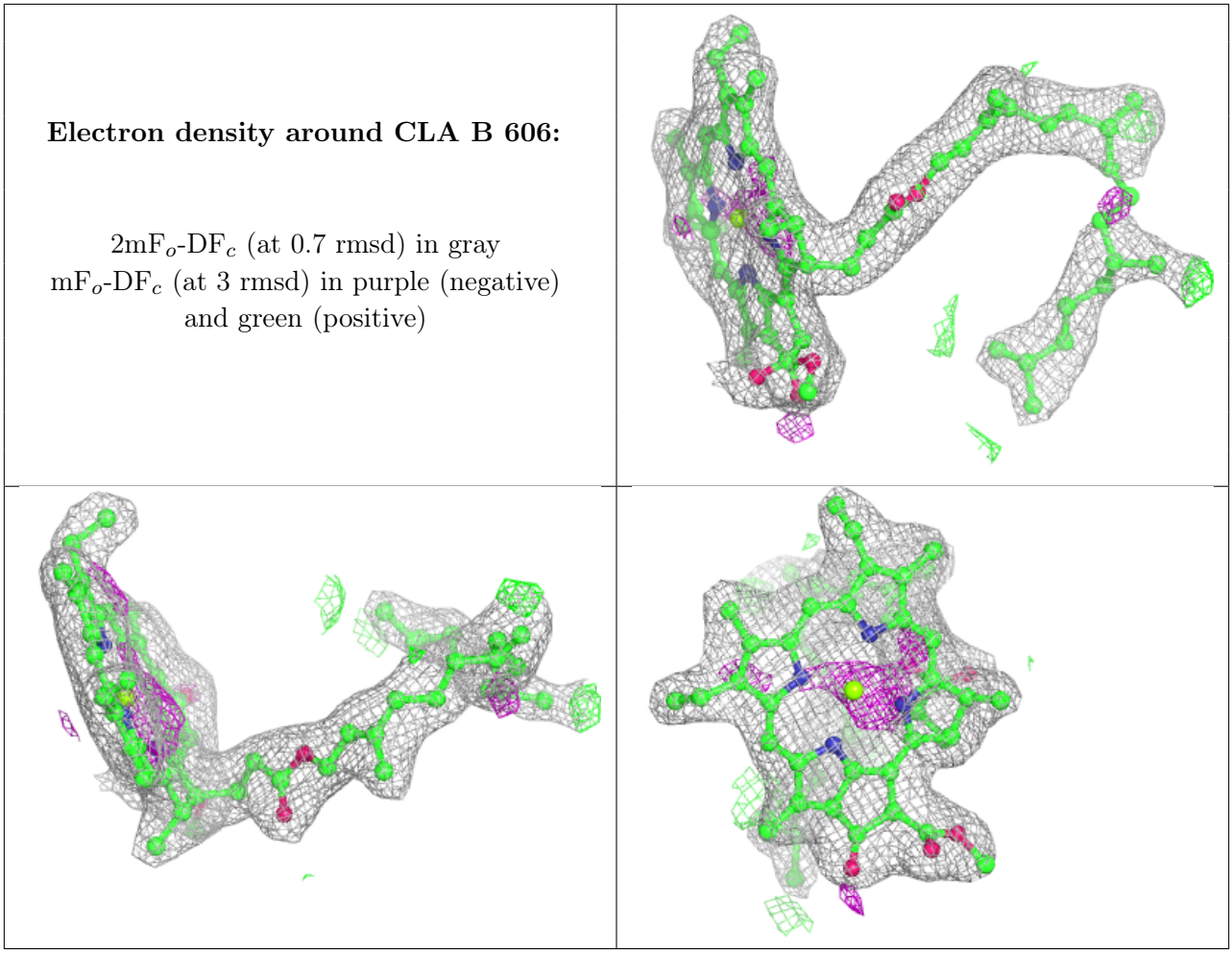
Electron density around SQD A 612:

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



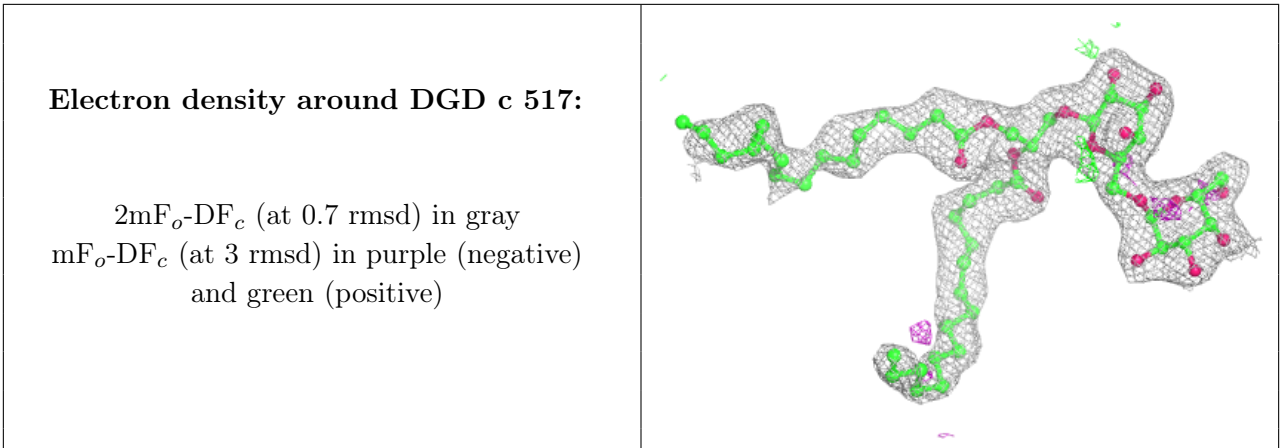
Electron density around CLA B 606:

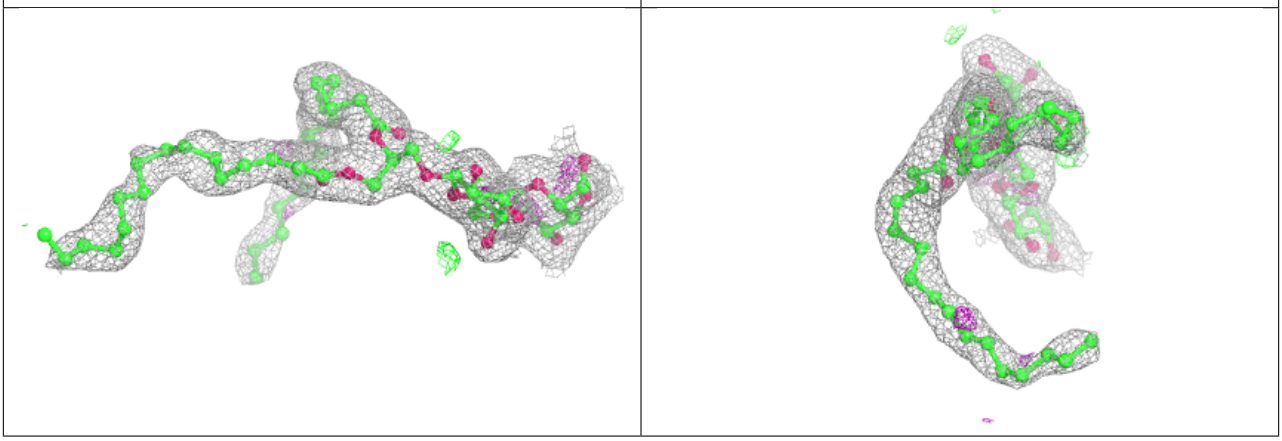
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD c 517:

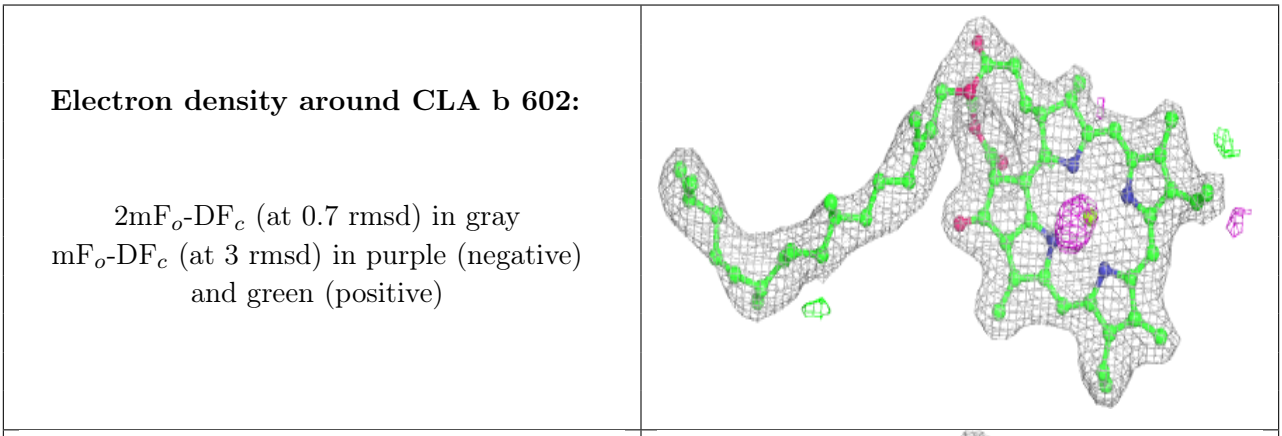
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

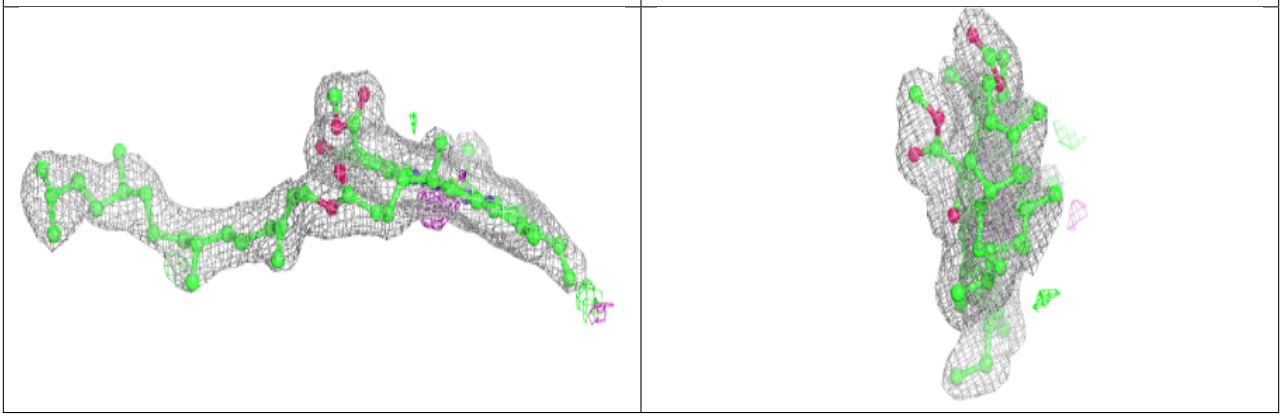




Electron density around CLA b 602:

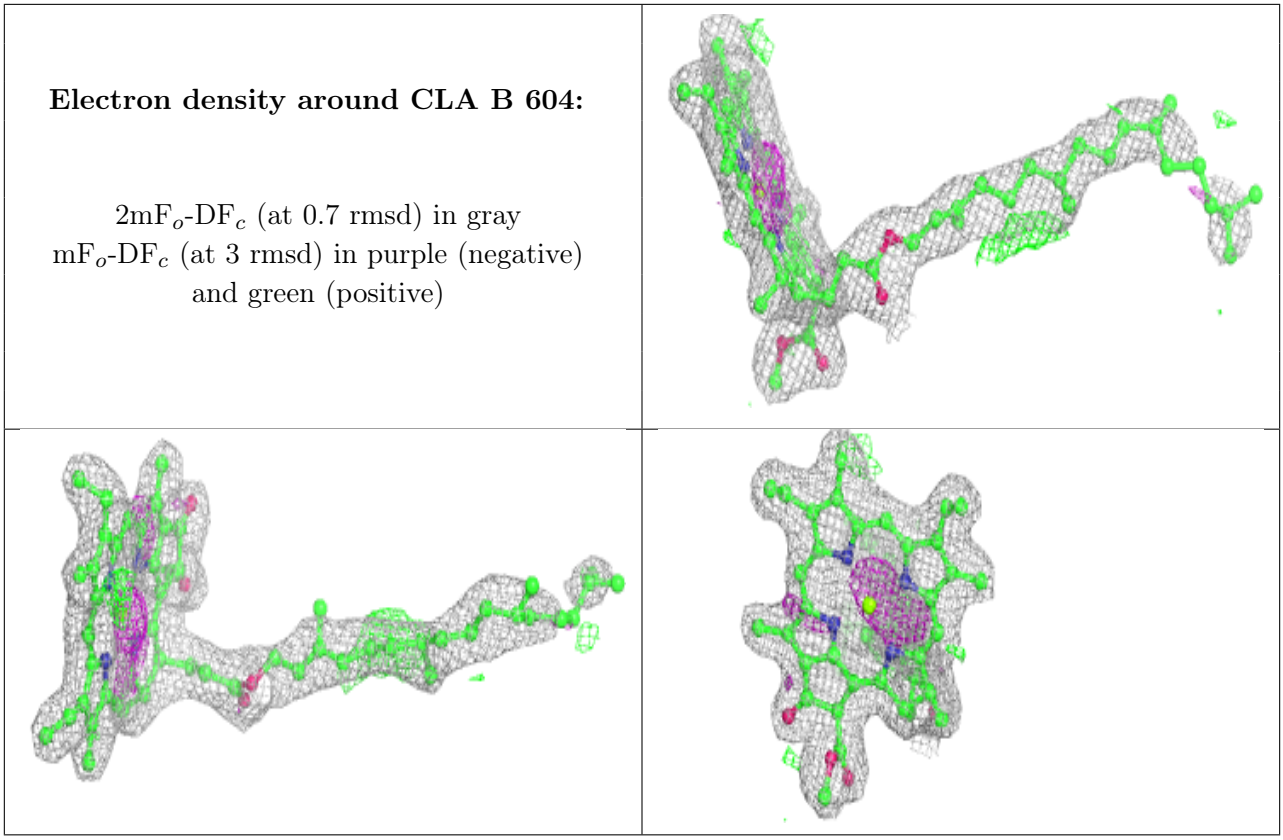
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





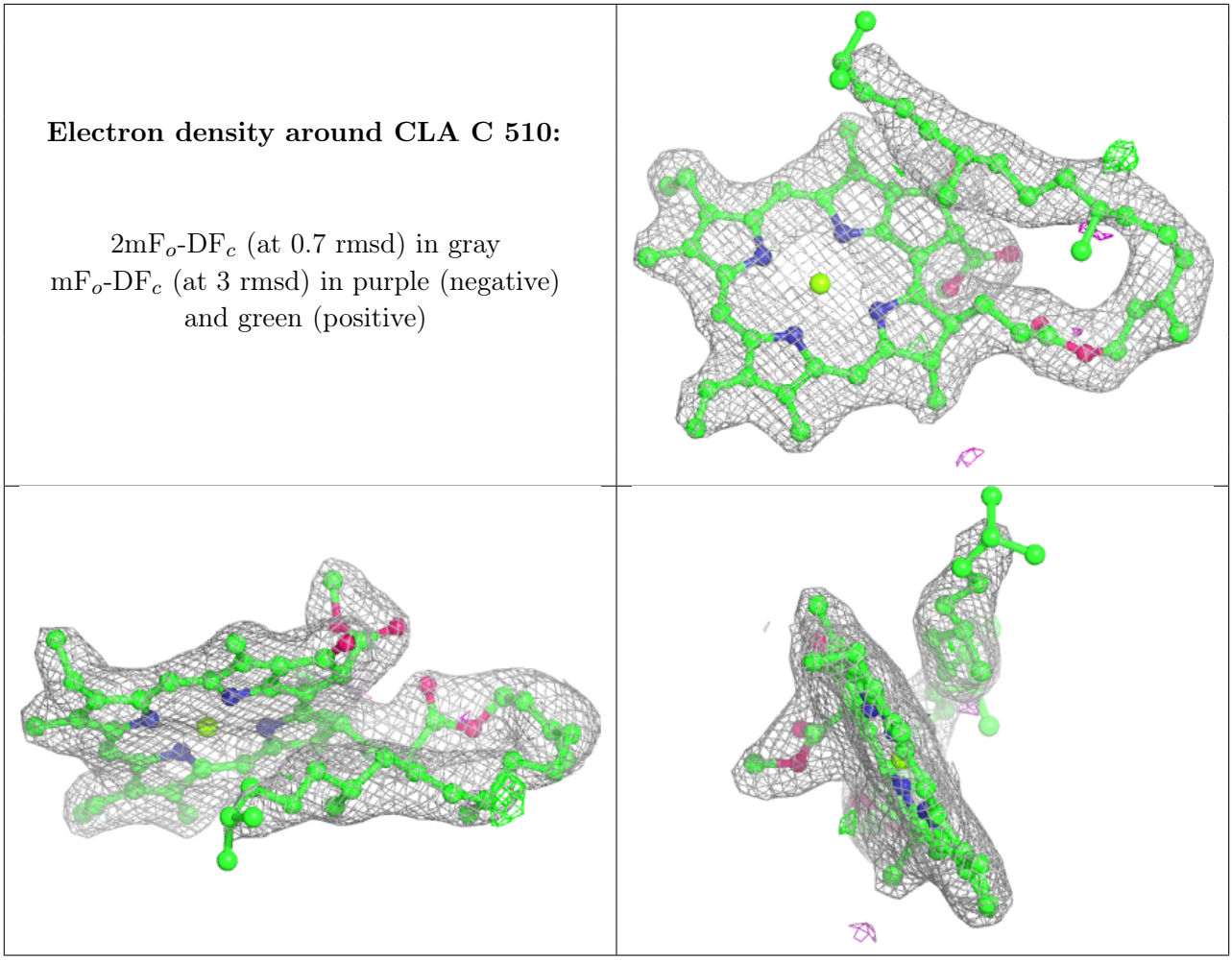
Electron density around CLA B 604:

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



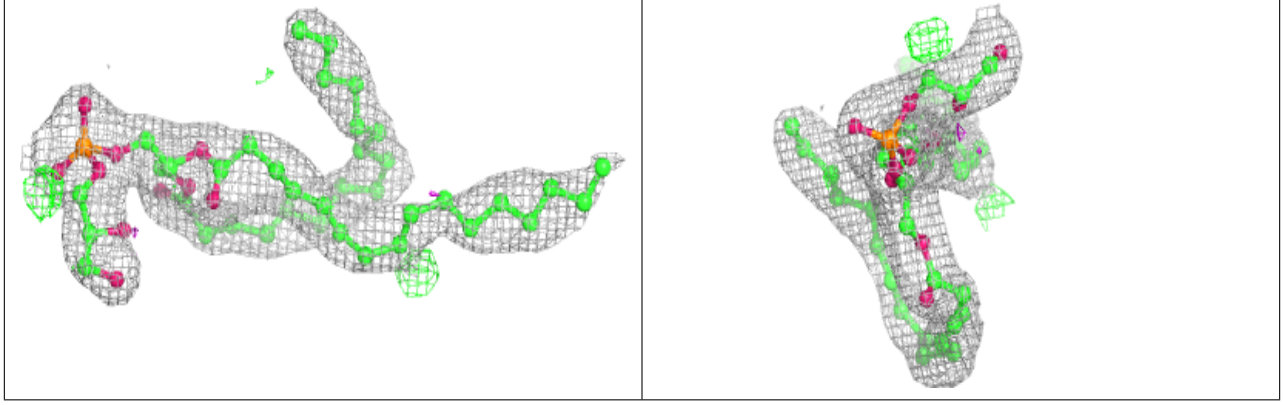
Electron density around CLA C 510:

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



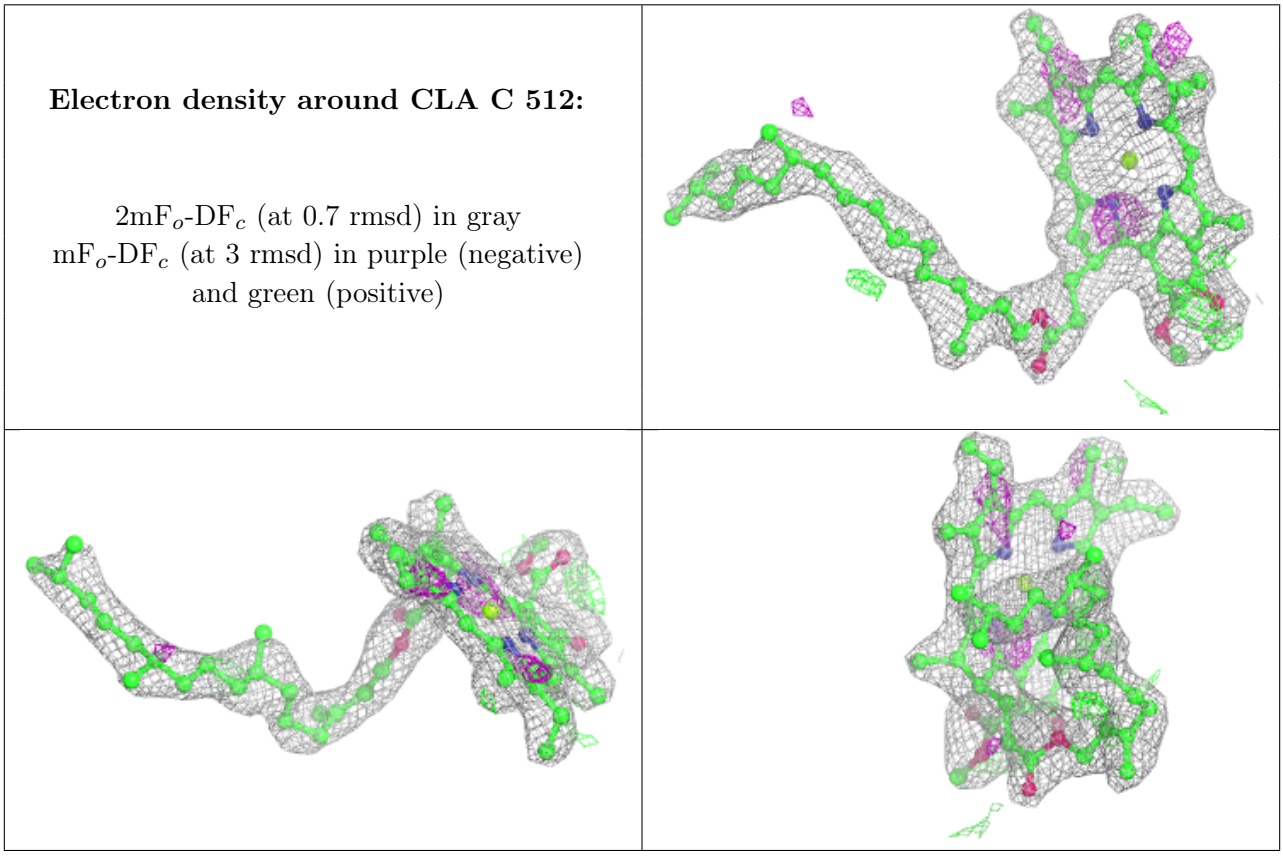
Electron density around LHG d 405:

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



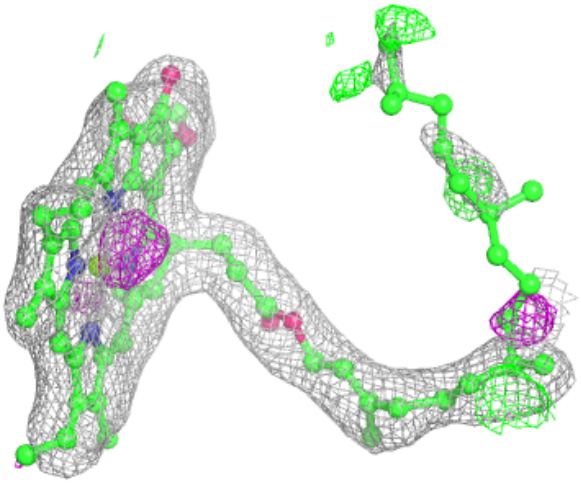
Electron density around CLA C 512:

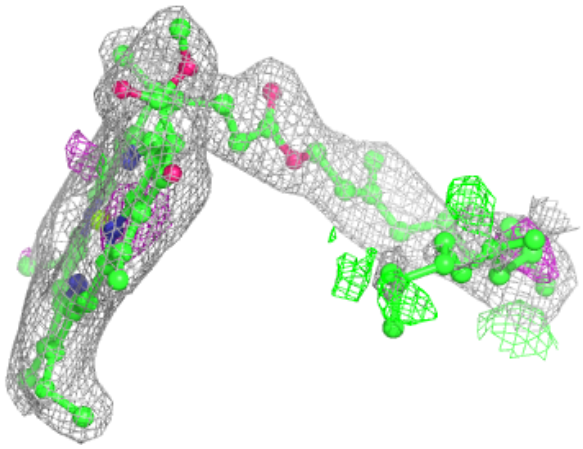
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

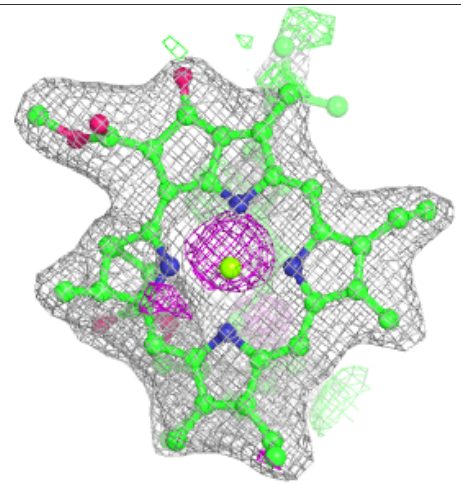


Electron density around CLA b 606 (A):

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

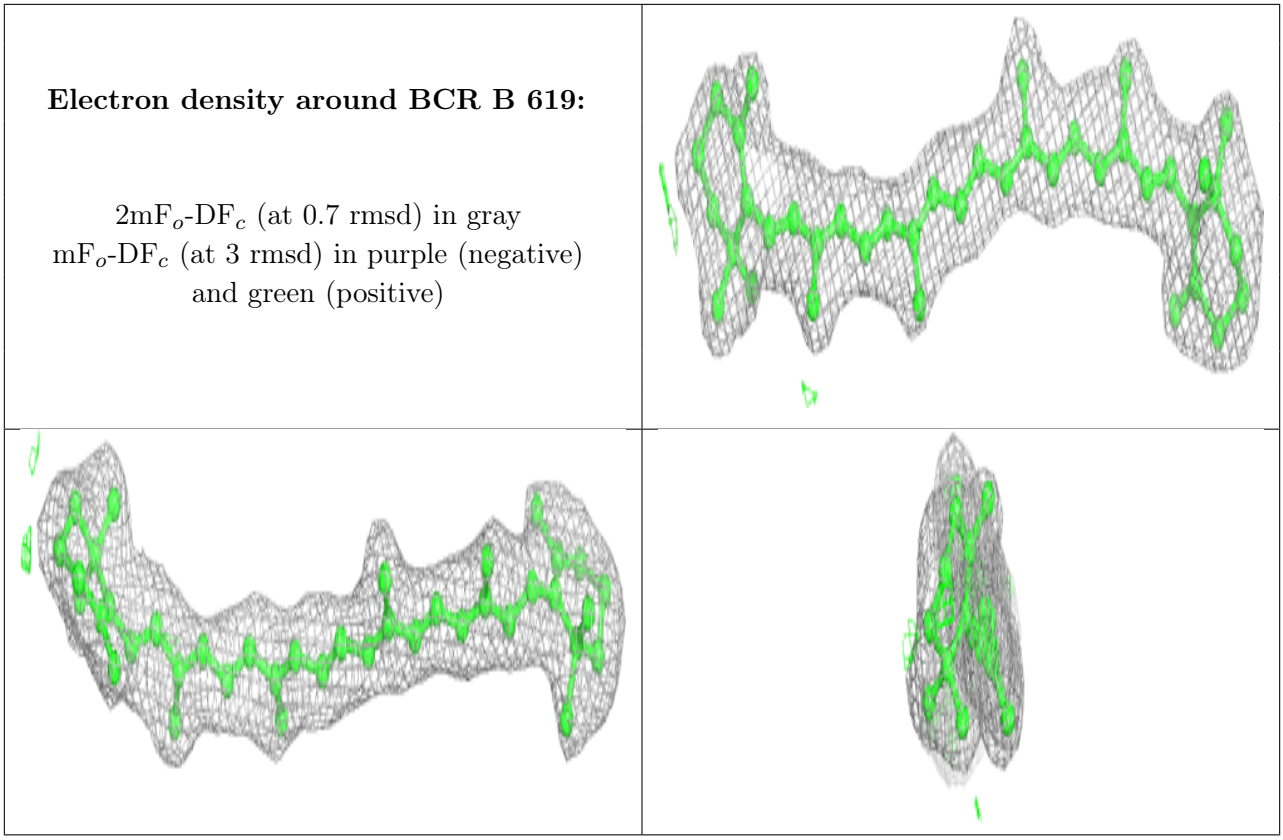






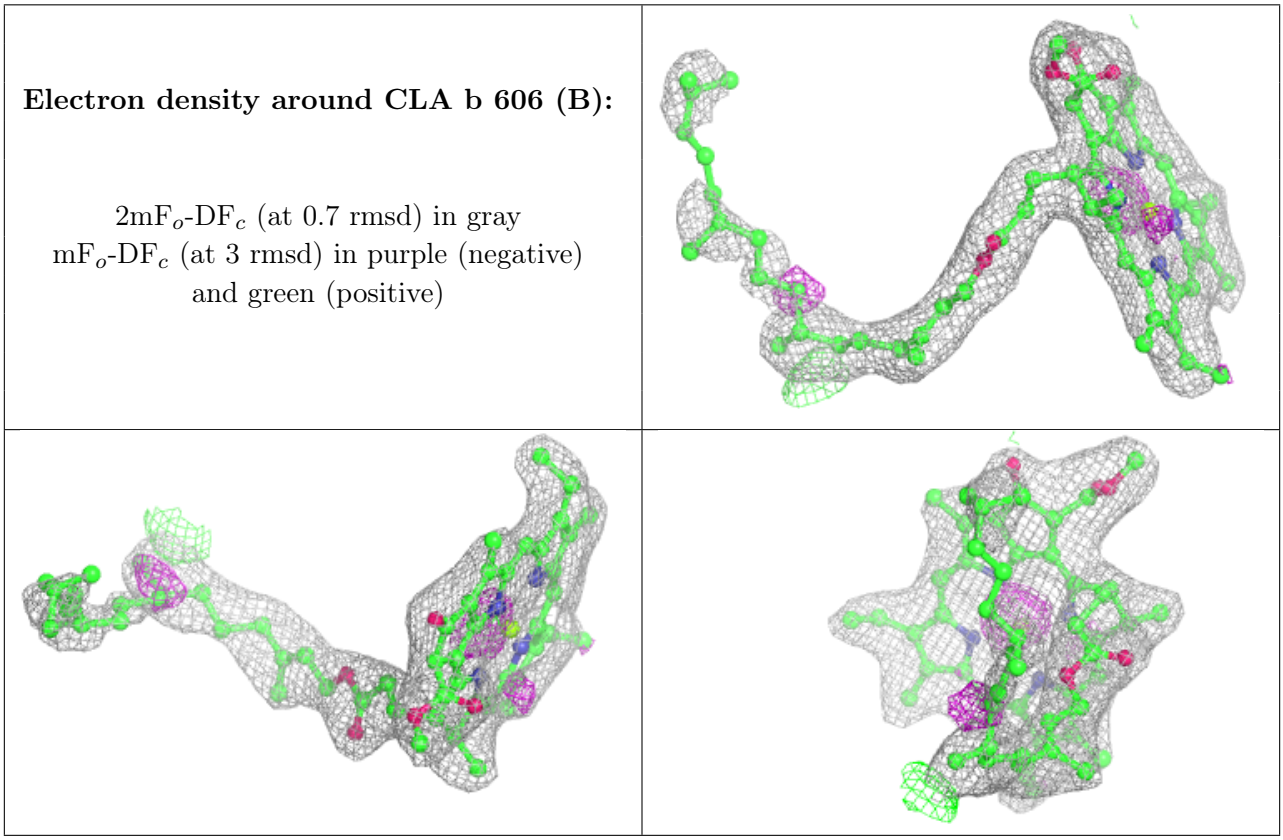
Electron density around BCR B 619:

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



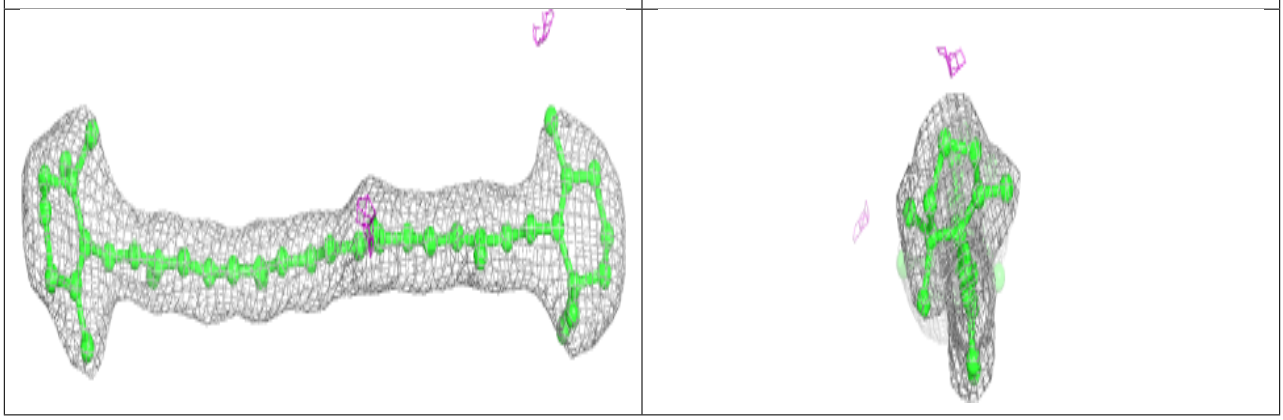
Electron density around CLA b 606 (B):

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



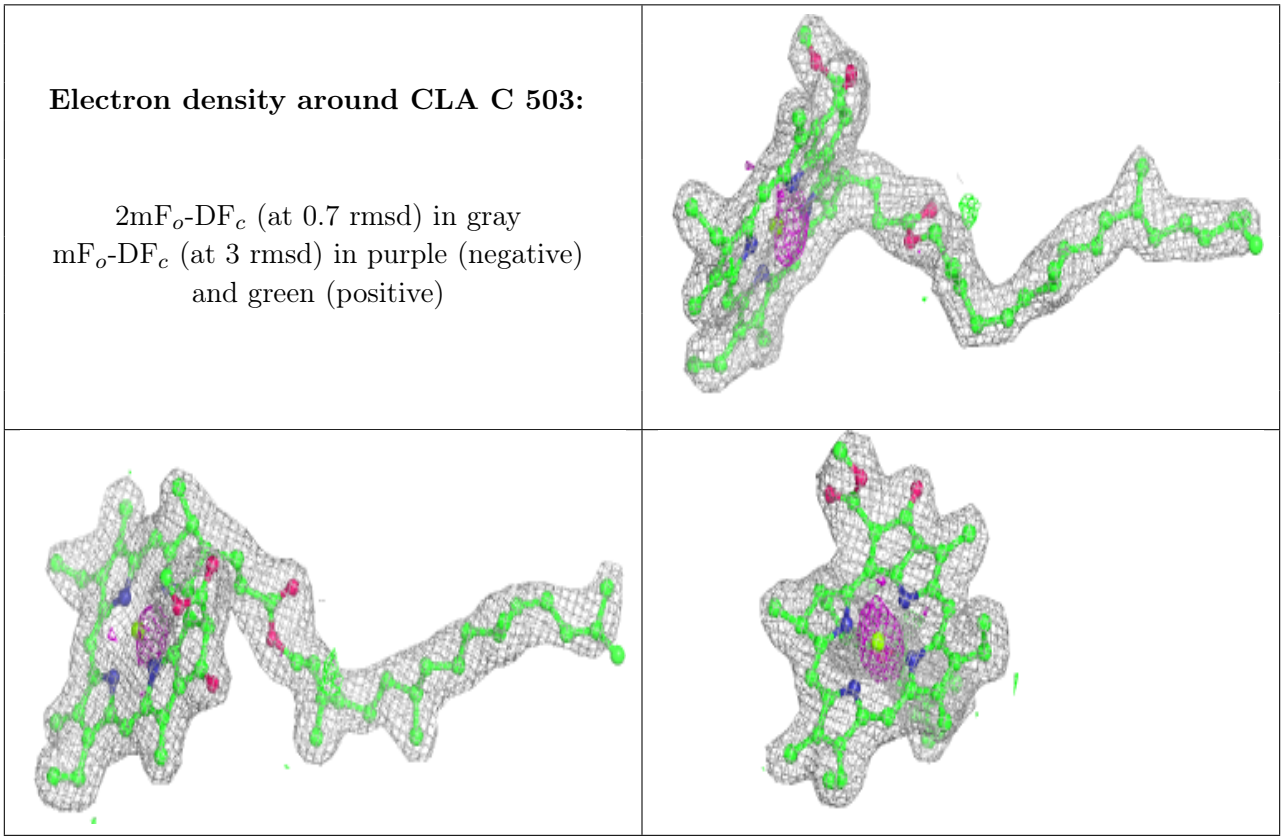
Electron density around BCR C 516:

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



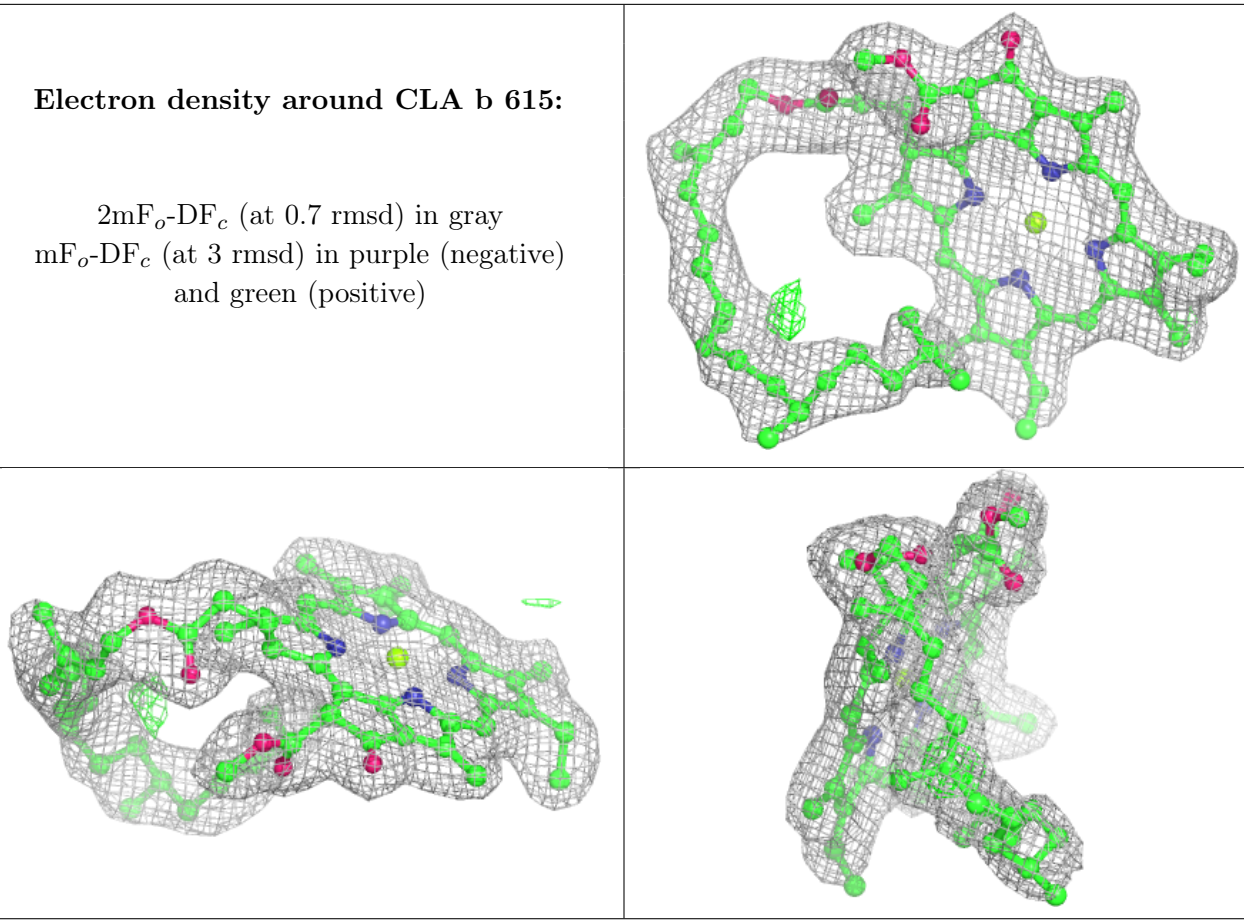
Electron density around CLA C 503:

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



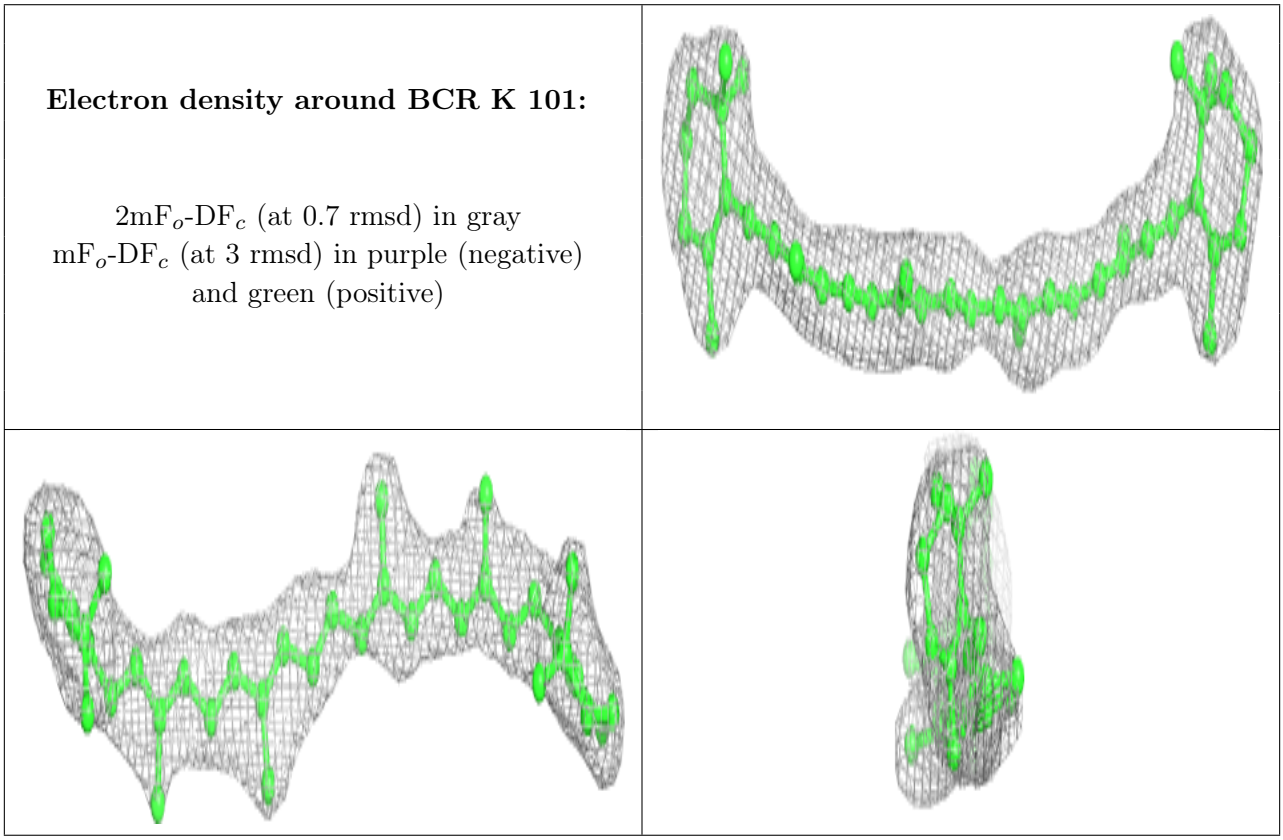
Electron density around CLA b 615:

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



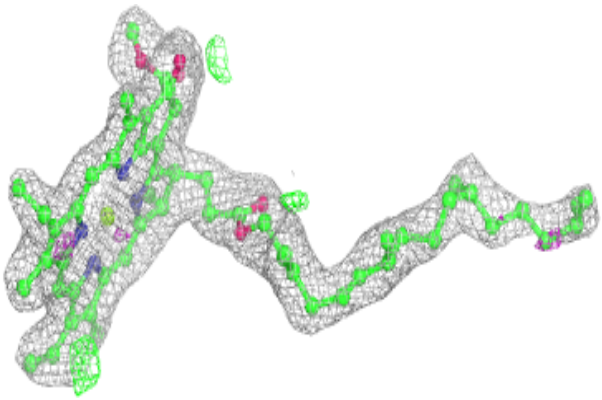
Electron density around BCR K 101:

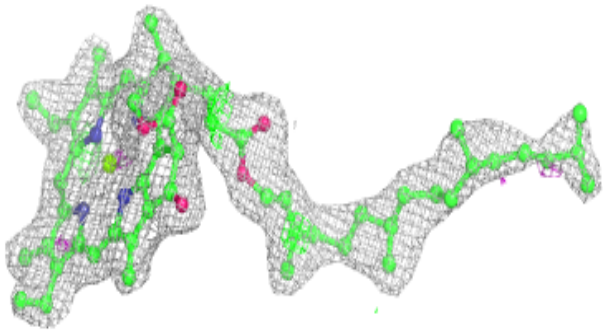
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

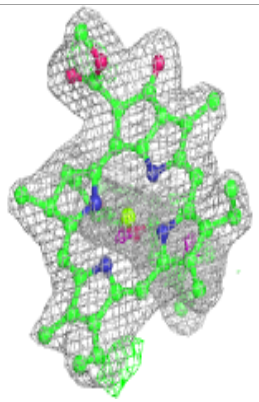


Electron density around CLA c 502:

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

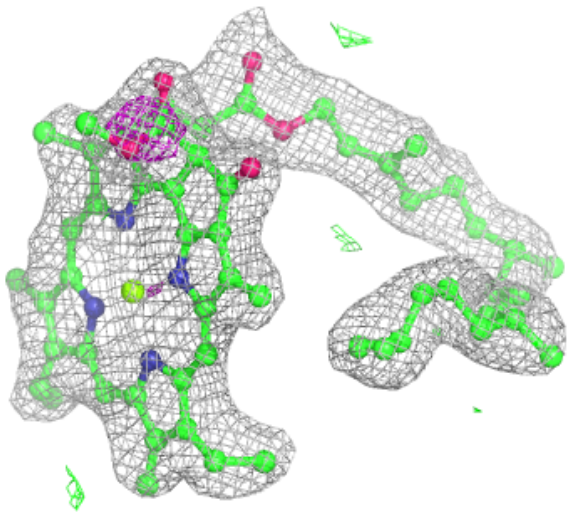


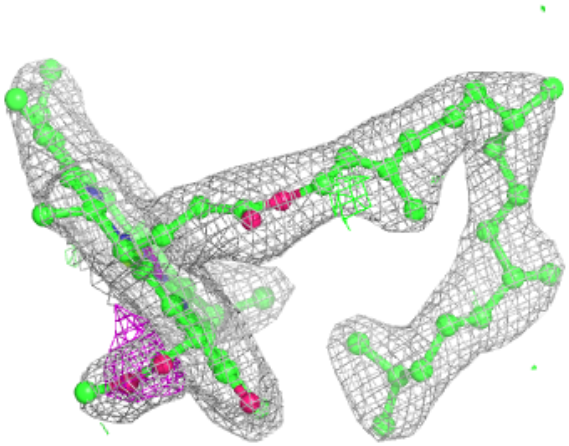


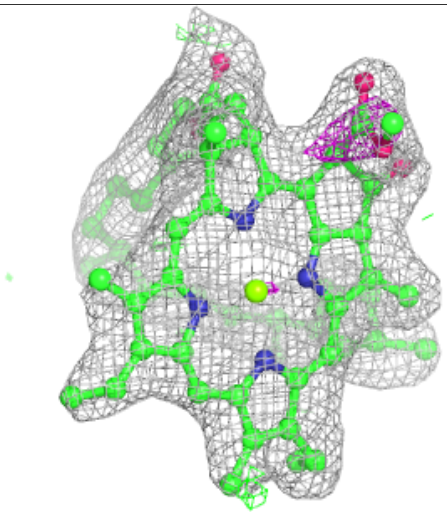


Electron density around CLA c 503:

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

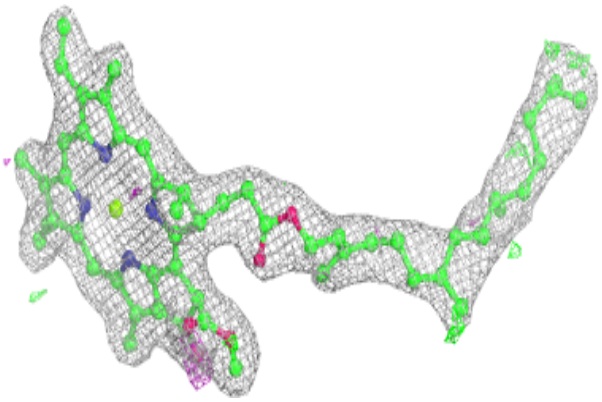


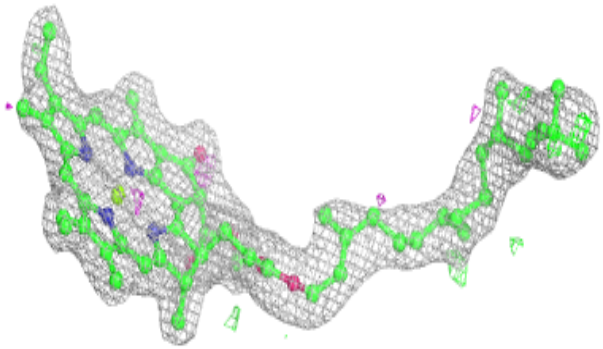


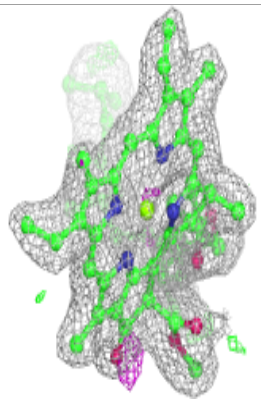


Electron density around CLA A 606:

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

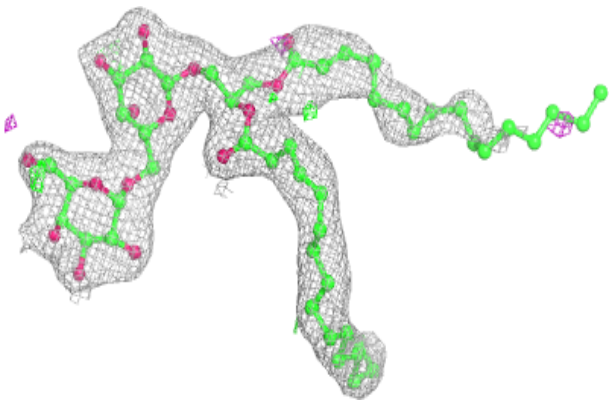


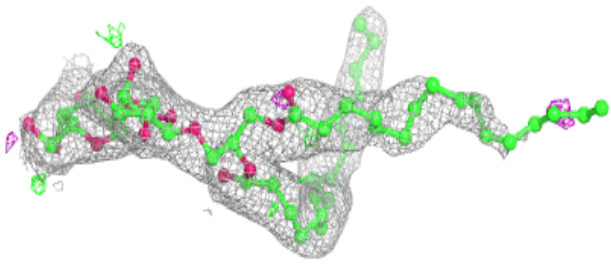


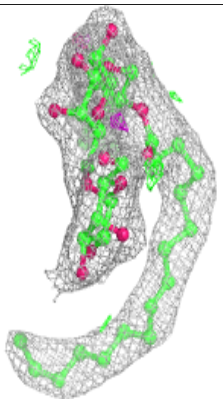


Electron density around DGD C 518:

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

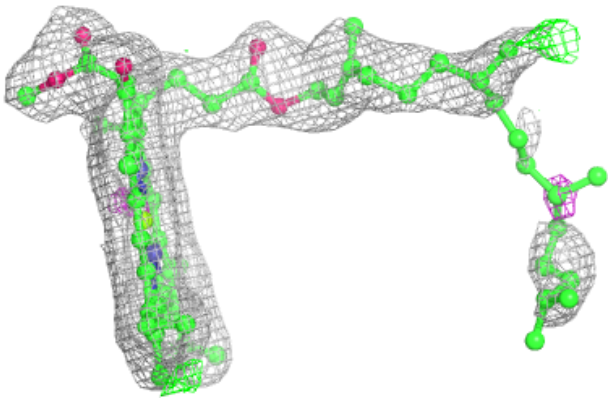


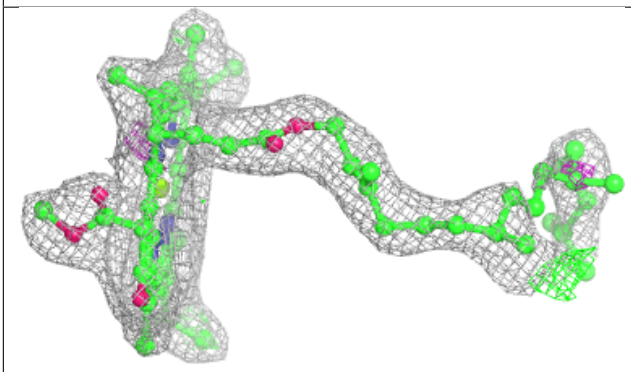


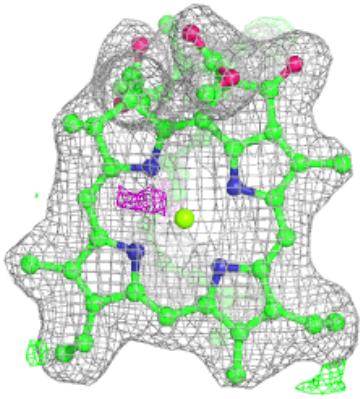


Electron density around CLA C 507:

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

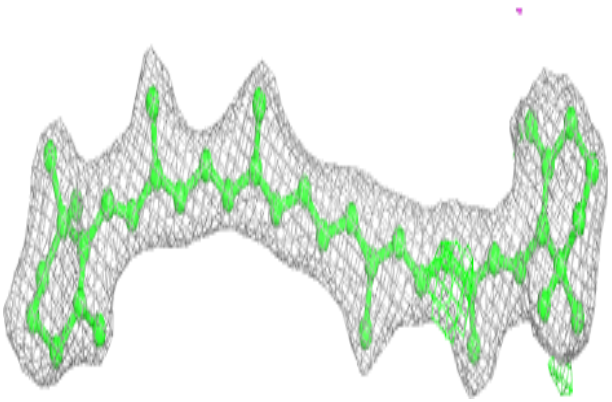


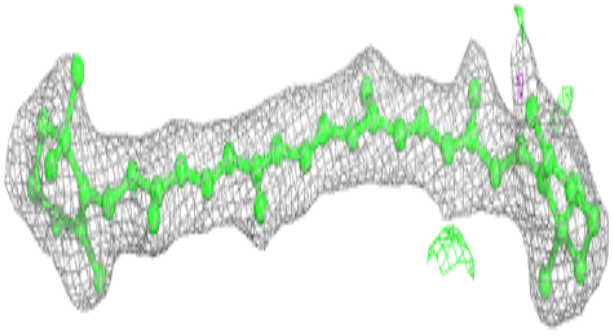


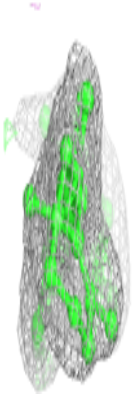


Electron density around BCR b 619:

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

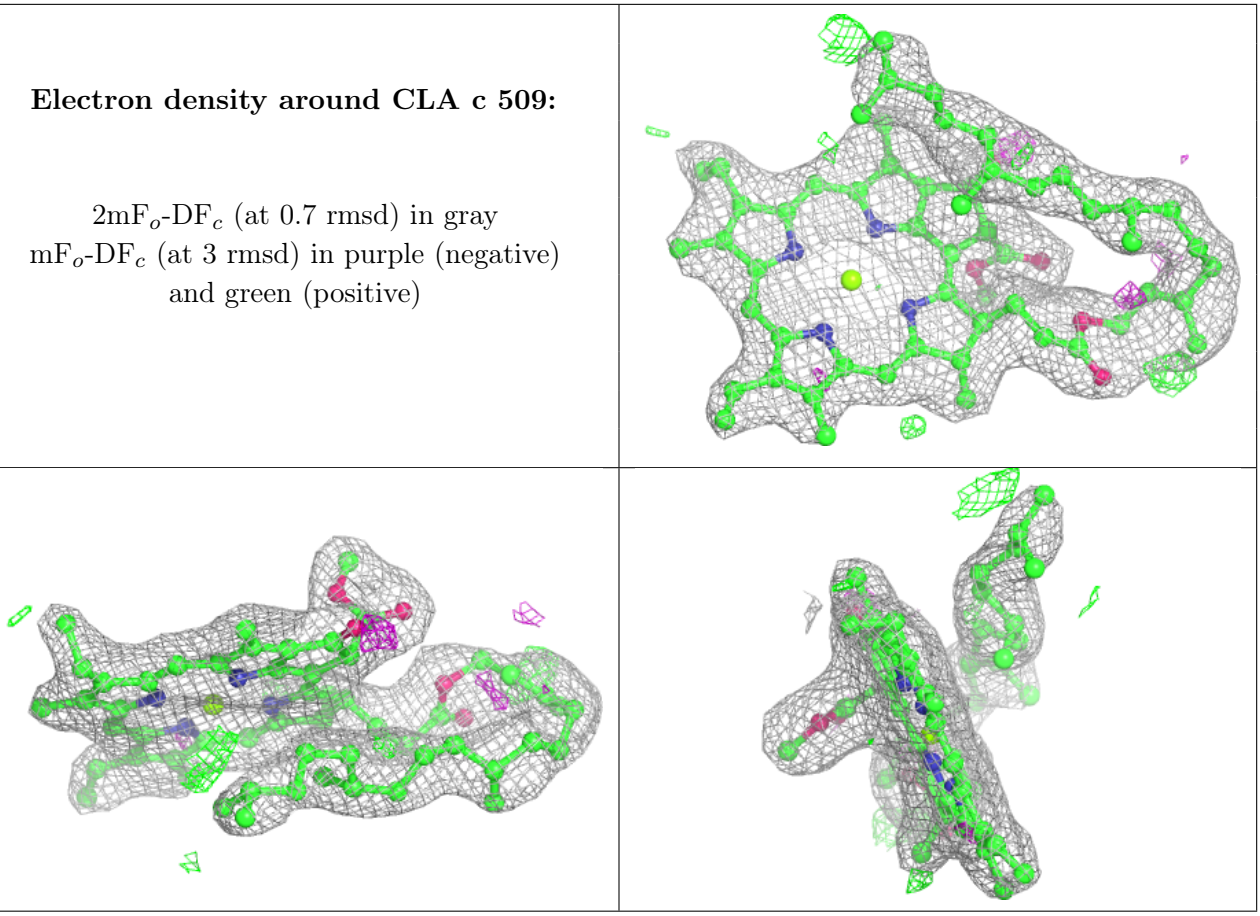






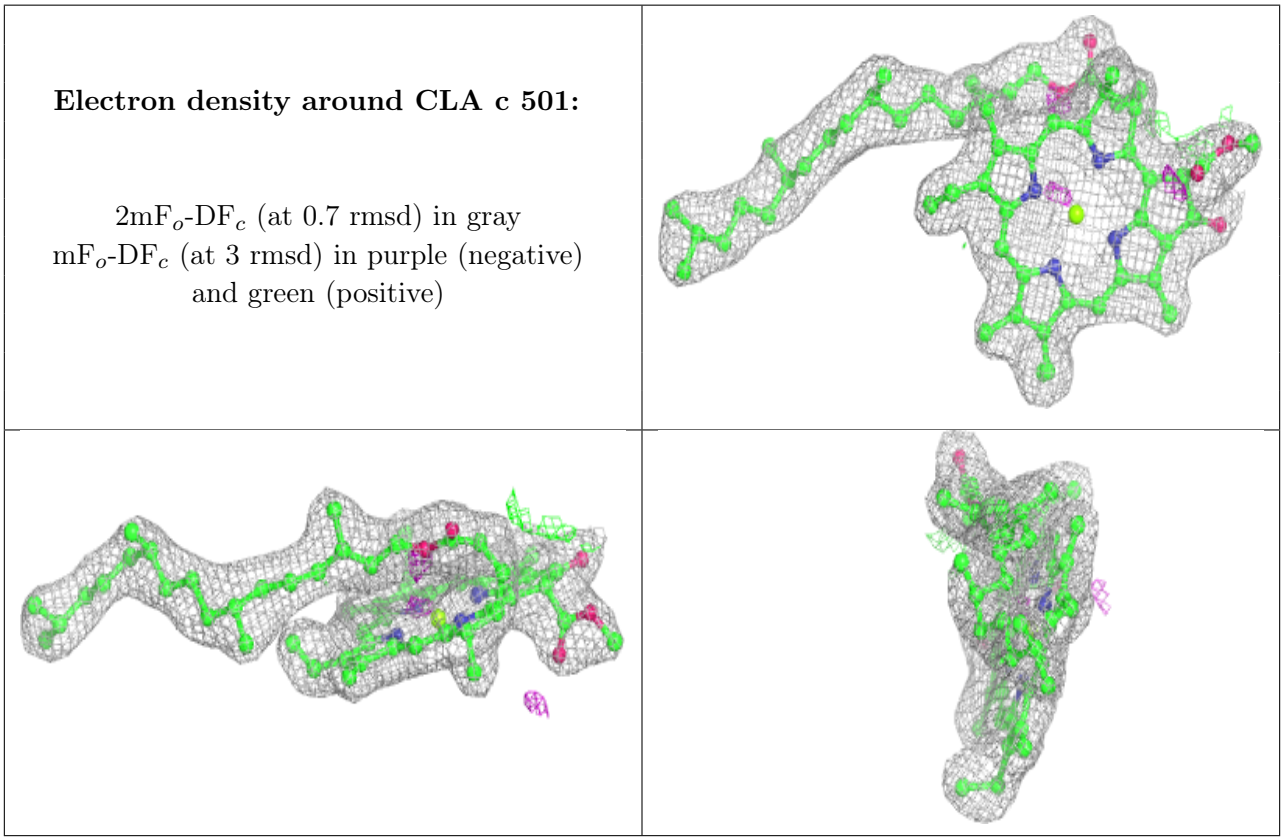
Electron density around CLA c 509:

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



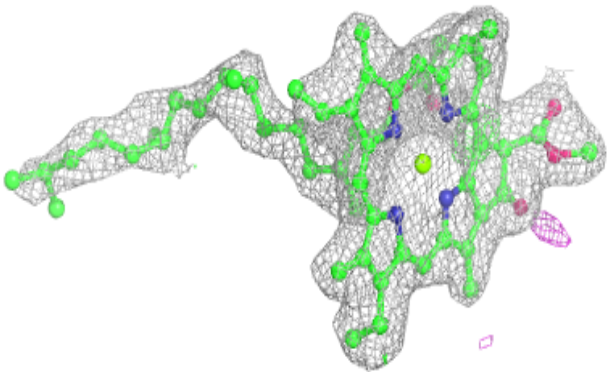
Electron density around CLA c 501:

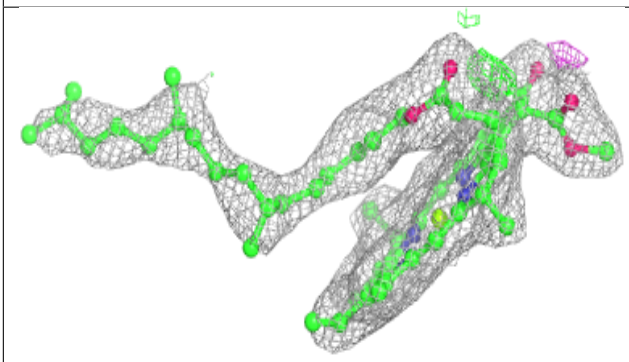
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

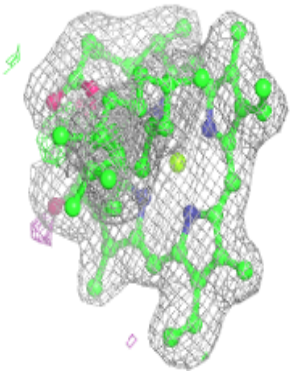


Electron density around CLA C 506:

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

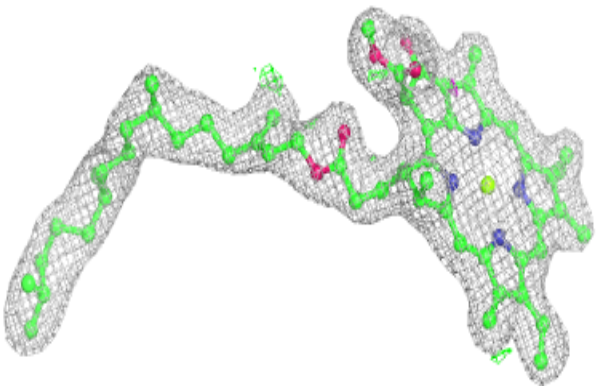


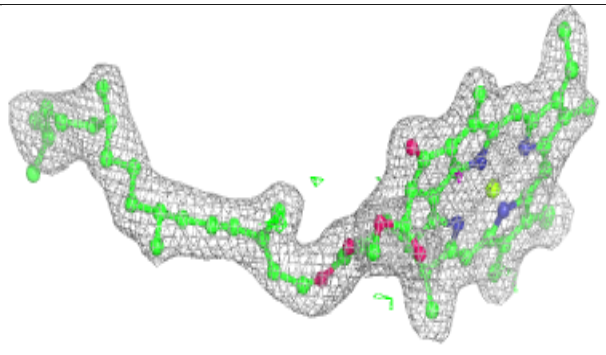


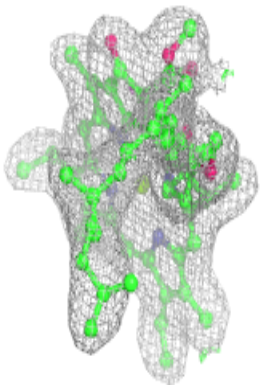


Electron density around CLA a 606:

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

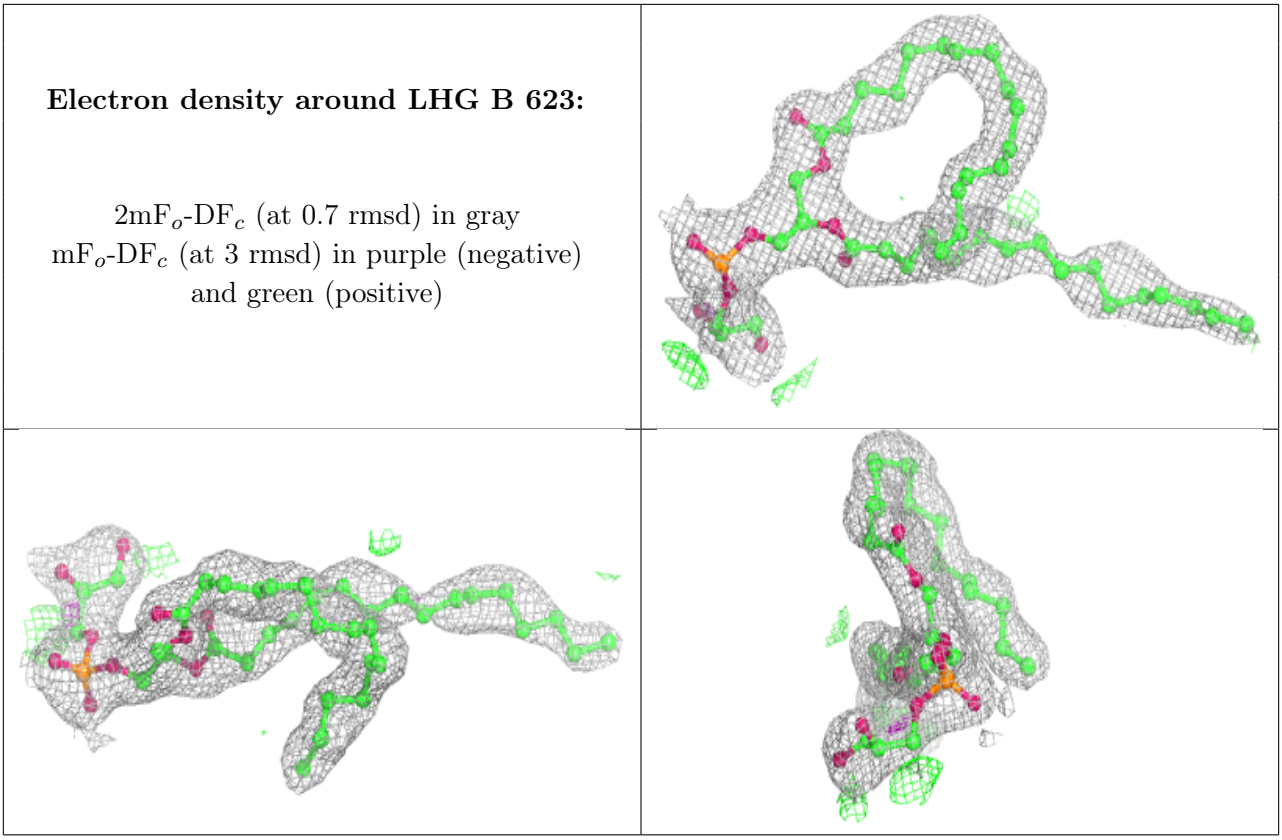






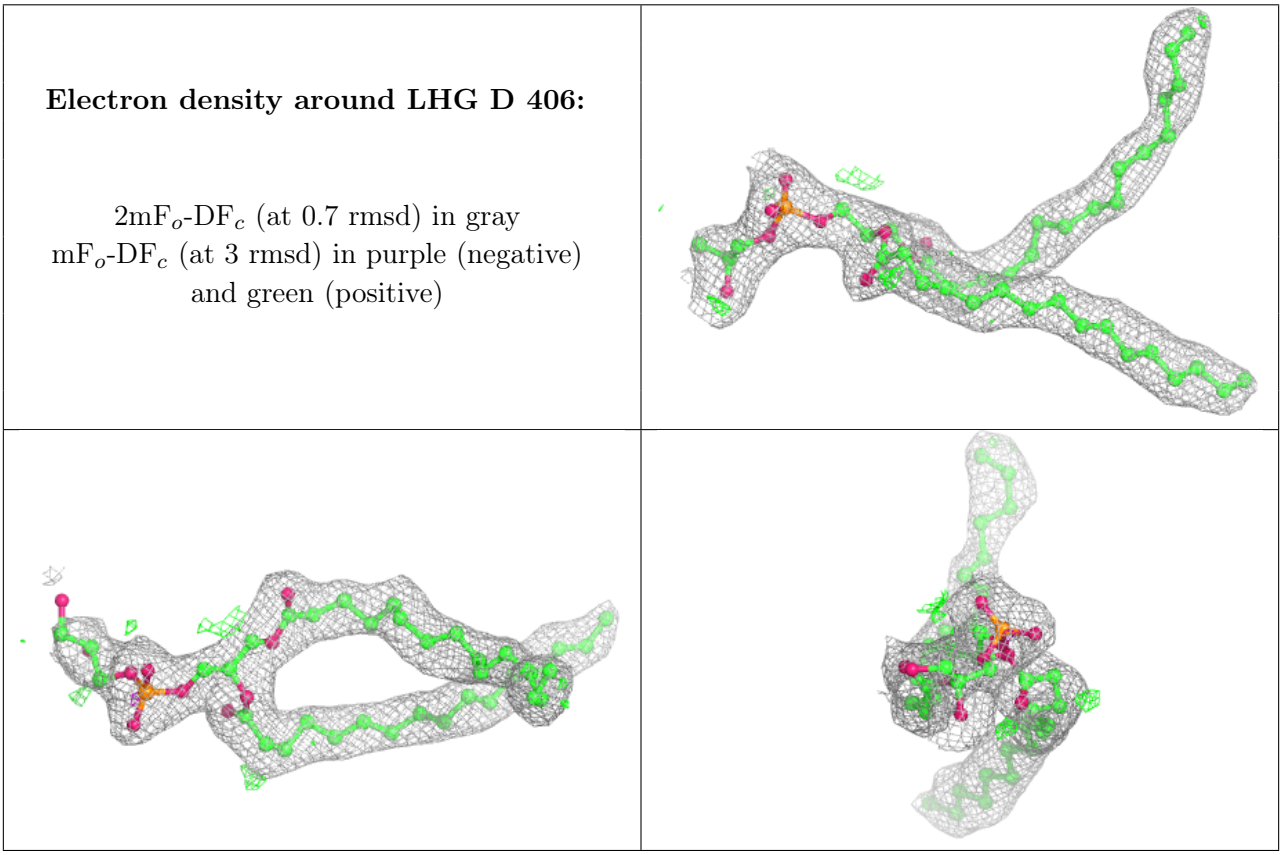
Electron density around LHG B 623:

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



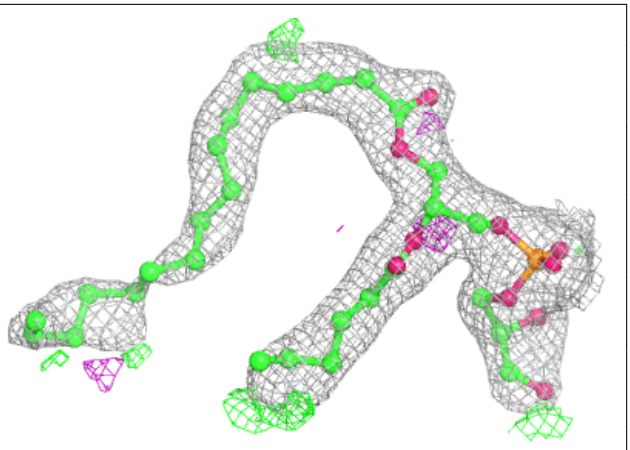
Electron density around LHG D 406:

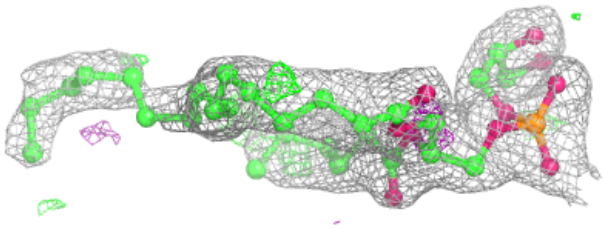
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

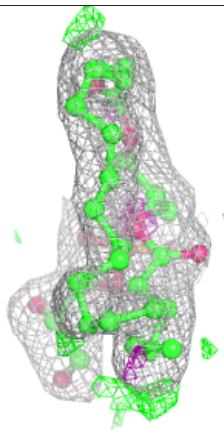


Electron density around LHG a 616:

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

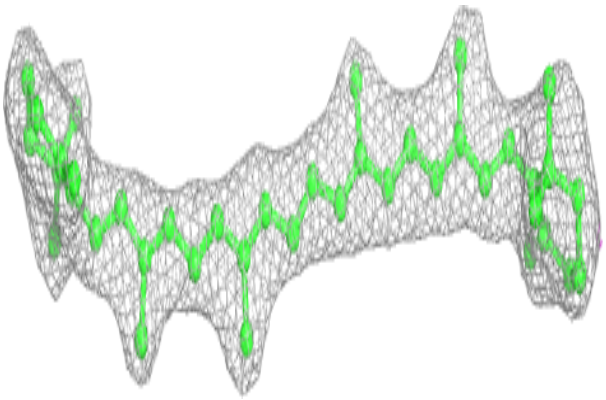


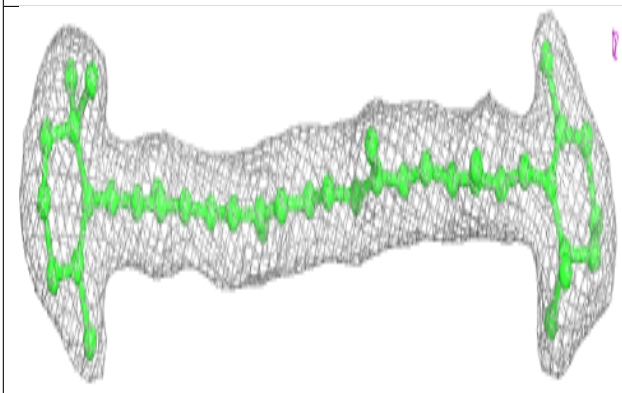


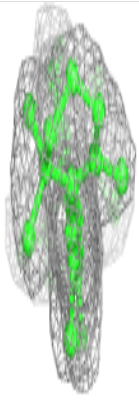


Electron density around BCR a 611:

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

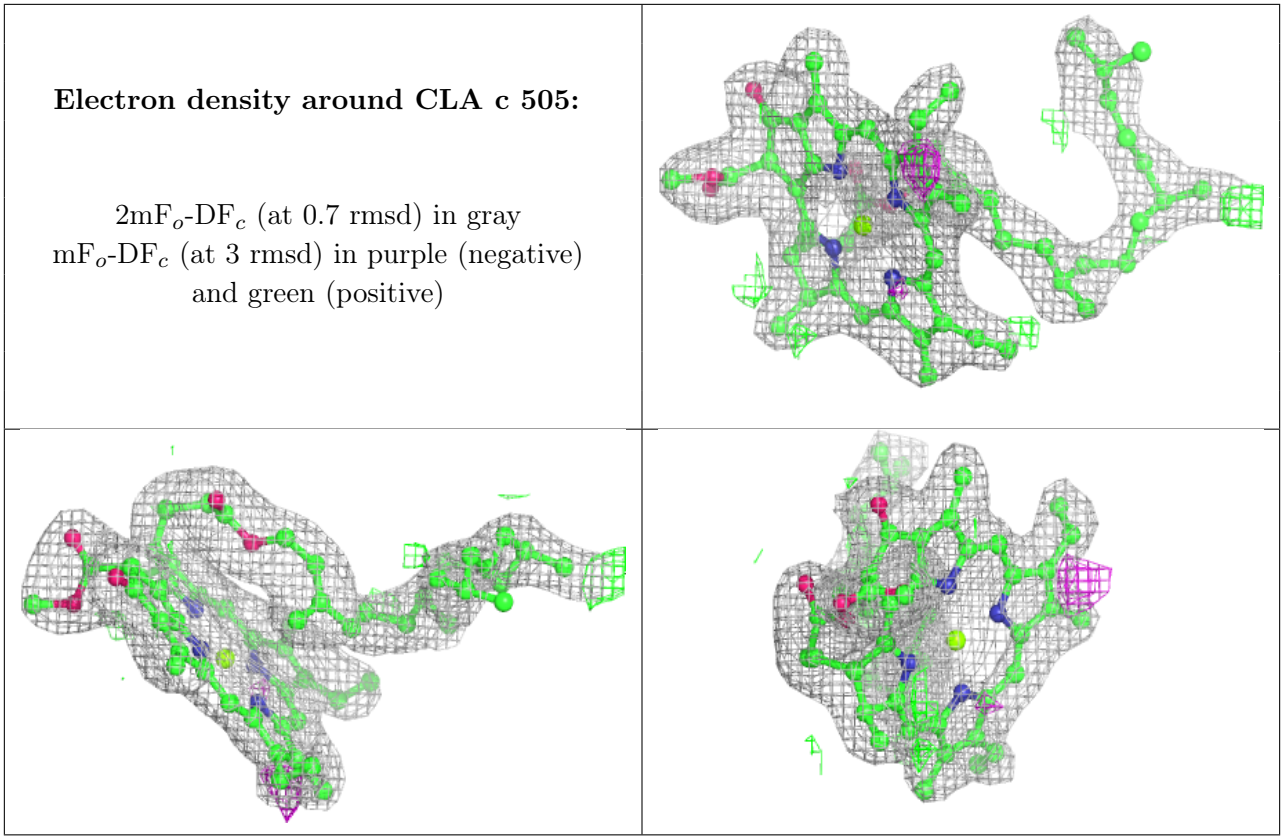






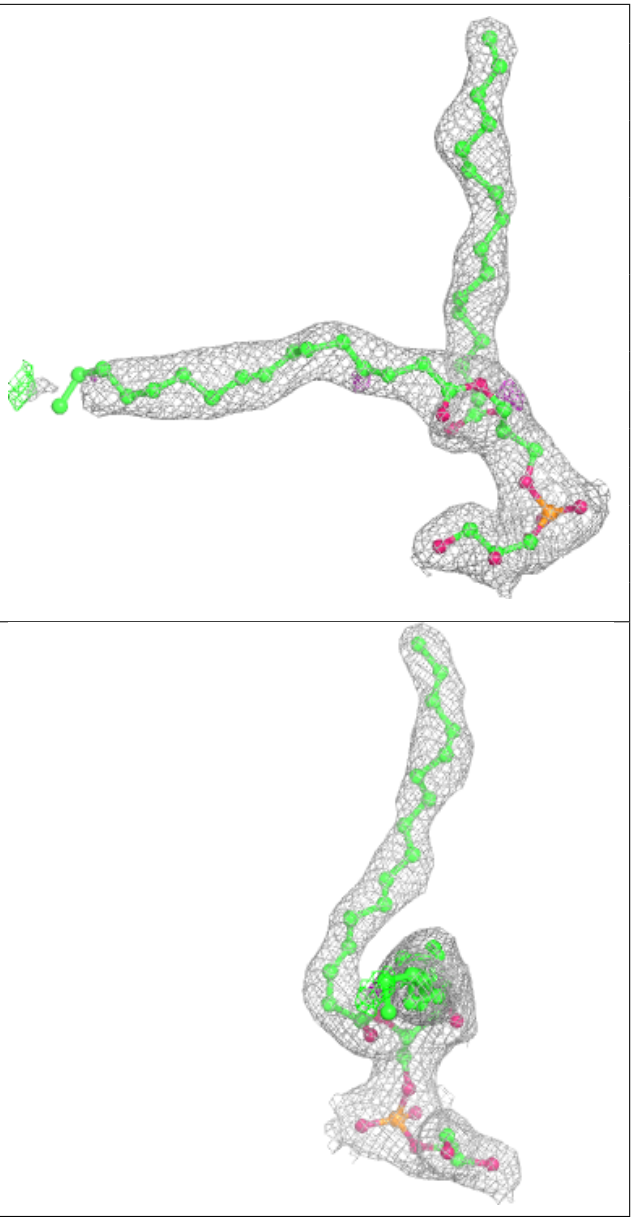
Electron density around CLA c 505:

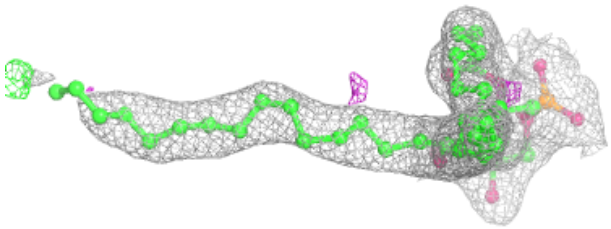
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG l 101:

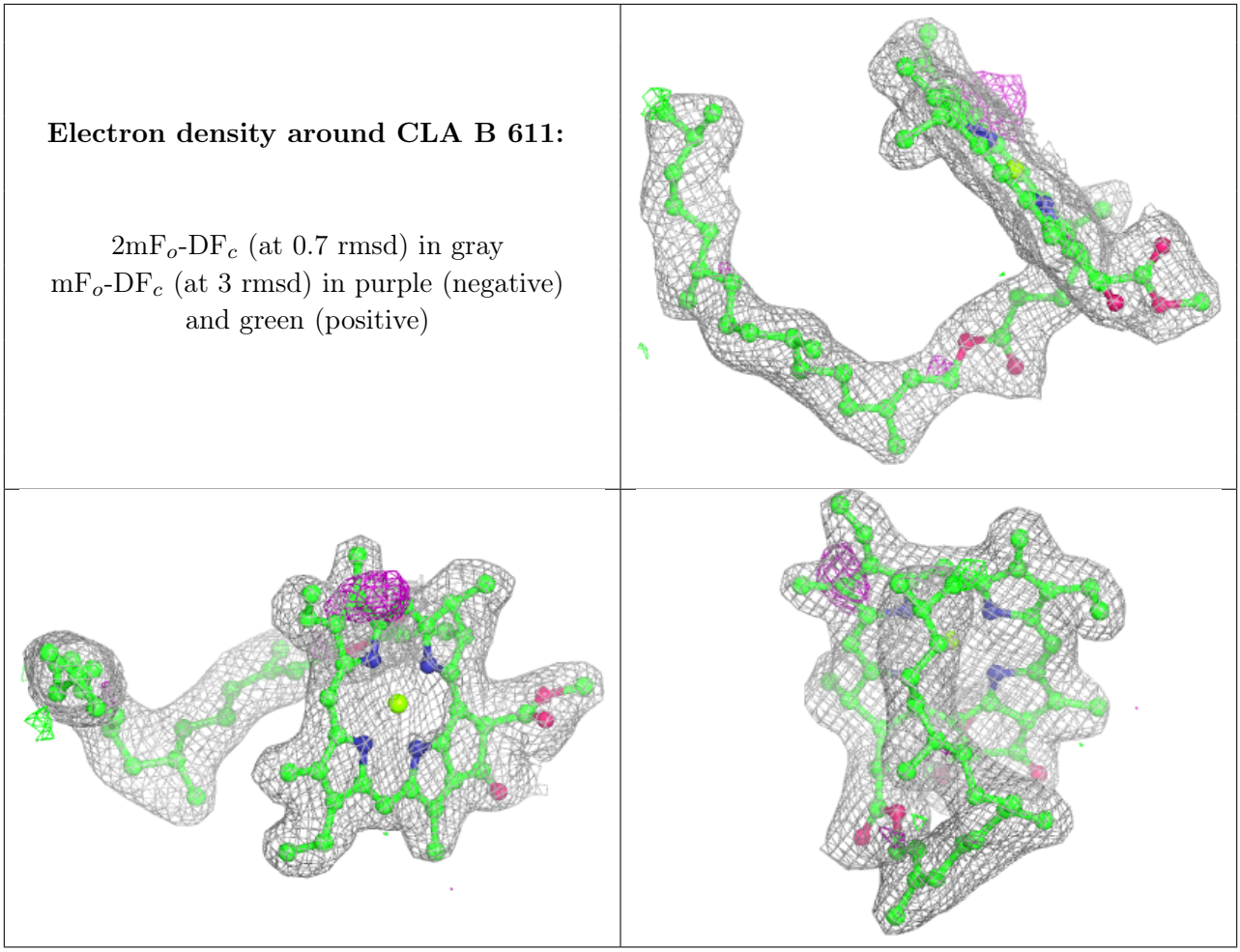
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





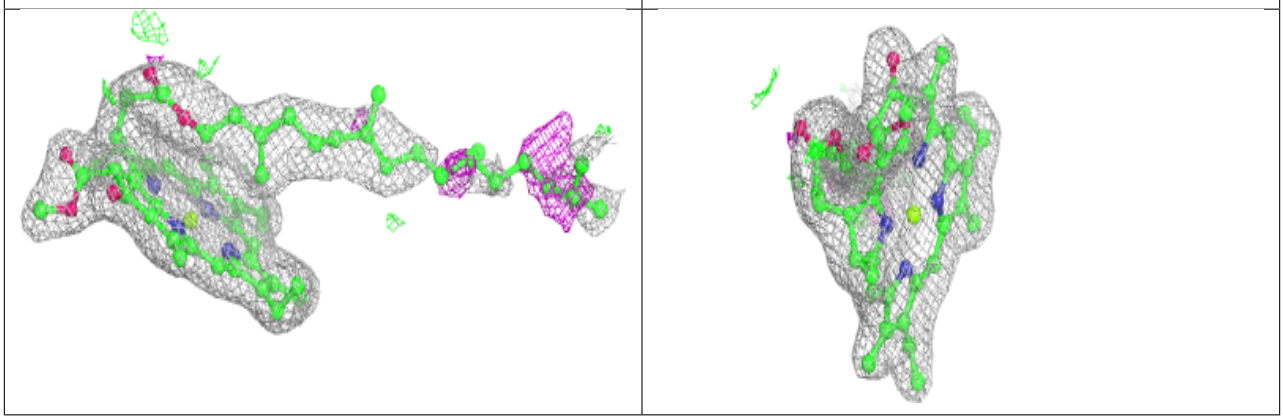
Electron density around CLA B 611:

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



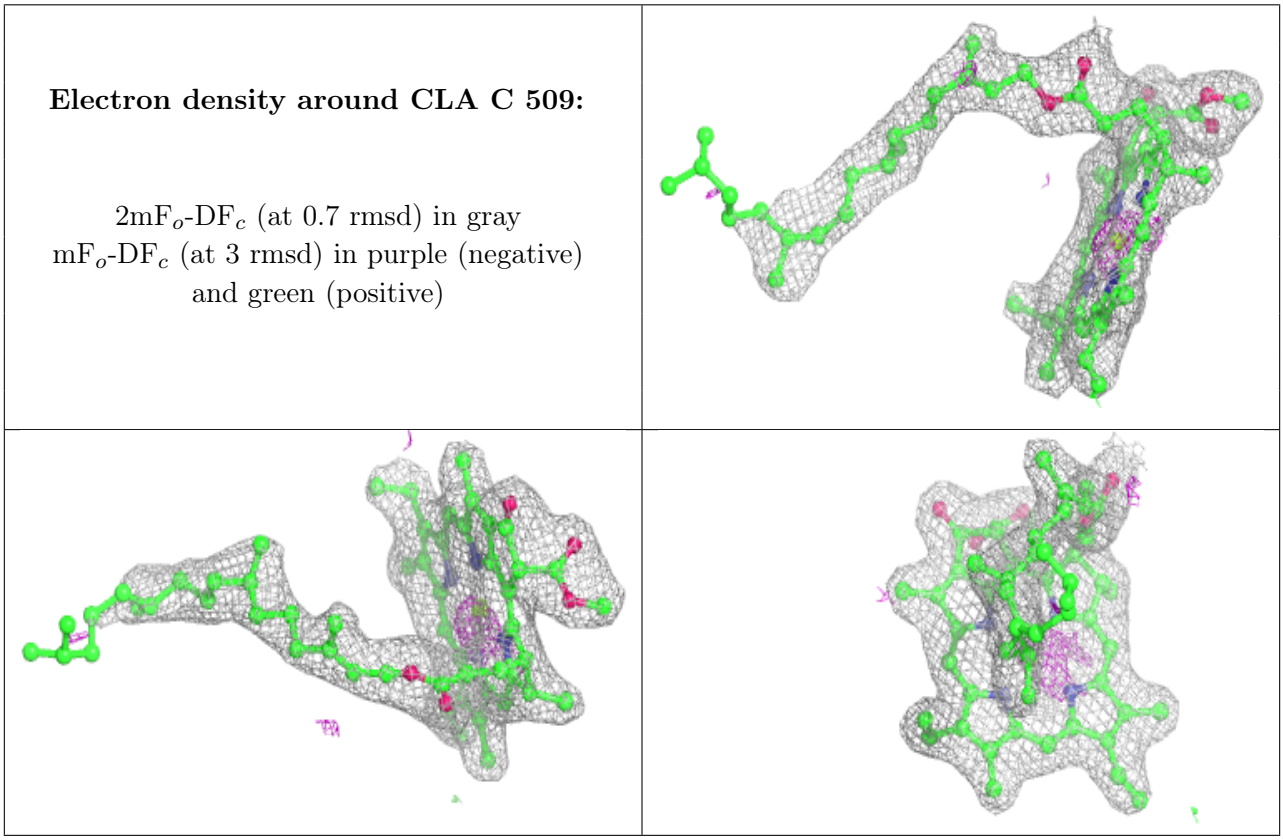
Electron density around CLA B 614:

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



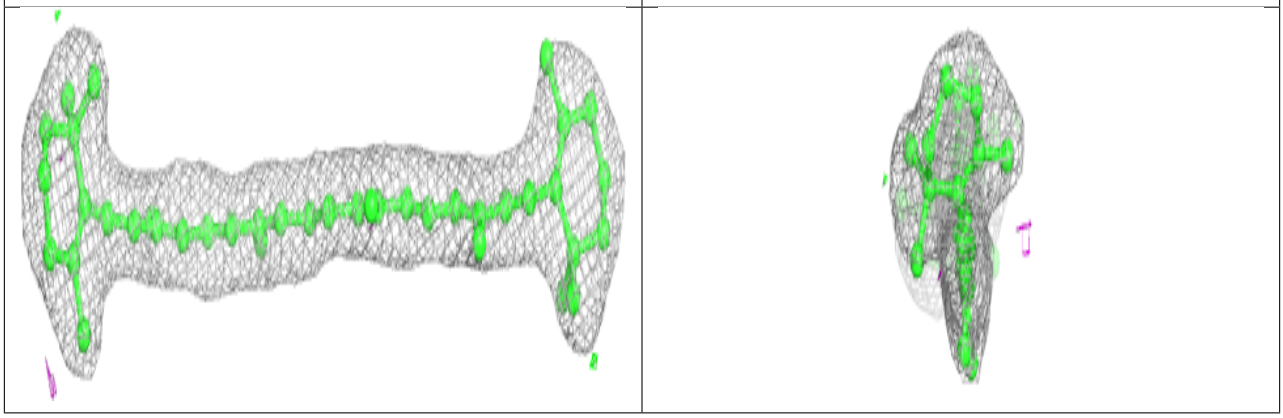
Electron density around CLA C 509:

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



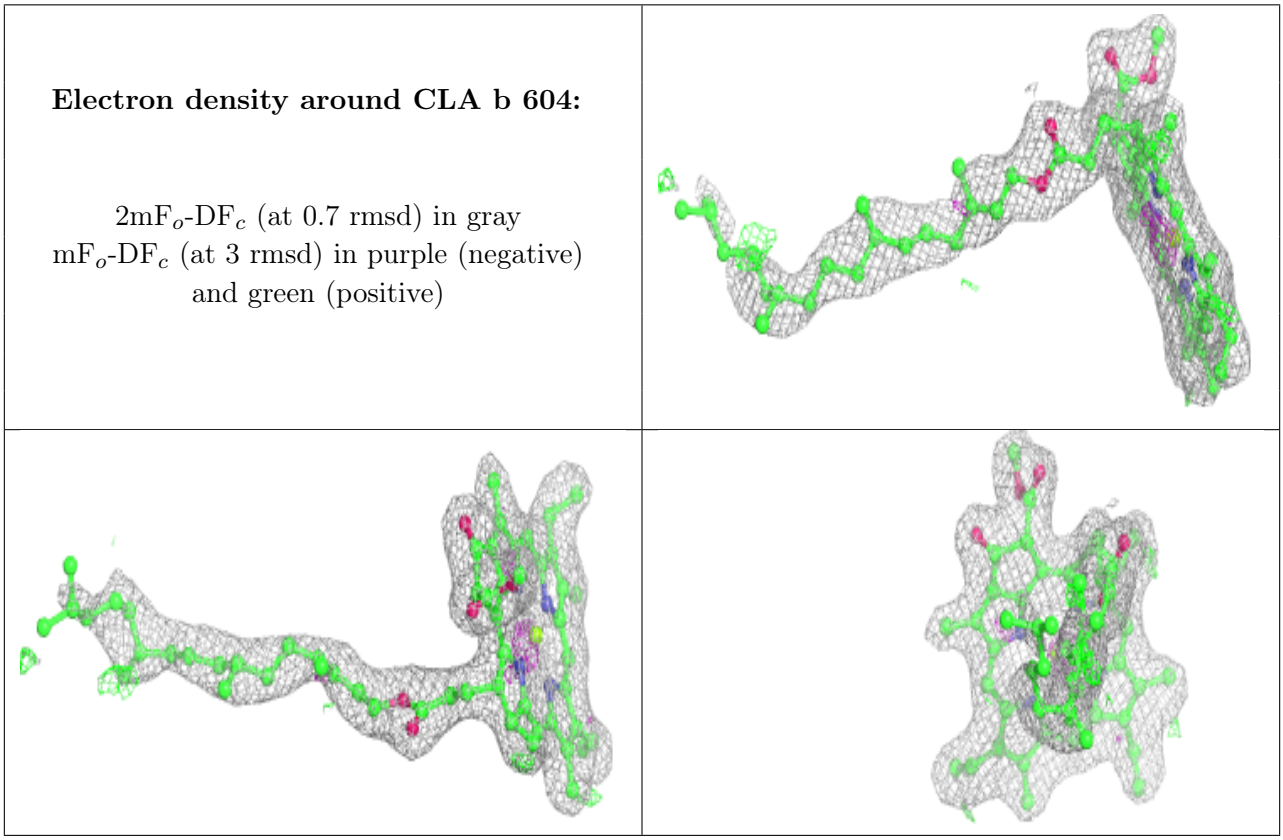
Electron density around BCR c 515:

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



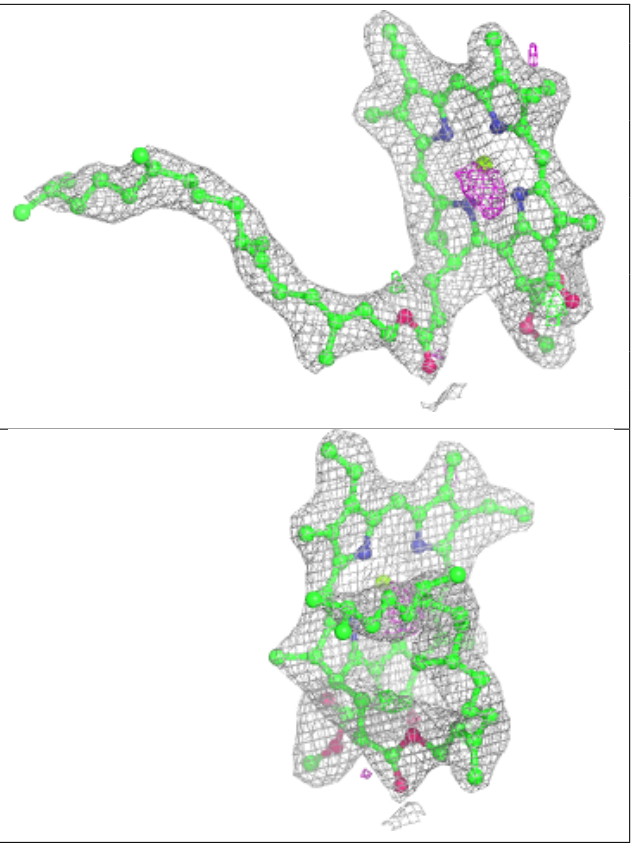
Electron density around CLA b 604:

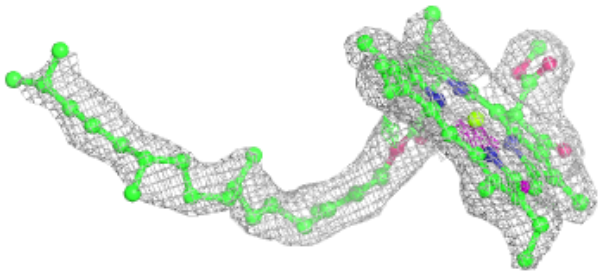
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA c 511:

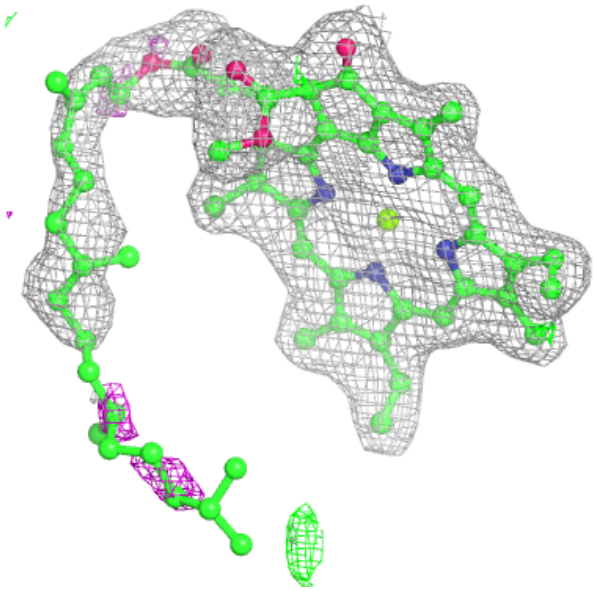
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

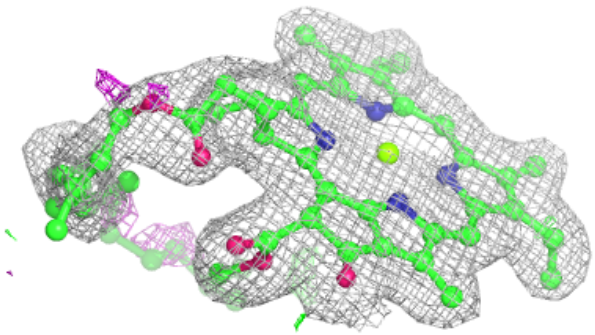


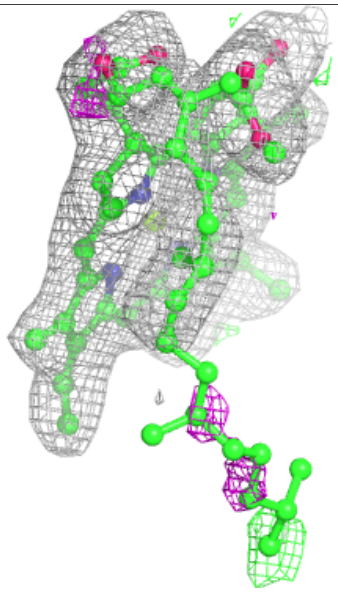


Electron density around CLA B 616:

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

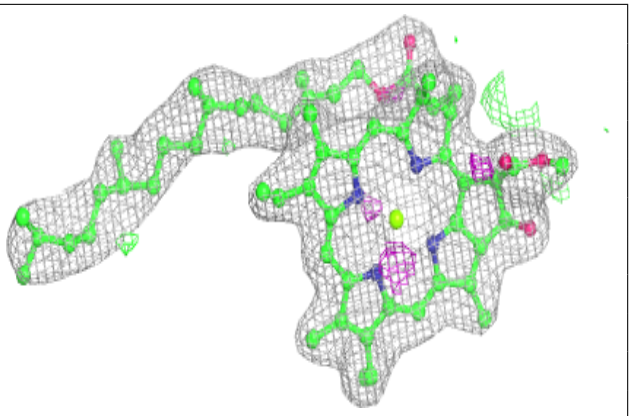


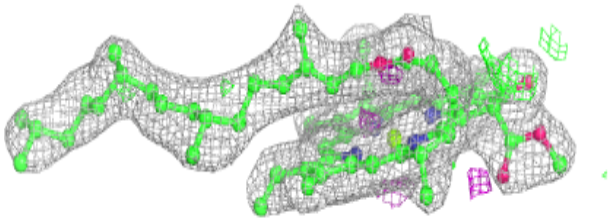


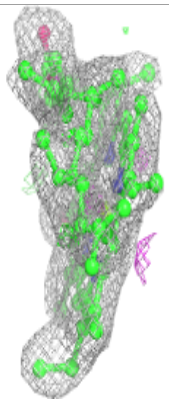


Electron density around CLA C 502:

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

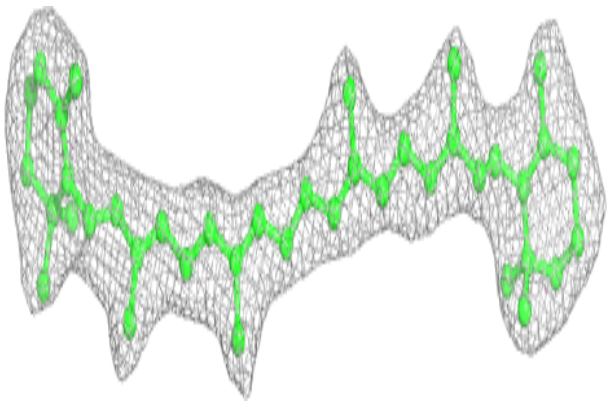


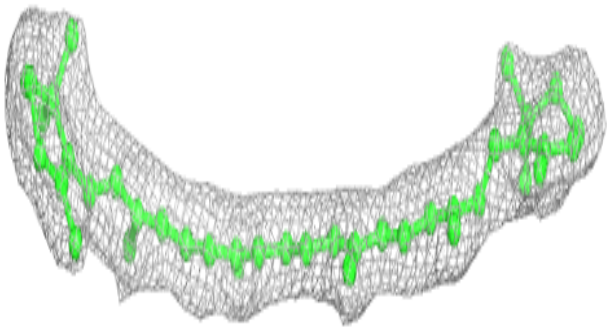


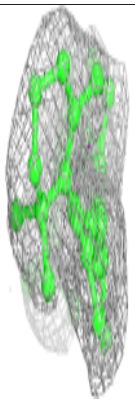


Electron density around BCR t 101:

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

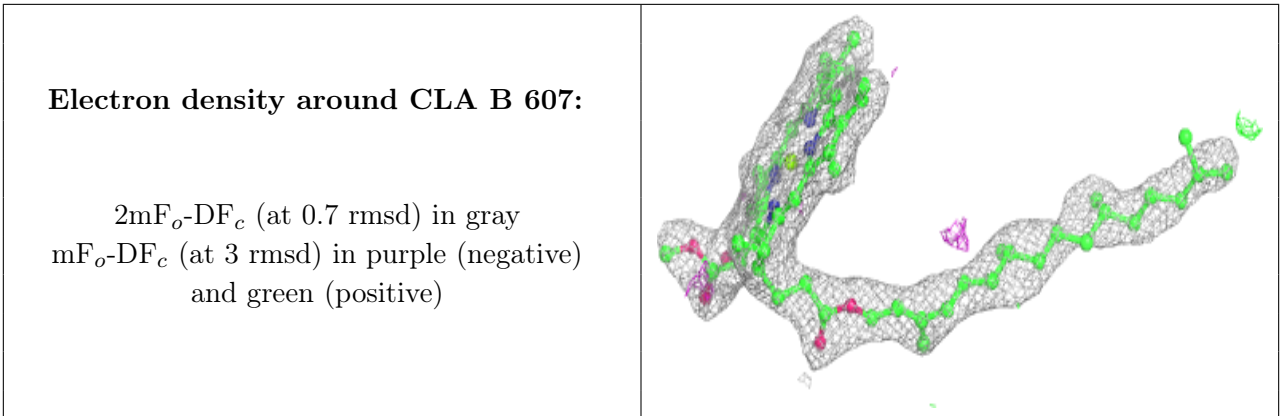


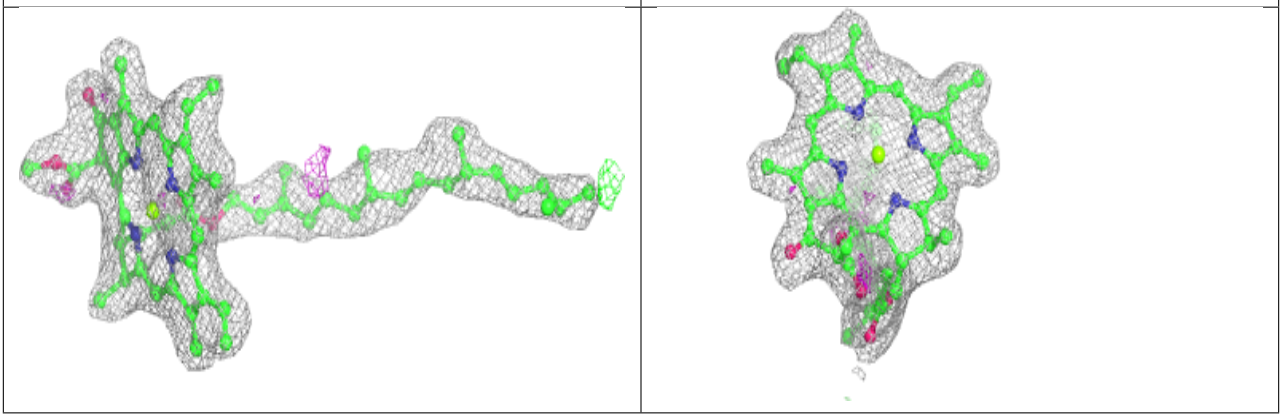




Electron density around CLA B 607:

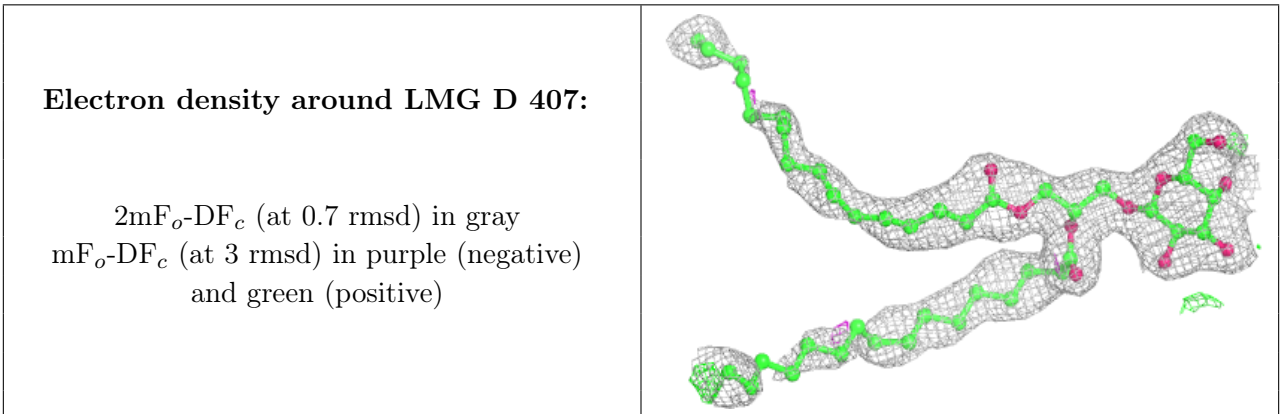
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

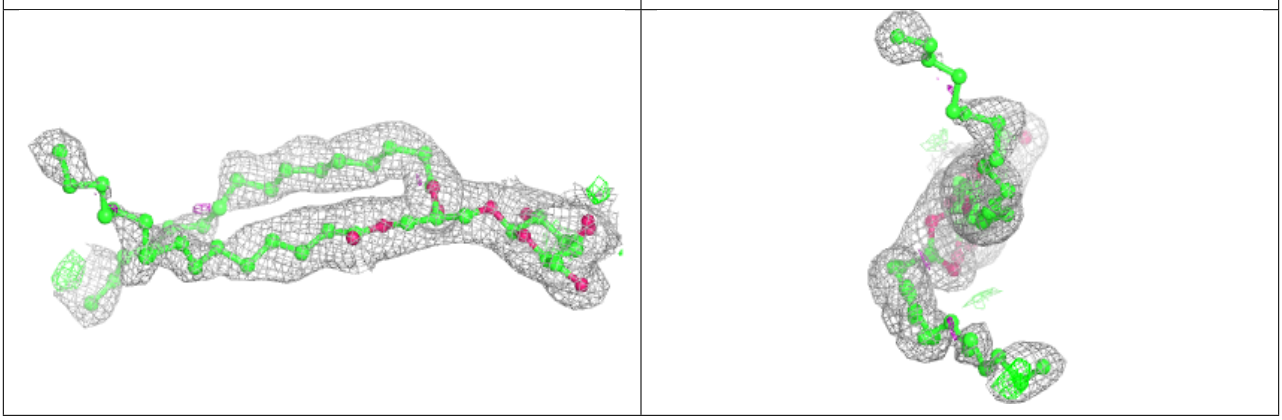




Electron density around LMG D 407:

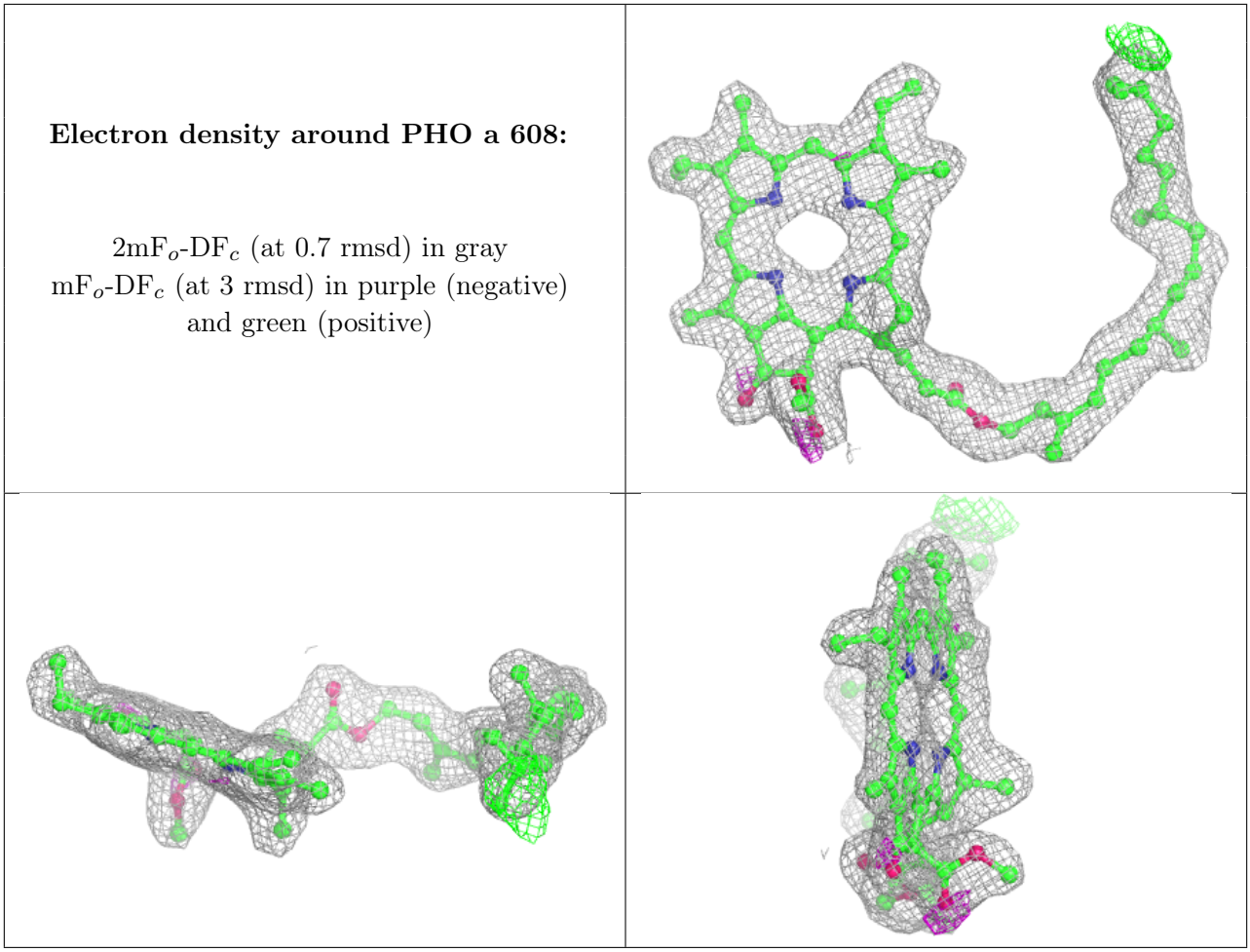
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





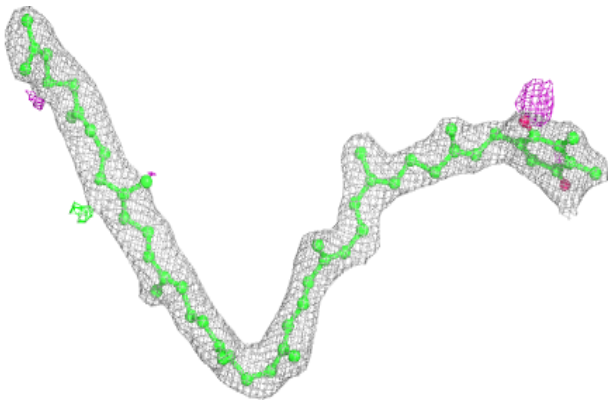
Electron density around PHO a 608:

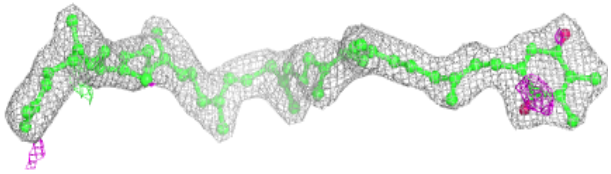
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

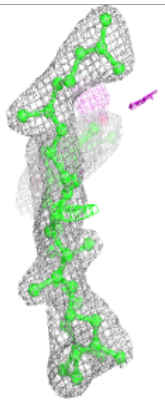


Electron density around PL9 d 404:

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

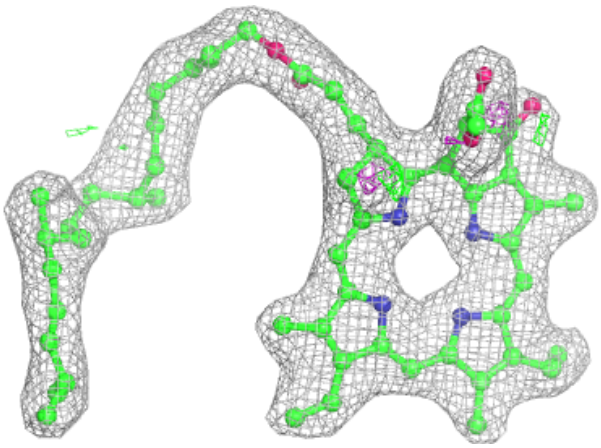


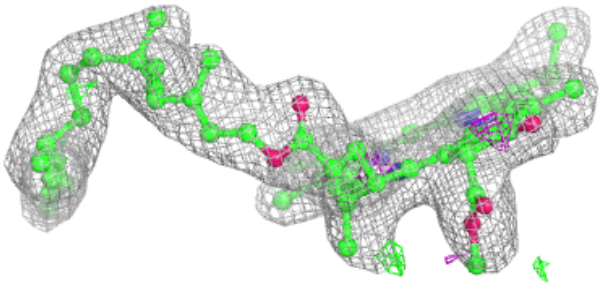


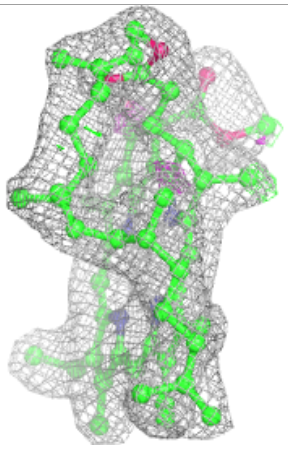


Electron density around PHO a 609:

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

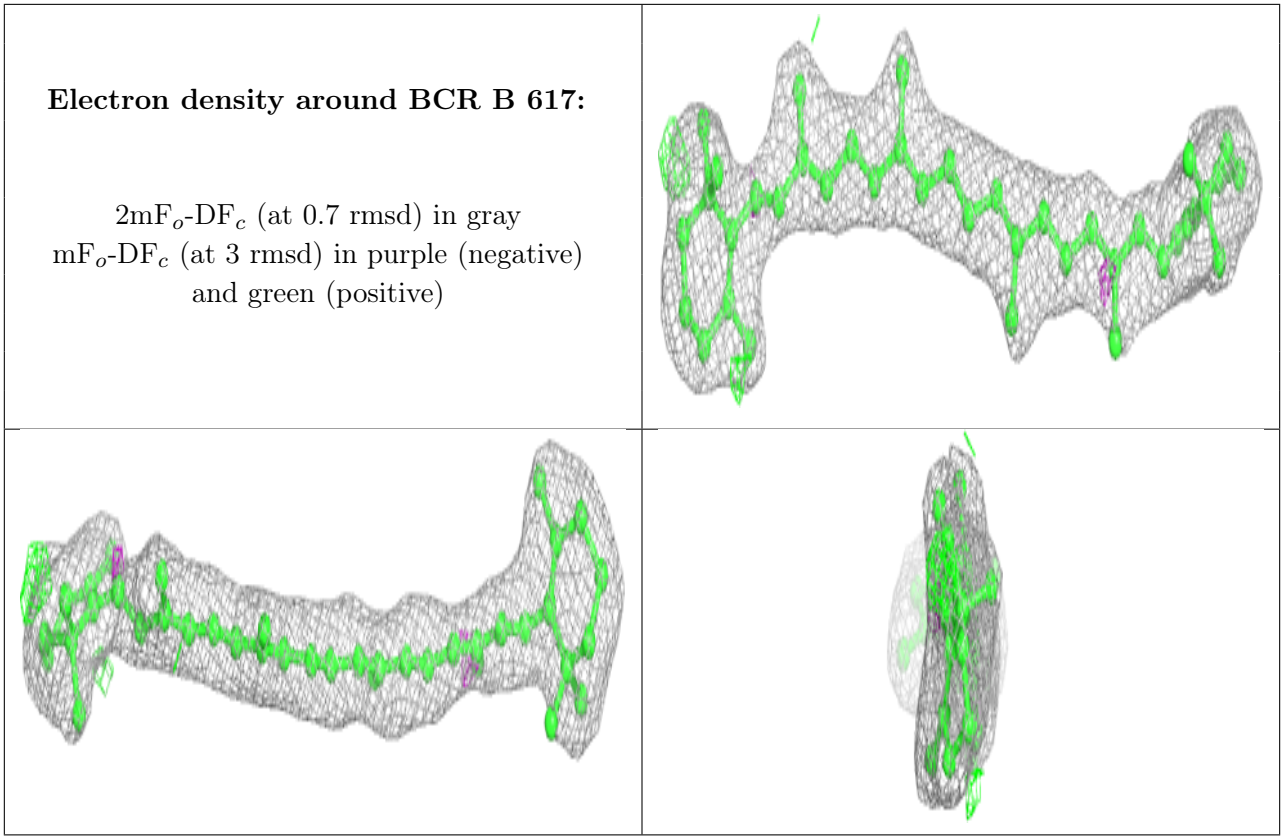






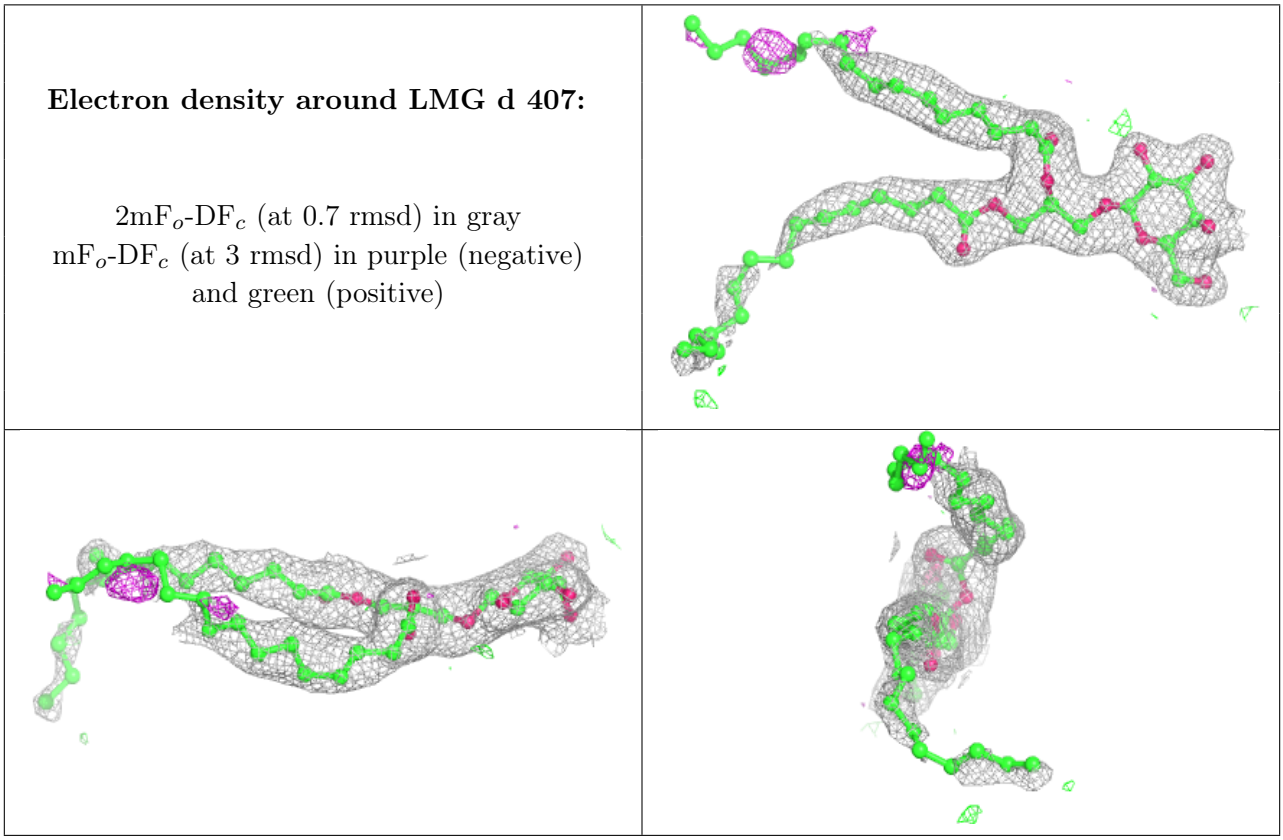
Electron density around BCR B 617:

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



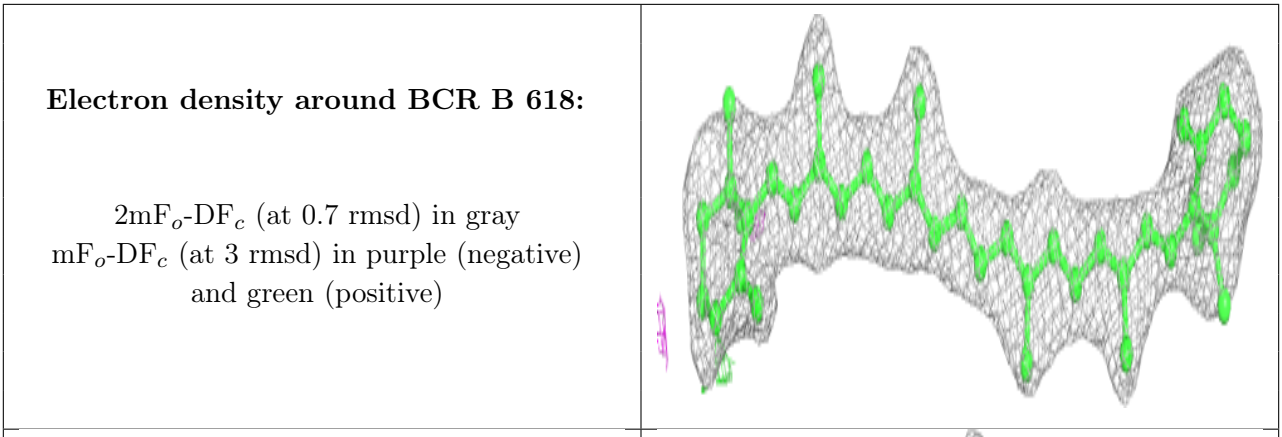
Electron density around LMG d 407:

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



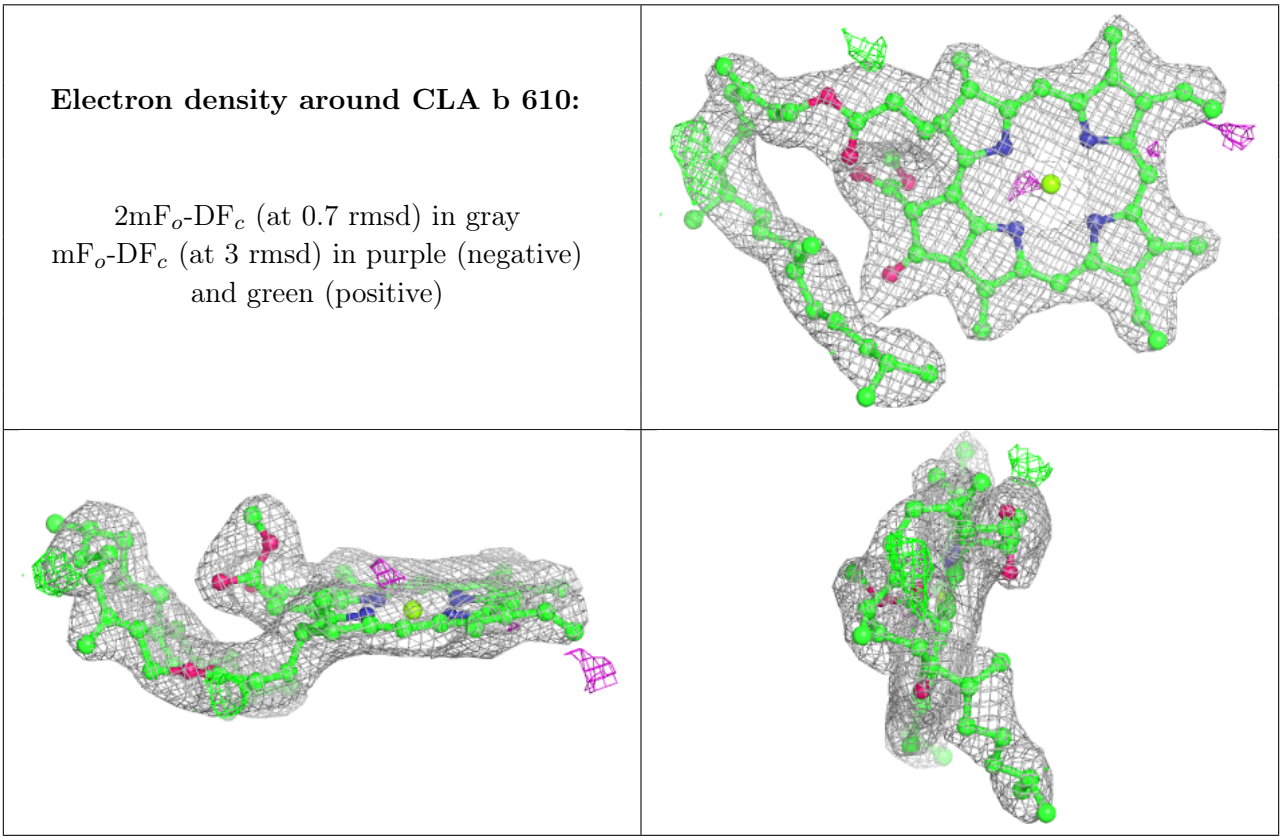
Electron density around BCR B 618:

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



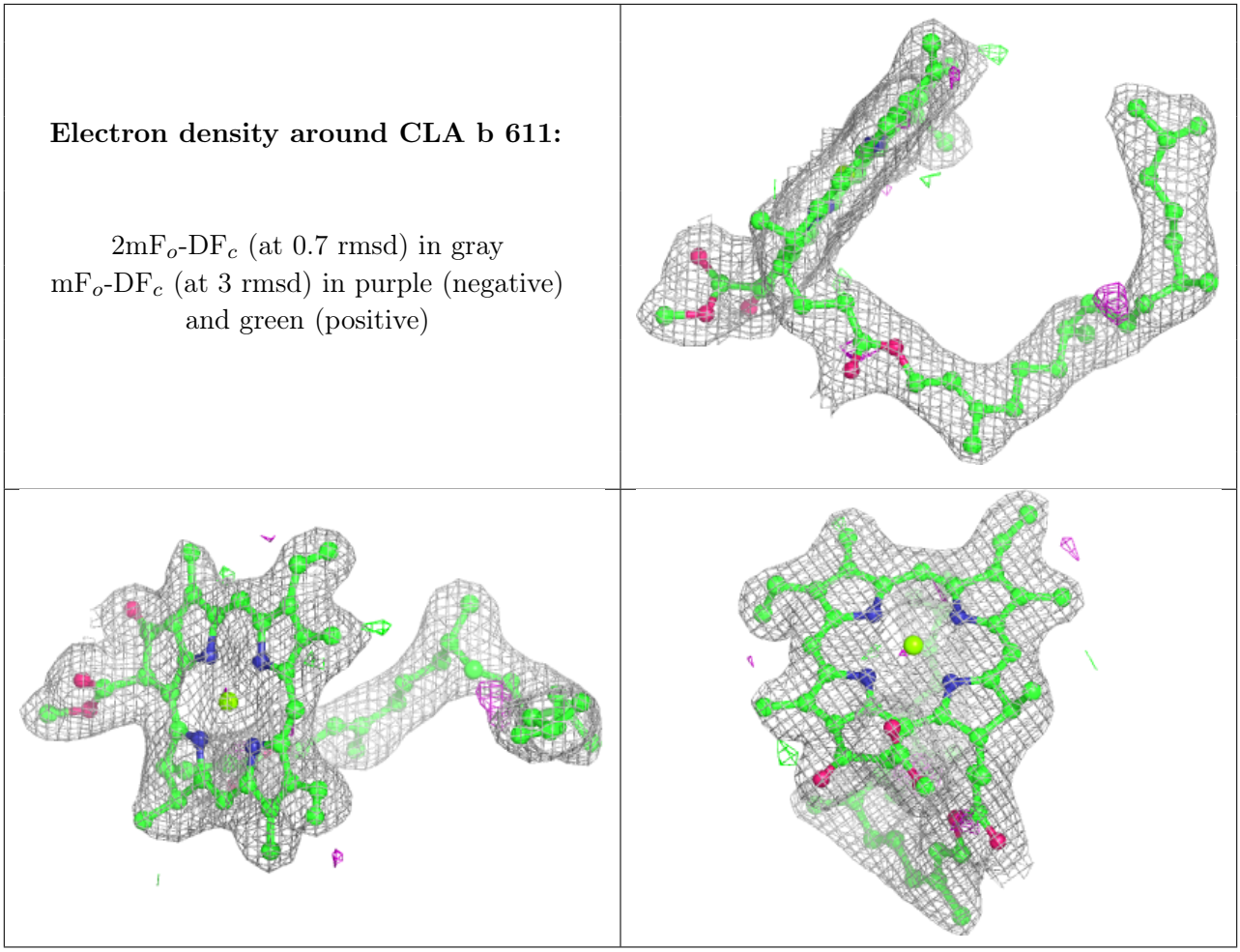
Electron density around CLA b 610:

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



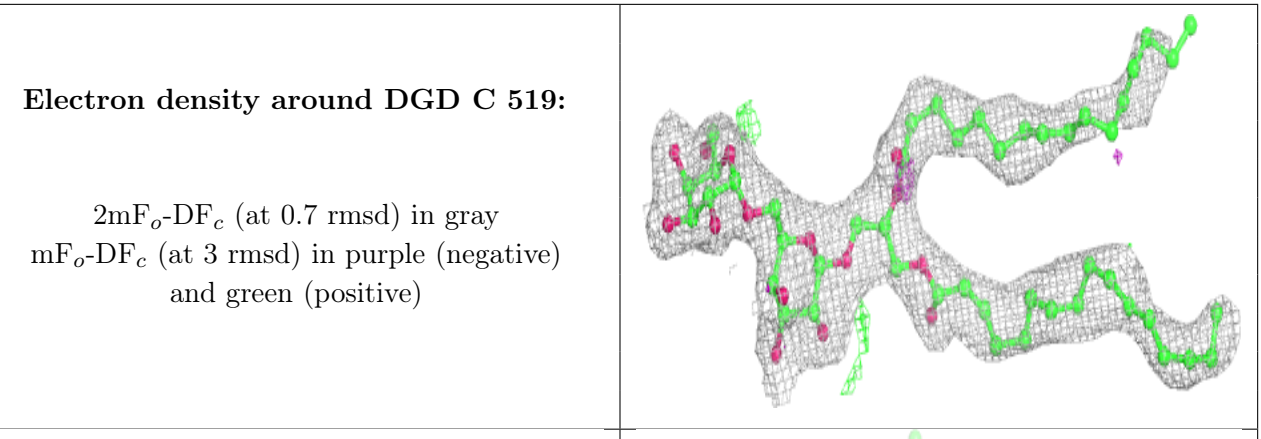
Electron density around CLA b 611:

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



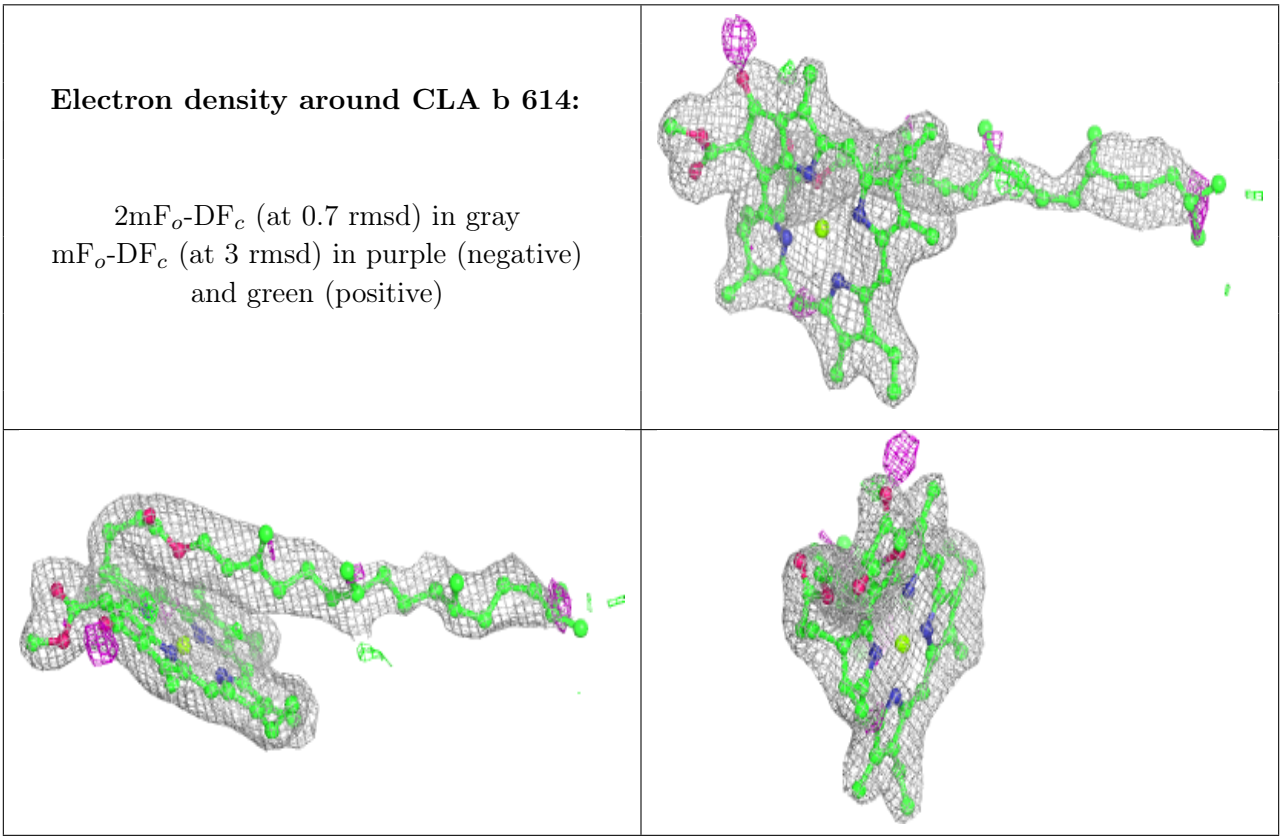
Electron density around DGD C 519:

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



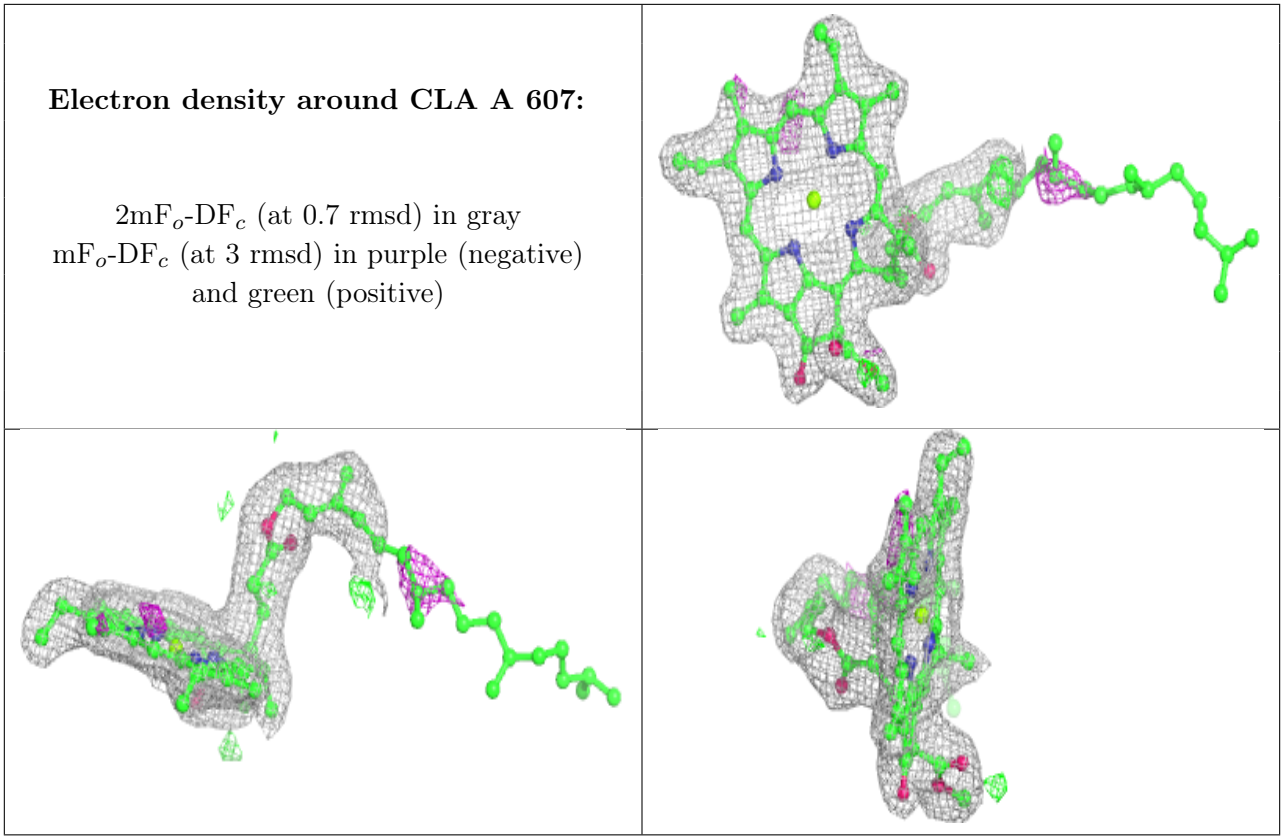
Electron density around CLA b 614:

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



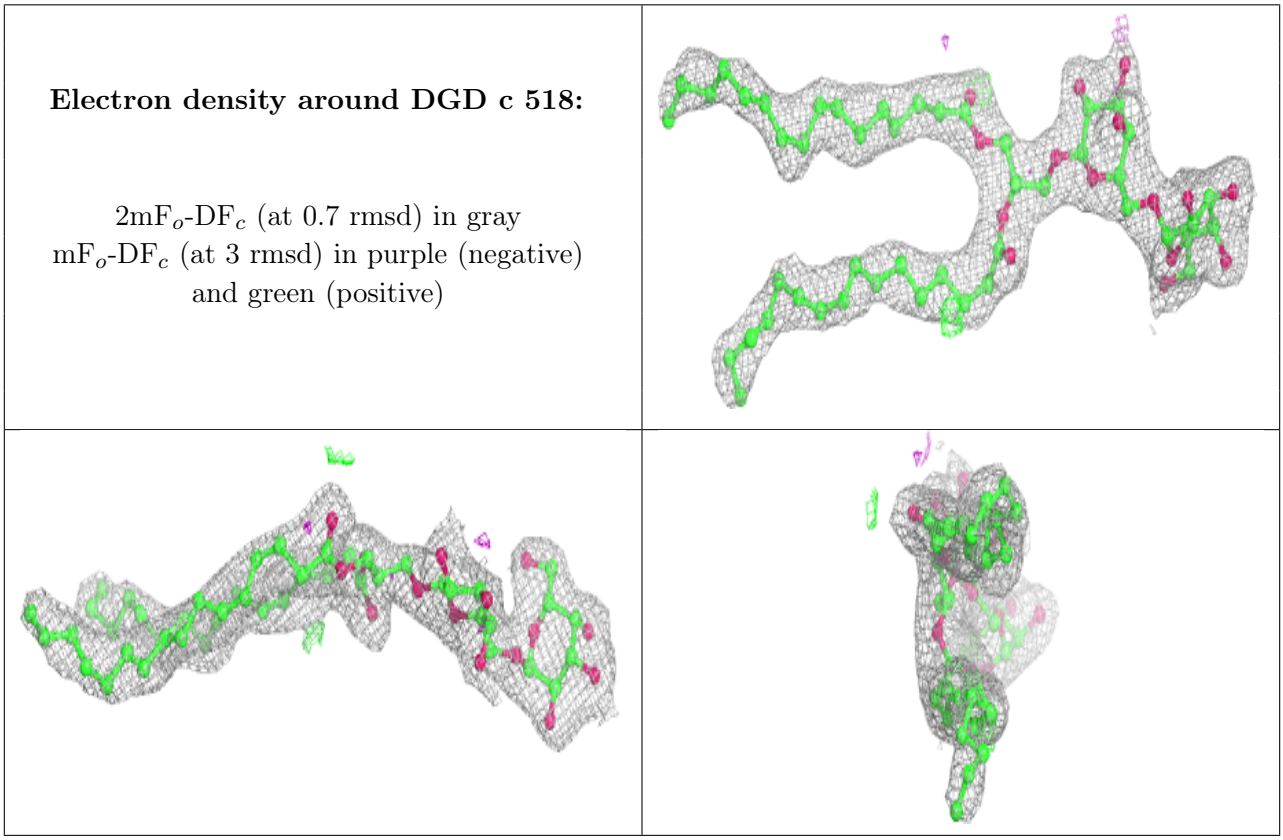
Electron density around CLA A 607:

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



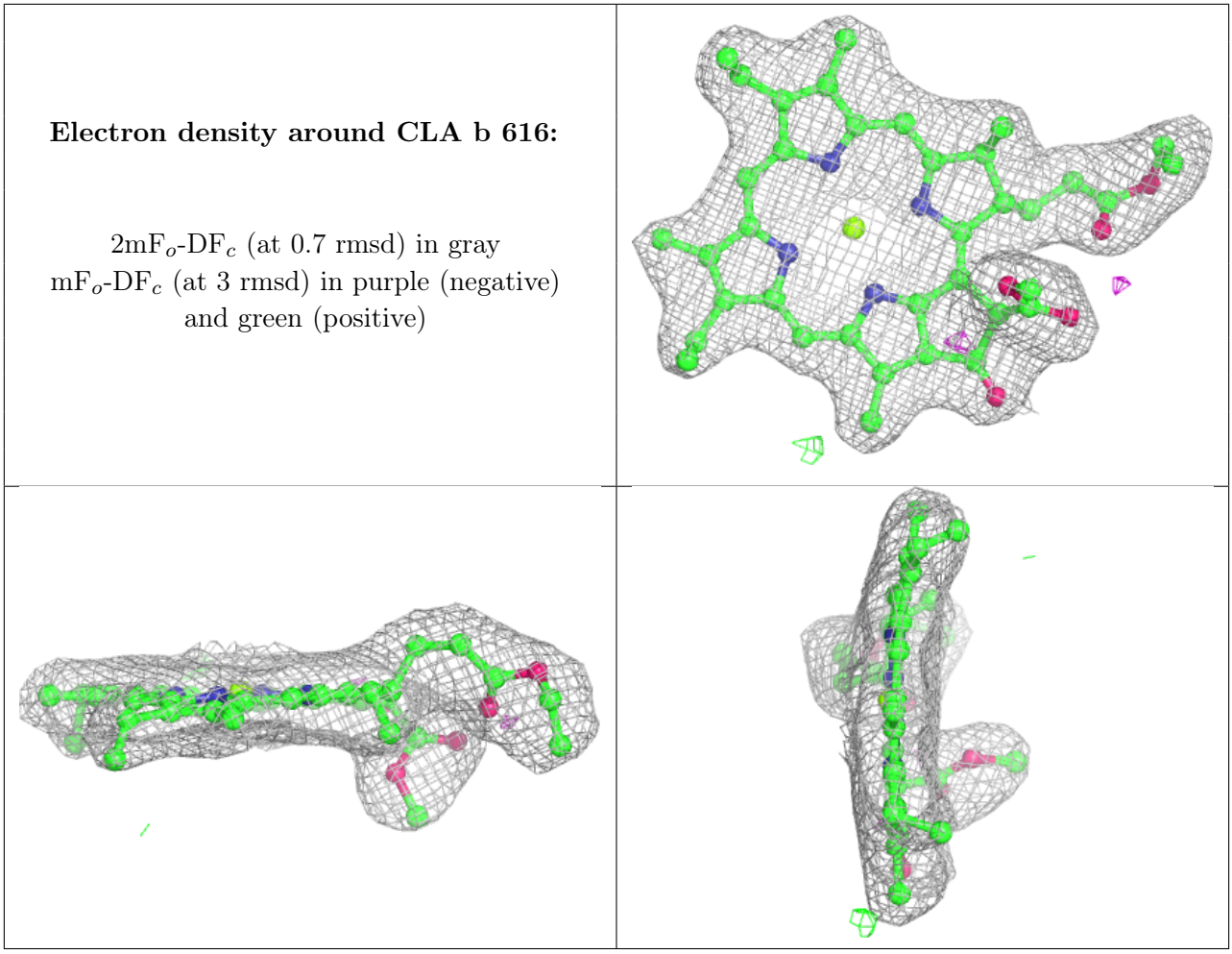
Electron density around DGD c 518:

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



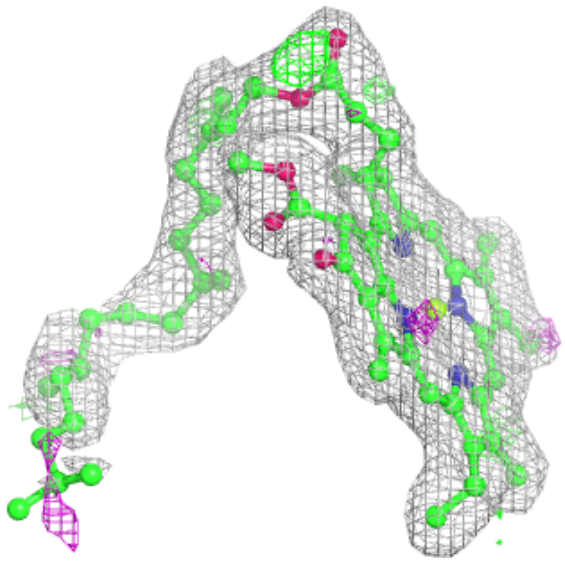
Electron density around CLA b 616:

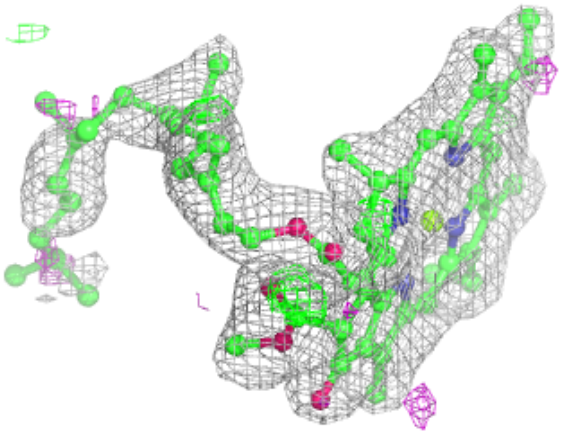
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

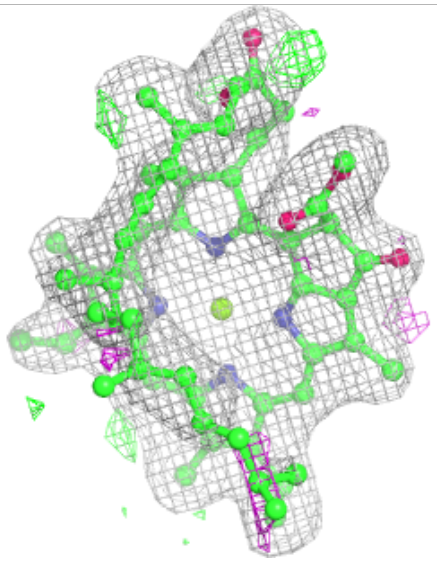


Electron density around CLA b 613:

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

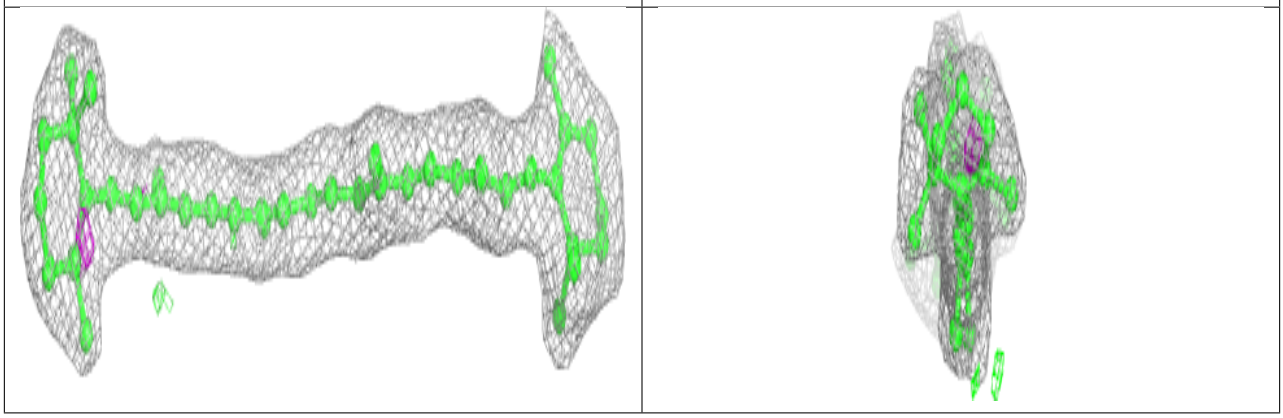






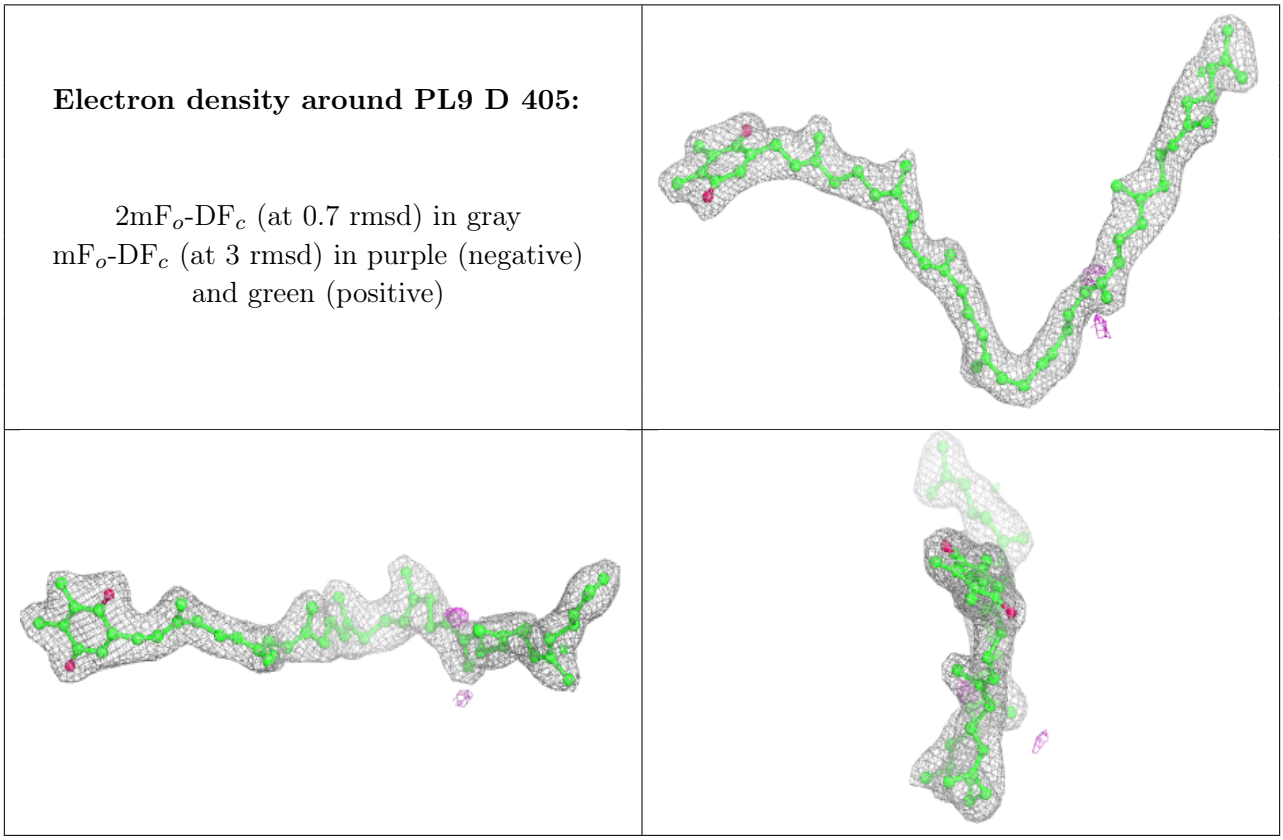
Electron density around BCR A 610:

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



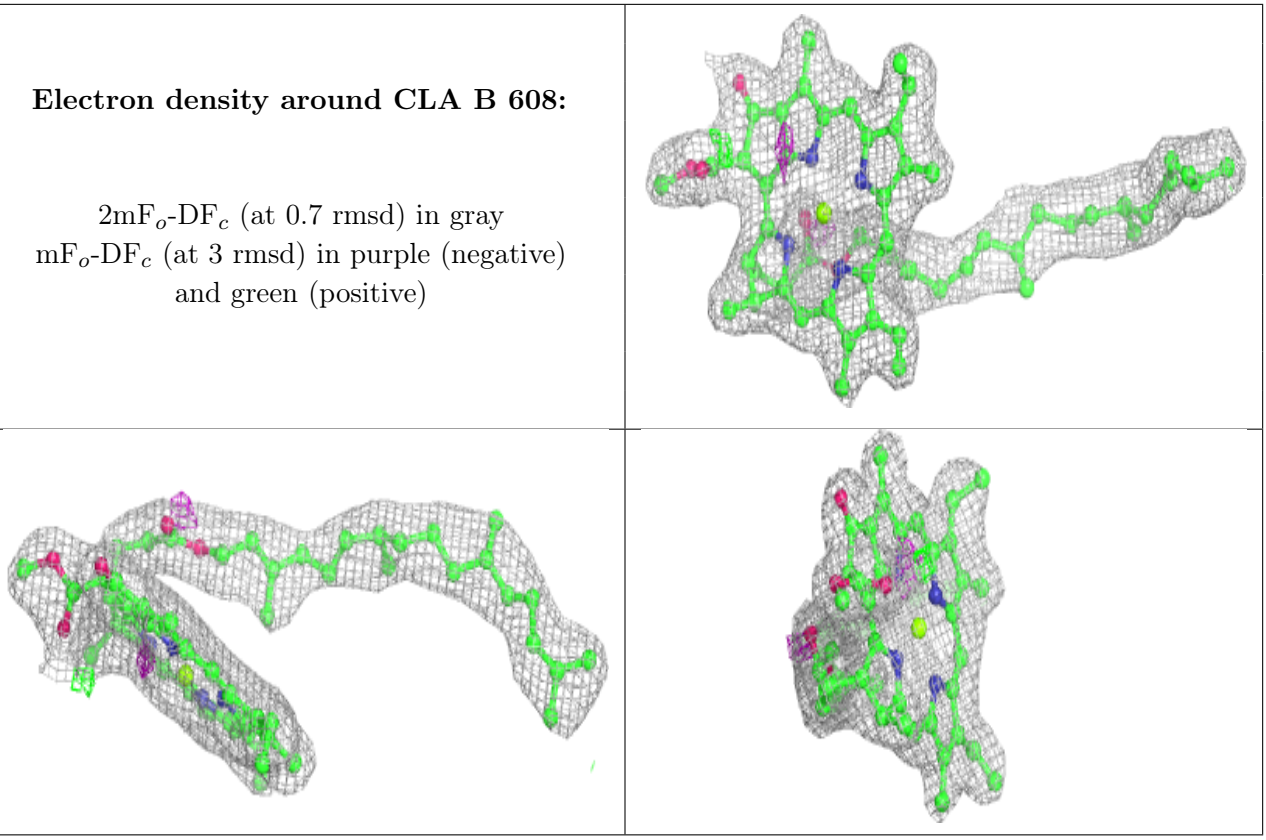
Electron density around PL9 D 405:

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



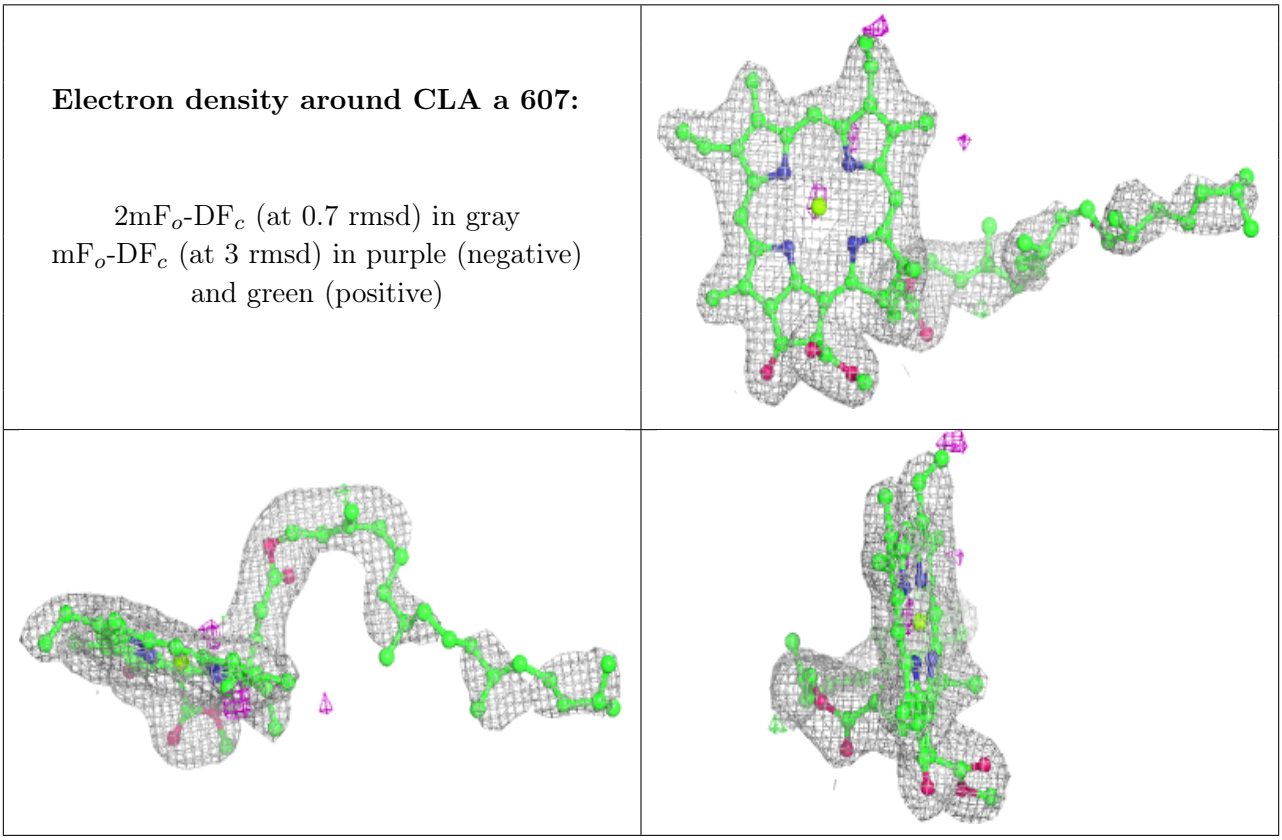
Electron density around CLA B 608:

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



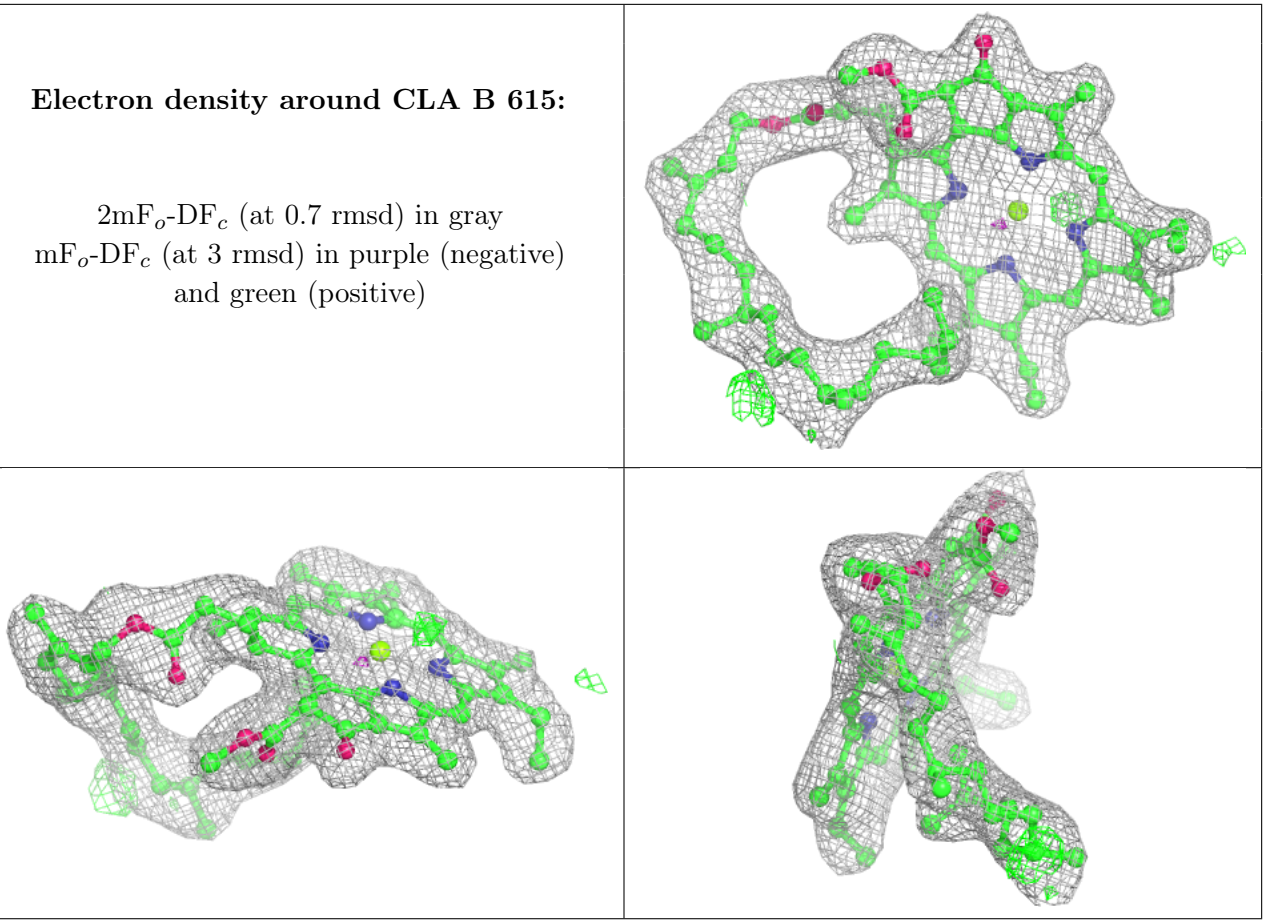
Electron density around CLA a 607:

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



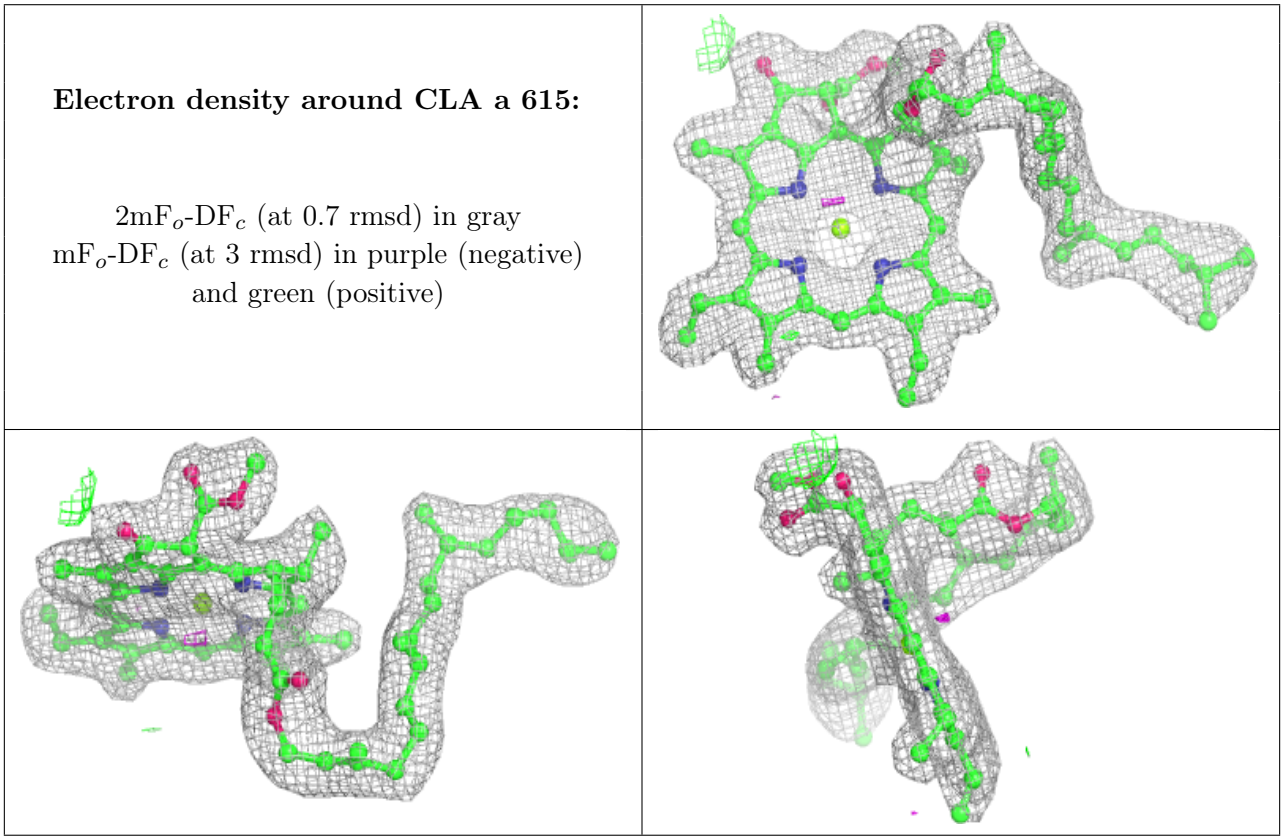
Electron density around CLA B 615:

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



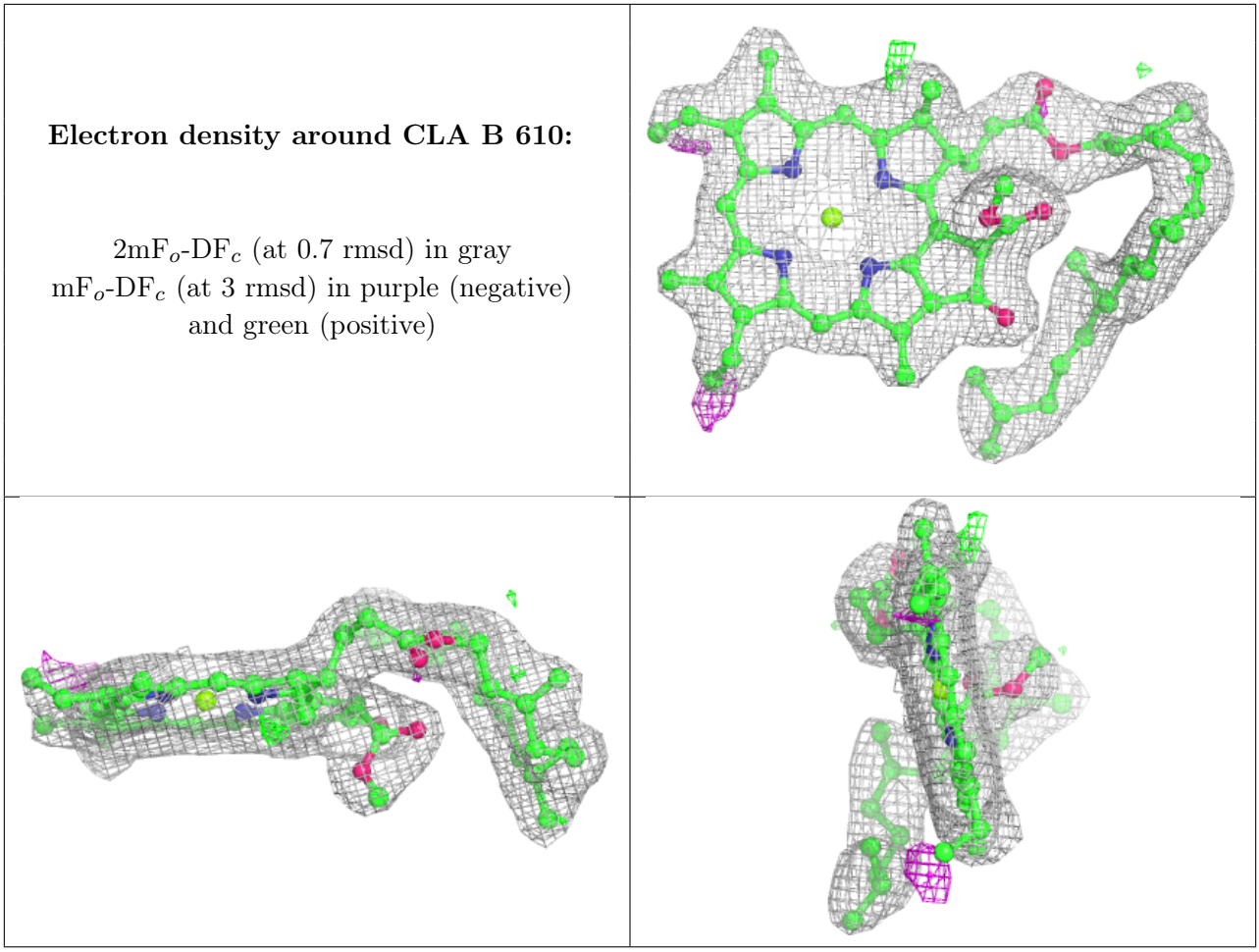
Electron density around CLA a 615:

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



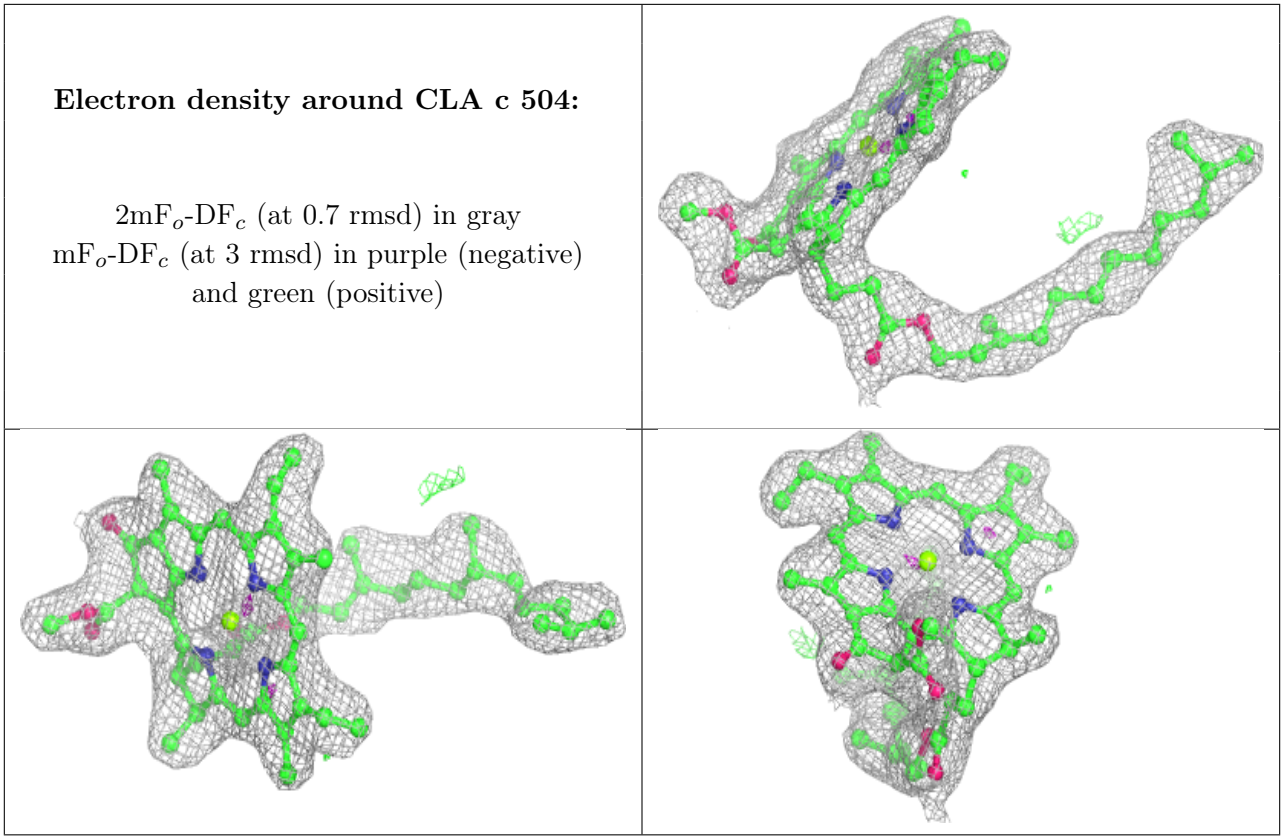
Electron density around CLA B 610:

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



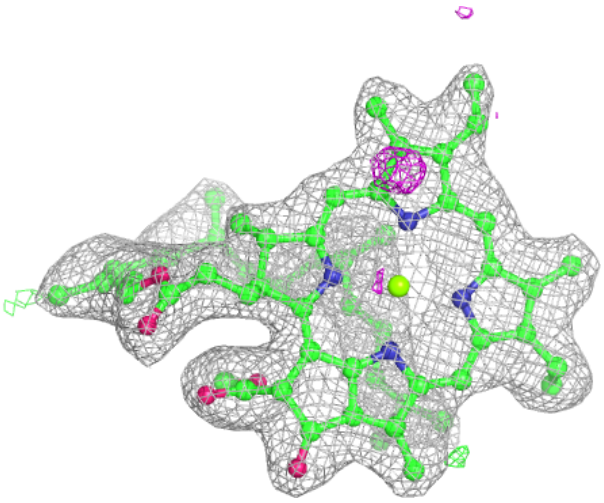
Electron density around CLA c 504:

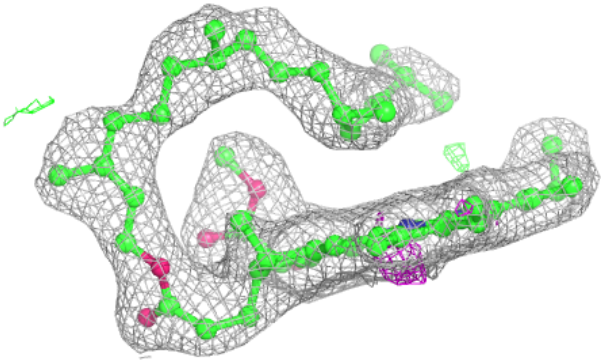
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

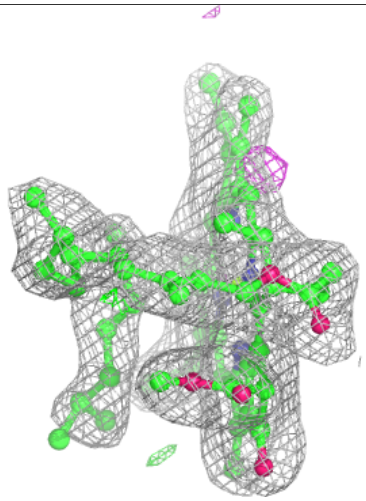


Electron density around CLA C 511:

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

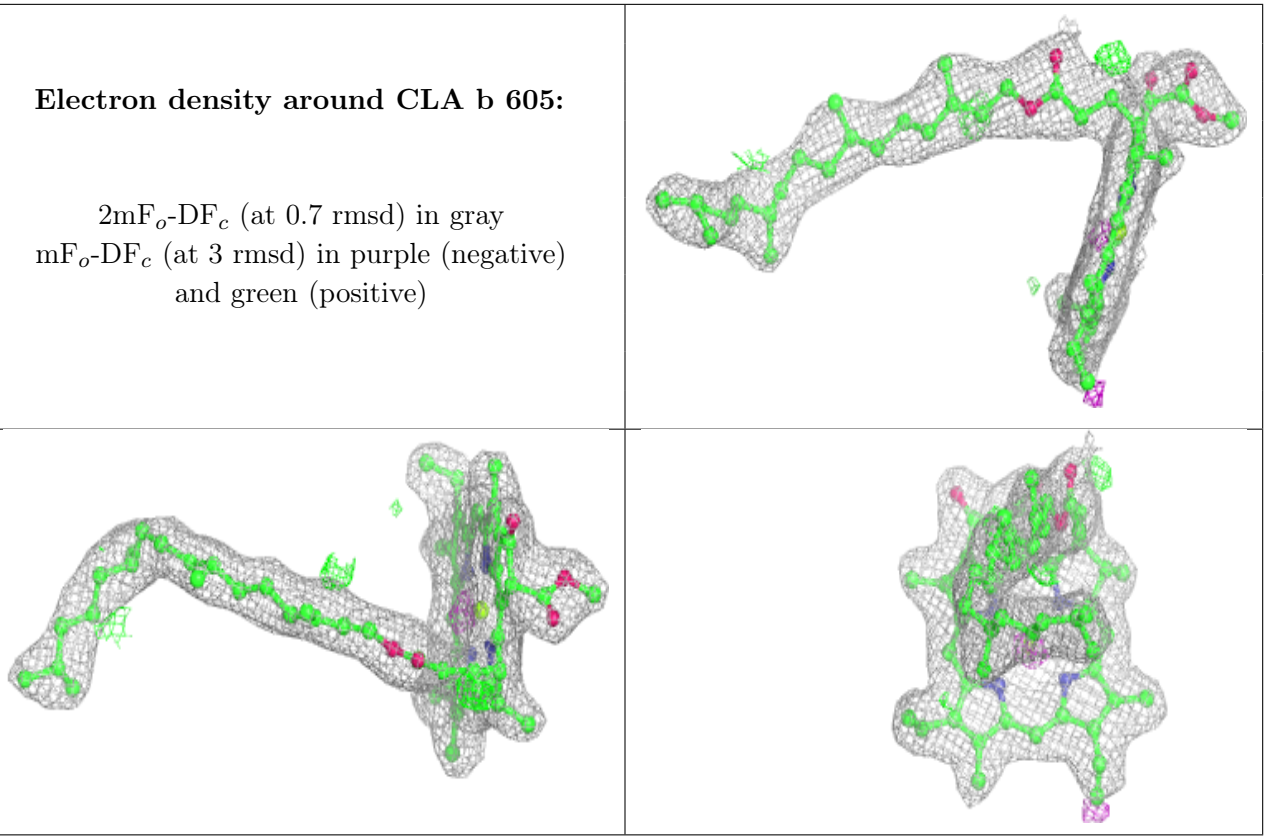






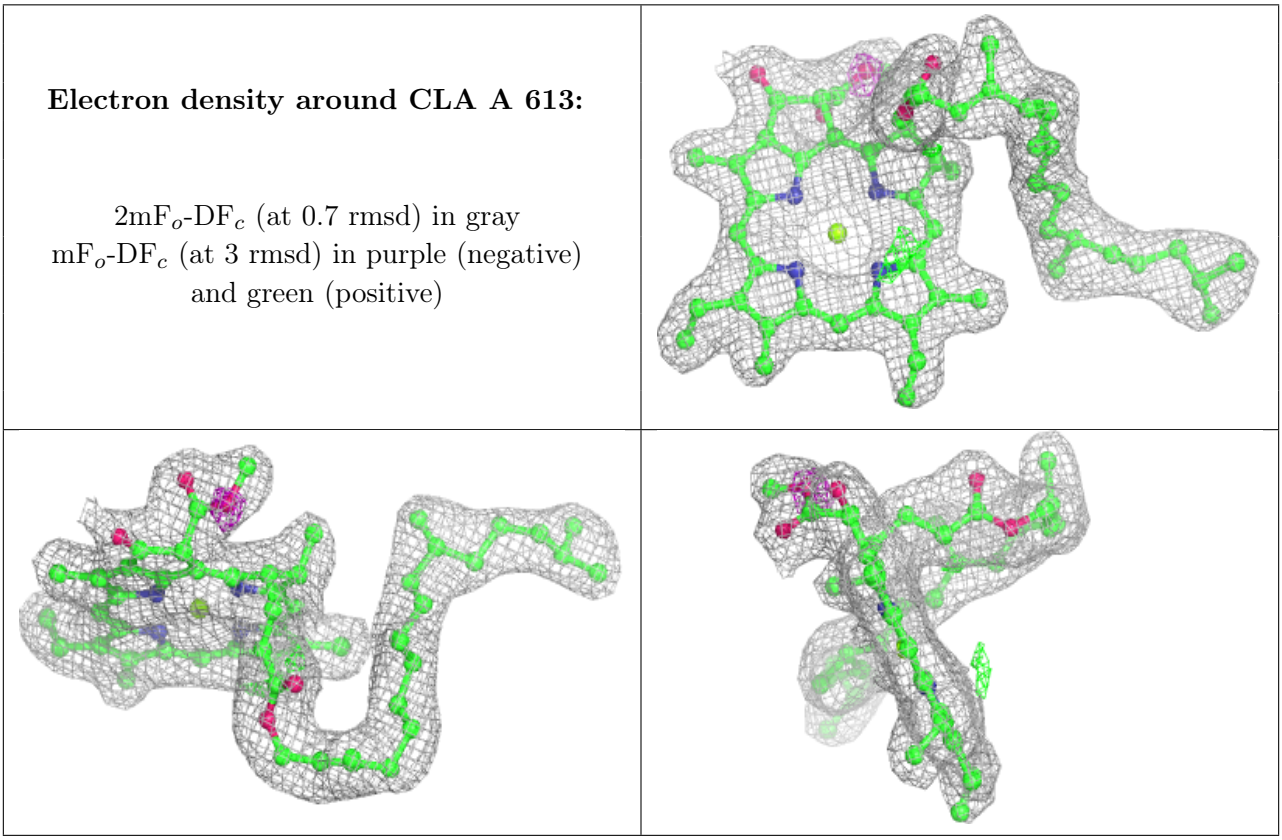
Electron density around CLA b 605:

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



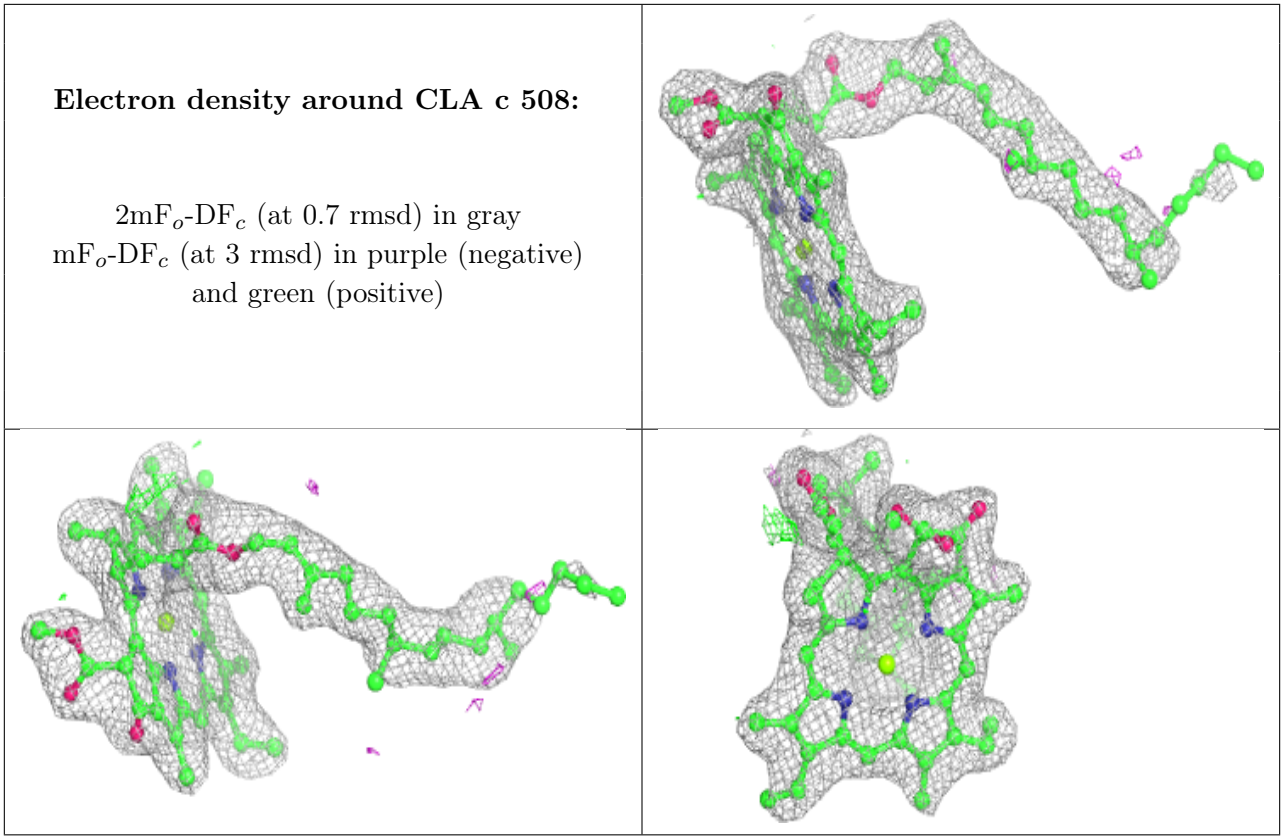
Electron density around CLA A 613:

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



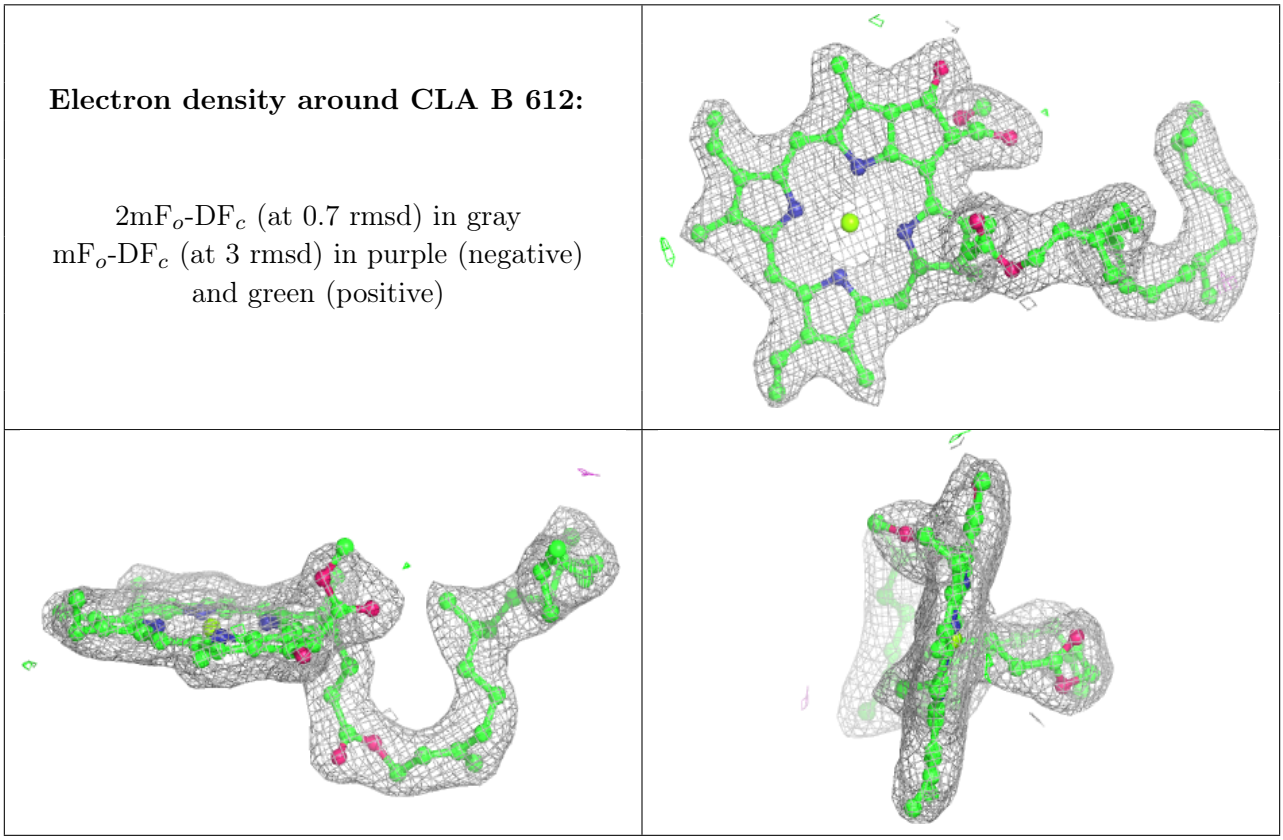
Electron density around CLA c 508:

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



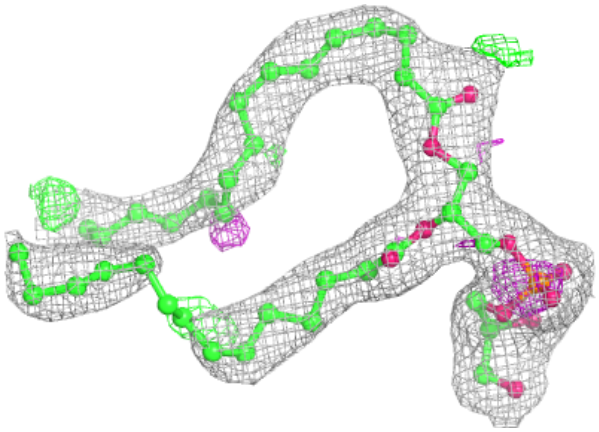
Electron density around CLA B 612:

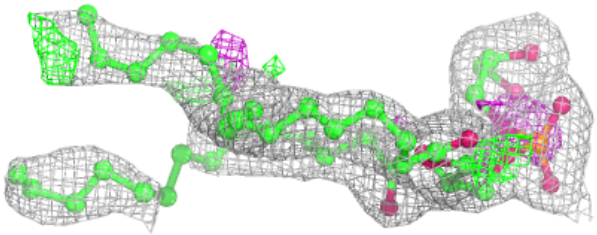
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

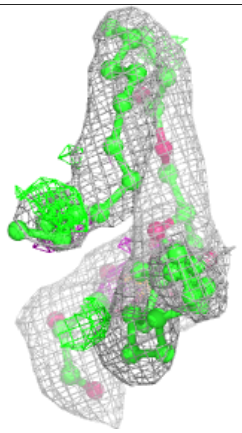


Electron density around LHG A 614:

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

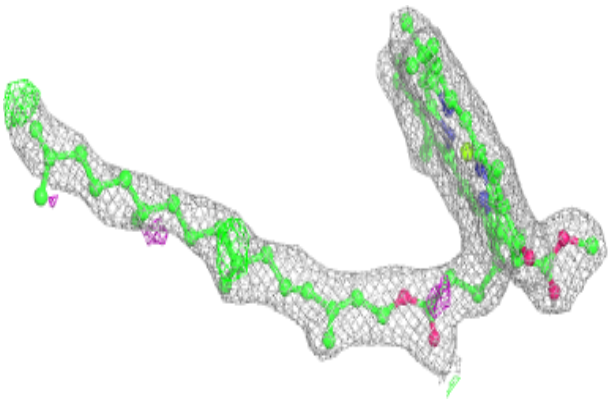


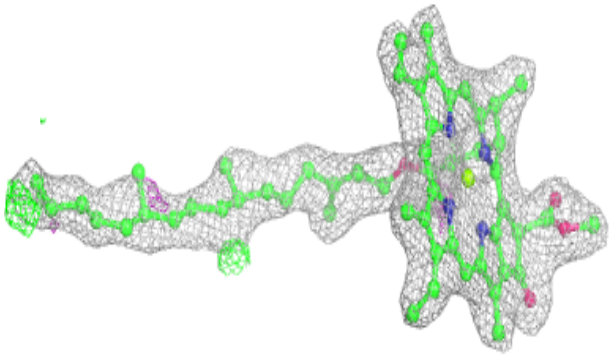


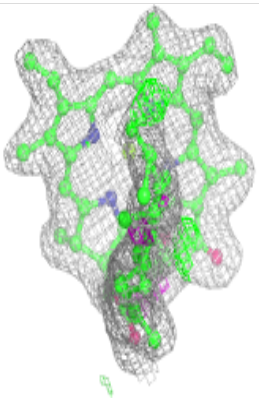


Electron density around CLA b 607:

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

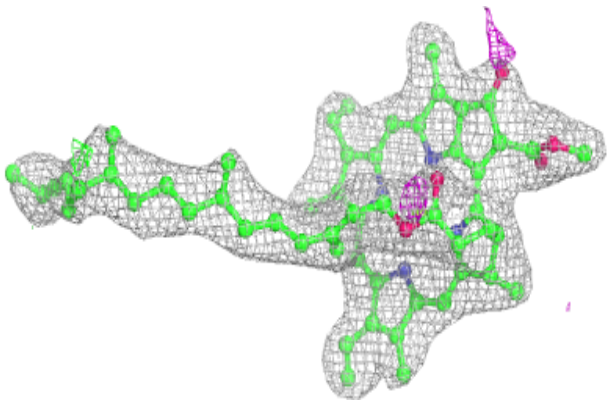


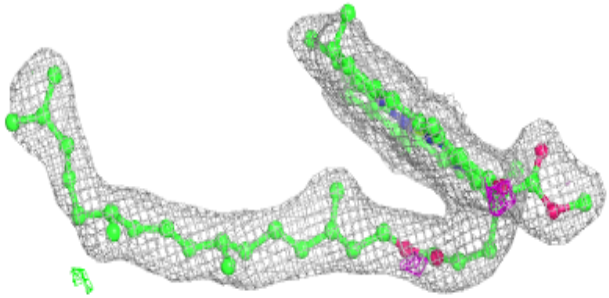


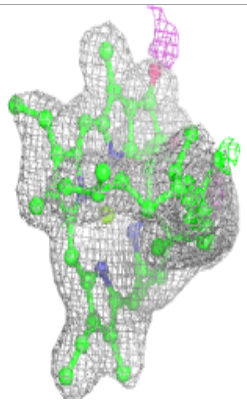


Electron density around CLA b 608:

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

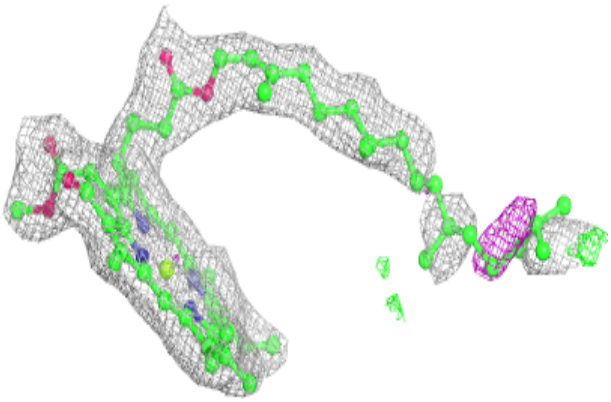


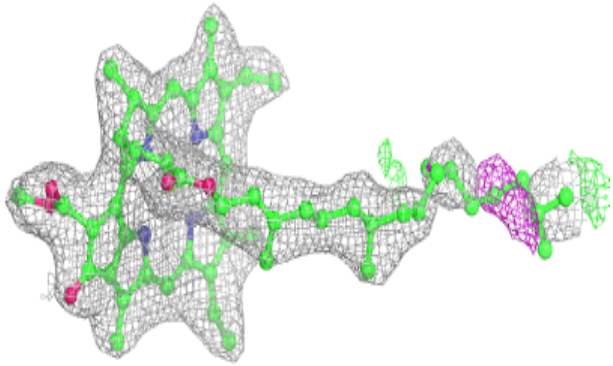


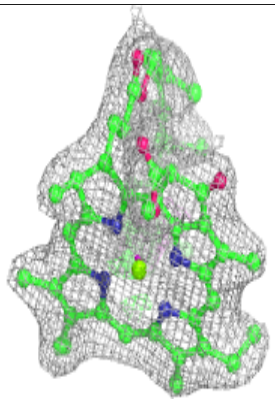


Electron density around CLA C 505:

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

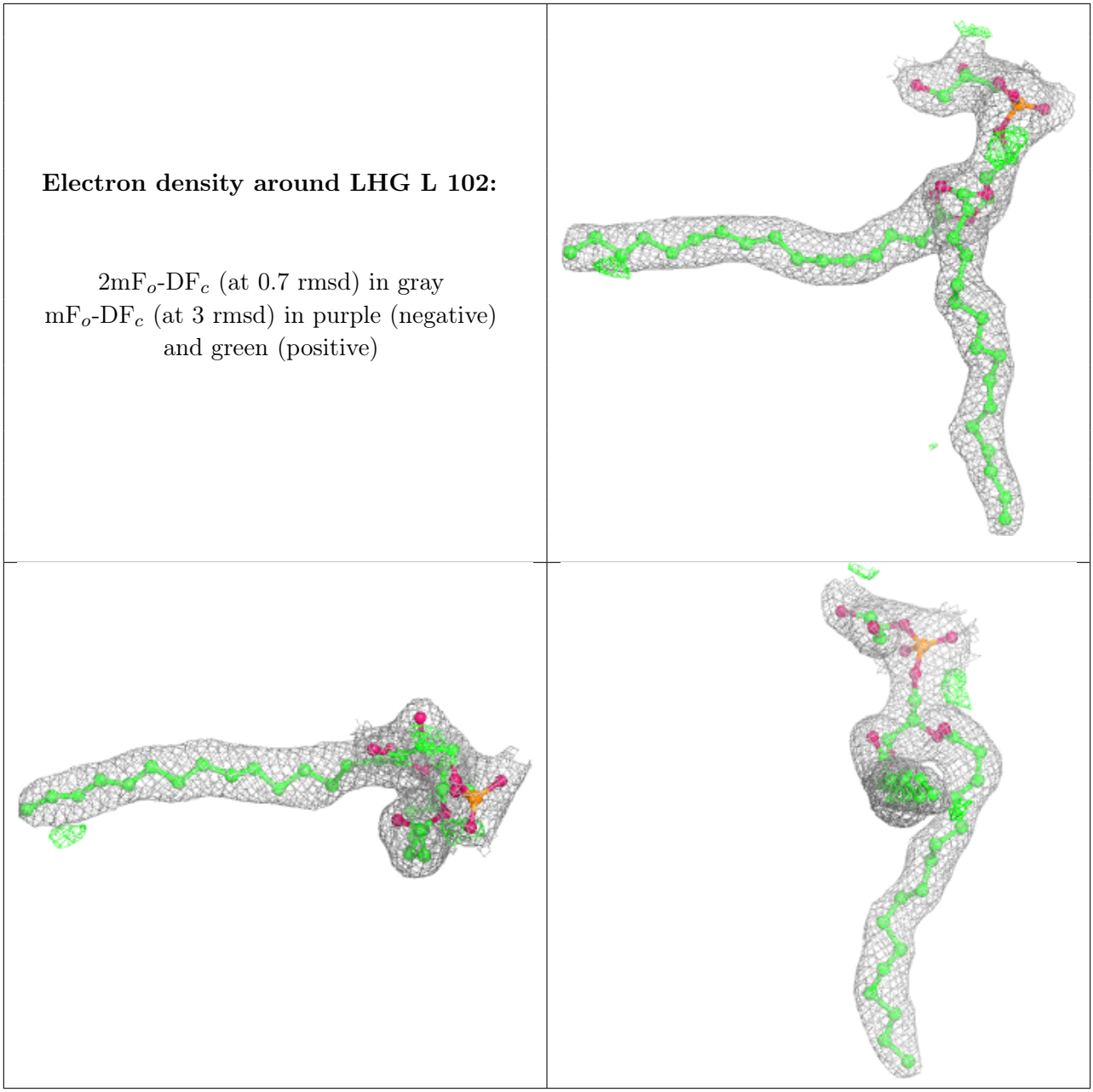






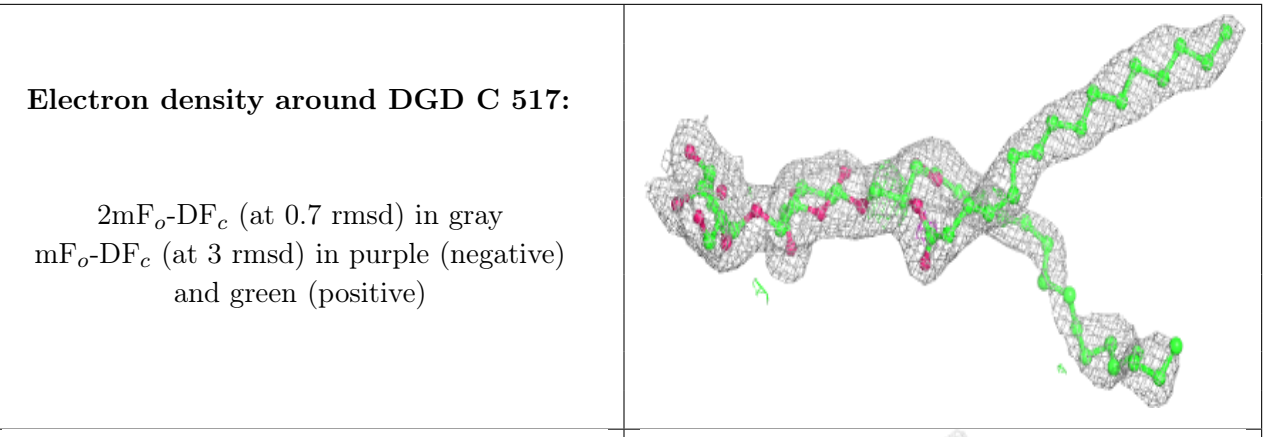
Electron density around LHG L 102:

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



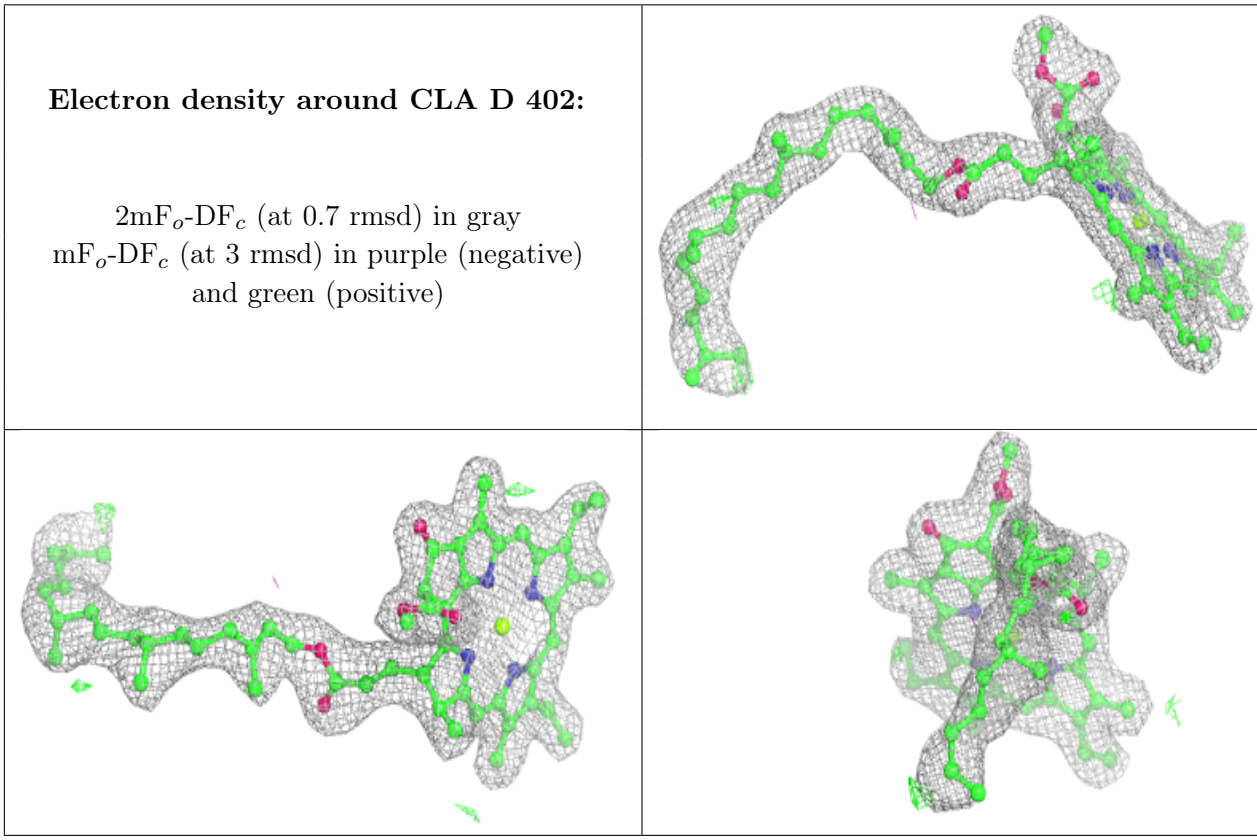
Electron density around DGD C 517:

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



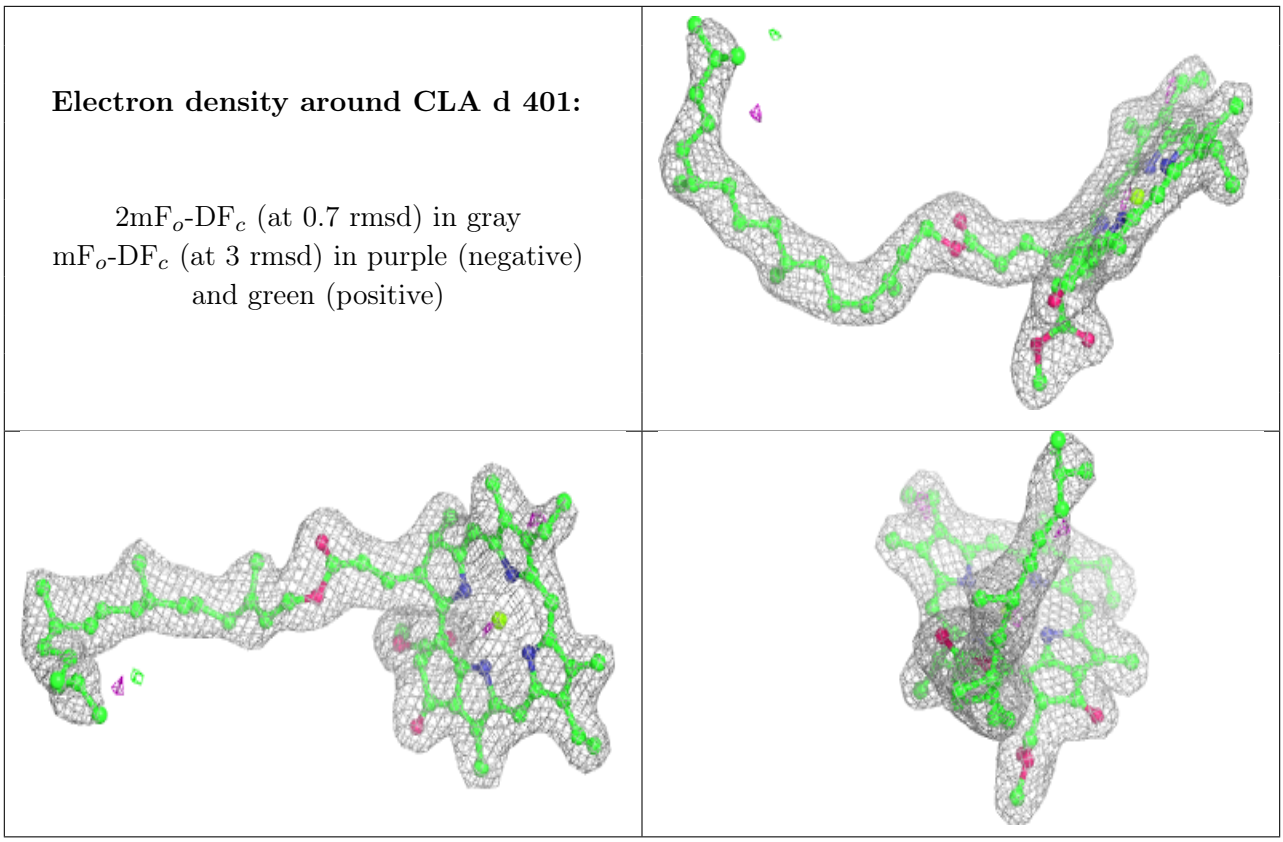
Electron density around CLA D 402:

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



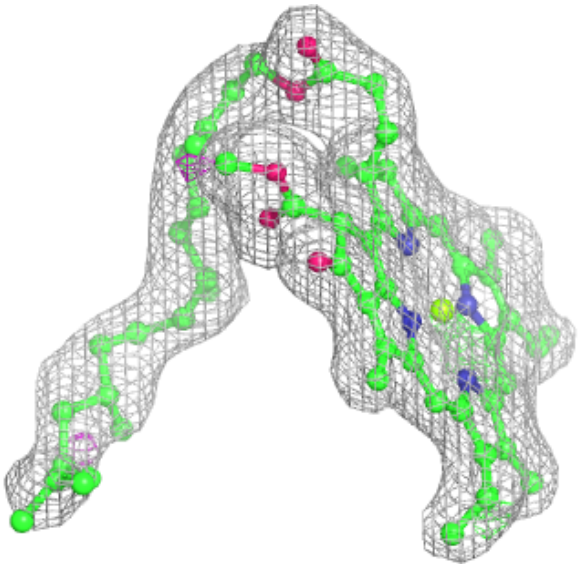
Electron density around CLA d 401:

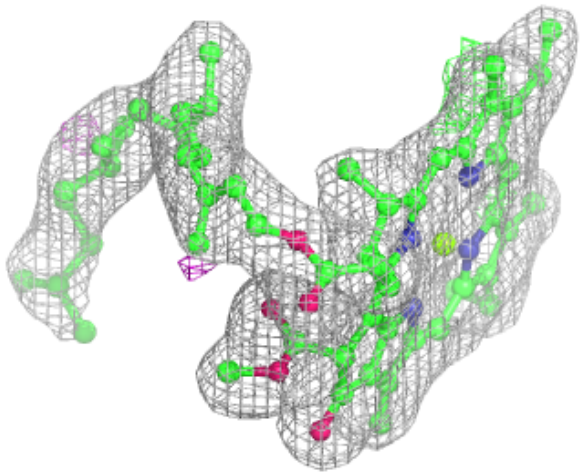
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

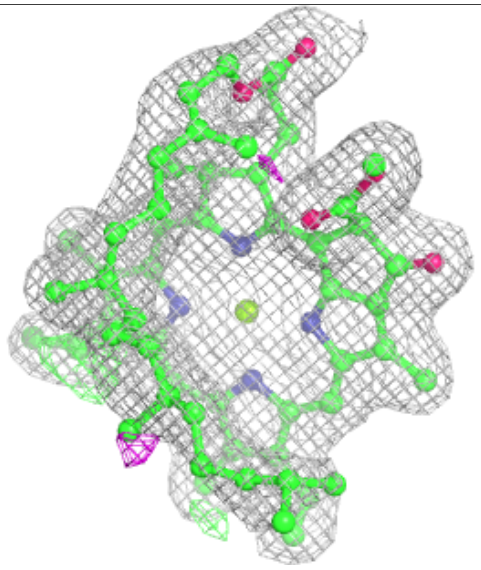


Electron density around CLA B 613:

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

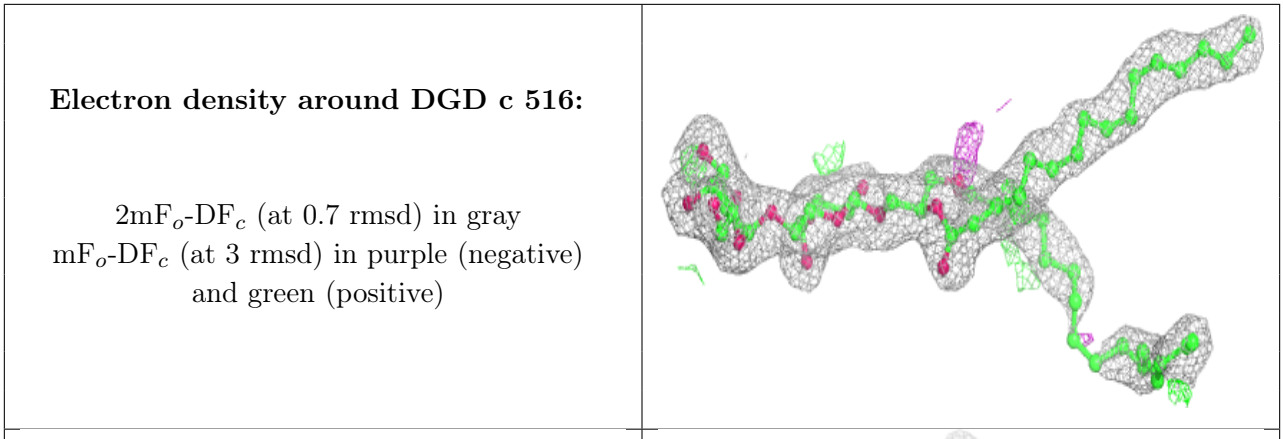






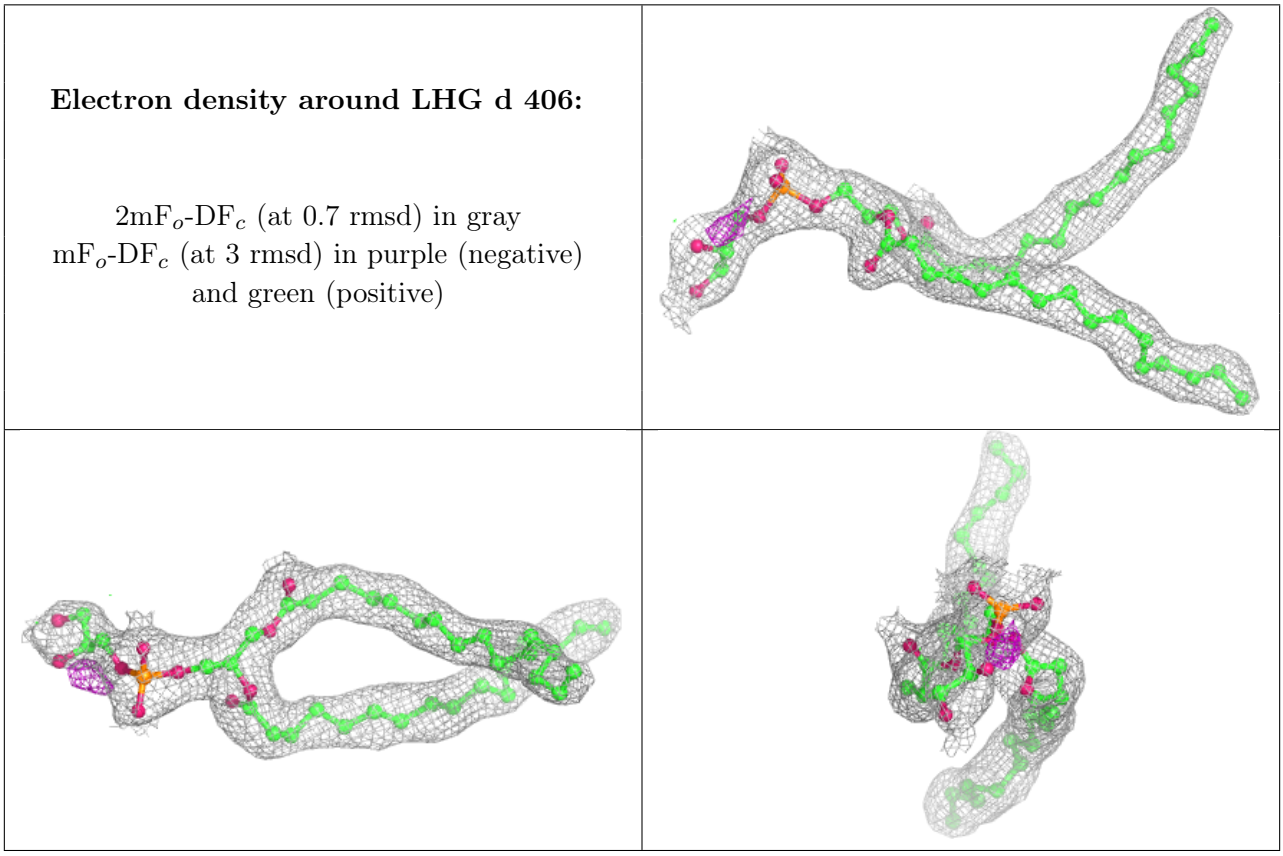
Electron density around DGD c 516:

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



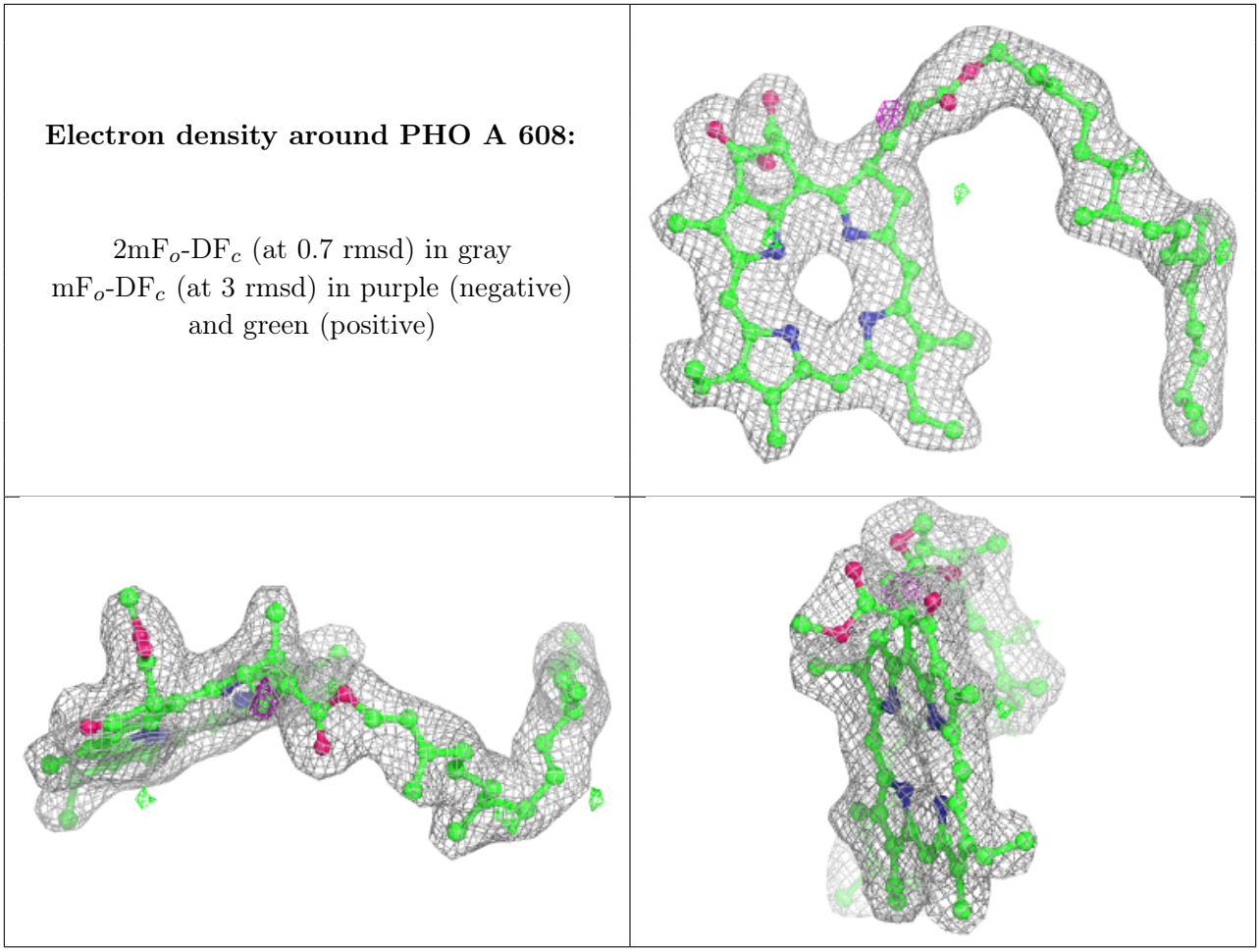
Electron density around LHG d 406:

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



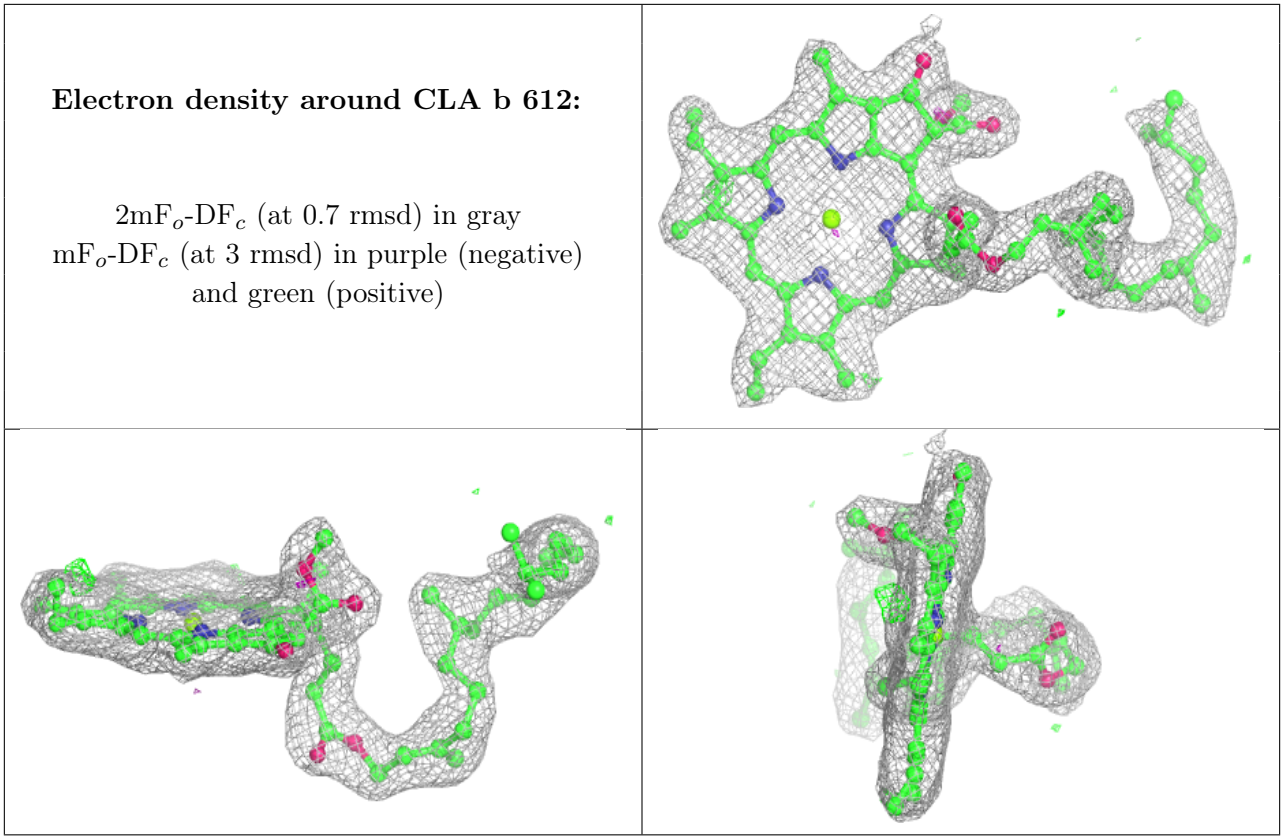
Electron density around PHO A 608:

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



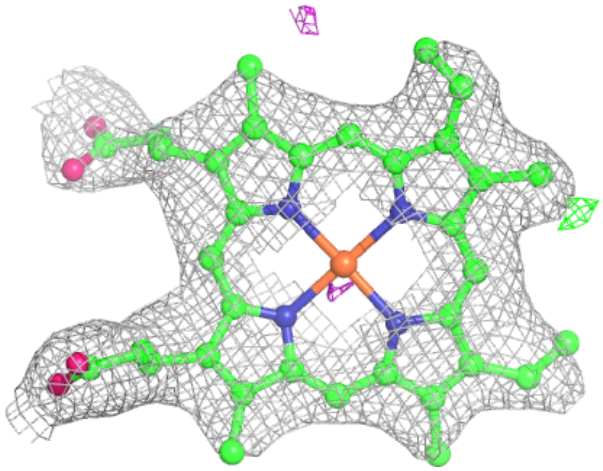
Electron density around CLA b 612:

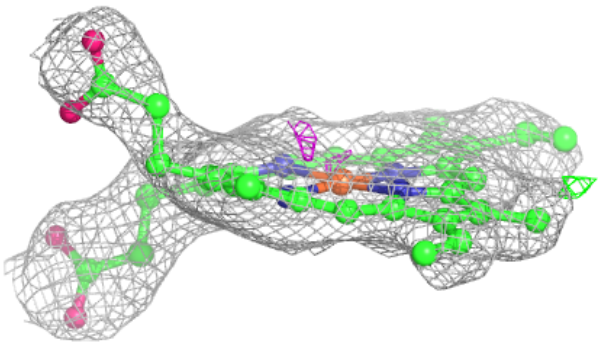
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

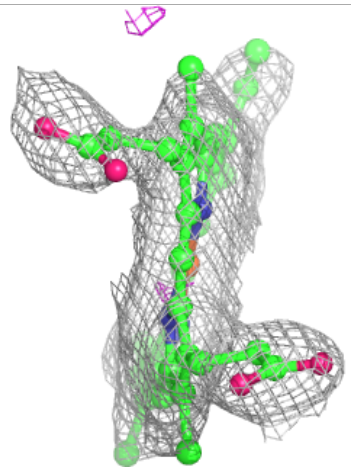


Electron density around HEM e 101:

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

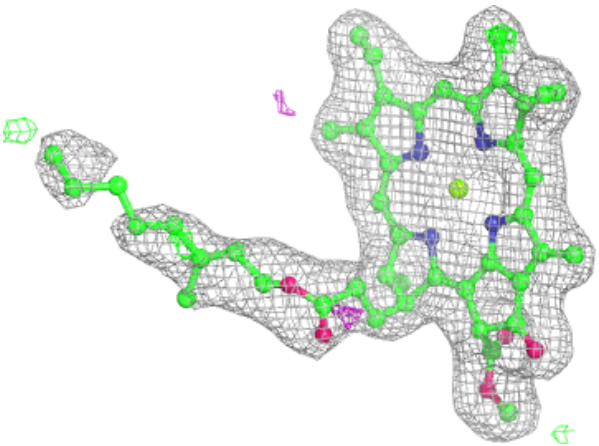


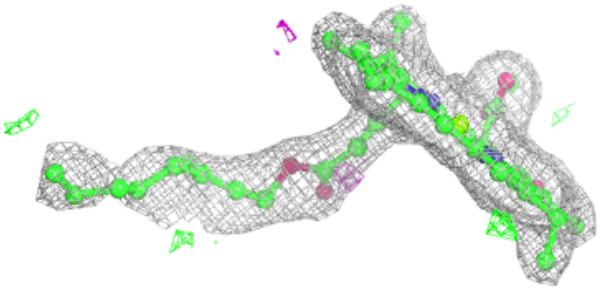


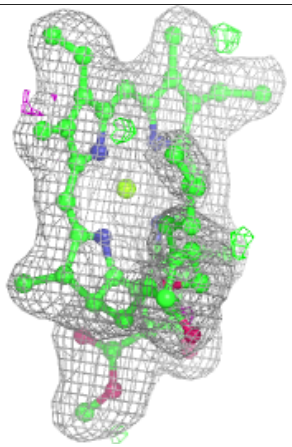


Electron density around CLA A 609:

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

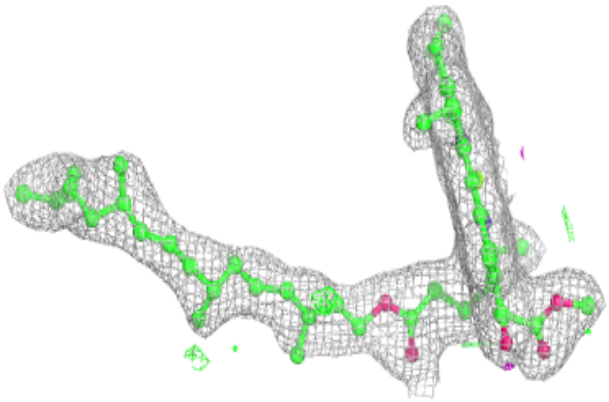


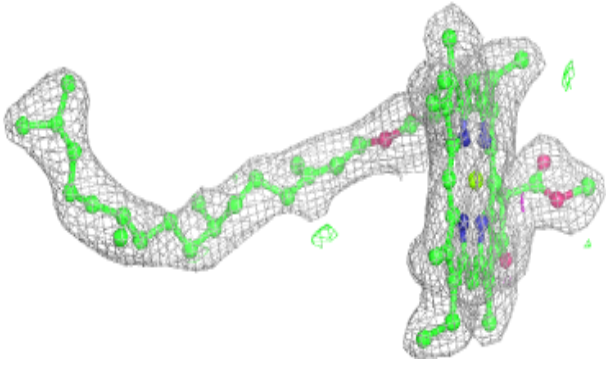


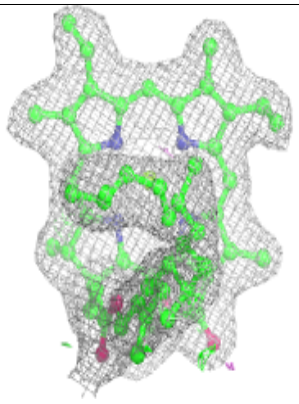


Electron density around CLA B 605:

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

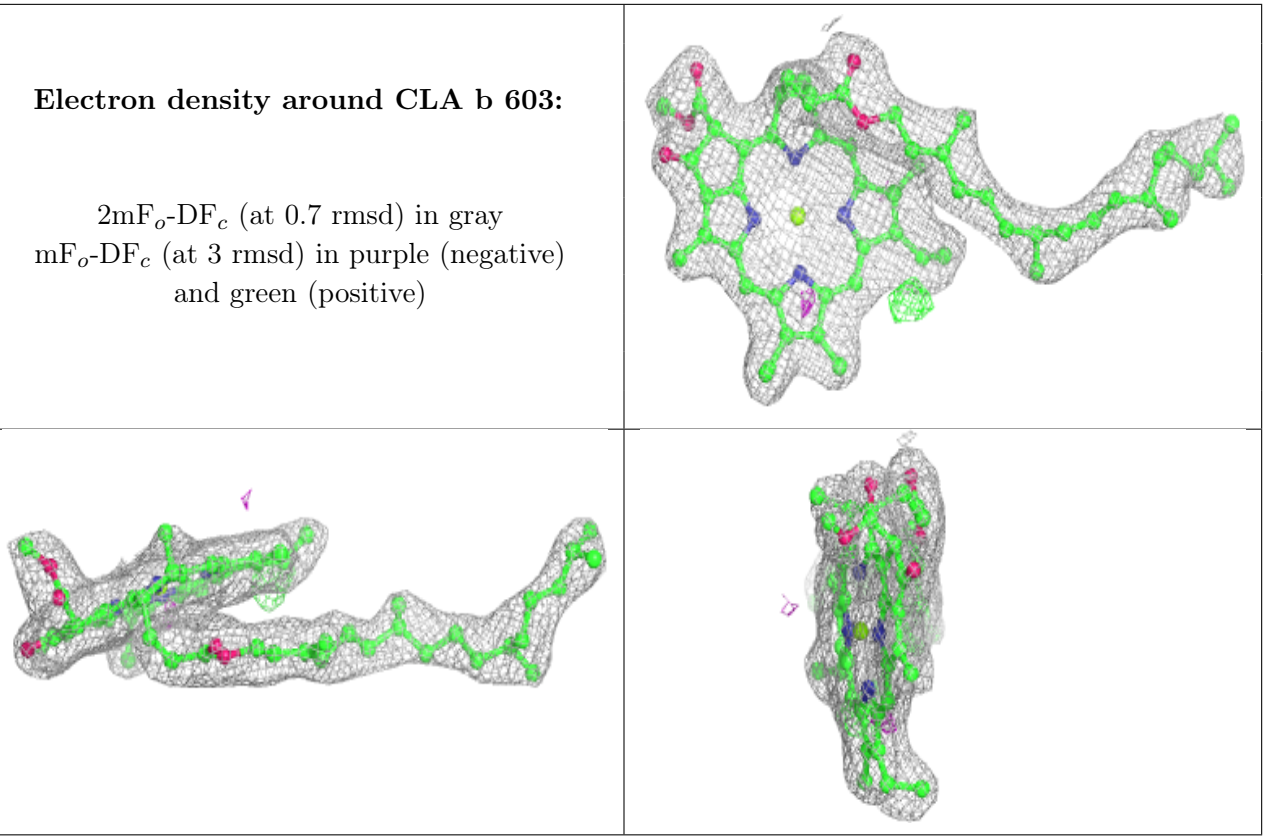






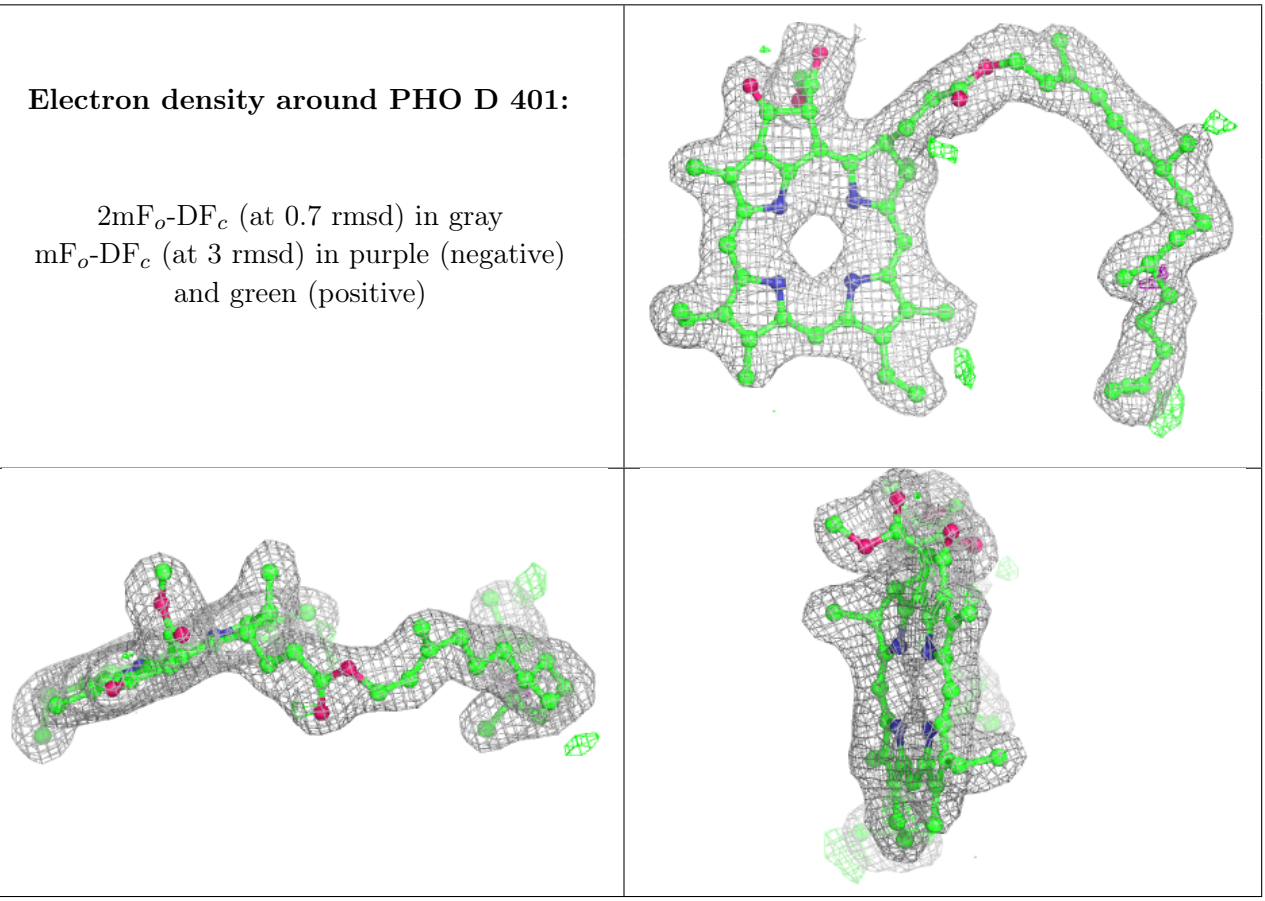
Electron density around CLA b 603:

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



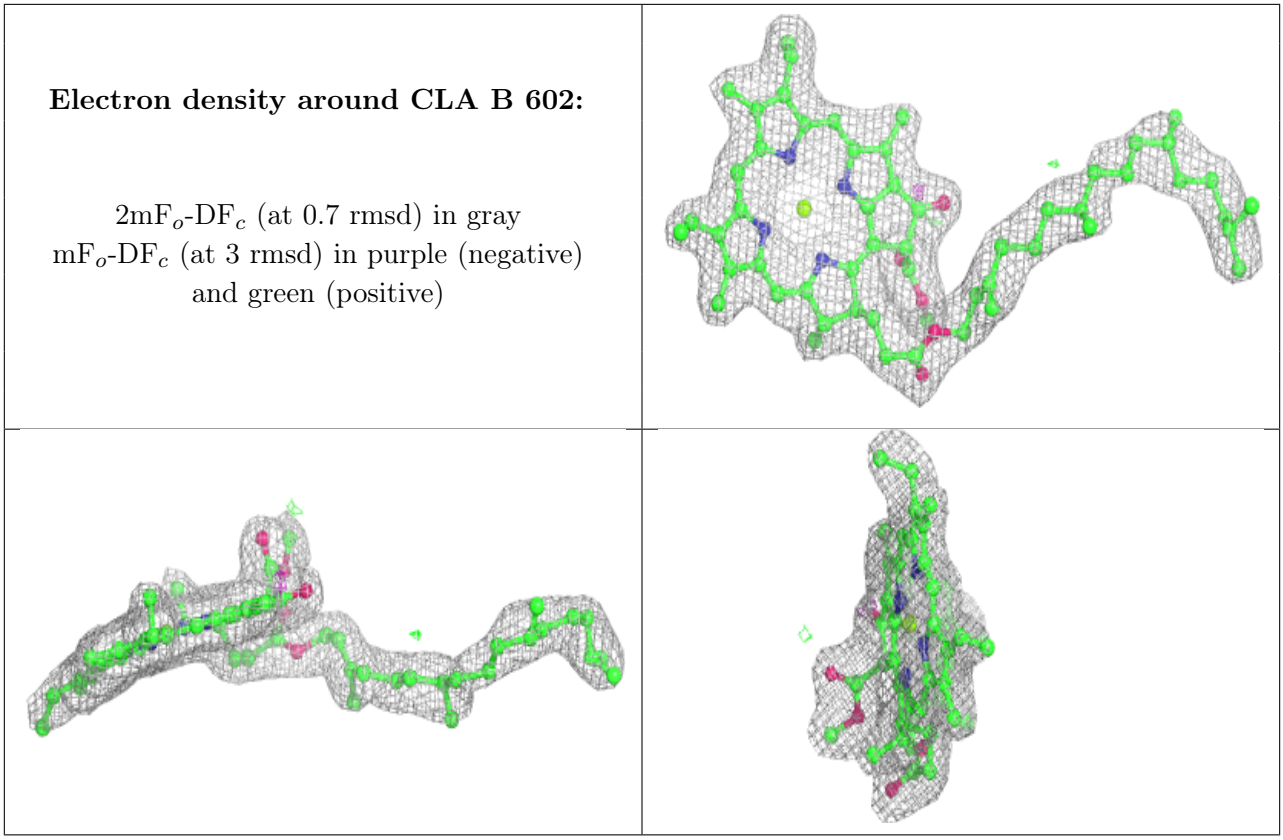
Electron density around PHO D 401:

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



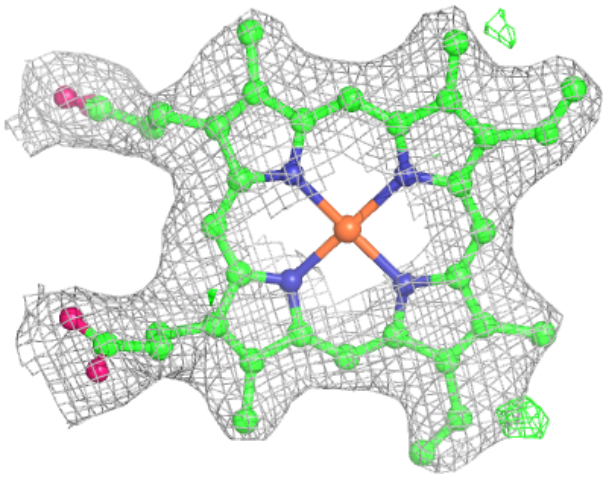
Electron density around CLA B 602:

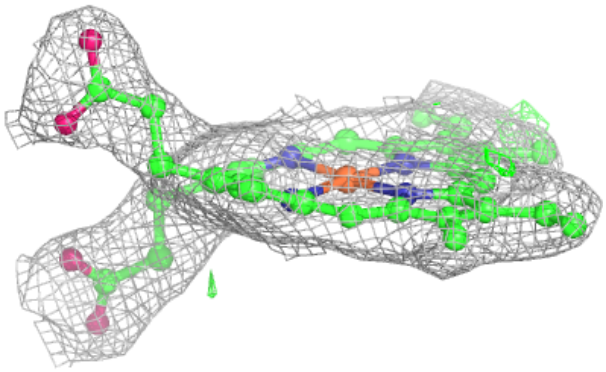
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

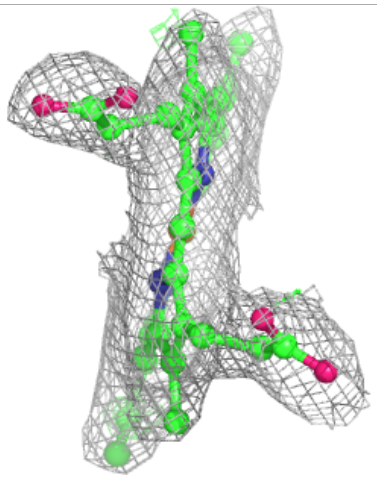


Electron density around HEM E 101:

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

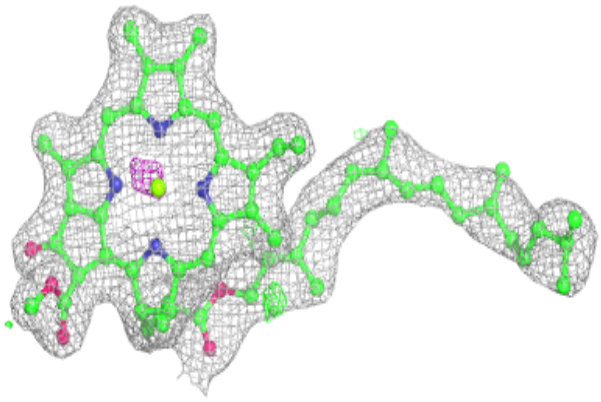


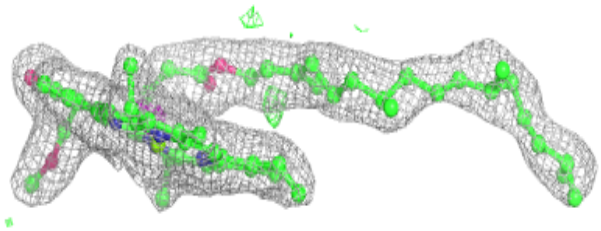


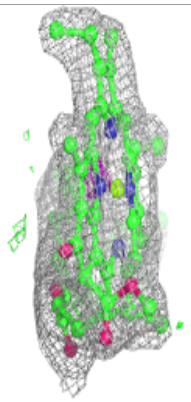


Electron density around CLA B 603:

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

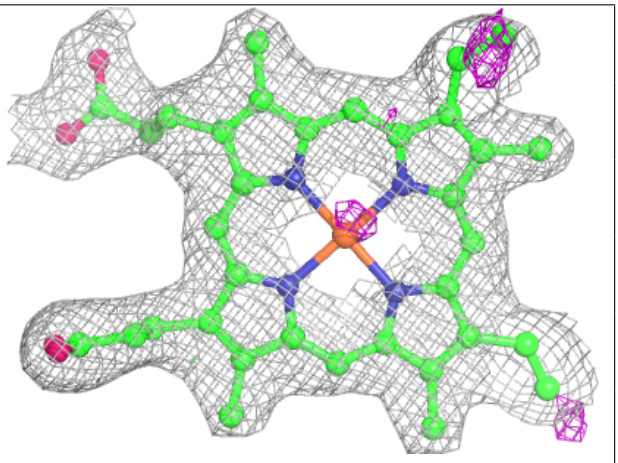


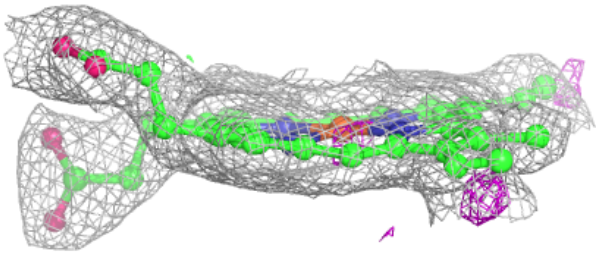


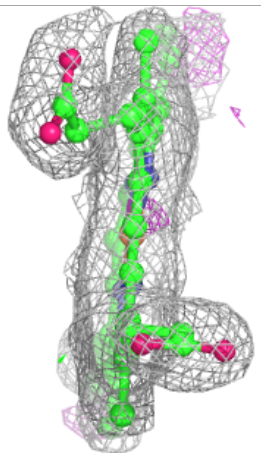


Electron density around HEC V 201:

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

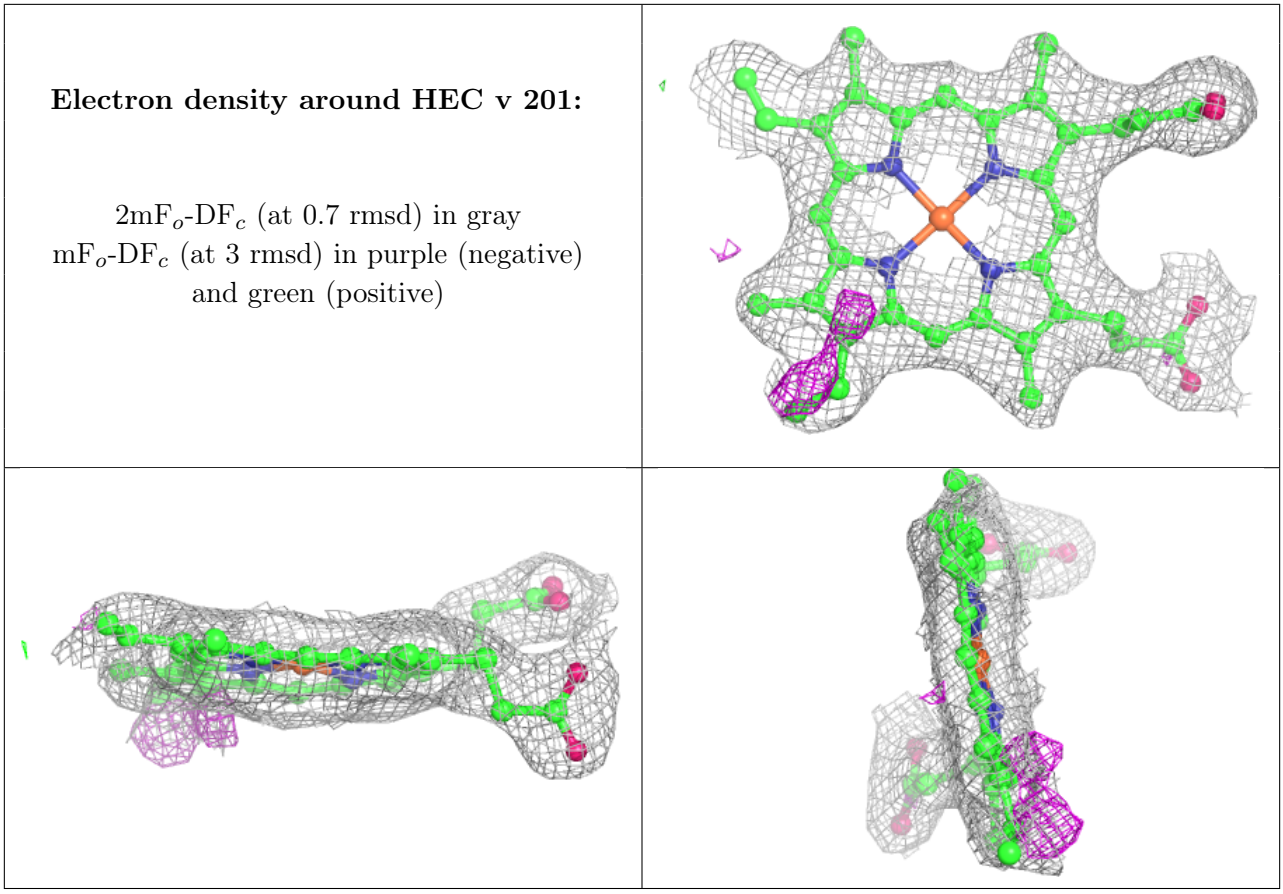






Electron density around HEC v 201:

$2mF_o$-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

There are no such residues in this entry.