Full wwPDB X-ray Structure Validation Report (i)

Aug 9, 2023 – 04:03 PM EDT

PDB ID	:	8F4E
Title	:	RT XFEL structure of Photosystem II 250 microseconds after the third illumination at 2.09 Angstrom resolution
Authors	:	Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on	:	2022-11-10
Resolution	:	2.09 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:

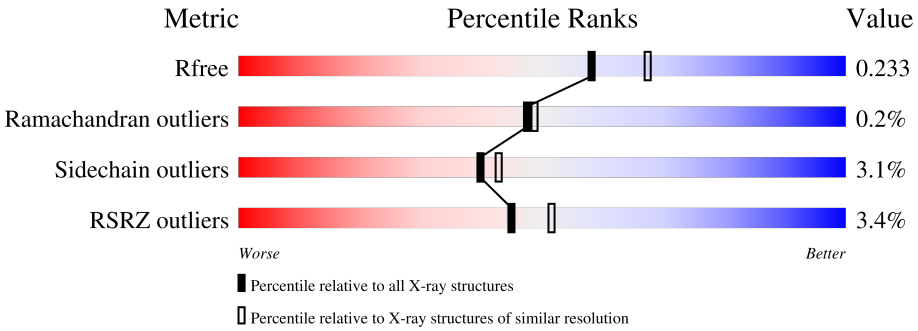
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35

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 2.09 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	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

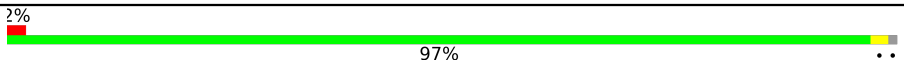
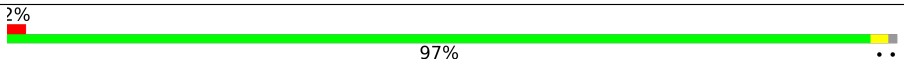
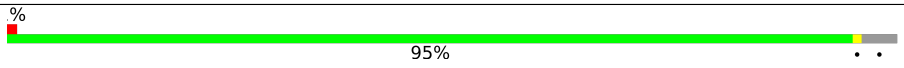
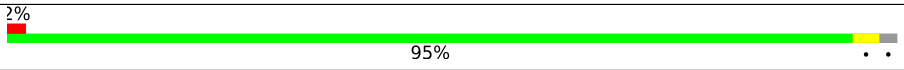
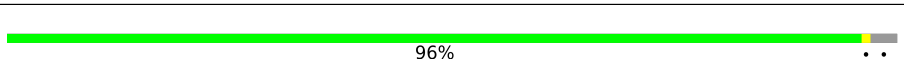
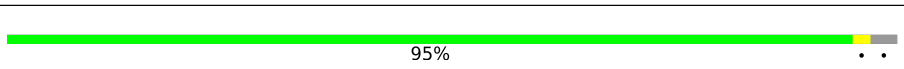
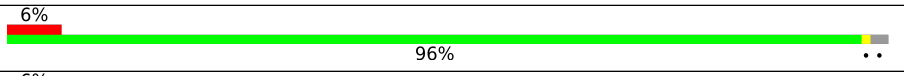
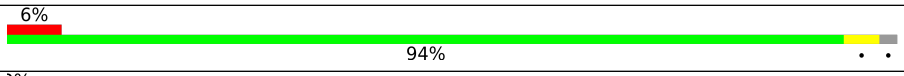
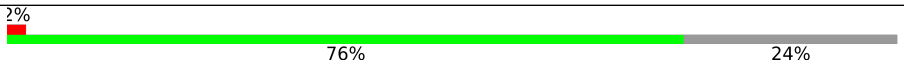
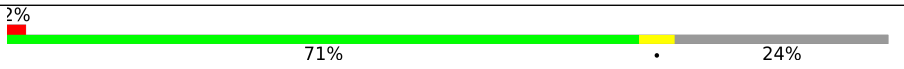
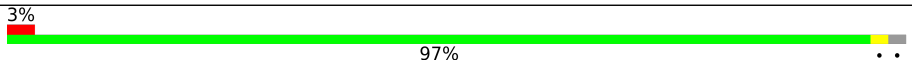
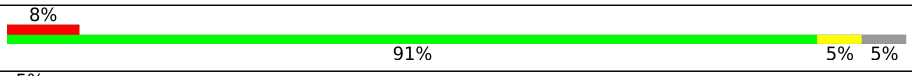
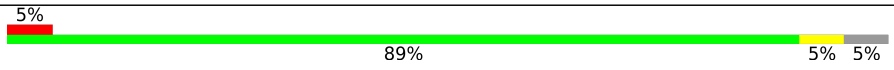
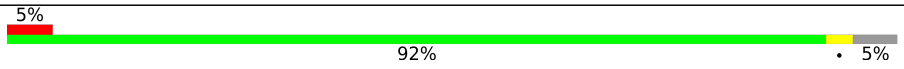
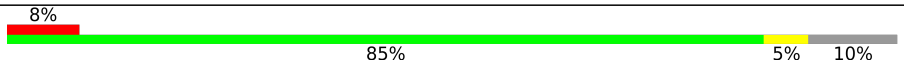
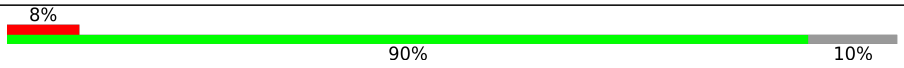
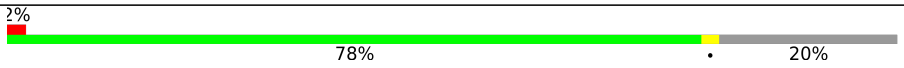
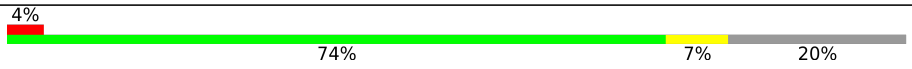
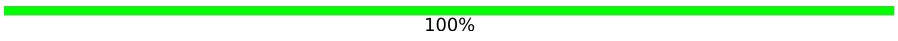
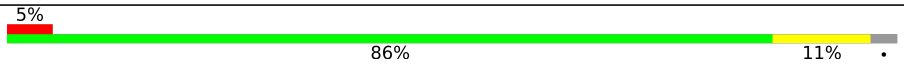
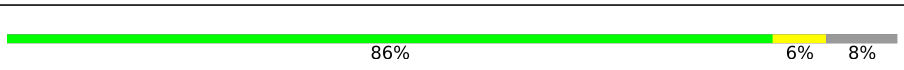
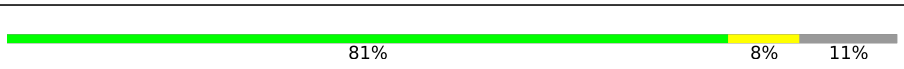
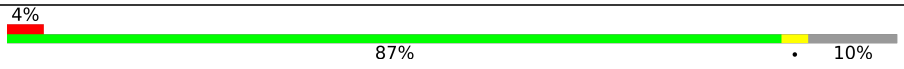
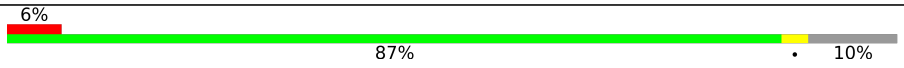
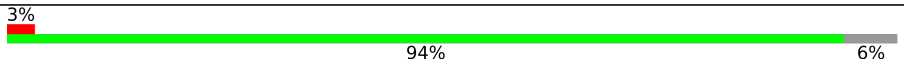
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	96%
1	a	344	94%

Continued on next page...

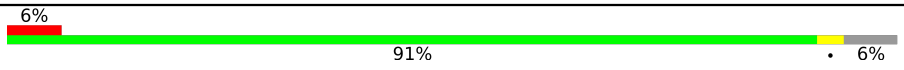
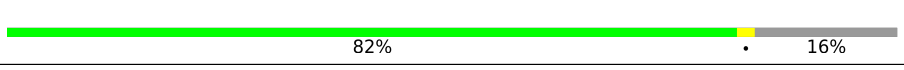
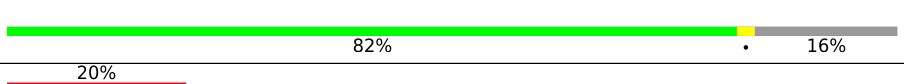
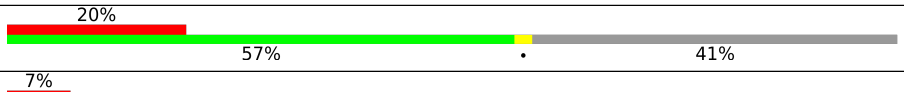
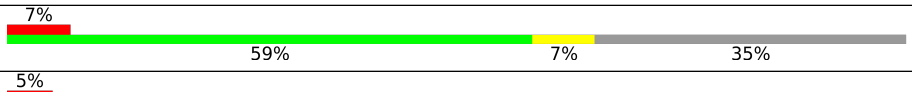
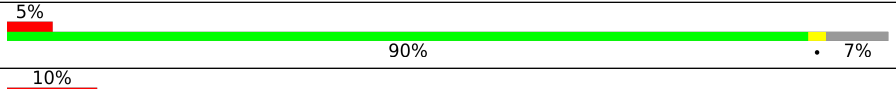
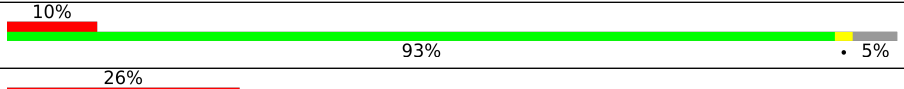
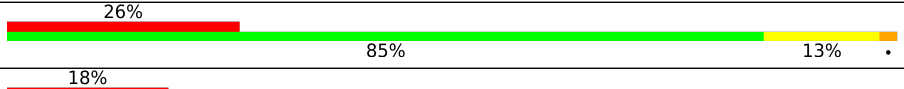
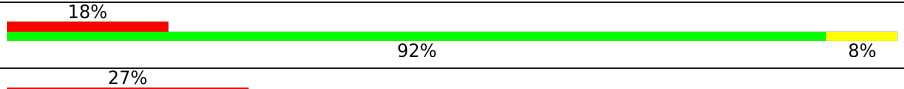
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	610	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	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	614	X	-	-	-
25	CLA	B	615	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	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	402	X	-	-	-
25	CLA	H	101	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	608	X	-	-	-
25	CLA	a	610	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	-	-	-
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	c	501	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	509	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	h	101	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 54466 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	64	0
			3604	2343	595	643	23			
1	a	334	Total	C	N	O	S	0	64	0
			3601	2340	595	643	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			4005	2631	666	695	13			
2	b	505	Total	C	N	O	S	0	0	0
			3978	2610	665	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	442	Total	C	N	O	S	0	11	0
			3592	2355	601	621	15			
3	c	451	Total	C	N	O	S	0	12	0
			3666	2396	617	638	15			

- 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	2	0
			2745	1818	448	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2751	1822	448	469	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total 666	C 436	N 107	O 123	0	1	0
5	e	82	Total 664	C 434	N 108	O 122	0	0	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	36	Total 296	C 200	N 46	O 49	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

Continued on next page...

Continued from previous page...

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	36	Total 296	C 197	N 47	O 52		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 256	C 171	N 37	O 47	S 1	0	0	0
12	m	32	Total 251	C 168	N 36	O 46	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 1870	C 1168	N 313	O 385	S 4	0	1	0
13	o	244	Total 1874	C 1170	N 317	O 383	S 4	0	0	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 256	C 180	N 36	O 38	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	0	0
			1064	675	177	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
			196	128	35	30	3			
17	y	30	Total	C	N	O	S	0	0	0
			218	144	35	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	39	Total	C	N	O	0	0	0
			286	191	46	49			

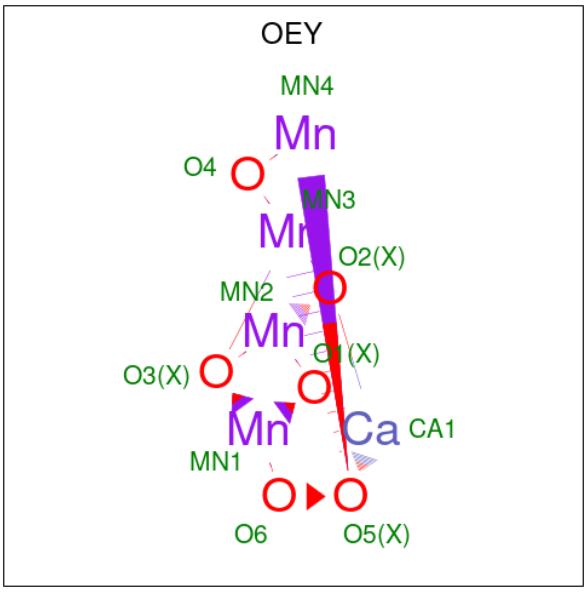
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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
			477	326	72	77	2			

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

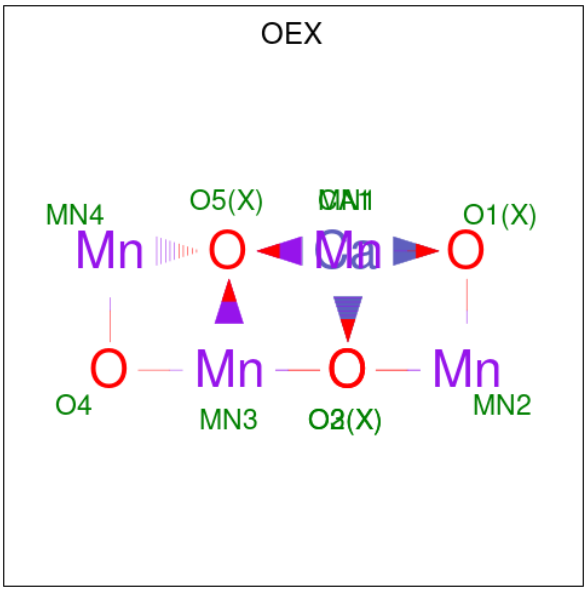
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: $CaMn_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			22	2	8	12		
21	a	1	Total	Ca	Mn	O	0	1
			22	2	8	12		

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

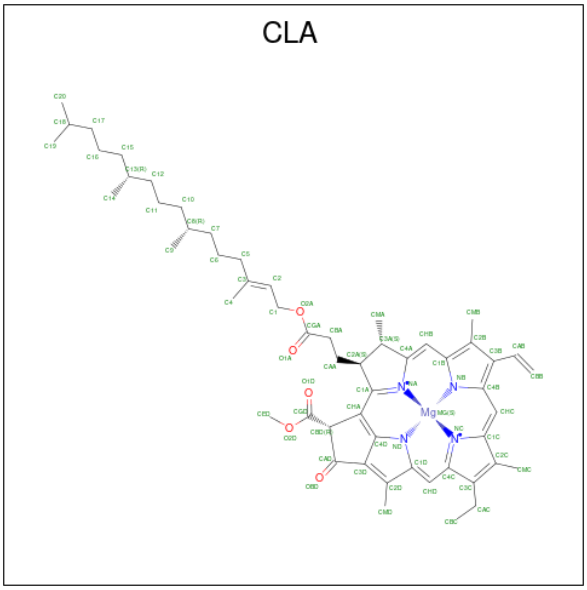
- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- 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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 54 44 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 60 50 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 65 55 1 4 5	0	0
25	C	1	Total C Mg N O 59 49 1 4 5	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

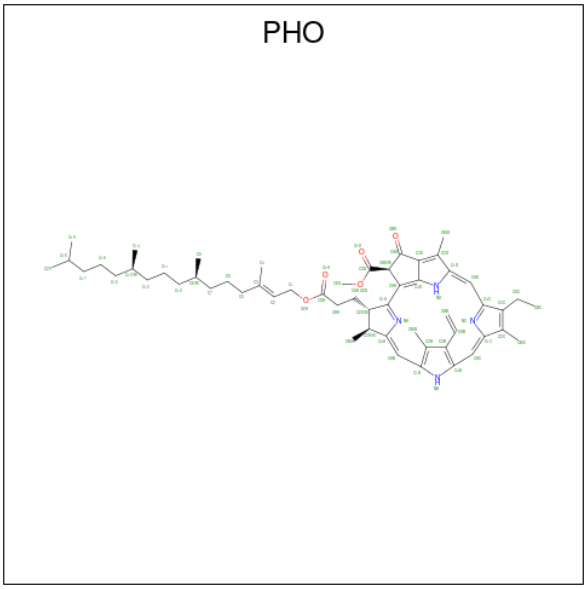
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4 5	0	0
25	b	1	Total C Mg N O 65 55 1 4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

Continued on next page...

Continued from previous page...

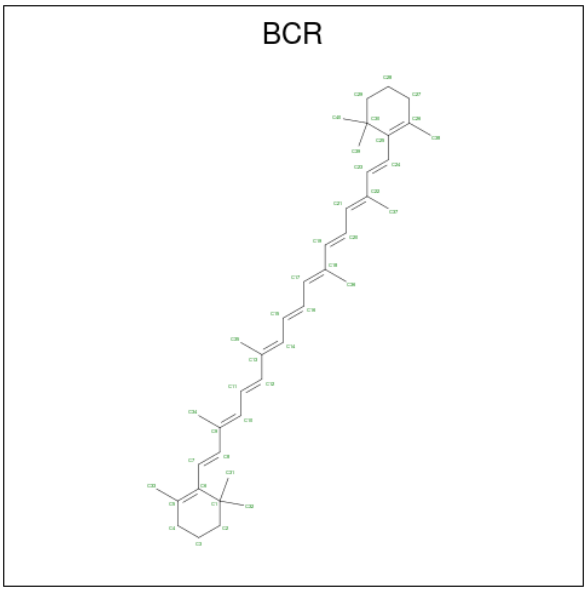
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	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		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



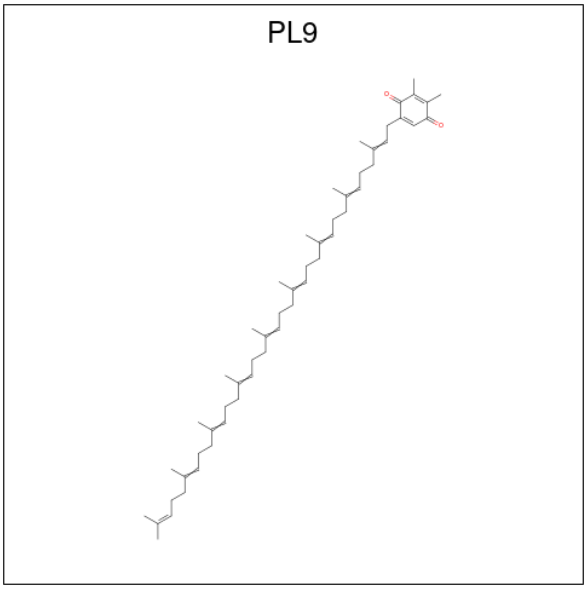
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

Continued on next page...

Continued from previous page...

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	d	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	x	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: $C_{53}H_{80}O_2$).



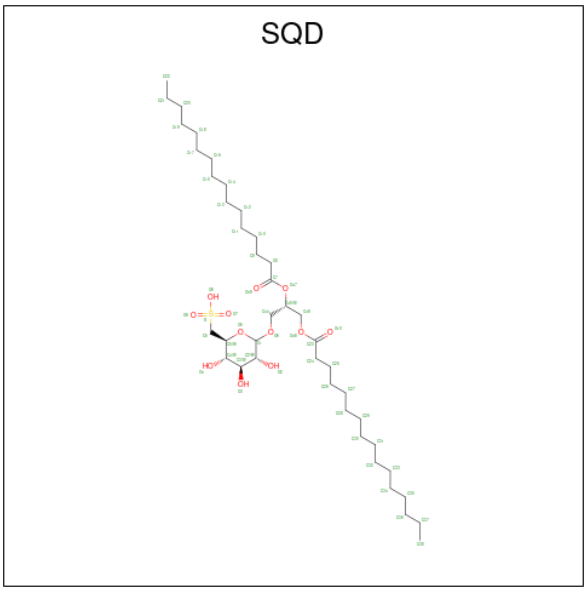
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0

Continued on next page...

Continued from previous page...

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

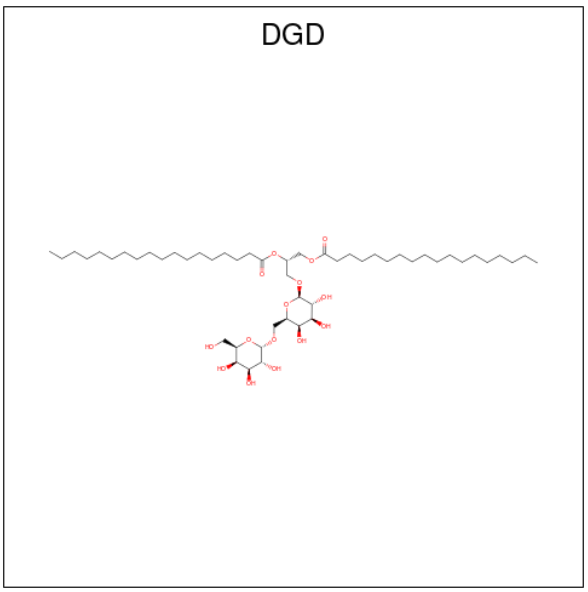
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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 39 35 4	0	0
29	F	1	Total C O S 36 25 10 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	a	1	Total C O 36 31 5	0	0
29	f	1	Total C O S 41 28 12 1	0	0
29	l	1	Total C O S 54 41 12 1	0	0

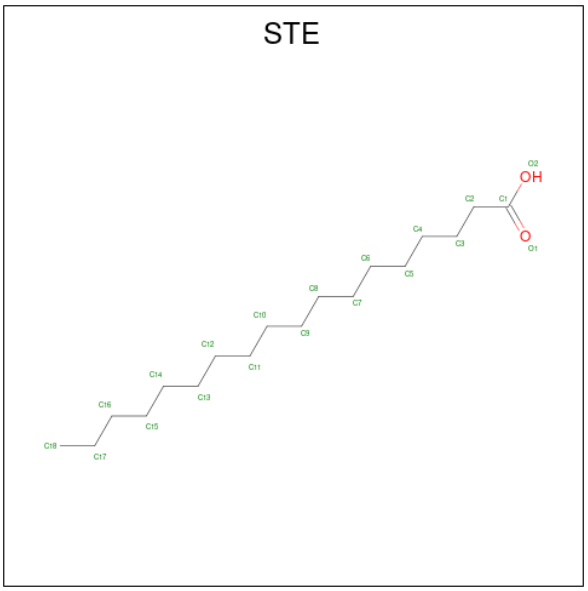
- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 66 51 15	0	0
30	C	1	Total C O 62 47 15	0	0
30	C	1	Total C O 62 47 15	0	0
30	C	1	Total C O 62 47 15	0	0
30	H	1	Total C O 62 47 15	0	0
30	a	1	Total C O 44 39 5	0	0
30	c	1	Total C O 62 47 15	0	0
30	c	1	Total C O 62 47 15	0	0
30	c	1	Total C O 62 47 15	0	0
30	h	1	Total C O 62 47 15	0	0

- Molecule 31 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



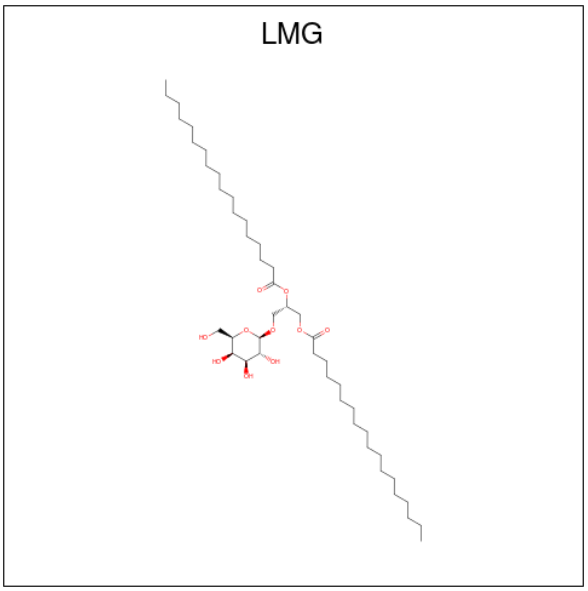
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 17 15 2	0	0
31	B	1	Total C O 12 10 2	0	0
31	B	1	Total C O 18 16 2	0	0
31	B	1	Total C O 12 10 2	0	0
31	B	1	Total C 16 16	0	0
31	C	1	Total C O 12 10 2	0	0
31	C	1	Total C O 12 10 2	0	0
31	C	1	Total C 16 16	0	0
31	D	1	Total C O 20 18 2	0	0
31	H	1	Total C 18 18	0	0
31	I	1	Total C 15 15	0	0
31	J	1	Total C O 12 10 2	0	0
31	M	1	Total C O 15 13 2	0	0
31	M	1	Total C 10 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	T	1	Total C 16 16	0	0
31	T	1	Total C 15 15	0	0
31	R	1	Total C O 12 10 2	0	0
31	a	1	Total C O 12 10 2	0	0
31	b	1	Total C O 20 18 2	0	0
31	b	1	Total C O 16 14 2	0	0
31	b	1	Total C O 20 18 2	0	0
31	b	1	Total C 10 10	0	0
31	c	1	Total C O 20 18 2	0	0
31	c	1	Total C O 12 10 2	0	0
31	d	1	Total C O 17 15 2	0	0
31	j	1	Total C O 12 10 2	0	0
31	l	1	Total C 18 18	0	0
31	m	1	Total C O 12 10 2	0	0
31	t	1	Total C O 14 12 2	0	0
31	t	1	Total C 10 10	0	0
31	x	1	Total C O 20 18 2	0	0

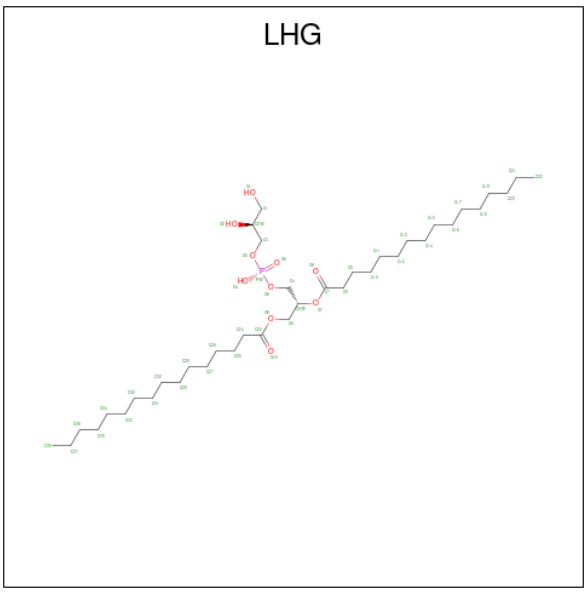
- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C O 28 24 4	0	0
32	C	1	Total C O 48 38 10	0	0
32	C	1	Total C O 48 38 10	0	0
32	D	1	Total C O 51 41 10	0	0
32	D	1	Total C O 33 27 6	0	0
32	M	1	Total C O 51 41 10	0	0
32	b	1	Total C O 55 45 10	0	0
32	c	1	Total C O 37 27 10	0	0
32	c	1	Total C O 48 38 10	0	0
32	c	1	Total C O 49 39 10	0	0
32	d	1	Total C O 23 21 2	0	0
32	d	1	Total C O 44 34 10	0	0
32	m	1	Total C O 51 41 10	0	0

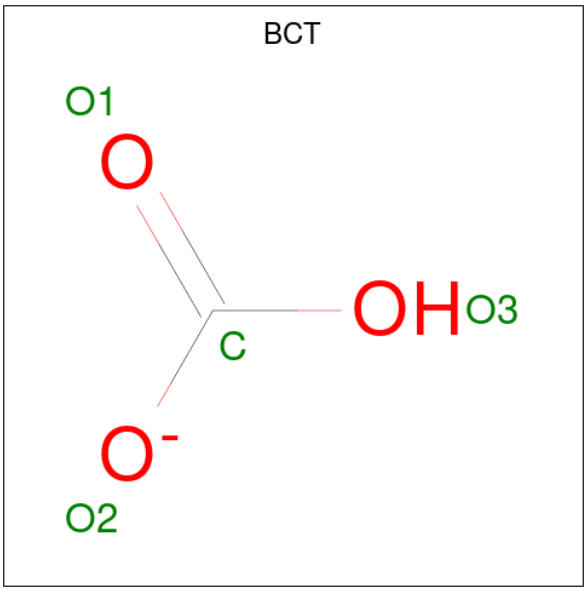
- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: $C_{38}H_{75}O_{10}P$).



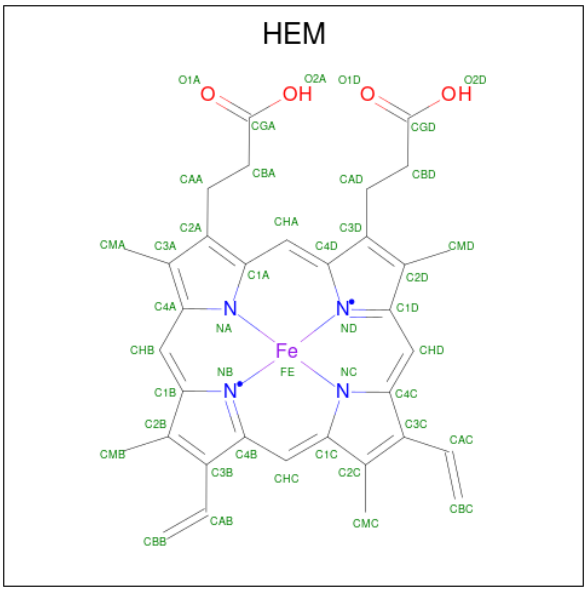
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	E	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			39	28	10	1		
33	e	1	Total	C	O	P	0	0
			42	31	10	1		
33	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



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

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



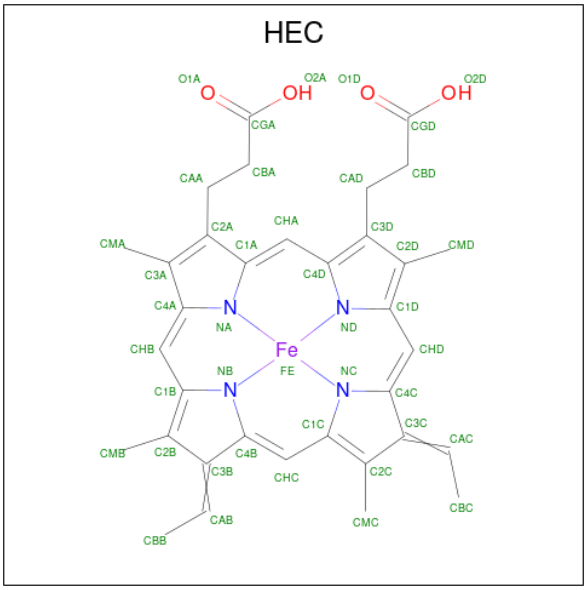
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

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

- Molecule 36 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	130	Total	O	0	4
			138	138		
37	B	191	Total	O	0	0
			191	191		
37	C	159	Total	O	0	0
			159	159		
37	D	119	Total	O	0	0
			119	119		
37	E	28	Total	O	0	0
			28	28		
37	F	9	Total	O	0	0
			9	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	33	Total O 33 33	0	0
37	I	21	Total O 21 21	0	0
37	J	10	Total O 10 10	0	0
37	K	5	Total O 5 5	0	0
37	L	7	Total O 7 7	0	0
37	M	4	Total O 4 4	0	0
37	O	91	Total O 91 91	0	0
37	T	13	Total O 13 13	0	0
37	U	46	Total O 46 46	0	0
37	V	58	Total O 58 58	0	0
37	Y	6	Total O 6 6	0	0
37	X	6	Total O 6 6	0	0
37	Z	8	Total O 8 8	0	0
37	R	7	Total O 7 7	0	0
37	a	117	Total O 125 125	0	4
37	b	184	Total O 184 184	0	0
37	c	166	Total O 166 166	0	0
37	d	105	Total O 105 105	0	0
37	e	26	Total O 26 26	0	0
37	f	7	Total O 7 7	0	0
37	h	23	Total O 23 23	0	0

Continued on next page...

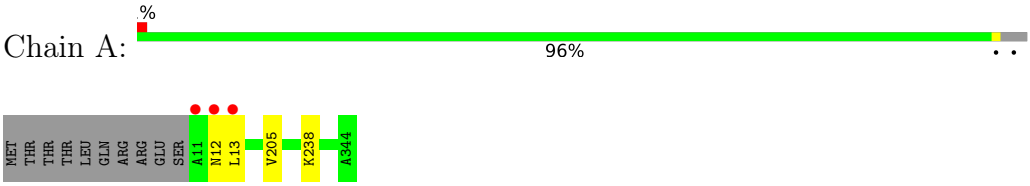
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	i	15	Total O 15 15	0	0
37	j	5	Total O 5 5	0	0
37	k	6	Total O 6 6	0	0
37	l	14	Total O 14 14	0	0
37	m	9	Total O 9 9	0	0
37	o	93	Total O 93 93	0	0
37	t	5	Total O 5 5	0	0
37	u	52	Total O 52 52	0	0
37	v	48	Total O 48 48	0	0
37	y	7	Total O 7 7	0	0
37	x	8	Total O 8 8	0	0
37	z	3	Total O 3 3	0	0
37	r	1	Total O 1 1	0	0

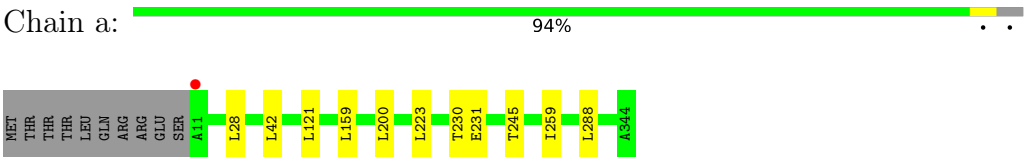
3 Residue-property plots (i)

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

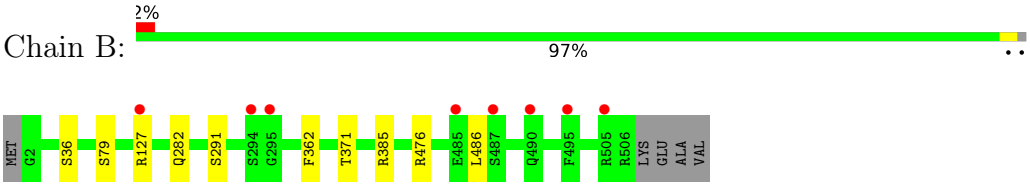
• Molecule 1: Photosystem II protein D1 1



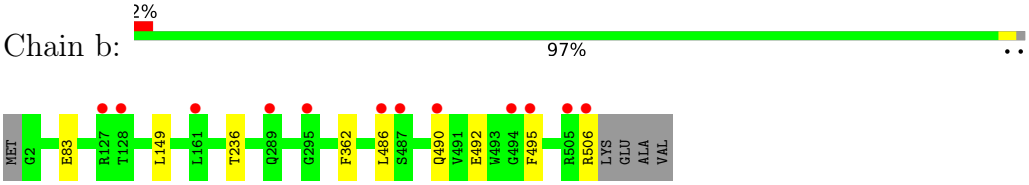
• Molecule 1: Photosystem II protein D1 1



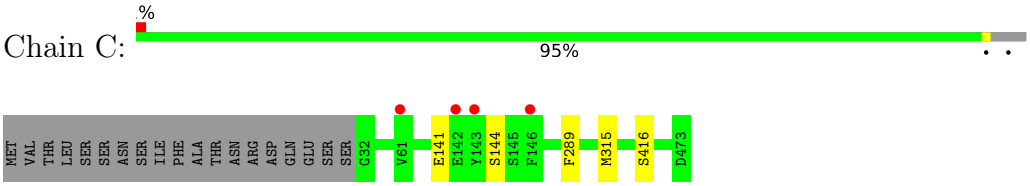
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

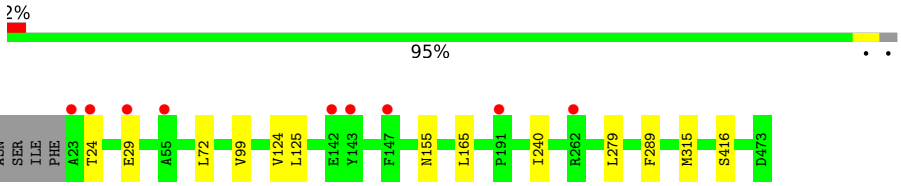


• Molecule 3: Photosystem II CP43 reaction center protein



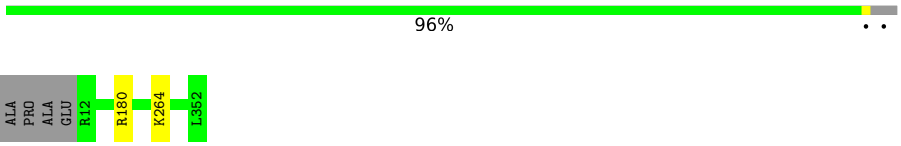
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



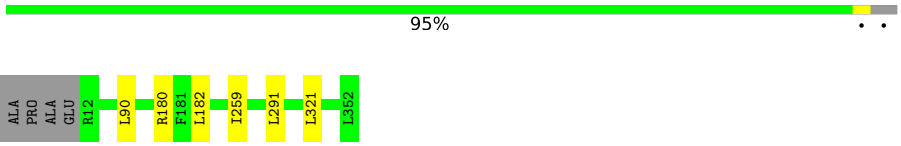
• Molecule 4: Photosystem II D2 protein

Chain D:



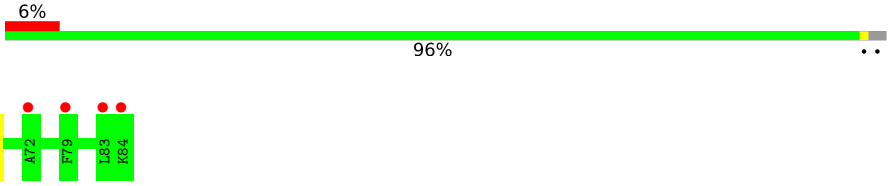
• Molecule 4: Photosystem II D2 protein

Chain d:



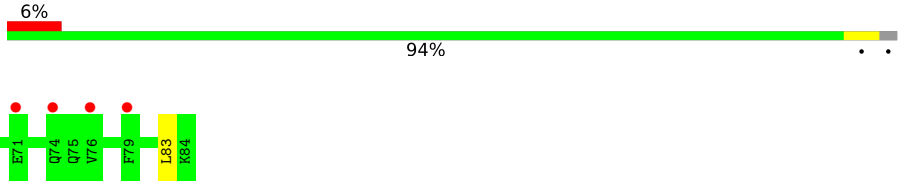
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



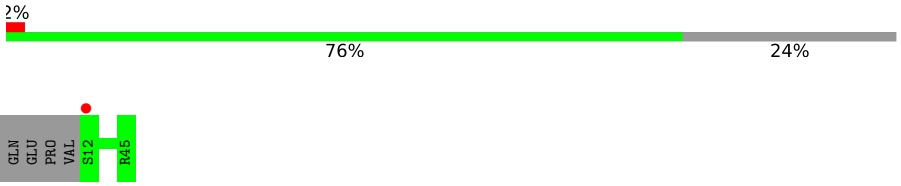
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



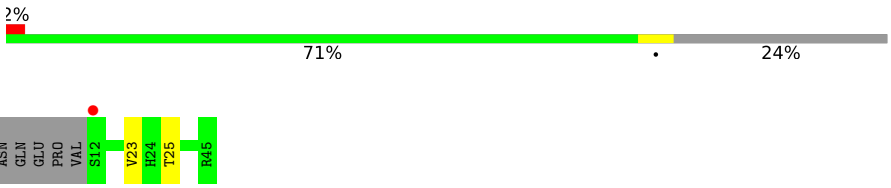
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



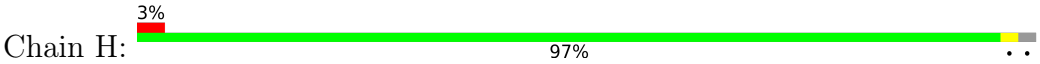
• Molecule 6: Cytochrome b559 subunit beta

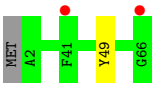
Chain f:



• Molecule 7: Photosystem II reaction center protein H

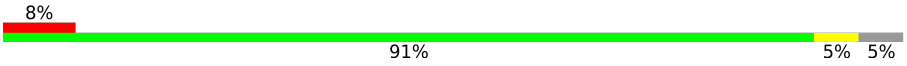
Chain H:

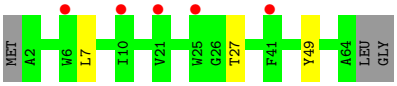




• Molecule 7: Photosystem II reaction center protein H

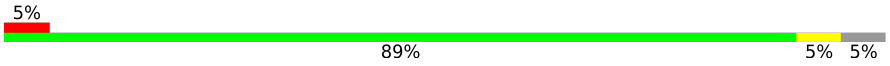
Chain h:

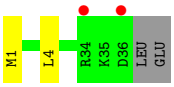




• Molecule 8: Photosystem II reaction center protein I

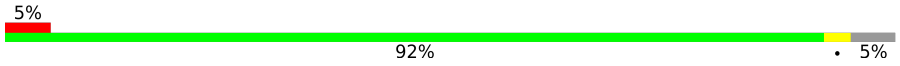
Chain I:

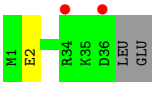




• Molecule 8: Photosystem II reaction center protein I

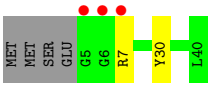
Chain i:





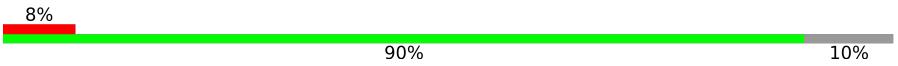
• Molecule 9: Photosystem II reaction center protein J

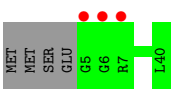
Chain J:



• Molecule 9: Photosystem II reaction center protein J

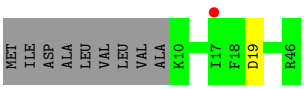
Chain j:





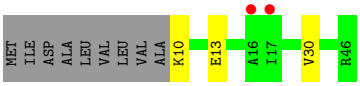
• Molecule 10: Photosystem II reaction center protein K

Chain K:



• Molecule 10: Photosystem II reaction center protein K

Chain k:



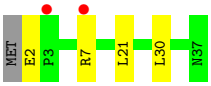
• Molecule 11: Photosystem II reaction center protein L

Chain L:

There are no outlier residues recorded for this chain.

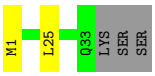
• Molecule 11: Photosystem II reaction center protein L

Chain l:



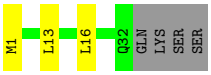
• Molecule 12: Photosystem II reaction center protein M

Chain M:



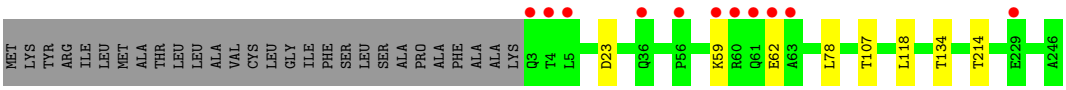
• Molecule 12: Photosystem II reaction center protein M

Chain m:



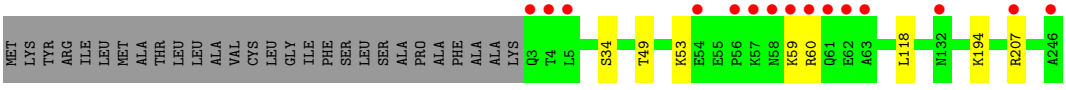
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



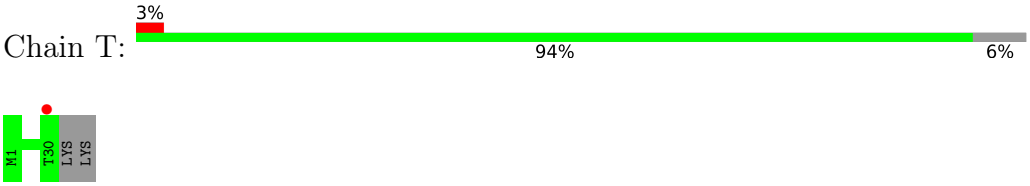
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



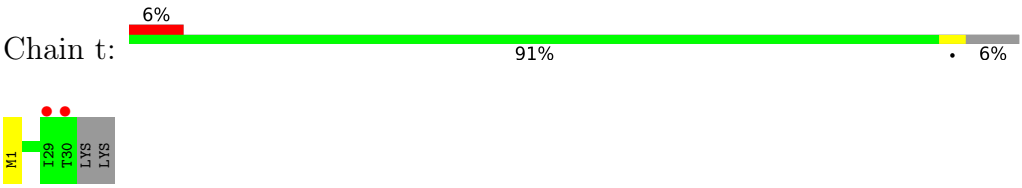
• Molecule 14: Photosystem II reaction center protein T

Chain T:



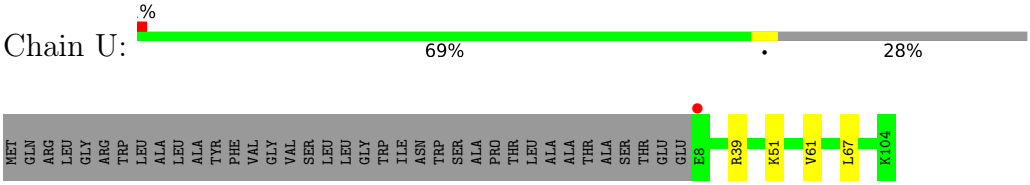
• Molecule 14: Photosystem II reaction center protein T

Chain t:



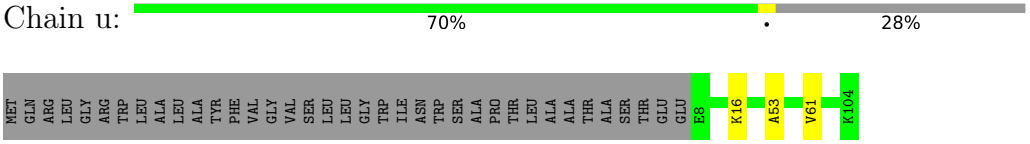
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



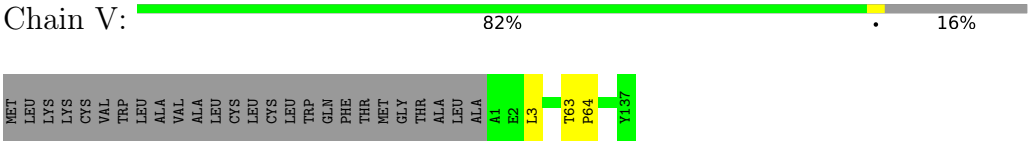
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



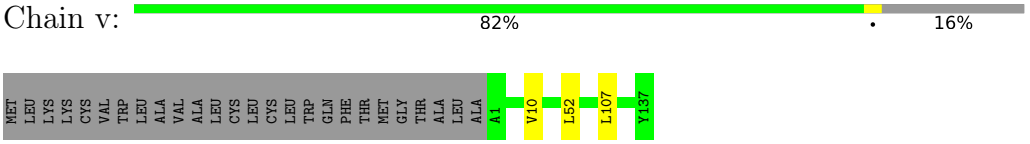
• Molecule 16: Cytochrome c-550

Chain V:



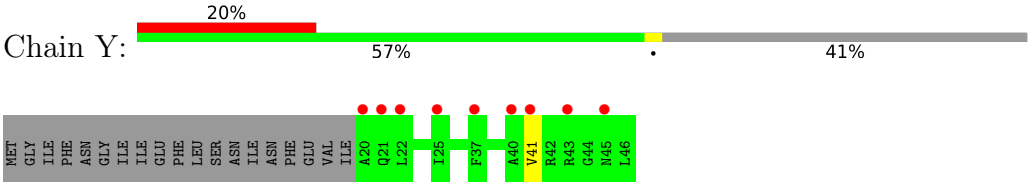
• Molecule 16: Cytochrome c-550

Chain v:



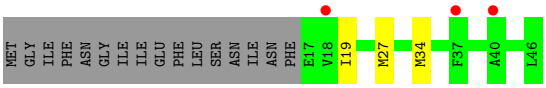
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



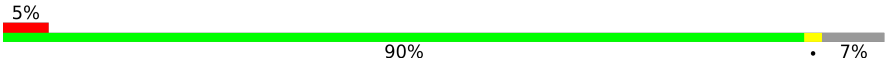
• Molecule 17: Photosystem II reaction center protein Ycf12

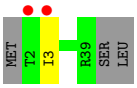
Chain y:



• Molecule 18: Photosystem II reaction center X protein

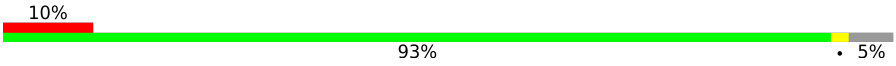
Chain X:

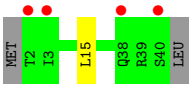




• Molecule 18: Photosystem II reaction center X protein

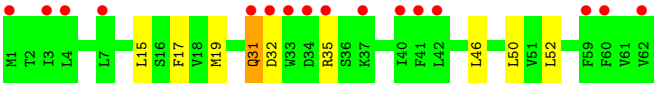
Chain x:





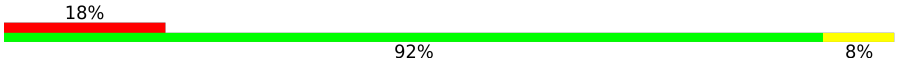
• Molecule 19: Photosystem II reaction center protein Z

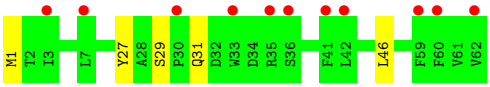
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

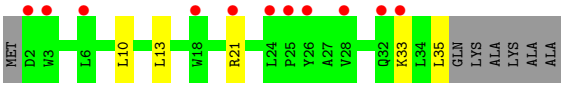
Chain z:





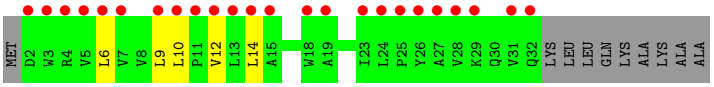
• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.05Å 221.92Å 308.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.58 – 2.09 33.70 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.58-2.09) 86.0 (33.70-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.41 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.233 0.182 , 0.233	Depositor DCC
R_{free} test set	4180 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 68.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	54466	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	0/3717	0.59	0/5060
1	a	0.43	0/3714	0.59	0/5056
2	B	0.42	0/4155	0.58	1/5661 (0.0%)
2	b	0.40	0/4118	0.57	0/5611
3	C	0.41	0/3711	0.57	0/5051
3	c	0.40	0/3791	0.55	0/5158
4	D	0.44	0/2838	0.57	0/3862
4	d	0.43	0/2847	0.58	0/3874
5	E	0.36	0/688	0.52	0/940
5	e	0.33	0/683	0.54	0/932
6	F	0.38	0/284	0.46	0/387
6	f	0.30	0/284	0.54	0/387
7	H	0.40	0/523	0.57	0/713
7	h	0.43	0/511	0.58	0/697
8	I	0.39	0/293	0.56	0/396
8	i	0.41	0/293	0.59	0/396
9	J	0.38	0/263	0.54	0/356
9	j	0.38	0/263	0.57	0/356
10	K	0.34	0/303	0.51	0/416
10	k	0.36	0/303	0.52	0/416
11	L	0.39	0/311	0.59	0/422
11	l	0.38	0/303	0.59	0/412
12	M	0.37	0/249	0.54	0/341
12	m	0.44	0/244	0.54	0/334
13	O	0.39	0/1904	0.62	0/2585
13	o	0.39	0/1905	0.62	0/2583
14	T	0.51	0/257	0.58	0/349
14	t	0.44	0/255	0.55	0/346
15	U	0.37	0/785	0.57	0/1064
15	u	0.39	0/785	0.60	0/1064
16	V	0.38	0/1085	0.58	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.37	0/1085	0.57	0/1473
17	Y	0.30	0/197	0.54	0/264
17	y	0.28	0/219	0.45	0/294
18	X	0.35	0/284	0.54	0/384
18	x	0.31	0/289	0.44	0/391
19	Z	0.32	0/490	0.47	0/669
19	z	0.30	0/488	0.43	0/666
20	R	0.34	0/277	0.59	0/380
20	r	0.30	0/252	0.53	0/347
All	All	0.40	0/45246	0.57	1/61566 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	V	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	486	LEU	C-N-CA	-5.24	108.59	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	V	63	THR	Peptide

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	458/344 (133%)	451 (98%)	7 (2%)	0	100	100
1	a	458/344 (133%)	449 (98%)	8 (2%)	1 (0%)	47	49
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	496 (99%)	7 (1%)	0	100	100
3	C	461/461 (100%)	451 (98%)	9 (2%)	1 (0%)	47	49
3	c	471/461 (102%)	460 (98%)	10 (2%)	1 (0%)	47	49
4	D	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
4	d	342/352 (97%)	334 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	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	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	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	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	230 (95%)	10 (4%)	3 (1%)	13	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	234 (97%)	8 (3%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
15	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	14	9
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	18
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
17	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	4
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100	100
20	r	29/41 (71%)	27 (93%)	2 (7%)	0	100	100
All	All	5534/5700 (97%)	5397 (98%)	128 (2%)	9 (0%)	47	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
16	V	64	PRO
19	Z	31	GLN
13	O	62	GLU
3	c	416	SER
15	u	53	ALA
13	O	134	THR
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	374/280 (134%)	370 (99%)	4 (1%)	73 79
1	a	373/280 (133%)	361 (97%)	12 (3%)	39 41
2	B	407/407 (100%)	398 (98%)	9 (2%)	52 57
2	b	402/407 (99%)	393 (98%)	9 (2%)	52 57
3	C	361/362 (100%)	357 (99%)	4 (1%)	73 79
3	c	370/362 (102%)	358 (97%)	12 (3%)	39 41
4	D	278/283 (98%)	276 (99%)	2 (1%)	84 88
4	d	279/283 (99%)	273 (98%)	6 (2%)	52 57
5	E	72/73 (99%)	70 (97%)	2 (3%)	43 47
5	e	71/73 (97%)	68 (96%)	3 (4%)	30 30
6	F	28/39 (72%)	28 (100%)	0	100 100
6	f	28/39 (72%)	26 (93%)	2 (7%)	14 11
7	H	54/55 (98%)	53 (98%)	1 (2%)	57 63
7	h	53/55 (96%)	50 (94%)	3 (6%)	20 18
8	I	32/34 (94%)	31 (97%)	1 (3%)	40 43
8	i	32/34 (94%)	31 (97%)	1 (3%)	40 43
9	J	24/28 (86%)	22 (92%)	2 (8%)	11 7
9	j	24/28 (86%)	24 (100%)	0	100 100
10	K	30/37 (81%)	29 (97%)	1 (3%)	38 40
10	k	30/37 (81%)	27 (90%)	3 (10%)	7 5
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5 2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35 36
12	m	28/32 (88%)	26 (93%)	2 (7%)	14 11
13	O	206/228 (90%)	201 (98%)	5 (2%)	49 53
13	o	207/228 (91%)	199 (96%)	8 (4%)	32 33
14	T	26/28 (93%)	26 (100%)	0	100 100
14	t	25/28 (89%)	25 (100%)	0	100 100
15	U	84/112 (75%)	80 (95%)	4 (5%)	25 24
15	u	84/112 (75%)	82 (98%)	2 (2%)	49 53
16	V	117/138 (85%)	116 (99%)	1 (1%)	78 84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	v	117/138 (85%)	114 (97%)	3 (3%)	46 50
17	Y	19/37 (51%)	18 (95%)	1 (5%)	22 20
17	y	22/37 (60%)	19 (86%)	3 (14%)	3 2
18	X	31/34 (91%)	30 (97%)	1 (3%)	39 41
18	x	31/34 (91%)	30 (97%)	1 (3%)	39 41
19	Z	52/52 (100%)	43 (83%)	9 (17%)	2 1
19	z	51/52 (98%)	46 (90%)	5 (10%)	8 5
20	R	28/33 (85%)	23 (82%)	5 (18%)	2 1
20	r	25/33 (76%)	20 (80%)	5 (20%)	1 0
All	All	4572/4654 (98%)	4435 (97%)	137 (3%)	40 44

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	205	VAL
1	A	238	LYS
2	B	36	SER
2	B	79	SER
2	B	127	ARG
2	B	282	GLN
2	B	291	SER
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	476	ARG
3	C	141	GLU
3	C	144	SER
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
4	D	264	LYS
5	E	22[A]	ILE
5	E	22[B]	ILE
7	H	49	TYR
8	I	4	LEU
9	J	7	ARG
9	J	30	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	K	19	ASP
12	M	25	LEU
13	O	23	ASP
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
15	U	39	ARG
15	U	51	LYS
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
17	Y	41	VAL
18	X	3	ILE
19	Z	15	LEU
19	Z	17	PHE
19	Z	19	MET
19	Z	31	GLN
19	Z	32	ASP
19	Z	35	ARG
19	Z	46	LEU
19	Z	50	LEU
19	Z	52	LEU
20	R	10	LEU
20	R	13	LEU
20	R	21	ARG
20	R	33	LYS
20	R	35	LEU
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	159[C]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	230	THR
1	a	231	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	149	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	236	THR
2	b	362	PHE
2	b	486	LEU
2	b	490	GLN
2	b	492	GLU
2	b	495	PHE
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	155	ASN
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU
4	d	321	LEU
5	e	4	THR
5	e	61	ARG
5	e	83	LEU
6	f	23	VAL
6	f	25	THR
7	h	7	LEU
7	h	27	THR
7	h	49	TYR
8	i	2	GLU
10	k	10	LYS
10	k	13	GLU
10	k	30	VAL
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	m	16	LEU
13	o	34	SER
13	o	49	THR
13	o	53	LYS
13	o	59	LYS
13	o	60	ARG
13	o	118	LEU
13	o	194	LYS
13	o	207	ARG
15	u	16	LYS
15	u	61	VAL
16	v	10	VAL
16	v	52	LEU
16	v	107	LEU
17	y	19	ILE
17	y	27	MET
17	y	34	MET
18	x	15	LEU
19	z	1	MET
19	z	27	TYR
19	z	29	SER
19	z	31	GLN
19	z	46	LEU
20	r	6	LEU
20	r	9	LEU
20	r	10	LEU
20	r	12	VAL
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
2	B	409	GLN
3	C	311	GLN
11	L	8	GLN
12	M	32	GLN
13	O	82	GLN
13	O	88	ASN
17	Y	21	GLN
18	X	38	GLN
19	Z	31	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	R	22	ASN
1	a	19	ASN
1	a	234	ASN
2	b	179	GLN
2	b	409	GLN
3	c	28	GLN
3	c	311	GLN
5	e	60	GLN
5	e	82	GLN
13	o	61	GLN
15	u	78	ASN
18	x	33	GLN
19	z	31	GLN
20	r	30	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	0.98	0	7,9,11	1.10	1 (14%)
12	FME	M	1	12	8,9,10	1.01	1 (12%)	7,9,11	1.19	1 (14%)
14	FME	T	1	14	8,9,10	1.01	0	7,9,11	0.87	0
14	FME	t	1	14	8,9,10	1.23	1 (12%)	7,9,11	1.10	0
12	FME	m	1	12	8,9,10	1.08	1 (12%)	7,9,11	0.53	0
8	FME	i	1	8	8,9,10	1.03	0	7,9,11	0.89	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	-	0/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.94	1.42	1.46
12	m	1	FME	CA-N	-2.24	1.43	1.46
12	M	1	FME	CA-N	-2.02	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	CA-N-CN	-2.33	119.23	122.82
12	M	1	FME	CA-N-CN	-2.02	119.71	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	t	1	FME	C-CA-CB-CG
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	N-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 - leaving 184 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	$\#\|Z\| > 2$
31	STE	b	619	-	19,19,19	0.63	0	19,19,19	0.99	0
25	CLA	C	506	-	65,73,73	1.62	7 (10%)	76,113,113	1.42	9 (11%)
36	HEC	v	201	16	32,50,50	2.16	3 (9%)	24,82,82	1.82	6 (25%)
27	BCR	t	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.44	10 (17%)
25	CLA	C	504	37	59,67,73	1.61	8 (13%)	68,105,113	1.49	11 (16%)
29	SQD	A	615	-	38,38,54	1.74	5 (13%)	40,40,65	1.31	3 (7%)
25	CLA	b	604	-	65,73,73	1.46	5 (7%)	76,113,113	1.42	11 (14%)
31	STE	c	523	-	11,11,19	0.75	0	11,11,19	1.21	1 (9%)
32	LMG	b	620	-	55,55,55	0.84	2 (3%)	63,63,63	1.36	9 (14%)
25	CLA	B	615	-	60,68,73	1.73	7 (11%)	70,107,113	1.63	11 (15%)
25	CLA	b	615	-	60,68,73	1.55	7 (11%)	70,107,113	1.52	8 (11%)
32	LMG	M	101	-	51,51,55	0.87	3 (5%)	59,59,63	1.40	8 (13%)
27	BCR	k	101	-	41,41,41	0.96	2 (4%)	56,56,56	1.08	3 (5%)
25	CLA	B	607	-	65,73,73	1.75	10 (15%)	76,113,113	1.43	7 (9%)
28	PL9	A	612	-	55,55,55	0.98	1 (1%)	68,69,69	1.56	14 (20%)
25	CLA	B	610	-	65,73,73	1.52	7 (10%)	76,113,113	1.66	12 (15%)
30	DGD	A	616	-	67,67,67	1.08	5 (7%)	81,81,81	1.31	12 (14%)
21	OEY	a	601[B]	37,3,1	0,16,16	-	-	-		
32	LMG	m	101	-	51,51,55	0.98	3 (5%)	59,59,63	1.38	8 (13%)
32	LMG	d	409	-	21,21,55	0.54	0	20,20,63	1.23	3 (15%)
31	STE	b	623	-	9,9,19	0.39	0	8,8,19	0.59	0
25	CLA	B	603	-	65,73,73	1.75	8 (12%)	76,113,113	1.64	10 (13%)
31	STE	d	411	-	16,16,19	0.64	0	16,16,19	1.14	1 (6%)
30	DGD	C	516	-	63,63,67	1.09	5 (7%)	77,77,81	1.36	10 (12%)
30	DGD	h	102	-	63,63,67	1.03	4 (6%)	77,77,81	1.45	13 (16%)
25	CLA	B	612	-	65,73,73	1.55	8 (12%)	76,113,113	1.50	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LHG	e	102	-	41,41,48	0.77	1 (2%)	44,47,54	1.28	5 (11%)
31	STE	x	102	-	19,19,19	0.65	0	19,19,19	0.94	1 (5%)
26	PHO	a	609	-	51,69,69	0.94	2 (3%)	47,99,99	1.28	8 (17%)
32	LMG	d	410	-	44,44,55	0.94	2 (4%)	52,52,63	1.30	6 (11%)
26	PHO	A	608	-	51,69,69	0.99	3 (5%)	47,99,99	1.23	5 (10%)
32	LMG	B	620	-	26,26,55	0.62	0	26,26,63	1.32	1 (3%)
25	CLA	B	601	-	65,73,73	1.58	7 (10%)	76,113,113	1.49	9 (11%)
21	OEY	A	601[C]	37,3,1	0,16,16	-	-	-		
26	PHO	d	401	-	51,69,69	0.98	3 (5%)	47,99,99	1.48	6 (12%)
25	CLA	A	607	37	65,73,73	1.53	6 (9%)	76,113,113	1.55	11 (14%)
33	LHG	B	621	-	48,48,48	0.71	1 (2%)	51,54,54	1.18	3 (5%)
25	CLA	D	402	-	65,73,73	1.53	6 (9%)	76,113,113	1.42	10 (13%)
31	STE	T	102	-	15,15,19	0.40	0	14,14,19	0.71	0
28	PL9	a	612	-	55,55,55	0.70	1 (1%)	68,69,69	1.54	12 (17%)
29	SQD	A	614	-	51,52,54	1.56	8 (15%)	60,63,65	1.93	13 (21%)
25	CLA	a	608	37	65,73,73	1.52	6 (9%)	76,113,113	1.37	9 (11%)
34	BCT	a	606	23	2,3,3	1.34	0	2,3,3	2.91	1 (50%)
25	CLA	b	603	-	65,73,73	1.63	6 (9%)	76,113,113	1.65	11 (14%)
31	STE	t	103	-	9,9,19	0.42	0	8,8,19	0.63	0
33	LHG	D	408	-	46,46,48	0.89	1 (2%)	49,52,54	1.29	6 (12%)
31	STE	B	625	-	11,11,19	0.63	0	11,11,19	1.36	2 (18%)
27	BCR	c	515	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
31	STE	B	623	-	11,11,19	0.82	0	11,11,19	1.08	0
26	PHO	A	609	-	51,69,69	0.95	4 (7%)	47,99,99	1.48	5 (10%)
25	CLA	C	502	-	65,73,73	1.42	6 (9%)	76,113,113	1.31	9 (11%)
25	CLA	B	604	-	65,73,73	1.40	7 (10%)	76,113,113	1.42	9 (11%)
31	STE	J	101	-	11,11,19	0.66	0	11,11,19	1.28	2 (18%)
30	DGD	c	518	-	63,63,67	0.95	2 (3%)	77,77,81	1.30	6 (7%)
25	CLA	c	512	-	65,73,73	1.55	9 (13%)	76,113,113	1.39	9 (11%)
27	BCR	K	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.44	10 (17%)
27	BCR	b	617	-	41,41,41	1.19	3 (7%)	56,56,56	1.19	6 (10%)
31	STE	H	104	-	17,17,19	0.42	0	16,16,19	0.57	0
25	CLA	b	613	-	65,73,73	1.64	7 (10%)	76,113,113	1.40	9 (11%)
25	CLA	c	504	37	60,68,73	1.56	6 (10%)	70,107,113	1.49	10 (14%)
32	LMG	D	406	-	51,51,55	0.90	2 (3%)	59,59,63	1.35	5 (8%)
25	CLA	c	513	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	STE	B	626	-	15,15,19	0.37	0	14,14,19	0.78	0
25	CLA	b	605	-	65,73,73	1.70	10 (15%)	76,113,113	1.61	9 (11%)
32	LMG	c	524	-	49,49,55	0.91	4 (8%)	57,57,63	1.25	3 (5%)
22	OEX	a	602[A]	37,3,1	0,15,15	-	-	-		
27	BCR	b	618	-	41,41,41	1.01	2 (4%)	56,56,56	1.27	6 (10%)
31	STE	C	522	-	15,15,19	0.37	0	14,14,19	0.74	0
25	CLA	b	612	-	65,73,73	1.55	9 (13%)	76,113,113	1.57	12 (15%)
33	LHG	d	408	-	38,38,48	0.76	1 (2%)	41,44,54	1.15	3 (7%)
25	CLA	B	611	-	65,73,73	1.50	7 (10%)	76,113,113	1.55	10 (13%)
32	LMG	D	409	-	31,31,55	0.66	1 (3%)	33,33,63	1.21	2 (6%)
27	BCR	b	616	-	41,41,41	0.95	2 (4%)	56,56,56	1.29	6 (10%)
27	BCR	C	514	-	41,41,41	1.05	3 (7%)	56,56,56	1.19	6 (10%)
27	BCR	D	404	-	41,41,41	1.01	2 (4%)	56,56,56	1.22	7 (12%)
32	LMG	c	520	-	37,37,55	0.96	1 (2%)	45,45,63	1.33	5 (11%)
27	BCR	x	101	-	41,41,41	0.94	1 (2%)	56,56,56	1.20	4 (7%)
25	CLA	B	605	-	65,73,73	1.59	9 (13%)	76,113,113	1.42	9 (11%)
31	STE	D	410	-	19,19,19	0.55	0	19,19,19	1.18	0
25	CLA	b	614	-	65,73,73	1.58	7 (10%)	76,113,113	1.40	7 (9%)
32	LMG	C	515	-	48,48,55	0.92	4 (8%)	56,56,63	1.31	5 (8%)
25	CLA	a	610	-	65,73,73	1.55	9 (13%)	76,113,113	1.31	9 (11%)
25	CLA	A	606	-	65,73,73	1.57	8 (12%)	76,113,113	1.23	9 (11%)
25	CLA	c	503	-	65,73,73	1.51	6 (9%)	76,113,113	1.50	8 (10%)
22	OEX	A	602[A]	37,3,1	0,15,15	-	-	-		
25	CLA	H	101	37	65,73,73	1.71	8 (12%)	76,113,113	1.39	6 (7%)
25	CLA	b	609	37	65,73,73	1.49	7 (10%)	76,113,113	1.47	10 (13%)
31	STE	I	101	-	14,14,19	0.40	0	13,13,19	0.71	0
31	STE	j	101	-	11,11,19	0.77	0	11,11,19	1.19	2 (18%)
33	LHG	D	407	-	48,48,48	0.75	1 (2%)	51,54,54	1.28	9 (17%)
27	BCR	B	617	-	41,41,41	0.99	1 (2%)	56,56,56	1.25	5 (8%)
31	STE	R	101	-	11,11,19	0.73	0	11,11,19	1.14	0
33	LHG	B	622	-	48,48,48	0.82	2 (4%)	51,54,54	1.33	7 (13%)
31	STE	l	103	-	17,17,19	0.29	0	16,16,19	0.93	0
25	CLA	C	510	-	65,73,73	1.54	10 (15%)	76,113,113	1.44	8 (10%)
32	LMG	C	519	-	48,48,55	0.91	2 (4%)	56,56,63	1.34	5 (8%)
31	STE	M	103	-	9,9,19	0.39	0	8,8,19	0.76	0
25	CLA	c	501	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	c	508	-	64,72,73	1.72	9 (14%)	74,111,113	1.51	13 (17%)
27	BCR	A	611	-	41,41,41	0.97	2 (4%)	56,56,56	1.33	8 (14%)
28	PL9	d	405	-	55,55,55	1.04	4 (7%)	68,69,69	1.54	10 (14%)
28	PL9	D	405	-	55,55,55	1.02	3 (5%)	68,69,69	1.63	17 (25%)
33	LHG	d	406	-	48,48,48	0.79	3 (6%)	51,54,54	1.33	7 (13%)
21	OEY	A	601[B]	37,3,1	0,16,16	-	-	-		
27	BCR	H	102	-	41,41,41	0.92	1 (2%)	56,56,56	1.20	4 (7%)
27	BCR	T	101	-	41,41,41	0.91	1 (2%)	56,56,56	1.22	6 (10%)
25	CLA	B	602	-	65,73,73	1.57	7 (10%)	76,113,113	1.52	12 (15%)
25	CLA	c	510	-	65,73,73	1.51	7 (10%)	76,113,113	1.43	9 (11%)
32	LMG	c	522	-	48,48,55	1.00	4 (8%)	56,56,63	1.30	7 (12%)
30	DGD	C	518	-	63,63,67	0.97	3 (4%)	77,77,81	1.42	7 (9%)
31	STE	C	520	-	11,11,19	0.65	0	11,11,19	1.40	2 (18%)
31	STE	B	619	-	16,16,19	0.70	0	16,16,19	1.11	0
25	CLA	C	509	-	65,73,73	1.76	10 (15%)	76,113,113	1.54	11 (14%)
31	STE	T	103	-	14,14,19	0.29	0	13,13,19	0.95	0
31	STE	M	102	-	14,14,19	0.65	0	14,14,19	1.26	1 (7%)
25	CLA	C	513	-	65,73,73	1.49	6 (9%)	76,113,113	1.51	10 (13%)
27	BCR	d	404	-	41,41,41	1.08	3 (7%)	56,56,56	1.18	5 (8%)
25	CLA	B	609	37	65,73,73	1.57	11 (16%)	76,113,113	1.53	14 (18%)
25	CLA	c	507	37	65,73,73	1.55	9 (13%)	76,113,113	1.36	9 (11%)
25	CLA	A	613	37	65,73,73	1.42	5 (7%)	76,113,113	1.40	9 (11%)
25	CLA	b	608	-	65,73,73	1.55	7 (10%)	76,113,113	1.44	10 (13%)
30	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.44	15 (19%)
34	BCT	D	401	23	2,3,3	1.21	0	2,3,3	3.13	1 (50%)
25	CLA	c	509	-	65,73,73	1.45	6 (9%)	76,113,113	1.56	6 (7%)
31	STE	m	102	-	11,11,19	0.72	0	11,11,19	1.39	2 (18%)
31	STE	b	621	-	15,15,19	0.69	0	15,15,19	0.91	0
25	CLA	c	506	-	65,73,73	1.60	8 (12%)	76,113,113	1.41	7 (9%)
29	SQD	L	101	-	48,49,54	1.65	10 (20%)	57,60,65	1.88	10 (17%)
25	CLA	b	602	-	65,73,73	1.52	7 (10%)	76,113,113	1.45	10 (13%)
25	CLA	a	607	-	65,73,73	1.69	8 (12%)	76,113,113	1.41	9 (11%)
31	STE	b	622	-	19,19,19	0.61	0	19,19,19	1.06	1 (5%)
25	CLA	b	611	-	65,73,73	1.60	8 (12%)	76,113,113	1.47	11 (14%)
25	CLA	b	607	-	65,73,73	1.74	8 (12%)	76,113,113	1.54	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	606	37	65,73,73	1.54	6 (9%)	76,113,113	1.54	9 (11%)
25	CLA	C	505	-	65,73,73	1.64	8 (12%)	76,113,113	1.34	5 (6%)
25	CLA	C	511	3	65,73,73	1.56	8 (12%)	76,113,113	1.47	8 (10%)
21	OEY	a	601[C]	37,3,1	0,16,16	-	-	-		
31	STE	c	521	-	19,19,19	0.64	0	19,19,19	0.94	0
30	DGD	a	616	-	43,43,67	0.77	2 (4%)	45,45,81	1.49	8 (17%)
29	SQD	l	101	-	53,54,54	1.57	10 (18%)	62,65,65	1.71	12 (19%)
27	BCR	a	611	-	41,41,41	0.93	2 (4%)	56,56,56	1.15	4 (7%)
29	SQD	f	101	-	40,41,54	1.69	10 (25%)	49,52,65	1.85	12 (24%)
25	CLA	c	505	-	65,73,73	1.49	7 (10%)	76,113,113	1.39	11 (14%)
25	CLA	c	511	3	65,73,73	1.64	6 (9%)	76,113,113	1.50	6 (7%)
31	STE	B	624	-	17,17,19	0.63	0	17,17,19	1.10	0
25	CLA	a	613	37	65,73,73	1.56	8 (12%)	76,113,113	1.45	11 (14%)
35	HEM	F	101	6,5	41,50,50	1.52	3 (7%)	45,82,82	1.34	4 (8%)
25	CLA	C	503	-	65,73,73	1.53	7 (10%)	76,113,113	1.60	11 (14%)
25	CLA	C	501	-	65,73,73	1.57	9 (13%)	76,113,113	1.40	9 (11%)
25	CLA	b	606	37	65,73,73	1.44	7 (10%)	76,113,113	1.45	10 (13%)
30	DGD	H	103	-	63,63,67	1.12	7 (11%)	77,77,81	1.42	11 (14%)
25	CLA	B	613	-	65,73,73	1.67	8 (12%)	76,113,113	1.37	9 (11%)
30	DGD	C	517	-	63,63,67	1.06	6 (9%)	77,77,81	1.46	11 (14%)
31	STE	t	102	-	13,13,19	0.62	0	13,13,19	1.31	2 (15%)
33	LHG	l	102	-	48,48,48	0.53	0	51,54,54	1.23	7 (13%)
25	CLA	h	101	37	65,73,73	1.65	9 (13%)	76,113,113	1.43	10 (13%)
27	BCR	K	103	-	41,41,41	1.05	2 (4%)	56,56,56	1.10	5 (8%)
25	CLA	C	512	-	65,73,73	1.62	9 (13%)	76,113,113	1.40	11 (14%)
33	LHG	E	101	-	48,48,48	0.73	1 (2%)	51,54,54	1.21	6 (11%)
25	CLA	B	608	-	65,73,73	1.54	6 (9%)	76,113,113	1.38	7 (9%)
25	CLA	b	610	-	65,73,73	1.47	6 (9%)	76,113,113	1.48	10 (13%)
27	BCR	c	514	-	41,41,41	1.03	2 (4%)	56,56,56	1.26	7 (12%)
36	HEC	V	201	16	32,50,50	1.97	3 (9%)	24,82,82	2.16	6 (25%)
25	CLA	A	610	-	54,62,73	1.62	5 (9%)	62,99,113	1.54	10 (16%)
27	BCR	c	516	-	41,41,41	1.05	2 (4%)	56,56,56	1.13	3 (5%)
25	CLA	d	403	-	65,73,73	1.64	8 (12%)	76,113,113	1.31	10 (13%)
31	STE	C	521	-	11,11,19	0.72	0	11,11,19	1.17	0
25	CLA	C	508	-	65,73,73	1.53	8 (12%)	76,113,113	1.62	10 (13%)
31	STE	a	617	-	11,11,19	0.76	0	11,11,19	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	DGD	c	517	-	63,63,67	0.87	3 (4%)	77,77,81	1.36	10 (12%)
29	SQD	a	615	-	35,35,54	1.72	6 (17%)	37,37,65	1.41	5 (13%)
25	CLA	d	402	-	65,73,73	1.60	7 (10%)	76,113,113	1.40	8 (10%)
29	SQD	a	614	-	53,54,54	1.54	7 (13%)	62,65,65	1.96	12 (19%)
27	BCR	K	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.18	5 (8%)
25	CLA	B	614	-	65,73,73	1.73	9 (13%)	76,113,113	1.35	7 (9%)
33	LHG	d	407	-	48,48,48	0.63	0	51,54,54	1.17	4 (7%)
25	CLA	c	502	-	65,73,73	1.42	8 (12%)	76,113,113	1.42	8 (10%)
35	HEM	e	101	6,5	41,50,50	1.44	5 (12%)	45,82,82	1.61	10 (22%)
25	CLA	C	507	37	65,73,73	1.50	7 (10%)	76,113,113	1.57	8 (10%)
29	SQD	F	102	-	35,36,54	1.55	7 (20%)	42,45,65	1.80	11 (26%)
25	CLA	b	601	-	65,73,73	1.39	6 (9%)	76,113,113	1.54	11 (14%)
25	CLA	D	403	-	65,73,73	1.58	10 (15%)	76,113,113	1.28	6 (7%)
27	BCR	B	616	-	41,41,41	1.03	3 (7%)	56,56,56	1.20	6 (10%)
27	BCR	B	618	-	41,41,41	1.01	2 (4%)	56,56,56	1.28	4 (7%)

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
31	STE	b	619	-	-	9/17/17/17	-
25	CLA	C	506	-	1/1/15/20	13/37/115/115	-
36	HEC	v	201	16	-	2/10/54/54	-
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
25	CLA	C	504	37	1/1/13/20	8/30/108/115	-
29	SQD	A	615	-	-	17/39/39/69	-
25	CLA	b	604	-	1/1/15/20	11/37/115/115	-
31	STE	c	523	-	-	4/9/9/17	-
32	LMG	b	620	-	-	31/50/70/70	0/1/1/1
25	CLA	B	615	-	1/1/14/20	7/31/109/115	-
25	CLA	b	615	-	1/1/14/20	6/31/109/115	-
32	LMG	M	101	-	-	24/46/66/70	0/1/1/1
27	BCR	k	101	-	-	6/29/63/63	0/2/2/2
25	CLA	B	607	-	1/1/15/20	2/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PL9	A	612	-	-	27/53/73/73	0/1/1/1
25	CLA	B	610	-	1/1/15/20	7/37/115/115	-
30	DGD	A	616	-	-	28/55/95/95	0/2/2/2
32	LMG	m	101	-	-	23/46/66/70	0/1/1/1
32	LMG	d	409	-	-	8/17/17/70	-
31	STE	b	623	-	-	2/7/7/17	-
25	CLA	B	603	-	1/1/15/20	12/37/115/115	-
31	STE	d	411	-	-	11/14/14/17	-
30	DGD	C	516	-	-	18/51/91/95	0/2/2/2
30	DGD	h	102	-	-	14/51/91/95	0/2/2/2
25	CLA	B	612	-	1/1/15/20	16/37/115/115	-
33	LHG	e	102	-	-	25/46/46/53	-
31	STE	x	102	-	-	6/17/17/17	-
26	PHO	a	609	-	-	2/37/103/103	0/5/6/6
32	LMG	d	410	-	-	8/39/59/70	0/1/1/1
26	PHO	A	608	-	-	2/37/103/103	0/5/6/6
32	LMG	B	620	-	-	14/22/22/70	-
25	CLA	B	601	-	1/1/15/20	8/37/115/115	-
26	PHO	d	401	-	-	7/37/103/103	0/5/6/6
25	CLA	A	607	37	-	10/37/115/115	-
33	LHG	B	621	-	-	22/53/53/53	-
25	CLA	D	402	-	1/1/15/20	4/37/115/115	-
31	STE	T	102	-	-	7/13/13/17	-
28	PL9	a	612	-	-	23/53/73/73	0/1/1/1
29	SQD	A	614	-	-	21/47/67/69	0/1/1/1
25	CLA	a	608	37	1/1/15/20	12/37/115/115	-
25	CLA	b	603	-	1/1/15/20	8/37/115/115	-
31	STE	t	103	-	-	4/7/7/17	-
33	LHG	D	408	-	-	23/51/51/53	-
31	STE	B	625	-	-	3/9/9/17	-
27	BCR	c	515	-	-	6/29/63/63	0/2/2/2
31	STE	B	623	-	-	7/9/9/17	-
26	PHO	A	609	-	-	2/37/103/103	0/5/6/6
25	CLA	C	502	-	1/1/15/20	7/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	604	-	1/1/15/20	5/37/115/115	-
31	STE	J	101	-	-	4/9/9/17	-
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
25	CLA	c	512	-	1/1/15/20	21/37/115/115	-
27	BCR	K	101	-	-	11/29/63/63	0/2/2/2
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
31	STE	H	104	-	-	9/15/15/17	-
25	CLA	b	613	-	1/1/15/20	15/37/115/115	-
25	CLA	c	504	37	1/1/14/20	9/31/109/115	-
32	LMG	D	406	-	-	18/46/66/70	0/1/1/1
25	CLA	c	513	-	1/1/15/20	10/37/115/115	-
31	STE	B	626	-	-	4/13/13/17	-
25	CLA	b	605	-	1/1/15/20	7/37/115/115	-
32	LMG	c	524	-	-	27/44/64/70	0/1/1/1
27	BCR	b	618	-	-	7/29/63/63	0/2/2/2
31	STE	C	522	-	-	4/13/13/17	-
25	CLA	b	612	-	1/1/15/20	4/37/115/115	-
33	LHG	d	408	-	-	13/43/43/53	-
25	CLA	B	611	-	1/1/15/20	10/37/115/115	-
32	LMG	D	409	-	-	18/33/33/70	-
27	BCR	b	616	-	-	4/29/63/63	0/2/2/2
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
27	BCR	D	404	-	-	7/29/63/63	0/2/2/2
32	LMG	c	520	-	-	14/31/51/70	0/1/1/1
27	BCR	x	101	-	-	5/29/63/63	0/2/2/2
25	CLA	B	605	-	1/1/15/20	15/37/115/115	-
31	STE	D	410	-	-	9/17/17/17	-
25	CLA	b	614	-	1/1/15/20	7/37/115/115	-
32	LMG	C	515	-	-	23/43/63/70	0/1/1/1
25	CLA	a	610	-	1/1/15/20	12/37/115/115	-
25	CLA	A	606	-	1/1/15/20	3/37/115/115	-
25	CLA	c	503	-	1/1/15/20	9/37/115/115	-
25	CLA	H	101	37	1/1/15/20	17/37/115/115	-
25	CLA	b	609	37	1/1/15/20	3/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	I	101	-	-	3/12/12/17	-
31	STE	j	101	-	-	3/9/9/17	-
33	LHG	D	407	-	-	24/53/53/53	-
27	BCR	B	617	-	-	6/29/63/63	0/2/2/2
31	STE	R	101	-	-	4/9/9/17	-
33	LHG	B	622	-	-	15/53/53/53	-
31	STE	l	103	-	-	8/15/15/17	-
25	CLA	C	510	-	1/1/15/20	10/37/115/115	-
32	LMG	C	519	-	-	22/43/63/70	0/1/1/1
31	STE	M	103	-	-	2/7/7/17	-
25	CLA	c	501	-	1/1/15/20	6/37/115/115	-
25	CLA	c	508	-	-	5/36/114/115	-
27	BCR	A	611	-	-	6/29/63/63	0/2/2/2
28	PL9	d	405	-	-	14/53/73/73	0/1/1/1
28	PL9	D	405	-	-	11/53/73/73	0/1/1/1
33	LHG	d	406	-	-	22/53/53/53	-
27	BCR	H	102	-	-	4/29/63/63	0/2/2/2
27	BCR	T	101	-	-	6/29/63/63	0/2/2/2
25	CLA	B	602	-	1/1/15/20	10/37/115/115	-
25	CLA	c	510	-	1/1/15/20	14/37/115/115	-
32	LMG	c	522	-	-	28/43/63/70	0/1/1/1
30	DGD	C	518	-	-	14/51/91/95	0/2/2/2
31	STE	C	520	-	-	1/9/9/17	-
31	STE	B	619	-	-	7/14/14/17	-
25	CLA	C	509	-	1/1/15/20	12/37/115/115	-
31	STE	T	103	-	-	11/12/12/17	-
31	STE	M	102	-	-	8/12/12/17	-
25	CLA	C	513	-	1/1/15/20	14/37/115/115	-
27	BCR	d	404	-	-	10/29/63/63	0/2/2/2
25	CLA	B	609	37	1/1/15/20	6/37/115/115	-
25	CLA	c	507	37	1/1/15/20	9/37/115/115	-
25	CLA	A	613	37	1/1/15/20	12/37/115/115	-
25	CLA	b	608	-	1/1/15/20	7/37/115/115	-
30	DGD	c	519	-	-	18/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	509	-	1/1/15/20	10/37/115/115	-
31	STE	m	102	-	-	4/9/9/17	-
31	STE	b	621	-	-	6/13/13/17	-
25	CLA	c	506	-	1/1/15/20	15/37/115/115	-
29	SQD	L	101	-	-	19/44/64/69	0/1/1/1
25	CLA	b	602	-	1/1/15/20	11/37/115/115	-
25	CLA	a	607	-	1/1/15/20	4/37/115/115	-
31	STE	b	622	-	-	9/17/17/17	-
25	CLA	b	611	-	1/1/15/20	10/37/115/115	-
25	CLA	b	607	-	1/1/15/20	3/37/115/115	-
25	CLA	B	606	37	1/1/15/20	12/37/115/115	-
25	CLA	C	505	-	1/1/15/20	15/37/115/115	-
25	CLA	C	511	3	1/1/15/20	8/37/115/115	-
31	STE	c	521	-	-	11/17/17/17	-
30	DGD	a	616	-	-	26/45/45/95	-
29	SQD	l	101	-	-	28/49/69/69	0/1/1/1
27	BCR	a	611	-	-	1/29/63/63	0/2/2/2
29	SQD	f	101	-	-	22/36/56/69	0/1/1/1
25	CLA	c	505	-	1/1/15/20	10/37/115/115	-
25	CLA	c	511	3	1/1/15/20	4/37/115/115	-
31	STE	B	624	-	-	8/15/15/17	-
25	CLA	a	613	37	1/1/15/20	3/37/115/115	-
35	HEM	F	101	6,5	-	2/12/54/54	-
25	CLA	C	503	-	1/1/15/20	7/37/115/115	-
25	CLA	C	501	-	1/1/15/20	6/37/115/115	-
25	CLA	b	606	37	1/1/15/20	14/37/115/115	-
30	DGD	H	103	-	-	16/51/91/95	0/2/2/2
25	CLA	B	613	-	1/1/15/20	16/37/115/115	-
30	DGD	C	517	-	-	24/51/91/95	0/2/2/2
31	STE	t	102	-	-	3/11/11/17	-
33	LHG	l	102	-	-	17/53/53/53	-
25	CLA	h	101	37	1/1/15/20	17/37/115/115	-
27	BCR	K	103	-	-	7/29/63/63	0/2/2/2
25	CLA	C	512	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	E	101	-	-	32/53/53/53	-
25	CLA	B	608	-	-	4/37/115/115	-
25	CLA	b	610	-	1/1/15/20	8/37/115/115	-
27	BCR	c	514	-	-	8/29/63/63	0/2/2/2
36	HEC	V	201	16	-	2/10/54/54	-
25	CLA	A	610	-	1/1/12/20	2/24/102/115	-
27	BCR	c	516	-	-	7/29/63/63	0/2/2/2
25	CLA	d	403	-	1/1/15/20	2/37/115/115	-
31	STE	C	521	-	-	5/9/9/17	-
25	CLA	C	508	-	-	10/37/115/115	-
31	STE	a	617	-	-	4/9/9/17	-
30	DGD	c	517	-	-	26/51/91/95	0/2/2/2
29	SQD	a	615	-	-	19/37/37/69	-
25	CLA	d	402	-	1/1/15/20	2/37/115/115	-
29	SQD	a	614	-	-	26/49/69/69	0/1/1/1
27	BCR	K	102	-	-	7/29/63/63	0/2/2/2
25	CLA	B	614	-	1/1/15/20	10/37/115/115	-
33	LHG	d	407	-	-	20/53/53/53	-
25	CLA	c	502	-	-	6/37/115/115	-
35	HEM	e	101	6,5	-	0/12/54/54	-
25	CLA	C	507	37	1/1/15/20	7/37/115/115	-
29	SQD	F	102	-	-	10/28/48/69	0/1/1/1
25	CLA	b	601	-	1/1/15/20	12/37/115/115	-
25	CLA	D	403	-	-	12/37/115/115	-
27	BCR	B	616	-	-	8/29/63/63	0/2/2/2
27	BCR	B	618	-	-	5/29/63/63	0/2/2/2

All (743) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	613	CLA	C4B-NB	8.79	1.43	1.35
25	b	603	CLA	C4B-NB	8.56	1.42	1.35
25	B	614	CLA	C4B-NB	8.32	1.42	1.35
25	B	607	CLA	C4B-NB	8.09	1.42	1.35
25	c	508	CLA	C4B-NB	8.09	1.42	1.35
25	H	101	CLA	C4B-NB	8.06	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	CLA	C4B-NB	8.03	1.42	1.35
25	C	505	CLA	C4B-NB	7.98	1.42	1.35
25	B	601	CLA	C4B-NB	7.81	1.42	1.35
25	B	612	CLA	C4B-NB	7.72	1.42	1.35
25	b	605	CLA	MG-NA	7.63	2.24	2.06
25	B	608	CLA	C4B-NB	7.62	1.42	1.35
25	A	610	CLA	C4B-NB	7.61	1.42	1.35
25	A	607	CLA	C4B-NB	7.60	1.42	1.35
25	c	513	CLA	C4B-NB	7.59	1.42	1.35
25	c	511	CLA	C4B-NB	7.56	1.42	1.35
25	h	101	CLA	C4B-NB	7.56	1.42	1.35
25	c	512	CLA	C4B-NB	7.54	1.41	1.35
25	C	510	CLA	C4B-NB	7.53	1.41	1.35
25	d	402	CLA	C4B-NB	7.52	1.41	1.35
25	b	614	CLA	C4B-NB	7.50	1.41	1.35
25	b	607	CLA	MG-NA	7.49	2.24	2.06
25	B	613	CLA	C4B-NB	7.48	1.41	1.35
25	B	609	CLA	C4B-NB	7.46	1.41	1.35
25	b	604	CLA	C4B-NB	7.45	1.41	1.35
25	c	506	CLA	C4B-NB	7.45	1.41	1.35
25	A	606	CLA	C4B-NB	7.45	1.41	1.35
25	b	608	CLA	C4B-NB	7.44	1.41	1.35
25	c	505	CLA	C4B-NB	7.44	1.41	1.35
25	B	615	CLA	MG-NA	7.43	2.23	2.06
25	c	504	CLA	C4B-NB	7.43	1.41	1.35
25	a	610	CLA	C4B-NB	7.38	1.41	1.35
25	C	512	CLA	C4B-NB	7.30	1.41	1.35
25	B	602	CLA	C4B-NB	7.25	1.41	1.35
25	a	608	CLA	C4B-NB	7.22	1.41	1.35
25	C	507	CLA	C4B-NB	7.20	1.41	1.35
25	B	611	CLA	C4B-NB	7.15	1.41	1.35
25	a	607	CLA	C4B-NB	7.13	1.41	1.35
25	C	513	CLA	C4B-NB	7.12	1.41	1.35
25	C	504	CLA	C4B-NB	7.10	1.41	1.35
25	c	510	CLA	C4B-NB	7.09	1.41	1.35
25	c	501	CLA	C4B-NB	7.04	1.41	1.35
25	B	603	CLA	MG-NA	7.01	2.22	2.06
25	a	613	CLA	C4B-NB	7.01	1.41	1.35
25	B	605	CLA	C4B-NB	6.96	1.41	1.35
25	b	602	CLA	C4B-NB	6.96	1.41	1.35
25	c	503	CLA	C4B-NB	6.91	1.41	1.35
25	C	508	CLA	C4B-NB	6.90	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	C4B-NB	6.87	1.41	1.35
25	C	501	CLA	C4B-NB	6.85	1.41	1.35
25	b	609	CLA	C4B-NB	6.81	1.41	1.35
25	b	606	CLA	C4B-NB	6.77	1.41	1.35
36	v	201	HEC	C2B-C3B	-6.76	1.33	1.40
25	B	603	CLA	C4B-NB	6.69	1.41	1.35
25	C	509	CLA	C4B-NB	6.69	1.41	1.35
25	c	507	CLA	C4B-NB	6.68	1.41	1.35
25	b	615	CLA	C4B-NB	6.66	1.41	1.35
25	B	610	CLA	C4B-NB	6.65	1.41	1.35
25	c	509	CLA	C4B-NB	6.62	1.41	1.35
25	C	503	CLA	C4B-NB	6.62	1.41	1.35
25	C	511	CLA	C4B-NB	6.61	1.41	1.35
25	b	607	CLA	C4B-NB	6.60	1.41	1.35
25	D	403	CLA	C4B-NB	6.60	1.41	1.35
25	B	606	CLA	C4B-NB	6.58	1.41	1.35
25	b	612	CLA	C4B-NB	6.55	1.41	1.35
25	C	509	CLA	MG-NA	6.48	2.21	2.06
25	A	613	CLA	C4B-NB	6.43	1.40	1.35
25	C	502	CLA	C4B-NB	6.36	1.40	1.35
25	b	605	CLA	C4B-NB	6.36	1.40	1.35
25	B	615	CLA	C4B-NB	6.34	1.40	1.35
25	b	611	CLA	C4B-NB	6.21	1.40	1.35
36	V	201	HEC	C2B-C3B	-6.16	1.34	1.40
25	H	101	CLA	MG-NA	6.14	2.20	2.06
25	b	610	CLA	C4B-NB	6.00	1.40	1.35
25	c	502	CLA	C4B-NB	5.97	1.40	1.35
25	B	604	CLA	C4B-NB	5.94	1.40	1.35
25	D	402	CLA	C4B-NB	5.89	1.40	1.35
25	B	605	CLA	MG-NA	5.77	2.20	2.06
25	b	611	CLA	MG-ND	-5.76	1.94	2.05
25	b	601	CLA	C4B-NB	5.76	1.40	1.35
25	c	511	CLA	MG-NA	5.73	2.19	2.06
25	B	607	CLA	MG-NA	5.51	2.19	2.06
25	a	607	CLA	MG-NC	5.49	2.19	2.06
36	v	201	HEC	C3C-C2C	-5.47	1.35	1.40
25	D	402	CLA	MG-NA	5.39	2.19	2.06
25	h	101	CLA	MG-NA	5.37	2.19	2.06
25	B	613	CLA	MG-ND	-5.24	1.95	2.05
25	b	610	CLA	MG-NA	5.23	2.18	2.06
25	b	612	CLA	MG-NA	5.20	2.18	2.06
29	A	615	SQD	O47-C45	-5.19	1.38	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	614	CLA	MG-NA	5.14	2.18	2.06
36	v	201	HEC	C3D-C2D	5.10	1.52	1.37
36	V	201	HEC	C3D-C2D	5.08	1.52	1.37
29	L	101	SQD	O48-C23	5.05	1.48	1.33
35	F	101	HEM	C3C-C2C	-4.99	1.33	1.40
29	a	614	SQD	O48-C23	4.89	1.47	1.33
29	a	615	SQD	O48-C23	4.87	1.47	1.33
25	B	602	CLA	MG-NA	4.84	2.17	2.06
29	F	102	SQD	O48-C23	4.84	1.47	1.33
36	V	201	HEC	C3C-C2C	-4.83	1.35	1.40
25	B	603	CLA	C1D-ND	4.80	1.43	1.37
25	B	606	CLA	MG-NA	4.78	2.17	2.06
29	A	615	SQD	O48-C23	4.75	1.47	1.33
25	C	511	CLA	MG-NA	4.73	2.17	2.06
29	f	101	SQD	O48-C23	4.71	1.47	1.33
25	C	506	CLA	MG-ND	-4.64	1.96	2.05
29	A	614	SQD	O48-C23	4.57	1.46	1.33
25	a	610	CLA	MG-ND	-4.56	1.96	2.05
29	l	101	SQD	O48-C23	4.54	1.46	1.33
25	b	603	CLA	MG-NA	4.51	2.17	2.06
25	d	402	CLA	MG-NA	4.48	2.16	2.06
25	C	505	CLA	MG-NA	4.46	2.16	2.06
25	B	609	CLA	C1D-ND	4.45	1.43	1.37
28	A	612	PL9	C7-C3	-4.43	1.46	1.51
25	c	506	CLA	C1D-ND	4.41	1.43	1.37
25	a	607	CLA	C1D-ND	4.41	1.43	1.37
25	C	503	CLA	MG-NA	4.40	2.16	2.06
25	b	602	CLA	MG-NA	4.38	2.16	2.06
25	C	504	CLA	MG-NA	4.38	2.16	2.06
25	C	501	CLA	MG-NA	4.30	2.16	2.06
25	b	609	CLA	C1D-ND	4.29	1.43	1.37
25	D	403	CLA	C1D-ND	4.29	1.43	1.37
25	B	610	CLA	MG-NA	4.28	2.16	2.06
25	B	608	CLA	C1D-ND	4.26	1.43	1.37
25	b	601	CLA	C1D-ND	4.24	1.43	1.37
25	b	611	CLA	C1D-ND	4.23	1.43	1.37
25	a	608	CLA	C4D-ND	-4.23	1.31	1.37
25	B	607	CLA	C1D-ND	4.20	1.43	1.37
25	C	506	CLA	MG-NA	4.19	2.16	2.06
25	a	608	CLA	C1D-ND	4.17	1.42	1.37
25	c	508	CLA	MG-ND	4.16	2.14	2.05
27	b	617	BCR	C30-C25	-4.15	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	613	CLA	MG-NA	4.14	2.16	2.06
25	b	613	CLA	C1D-ND	4.12	1.42	1.37
25	a	613	CLA	MG-NA	4.11	2.16	2.06
25	C	508	CLA	MG-NA	4.10	2.16	2.06
25	B	606	CLA	C1D-ND	4.09	1.42	1.37
25	c	503	CLA	MG-NA	4.07	2.15	2.06
25	B	615	CLA	C1D-ND	4.07	1.42	1.37
25	d	403	CLA	C1D-ND	4.04	1.42	1.37
25	C	512	CLA	MG-ND	-4.03	1.97	2.05
25	d	402	CLA	C1D-ND	4.02	1.42	1.37
25	C	506	CLA	C1D-ND	4.00	1.42	1.37
25	C	509	CLA	C1D-ND	3.95	1.42	1.37
25	b	614	CLA	MG-NC	3.95	2.15	2.06
25	c	507	CLA	C1D-ND	3.94	1.42	1.37
25	c	509	CLA	C1D-ND	3.93	1.42	1.37
25	D	402	CLA	C1D-ND	3.93	1.42	1.37
25	b	615	CLA	C1D-ND	3.92	1.42	1.37
25	A	606	CLA	C1D-ND	3.91	1.42	1.37
25	D	403	CLA	MG-ND	-3.91	1.98	2.05
25	B	604	CLA	C4D-ND	-3.90	1.32	1.37
25	C	509	CLA	MG-ND	3.89	2.13	2.05
25	c	505	CLA	C4D-ND	-3.87	1.32	1.37
25	C	513	CLA	C1D-ND	3.86	1.42	1.37
29	a	615	SQD	O47-C7	3.85	1.45	1.34
25	b	614	CLA	C1D-ND	3.84	1.42	1.37
25	C	501	CLA	C1D-ND	3.84	1.42	1.37
25	b	610	CLA	C1D-ND	3.83	1.42	1.37
25	C	505	CLA	C1D-ND	3.82	1.42	1.37
25	H	101	CLA	C1D-ND	3.80	1.42	1.37
25	b	612	CLA	C1D-ND	3.79	1.42	1.37
27	c	515	BCR	C1-C6	-3.79	1.48	1.53
25	b	603	CLA	C1D-ND	3.77	1.42	1.37
25	c	508	CLA	C4D-ND	-3.75	1.32	1.37
25	c	503	CLA	C1D-ND	3.75	1.42	1.37
33	D	408	LHG	P-O6	3.74	1.74	1.59
25	B	604	CLA	C1D-ND	3.73	1.42	1.37
25	c	508	CLA	C1D-ND	3.72	1.42	1.37
25	c	512	CLA	C1D-ND	3.72	1.42	1.37
25	C	511	CLA	C1D-ND	3.71	1.42	1.37
29	f	101	SQD	O47-C7	3.71	1.44	1.34
25	A	613	CLA	C1D-ND	3.71	1.42	1.37
28	D	405	PL9	C3-C4	-3.70	1.43	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	607	CLA	MG-NC	-3.70	1.97	2.06
25	B	612	CLA	C1D-ND	3.69	1.42	1.37
25	A	607	CLA	C1D-ND	3.69	1.42	1.37
25	b	606	CLA	MG-NC	3.69	2.15	2.06
25	D	403	CLA	MG-NA	3.68	2.15	2.06
29	A	615	SQD	O47-C7	3.68	1.44	1.34
25	c	501	CLA	C1D-ND	3.67	1.42	1.37
29	l	101	SQD	O47-C7	3.65	1.44	1.34
25	c	510	CLA	C1D-ND	3.65	1.42	1.37
25	d	403	CLA	MG-ND	-3.65	1.98	2.05
35	e	101	HEM	C3C-C2C	-3.65	1.35	1.40
27	C	514	BCR	C1-C6	-3.64	1.48	1.53
25	a	613	CLA	C1D-ND	3.63	1.42	1.37
35	e	101	HEM	C3C-CAC	3.63	1.55	1.47
25	C	510	CLA	CHC-C1C	3.63	1.44	1.35
27	b	617	BCR	C1-C6	-3.61	1.48	1.53
25	B	601	CLA	C1D-ND	3.61	1.42	1.37
25	c	511	CLA	C1D-ND	3.61	1.42	1.37
25	B	614	CLA	CHC-C1C	3.60	1.44	1.35
25	c	502	CLA	C4D-ND	-3.58	1.32	1.37
25	C	512	CLA	MG-NA	3.57	2.14	2.06
30	C	516	DGD	C4E-C3E	3.57	1.61	1.52
25	c	504	CLA	C4D-ND	-3.57	1.32	1.37
29	F	102	SQD	C24-C23	3.56	1.61	1.50
25	c	508	CLA	CHC-C1C	3.56	1.44	1.35
25	c	507	CLA	MG-NA	3.56	2.14	2.06
25	b	604	CLA	C4D-ND	-3.56	1.32	1.37
25	B	610	CLA	C1D-ND	3.56	1.42	1.37
25	B	605	CLA	CHC-C1C	3.56	1.44	1.35
25	C	505	CLA	CHC-C1C	3.55	1.44	1.35
25	b	608	CLA	C1D-ND	3.55	1.42	1.37
25	C	507	CLA	MG-NA	3.54	2.14	2.06
25	B	603	CLA	C4D-ND	-3.54	1.32	1.37
25	B	601	CLA	CHC-C1C	3.54	1.44	1.35
25	b	605	CLA	C1D-ND	3.54	1.42	1.37
29	L	101	SQD	O47-C7	3.53	1.44	1.34
25	c	509	CLA	C4D-ND	-3.53	1.32	1.37
25	A	607	CLA	C4D-ND	-3.53	1.32	1.37
25	C	507	CLA	C1D-ND	3.52	1.42	1.37
25	B	611	CLA	C1D-ND	3.52	1.42	1.37
25	c	507	CLA	C4D-ND	-3.51	1.32	1.37
25	B	611	CLA	CHC-C1C	3.51	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	610	CLA	C1D-ND	3.50	1.42	1.37
28	d	405	PL9	C6-C1	-3.50	1.42	1.48
25	a	613	CLA	CHC-C1C	3.50	1.43	1.35
25	B	614	CLA	C1D-ND	3.48	1.42	1.37
25	b	607	CLA	CHC-C1C	3.48	1.43	1.35
25	c	511	CLA	CHC-C1C	3.48	1.43	1.35
29	a	615	SQD	C24-C23	3.48	1.60	1.50
25	D	402	CLA	C4D-ND	-3.47	1.32	1.37
25	h	101	CLA	CHC-C1C	3.47	1.43	1.35
25	C	512	CLA	C1D-ND	3.47	1.42	1.37
25	b	614	CLA	CHC-C1C	3.46	1.43	1.35
25	C	508	CLA	C1D-ND	3.46	1.42	1.37
25	C	510	CLA	C1D-ND	3.46	1.42	1.37
27	K	102	BCR	C1-C6	-3.45	1.49	1.53
35	F	101	HEM	C3C-CAC	3.45	1.54	1.47
29	a	614	SQD	O47-C7	3.44	1.44	1.34
25	B	613	CLA	C4D-ND	-3.42	1.33	1.37
25	b	608	CLA	C4D-ND	-3.42	1.33	1.37
25	A	606	CLA	C4D-ND	-3.41	1.33	1.37
25	C	501	CLA	CHC-C1C	3.40	1.43	1.35
25	b	615	CLA	C4D-ND	-3.39	1.33	1.37
29	a	614	SQD	O47-C45	-3.39	1.38	1.46
25	A	606	CLA	MG-ND	-3.38	1.99	2.05
25	C	502	CLA	C4D-ND	-3.37	1.33	1.37
25	B	602	CLA	CHC-C1C	3.36	1.43	1.35
25	B	610	CLA	CHC-C1C	3.35	1.43	1.35
25	C	502	CLA	C1D-ND	3.35	1.41	1.37
25	b	609	CLA	MG-NC	3.35	2.14	2.06
25	C	503	CLA	C1D-ND	3.34	1.41	1.37
32	c	522	LMG	C3-C2	3.34	1.60	1.52
25	b	603	CLA	C4D-ND	-3.34	1.33	1.37
25	b	611	CLA	CHC-C1C	3.33	1.43	1.35
25	c	503	CLA	CHC-C1C	3.32	1.43	1.35
25	D	402	CLA	CHC-C1C	3.32	1.43	1.35
29	L	101	SQD	O5-C1	3.30	1.50	1.41
25	c	513	CLA	C4D-ND	-3.30	1.33	1.37
25	c	513	CLA	C1D-ND	3.29	1.41	1.37
25	a	607	CLA	C4D-ND	-3.29	1.33	1.37
25	b	602	CLA	C1D-ND	3.29	1.41	1.37
25	B	608	CLA	C4D-ND	-3.29	1.33	1.37
25	h	101	CLA	C1D-ND	3.29	1.41	1.37
25	A	613	CLA	CHC-C1C	3.28	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	m	101	LMG	C4-C3	3.28	1.60	1.52
25	c	502	CLA	C1D-ND	3.28	1.41	1.37
25	A	613	CLA	C4D-ND	-3.27	1.33	1.37
25	c	510	CLA	MG-NA	3.27	2.14	2.06
25	B	613	CLA	C1D-ND	3.27	1.41	1.37
25	c	513	CLA	CHC-C1C	3.27	1.43	1.35
25	C	505	CLA	C4D-ND	-3.24	1.33	1.37
25	A	610	CLA	C4D-ND	-3.24	1.33	1.37
25	B	612	CLA	C4D-ND	-3.24	1.33	1.37
25	A	607	CLA	CHC-C1C	3.24	1.43	1.35
27	B	617	BCR	C30-C25	-3.24	1.49	1.53
25	b	611	CLA	C4D-ND	-3.23	1.33	1.37
29	l	101	SQD	O47-C45	-3.23	1.38	1.46
25	H	101	CLA	CHC-C1C	3.22	1.43	1.35
25	C	504	CLA	CHC-C1C	3.22	1.43	1.35
25	d	403	CLA	CHC-C1C	3.22	1.43	1.35
25	b	602	CLA	C4D-ND	-3.22	1.33	1.37
25	B	606	CLA	C4D-ND	-3.22	1.33	1.37
25	C	503	CLA	C4D-ND	-3.22	1.33	1.37
25	C	512	CLA	CHC-C1C	3.22	1.43	1.35
25	c	501	CLA	CHC-C1C	3.22	1.43	1.35
25	c	506	CLA	C4D-ND	-3.21	1.33	1.37
25	a	608	CLA	CHC-C1C	3.21	1.43	1.35
25	A	610	CLA	C1D-ND	3.21	1.41	1.37
25	b	603	CLA	CHC-C1C	3.20	1.43	1.35
25	c	505	CLA	CHC-C1C	3.20	1.43	1.35
25	c	510	CLA	CHC-C1C	3.20	1.43	1.35
30	C	518	DGD	O1G-C1G	-3.20	1.37	1.45
25	C	507	CLA	CHC-C1C	3.20	1.43	1.35
25	c	509	CLA	CHC-C1C	3.20	1.43	1.35
33	B	622	LHG	O7-C5	-3.20	1.38	1.46
25	B	603	CLA	CHC-C1C	3.20	1.43	1.35
29	A	614	SQD	C24-C23	3.20	1.60	1.50
25	c	503	CLA	C4D-ND	-3.19	1.33	1.37
25	B	608	CLA	MG-NA	3.19	2.13	2.06
25	B	609	CLA	CHC-C1C	3.18	1.43	1.35
25	a	607	CLA	MG-ND	-3.18	1.99	2.05
29	A	614	SQD	O47-C45	-3.18	1.38	1.46
25	C	513	CLA	C4D-ND	-3.18	1.33	1.37
25	b	613	CLA	CHC-C1C	3.17	1.43	1.35
25	c	512	CLA	CHC-C1C	3.17	1.43	1.35
27	K	103	BCR	C1-C6	-3.17	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	511	CLA	CHC-C1C	3.17	1.43	1.35
25	b	607	CLA	C1D-ND	3.16	1.41	1.37
25	C	506	CLA	CHC-C1C	3.16	1.43	1.35
29	f	101	SQD	C24-C23	3.16	1.59	1.50
25	C	508	CLA	CHC-C1C	3.15	1.43	1.35
27	t	101	BCR	C30-C25	-3.15	1.49	1.53
25	A	610	CLA	CHC-C1C	3.14	1.43	1.35
33	d	406	LHG	O7-C5	-3.14	1.38	1.46
30	A	616	DGD	C4D-C5D	3.13	1.59	1.53
25	b	615	CLA	MG-NA	3.12	2.13	2.06
29	A	614	SQD	O47-C7	3.12	1.43	1.34
25	C	512	CLA	C4D-ND	-3.12	1.33	1.37
25	b	601	CLA	C4D-ND	-3.12	1.33	1.37
25	B	607	CLA	CHC-C1C	3.11	1.42	1.35
25	c	504	CLA	CHC-C1C	3.10	1.42	1.35
25	B	607	CLA	MG-NC	3.10	2.13	2.06
25	c	501	CLA	C4D-ND	-3.09	1.33	1.37
27	d	404	BCR	C1-C6	-3.09	1.49	1.53
25	C	504	CLA	C1D-ND	3.09	1.41	1.37
32	c	522	LMG	C4-C3	3.09	1.60	1.52
25	C	513	CLA	CHC-C1C	3.09	1.42	1.35
27	B	616	BCR	C1-C6	-3.08	1.49	1.53
27	c	516	BCR	C30-C25	-3.08	1.49	1.53
25	c	508	CLA	MG-NC	3.08	2.13	2.06
25	b	604	CLA	C1D-ND	3.07	1.41	1.37
30	H	103	DGD	O5D-C1E	3.07	1.45	1.40
25	A	606	CLA	CHC-C1C	3.07	1.42	1.35
25	d	403	CLA	C4D-ND	-3.07	1.33	1.37
25	C	503	CLA	CHC-C1C	3.06	1.42	1.35
29	A	615	SQD	C24-C23	3.06	1.59	1.50
25	B	601	CLA	MG-NA	3.06	2.13	2.06
25	a	607	CLA	CHC-C1C	3.05	1.42	1.35
29	A	614	SQD	O5-C1	3.05	1.49	1.41
25	a	610	CLA	C4D-ND	-3.05	1.33	1.37
35	F	101	HEM	CAB-C3B	3.04	1.55	1.47
25	b	613	CLA	MG-NA	3.04	2.13	2.06
25	B	611	CLA	C4D-ND	-3.03	1.33	1.37
25	c	506	CLA	CHC-C1C	3.02	1.42	1.35
25	a	613	CLA	C4D-ND	-3.01	1.33	1.37
25	c	507	CLA	CHC-C1C	3.01	1.42	1.35
25	c	504	CLA	C1D-ND	3.01	1.41	1.37
27	d	404	BCR	C30-C25	-3.01	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	C4D-ND	-3.00	1.33	1.37
25	b	609	CLA	C4D-ND	-3.00	1.33	1.37
29	f	101	SQD	O5-C1	3.00	1.49	1.41
29	l	101	SQD	O5-C1	3.00	1.49	1.41
25	c	502	CLA	CHC-C1C	2.99	1.42	1.35
25	B	612	CLA	CHC-C1C	2.99	1.42	1.35
29	f	101	SQD	O47-C45	-2.98	1.39	1.46
29	F	102	SQD	O5-C1	2.98	1.49	1.41
25	B	612	CLA	MG-ND	-2.97	1.99	2.05
25	b	610	CLA	CHC-C1C	2.97	1.42	1.35
29	L	101	SQD	C24-C23	2.96	1.59	1.50
25	C	509	CLA	CHC-C1C	2.96	1.42	1.35
25	B	613	CLA	CHC-C1C	2.96	1.42	1.35
25	B	601	CLA	C4D-ND	-2.96	1.33	1.37
25	b	604	CLA	CHC-C1C	2.96	1.42	1.35
25	B	605	CLA	C1D-ND	2.95	1.41	1.37
25	B	602	CLA	C4D-ND	-2.95	1.33	1.37
25	b	605	CLA	CHC-C1C	2.94	1.42	1.35
25	C	509	CLA	C4D-ND	-2.94	1.33	1.37
28	D	405	PL9	C7-C3	-2.93	1.48	1.51
30	c	517	DGD	C3G-C2G	2.93	1.59	1.50
25	b	606	CLA	C1D-ND	2.93	1.41	1.37
25	c	506	CLA	MG-NC	2.92	2.13	2.06
25	b	607	CLA	C4D-ND	-2.92	1.33	1.37
27	c	516	BCR	C1-C6	-2.92	1.49	1.53
25	c	504	CLA	MG-NC	2.92	2.13	2.06
25	b	615	CLA	CHC-C1C	2.91	1.42	1.35
25	C	501	CLA	C4D-ND	-2.90	1.33	1.37
27	K	101	BCR	C1-C6	-2.90	1.49	1.53
25	B	614	CLA	C4D-ND	-2.90	1.33	1.37
25	C	511	CLA	C4D-ND	-2.89	1.33	1.37
28	d	405	PL9	C53-C6	-2.88	1.44	1.50
27	K	103	BCR	C30-C25	-2.88	1.49	1.53
25	b	602	CLA	CHC-C1C	2.88	1.42	1.35
25	B	615	CLA	CHC-C1C	2.88	1.42	1.35
25	b	608	CLA	CHC-C1C	2.88	1.42	1.35
27	B	618	BCR	C1-C6	-2.88	1.49	1.53
29	a	614	SQD	C24-C23	2.87	1.59	1.50
25	b	606	CLA	C4D-ND	-2.87	1.33	1.37
32	C	515	LMG	C4-C3	2.87	1.59	1.52
25	b	613	CLA	C4D-ND	-2.87	1.33	1.37
25	B	610	CLA	C4D-ND	-2.86	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	C4D-ND	-2.86	1.33	1.37
25	h	101	CLA	C4D-ND	-2.86	1.33	1.37
25	B	607	CLA	MG-ND	-2.86	2.00	2.05
33	d	408	LHG	P-O6	2.86	1.70	1.59
27	c	514	BCR	C1-C6	-2.85	1.49	1.53
27	C	514	BCR	C30-C25	-2.85	1.49	1.53
32	c	524	LMG	C1-C2	2.85	1.60	1.52
32	D	406	LMG	C4-C5	2.84	1.59	1.53
25	C	510	CLA	C4D-ND	-2.84	1.33	1.37
25	D	403	CLA	C4D-ND	-2.84	1.33	1.37
29	L	101	SQD	O47-C45	-2.84	1.39	1.46
25	b	608	CLA	CMB-C2B	-2.84	1.45	1.51
25	B	612	CLA	MG-NA	2.83	2.13	2.06
25	b	606	CLA	CHC-C1C	2.82	1.42	1.35
25	B	615	CLA	C4D-ND	-2.82	1.33	1.37
32	C	519	LMG	C4-C3	2.82	1.59	1.52
27	K	102	BCR	C30-C25	-2.81	1.49	1.53
25	C	503	CLA	MG-NC	2.81	2.12	2.06
25	c	510	CLA	C4D-ND	-2.80	1.33	1.37
27	b	618	BCR	C1-C6	-2.80	1.49	1.53
25	B	609	CLA	MG-NA	2.80	2.12	2.06
25	c	511	CLA	C4D-ND	-2.80	1.33	1.37
32	d	410	LMG	C4-C5	2.79	1.58	1.53
29	A	615	SQD	C46-C45	2.79	1.57	1.50
27	k	101	BCR	C1-C6	-2.79	1.49	1.53
25	C	502	CLA	CHC-C1C	2.78	1.42	1.35
27	a	611	BCR	C1-C6	-2.78	1.50	1.53
25	c	512	CLA	C4D-ND	-2.77	1.33	1.37
25	B	607	CLA	C4D-ND	-2.76	1.33	1.37
27	K	101	BCR	C30-C25	-2.76	1.50	1.53
25	b	601	CLA	CHC-C1C	2.76	1.42	1.35
27	A	611	BCR	C1-C6	-2.76	1.50	1.53
25	B	602	CLA	C1D-ND	2.76	1.41	1.37
25	c	509	CLA	MG-NA	2.76	2.12	2.06
32	c	520	LMG	C1-C2	2.76	1.60	1.52
32	b	620	LMG	C3-C2	2.75	1.59	1.52
25	C	504	CLA	C4D-ND	-2.75	1.33	1.37
25	d	402	CLA	CHC-C1C	2.75	1.42	1.35
28	d	405	PL9	C3-C4	-2.74	1.45	1.49
25	a	610	CLA	CHC-C1C	2.74	1.42	1.35
30	A	616	DGD	C3E-C2E	2.74	1.59	1.52
25	b	605	CLA	C4D-ND	-2.74	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	C4D-ND	-2.73	1.33	1.37
25	a	607	CLA	CMB-C2B	-2.72	1.46	1.51
25	C	513	CLA	MG-NA	2.71	2.12	2.06
27	b	618	BCR	C30-C25	-2.70	1.50	1.53
29	a	614	SQD	O5-C1	2.70	1.48	1.41
29	a	615	SQD	O47-C45	-2.70	1.39	1.46
25	B	609	CLA	CMB-C2B	-2.69	1.46	1.51
30	C	517	DGD	C4D-C3D	2.69	1.59	1.52
25	B	609	CLA	C4D-ND	-2.68	1.34	1.37
26	d	401	PHO	CAC-C3C	-2.68	1.47	1.52
25	C	509	CLA	MG-NC	-2.68	1.99	2.06
25	A	606	CLA	MG-NA	2.68	2.12	2.06
29	l	101	SQD	C24-C23	2.67	1.58	1.50
25	c	505	CLA	C1D-ND	2.67	1.41	1.37
27	H	102	BCR	C30-C25	-2.67	1.50	1.53
33	E	101	LHG	P-O6	2.66	1.70	1.59
25	C	507	CLA	C4D-ND	-2.66	1.34	1.37
25	B	604	CLA	MG-ND	-2.66	2.00	2.05
27	x	101	BCR	C30-C25	-2.66	1.50	1.53
25	b	604	CLA	MG-NA	2.66	2.12	2.06
25	C	511	CLA	CMB-C2B	-2.65	1.46	1.51
25	b	608	CLA	MG-NC	2.64	2.12	2.06
25	a	613	CLA	CMB-C2B	-2.64	1.46	1.51
25	B	606	CLA	CHC-C1C	2.64	1.41	1.35
25	B	601	CLA	MG-ND	-2.64	2.00	2.05
25	b	612	CLA	C4D-ND	-2.62	1.34	1.37
25	b	612	CLA	MG-ND	-2.62	2.00	2.05
27	b	616	BCR	C1-C6	-2.61	1.50	1.53
25	D	403	CLA	CMB-C2B	-2.61	1.46	1.51
25	b	605	CLA	C1B-NB	2.61	1.37	1.35
25	d	402	CLA	C4D-ND	-2.60	1.34	1.37
25	C	501	CLA	MG-ND	-2.60	2.00	2.05
25	c	502	CLA	MG-ND	2.60	2.10	2.05
30	A	616	DGD	O5D-C6D	-2.60	1.39	1.43
26	A	608	PHO	CMC-C2C	-2.59	1.45	1.51
25	c	512	CLA	MG-NA	2.59	2.12	2.06
30	H	103	DGD	C4D-C5D	2.59	1.58	1.53
27	B	616	BCR	C30-C25	-2.59	1.50	1.53
27	c	514	BCR	C30-C25	-2.59	1.50	1.53
25	b	614	CLA	CMD-C2D	-2.59	1.45	1.50
28	a	612	PL9	C53-C6	-2.59	1.45	1.50
25	C	509	CLA	CMB-C2B	-2.58	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	615	CLA	MG-ND	-2.58	2.00	2.05
25	B	608	CLA	CHC-C1C	2.58	1.41	1.35
25	b	602	CLA	CMD-C2D	-2.58	1.45	1.50
30	C	517	DGD	C1E-C2E	2.57	1.59	1.52
25	C	505	CLA	MG-ND	-2.57	2.00	2.05
35	e	101	HEM	CAB-C3B	2.56	1.54	1.47
27	B	618	BCR	C30-C25	-2.56	1.50	1.53
25	B	604	CLA	CHC-C1C	2.56	1.41	1.35
25	d	402	CLA	CMB-C2B	-2.55	1.46	1.51
25	c	507	CLA	C3B-CAB	-2.54	1.42	1.47
30	h	102	DGD	C4D-C3D	2.54	1.58	1.52
30	C	518	DGD	O2G-C2G	-2.53	1.40	1.46
25	B	606	CLA	CMB-C2B	-2.52	1.46	1.51
30	C	516	DGD	O2G-C2G	-2.52	1.40	1.46
25	B	605	CLA	C3B-CAB	-2.52	1.42	1.47
25	d	403	CLA	CMB-C2B	-2.51	1.46	1.51
26	A	608	PHO	CAC-C3C	-2.51	1.47	1.52
25	B	611	CLA	MG-ND	-2.50	2.00	2.05
25	B	601	CLA	CMB-C2B	-2.50	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.50	1.46	1.51
25	D	403	CLA	C3B-C2B	-2.50	1.36	1.40
25	b	607	CLA	CMB-C2B	-2.50	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.50	1.46	1.51
27	T	101	BCR	C30-C25	-2.49	1.50	1.53
30	c	519	DGD	O2G-C2G	-2.49	1.40	1.46
27	D	404	BCR	C1-C6	-2.49	1.50	1.53
25	b	609	CLA	CHC-C1C	2.49	1.41	1.35
25	c	506	CLA	MG-ND	-2.48	2.00	2.05
25	H	101	CLA	C3B-C2B	-2.48	1.36	1.40
25	c	512	CLA	MG-ND	-2.48	2.00	2.05
25	b	612	CLA	CMB-C2B	-2.48	1.46	1.51
25	H	101	CLA	CMB-C2B	-2.48	1.46	1.51
25	c	506	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	611	CLA	MG-NC	2.47	2.12	2.06
25	B	610	CLA	CMB-C2B	-2.46	1.46	1.51
30	H	103	DGD	C1E-C2E	2.46	1.59	1.52
25	C	502	CLA	CMB-C2B	-2.46	1.46	1.51
26	A	609	PHO	CAC-C3C	-2.46	1.47	1.52
25	b	612	CLA	CHC-C1C	2.46	1.41	1.35
25	B	614	CLA	MG-NC	2.45	2.12	2.06
25	B	610	CLA	MG-ND	2.45	2.10	2.05
25	b	614	CLA	CMB-C2B	-2.44	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	609	CLA	CMB-C2B	-2.44	1.46	1.51
33	D	407	LHG	O7-C5	-2.43	1.40	1.46
25	B	603	CLA	CMB-C2B	-2.43	1.46	1.51
25	a	607	CLA	MG-NA	2.43	2.12	2.06
33	B	622	LHG	C24-C23	2.43	1.57	1.50
27	k	101	BCR	C30-C25	-2.43	1.50	1.53
25	B	602	CLA	CMD-C2D	-2.42	1.45	1.50
25	D	403	CLA	CMD-C2D	-2.42	1.45	1.50
25	b	605	CLA	CMB-C2B	-2.42	1.46	1.51
32	m	101	LMG	C9-C8	2.42	1.58	1.50
28	d	405	PL9	C31-C29	-2.42	1.46	1.51
25	c	505	CLA	MG-NA	2.41	2.12	2.06
25	B	603	CLA	C1B-NB	2.41	1.37	1.35
25	C	511	CLA	C1B-NB	2.41	1.37	1.35
25	C	512	CLA	CMB-C2B	-2.41	1.46	1.51
25	C	501	CLA	C3B-C2B	-2.40	1.37	1.40
32	D	406	LMG	C7-C8	2.40	1.58	1.50
25	B	613	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	508	CLA	CMB-C2B	-2.40	1.46	1.51
32	d	410	LMG	O7-C8	-2.40	1.40	1.46
27	D	404	BCR	C30-C25	-2.39	1.50	1.53
32	C	519	LMG	O7-C8	-2.39	1.40	1.46
25	b	613	CLA	CMB-C2B	-2.39	1.46	1.51
29	l	101	SQD	O9-S	2.39	1.52	1.45
30	C	517	DGD	C1G-C2G	2.38	1.58	1.50
30	h	102	DGD	C4E-C3E	2.38	1.58	1.52
33	B	621	LHG	O7-C5	-2.38	1.40	1.46
25	A	610	CLA	MG-ND	-2.38	2.01	2.05
27	b	616	BCR	C30-C25	-2.37	1.50	1.53
25	b	611	CLA	CMC-C2C	-2.37	1.45	1.50
25	C	510	CLA	MG-NA	2.37	2.11	2.06
25	C	508	CLA	C1D-C2D	2.37	1.50	1.45
25	b	610	CLA	C4D-ND	-2.37	1.34	1.37
30	h	102	DGD	C1E-C2E	2.36	1.59	1.52
25	h	101	CLA	MG-NC	-2.36	2.00	2.06
25	C	507	CLA	MG-NC	2.36	2.11	2.06
25	b	606	CLA	CMB-C2B	-2.36	1.46	1.51
30	a	616	DGD	C1G-C2G	2.36	1.57	1.50
32	M	101	LMG	C4-C3	2.36	1.58	1.52
29	A	614	SQD	O9-S	2.36	1.52	1.45
25	B	604	CLA	C4B-CHC	-2.36	1.34	1.41
25	A	606	CLA	CMB-C2B	-2.35	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	509	CLA	CMB-C2B	-2.35	1.46	1.51
25	H	101	CLA	C4D-ND	-2.35	1.34	1.37
29	a	614	SQD	O7-S	2.34	1.51	1.45
25	C	512	CLA	MG-NC	2.34	2.11	2.06
25	C	507	CLA	CMB-C2B	-2.34	1.46	1.51
29	L	101	SQD	O7-S	2.34	1.51	1.45
25	C	510	CLA	CMB-C2B	-2.34	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.34	1.46	1.51
25	c	508	CLA	CMD-C2D	-2.33	1.45	1.50
25	a	610	CLA	CMC-C2C	-2.33	1.45	1.50
25	C	504	CLA	CMB-C2B	-2.33	1.46	1.51
25	d	402	CLA	MG-NC	2.33	2.11	2.06
25	C	508	CLA	CMB-C2B	-2.32	1.46	1.51
25	a	608	CLA	CMB-C2B	-2.32	1.46	1.51
29	f	101	SQD	O7-S	2.32	1.51	1.45
25	c	512	CLA	CMB-C2B	-2.32	1.46	1.51
25	C	505	CLA	MG-NC	2.32	2.11	2.06
25	B	615	CLA	CMC-C2C	-2.31	1.45	1.50
32	C	515	LMG	O1-C7	-2.31	1.39	1.43
25	C	504	CLA	MG-ND	-2.31	2.01	2.05
25	c	506	CLA	CMD-C2D	-2.31	1.45	1.50
27	c	515	BCR	C30-C25	-2.30	1.50	1.53
25	D	403	CLA	CHC-C1C	2.30	1.40	1.35
29	L	101	SQD	O9-S	2.30	1.51	1.45
29	l	101	SQD	C44-C45	2.30	1.57	1.50
30	C	516	DGD	C6E-C5E	2.30	1.59	1.51
25	B	602	CLA	CMB-C2B	-2.30	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.29	1.46	1.51
25	B	609	CLA	MG-ND	-2.29	2.01	2.05
25	C	510	CLA	MG-NC	2.29	2.11	2.06
33	e	102	LHG	P-O6	2.29	1.68	1.59
32	C	515	LMG	C7-C8	2.28	1.57	1.50
25	b	602	CLA	CMB-C2B	-2.28	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.28	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.28	1.46	1.51
25	b	606	CLA	C3B-C2B	-2.27	1.37	1.40
25	C	512	CLA	CMD-C2D	-2.27	1.46	1.50
25	c	503	CLA	CMB-C2B	-2.26	1.46	1.51
25	B	613	CLA	C3B-CAB	-2.26	1.43	1.47
25	B	605	CLA	C3B-C2B	-2.25	1.37	1.40
30	C	517	DGD	O6D-C5D	-2.25	1.38	1.44
25	B	615	CLA	CMB-C2B	-2.25	1.47	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	612	CLA	MG-NC	2.24	2.11	2.06
29	a	614	SQD	C6-S	2.24	1.85	1.77
29	L	101	SQD	C6-S	2.24	1.85	1.77
25	C	509	CLA	CMD-C2D	-2.24	1.46	1.50
32	m	101	LMG	C4-C5	2.24	1.57	1.53
25	b	608	CLA	MG-NA	2.23	2.11	2.06
25	C	510	CLA	CMD-C2D	-2.22	1.46	1.50
25	b	609	CLA	C3B-C2B	-2.22	1.37	1.40
29	L	101	SQD	O5-C5	2.22	1.49	1.44
25	b	601	CLA	CMD-C2D	-2.22	1.46	1.50
25	b	612	CLA	CMD-C2D	-2.22	1.46	1.50
26	A	609	PHO	CMB-C2B	-2.22	1.46	1.51
25	C	508	CLA	MG-ND	2.21	2.10	2.05
27	a	611	BCR	C30-C25	-2.21	1.50	1.53
25	B	611	CLA	MG-NA	2.21	2.11	2.06
35	e	101	HEM	C3B-C2B	-2.21	1.32	1.37
33	d	406	LHG	P-O6	2.21	1.68	1.59
25	a	613	CLA	C1D-C2D	2.20	1.49	1.45
25	d	403	CLA	C3B-CAB	-2.20	1.43	1.47
25	c	507	CLA	C3D-C4D	2.20	1.49	1.44
32	C	515	LMG	C1-C2	2.20	1.58	1.52
25	b	615	CLA	CMB-C2B	-2.19	1.47	1.51
26	A	609	PHO	CMC-C2C	-2.19	1.46	1.51
25	a	610	CLA	CMD-C2D	-2.19	1.46	1.50
25	a	613	CLA	C3B-C2B	-2.19	1.37	1.40
30	c	519	DGD	O4E-C4E	-2.19	1.37	1.43
30	H	103	DGD	C6D-C5D	2.19	1.58	1.51
32	D	409	LMG	C7-C8	2.19	1.56	1.51
29	a	615	SQD	C44-C45	2.19	1.56	1.51
25	c	501	CLA	CMD-C2D	-2.18	1.46	1.50
25	A	607	CLA	MG-ND	2.18	2.10	2.05
25	c	501	CLA	CMB-C2B	-2.18	1.47	1.51
30	a	616	DGD	O1G-C1A	2.18	1.39	1.33
32	c	524	LMG	C4-C3	2.18	1.57	1.52
25	D	402	CLA	CMC-C2C	-2.18	1.46	1.50
29	L	101	SQD	C46-C45	2.18	1.57	1.50
25	H	101	CLA	CMC-C2C	-2.18	1.46	1.50
25	a	610	CLA	CMB-C2B	-2.17	1.47	1.51
30	C	516	DGD	C3G-C2G	2.17	1.57	1.50
25	b	613	CLA	CMC-C2C	-2.17	1.46	1.50
25	c	512	CLA	C1D-C2D	2.17	1.49	1.45
30	A	616	DGD	C3G-C2G	2.17	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	101	CLA	O2A-CGA	2.16	1.39	1.33
25	b	601	CLA	CMB-C2B	-2.16	1.47	1.51
25	B	609	CLA	C3B-C2B	-2.16	1.37	1.40
29	f	101	SQD	O5-C5	2.16	1.49	1.44
30	c	517	DGD	C4D-C3D	2.16	1.57	1.52
26	a	609	PHO	CAC-C3C	-2.16	1.48	1.52
26	d	401	PHO	CMC-C2C	-2.15	1.46	1.51
29	l	101	SQD	C8-C7	2.15	1.57	1.50
29	a	615	SQD	C46-C45	2.15	1.57	1.50
32	M	101	LMG	C4-C5	2.15	1.57	1.53
25	B	605	CLA	CMB-C2B	-2.15	1.47	1.51
25	C	501	CLA	CMB-C2B	-2.15	1.47	1.51
25	B	614	CLA	C3B-C2B	-2.15	1.37	1.40
30	C	518	DGD	O2E-C2E	-2.15	1.37	1.43
30	c	518	DGD	O6D-C5D	-2.15	1.39	1.44
25	B	607	CLA	C1B-NB	2.15	1.37	1.35
25	C	509	CLA	C1B-NB	2.15	1.37	1.35
25	b	611	CLA	CMB-C2B	-2.15	1.47	1.51
25	B	605	CLA	CMD-C2D	-2.15	1.46	1.50
32	c	524	LMG	C4-C5	2.14	1.57	1.53
25	b	605	CLA	CMD-C2D	-2.14	1.46	1.50
25	a	608	CLA	MG-ND	-2.14	2.01	2.05
25	A	607	CLA	CMB-C2B	-2.14	1.47	1.51
27	d	404	BCR	C38-C26	-2.14	1.47	1.50
25	B	607	CLA	C3B-CAB	-2.14	1.43	1.47
25	c	502	CLA	CMD-C2D	-2.14	1.46	1.50
27	A	611	BCR	C33-C5	-2.13	1.47	1.50
25	C	501	CLA	C1D-C2D	2.13	1.49	1.45
29	f	101	SQD	O9-S	2.13	1.51	1.45
25	b	612	CLA	C3C-C2C	2.13	1.41	1.36
26	d	401	PHO	CMD-C2D	-2.12	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.11	1.47	1.51
27	t	101	BCR	C1-C6	-2.11	1.50	1.53
25	b	603	CLA	CMB-C2B	-2.11	1.47	1.51
25	B	605	CLA	C4D-ND	-2.11	1.34	1.37
29	l	101	SQD	O7-S	2.11	1.51	1.45
30	A	616	DGD	C3D-C2D	2.11	1.57	1.52
25	h	101	CLA	CMB-C2B	-2.11	1.47	1.51
25	B	608	CLA	CMD-C2D	-2.10	1.46	1.50
25	A	606	CLA	CMC-C2C	-2.10	1.46	1.50
27	b	617	BCR	C38-C26	-2.10	1.47	1.50
32	b	620	LMG	O1-C7	-2.10	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	C3D-C4D	2.09	1.48	1.44
35	e	101	HEM	CMB-C2B	2.09	1.55	1.50
29	A	614	SQD	C6-S	2.09	1.85	1.77
25	C	504	CLA	CMD-C2D	-2.09	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.09	1.46	1.50
30	H	103	DGD	O6E-C1E	2.08	1.47	1.41
29	f	101	SQD	C46-C45	2.08	1.57	1.50
33	d	406	LHG	C24-C23	2.08	1.56	1.50
25	B	614	CLA	C3B-CAB	-2.08	1.43	1.47
30	c	517	DGD	O2G-C2G	-2.08	1.41	1.46
30	c	518	DGD	C4D-C3D	2.08	1.57	1.52
26	A	608	PHO	CMD-C2D	-2.08	1.46	1.51
30	h	102	DGD	C4E-C5E	2.07	1.57	1.53
25	A	613	CLA	C1D-C2D	2.07	1.49	1.45
25	C	511	CLA	CMD-C2D	-2.07	1.46	1.50
29	F	102	SQD	O9-S	2.07	1.51	1.45
28	D	405	PL9	C41-C39	-2.07	1.47	1.51
25	d	403	CLA	MG-NA	2.07	2.11	2.06
26	A	609	PHO	CMD-C2D	-2.07	1.46	1.51
25	h	101	CLA	CMC-C2C	-2.07	1.46	1.50
25	c	502	CLA	CMC-C2C	-2.07	1.46	1.50
25	b	605	CLA	C4B-CHC	-2.06	1.35	1.41
26	a	609	PHO	O2D-CGD	2.06	1.38	1.33
25	C	503	CLA	CMB-C2B	-2.06	1.47	1.51
25	b	605	CLA	CMC-C2C	-2.06	1.46	1.50
25	b	607	CLA	C1D-C2D	2.05	1.49	1.45
32	c	524	LMG	C7-C8	2.05	1.57	1.50
25	C	505	CLA	C3B-CAB	-2.05	1.43	1.47
32	c	522	LMG	O1-C1	2.05	1.43	1.40
25	b	611	CLA	MG-NC	2.05	2.11	2.06
25	B	603	CLA	MG-NC	2.04	2.11	2.06
30	C	516	DGD	O4D-C4D	-2.04	1.38	1.43
30	C	517	DGD	O3D-C3D	-2.04	1.38	1.43
25	B	612	CLA	CMB-C2B	-2.04	1.47	1.51
25	c	505	CLA	C3B-CAB	-2.04	1.43	1.47
32	M	101	LMG	C9-C8	2.04	1.57	1.50
25	B	604	CLA	CMD-C2D	-2.04	1.46	1.50
25	C	502	CLA	C3B-C2B	-2.04	1.37	1.40
25	c	502	CLA	CMB-C2B	-2.04	1.47	1.51
27	C	514	BCR	C33-C5	-2.03	1.47	1.50
30	H	103	DGD	C1G-C2G	2.03	1.56	1.50
25	B	607	CLA	CMB-C2B	-2.03	1.47	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	504	CLA	O2D-CGD	2.03	1.38	1.33
29	l	101	SQD	O5-C5	2.03	1.49	1.44
30	C	517	DGD	O3G-C3G	-2.02	1.40	1.43
29	A	614	SQD	C8-C7	2.02	1.56	1.50
25	B	609	CLA	C3D-C4D	2.02	1.48	1.44
25	D	403	CLA	C4B-CHC	-2.02	1.35	1.41
29	F	102	SQD	O5-C5	2.02	1.49	1.44
25	C	510	CLA	CMC-C2C	-2.02	1.46	1.50
27	B	616	BCR	C33-C5	-2.02	1.47	1.50
29	F	102	SQD	O7-S	2.01	1.51	1.45
25	a	610	CLA	C4B-CHC	-2.01	1.35	1.41
25	B	609	CLA	CMC-C2C	-2.01	1.46	1.50
29	f	101	SQD	C44-C45	2.01	1.56	1.50
32	c	522	LMG	C1-C2	2.01	1.58	1.52
29	F	102	SQD	C6-S	2.01	1.84	1.77
25	B	609	CLA	C1D-C2D	2.01	1.49	1.45
25	C	506	CLA	CMC-C2C	-2.01	1.46	1.50
25	b	610	CLA	C1D-C2D	2.01	1.49	1.45
25	c	501	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	507	CLA	CMC-C2C	-2.01	1.46	1.50
25	c	508	CLA	CMC-C2C	-2.01	1.46	1.50
30	H	103	DGD	C4E-C5E	2.00	1.57	1.53
25	C	510	CLA	C3C-C2C	2.00	1.41	1.36

All (1209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	509	CLA	C4A-NA-C1A	8.94	110.73	106.71
25	c	511	CLA	C4A-NA-C1A	8.67	110.60	106.71
25	C	507	CLA	C4A-NA-C1A	8.61	110.58	106.71
25	B	603	CLA	C4A-NA-C1A	8.47	110.51	106.71
25	b	603	CLA	C4A-NA-C1A	7.88	110.25	106.71
25	b	605	CLA	C4A-NA-C1A	7.86	110.24	106.71
25	C	511	CLA	C4A-NA-C1A	7.85	110.23	106.71
25	C	508	CLA	C4A-NA-C1A	7.75	110.19	106.71
25	c	503	CLA	C4A-NA-C1A	7.68	110.16	106.71
25	H	101	CLA	C4A-NA-C1A	7.50	110.08	106.71
25	C	503	CLA	C4A-NA-C1A	7.42	110.04	106.71
25	B	614	CLA	C4A-NA-C1A	7.38	110.03	106.71
25	C	513	CLA	C4A-NA-C1A	7.36	110.02	106.71
25	B	615	CLA	C4A-NA-C1A	7.26	109.97	106.71
25	C	506	CLA	C4A-NA-C1A	7.15	109.92	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	506	CLA	C4A-NA-C1A	7.02	109.86	106.71
25	b	606	CLA	C4A-NA-C1A	6.92	109.82	106.71
25	B	608	CLA	C4A-NA-C1A	6.86	109.79	106.71
25	B	610	CLA	C4A-NA-C1A	6.79	109.76	106.71
25	A	607	CLA	C4A-NA-C1A	6.78	109.76	106.71
25	b	615	CLA	C4A-NA-C1A	6.77	109.75	106.71
25	b	610	CLA	C4A-NA-C1A	6.71	109.72	106.71
25	C	510	CLA	C4A-NA-C1A	6.67	109.71	106.71
25	B	606	CLA	C4A-NA-C1A	6.65	109.69	106.71
25	B	607	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	c	501	CLA	C4A-NA-C1A	6.53	109.64	106.71
25	c	507	CLA	C4A-NA-C1A	6.51	109.63	106.71
25	b	614	CLA	C4A-NA-C1A	6.49	109.62	106.71
29	a	614	SQD	C1-O5-C5	-6.47	100.98	113.69
29	a	614	SQD	O6-C1-C2	6.37	118.24	108.30
25	a	607	CLA	C4A-NA-C1A	6.34	109.56	106.71
25	B	611	CLA	C4A-NA-C1A	6.33	109.55	106.71
25	b	609	CLA	C4A-NA-C1A	6.31	109.54	106.71
25	B	612	CLA	C4A-NA-C1A	6.19	109.49	106.71
25	B	605	CLA	C4A-NA-C1A	6.17	109.48	106.71
25	h	101	CLA	C4A-NA-C1A	6.11	109.45	106.71
25	C	505	CLA	C4A-NA-C1A	6.05	109.42	106.71
25	c	510	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	C	509	CLA	C4A-NA-C1A	6.01	109.41	106.71
29	A	614	SQD	O6-C1-C2	5.96	117.61	108.30
25	D	402	CLA	C4A-NA-C1A	5.95	109.38	106.71
28	a	612	PL9	C7-C3-C4	5.90	121.67	116.88
25	b	612	CLA	C4A-NA-C1A	5.87	109.34	106.71
25	C	501	CLA	C4A-NA-C1A	5.77	109.30	106.71
29	L	101	SQD	O6-C1-C2	5.74	117.26	108.30
25	c	502	CLA	C4A-NA-C1A	5.73	109.28	106.71
29	L	101	SQD	O7-S-C6	5.73	113.75	106.94
25	b	602	CLA	C4A-NA-C1A	5.61	109.23	106.71
25	d	402	CLA	C4A-NA-C1A	5.60	109.22	106.71
25	c	504	CLA	C4A-NA-C1A	5.48	109.17	106.71
28	A	612	PL9	C7-C3-C4	5.38	121.25	116.88
25	b	604	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	a	608	CLA	C4A-NA-C1A	5.34	109.11	106.71
29	f	101	SQD	O7-S-C6	5.33	113.27	106.94
25	A	613	CLA	C4A-NA-C1A	5.26	109.07	106.71
29	l	101	SQD	O6-C1-C2	5.26	116.52	108.30
25	c	505	CLA	C4A-NA-C1A	5.19	109.04	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	606	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
25	b	608	CLA	C4A-NA-C1A	5.16	109.03	106.71
25	b	611	CLA	C4A-NA-C1A	5.13	109.01	106.71
25	c	512	CLA	C4A-NA-C1A	5.12	109.01	106.71
29	a	615	SQD	O47-C7-C8	5.11	122.52	111.50
25	c	513	CLA	C4A-NA-C1A	5.09	109.00	106.71
25	D	403	CLA	C4A-NA-C1A	5.07	108.99	106.71
25	B	604	CLA	C4A-NA-C1A	5.06	108.98	106.71
29	l	101	SQD	O47-C7-C8	5.05	122.39	111.50
28	d	405	PL9	C7-C3-C4	4.93	120.89	116.88
36	V	201	HEC	CBD-CAD-C3D	-4.92	104.22	112.62
29	A	614	SQD	O47-C7-C8	4.89	122.05	111.50
29	A	614	SQD	O7-S-C6	4.89	112.76	106.94
25	b	605	CLA	O2D-CGD-O1D	-4.89	114.27	123.84
25	b	608	CLA	CMB-C2B-C1B	-4.89	120.94	128.46
29	A	614	SQD	C1-C2-C3	-4.83	99.93	110.00
25	B	601	CLA	C4A-NA-C1A	4.83	108.88	106.71
25	C	504	CLA	C4A-NA-C1A	4.80	108.86	106.71
25	C	504	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
25	b	601	CLA	C4A-NA-C1A	4.75	108.84	106.71
25	a	613	CLA	C4A-NA-C1A	4.75	108.84	106.71
25	B	613	CLA	C4A-NA-C1A	4.74	108.84	106.71
25	B	611	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
25	c	508	CLA	C4A-NA-C1A	4.69	108.82	106.71
25	A	606	CLA	C4A-NA-C1A	4.67	108.81	106.71
25	b	607	CLA	C4A-NA-C1A	4.67	108.81	106.71
25	c	501	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
25	B	609	CLA	C4A-NA-C1A	4.65	108.80	106.71
29	F	102	SQD	O9-S-C6	4.64	112.46	106.94
29	F	102	SQD	C1-O5-C5	-4.62	104.62	113.69
30	C	518	DGD	O3G-C3G-C2G	-4.61	99.77	110.90
25	c	508	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
25	b	607	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
25	C	512	CLA	C4A-NA-C1A	4.59	108.77	106.71
25	C	509	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
25	B	601	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
26	A	609	PHO	C1-C2-C3	-4.54	118.19	126.04
25	c	504	CLA	CMB-C2B-C1B	-4.51	121.54	128.46
25	A	610	CLA	CMB-C2B-C1B	-4.49	121.57	128.46
25	C	508	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
25	B	607	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
25	d	402	CLA	CMB-C2B-C1B	-4.43	121.66	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	610	CLA	CHD-C1D-ND	-4.40	120.41	124.45
25	b	613	CLA	CMB-C2B-C1B	-4.38	121.72	128.46
25	B	602	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
25	C	510	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
25	B	606	CLA	CMB-C2B-C3B	4.35	132.81	124.68
33	d	407	LHG	O4-P-O5	4.34	133.71	112.24
25	c	513	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
25	b	612	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
25	C	509	CLA	CHD-C1D-ND	-4.26	120.54	124.45
30	C	517	DGD	O3G-C3G-C2G	-4.26	100.61	110.90
25	B	611	CLA	CMB-C2B-C3B	4.25	132.64	124.68
25	b	606	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
25	C	502	CLA	C4A-NA-C1A	4.24	108.61	106.71
25	b	613	CLA	C4A-NA-C1A	4.24	108.61	106.71
33	e	102	LHG	O4-P-O5	4.23	133.13	112.24
25	a	610	CLA	C4A-NA-C1A	4.19	108.59	106.71
34	D	401	BCT	O2-C-O1	4.19	130.41	119.55
28	D	405	PL9	C7-C3-C4	4.17	120.27	116.88
25	B	609	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
26	A	608	PHO	CMB-C2B-C3B	4.14	132.43	124.68
25	B	615	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
25	B	612	CLA	C1-C2-C3	-4.14	118.89	126.04
29	f	101	SQD	O6-C1-C2	4.12	114.73	108.30
33	B	621	LHG	O4-P-O5	4.10	132.51	112.24
26	d	401	PHO	C1-C2-C3	-4.09	118.97	126.04
25	c	504	CLA	CMB-C2B-C3B	4.08	132.32	124.68
25	c	510	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
33	E	101	LHG	O4-P-O5	4.08	132.39	112.24
33	B	622	LHG	O4-P-O5	4.07	132.38	112.24
25	d	403	CLA	C4A-NA-C1A	4.07	108.54	106.71
25	C	506	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
33	D	408	LHG	O4-P-O5	4.04	132.21	112.24
33	d	406	LHG	O4-P-O5	4.04	132.20	112.24
29	f	101	SQD	O9-S-O7	-4.01	100.08	113.95
33	D	407	LHG	O4-P-O5	4.01	132.04	112.24
30	H	103	DGD	O3G-C3G-C2G	-3.99	101.27	110.90
25	B	615	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
25	b	603	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
30	c	519	DGD	O3G-C3G-C2G	-3.98	101.29	110.90
33	l	102	LHG	O4-P-O5	3.98	131.92	112.24
25	B	610	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
25	B	613	CLA	CMB-C2B-C1B	-3.97	122.36	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	614	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
25	C	505	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
25	b	609	CLA	C1-C2-C3	-3.96	119.19	126.04
25	D	402	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
25	b	615	CLA	CMB-C2B-C1B	-3.96	122.39	128.46
25	A	610	CLA	CMB-C2B-C3B	3.95	132.07	124.68
29	l	101	SQD	O7-S-C6	3.95	111.63	106.94
25	B	601	CLA	CMB-C2B-C3B	3.94	132.05	124.68
25	C	509	CLA	CMB-C2B-C3B	3.94	132.05	124.68
29	f	101	SQD	O5-C5-C4	3.94	116.84	109.69
33	d	408	LHG	O4-P-O5	3.93	131.68	112.24
36	V	201	HEC	CMC-C2C-C1C	-3.93	122.43	128.46
29	A	614	SQD	C1-O5-C5	-3.93	105.98	113.69
34	a	606	BCT	O2-C-O1	3.93	129.73	119.55
36	V	201	HEC	C1D-C2D-C3D	-3.93	104.27	107.00
25	b	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	B	610	CLA	O2D-CGD-CBD	3.92	118.23	111.27
25	b	607	CLA	CMB-C2B-C3B	3.91	131.99	124.68
26	d	401	PHO	CMB-C2B-C3B	3.91	131.99	124.68
36	v	201	HEC	CBD-CAD-C3D	-3.89	105.98	112.62
29	a	614	SQD	O47-C7-C8	3.86	119.83	111.50
25	c	509	CLA	O2A-CGA-O1A	-3.86	113.84	123.59
25	c	512	CLA	C1-C2-C3	-3.85	119.38	126.04
29	a	614	SQD	O8-S-C6	3.85	111.88	105.74
27	B	616	BCR	C2-C1-C6	3.84	116.39	110.48
25	A	613	CLA	CMB-C2B-C3B	3.84	131.85	124.68
25	b	608	CLA	CMB-C2B-C3B	3.83	131.85	124.68
29	L	101	SQD	C1-C2-C3	-3.83	102.01	110.00
28	A	612	PL9	C7-C3-C2	-3.83	118.26	123.30
25	d	403	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
25	B	612	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
26	A	609	PHO	O2D-CGD-O1D	-3.82	116.36	123.84
25	B	602	CLA	CMB-C2B-C3B	3.81	131.81	124.68
25	b	615	CLA	O2D-CGD-O1D	-3.81	116.39	123.84
30	a	616	DGD	O3G-C3G-C2G	-3.81	101.68	111.78
25	d	402	CLA	CMB-C2B-C3B	3.79	131.77	124.68
25	c	502	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
30	h	102	DGD	O3G-C3G-C2G	-3.78	101.77	110.90
25	b	605	CLA	O2D-CGD-CBD	3.77	117.97	111.27
35	e	101	HEM	CBA-CAA-C2A	-3.76	106.20	112.62
25	b	605	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
25	h	101	CLA	CMB-C2B-C1B	-3.76	122.69	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	607	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
25	a	613	CLA	C1-C2-C3	-3.75	119.55	126.04
27	K	101	BCR	C15-C16-C17	-3.74	115.81	123.47
25	C	513	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
25	A	610	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
25	a	607	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
25	A	613	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
25	c	508	CLA	CMB-C2B-C3B	3.72	131.64	124.68
27	K	101	BCR	C11-C10-C9	-3.70	122.03	127.31
25	c	508	CLA	CHD-C1D-ND	-3.68	121.07	124.45
25	B	601	CLA	O2D-CGD-CBD	3.68	117.81	111.27
25	C	510	CLA	CMB-C2B-C3B	3.68	131.56	124.68
25	c	513	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
25	C	508	CLA	CMB-C2B-C3B	3.66	131.53	124.68
27	B	617	BCR	C15-C14-C13	-3.66	122.08	127.31
25	c	513	CLA	CMB-C2B-C3B	3.64	131.50	124.68
25	d	402	CLA	O2D-CGD-O1D	-3.64	116.71	123.84
25	B	607	CLA	CMB-C2B-C3B	3.64	131.49	124.68
35	e	101	HEM	CBD-CAD-C3D	-3.63	102.54	112.63
25	B	615	CLA	CMB-C2B-C3B	3.63	131.47	124.68
25	h	101	CLA	CHD-C1D-ND	-3.62	121.13	124.45
25	C	504	CLA	CMB-C2B-C3B	3.62	131.45	124.68
25	C	508	CLA	CHD-C1D-ND	-3.61	121.14	124.45
25	C	508	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
29	a	614	SQD	O9-S-O7	-3.60	101.48	113.95
29	L	101	SQD	O5-C5-C4	3.59	116.21	109.69
28	a	612	PL9	C7-C3-C2	-3.59	118.58	123.30
29	L	101	SQD	O47-C7-C8	3.59	119.23	111.50
30	C	516	DGD	O3G-C3G-C2G	-3.59	102.25	110.90
25	b	601	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
25	B	607	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
36	v	201	HEC	CMB-C2B-C1B	-3.58	122.96	128.46
26	d	401	PHO	O1D-CGD-CBD	3.58	130.70	124.74
27	b	616	BCR	C2-C1-C6	3.58	115.98	110.48
25	B	603	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
25	C	501	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
25	C	513	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
25	b	612	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
29	A	614	SQD	O9-S-O7	-3.56	101.61	113.95
25	C	507	CLA	O2D-CGD-O1D	-3.56	116.87	123.84
25	C	506	CLA	CMB-C2B-C3B	3.55	131.32	124.68
25	A	610	CLA	C4A-NA-C1A	3.55	108.30	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	512	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
29	A	615	SQD	O47-C7-C8	3.55	119.15	111.50
25	c	501	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
29	A	615	SQD	O48-C23-C24	3.54	123.03	111.91
29	L	101	SQD	O48-C23-C24	3.54	123.03	111.91
35	F	101	HEM	CBA-CAA-C2A	-3.53	106.60	112.62
25	C	507	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
25	c	510	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
25	D	402	CLA	CMB-C2B-C3B	3.51	131.25	124.68
25	c	501	CLA	O2D-CGD-CBD	3.51	117.50	111.27
25	b	601	CLA	CHB-C4A-NA	3.50	129.36	124.51
25	b	601	CLA	CMB-C2B-C3B	3.50	131.22	124.68
27	K	101	BCR	C15-C14-C13	-3.49	122.33	127.31
25	B	608	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
25	B	609	CLA	CHB-C4A-NA	3.48	129.32	124.51
36	V	201	HEC	CMC-C2C-C3C	3.48	129.91	125.82
25	b	611	CLA	CMB-C2B-C3B	3.47	131.18	124.68
25	C	510	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
25	b	602	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
25	b	602	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
26	A	609	PHO	CMB-C2B-C3B	3.46	131.16	124.68
25	B	603	CLA	C1-C2-C3	-3.46	120.06	126.04
25	c	505	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
30	c	517	DGD	O3G-C3G-C2G	-3.46	102.56	110.90
32	m	101	LMG	O1-C7-C8	-3.45	102.57	110.90
25	b	604	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
25	D	403	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
25	b	606	CLA	CMB-C2B-C3B	3.44	131.12	124.68
25	A	610	CLA	CHD-C1D-ND	-3.44	121.29	124.45
25	B	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
27	t	101	BCR	C3-C4-C5	-3.43	107.95	114.08
36	V	201	HEC	CMB-C2B-C1B	-3.43	123.19	128.46
29	a	614	SQD	O7-S-C6	3.43	111.01	106.94
25	b	609	CLA	CAA-CBA-CGA	-3.42	103.25	113.25
29	a	614	SQD	C44-O6-C1	-3.42	107.05	113.74
25	b	610	CLA	O2D-CGD-CBD	3.42	117.34	111.27
25	b	615	CLA	CMB-C2B-C3B	3.41	131.06	124.68
25	B	602	CLA	C4A-NA-C1A	3.41	108.24	106.71
26	d	401	PHO	CMC-C2C-C3C	3.41	131.37	124.94
25	b	612	CLA	CMB-C2B-C3B	3.41	131.06	124.68
25	c	507	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
25	B	603	CLA	O2D-CGD-O1D	-3.41	117.18	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	406	LHG	O8-C23-C24	3.40	122.57	111.91
25	a	608	CLA	CHB-C4A-NA	3.40	129.21	124.51
29	L	101	SQD	O9-S-O7	-3.40	102.20	113.95
25	c	502	CLA	CMB-C2B-C3B	3.39	131.02	124.68
25	C	512	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
25	d	403	CLA	CMB-C2B-C3B	3.38	131.00	124.68
25	c	512	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
27	c	515	BCR	C11-C10-C9	-3.38	122.49	127.31
32	c	524	LMG	O6-C1-O1	-3.37	101.98	109.97
25	H	101	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
25	C	511	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
26	A	609	PHO	O1D-CGD-CBD	3.37	130.35	124.74
25	b	611	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
29	a	615	SQD	O48-C23-C24	3.36	122.45	111.91
36	v	201	HEC	CMC-C2C-C1C	-3.35	123.31	128.46
35	F	101	HEM	CBD-CAD-C3D	-3.35	103.33	112.63
25	B	609	CLA	O2A-CGA-O1A	-3.34	115.15	123.59
29	a	614	SQD	O48-C23-C24	3.34	122.40	111.91
25	a	613	CLA	CHD-C1D-ND	-3.34	121.39	124.45
30	C	517	DGD	O6D-C1D-O3G	-3.33	102.08	109.97
25	A	613	CLA	CHD-C1D-ND	-3.32	121.40	124.45
28	D	405	PL9	C22-C23-C24	-3.32	119.67	127.66
25	a	608	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
25	c	506	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
27	b	617	BCR	C15-C14-C13	-3.31	122.59	127.31
25	a	610	CLA	C1-C2-C3	-3.31	120.33	126.04
25	c	502	CLA	CHD-C1D-ND	-3.30	121.42	124.45
25	A	607	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	a	610	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	b	602	CLA	CHD-C1D-ND	-3.29	121.43	124.45
25	B	613	CLA	CMB-C2B-C3B	3.29	130.83	124.68
25	C	503	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
25	B	604	CLA	CHD-C1D-ND	-3.29	121.43	124.45
25	C	502	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
25	C	512	CLA	CHB-C4A-NA	3.28	129.05	124.51
25	B	610	CLA	CHD-C4C-NC	3.28	129.37	124.20
25	b	601	CLA	C1-C2-C3	-3.28	120.38	126.04
25	B	604	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
25	b	611	CLA	C1-C2-C3	-3.27	120.39	126.04
25	c	511	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
30	c	518	DGD	O3G-C3G-C2G	-3.25	103.06	110.90
25	b	609	CLA	O2D-CGD-O1D	-3.24	117.50	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	501	CLA	CHD-C1D-ND	-3.24	121.48	124.45
25	c	503	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
25	b	613	CLA	CMB-C2B-C3B	3.24	130.74	124.68
26	d	401	PHO	O2D-CGD-O1D	-3.24	117.51	123.84
29	F	102	SQD	O8-S-C6	3.23	110.89	105.74
25	C	505	CLA	CMB-C2B-C3B	3.23	130.72	124.68
30	h	102	DGD	C1D-C2D-C3D	-3.23	103.28	110.00
25	B	610	CLA	CHB-C4A-NA	3.22	128.97	124.51
25	b	609	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
25	b	604	CLA	CHD-C1D-ND	-3.22	121.50	124.45
30	a	616	DGD	C1G-C2G-C3G	-3.21	104.28	111.80
25	c	502	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
25	b	613	CLA	CHD-C1D-ND	-3.20	121.51	124.45
25	b	610	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
25	c	503	CLA	C1-C2-C3	-3.20	120.52	126.04
29	f	101	SQD	O47-C7-C8	3.19	119.71	110.80
29	l	101	SQD	O48-C23-C24	3.19	121.92	111.91
25	B	601	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
31	x	102	STE	C3-C2-C1	-3.19	106.44	114.47
32	d	410	LMG	O6-C1-O1	-3.19	102.43	109.97
30	c	518	DGD	O6D-C1D-O3G	-3.18	102.43	109.97
25	C	503	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
25	c	510	CLA	CMB-C2B-C3B	3.18	130.62	124.68
25	C	513	CLA	CMB-C2B-C3B	3.17	130.62	124.68
25	B	612	CLA	CMB-C2B-C3B	3.16	130.60	124.68
25	b	603	CLA	CMB-C2B-C3B	3.16	130.59	124.68
25	c	508	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
25	b	614	CLA	CMB-C2B-C3B	3.16	130.59	124.68
25	B	604	CLA	C7-C6-C5	-3.15	104.79	113.36
25	b	602	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
31	M	102	STE	C3-C2-C1	-3.15	106.53	114.47
25	A	607	CLA	CHB-C4A-NA	3.14	128.86	124.51
25	h	101	CLA	CMB-C2B-C3B	3.14	130.56	124.68
25	b	604	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	B	602	CLA	O2A-CGA-O1A	-3.14	115.68	123.59
30	H	103	DGD	C1D-C2D-C3D	-3.13	103.47	110.00
25	b	601	CLA	C2D-C1D-ND	-3.13	107.80	110.10
25	B	601	CLA	CHB-C4A-NA	3.13	128.84	124.51
25	B	602	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	b	605	CLA	CMB-C2B-C3B	3.11	130.50	124.68
25	B	611	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
25	b	602	CLA	CMB-C2B-C3B	3.11	130.50	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	504	CLA	O2A-CGA-O1A	-3.11	115.75	123.59
28	D	405	PL9	C36-C34-C33	-3.11	114.83	121.12
25	A	610	CLA	O2D-CGD-CBD	3.10	116.77	111.27
25	C	511	CLA	C1-C2-C3	-3.09	120.69	126.04
25	B	609	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
25	D	403	CLA	CMB-C2B-C3B	3.08	130.44	124.68
30	h	102	DGD	C3D-C4D-C5D	-3.07	104.76	110.24
29	l	101	SQD	C1-C2-C3	-3.06	103.62	110.00
25	c	505	CLA	CMB-C2B-C3B	3.06	130.40	124.68
25	C	513	CLA	CHD-C1D-ND	-3.06	121.64	124.45
25	A	613	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	b	613	CLA	C1-C2-C3	-3.05	120.76	126.04
28	d	405	PL9	C37-C38-C39	-3.05	120.31	127.66
25	b	610	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
30	C	518	DGD	O6D-C1D-O3G	-3.04	102.76	109.97
29	a	614	SQD	O9-S-C6	3.04	110.56	106.94
25	C	501	CLA	O2A-CGA-O1A	-3.04	115.93	123.59
25	b	612	CLA	O2D-CGD-CBD	3.04	116.66	111.27
25	b	610	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	a	614	SQD	C1-C2-C3	-3.04	103.67	110.00
25	b	607	CLA	CHD-C1D-ND	-3.03	121.67	124.45
25	C	507	CLA	CMB-C2B-C3B	3.03	130.36	124.68
36	v	201	HEC	CBA-CAA-C2A	-3.03	107.50	112.60
25	h	101	CLA	CHB-C4A-NA	3.03	128.70	124.51
25	a	607	CLA	CMB-C2B-C3B	3.03	130.34	124.68
25	c	509	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
25	c	501	CLA	CMB-C2B-C3B	3.03	130.34	124.68
27	x	101	BCR	C27-C26-C25	3.03	127.13	122.73
25	c	507	CLA	CMB-C2B-C3B	3.03	130.34	124.68
25	C	504	CLA	CHD-C1D-ND	-3.03	121.67	124.45
27	T	101	BCR	C3-C4-C5	-3.02	108.68	114.08
30	C	517	DGD	O2D-C2D-C1D	-3.02	102.72	110.05
25	b	608	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
25	B	605	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
28	d	405	PL9	C7-C8-C9	-3.01	121.78	126.79
25	C	505	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
29	F	102	SQD	O9-S-O7	-3.00	103.55	113.95
25	a	610	CLA	CMB-C2B-C3B	3.00	130.30	124.68
29	l	101	SQD	O9-S-O7	-3.00	103.57	113.95
25	c	508	CLA	C1-C2-C3	-3.00	120.86	126.04
27	A	611	BCR	C27-C26-C25	3.00	127.08	122.73
25	B	613	CLA	O2D-CGD-O1D	-3.00	117.98	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	607	CLA	CMB-C2B-C3B	2.99	130.27	124.68
27	B	618	BCR	C29-C30-C25	2.99	115.08	110.48
27	C	514	BCR	C15-C16-C17	-2.98	117.36	123.47
25	d	403	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
27	T	101	BCR	C2-C1-C6	2.98	115.07	110.48
25	B	603	CLA	CMB-C2B-C3B	2.98	130.25	124.68
25	b	603	CLA	C1-C2-C3	-2.97	120.90	126.04
32	D	406	LMG	O1-C1-C2	-2.97	103.66	108.30
31	b	622	STE	C3-C2-C1	-2.97	106.98	114.47
25	h	101	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
25	C	512	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	C	507	CLA	CHB-C4A-NA	2.96	128.61	124.51
25	b	613	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
32	C	515	LMG	C1-O6-C5	-2.96	107.88	113.69
25	a	613	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	B	605	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
25	C	503	CLA	CMB-C2B-C3B	2.96	130.21	124.68
27	T	101	BCR	C27-C26-C25	2.95	127.02	122.73
25	C	503	CLA	C7-C6-C5	-2.95	105.35	113.36
25	A	606	CLA	CHB-C4A-NA	2.95	128.59	124.51
32	b	620	LMG	O2-C2-C1	-2.95	102.89	110.05
33	d	408	LHG	O8-C23-C24	2.95	121.15	111.91
29	F	102	SQD	C1-C2-C3	-2.94	103.86	110.00
29	A	614	SQD	O5-C1-C2	-2.94	104.12	110.35
27	d	404	BCR	C27-C26-C25	2.92	126.97	122.73
25	b	612	CLA	C2D-C1D-ND	-2.92	107.95	110.10
25	b	601	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
25	c	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	a	613	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
25	C	502	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
29	F	102	SQD	O6-C1-C2	2.90	112.83	108.30
28	A	612	PL9	C20-C19-C21	2.90	120.15	115.27
28	D	405	PL9	C35-C34-C36	2.90	120.14	115.27
33	D	407	LHG	O8-C23-C24	2.89	120.99	111.91
29	f	101	SQD	O48-C23-C24	2.89	120.98	111.91
25	c	505	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
32	b	620	LMG	O1-C1-C2	-2.88	103.80	108.30
30	C	516	DGD	O6D-C1D-O3G	-2.88	103.15	109.97
27	d	404	BCR	C11-C10-C9	-2.88	123.20	127.31
25	A	613	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	a	610	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
25	A	607	CLA	CHD-C1D-ND	-2.88	121.81	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	520	LMG	O6-C1-O1	-2.87	103.17	109.97
25	c	513	CLA	O2D-CGD-CBD	2.87	116.37	111.27
32	m	101	LMG	O7-C10-O9	-2.87	116.76	123.70
25	b	612	CLA	CHB-C4A-NA	2.87	128.48	124.51
33	e	102	LHG	O8-C23-C24	2.87	120.90	111.91
25	b	610	CLA	C2D-C1D-ND	-2.87	107.99	110.10
25	c	512	CLA	CHD-C1D-ND	-2.86	121.82	124.45
32	b	620	LMG	C1-O6-C5	-2.86	108.08	113.69
25	C	501	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	a	608	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
25	a	608	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	B	606	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
25	B	611	CLA	C1-C2-C3	-2.85	121.11	126.04
29	L	101	SQD	C3-C4-C5	2.85	115.32	110.24
32	M	101	LMG	C38-C37-C36	-2.85	99.97	114.42
26	a	609	PHO	CMB-C2B-C3B	2.85	130.00	124.68
29	f	101	SQD	O9-S-C6	2.85	110.32	106.94
25	C	508	CLA	O2D-CGD-CBD	2.85	116.32	111.27
25	b	611	CLA	CHB-C4A-NA	2.84	128.45	124.51
28	d	405	PL9	C40-C39-C41	2.84	120.06	115.27
25	B	605	CLA	O2D-CGD-CBD	2.84	116.32	111.27
27	B	617	BCR	C35-C13-C14	-2.84	118.95	122.92
25	c	512	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	c	504	CLA	CHD-C1D-ND	-2.84	121.85	124.45
28	d	405	PL9	C12-C13-C14	-2.84	120.83	127.66
27	x	101	BCR	C2-C1-C6	2.83	114.84	110.48
25	d	403	CLA	CHD-C1D-ND	-2.83	121.85	124.45
25	b	601	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
25	b	607	CLA	CHB-C4A-NA	2.82	128.42	124.51
25	B	610	CLA	CMB-C2B-C3B	2.82	129.96	124.68
28	d	405	PL9	C22-C23-C24	-2.82	120.87	127.66
27	c	515	BCR	C15-C16-C17	-2.82	117.69	123.47
25	D	403	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	B	614	CLA	C7-C6-C5	-2.82	105.70	113.36
28	d	405	PL9	C7-C3-C2	-2.82	119.59	123.30
27	H	102	BCR	C16-C15-C14	-2.81	117.71	123.47
33	B	622	LHG	C11-C10-C9	-2.81	100.15	114.42
30	H	103	DGD	O2D-C2D-C1D	-2.80	103.23	110.05
25	B	603	CLA	O2D-CGD-CBD	2.80	116.24	111.27
25	c	513	CLA	CHB-C4A-NA	2.80	128.38	124.51
31	m	102	STE	O2-C1-C2	2.80	123.01	114.03
25	A	607	CLA	O2A-CGA-O1A	-2.80	116.54	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	A	616	DGD	O6D-C1D-O3G	-2.80	103.35	109.97
29	F	102	SQD	O48-C23-C24	2.80	120.68	111.91
30	C	517	DGD	C6D-O5D-C1E	2.79	119.20	113.74
27	b	617	BCR	C27-C26-C25	2.79	126.78	122.73
25	b	606	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
26	A	608	PHO	CMA-C3A-C4A	-2.78	108.28	114.38
27	c	514	BCR	C33-C5-C6	-2.78	121.40	124.53
25	c	509	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	B	608	CLA	CMB-C2B-C3B	2.78	129.88	124.68
29	L	101	SQD	O9-S-C6	2.78	110.24	106.94
28	D	405	PL9	C7-C3-C2	-2.77	119.66	123.30
33	B	622	LHG	O8-C23-C24	2.77	120.59	111.91
27	K	102	BCR	C33-C5-C6	-2.76	121.42	124.53
25	C	504	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	B	611	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	d	402	CLA	O2A-CGA-O1A	-2.76	116.64	123.59
25	b	610	CLA	CMB-C2B-C3B	2.75	129.83	124.68
25	b	604	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	C	512	CLA	O2D-CGD-CBD	2.75	116.16	111.27
25	b	615	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	C	514	BCR	C2-C1-C6	2.75	114.71	110.48
27	A	611	BCR	C11-C10-C9	-2.75	123.39	127.31
28	D	405	PL9	C7-C8-C9	-2.75	122.22	126.79
25	a	607	CLA	C1B-CHB-C4A	-2.74	124.68	130.12
25	c	509	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	b	606	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	A	606	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
33	B	622	LHG	O8-C23-O10	-2.74	116.69	123.59
31	t	102	STE	C3-C2-C1	-2.73	107.58	114.47
25	c	506	CLA	CMB-C2B-C3B	2.73	129.79	124.68
36	v	201	HEC	C1D-C2D-C3D	-2.73	105.10	107.00
27	c	514	BCR	C2-C1-C6	2.73	114.68	110.48
25	b	607	CLA	O2D-CGD-CBD	2.72	116.11	111.27
28	D	405	PL9	C20-C19-C21	2.72	119.85	115.27
25	b	604	CLA	C1-C2-C3	-2.72	121.34	126.04
25	b	607	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
27	K	102	BCR	C27-C26-C25	2.72	126.68	122.73
25	b	613	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
27	K	101	BCR	C2-C1-C6	2.72	114.66	110.48
27	H	102	BCR	C2-C1-C6	2.71	114.66	110.48
30	A	616	DGD	O5D-C6D-C5D	-2.71	104.03	109.05
27	D	404	BCR	C3-C4-C5	-2.71	109.24	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	503	CLA	CHD-C1D-ND	-2.71	121.96	124.45
25	B	609	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
35	e	101	HEM	C3B-C2B-C1B	2.71	108.50	106.49
29	A	614	SQD	C45-O47-C7	-2.71	111.12	117.79
25	a	608	CLA	CMB-C2B-C3B	2.71	129.74	124.68
32	d	410	LMG	O2-C2-C1	-2.70	103.48	110.05
25	c	501	CLA	C2D-C1D-ND	-2.70	108.11	110.10
32	D	406	LMG	O3-C3-C2	-2.70	104.11	110.35
25	b	602	CLA	CHB-C4A-NA	2.70	128.24	124.51
32	C	519	LMG	O6-C1-O1	-2.69	103.60	109.97
26	a	609	PHO	OBD-CAD-CBD	-2.69	121.88	125.82
32	m	101	LMG	C1-O6-C5	-2.69	108.41	113.69
27	b	616	BCR	C35-C13-C14	-2.69	119.16	122.92
27	c	514	BCR	C27-C26-C25	2.68	126.63	122.73
25	B	611	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	C	513	CLA	CHB-C4A-NA	2.68	128.21	124.51
25	B	607	CLA	O2D-CGD-CBD	2.68	116.03	111.27
25	a	608	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
25	C	506	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
35	e	101	HEM	C1B-NB-C4B	2.67	107.83	105.07
27	b	618	BCR	C15-C16-C17	-2.67	118.01	123.47
25	b	604	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
30	c	517	DGD	O6D-C1D-O3G	-2.67	103.66	109.97
29	A	614	SQD	O8-S-C6	2.67	109.99	105.74
25	C	503	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	B	608	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
30	c	517	DGD	O3E-C3E-C2E	-2.66	104.19	110.35
25	c	511	CLA	CMB-C2B-C3B	2.66	129.66	124.68
25	a	607	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
32	C	519	LMG	O1-C7-C8	-2.65	104.49	110.90
25	b	608	CLA	CHD-C1D-ND	-2.65	122.02	124.45
25	c	505	CLA	O2D-CGD-CBD	2.65	115.98	111.27
28	D	405	PL9	C40-C39-C41	2.65	119.73	115.27
25	a	610	CLA	O2D-CGD-CBD	2.65	115.97	111.27
30	C	517	DGD	O5D-C6D-C5D	-2.65	104.15	109.05
26	a	609	PHO	O2A-CGA-O1A	-2.65	116.91	123.59
25	C	511	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	c	512	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
27	c	515	BCR	C33-C5-C6	-2.64	121.56	124.53
25	c	505	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
25	D	403	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
36	V	201	HEC	CAD-CBD-CGD	-2.64	106.37	113.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	H	103	DGD	C3E-C4E-C5E	-2.63	105.54	110.24
25	c	503	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	f	101	SQD	C1-C2-C3	-2.63	104.51	110.00
25	A	606	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
25	b	614	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	A	610	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
25	B	601	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
33	d	406	LHG	O8-C23-O10	-2.63	116.96	123.59
25	c	503	CLA	CMB-C2B-C3B	2.63	129.59	124.68
29	l	101	SQD	O5-C5-C4	2.63	114.47	109.69
25	C	511	CLA	CMB-C2B-C3B	2.62	129.59	124.68
33	D	407	LHG	C27-C26-C25	-2.62	101.11	114.42
25	B	615	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
25	B	602	CLA	O2D-CGD-CBD	2.62	115.93	111.27
25	D	402	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
27	b	617	BCR	C8-C7-C6	-2.62	119.84	127.20
25	D	402	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
30	h	102	DGD	CDB-CCB-CBB	-2.62	101.14	114.42
25	B	613	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
25	c	512	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
30	C	516	DGD	CDB-CCB-CBB	-2.61	101.16	114.42
25	B	605	CLA	CGD-CBD-CAD	-2.61	102.27	110.73
27	b	616	BCR	C15-C14-C13	-2.61	123.58	127.31
25	B	609	CLA	CHC-C1C-NC	2.61	128.17	124.20
25	C	504	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
27	K	101	BCR	C24-C23-C22	-2.61	122.29	126.23
25	b	611	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
25	B	602	CLA	CHD-C1D-ND	-2.61	122.06	124.45
30	C	516	DGD	O5D-C6D-C5D	-2.60	104.23	109.05
30	a	616	DGD	CDB-CCB-CBB	-2.60	101.20	114.42
28	A	612	PL9	C36-C34-C33	-2.60	115.85	121.12
36	v	201	HEC	CAD-CBD-CGD	-2.60	106.46	113.76
33	D	407	LHG	C18-C17-C16	-2.60	101.21	114.42
29	a	614	SQD	C3-C4-C5	2.60	114.88	110.24
25	B	604	CLA	CAA-CBA-CGA	-2.60	105.65	113.25
25	b	612	CLA	C1D-ND-C4D	2.60	108.18	106.33
27	t	101	BCR	C2-C1-C6	2.60	114.48	110.48
31	B	625	STE	O2-C1-C2	2.59	122.37	114.03
27	b	616	BCR	C3-C4-C5	-2.59	109.44	114.08
27	H	102	BCR	C27-C26-C25	2.59	126.50	122.73
30	C	517	DGD	CDB-CCB-CBB	-2.59	101.28	114.42
25	B	611	CLA	C11-C12-C13	-2.59	107.55	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	609	PHO	CMC-C2C-C3C	2.59	129.82	124.94
27	c	514	BCR	C15-C14-C13	-2.58	123.62	127.31
27	k	101	BCR	C33-C5-C6	-2.58	121.63	124.53
27	D	404	BCR	C28-C27-C26	-2.58	109.47	114.08
28	A	612	PL9	C27-C28-C29	-2.58	121.44	127.66
33	E	101	LHG	O8-C23-C24	2.58	120.00	111.91
25	A	613	CLA	O2D-CGD-CBD	2.58	115.85	111.27
25	c	502	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
25	c	510	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	B	605	CLA	CMB-C2B-C3B	2.58	129.50	124.68
30	c	519	DGD	C3G-C2G-C1G	-2.58	105.69	111.79
30	c	517	DGD	C3D-C4D-C5D	-2.57	105.65	110.24
25	C	502	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
32	b	620	LMG	C3-C4-C5	-2.57	105.65	110.24
27	c	516	BCR	C27-C26-C25	2.57	126.47	122.73
25	c	506	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
25	b	602	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
25	C	503	CLA	O2A-C1-C2	-2.57	101.88	108.64
27	A	611	BCR	C37-C22-C21	-2.57	119.32	122.92
25	D	402	CLA	C4-C3-C5	2.57	119.59	115.27
30	C	517	DGD	C1D-C2D-C3D	-2.57	104.65	110.00
30	c	519	DGD	O5D-C1E-C2E	2.57	112.31	108.30
30	C	518	DGD	CDB-CCB-CBB	-2.57	101.40	114.42
29	A	614	SQD	O9-S-C6	2.57	109.99	106.94
25	b	611	CLA	C11-C12-C13	-2.56	107.63	115.92
25	B	612	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
25	b	603	CLA	C11-C12-C13	-2.56	107.65	115.92
25	c	510	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
25	a	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
30	h	102	DGD	O6D-C1D-O3G	-2.55	103.92	109.97
30	c	517	DGD	O5D-C6D-C5D	-2.55	104.32	109.05
25	A	607	CLA	C1-C2-C3	-2.55	121.63	126.04
25	B	604	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
27	B	618	BCR	C2-C1-C6	2.55	114.41	110.48
27	b	618	BCR	C11-C10-C9	-2.54	123.68	127.31
25	a	613	CLA	O2D-CGD-CBD	2.54	115.79	111.27
27	B	618	BCR	C37-C22-C21	-2.54	119.36	122.92
30	A	616	DGD	C3G-C2G-C1G	-2.54	105.78	111.79
27	K	101	BCR	C27-C26-C25	2.54	126.42	122.73
30	A	616	DGD	C4E-C3E-C2E	-2.54	106.39	110.82
28	D	405	PL9	C27-C28-C29	-2.54	121.55	127.66
33	E	101	LHG	C11-C10-C9	-2.54	101.54	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	502	CLA	CMB-C2B-C3B	2.54	129.42	124.68
29	l	101	SQD	C1-O5-C5	-2.53	108.71	113.69
27	b	616	BCR	C27-C26-C25	2.53	126.41	122.73
25	C	509	CLA	CHD-C1D-C2D	2.53	130.78	125.48
30	c	517	DGD	CDB-CCB-CBB	-2.53	101.59	114.42
29	A	614	SQD	O47-C7-O49	-2.53	117.59	123.70
25	c	506	CLA	CHB-C4A-NA	2.53	128.01	124.51
35	e	101	HEM	CHB-C1B-NB	2.52	127.50	124.38
25	B	614	CLA	CMB-C2B-C1B	-2.52	124.58	128.46
33	l	102	LHG	C20-C19-C18	-2.52	101.61	114.42
30	A	616	DGD	CDB-CCB-CBB	-2.52	101.62	114.42
32	c	522	LMG	C4-C3-C2	2.52	115.22	110.82
25	C	512	CLA	C1-C2-C3	-2.52	121.68	126.04
25	C	502	CLA	CHD-C1D-ND	-2.52	122.14	124.45
25	c	512	CLA	CMB-C2B-C3B	2.52	129.39	124.68
27	B	617	BCR	C2-C1-C6	2.52	114.36	110.48
30	h	102	DGD	O6E-C1E-O5D	-2.51	104.02	109.97
33	D	408	LHG	O8-C23-C24	2.51	119.80	111.91
25	c	505	CLA	C1-C2-C3	-2.51	121.70	126.04
32	D	406	LMG	O6-C1-O1	-2.51	104.02	109.97
33	d	406	LHG	C11-C10-C9	-2.51	101.67	114.42
30	c	519	DGD	CAB-C9B-C8B	-2.51	101.68	114.42
25	D	403	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	A	613	CLA	C16-C15-C13	-2.51	107.81	115.92
25	B	606	CLA	CED-O2D-CGD	2.51	121.61	115.94
32	b	620	LMG	O7-C10-O9	-2.51	117.64	123.70
25	d	403	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
25	C	502	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
26	a	609	PHO	CMD-C2D-C3D	2.49	129.34	124.68
27	a	611	BCR	C27-C26-C25	2.49	126.35	122.73
25	C	503	CLA	CHB-C4A-NA	2.49	127.96	124.51
32	c	522	LMG	O6-C1-O1	-2.49	104.08	109.97
29	l	101	SQD	O8-S-C6	2.49	109.71	105.74
25	B	615	CLA	CHD-C1D-ND	-2.49	122.17	124.45
30	C	518	DGD	C3G-C2G-C1G	-2.49	105.91	111.79
25	b	607	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
25	c	506	CLA	C1-C2-C3	-2.48	121.75	126.04
25	B	615	CLA	CAA-CBA-CGA	-2.48	106.00	113.25
29	f	101	SQD	C3-C4-C5	2.48	114.66	110.24
28	a	612	PL9	C7-C8-C9	-2.48	122.66	126.79
27	H	102	BCR	C35-C13-C14	-2.48	119.45	122.92
25	a	610	CLA	CHB-C4A-NA	2.48	127.94	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	613	CLA	C2D-C1D-ND	-2.48	108.28	110.10
25	C	508	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	B	608	CLA	CHD-C1D-ND	-2.48	122.18	124.45
30	H	103	DGD	O6D-C1D-O3G	-2.47	104.12	109.97
27	t	101	BCR	C33-C5-C6	-2.47	121.75	124.53
25	b	603	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
25	A	610	CLA	CHB-C4A-NA	2.47	127.93	124.51
28	D	405	PL9	C42-C43-C44	-2.47	121.71	127.66
30	H	103	DGD	CDB-CCB-CBB	-2.47	101.89	114.42
25	b	603	CLA	CHD-C1D-ND	-2.47	122.19	124.45
27	K	101	BCR	C35-C13-C14	-2.47	119.47	122.92
25	a	610	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
29	f	101	SQD	C1-O5-C5	-2.47	108.85	113.69
30	a	616	DGD	CBB-CAB-C9B	-2.46	101.92	114.42
27	c	515	BCR	C27-C26-C25	2.46	126.31	122.73
27	k	101	BCR	C27-C26-C25	2.46	126.31	122.73
25	a	608	CLA	O2D-CGD-CBD	2.46	115.64	111.27
27	c	516	BCR	C33-C5-C6	-2.46	121.77	124.53
31	C	520	STE	C3-C2-C1	-2.45	108.30	114.47
25	C	508	CLA	C3C-C4C-NC	-2.45	107.83	110.57
25	B	612	CLA	CED-O2D-CGD	2.44	121.47	115.94
29	A	614	SQD	O48-C23-C24	2.44	119.58	111.91
33	l	102	LHG	O8-C23-C24	2.44	119.57	111.91
25	B	602	CLA	C2D-C1D-ND	-2.44	108.30	110.10
28	a	612	PL9	C37-C38-C39	-2.44	121.78	127.66
25	a	607	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	c	514	BCR	C15-C16-C17	-2.44	118.47	123.47
25	b	608	CLA	C1-C2-C3	-2.44	121.82	126.04
28	a	612	PL9	C22-C23-C24	-2.44	121.78	127.66
28	A	612	PL9	C12-C13-C14	-2.44	121.79	127.66
25	B	601	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
32	m	101	LMG	O3-C3-C2	-2.44	104.71	110.35
32	M	101	LMG	C40-C39-C38	-2.44	102.04	114.42
25	c	501	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	C	501	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
25	C	503	CLA	O1D-CGD-CBD	2.44	129.47	124.48
27	b	618	BCR	C37-C22-C21	-2.44	119.51	122.92
28	A	612	PL9	C31-C32-C33	-2.43	103.90	111.88
25	C	512	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
30	C	517	DGD	C5B-C4B-C3B	-2.43	102.11	114.42
33	D	408	LHG	C27-C26-C25	-2.43	102.11	114.42
30	C	517	DGD	O2G-C1B-O1B	-2.42	117.85	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	f	101	SQD	O8-S-C6	2.42	109.60	105.74
33	l	102	LHG	C18-C17-C16	-2.42	102.14	114.42
27	C	514	BCR	C33-C5-C6	-2.42	121.81	124.53
25	B	610	CLA	CHD-C1D-C2D	2.41	130.54	125.48
25	c	504	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
27	B	617	BCR	C3-C4-C5	-2.41	109.78	114.08
25	B	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	c	507	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
25	C	506	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
25	C	507	CLA	C2A-C1A-CHA	2.40	128.05	123.86
30	c	519	DGD	CDB-CCB-CBB	-2.40	102.26	114.42
25	c	507	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
25	d	403	CLA	CHB-C4A-NA	2.40	127.82	124.51
28	A	612	PL9	C7-C8-C9	-2.39	122.81	126.79
29	a	615	SQD	C9-C8-C7	-2.39	104.92	113.62
27	C	514	BCR	C27-C26-C25	2.39	126.20	122.73
32	d	410	LMG	O1-C1-C2	-2.39	104.57	108.30
25	c	505	CLA	C11-C10-C8	-2.39	108.20	115.92
28	A	612	PL9	C22-C23-C24	-2.39	121.91	127.66
32	m	101	LMG	C40-C39-C38	-2.39	102.31	114.42
25	c	507	CLA	CHB-C4A-NA	2.39	127.81	124.51
25	c	513	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
33	D	408	LHG	C11-C10-C9	-2.39	102.31	114.42
27	c	515	BCR	C7-C8-C9	-2.39	122.63	126.23
25	b	612	CLA	C1-C2-C3	-2.38	121.92	126.04
25	b	601	CLA	O2D-CGD-CBD	2.38	115.50	111.27
27	K	102	BCR	C8-C7-C6	-2.38	120.51	127.20
25	B	604	CLA	O1D-CGD-CBD	2.38	129.36	124.48
25	B	603	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
28	A	612	PL9	O2-C1-C2	-2.38	116.33	121.78
26	A	608	PHO	CMC-C2C-C3C	2.38	129.42	124.94
25	B	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
27	t	101	BCR	C11-C10-C9	-2.37	123.92	127.31
25	C	510	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	b	614	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	c	518	DGD	CDB-CCB-CBB	-2.37	102.40	114.42
25	b	602	CLA	O2D-CGD-CBD	2.37	115.47	111.27
25	c	502	CLA	C1-C2-C3	-2.37	121.95	126.04
35	e	101	HEM	CAB-C3B-C2B	-2.36	120.81	128.60
30	c	519	DGD	O6E-C5E-C4E	2.36	113.99	109.69
25	C	512	CLA	C2D-C1D-ND	-2.36	108.36	110.10
25	H	101	CLA	O2D-CGD-CBD	2.36	115.46	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	609	CLA	O2D-CGD-CBD	2.36	115.46	111.27
25	C	509	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
32	C	515	LMG	C38-C37-C36	-2.36	102.46	114.42
25	c	508	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
30	c	517	DGD	O1G-C1A-O1A	-2.36	117.65	123.59
25	B	609	CLA	CMB-C2B-C3B	2.35	129.08	124.68
25	C	511	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
25	b	615	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
29	f	101	SQD	O5-C1-C2	-2.35	105.37	110.35
33	l	102	LHG	C11-C10-C9	-2.35	102.48	114.42
28	D	405	PL9	C31-C32-C33	-2.35	104.15	111.88
30	C	517	DGD	C7B-C6B-C5B	-2.35	102.49	114.42
29	L	101	SQD	O8-S-C6	2.35	109.48	105.74
25	B	615	CLA	C1-C2-C3	2.35	130.10	126.04
25	A	606	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
25	A	613	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	b	603	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	D	402	CLA	C1-C2-C3	-2.34	122.00	126.04
30	C	516	DGD	C3D-C4D-C5D	-2.34	106.07	110.24
27	t	101	BCR	C35-C13-C14	-2.34	119.65	122.92
25	b	603	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	C	506	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	D	402	CLA	C2D-C1D-ND	-2.33	108.39	110.10
25	b	610	CLA	CHB-C4A-NA	2.33	127.73	124.51
27	c	516	BCR	C11-C10-C9	-2.33	123.99	127.31
25	c	508	CLA	CHD-C1D-C2D	2.33	130.36	125.48
25	C	509	CLA	C1-C2-C3	-2.33	122.02	126.04
25	h	101	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
25	C	508	CLA	CHD-C1D-C2D	2.32	130.35	125.48
25	c	503	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
33	E	101	LHG	C20-C19-C18	-2.32	102.65	114.42
28	D	405	PL9	C50-C49-C48	-2.32	115.94	122.65
25	A	610	CLA	CHD-C4C-NC	2.32	127.86	124.20
27	t	101	BCR	C15-C14-C13	-2.32	124.00	127.31
32	c	520	LMG	C38-C37-C36	-2.32	102.65	114.42
25	b	610	CLA	CHD-C1D-C2D	2.32	130.34	125.48
30	c	518	DGD	O2E-C2E-C1E	-2.32	104.41	110.05
27	x	101	BCR	C3-C4-C5	-2.32	109.94	114.08
25	c	508	CLA	O2D-CGD-CBD	2.32	115.39	111.27
27	d	404	BCR	C38-C26-C25	-2.32	121.93	124.53
27	T	101	BCR	C7-C8-C9	-2.32	122.73	126.23
25	c	506	CLA	O2D-CGD-O1D	-2.32	119.31	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	407	LHG	C20-C19-C18	-2.31	102.67	114.42
30	C	516	DGD	CAB-C9B-C8B	-2.31	102.68	114.42
35	e	101	HEM	C4B-CHC-C1C	2.31	125.61	122.56
32	d	410	LMG	C40-C39-C38	-2.31	102.69	114.42
25	a	613	CLA	CHD-C1D-C2D	2.31	130.33	125.48
27	d	404	BCR	C30-C25-C26	-2.31	119.36	122.61
26	A	608	PHO	O2A-CGA-O1A	-2.31	117.76	123.59
27	D	404	BCR	C38-C26-C25	-2.31	121.93	124.53
25	c	513	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
25	B	613	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	b	601	CLA	C11-C10-C8	-2.31	108.46	115.92
27	A	611	BCR	C16-C15-C14	-2.31	118.75	123.47
25	B	612	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
25	b	612	CLA	C16-C15-C13	-2.30	108.47	115.92
27	a	611	BCR	C11-C10-C9	-2.30	124.02	127.31
27	b	618	BCR	C7-C8-C9	-2.30	122.75	126.23
32	B	620	LMG	C38-C37-C36	-2.30	102.73	114.42
25	c	505	CLA	CMD-C2D-C3D	2.30	132.91	127.61
25	C	510	CLA	O2D-CGD-CBD	2.30	115.36	111.27
25	C	507	CLA	C1-C2-C3	-2.30	122.06	126.04
32	D	406	LMG	C38-C37-C36	-2.30	102.75	114.42
33	e	102	LHG	C11-C10-C9	-2.30	102.75	114.42
28	D	405	PL9	C37-C38-C39	-2.30	122.12	127.66
28	a	612	PL9	C40-C39-C41	2.30	119.14	115.27
27	D	404	BCR	C2-C1-C6	2.29	114.01	110.48
25	a	607	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
25	c	501	CLA	C1-C2-C3	-2.29	122.08	126.04
28	d	405	PL9	C32-C33-C34	-2.29	122.14	127.66
30	c	518	DGD	O5D-C6D-C5D	-2.29	104.81	109.05
32	c	522	LMG	O3-C3-C2	-2.29	105.05	110.35
30	c	519	DGD	C8B-C7B-C6B	-2.29	102.81	114.42
25	d	403	CLA	C1-C2-C3	-2.29	122.08	126.04
25	b	609	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
28	a	612	PL9	C27-C28-C29	-2.28	122.16	127.66
30	c	519	DGD	O6D-C1D-O3G	-2.28	104.57	109.97
27	B	616	BCR	C3-C4-C5	-2.28	110.00	114.08
25	A	607	CLA	C3C-C4C-NC	-2.28	108.01	110.57
25	b	605	CLA	CHB-C4A-NA	2.28	127.66	124.51
27	K	102	BCR	C16-C15-C14	-2.28	118.81	123.47
25	c	508	CLA	CHD-C4C-NC	2.28	127.79	124.20
27	D	404	BCR	C7-C8-C9	-2.28	122.80	126.23
25	B	604	CLA	C1B-CHB-C4A	-2.28	125.61	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	614	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
25	B	602	CLA	C7-C6-C5	-2.27	107.18	113.36
25	C	512	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
25	B	612	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	b	612	CLA	C7-C6-C5	-2.27	107.20	113.36
25	B	605	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
32	c	520	LMG	C40-C39-C38	-2.27	102.92	114.42
29	l	101	SQD	O6-C44-C45	2.27	116.37	110.90
25	A	606	CLA	C7-C6-C5	-2.27	107.20	113.36
33	B	622	LHG	C18-C17-C16	-2.27	102.92	114.42
30	c	519	DGD	O3D-C3D-C4D	-2.26	105.11	110.35
33	D	408	LHG	C18-C17-C16	-2.26	102.93	114.42
25	C	512	CLA	CAA-CBA-CGA	-2.26	106.64	113.25
33	d	407	LHG	O8-C23-C24	2.26	119.00	111.91
32	M	101	LMG	C1-O6-C5	-2.26	109.25	113.69
27	B	618	BCR	C15-C16-C17	-2.26	118.85	123.47
25	B	602	CLA	C4-C3-C5	2.26	119.07	115.27
27	t	101	BCR	C27-C26-C25	2.26	126.01	122.73
25	C	513	CLA	O2D-CGD-CBD	2.26	115.28	111.27
26	a	609	PHO	O1D-CGD-CBD	2.26	128.50	124.74
30	h	102	DGD	O3E-C3E-C2E	-2.25	105.14	110.35
27	t	101	BCR	C15-C16-C17	-2.25	118.86	123.47
25	c	510	CLA	C16-C15-C13	-2.25	108.63	115.92
25	b	609	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
32	b	620	LMG	O8-C28-O10	-2.25	117.91	123.59
27	K	102	BCR	C30-C25-C26	-2.25	119.45	122.61
31	J	101	STE	C3-C2-C1	-2.25	108.81	114.47
25	a	607	CLA	O1D-CGD-CBD	2.25	129.08	124.48
25	B	605	CLA	CHB-C4A-NA	2.25	127.62	124.51
33	D	407	LHG	O8-C23-O10	-2.25	117.92	123.59
30	h	102	DGD	O5D-C6D-C5D	-2.24	104.89	109.05
27	K	103	BCR	C24-C23-C22	-2.24	122.84	126.23
25	B	605	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
25	c	505	CLA	CHB-C4A-NA	2.24	127.61	124.51
25	B	609	CLA	CHD-C1D-ND	-2.24	122.39	124.45
32	b	620	LMG	C40-C39-C38	-2.24	103.05	114.42
27	b	616	BCR	C33-C5-C6	-2.24	122.01	124.53
33	d	408	LHG	C27-C26-C25	-2.24	103.05	114.42
25	A	606	CLA	CMB-C2B-C3B	2.24	128.87	124.68
25	H	101	CLA	CHD-C1D-ND	-2.24	122.40	124.45
32	d	409	LMG	O7-C10-O9	-2.24	117.72	123.30
28	D	405	PL9	C12-C13-C14	-2.24	122.27	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	101	CLA	CHD-C4C-NC	2.24	127.73	124.20
25	C	501	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
27	K	103	BCR	C27-C26-C25	2.24	125.98	122.73
31	j	101	STE	O2-C1-C2	2.23	121.21	114.03
25	C	513	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
25	c	504	CLA	CHB-C4A-NA	2.23	127.60	124.51
28	d	405	PL9	C36-C34-C33	-2.23	116.60	121.12
28	D	405	PL9	C11-C12-C13	-2.23	104.55	111.88
25	b	609	CLA	CMB-C2B-C3B	2.23	128.85	124.68
27	a	611	BCR	C7-C8-C9	-2.23	122.87	126.23
32	M	101	LMG	C1-C2-C3	-2.23	105.36	110.00
25	B	604	CLA	CHB-C4A-NA	2.22	127.58	124.51
28	a	612	PL9	O2-C1-C2	-2.22	116.69	121.78
25	b	611	CLA	C11-C10-C8	-2.22	108.74	115.92
27	c	514	BCR	C11-C10-C9	-2.22	124.14	127.31
33	B	621	LHG	C20-C19-C18	-2.22	103.15	114.42
32	C	519	LMG	C40-C39-C38	-2.22	103.16	114.42
30	C	517	DGD	CBB-CAB-C9B	-2.22	103.16	114.42
31	d	411	STE	O2-C1-C2	2.22	121.16	114.03
28	d	405	PL9	C20-C19-C21	2.22	119.00	115.27
30	c	519	DGD	O3G-C1D-C2D	-2.22	104.84	108.30
25	c	512	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
25	d	402	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
25	B	610	CLA	C3C-C4C-NC	-2.22	108.08	110.57
35	e	101	HEM	C4D-ND-C1D	2.22	107.36	105.07
25	C	504	CLA	CHD-C4C-NC	2.21	127.69	124.20
27	B	616	BCR	C29-C30-C25	2.21	113.89	110.48
28	D	405	PL9	O2-C1-C6	2.21	124.42	120.59
32	M	101	LMG	O3-C3-C2	-2.21	105.23	110.35
28	A	612	PL9	O2-C1-C6	2.21	124.42	120.59
33	l	102	LHG	C5-O7-C7	-2.21	112.35	117.79
25	C	510	CLA	CHD-C1D-ND	-2.21	122.42	124.45
32	C	519	LMG	C38-C37-C36	-2.21	103.21	114.42
31	J	101	STE	O2-C1-C2	2.21	121.13	114.03
27	b	618	BCR	C27-C26-C25	2.21	125.94	122.73
27	B	616	BCR	C33-C5-C6	-2.21	122.05	124.53
25	B	614	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
25	b	606	CLA	O2A-C1-C2	-2.21	102.83	108.64
33	E	101	LHG	C18-C17-C16	-2.21	103.23	114.42
30	A	616	DGD	CBB-CAB-C9B	-2.21	103.23	114.42
30	c	519	DGD	C6B-C5B-C4B	-2.20	103.23	114.42
27	B	617	BCR	C15-C16-C17	-2.20	118.96	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	H	103	DGD	CAB-C9B-C8B	-2.20	103.24	114.42
29	A	615	SQD	O48-C23-O10	-2.20	118.03	123.59
25	a	613	CLA	CMB-C2B-C3B	2.20	128.79	124.68
27	A	611	BCR	C8-C7-C6	-2.20	121.02	127.20
25	b	603	CLA	C4-C3-C5	2.20	118.97	115.27
25	c	511	CLA	CHB-C4A-NA	2.20	127.55	124.51
25	C	504	CLA	O2D-CGD-CBD	2.20	115.17	111.27
27	K	101	BCR	C33-C5-C6	-2.20	122.06	124.53
25	a	613	CLA	C3C-C4C-NC	-2.19	108.11	110.57
25	B	610	CLA	C11-C12-C13	-2.19	108.83	115.92
25	B	609	CLA	CHA-C1A-NA	-2.19	121.38	126.40
25	B	607	CLA	C6-C7-C8	-2.19	108.85	115.92
35	e	101	HEM	CHC-C4B-C3B	2.19	127.92	124.57
25	C	506	CLA	C1-C2-C3	-2.19	122.26	126.04
25	C	511	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
25	B	615	CLA	O1D-CGD-CBD	2.18	128.95	124.48
30	a	616	DGD	C5B-C4B-C3B	-2.18	103.36	114.42
25	B	613	CLA	C1-C2-C3	-2.18	122.27	126.04
32	d	410	LMG	O1-C7-C8	-2.18	105.64	110.90
25	b	604	CLA	O1D-CGD-CBD	2.18	128.94	124.48
33	e	102	LHG	C20-C19-C18	-2.18	103.37	114.42
32	D	409	LMG	O1-C7-C8	-2.18	106.01	111.78
25	B	606	CLA	O2A-C1-C2	-2.18	102.91	108.64
33	B	622	LHG	C20-C19-C18	-2.18	103.38	114.42
25	b	605	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
30	C	516	DGD	C6B-C5B-C4B	-2.18	103.38	114.42
31	t	102	STE	O2-C1-C2	2.17	121.02	114.03
25	a	607	CLA	C2D-C1D-ND	-2.17	108.50	110.10
25	c	510	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
25	B	609	CLA	C2A-C1A-CHA	2.17	127.65	123.86
30	h	102	DGD	CBB-CAB-C9B	-2.17	103.42	114.42
32	C	519	LMG	O3-C3-C2	-2.17	105.34	110.35
30	c	518	DGD	CBB-CAB-C9B	-2.17	103.42	114.42
25	b	604	CLA	CHB-C4A-NA	2.17	127.51	124.51
30	a	616	DGD	CFB-CEB-CDB	-2.17	103.42	114.42
26	a	609	PHO	O2D-CGD-O1D	-2.17	119.60	123.84
25	C	508	CLA	C2D-C1D-ND	-2.17	108.51	110.10
26	A	608	PHO	O1D-CGD-CBD	2.17	128.35	124.74
25	c	501	CLA	CHB-C4A-NA	2.17	127.51	124.51
25	b	608	CLA	CED-O2D-CGD	2.17	120.83	115.94
29	l	101	SQD	C25-C24-C23	-2.16	105.75	113.62
25	A	610	CLA	C1-C2-C3	-2.16	122.30	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	K	103	BCR	C15-C14-C13	-2.16	124.22	127.31
27	K	101	BCR	C7-C8-C9	-2.16	122.97	126.23
25	c	513	CLA	CHD-C1D-ND	-2.16	122.47	124.45
26	a	609	PHO	C1-C2-C3	-2.16	122.31	126.04
25	C	503	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
25	c	505	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
27	C	514	BCR	C7-C8-C9	-2.15	122.98	126.23
25	C	504	CLA	CHC-C1C-NC	2.15	127.47	124.20
25	B	610	CLA	C1-C2-C3	-2.15	122.32	126.04
25	B	601	CLA	CHD-C1D-ND	-2.15	122.48	124.45
25	b	606	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
25	b	614	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
25	C	509	CLA	CHB-C4A-NA	2.15	127.49	124.51
25	C	502	CLA	C1-C2-C3	-2.15	122.32	126.04
33	d	406	LHG	C20-C19-C18	-2.15	103.51	114.42
25	c	503	CLA	C7-C6-C5	-2.15	107.52	113.36
32	D	406	LMG	O2-C2-C1	-2.15	104.83	110.05
32	c	522	LMG	C6-C5-C4	-2.15	107.98	113.00
27	T	101	BCR	C30-C25-C26	-2.15	119.59	122.61
29	F	102	SQD	O5-C1-C2	-2.15	105.81	110.35
31	B	625	STE	C3-C2-C1	-2.14	109.07	114.47
30	A	616	DGD	C5B-C4B-C3B	-2.14	103.54	114.42
25	b	611	CLA	O1D-CGD-CBD	2.14	128.87	124.48
30	h	102	DGD	O6E-C5E-C6E	-2.14	101.11	106.44
25	C	509	CLA	CHD-C4C-NC	2.14	127.58	124.20
35	F	101	HEM	C4B-CHC-C1C	2.14	125.38	122.56
25	b	603	CLA	CHB-C4A-NA	2.14	127.47	124.51
25	A	607	CLA	O2D-CGD-CBD	2.14	115.07	111.27
25	C	511	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
30	c	519	DGD	C3D-C4D-C5D	-2.14	106.42	110.24
25	c	501	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	B	615	CLA	O2A-C1-C2	2.14	114.25	108.64
25	A	607	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
28	A	612	PL9	C11-C9-C8	-2.14	116.79	121.12
25	B	612	CLA	CAC-C3C-C4C	2.14	127.58	124.81
25	b	604	CLA	O2A-C1-C2	-2.14	103.02	108.64
25	B	611	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	d	402	CLA	C4-C3-C5	2.13	118.86	115.27
25	C	509	CLA	C3C-C4C-NC	-2.13	108.18	110.57
30	A	616	DGD	CFB-CEB-CDB	-2.13	103.59	114.42
25	C	507	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
25	c	508	CLA	C1B-CHB-C4A	-2.13	125.89	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	t	101	BCR	C7-C8-C9	-2.13	123.01	126.23
27	b	617	BCR	C33-C5-C6	-2.13	122.13	124.53
33	D	407	LHG	C11-C10-C9	-2.13	103.61	114.42
25	C	504	CLA	C4-C3-C5	2.13	118.85	115.27
28	a	612	PL9	C11-C12-C13	-2.13	104.88	111.88
29	a	615	SQD	O49-C7-C8	-2.13	115.43	123.73
25	B	614	CLA	CHD-C1D-ND	-2.13	122.50	124.45
27	C	514	BCR	C15-C14-C13	-2.13	124.27	127.31
29	F	102	SQD	C3-C4-C5	2.13	114.03	110.24
25	b	606	CLA	CHD-C1D-ND	-2.13	122.50	124.45
33	l	102	LHG	O8-C23-O10	-2.12	118.23	123.59
25	b	608	CLA	C7-C6-C5	-2.12	107.59	113.36
25	c	504	CLA	C6-C7-C8	-2.12	109.05	115.92
25	C	502	CLA	O2D-CGD-CBD	2.12	115.04	111.27
25	C	505	CLA	CHB-C4A-NA	2.12	127.45	124.51
27	b	617	BCR	C11-C10-C9	-2.12	124.28	127.31
25	B	614	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
27	b	617	BCR	C36-C18-C17	-2.12	119.96	122.92
27	T	101	BCR	C38-C26-C27	-2.12	109.55	113.62
32	d	409	LMG	C38-C37-C36	-2.12	103.68	114.42
32	C	515	LMG	O8-C28-O10	-2.12	118.25	123.59
30	h	102	DGD	C7B-C6B-C5B	-2.12	103.69	114.42
25	b	604	CLA	C4-C3-C5	2.11	118.83	115.27
27	A	611	BCR	C15-C14-C13	-2.11	124.29	127.31
27	A	611	BCR	C33-C5-C6	-2.11	122.16	124.53
32	c	522	LMG	C40-C39-C38	-2.11	103.70	114.42
25	b	607	CLA	CHD-C4C-NC	2.11	127.53	124.20
25	B	606	CLA	CHD-C1D-ND	-2.11	122.51	124.45
33	B	621	LHG	C11-C10-C9	-2.11	103.70	114.42
32	D	409	LMG	C38-C37-C36	-2.11	103.70	114.42
33	B	622	LHG	O3-P-O5	-2.11	100.82	109.07
27	K	103	BCR	C28-C27-C26	-2.11	110.31	114.08
25	A	606	CLA	C11-C12-C13	-2.11	109.10	115.92
33	E	101	LHG	C27-C26-C25	-2.11	103.71	114.42
25	B	609	CLA	O1D-CGD-CBD	2.11	128.80	124.48
28	a	612	PL9	C20-C19-C21	2.11	118.82	115.27
32	C	515	LMG	C40-C39-C38	-2.11	103.73	114.42
25	D	402	CLA	O2D-CGD-CBD	2.10	115.01	111.27
27	d	404	BCR	C3-C4-C5	-2.10	110.32	114.08
25	B	615	CLA	O2D-CGD-CBD	2.10	115.01	111.27
27	D	404	BCR	C27-C26-C25	2.10	125.78	122.73
25	b	605	CLA	CHD-C1D-ND	-2.10	122.52	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	603	CLA	C11-C10-C8	-2.10	109.12	115.92
30	a	616	DGD	CAB-C9B-C8B	-2.10	103.75	114.42
30	H	103	DGD	C4E-C3E-C2E	-2.10	107.15	110.82
32	M	101	LMG	O2-C2-C1	-2.10	104.94	110.05
25	a	610	CLA	CHA-C1A-NA	-2.10	121.59	126.40
32	m	101	LMG	C6-C5-C4	-2.10	108.09	113.00
30	h	102	DGD	C1D-O6D-C5D	-2.10	109.57	113.69
32	c	522	LMG	C38-C37-C36	-2.10	103.77	114.42
25	b	609	CLA	O1D-CGD-CBD	2.10	128.78	124.48
25	b	606	CLA	C4-C3-C5	2.10	118.80	115.27
27	B	616	BCR	C30-C25-C26	-2.10	119.66	122.61
25	b	608	CLA	CHB-C4A-NA	2.10	127.41	124.51
35	e	101	HEM	CMC-C2C-C3C	2.09	128.60	124.68
28	D	405	PL9	C36-C37-C38	-2.09	105.00	111.88
30	A	616	DGD	O3G-C3G-C2G	-2.09	105.85	110.90
25	b	615	CLA	O2D-CGD-CBD	2.09	114.99	111.27
33	d	407	LHG	O8-C23-O10	-2.09	118.31	123.59
29	F	102	SQD	C46-C45-C44	-2.09	106.75	113.70
25	c	508	CLA	C2D-C1D-ND	-2.09	108.56	110.10
32	b	620	LMG	O6-C5-C6	2.09	111.63	106.44
30	H	103	DGD	C3G-C2G-C1G	-2.09	106.85	111.79
30	a	616	DGD	C7B-C6B-C5B	-2.09	103.83	114.42
25	b	601	CLA	C11-C12-C13	-2.09	109.17	115.92
29	A	614	SQD	O6-C44-C45	-2.09	105.86	110.90
29	F	102	SQD	O5-C5-C4	2.09	113.48	109.69
25	H	101	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
25	c	510	CLA	C2D-C1D-ND	-2.09	108.57	110.10
30	C	516	DGD	C6D-O5D-C1E	2.08	117.81	113.74
27	K	103	BCR	C2-C1-C6	2.08	113.68	110.48
30	c	519	DGD	O2D-C2D-C1D	-2.08	105.00	110.05
30	H	103	DGD	C8B-C7B-C6B	-2.08	103.88	114.42
25	b	607	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
32	c	524	LMG	C40-C39-C38	-2.08	103.88	114.42
30	c	519	DGD	O3E-C3E-C2E	-2.08	105.55	110.35
30	h	102	DGD	CAB-C9B-C8B	-2.07	103.90	114.42
30	c	519	DGD	C7A-C6A-C5A	-2.07	103.90	114.42
29	a	615	SQD	O48-C23-O10	-2.07	118.36	123.59
25	C	506	CLA	CHA-C1A-NA	-2.07	121.66	126.40
32	c	524	LMG	C38-C37-C36	-2.07	103.92	114.42
29	a	614	SQD	O4-C4-C3	-2.07	105.56	110.35
31	m	102	STE	O2-C1-O1	-2.07	118.14	123.30
25	c	507	CLA	O2A-CGA-O1A	-2.07	118.38	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	520	LMG	O8-C28-O10	-2.07	118.38	123.59
25	a	608	CLA	CHD-C1D-ND	-2.07	122.56	124.45
30	c	517	DGD	C5B-C4B-C3B	-2.06	103.94	114.42
25	C	506	CLA	CHA-C4D-ND	2.06	136.82	132.50
28	A	612	PL9	C35-C34-C36	2.06	118.74	115.27
32	d	409	LMG	C40-C39-C38	-2.06	103.95	114.42
25	d	403	CLA	CHA-C1A-NA	-2.06	121.68	126.40
25	b	613	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
25	C	501	CLA	CHB-C4A-NA	2.06	127.36	124.51
25	H	101	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
25	b	612	CLA	CHA-C1A-NA	-2.06	121.68	126.40
25	c	504	CLA	O1A-CGA-CBA	2.06	131.76	123.73
30	c	517	DGD	O6E-C5E-C4E	2.06	113.43	109.69
25	b	608	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
25	C	513	CLA	C2D-C1D-ND	-2.05	108.59	110.10
25	B	602	CLA	CHA-C1A-NA	-2.05	121.69	126.40
25	B	602	CLA	C3C-C4C-NC	-2.05	108.27	110.57
28	a	612	PL9	C35-C34-C36	2.05	118.72	115.27
25	C	510	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
30	C	516	DGD	O3D-C3D-C4D	-2.05	105.61	110.35
25	B	603	CLA	CHA-C4D-ND	2.05	136.79	132.50
27	b	618	BCR	C31-C1-C6	2.05	113.62	110.30
32	m	101	LMG	C1-C2-C3	-2.05	105.73	110.00
27	A	611	BCR	C2-C1-C6	2.05	113.64	110.48
32	c	522	LMG	C42-C41-C40	-2.05	104.02	114.42
33	D	407	LHG	C29-C28-C27	-2.05	104.02	114.42
32	M	101	LMG	O1-C7-C8	-2.05	105.96	110.90
25	A	606	CLA	CHA-C1A-NA	-2.05	121.71	126.40
32	b	620	LMG	C8-O7-C10	2.05	122.83	117.79
25	c	504	CLA	CHD-C4C-NC	2.04	127.43	124.20
25	B	608	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	B	613	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	b	613	CLA	CED-O2D-CGD	2.04	120.56	115.94
25	C	513	CLA	CHD-C1D-C2D	2.04	129.76	125.48
25	B	606	CLA	CHB-C4A-NA	2.04	127.34	124.51
27	K	101	BCR	C3-C4-C5	-2.04	110.43	114.08
26	A	609	PHO	CMD-C2D-C3D	2.04	128.50	124.68
33	D	408	LHG	C29-C28-C27	-2.04	104.07	114.42
25	c	509	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
30	H	103	DGD	C7B-C6B-C5B	-2.04	104.07	114.42
25	d	403	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
25	c	502	CLA	CHB-C4A-NA	2.04	127.33	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	612	PL9	O1-C4-C3	-2.04	118.47	120.72
30	A	616	DGD	CAB-C9B-C8B	-2.04	104.08	114.42
28	a	612	PL9	C32-C33-C34	-2.04	122.75	127.66
32	m	101	LMG	C38-C37-C36	-2.04	104.08	114.42
25	b	610	CLA	CHC-C1C-NC	2.04	127.29	124.20
25	c	501	CLA	CHC-C1C-NC	2.04	127.29	124.20
31	c	523	STE	O2-C1-C2	2.04	120.57	114.03
27	c	514	BCR	C7-C8-C9	-2.04	123.16	126.23
25	c	507	CLA	CHA-C1A-NA	-2.04	121.74	126.40
25	B	607	CLA	CHA-C1A-NA	-2.04	121.74	126.40
31	j	101	STE	O2-C1-O1	-2.03	118.23	123.30
32	C	515	LMG	O5-C6-C5	-2.03	104.31	111.29
30	C	516	DGD	O2D-C2D-C1D	-2.03	105.10	110.05
33	d	407	LHG	C27-C26-C25	-2.03	104.10	114.42
31	C	520	STE	C4-C3-C2	-2.03	105.88	113.19
25	b	609	CLA	CHB-C4A-NA	2.03	127.32	124.51
33	d	406	LHG	C27-C26-C25	-2.03	104.11	114.42
25	B	603	CLA	CGD-CBD-CAD	-2.03	104.16	110.73
25	B	612	CLA	CHD-C1D-ND	-2.03	122.59	124.45
32	d	410	LMG	O7-C10-O9	-2.03	118.80	123.70
25	c	508	CLA	C3C-C4C-NC	-2.03	108.30	110.57
25	B	609	CLA	C1-C2-C3	-2.03	122.53	126.04
33	D	407	LHG	O8-C6-C5	-2.03	102.53	108.43
25	b	606	CLA	C1-O2A-CGA	2.03	121.76	116.44
26	d	401	PHO	C1B-NB-C4B	2.03	111.25	107.09
32	c	520	LMG	O1-C7-C8	-2.03	106.01	110.90
25	b	602	CLA	CHD-C1D-C2D	2.02	129.73	125.48
30	C	518	DGD	O6E-C5E-C4E	2.02	113.37	109.69
25	D	402	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
25	C	503	CLA	C6-C5-C3	2.02	118.76	113.45
25	d	402	CLA	O2D-CGD-CBD	2.02	114.86	111.27
32	M	101	LMG	C6-C5-C4	-2.02	108.27	113.00
27	D	404	BCR	C2-C3-C4	-2.02	106.86	111.38
25	c	507	CLA	CHD-C1D-ND	-2.02	122.60	124.45
27	k	101	BCR	C38-C26-C25	-2.02	122.26	124.53
27	B	616	BCR	C27-C26-C25	2.02	125.66	122.73
27	a	611	BCR	C29-C30-C25	2.02	113.58	110.48
35	F	101	HEM	CAD-CBD-CGD	2.01	117.94	113.60
30	c	517	DGD	C4A-C3A-C2A	-2.01	105.95	113.19
30	A	616	DGD	C1D-C2D-C3D	-2.01	105.81	110.00
25	h	101	CLA	CHD-C1D-C2D	2.01	129.70	125.48
25	B	608	CLA	C1B-CHB-C4A	-2.01	126.14	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	611	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	h	101	CLA	O2D-CGD-CBD	2.01	114.84	111.27
30	C	518	DGD	C5B-C4B-C3B	-2.01	104.23	114.42
25	B	606	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
33	d	406	LHG	C18-C17-C16	-2.01	104.24	114.42
27	x	101	BCR	C11-C10-C9	-2.01	124.45	127.31
25	b	605	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
25	c	511	CLA	C2A-C1A-CHA	2.01	127.37	123.86
30	A	616	DGD	O3D-C3D-C4D	-2.01	105.71	110.35
27	t	101	BCR	C31-C1-C6	2.01	113.55	110.30
33	e	102	LHG	C18-C17-C16	-2.01	104.24	114.42
30	C	518	DGD	O3E-C3E-C2E	-2.00	105.72	110.35
25	B	611	CLA	O1D-CGD-CBD	2.00	128.58	124.48
25	C	509	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
25	b	615	CLA	O1D-CGD-CBD	2.00	128.58	124.48
25	C	501	CLA	CHD-C1D-C2D	2.00	129.68	125.48
29	l	101	SQD	O5-C1-C2	-2.00	106.11	110.35
25	C	504	CLA	CHA-C1A-NA	-2.00	121.82	126.40

All (64) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	610	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	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	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	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	402	CLA	ND
25	H	101	CLA	ND
25	a	607	CLA	ND
25	a	608	CLA	ND
25	a	610	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
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	c	501	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	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	402	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	d	403	CLA	ND
25	h	101	CLA	ND

All (1881) 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	605	CLA	CHA-CBD-CGD-O1D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	B	613	CLA	CHA-CBD-CGD-O1D
25	B	613	CLA	CHA-CBD-CGD-O2D
25	B	613	CLA	CAD-CBD-CGD-O1D
25	B	613	CLA	C14-C13-C15-C16
25	C	504	CLA	C4-C3-C5-C6
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	H	101	CLA	C1A-C2A-CAA-CBA
25	H	101	CLA	CHA-CBD-CGD-O1D
25	H	101	CLA	C6-C7-C8-C9
25	a	613	CLA	CHA-CBD-CGD-O1D
25	a	613	CLA	CHA-CBD-CGD-O2D
25	b	604	CLA	C4-C3-C5-C6
25	b	613	CLA	CHA-CBD-CGD-O1D
25	b	613	CLA	CHA-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	C2-C3-C5-C6
25	b	613	CLA	C4-C3-C5-C6
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	512	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	CAD-CBD-CGD-O1D
25	c	513	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CBD-CGD-O2D-CED
25	h	101	CLA	C1A-C2A-CAA-CBA
25	h	101	CLA	C3A-C2A-CAA-CBA
27	B	616	BCR	C1-C6-C7-C8
27	B	616	BCR	C7-C8-C9-C34
27	B	617	BCR	C7-C8-C9-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B	618	BCR	C35-C13-C14-C15
27	B	618	BCR	C20-C21-C22-C37
27	B	618	BCR	C37-C22-C23-C24
27	C	514	BCR	C11-C12-C13-C14
27	D	404	BCR	C37-C22-C23-C24
27	D	404	BCR	C22-C23-C24-C25
27	K	101	BCR	C7-C8-C9-C34
27	K	101	BCR	C11-C10-C9-C8
27	K	101	BCR	C16-C17-C18-C36
27	K	102	BCR	C11-C12-C13-C35
27	K	102	BCR	C37-C22-C23-C24
27	K	103	BCR	C37-C22-C23-C24
27	K	103	BCR	C23-C24-C25-C30
27	T	101	BCR	C7-C8-C9-C10
27	T	101	BCR	C7-C8-C9-C34
27	b	617	BCR	C7-C8-C9-C34
27	b	618	BCR	C11-C12-C13-C14
27	b	618	BCR	C11-C12-C13-C35
27	b	618	BCR	C37-C22-C23-C24
27	c	515	BCR	C7-C8-C9-C10
27	c	515	BCR	C7-C8-C9-C34
27	c	515	BCR	C11-C12-C13-C35
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C17-C18-C19-C20
27	t	101	BCR	C7-C8-C9-C34
27	x	101	BCR	C7-C8-C9-C34
28	A	612	PL9	C12-C13-C14-C15
28	A	612	PL9	C12-C13-C14-C16
28	A	612	PL9	C17-C18-C19-C21
28	A	612	PL9	C18-C19-C21-C22
28	A	612	PL9	C22-C23-C24-C26
28	A	612	PL9	C25-C24-C26-C27
28	A	612	PL9	C32-C33-C34-C35
28	A	612	PL9	C32-C33-C34-C36
28	A	612	PL9	C35-C34-C36-C37
28	A	612	PL9	C37-C38-C39-C40
28	A	612	PL9	C40-C39-C41-C42
28	A	612	PL9	C43-C44-C46-C47
28	A	612	PL9	C45-C44-C46-C47
28	D	405	PL9	C32-C33-C34-C36
28	D	405	PL9	C33-C34-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	a	612	PL9	C22-C23-C24-C26
28	a	612	PL9	C27-C28-C29-C31
28	a	612	PL9	C28-C29-C31-C32
28	a	612	PL9	C32-C33-C34-C36
28	a	612	PL9	C42-C43-C44-C45
28	a	612	PL9	C47-C48-C49-C51
28	d	405	PL9	C27-C28-C29-C31
28	d	405	PL9	C38-C39-C41-C42
28	d	405	PL9	C40-C39-C41-C42
29	A	615	SQD	C44-C45-C46-O48
29	A	615	SQD	O47-C45-C46-O48
29	F	102	SQD	C45-C44-O6-C1
29	F	102	SQD	O10-C23-O48-C46
29	F	102	SQD	C24-C23-O48-C46
29	L	101	SQD	C8-C7-O47-C45
29	L	101	SQD	O10-C23-O48-C46
29	L	101	SQD	C24-C23-O48-C46
29	a	614	SQD	O6-C44-C45-O47
29	a	615	SQD	O47-C45-C46-O48
29	a	615	SQD	O49-C7-O47-C45
29	a	615	SQD	C8-C7-O47-C45
29	f	101	SQD	C2-C1-O6-C44
29	f	101	SQD	O5-C1-O6-C44
29	f	101	SQD	C8-C7-O47-C45
29	f	101	SQD	C5-C6-S-O7
29	l	101	SQD	C2-C1-O6-C44
29	l	101	SQD	O5-C1-O6-C44
29	l	101	SQD	O6-C44-C45-O47
29	l	101	SQD	O49-C7-O47-C45
29	l	101	SQD	C8-C7-O47-C45
30	A	616	DGD	O1B-C1B-O2G-C2G
30	a	616	DGD	C1G-C2G-C3G-O3G
30	a	616	DGD	O2G-C2G-C3G-O3G
32	C	515	LMG	O6-C1-O1-C7
32	C	515	LMG	O9-C10-O7-C8
32	D	409	LMG	O1-C7-C8-C9
32	D	409	LMG	O1-C7-C8-O7
32	c	522	LMG	C11-C10-O7-C8
32	c	524	LMG	C2-C1-O1-C7
32	c	524	LMG	O6-C1-O1-C7
32	c	524	LMG	C29-C28-O8-C9
32	m	101	LMG	C2-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	m	101	LMG	O6-C1-O1-C7
33	B	621	LHG	C4-O6-P-O4
33	B	622	LHG	O1-C1-C2-C3
33	B	622	LHG	C3-O3-P-O4
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C3-O3-P-O4
33	D	407	LHG	C3-O3-P-O6
33	D	407	LHG	C4-O6-P-O4
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	O2-C2-C3-O3
33	D	408	LHG	C3-O3-P-O5
33	D	408	LHG	C3-O3-P-O6
33	E	101	LHG	O1-C1-C2-C3
33	E	101	LHG	C4-O6-P-O3
33	E	101	LHG	C4-O6-P-O4
33	E	101	LHG	C4-O6-P-O5
33	d	406	LHG	C3-O3-P-O4
33	d	407	LHG	O1-C1-C2-C3
33	d	407	LHG	C4-O6-P-O3
33	d	407	LHG	C4-O6-P-O4
33	d	407	LHG	C4-O6-P-O5
33	d	408	LHG	C4-O6-P-O4
33	e	102	LHG	O1-C1-C2-C3
33	e	102	LHG	C1-C2-C3-O3
33	e	102	LHG	C3-O3-P-O4
33	e	102	LHG	C3-O3-P-O5
33	e	102	LHG	C3-O3-P-O6
33	e	102	LHG	O10-C23-O8-C6
33	e	102	LHG	C24-C23-O8-C6
25	h	101	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	h	101	CLA	CBD-CGD-O2D-CED
32	c	524	LMG	O10-C28-O8-C9
32	c	522	LMG	C29-C28-O8-C9
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	513	CLA	CBD-CGD-O2D-CED
25	a	608	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	H	101	CLA	O1A-CGA-O2A-C1
29	f	101	SQD	O10-C23-O48-C46
32	M	101	LMG	O10-C28-O8-C9
32	c	522	LMG	O10-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	513	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
29	L	101	SQD	O49-C7-O47-C45
29	f	101	SQD	O49-C7-O47-C45
32	c	520	LMG	C11-C10-O7-C8
25	B	615	CLA	C3-C5-C6-C7
25	b	613	CLA	C3-C5-C6-C7
25	H	101	CLA	CBA-CGA-O2A-C1
29	a	615	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
30	A	616	DGD	C2B-C1B-O2G-C2G
32	C	515	LMG	C11-C10-O7-C8
32	D	409	LMG	C11-C10-O7-C8
28	D	405	PL9	C47-C48-C49-C50
28	D	405	PL9	C47-C48-C49-C51
28	a	612	PL9	C40-C39-C41-C42
25	C	504	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	B	605	CLA	C2A-CAA-CBA-CGA
25	b	605	CLA	C2A-CAA-CBA-CGA
25	h	101	CLA	C2A-CAA-CBA-CGA
25	h	101	CLA	C3-C5-C6-C7
32	M	101	LMG	C29-C28-O8-C9
32	d	410	LMG	C10-C11-C12-C13
28	d	405	PL9	C47-C48-C49-C51
28	a	612	PL9	C22-C23-C24-C25
25	c	511	CLA	O1D-CGD-O2D-CED
32	D	409	LMG	O9-C10-O7-C8
32	b	620	LMG	O9-C10-O7-C8
32	c	522	LMG	O9-C10-O7-C8
28	A	612	PL9	C37-C38-C39-C41
28	a	612	PL9	C42-C43-C44-C46
29	a	615	SQD	O10-C23-O48-C46
25	C	511	CLA	CBD-CGD-O2D-CED
25	D	403	CLA	CBD-CGD-O2D-CED
25	H	101	CLA	CBD-CGD-O2D-CED
33	D	407	LHG	O2-C2-C3-O3
30	A	616	DGD	O6E-C5E-C6E-O5E
25	b	603	CLA	C13-C15-C16-C17
32	C	519	LMG	C11-C10-O7-C8
32	b	620	LMG	C11-C10-O7-C8
25	B	611	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	406	LHG	C28-C29-C30-C31
33	d	407	LHG	C28-C29-C30-C31
30	A	616	DGD	C4E-C5E-C6E-O5E
32	c	524	LMG	C4-C5-C6-O5
31	H	104	STE	C11-C12-C13-C14
31	b	622	STE	C4-C5-C6-C7
28	a	612	PL9	C47-C48-C49-C50
32	C	515	LMG	O6-C5-C6-O5
25	b	606	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	b	606	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	A	612	PL9	C38-C39-C41-C42
28	a	612	PL9	C38-C39-C41-C42
32	b	620	LMG	O10-C28-O8-C9
28	A	612	PL9	C39-C41-C42-C43
28	A	612	PL9	C44-C46-C47-C48
29	a	614	SQD	C11-C12-C13-C14
32	m	101	LMG	C29-C28-O8-C9
33	E	101	LHG	C27-C28-C29-C30
32	c	520	LMG	O6-C5-C6-O5
33	E	101	LHG	O10-C23-O8-C6
31	B	623	STE	C4-C5-C6-C7
28	a	612	PL9	C32-C33-C34-C35
25	b	615	CLA	O1D-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
32	c	524	LMG	O6-C5-C6-O5
28	a	612	PL9	C37-C38-C39-C41
25	H	101	CLA	C3-C5-C6-C7
33	E	101	LHG	C24-C23-O8-C6
32	c	524	LMG	C15-C16-C17-C18
25	b	604	CLA	C5-C6-C7-C8
25	B	606	CLA	C8-C10-C11-C12
25	C	507	CLA	C13-C15-C16-C17
25	C	512	CLA	C5-C6-C7-C8
25	c	509	CLA	C13-C15-C16-C17
33	e	102	LHG	O2-C2-C3-O3
30	A	616	DGD	O2G-C2G-C3G-O3G
25	A	607	CLA	C14-C13-C15-C16
25	B	609	CLA	C14-C13-C15-C16
25	B	612	CLA	C11-C12-C13-C14
25	B	613	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	614	CLA	C11-C10-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	512	CLA	C6-C7-C8-C9
25	d	403	CLA	C11-C12-C13-C14
25	h	101	CLA	C11-C10-C8-C9
25	h	101	CLA	C14-C13-C15-C16
25	a	608	CLA	O1D-CGD-O2D-CED
27	C	514	BCR	C7-C8-C9-C34
27	C	514	BCR	C11-C12-C13-C35
27	H	102	BCR	C11-C12-C13-C35
27	K	102	BCR	C7-C8-C9-C34
27	d	404	BCR	C7-C8-C9-C34
27	d	404	BCR	C37-C22-C23-C24
27	x	101	BCR	C11-C12-C13-C35
29	A	614	SQD	C23-C24-C25-C26
29	a	614	SQD	C23-C24-C25-C26
31	B	624	STE	C1-C2-C3-C4
32	d	410	LMG	C28-C29-C30-C31
33	E	101	LHG	C23-C24-C25-C26
30	a	616	DGD	O1A-C1A-O1G-C1G
25	C	506	CLA	C13-C15-C16-C17
25	a	610	CLA	C10-C11-C12-C13
25	b	604	CLA	C10-C11-C12-C13
25	c	512	CLA	C15-C16-C17-C18
29	l	101	SQD	C11-C10-C9-C8
32	C	515	LMG	C4-C5-C6-O5
25	C	509	CLA	C3-C5-C6-C7
25	B	601	CLA	C13-C15-C16-C17
25	C	513	CLA	C15-C16-C17-C18
25	H	101	CLA	C13-C15-C16-C17
25	b	606	CLA	C10-C11-C12-C13
30	a	616	DGD	C1A-C2A-C3A-C4A
31	T	102	STE	C5-C6-C7-C8
25	B	612	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	615	CLA	C5-C6-C7-C8
25	C	503	CLA	C5-C6-C7-C8
25	C	506	CLA	C8-C10-C11-C12
25	C	507	CLA	C10-C11-C12-C13
25	C	509	CLA	C5-C6-C7-C8
25	C	509	CLA	C8-C10-C11-C12
25	b	611	CLA	C15-C16-C17-C18
25	b	614	CLA	C15-C16-C17-C18
25	c	509	CLA	C10-C11-C12-C13
25	c	510	CLA	C10-C11-C12-C13
29	A	614	SQD	C7-C8-C9-C10
29	L	101	SQD	C23-C24-C25-C26
32	D	409	LMG	C10-C11-C12-C13
32	D	409	LMG	C28-C29-C30-C31
32	b	620	LMG	C28-C29-C30-C31
32	c	522	LMG	C10-C11-C12-C13
33	d	406	LHG	C23-C24-C25-C26
33	l	102	LHG	C23-C24-C25-C26
32	c	522	LMG	O6-C5-C6-O5
25	b	602	CLA	C5-C6-C7-C8
25	c	512	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	O1D-CGD-O2D-CED
28	d	405	PL9	C42-C43-C44-C46
25	B	612	CLA	C8-C10-C11-C12
25	C	505	CLA	C5-C6-C7-C8
29	A	615	SQD	C7-C8-C9-C10
29	A	615	SQD	C23-C24-C25-C26
32	c	520	LMG	C28-C29-C30-C31
33	d	406	LHG	C7-C8-C9-C10
25	b	601	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C10-C11-C12-C13
25	A	607	CLA	C12-C13-C15-C16
25	B	610	CLA	C12-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C15
25	C	503	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	C	513	CLA	C11-C10-C8-C7
25	D	403	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C10-C8-C7
25	b	608	CLA	C11-C12-C13-C15
25	b	614	CLA	C11-C12-C13-C15
25	C	501	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	606	CLA	O1D-CGD-O2D-CED
25	A	613	CLA	C15-C16-C17-C18
25	h	101	CLA	C13-C15-C16-C17
30	C	518	DGD	O1A-C1A-O1G-C1G
29	L	101	SQD	O5-C1-O6-C44
25	B	603	CLA	C15-C16-C17-C18
25	b	602	CLA	C13-C15-C16-C17
28	A	612	PL9	C34-C36-C37-C38
29	l	101	SQD	C29-C30-C31-C32
27	B	617	BCR	C18-C19-C20-C21
33	d	408	LHG	C33-C34-C35-C36
33	d	406	LHG	O2-C2-C3-O3
25	B	613	CLA	C5-C6-C7-C8
25	c	512	CLA	C8-C10-C11-C12
32	b	620	LMG	C29-C28-O8-C9
33	e	102	LHG	C23-C24-C25-C26
31	b	622	STE	C2-C3-C4-C5
25	B	609	CLA	C15-C16-C17-C18
25	B	610	CLA	C8-C10-C11-C12
25	B	610	CLA	C13-C15-C16-C17
25	C	506	CLA	C15-C16-C17-C18
25	C	508	CLA	C10-C11-C12-C13
25	a	607	CLA	C15-C16-C17-C18
25	a	608	CLA	C8-C10-C11-C12
25	b	613	CLA	C13-C15-C16-C17
25	c	503	CLA	C5-C6-C7-C8
25	c	505	CLA	C15-C16-C17-C18
25	C	510	CLA	CBD-CGD-O2D-CED
32	m	101	LMG	O10-C28-O8-C9
25	b	610	CLA	C8-C10-C11-C12
33	B	621	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O3
33	d	406	LHG	C3-O3-P-O6
33	l	102	LHG	C4-O6-P-O3
25	b	608	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7
32	c	520	LMG	O9-C10-O7-C8
25	B	605	CLA	C13-C15-C16-C17
25	b	606	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
31	B	623	STE	C1-C2-C3-C4
33	d	406	LHG	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	C	519	LMG	O9-C10-O7-C8
25	B	605	CLA	C15-C16-C17-C18
25	b	613	CLA	C8-C10-C11-C12
28	d	405	PL9	C47-C48-C49-C50
32	C	519	LMG	C29-C28-O8-C9
25	c	510	CLA	C15-C16-C17-C18
25	c	512	CLA	C13-C15-C16-C17
30	C	517	DGD	C8A-C9A-CAA-CBA
31	H	104	STE	C7-C8-C9-C10
32	C	519	LMG	C17-C18-C19-C20
33	d	406	LHG	C17-C18-C19-C20
27	B	616	BCR	C16-C17-C18-C36
27	B	616	BCR	C20-C21-C22-C37
27	B	617	BCR	C20-C21-C22-C37
27	D	404	BCR	C20-C21-C22-C37
27	K	101	BCR	C35-C13-C14-C15
27	K	102	BCR	C20-C21-C22-C37
27	T	101	BCR	C20-C21-C22-C37
27	c	514	BCR	C16-C17-C18-C36
27	c	515	BCR	C35-C13-C14-C15
27	c	516	BCR	C20-C21-C22-C37
27	d	404	BCR	C16-C17-C18-C36
27	t	101	BCR	C35-C13-C14-C15
30	C	517	DGD	C5A-C6A-C7A-C8A
30	h	102	DGD	C2B-C3B-C4B-C5B
31	B	624	STE	C2-C3-C4-C5
31	T	103	STE	C11-C12-C13-C14
31	c	523	STE	C5-C6-C7-C8
32	C	519	LMG	C12-C13-C14-C15
32	C	519	LMG	C30-C31-C32-C33
32	M	101	LMG	C29-C30-C31-C32
32	c	522	LMG	C39-C40-C41-C42
33	B	621	LHG	C31-C32-C33-C34
33	D	408	LHG	C11-C12-C13-C14
33	D	408	LHG	C27-C28-C29-C30
33	D	408	LHG	C33-C34-C35-C36
25	A	613	CLA	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C20
25	B	613	CLA	C16-C17-C18-C20
25	b	613	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
29	A	614	SQD	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	614	SQD	C17-C18-C19-C20
29	f	101	SQD	C32-C33-C34-C35
29	l	101	SQD	C11-C12-C13-C14
30	A	616	DGD	CEA-CFA-CGA-CHA
30	c	517	DGD	C9B-CAB-CBB-CCB
30	c	519	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	C6B-C7B-C8B-C9B
31	H	104	STE	C5-C6-C7-C8
31	c	523	STE	C3-C4-C5-C6
31	x	102	STE	C4-C5-C6-C7
32	b	620	LMG	C17-C18-C19-C20
33	B	621	LHG	C27-C28-C29-C30
33	d	407	LHG	C33-C34-C35-C36
29	L	101	SQD	C46-C45-O47-C7
32	D	409	LMG	C9-C8-O7-C10
30	a	616	DGD	O1B-C1B-O2G-C2G
25	b	603	CLA	C15-C16-C17-C18
31	c	521	STE	C1-C2-C3-C4
29	F	102	SQD	C30-C31-C32-C33
30	c	517	DGD	C2A-C3A-C4A-C5A
30	c	517	DGD	C7B-C8B-C9B-CAB
31	H	104	STE	C2-C3-C4-C5
31	x	102	STE	C11-C12-C13-C14
32	M	101	LMG	C13-C14-C15-C16
32	b	620	LMG	C34-C35-C36-C37
33	D	408	LHG	C9-C10-C11-C12
33	D	408	LHG	C32-C33-C34-C35
33	E	101	LHG	C18-C19-C20-C21
33	E	101	LHG	C26-C27-C28-C29
33	E	101	LHG	C30-C31-C32-C33
33	e	102	LHG	C11-C10-C9-C8
25	c	512	CLA	O1A-CGA-O2A-C1
29	A	615	SQD	C25-C26-C27-C28
29	A	615	SQD	C26-C27-C28-C29
29	L	101	SQD	C26-C27-C28-C29
30	A	616	DGD	CBA-CCA-CDA-CEA
30	C	517	DGD	C3B-C4B-C5B-C6B
30	c	517	DGD	C3A-C4A-C5A-C6A
31	T	103	STE	C9-C10-C11-C12
31	d	411	STE	C10-C11-C12-C13
32	c	524	LMG	C19-C20-C21-C22
32	c	524	LMG	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	d	409	LMG	C34-C35-C36-C37
33	B	622	LHG	C28-C29-C30-C31
33	D	408	LHG	C30-C31-C32-C33
33	e	102	LHG	C27-C28-C29-C30
30	c	517	DGD	CAB-CBB-CCB-CDB
31	T	102	STE	C6-C7-C8-C9
31	d	411	STE	C3-C4-C5-C6
31	d	411	STE	C5-C6-C7-C8
32	D	406	LMG	C30-C31-C32-C33
32	M	101	LMG	C35-C36-C37-C38
32	b	620	LMG	C40-C41-C42-C43
32	d	409	LMG	C37-C38-C39-C40
31	J	101	STE	C1-C2-C3-C4
33	D	408	LHG	C7-C8-C9-C10
27	B	618	BCR	C12-C13-C14-C15
27	K	101	BCR	C16-C17-C18-C19
27	b	618	BCR	C12-C13-C14-C15
27	c	514	BCR	C12-C13-C14-C15
27	d	404	BCR	C16-C17-C18-C19
27	x	101	BCR	C11-C10-C9-C8
30	c	518	DGD	C2E-C1E-O5D-C6D
32	C	519	LMG	C2-C1-O1-C7
30	a	616	DGD	C2A-C1A-O1G-C1G
29	A	614	SQD	C27-C28-C29-C30
29	a	614	SQD	C10-C11-C12-C13
29	a	614	SQD	C29-C30-C31-C32
29	f	101	SQD	C30-C31-C32-C33
30	c	517	DGD	C5B-C6B-C7B-C8B
31	t	102	STE	C11-C10-C9-C8
31	x	102	STE	C2-C3-C4-C5
31	x	102	STE	C3-C4-C5-C6
32	M	101	LMG	C32-C33-C34-C35
32	c	522	LMG	C36-C37-C38-C39
33	D	407	LHG	C13-C14-C15-C16
33	D	408	LHG	C29-C30-C31-C32
33	d	406	LHG	C11-C10-C9-C8
25	c	503	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
25	B	604	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C19
29	l	101	SQD	C33-C34-C35-C36
30	C	518	DGD	CBB-CCB-CDB-CEB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	H	103	DGD	CCA-CDA-CEA-CFA
30	c	519	DGD	C3A-C4A-C5A-C6A
32	b	620	LMG	C16-C17-C18-C19
33	D	407	LHG	C32-C33-C34-C35
33	E	101	LHG	C32-C33-C34-C35
33	d	406	LHG	C16-C17-C18-C19
25	B	610	CLA	C2-C3-C5-C6
28	d	405	PL9	C43-C44-C46-C47
25	B	606	CLA	C11-C12-C13-C14
25	C	502	CLA	C11-C12-C13-C14
25	C	511	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	605	CLA	C14-C13-C15-C16
25	b	614	CLA	C11-C12-C13-C14
32	m	101	LMG	C10-C11-C12-C13
29	f	101	SQD	C28-C29-C30-C31
30	A	616	DGD	CBB-CCB-CDB-CEB
30	C	516	DGD	C4B-C5B-C6B-C7B
30	C	518	DGD	CAB-CBB-CCB-CDB
30	a	616	DGD	CEA-CFA-CGA-CHA
31	H	104	STE	C4-C5-C6-C7
31	T	102	STE	C7-C8-C9-C10
31	c	521	STE	C5-C6-C7-C8
32	B	620	LMG	C31-C32-C33-C34
32	B	620	LMG	C36-C37-C38-C39
32	D	406	LMG	C17-C18-C19-C20
32	c	520	LMG	C33-C34-C35-C36
32	d	410	LMG	C34-C35-C36-C37
33	B	621	LHG	C12-C13-C14-C15
33	B	622	LHG	C11-C12-C13-C14
33	D	408	LHG	C14-C15-C16-C17
33	d	408	LHG	C25-C26-C27-C28
33	l	102	LHG	C32-C33-C34-C35
25	b	601	CLA	C15-C16-C17-C18
25	b	614	CLA	C10-C11-C12-C13
29	a	615	SQD	C14-C15-C16-C17
31	b	622	STE	C13-C14-C15-C16
32	C	515	LMG	C16-C17-C18-C19
32	c	522	LMG	C14-C15-C16-C17
33	l	102	LHG	C14-C15-C16-C17
33	l	102	LHG	C25-C26-C27-C28
33	d	406	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	408	LHG	O1-C1-C2-C3
25	b	609	CLA	C13-C15-C16-C17
25	c	504	CLA	C8-C10-C11-C12
29	l	101	SQD	C25-C26-C27-C28
31	J	101	STE	C5-C6-C7-C8
31	c	523	STE	C2-C3-C4-C5
31	d	411	STE	C11-C12-C13-C14
32	B	620	LMG	C33-C34-C35-C36
29	l	101	SQD	C7-C8-C9-C10
30	c	518	DGD	C1B-C2B-C3B-C4B
29	a	615	SQD	C11-C10-C9-C8
29	f	101	SQD	C31-C32-C33-C34
30	A	616	DGD	C2A-C3A-C4A-C5A
30	C	518	DGD	C2A-C3A-C4A-C5A
30	H	103	DGD	CCB-CDB-CEB-CFB
30	a	616	DGD	C7B-C8B-C9B-CAB
31	B	625	STE	C5-C6-C7-C8
31	C	521	STE	C3-C4-C5-C6
31	D	410	STE	C2-C3-C4-C5
31	T	103	STE	C7-C8-C9-C10
31	T	103	STE	C10-C11-C12-C13
31	b	621	STE	C5-C6-C7-C8
31	c	521	STE	C3-C4-C5-C6
31	d	411	STE	C9-C10-C11-C12
32	D	406	LMG	C14-C15-C16-C17
32	M	101	LMG	C12-C13-C14-C15
32	b	620	LMG	C11-C12-C13-C14
32	b	620	LMG	C14-C15-C16-C17
33	d	406	LHG	C29-C30-C31-C32
33	l	102	LHG	C11-C12-C13-C14
30	C	516	DGD	O6E-C5E-C6E-O5E
32	b	620	LMG	O6-C5-C6-O5
25	B	603	CLA	C16-C17-C18-C20
25	b	613	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C19
30	c	518	DGD	O6E-C1E-O5D-C6D
32	C	519	LMG	O6-C1-O1-C7
25	b	613	CLA	C5-C6-C7-C8
30	C	517	DGD	C8B-C9B-CAB-CBB
30	a	616	DGD	C8B-C9B-CAB-CBB
30	a	616	DGD	CAB-CBB-CCB-CDB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	c	518	DGD	CBB-CCB-CDB-CEB
31	B	624	STE	C7-C8-C9-C10
31	b	619	STE	C6-C7-C8-C9
31	b	621	STE	C4-C5-C6-C7
31	c	521	STE	C9-C10-C11-C12
32	C	519	LMG	C32-C33-C34-C35
32	c	522	LMG	C34-C35-C36-C37
32	m	101	LMG	C30-C31-C32-C33
33	E	101	LHG	C24-C25-C26-C27
25	C	511	CLA	O1D-CGD-O2D-CED
29	A	614	SQD	C14-C15-C16-C17
29	A	615	SQD	C18-C19-C20-C21
30	C	518	DGD	C5A-C6A-C7A-C8A
30	a	616	DGD	C3B-C4B-C5B-C6B
32	m	101	LMG	C15-C16-C17-C18
33	D	407	LHG	C11-C10-C9-C8
33	D	408	LHG	C11-C10-C9-C8
33	d	408	LHG	C30-C31-C32-C33
31	x	102	STE	C1-C2-C3-C4
32	C	519	LMG	C28-C29-C30-C31
33	B	621	LHG	C23-C24-C25-C26
25	B	613	CLA	C8-C10-C11-C12
29	a	615	SQD	C10-C11-C12-C13
30	C	518	DGD	C3A-C4A-C5A-C6A
30	a	616	DGD	CEB-CFB-CGB-CHB
31	H	104	STE	C3-C4-C5-C6
31	c	521	STE	C11-C12-C13-C14
32	c	524	LMG	C30-C31-C32-C33
32	c	524	LMG	C33-C34-C35-C36
33	E	101	LHG	C15-C16-C17-C18
30	c	519	DGD	C2A-C1A-O1G-C1G
29	A	615	SQD	C10-C11-C12-C13
31	T	103	STE	C13-C14-C15-C16
32	M	101	LMG	C33-C34-C35-C36
33	E	101	LHG	C11-C10-C9-C8
33	E	101	LHG	C12-C13-C14-C15
33	e	102	LHG	C11-C12-C13-C14
25	D	403	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	C3A-C2A-CAA-CBA
26	d	401	PHO	C3A-C2A-CAA-CBA
29	a	614	SQD	C27-C28-C29-C30
30	A	616	DGD	C2B-C3B-C4B-C5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	C	518	DGD	C6A-C7A-C8A-C9A
30	c	518	DGD	CCA-CDA-CEA-CFA
30	c	519	DGD	CBB-CCB-CDB-CEB
32	c	520	LMG	C31-C32-C33-C34
32	c	520	LMG	C38-C39-C40-C41
33	D	407	LHG	C29-C30-C31-C32
33	d	407	LHG	C29-C30-C31-C32
25	B	603	CLA	C16-C17-C18-C19
25	B	604	CLA	C16-C17-C18-C20
25	B	613	CLA	C16-C17-C18-C19
25	b	606	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
29	l	101	SQD	C28-C29-C30-C31
30	A	616	DGD	CCA-CDA-CEA-CFA
30	A	616	DGD	C4B-C5B-C6B-C7B
30	a	616	DGD	C4B-C5B-C6B-C7B
30	h	102	DGD	C3B-C4B-C5B-C6B
33	D	408	LHG	C15-C16-C17-C18
25	b	610	CLA	C13-C15-C16-C17
29	L	101	SQD	C13-C14-C15-C16
30	h	102	DGD	C5B-C6B-C7B-C8B
31	a	617	STE	C3-C4-C5-C6
25	B	611	CLA	O1D-CGD-O2D-CED
29	a	614	SQD	C15-C16-C17-C18
31	m	102	STE	C5-C6-C7-C8
32	c	524	LMG	C12-C13-C14-C15
33	e	102	LHG	O1-C1-C2-O2
29	l	101	SQD	C18-C19-C20-C21
30	C	516	DGD	C6B-C7B-C8B-C9B
30	a	616	DGD	C5B-C6B-C7B-C8B
31	C	522	STE	C7-C8-C9-C10
31	T	103	STE	C12-C13-C14-C15
31	j	101	STE	C2-C3-C4-C5
33	d	408	LHG	C32-C33-C34-C35
25	b	602	CLA	C16-C17-C18-C20
30	C	517	DGD	C6A-C7A-C8A-C9A
31	B	619	STE	C2-C3-C4-C5
29	a	614	SQD	C24-C25-C26-C27
30	c	517	DGD	C4B-C5B-C6B-C7B
32	d	409	LMG	C36-C37-C38-C39
33	E	101	LHG	C11-C12-C13-C14
29	L	101	SQD	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	615	SQD	C14-C15-C16-C17
29	F	102	SQD	C25-C26-C27-C28
32	C	515	LMG	C34-C35-C36-C37
33	D	407	LHG	C16-C17-C18-C19
33	d	406	LHG	C31-C32-C33-C34
32	c	524	LMG	O9-C10-O7-C8
30	A	616	DGD	O6D-C5D-C6D-O5D
29	a	615	SQD	C30-C31-C32-C33
30	c	518	DGD	C7B-C8B-C9B-CAB
31	T	103	STE	C14-C15-C16-C17
33	B	622	LHG	C25-C26-C27-C28
33	d	407	LHG	C32-C33-C34-C35
25	B	606	CLA	C5-C6-C7-C8
25	b	601	CLA	C13-C15-C16-C17
29	F	102	SQD	C27-C28-C29-C30
29	a	614	SQD	C18-C19-C20-C21
29	l	101	SQD	C16-C17-C18-C19
32	B	620	LMG	C28-C29-C30-C31
33	D	407	LHG	C23-C24-C25-C26
27	B	616	BCR	C5-C6-C7-C8
27	D	404	BCR	C23-C24-C25-C26
27	D	404	BCR	C23-C24-C25-C30
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C5-C6-C7-C8
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
31	T	102	STE	C14-C15-C16-C17
31	c	521	STE	C10-C11-C12-C13
31	l	103	STE	C14-C15-C16-C17
32	C	519	LMG	C31-C32-C33-C34
33	d	406	LHG	C25-C26-C27-C28
33	d	408	LHG	C27-C28-C29-C30
33	l	102	LHG	C29-C30-C31-C32
30	C	518	DGD	C2A-C1A-O1G-C1G
25	C	509	CLA	C10-C11-C12-C13
31	t	103	STE	C2-C3-C4-C5
32	c	522	LMG	C30-C31-C32-C33
32	C	515	LMG	C38-C39-C40-C41
25	b	602	CLA	C8-C10-C11-C12
30	A	616	DGD	C7B-C8B-C9B-CAB
30	c	519	DGD	C9B-CAB-CBB-CCB
32	C	515	LMG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	610	CLA	C4-C3-C5-C6
28	A	612	PL9	C20-C19-C21-C22
28	D	405	PL9	C35-C34-C36-C37
25	A	607	CLA	C6-C7-C8-C10
25	B	605	CLA	C6-C7-C8-C10
25	B	605	CLA	C12-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C15
25	C	506	CLA	C6-C7-C8-C10
25	C	511	CLA	C6-C7-C8-C10
25	a	610	CLA	C6-C7-C8-C10
25	b	604	CLA	C11-C12-C13-C15
25	b	605	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C10-C8-C7
25	c	510	CLA	C11-C10-C8-C7
25	h	101	CLA	C12-C13-C15-C16
31	B	624	STE	C4-C5-C6-C7
32	B	620	LMG	C32-C33-C34-C35
33	B	622	LHG	C29-C30-C31-C32
25	B	605	CLA	C8-C10-C11-C12
25	b	610	CLA	C15-C16-C17-C18
25	b	615	CLA	C5-C6-C7-C8
27	k	101	BCR	C19-C20-C21-C22
29	a	614	SQD	C7-C8-C9-C10
33	D	407	LHG	C25-C26-C27-C28
25	b	609	CLA	C2A-CAA-CBA-CGA
25	h	101	CLA	C8-C10-C11-C12
29	A	615	SQD	C12-C13-C14-C15
30	A	616	DGD	C8B-C9B-CAB-CBB
31	C	521	STE	C5-C6-C7-C8
31	b	621	STE	C2-C3-C4-C5
25	H	101	CLA	O1D-CGD-O2D-CED
29	L	101	SQD	C27-C28-C29-C30
29	a	614	SQD	C25-C26-C27-C28
31	a	617	STE	C5-C6-C7-C8
33	D	407	LHG	C28-C29-C30-C31
33	d	406	LHG	C32-C33-C34-C35
30	H	103	DGD	C1A-C2A-C3A-C4A
25	c	507	CLA	C8-C10-C11-C12
30	C	516	DGD	CCB-CDB-CEB-CFB
30	H	103	DGD	C7B-C8B-C9B-CAB
31	D	410	STE	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	C	515	LMG	C36-C37-C38-C39
32	D	406	LMG	C35-C36-C37-C38
32	m	101	LMG	C11-C12-C13-C14
33	d	407	LHG	C11-C12-C13-C14
33	e	102	LHG	C18-C19-C20-C21
33	l	102	LHG	C16-C17-C18-C19
25	B	603	CLA	C3-C5-C6-C7
25	b	607	CLA	C2C-C3C-CAC-CBC
32	b	620	LMG	C23-C24-C25-C26
33	e	102	LHG	C14-C15-C16-C17
29	l	101	SQD	C24-C23-O48-C46
25	c	506	CLA	C16-C17-C18-C20
30	C	517	DGD	O6D-C1D-O3G-C3G
25	B	611	CLA	C10-C11-C12-C13
25	C	509	CLA	C13-C15-C16-C17
29	A	615	SQD	C24-C25-C26-C27
31	d	411	STE	C2-C3-C4-C5
31	l	103	STE	C7-C8-C9-C10
32	c	524	LMG	C14-C15-C16-C17
33	B	621	LHG	C15-C16-C17-C18
27	d	404	BCR	C18-C19-C20-C21
29	L	101	SQD	C24-C25-C26-C27
30	c	517	DGD	CCA-CDA-CEA-CFA
30	c	519	DGD	CAA-CBA-CCA-CDA
33	B	621	LHG	C11-C12-C13-C14
33	B	621	LHG	C17-C18-C19-C20
25	B	607	CLA	C15-C16-C17-C18
25	C	508	CLA	C13-C15-C16-C17
25	C	512	CLA	C13-C15-C16-C17
30	c	517	DGD	C8A-C9A-CAA-CBA
32	c	520	LMG	C36-C37-C38-C39
33	B	621	LHG	C13-C14-C15-C16
32	d	409	LMG	C31-C32-C33-C34
32	C	515	LMG	O1-C7-C8-O7
30	c	517	DGD	O6E-C5E-C6E-O5E
32	d	410	LMG	O6-C5-C6-O5
30	A	616	DGD	CEB-CFB-CGB-CHB
29	l	101	SQD	C26-C27-C28-C29
30	c	517	DGD	CCB-CDB-CEB-CFB
32	C	515	LMG	C33-C34-C35-C36
32	D	406	LMG	C18-C19-C20-C21
32	D	409	LMG	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	c	522	LMG	C33-C34-C35-C36
33	E	101	LHG	C31-C32-C33-C34
33	d	407	LHG	C10-C11-C12-C13
25	B	604	CLA	C13-C15-C16-C17
25	C	512	CLA	C15-C16-C17-C18
25	C	505	CLA	C2-C3-C5-C6
28	a	612	PL9	C33-C34-C36-C37
28	a	612	PL9	C43-C44-C46-C47
28	D	405	PL9	C4-C3-C7-C8
31	T	103	STE	C5-C6-C7-C8
25	B	602	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C10-C8-C9
25	B	603	CLA	C14-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C9
25	C	503	CLA	C14-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	a	610	CLA	C6-C7-C8-C9
25	b	613	CLA	C6-C7-C8-C9
25	c	502	CLA	C6-C7-C8-C9
25	c	505	CLA	C11-C10-C8-C9
25	c	510	CLA	C14-C13-C15-C16
29	A	615	SQD	C28-C29-C30-C31
30	C	516	DGD	C2B-C3B-C4B-C5B
30	C	517	DGD	C3A-C4A-C5A-C6A
33	D	407	LHG	C17-C18-C19-C20
31	D	410	STE	C11-C10-C9-C8
32	C	515	LMG	C30-C31-C32-C33
25	B	604	CLA	C8-C10-C11-C12
31	b	623	STE	C4-C5-C6-C7
27	b	616	BCR	C21-C22-C23-C24
25	C	508	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	A	613	CLA	C16-C17-C18-C19
25	B	602	CLA	C16-C17-C18-C19
25	B	602	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
33	e	102	LHG	O9-C7-O7-C5
29	A	615	SQD	C17-C18-C19-C20
30	A	616	DGD	C5B-C6B-C7B-C8B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	a	616	DGD	C9A-CAA-CBA-CCA
31	a	617	STE	C4-C5-C6-C7
31	b	619	STE	C11-C12-C13-C14
33	d	407	LHG	C13-C14-C15-C16
25	A	607	CLA	C10-C11-C12-C13
25	B	612	CLA	C10-C11-C12-C13
25	b	601	CLA	C10-C11-C12-C13
29	a	615	SQD	C17-C18-C19-C20
30	c	518	DGD	C6A-C7A-C8A-C9A
32	M	101	LMG	C38-C39-C40-C41
33	D	407	LHG	C14-C15-C16-C17
29	l	101	SQD	C23-C24-C25-C26
32	m	101	LMG	C19-C20-C21-C22
33	D	407	LHG	C15-C16-C17-C18
25	B	613	CLA	C15-C16-C17-C18
33	E	101	LHG	O6-C4-C5-C6
33	l	102	LHG	O6-C4-C5-C6
30	c	519	DGD	CCA-CDA-CEA-CFA
33	E	101	LHG	C33-C34-C35-C36
25	b	606	CLA	C16-C17-C18-C19
30	a	616	DGD	C8A-C9A-CAA-CBA
31	x	102	STE	C5-C6-C7-C8
32	D	409	LMG	C12-C13-C14-C15
33	E	101	LHG	C17-C18-C19-C20
25	C	509	CLA	CBD-CGD-O2D-CED
29	l	101	SQD	C9-C10-C11-C12
30	c	518	DGD	C4A-C5A-C6A-C7A
33	E	101	LHG	C10-C11-C12-C13
28	d	405	PL9	C30-C29-C31-C32
28	A	612	PL9	C23-C24-C26-C27
30	C	516	DGD	C4A-C5A-C6A-C7A
30	h	102	DGD	CCA-CDA-CEA-CFA
32	b	620	LMG	C22-C23-C24-C25
32	c	524	LMG	C31-C32-C33-C34
33	B	621	LHG	C18-C19-C20-C21
32	c	522	LMG	C40-C41-C42-C43
33	B	621	LHG	C29-C30-C31-C32
30	c	518	DGD	C8A-C9A-CAA-CBA
25	c	504	CLA	C11-C12-C13-C14
29	a	614	SQD	O6-C44-C45-C46
29	a	615	SQD	C44-C45-C46-O48
29	l	101	SQD	O6-C44-C45-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	616	DGD	C1G-C2G-C3G-O3G
31	B	625	STE	C4-C5-C6-C7
32	C	519	LMG	O1-C7-C8-C9
32	b	620	LMG	C38-C39-C40-C41
32	c	522	LMG	C7-C8-C9-O8
32	m	101	LMG	C7-C8-C9-O8
25	C	502	CLA	C13-C15-C16-C17
30	c	518	DGD	CBA-CCA-CDA-CEA
30	c	519	DGD	CBA-CCA-CDA-CEA
31	b	622	STE	C10-C11-C12-C13
32	D	406	LMG	C39-C40-C41-C42
33	B	622	LHG	C27-C28-C29-C30
29	l	101	SQD	C45-C44-O6-C1
30	C	517	DGD	C5D-C6D-O5D-C1E
30	c	518	DGD	C5D-C6D-O5D-C1E
29	A	614	SQD	C17-C18-C19-C20
31	B	619	STE	C9-C10-C11-C12
31	b	619	STE	C15-C16-C17-C18
31	l	103	STE	C1-C2-C3-C4
32	b	620	LMG	C24-C25-C26-C27
30	c	518	DGD	C4E-C5E-C6E-O5E
33	d	406	LHG	C12-C13-C14-C15
30	C	517	DGD	C1B-C2B-C3B-C4B
29	A	615	SQD	C11-C12-C13-C14
29	l	101	SQD	C13-C14-C15-C16
31	b	623	STE	C7-C8-C9-C10
32	M	101	LMG	C17-C18-C19-C20
32	c	522	LMG	C42-C43-C44-C45
29	F	102	SQD	O5-C1-O6-C44
28	A	612	PL9	C19-C21-C22-C23
32	d	409	LMG	C33-C34-C35-C36
33	B	622	LHG	O1-C1-C2-O2
33	D	407	LHG	O1-C1-C2-O2
32	c	524	LMG	C20-C21-C22-C23
25	A	610	CLA	C5-C6-C7-C8
30	a	616	DGD	CDA-CEA-CFA-CGA
30	a	616	DGD	C2B-C1B-O2G-C2G
32	B	620	LMG	C37-C38-C39-C40
25	a	610	CLA	C5-C6-C7-C8
27	A	611	BCR	C35-C13-C14-C15
27	c	514	BCR	C35-C13-C14-C15
27	d	404	BCR	C20-C21-C22-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	t	101	BCR	C20-C21-C22-C37
30	h	102	DGD	O6E-C5E-C6E-O5E
25	C	505	CLA	C4-C3-C5-C6
25	b	610	CLA	C4-C3-C5-C6
28	A	612	PL9	C15-C14-C16-C17
28	d	405	PL9	C45-C44-C46-C47
29	l	101	SQD	C19-C20-C21-C22
30	c	519	DGD	CDA-CEA-CFA-CGA
31	b	621	STE	C10-C11-C12-C13
33	B	622	LHG	C23-C24-C25-C26
25	B	603	CLA	CBA-CGA-O2A-C1
30	c	517	DGD	CDB-CEB-CFB-CGB
30	c	518	DGD	CDA-CEA-CFA-CGA
25	C	504	CLA	C11-C12-C13-C14
29	A	614	SQD	C26-C27-C28-C29
31	B	623	STE	C2-C3-C4-C5
32	c	522	LMG	C38-C39-C40-C41
25	B	615	CLA	C2-C1-O2A-CGA
31	H	104	STE	C12-C13-C14-C15
33	d	406	LHG	C27-C28-C29-C30
30	a	616	DGD	C1B-C2B-C3B-C4B
32	D	406	LMG	O6-C5-C6-O5
30	c	517	DGD	C5A-C6A-C7A-C8A
30	h	102	DGD	C7A-C8A-C9A-CAA
30	C	518	DGD	CAA-CBA-CCA-CDA
31	B	623	STE	C6-C7-C8-C9
33	B	621	LHG	C30-C31-C32-C33
25	C	511	CLA	CBA-CGA-O2A-C1
25	c	509	CLA	CAA-CBA-CGA-O2A
33	E	101	LHG	C9-C10-C11-C12
25	b	601	CLA	O1D-CGD-O2D-CED
29	a	614	SQD	C12-C13-C14-C15
31	t	103	STE	C7-C8-C9-C10
27	A	611	BCR	C16-C17-C18-C19
27	B	617	BCR	C11-C10-C9-C8
27	c	516	BCR	C11-C10-C9-C8
30	A	616	DGD	C2E-C1E-O5D-C6D
31	m	102	STE	C3-C4-C5-C6
31	B	626	STE	C5-C6-C7-C8
32	D	406	LMG	C36-C37-C38-C39
32	c	522	LMG	C29-C30-C31-C32
32	c	524	LMG	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	c	517	DGD	O6D-C5D-C6D-O5D
29	l	101	SQD	O10-C23-O48-C46
30	c	517	DGD	CBB-CCB-CDB-CEB
30	c	518	DGD	CDB-CEB-CFB-CGB
33	E	101	LHG	C35-C36-C37-C38
31	R	101	STE	C3-C4-C5-C6
25	B	602	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	603	CLA	C11-C10-C8-C7
25	B	603	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C15
25	B	606	CLA	C6-C7-C8-C10
25	B	610	CLA	C11-C10-C8-C7
25	B	612	CLA	C12-C13-C15-C16
25	B	614	CLA	C6-C7-C8-C10
25	B	614	CLA	C11-C10-C8-C7
25	C	503	CLA	C11-C10-C8-C7
25	C	505	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	505	CLA	C12-C13-C15-C16
25	C	509	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	C	511	CLA	C11-C12-C13-C15
25	C	512	CLA	C6-C7-C8-C10
25	D	403	CLA	C6-C7-C8-C10
25	a	610	CLA	C12-C13-C15-C16
25	b	601	CLA	C12-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C7
25	c	505	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C15
25	c	509	CLA	C6-C7-C8-C10
25	c	510	CLA	C6-C7-C8-C10
25	c	510	CLA	C12-C13-C15-C16
25	c	512	CLA	C12-C13-C15-C16
25	h	101	CLA	C11-C12-C13-C15
30	C	516	DGD	O1G-C1A-C2A-C3A
25	A	607	CLA	C6-C7-C8-C9
25	B	602	CLA	C6-C7-C8-C9
25	B	605	CLA	C11-C12-C13-C14
25	B	610	CLA	C14-C13-C15-C16
25	C	505	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	D	403	CLA	C11-C10-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	a	608	CLA	C14-C13-C15-C16
25	b	601	CLA	C6-C7-C8-C9
25	b	601	CLA	C14-C13-C15-C16
25	b	603	CLA	C14-C13-C15-C16
25	b	608	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
25	c	510	CLA	C6-C7-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	h	101	CLA	C11-C12-C13-C14
29	A	614	SQD	C9-C10-C11-C12
31	l	103	STE	C4-C5-C6-C7
32	M	101	LMG	C31-C32-C33-C34
25	c	501	CLA	O1D-CGD-O2D-CED
33	d	407	LHG	C35-C36-C37-C38
30	A	616	DGD	C4D-C5D-C6D-O5D
25	C	513	CLA	C16-C17-C18-C19
25	c	506	CLA	C16-C17-C18-C19
30	C	517	DGD	CBB-CCB-CDB-CEB
27	K	101	BCR	C7-C8-C9-C10
30	C	517	DGD	CDA-CEA-CFA-CGA
31	J	101	STE	C6-C7-C8-C9
31	t	103	STE	C5-C6-C7-C8
33	B	622	LHG	C1-C2-C3-O3
25	C	505	CLA	C10-C11-C12-C13
25	C	508	CLA	C15-C16-C17-C18
29	A	614	SQD	C8-C7-O47-C45
29	l	101	SQD	C35-C36-C37-C38
32	D	409	LMG	C34-C35-C36-C37
29	a	614	SQD	C26-C27-C28-C29
31	M	103	STE	C1-C2-C3-C4
31	b	622	STE	C11-C12-C13-C14
25	A	607	CLA	C15-C16-C17-C18
32	c	520	LMG	C4-C5-C6-O5
32	C	519	LMG	C18-C19-C20-C21
32	C	519	LMG	C37-C38-C39-C40
33	B	622	LHG	C16-C17-C18-C19
27	b	618	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	614	SQD	C10-C11-C12-C13
29	l	101	SQD	C17-C18-C19-C20
32	C	519	LMG	C40-C41-C42-C43
33	E	101	LHG	C28-C29-C30-C31
32	d	409	LMG	C35-C36-C37-C38
25	D	402	CLA	C2C-C3C-CAC-CBC
30	C	517	DGD	C5B-C6B-C7B-C8B
30	h	102	DGD	O2G-C1B-C2B-C3B
30	C	518	DGD	C2B-C3B-C4B-C5B
30	a	616	DGD	CBB-CCB-CDB-CEB
32	C	515	LMG	C32-C33-C34-C35
25	C	510	CLA	C4-C3-C5-C6
31	T	102	STE	C3-C4-C5-C6
32	c	524	LMG	C17-C18-C19-C20
25	b	605	CLA	C15-C16-C17-C18
29	a	615	SQD	C11-C12-C13-C14
31	b	621	STE	C9-C10-C11-C12
33	d	407	LHG	C9-C10-C11-C12
30	C	518	DGD	C4B-C5B-C6B-C7B
33	l	102	LHG	C34-C35-C36-C37
32	d	410	LMG	C11-C10-O7-C8
29	A	614	SQD	C24-C25-C26-C27
32	c	522	LMG	C32-C33-C34-C35
25	b	601	CLA	C3-C5-C6-C7
31	B	619	STE	C10-C11-C12-C13
25	C	513	CLA	CBA-CGA-O2A-C1
29	f	101	SQD	C26-C27-C28-C29
30	A	616	DGD	CDB-CEB-CFB-CGB
32	D	409	LMG	C7-C8-C9-O8
29	l	101	SQD	C34-C35-C36-C37
30	A	616	DGD	CFA-CGA-CHA-CIA
31	b	619	STE	C4-C5-C6-C7
31	m	102	STE	C4-C5-C6-C7
33	l	102	LHG	C24-C25-C26-C27
29	a	614	SQD	C11-C10-C9-C8
32	c	522	LMG	C15-C16-C17-C18
29	a	615	SQD	C15-C16-C17-C18
28	a	612	PL9	C18-C19-C21-C22
31	M	103	STE	C4-C5-C6-C7
33	e	102	LHG	C4-O6-P-O3
32	c	524	LMG	C10-C11-C12-C13
30	c	517	DGD	C7A-C8A-C9A-CAA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	T	102	STE	C10-C11-C12-C13
32	c	524	LMG	C11-C12-C13-C14
33	d	407	LHG	O1-C1-C2-O2
25	c	503	CLA	C15-C16-C17-C18
31	c	521	STE	C11-C10-C9-C8
32	D	406	LMG	C34-C35-C36-C37
29	a	614	SQD	C24-C23-O48-C46
28	d	405	PL9	C42-C43-C44-C45
25	B	603	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	C	510	CLA	C16-C17-C18-C20
25	a	608	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C15
31	D	410	STE	C7-C8-C9-C10
32	c	522	LMG	C31-C32-C33-C34
31	d	411	STE	C12-C13-C14-C15
32	C	519	LMG	C14-C15-C16-C17
33	d	406	LHG	C33-C34-C35-C36
29	a	614	SQD	O47-C45-C46-O48
32	C	519	LMG	O1-C7-C8-O7
32	D	409	LMG	O7-C8-C9-O8
32	M	101	LMG	O7-C8-C9-O8
32	c	522	LMG	O7-C8-C9-O8
32	m	101	LMG	O7-C8-C9-O8
25	A	606	CLA	C15-C16-C17-C18
29	A	615	SQD	C19-C20-C21-C22
29	L	101	SQD	C25-C26-C27-C28
30	c	517	DGD	C1A-C2A-C3A-C4A
30	C	517	DGD	O6E-C1E-O5D-C6D
33	D	407	LHG	C1-C2-C3-O3
30	C	517	DGD	C7B-C8B-C9B-CAB
31	a	617	STE	C2-C3-C4-C5
31	c	521	STE	C15-C16-C17-C18
25	d	402	CLA	C2-C1-O2A-CGA
25	C	510	CLA	C2-C3-C5-C6
29	F	102	SQD	C28-C29-C30-C31
25	c	505	CLA	C5-C6-C7-C8
25	c	507	CLA	C15-C16-C17-C18
25	B	601	CLA	C11-C12-C13-C14
25	B	612	CLA	C14-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C9
25	b	604	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C11-C12-C13-C14
25	c	506	CLA	C11-C10-C8-C9
25	c	512	CLA	C11-C12-C13-C14
30	H	103	DGD	C3A-C4A-C5A-C6A
32	b	620	LMG	C15-C16-C17-C18
29	A	614	SQD	C11-C10-C9-C8
31	B	624	STE	C9-C10-C11-C12
32	D	409	LMG	C37-C38-C39-C40
26	d	401	PHO	C1A-C2A-CAA-CBA
33	d	408	LHG	C2-C3-O3-P
30	c	517	DGD	C4A-C5A-C6A-C7A
25	C	506	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C19
27	A	611	BCR	C23-C24-C25-C26
27	B	617	BCR	C23-C24-C25-C26
27	C	514	BCR	C23-C24-C25-C26
27	C	514	BCR	C23-C24-C25-C30
27	H	102	BCR	C23-C24-C25-C26
27	H	102	BCR	C23-C24-C25-C30
27	K	103	BCR	C1-C6-C7-C8
27	K	103	BCR	C5-C6-C7-C8
27	K	103	BCR	C23-C24-C25-C26
27	b	616	BCR	C1-C6-C7-C8
27	b	616	BCR	C5-C6-C7-C8
27	c	514	BCR	C1-C6-C7-C8
27	c	514	BCR	C5-C6-C7-C8
27	c	515	BCR	C1-C6-C7-C8
27	c	515	BCR	C5-C6-C7-C8
27	d	404	BCR	C23-C24-C25-C26
31	B	623	STE	C7-C8-C9-C10
25	C	510	CLA	O1D-CGD-O2D-CED
32	M	101	LMG	C28-C29-C30-C31
30	C	518	DGD	O6D-C5D-C6D-O5D
27	d	404	BCR	C14-C15-C16-C17
32	m	101	LMG	C29-C30-C31-C32
30	C	517	DGD	C9A-CAA-CBA-CCA
25	B	609	CLA	C16-C17-C18-C19
30	H	103	DGD	C1B-C2B-C3B-C4B
30	a	616	DGD	C2B-C3B-C4B-C5B
31	T	103	STE	C11-C10-C9-C8
33	D	408	LHG	C16-C17-C18-C19
33	d	407	LHG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	605	CLA	CBD-CGD-O2D-CED
33	d	407	LHG	O6-C4-C5-C6
28	d	405	PL9	C15-C14-C16-C17
30	C	516	DGD	C6A-C7A-C8A-C9A
32	D	406	LMG	C20-C21-C22-C23
30	H	103	DGD	C4E-C5E-C6E-O5E
25	A	607	CLA	C11-C12-C13-C15
25	B	601	CLA	C11-C12-C13-C15
25	B	603	CLA	C11-C12-C13-C15
25	B	613	CLA	C12-C13-C15-C16
25	B	614	CLA	C11-C12-C13-C15
25	C	506	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10
25	H	101	CLA	C6-C7-C8-C10
25	a	608	CLA	C11-C10-C8-C7
25	a	608	CLA	C12-C13-C15-C16
25	b	601	CLA	C6-C7-C8-C10
25	b	603	CLA	C12-C13-C15-C16
25	b	604	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C15
25	b	608	CLA	C12-C13-C15-C16
25	b	611	CLA	C12-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C7
25	c	505	CLA	C6-C7-C8-C10
25	c	512	CLA	C6-C7-C8-C10
25	c	512	CLA	C11-C12-C13-C15
32	d	409	LMG	C40-C41-C42-C43
25	B	608	CLA	C16-C17-C18-C19
31	D	410	STE	C9-C10-C11-C12
33	B	621	LHG	C16-C17-C18-C19
33	e	102	LHG	C26-C27-C28-C29
25	c	510	CLA	C5-C6-C7-C8
30	h	102	DGD	C5A-C6A-C7A-C8A
27	K	103	BCR	C16-C17-C18-C36
27	a	611	BCR	C16-C17-C18-C36
27	b	616	BCR	C20-C21-C22-C37
27	b	617	BCR	C16-C17-C18-C36
27	b	618	BCR	C20-C21-C22-C37
27	k	101	BCR	C35-C13-C14-C15
32	D	406	LMG	C37-C38-C39-C40
33	E	101	LHG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	513	CLA	C16-C17-C18-C20
25	a	608	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C20
25	D	403	CLA	C8-C10-C11-C12
26	d	401	PHO	C5-C6-C7-C8
30	H	103	DGD	O2G-C1B-C2B-C3B
29	L	101	SQD	C19-C20-C21-C22
31	I	101	STE	C4-C5-C6-C7
31	m	102	STE	C6-C7-C8-C9
29	a	615	SQD	C18-C19-C20-C21
31	M	102	STE	C5-C6-C7-C8
32	m	101	LMG	C16-C17-C18-C19
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	615	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	b	603	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
26	a	609	PHO	CAD-CBD-CGD-O2D
30	a	616	DGD	C3A-C4A-C5A-C6A
30	c	518	DGD	O6E-C5E-C6E-O5E
30	A	616	DGD	C2A-C1A-O1G-C1G
28	A	612	PL9	C47-C48-C49-C50
25	B	612	CLA	C4-C3-C5-C6
25	c	502	CLA	C16-C17-C18-C19
31	M	102	STE	C11-C10-C9-C8
30	A	616	DGD	O6E-C1E-O5D-C6D
25	c	510	CLA	C2-C3-C5-C6
26	A	609	PHO	C2C-C3C-CAC-CBC
30	C	516	DGD	O1G-C1G-C2G-C3G
32	M	101	LMG	C7-C8-C9-O8
32	m	101	LMG	O1-C7-C8-C9
29	a	614	SQD	C19-C20-C21-C22
33	l	102	LHG	O6-C4-C5-O7
25	C	512	CLA	C3-C5-C6-C7
33	D	408	LHG	C25-C26-C27-C28
32	d	410	LMG	C40-C41-C42-C43
25	C	513	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	622	STE	C6-C7-C8-C9
33	D	408	LHG	C13-C14-C15-C16
25	C	509	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	H	101	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O1D
32	C	519	LMG	O10-C28-O8-C9
25	b	607	CLA	C4C-C3C-CAC-CBC
29	a	614	SQD	C13-C14-C15-C16
30	a	616	DGD	C5A-C6A-C7A-C8A
32	m	101	LMG	C17-C18-C19-C20
30	C	517	DGD	C2E-C1E-O5D-C6D
32	C	515	LMG	C40-C41-C42-C43
32	D	409	LMG	C30-C31-C32-C33
29	A	614	SQD	O6-C44-C45-O47
30	C	516	DGD	O1G-C1G-C2G-O2G
32	m	101	LMG	O1-C7-C8-O7
32	D	409	LMG	C36-C37-C38-C39
25	b	614	CLA	C8-C10-C11-C12
29	a	614	SQD	O10-C23-O48-C46
32	D	406	LMG	C11-C12-C13-C14
25	c	502	CLA	C16-C17-C18-C20
33	E	101	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
30	c	519	DGD	CDB-CEB-CFB-CGB
25	C	506	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
25	b	610	CLA	C2-C3-C5-C6
28	A	612	PL9	C4-C3-C7-C8
28	a	612	PL9	C4-C3-C7-C8
25	A	607	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C12-C13-C14
25	a	608	CLA	C11-C10-C8-C9
25	c	504	CLA	C11-C10-C8-C9
31	I	101	STE	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	b	620	LMG	C30-C31-C32-C33
32	c	524	LMG	C37-C38-C39-C40
33	D	407	LHG	C35-C36-C37-C38
29	f	101	SQD	C5-C6-S-O8
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	CBA-CGA-O2A-C1
30	c	517	DGD	C4D-C5D-C6D-O5D
27	D	404	BCR	C7-C8-C9-C10
29	a	615	SQD	C29-C30-C31-C32
30	c	519	DGD	C5B-C6B-C7B-C8B
25	C	503	CLA	C1A-C2A-CAA-CBA
25	a	613	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
33	B	622	LHG	C7-C8-C9-C10
29	A	614	SQD	O49-C7-O47-C45
33	d	407	LHG	C31-C32-C33-C34
30	H	103	DGD	C7A-C8A-C9A-CAA
31	B	619	STE	C7-C8-C9-C10
31	B	619	STE	C11-C12-C13-C14
32	C	519	LMG	C11-C12-C13-C14
25	a	610	CLA	C4-C3-C5-C6
28	d	405	PL9	C28-C29-C31-C32
30	c	517	DGD	C8B-C9B-CAB-CBB
32	b	620	LMG	C37-C38-C39-C40
32	b	620	LMG	C39-C40-C41-C42
25	b	602	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	O1A-CGA-O2A-C1
33	B	621	LHG	C4-O6-P-O5
33	D	407	LHG	C4-O6-P-O5
33	d	406	LHG	C3-O3-P-O5
33	e	102	LHG	C4-O6-P-O5
33	l	102	LHG	C4-O6-P-O5
25	C	510	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
25	b	610	CLA	C16-C17-C18-C19
30	c	518	DGD	C8B-C9B-CAB-CBB
32	b	620	LMG	O6-C1-O1-C7
25	D	403	CLA	C13-C15-C16-C17
25	c	506	CLA	CBA-CGA-O2A-C1
33	e	102	LHG	O6-C4-C5-C6
31	M	102	STE	C1-C2-C3-C4
25	A	607	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	408	LHG	C34-C35-C36-C37
32	C	519	LMG	C16-C17-C18-C19
29	a	615	SQD	C31-C32-C33-C34
32	c	522	LMG	C16-C17-C18-C19
25	B	606	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	H	101	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
31	B	625	STE	C1-C2-C3-C4
30	c	517	DGD	C2B-C3B-C4B-C5B
30	a	616	DGD	CFA-CGA-CHA-CIA
32	B	620	LMG	C34-C35-C36-C37
30	C	517	DGD	C4A-C5A-C6A-C7A
30	c	519	DGD	C8B-C9B-CAB-CBB
29	A	614	SQD	C29-C30-C31-C32
31	c	523	STE	C7-C8-C9-C10
32	d	409	LMG	C39-C40-C41-C42
25	B	601	CLA	C16-C17-C18-C20
25	A	613	CLA	C12-C13-C15-C16
25	B	612	CLA	C6-C7-C8-C10
25	B	612	CLA	C11-C12-C13-C15
25	B	614	CLA	C12-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C10
25	C	504	CLA	C6-C7-C8-C10
25	C	509	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C12-C13-C15
25	H	101	CLA	C11-C10-C8-C7
25	b	605	CLA	C11-C10-C8-C7
25	b	615	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C10-C8-C7
25	c	513	CLA	C11-C12-C13-C15
33	E	101	LHG	O6-C4-C5-O7
33	d	407	LHG	O6-C4-C5-O7
30	c	519	DGD	C7B-C8B-C9B-CAB
31	B	619	STE	C12-C13-C14-C15
30	H	103	DGD	C6B-C7B-C8B-C9B
32	D	409	LMG	C13-C14-C15-C16
31	C	520	STE	C7-C8-C9-C10
31	j	101	STE	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	M	101	LMG	C14-C15-C16-C17
30	h	102	DGD	C9A-CAA-CBA-CCA
25	b	615	CLA	C11-C12-C13-C15
32	M	101	LMG	C10-C11-C12-C13
32	C	515	LMG	O1-C7-C8-C9
32	b	620	LMG	O1-C7-C8-C9
33	e	102	LHG	C4-C5-C6-O8
32	b	620	LMG	O1-C7-C8-O7
29	f	101	SQD	C29-C30-C31-C32
31	l	103	STE	C10-C11-C12-C13
32	C	519	LMG	C13-C14-C15-C16
33	d	406	LHG	C30-C31-C32-C33
32	C	515	LMG	C39-C40-C41-C42
30	C	517	DGD	C2G-C3G-O3G-C1D
29	L	101	SQD	C30-C31-C32-C33
32	M	101	LMG	C30-C31-C32-C33
31	t	102	STE	C5-C6-C7-C8
31	l	103	STE	C15-C16-C17-C18
25	c	508	CLA	C10-C11-C12-C13
25	B	612	CLA	C6-C7-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	C	508	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C12-C13-C14
25	b	614	CLA	C6-C7-C8-C9
25	c	505	CLA	C6-C7-C8-C9
31	b	619	STE	C2-C3-C4-C5
32	b	620	LMG	C32-C33-C34-C35
33	d	406	LHG	O1-C1-C2-O2
32	D	406	LMG	C33-C34-C35-C36
32	c	520	LMG	C40-C41-C42-C43
28	d	405	PL9	C27-C28-C29-C30
25	B	608	CLA	C16-C17-C18-C20
25	C	506	CLA	C16-C17-C18-C19
29	f	101	SQD	C24-C25-C26-C27
30	c	517	DGD	C6B-C7B-C8B-C9B
27	T	101	BCR	C21-C22-C23-C24
29	A	615	SQD	C27-C28-C29-C30
32	b	620	LMG	C13-C14-C15-C16
32	D	406	LMG	C16-C17-C18-C19
32	c	524	LMG	C40-C41-C42-C43
32	m	101	LMG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C2-C3-C5-C6
30	C	516	DGD	C9B-CAB-CBB-CCB
30	A	616	DGD	C3B-C4B-C5B-C6B
32	C	515	LMG	C19-C20-C21-C22
29	f	101	SQD	C44-C45-O47-C7
32	b	620	LMG	C9-C8-O7-C10
32	c	524	LMG	C9-C8-O7-C10
25	C	501	CLA	C2A-CAA-CBA-CGA
25	C	506	CLA	C2-C1-O2A-CGA
29	l	101	SQD	C27-C28-C29-C30
32	D	406	LMG	C19-C20-C21-C22
30	A	616	DGD	CFB-CGB-CHB-CIB
33	B	621	LHG	O10-C23-O8-C6
33	e	102	LHG	O6-C4-C5-O7
31	b	619	STE	C3-C4-C5-C6
25	B	612	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19
32	C	515	LMG	C17-C18-C19-C20
27	A	611	BCR	C1-C6-C7-C8
27	A	611	BCR	C5-C6-C7-C8
27	B	617	BCR	C23-C24-C25-C30
27	d	404	BCR	C23-C24-C25-C30
31	l	103	STE	C13-C14-C15-C16
25	C	512	CLA	C10-C11-C12-C13
25	b	607	CLA	C13-C15-C16-C17
27	C	514	BCR	C11-C10-C9-C8
27	H	102	BCR	C11-C10-C9-C8
32	b	620	LMG	C2-C1-O1-C7
32	b	620	LMG	O7-C8-C9-O8
33	e	102	LHG	O7-C5-C6-O8
31	T	103	STE	C15-C16-C17-C18
31	b	621	STE	C3-C4-C5-C6
32	M	101	LMG	C18-C19-C20-C21
33	d	407	LHG	C3-O3-P-O6
32	c	524	LMG	C18-C19-C20-C21
30	C	516	DGD	O6D-C5D-C6D-O5D
25	a	607	CLA	C16-C17-C18-C19
30	h	102	DGD	CDB-CEB-CFB-CGB
29	A	615	SQD	O48-C23-C24-C25
30	c	519	DGD	C1B-C2B-C3B-C4B
31	d	411	STE	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	624	STE	C11-C12-C13-C14
32	c	522	LMG	O1-C7-C8-C9
32	B	620	LMG	C35-C36-C37-C38
25	b	613	CLA	C6-C7-C8-C10
25	b	613	CLA	C11-C12-C13-C15
32	M	101	LMG	C34-C35-C36-C37
33	D	407	LHG	C30-C31-C32-C33
25	A	613	CLA	C11-C12-C13-C14
25	A	613	CLA	C14-C13-C15-C16
25	B	606	CLA	C6-C7-C8-C9
25	B	614	CLA	C14-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C9
25	C	505	CLA	C6-C7-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C12-C13-C14
25	D	403	CLA	C6-C7-C8-C9
25	a	610	CLA	C14-C13-C15-C16
25	b	605	CLA	C11-C10-C8-C9
25	b	611	CLA	C14-C13-C15-C16
25	c	505	CLA	C14-C13-C15-C16
25	A	606	CLA	C13-C15-C16-C17
27	K	101	BCR	C13-C14-C15-C16
29	F	102	SQD	C44-C45-C46-O48
32	d	410	LMG	C11-C12-C13-C14
30	h	102	DGD	CBB-CCB-CDB-CEB
30	C	517	DGD	C7A-C8A-C9A-CAA
31	I	101	STE	C11-C10-C9-C8
30	C	516	DGD	C4D-C5D-C6D-O5D
25	C	513	CLA	C8-C10-C11-C12
30	a	616	DGD	C6B-C7B-C8B-C9B
32	M	101	LMG	C15-C16-C17-C18
25	c	513	CLA	C3-C5-C6-C7
25	C	513	CLA	C13-C15-C16-C17
30	C	516	DGD	CBA-CCA-CDA-CEA
25	B	612	CLA	C16-C17-C18-C20
25	a	610	CLA	CBA-CGA-O2A-C1
32	c	520	LMG	C29-C28-O8-C9
25	b	603	CLA	C8-C10-C11-C12
25	B	607	CLA	C10-C11-C12-C13
31	D	410	STE	O2-C1-C2-C3
30	H	103	DGD	CAA-CBA-CCA-CDA
32	D	406	LMG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	612	CLA	C13-C15-C16-C17
30	c	519	DGD	O6D-C5D-C6D-O5D
25	C	505	CLA	CBD-CGD-O2D-CED
27	K	101	BCR	C9-C10-C11-C12
27	d	404	BCR	C13-C14-C15-C16
32	B	620	LMG	C30-C31-C32-C33
31	D	410	STE	C5-C6-C7-C8
33	B	622	LHG	C13-C14-C15-C16
25	B	613	CLA	C4-C3-C5-C6
28	a	612	PL9	C30-C29-C31-C32
25	A	613	CLA	C13-C15-C16-C17
25	B	611	CLA	C8-C10-C11-C12
25	D	402	CLA	C2-C1-O2A-CGA
32	m	101	LMG	C18-C19-C20-C21
30	C	517	DGD	C2D-C1D-O3G-C3G
25	B	601	CLA	C2A-CAA-CBA-CGA
31	B	626	STE	C4-C5-C6-C7
25	H	101	CLA	C3A-C2A-CAA-CBA
25	c	505	CLA	C13-C15-C16-C17
25	c	509	CLA	C16-C17-C18-C19
32	c	520	LMG	C34-C35-C36-C37
27	B	616	BCR	C9-C10-C11-C12
25	b	611	CLA	C10-C11-C12-C13
28	D	405	PL9	C30-C29-C31-C32
30	h	102	DGD	CBA-CCA-CDA-CEA
32	c	524	LMG	C38-C39-C40-C41
30	h	102	DGD	CAB-CBB-CCB-CDB
25	B	605	CLA	C6-C7-C8-C9
25	B	605	CLA	C11-C10-C8-C9
25	B	613	CLA	C6-C7-C8-C9
25	C	507	CLA	C14-C13-C15-C16
25	c	503	CLA	C11-C12-C13-C14
25	c	513	CLA	C11-C12-C13-C14
33	D	408	LHG	C35-C36-C37-C38
31	b	619	STE	O1-C1-C2-C3
31	B	619	STE	C1-C2-C3-C4
32	D	406	LMG	C38-C39-C40-C41
27	K	101	BCR	C20-C21-C22-C37
27	x	101	BCR	C20-C21-C22-C37
29	a	614	SQD	C44-C45-C46-O48
35	F	101	HEM	CAD-CBD-CGD-O1D
25	B	601	CLA	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	512	CLA	O2A-C1-C2-C3
25	D	403	CLA	O2A-C1-C2-C3
26	A	608	PHO	O2A-C1-C2-C3
26	a	609	PHO	O2A-C1-C2-C3
29	A	614	SQD	C24-C23-O48-C46
30	c	517	DGD	O6E-C1E-O5D-C6D
31	B	624	STE	O1-C1-C2-C3
31	J	101	STE	C3-C4-C5-C6
33	D	408	LHG	C12-C13-C14-C15
32	m	101	LMG	C28-C29-C30-C31
29	A	614	SQD	C11-C12-C13-C14
29	f	101	SQD	C46-C45-O47-C7
32	C	515	LMG	C9-C8-O7-C10
25	A	613	CLA	C11-C12-C13-C15
25	B	602	CLA	C11-C10-C8-C7
25	B	609	CLA	C12-C13-C15-C16
25	b	612	CLA	C11-C10-C8-C7
25	c	501	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C10-C8-C7
29	A	614	SQD	O10-C23-O48-C46
32	B	620	LMG	O7-C10-C11-C12
27	c	516	BCR	C15-C16-C17-C18
31	j	101	STE	C7-C8-C9-C10
33	B	622	LHG	C24-C25-C26-C27
32	C	515	LMG	C12-C13-C14-C15
30	C	518	DGD	CBA-CCA-CDA-CEA
32	C	519	LMG	C38-C39-C40-C41
31	D	410	STE	O1-C1-C2-C3
32	B	620	LMG	C11-C12-C13-C14
31	D	410	STE	C10-C11-C12-C13
30	H	103	DGD	C9A-CAA-CBA-CCA
31	b	622	STE	C14-C15-C16-C17
32	c	520	LMG	C39-C40-C41-C42
30	C	517	DGD	C2B-C3B-C4B-C5B
25	H	101	CLA	C15-C16-C17-C18
33	B	621	LHG	C35-C36-C37-C38
31	d	411	STE	O2-C1-C2-C3
30	C	516	DGD	C5B-C6B-C7B-C8B
30	H	103	DGD	CBB-CCB-CDB-CEB
25	c	509	CLA	CAA-CBA-CGA-O1A
29	A	614	SQD	C15-C16-C17-C18
31	l	103	STE	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	M	101	LMG	C16-C17-C18-C19
33	D	408	LHG	C23-C24-C25-C26
25	c	506	CLA	C8-C10-C11-C12
25	C	508	CLA	O1A-CGA-O2A-C1
25	a	610	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	C4-C3-C5-C6
28	a	612	PL9	C7-C8-C9-C10
25	B	612	CLA	C2-C1-O2A-CGA
25	a	607	CLA	C2-C1-O2A-CGA
28	A	612	PL9	C13-C14-C16-C17
33	D	408	LHG	C31-C32-C33-C34
31	B	624	STE	O2-C1-C2-C3
31	b	619	STE	O2-C1-C2-C3
25	b	610	CLA	C11-C12-C13-C14
31	b	622	STE	C12-C13-C14-C15
25	B	608	CLA	C15-C16-C17-C18
35	F	101	HEM	CAD-CBD-CGD-O2D
31	M	102	STE	C7-C8-C9-C10
31	H	104	STE	C11-C10-C9-C8
32	B	620	LMG	C12-C13-C14-C15
33	l	102	LHG	C17-C18-C19-C20
27	A	611	BCR	C23-C24-C25-C30
27	K	101	BCR	C23-C24-C25-C30
27	K	102	BCR	C23-C24-C25-C30
27	b	617	BCR	C23-C24-C25-C30
27	c	514	BCR	C23-C24-C25-C30
27	c	516	BCR	C1-C6-C7-C8
27	c	516	BCR	C23-C24-C25-C30
27	k	101	BCR	C23-C24-C25-C30
27	t	101	BCR	C1-C6-C7-C8
27	x	101	BCR	C23-C24-C25-C30
32	b	620	LMG	C7-C8-C9-O8
32	c	522	LMG	C11-C12-C13-C14
25	H	101	CLA	C4-C3-C5-C6
27	t	101	BCR	C7-C8-C9-C10
30	c	518	DGD	C2G-C3G-O3G-C1D
31	d	411	STE	O1-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
25	C	505	CLA	C16-C17-C18-C19
25	C	511	CLA	C16-C17-C18-C19
25	b	601	CLA	C16-C17-C18-C19
25	b	608	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	L	101	SQD	C12-C13-C14-C15
30	H	103	DGD	CBA-CCA-CDA-CEA
31	d	411	STE	C6-C7-C8-C9
32	C	515	LMG	C28-C29-C30-C31
25	c	504	CLA	C4-C3-C5-C6
28	D	405	PL9	C24-C26-C27-C28
28	D	405	PL9	C44-C46-C47-C48
25	c	506	CLA	C10-C11-C12-C13
30	a	616	DGD	CCB-CDB-CEB-CFB
32	c	524	LMG	C16-C17-C18-C19
30	c	517	DGD	O1G-C1A-C2A-C3A
25	a	607	CLA	C16-C17-C18-C20
31	M	102	STE	C9-C10-C11-C12
29	f	101	SQD	O6-C44-C45-O47
32	c	522	LMG	O1-C7-C8-O7
25	b	614	CLA	C13-C15-C16-C17
25	h	101	CLA	C10-C11-C12-C13
25	c	507	CLA	C3-C5-C6-C7
25	c	501	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	C5-C6-C7-C8
29	F	102	SQD	C31-C32-C33-C34
25	b	612	CLA	C16-C17-C18-C19
33	d	406	LHG	C26-C27-C28-C29
36	V	201	HEC	CAD-CBD-CGD-O1D
25	C	508	CLA	CBA-CGA-O2A-C1
27	B	616	BCR	C11-C10-C9-C34
27	K	103	BCR	C11-C10-C9-C34
27	b	618	BCR	C35-C13-C14-C15
31	B	626	STE	C11-C10-C9-C8
31	c	521	STE	C4-C5-C6-C7
29	a	615	SQD	O48-C23-C24-C25
25	A	610	CLA	C4-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
28	A	612	PL9	C12-C11-C9-C10
28	a	612	PL9	C35-C34-C36-C37
28	a	612	PL9	C45-C44-C46-C47
31	B	623	STE	O2-C1-C2-C3
25	B	612	CLA	C2-C3-C5-C6
29	l	101	SQD	C24-C25-C26-C27
25	B	602	CLA	C11-C10-C8-C9
25	B	605	CLA	C14-C13-C15-C16
25	B	608	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	501	CLA	C14-C13-C15-C16
25	C	504	CLA	C6-C7-C8-C9
25	H	101	CLA	C11-C10-C8-C9
25	c	510	CLA	C11-C10-C8-C9
32	b	620	LMG	C18-C19-C20-C21
31	M	102	STE	O1-C1-C2-C3
36	v	201	HEC	CAD-CBD-CGD-O2D
31	H	104	STE	C15-C16-C17-C18
26	d	401	PHO	O1D-CGD-O2D-CED
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	611	CLA	CAA-CBA-CGA-O2A
30	c	517	DGD	O2G-C1B-C2B-C3B
30	C	517	DGD	C9B-CAB-CBB-CCB
25	B	611	CLA	CAD-CBD-CGD-O2D
25	C	512	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	b	602	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	606	CLA	CAD-CBD-CGD-O2D
25	b	609	CLA	CAD-CBD-CGD-O2D
25	h	101	CLA	CAD-CBD-CGD-O2D
29	a	615	SQD	C9-C10-C11-C12
31	C	522	STE	C12-C13-C14-C15
33	E	101	LHG	O9-C7-O7-C5
31	B	626	STE	C6-C7-C8-C9
31	T	103	STE	C6-C7-C8-C9
33	B	621	LHG	C19-C20-C21-C22
30	c	519	DGD	O1G-C1A-C2A-C3A
31	R	101	STE	C2-C3-C4-C5
25	B	614	CLA	C16-C17-C18-C19
31	M	102	STE	O2-C1-C2-C3
31	C	522	STE	C4-C5-C6-C7
30	c	518	DGD	O6D-C1D-O3G-C3G
29	L	101	SQD	C28-C29-C30-C31
28	a	612	PL9	C24-C26-C27-C28
31	C	522	STE	C3-C4-C5-C6
32	m	101	LMG	C38-C39-C40-C41
31	C	521	STE	C1-C2-C3-C4
33	E	101	LHG	C4-C5-C6-O8
31	R	101	STE	O1-C1-C2-C3
25	B	611	CLA	CBA-CGA-O2A-C1
25	B	609	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	A	616	DGD	C6A-C7A-C8A-C9A
33	B	621	LHG	C11-C10-C9-C8
33	D	407	LHG	C33-C34-C35-C36
29	a	614	SQD	O47-C7-C8-C9
29	f	101	SQD	O48-C23-C24-C25
25	B	615	CLA	O2A-C1-C2-C3
25	C	513	CLA	O2A-C1-C2-C3
25	d	402	CLA	O2A-C1-C2-C3
27	B	616	BCR	C14-C15-C16-C17
27	K	101	BCR	C14-C15-C16-C17
32	d	410	LMG	O7-C10-C11-C12
31	c	521	STE	O1-C1-C2-C3
31	c	521	STE	O2-C1-C2-C3
32	B	620	LMG	O9-C10-C11-C12
25	c	512	CLA	O1D-CGD-O2D-CED
32	c	520	LMG	C30-C31-C32-C33
33	B	622	LHG	O2-C2-C3-O3
26	d	401	PHO	CBD-CGD-O2D-CED
25	A	607	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	a	608	CLA	CHA-CBD-CGD-O1D
25	a	608	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	506	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O1D
36	v	201	HEC	CAD-CBD-CGD-O1D
25	C	512	CLA	C4-C3-C5-C6
33	d	408	LHG	C35-C36-C37-C38
30	H	103	DGD	C5A-C6A-C7A-C8A
30	c	519	DGD	C8A-C9A-CAA-CBA
33	d	408	LHG	C31-C32-C33-C34
25	c	511	CLA	C3-C5-C6-C7
32	m	101	LMG	C11-C10-O7-C8
32	D	406	LMG	C12-C13-C14-C15
32	M	101	LMG	C36-C37-C38-C39
29	L	101	SQD	C11-C10-C9-C8
32	D	409	LMG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	h	101	CLA	C15-C16-C17-C18
32	b	620	LMG	O7-C10-C11-C12
33	E	101	LHG	O7-C5-C6-O8
31	R	101	STE	O2-C1-C2-C3
32	D	409	LMG	C31-C32-C33-C34
31	t	103	STE	C4-C5-C6-C7
29	A	614	SQD	O47-C7-C8-C9
32	m	101	LMG	O8-C28-C29-C30
31	C	521	STE	O2-C1-C2-C3
26	A	608	PHO	CHA-CBD-CGD-O1D
26	A	609	PHO	CHA-CBD-CGD-O1D
31	t	102	STE	C2-C3-C4-C5
25	B	611	CLA	CAA-CBA-CGA-O2A
30	C	517	DGD	O2G-C1B-C2B-C3B
32	B	620	LMG	O10-C28-C29-C30
31	b	622	STE	C9-C10-C11-C12
33	B	621	LHG	C10-C11-C12-C13
25	C	507	CLA	C6-C7-C8-C10
25	a	610	CLA	C2-C3-C5-C6
25	c	509	CLA	C11-C12-C13-C15
25	c	505	CLA	C10-C11-C12-C13
25	A	613	CLA	C4C-C3C-CAC-CBC
25	c	507	CLA	C11-C10-C8-C9
31	B	623	STE	O1-C1-C2-C3
33	l	102	LHG	C24-C23-O8-C6
29	f	101	SQD	C4-C5-C6-S
29	a	614	SQD	C34-C35-C36-C37
28	D	405	PL9	C46-C47-C48-C49
25	B	601	CLA	C15-C16-C17-C18
29	L	101	SQD	C16-C17-C18-C19
25	h	101	CLA	C16-C17-C18-C19
26	d	401	PHO	C16-C17-C18-C20
33	B	621	LHG	C28-C29-C30-C31
31	T	102	STE	C4-C5-C6-C7
32	M	101	LMG	C39-C40-C41-C42
30	H	103	DGD	O1A-C1A-O1G-C1G
28	d	405	PL9	C13-C14-C16-C17
33	E	101	LHG	C25-C26-C27-C28
27	B	618	BCR	C11-C12-C13-C14
25	B	601	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	614	SQD	O49-C7-C8-C9
25	c	512	CLA	C2-C1-O2A-CGA
29	a	614	SQD	C9-C10-C11-C12
25	B	612	CLA	CAA-CBA-CGA-O1A
29	a	615	SQD	O10-C23-C24-C25
32	M	101	LMG	C20-C21-C22-C23
33	l	102	LHG	C28-C29-C30-C31
25	b	602	CLA	C2A-CAA-CBA-CGA
25	A	606	CLA	C16-C17-C18-C20
25	B	611	CLA	CAA-CBA-CGA-O1A
25	b	611	CLA	CAA-CBA-CGA-O1A
29	A	614	SQD	O49-C7-C8-C9
32	m	101	LMG	O10-C28-C29-C30
32	c	524	LMG	C36-C37-C38-C39
30	C	518	DGD	C8B-C9B-CAB-CBB
31	b	619	STE	C14-C15-C16-C17
33	d	407	LHG	C3-O3-P-O5
33	l	102	LHG	C3-O3-P-O4
25	B	606	CLA	C16-C17-C18-C19
25	b	601	CLA	C16-C17-C18-C20
30	C	516	DGD	O1B-C1B-C2B-C3B
30	c	517	DGD	O1B-C1B-C2B-C3B
33	e	102	LHG	O10-C23-C24-C25
27	c	514	BCR	C11-C10-C9-C34
28	D	405	PL9	C32-C33-C34-C35
27	c	514	BCR	C23-C24-C25-C26
27	c	516	BCR	C5-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
30	C	516	DGD	C1B-C2B-C3B-C4B
25	B	611	CLA	O1A-CGA-O2A-C1
25	B	613	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	C13-C15-C16-C17
25	C	505	CLA	C15-C16-C17-C18
25	B	605	CLA	C4-C3-C5-C6
28	A	612	PL9	C33-C34-C36-C37
25	B	604	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	b	608	CLA	CAD-CBD-CGD-O1D
25	b	611	CLA	CAD-CBD-CGD-O1D
29	f	101	SQD	O5-C5-C6-S
29	f	101	SQD	O10-C23-C24-C25
30	C	517	DGD	C2A-C3A-C4A-C5A

Continued on next page...

Continued from previous page...

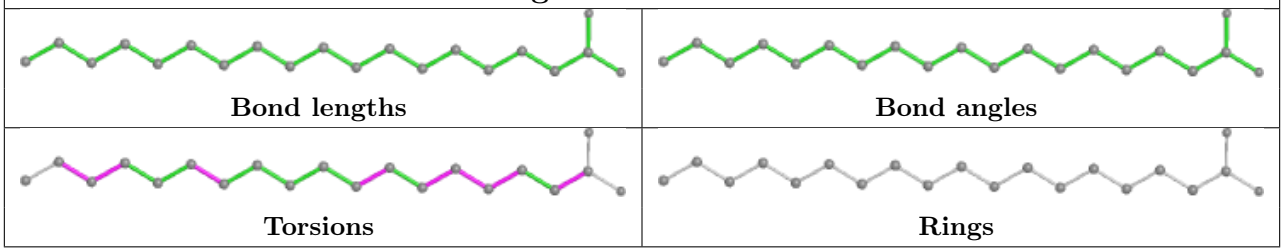
Mol	Chain	Res	Type	Atoms
32	c	522	LMG	C12-C13-C14-C15
33	e	102	LHG	O8-C23-C24-C25
25	A	613	CLA	C8-C10-C11-C12
25	B	606	CLA	C14-C13-C15-C16
25	a	610	CLA	C11-C10-C8-C9
25	b	606	CLA	C14-C13-C15-C16
25	c	501	CLA	C11-C12-C13-C14
30	c	518	DGD	C9A-CAA-CBA-CCA
32	c	522	LMG	C17-C18-C19-C20
30	C	516	DGD	CDB-CEB-CFB-CGB
33	d	408	LHG	O8-C23-C24-C25
31	C	521	STE	O1-C1-C2-C3
25	B	602	CLA	C13-C15-C16-C17
25	b	612	CLA	CAA-CBA-CGA-O2A
32	c	522	LMG	C35-C36-C37-C38
25	C	502	CLA	C16-C17-C18-C19
25	D	402	CLA	C15-C16-C17-C18
25	B	606	CLA	C12-C13-C15-C16
25	C	501	CLA	C12-C13-C15-C16
25	D	402	CLA	C12-C13-C15-C16
25	a	608	CLA	C11-C12-C13-C15
25	a	610	CLA	C11-C10-C8-C7
25	b	605	CLA	C6-C7-C8-C10
25	b	611	CLA	C6-C7-C8-C10
25	c	512	CLA	C11-C10-C8-C7
25	c	513	CLA	C12-C13-C15-C16
26	d	401	PHO	C11-C10-C8-C7
30	A	616	DGD	O1B-C1B-C2B-C3B
33	B	621	LHG	O7-C7-C8-C9
32	C	515	LMG	C29-C28-O8-C9
27	D	404	BCR	C21-C22-C23-C24
33	d	408	LHG	O10-C23-C24-C25
27	c	516	BCR	C13-C14-C15-C16
25	c	510	CLA	CAA-CBA-CGA-O2A
31	M	102	STE	C10-C11-C12-C13
25	B	614	CLA	C10-C11-C12-C13
28	a	612	PL9	C12-C13-C14-C15
30	c	519	DGD	CAB-CBB-CCB-CDB
33	D	407	LHG	C31-C32-C33-C34

There are no ring outliers.

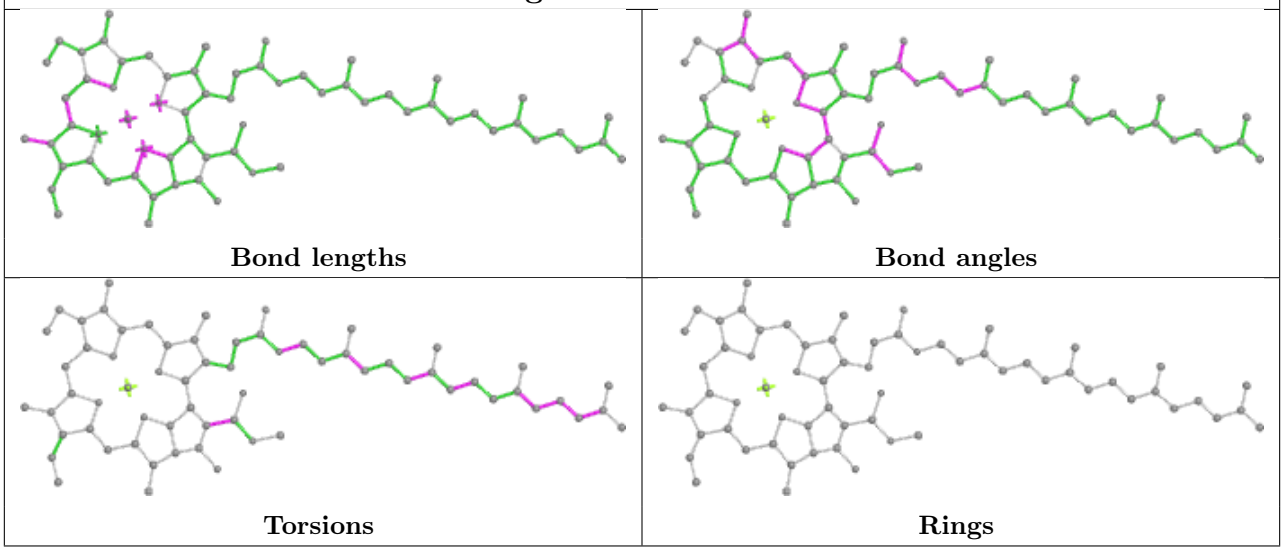
No monomer is involved in short contacts.

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.

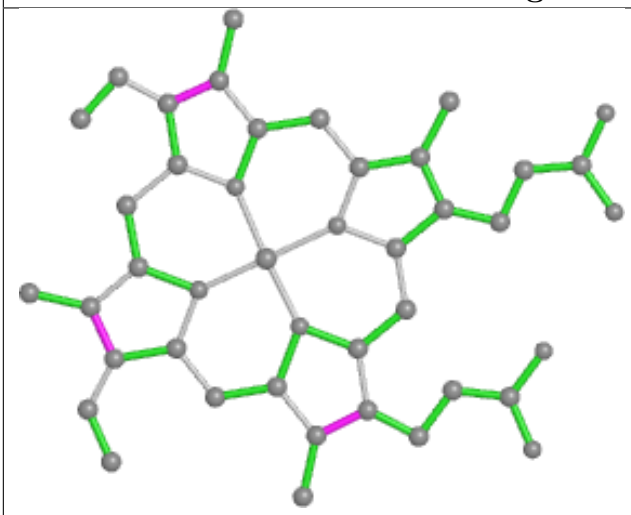
Ligand STE b 619



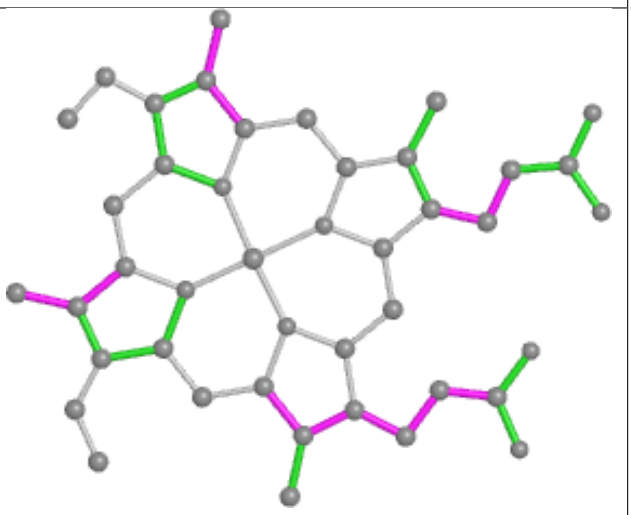
Ligand CLA C 506



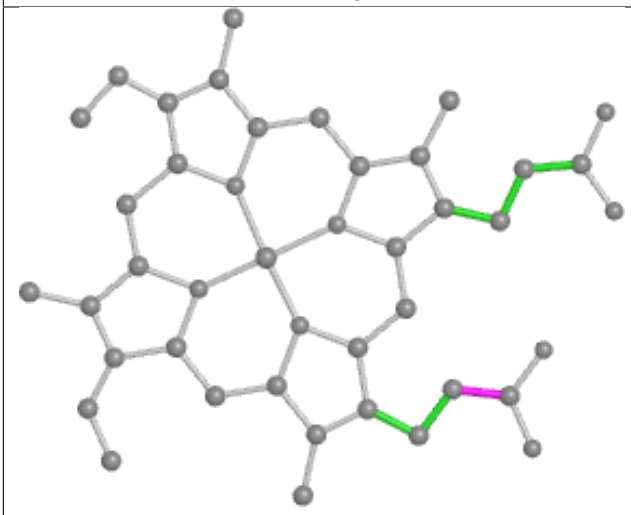
Ligand HEC v 201



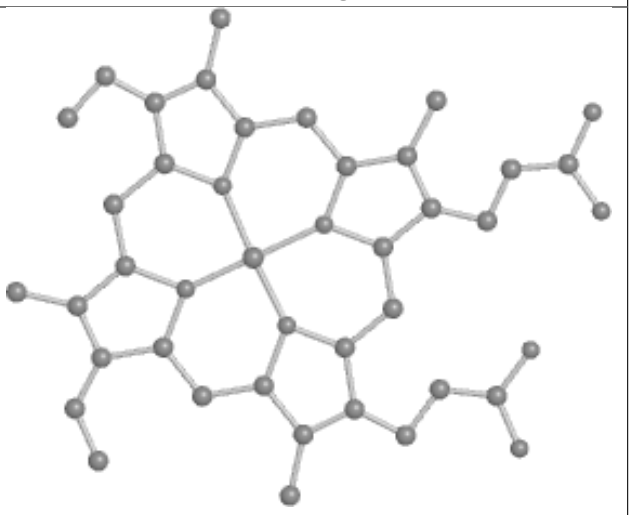
Bond lengths



Bond angles

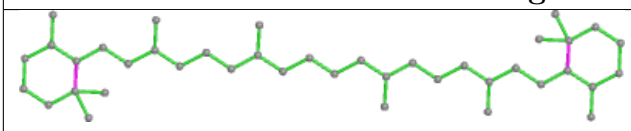


Torsions

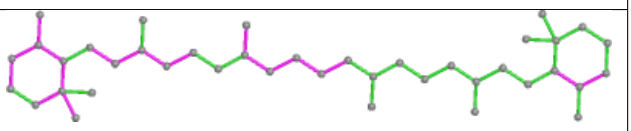


Rings

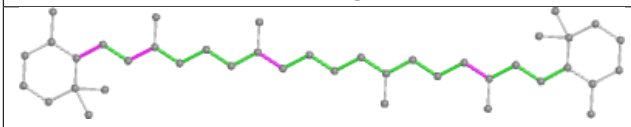
Ligand BCR t 101



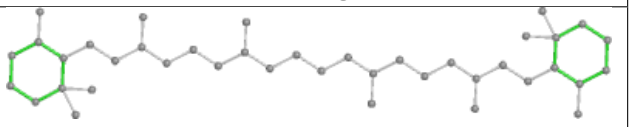
Bond lengths



Bond angles

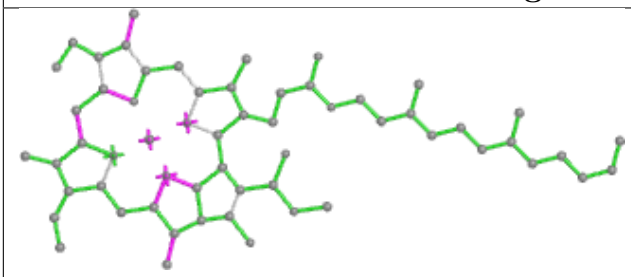


Torsions

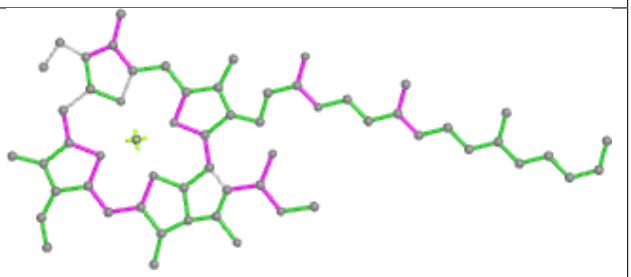


Rings

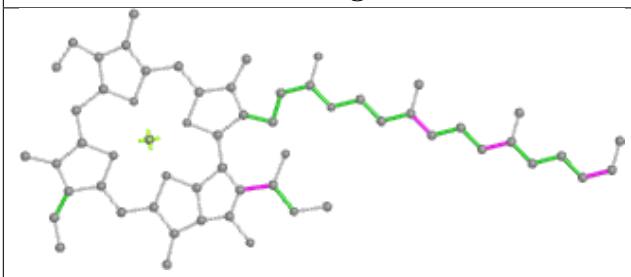
Ligand CLA C 504



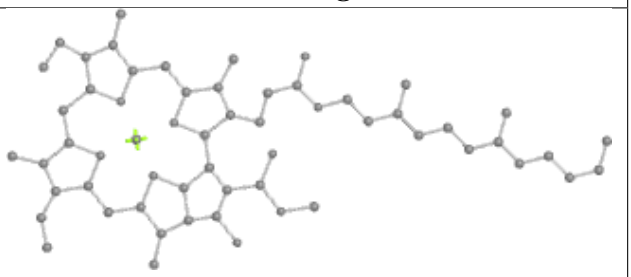
Bond lengths



Bond angles

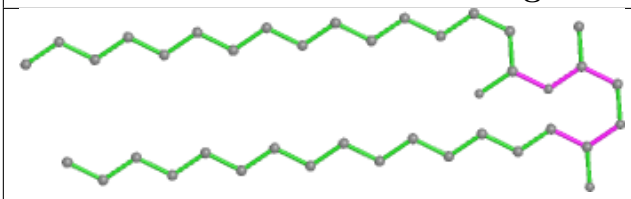


Torsions

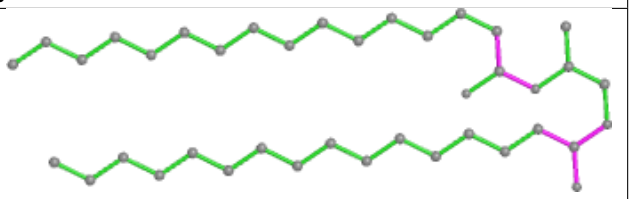


Rings

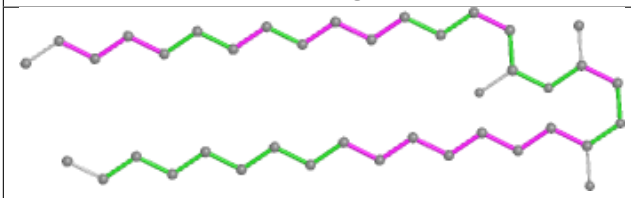
Ligand SQD A 615



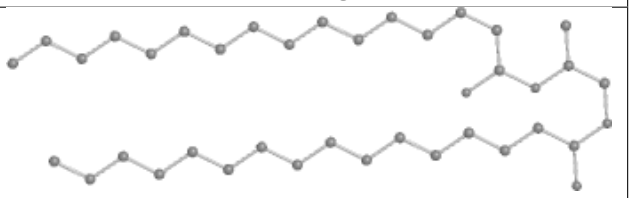
Bond lengths



Bond angles

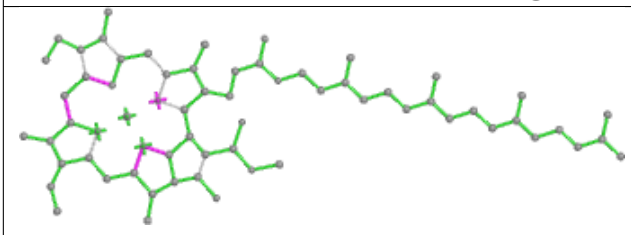


Torsions

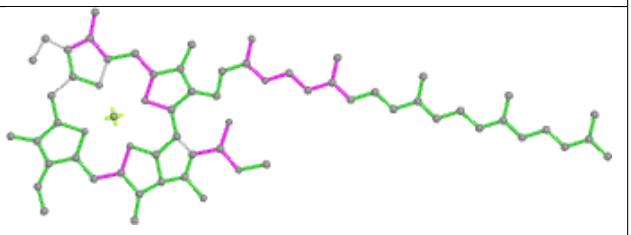


Rings

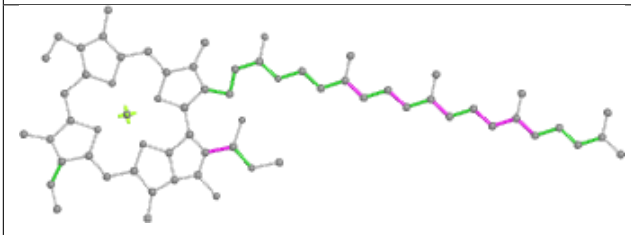
Ligand CLA b 604



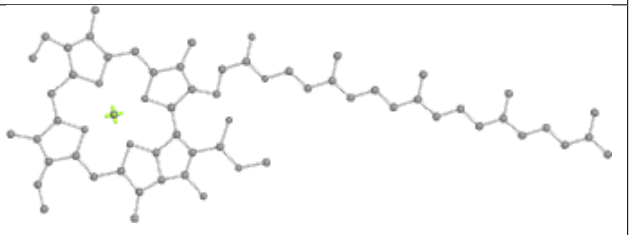
Bond lengths



Bond angles

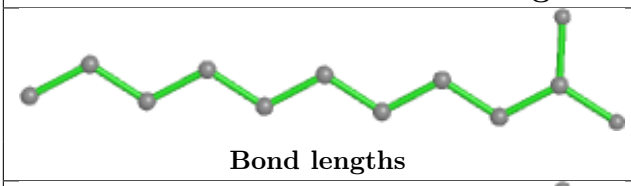


Torsions

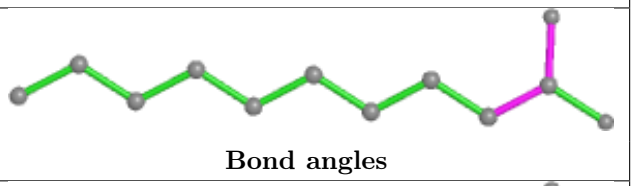


Rings

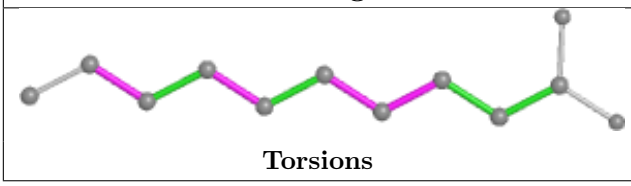
Ligand STE c 523



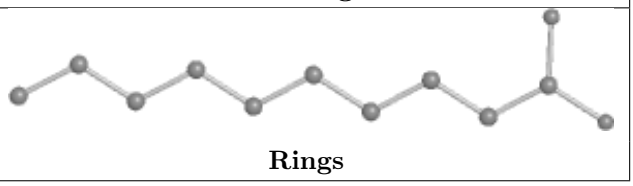
Bond lengths



Bond angles

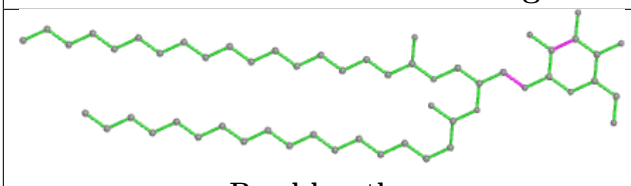


Torsions

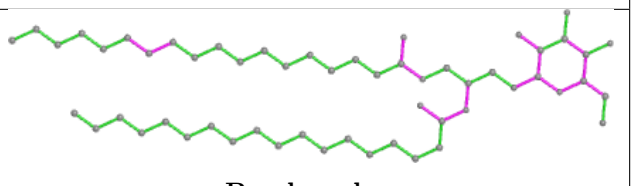


Rings

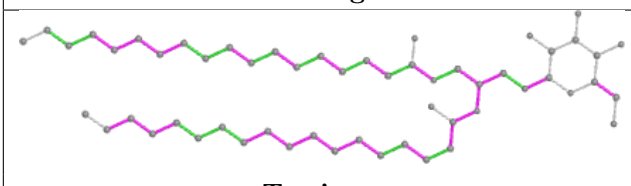
Ligand LMG b 620



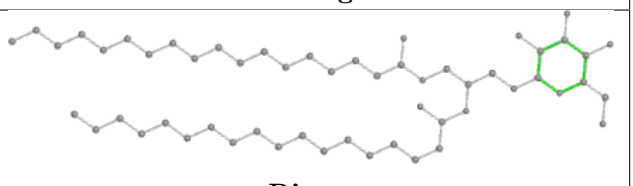
Bond lengths



Bond angles

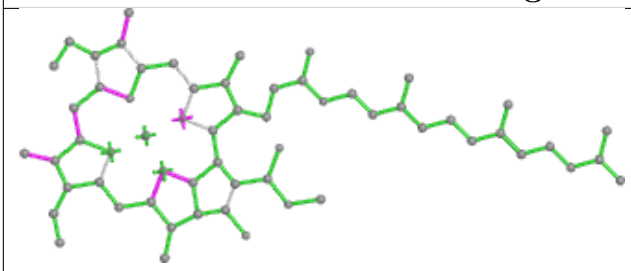


Torsions

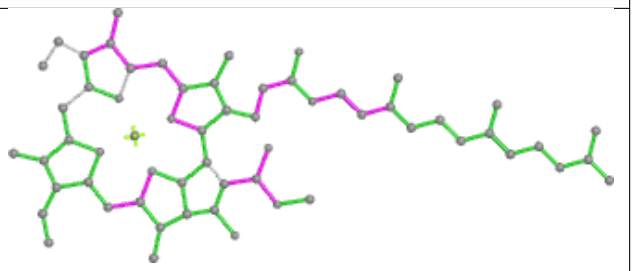


Rings

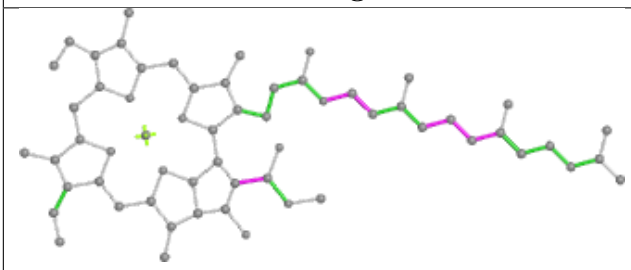
Ligand CLA B 615



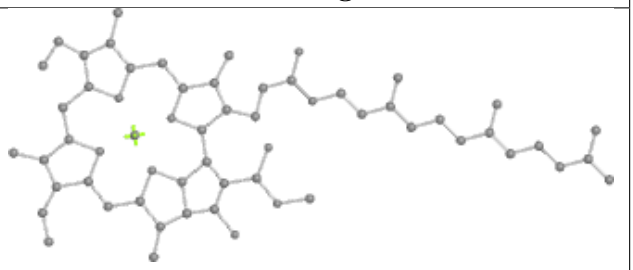
Bond lengths



Bond angles

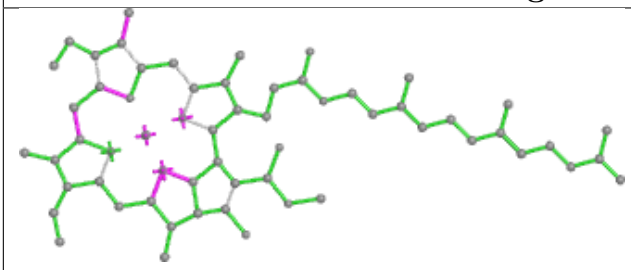


Torsions

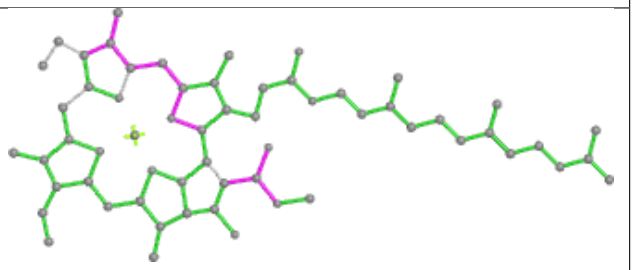


Rings

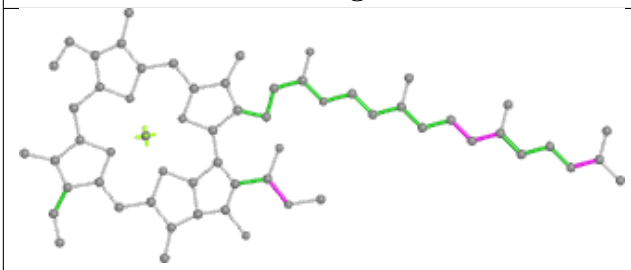
Ligand CLA b 615



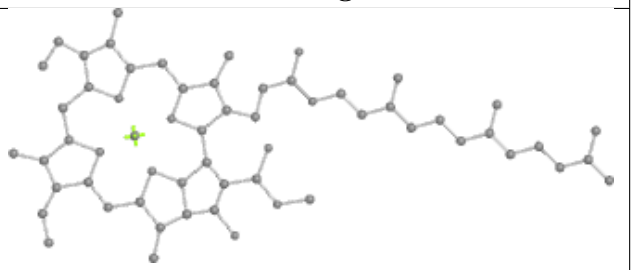
Bond lengths



Bond angles

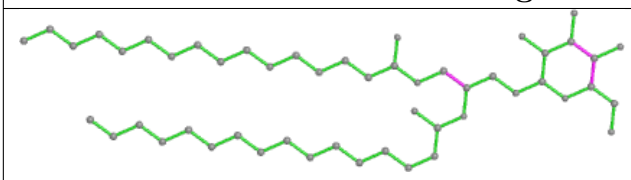


Torsions

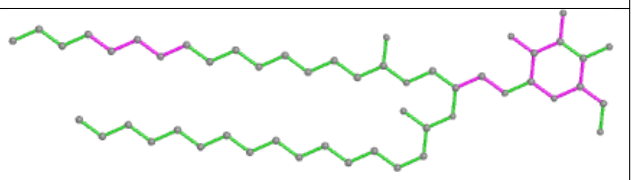


Rings

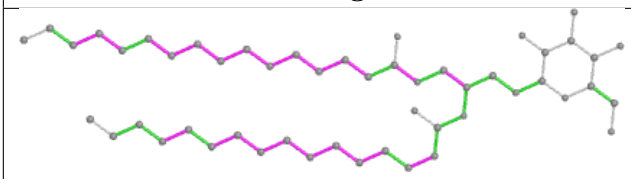
Ligand LMG M 101



Bond lengths



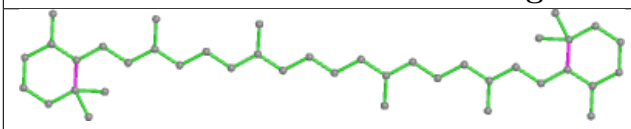
Bond angles



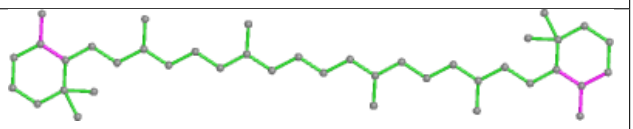
Torsions

Rings

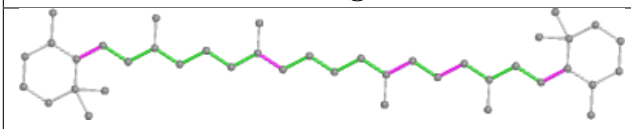
Ligand BCR k 101



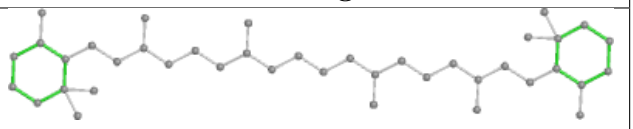
Bond lengths



Bond angles

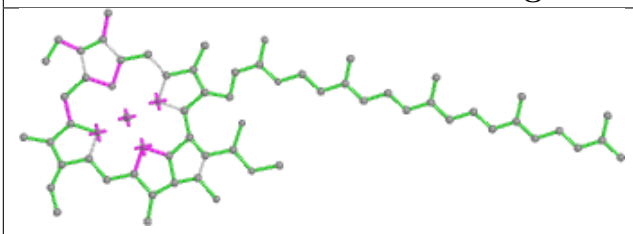


Torsions

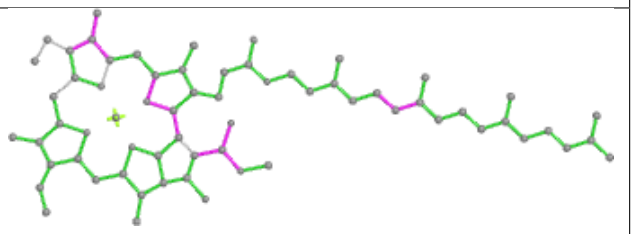


Rings

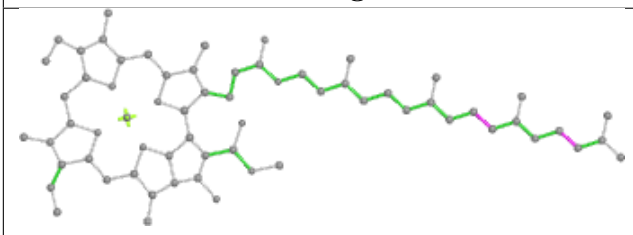
Ligand CLA B 607



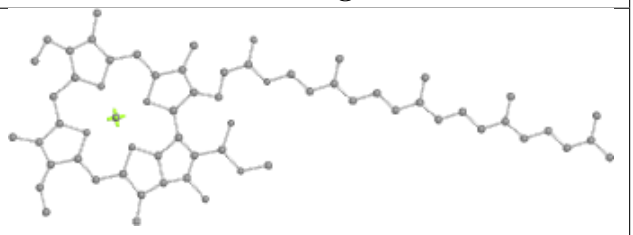
Bond lengths



Bond angles

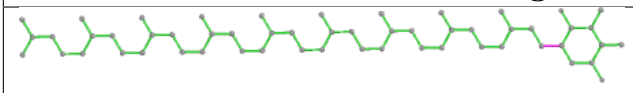


Torsions

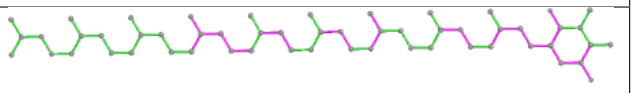


Rings

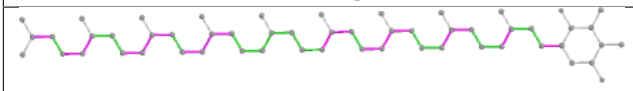
Ligand PL9 A 612



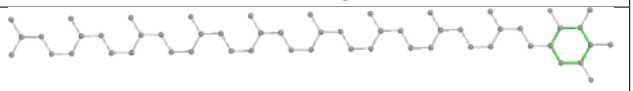
Bond lengths



Bond angles

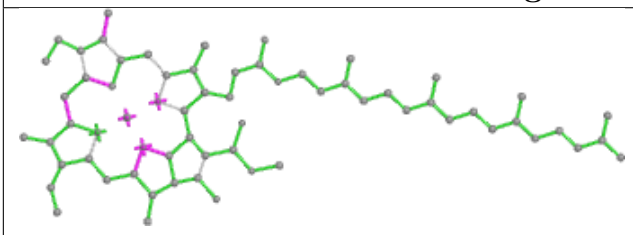


Torsions

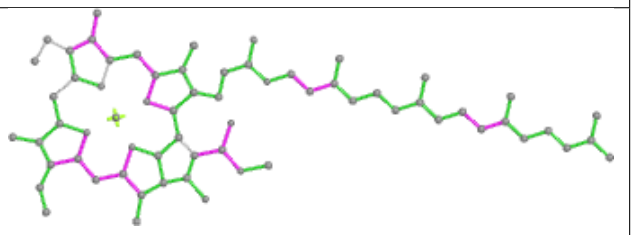


Rings

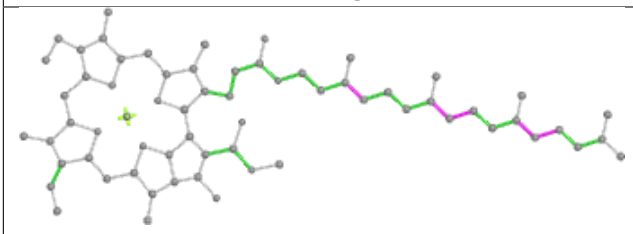
Ligand CLA B 610



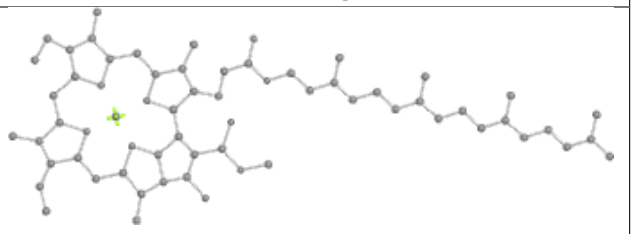
Bond lengths



Bond angles

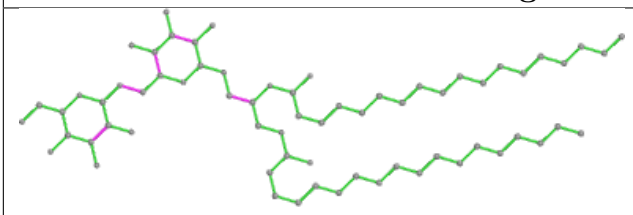


Torsions

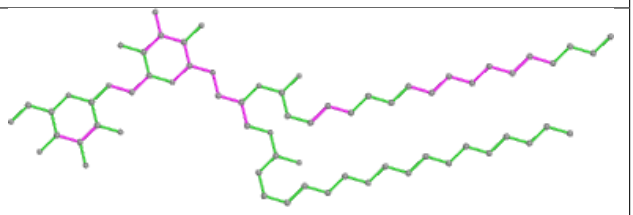


Rings

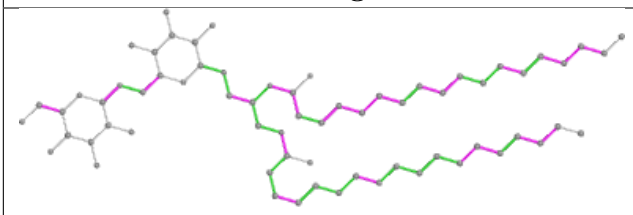
Ligand DGD A 616



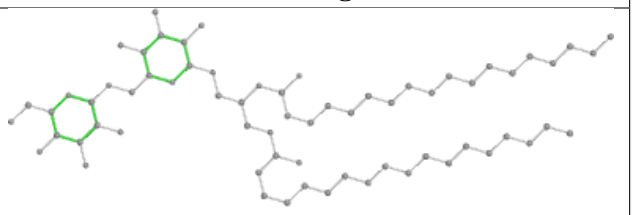
Bond lengths



Bond angles

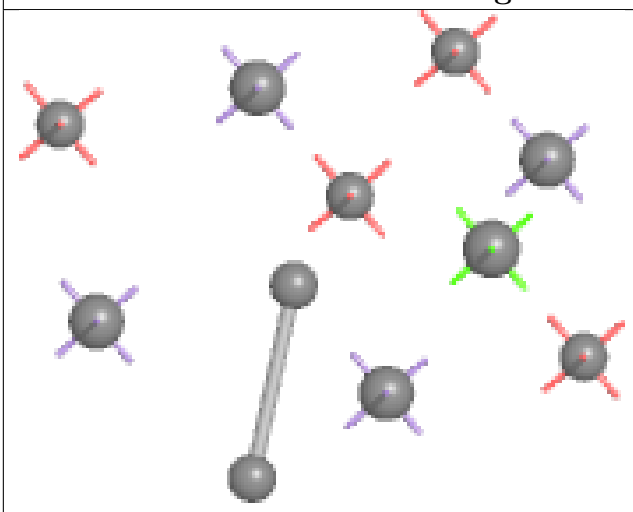


Torsions

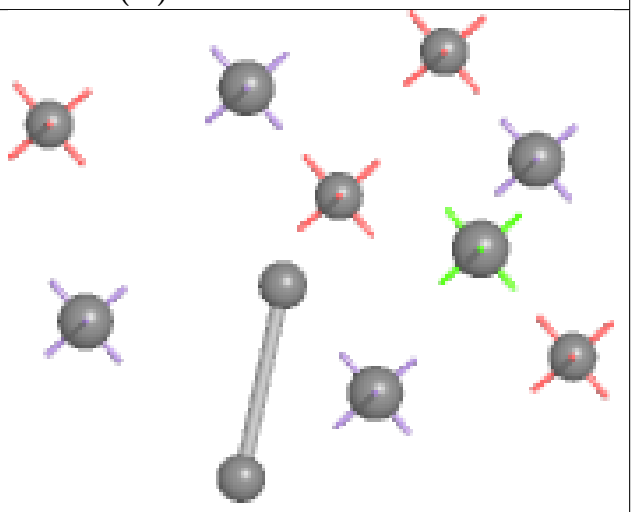


Rings

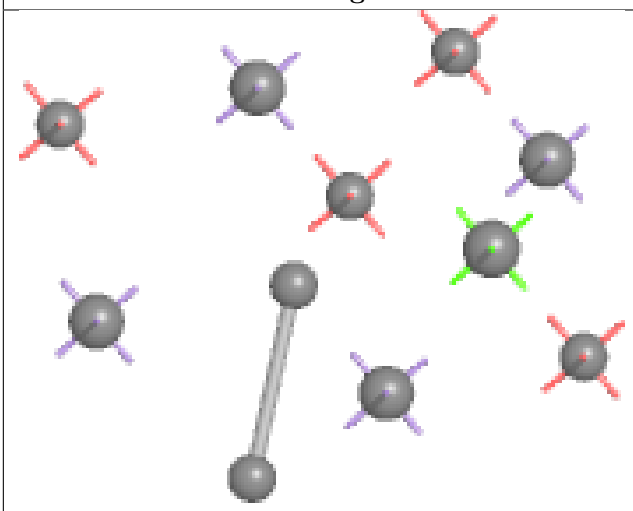
Ligand OEY a 601 (B)



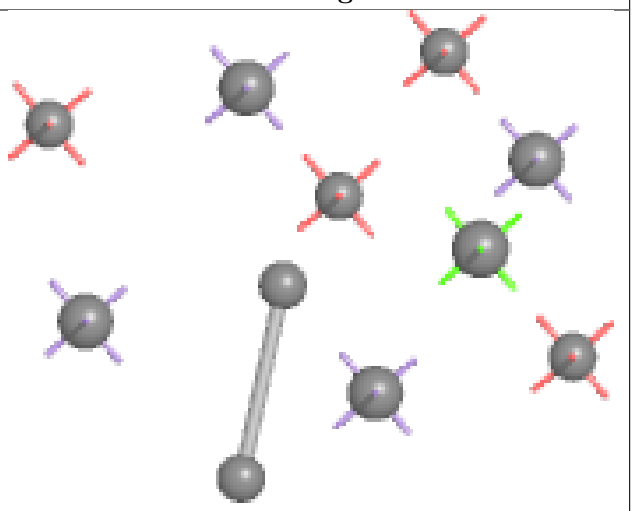
Bond lengths



Bond angles

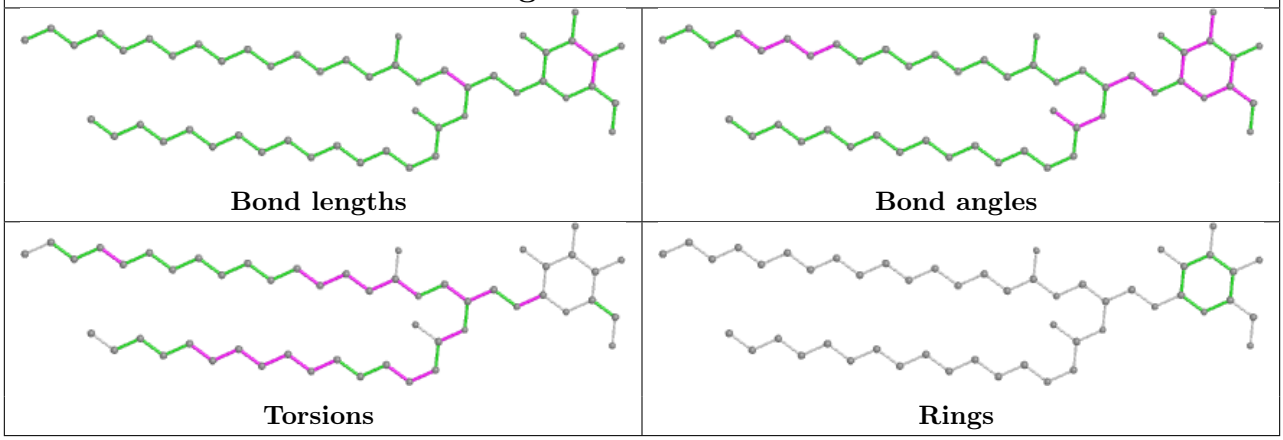


Torsions

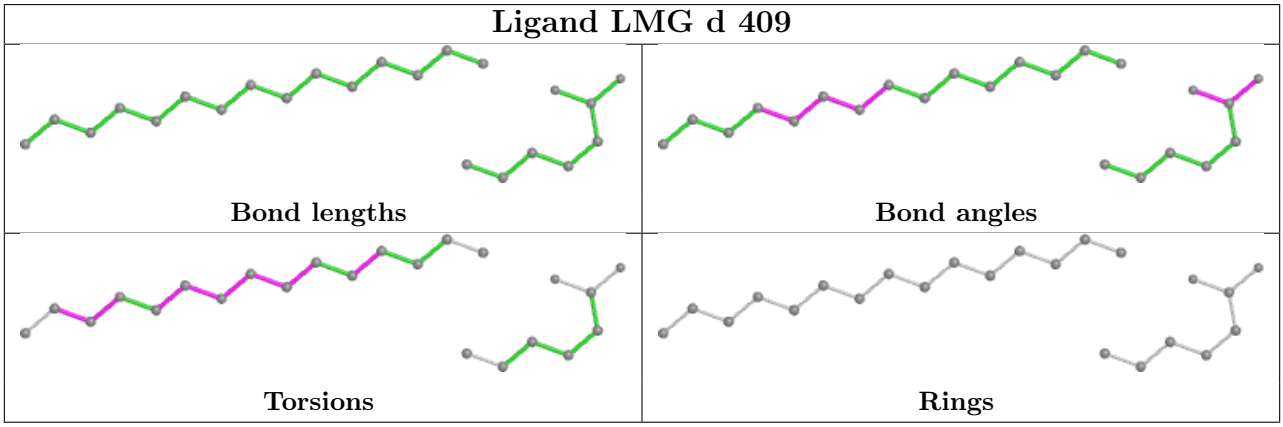


Rings

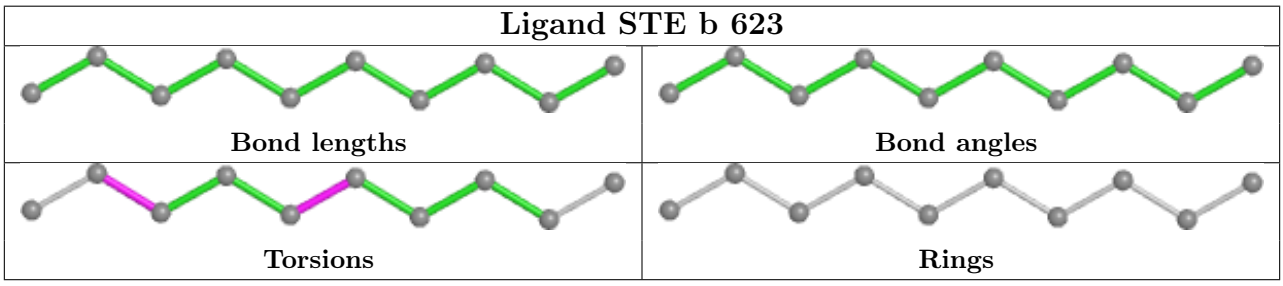
Ligand LMG m 101



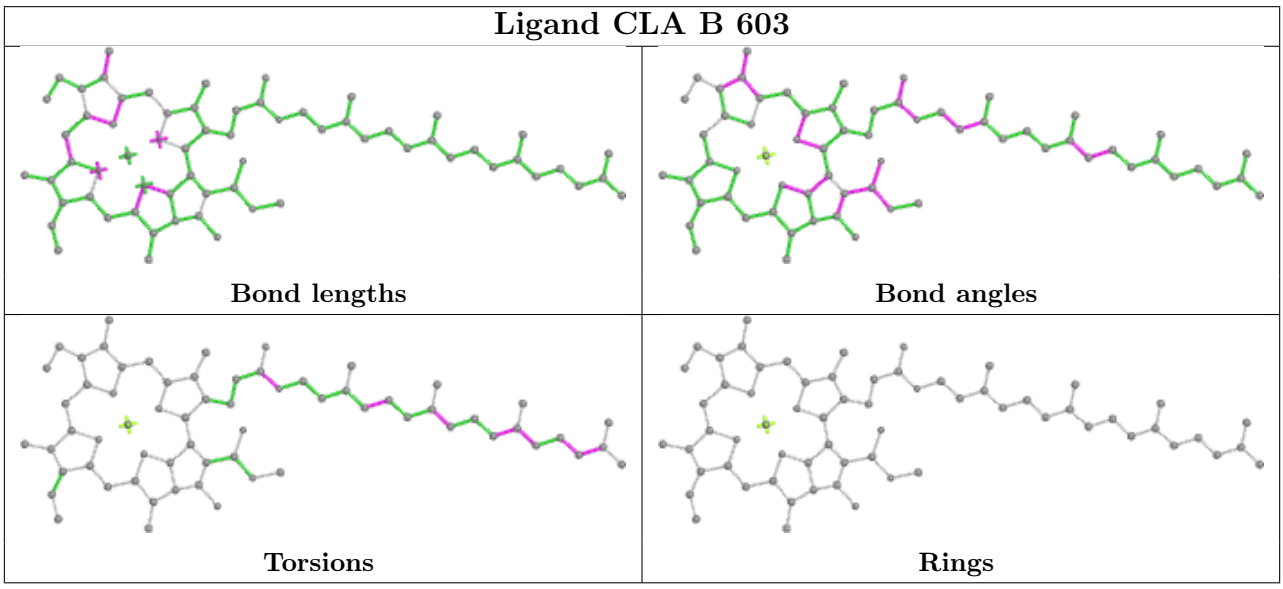
Ligand LMG d 409



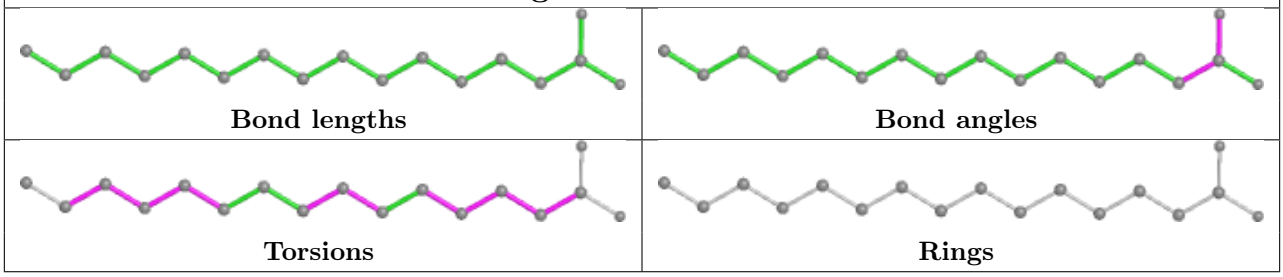
Ligand STE b 623



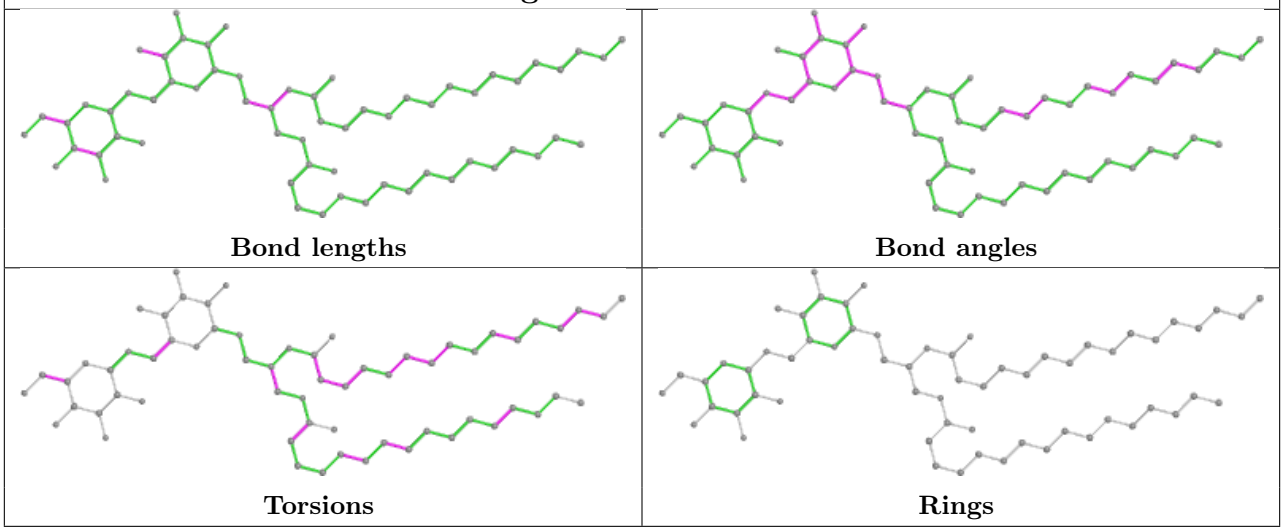
Ligand CLA B 603



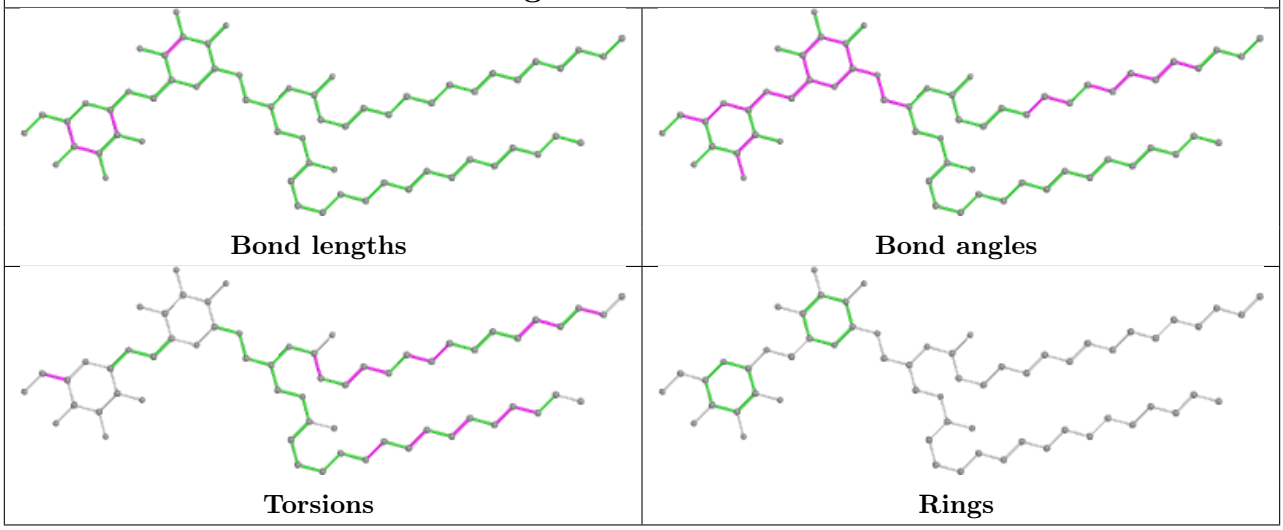
Ligand STE d 411



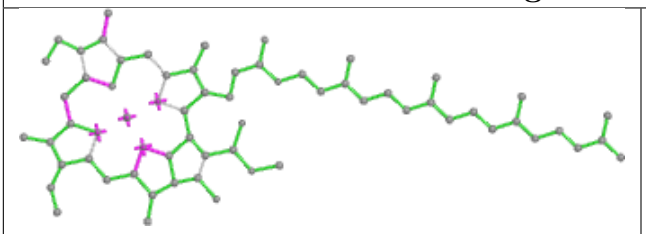
Ligand DGD C 516



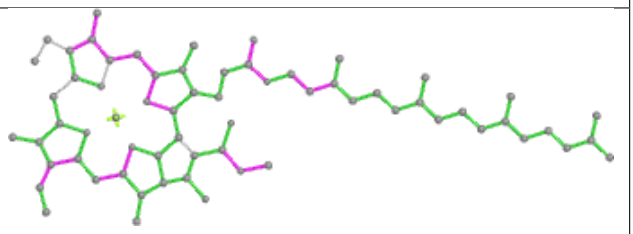
Ligand DGD h 102



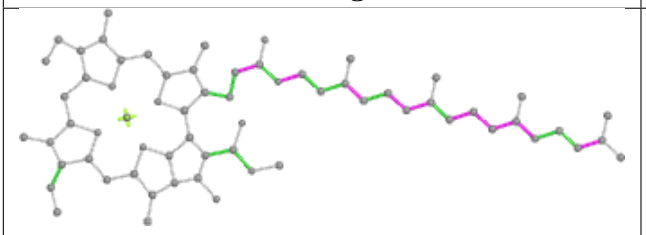
Ligand CLA B 612



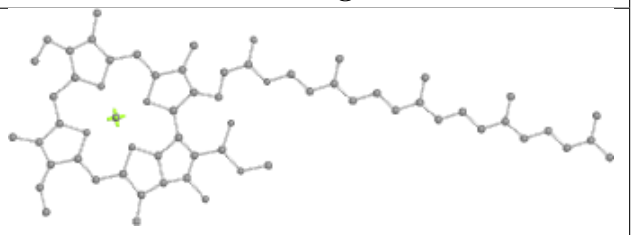
Bond lengths



Bond angles

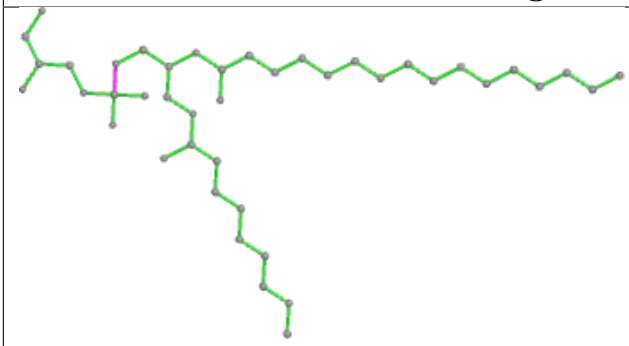


Torsions

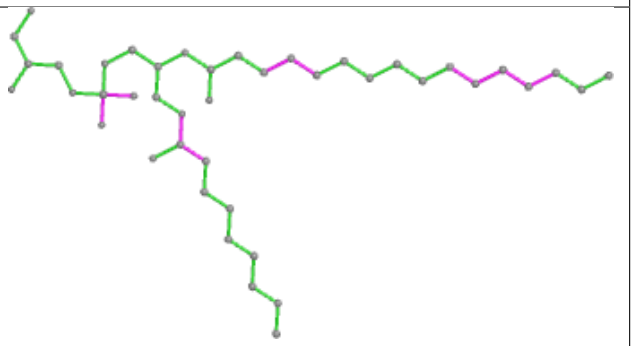


Rings

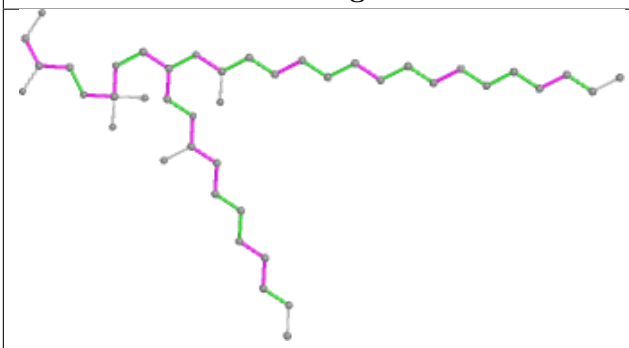
Ligand LHG e 102



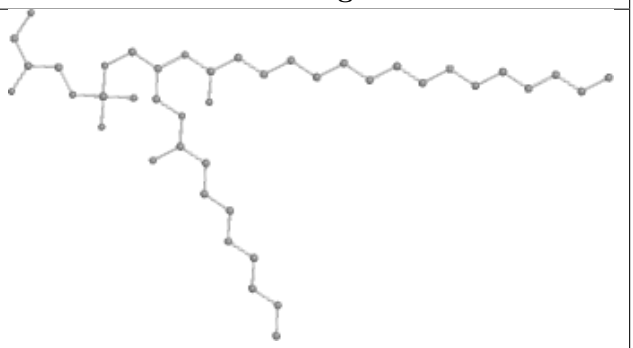
Bond lengths



Bond angles

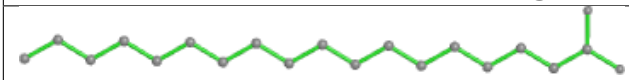


Torsions

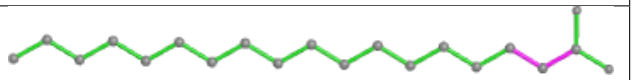


Rings

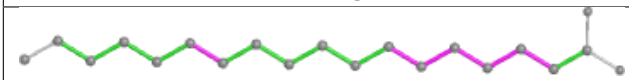
Ligand STE x 102



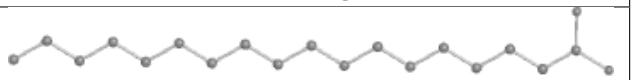
Bond lengths



Bond angles

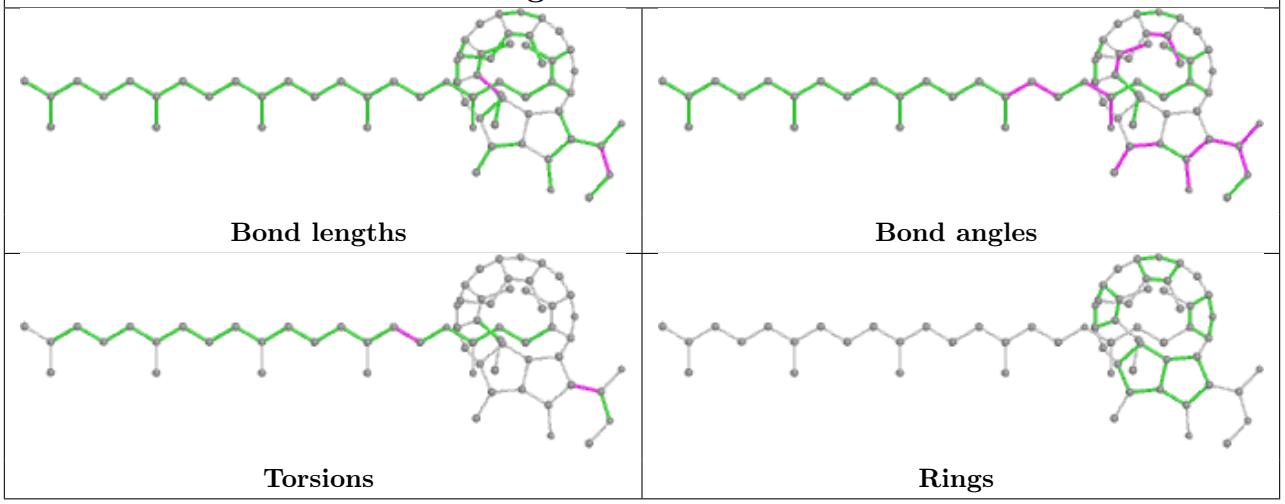


Torsions

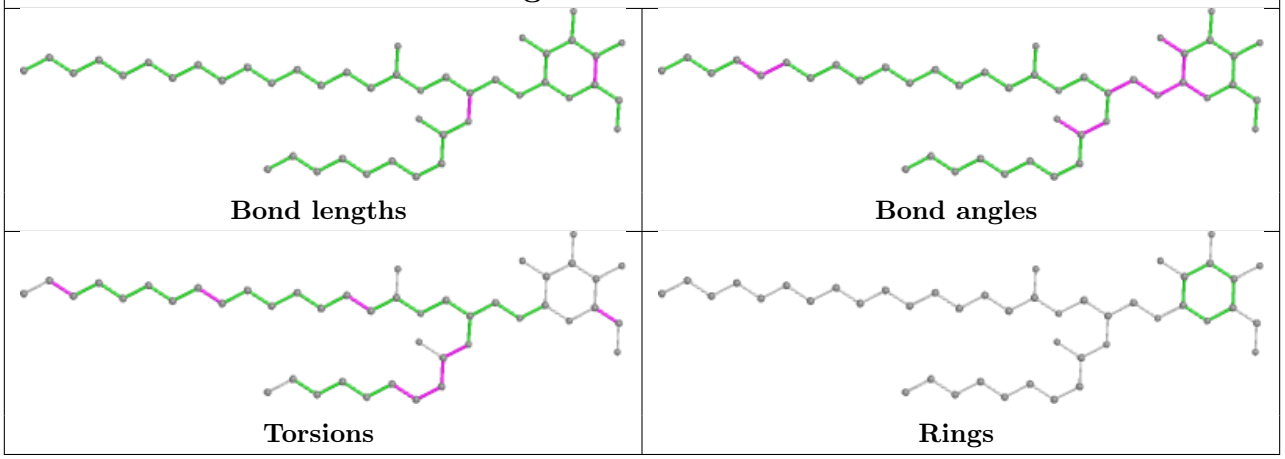


Rings

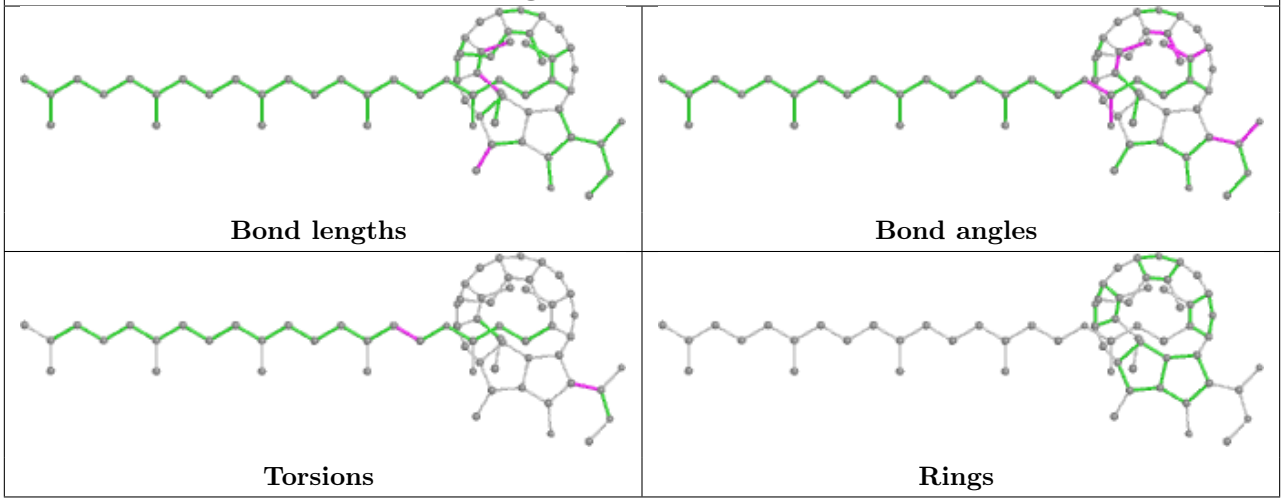
Ligand PHO a 609



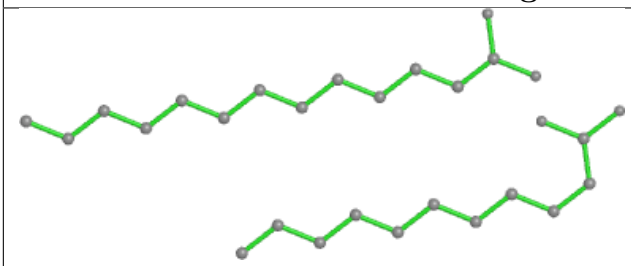
Ligand LMG d 410



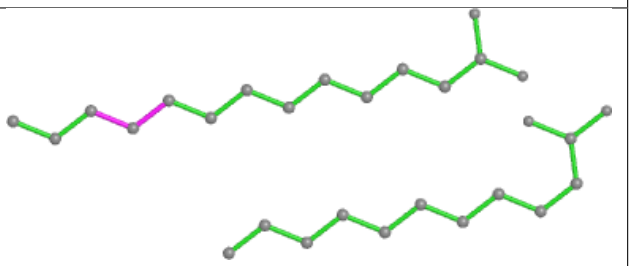
Ligand PHO A 608



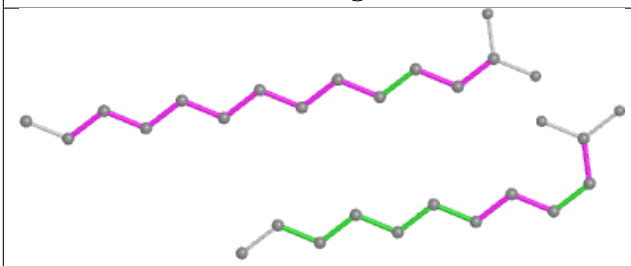
Ligand LMG B 620



Bond lengths



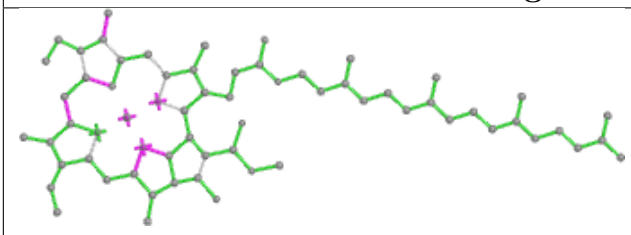
Bond angles



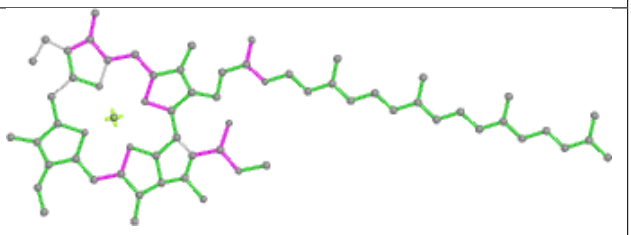
Torsions

Rings

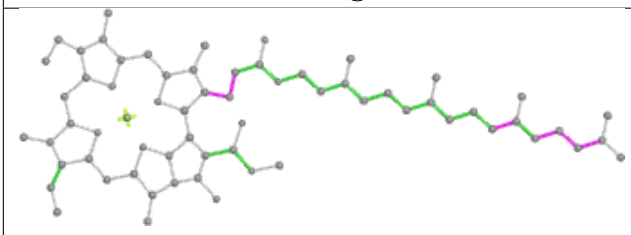
Ligand CLA B 601



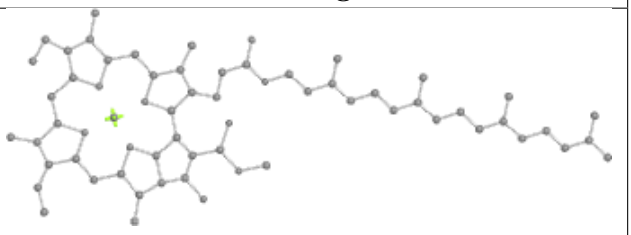
Bond lengths



Bond angles

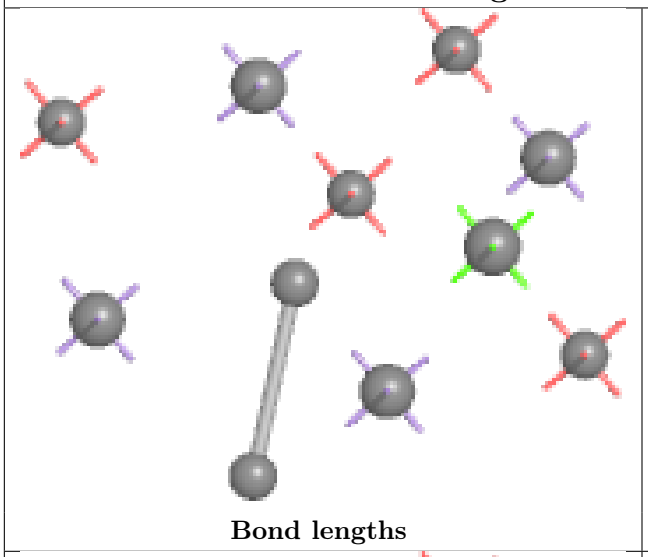


Torsions

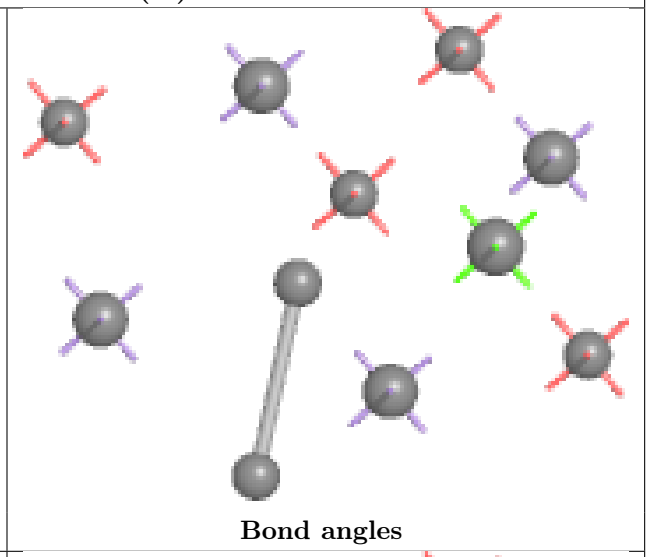


Rings

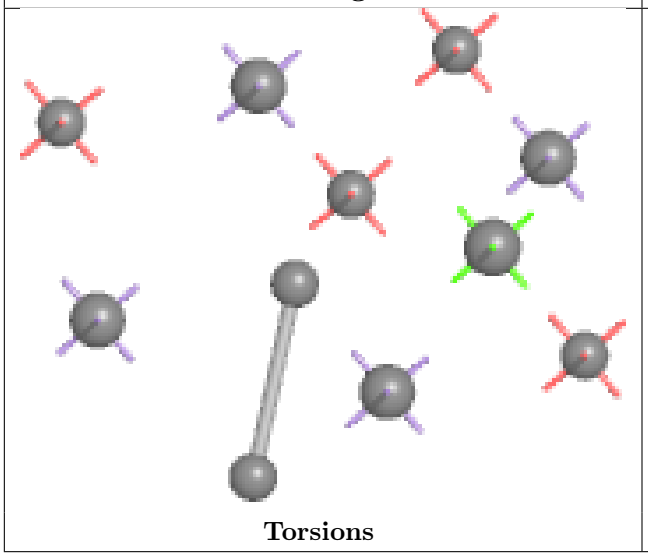
Ligand OEY A 601 (C)



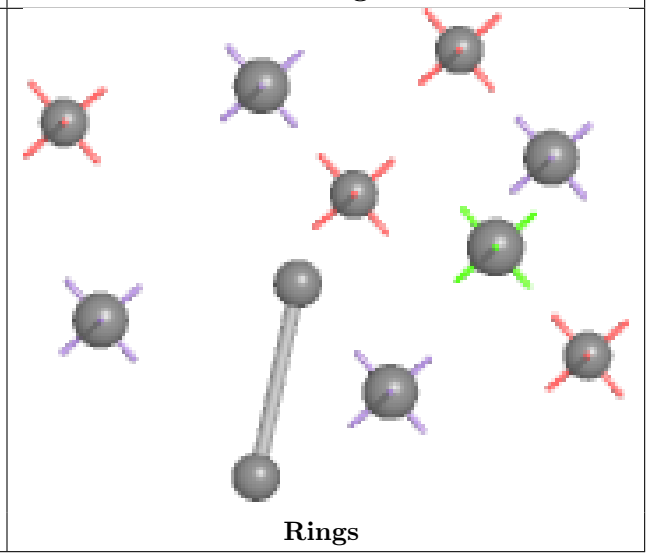
Bond lengths



Bond angles

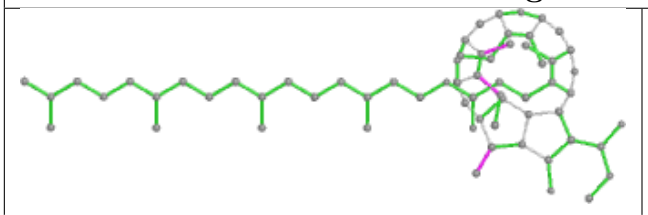


Torsions

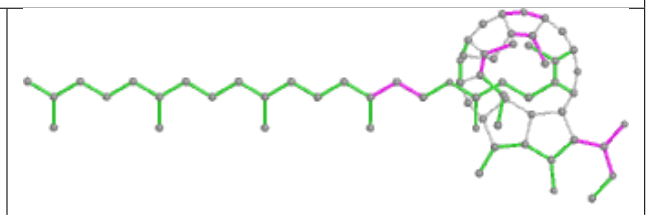


Rings

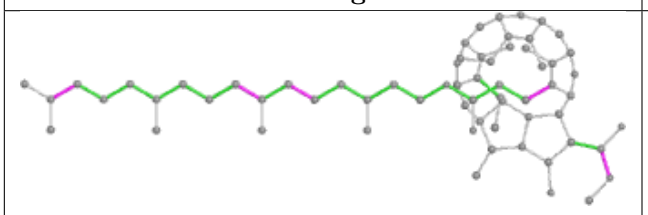
Ligand PHO d 401



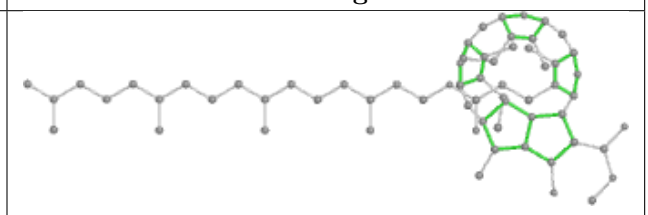
Bond lengths



Bond angles

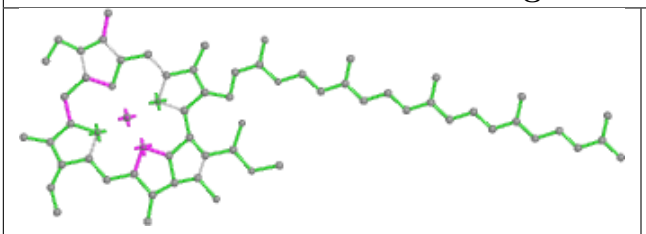


Torsions

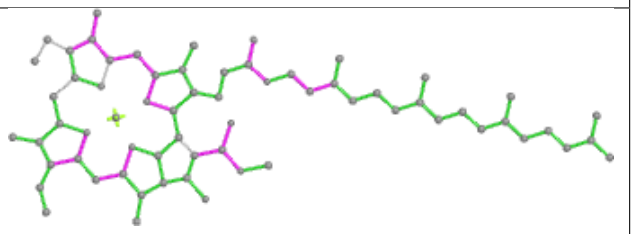


Rings

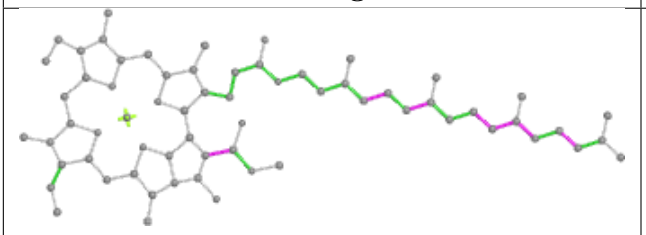
Ligand CLA A 607



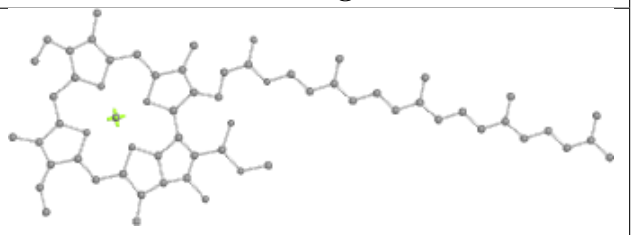
Bond lengths



Bond angles

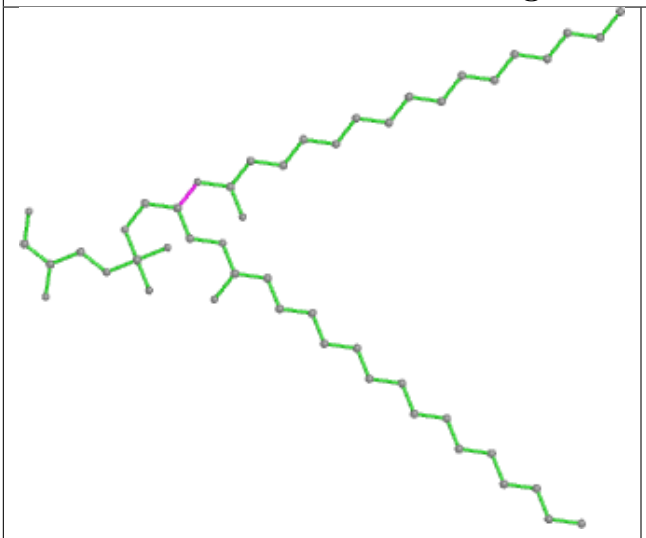


Torsions

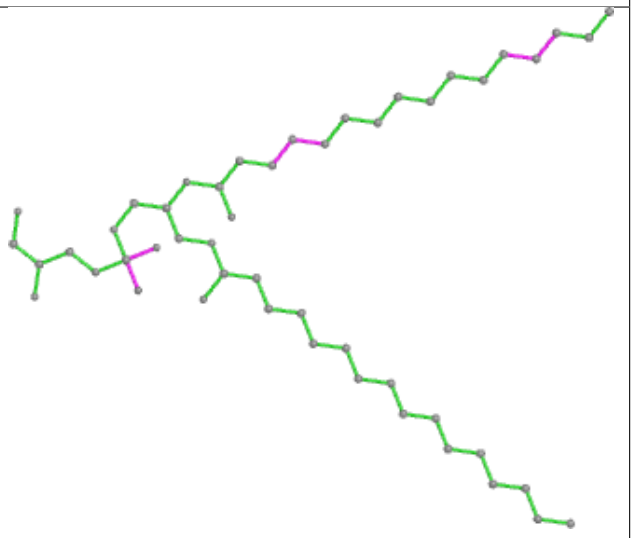


Rings

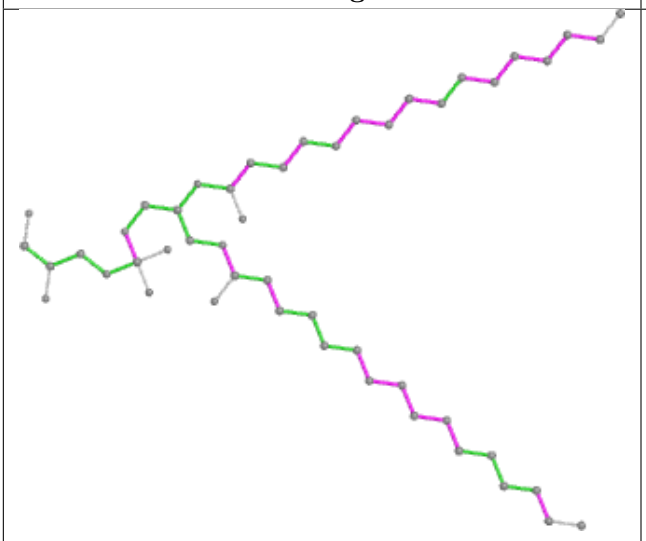
Ligand LHG B 621



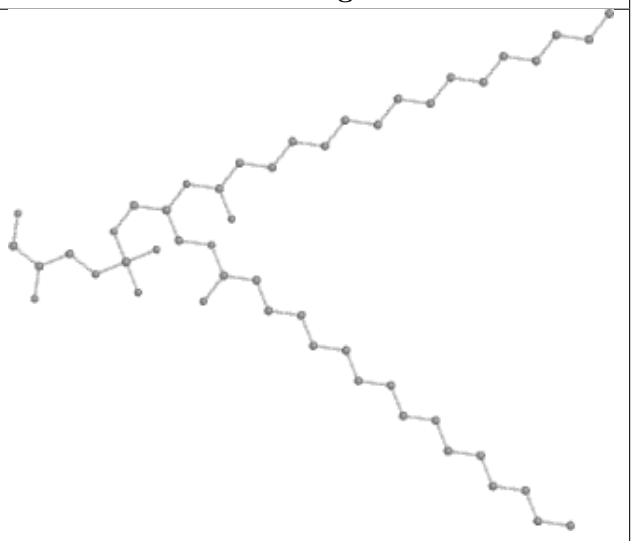
Bond lengths



Bond angles

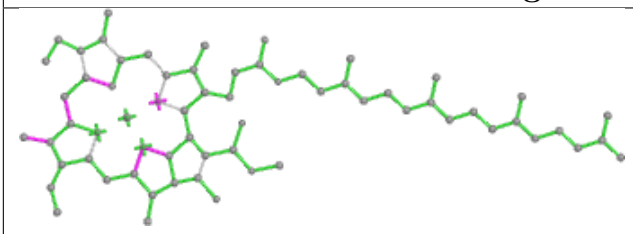


Torsions

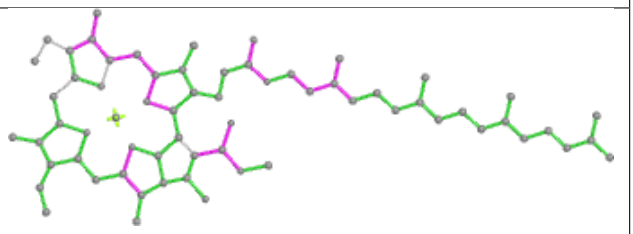


Rings

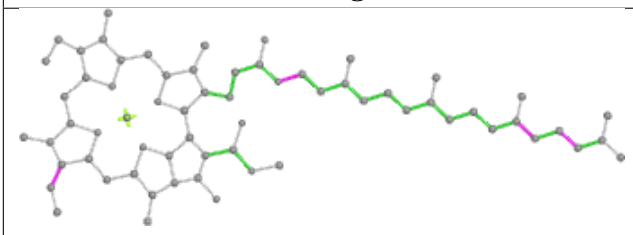
Ligand CLA D 402



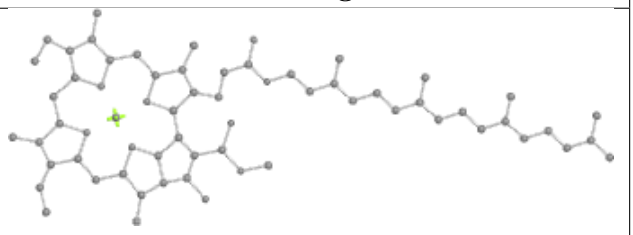
Bond lengths



Bond angles

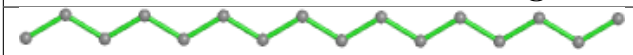


Torsions



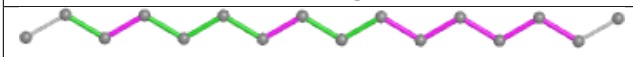
Rings

Ligand STE T 102

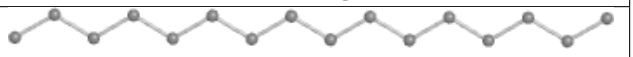


Bond lengths

Bond angles

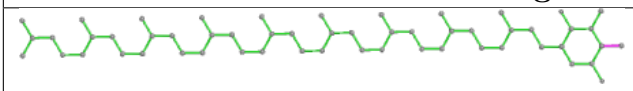


Torsions

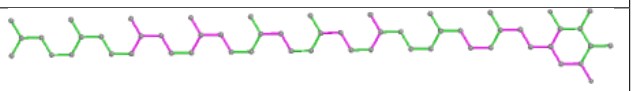


Rings

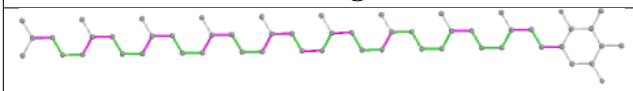
Ligand PL9 a 612



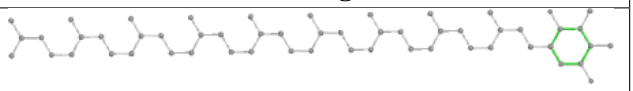
Bond lengths



Bond angles

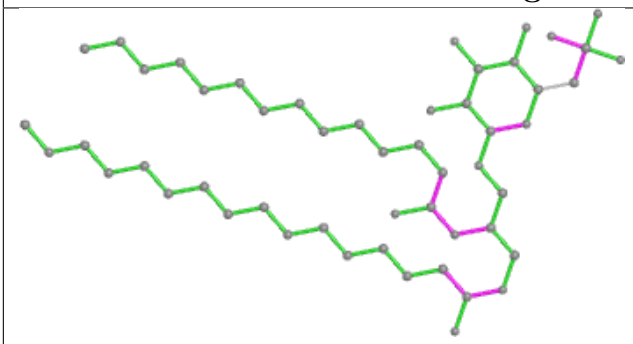


Torsions

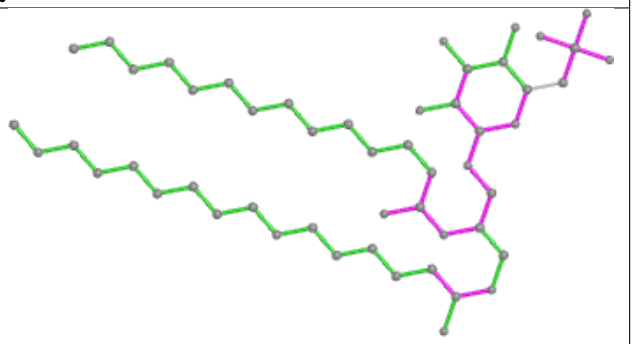


Rings

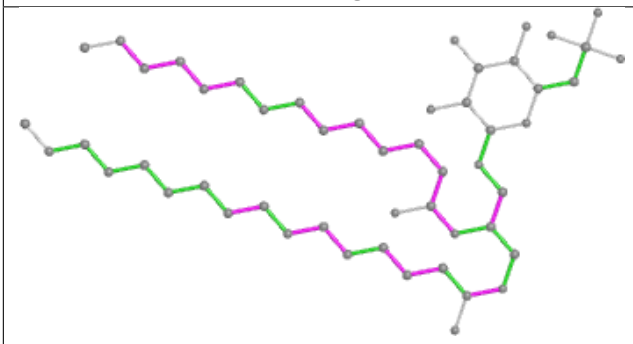
Ligand SQD A 614



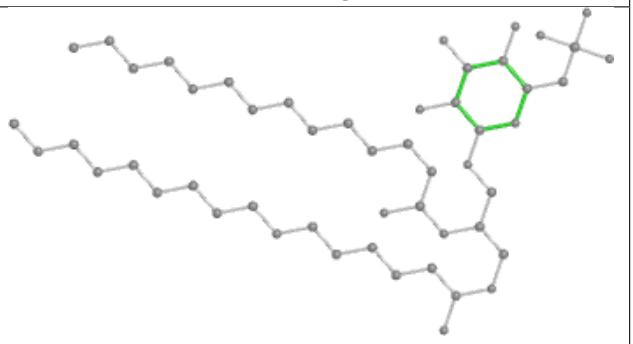
Bond lengths



Bond angles

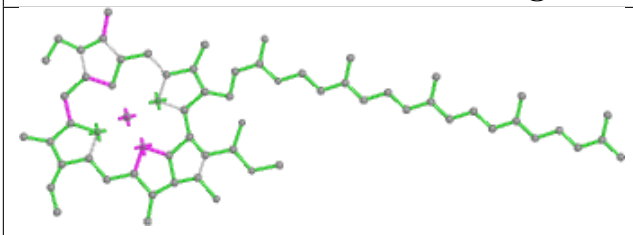


Torsions

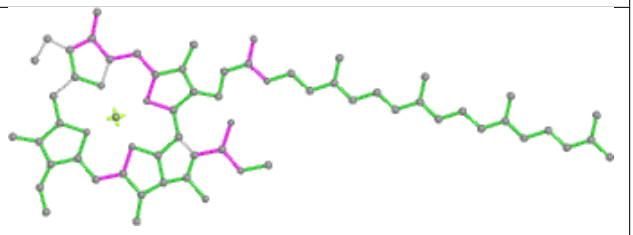


Rings

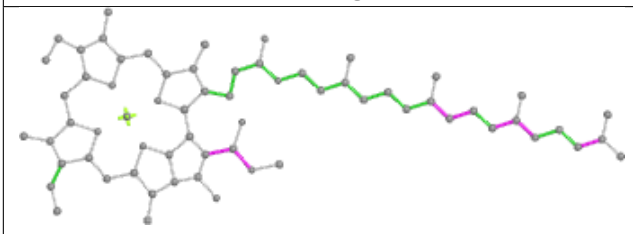
Ligand CLA a 608



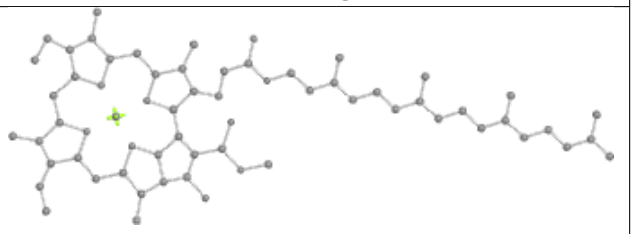
Bond lengths



Bond angles

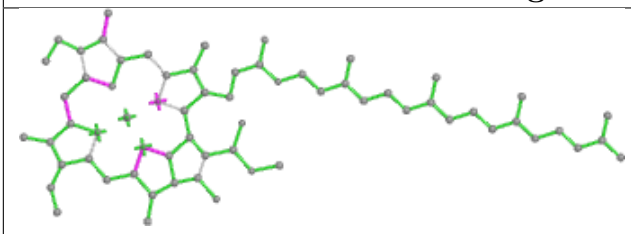


Torsions

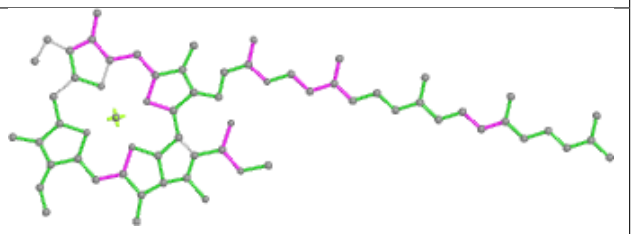


Rings

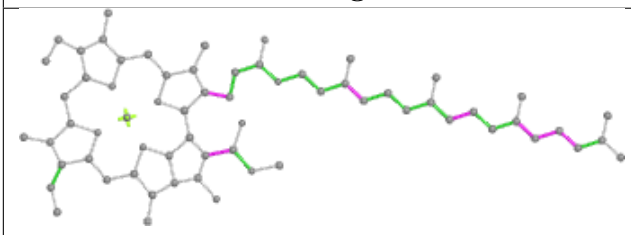
Ligand CLA b 603



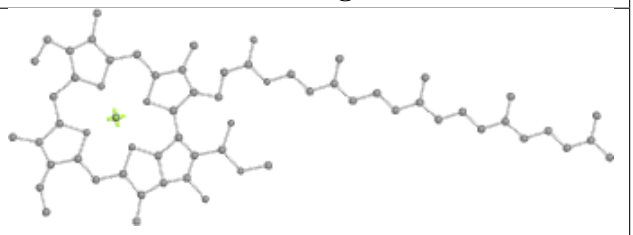
Bond lengths



Bond angles

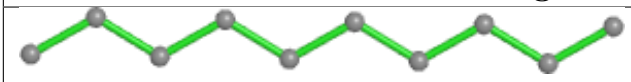


Torsions

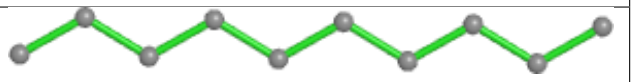


Rings

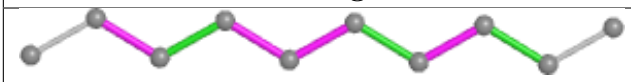
Ligand STE t 103



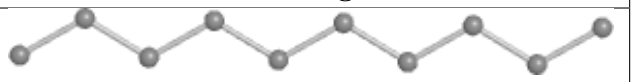
Bond lengths



Bond angles

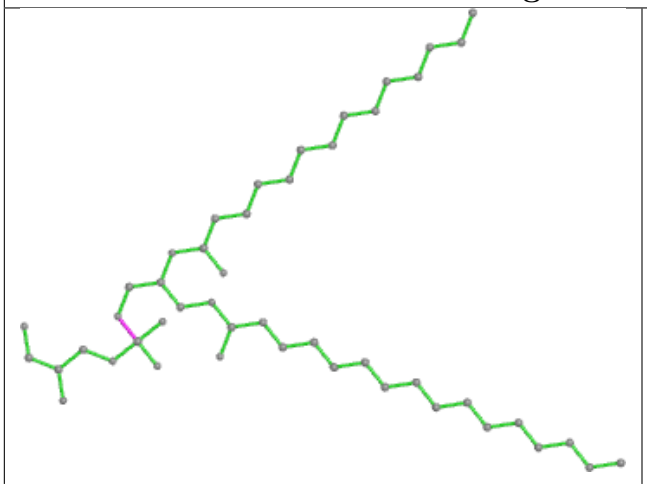


Torsions

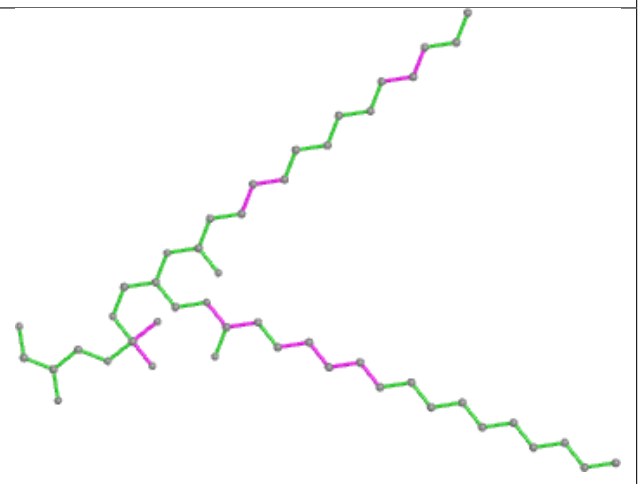


Rings

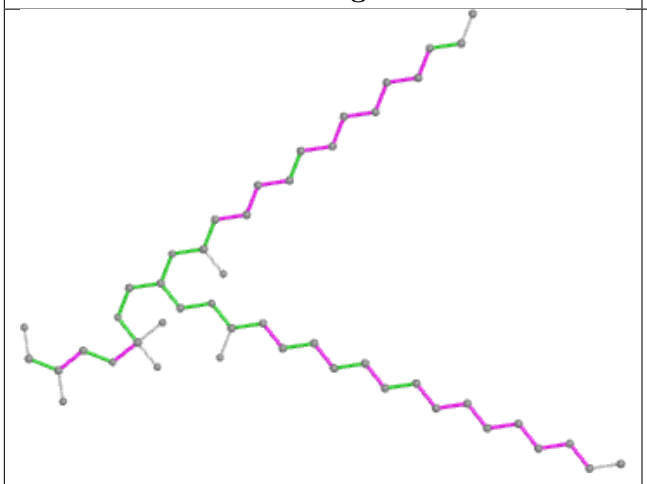
Ligand LHG D 408



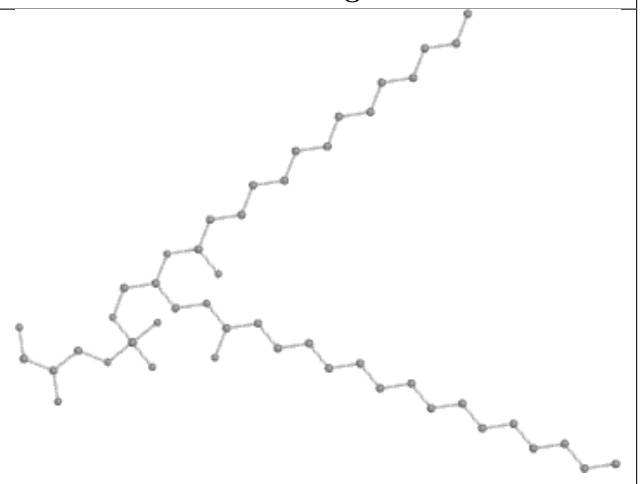
Bond lengths



Bond angles

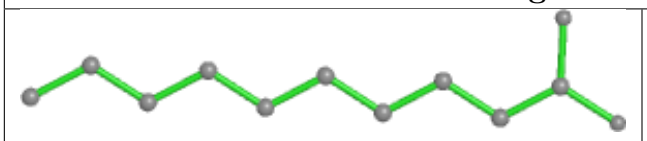


Torsions

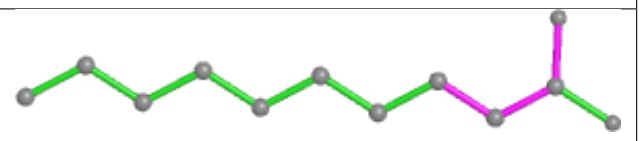


Rings

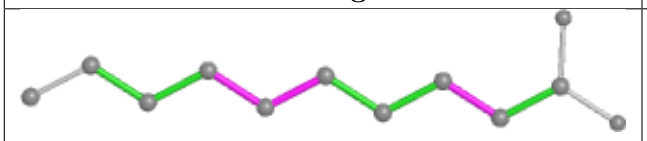
Ligand STE B 625



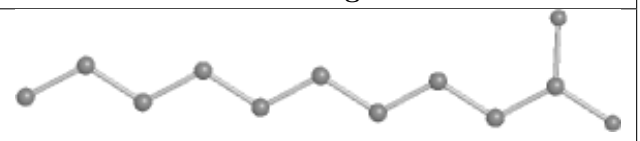
Bond lengths



Bond angles

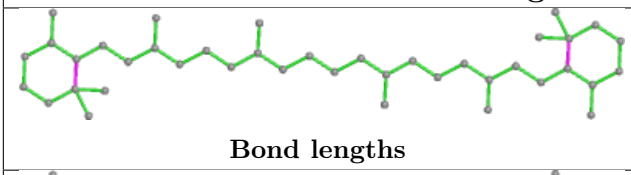


Torsions

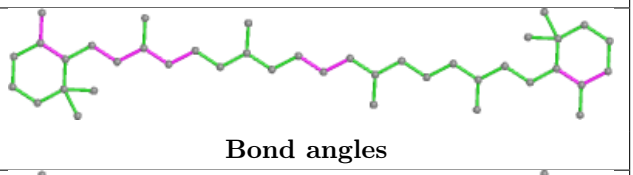


Rings

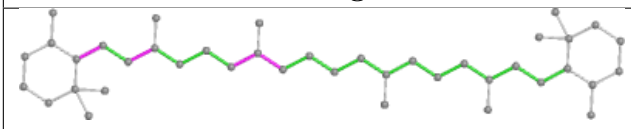
Ligand BCR c 515



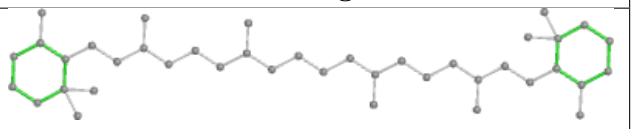
Bond lengths



Bond angles

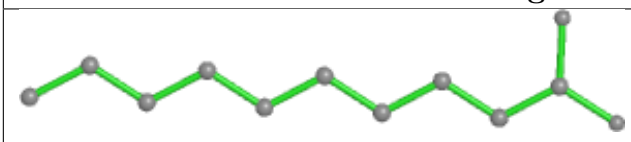


Torsions

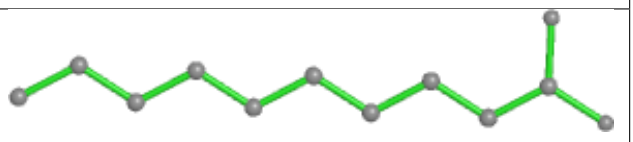


Rings

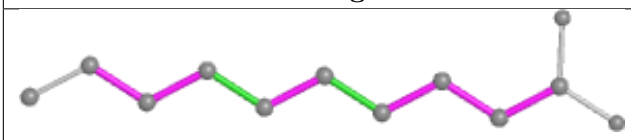
Ligand STE B 623



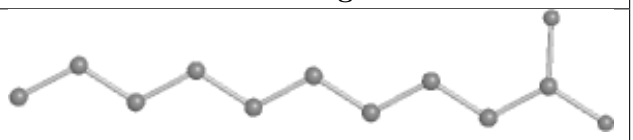
Bond lengths



Bond angles

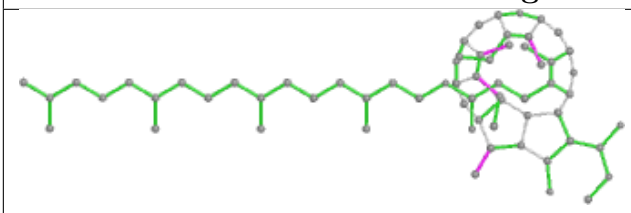


Torsions

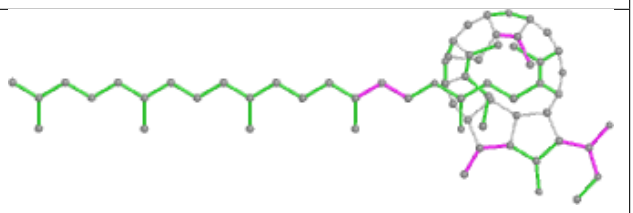


Rings

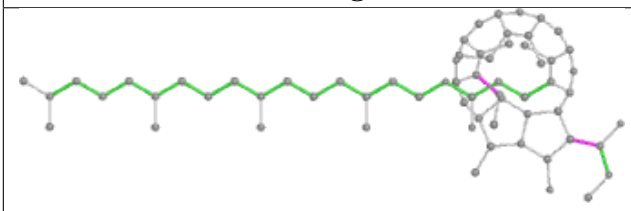
Ligand PHO A 609



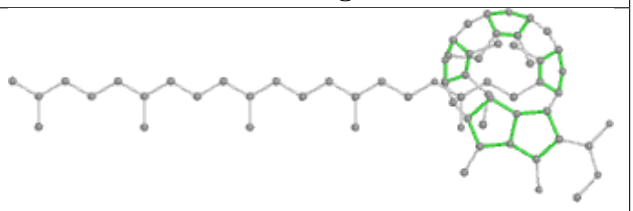
Bond lengths



Bond angles

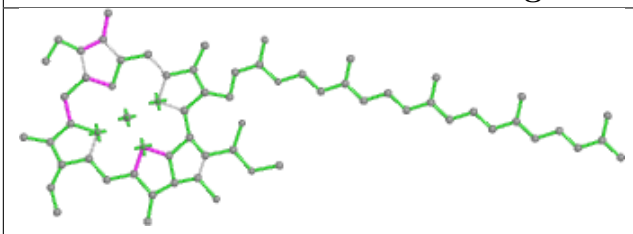


Torsions

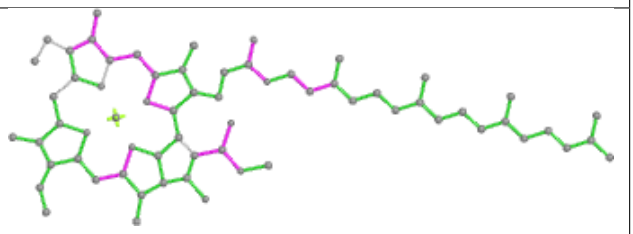


Rings

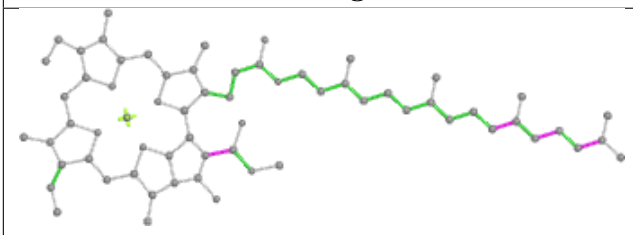
Ligand CLA C 502



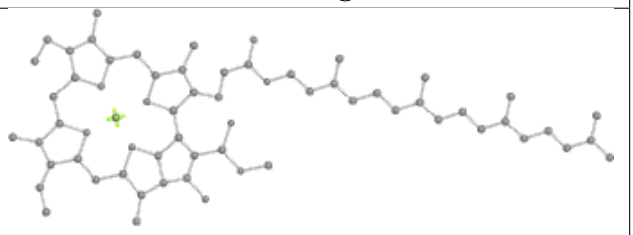
Bond lengths



Bond angles

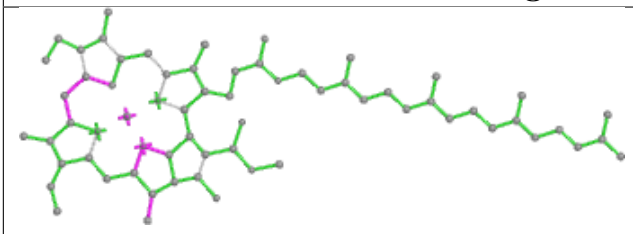


Torsions

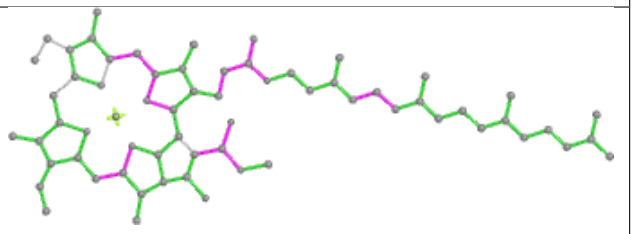


Rings

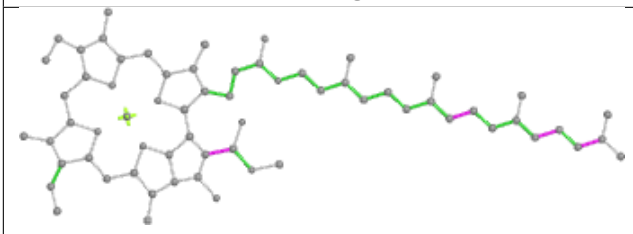
Ligand CLA B 604



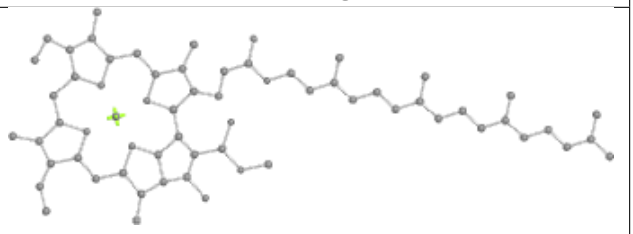
Bond lengths



Bond angles

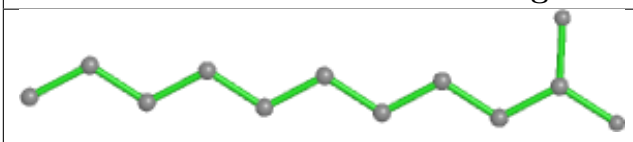


Torsions

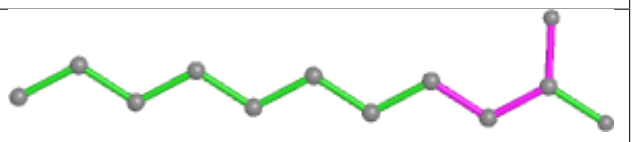


Rings

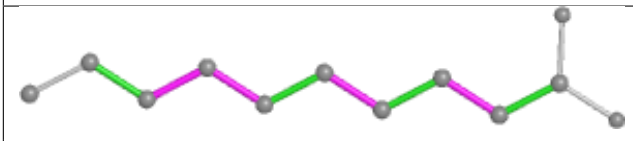
Ligand STE J 101



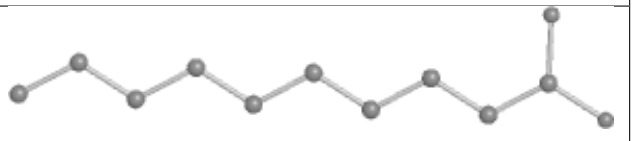
Bond lengths



Bond angles

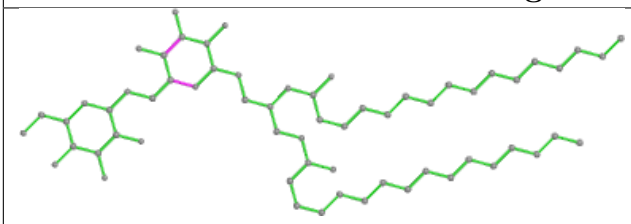


Torsions

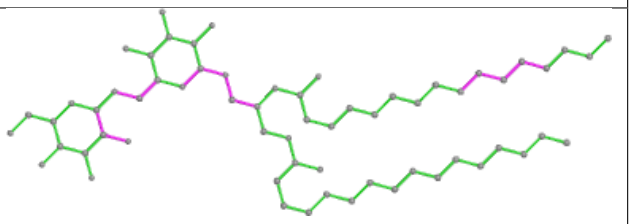


Rings

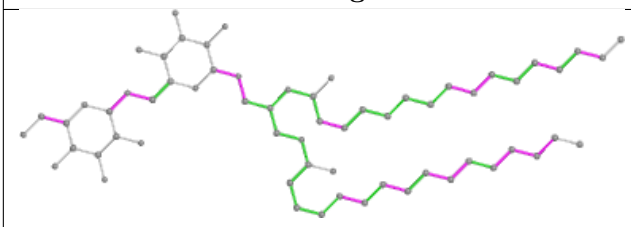
Ligand DGD c 518



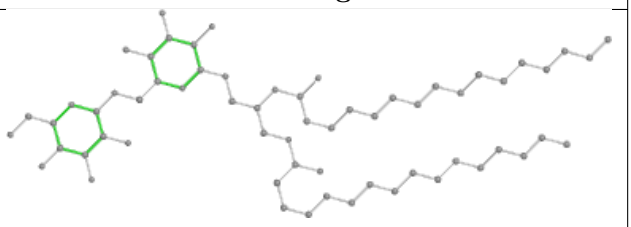
Bond lengths



Bond angles

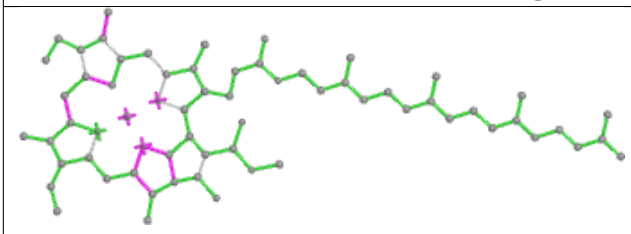


Torsions

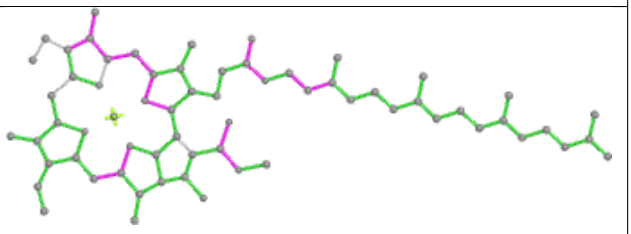


Rings

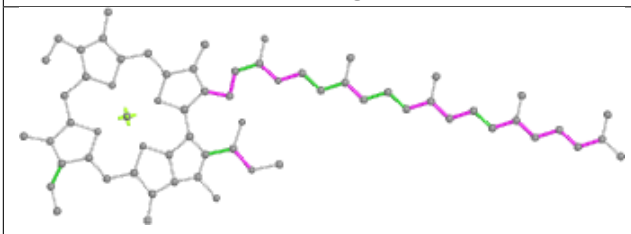
Ligand CLA c 512



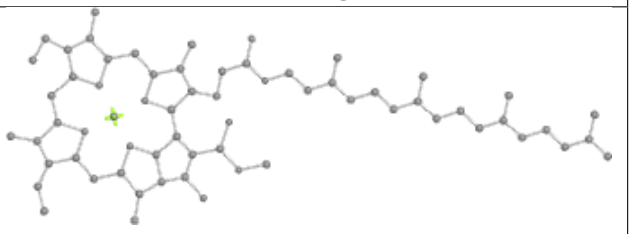
Bond lengths



Bond angles

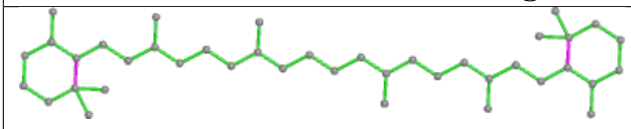


Torsions

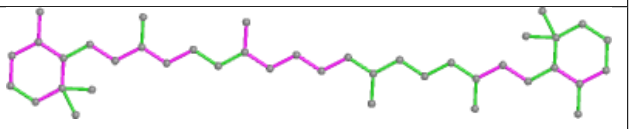


Rings

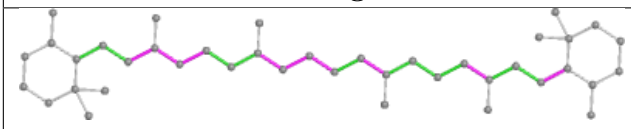
Ligand BCR K 101



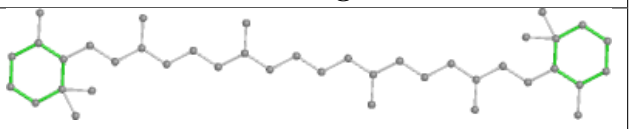
Bond lengths



Bond angles

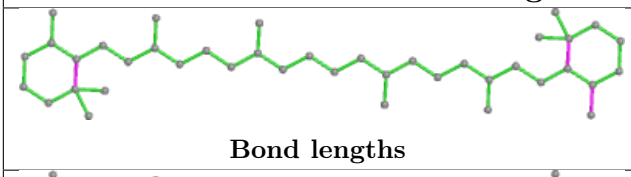


Torsions

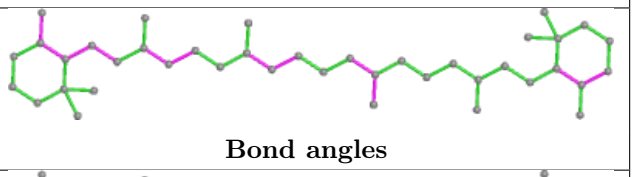


Rings

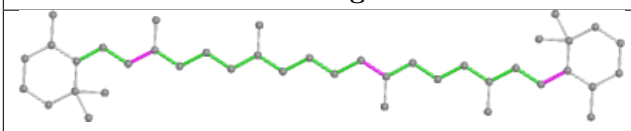
Ligand BCR b 617



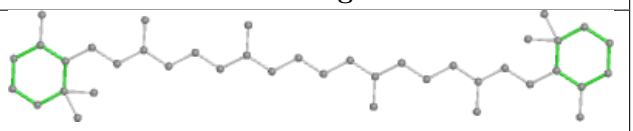
Bond lengths



Bond angles

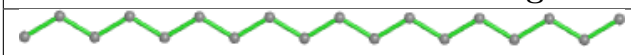


Torsions



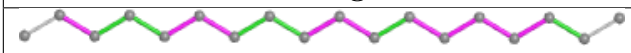
Rings

Ligand STE H 104

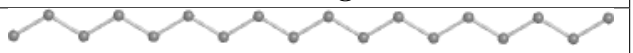


Bond lengths

Bond angles

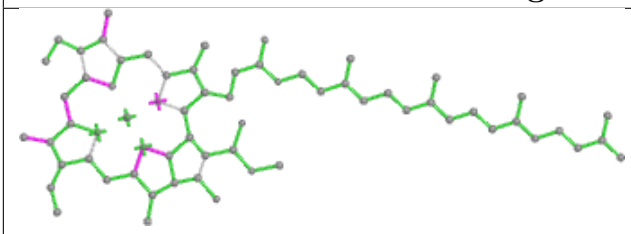


Torsions

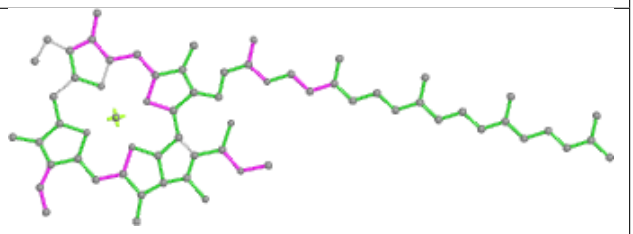


Rings

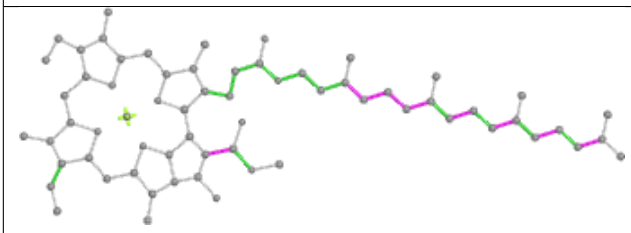
Ligand CLA b 613



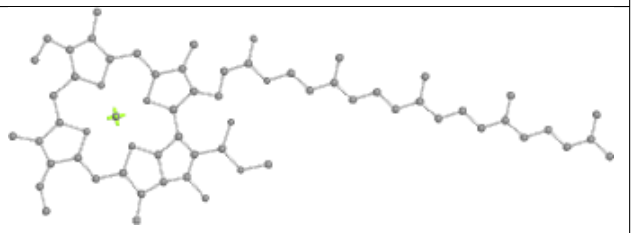
Bond lengths



Bond angles

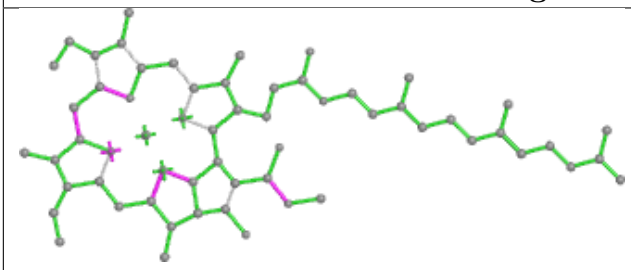


Torsions

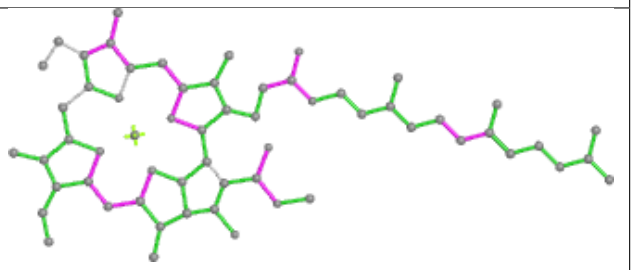


Rings

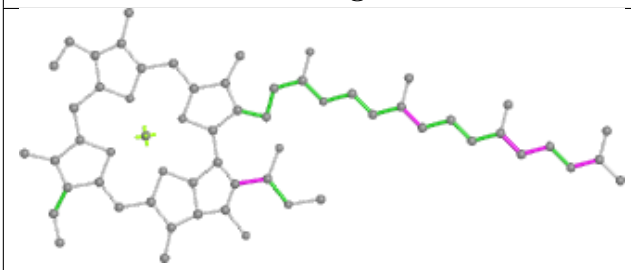
Ligand CLA c 504



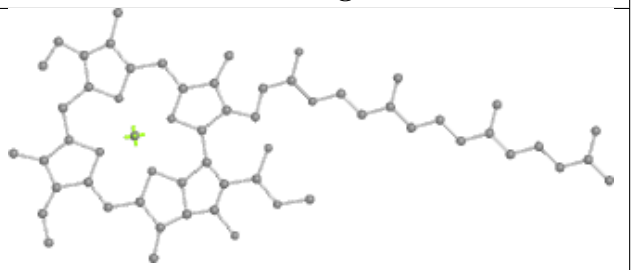
Bond lengths



Bond angles

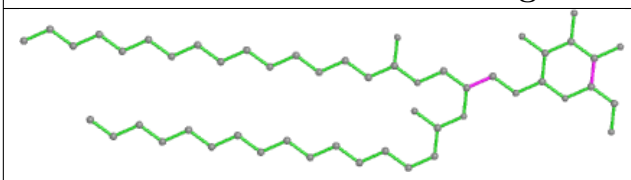


Torsions

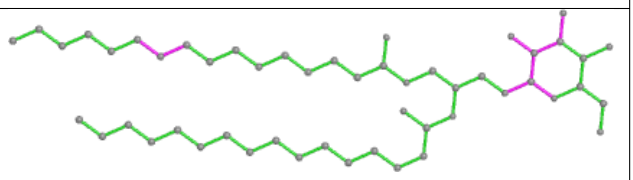


Rings

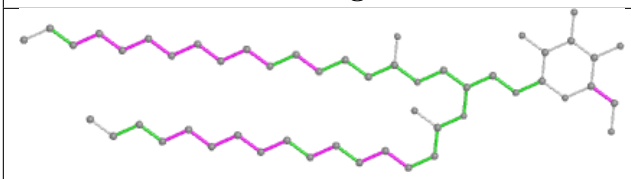
Ligand LMG D 406



Bond lengths



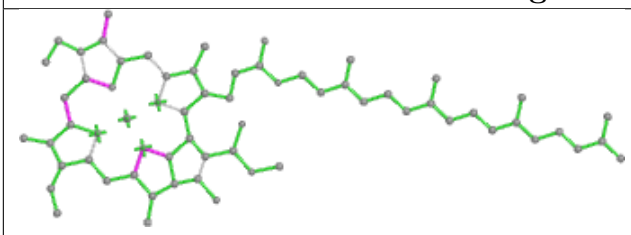
Bond angles



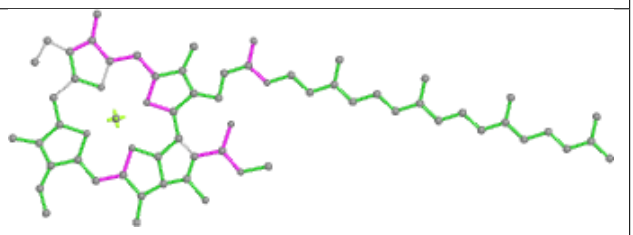
Torsions

Rings

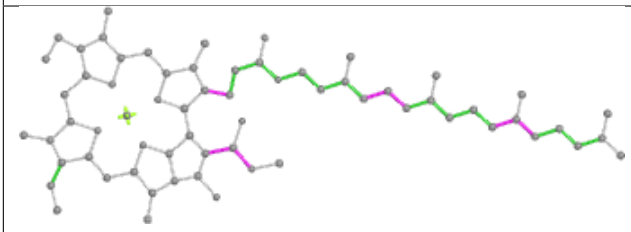
Ligand CLA c 513



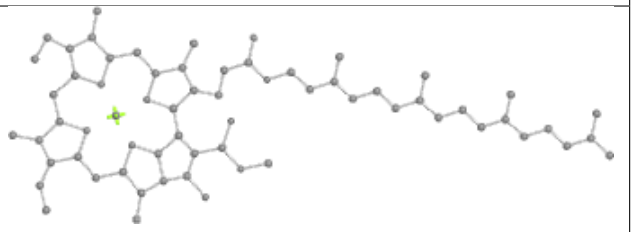
Bond lengths



Bond angles

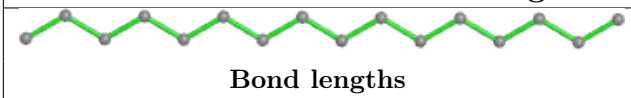


Torsions

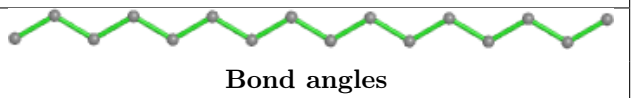


Rings

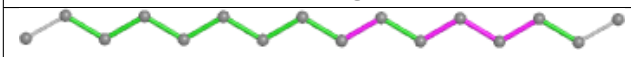
Ligand STE B 626



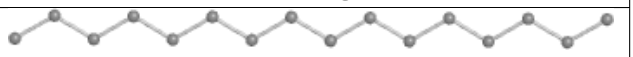
Bond lengths



Bond angles

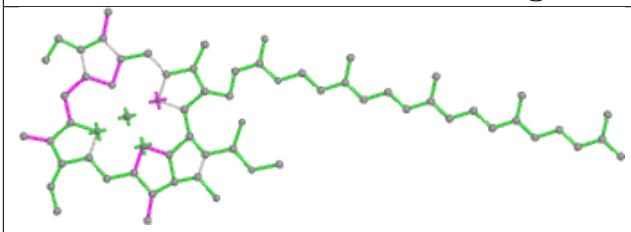


Torsions

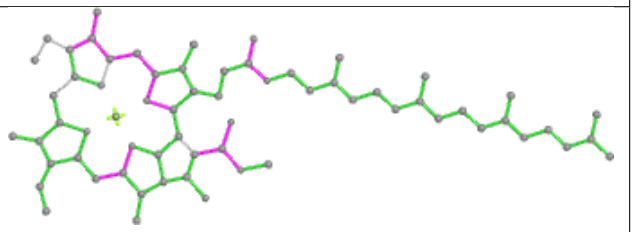


Rings

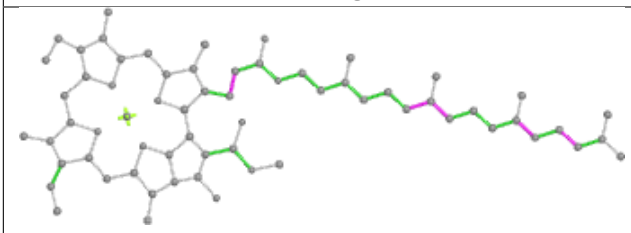
Ligand CLA b 605



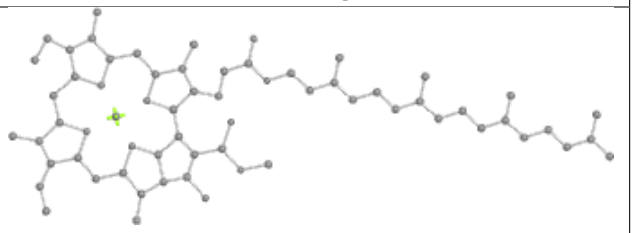
Bond lengths



Bond angles

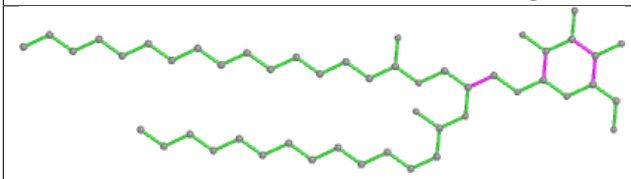


Torsions

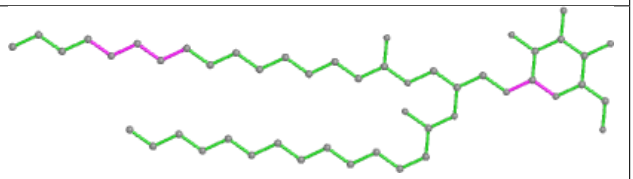


Rings

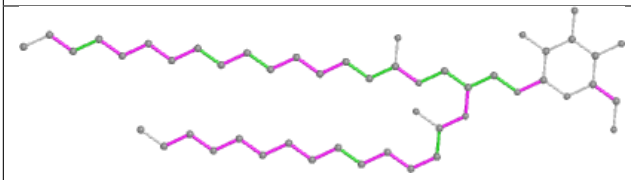
Ligand LMG c 524



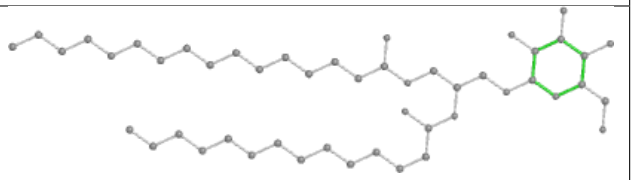
Bond lengths



Bond angles

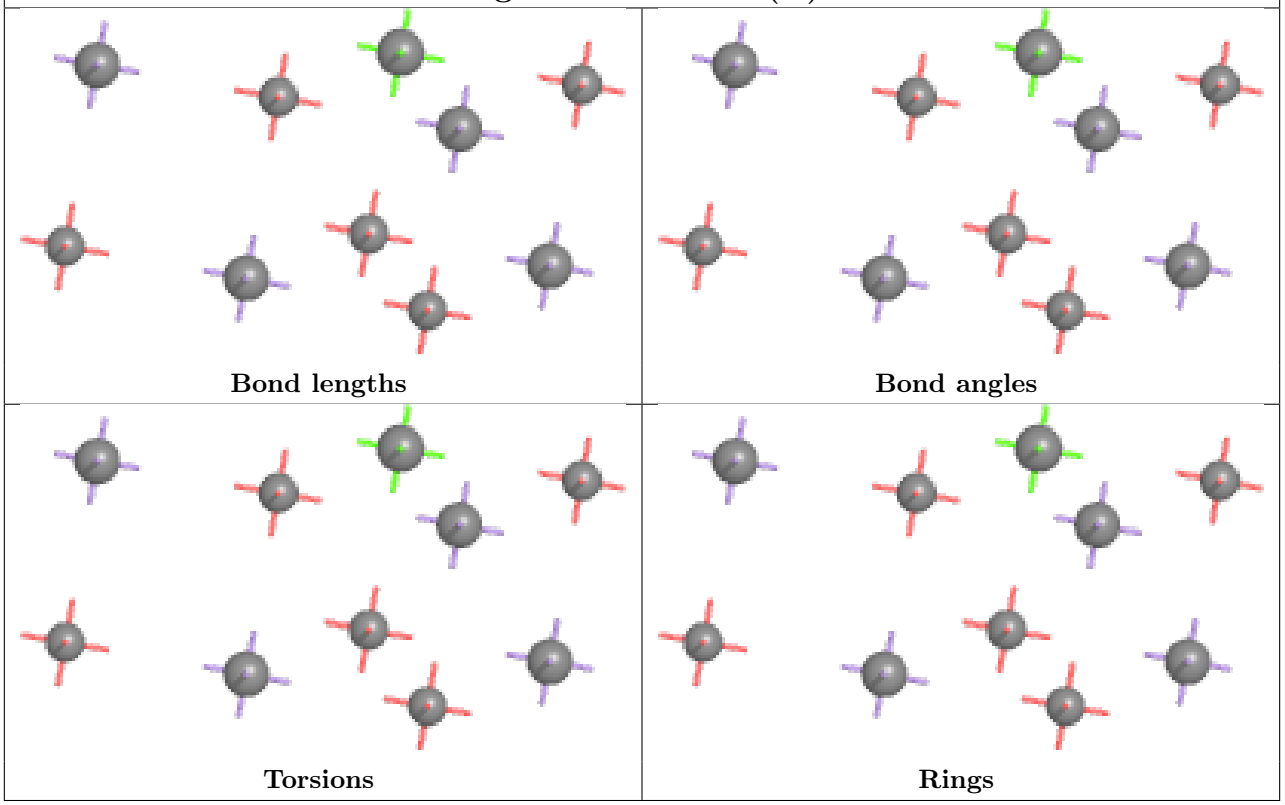


Torsions

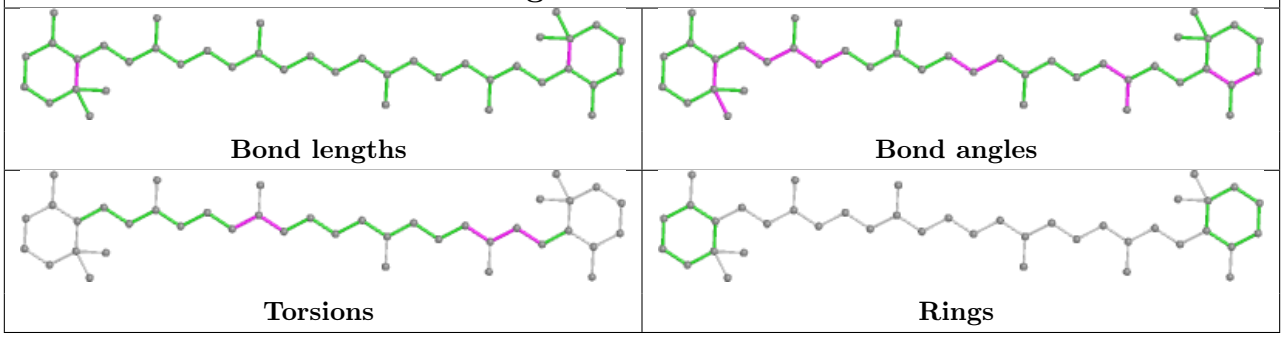


Rings

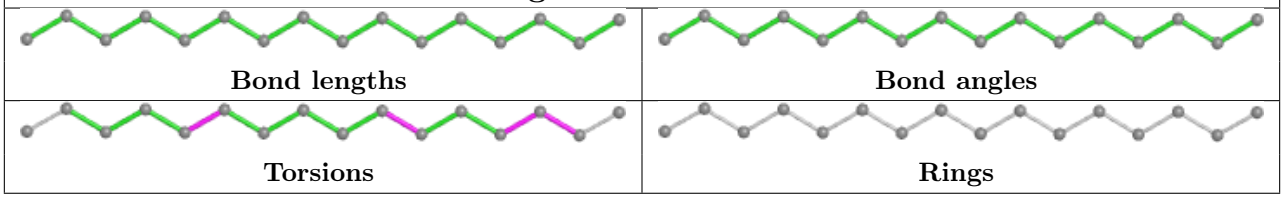
Ligand OEX a 602 (A)



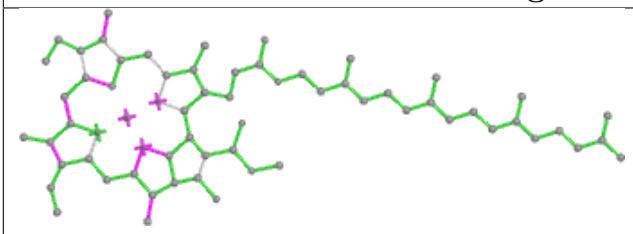
Ligand BCR b 618



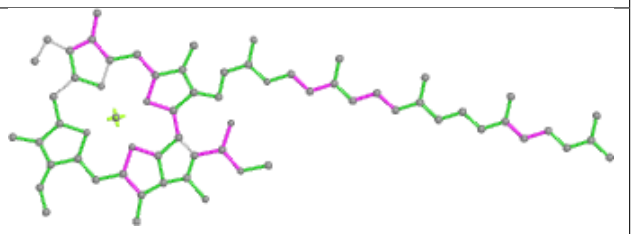
Ligand STE C 522



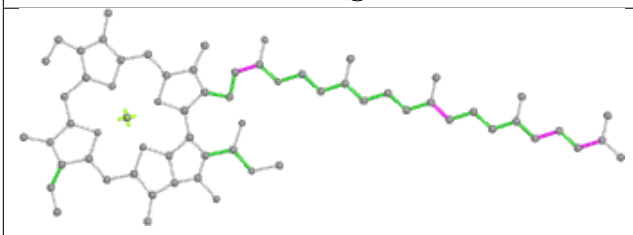
Ligand CLA b 612



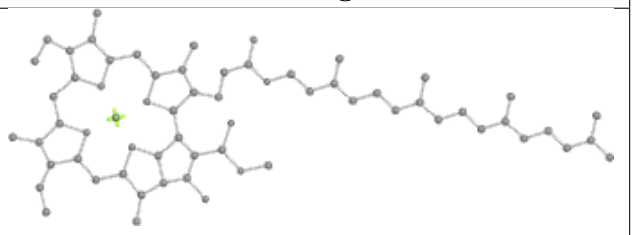
Bond lengths



Bond angles

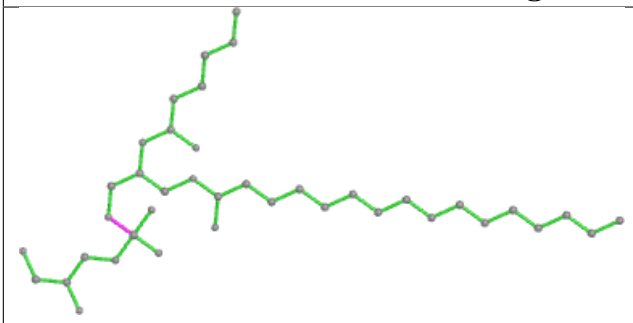


Torsions

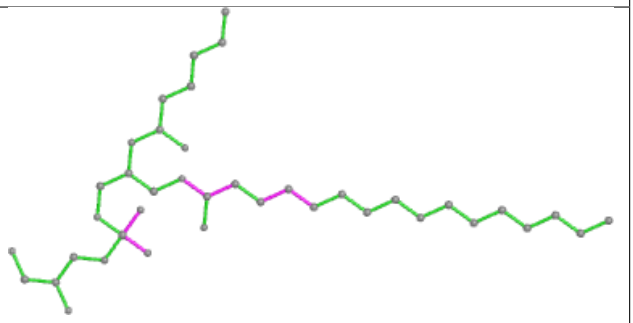


Rings

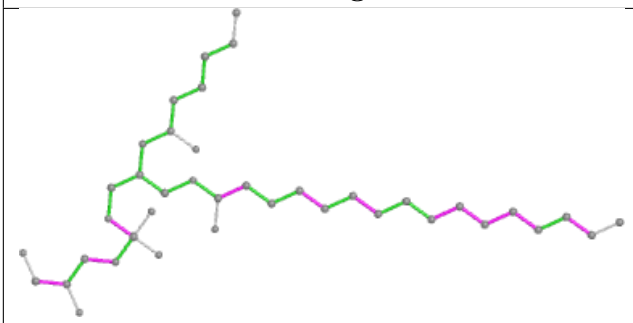
Ligand LHG d 408



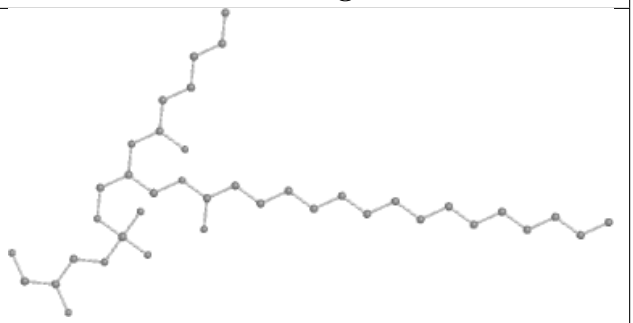
Bond lengths



Bond angles

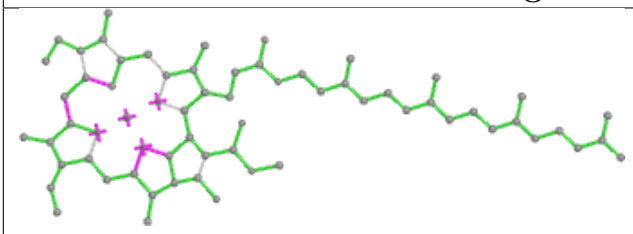


Torsions

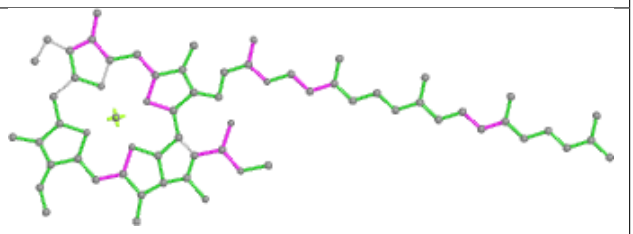


Rings

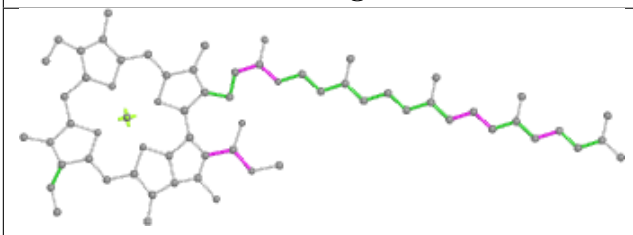
Ligand CLA B 611



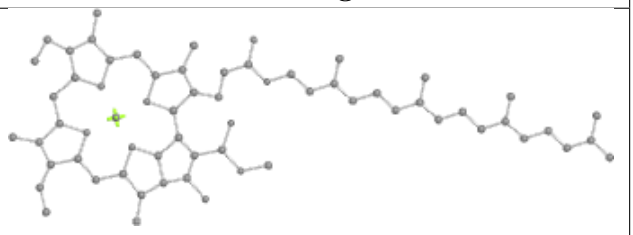
Bond lengths



Bond angles

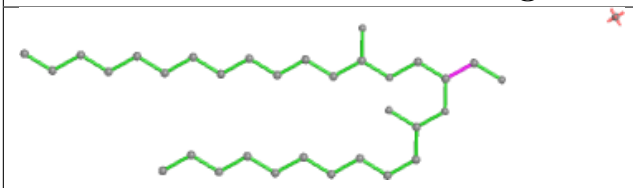


Torsions

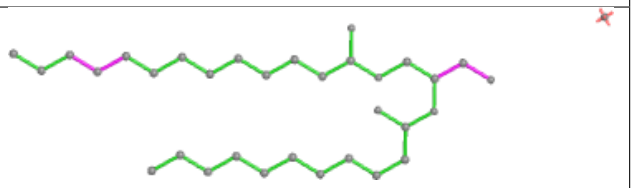


Rings

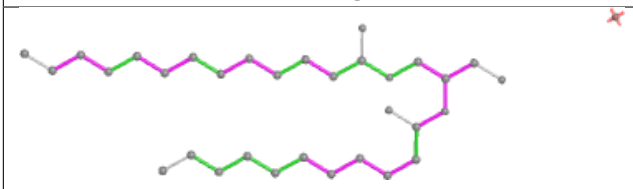
Ligand LMG D 409



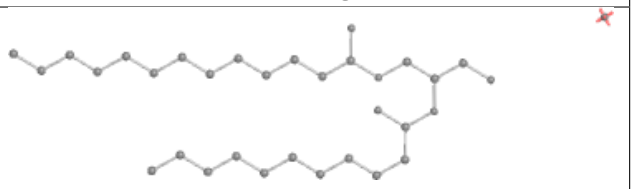
Bond lengths



Bond angles

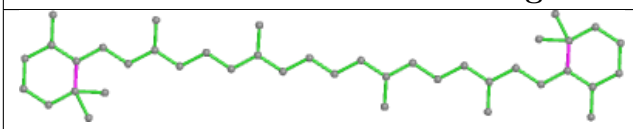


Torsions

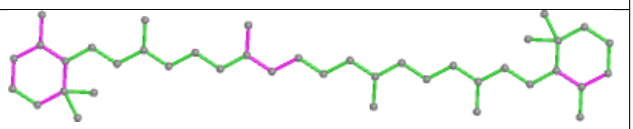


Rings

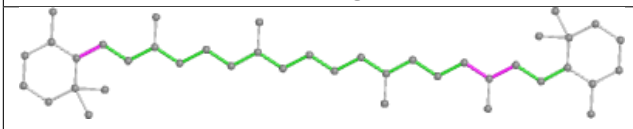
Ligand BCR b 616



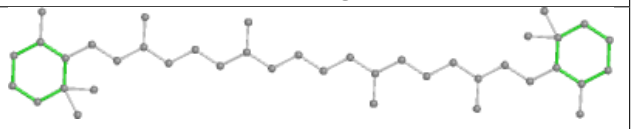
Bond lengths



Bond angles

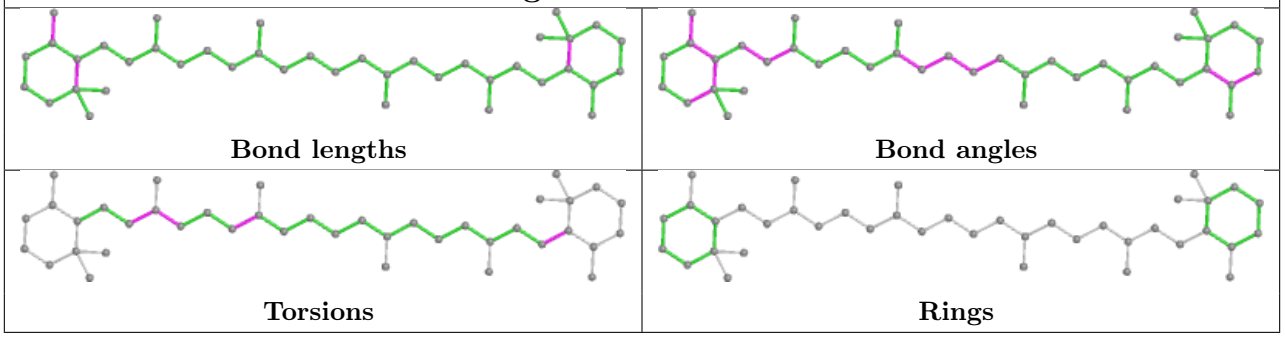


Torsions

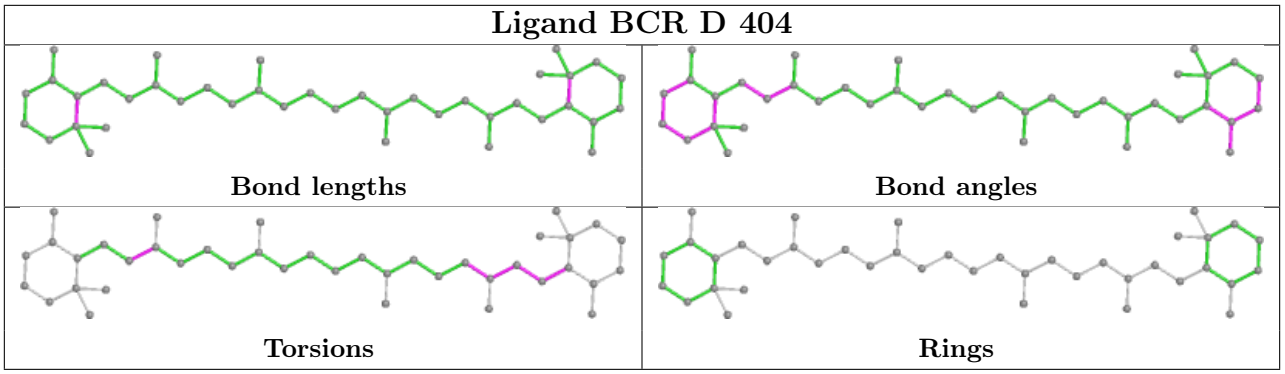


Rings

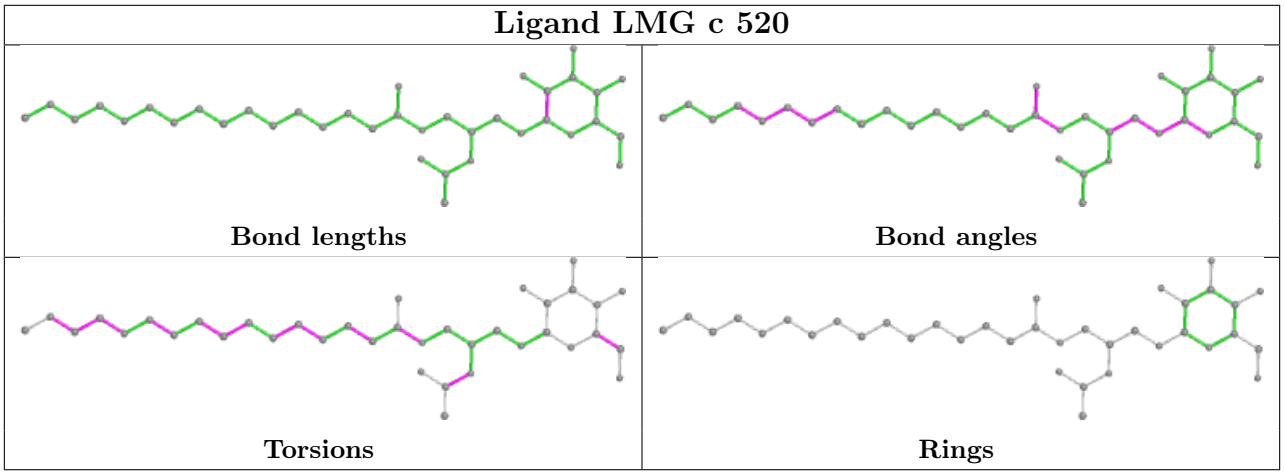
Ligand BCR C 514



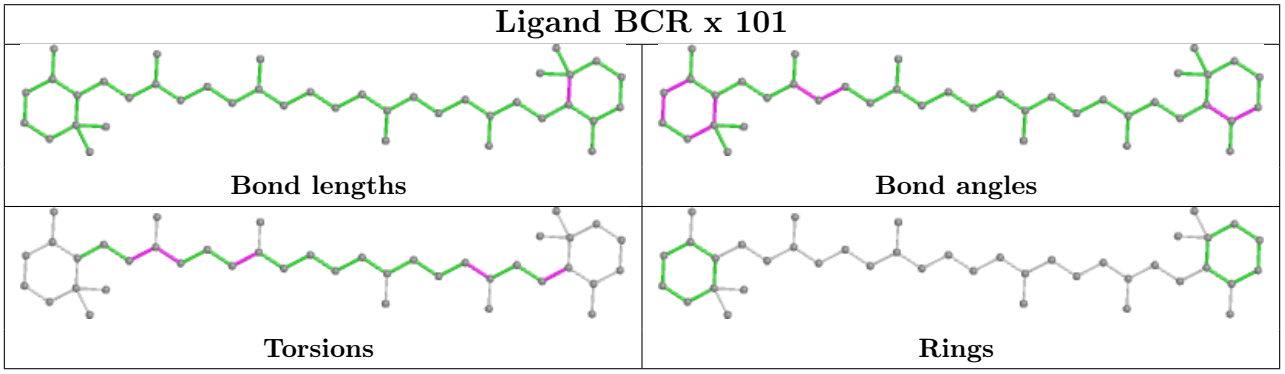
Ligand BCR D 404



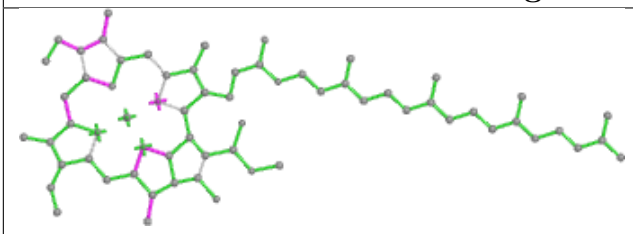
Ligand LMG c 520



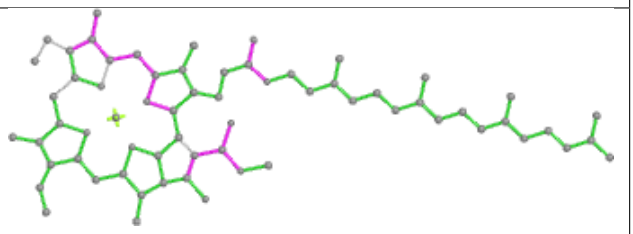
Ligand BCR x 101



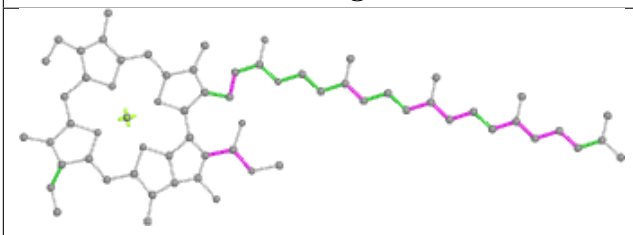
Ligand CLA B 605



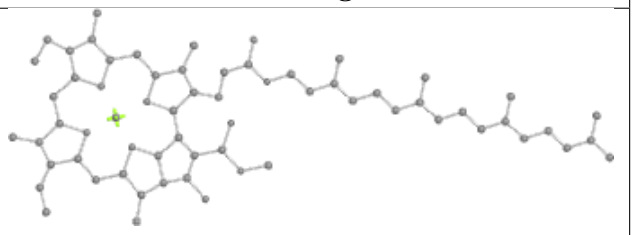
Bond lengths



Bond angles

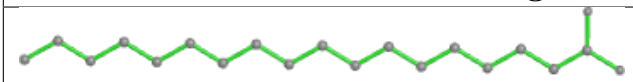


Torsions

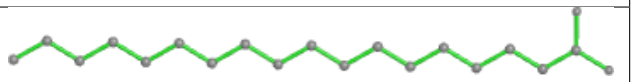


Rings

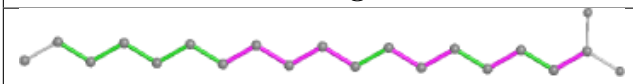
Ligand STE D 410



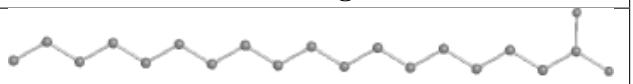
Bond lengths



Bond angles

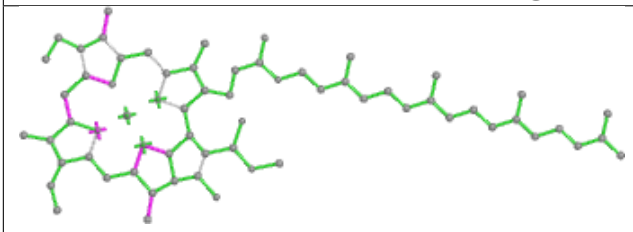


Torsions

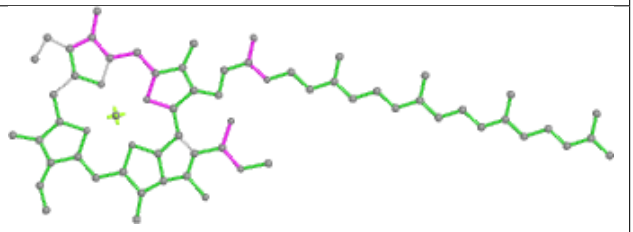


Rings

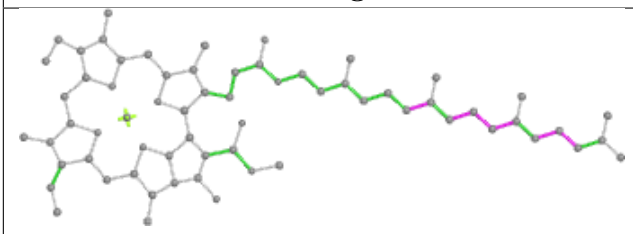
Ligand CLA b 614



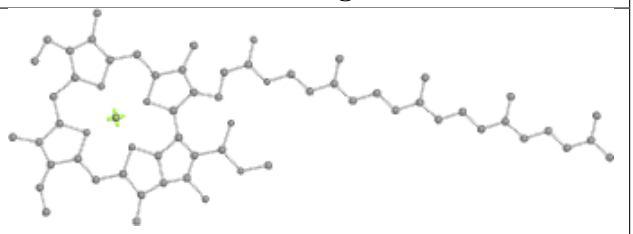
Bond lengths



Bond angles

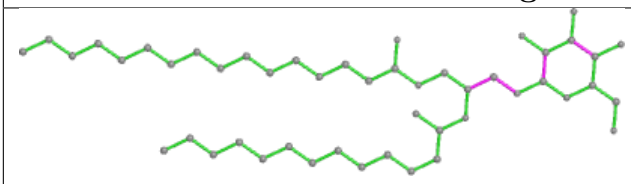


Torsions

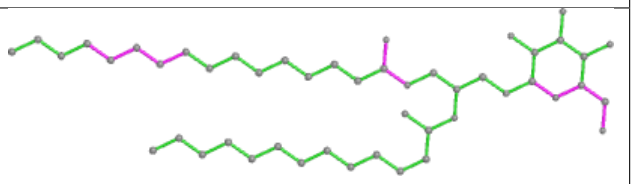


Rings

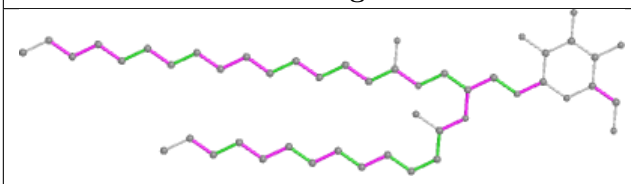
Ligand LMG C 515



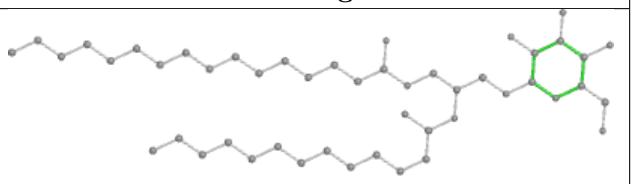
Bond lengths



Bond angles

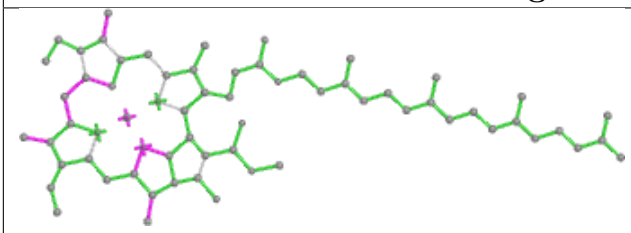


Torsions

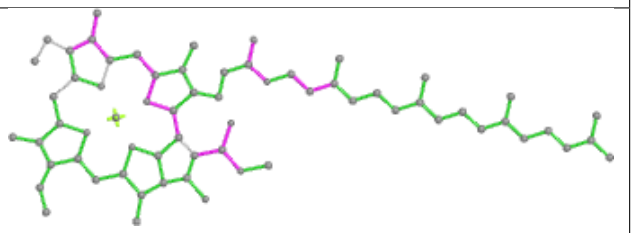


Rings

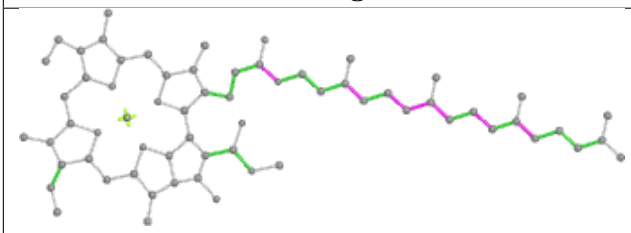
Ligand CLA a 610



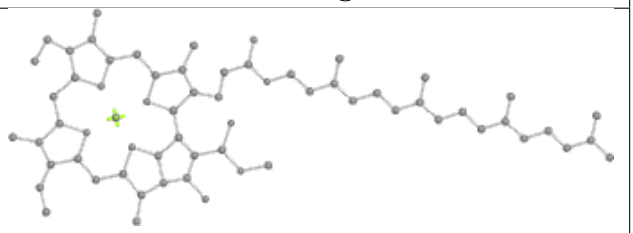
Bond lengths



Bond angles

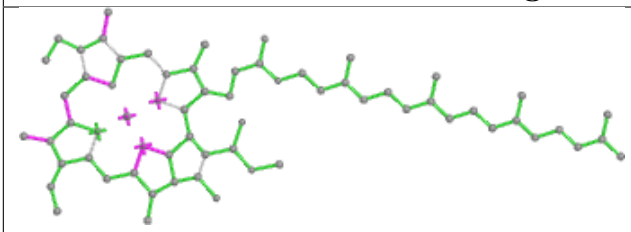


Torsions

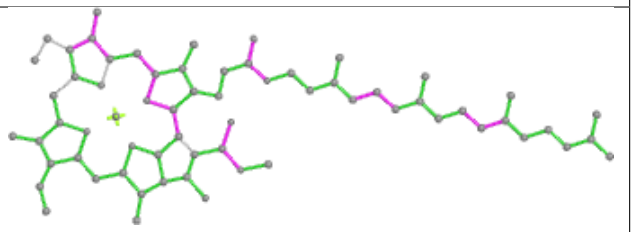


Rings

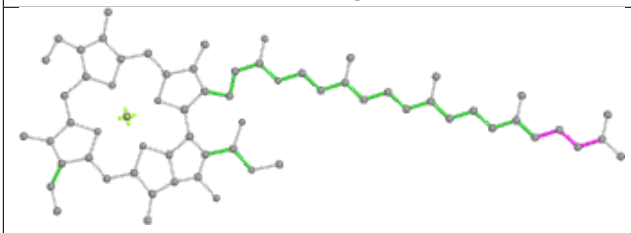
Ligand CLA A 606



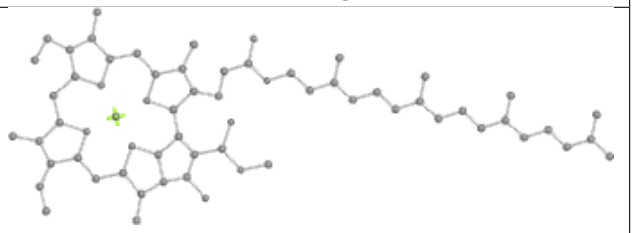
Bond lengths



Bond angles

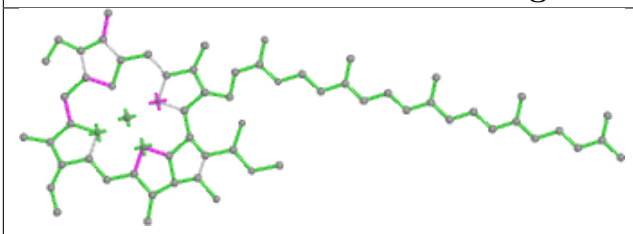


Torsions

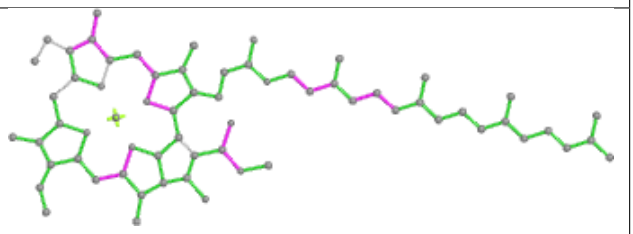


Rings

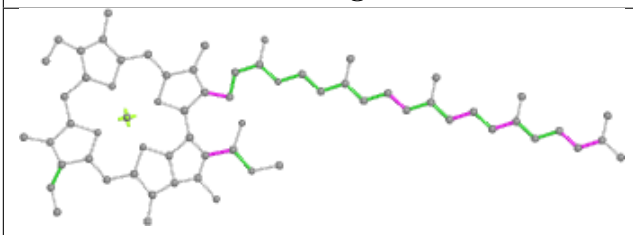
Ligand CLA c 503



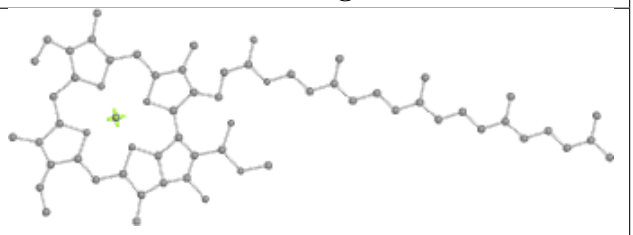
Bond lengths



Bond angles

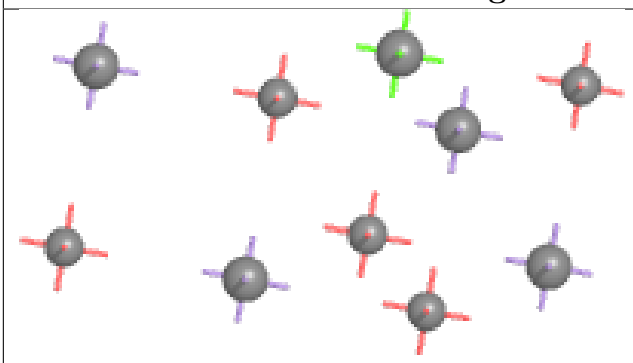


Torsions

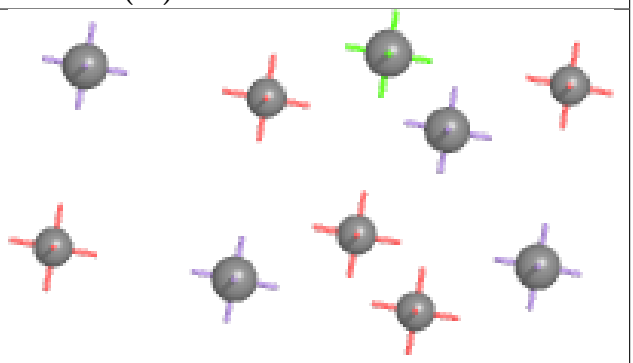


Rings

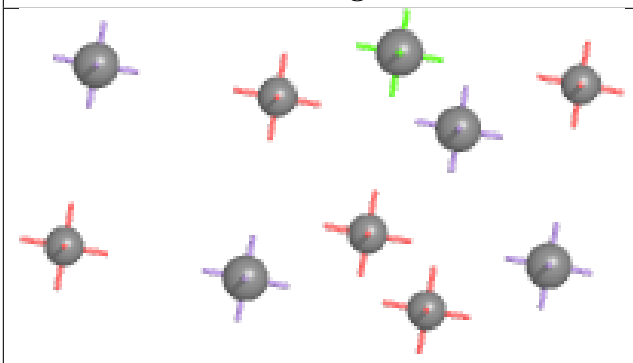
Ligand OEX A 602 (A)



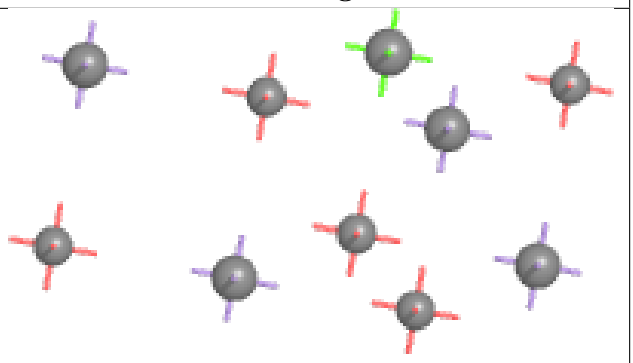
Bond lengths



Bond angles

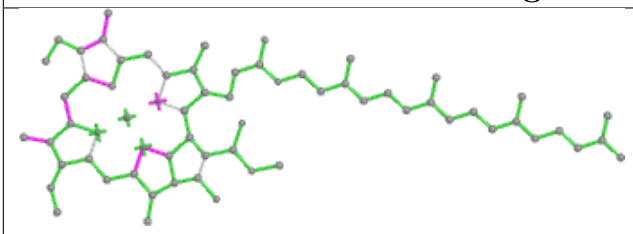


Torsions

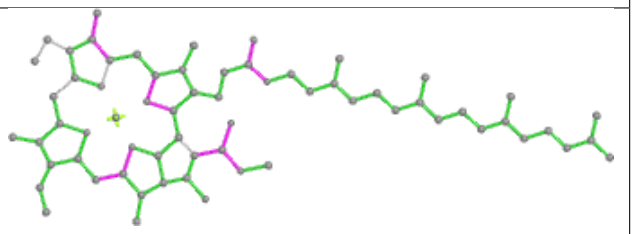


Rings

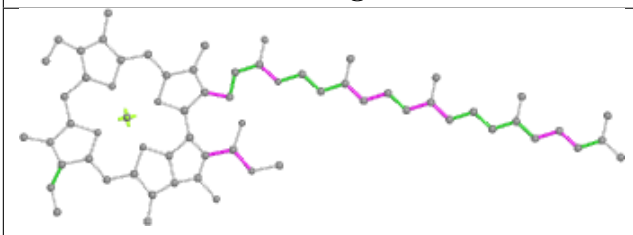
Ligand CLA H 101



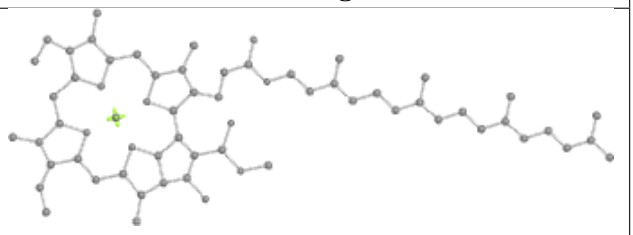
Bond lengths



Bond angles

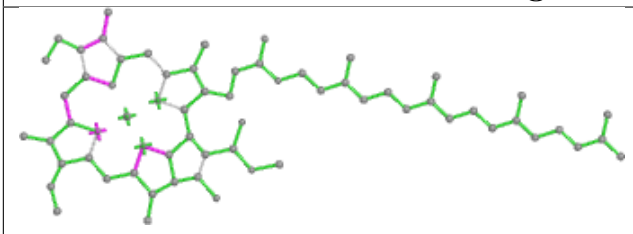


Torsions

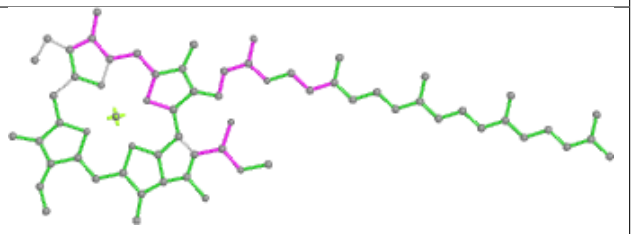


Rings

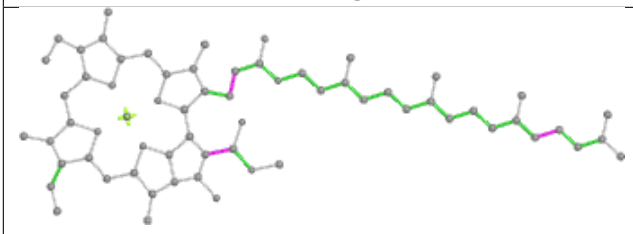
Ligand CLA b 609



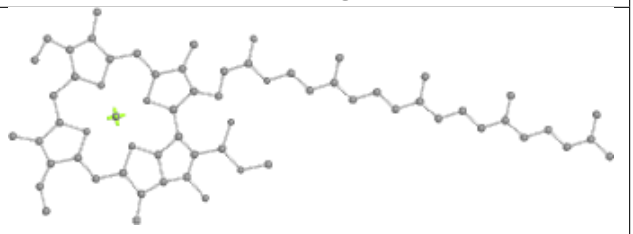
Bond lengths



Bond angles



Torsions



Rings

Ligand STE I 101

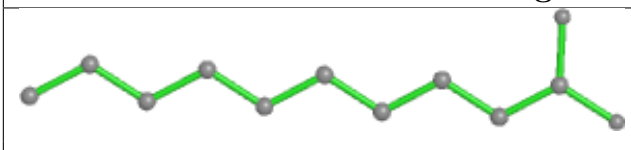
Bond lengths

Bond angles

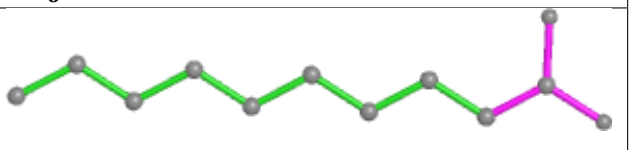
Torsions

Rings

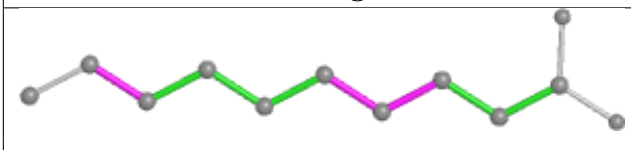
Ligand STE j 101



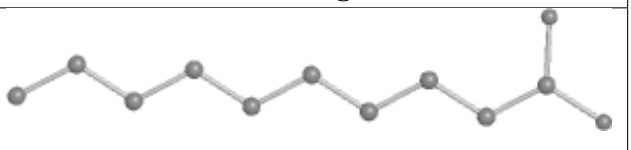
Bond lengths



Bond angles

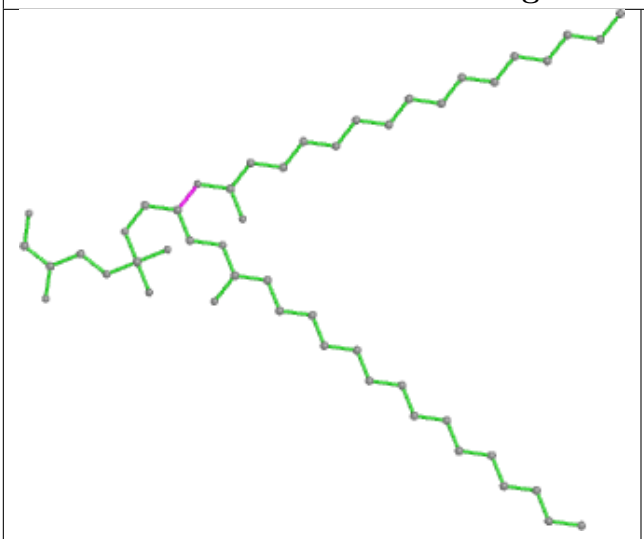


Torsions

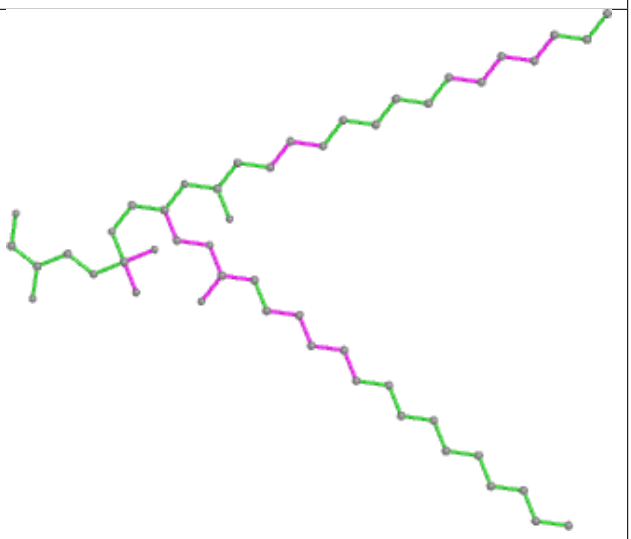


Rings

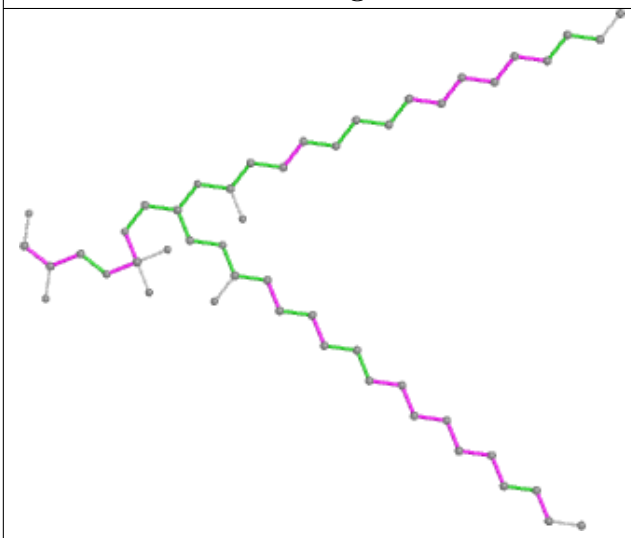
Ligand LHG D 407



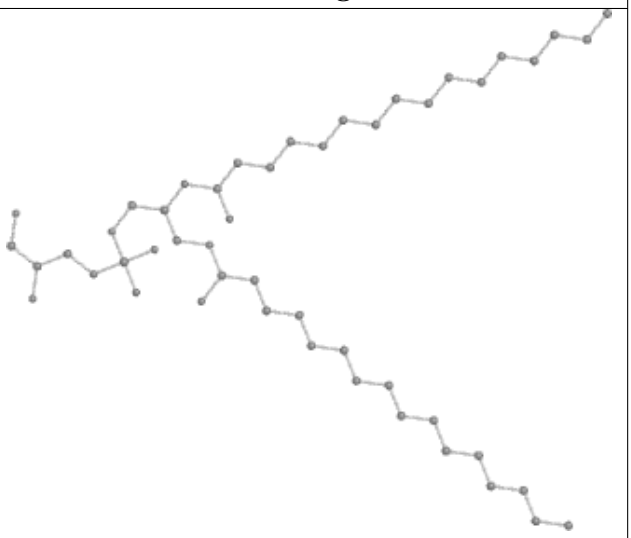
Bond lengths



Bond angles

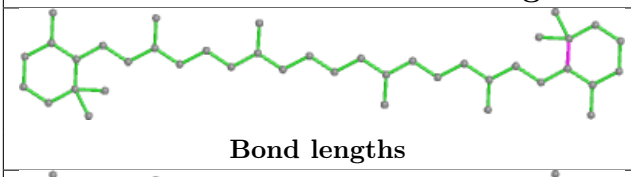


Torsions

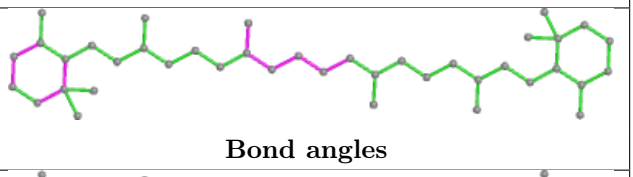


Rings

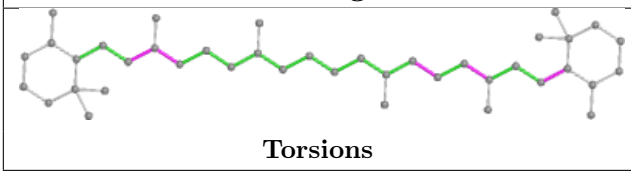
Ligand BCR B 617



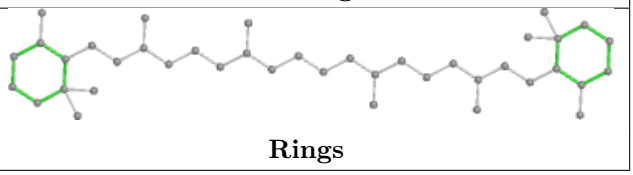
Bond lengths



Bond angles

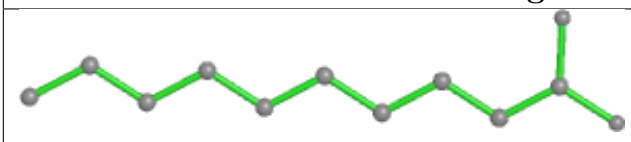


Torsions

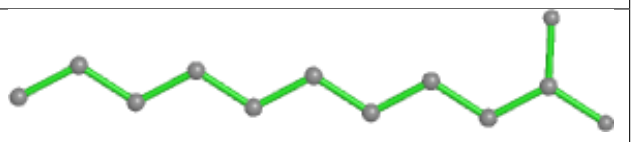


Rings

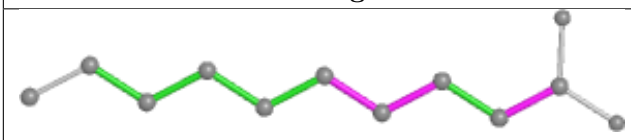
Ligand STE R 101



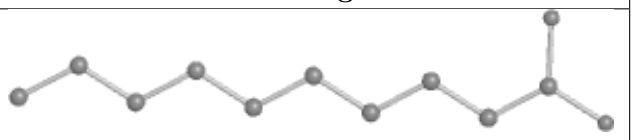
Bond lengths



Bond angles

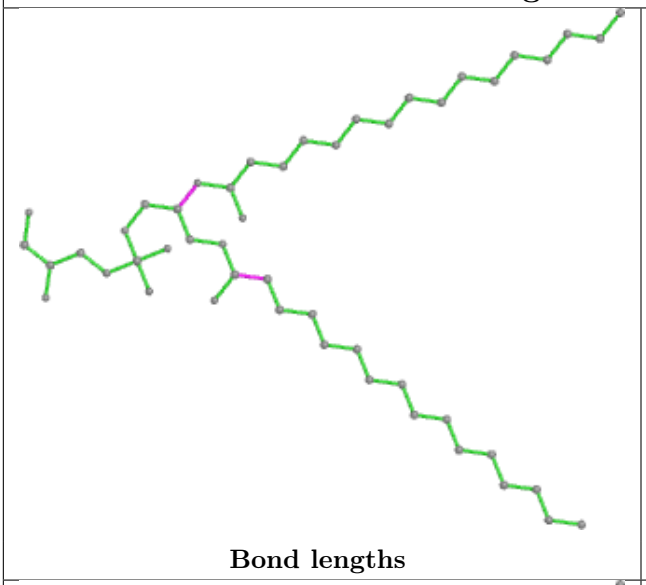


Torsions

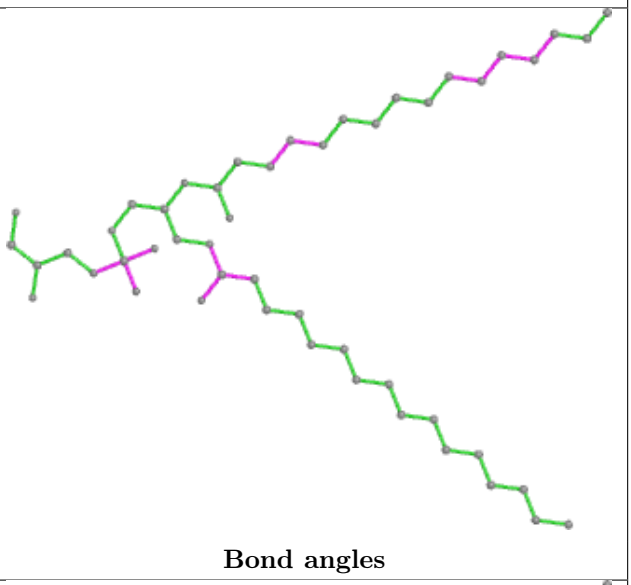


Rings

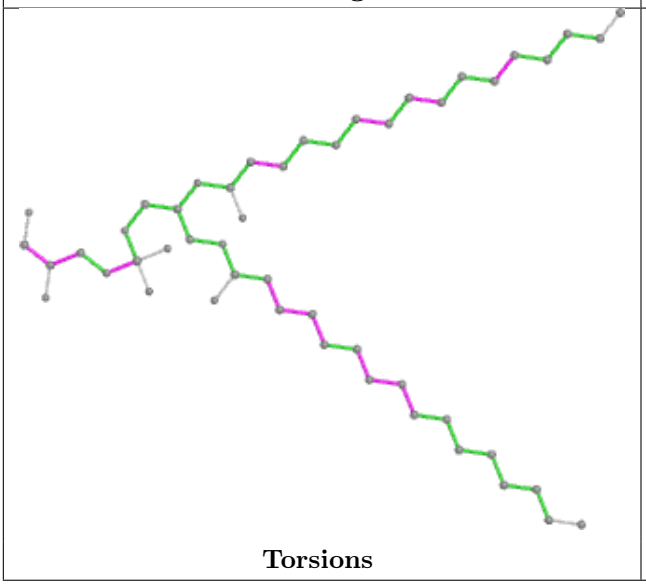
Ligand LHG B 622



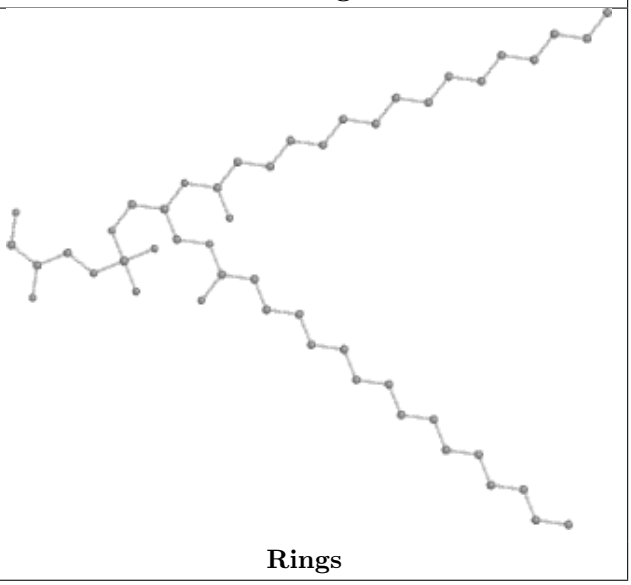
Bond lengths



Bond angles



Torsions

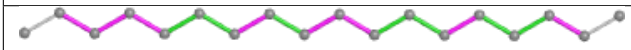


Rings

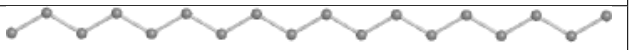
Ligand STE l 103

Bond lengths

Bond angles

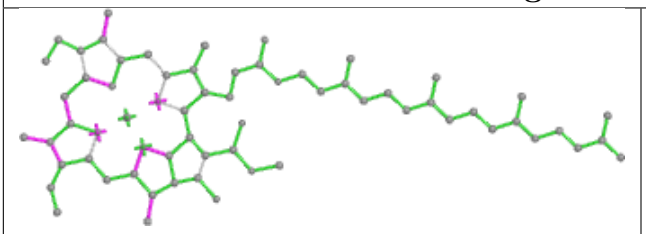


Torsions

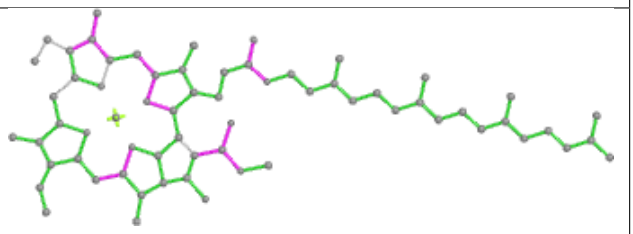


Rings

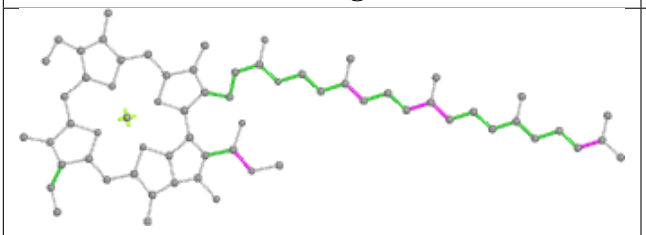
Ligand CLA C 510



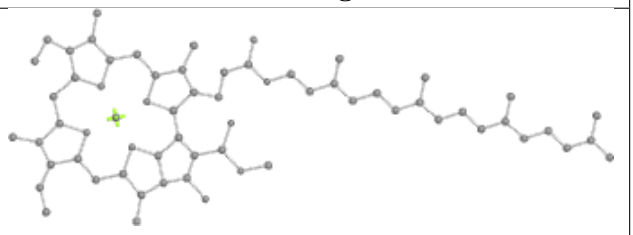
Bond lengths



Bond angles

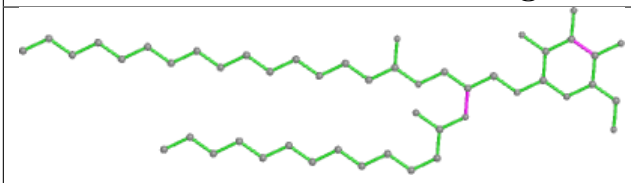


Torsions

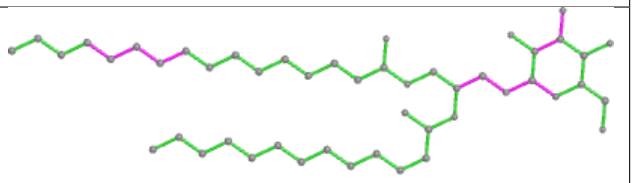


Rings

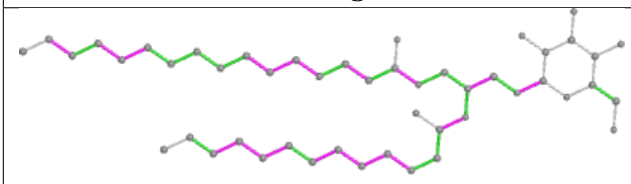
Ligand LMG C 519



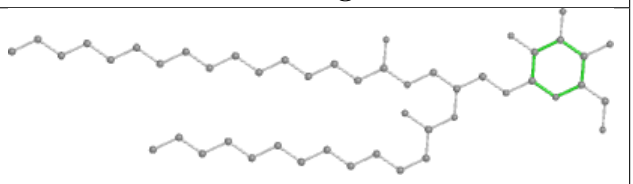
Bond lengths



Bond angles

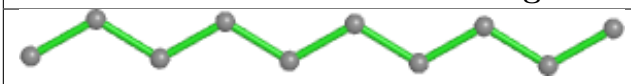


Torsions



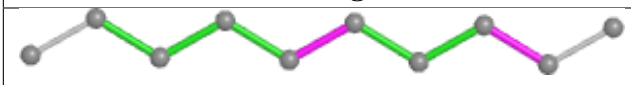
Rings

Ligand STE M 103

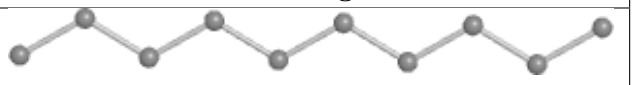


Bond lengths

Bond angles

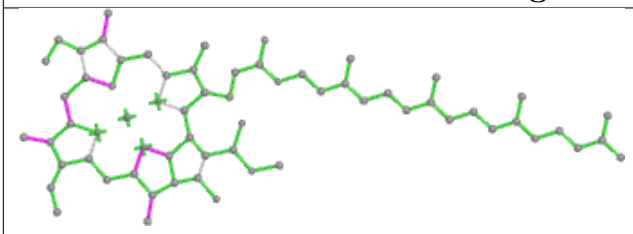


Torsions

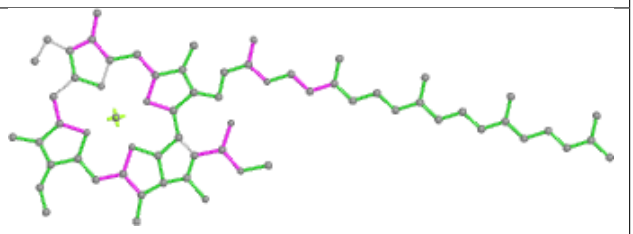


Rings

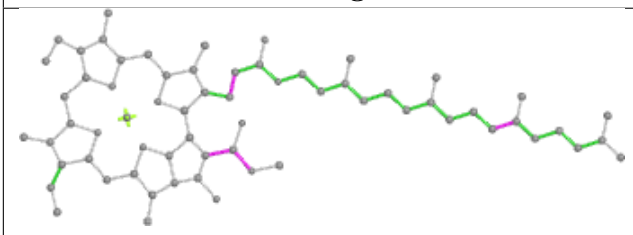
Ligand CLA c 501



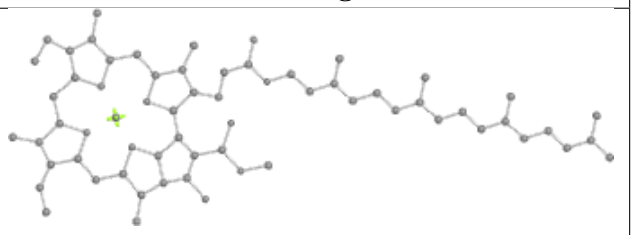
Bond lengths



Bond angles

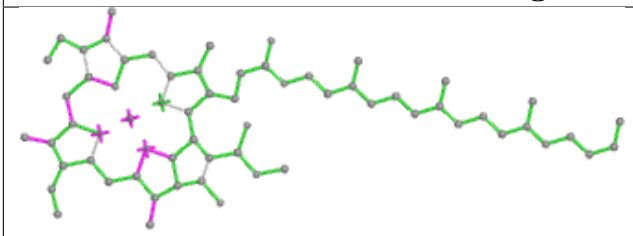


Torsions

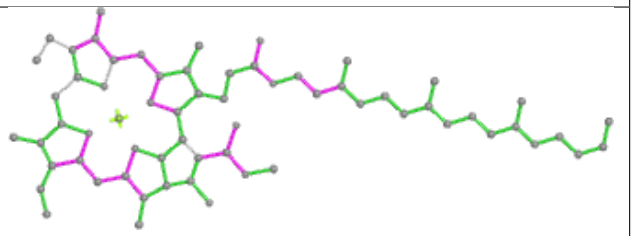


Rings

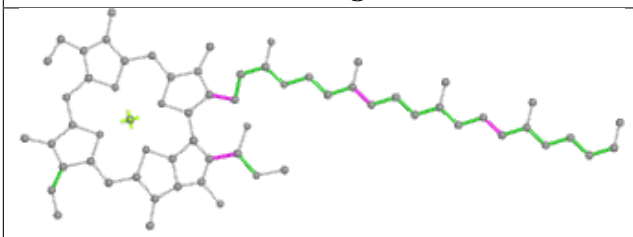
Ligand CLA c 508



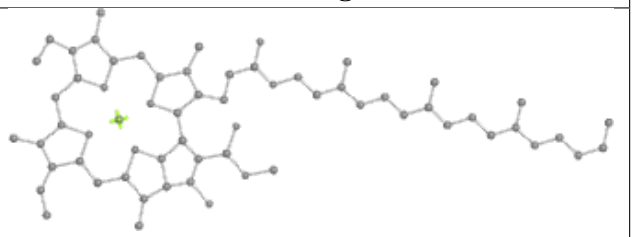
Bond lengths



Bond angles

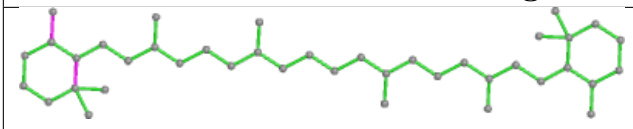


Torsions

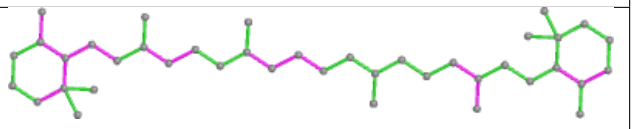


Rings

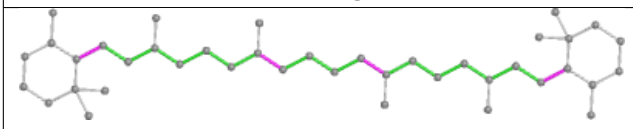
Ligand BCR A 611



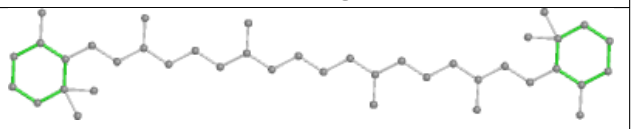
Bond lengths



Bond angles

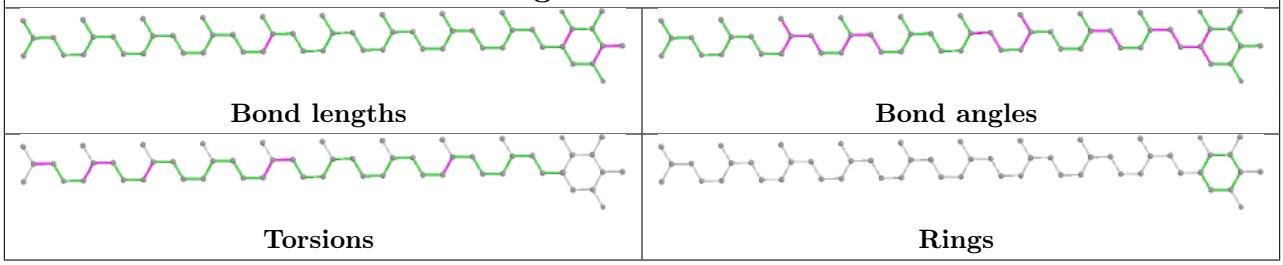


Torsions

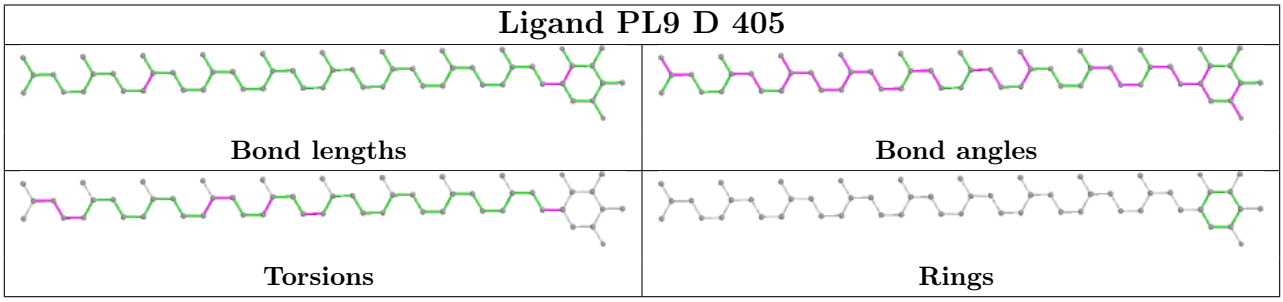


Rings

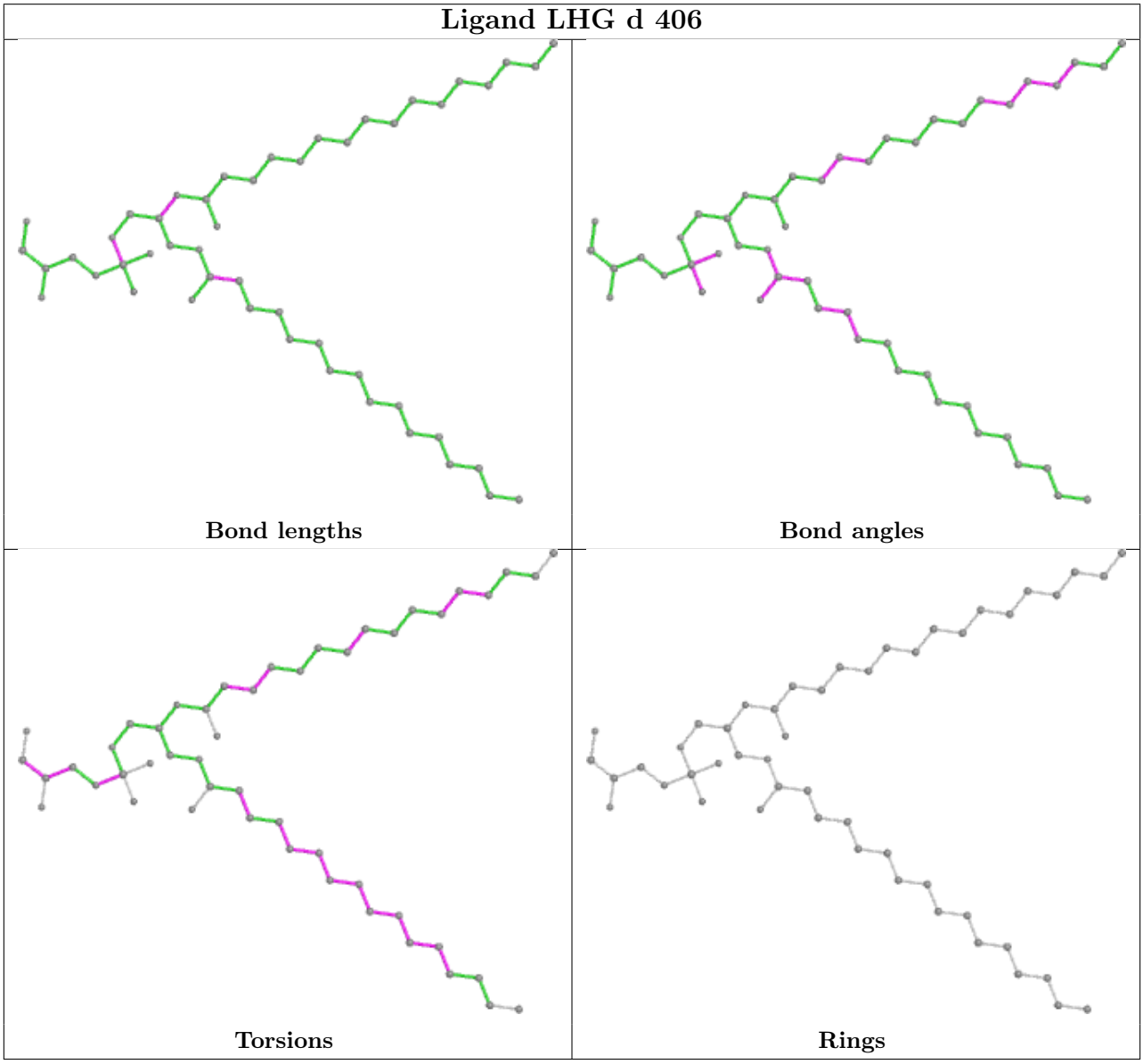
Ligand PL9 d 405



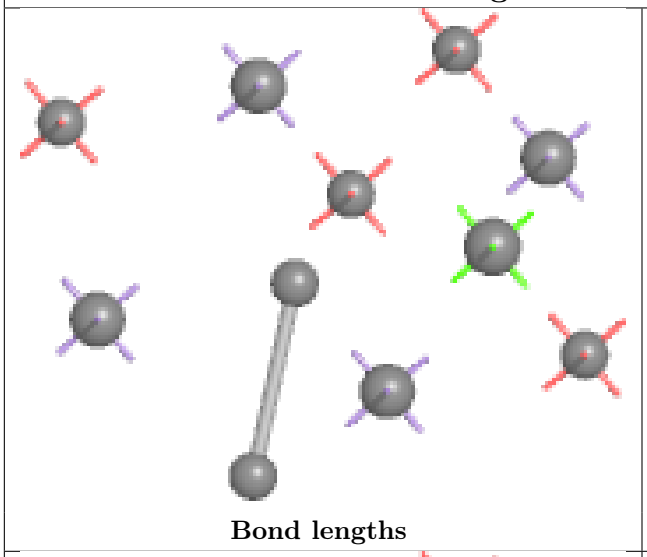
Ligand PL9 D 405



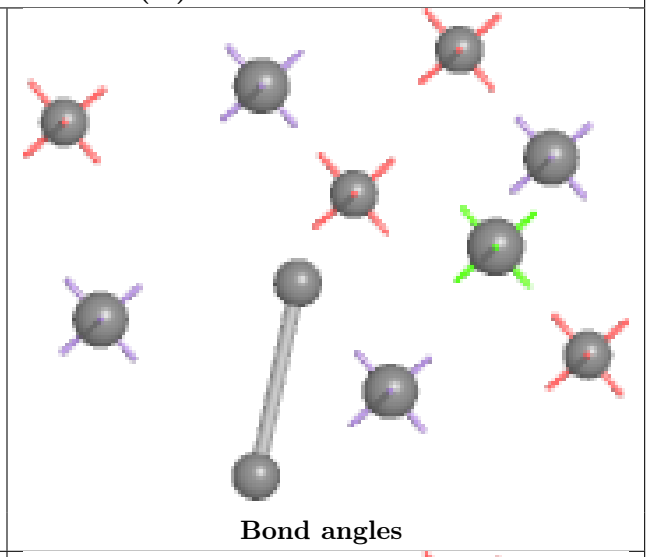
Ligand LHG d 406



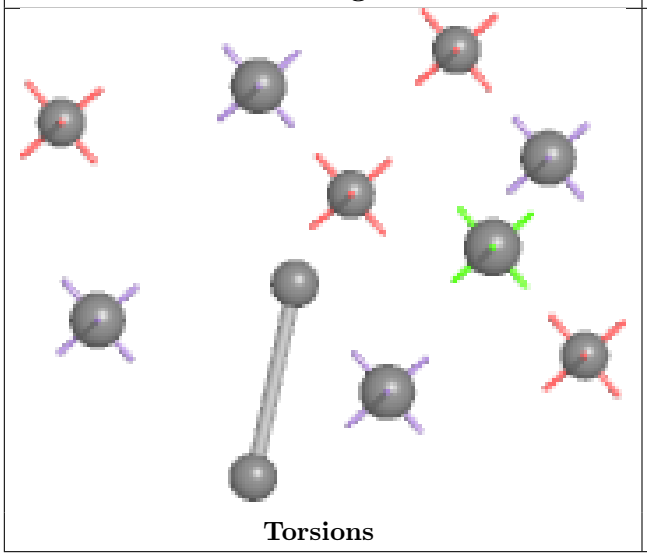
Ligand OEY A 601 (B)



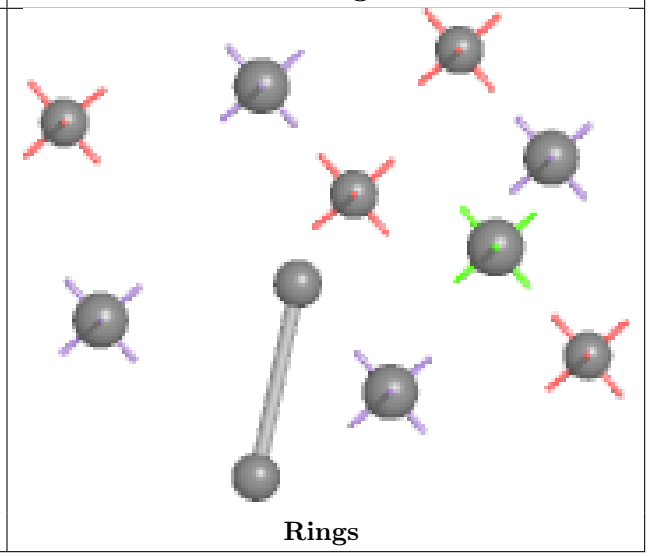
Bond lengths



Bond angles



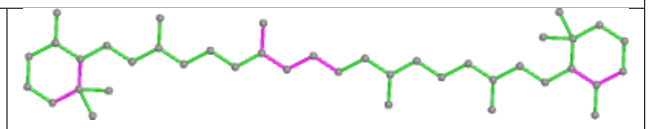
Torsions



Rings

Ligand BCR H 102

Bond lengths

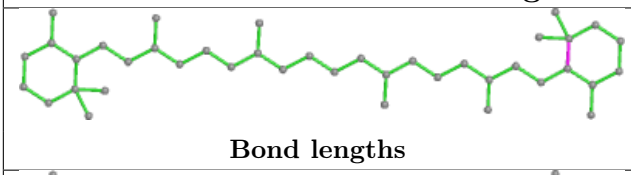


Bond angles

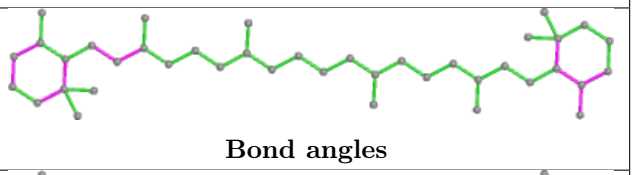
Torsions

Rings

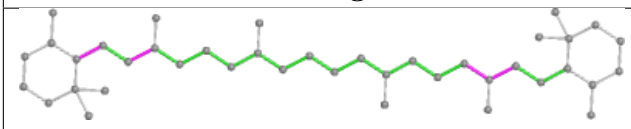
Ligand BCR T 101



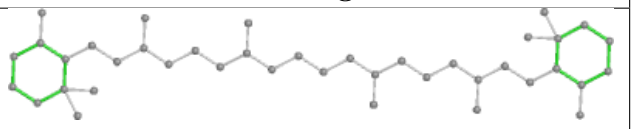
Bond lengths



Bond angles

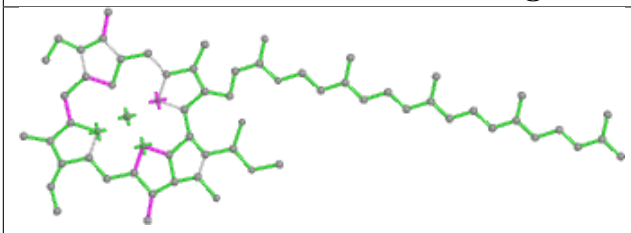


Torsions

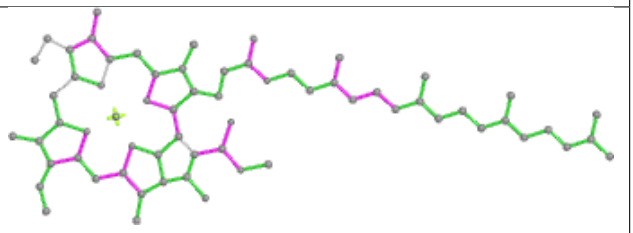


Rings

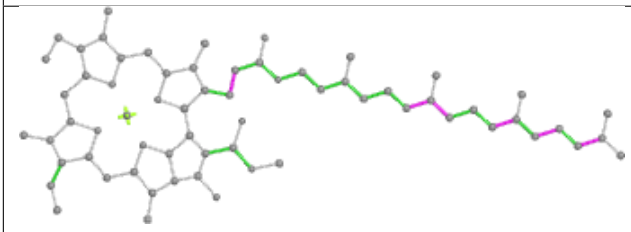
Ligand CLA B 602



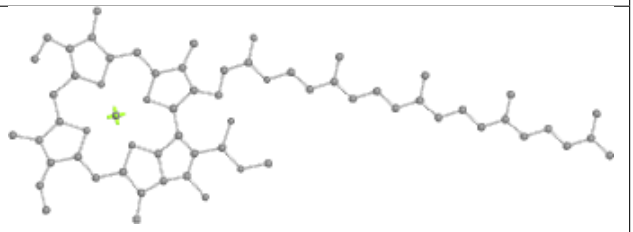
Bond lengths



Bond angles

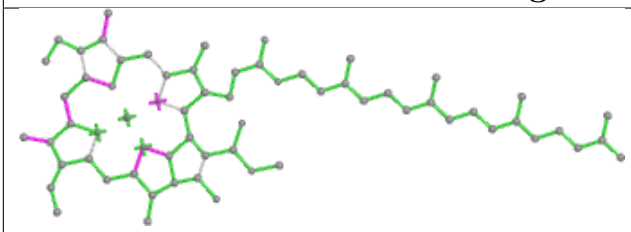


Torsions

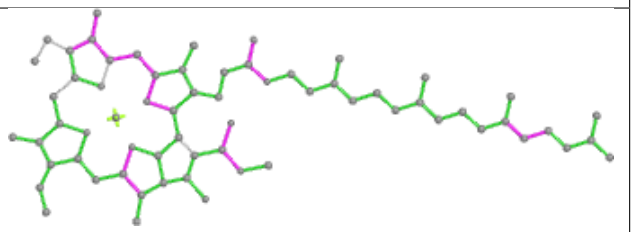


Rings

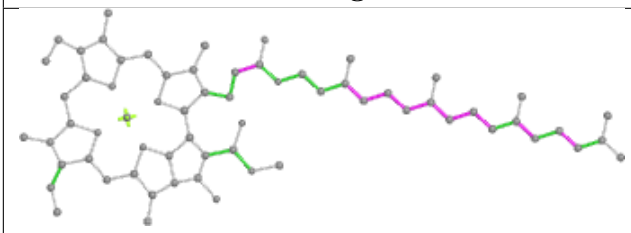
Ligand CLA c 510



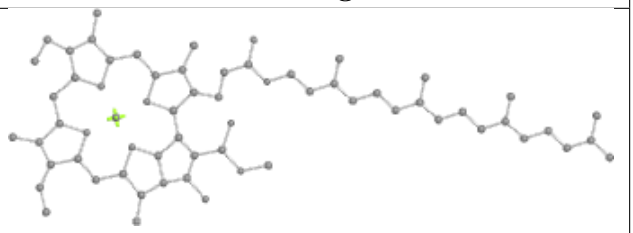
Bond lengths



Bond angles

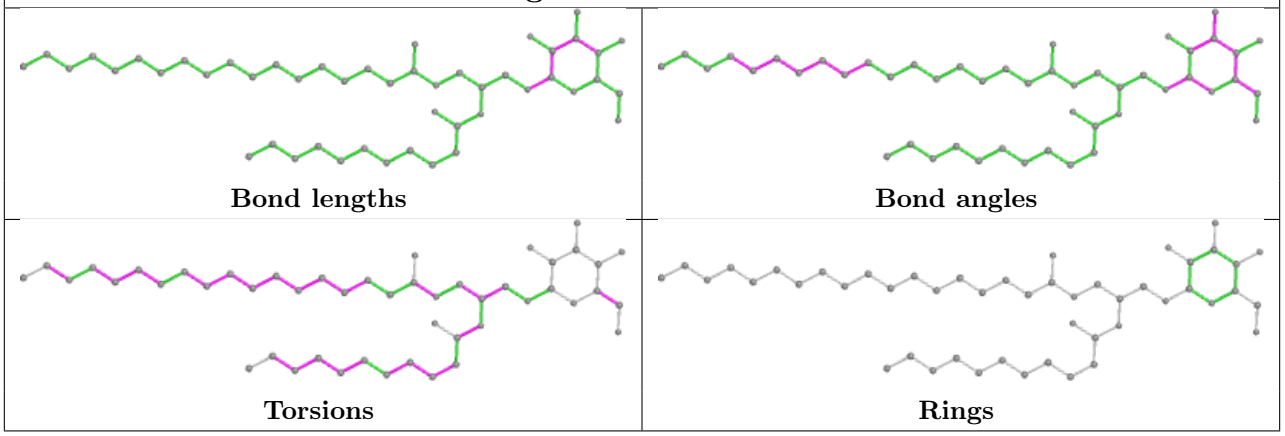


Torsions

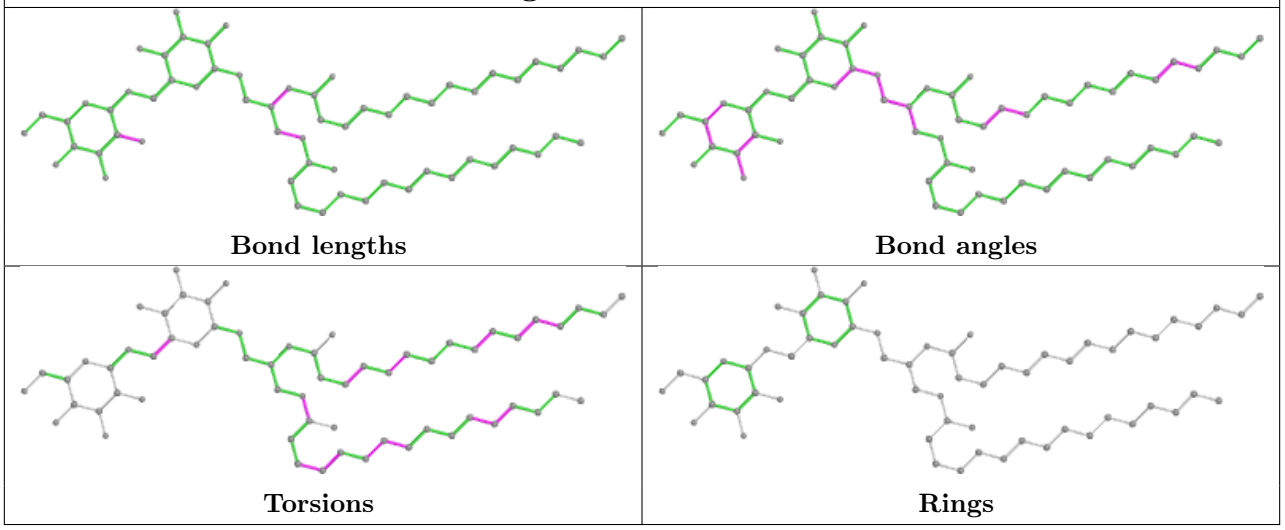


Rings

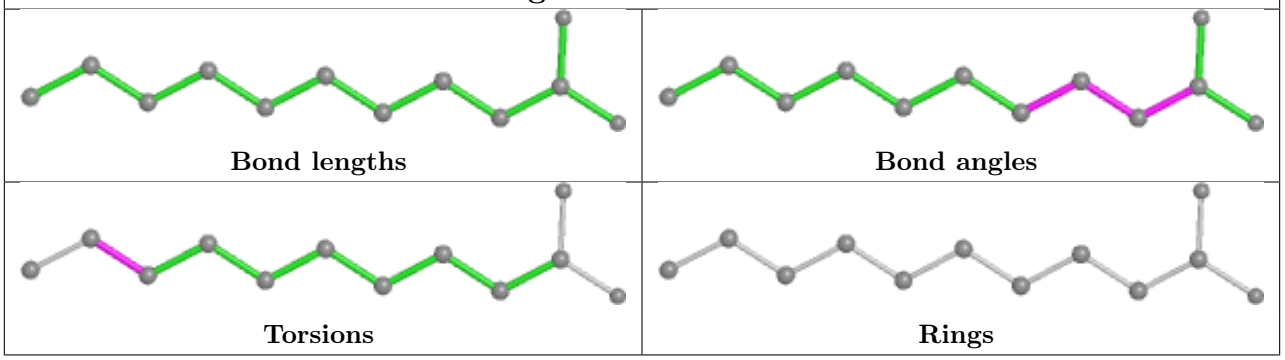
Ligand LMG c 522



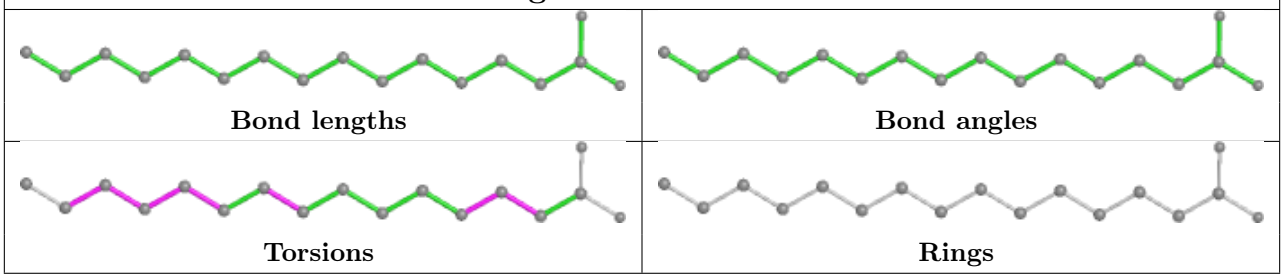
Ligand DGD C 518



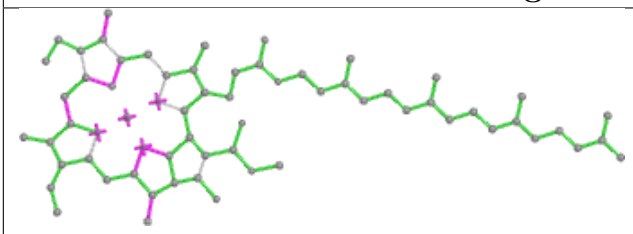
Ligand STE C 520

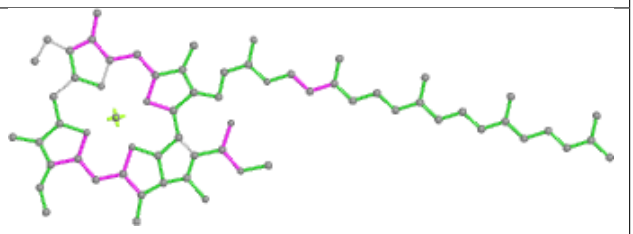


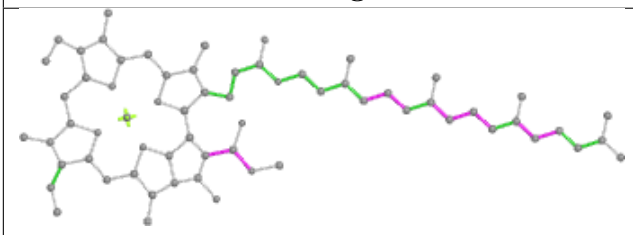
Ligand STE B 619

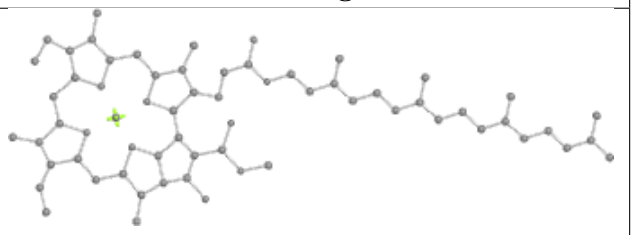


Ligand CLA C 509


Bond lengths

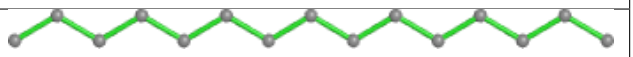

Bond angles


Torsions


Rings

Ligand STE T 103

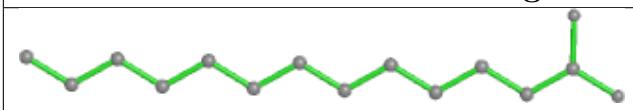

Bond lengths

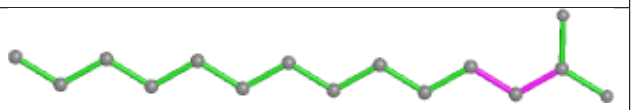

Bond angles

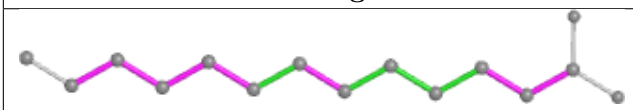

Torsions

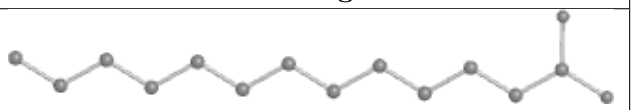

Rings

Ligand STE M 102

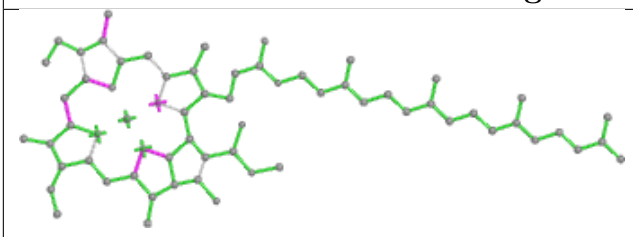

Bond lengths

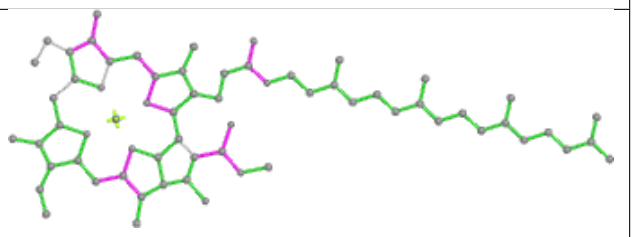

Bond angles

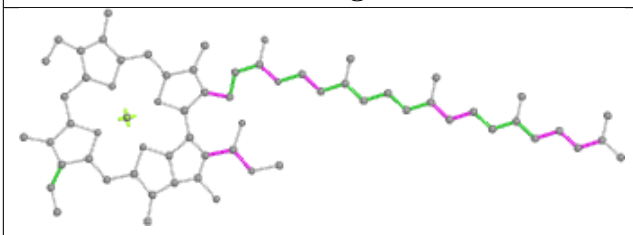

Torsions

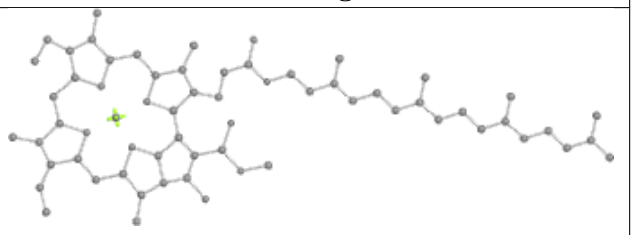

Rings

Ligand CLA C 513

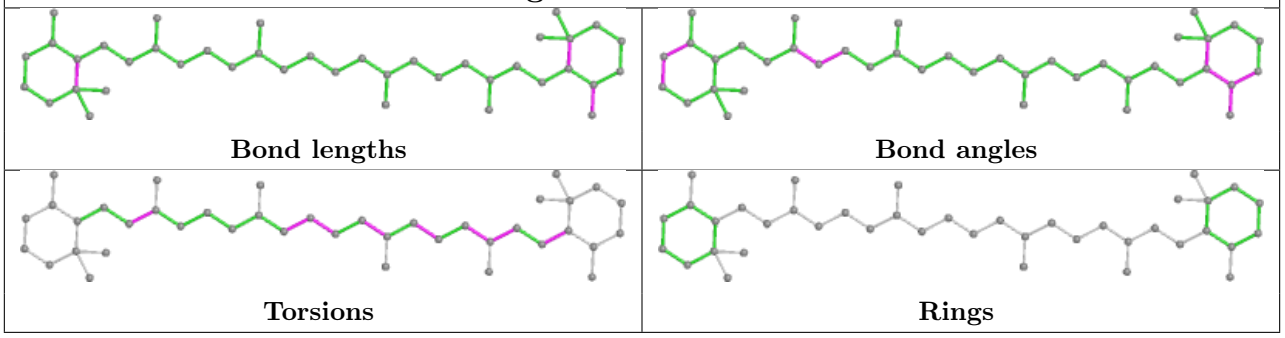

Bond lengths


Bond angles

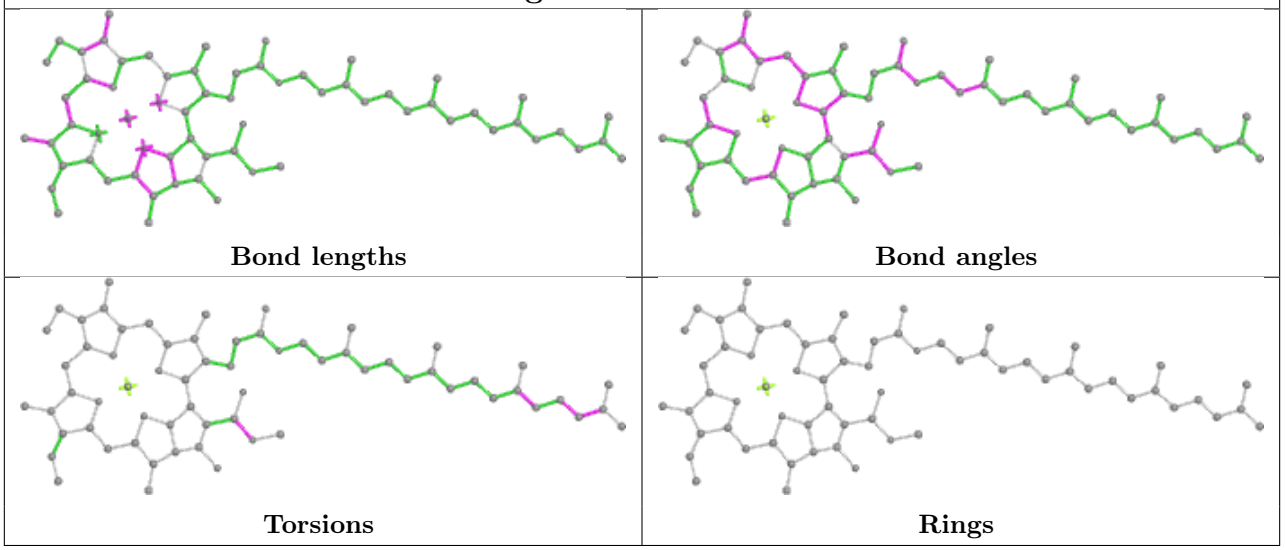

Torsions


Rings

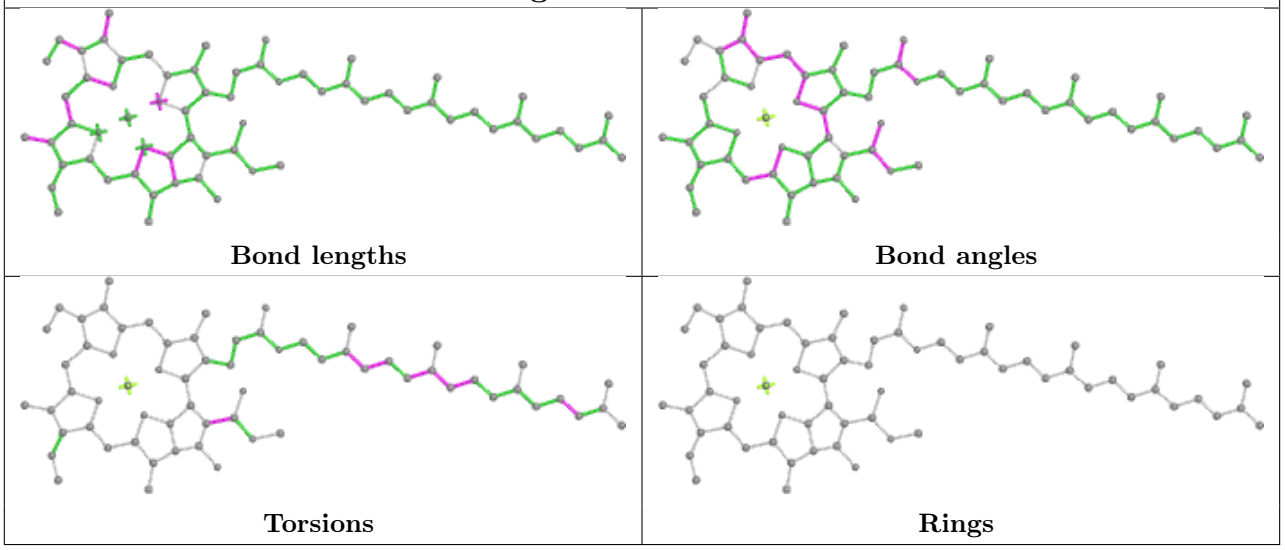
Ligand BCR d 404



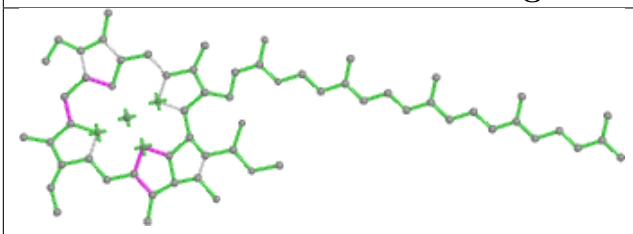
Ligand CLA B 609



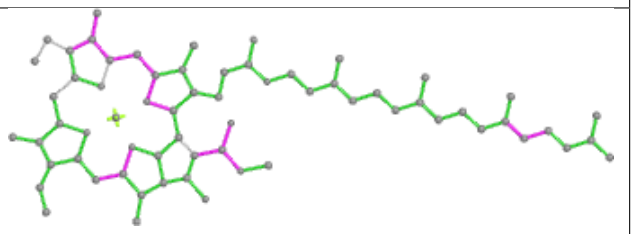
Ligand CLA c 507



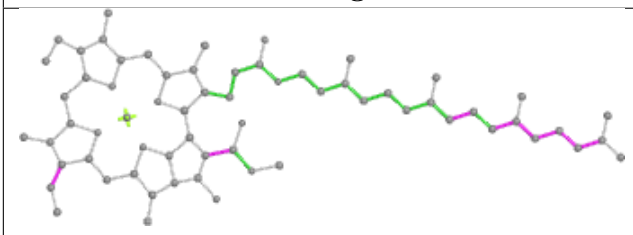
Ligand CLA A 613



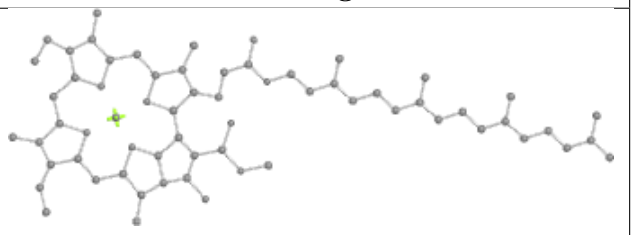
Bond lengths



Bond angles

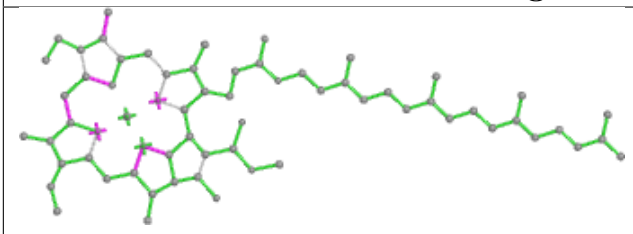


Torsions

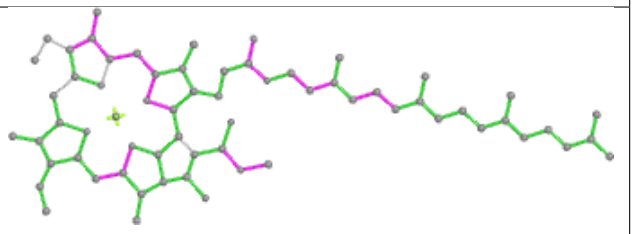


Rings

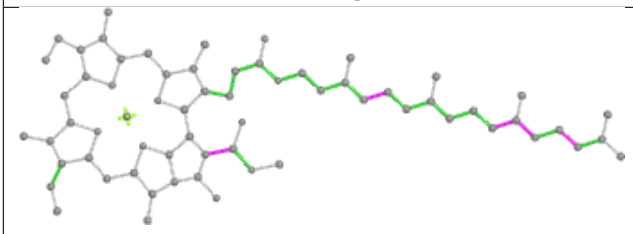
Ligand CLA b 608



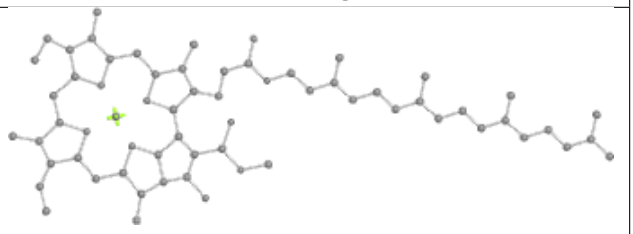
Bond lengths



Bond angles

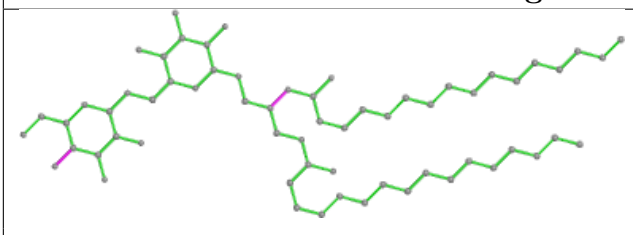


Torsions

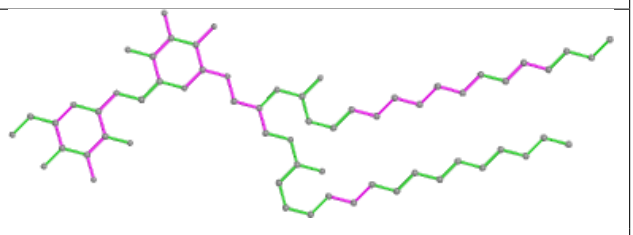


Rings

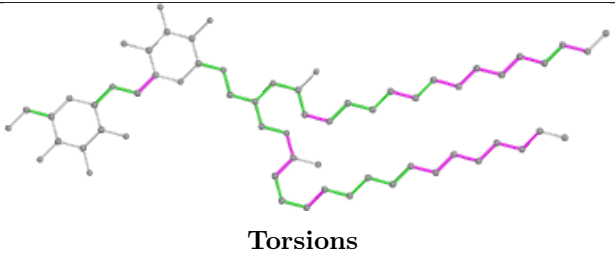
Ligand DGD c 519



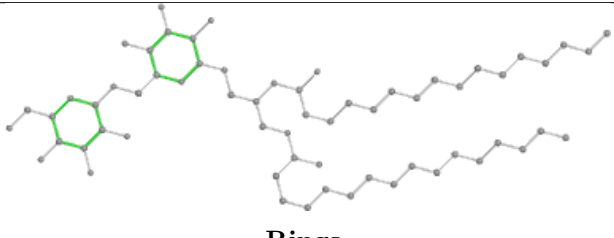
Bond lengths



Bond angles

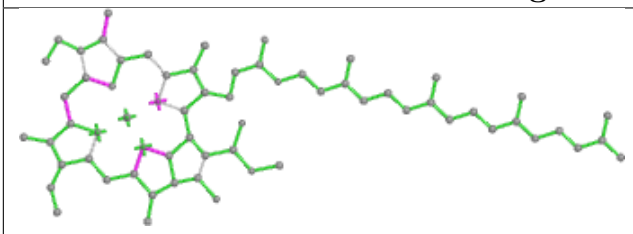


Torsions

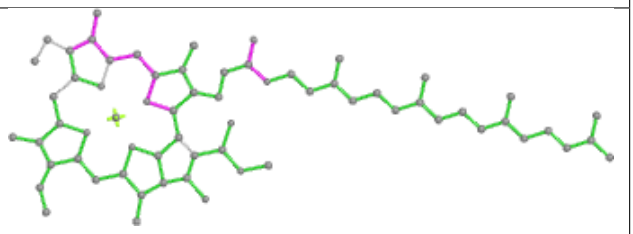


Rings

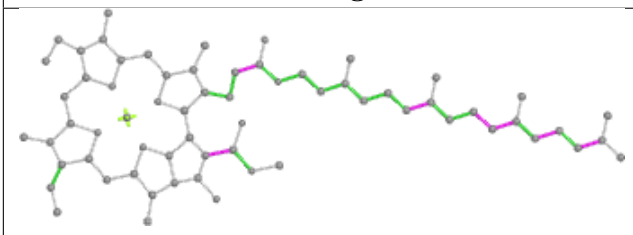
Ligand CLA c 509



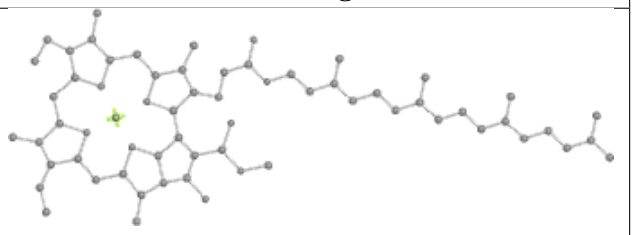
Bond lengths



Bond angles

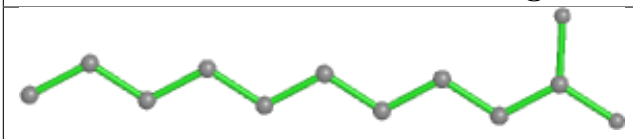


Torsions

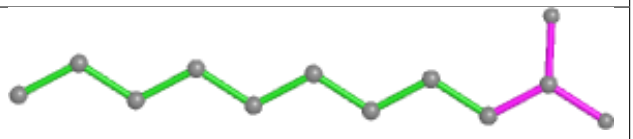


Rings

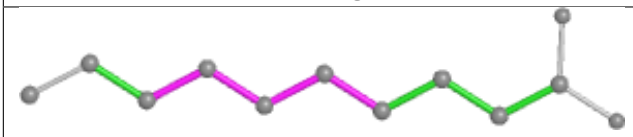
Ligand STE m 102



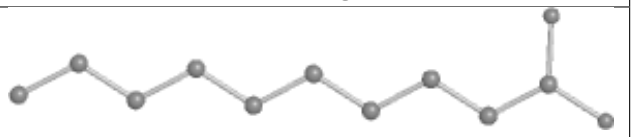
Bond lengths



Bond angles

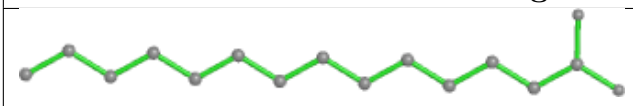


Torsions



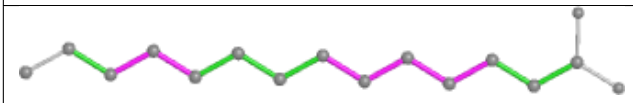
Rings

Ligand STE b 621

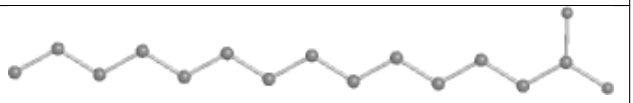


Bond lengths

Bond angles

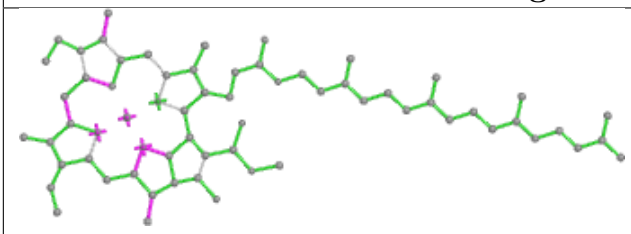


Torsions

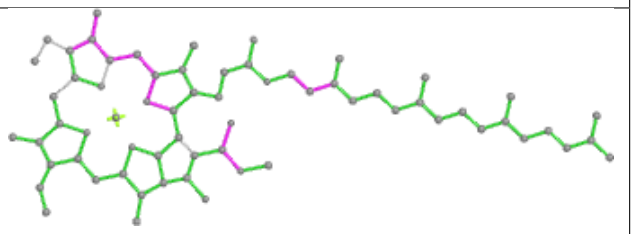


Rings

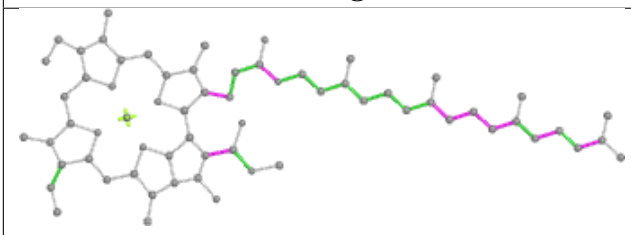
Ligand CLA c 506



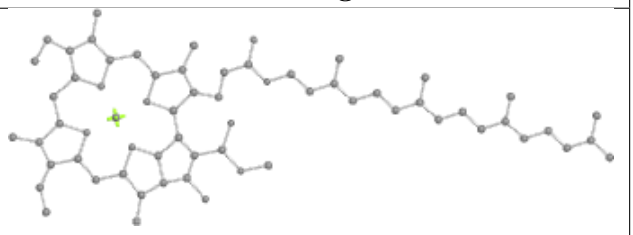
Bond lengths



Bond angles

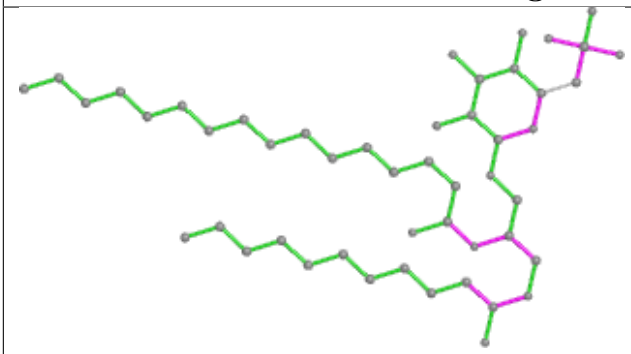


Torsions

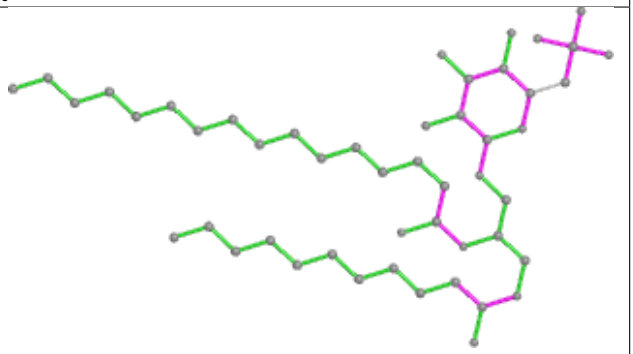


Rings

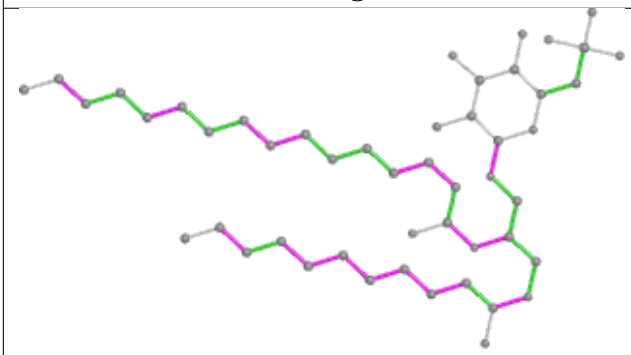
Ligand SQD L 101



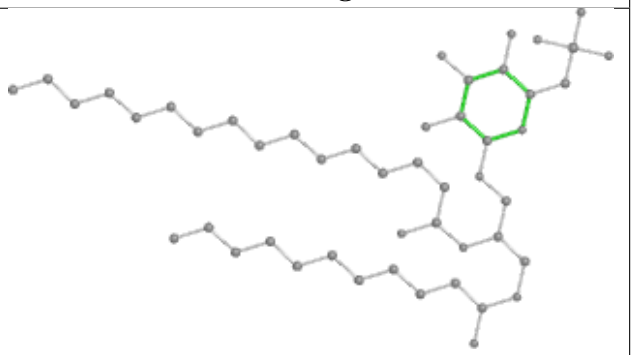
Bond lengths



Bond angles

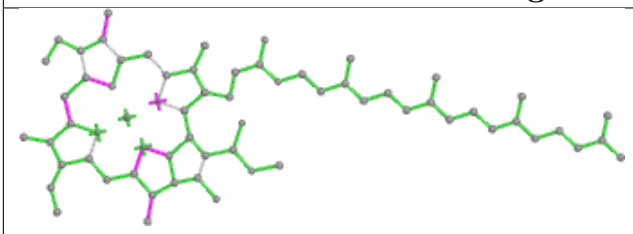


Torsions

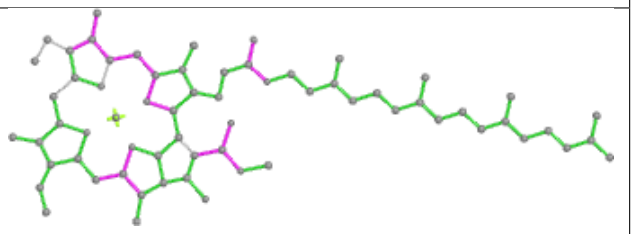


Rings

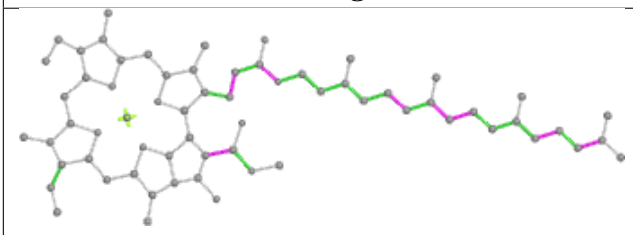
Ligand CLA b 602



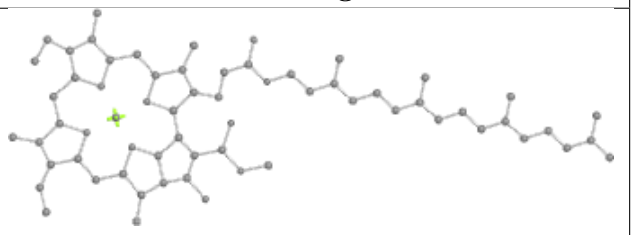
Bond lengths



Bond angles

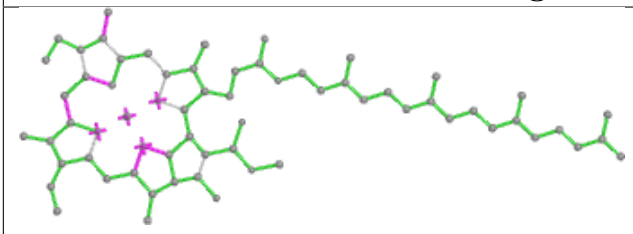


Torsions

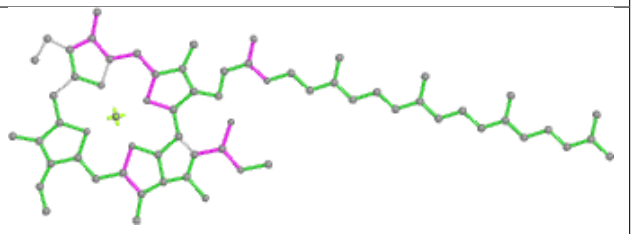


Rings

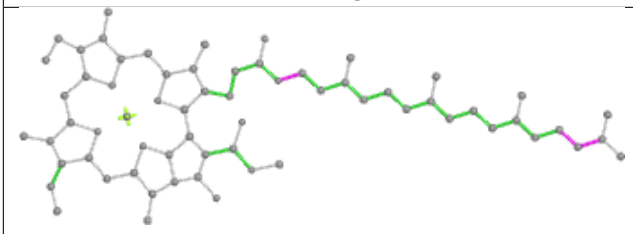
Ligand CLA a 607



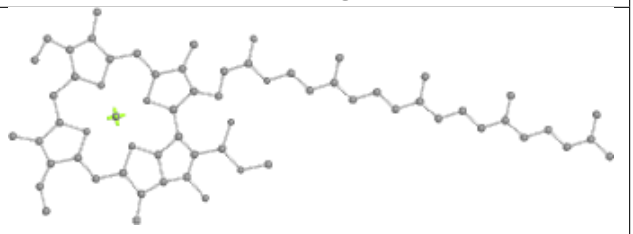
Bond lengths



Bond angles

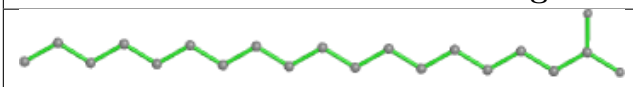


Torsions

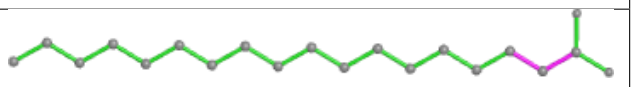


Rings

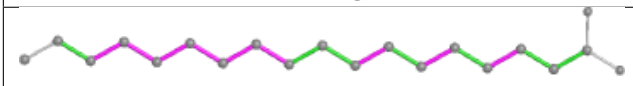
Ligand STE b 622



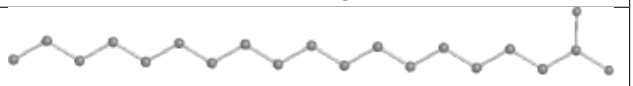
Bond lengths



Bond angles

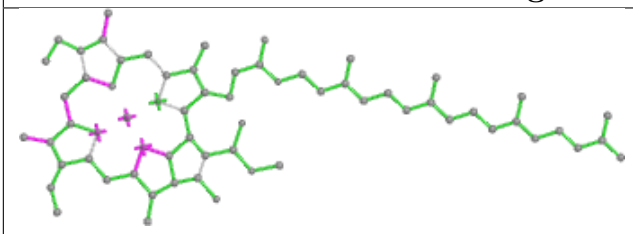


Torsions

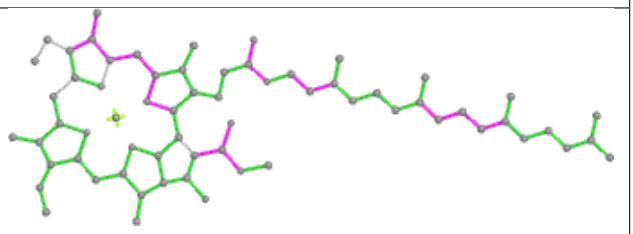


Rings

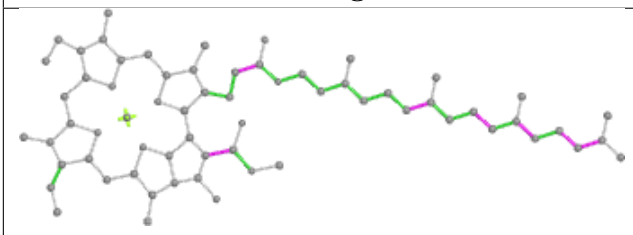
Ligand CLA b 611



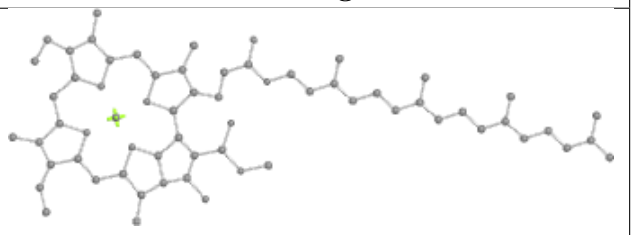
Bond lengths



Bond angles

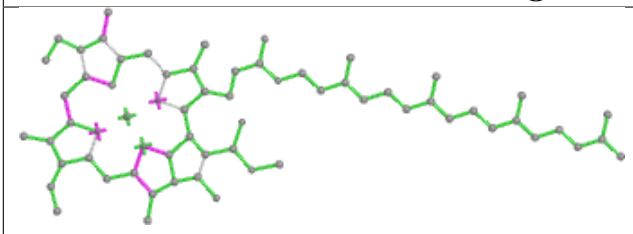


Torsions

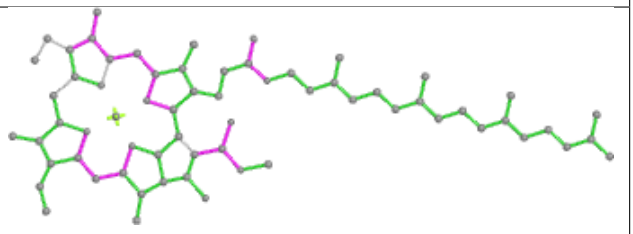


Rings

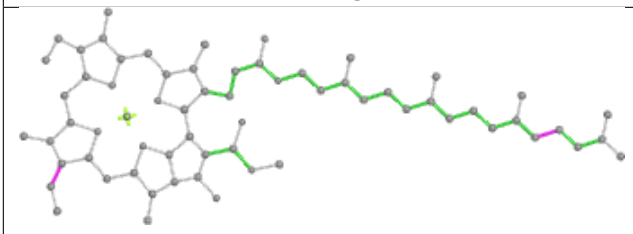
Ligand CLA b 607



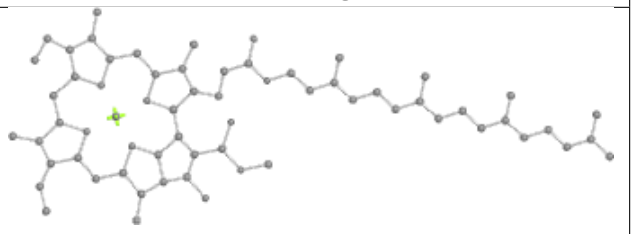
Bond lengths



Bond angles

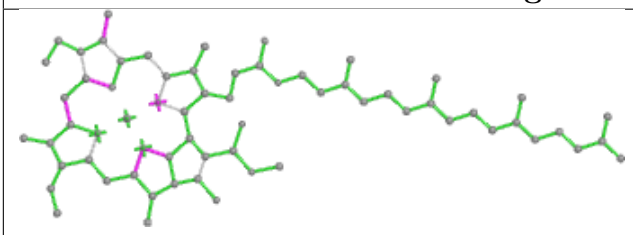


Torsions

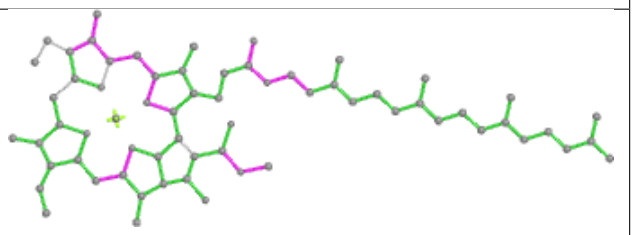


Rings

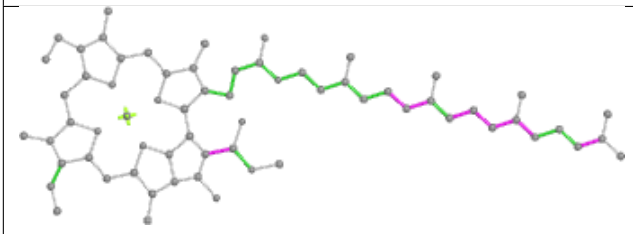
Ligand CLA B 606



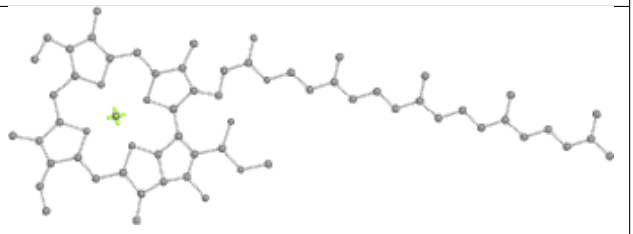
Bond lengths



Bond angles

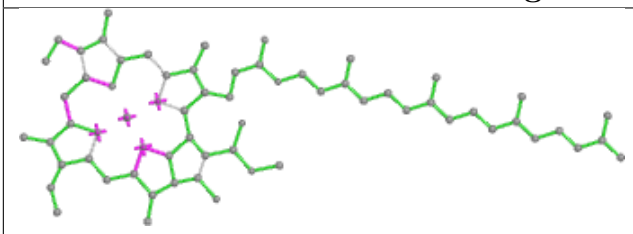


Torsions

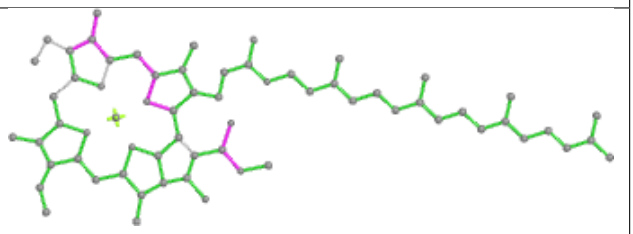


Rings

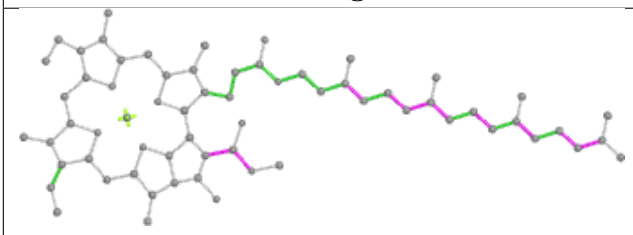
Ligand CLA C 505



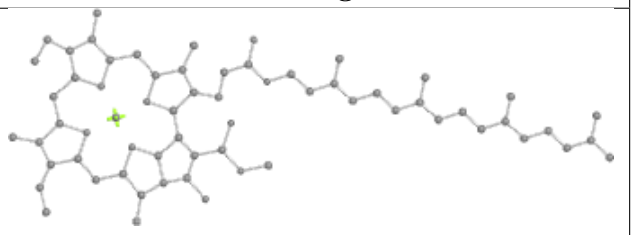
Bond lengths



Bond angles

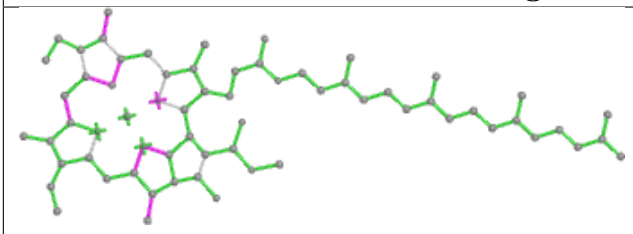


Torsions

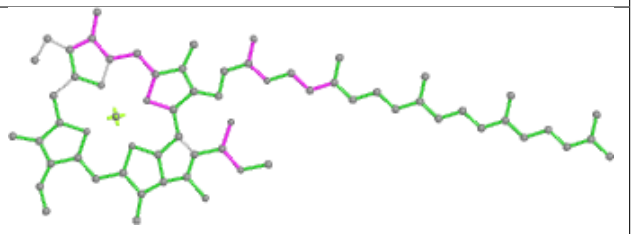


Rings

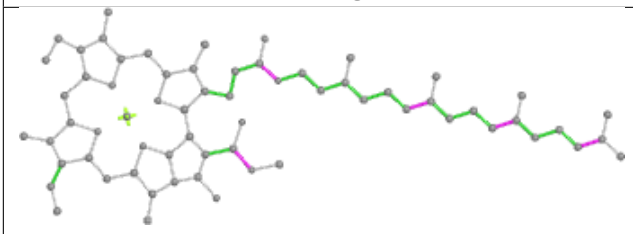
Ligand CLA C 511



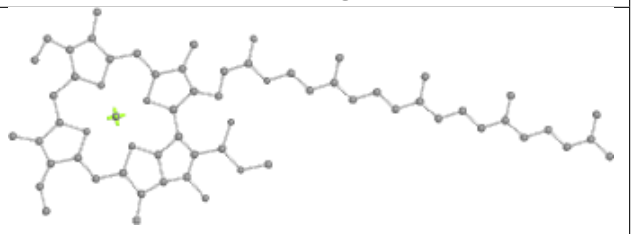
Bond lengths



Bond angles

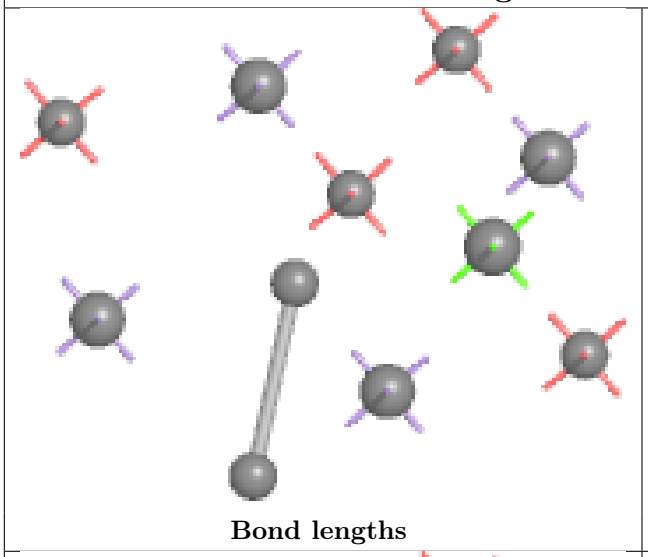


Torsions

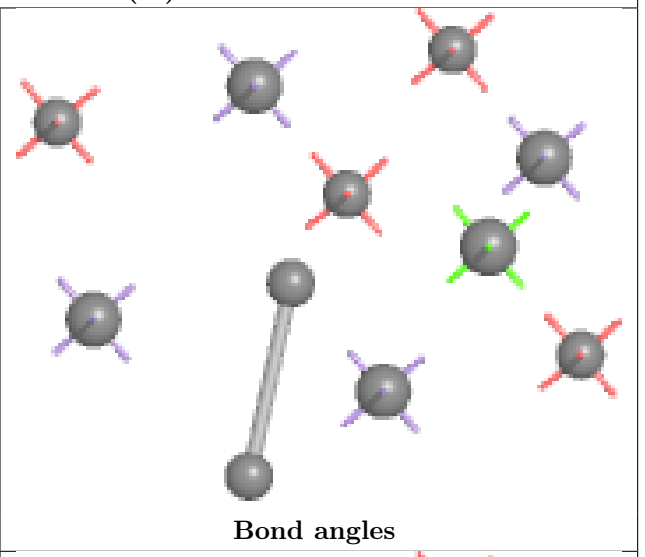


Rings

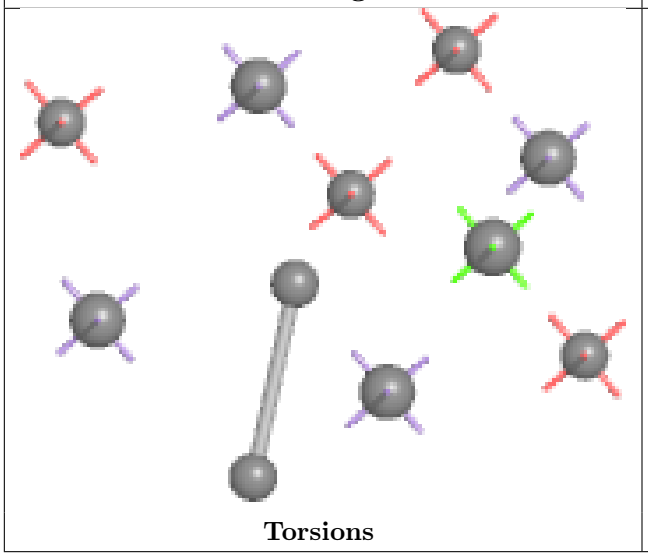
Ligand OEY a 601 (C)



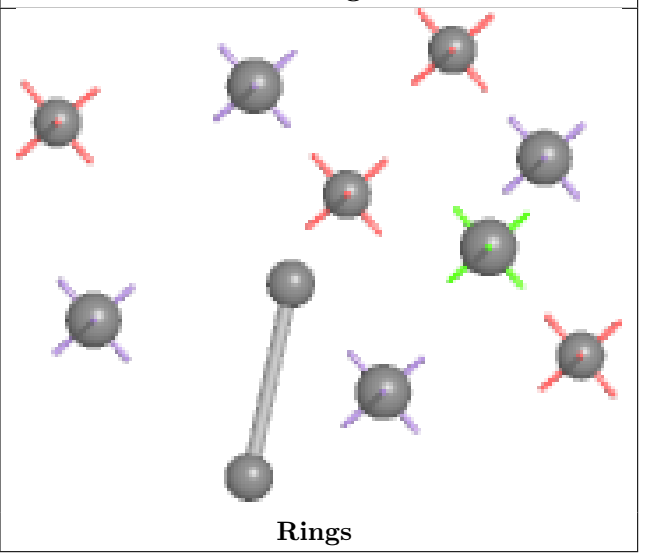
Bond lengths



Bond angles

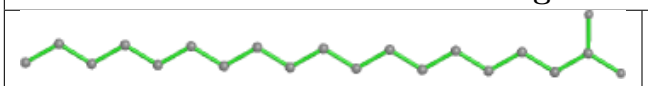


Torsions

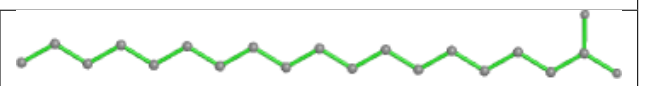


Rings

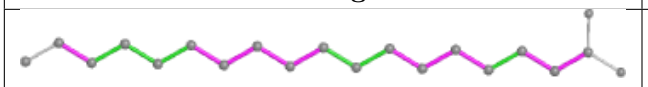
Ligand STE c 521



Bond lengths



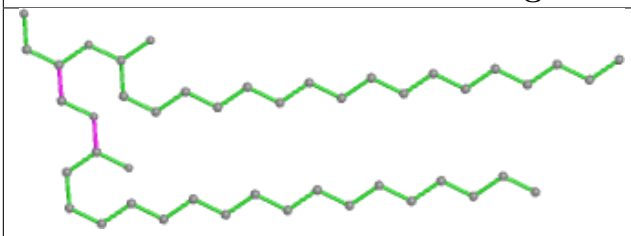
Bond angles



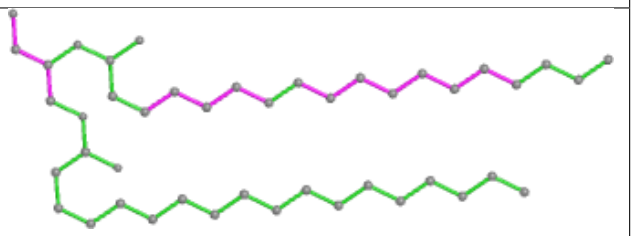
Torsions

Rings

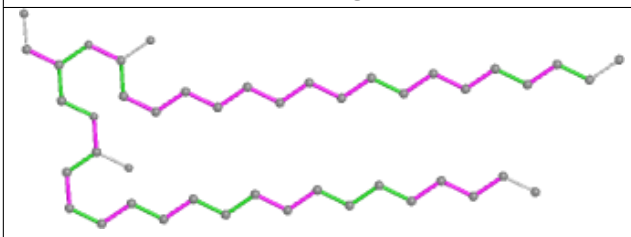
Ligand DGD a 616



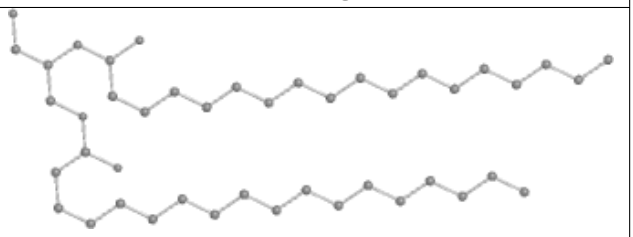
Bond lengths



Bond angles

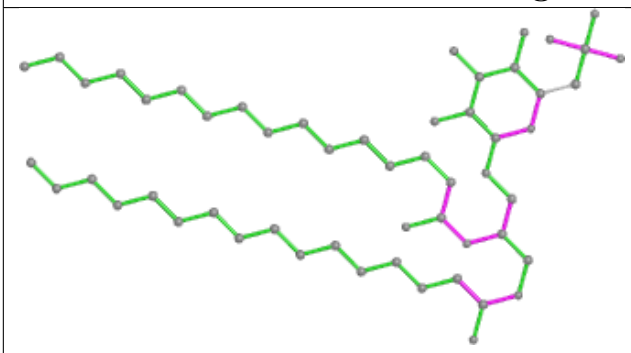


Torsions

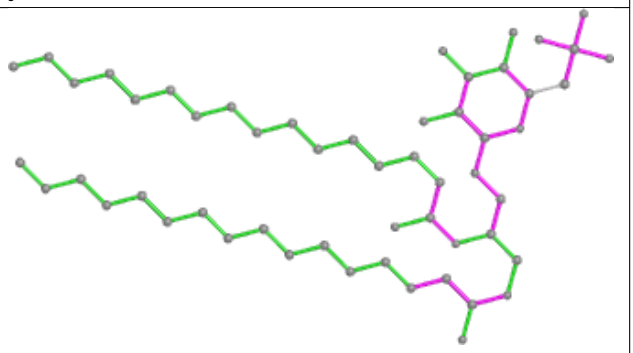


Rings

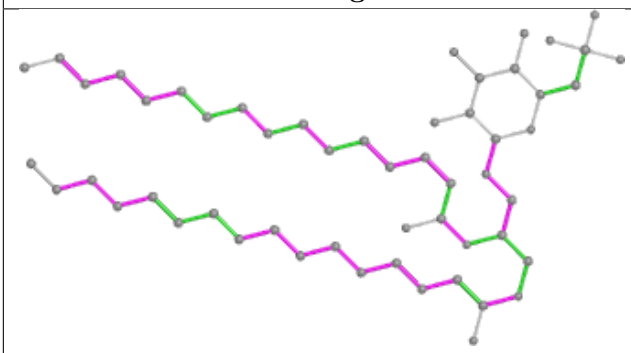
Ligand SQD l 101



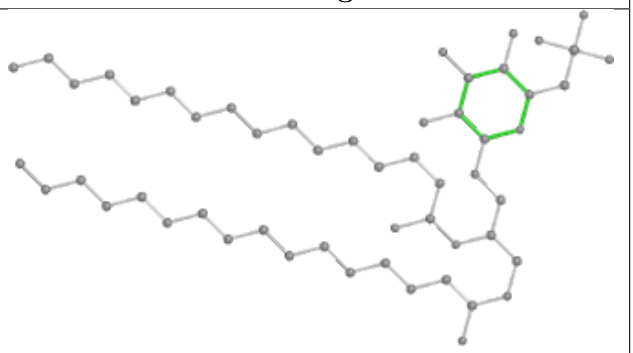
Bond lengths



Bond angles

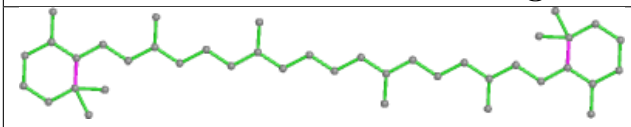


Torsions

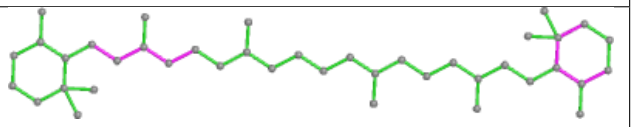


Rings

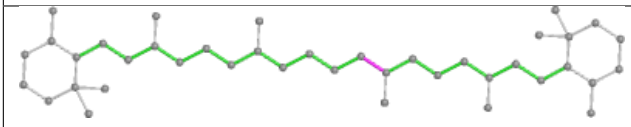
Ligand BCR a 611



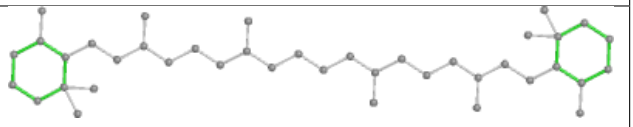
Bond lengths



Bond angles

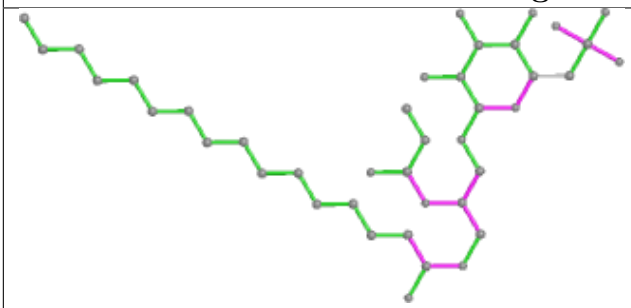


Torsions

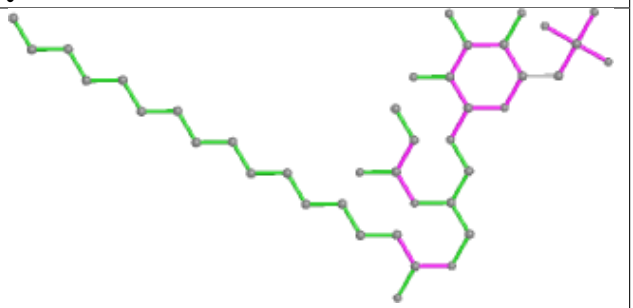


Rings

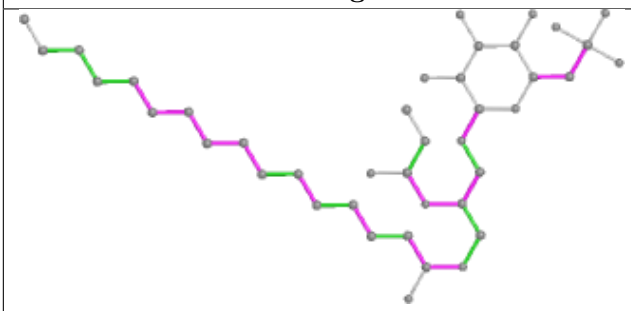
Ligand SQD f 101



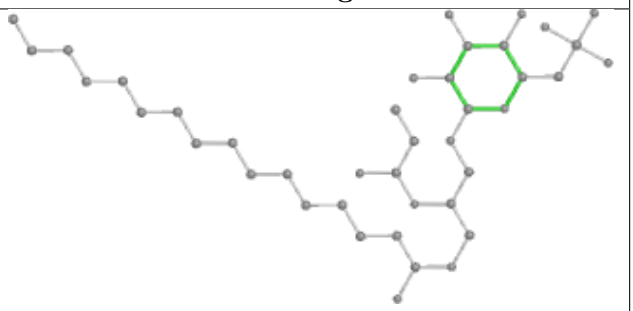
Bond lengths



Bond angles

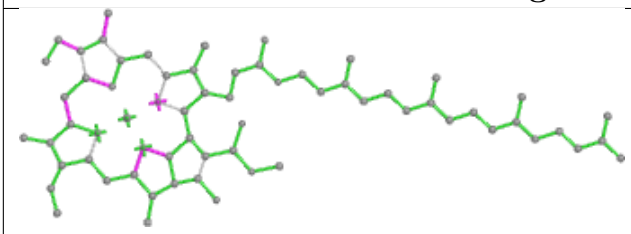


Torsions

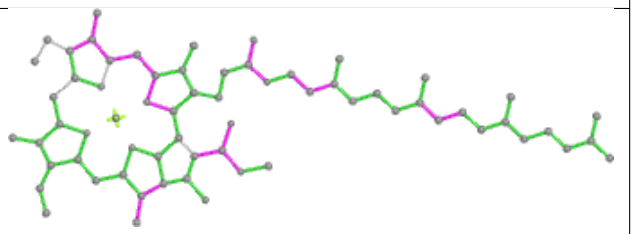


Rings

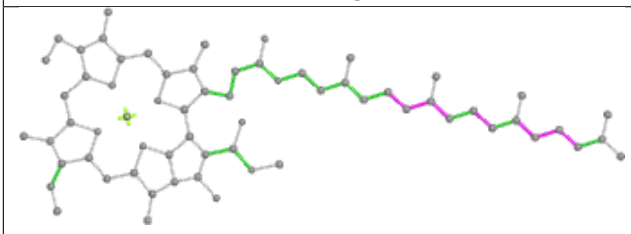
Ligand CLA c 505



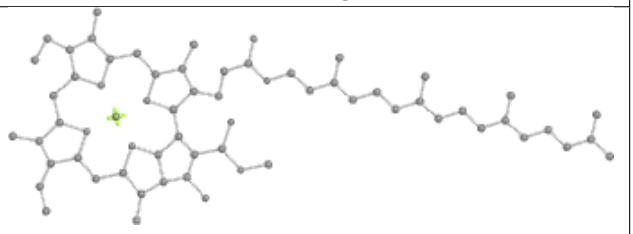
Bond lengths



Bond angles

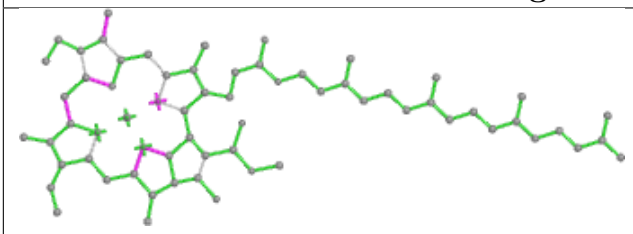


Torsions

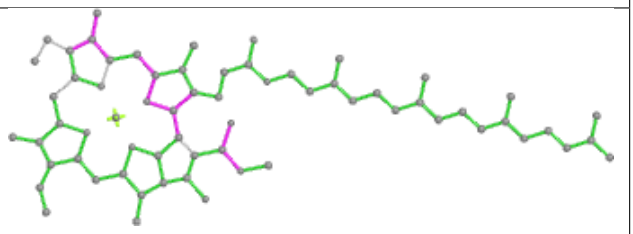


Rings

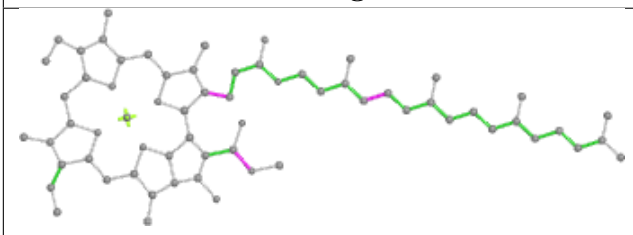
Ligand CLA c 511



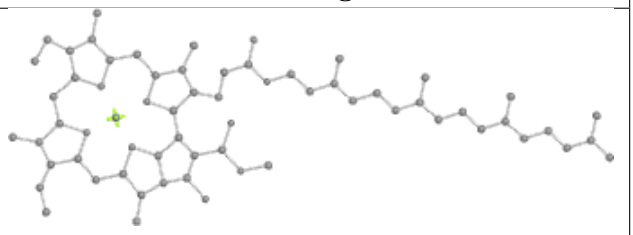
Bond lengths



Bond angles

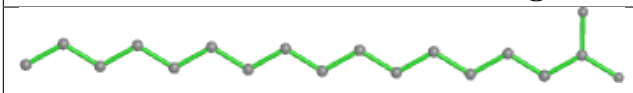


Torsions

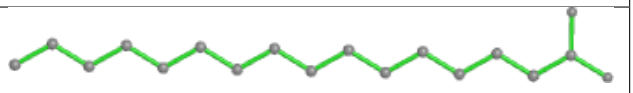


Rings

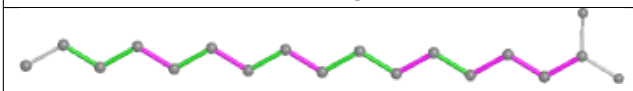
Ligand STE B 624



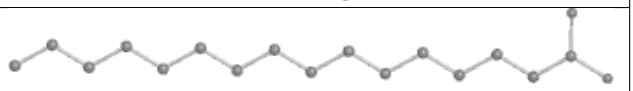
Bond lengths



Bond angles

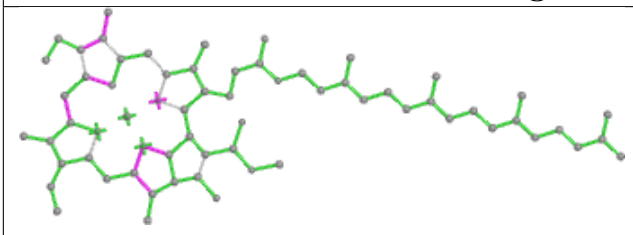


Torsions

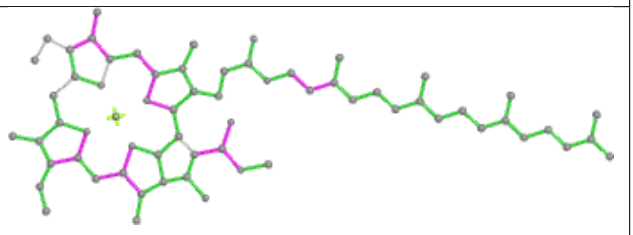


Rings

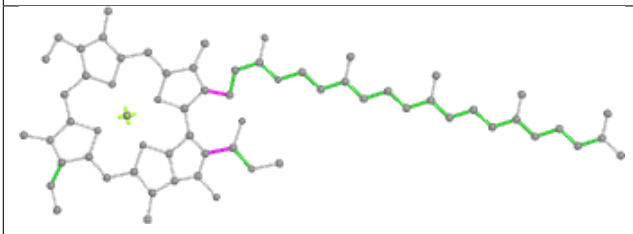
Ligand CLA a 613



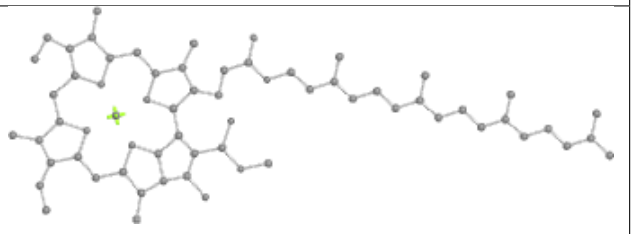
Bond lengths



Bond angles

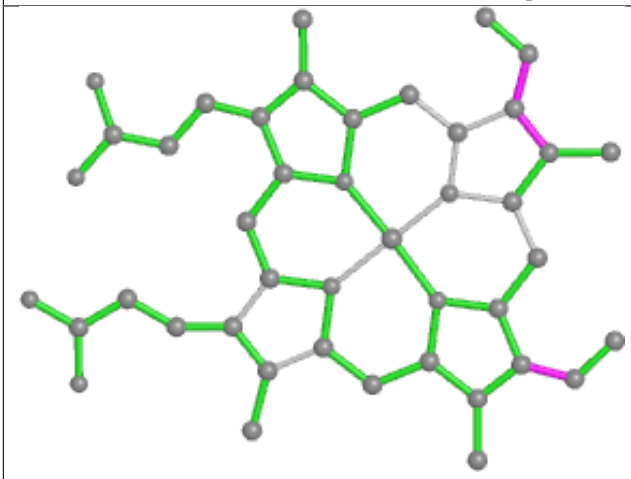


Torsions

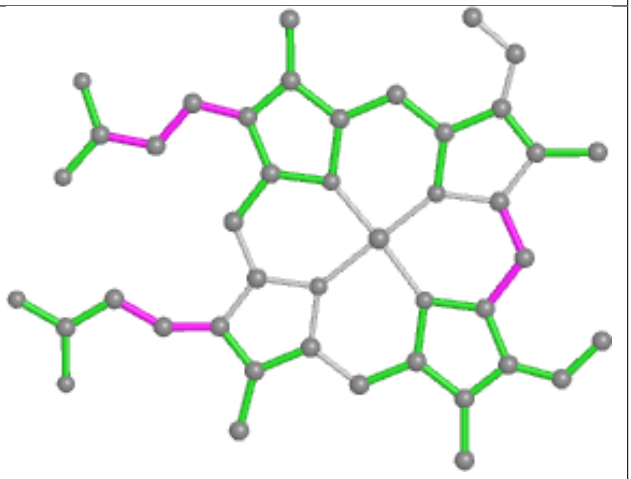


Rings

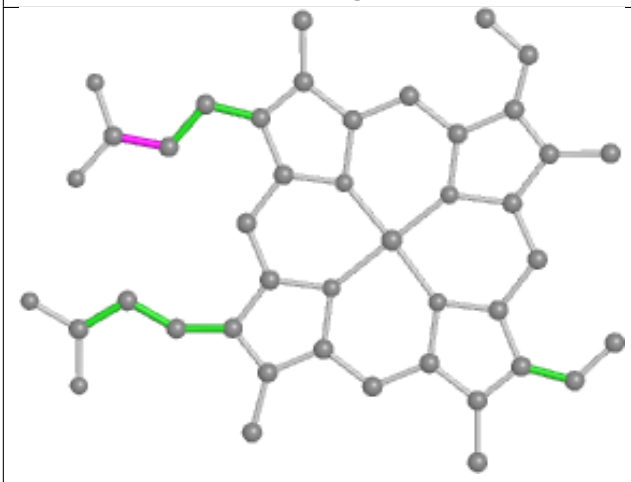
Ligand HEM F 101



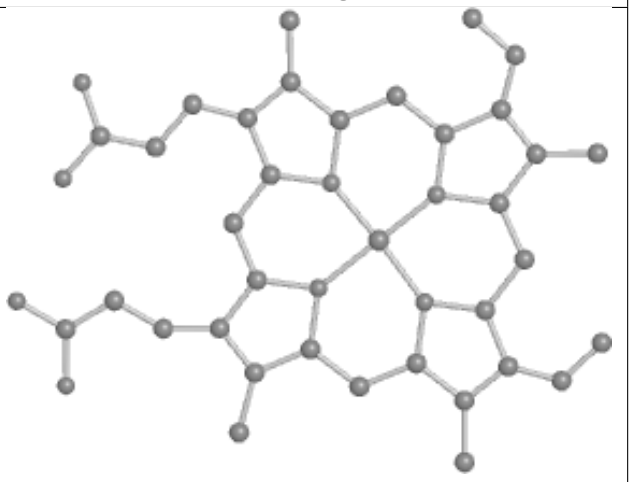
Bond lengths



Bond angles

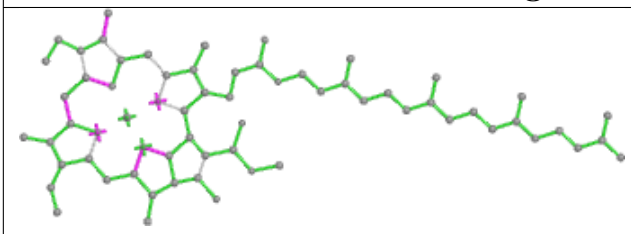


Torsions

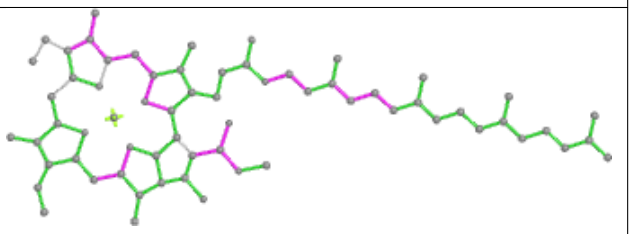


Rings

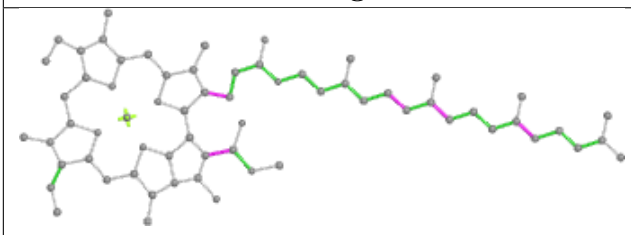
Ligand CLA C 503



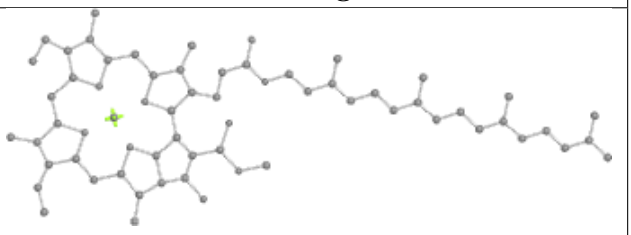
Bond lengths



Bond angles

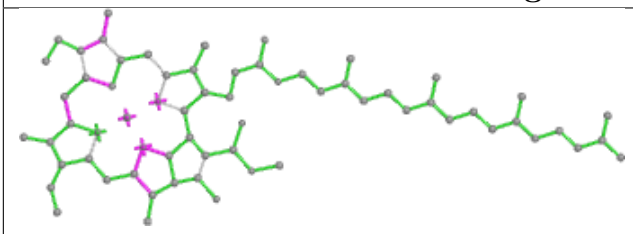


Torsions

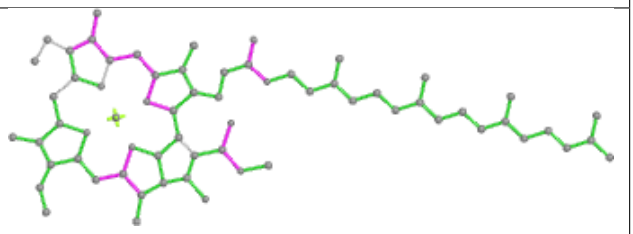


Rings

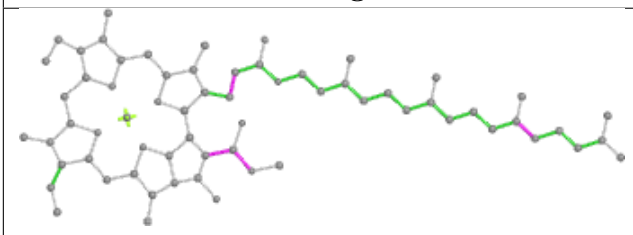
Ligand CLA C 501



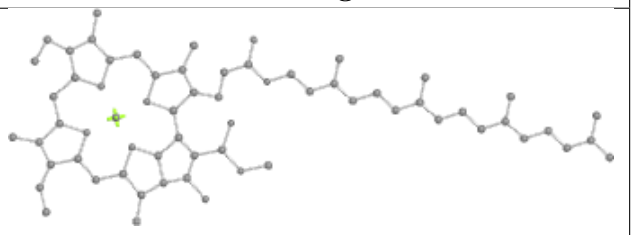
Bond lengths



Bond angles

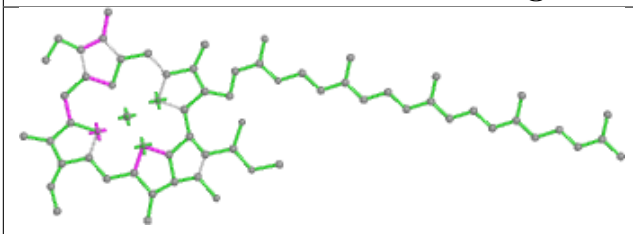


Torsions

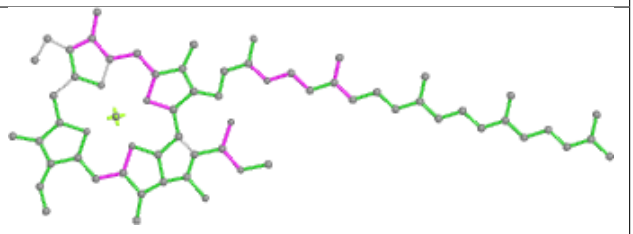


Rings

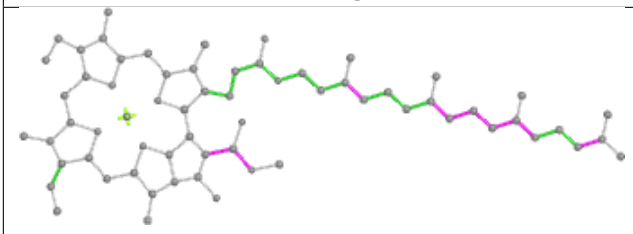
Ligand CLA b 606



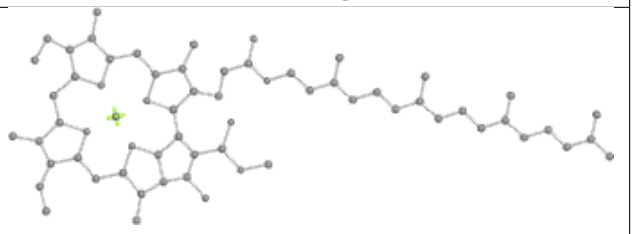
Bond lengths



Bond angles

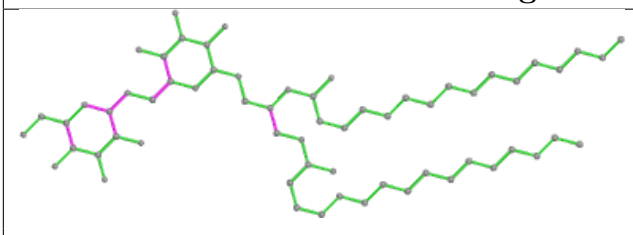


Torsions

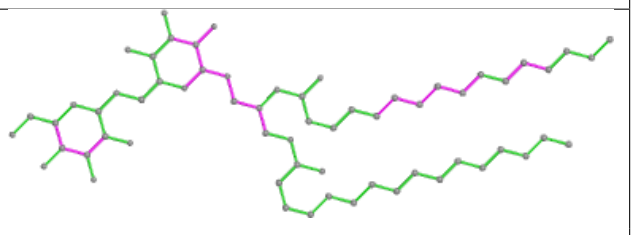


Rings

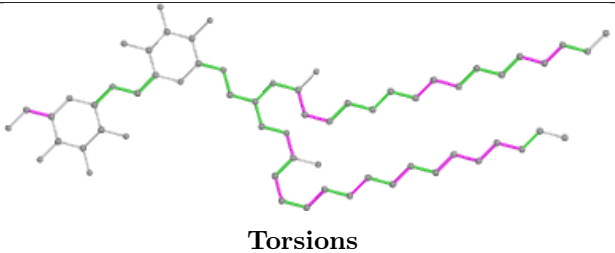
Ligand DGD H 103



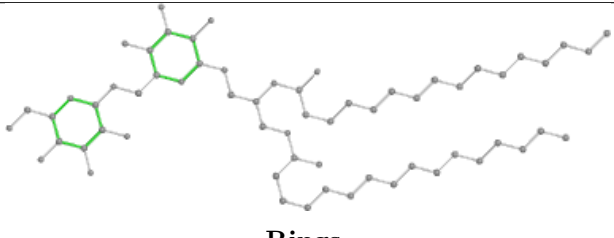
Bond lengths



Bond angles

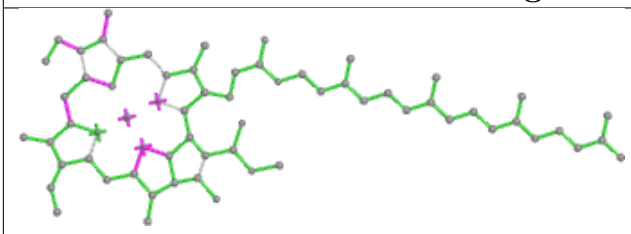


Torsions

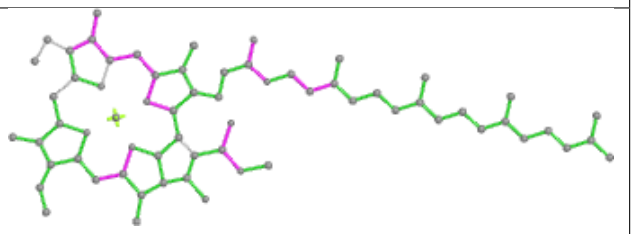


Rings

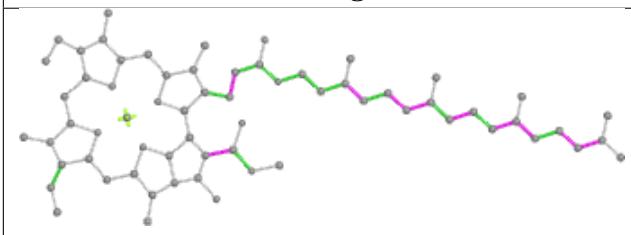
Ligand CLA B 613



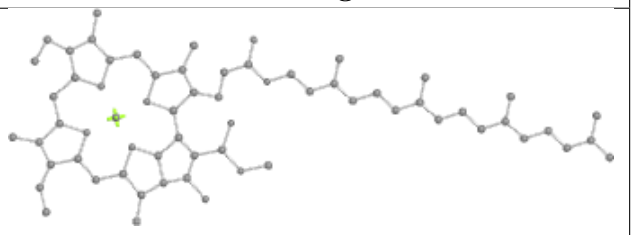
Bond lengths



Bond angles

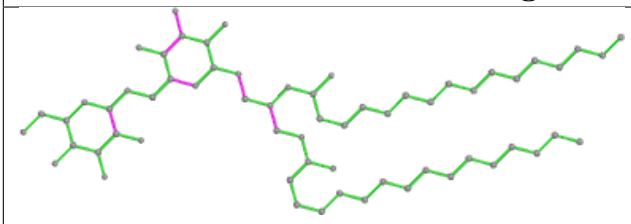


Torsions

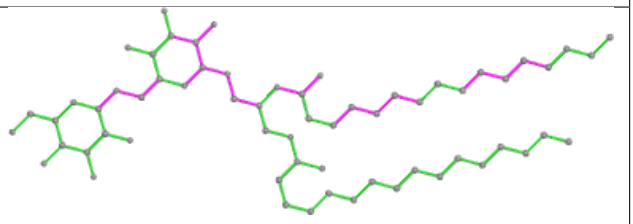


Rings

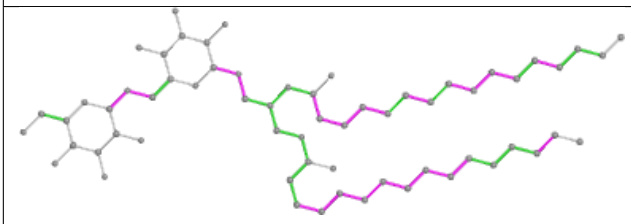
Ligand DGD C 517



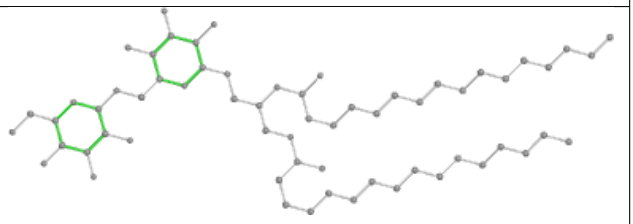
Bond lengths



Bond angles

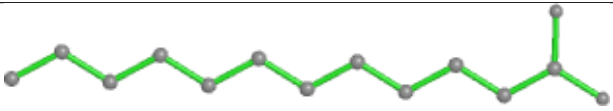


Torsions

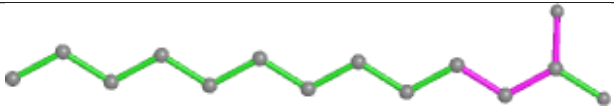


Rings

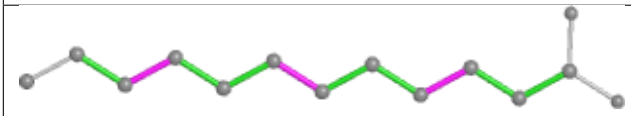
Ligand STE t 102



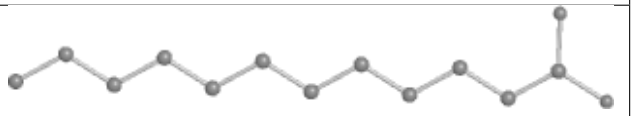
Bond lengths



Bond angles

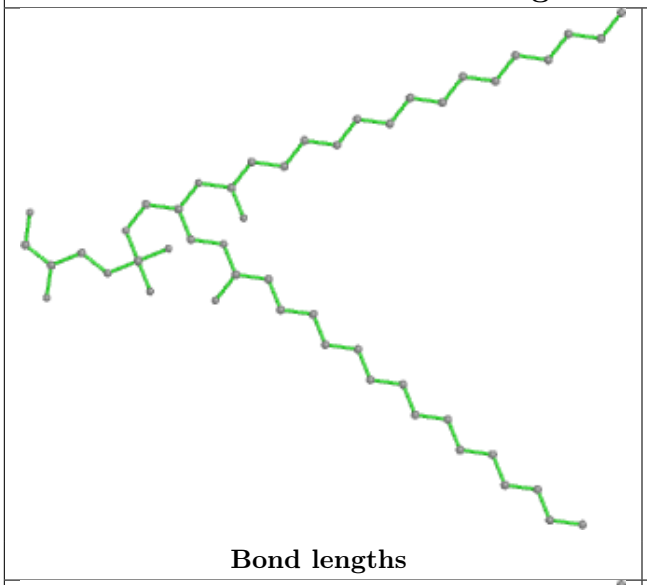


Torsions

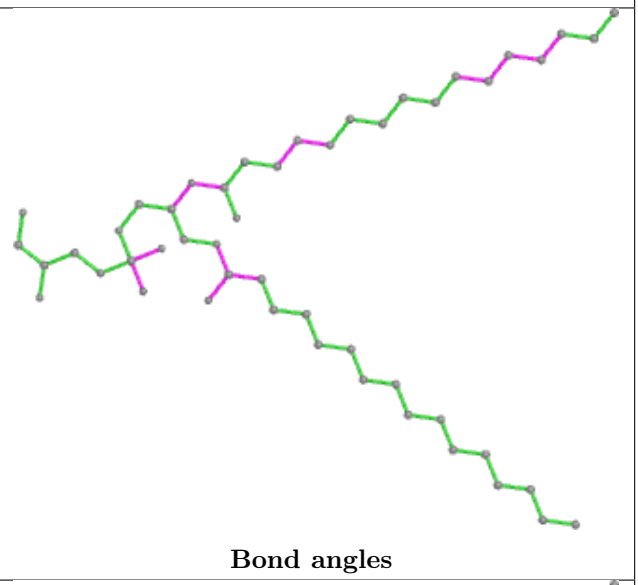


Rings

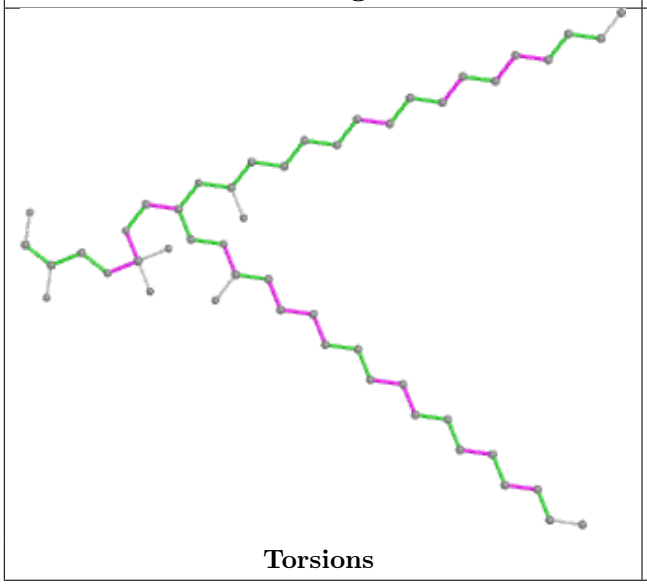
Ligand LHG l 102



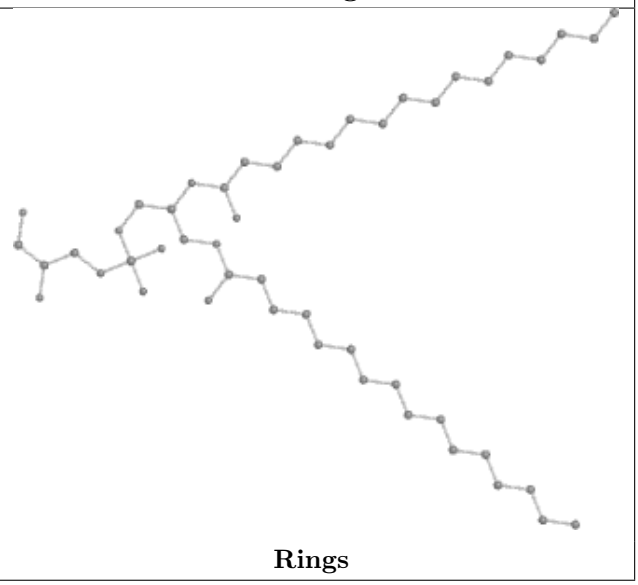
Bond lengths



Bond angles

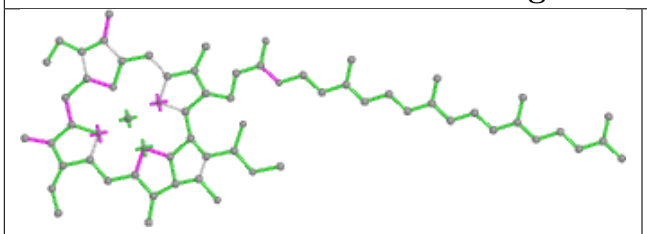


Torsions

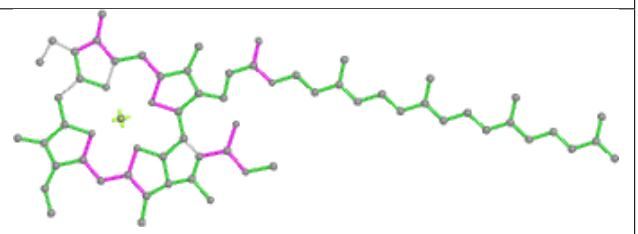


Rings

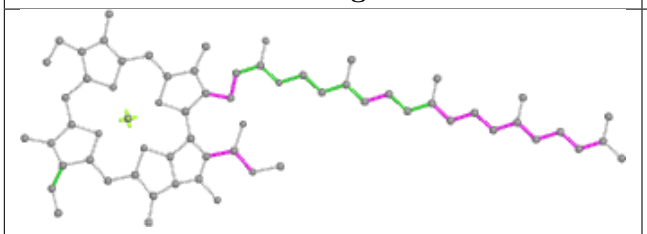
Ligand CLA h 101



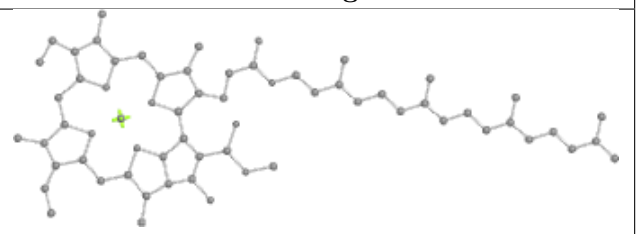
Bond lengths



Bond angles

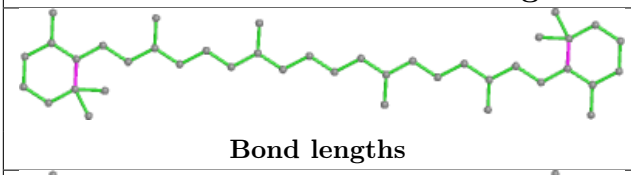


Torsions

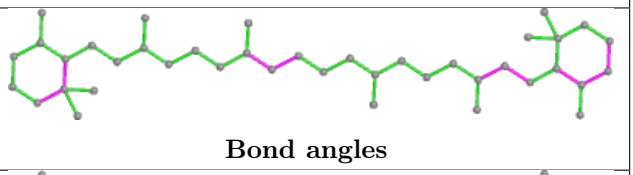


Rings

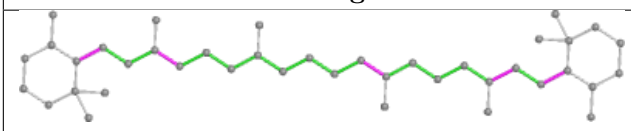
Ligand BCR K 103



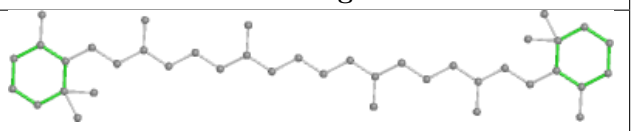
Bond lengths



Bond angles

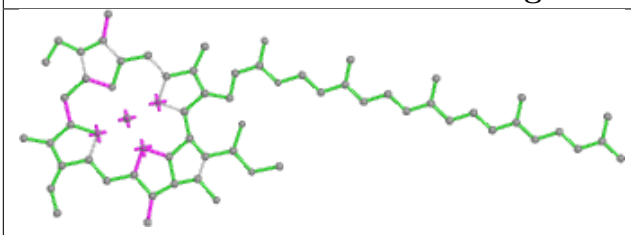


Torsions

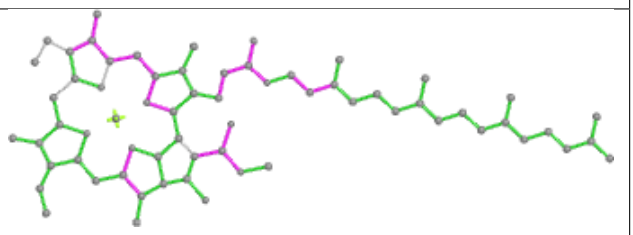


Rings

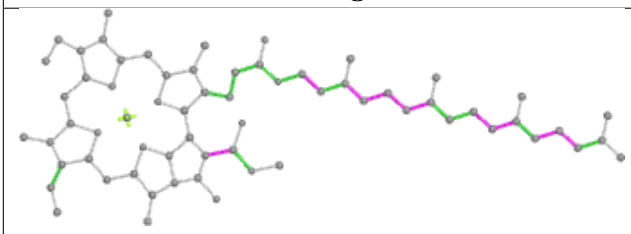
Ligand CLA C 512



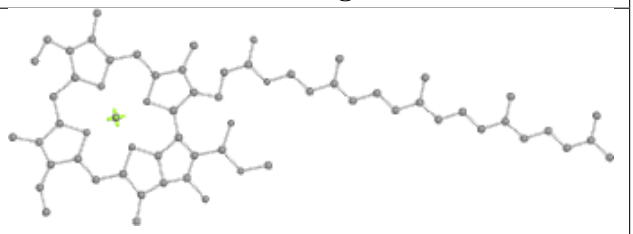
Bond lengths



Bond angles

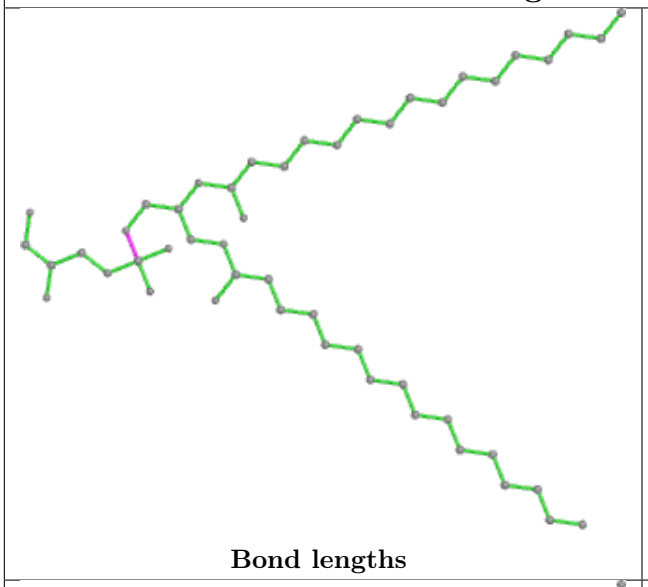


Torsions

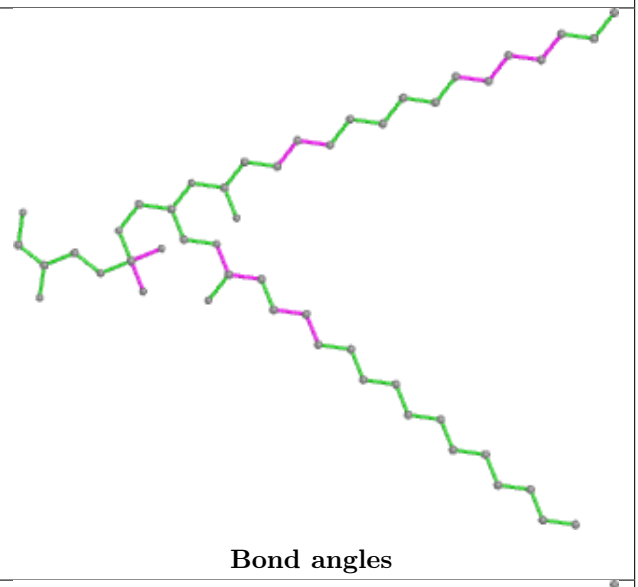


Rings

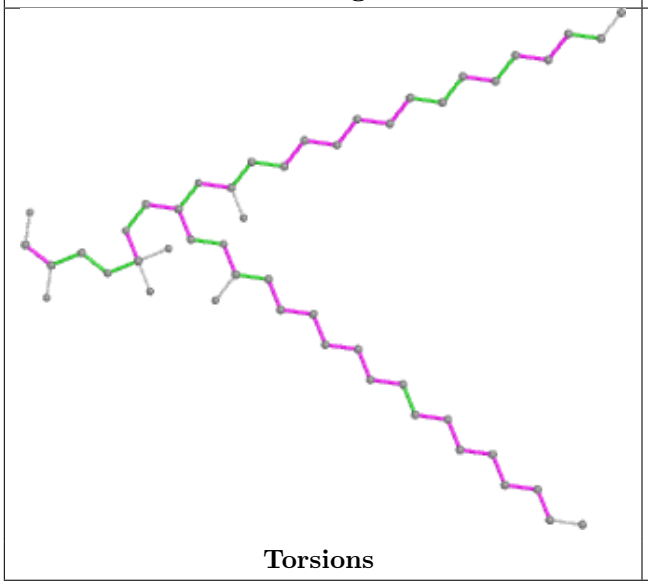
Ligand LHG E 101



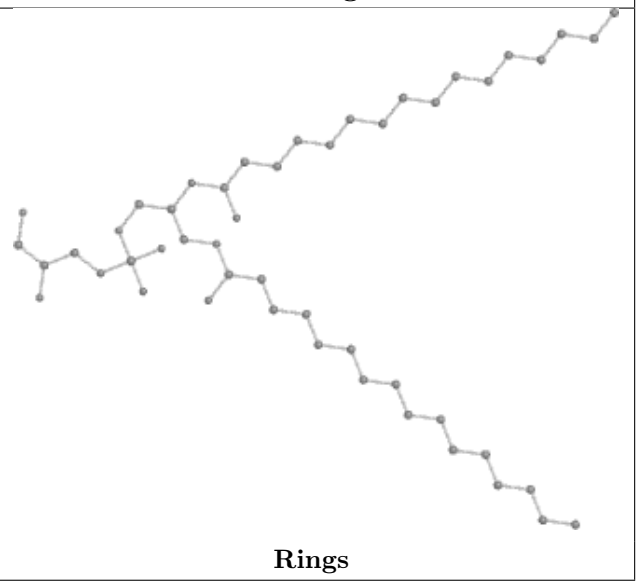
Bond lengths



Bond angles

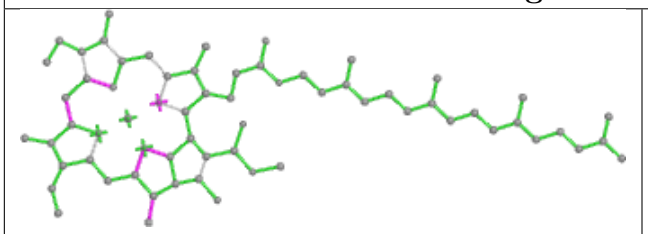


Torsions

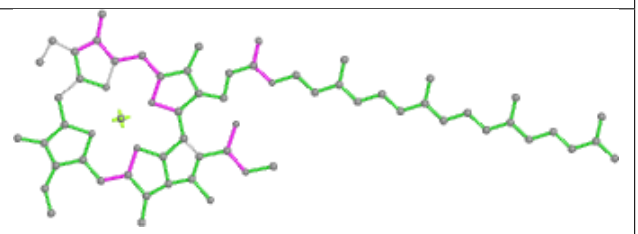


Rings

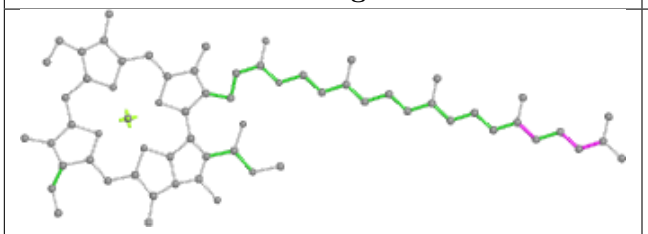
Ligand CLA B 608



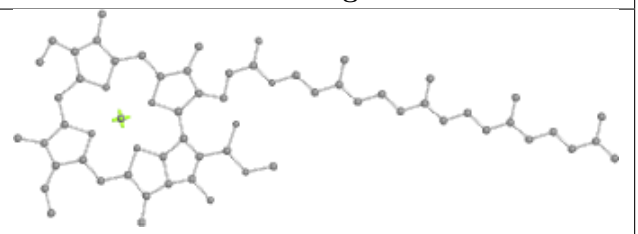
Bond lengths



Bond angles

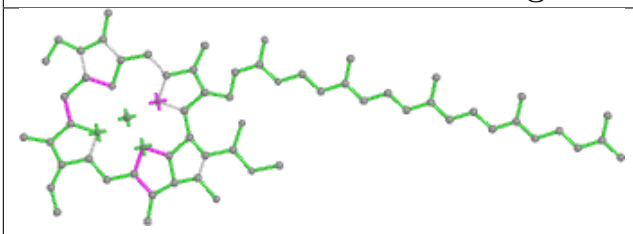


Torsions

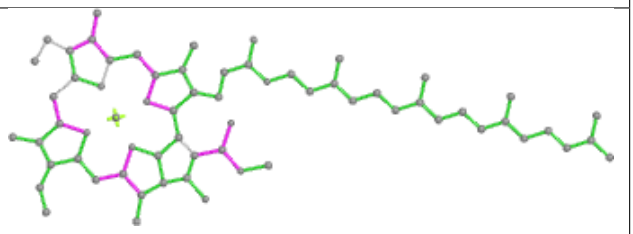


Rings

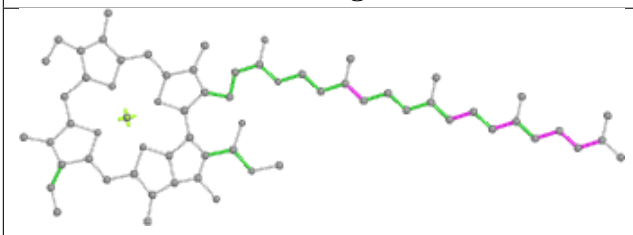
Ligand CLA b 610



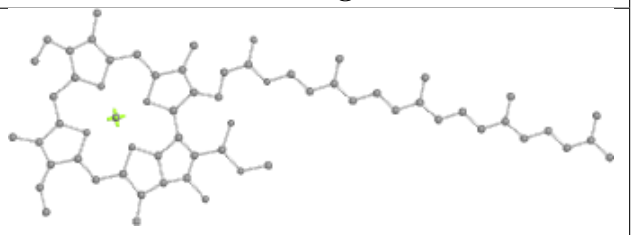
Bond lengths



Bond angles

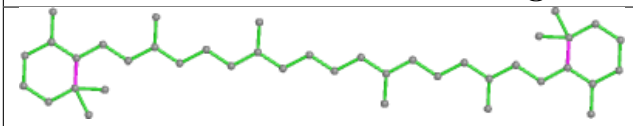


Torsions

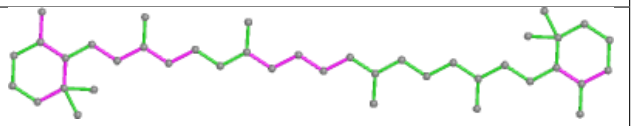


Rings

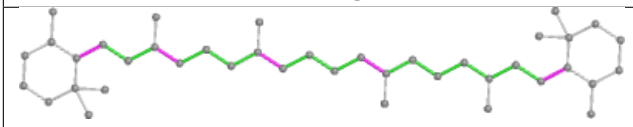
Ligand BCR c 514



Bond lengths



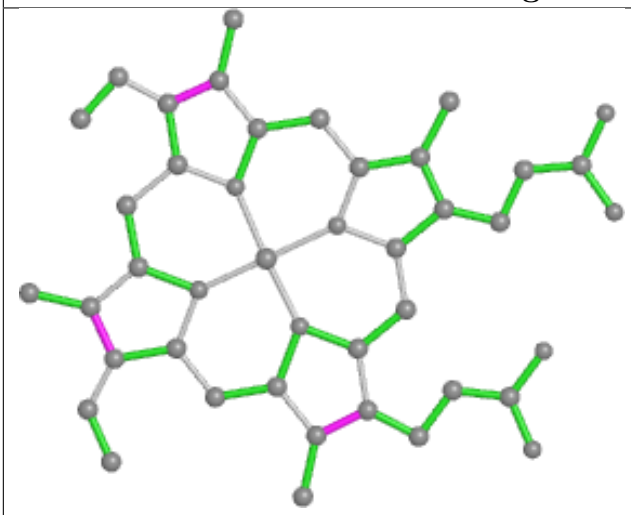
Bond angles



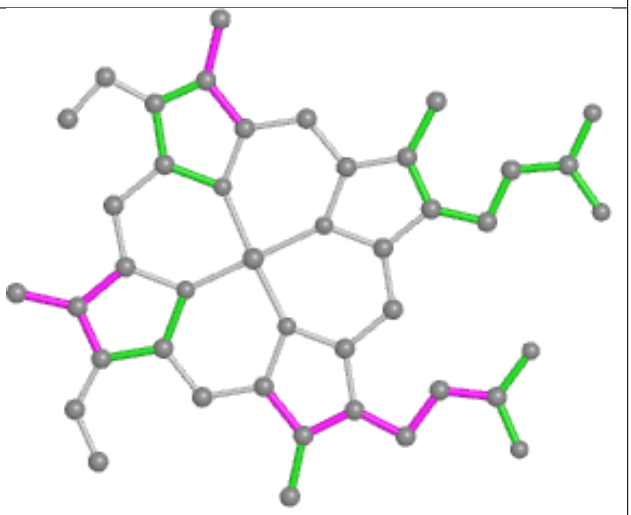
Torsions

Rings

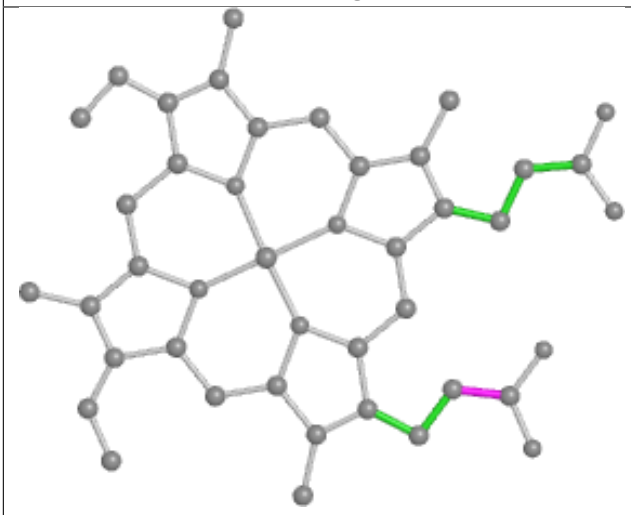
Ligand HEC V 201



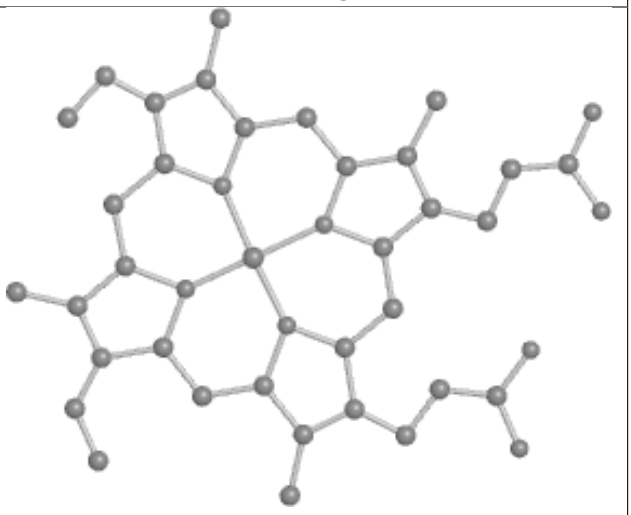
Bond lengths



Bond angles

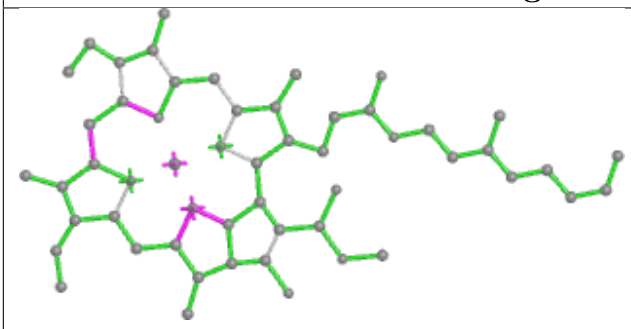


Torsions

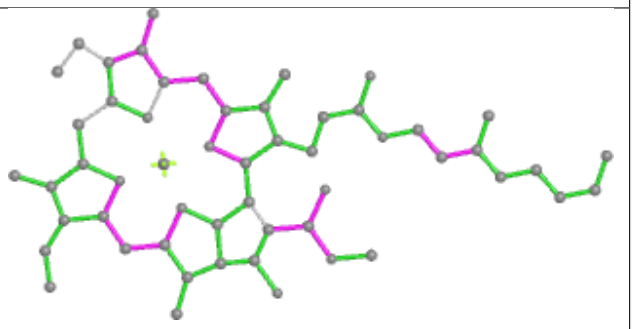


Rings

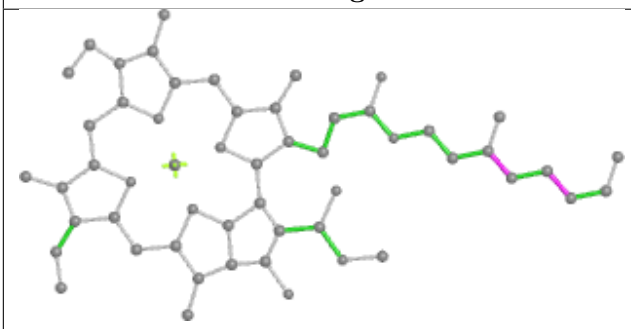
Ligand CLA A 610



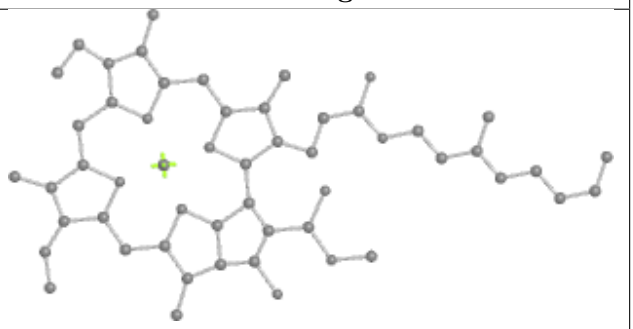
Bond lengths



Bond angles

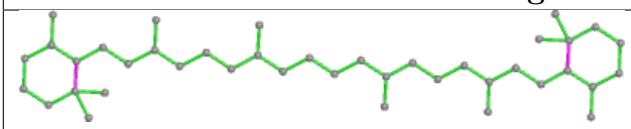


Torsions

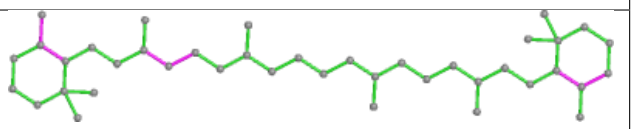


Rings

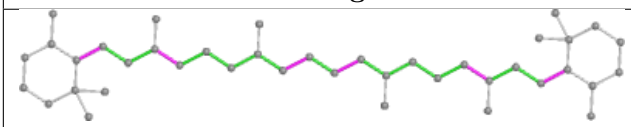
Ligand BCR c 516



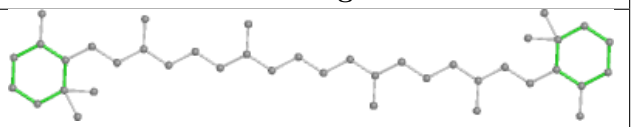
Bond lengths



Bond angles

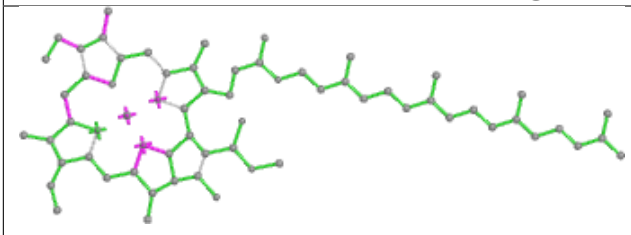


Torsions

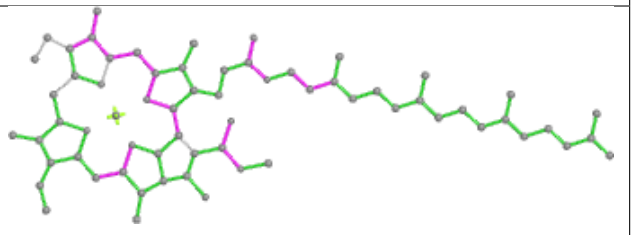


Rings

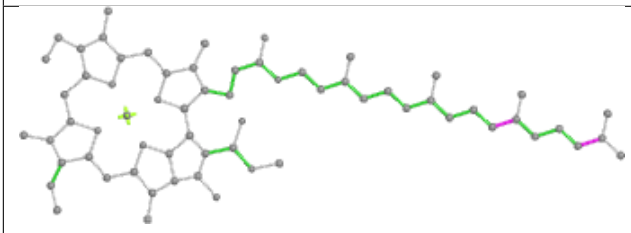
Ligand CLA d 403



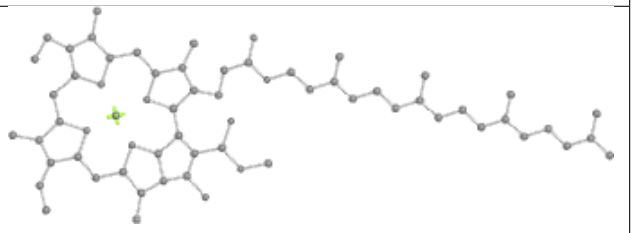
Bond lengths



Bond angles

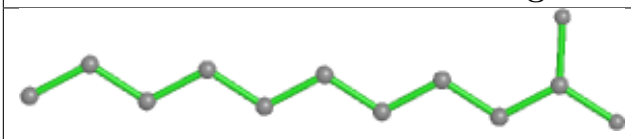


Torsions

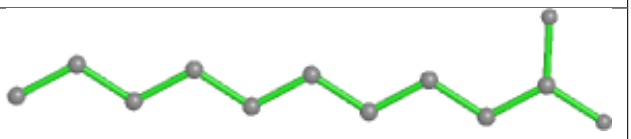


Rings

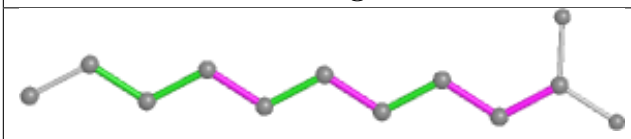
Ligand STE C 521



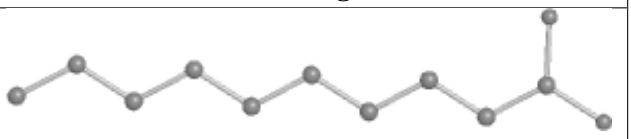
Bond lengths



Bond angles

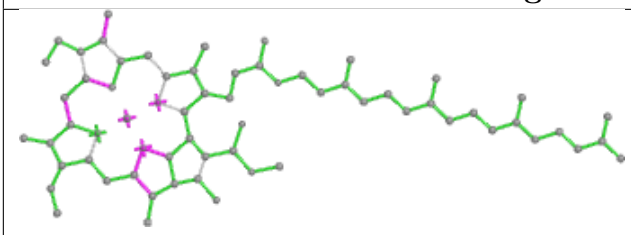


Torsions

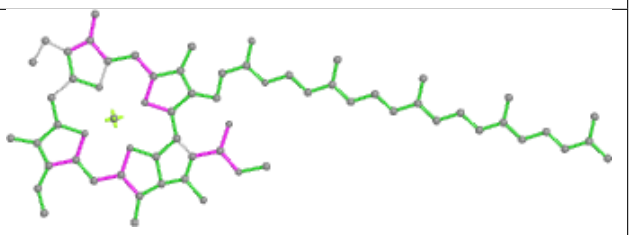


Rings

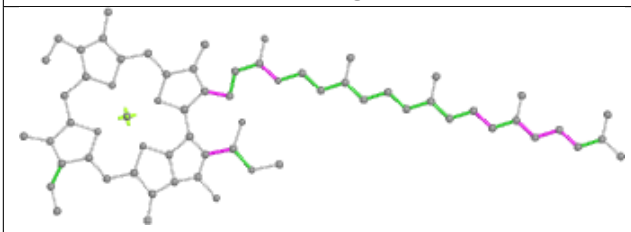
Ligand CLA C 508



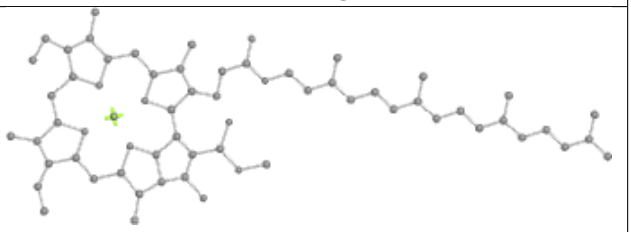
Bond lengths



Bond angles

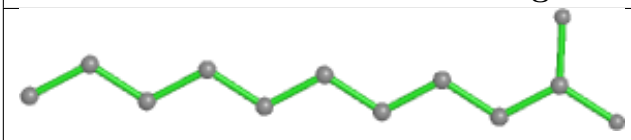


Torsions

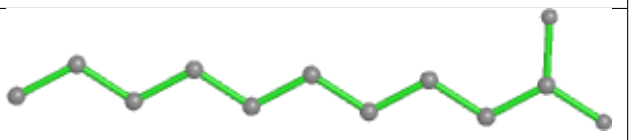


Rings

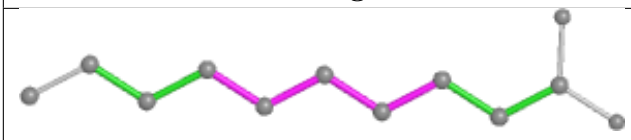
Ligand STE a 617



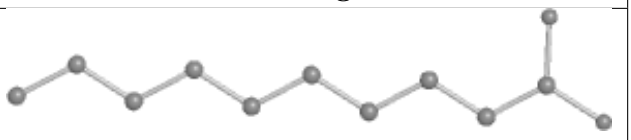
Bond lengths



Bond angles

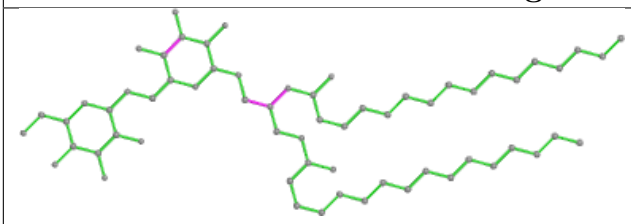


Torsions

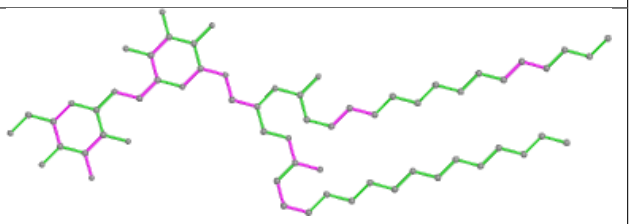


Rings

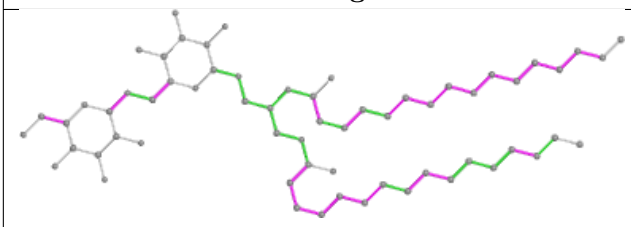
Ligand DGD c 517



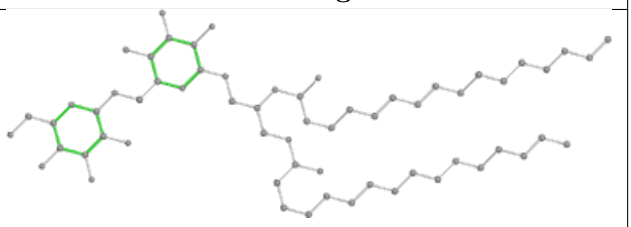
Bond lengths



Bond angles

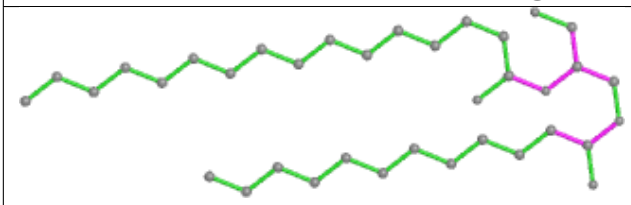


Torsions

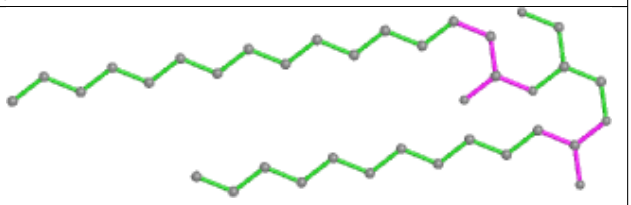


Rings

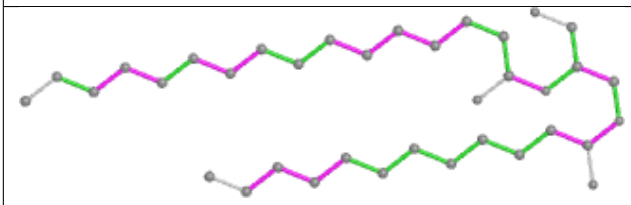
Ligand SQD a 615



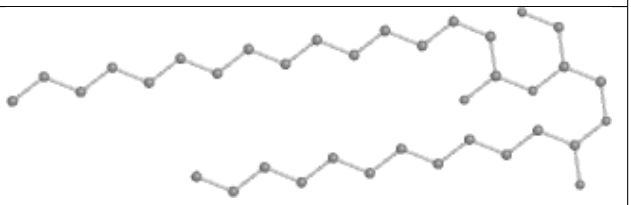
Bond lengths



Bond angles

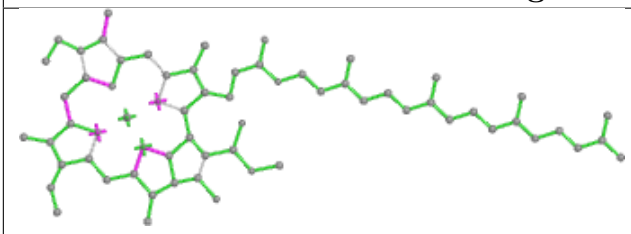


Torsions

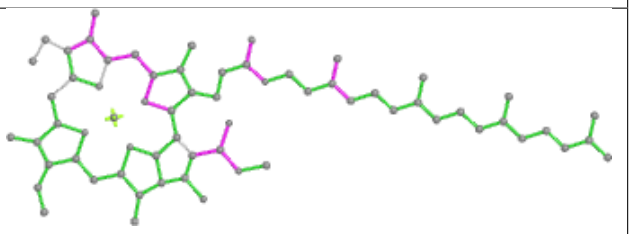


Rings

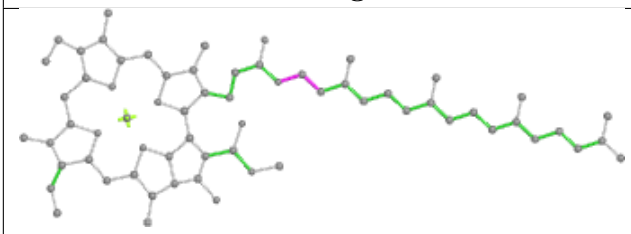
Ligand CLA d 402



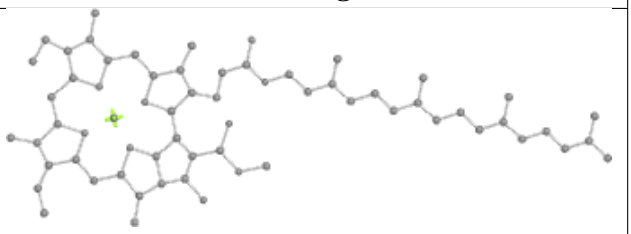
Bond lengths



Bond angles

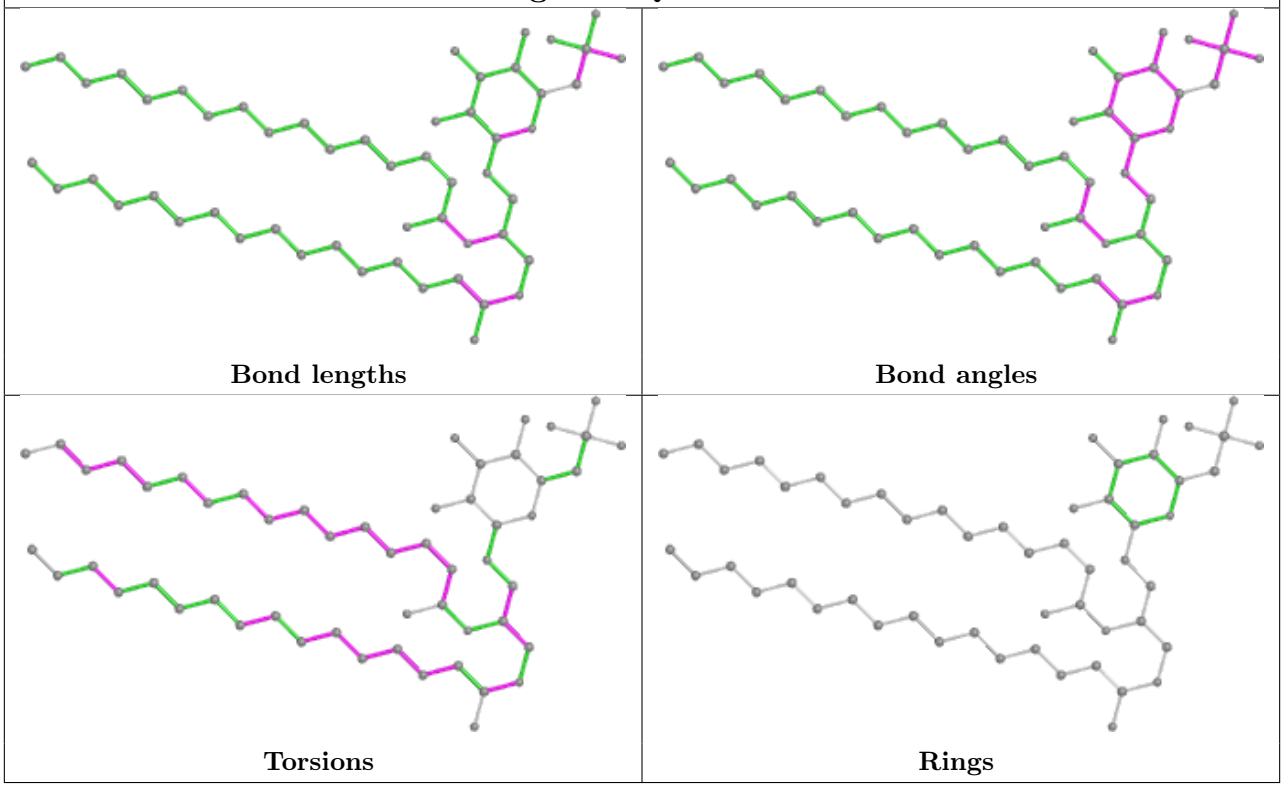


Torsions

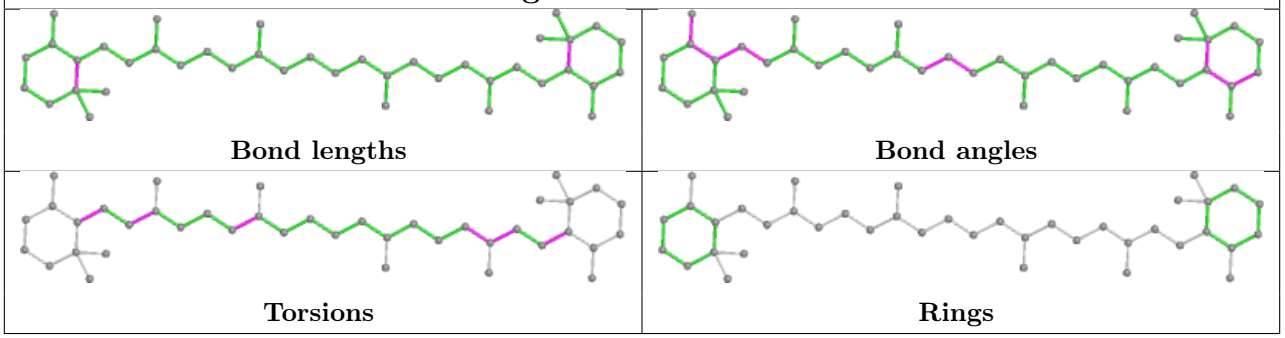


Rings

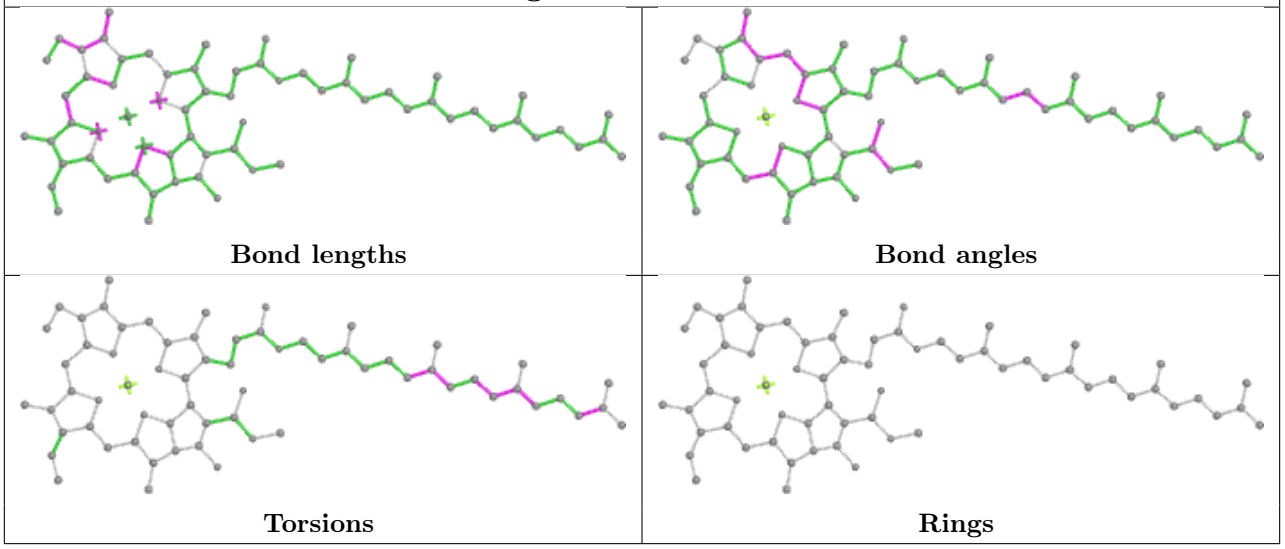
Ligand SQD a 614



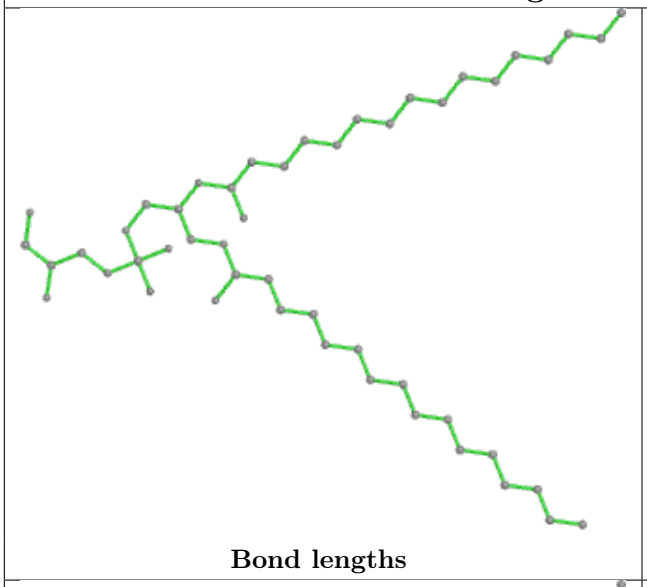
Ligand BCR K 102



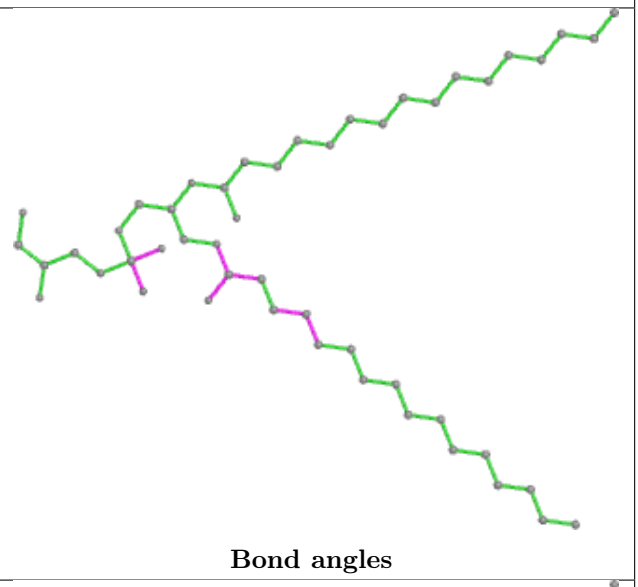
Ligand CLA B 614



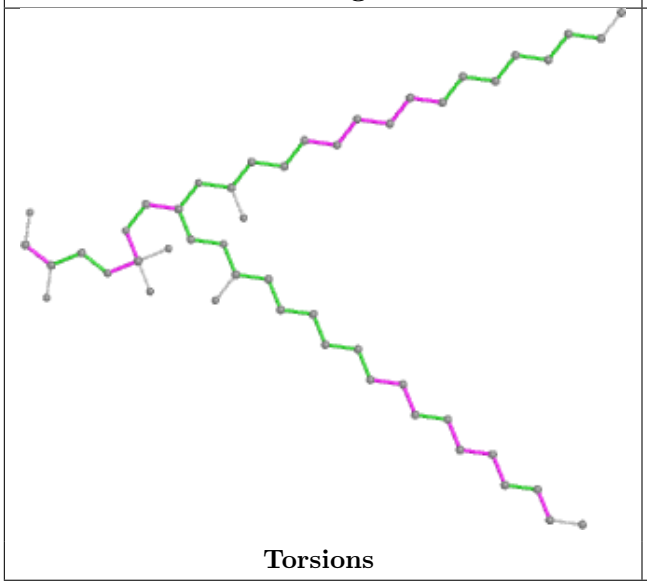
Ligand LHG d 407



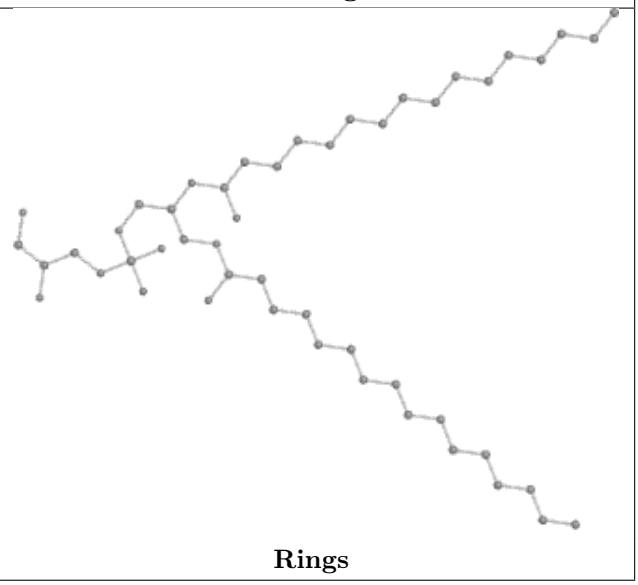
Bond lengths



Bond angles

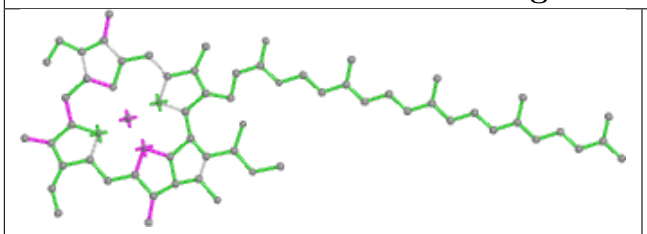


Torsions

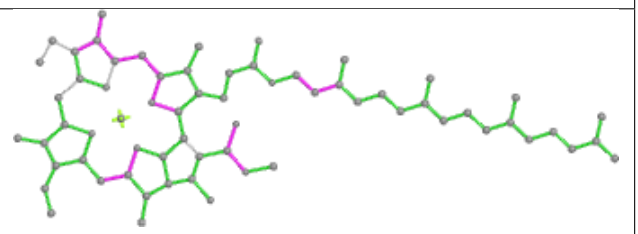


Rings

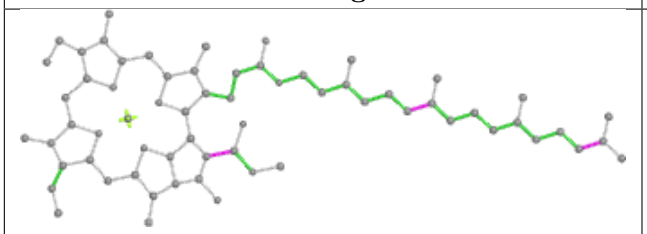
Ligand CLA c 502



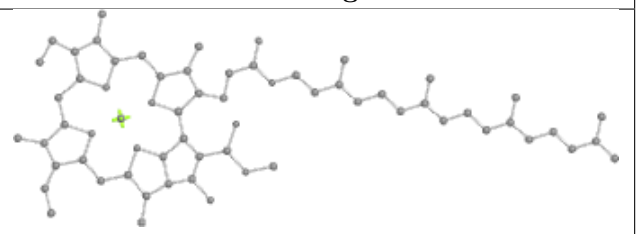
Bond lengths



Bond angles

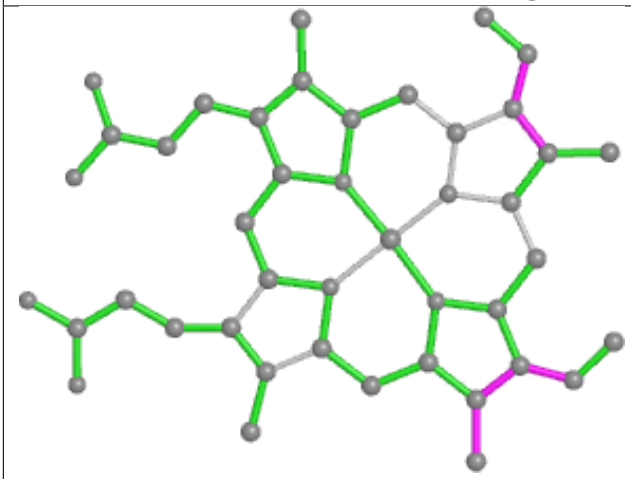


Torsions

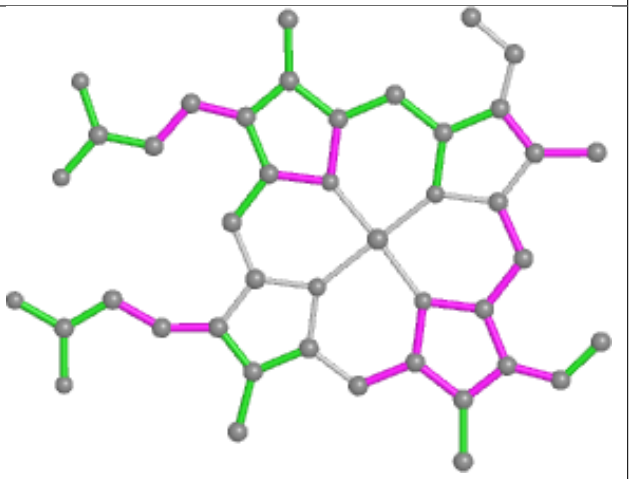


Rings

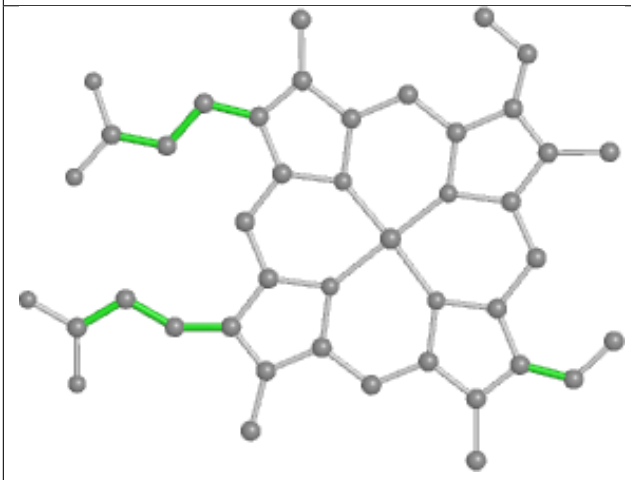
Ligand HEM e 101



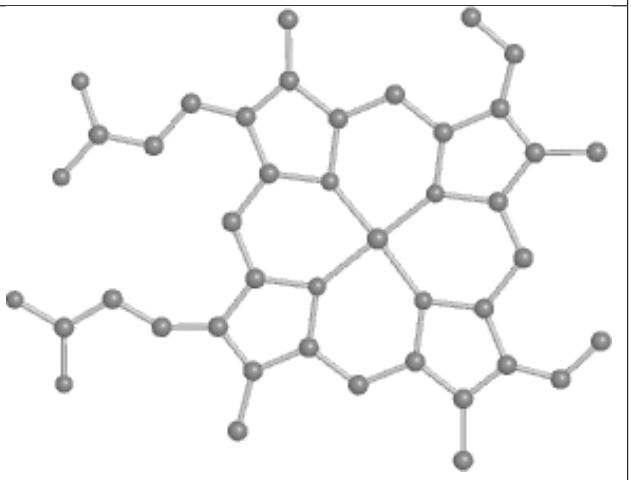
Bond lengths



Bond angles

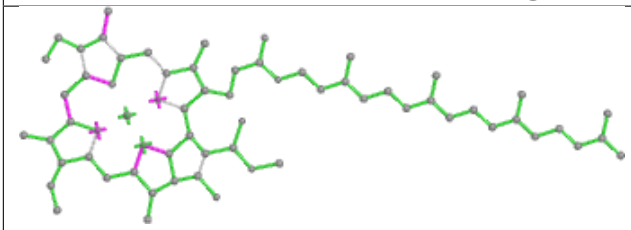


Torsions

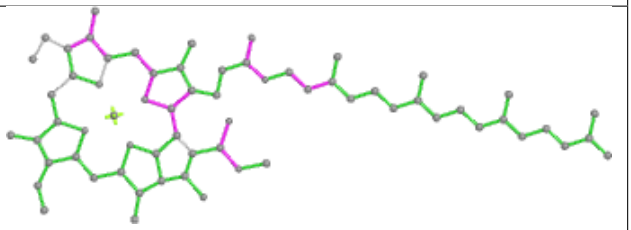


Rings

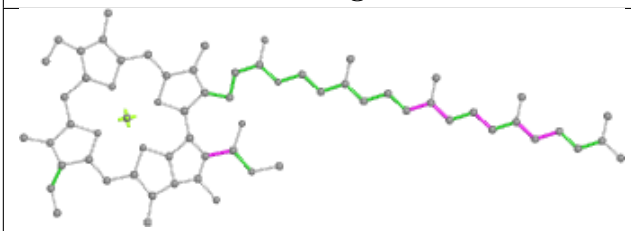
Ligand CLA C 507



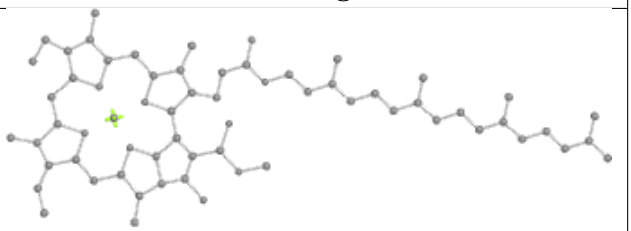
Bond lengths



Bond angles

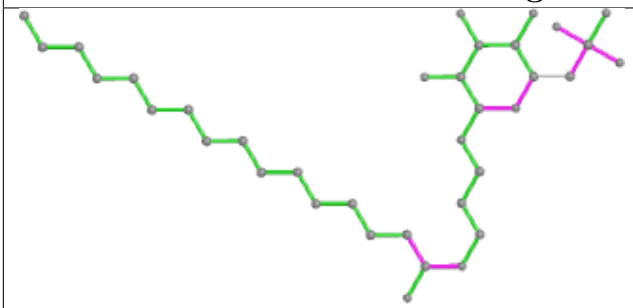


Torsions

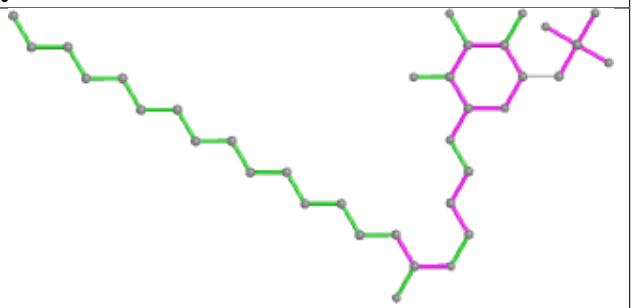


Rings

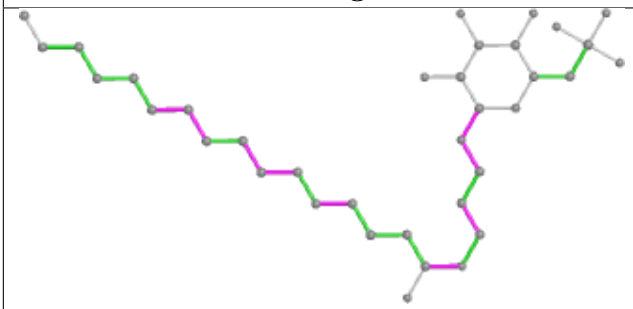
Ligand SQD F 102



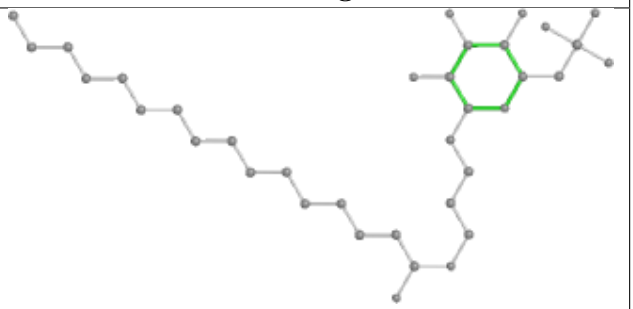
Bond lengths



Bond angles

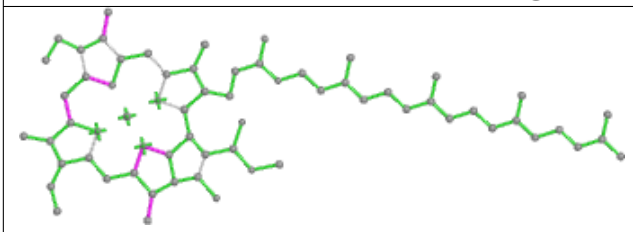


Torsions

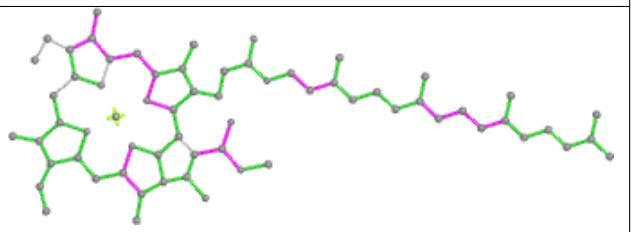


Rings

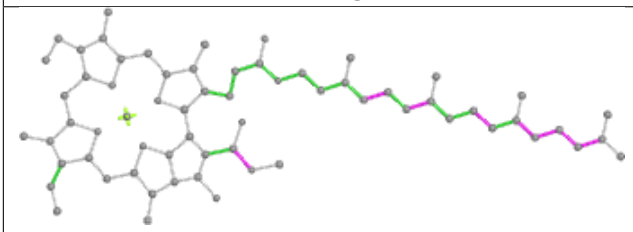
Ligand CLA b 601



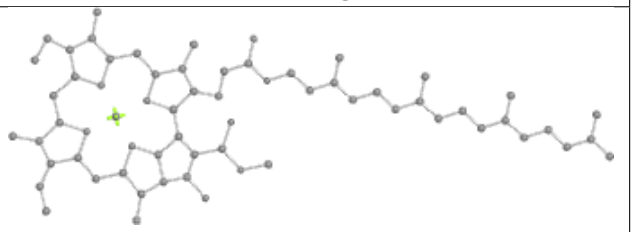
Bond lengths



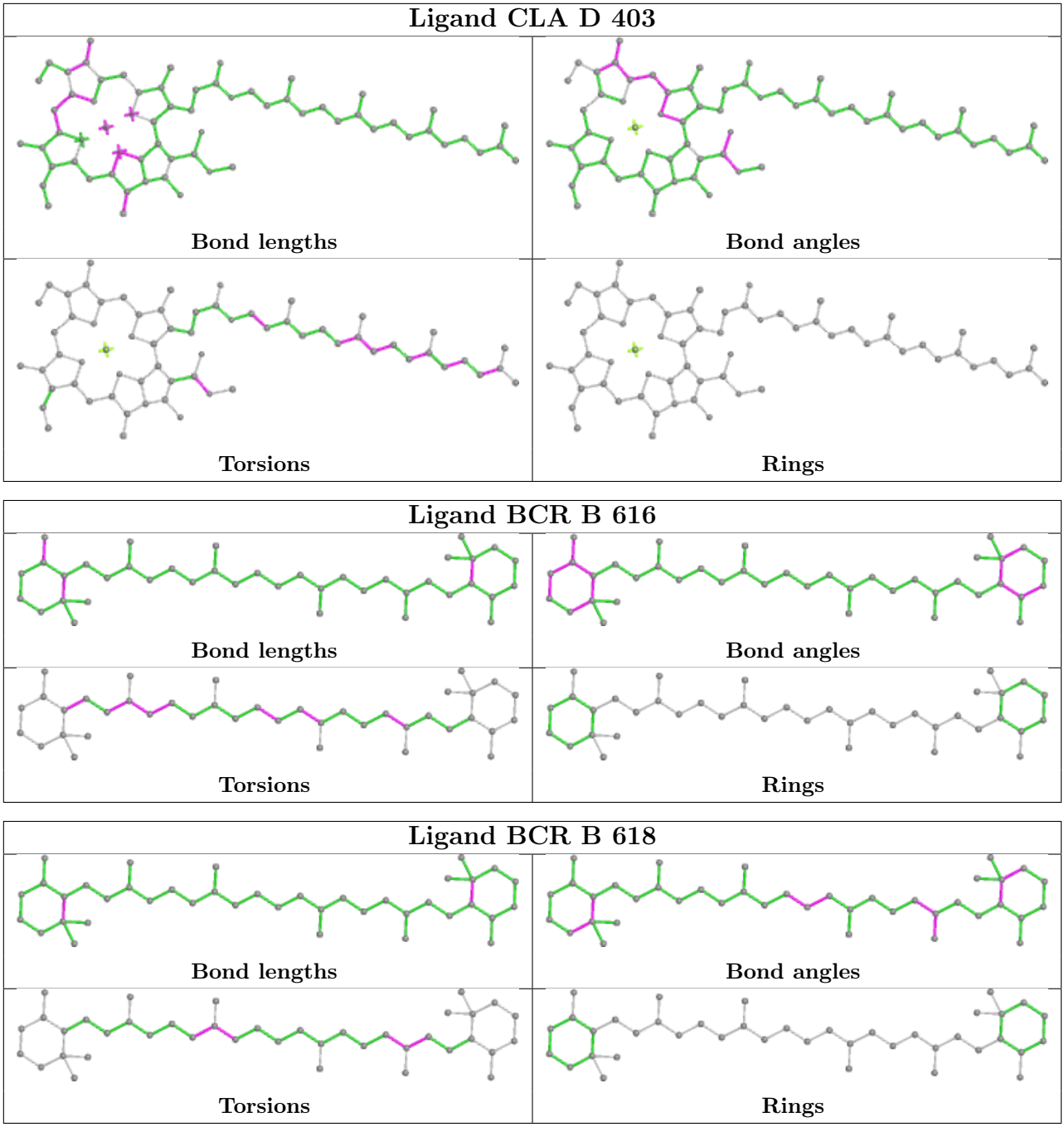
Bond angles



Torsions



Rings



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 86	26, 31, 50, 82	0
1	a	334/344 (97%)	-0.38	1 (0%) 94 94	26, 33, 58, 81	0
2	B	505/510 (99%)	-0.39	8 (1%) 72 75	25, 35, 62, 88	0
2	b	505/510 (99%)	-0.23	12 (2%) 59 64	27, 39, 71, 112	0
3	C	442/461 (95%)	-0.31	4 (0%) 84 86	28, 38, 54, 75	0
3	c	451/461 (97%)	-0.21	9 (1%) 65 69	29, 42, 62, 99	0
4	D	341/352 (96%)	-0.36	0 100 100	25, 32, 49, 73	0
4	d	341/352 (96%)	-0.32	0 100 100	26, 36, 60, 80	0
5	E	82/84 (97%)	0.10	5 (6%) 21 26	36, 54, 70, 85	0
5	e	82/84 (97%)	0.16	5 (6%) 21 26	42, 60, 78, 86	0
6	F	34/45 (75%)	-0.43	1 (2%) 51 57	40, 45, 59, 87	0
6	f	34/45 (75%)	-0.19	1 (2%) 51 57	44, 52, 79, 92	0
7	H	65/66 (98%)	-0.13	2 (3%) 49 55	35, 42, 58, 72	0
7	h	63/66 (95%)	0.32	5 (7%) 12 16	42, 51, 62, 66	0
8	I	35/38 (92%)	-0.38	2 (5%) 23 29	35, 41, 68, 77	0
8	i	35/38 (92%)	-0.19	2 (5%) 23 29	34, 43, 77, 88	0
9	J	36/40 (90%)	-0.05	3 (8%) 11 14	38, 51, 78, 86	0
9	j	36/40 (90%)	0.25	3 (8%) 11 14	41, 54, 87, 92	0
10	K	37/46 (80%)	0.14	1 (2%) 54 60	46, 52, 69, 77	0
10	k	37/46 (80%)	-0.09	2 (5%) 25 31	51, 57, 72, 78	0
11	L	37/37 (100%)	-0.41	0 100 100	27, 31, 61, 68	0
11	l	36/37 (97%)	-0.31	2 (5%) 24 29	30, 33, 68, 88	0
12	M	32/36 (88%)	-0.05	0 100 100	30, 35, 58, 71	0
12	m	31/36 (86%)	-0.20	0 100 100	31, 36, 54, 65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.07	11 (4%) 33 38	27, 44, 80, 133	0
13	o	244/272 (89%)	-0.12	15 (6%) 21 26	29, 42, 79, 123	0
14	T	29/32 (90%)	-0.35	1 (3%) 45 51	28, 33, 57, 71	0
14	t	29/32 (90%)	-0.30	2 (6%) 16 21	30, 34, 71, 87	0
15	U	97/134 (72%)	-0.33	1 (1%) 82 85	34, 45, 71, 88	0
15	u	97/134 (72%)	-0.47	0 100 100	33, 42, 58, 84	0
16	V	137/163 (84%)	-0.50	0 100 100	33, 42, 58, 77	0
16	v	137/163 (84%)	-0.17	0 100 100	36, 48, 66, 86	0
17	Y	27/46 (58%)	1.22	9 (33%) 0 0	55, 75, 93, 95	0
17	y	30/46 (65%)	0.51	3 (10%) 7 9	64, 76, 89, 104	0
18	X	38/41 (92%)	0.06	2 (5%) 26 32	41, 53, 67, 74	0
18	x	39/41 (95%)	0.32	4 (10%) 6 8	50, 60, 87, 102	0
19	Z	62/62 (100%)	0.88	16 (25%) 0 0	57, 69, 111, 126	0
19	z	62/62 (100%)	0.64	11 (17%) 1 1	61, 72, 115, 119	0
20	R	34/41 (82%)	1.70	11 (32%) 0 0	61, 69, 81, 84	0
20	r	31/41 (75%)	3.39	24 (77%) 0 0	73, 88, 108, 116	0
All	All	5302/5700 (93%)	-0.18	181 (3%) 45 51	25, 40, 73, 133	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	r	29	LYS	8.1
13	o	58	ASN	7.9
3	c	23	ALA	7.5
19	Z	33	TRP	7.1
20	r	28	VAL	7.0
9	j	6	GLY	6.6
13	O	60	ARG	6.3
19	Z	32	ASP	5.9
20	R	6	LEU	5.8
20	r	3	TRP	5.7
18	X	2	THR	5.7
20	r	10	LEU	5.7
20	r	2	ASP	5.5
13	O	56	PRO	5.3
20	r	31	VAL	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	j	5	GLY	5.1
20	r	26	TYR	5.0
14	T	30	THR	5.0
17	y	40	ALA	5.0
13	O	3	GLN	5.0
13	o	3	GLN	5.0
2	b	495	PHE	4.9
13	O	62	GLU	4.8
20	r	14	LEU	4.8
13	O	4	THR	4.8
20	R	3	TRP	4.7
13	o	57	LYS	4.7
13	o	56	PRO	4.7
18	x	2	THR	4.7
17	Y	25	ILE	4.6
13	o	60	ARG	4.5
20	r	18	TRP	4.5
6	f	12	SER	4.4
14	t	30	THR	4.3
20	R	32	GLN	4.3
19	z	33	TRP	4.3
19	Z	41	PHE	4.3
20	r	9	LEU	4.3
19	z	35	ARG	4.2
13	o	4	THR	4.2
20	r	13	LEU	4.2
13	o	62	GLU	4.2
2	b	127	ARG	4.0
3	c	143	TYR	4.0
5	E	79	PHE	4.0
8	i	36	ASP	3.9
20	r	25	PRO	3.9
1	A	11	ALA	3.8
1	A	13	LEU	3.8
20	R	28	VAL	3.7
18	x	38	GLN	3.6
19	Z	35	ARG	3.6
19	Z	62	VAL	3.6
5	e	61	ARG	3.5
18	X	3	ILE	3.5
20	r	24	LEU	3.5
13	O	61	GLN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	Y	20	ALA	3.5
19	z	36	SER	3.4
10	K	17	ILE	3.4
20	R	26	TYR	3.4
13	O	59	LYS	3.3
5	e	79	PHE	3.3
17	Y	22	LEU	3.3
17	Y	43	ARG	3.3
20	r	7	VAL	3.3
13	O	63	ALA	3.3
20	R	18	TRP	3.3
9	J	5	GLY	3.2
6	F	12	SER	3.2
20	R	2	ASP	3.2
20	r	32	GLN	3.2
2	b	161	LEU	3.2
20	r	6	LEU	3.2
13	O	5	LEU	3.1
2	b	289	GLN	3.1
7	h	6	TRP	3.1
20	r	19	ALA	3.1
2	B	487	SER	3.1
9	j	7	ARG	3.0
20	R	24	LEU	3.0
20	r	27	ALA	3.0
19	Z	7	LEU	2.9
8	I	36	ASP	2.9
19	Z	40	ILE	2.9
13	o	59	LYS	2.9
8	I	34	ARG	2.9
8	i	34	ARG	2.9
9	J	7	ARG	2.8
2	B	490	GLN	2.8
19	Z	1	MET	2.8
2	b	506	ARG	2.8
7	h	21	VAL	2.8
20	r	11	PRO	2.8
19	z	60	PHE	2.8
3	C	143	TYR	2.8
19	Z	31	GLN	2.7
2	B	127	ARG	2.7
13	o	246	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	J	6	GLY	2.7
19	z	30	PRO	2.7
17	y	18	VAL	2.7
18	x	40	SER	2.7
10	k	16	ALA	2.7
7	h	25	TRP	2.7
19	Z	37	LYS	2.7
20	R	33	LYS	2.7
1	a	11	ALA	2.6
5	E	83	LEU	2.6
13	o	61	GLN	2.6
17	Y	37	PHE	2.6
17	y	37	PHE	2.6
2	B	505	ARG	2.6
3	c	191	PRO	2.6
11	l	7	ARG	2.6
13	o	63	ALA	2.6
3	c	24	THR	2.6
18	x	3	ILE	2.5
2	b	505	ARG	2.5
20	R	25	PRO	2.5
2	B	495	PHE	2.5
7	h	41	PHE	2.5
19	Z	3	ILE	2.5
20	R	21	ARG	2.5
3	c	147	PHE	2.5
19	Z	34	ASP	2.5
19	Z	4	LEU	2.4
7	h	10	ILE	2.4
1	A	12	ASN	2.4
19	Z	60	PHE	2.4
5	e	74	GLN	2.4
17	Y	21	GLN	2.4
5	E	84	LYS	2.4
14	t	29	ILE	2.4
3	c	29	GLU	2.4
2	b	295	GLY	2.4
2	b	494	GLY	2.4
5	E	72	ALA	2.3
20	r	15	ALA	2.3
2	B	485	GLU	2.3
19	z	3	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	H	66	GLY	2.3
3	C	146	PHE	2.3
19	Z	59	PHE	2.3
2	b	486	LEU	2.2
5	e	76	VAL	2.2
3	c	142	GLU	2.2
15	U	8	GLU	2.2
20	r	5	VAL	2.2
7	H	41	PHE	2.2
13	o	207	ARG	2.2
19	Z	42	LEU	2.2
3	C	142	GLU	2.2
11	l	3	PRO	2.2
17	Y	40	ALA	2.2
2	b	487	SER	2.2
13	o	5	LEU	2.2
19	z	59	PHE	2.2
2	b	128	THR	2.2
10	k	17	ILE	2.1
13	O	36	GLN	2.1
3	C	61	VAL	2.1
2	b	490	GLN	2.1
3	c	55	ALA	2.1
20	r	4	ARG	2.1
5	e	71	GLU	2.1
3	c	262	ARG	2.1
20	r	12	VAL	2.1
19	z	41	PHE	2.1
13	O	229[A]	GLU	2.1
2	B	295	GLY	2.1
19	z	42	LEU	2.1
17	Y	45	ASN	2.1
2	B	294	SER	2.0
13	o	54	GLU	2.0
13	o	132	ASN	2.0
19	z	7	LEU	2.0
5	E	5	THR	2.0
19	z	62	VAL	2.0
20	r	23	ILE	2.0
17	Y	41	VAL	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
14	FME	t	1	10/11	0.91	0.11	33,38,54,78	0
12	FME	M	1	10/11	0.93	0.17	44,51,67,72	0
14	FME	T	1	10/11	0.95	0.10	33,41,57,63	0
12	FME	m	1	10/11	0.95	0.16	33,45,62,66	0
8	FME	I	1	10/11	0.95	0.11	39,49,57,57	0
8	FME	i	1	10/11	0.96	0.18	37,50,52,53	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	STE	H	104	18/20	0.69	0.29	52,68,74,75	0
31	STE	c	521	20/20	0.74	0.20	44,55,77,78	0
32	LMG	d	409	23/55	0.74	0.25	49,63,69,72	0
31	STE	B	626	16/20	0.75	0.26	48,58,64,69	0
33	LHG	E	101	49/49	0.76	0.24	52,74,93,101	0
31	STE	b	622	20/20	0.77	0.19	47,57,75,76	0
31	STE	B	624	18/20	0.77	0.15	41,50,72,75	0
31	STE	B	619	17/20	0.78	0.16	37,49,69,70	0
31	STE	a	617	12/20	0.78	0.24	50,56,71,72	0
32	LMG	c	522	48/55	0.79	0.22	51,71,81,87	0
32	LMG	b	620	55/55	0.80	0.29	50,66,81,84	0
31	STE	R	101	12/20	0.80	0.31	63,68,83,84	0
30	DGD	a	616	44/66	0.80	0.16	36,52,82,85	0
31	STE	x	102	20/20	0.80	0.21	43,54,63,69	0
31	STE	b	621	16/20	0.81	0.19	53,59,78,79	0
31	STE	t	103	10/20	0.81	0.20	43,53,58,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	SQD	a	615	36/54	0.81	0.17	30,52,69,74	0
32	LMG	D	409	33/55	0.81	0.18	37,52,69,72	0
28	PL9	A	612	55/55	0.82	0.26	39,62,73,75	0
31	STE	c	523	12/20	0.82	0.18	57,67,75,76	0
28	PL9	a	612	55/55	0.82	0.24	46,67,79,83	0
25	CLA	h	101	65/65	0.83	0.17	52,66,86,94	0
31	STE	m	102	12/20	0.83	0.16	48,52,66,67	0
31	STE	D	410	20/20	0.83	0.16	35,45,64,73	0
31	STE	J	101	12/20	0.84	0.12	49,54,61,65	0
31	STE	b	623	10/20	0.84	0.20	44,50,52,55	0
31	STE	T	102	16/20	0.84	0.16	36,45,56,61	0
31	STE	C	522	16/20	0.84	0.13	37,52,58,59	0
27	BCR	H	102	40/40	0.84	0.15	34,45,55,57	0
29	SQD	l	101	54/54	0.84	0.17	38,60,76,82	0
33	LHG	e	102	42/49	0.84	0.24	58,80,99,107	0
31	STE	C	520	12/20	0.85	0.13	34,44,52,56	0
27	BCR	x	101	40/40	0.85	0.14	38,53,61,64	0
31	STE	b	619	20/20	0.85	0.22	40,52,66,68	0
32	LMG	C	515	48/55	0.85	0.16	40,54,65,71	0
31	STE	T	103	15/20	0.85	0.15	45,53,69,73	0
31	STE	B	625	12/20	0.86	0.36	49,56,65,65	0
30	DGD	A	616	66/66	0.86	0.15	47,57,66,70	0
32	LMG	c	524	49/55	0.86	0.15	39,54,70,76	0
32	LMG	B	620	28/55	0.86	0.16	37,48,61,67	0
31	STE	l	103	18/20	0.86	0.16	37,44,63,64	0
29	SQD	A	615	39/54	0.86	0.18	40,51,77,78	0
25	CLA	H	101	65/65	0.87	0.15	39,53,77,84	0
31	STE	B	623	12/20	0.87	0.12	39,47,59,59	0
31	STE	j	101	12/20	0.87	0.11	51,57,60,61	0
27	BCR	K	102	40/40	0.87	0.13	43,51,61,62	0
29	SQD	L	101	49/54	0.88	0.14	42,58,80,82	0
31	STE	M	102	15/20	0.88	0.15	36,43,60,62	0
27	BCR	d	404	40/40	0.88	0.14	38,47,79,85	0
29	SQD	f	101	41/54	0.88	0.20	65,78,88,91	0
27	BCR	k	101	40/40	0.88	0.12	50,57,65,70	0
25	CLA	C	512	65/65	0.88	0.16	39,48,69,79	0
31	STE	d	411	17/20	0.88	0.16	49,52,64,66	0
25	CLA	C	513	65/65	0.89	0.18	45,55,79,83	0
25	CLA	c	512	65/65	0.89	0.15	47,55,78,83	0
32	LMG	m	101	51/55	0.89	0.12	34,49,63,71	0
25	CLA	c	513	65/65	0.89	0.18	48,60,86,92	0
27	BCR	c	516	40/40	0.89	0.17	47,52,61,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	BCR	D	404	40/40	0.90	0.13	33,43,70,79	0
32	LMG	C	519	48/55	0.90	0.14	43,65,81,85	0
31	STE	I	101	15/20	0.90	0.11	43,51,64,65	0
32	LMG	M	101	51/55	0.90	0.12	33,46,61,62	0
31	STE	C	521	12/20	0.90	0.14	43,50,56,61	0
32	LMG	c	520	37/55	0.90	0.15	49,59,71,73	0
31	STE	M	103	10/20	0.91	0.13	35,46,53,54	0
27	BCR	K	101	40/40	0.91	0.13	41,53,58,60	0
25	CLA	b	615	60/65	0.92	0.12	33,40,77,79	0
25	CLA	c	502	65/65	0.92	0.13	33,41,53,59	0
25	CLA	c	503	65/65	0.92	0.14	36,44,50,55	0
32	LMG	D	406	51/55	0.92	0.16	32,47,64,68	0
27	BCR	b	618	40/40	0.92	0.10	33,43,53,55	0
27	BCR	c	514	40/40	0.92	0.15	46,56,63,65	0
25	CLA	C	502	65/65	0.92	0.12	33,39,49,58	0
30	DGD	C	517	62/66	0.92	0.12	36,45,83,98	0
30	DGD	H	103	62/66	0.92	0.11	34,42,50,52	0
25	CLA	D	403	65/65	0.92	0.12	28,34,77,92	0
25	CLA	B	605	65/65	0.92	0.11	26,34,63,72	0
27	BCR	B	618	40/40	0.92	0.10	31,42,50,52	0
27	BCR	C	514	40/40	0.92	0.11	31,41,49,50	0
25	CLA	a	610	65/65	0.92	0.12	24,31,66,74	0
31	STE	t	102	14/20	0.93	0.10	38,43,50,54	0
28	PL9	D	405	55/55	0.93	0.11	24,31,40,42	0
30	DGD	c	518	62/66	0.93	0.11	39,47,75,81	0
30	DGD	c	519	62/66	0.93	0.13	33,46,66,68	0
30	DGD	h	102	62/66	0.93	0.11	34,45,52,54	0
25	CLA	b	608	65/65	0.93	0.13	32,43,54,64	0
25	CLA	b	614	65/65	0.93	0.12	29,39,51,56	0
25	CLA	d	403	65/65	0.93	0.12	34,42,70,74	0
29	SQD	a	614	54/54	0.93	0.13	38,59,75,81	0
25	CLA	C	511	65/65	0.93	0.11	36,48,57,62	0
27	BCR	B	617	40/40	0.93	0.09	27,36,46,48	0
25	CLA	B	603	65/65	0.93	0.12	25,30,63,65	0
25	CLA	C	506	65/65	0.93	0.12	30,41,74,79	0
30	DGD	C	516	62/66	0.93	0.14	30,35,70,79	0
25	CLA	c	509	65/65	0.93	0.15	38,46,56,58	0
30	DGD	C	518	62/66	0.93	0.11	31,43,61,66	0
25	CLA	c	510	65/65	0.93	0.15	33,45,52,54	0
25	CLA	b	603	65/65	0.94	0.12	25,33,62,71	0
25	CLA	C	505	65/65	0.94	0.14	28,36,58,65	0
25	CLA	b	613	65/65	0.94	0.12	27,37,63,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	A	610	54/65	0.94	0.11	22,30,58,60	0
25	CLA	C	507	65/65	0.94	0.12	29,38,49,51	0
25	CLA	C	508	65/65	0.94	0.11	33,39,83,94	0
27	BCR	K	103	40/40	0.94	0.14	42,48,58,59	0
27	BCR	T	101	40/40	0.94	0.08	29,38,47,48	0
27	BCR	b	616	40/40	0.94	0.09	28,42,48,51	0
25	CLA	C	510	65/65	0.94	0.12	31,43,51,53	0
25	CLA	c	506	65/65	0.94	0.11	37,43,71,77	0
25	CLA	c	507	65/65	0.94	0.11	32,40,49,55	0
25	CLA	c	508	64/65	0.94	0.12	36,42,77,93	0
25	CLA	B	608	65/65	0.94	0.12	28,37,49,52	0
27	BCR	t	101	40/40	0.94	0.09	27,39,48,48	0
25	CLA	B	613	65/65	0.94	0.15	26,36,57,67	0
25	CLA	c	511	65/65	0.94	0.11	44,53,59,63	0
25	CLA	B	614	65/65	0.94	0.10	25,35,51,62	0
25	CLA	B	615	60/65	0.94	0.13	28,35,74,82	0
29	SQD	A	614	52/54	0.94	0.14	33,52,68,74	0
25	CLA	d	402	65/65	0.94	0.10	21,32,51,55	0
29	SQD	F	102	36/54	0.94	0.15	48,64,72,75	0
25	CLA	C	501	65/65	0.94	0.11	26,35,45,45	0
25	CLA	A	607	65/65	0.94	0.12	23,32,80,84	0
32	LMG	d	410	44/55	0.94	0.11	38,48,71,76	0
27	BCR	A	611	40/40	0.94	0.09	26,34,38,39	0
33	LHG	D	408	47/49	0.94	0.11	31,40,69,74	0
27	BCR	B	616	40/40	0.94	0.11	31,36,46,55	0
25	CLA	b	601	65/65	0.94	0.13	31,39,52,55	0
26	PHO	d	401	64/64	0.95	0.09	28,38,44,46	0
25	CLA	b	607	65/65	0.95	0.11	32,40,53,56	0
25	CLA	A	606	65/65	0.95	0.09	21,27,37,41	0
25	CLA	b	609	65/65	0.95	0.16	30,37,43,49	0
25	CLA	b	610	65/65	0.95	0.12	25,33,45,50	0
25	CLA	b	612	65/65	0.95	0.12	26,31,64,67	0
25	CLA	C	509	65/65	0.95	0.15	32,40,53,55	0
25	CLA	B	604	65/65	0.95	0.13	26,31,39,42	0
25	CLA	B	601	65/65	0.95	0.12	28,36,49,54	0
25	CLA	c	501	65/65	0.95	0.12	29,38,46,48	0
25	CLA	B	606	65/65	0.95	0.10	21,30,54,57	0
30	DGD	c	517	62/66	0.95	0.11	27,38,58,67	0
25	CLA	B	602	65/65	0.95	0.14	25,31,52,54	0
27	BCR	a	611	40/40	0.95	0.08	23,32,42,45	0
25	CLA	c	504	60/65	0.95	0.09	30,42,68,72	0
27	BCR	b	617	40/40	0.95	0.09	29,39,45,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	c	505	65/65	0.95	0.14	31,39,58,60	0
25	CLA	C	503	65/65	0.95	0.12	35,41,45,52	0
27	BCR	c	515	40/40	0.95	0.10	32,44,50,53	0
25	CLA	C	504	59/65	0.95	0.10	35,41,66,72	0
25	CLA	a	607	65/65	0.95	0.09	24,29,37,47	0
25	CLA	a	608	65/65	0.95	0.11	28,37,85,93	0
25	CLA	B	609	65/65	0.95	0.12	25,32,37,42	0
25	CLA	a	613	65/65	0.95	0.09	25,30,40,42	0
25	CLA	B	611	65/65	0.95	0.13	24,31,40,47	0
25	CLA	b	602	65/65	0.95	0.12	27,33,56,68	0
25	CLA	B	612	65/65	0.95	0.12	22,30,56,65	0
28	PL9	d	405	55/55	0.95	0.11	25,34,39,41	0
33	LHG	B	622	49/49	0.95	0.12	32,41,53,61	0
25	CLA	b	604	65/65	0.95	0.11	25,34,42,45	0
25	CLA	b	605	65/65	0.95	0.10	30,37,62,65	0
33	LHG	d	406	49/49	0.95	0.13	32,45,59,65	0
26	PHO	a	609	64/64	0.95	0.11	26,31,36,39	0
33	LHG	l	102	49/49	0.95	0.10	32,41,46,49	0
25	CLA	A	613	65/65	0.96	0.08	21,28,41,45	0
25	CLA	B	607	65/65	0.96	0.10	25,33,47,50	0
33	LHG	B	621	49/49	0.96	0.12	30,36,45,53	0
25	CLA	B	610	65/65	0.96	0.13	23,30,40,43	0
33	LHG	D	407	49/49	0.96	0.11	25,35,45,46	0
25	CLA	b	611	65/65	0.96	0.15	25,33,39,45	0
25	CLA	b	606	65/65	0.96	0.11	25,33,54,60	0
25	CLA	D	402	65/65	0.96	0.10	22,28,47,52	0
33	LHG	d	407	49/49	0.96	0.12	30,40,47,52	0
33	LHG	d	408	39/49	0.96	0.10	34,44,55,60	0
26	PHO	A	608	64/64	0.96	0.08	21,27,33,37	0
26	PHO	A	609	64/64	0.96	0.13	27,32,38,42	0
35	HEM	F	101	43/43	0.96	0.11	42,48,58,63	0
35	HEM	e	101	43/43	0.96	0.11	54,58,72,85	0
34	BCT	D	401	4/4	0.97	0.15	35,37,38,38	0
36	HEC	V	201	43/43	0.97	0.11	29,36,44,52	0
36	HEC	v	201	43/43	0.97	0.11	29,38,41,44	0
24	CL	A	605	1/1	0.98	0.07	31,31,31,31	0
24	CL	a	604	1/1	0.98	0.04	32,32,32,32	0
24	CL	a	605	1/1	0.98	0.04	34,34,34,34	0
21	OEY	A	601[B]	11/11	0.98	0.11	20,24,27,30	11
21	OEY	A	601[C]	11/11	0.98	0.11	29,31,35,37	11
21	OEY	a	601[B]	11/11	0.98	0.09	20,25,29,30	11
34	BCT	a	606	4/4	0.98	0.13	33,36,41,45	0

Continued on next page...

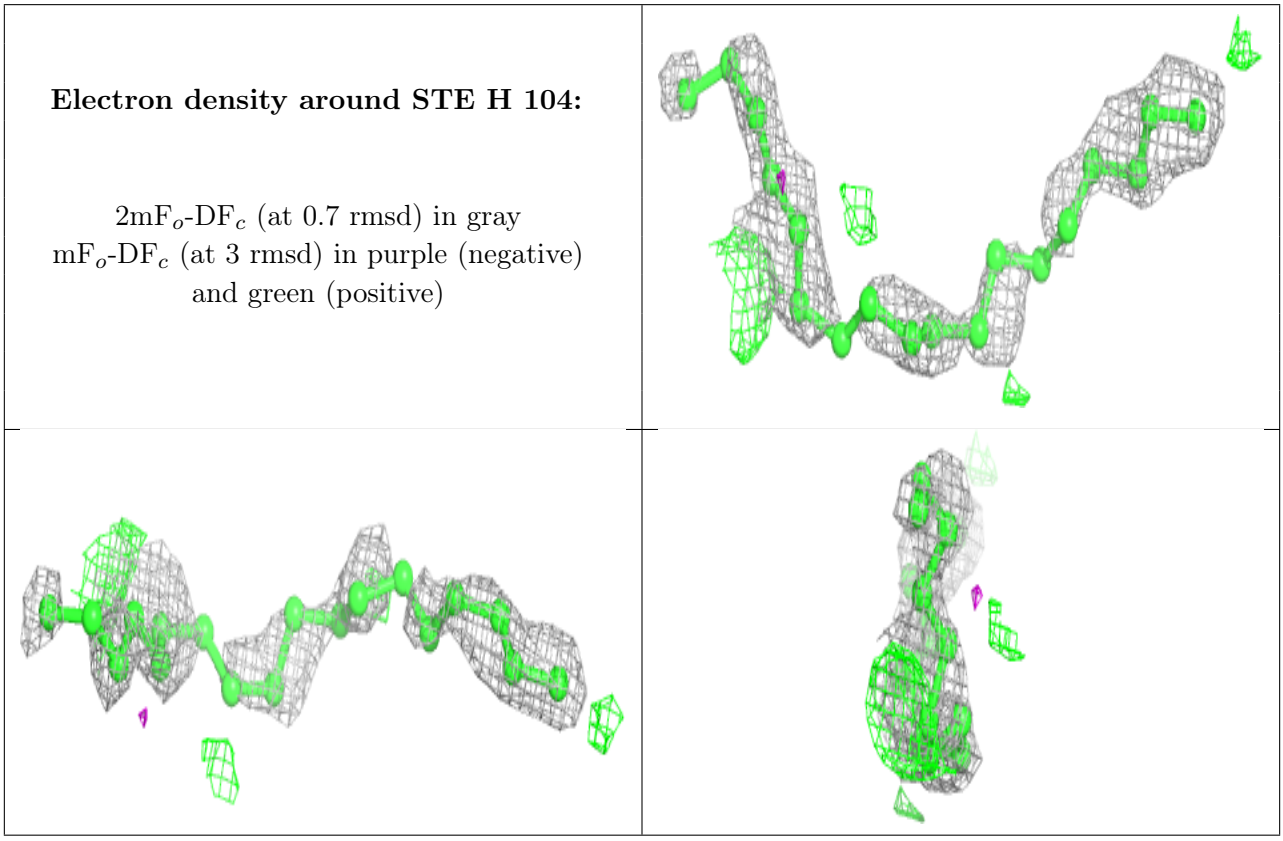
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	OEY	a	601[C]	11/11	0.98	0.09	30,32,34,36	11
22	OEX	A	602[A]	10/10	0.98	0.11	36,38,41,43	10
22	OEX	a	602[A]	10/10	0.98	0.09	35,37,42,42	10
24	CL	A	604	1/1	0.98	0.05	34,34,34,34	0
23	FE2	a	603	1/1	0.99	0.05	36,36,36,36	0
23	FE2	A	603	1/1	1.00	0.05	28,28,28,28	0

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

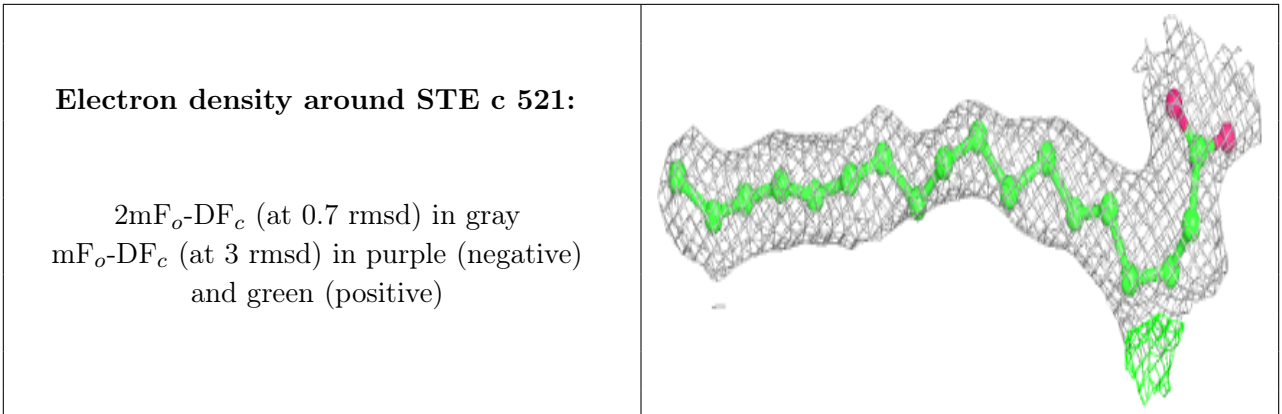
Electron density around STE H 104:

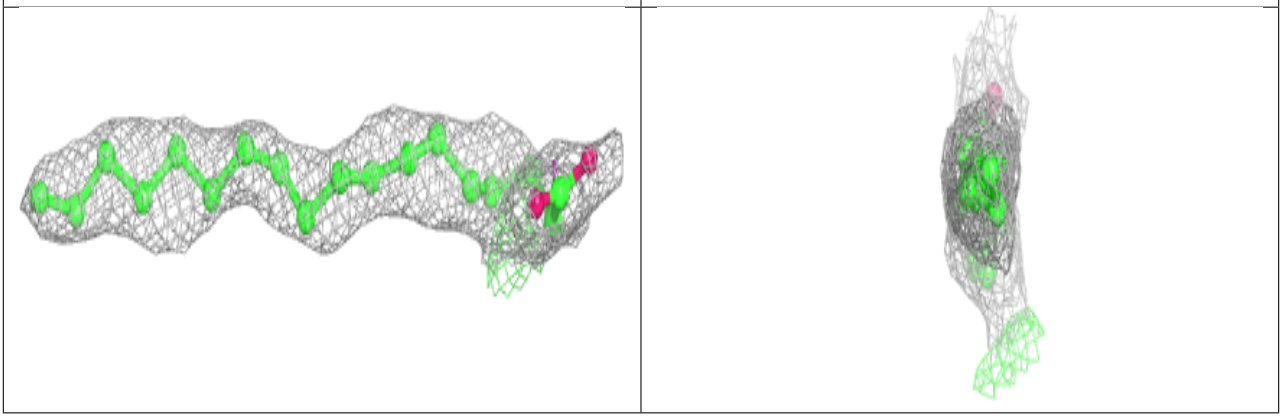
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around STE c 521:

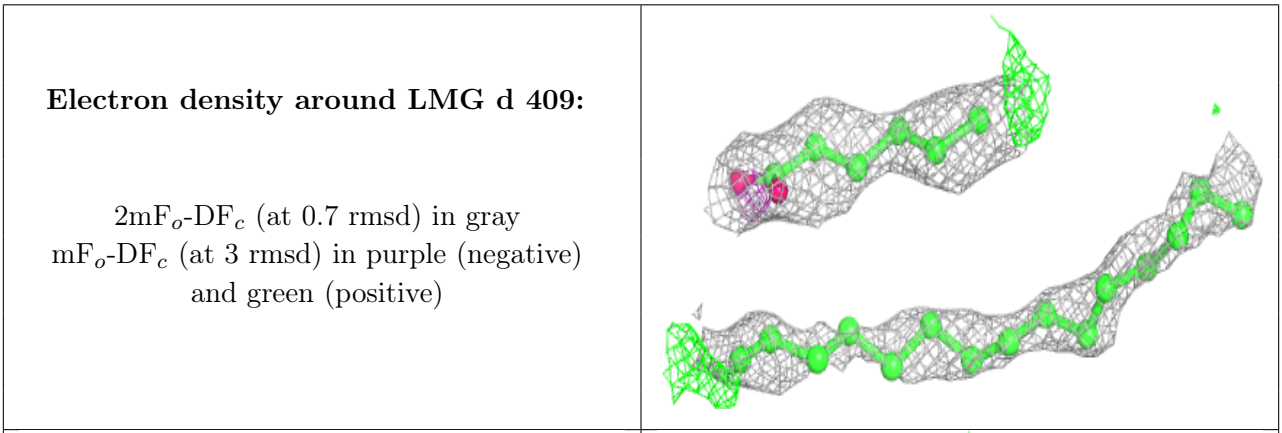
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

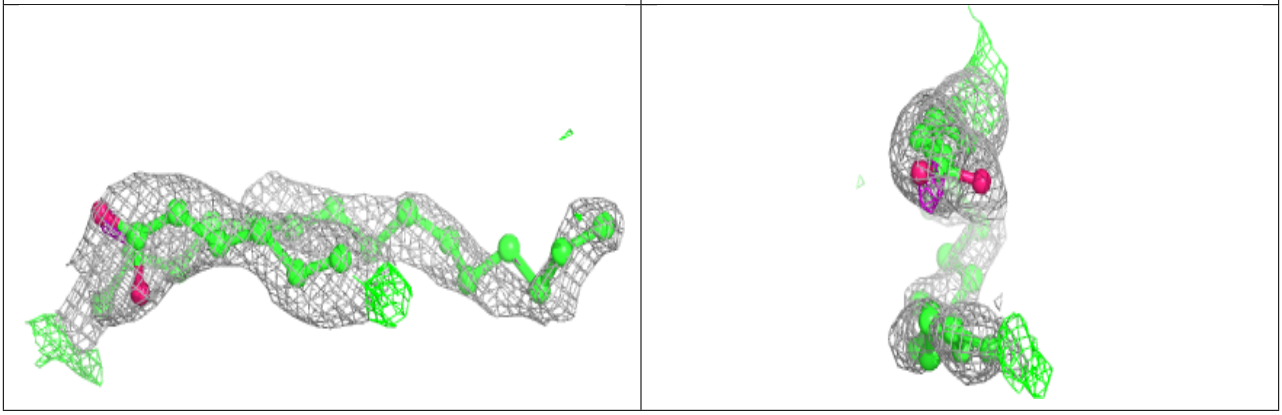




Electron density around LMG d 409:

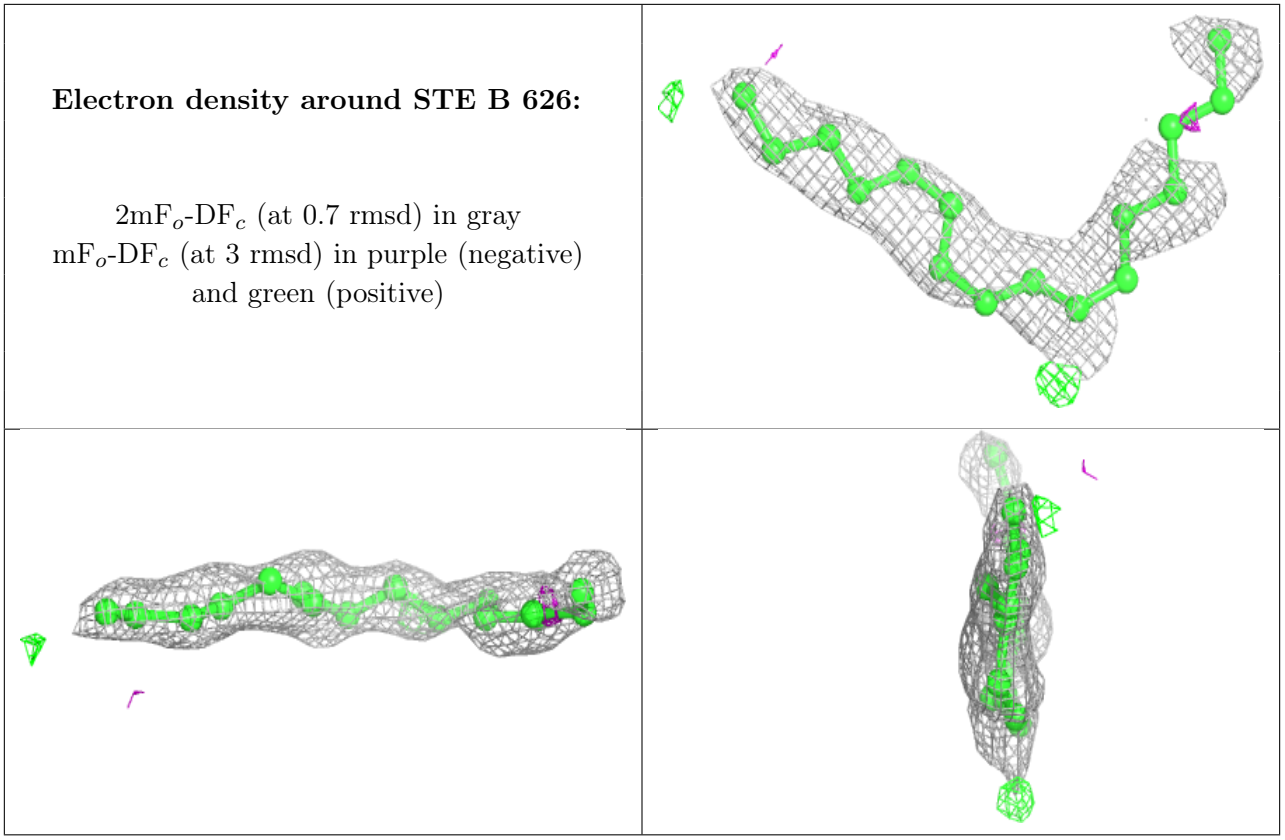
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





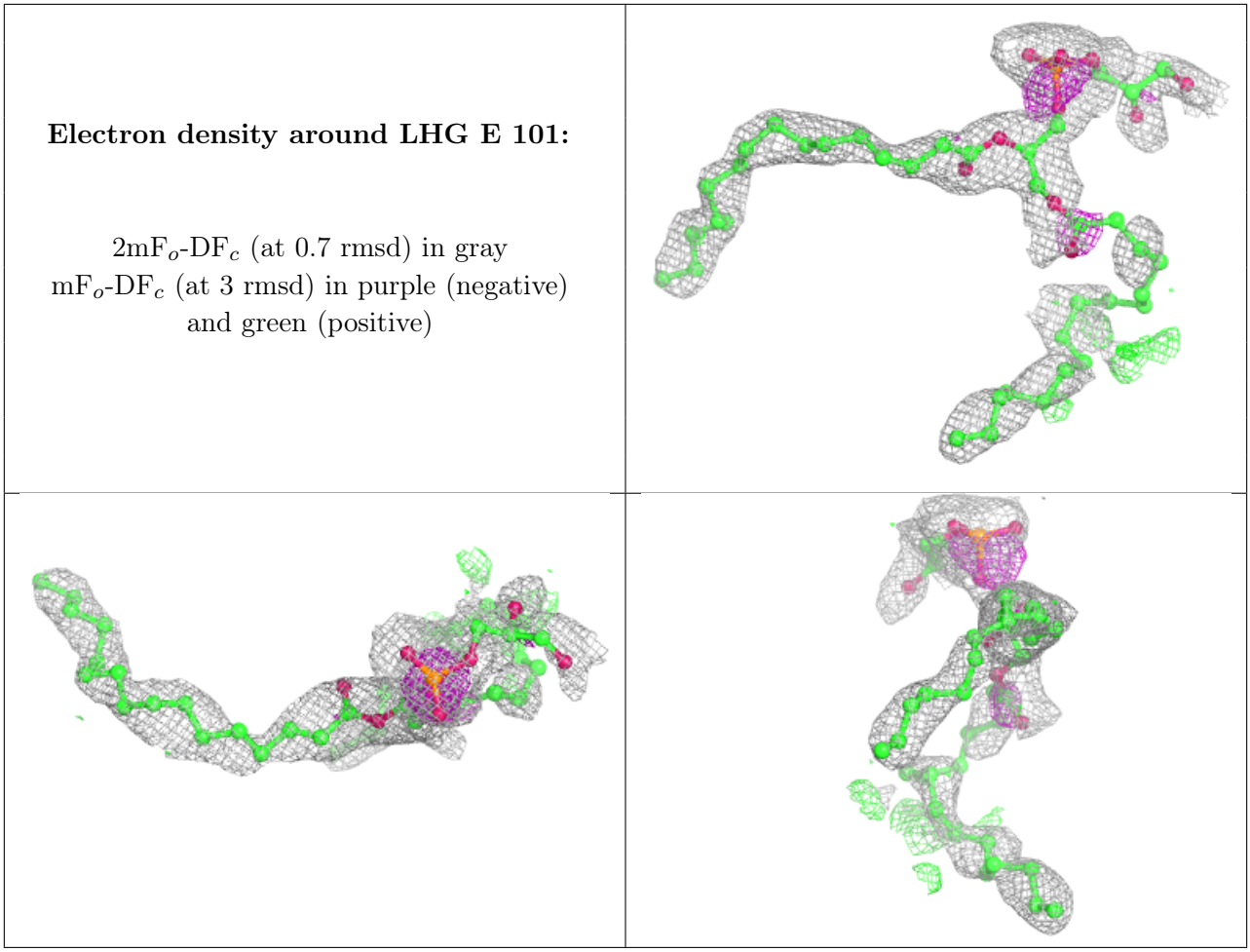
Electron density around STE B 626:

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



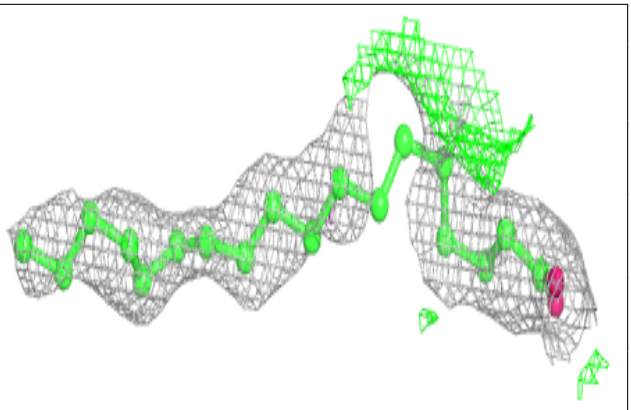
Electron density around LHG E 101:

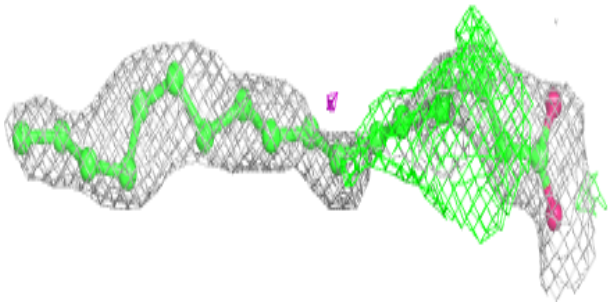
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

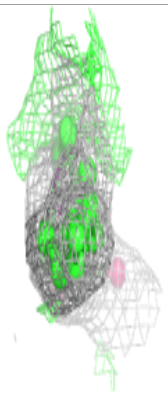


Electron density around STE b 622:

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

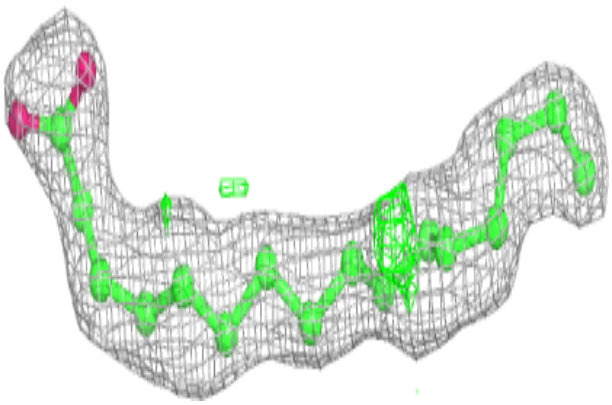


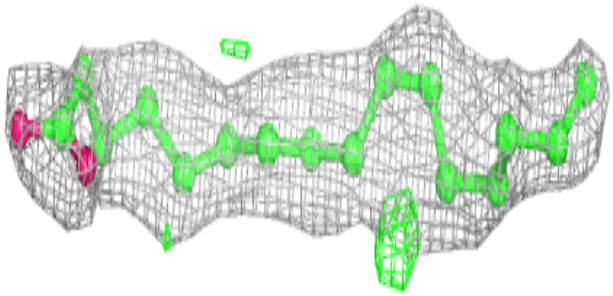


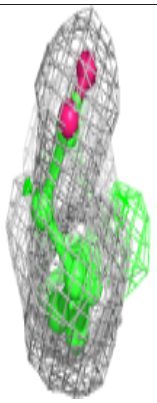


Electron density around STE B 624:

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

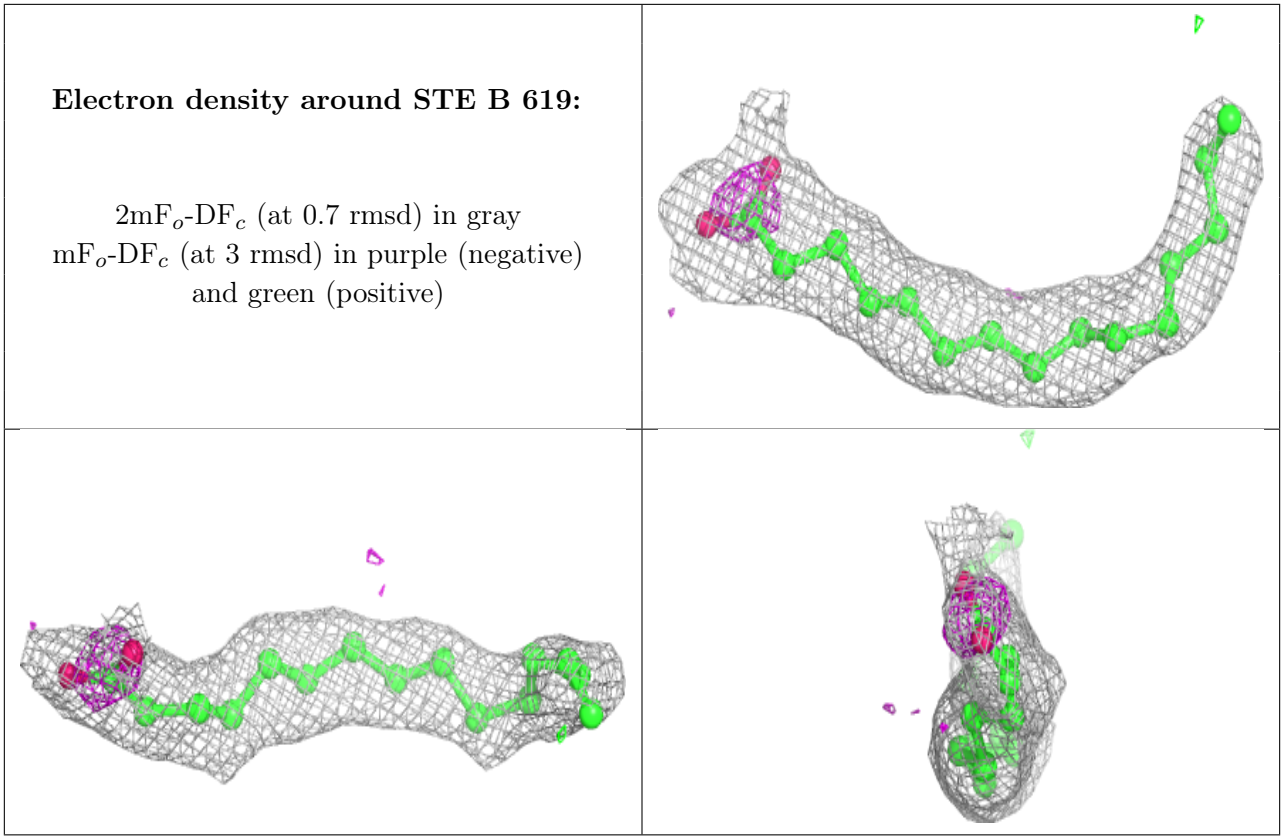






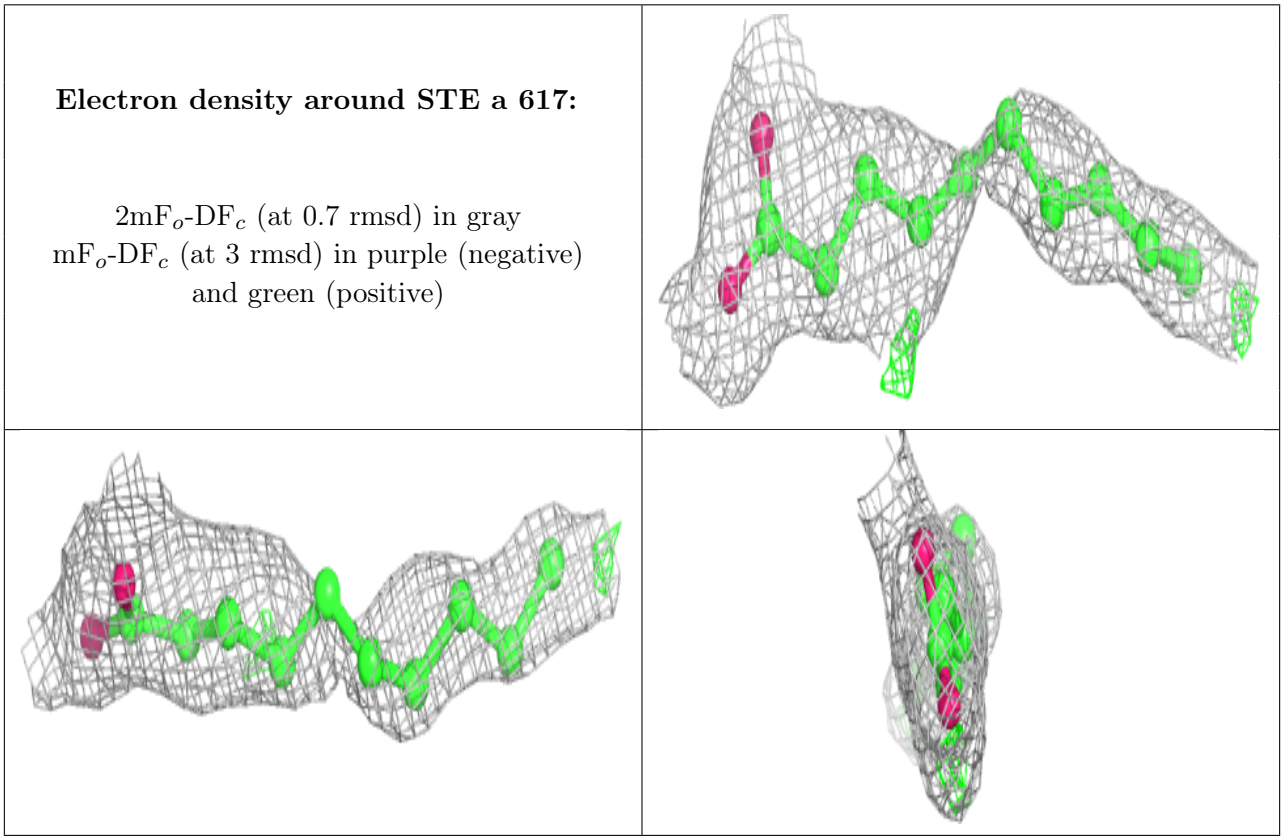
Electron density around STE B 619:

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



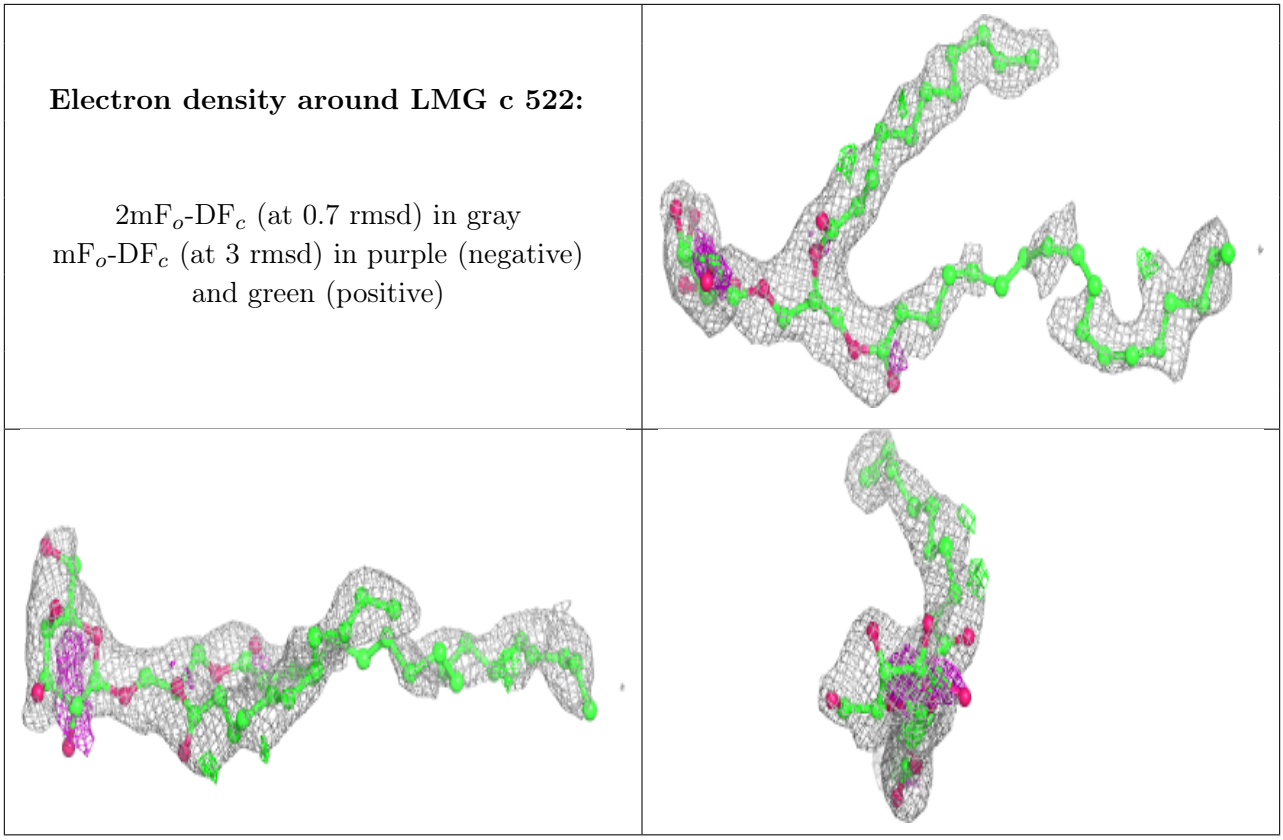
Electron density around STE a 617:

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



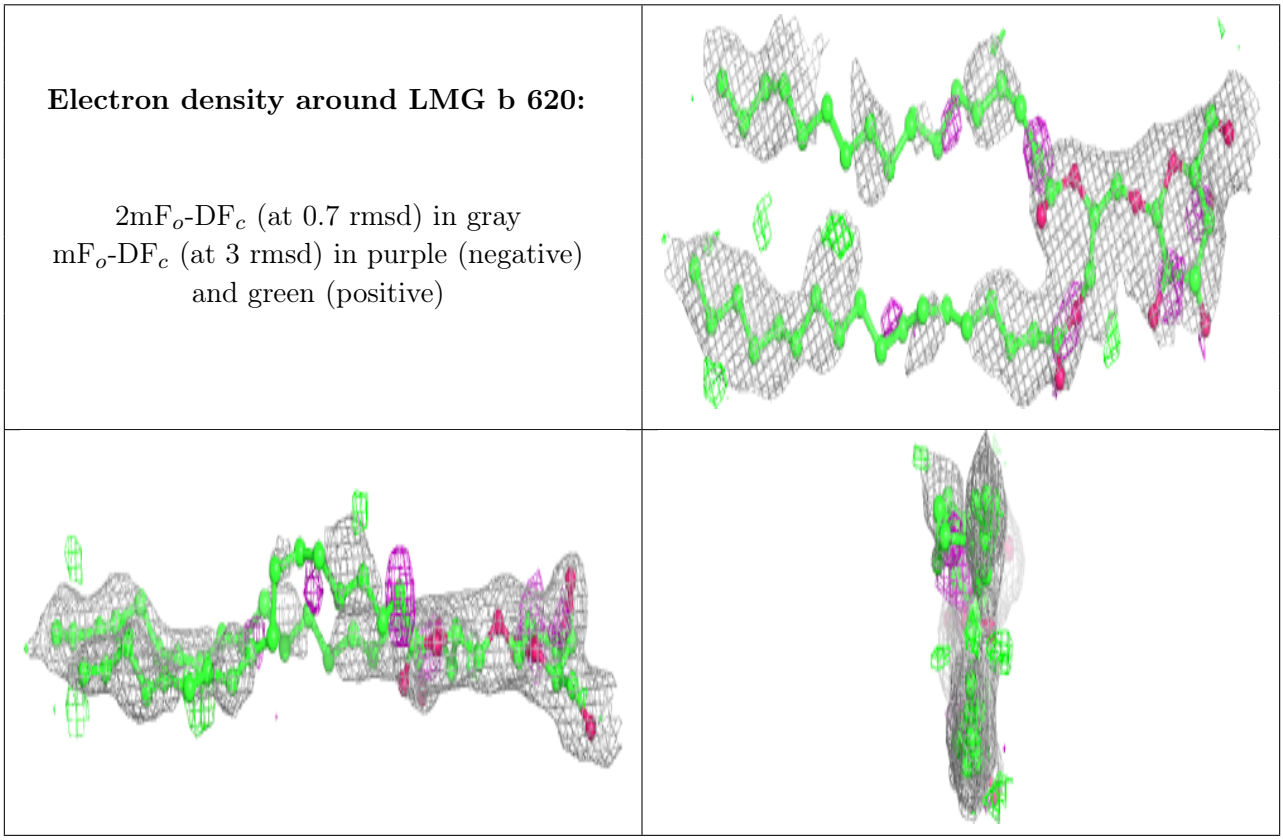
Electron density around LMG c 522:

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



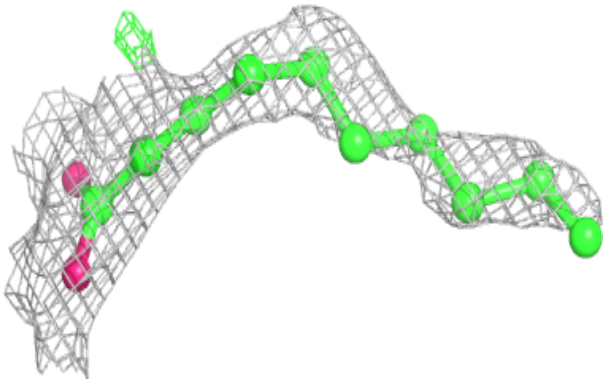
Electron density around LMG b 620:

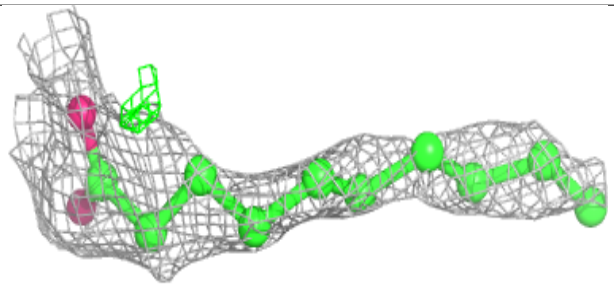
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

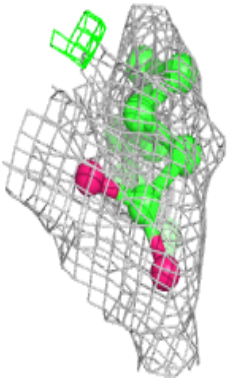


Electron density around STE R 101:

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

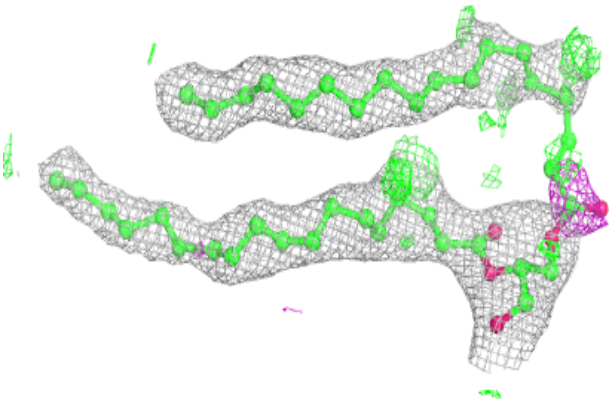


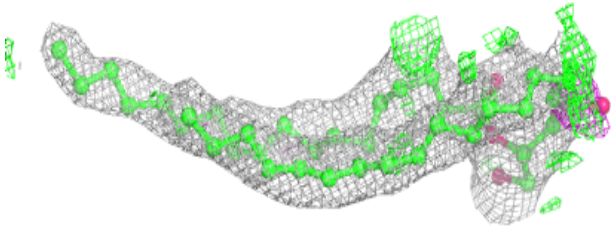


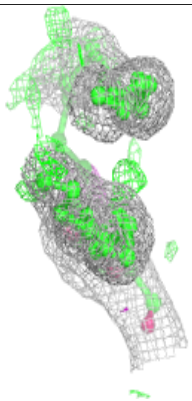


Electron density around DGD a 616:

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

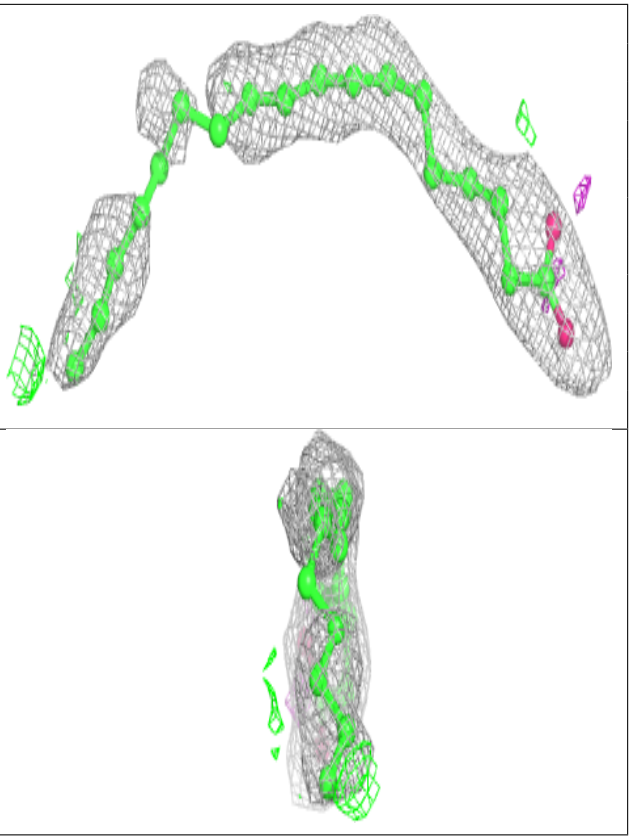






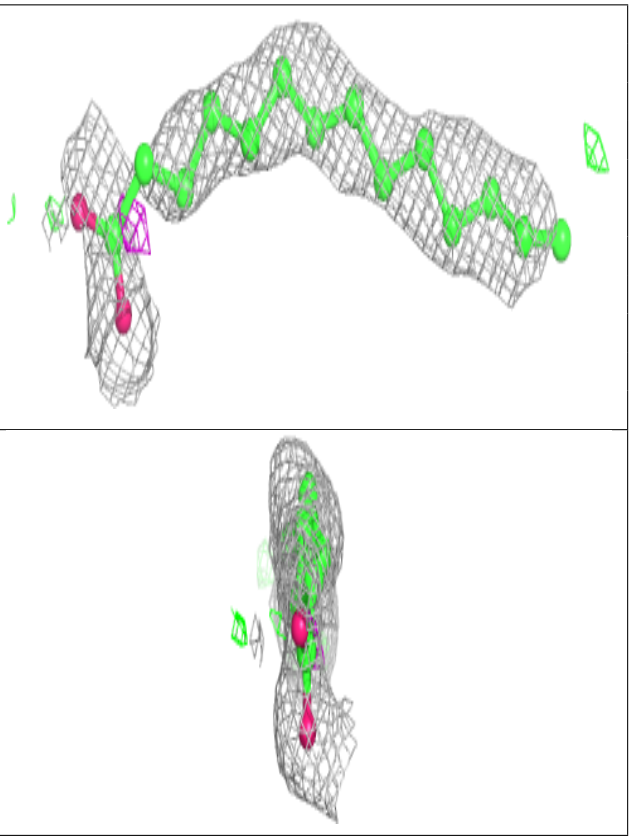
Electron density around STE x 102:

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



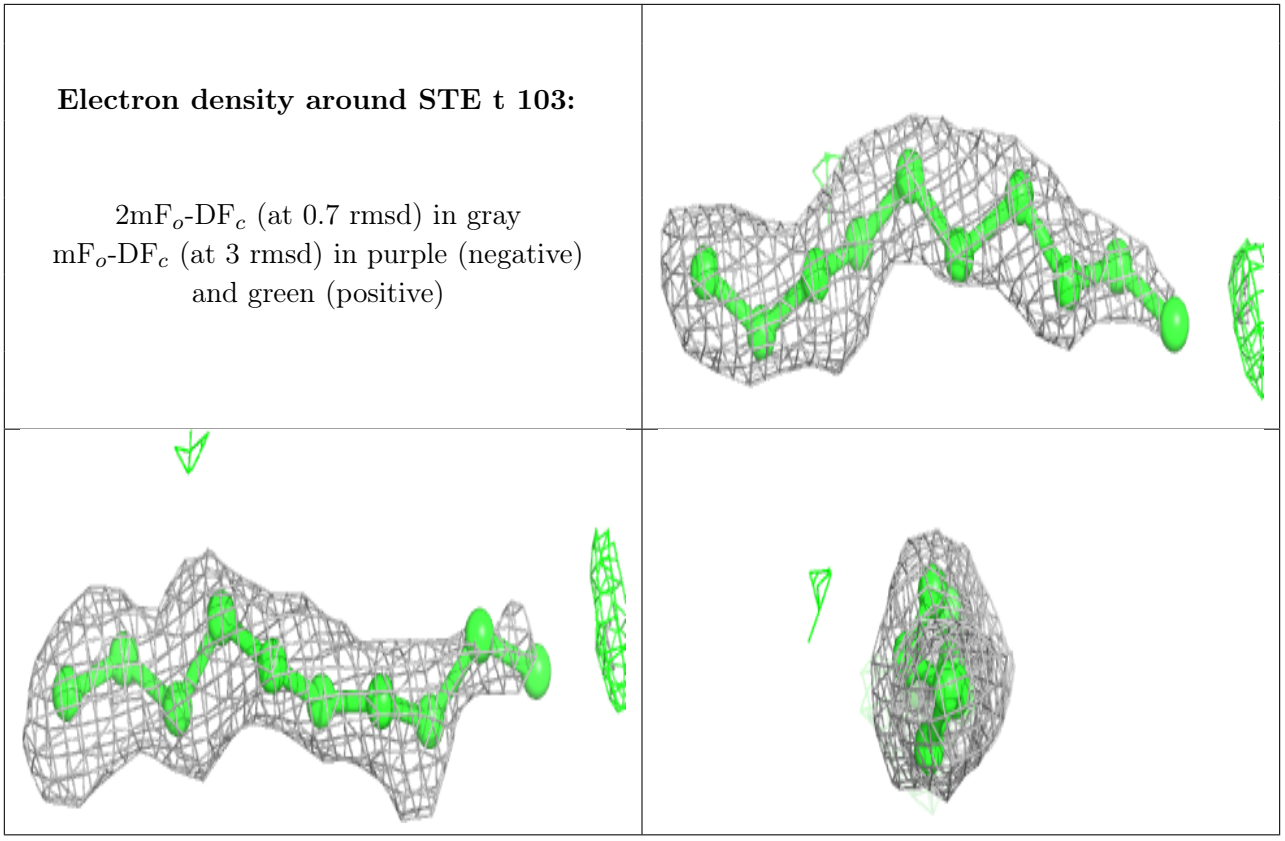
Electron density around STE b 621:

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



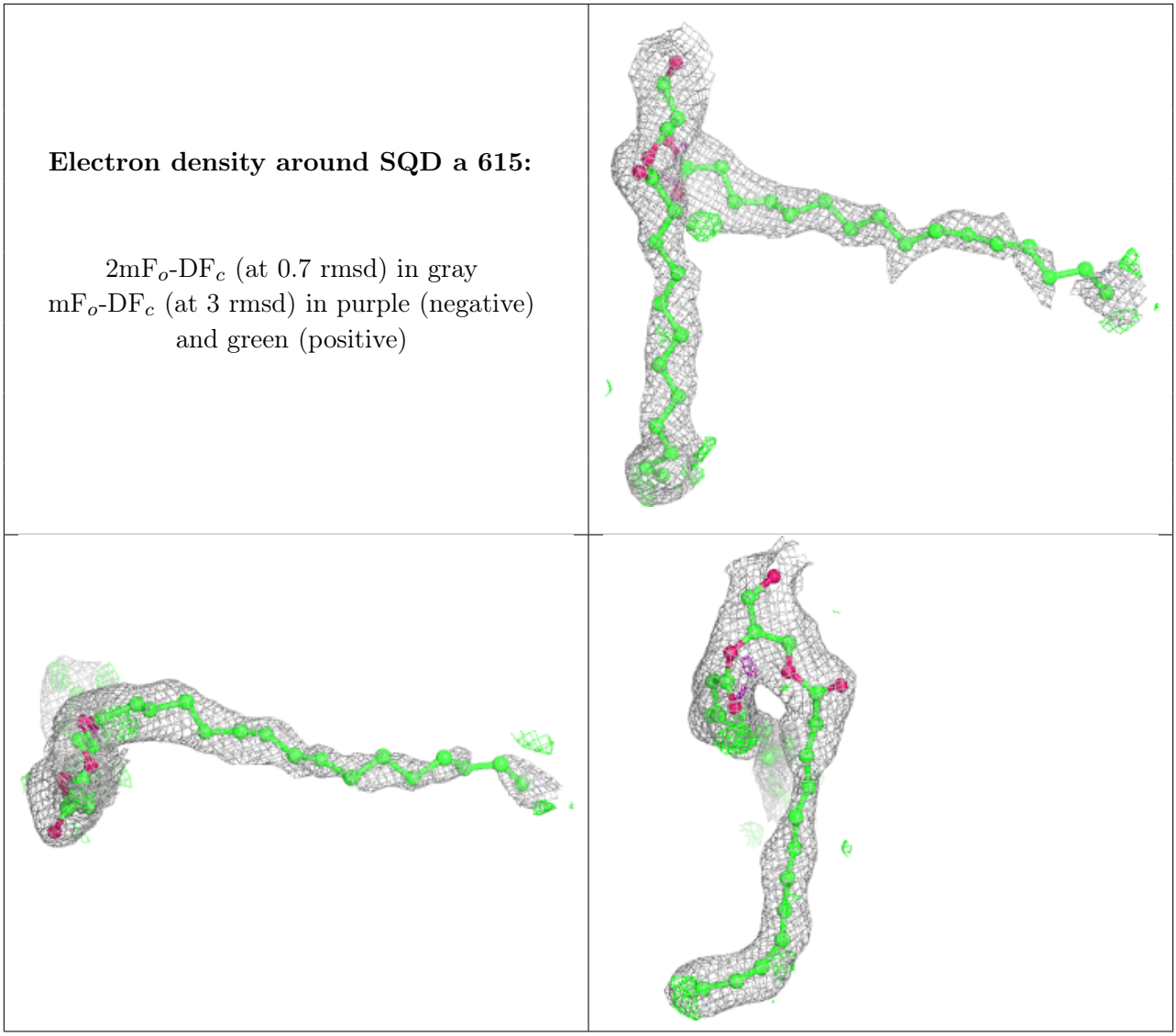
Electron density around STE t 103:

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



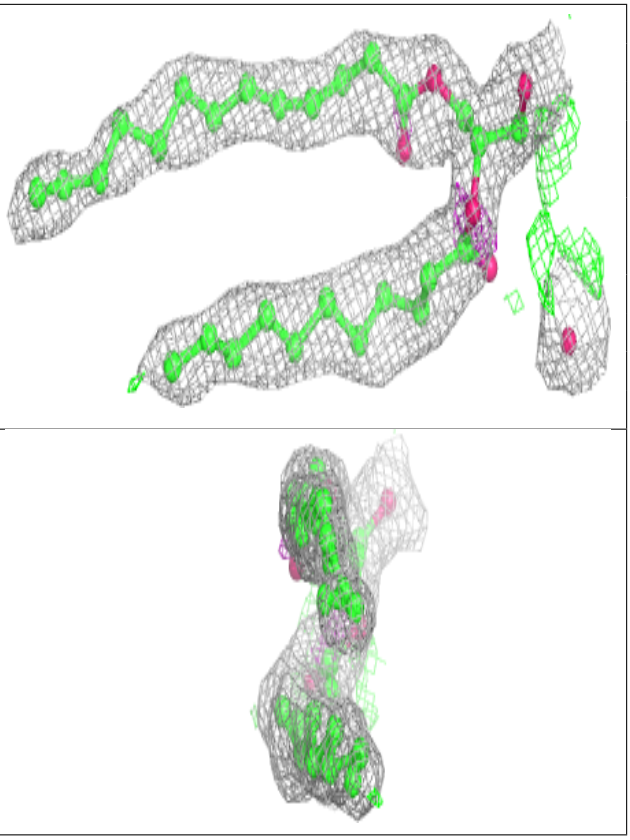
Electron density around SQD a 615:

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



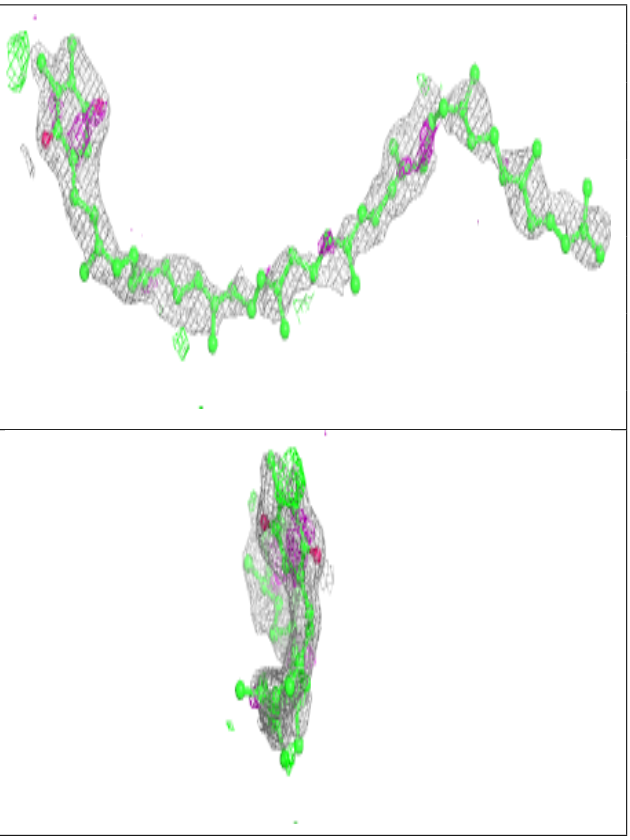
Electron density around LMG D 409:

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



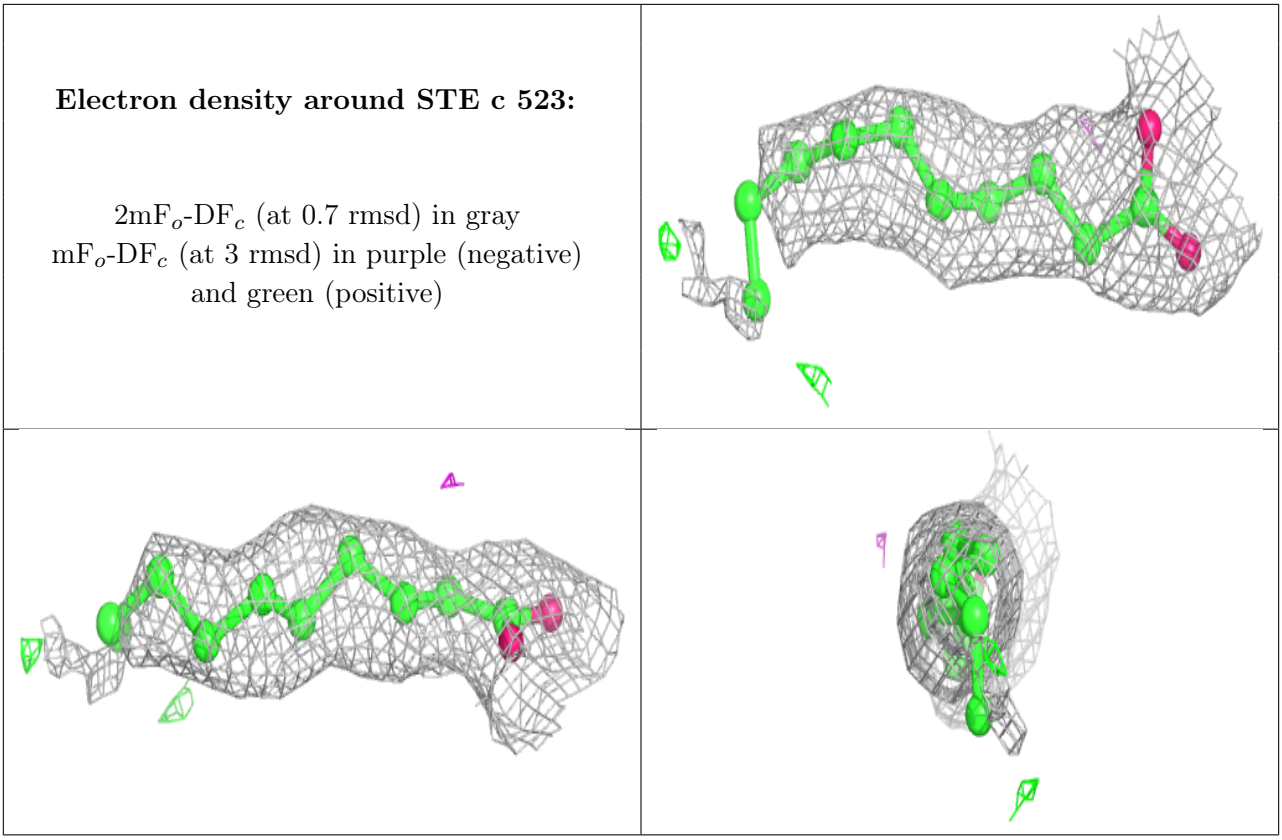
Electron density around PL9 A 612:

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



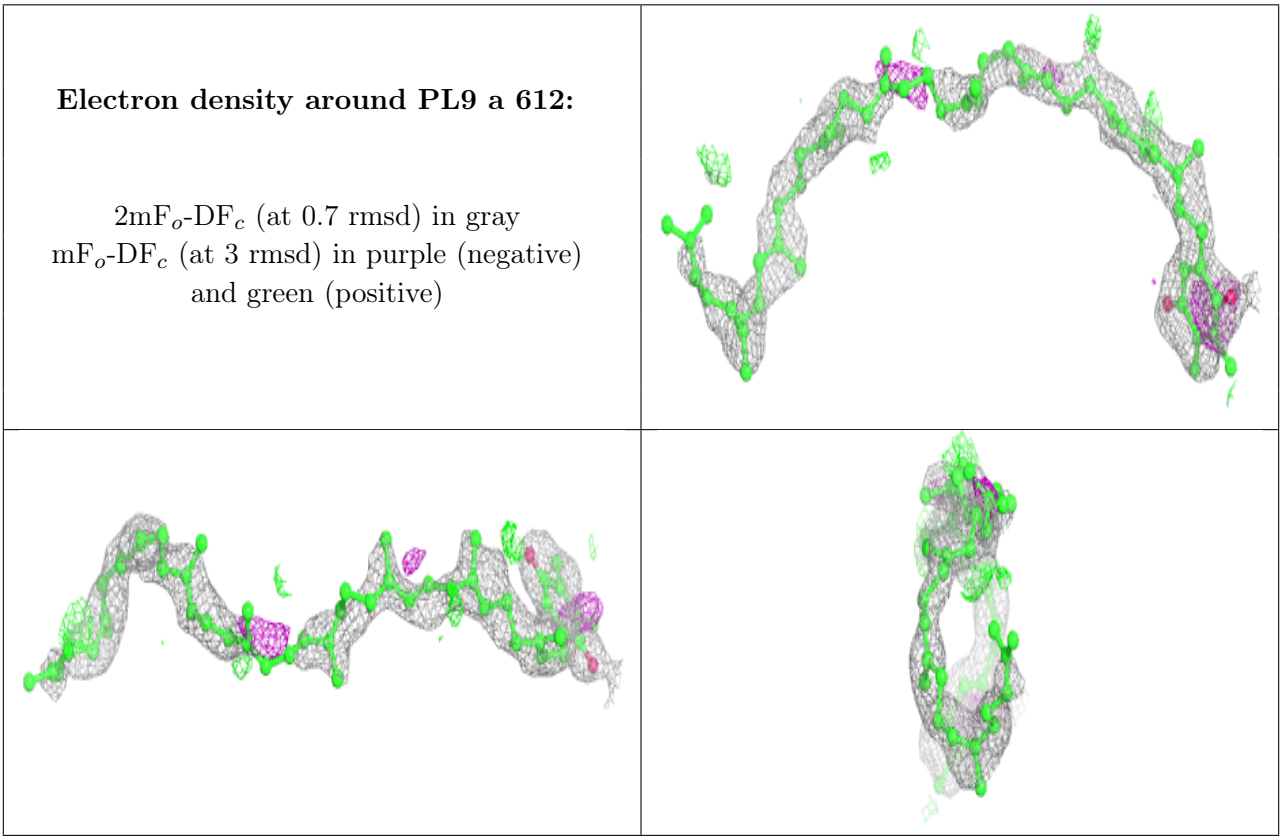
Electron density around STE c 523:

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



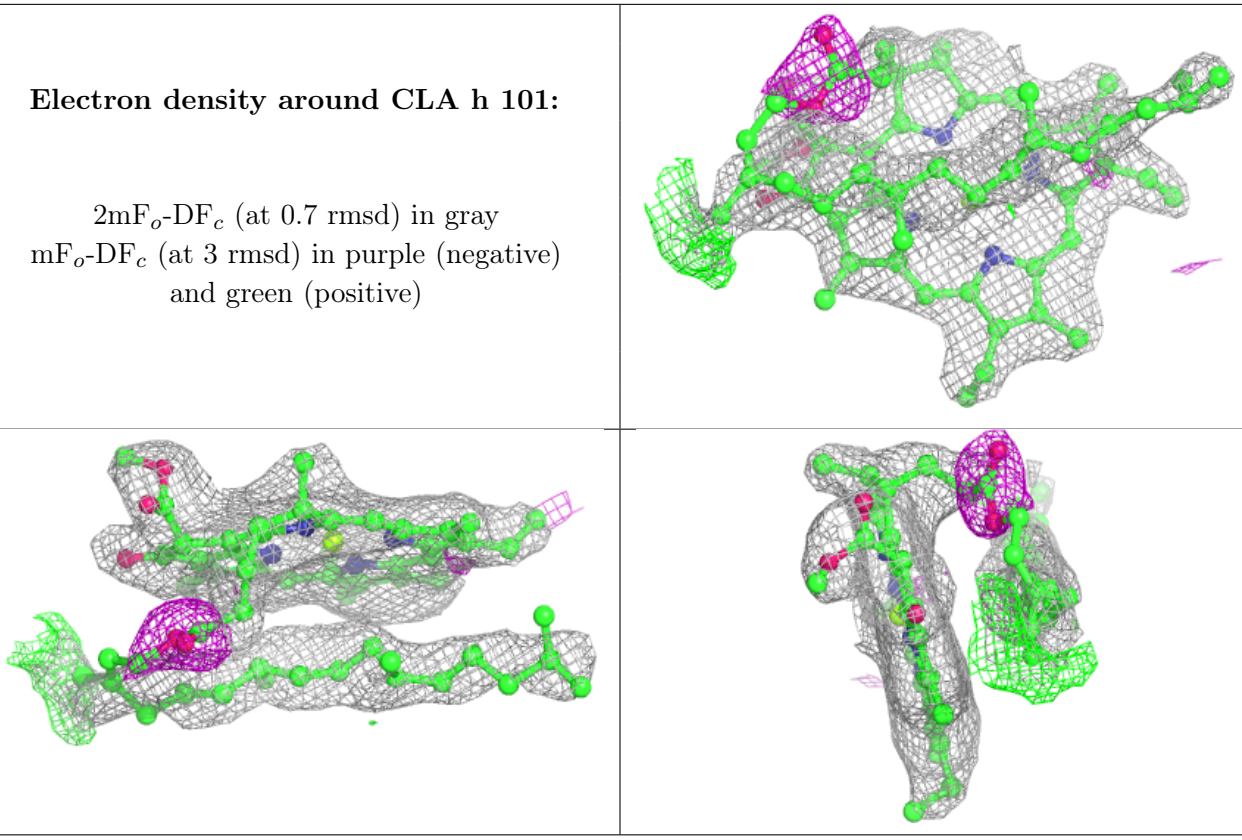
Electron density around PL9 a 612:

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



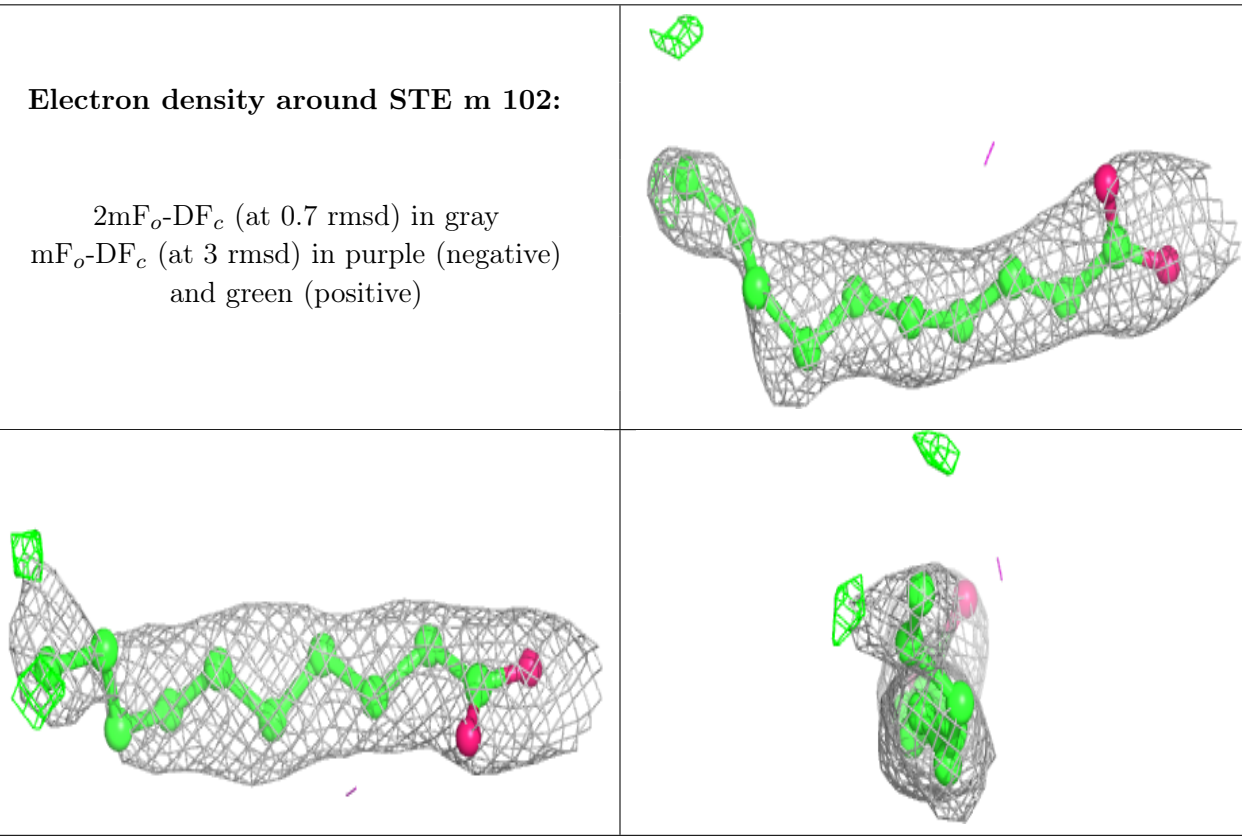
Electron density around CLA h 101:

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



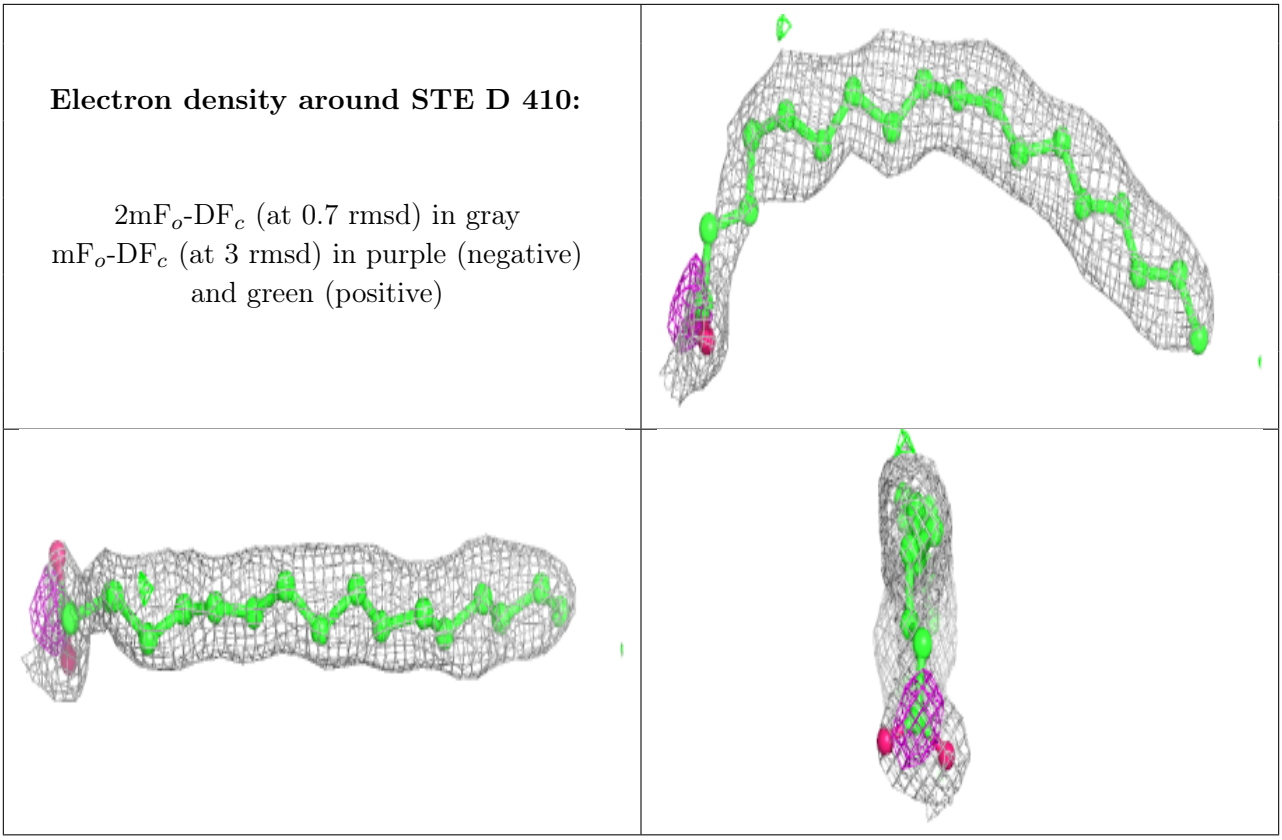
Electron density around STE m 102:

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



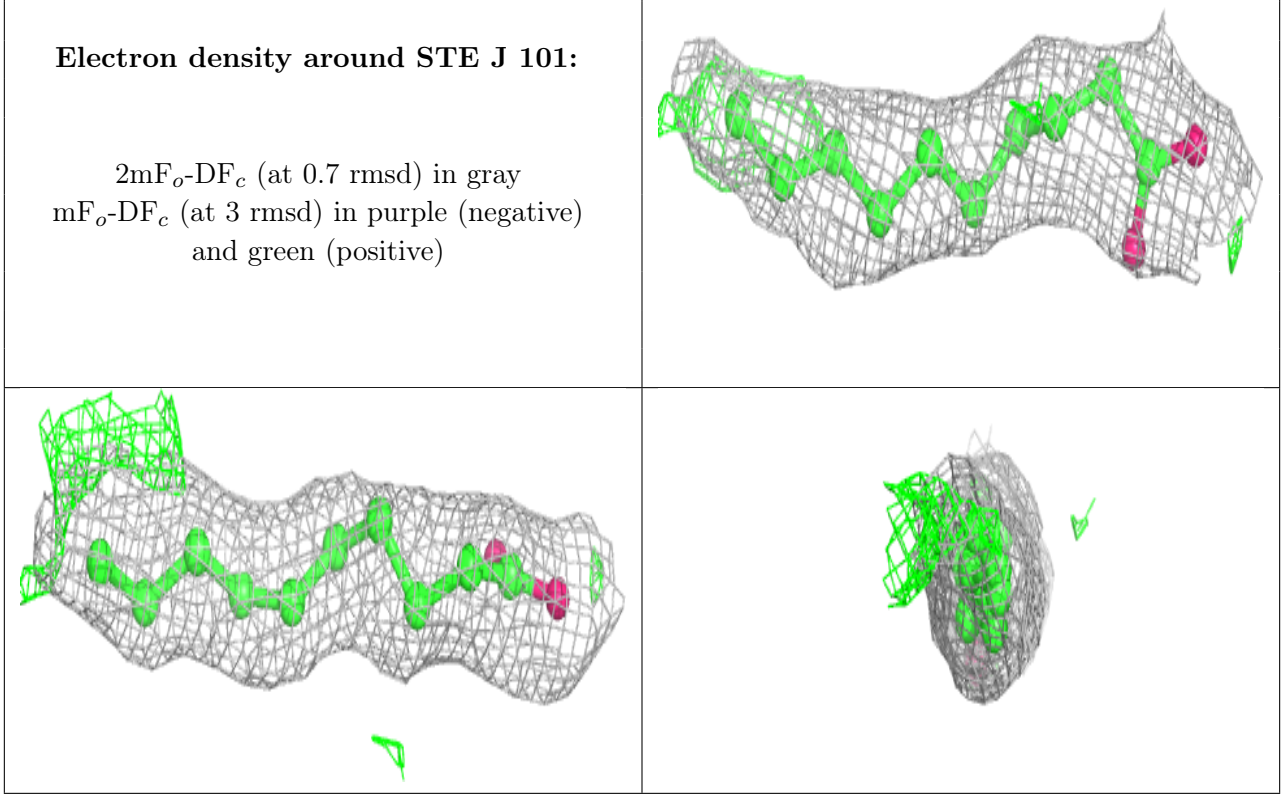
Electron density around STE D 410:

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



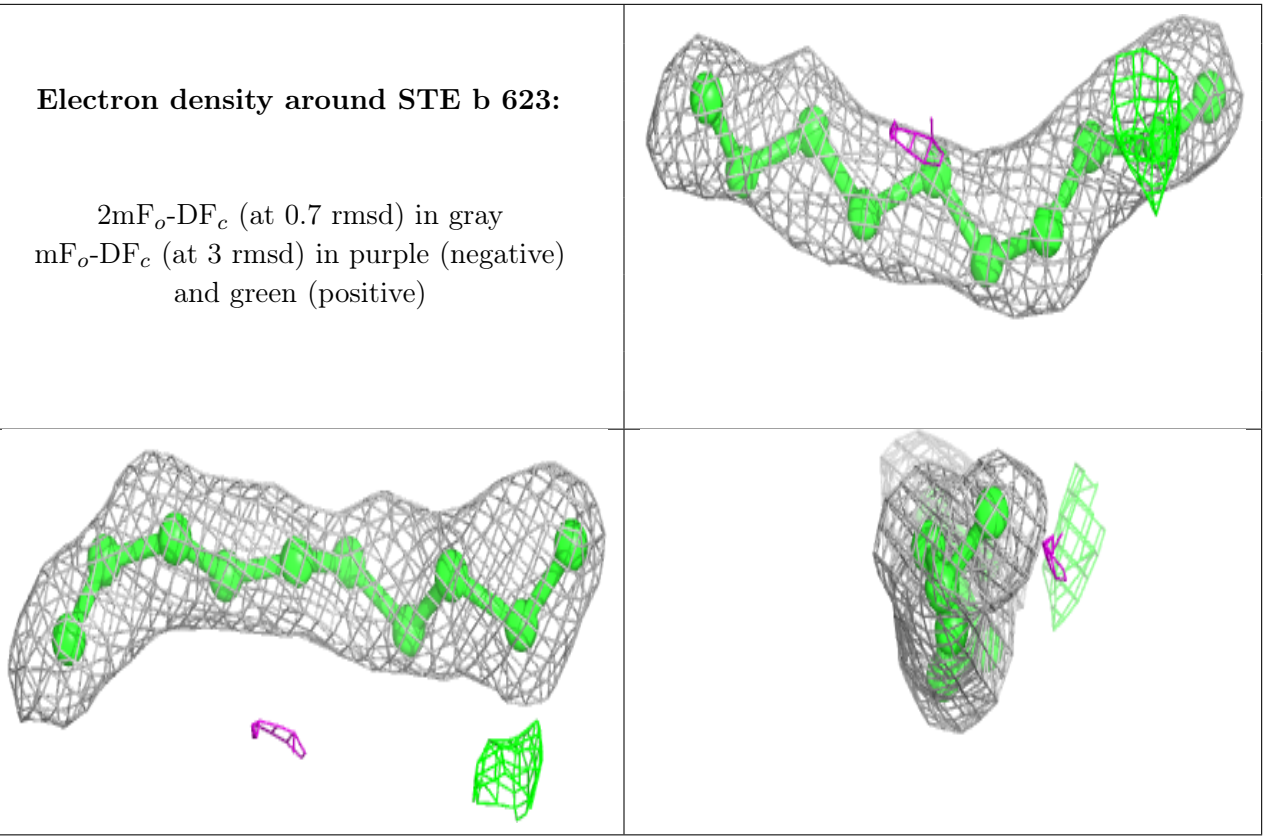
Electron density around STE J 101:

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



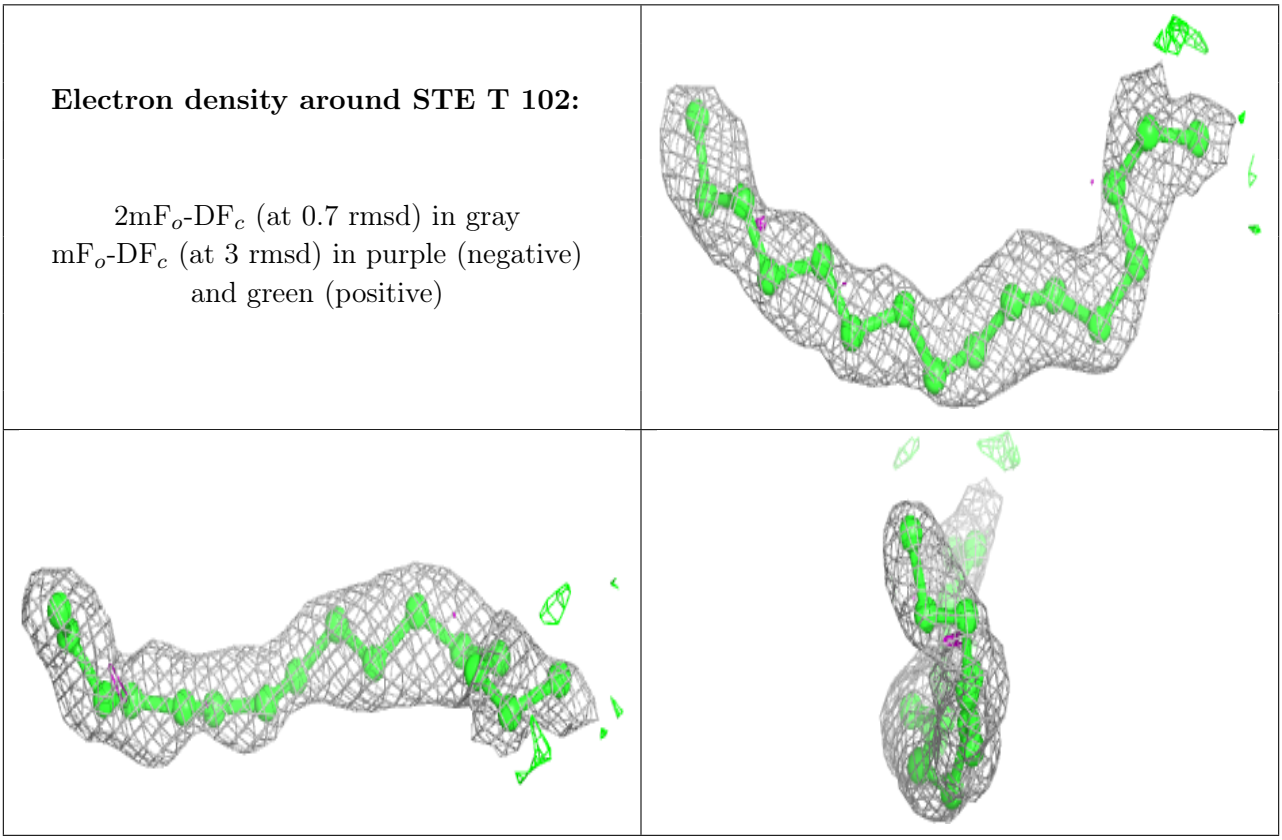
Electron density around STE b 623:

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



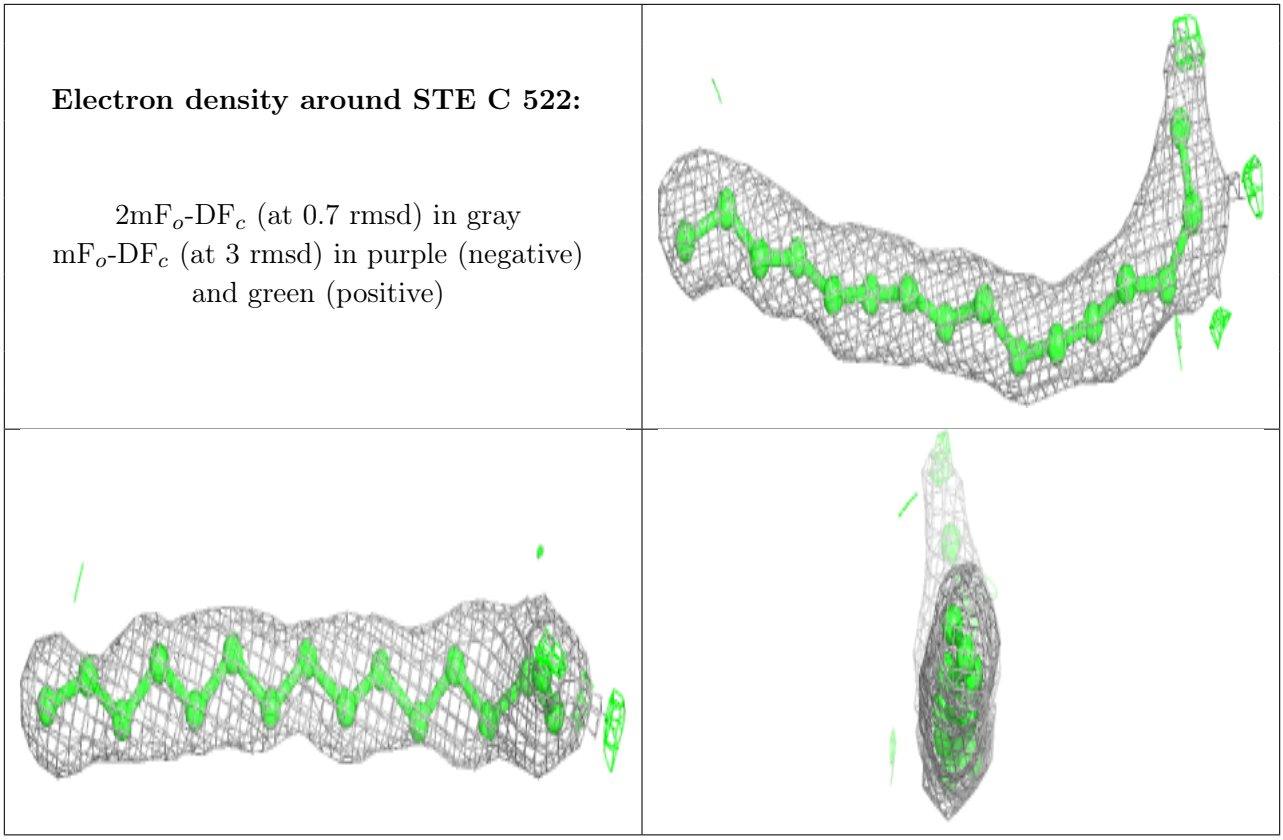
Electron density around STE T 102:

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



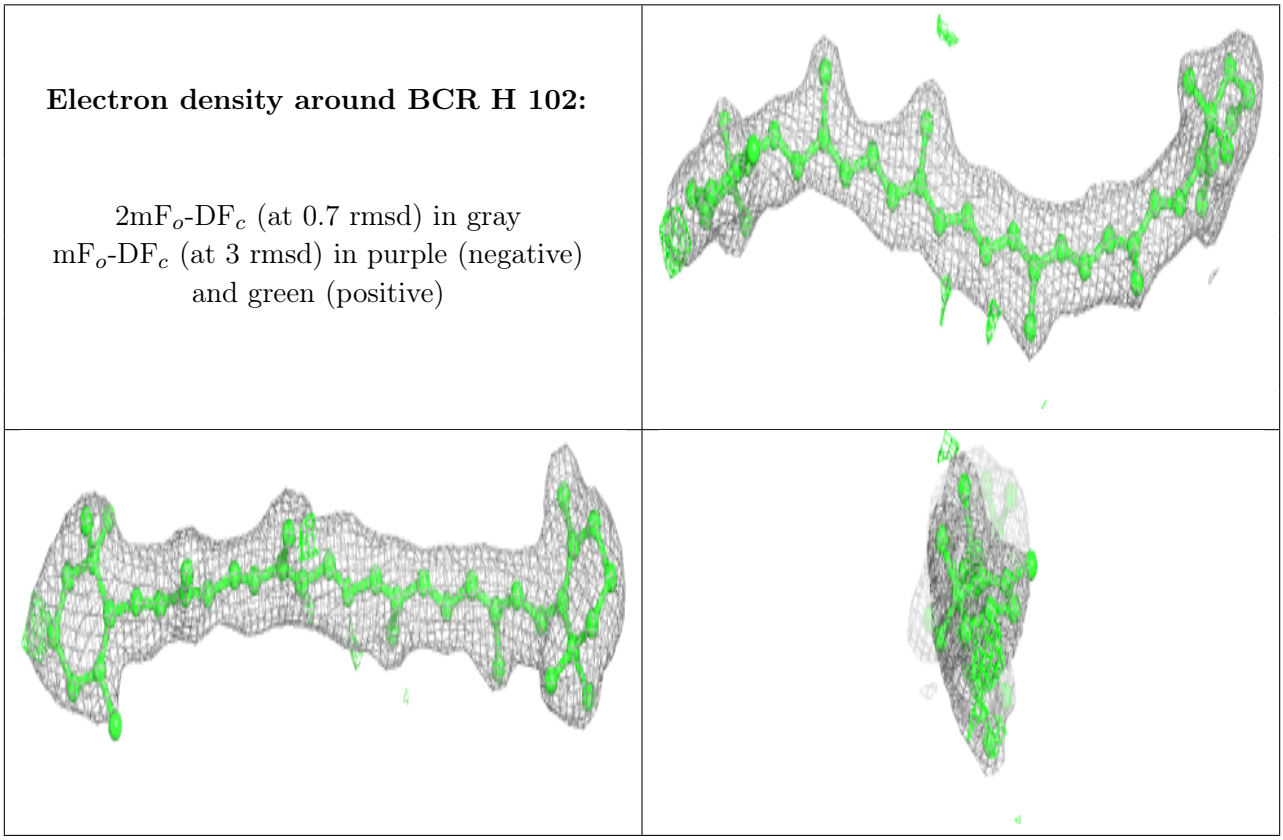
Electron density around STE C 522:

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



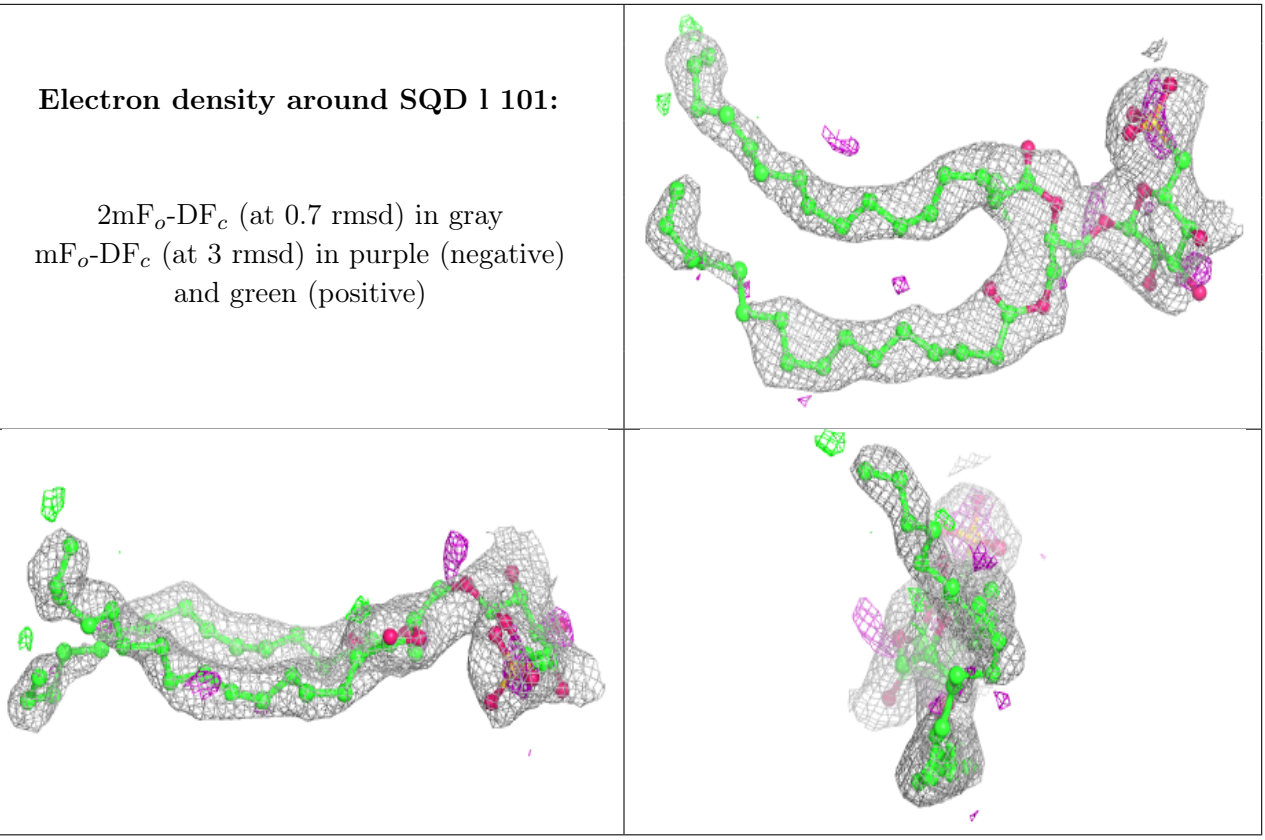
Electron density around BCR H 102:

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



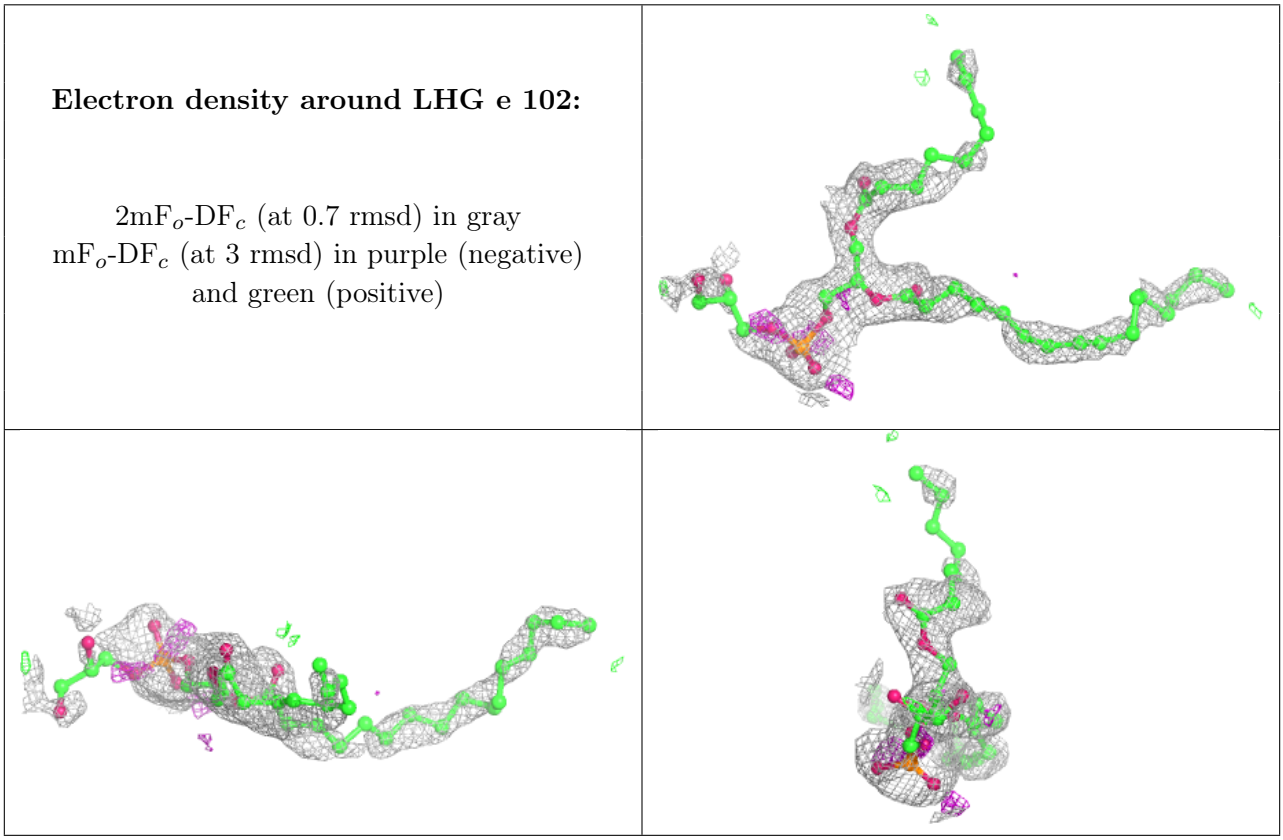
Electron density around SQD l 101:

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



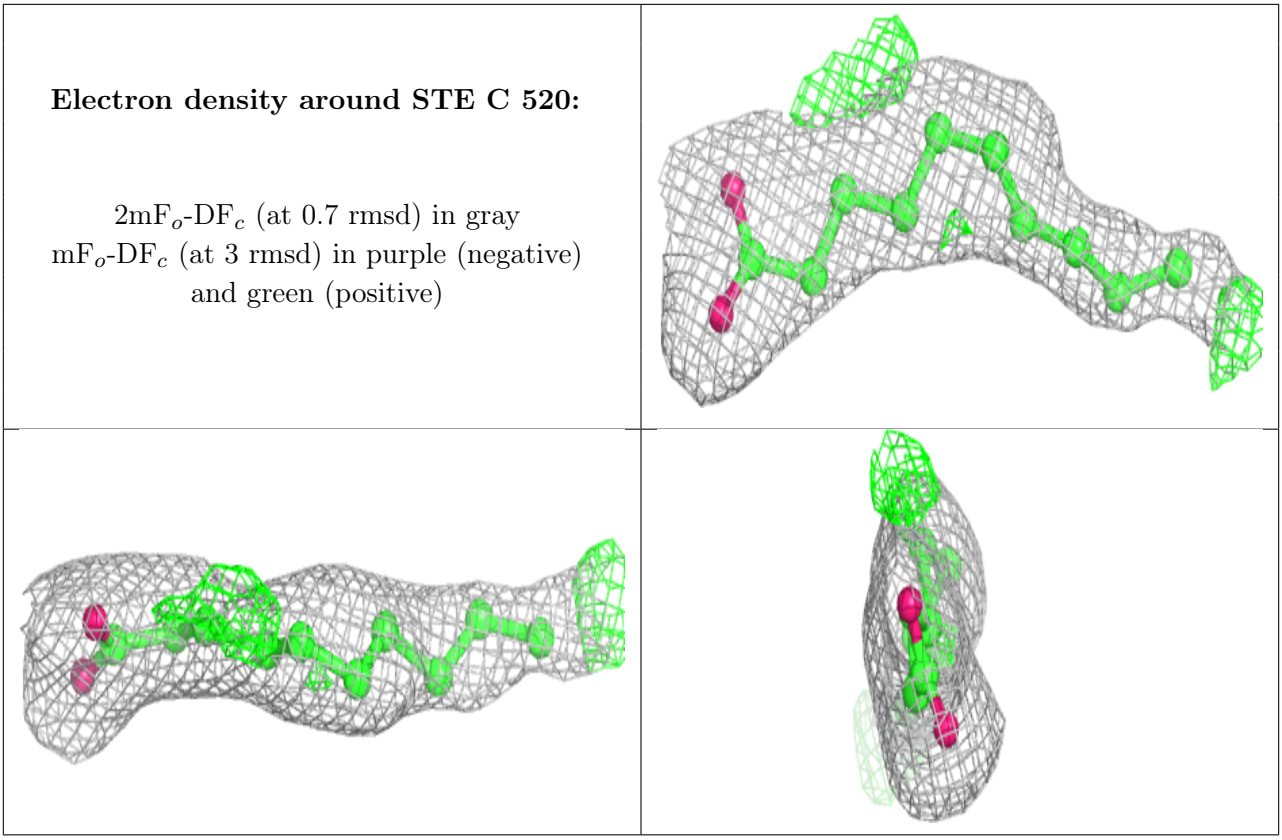
Electron density around LHG e 102:

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



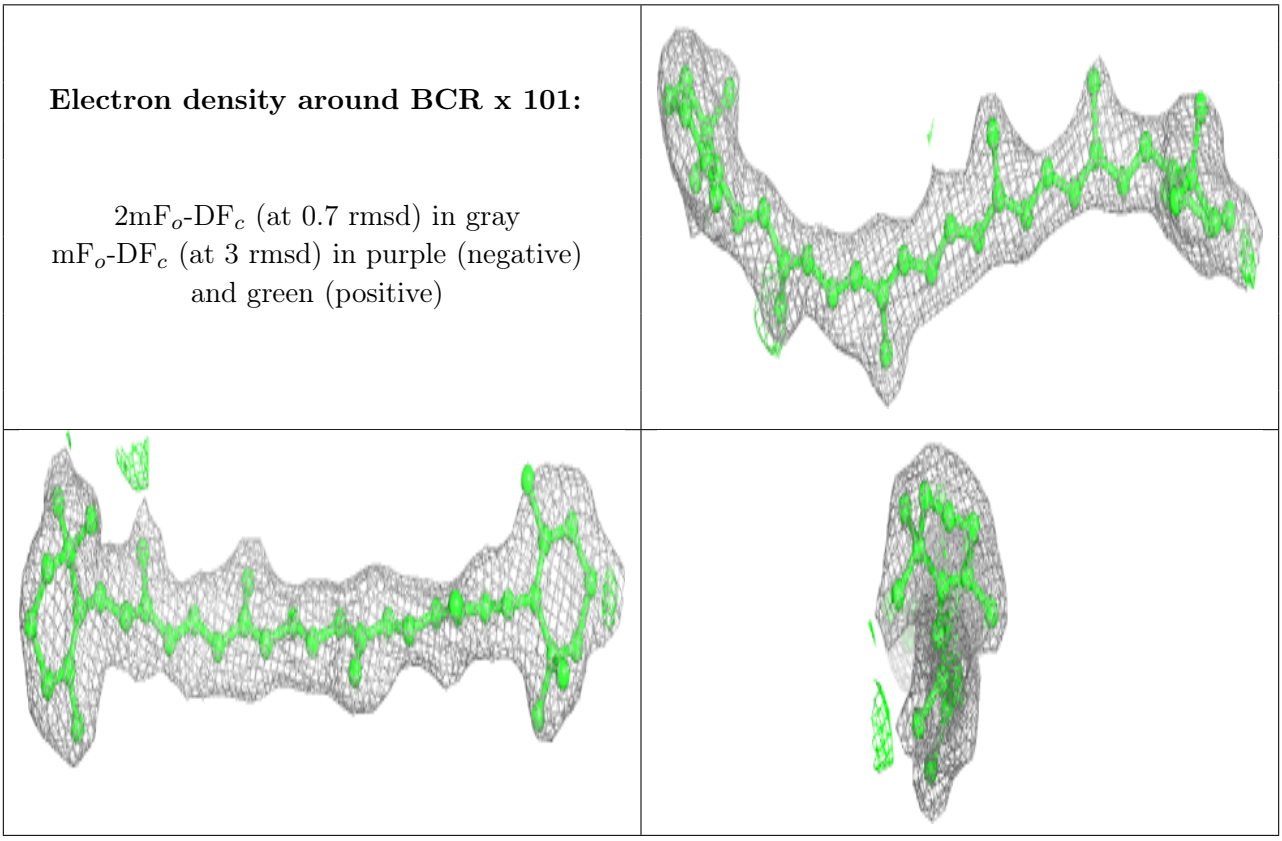
Electron density around STE C 520:

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



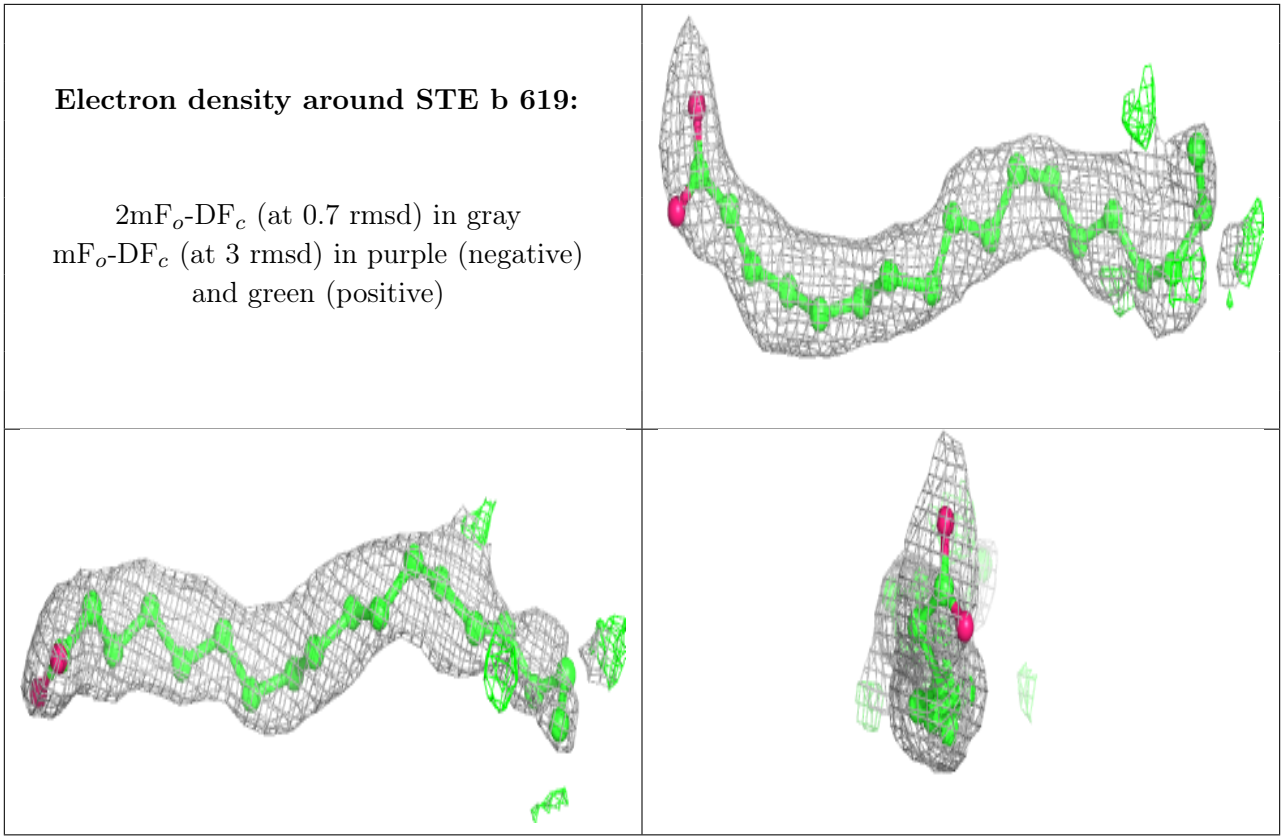
Electron density around BCR x 101:

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



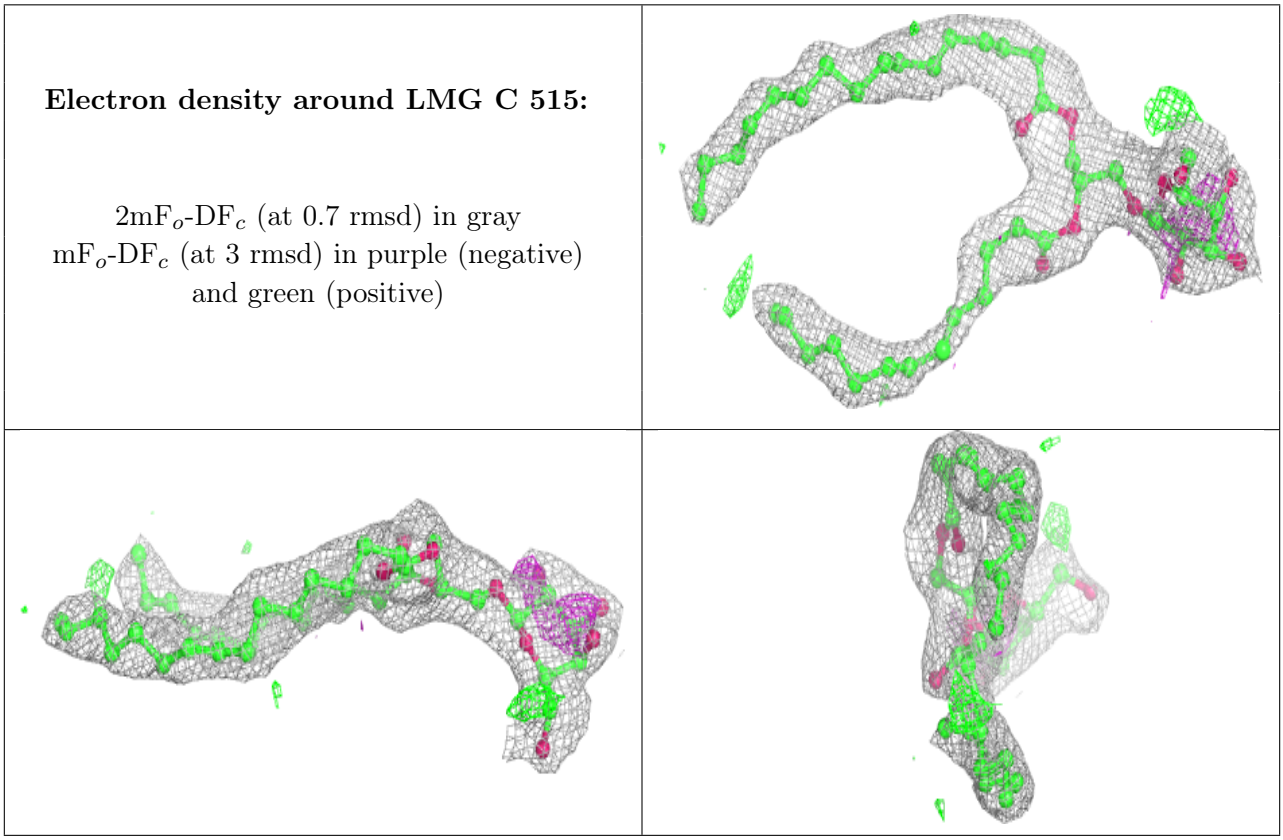
Electron density around STE b 619:

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



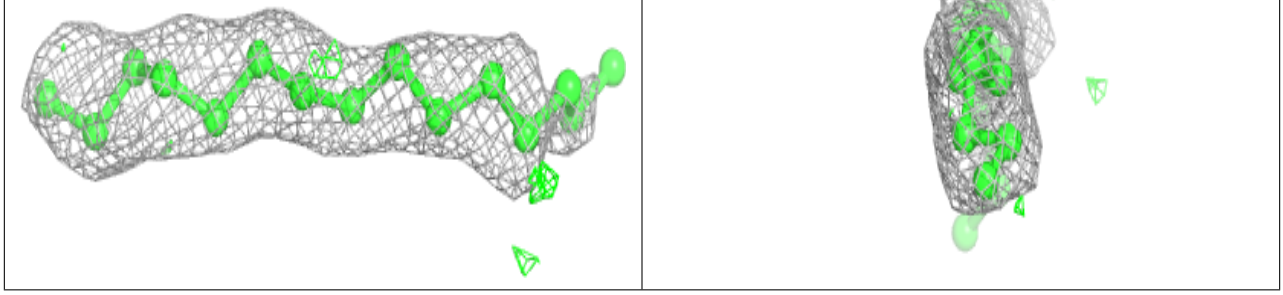
Electron density around LMG C 515:

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



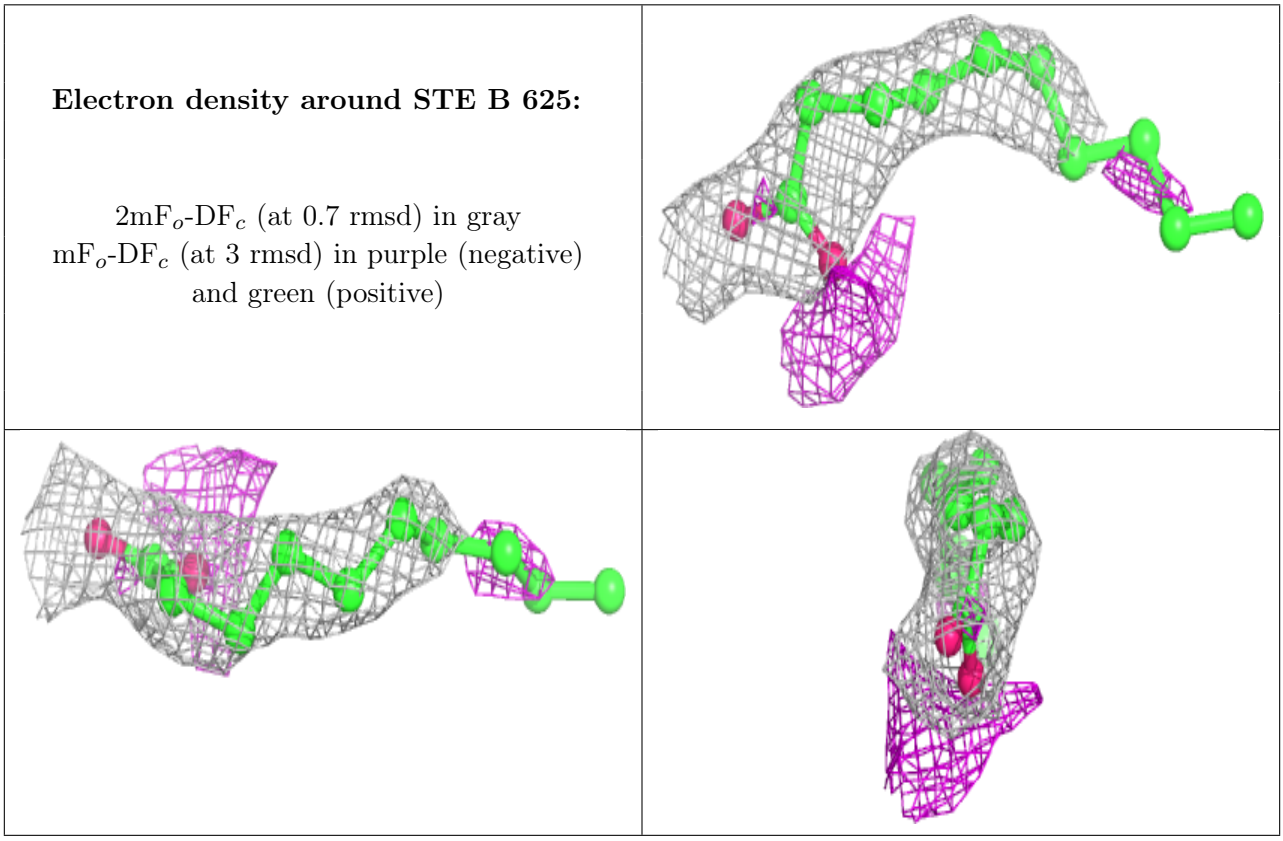
Electron density around STE T 103:

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



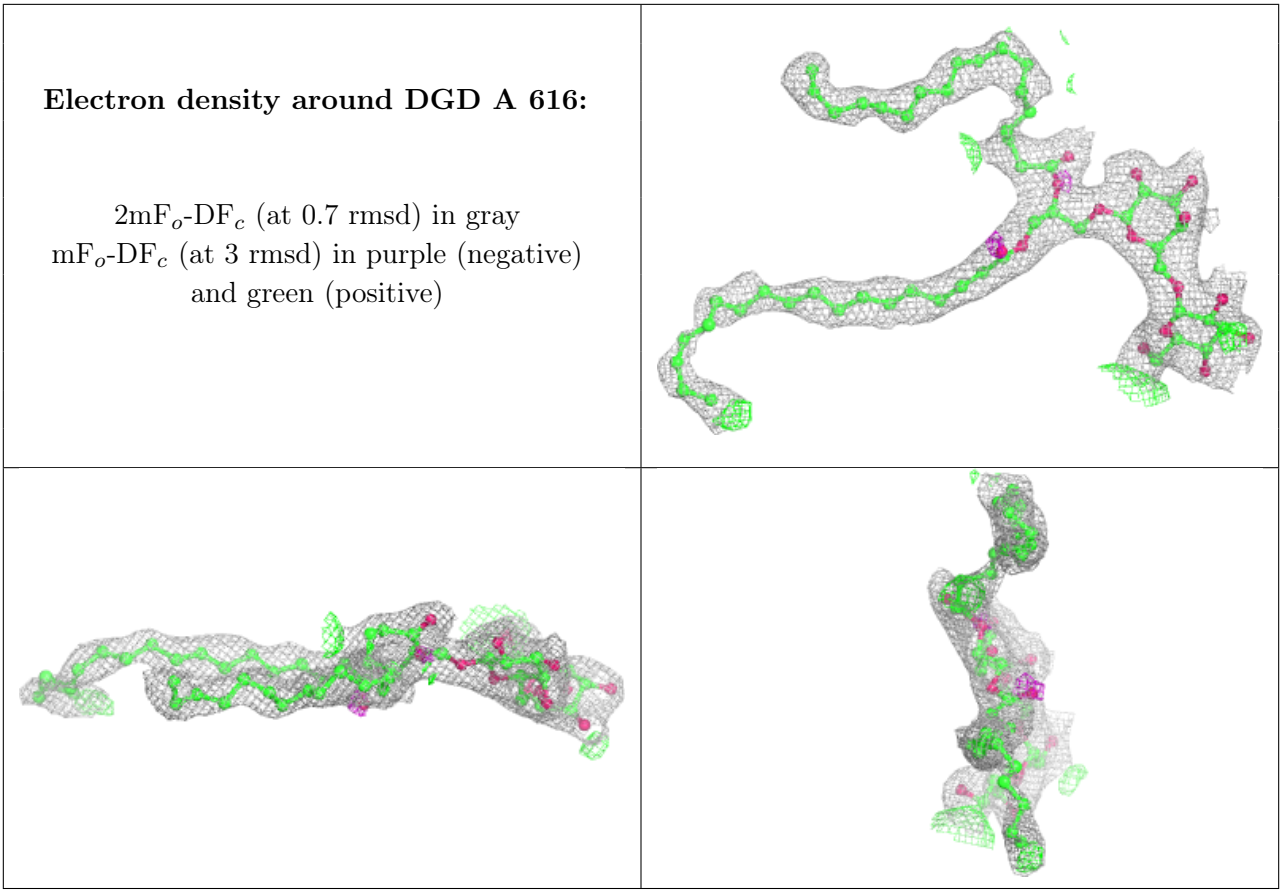
Electron density around STE B 625:

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



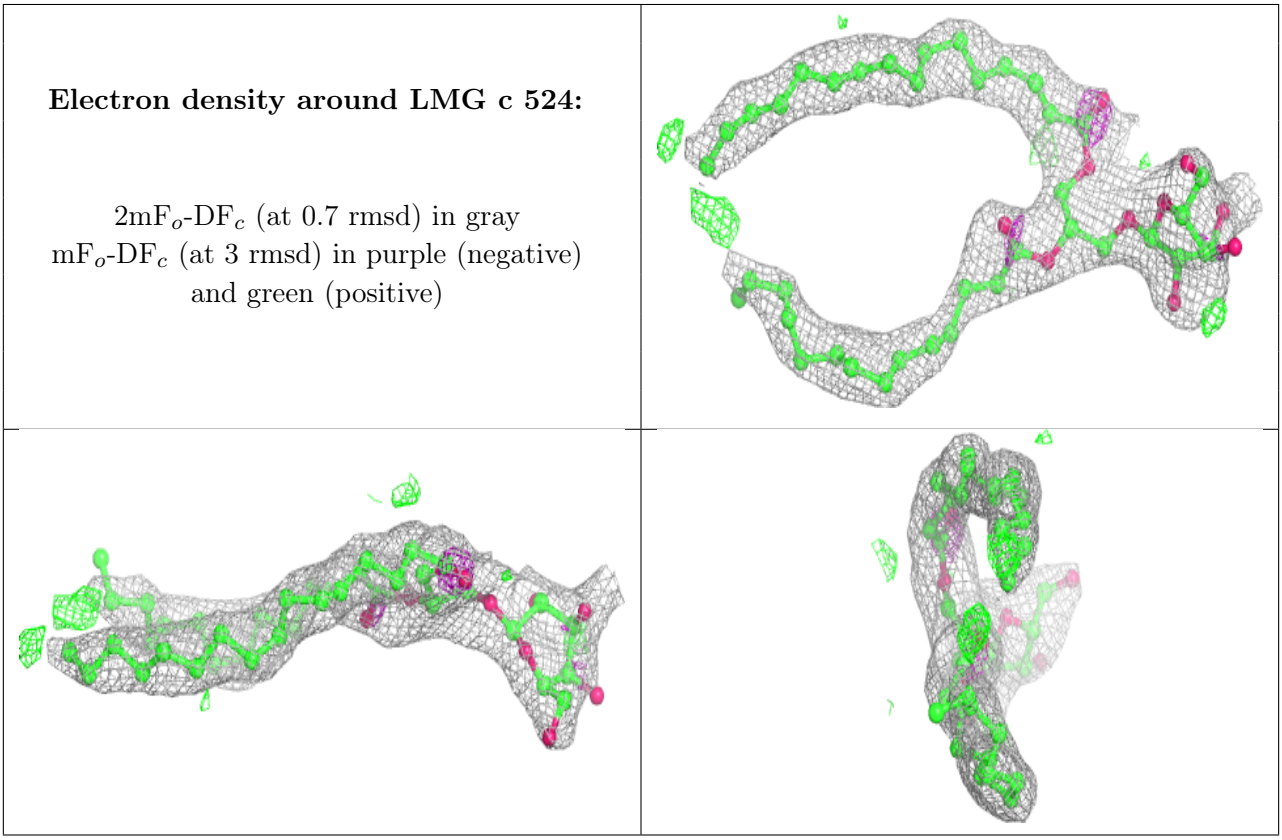
Electron density around DGD A 616:

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



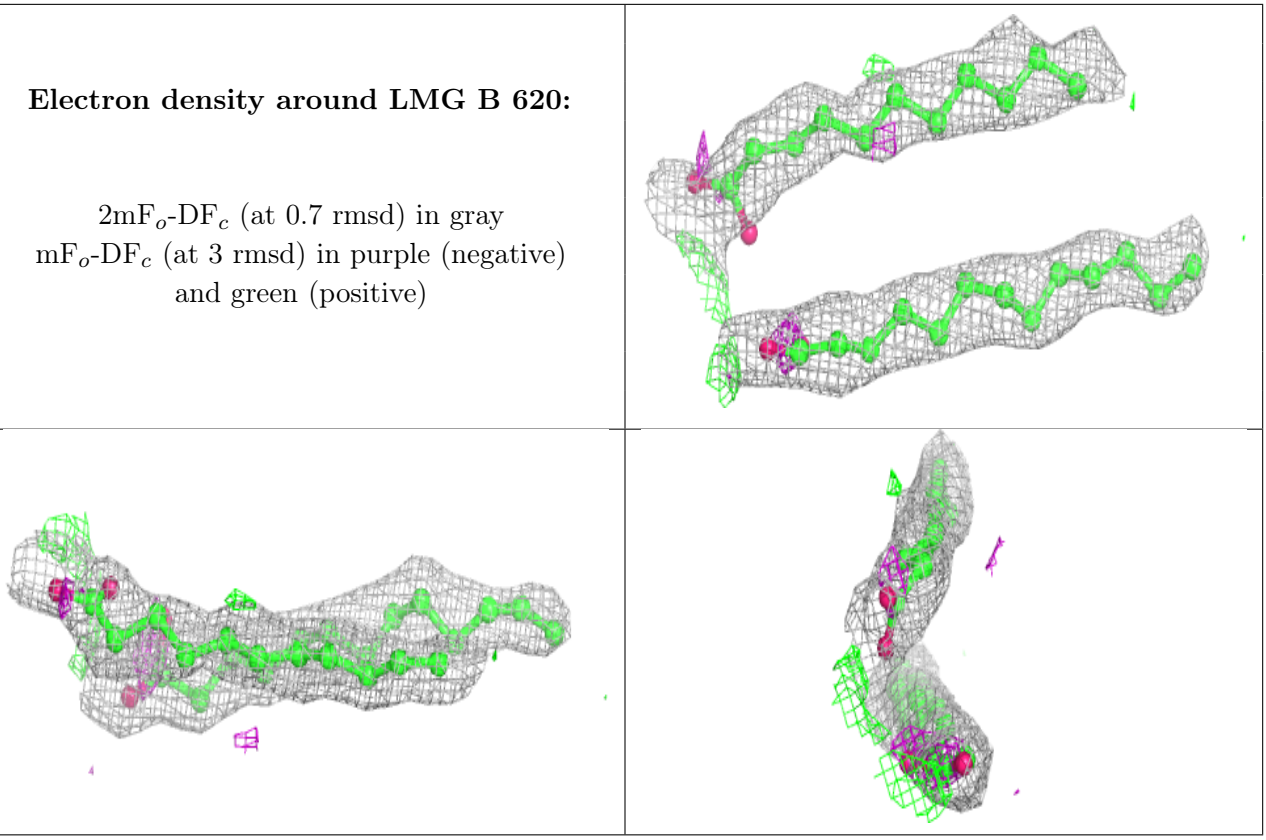
Electron density around LMG c 524:

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



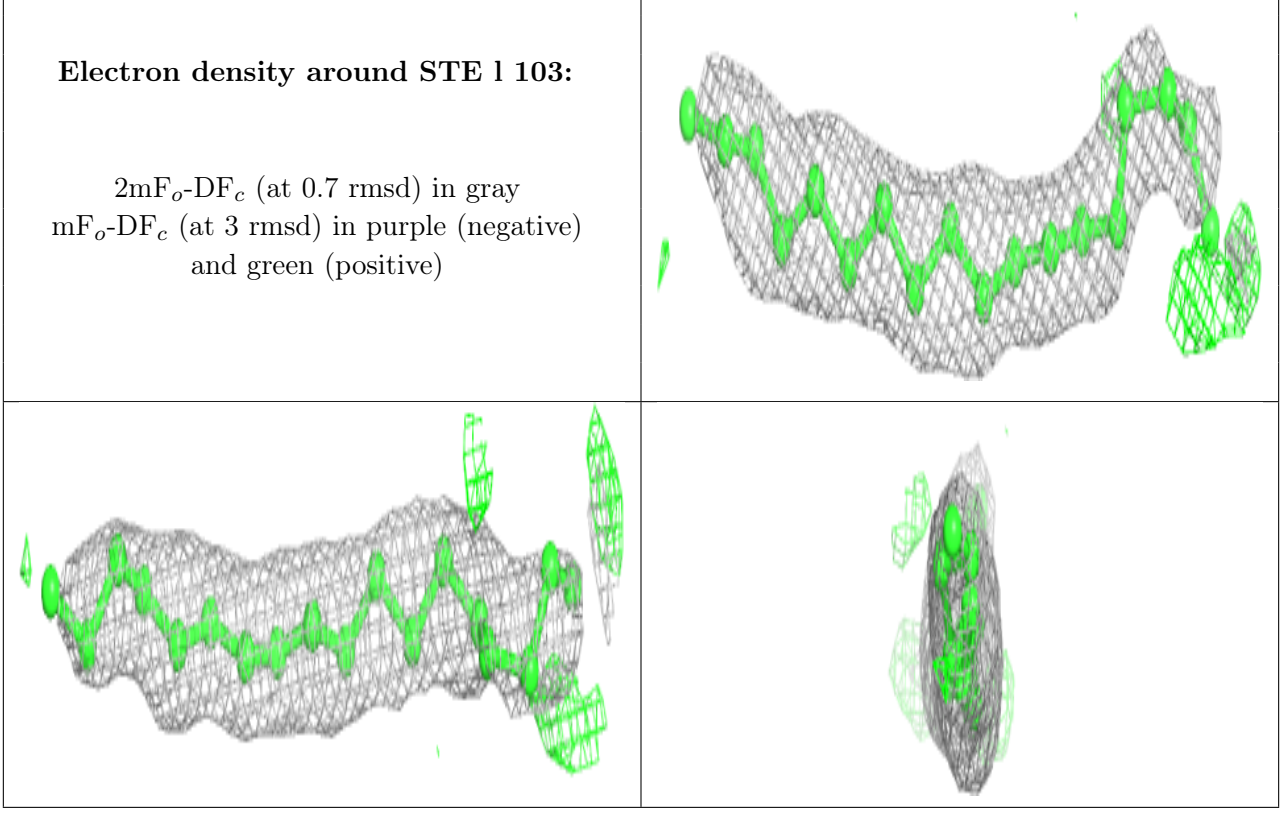
Electron density around LMG B 620:

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



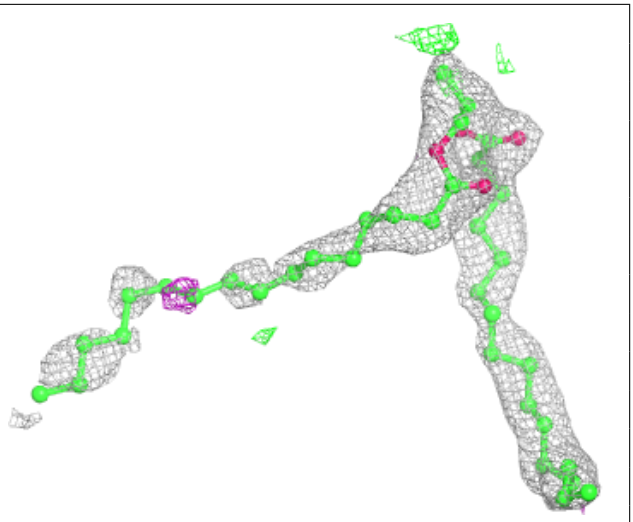
Electron density around STE l 103:

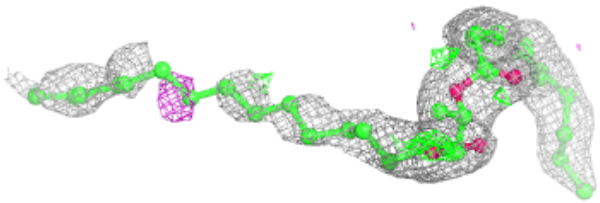
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

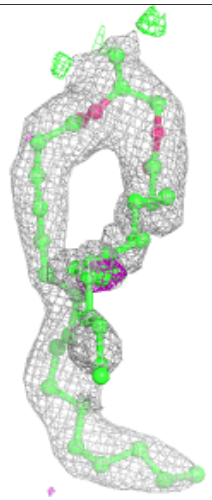


Electron density around SQD A 615:

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

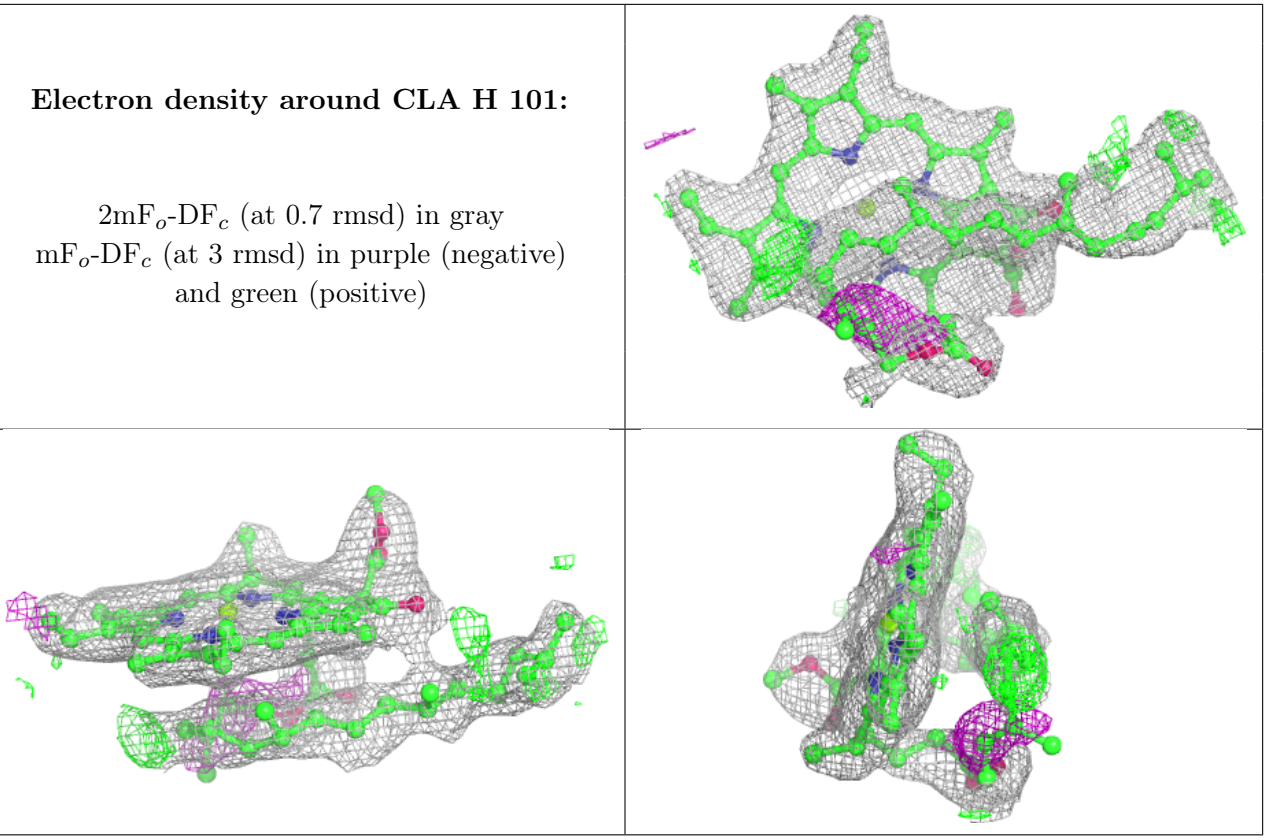






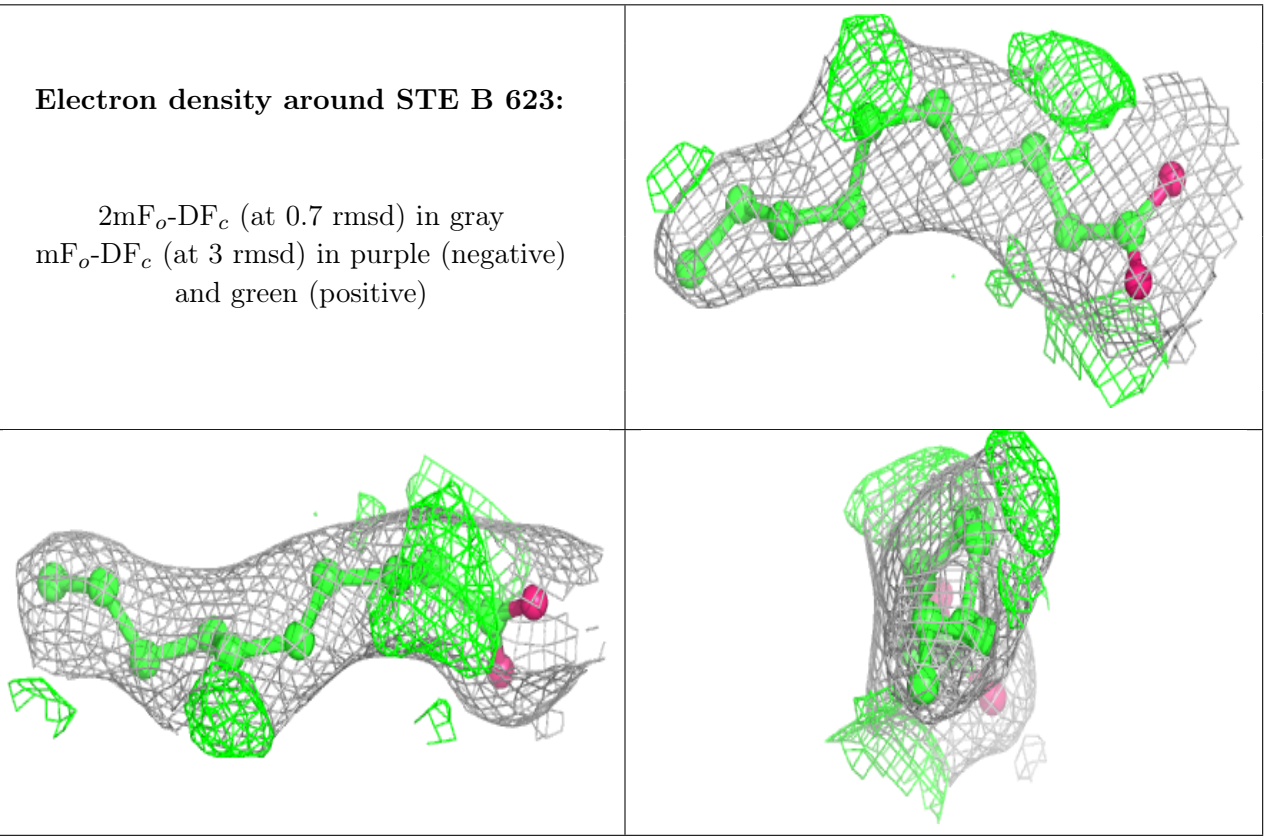
Electron density around CLA H 101:

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



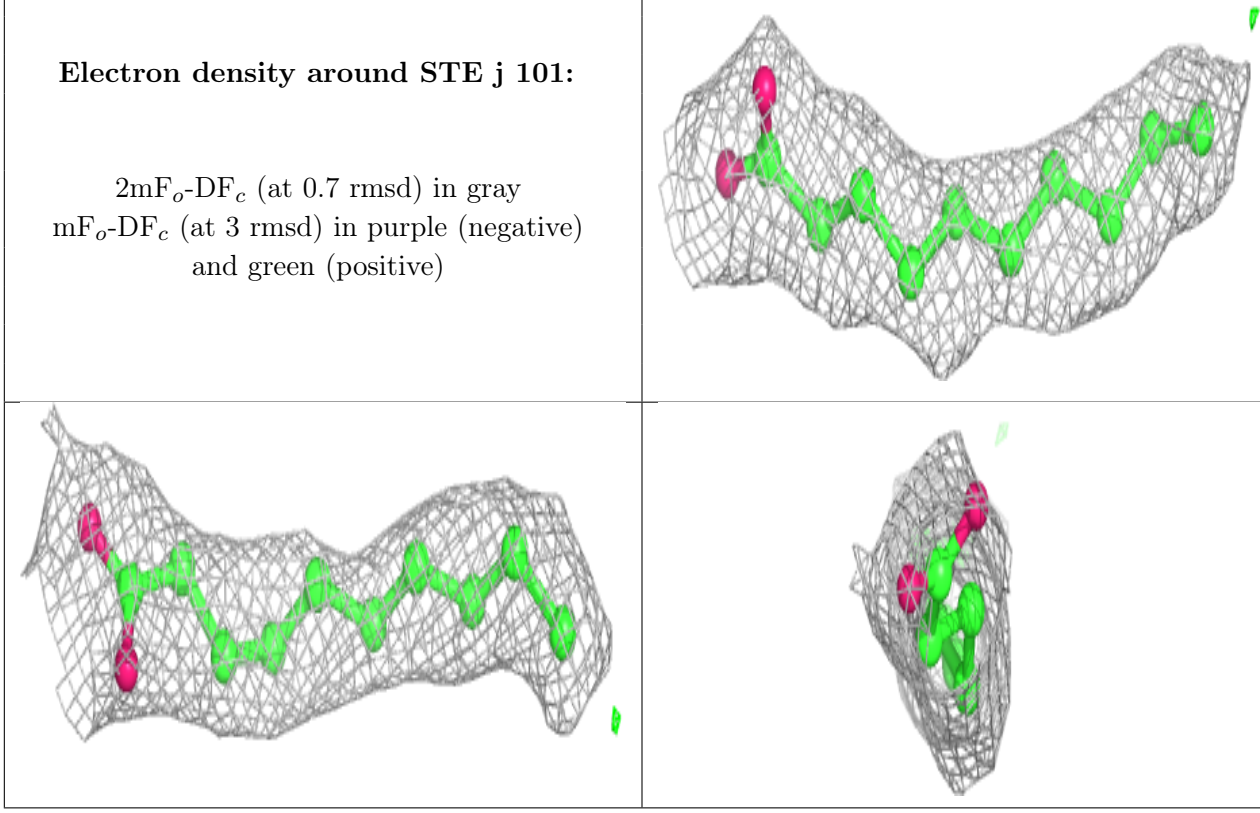
Electron density around STE B 623:

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



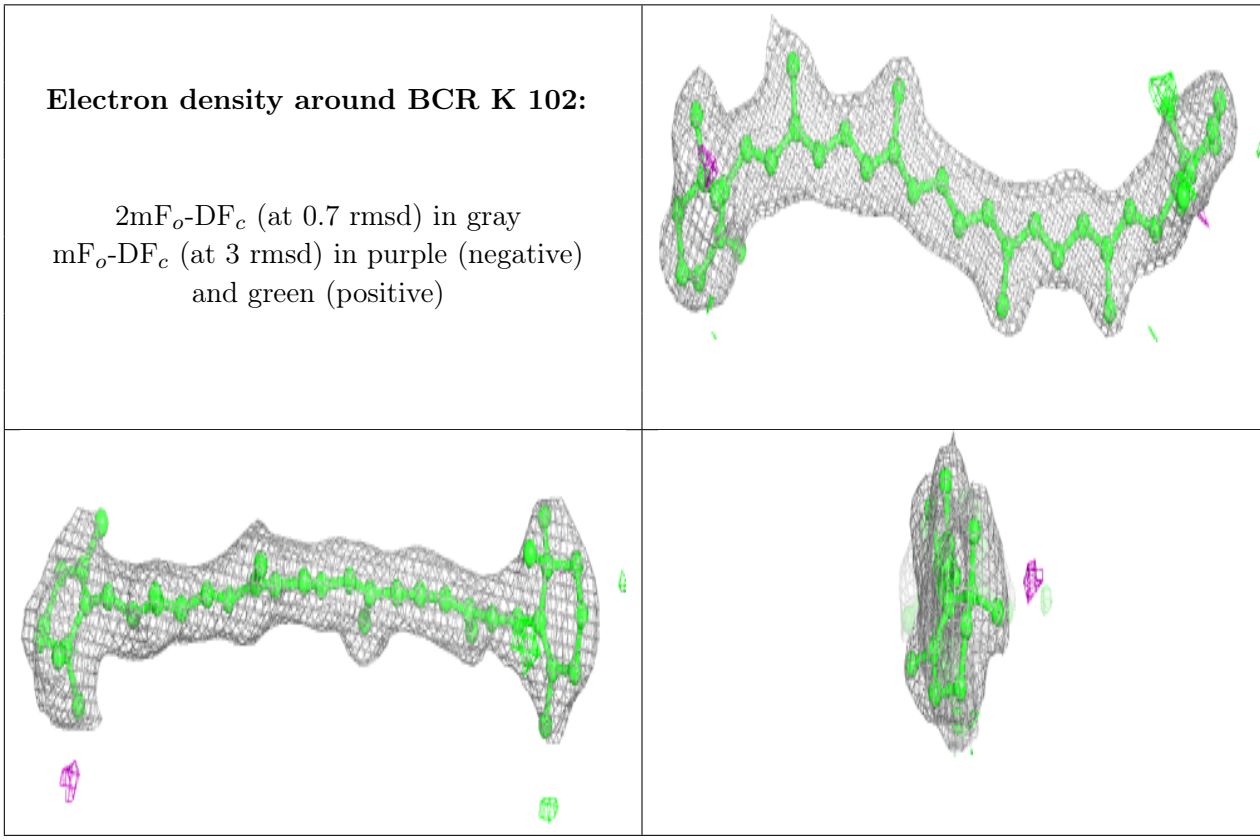
Electron density around STE j 101:

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



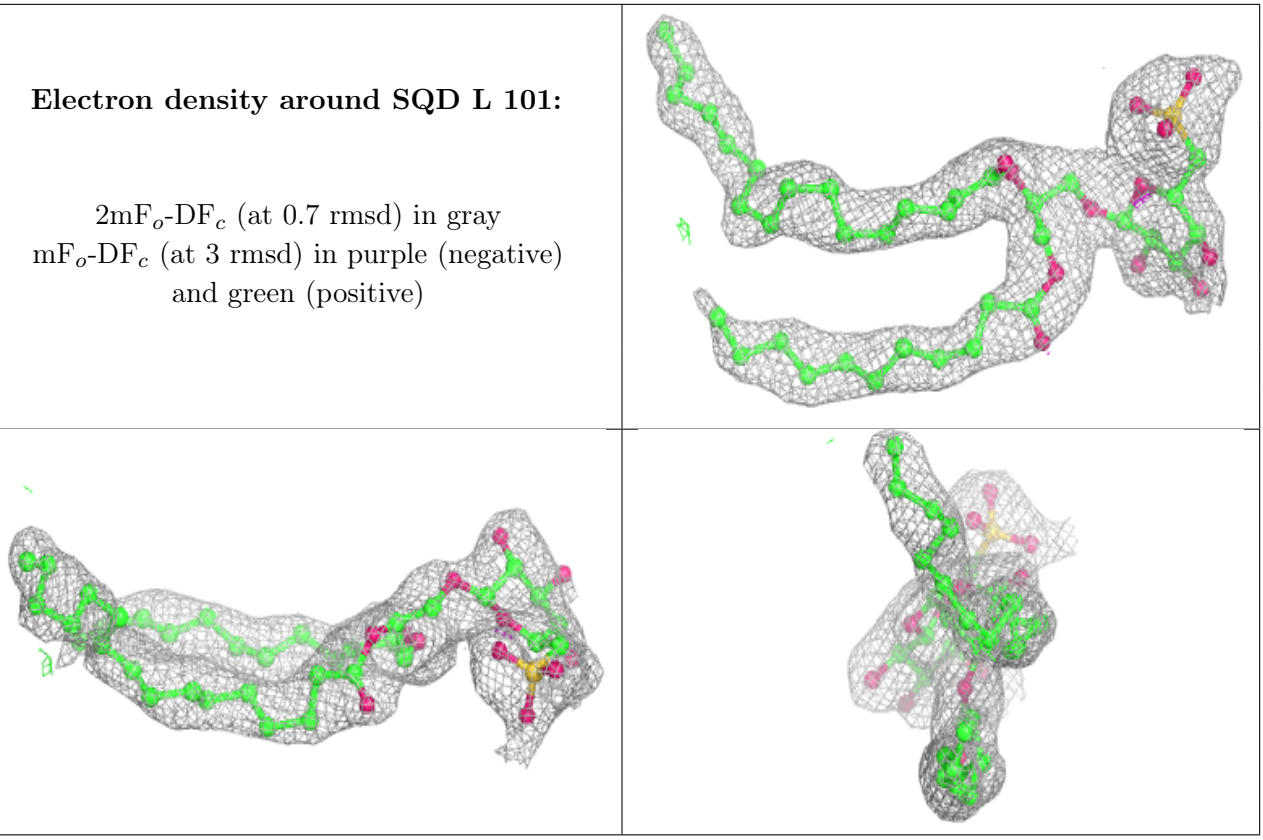
Electron density around BCR K 102:

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



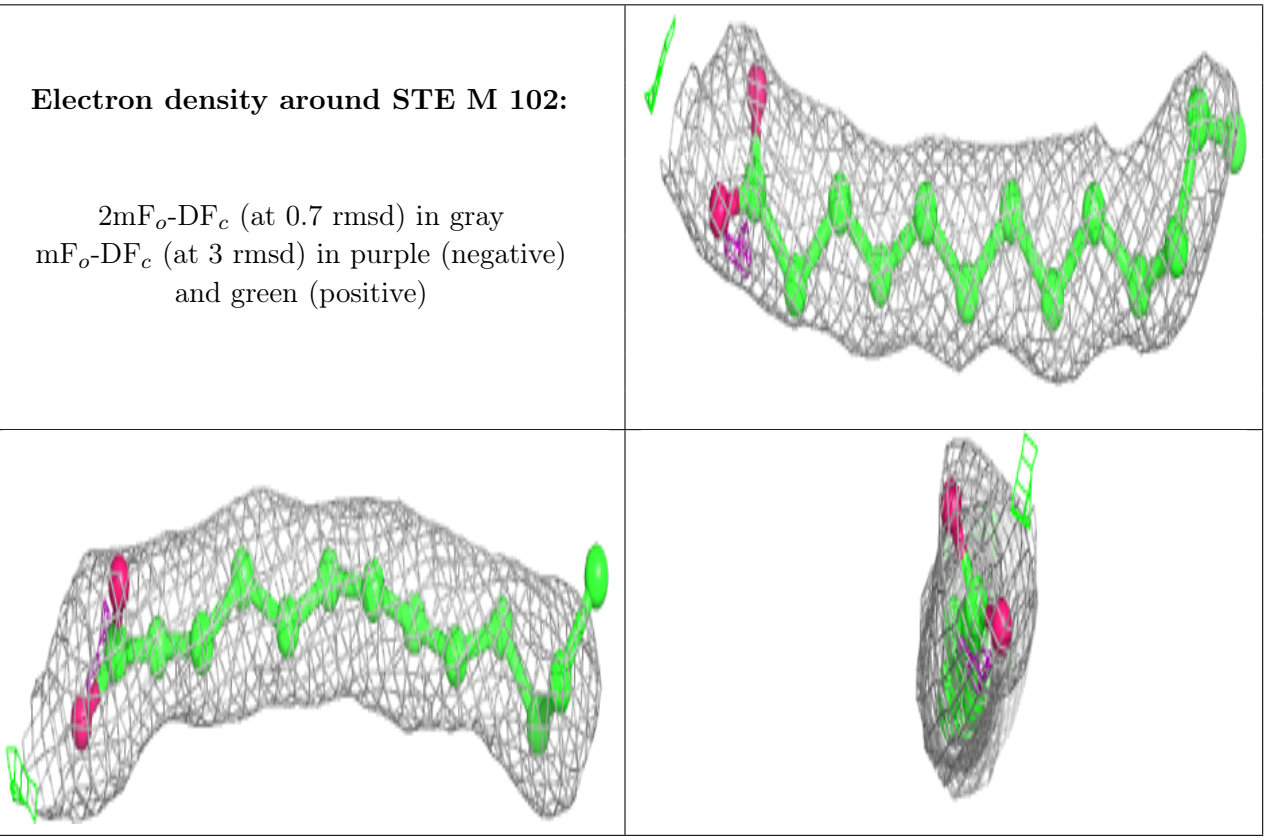
Electron density around SQD L 101:

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



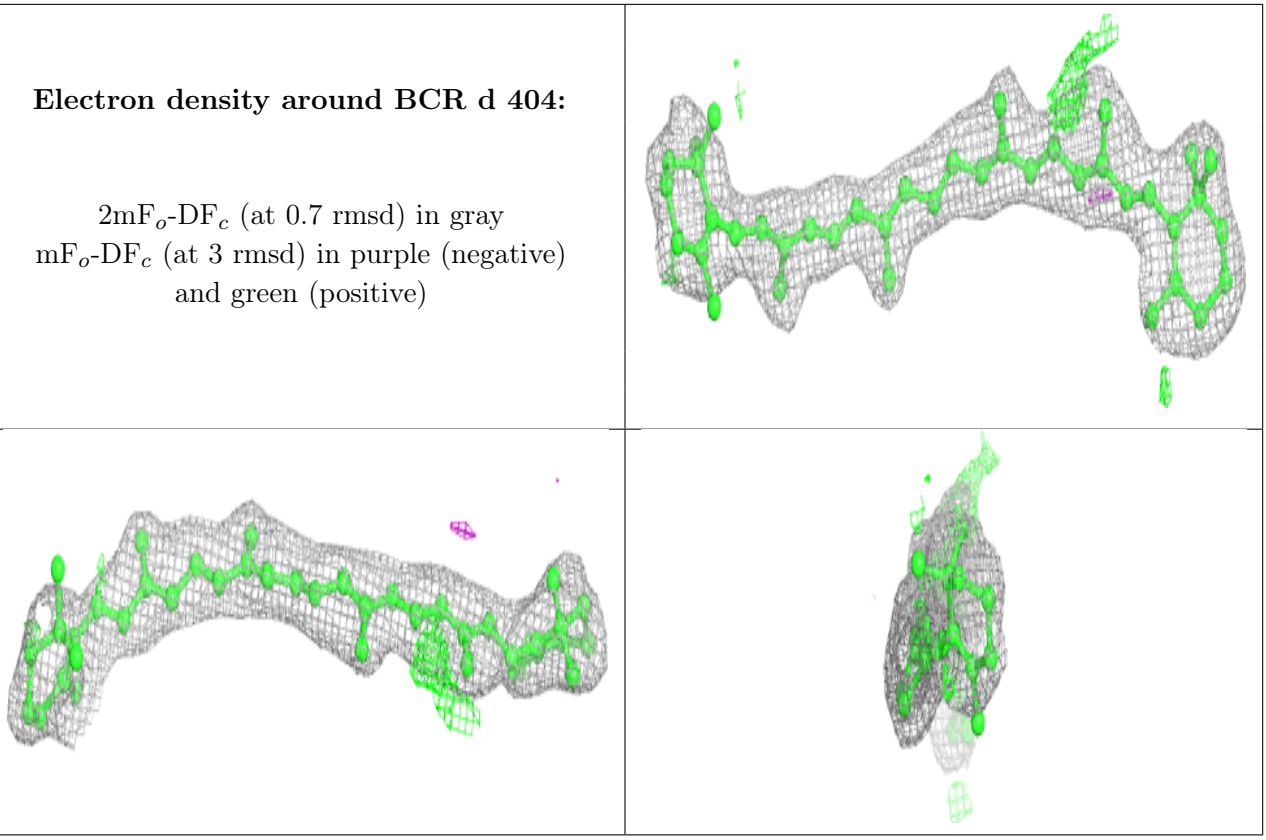
Electron density around STE M 102:

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



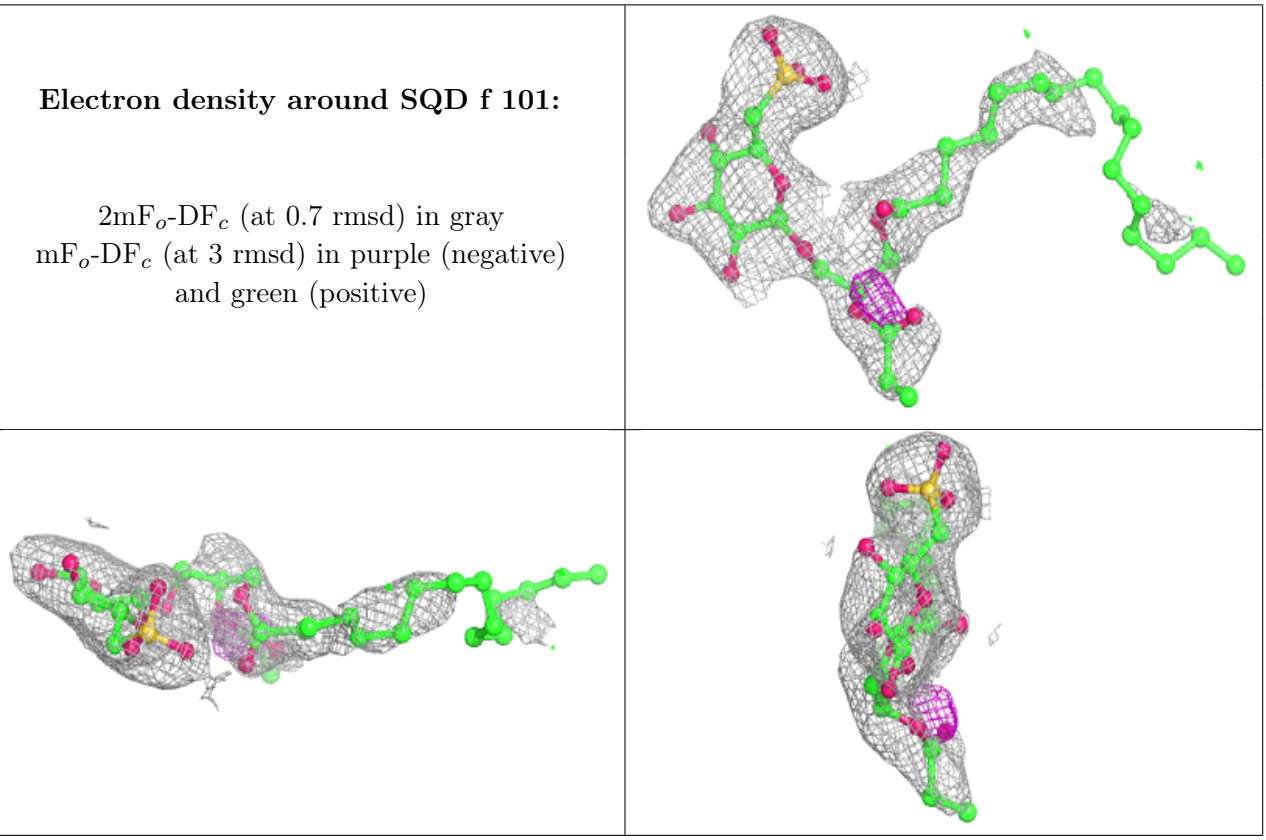
Electron density around BCR d 404:

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



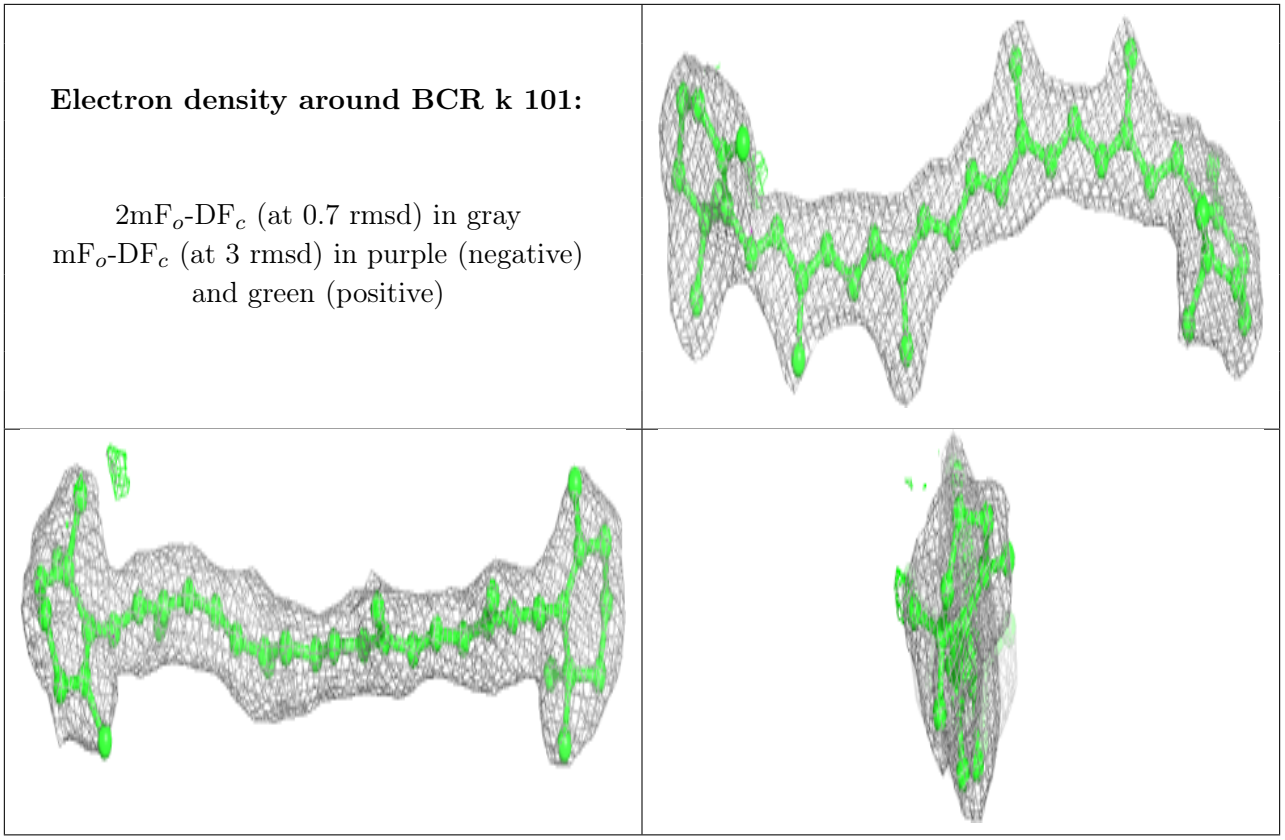
Electron density around SQD f 101:

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



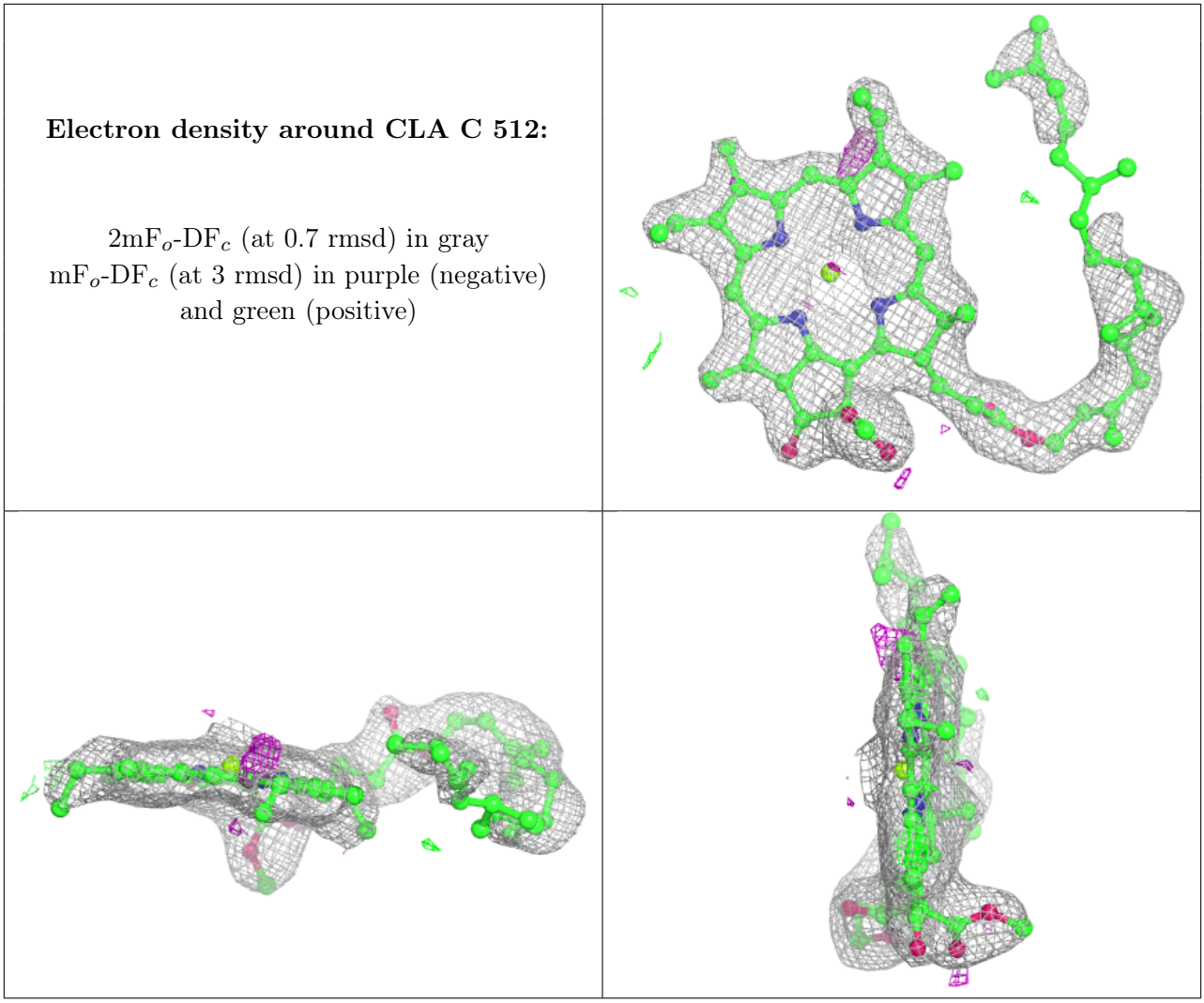
Electron density around BCR k 101:

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



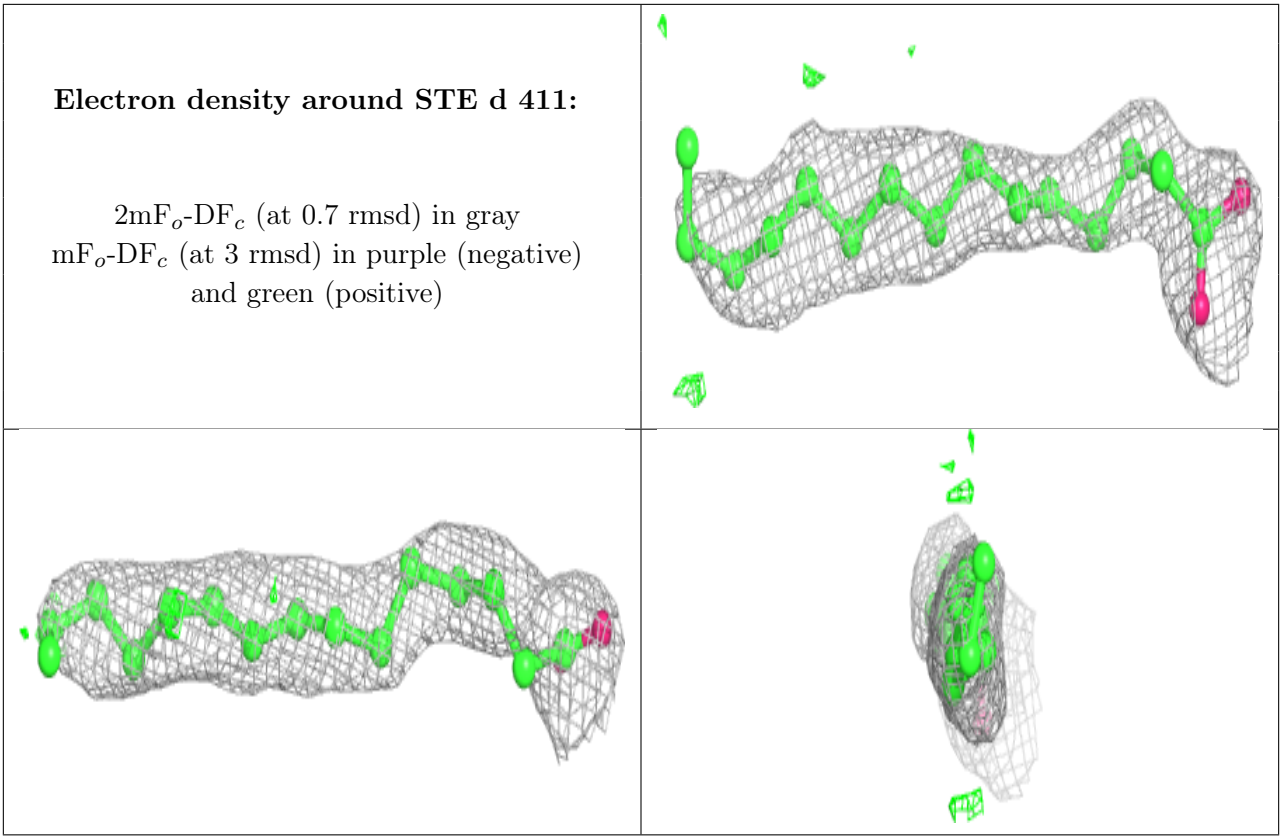
Electron density around CLA C 512:

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



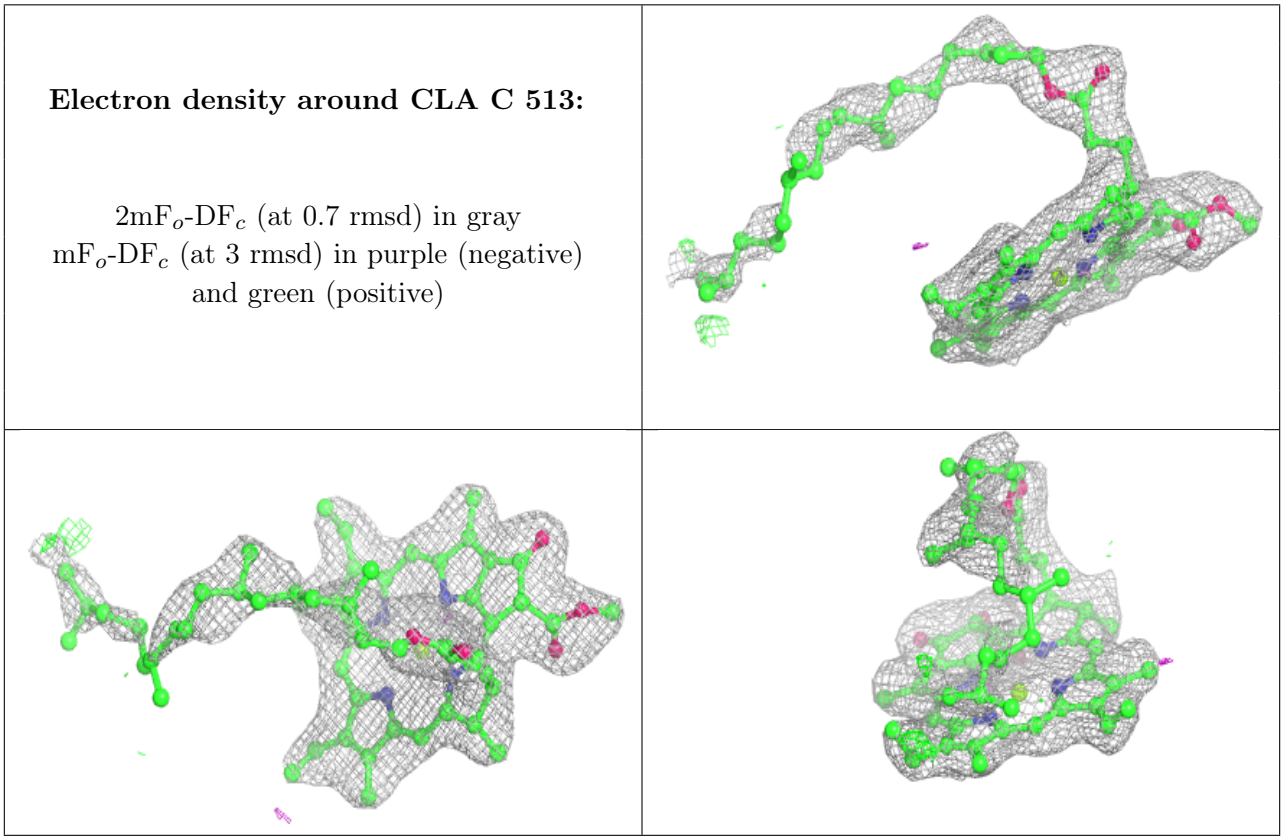
Electron density around STE d 411:

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



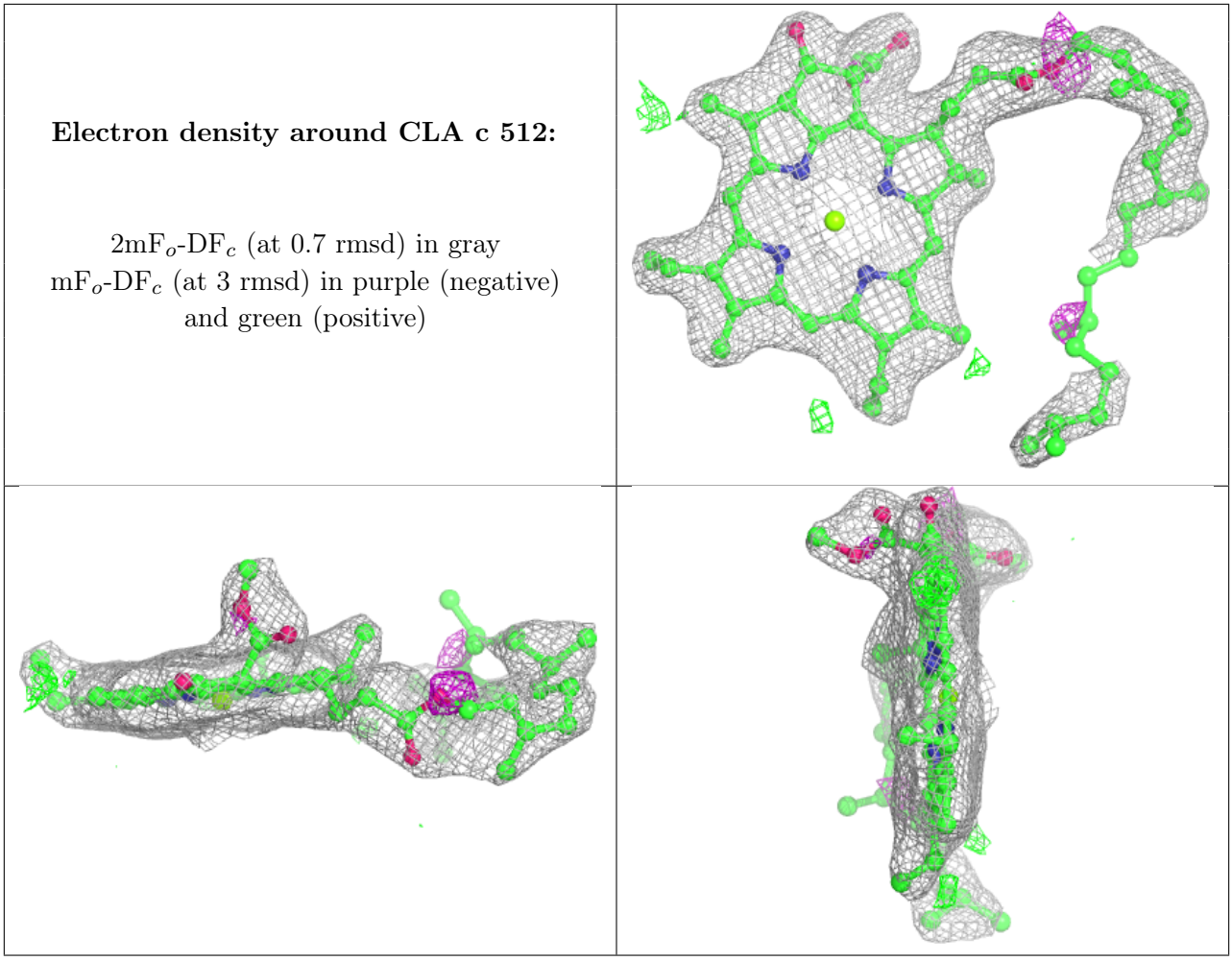
Electron density around CLA C 513:

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



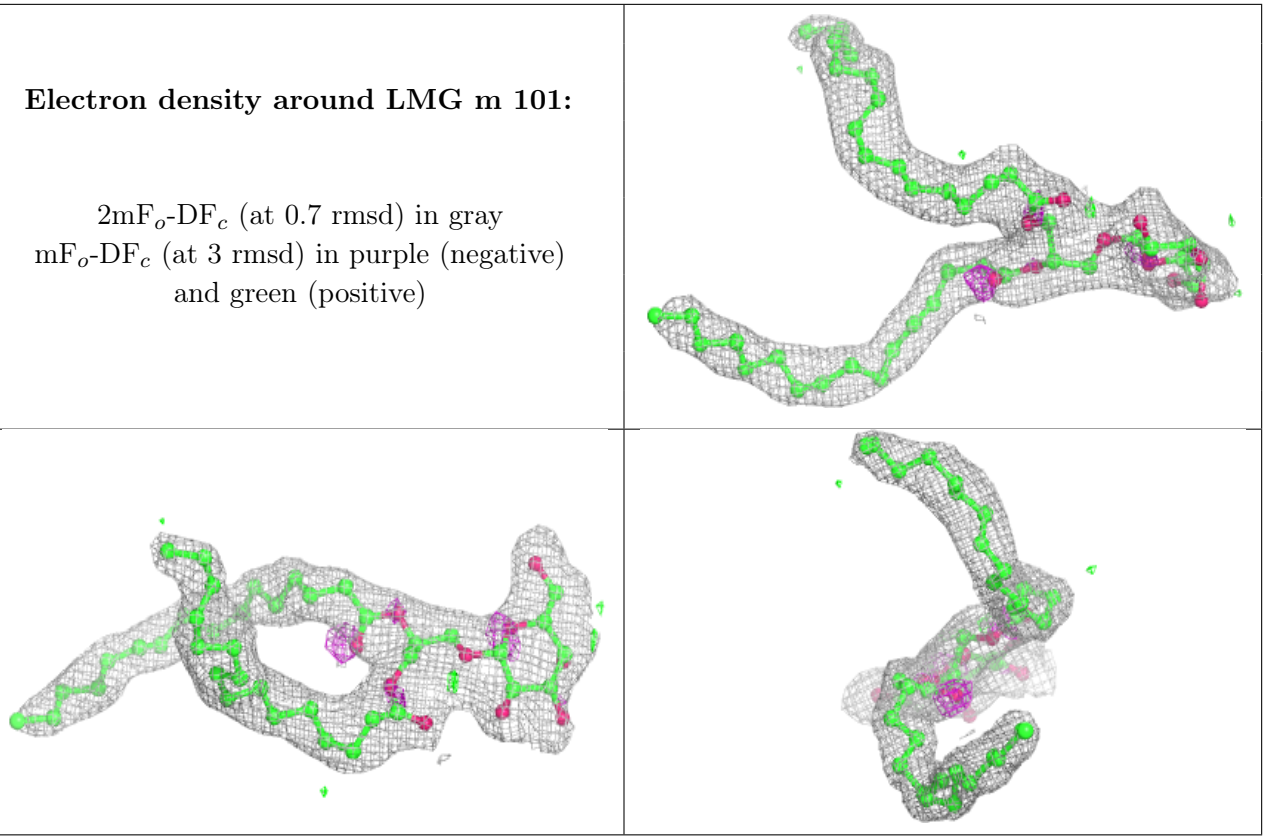
Electron density around CLA c 512:

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



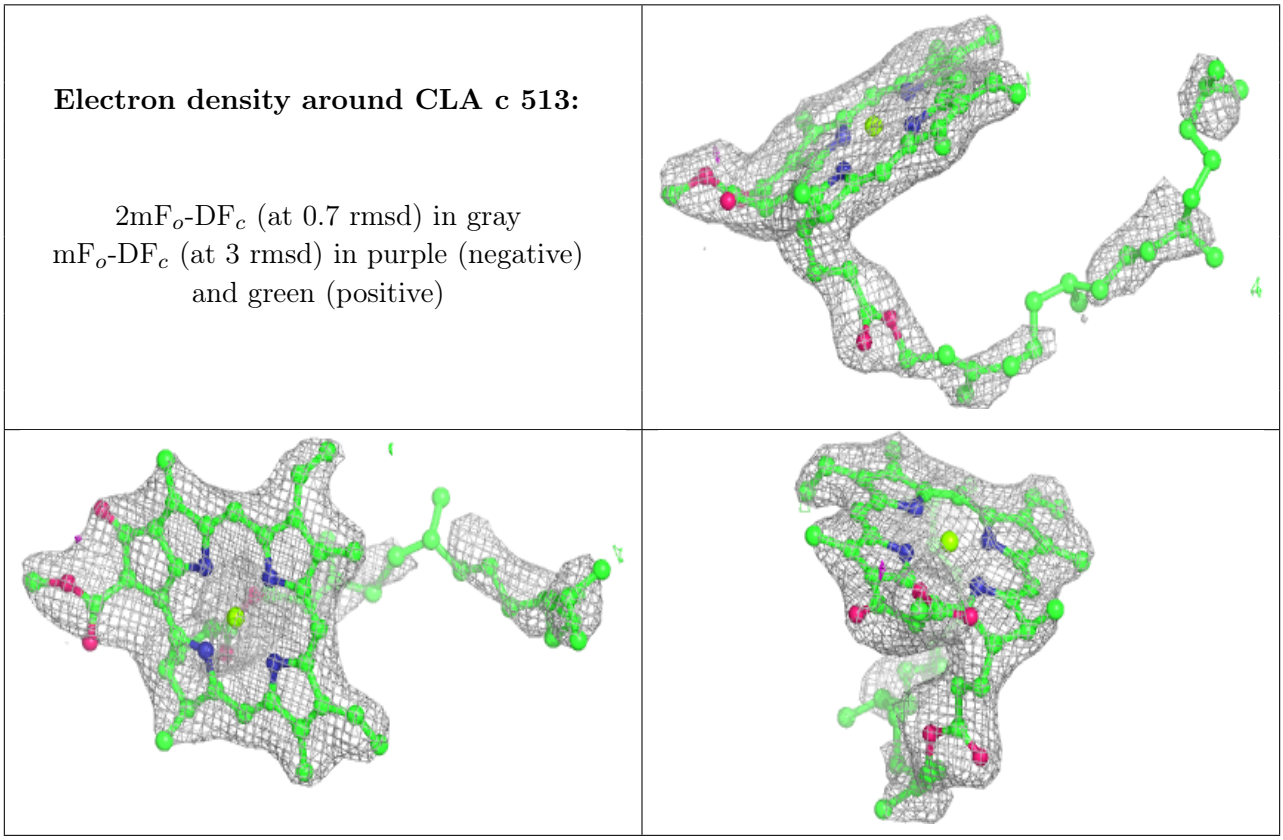
Electron density around LMG m 101:

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



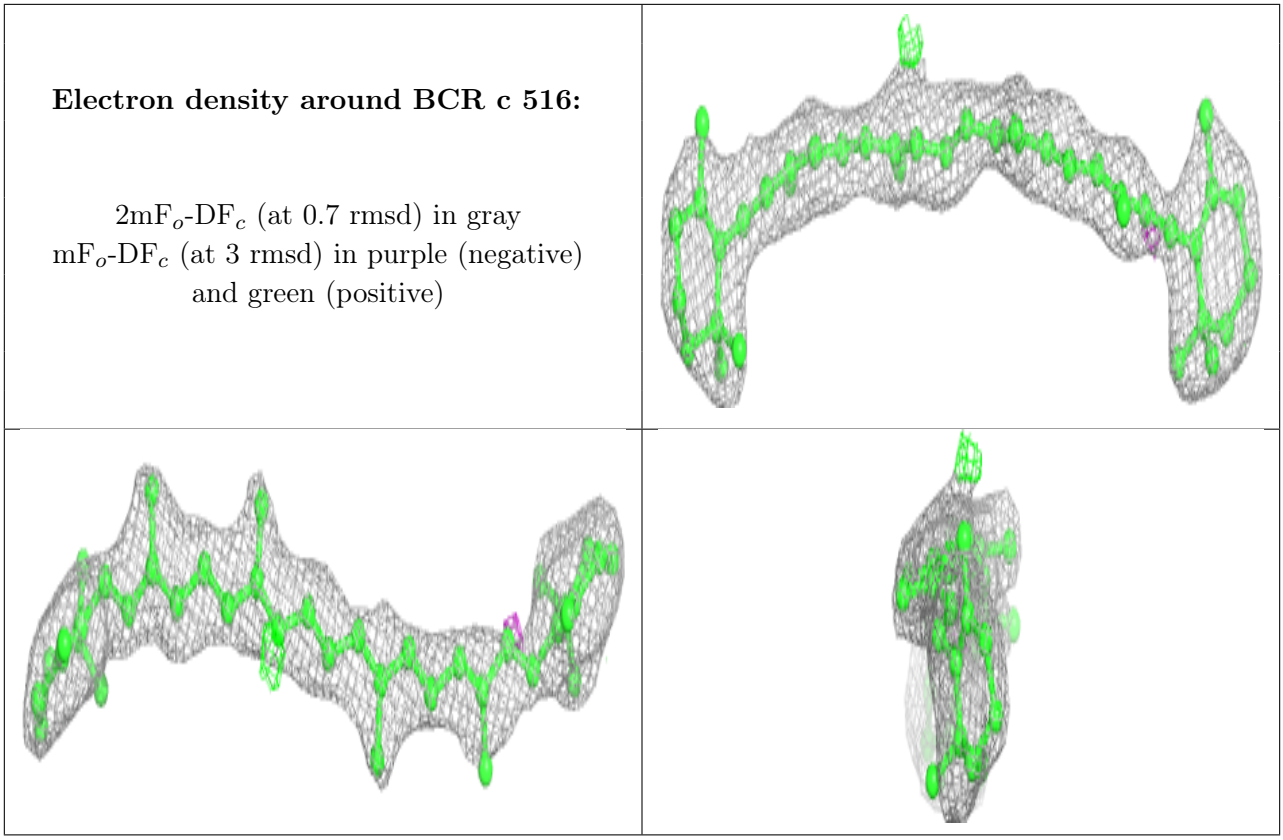
Electron density around CLA c 513:

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



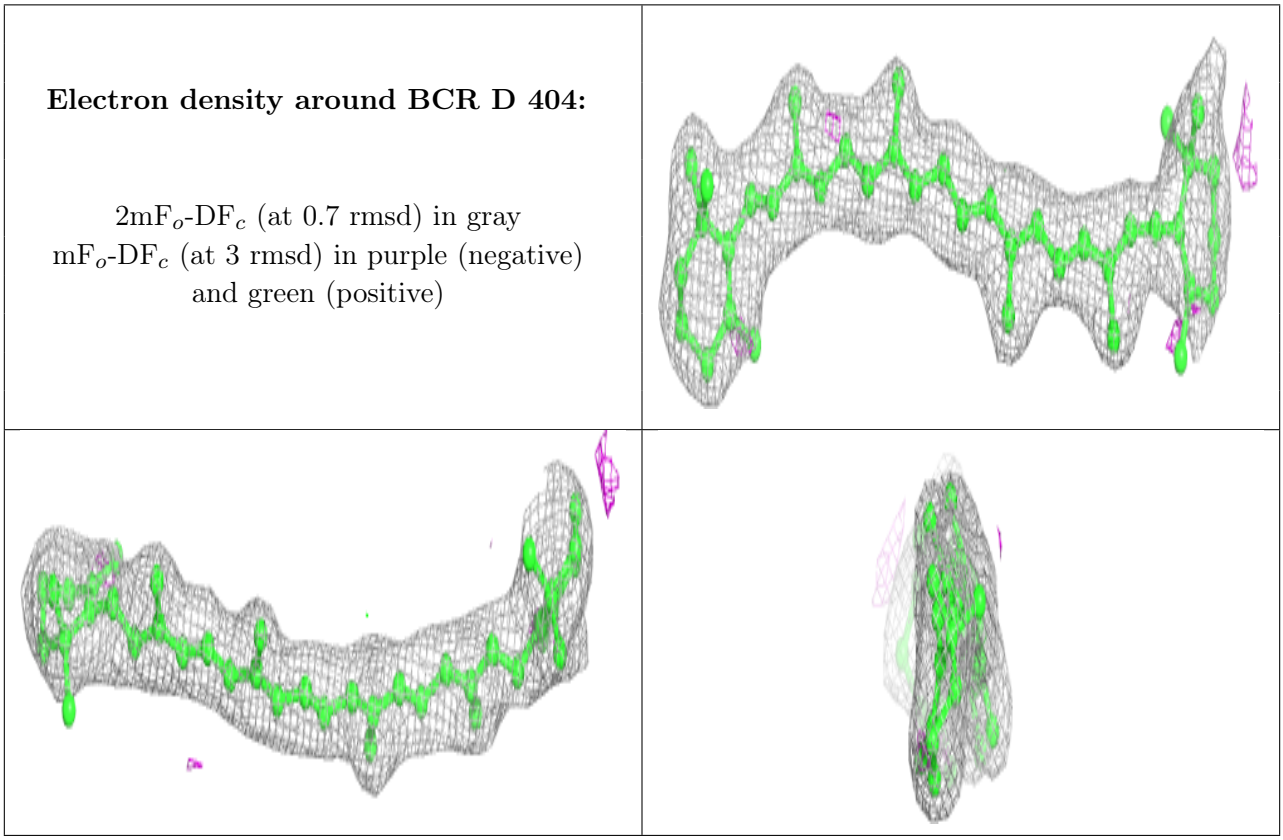
Electron density around BCR c 516:

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



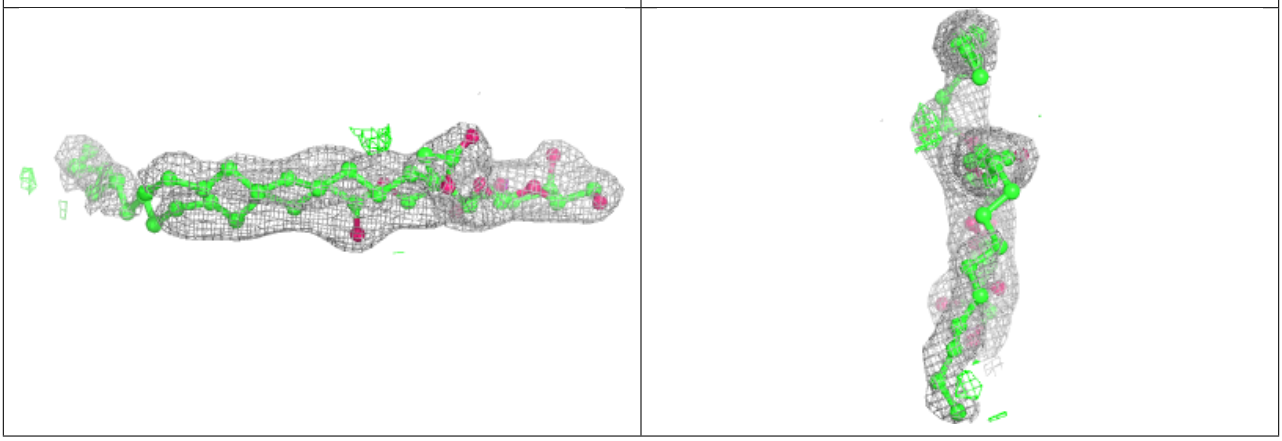
Electron density around BCR D 404:

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



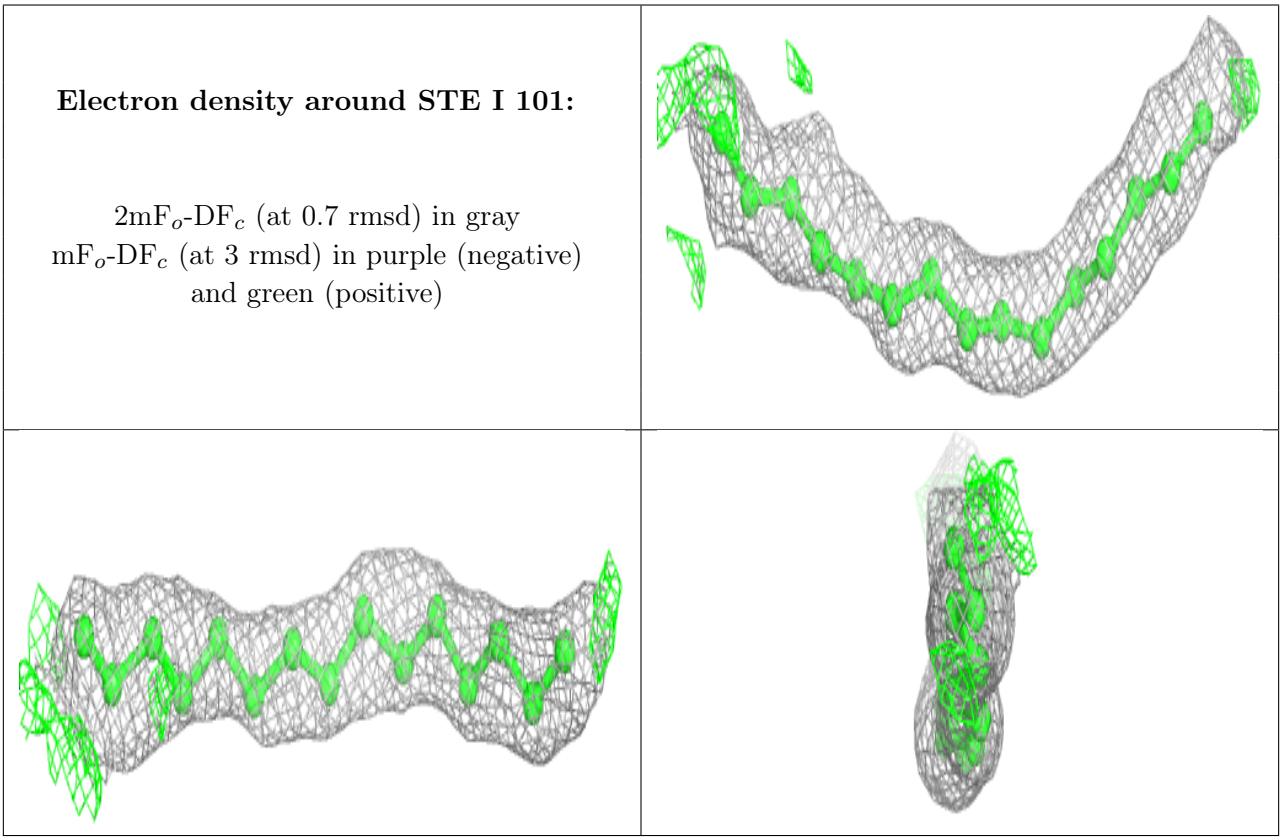
Electron density around LMG C 519:

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



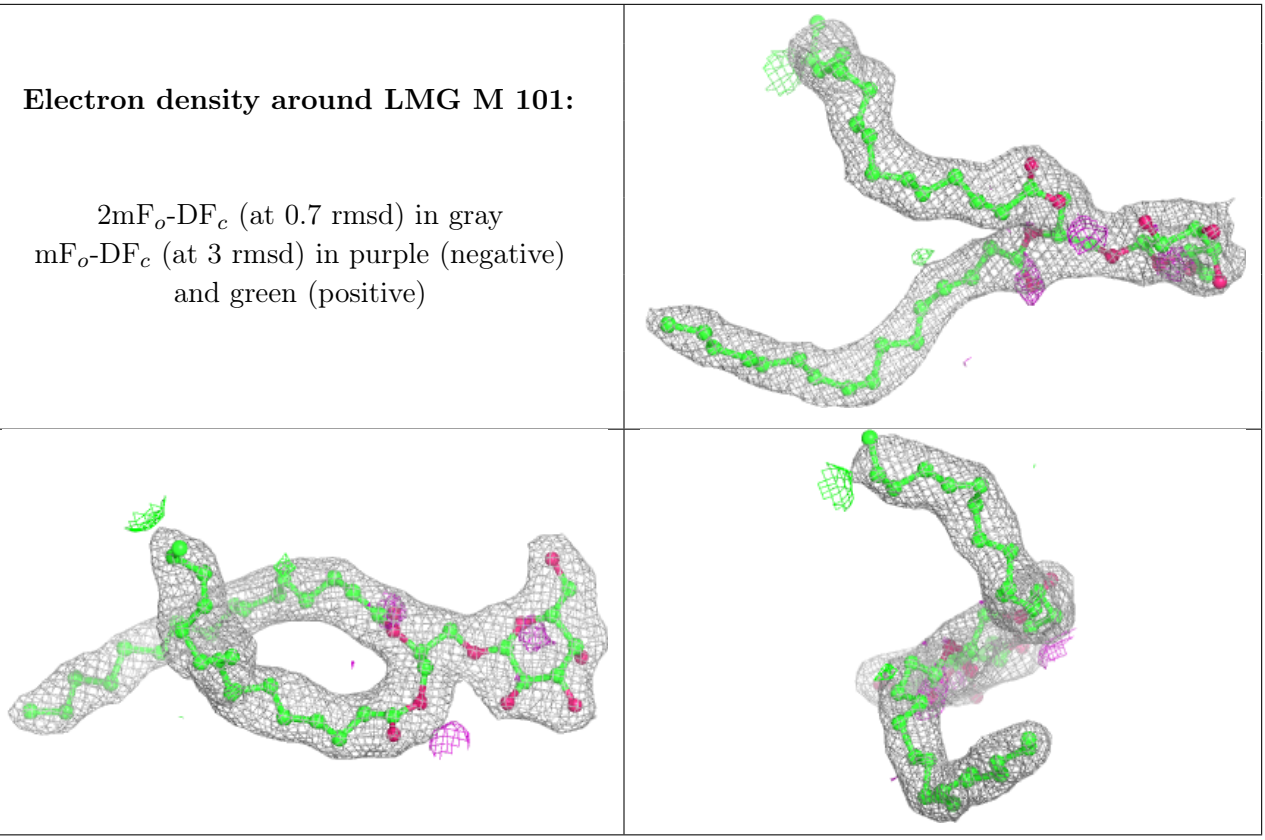
Electron density around STE I 101:

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



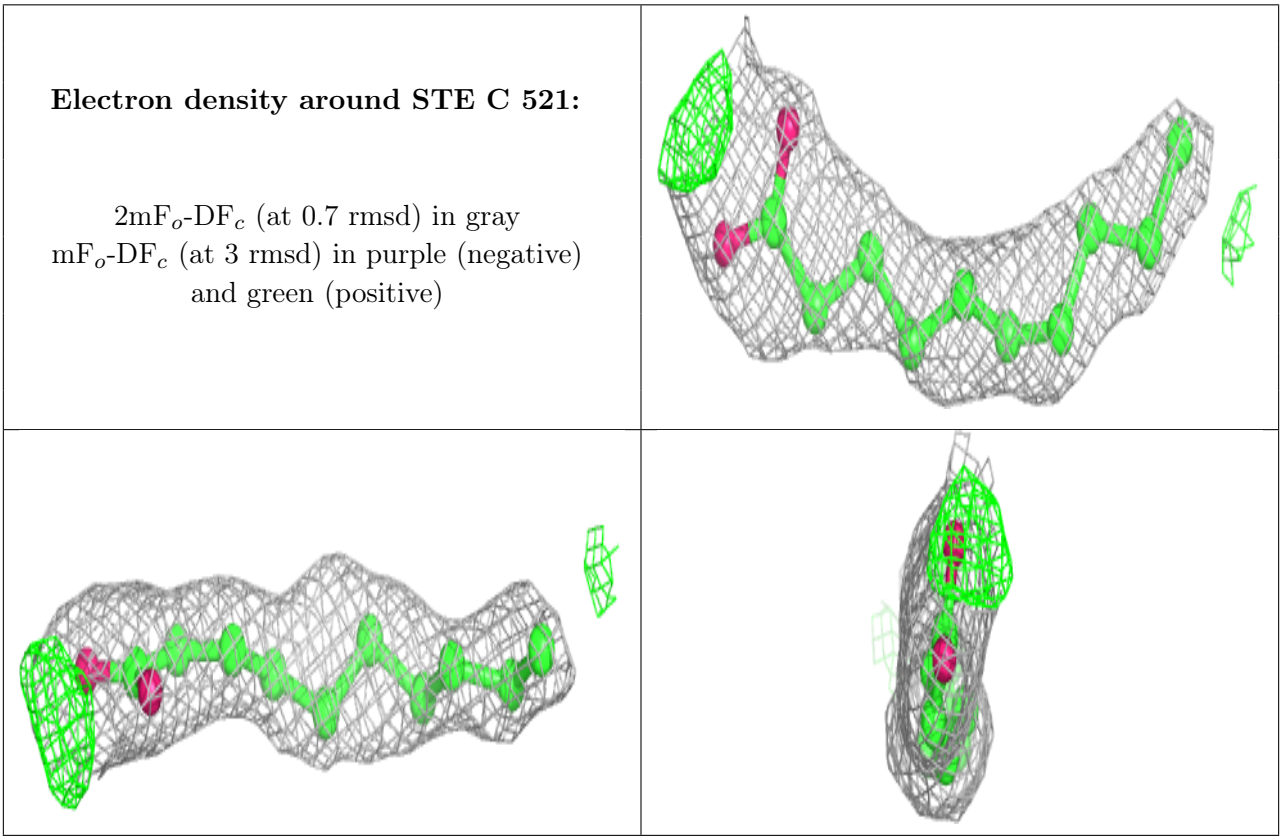
Electron density around LMG M 101:

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



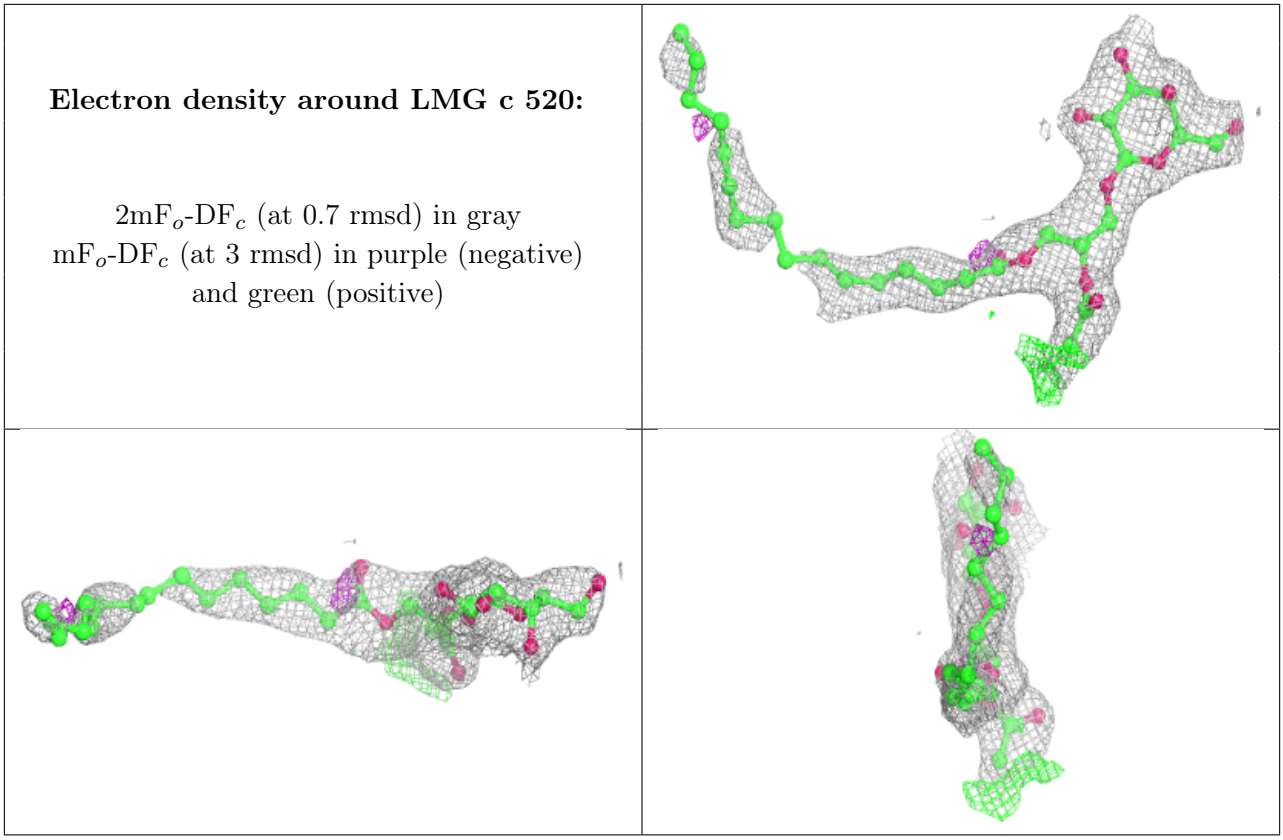
Electron density around STE C 521:

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



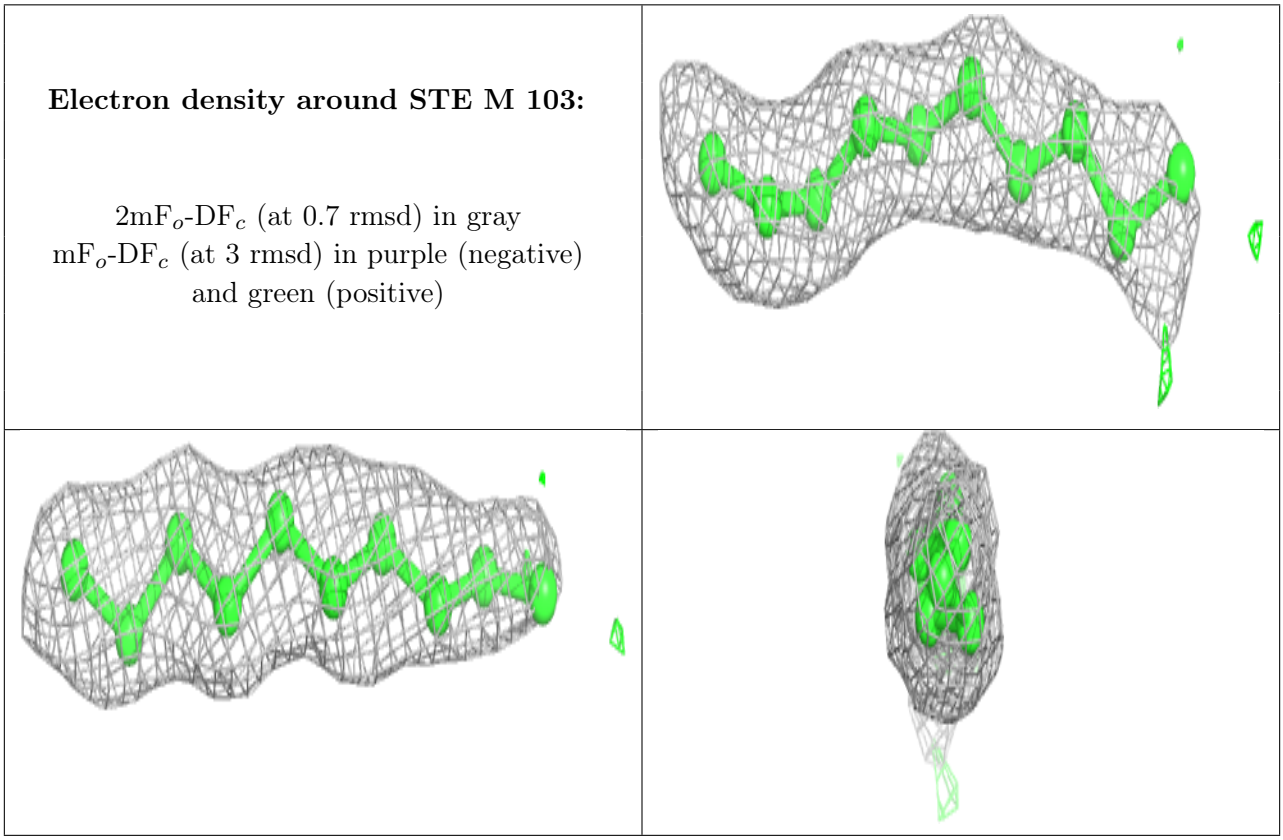
Electron density around LMG c 520:

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



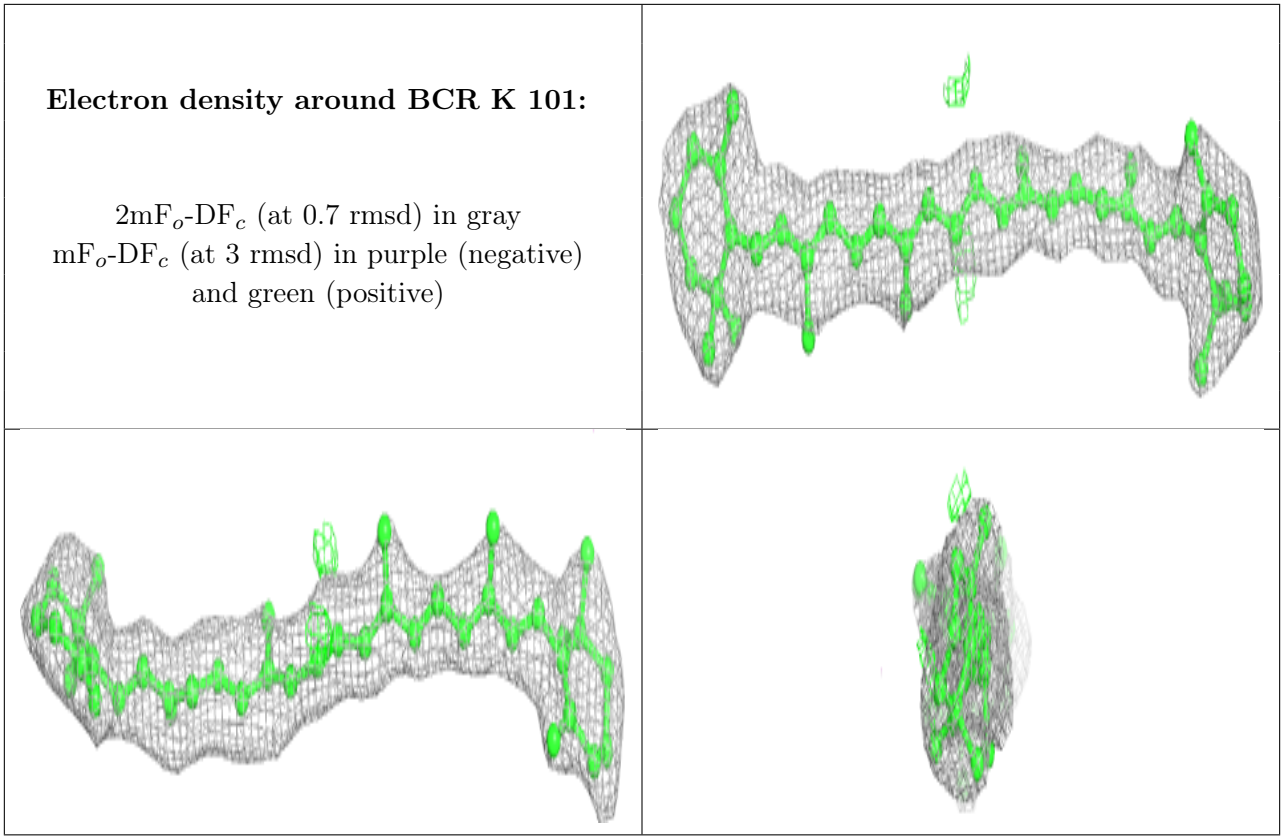
Electron density around STE M 103:

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



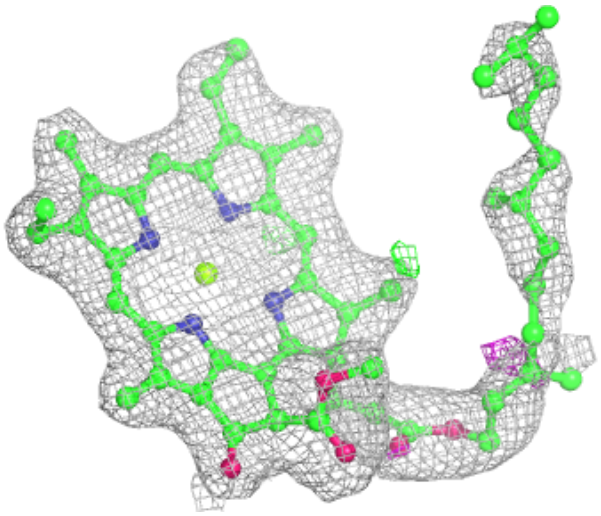
Electron density around BCR K 101:

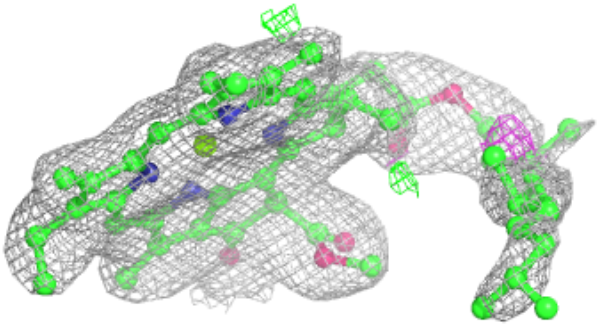
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

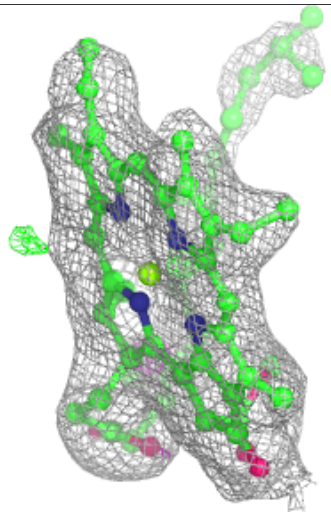


Electron density around CLA b 615:

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

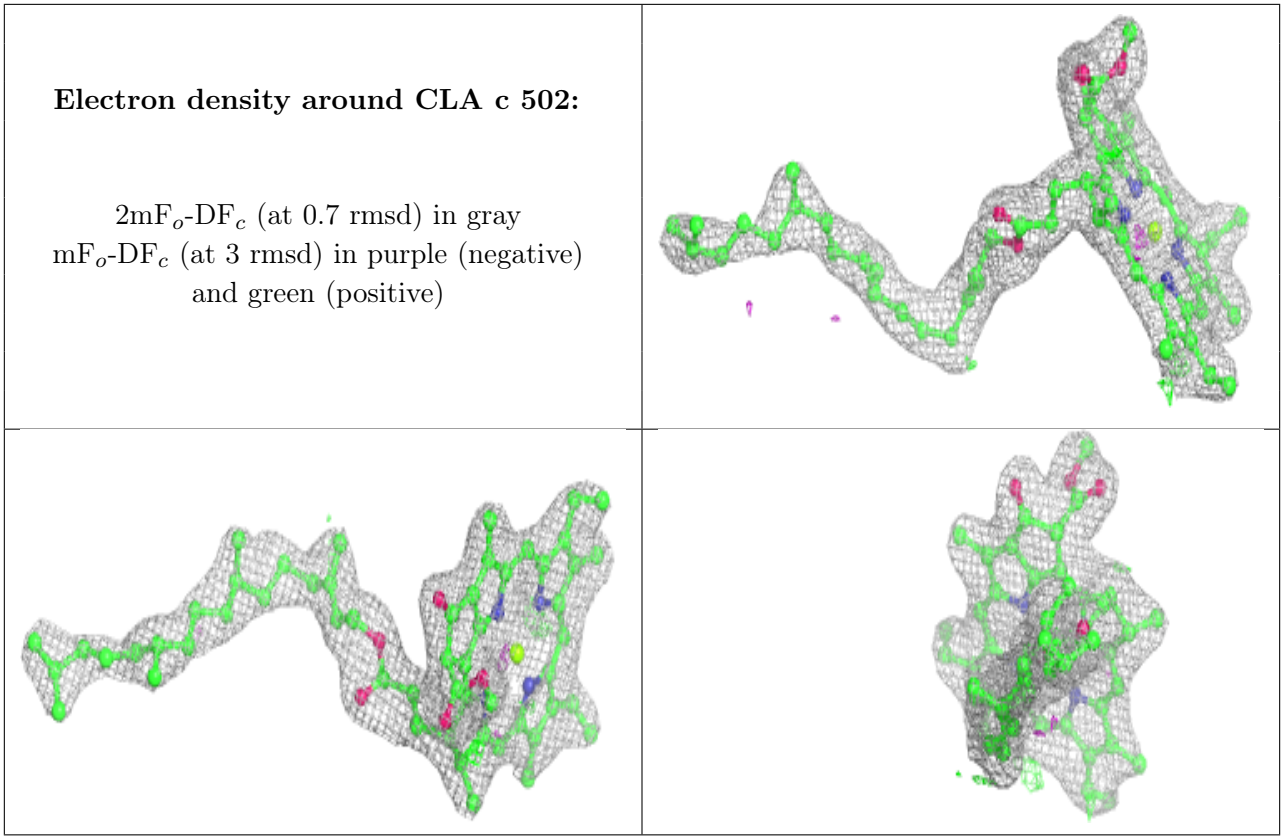






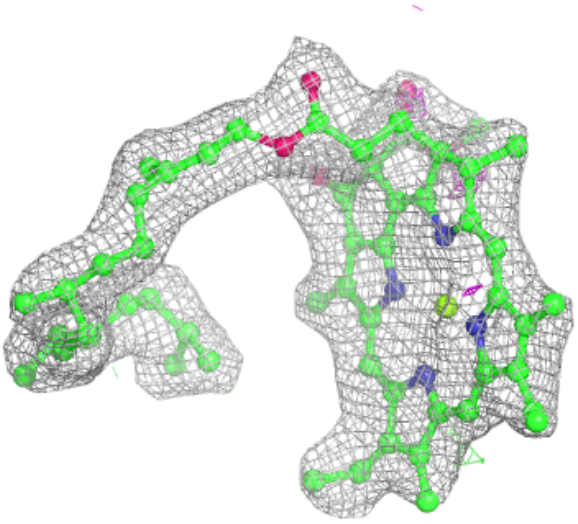
Electron density around CLA c 502:

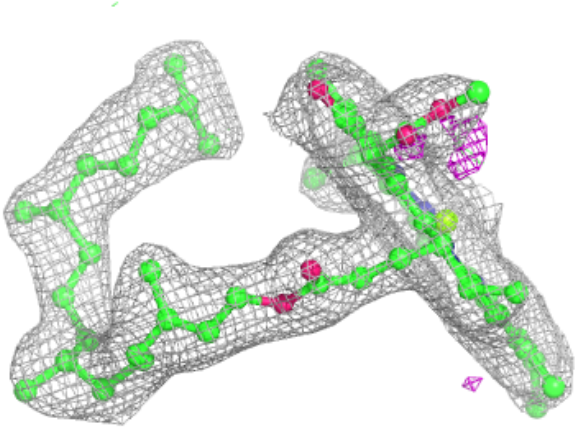
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

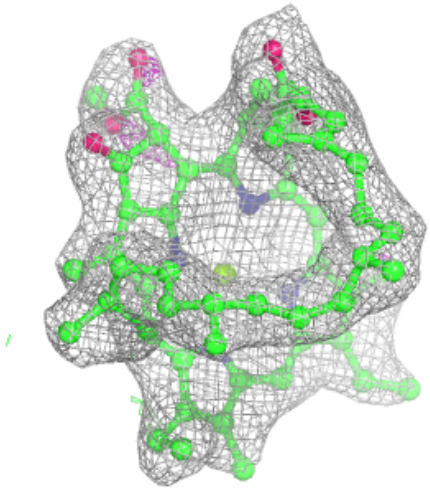


Electron density around CLA c 503:

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

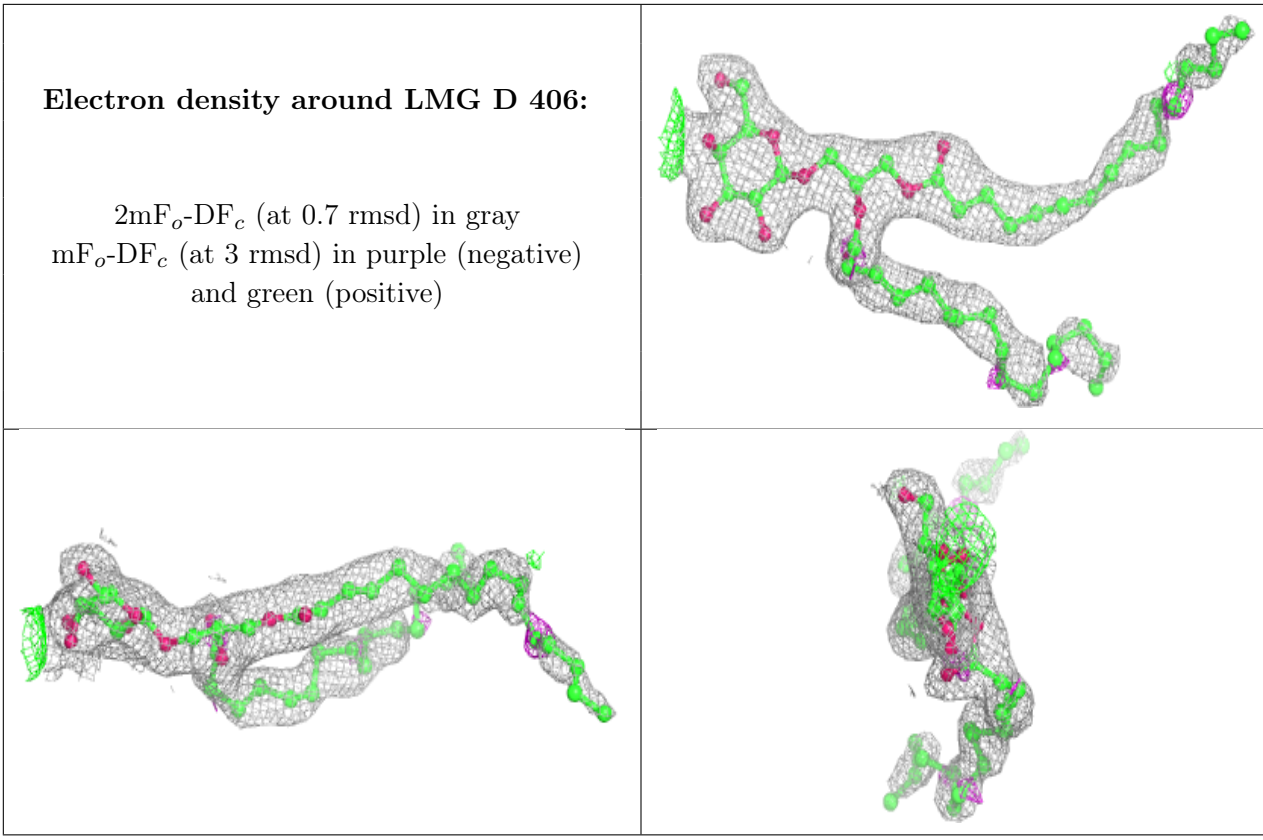






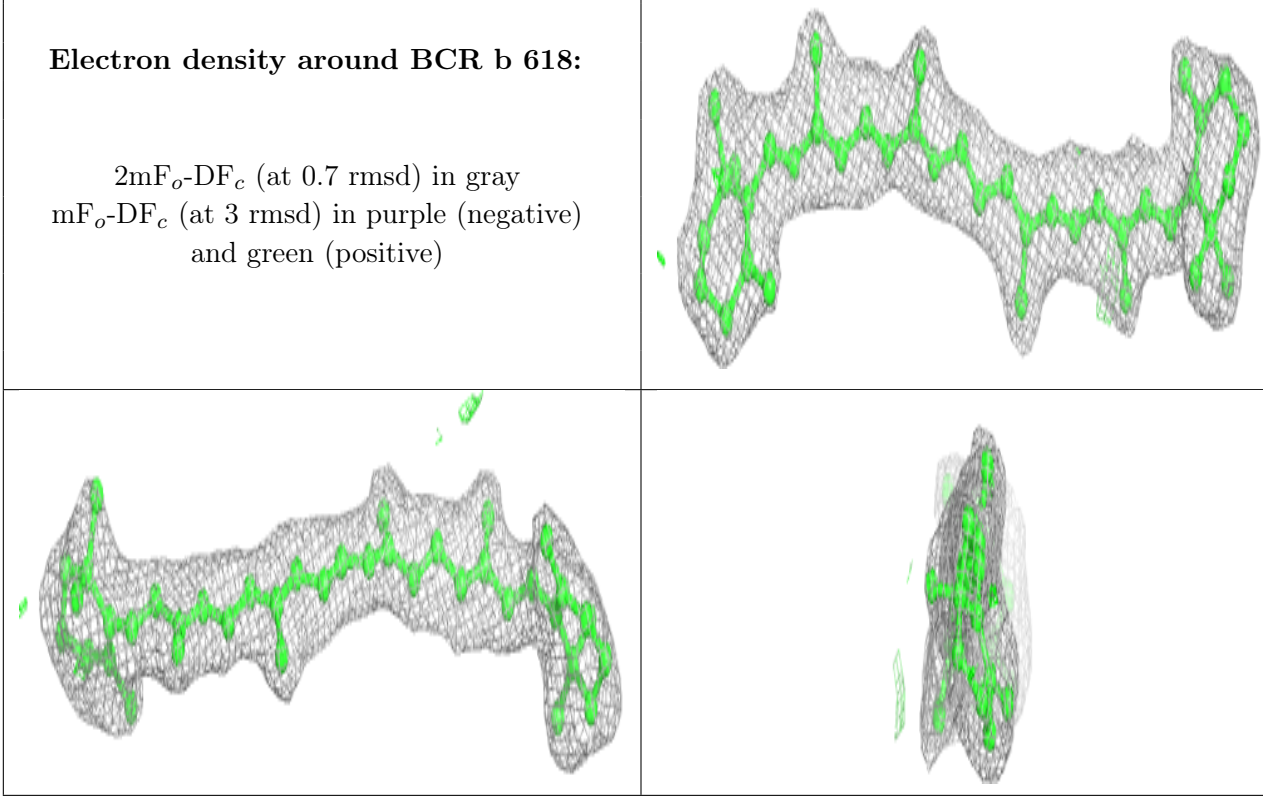
Electron density around LMG D 406:

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



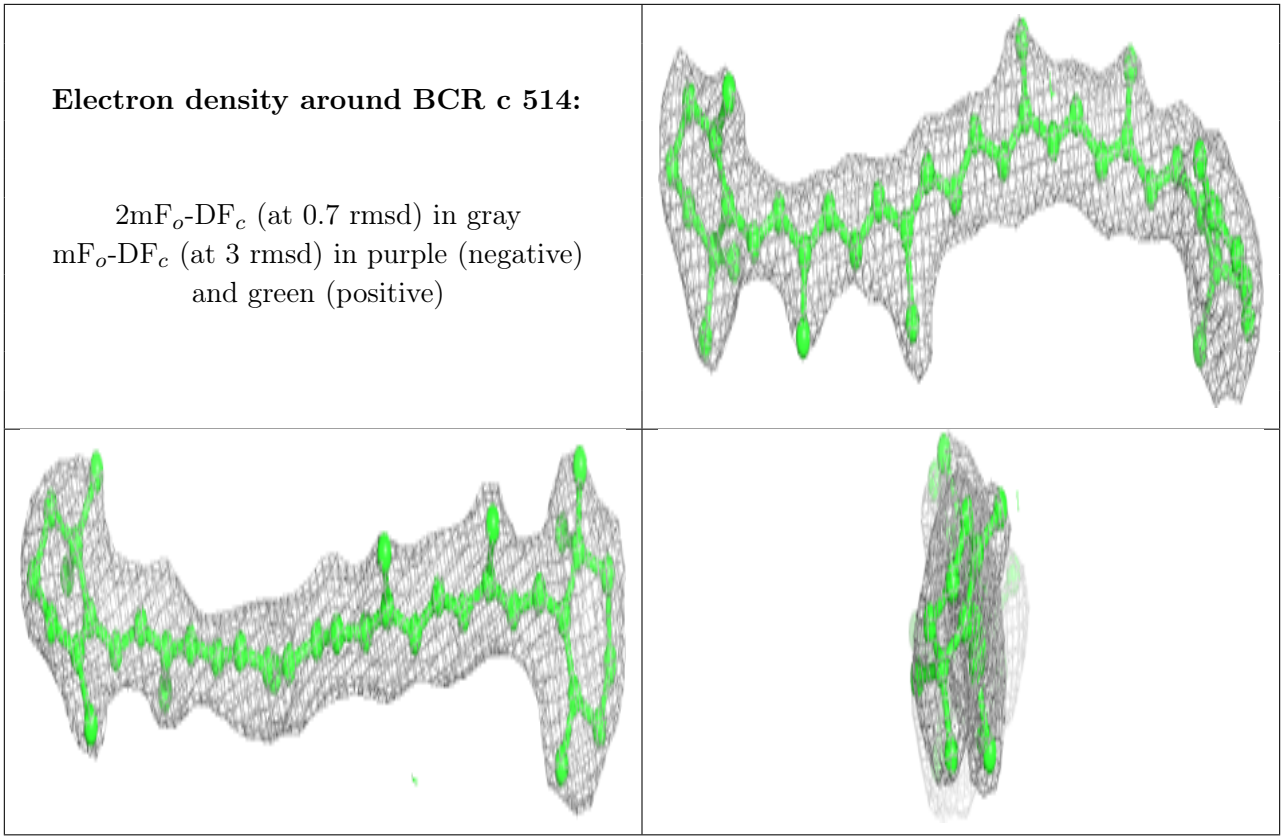
Electron density around BCR b 618:

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



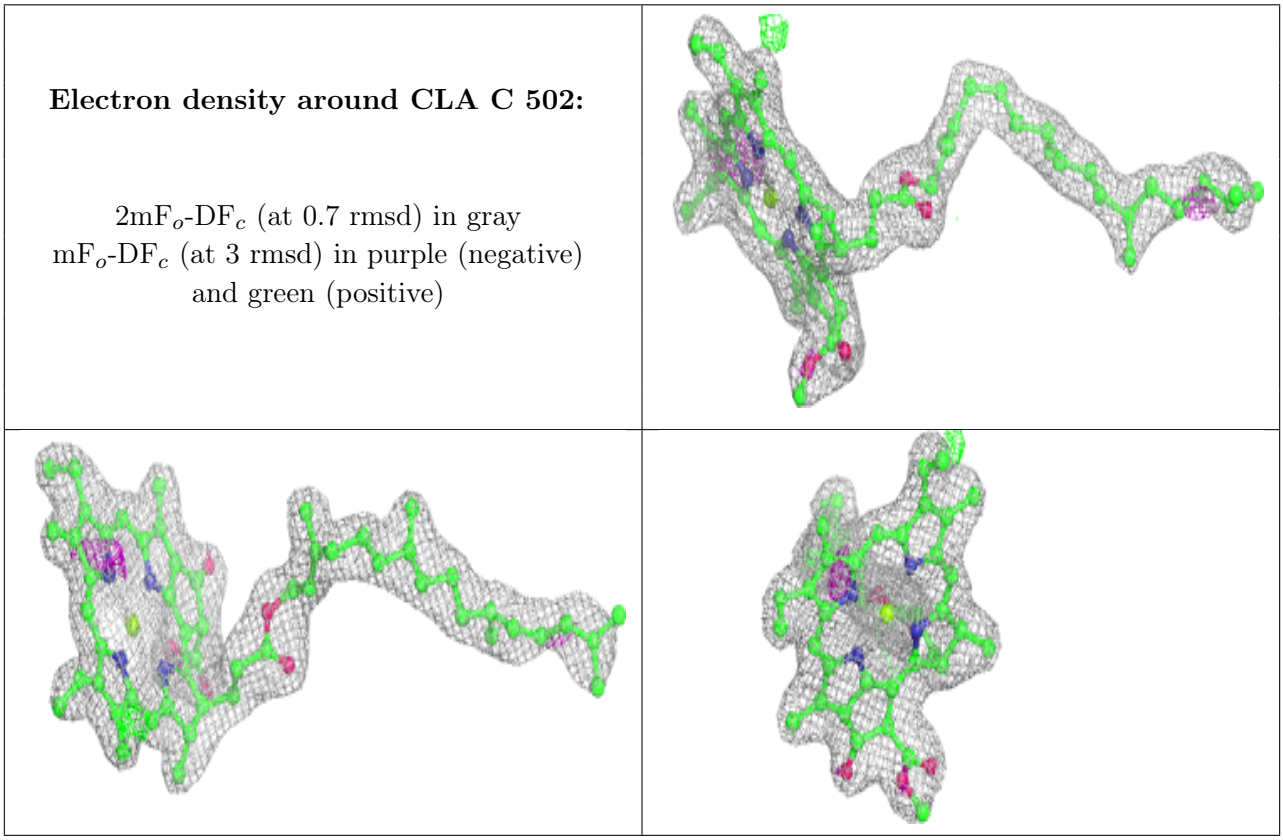
Electron density around BCR c 514:

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



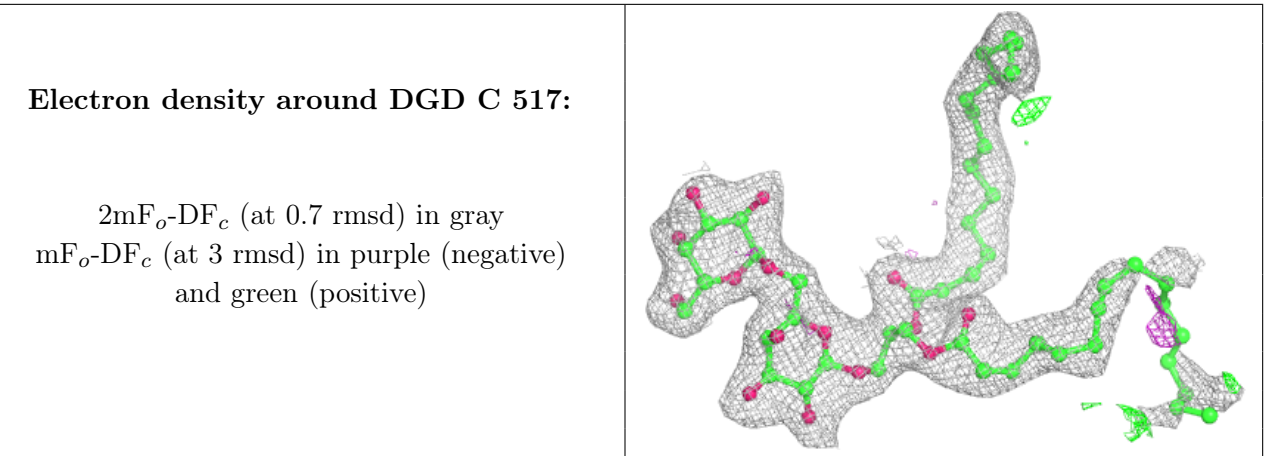
Electron density around CLA C 502:

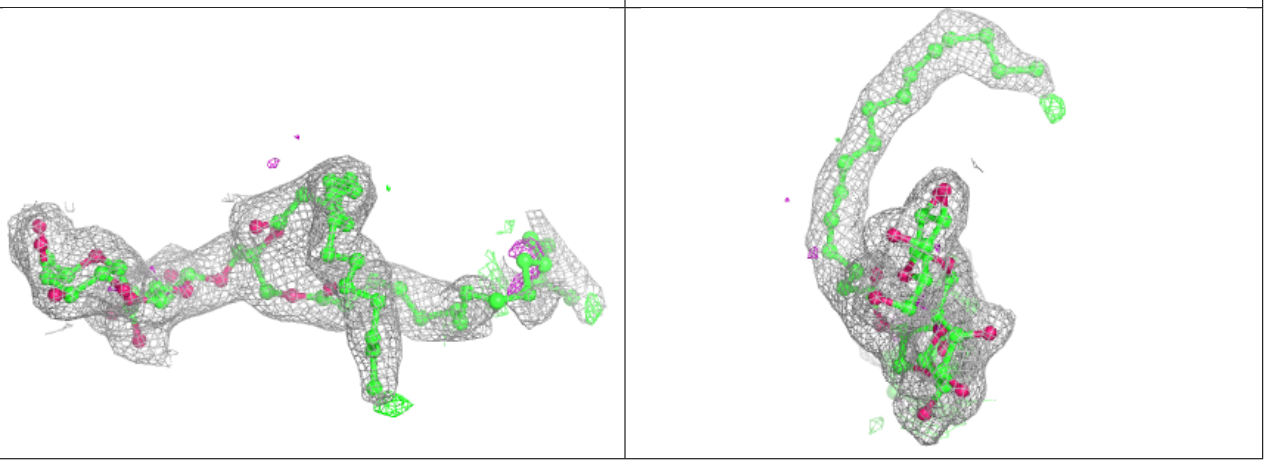
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD C 517:

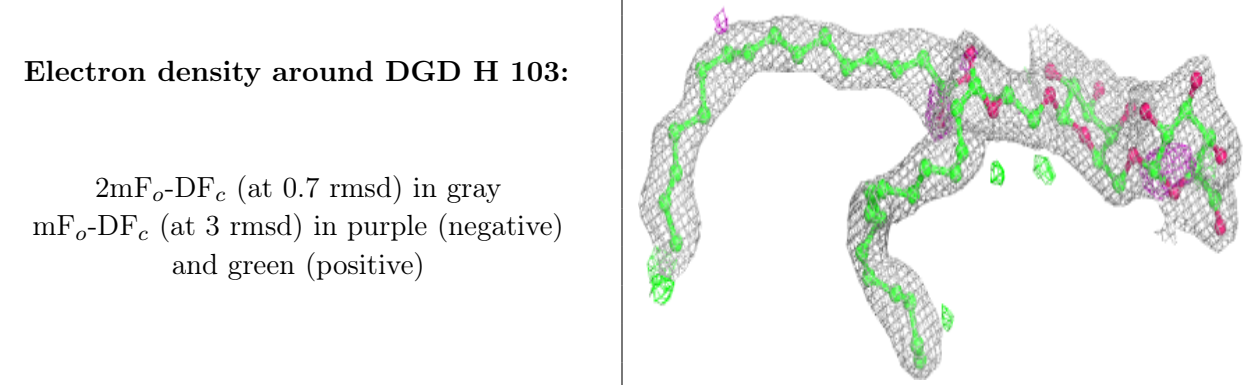
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

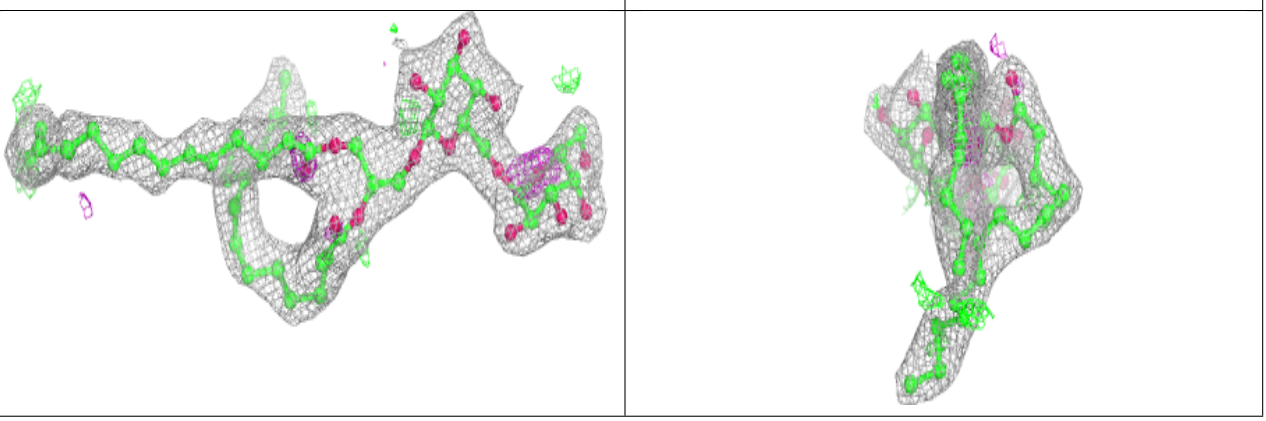




Electron density around DGD H 103:

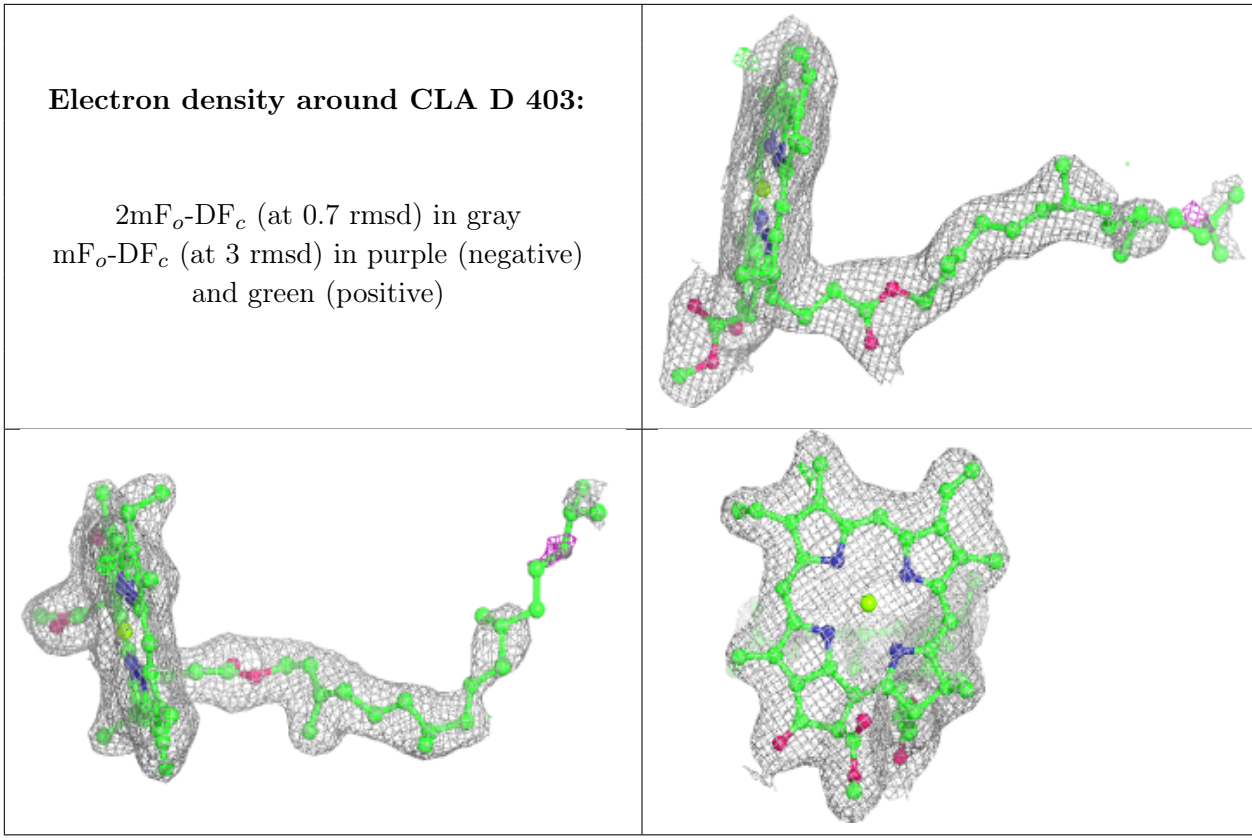
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





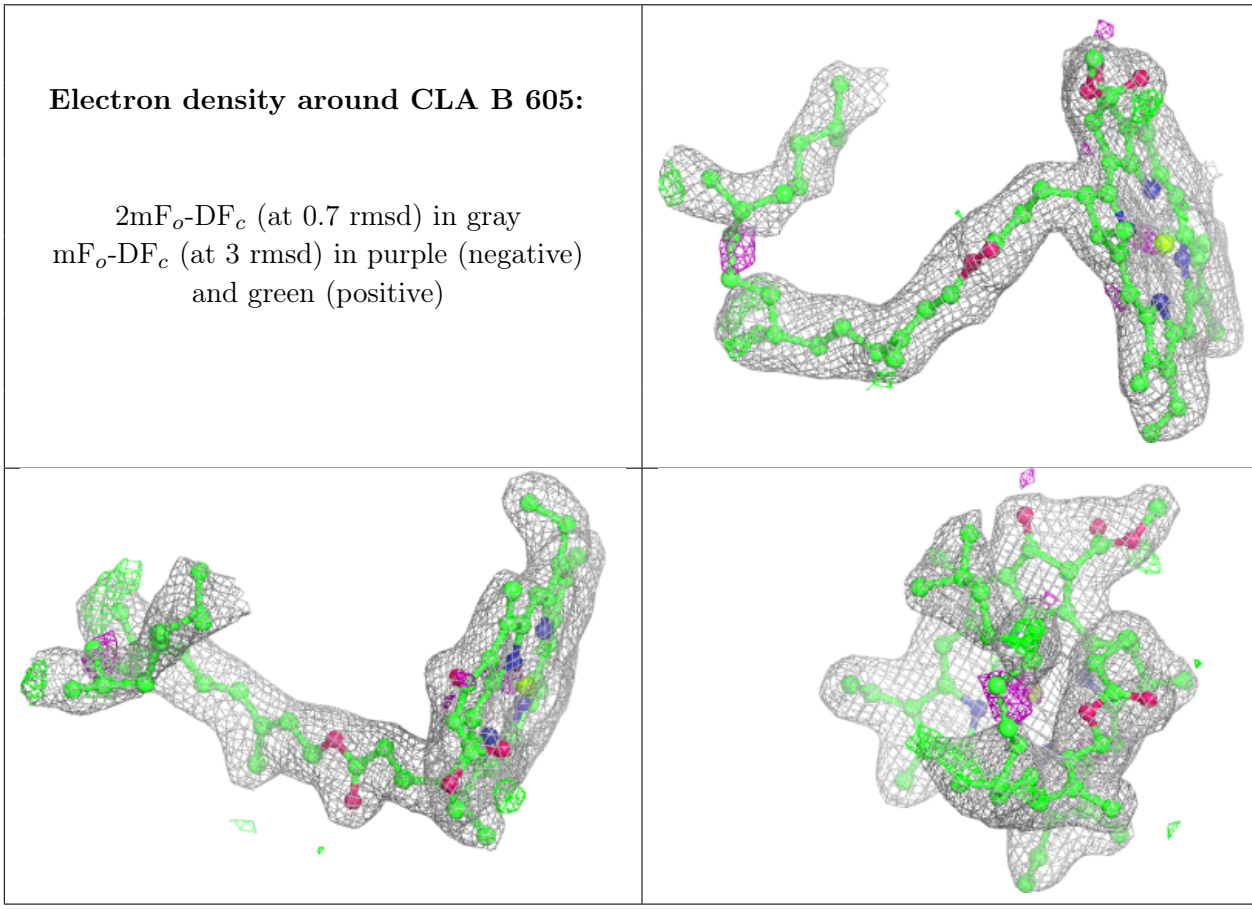
Electron density around CLA D 403:

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



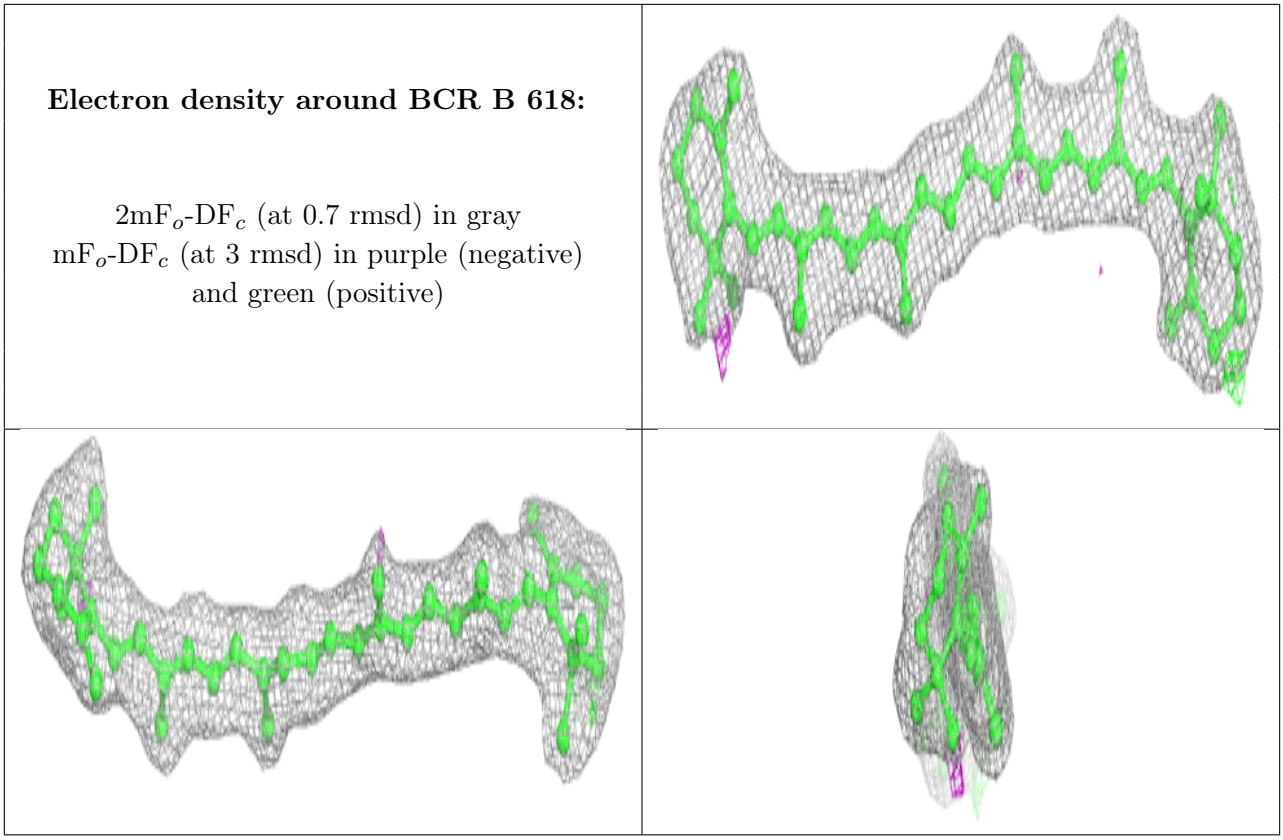
Electron density around CLA B 605:

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



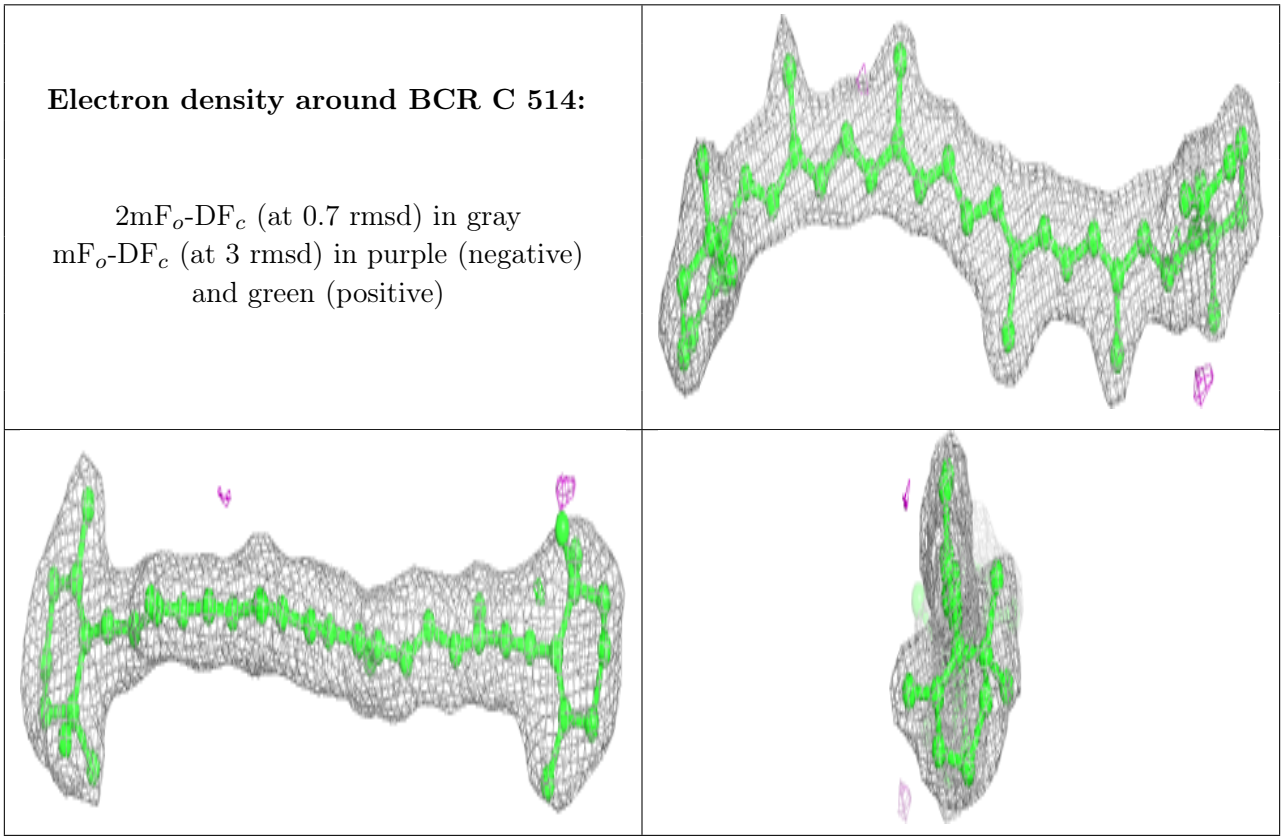
Electron density around BCR B 618:

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



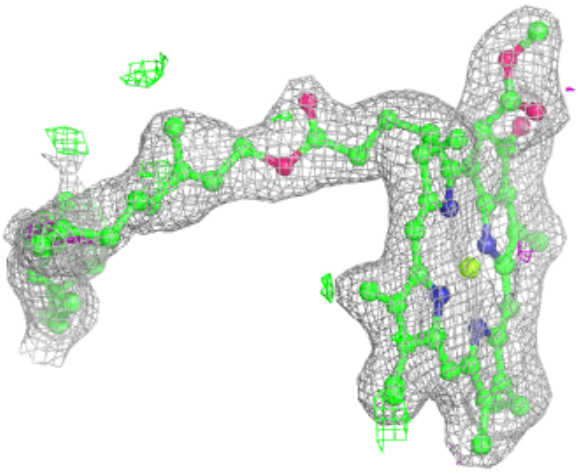
Electron density around BCR C 514:

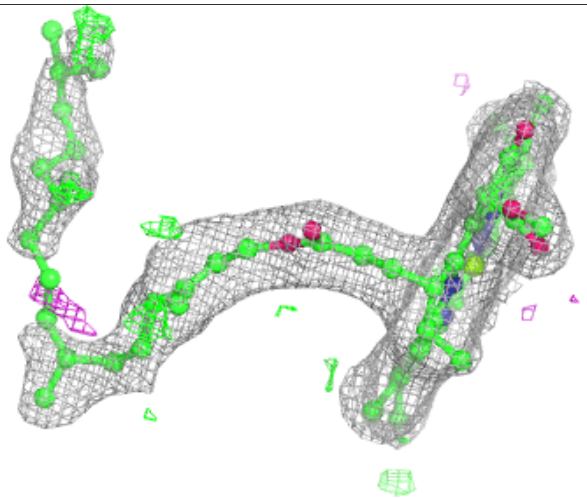
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

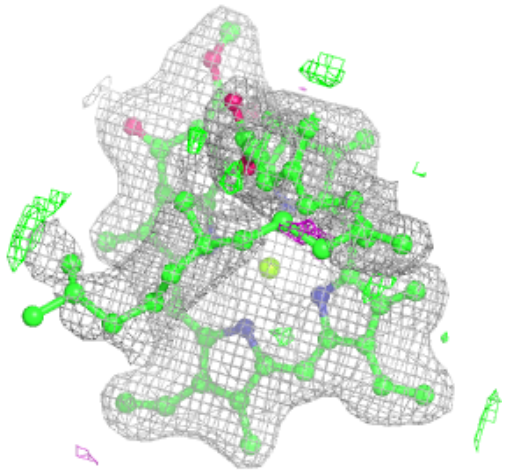


Electron density around CLA a 610:

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

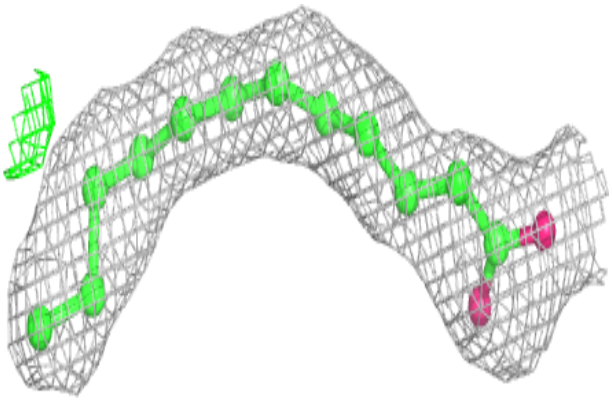


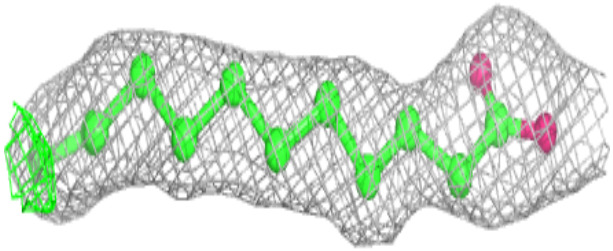


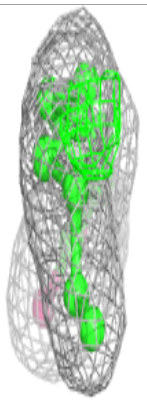


Electron density around STE t 102:

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

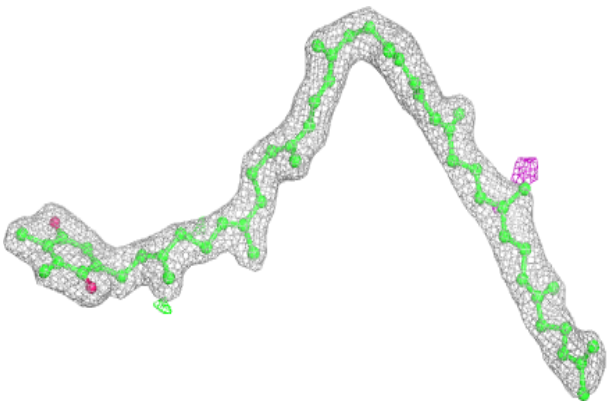


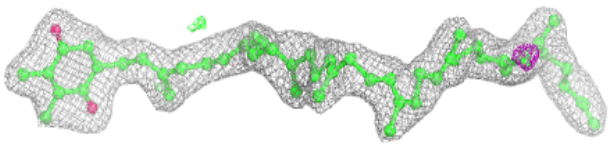


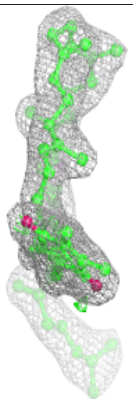


Electron density around PL9 D 405:

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

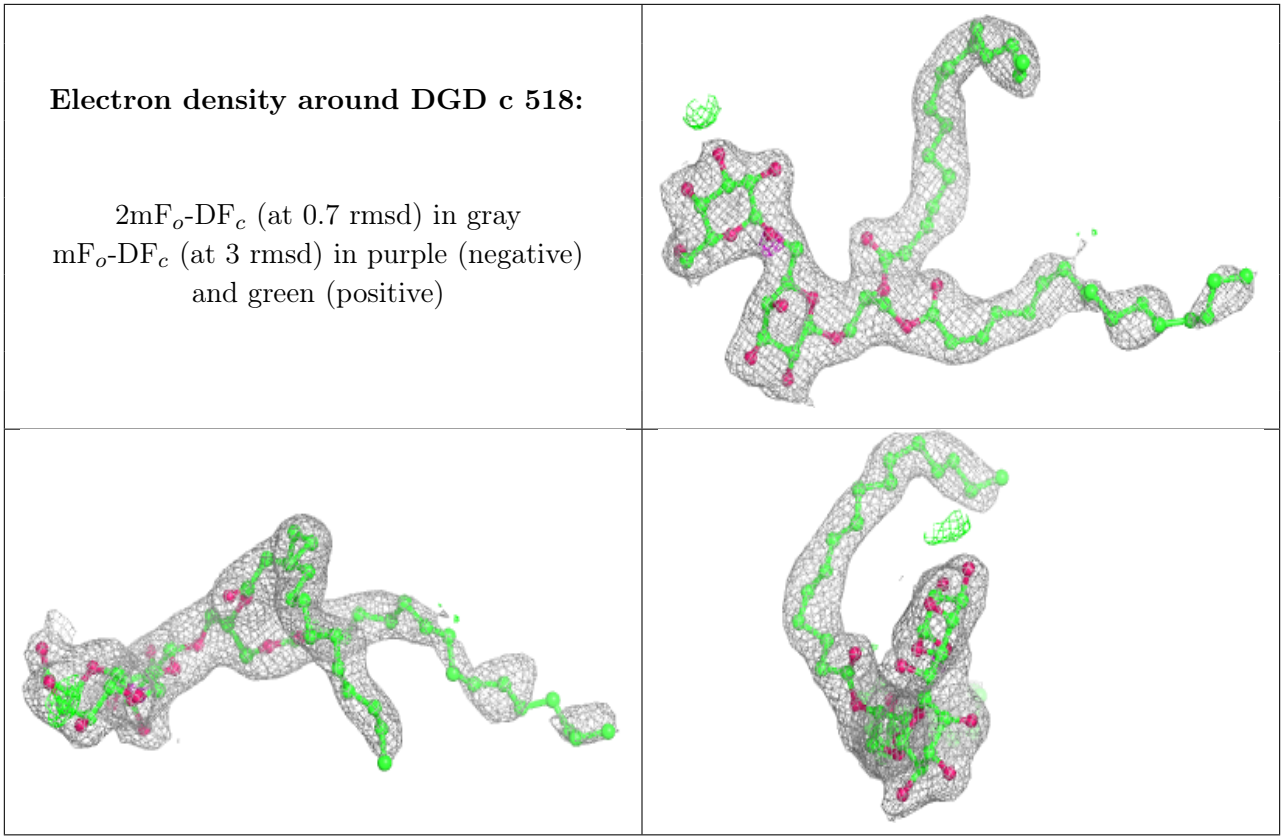






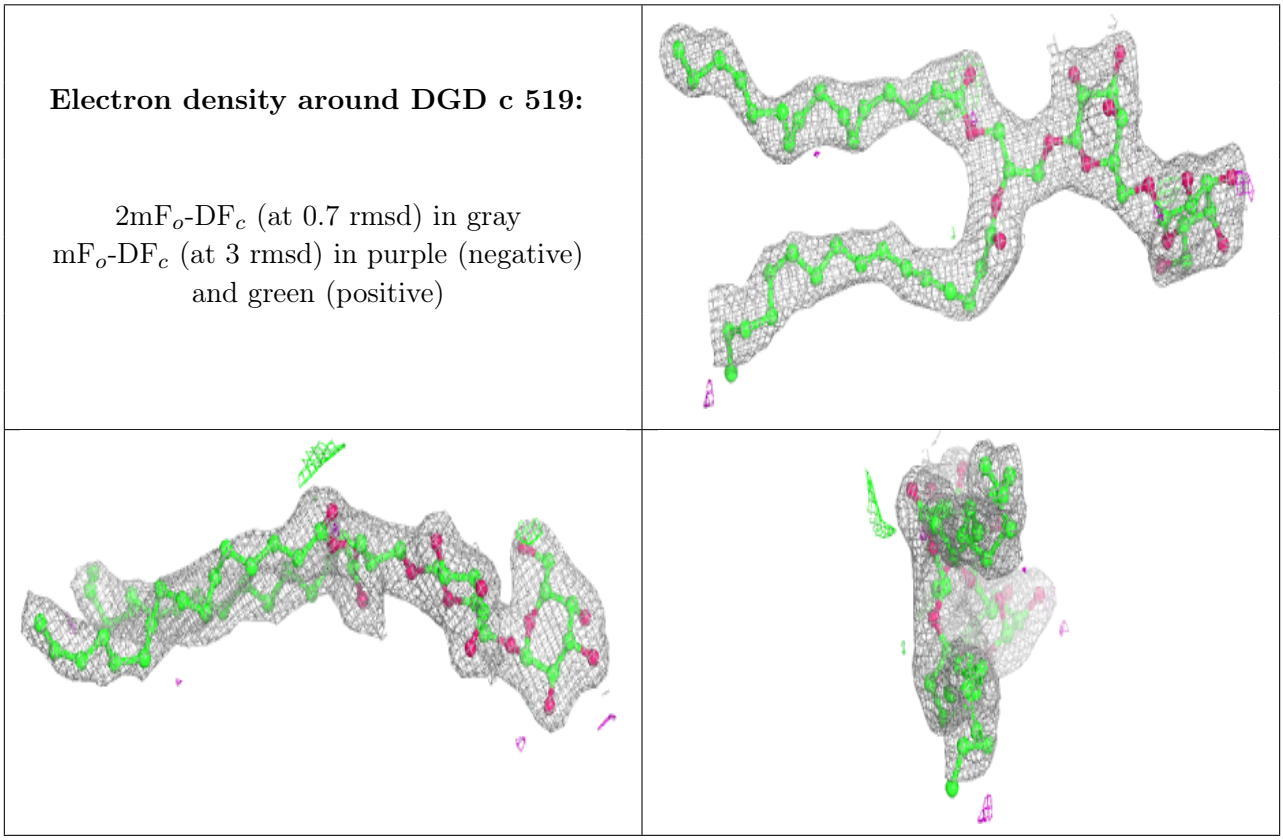
Electron density around DGD c 518:

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



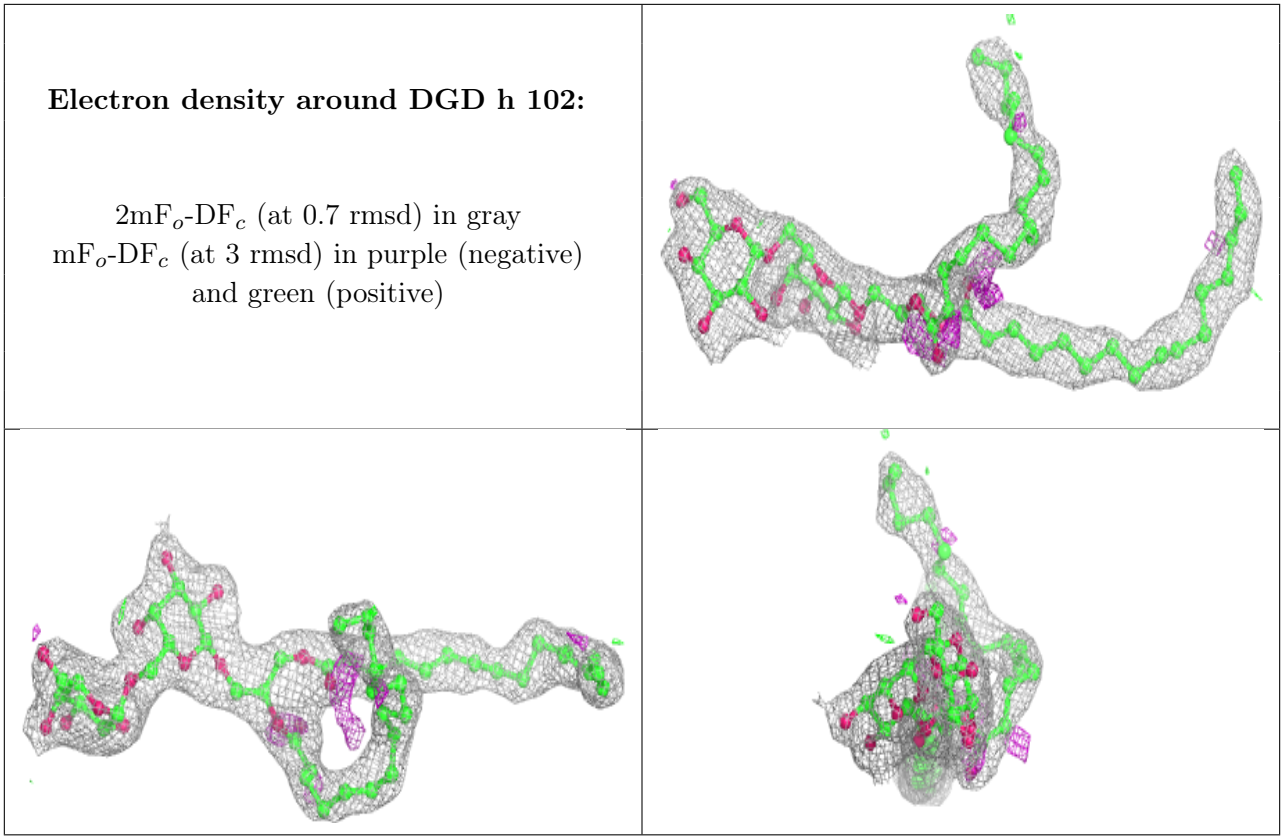
Electron density around DGD c 519:

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



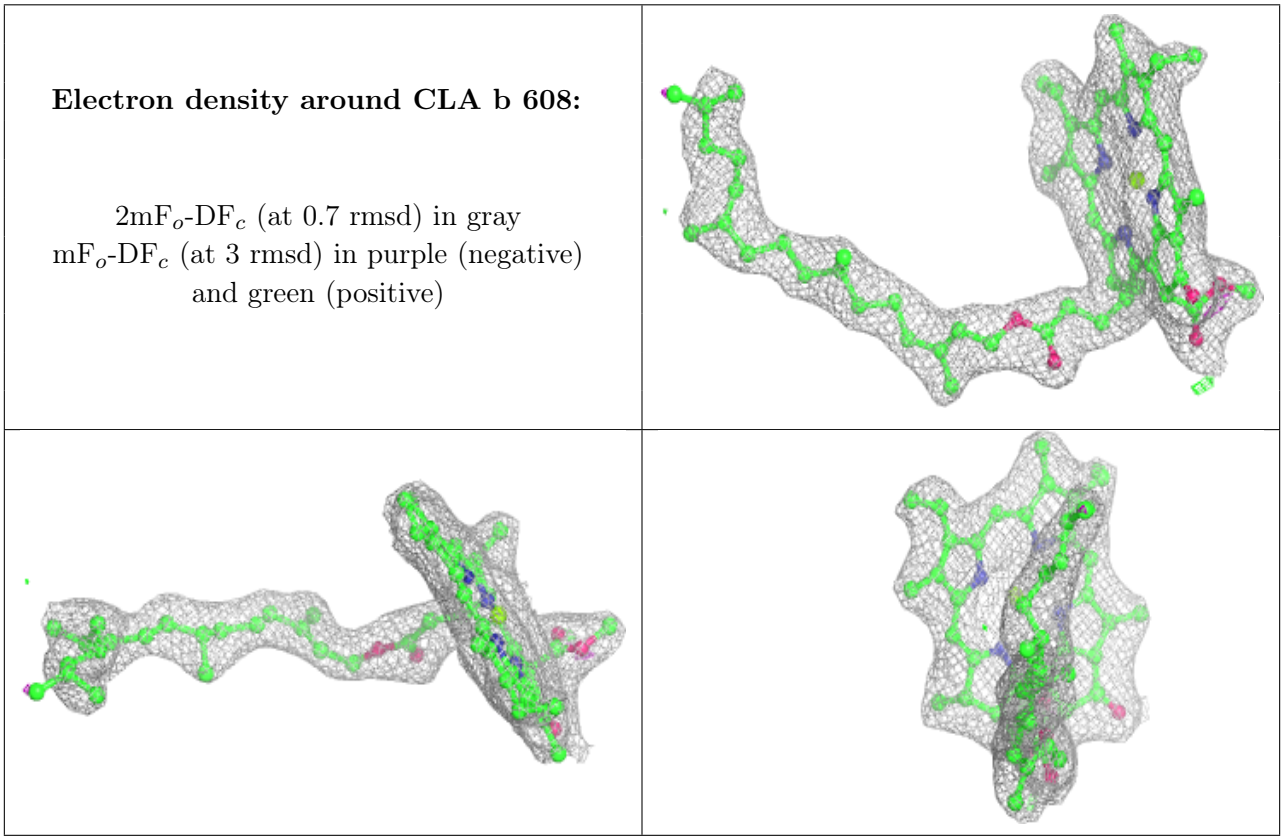
Electron density around DGD h 102:

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



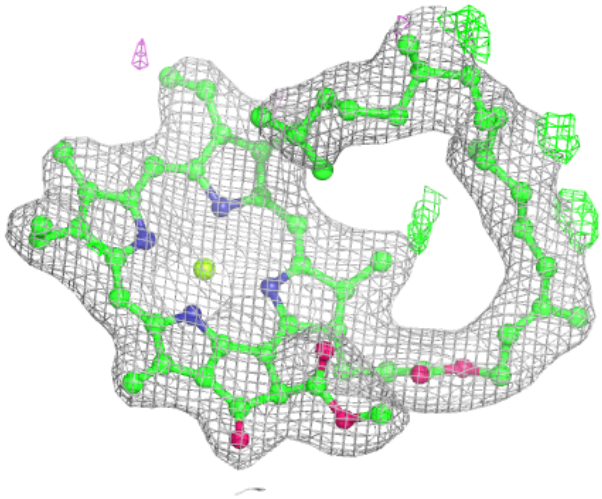
Electron density around CLA b 608:

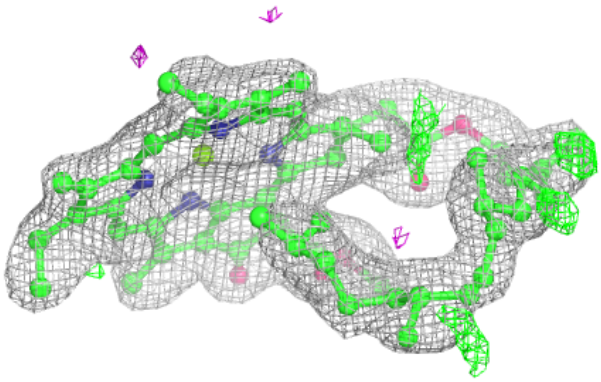
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

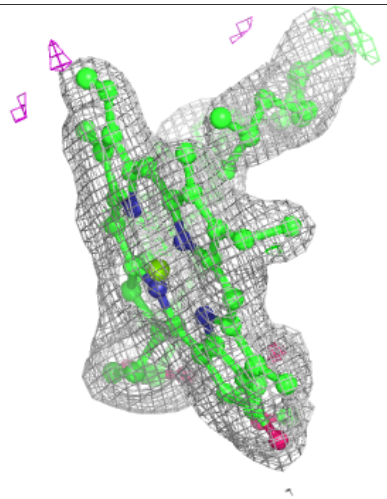


Electron density around CLA b 614:

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

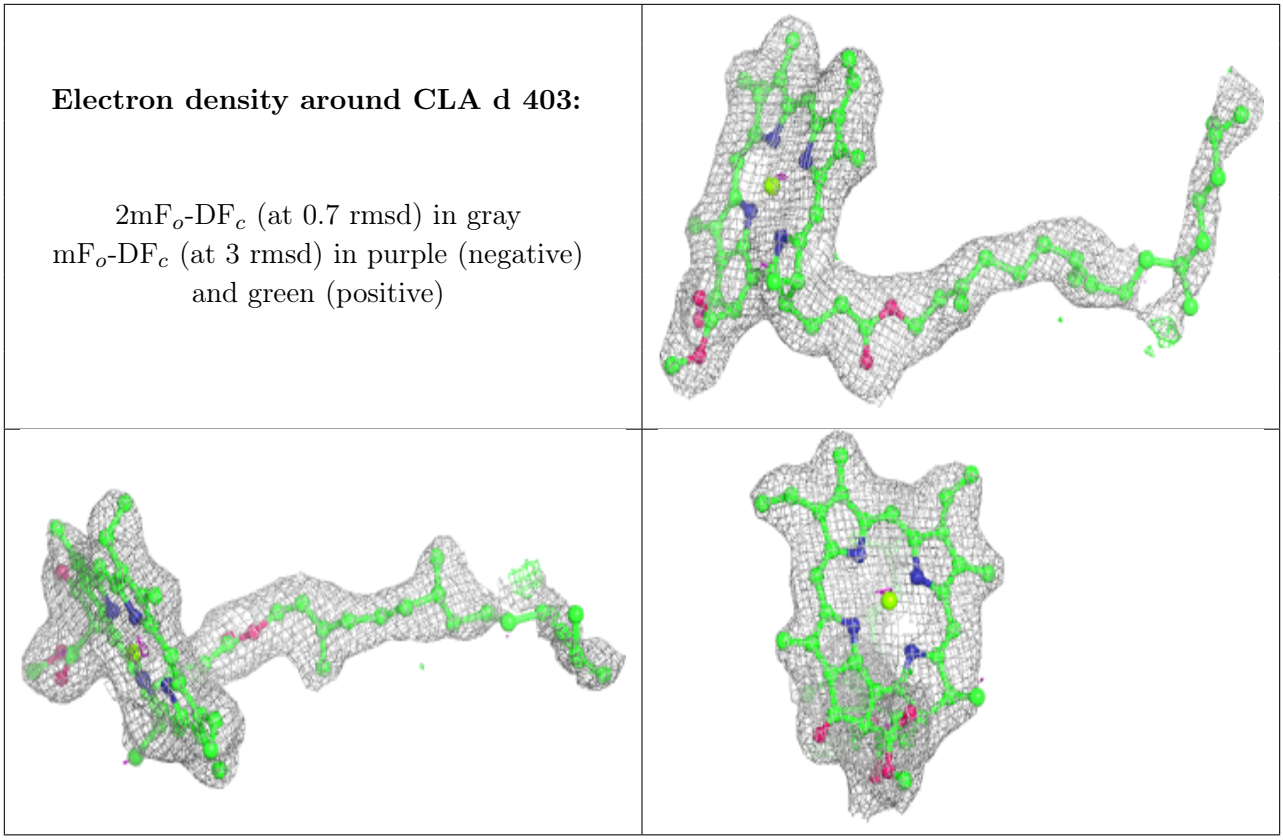






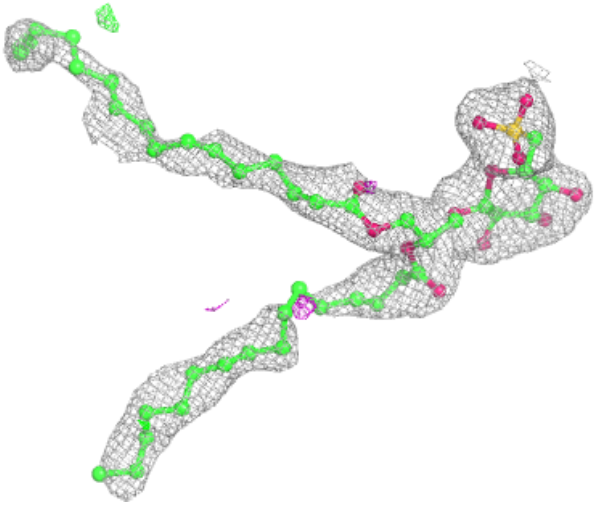
Electron density around CLA d 403:

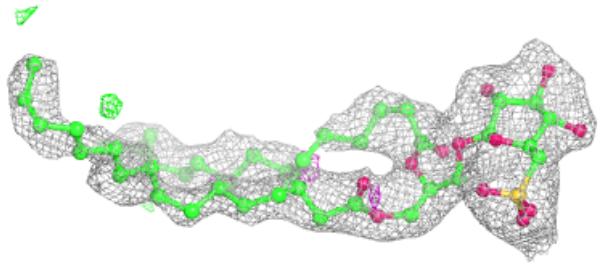
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

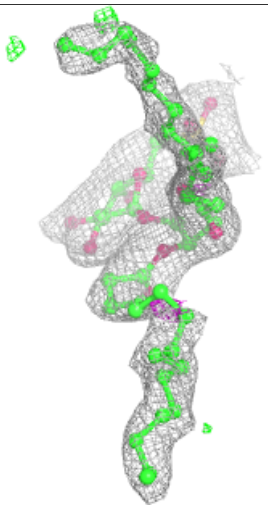


Electron density around SQD a 614:

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

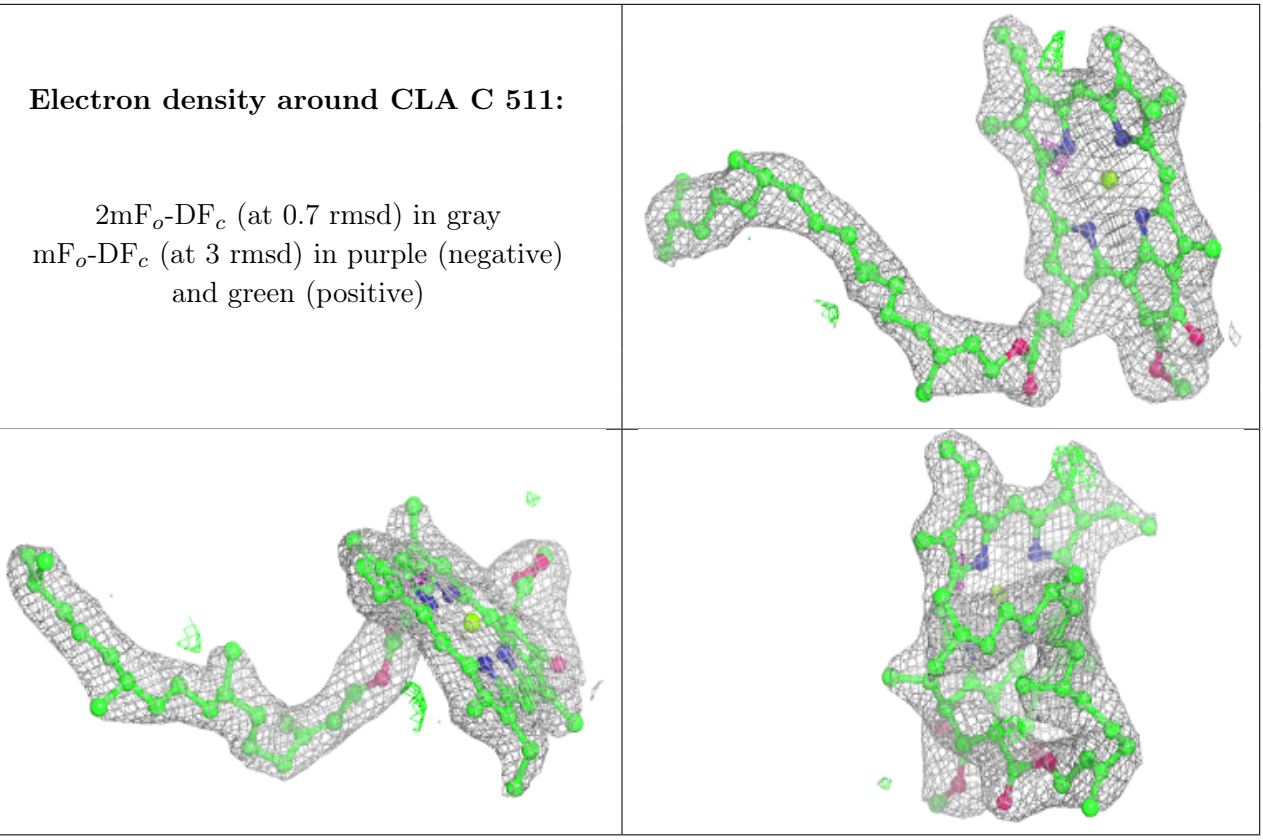






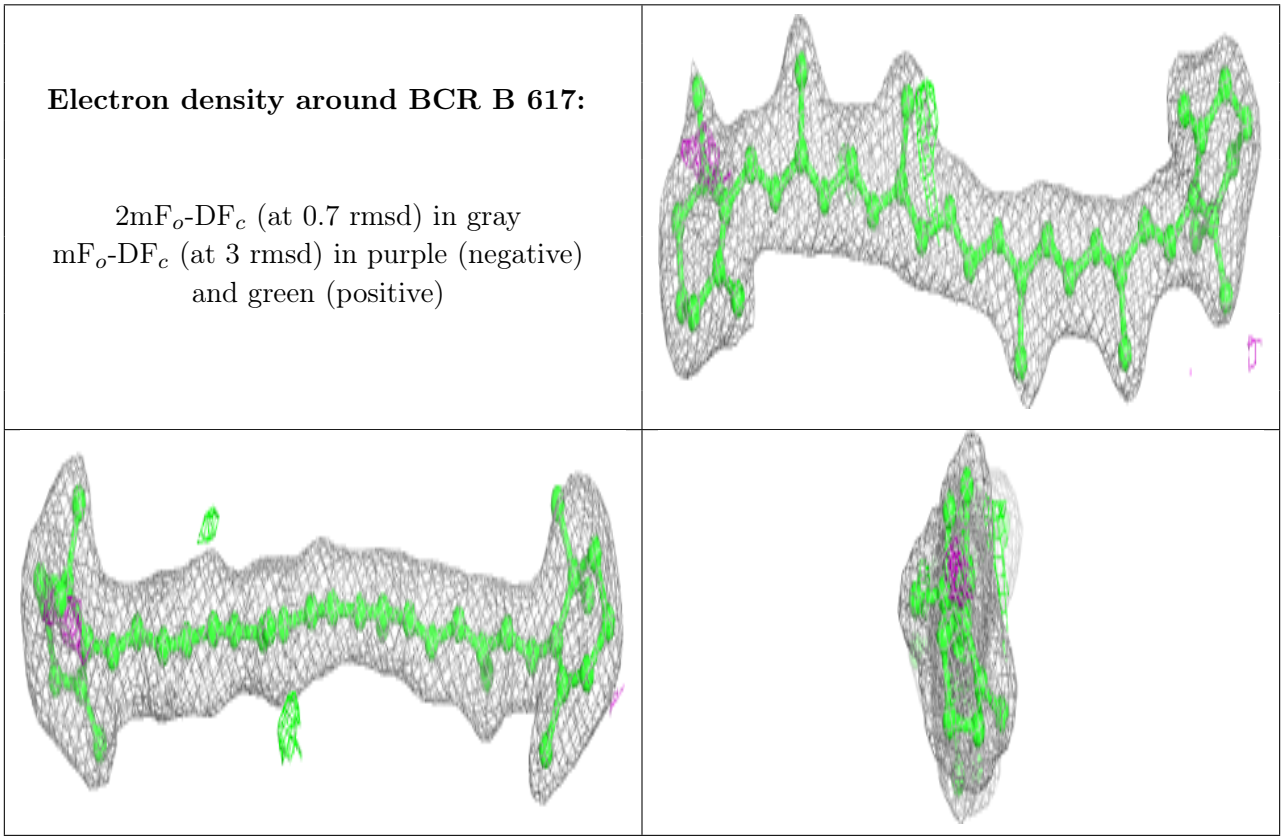
Electron density around CLA C 511:

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



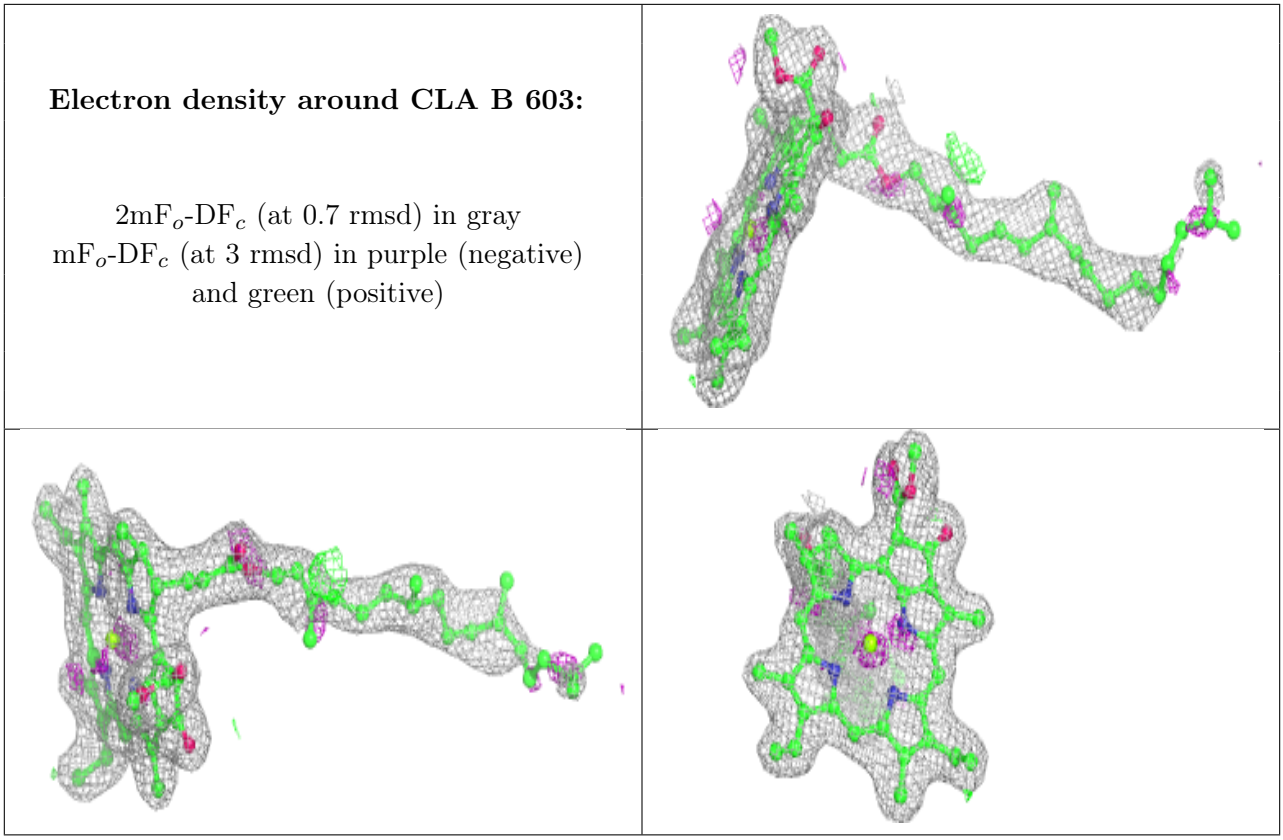
Electron density around BCR B 617:

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



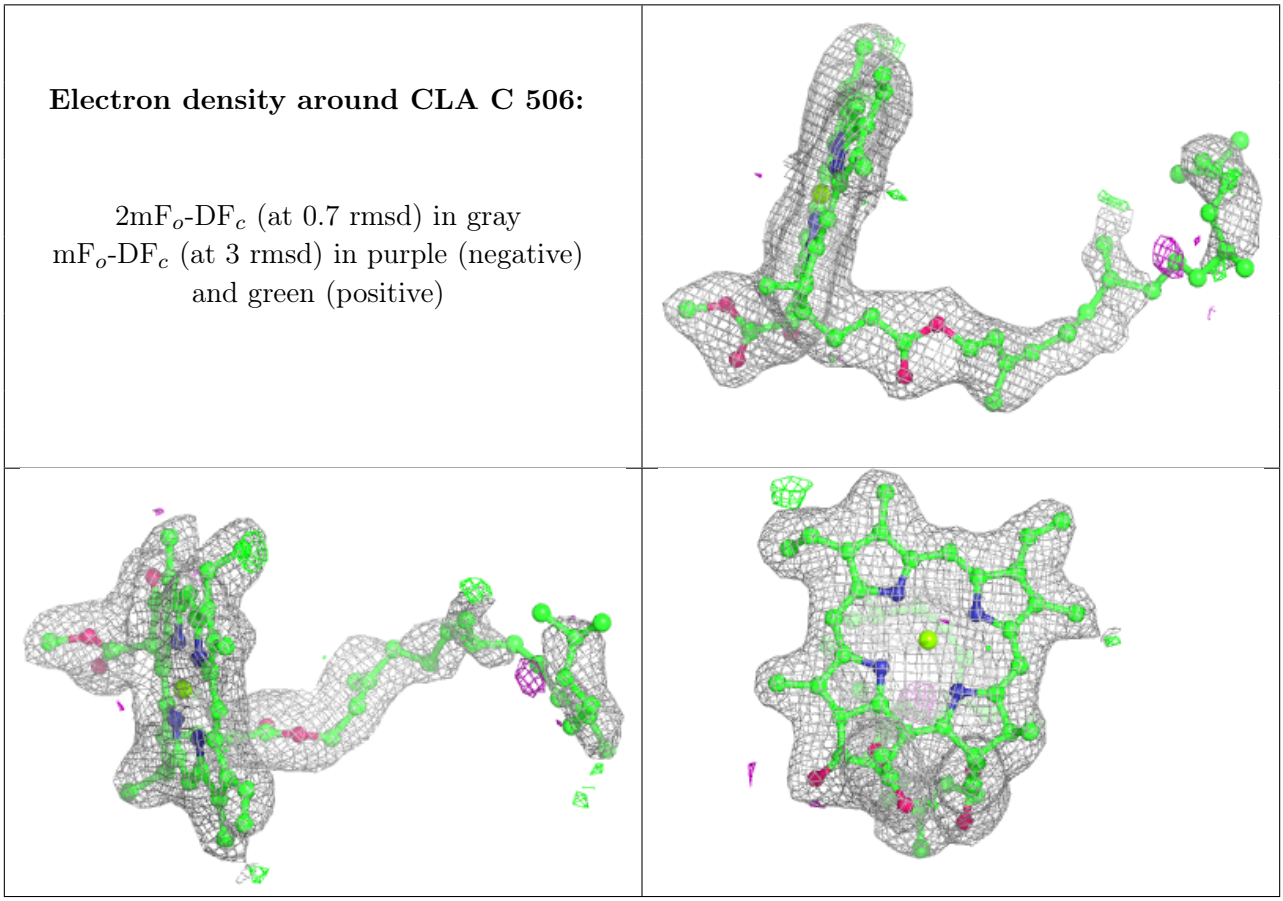
Electron density around CLA B 603:

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



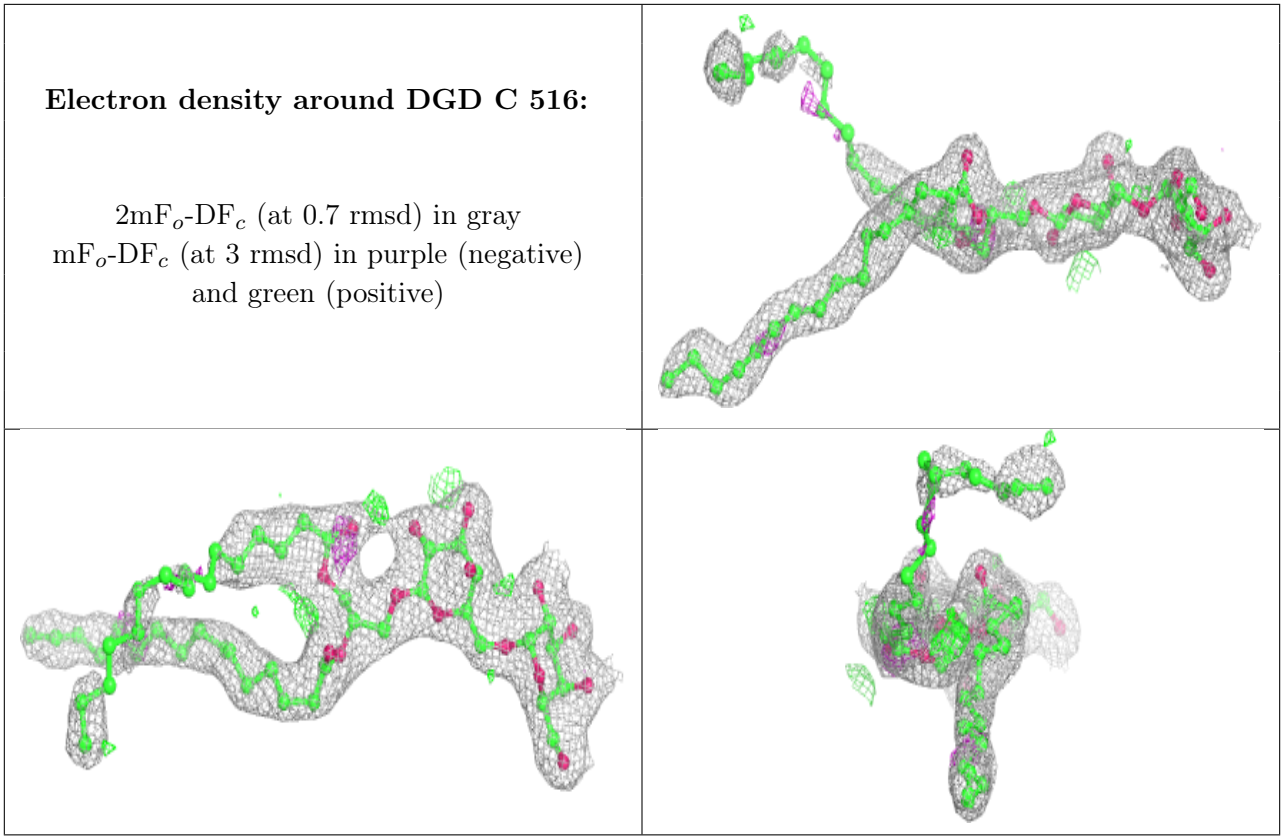
Electron density around CLA C 506:

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



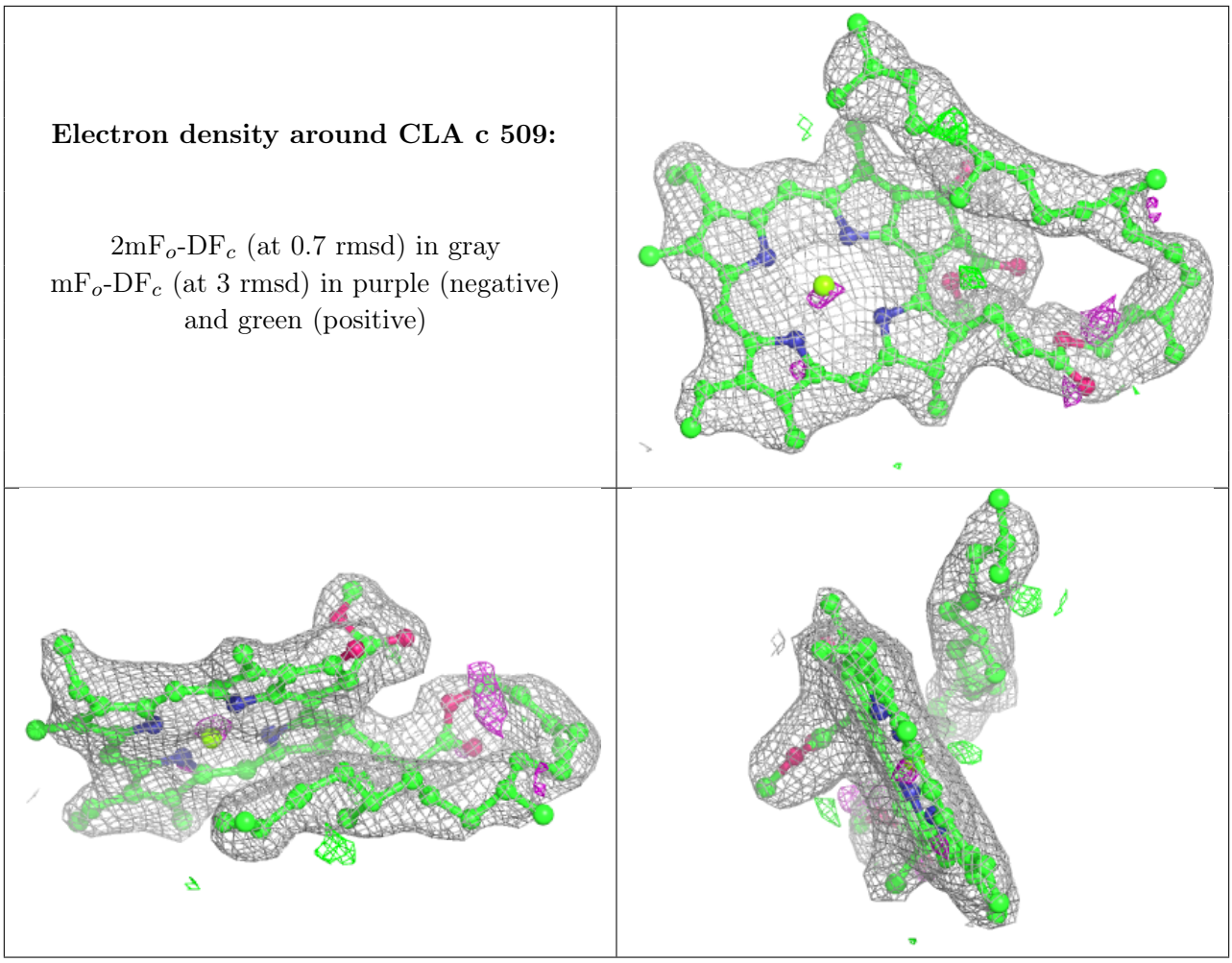
Electron density around DGD C 516:

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



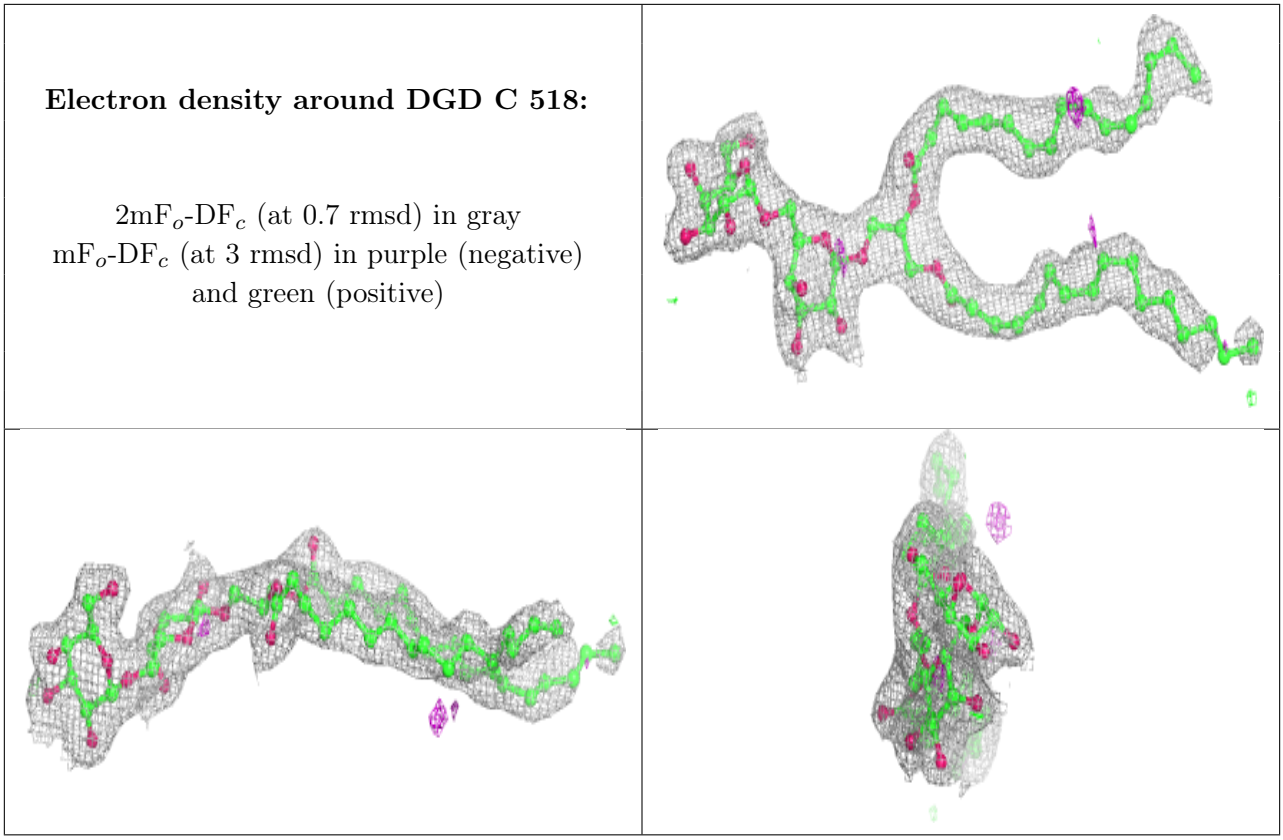
Electron density around CLA c 509:

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



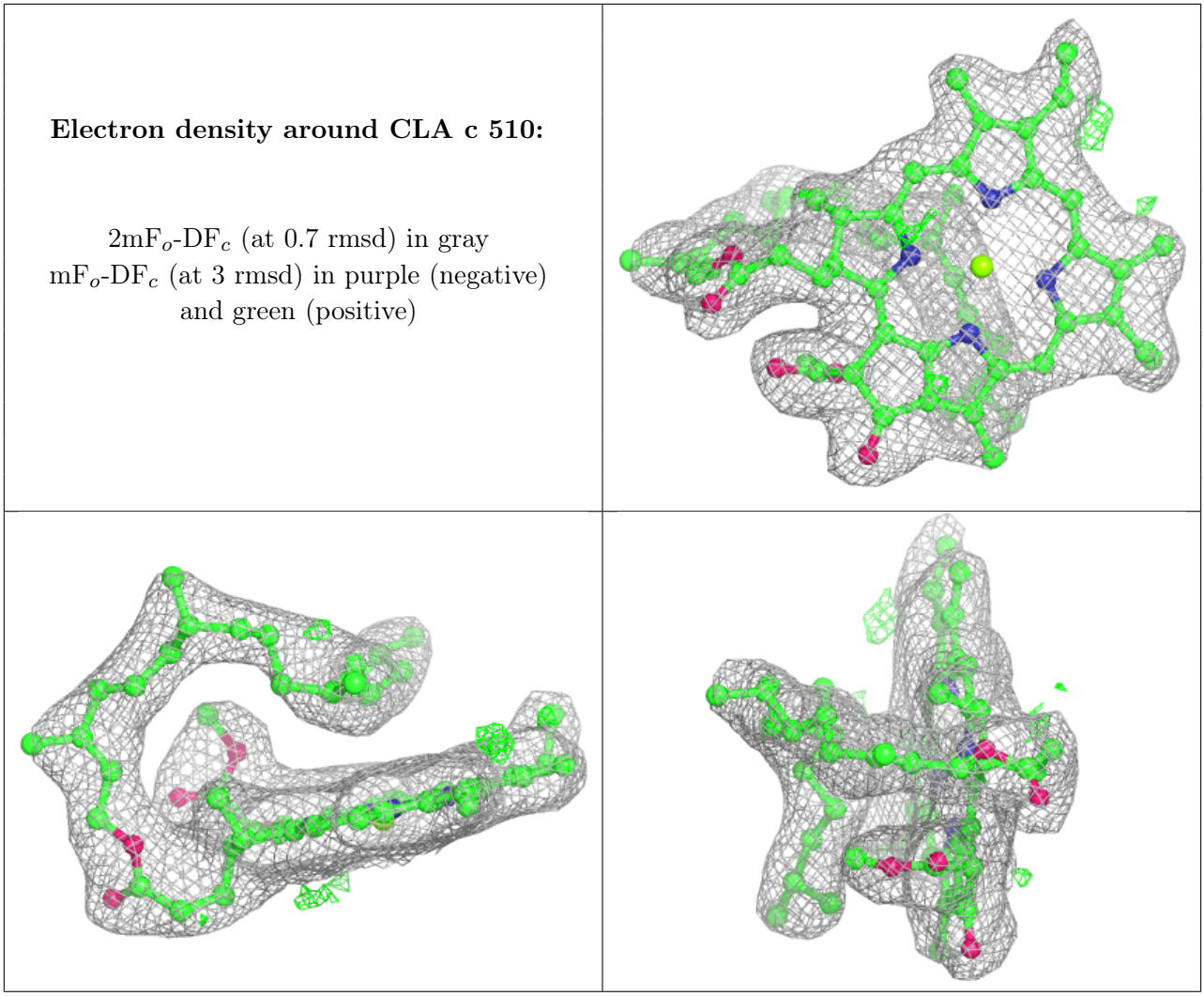
Electron density around DGD C 518:

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



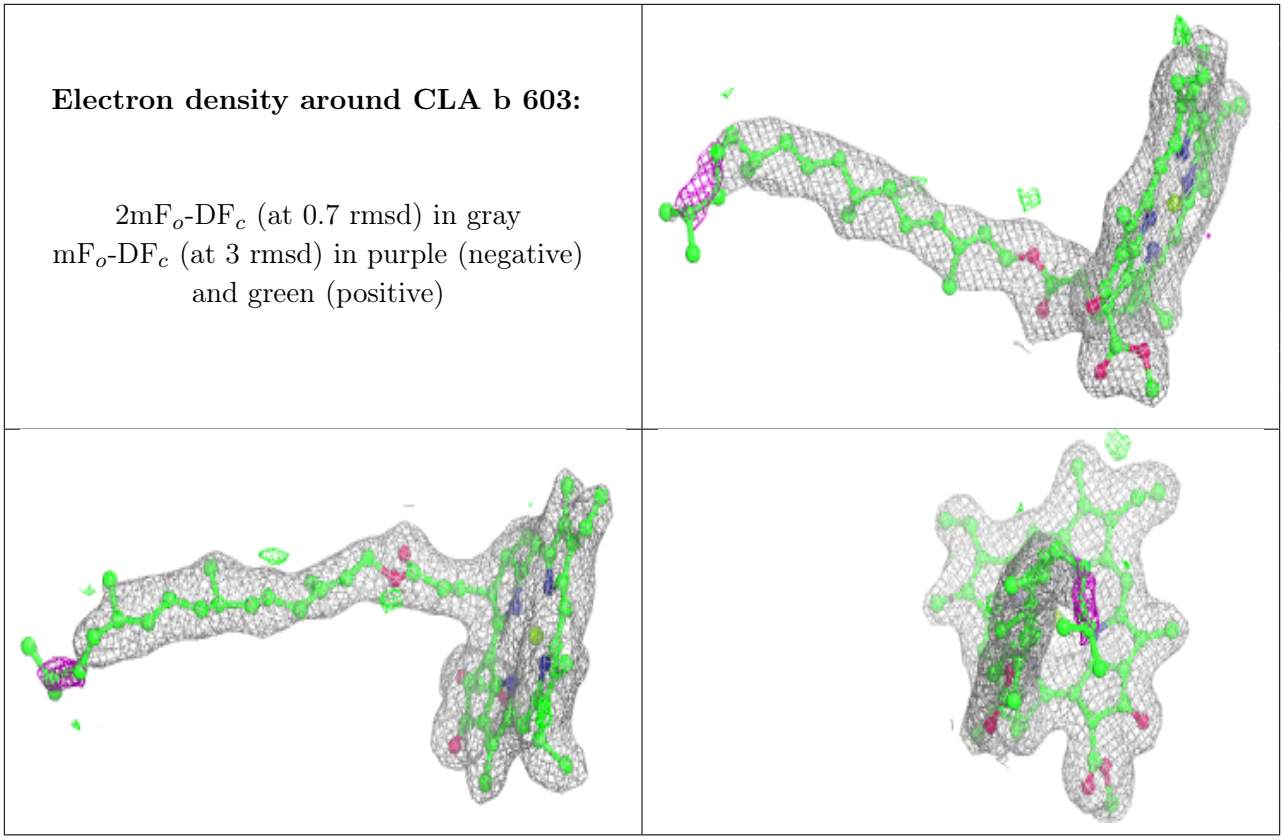
Electron density around CLA c 510:

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



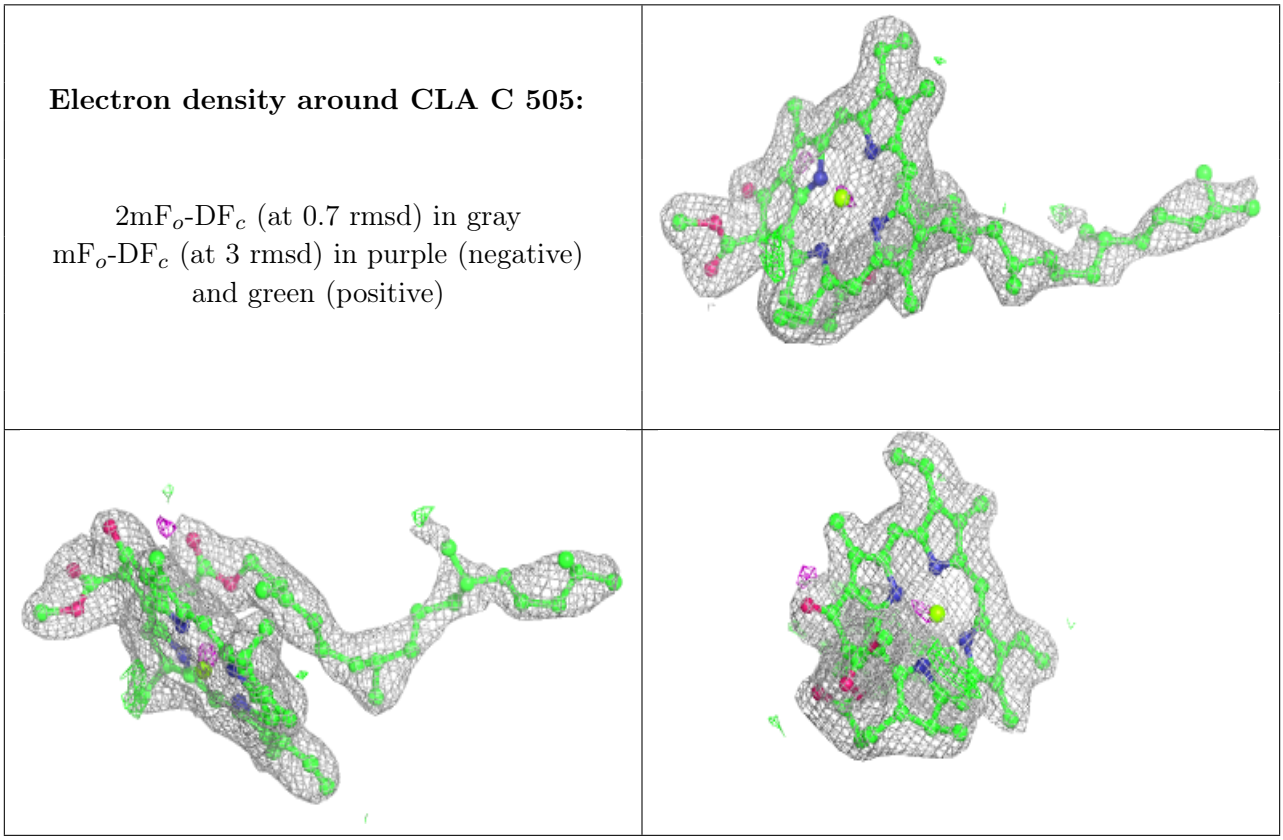
Electron density around CLA b 603:

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



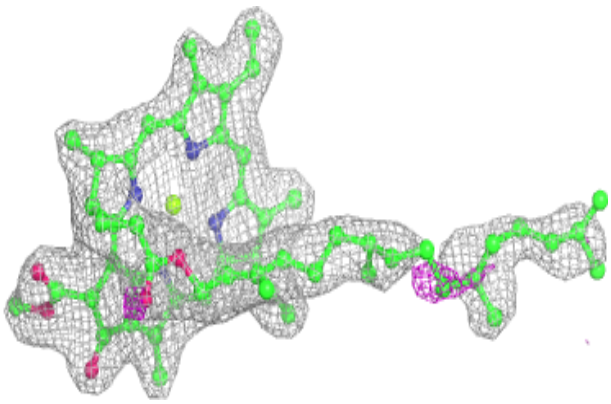
Electron density around CLA C 505:

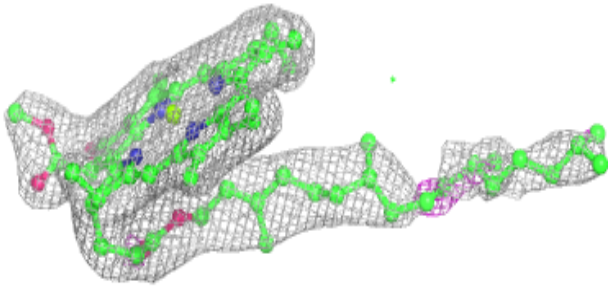
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

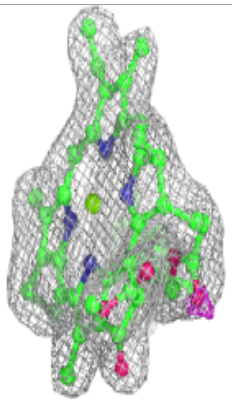


Electron density around CLA b 613:

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

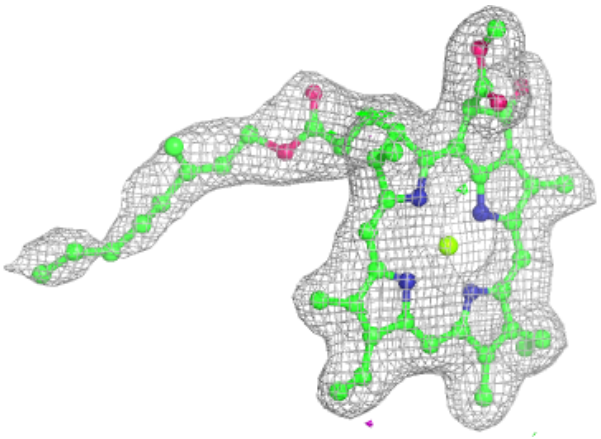


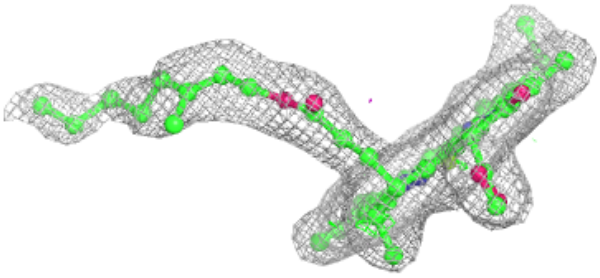


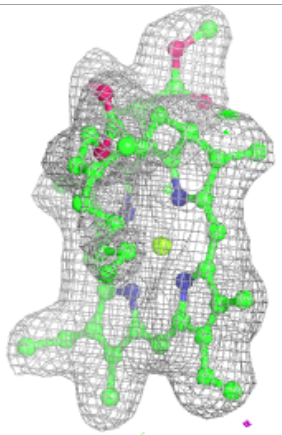


Electron density around CLA A 610:

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

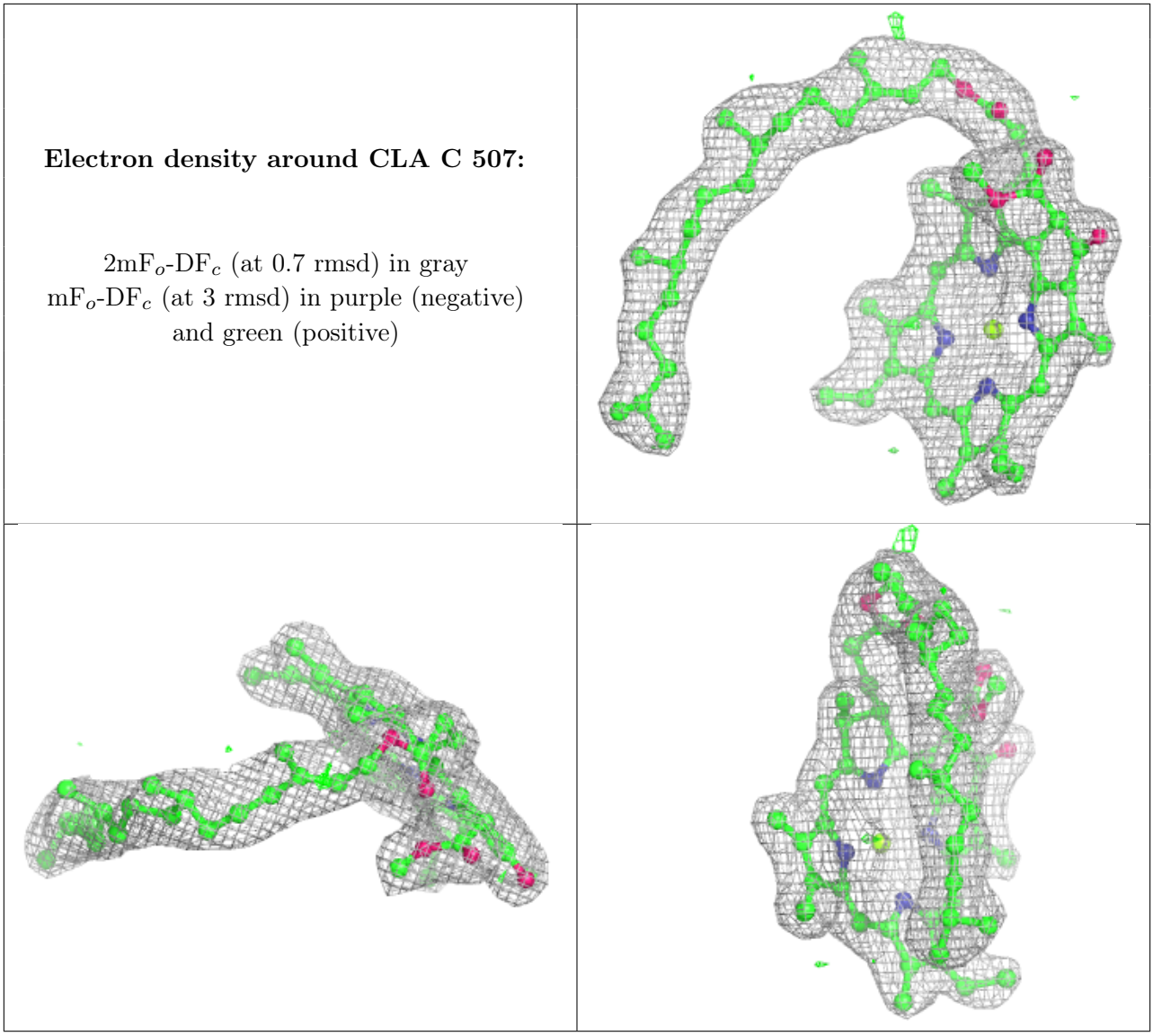






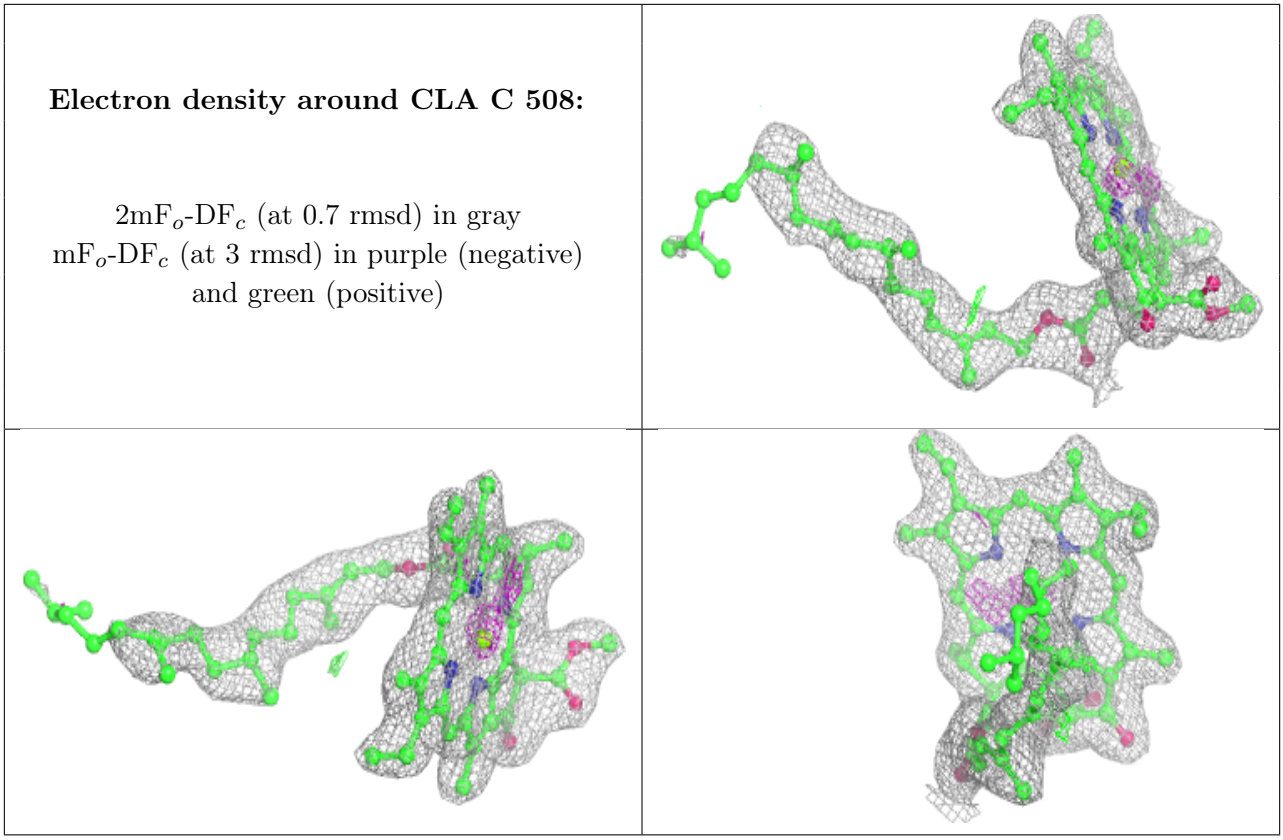
Electron density around CLA C 507:

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



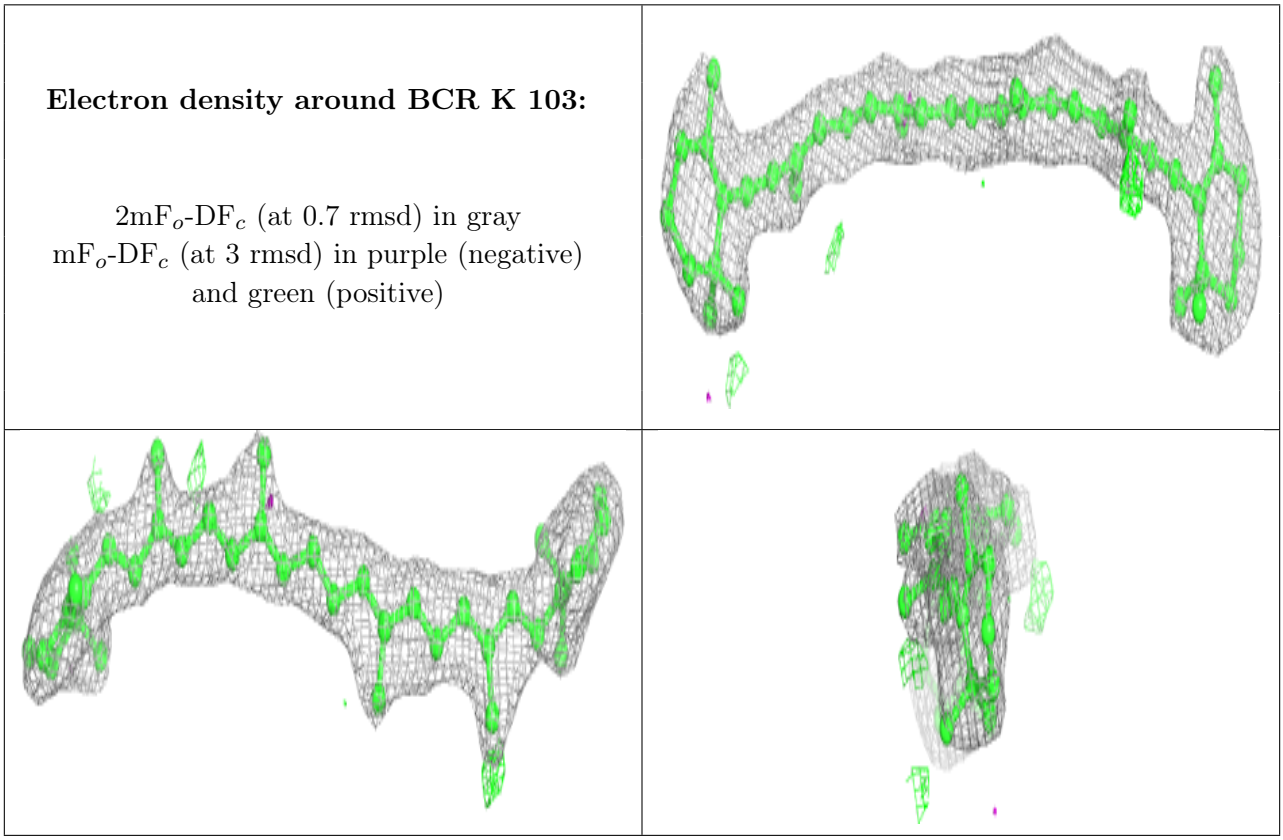
Electron density around CLA C 508:

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



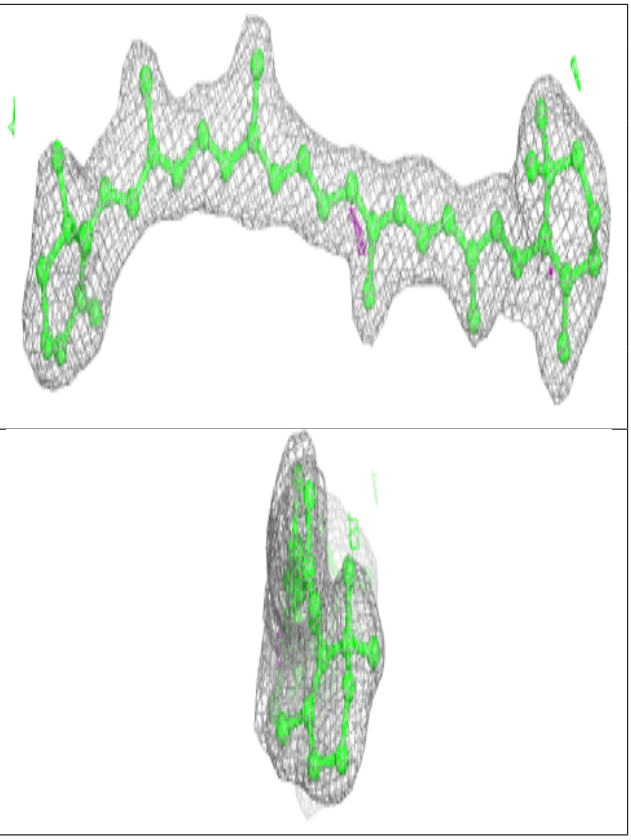
Electron density around BCR K 103:

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



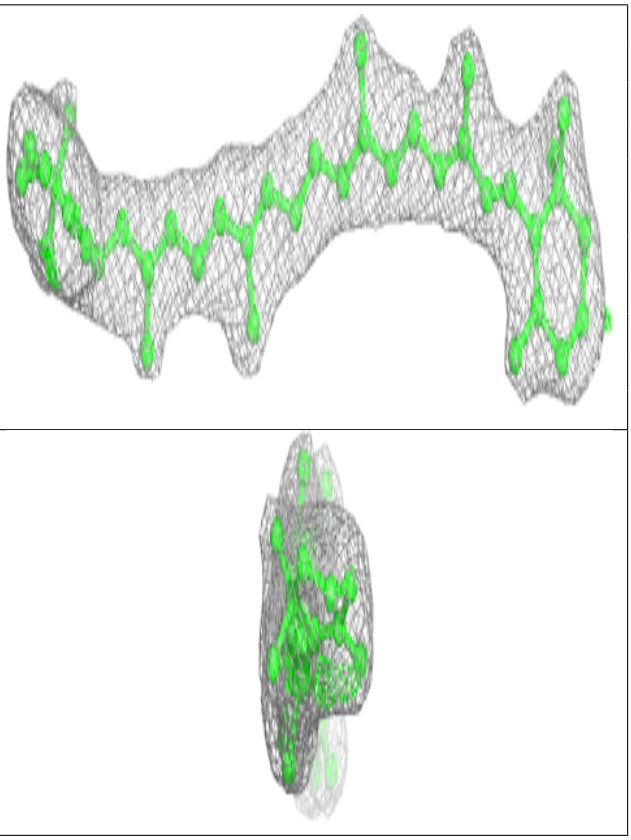
Electron density around BCR T 101:

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



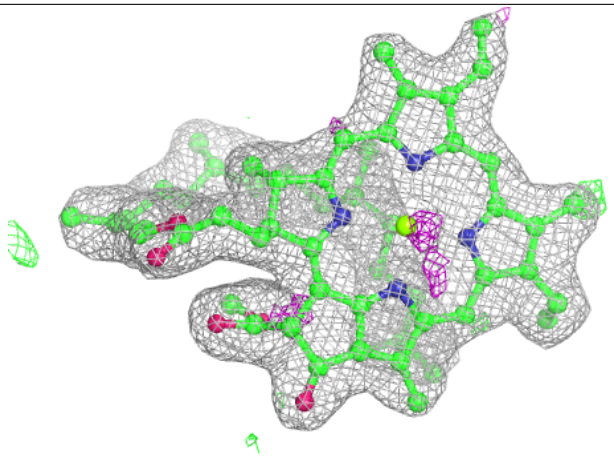
Electron density around BCR b 616:

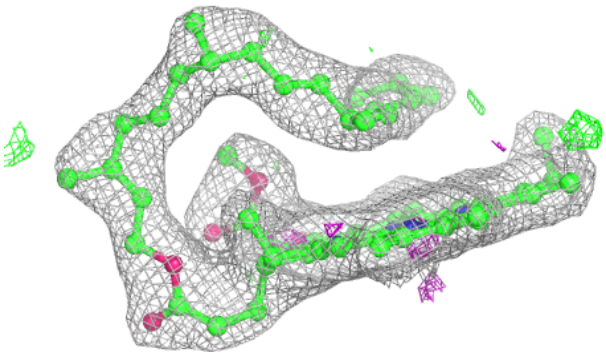
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

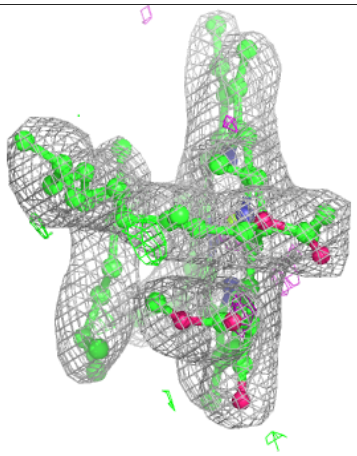


Electron density around CLA C 510:

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

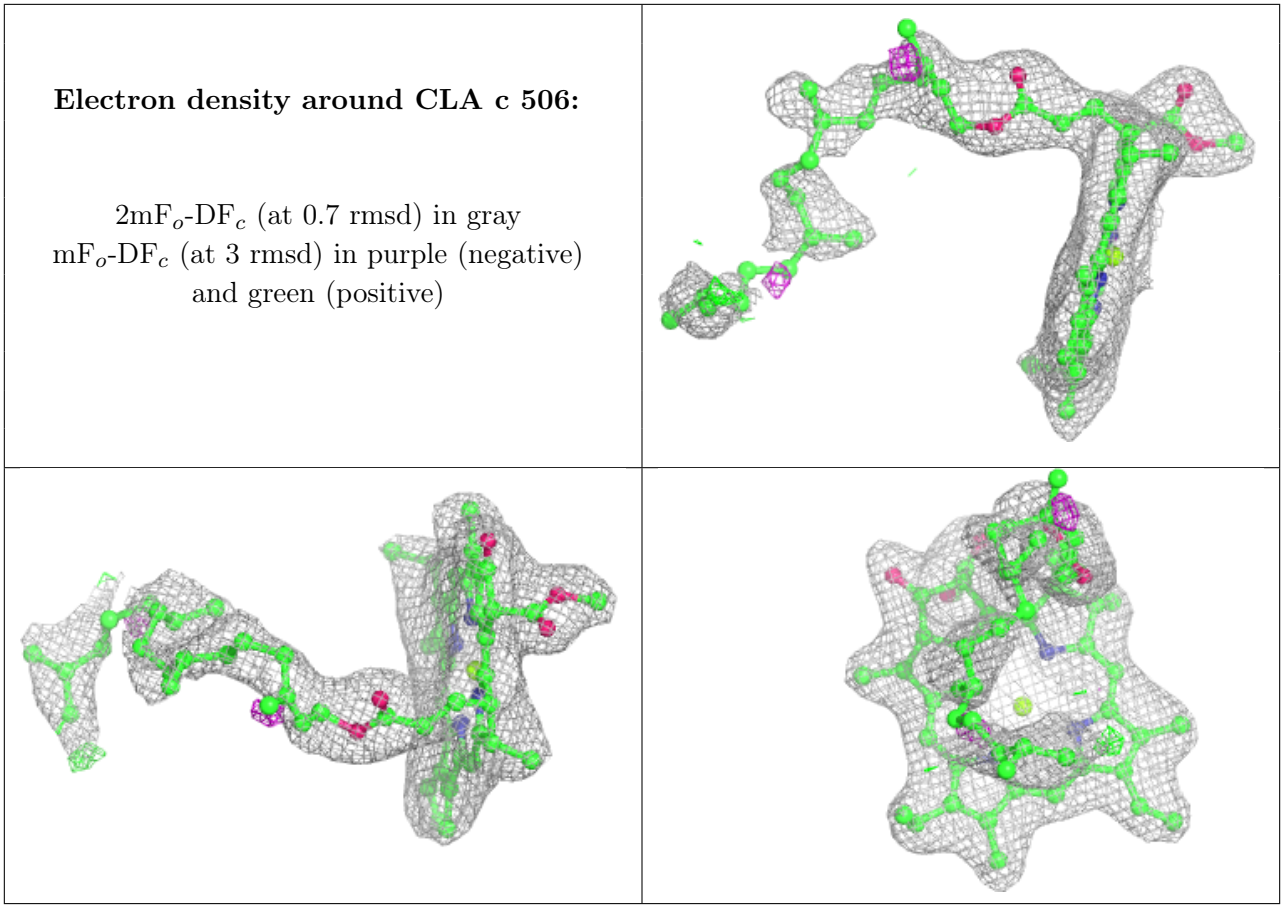






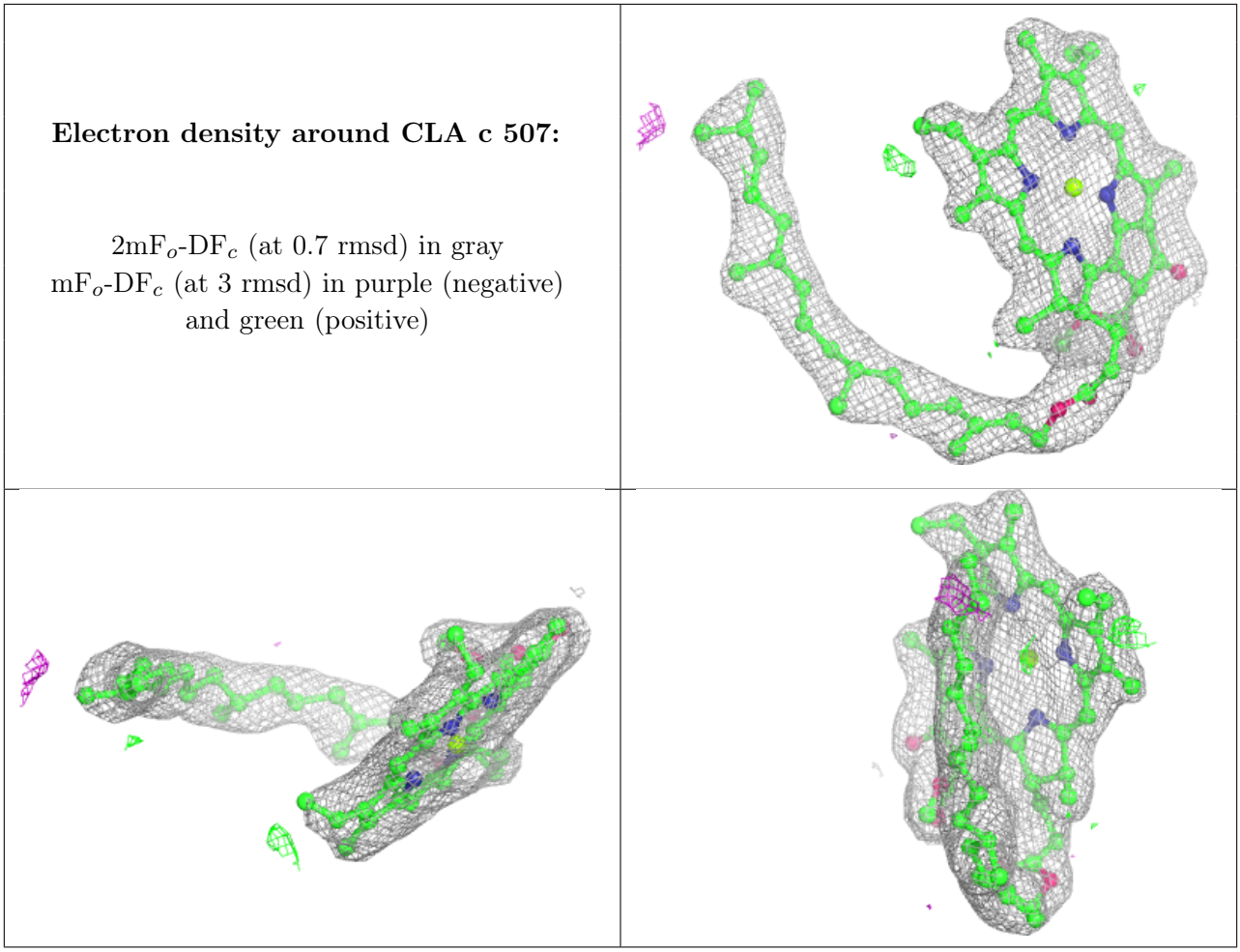
Electron density around CLA c 506:

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



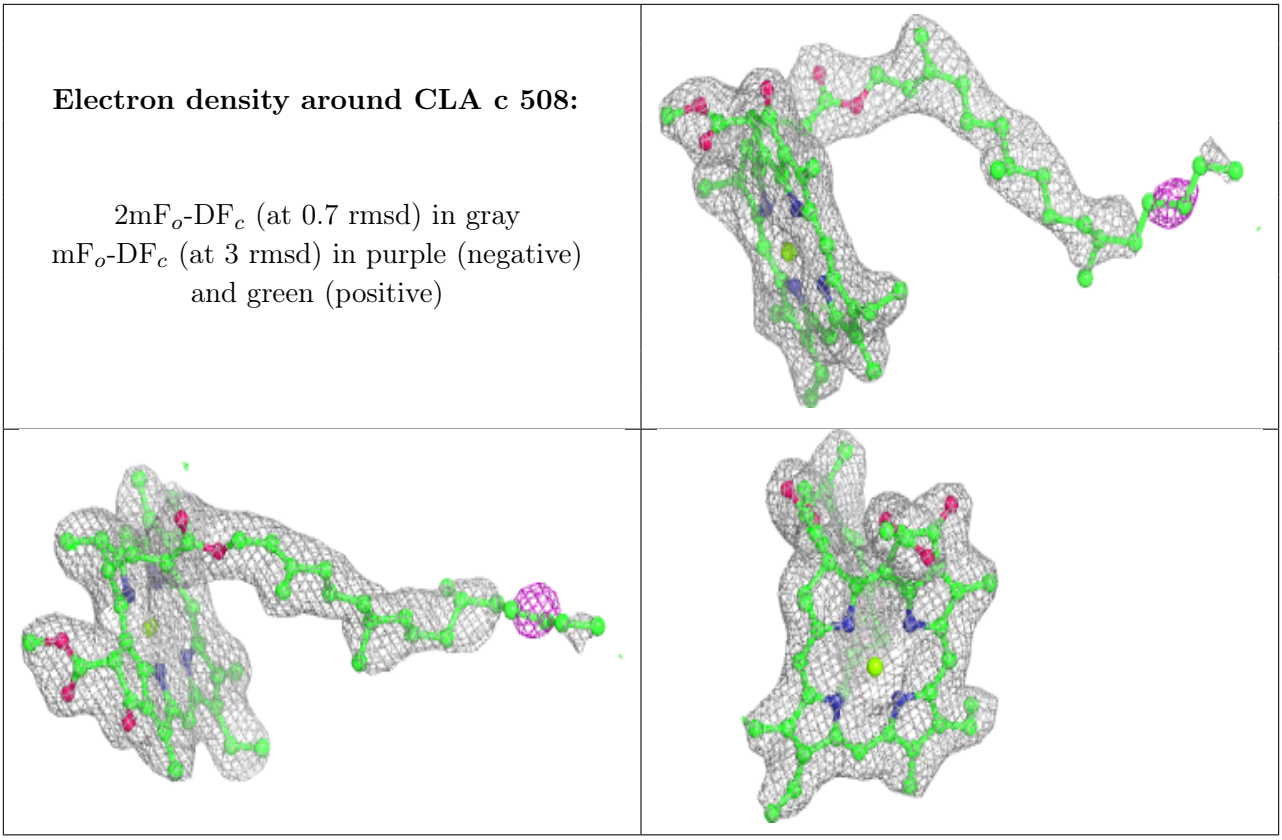
Electron density around CLA c 507:

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



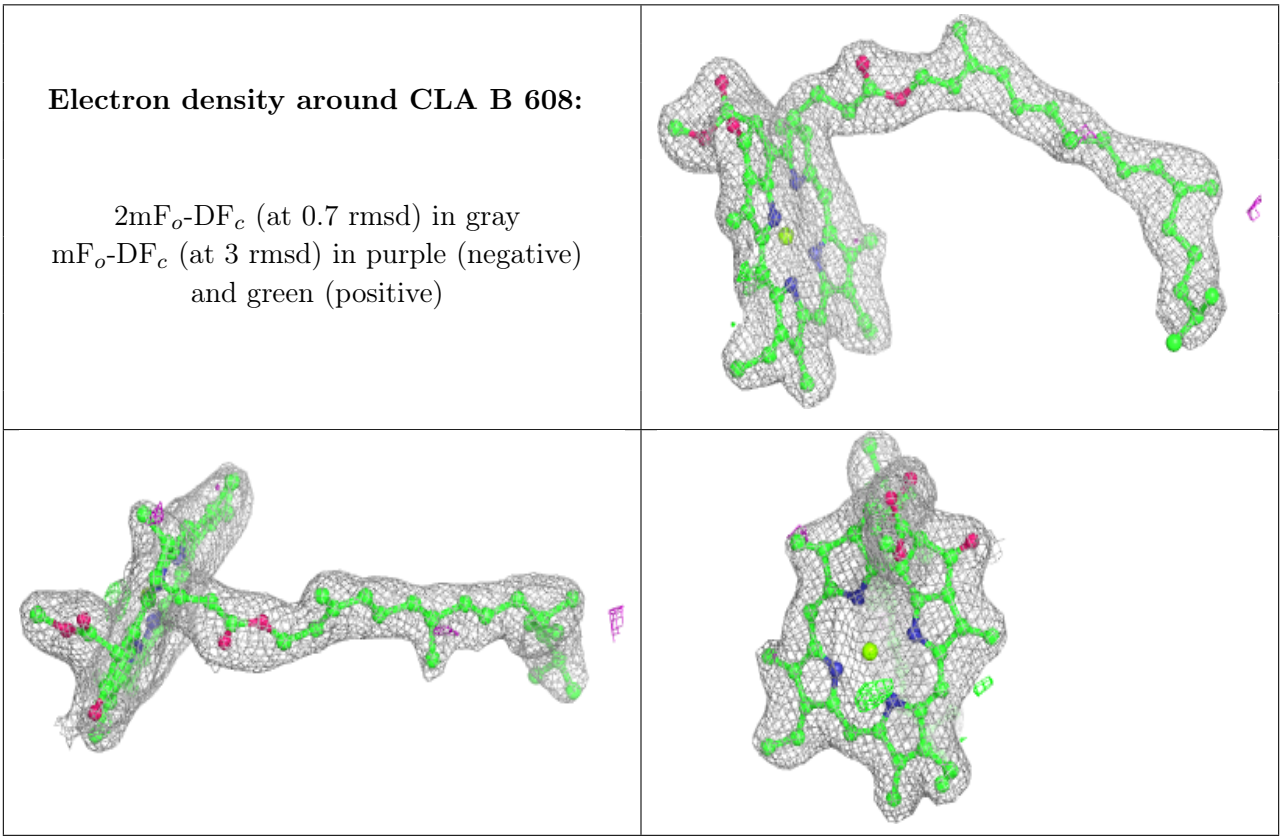
Electron density around CLA c 508:

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



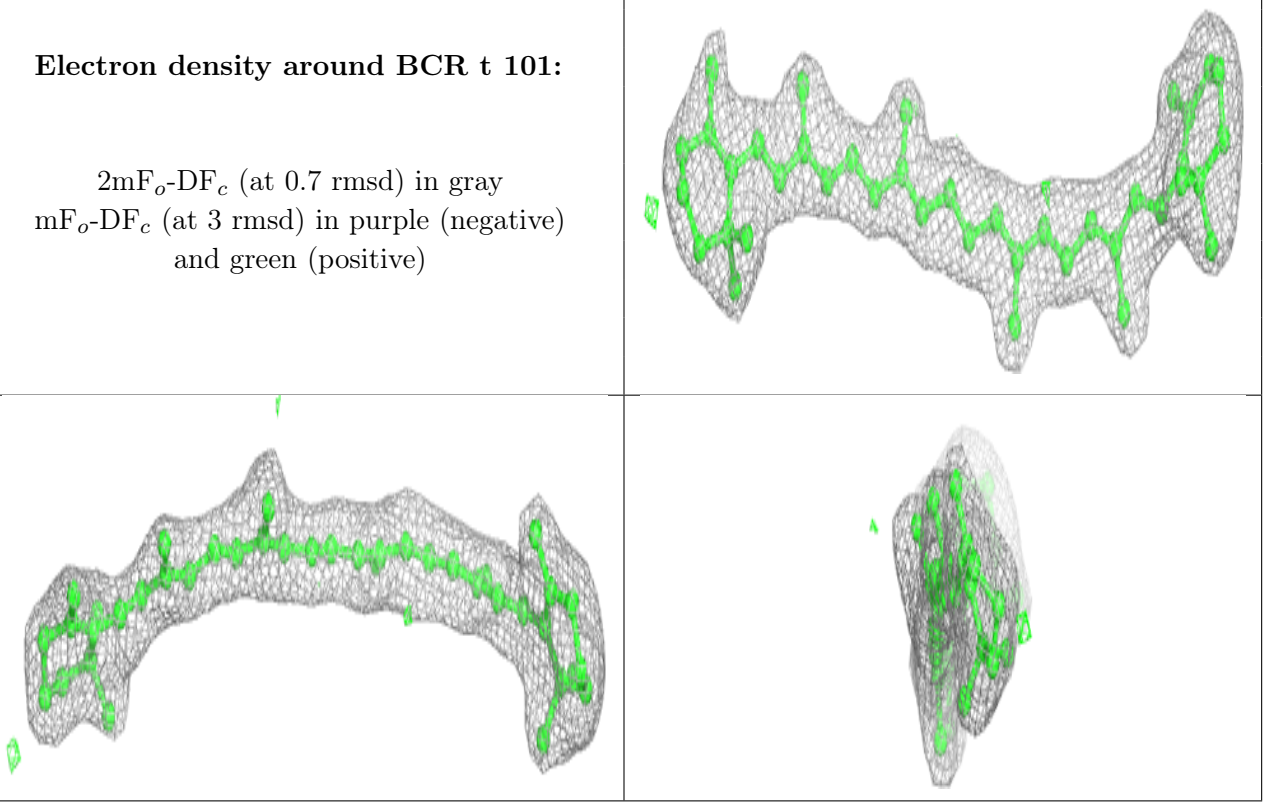
Electron density around CLA B 608:

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



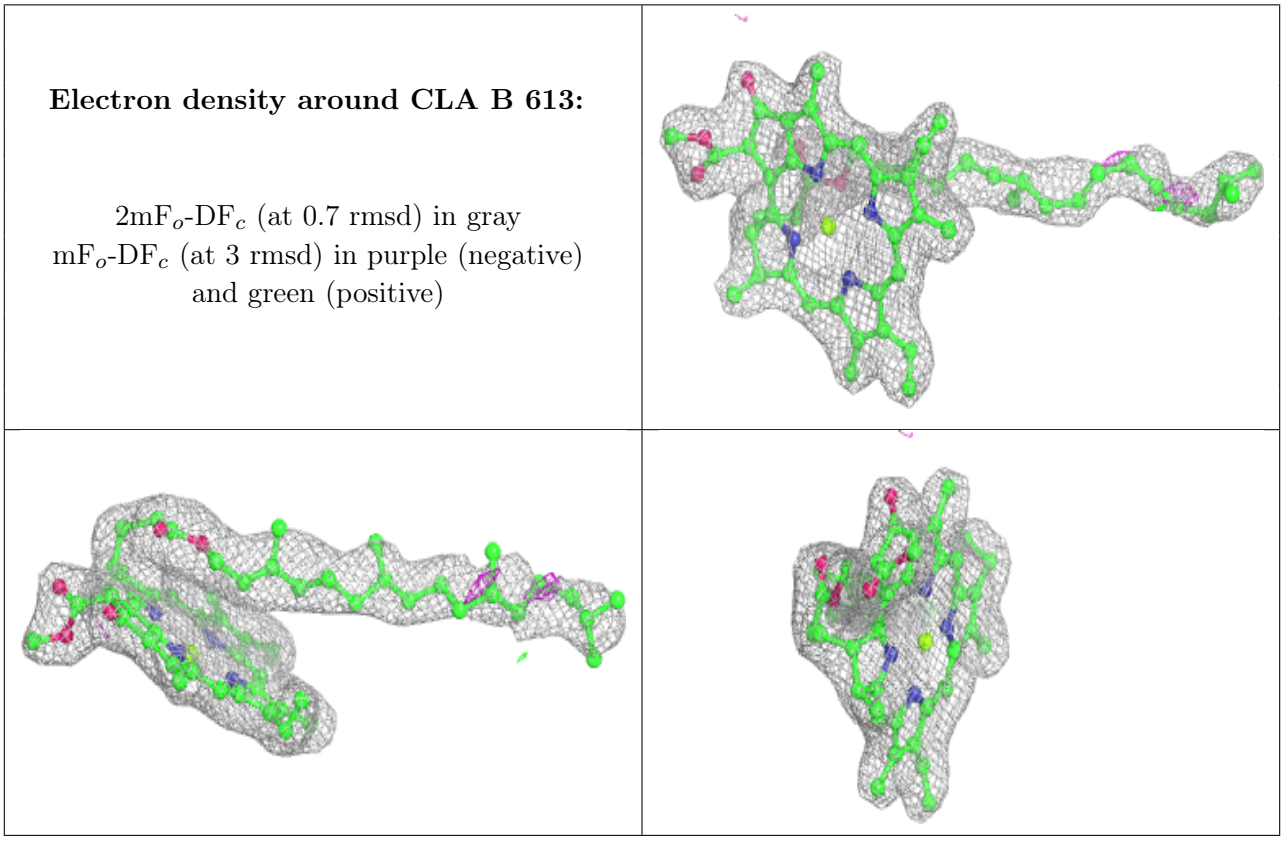
Electron density around BCR t 101:

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



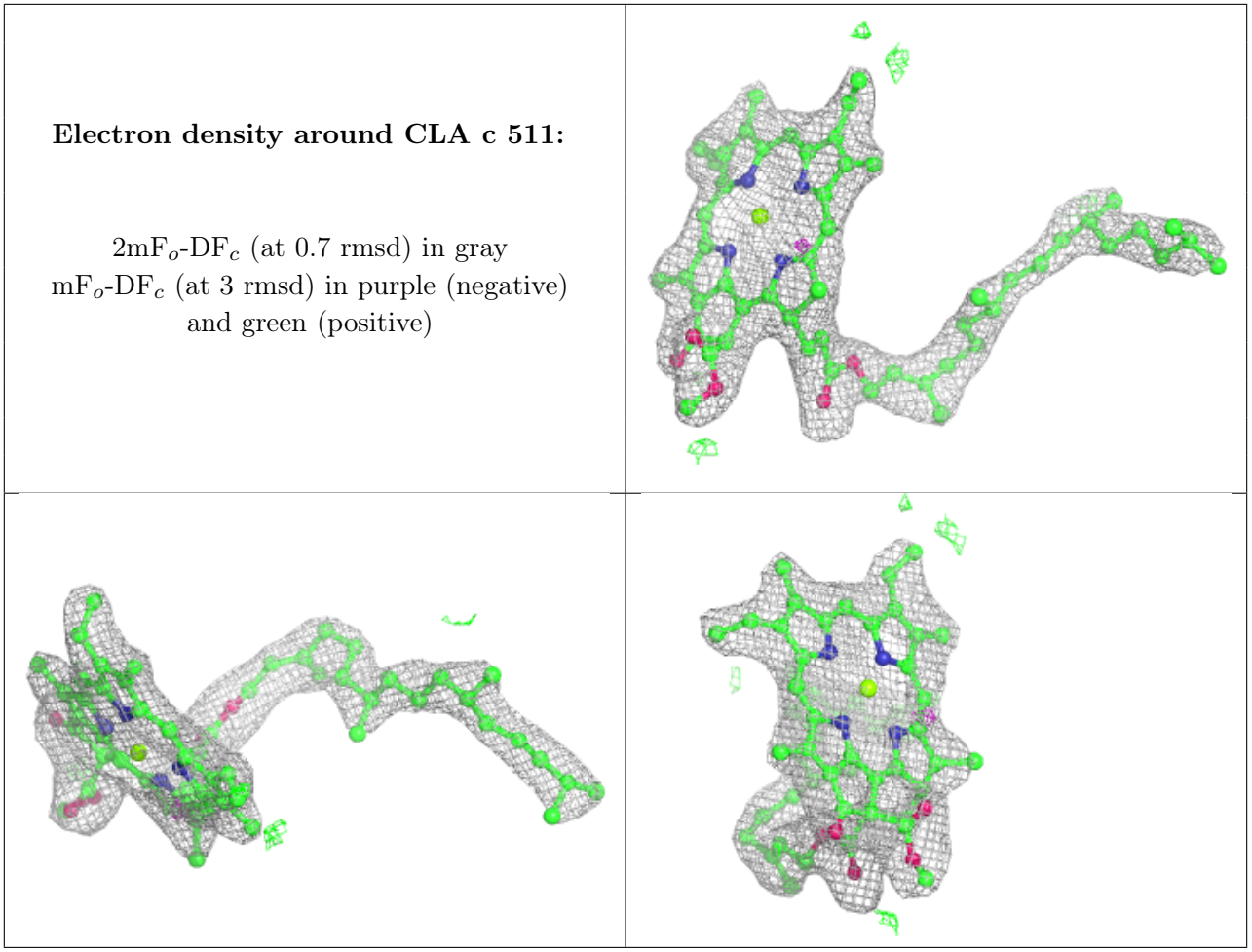
Electron density around CLA B 613:

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



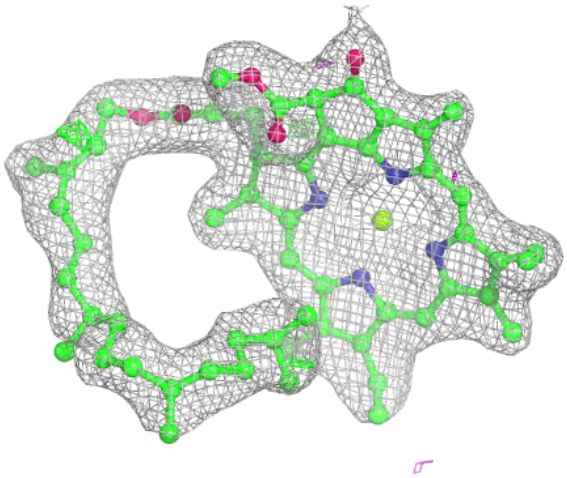
Electron density around CLA c 511:

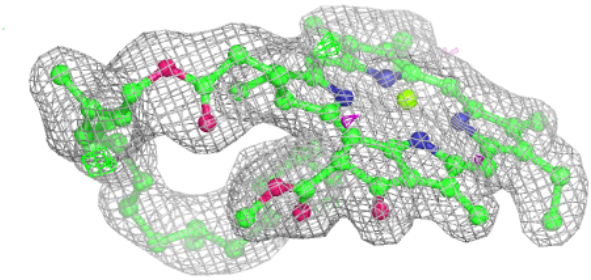
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

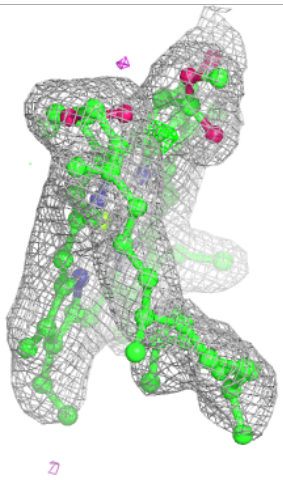


Electron density around CLA B 614:

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

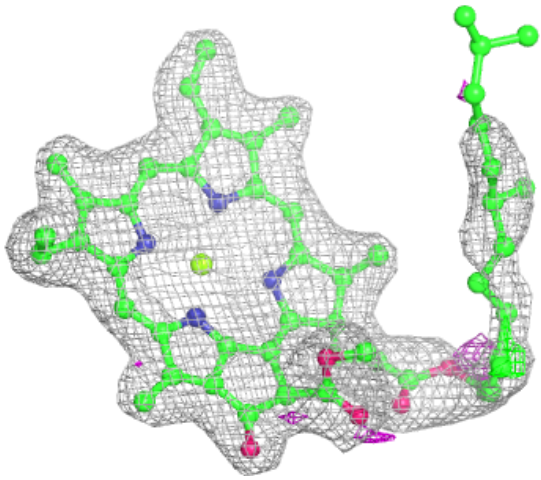


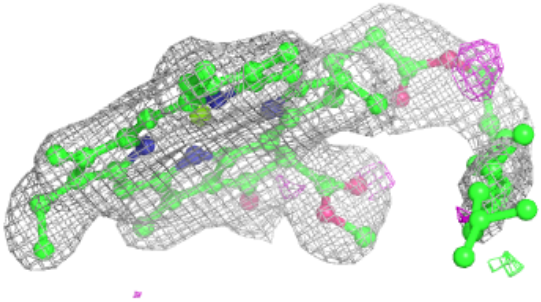


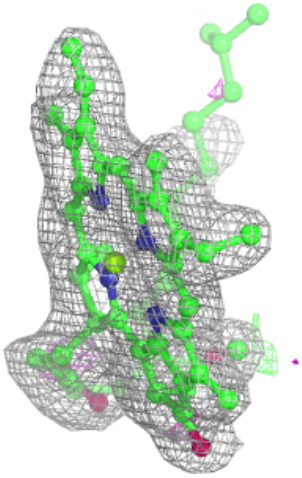


Electron density around CLA B 615:

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

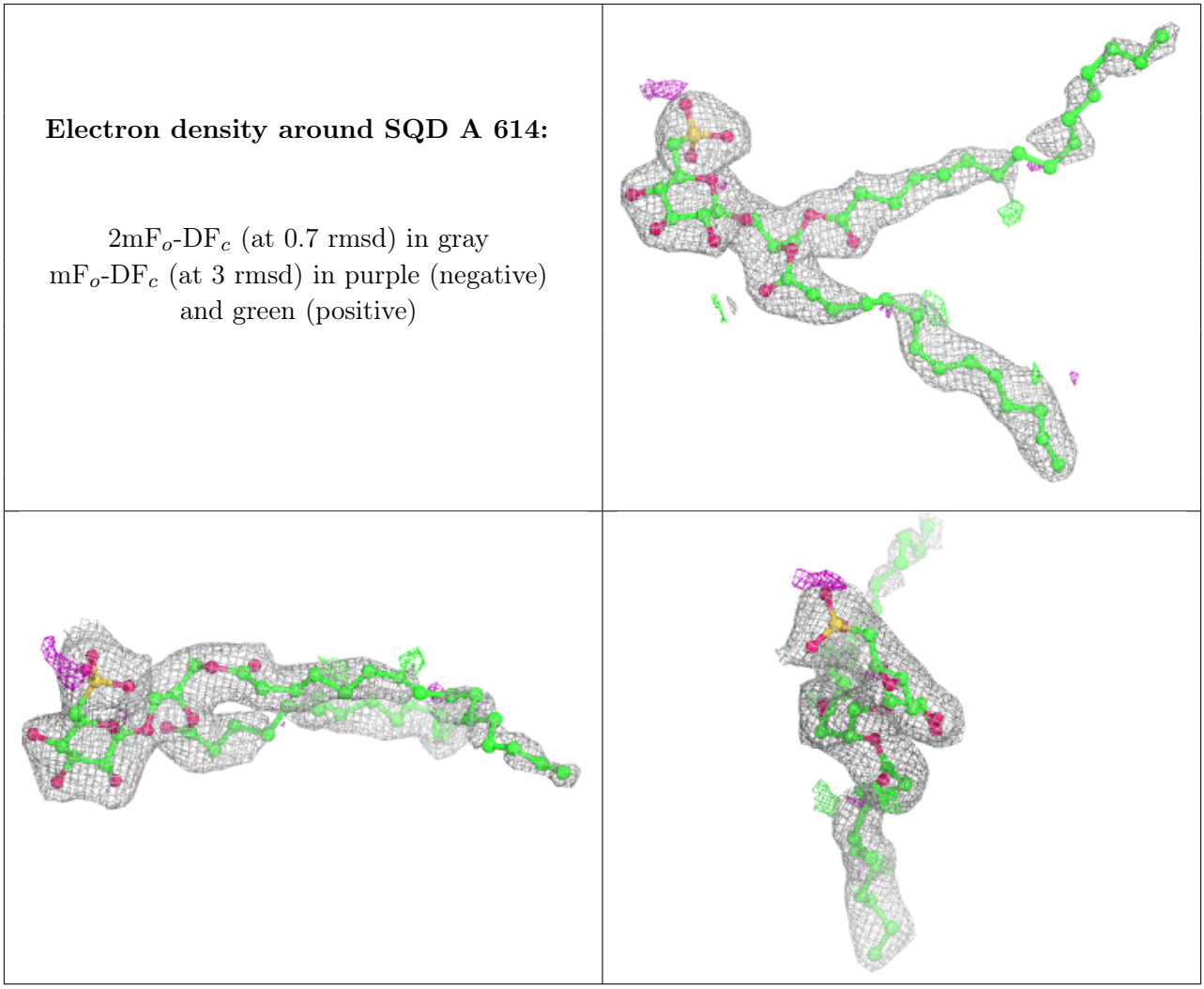






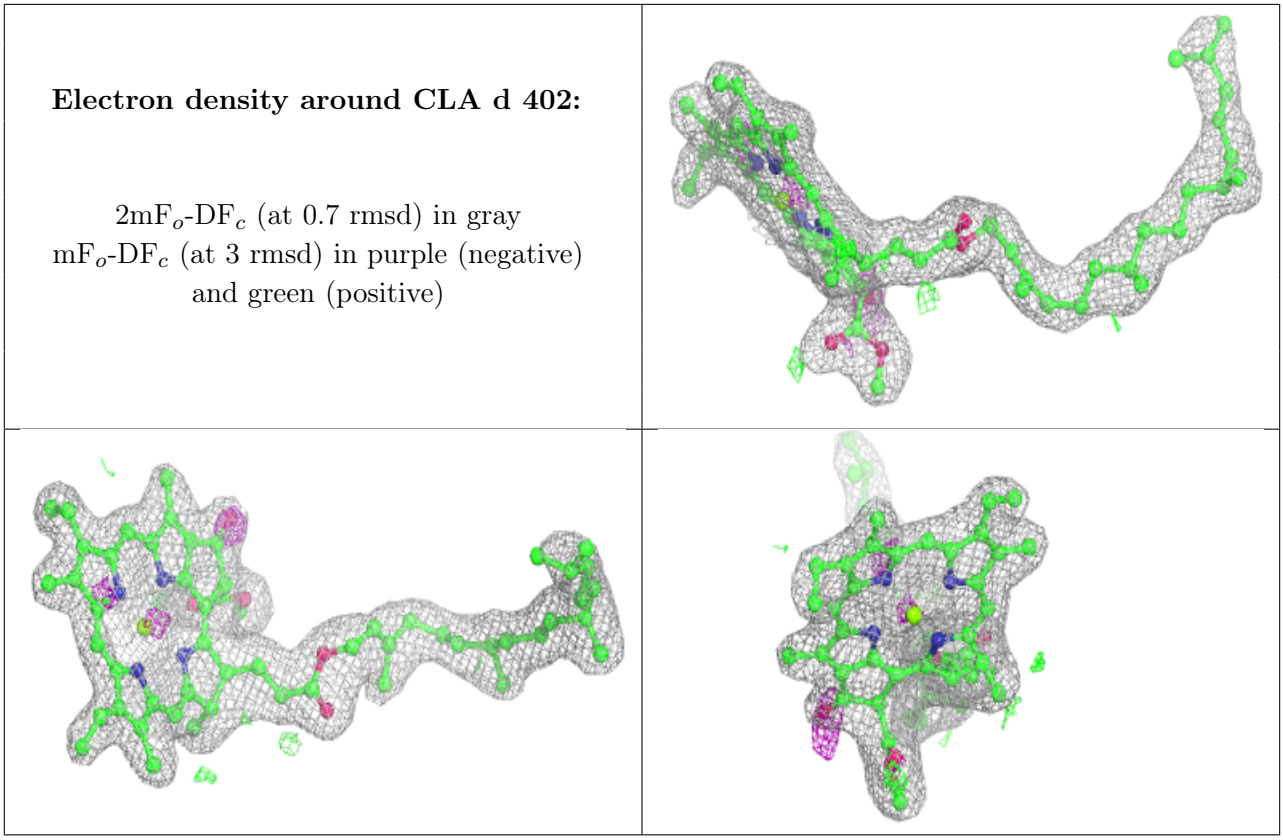
Electron density around SQD A 614:

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



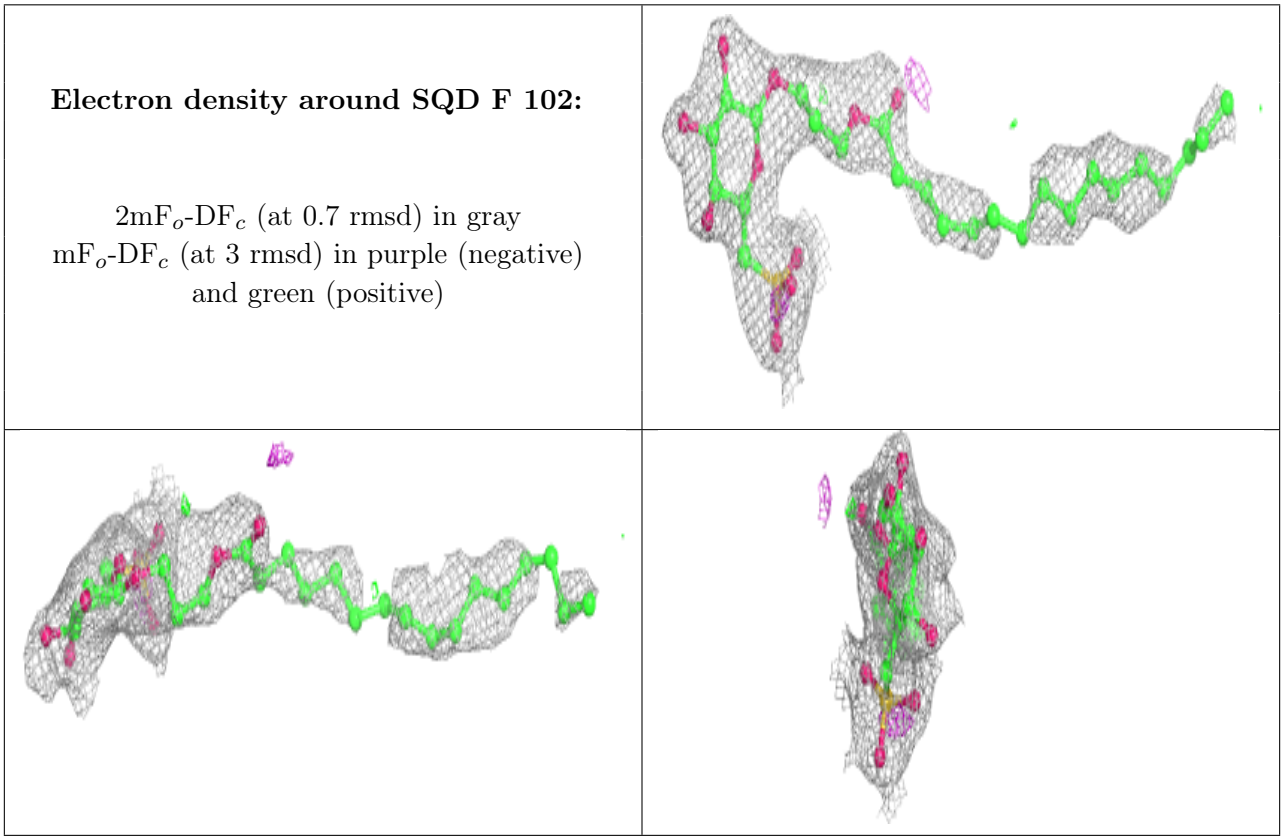
Electron density around CLA d 402:

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



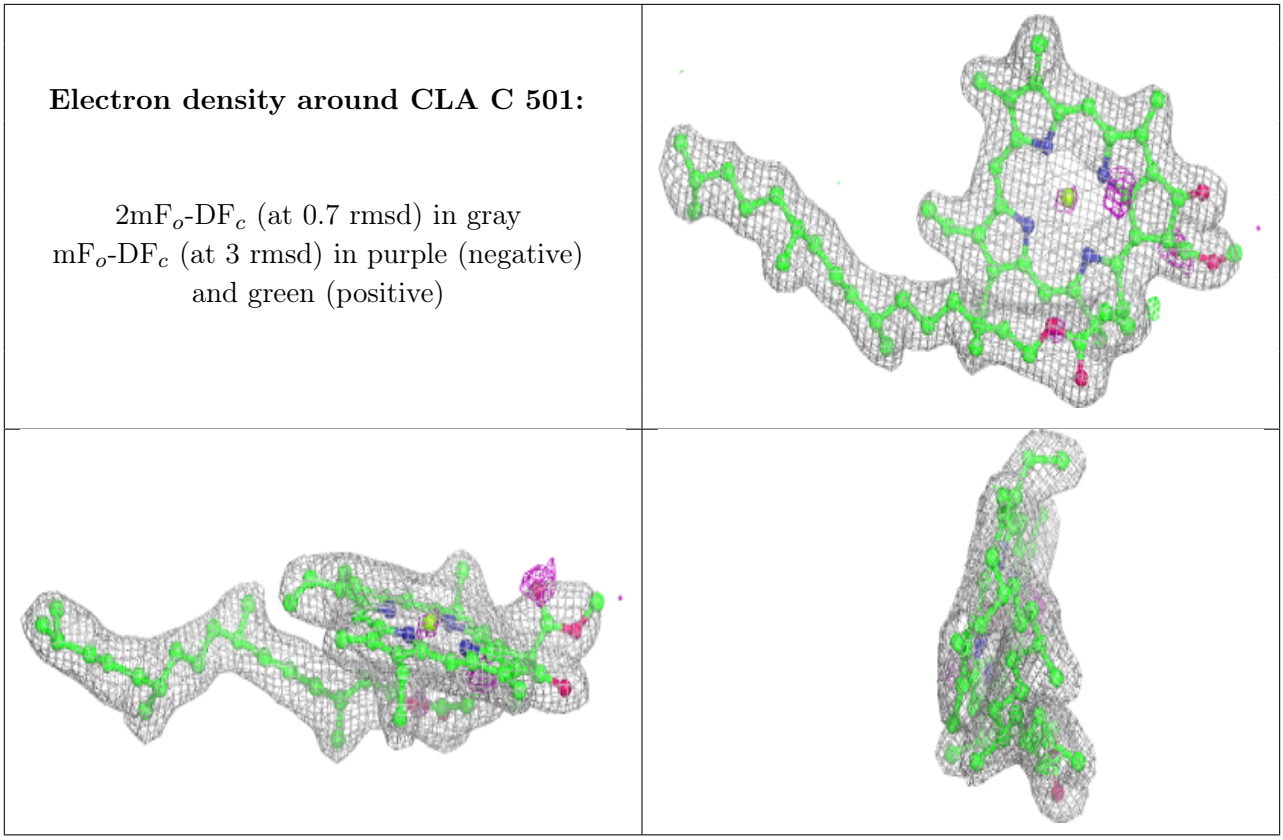
Electron density around SQD F 102:

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



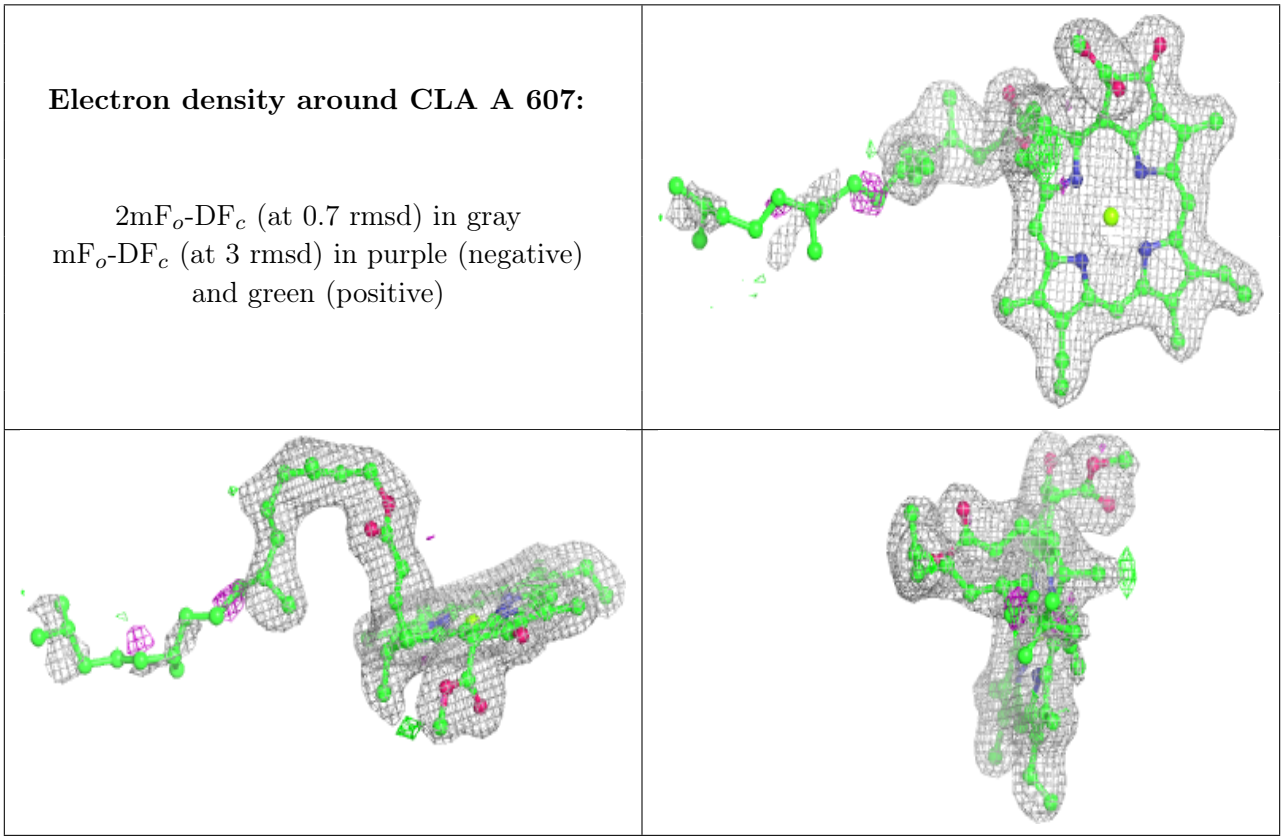
Electron density around CLA C 501:

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



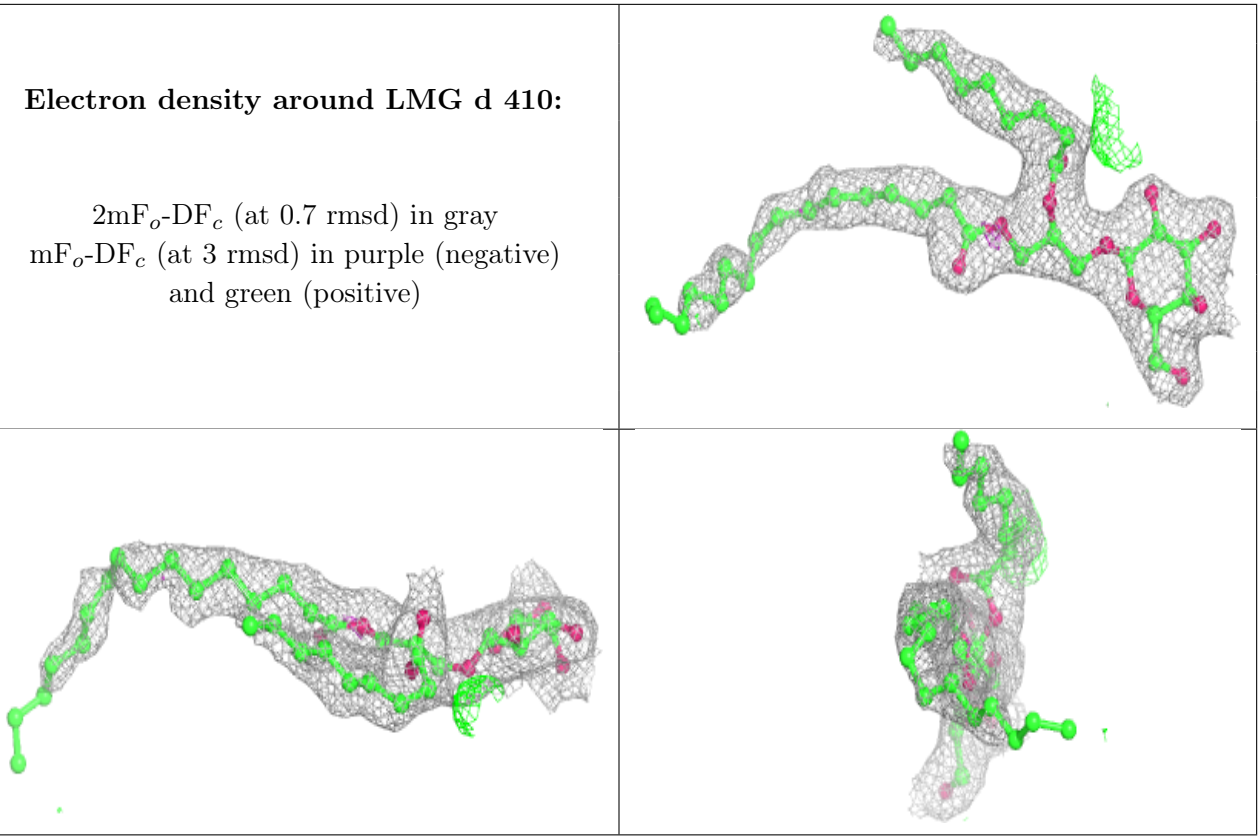
Electron density around CLA A 607:

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



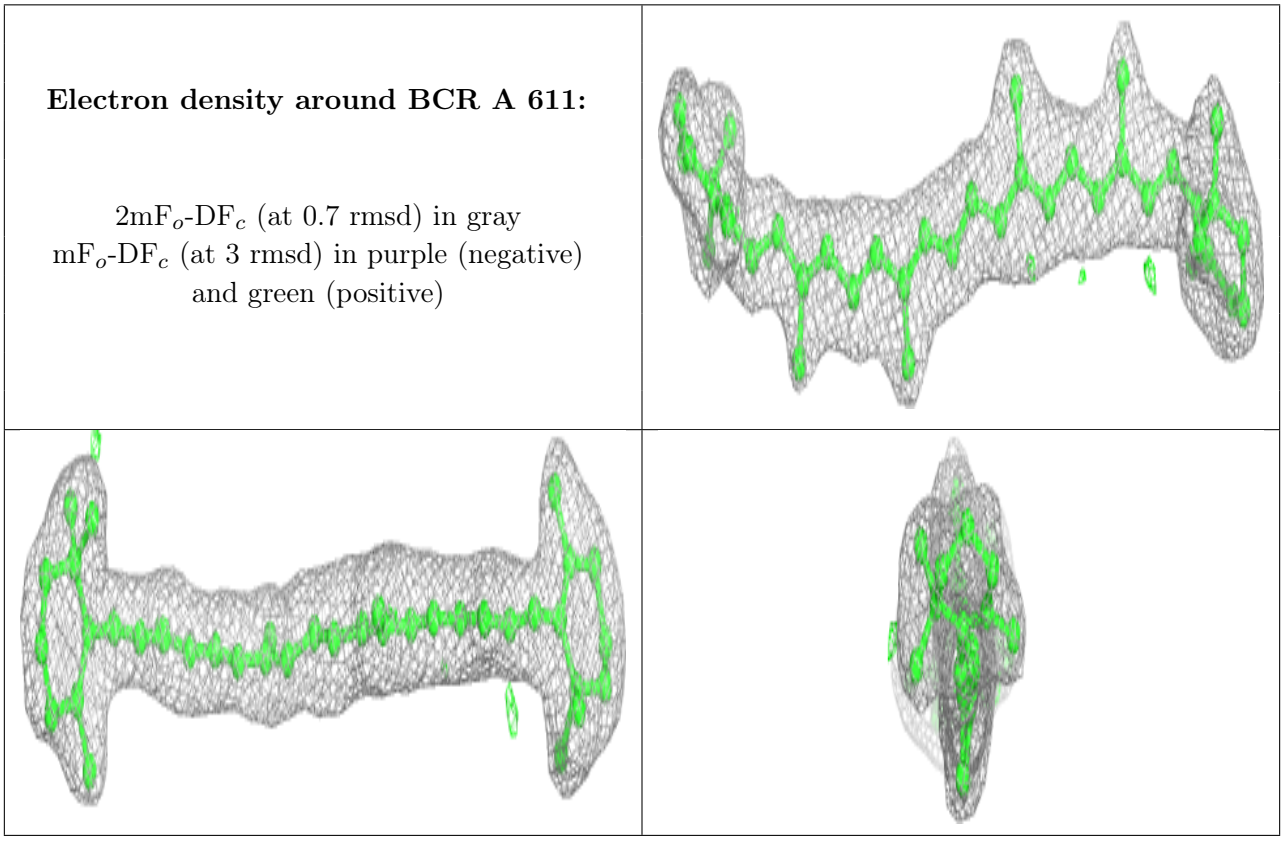
Electron density around LMG d 410:

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



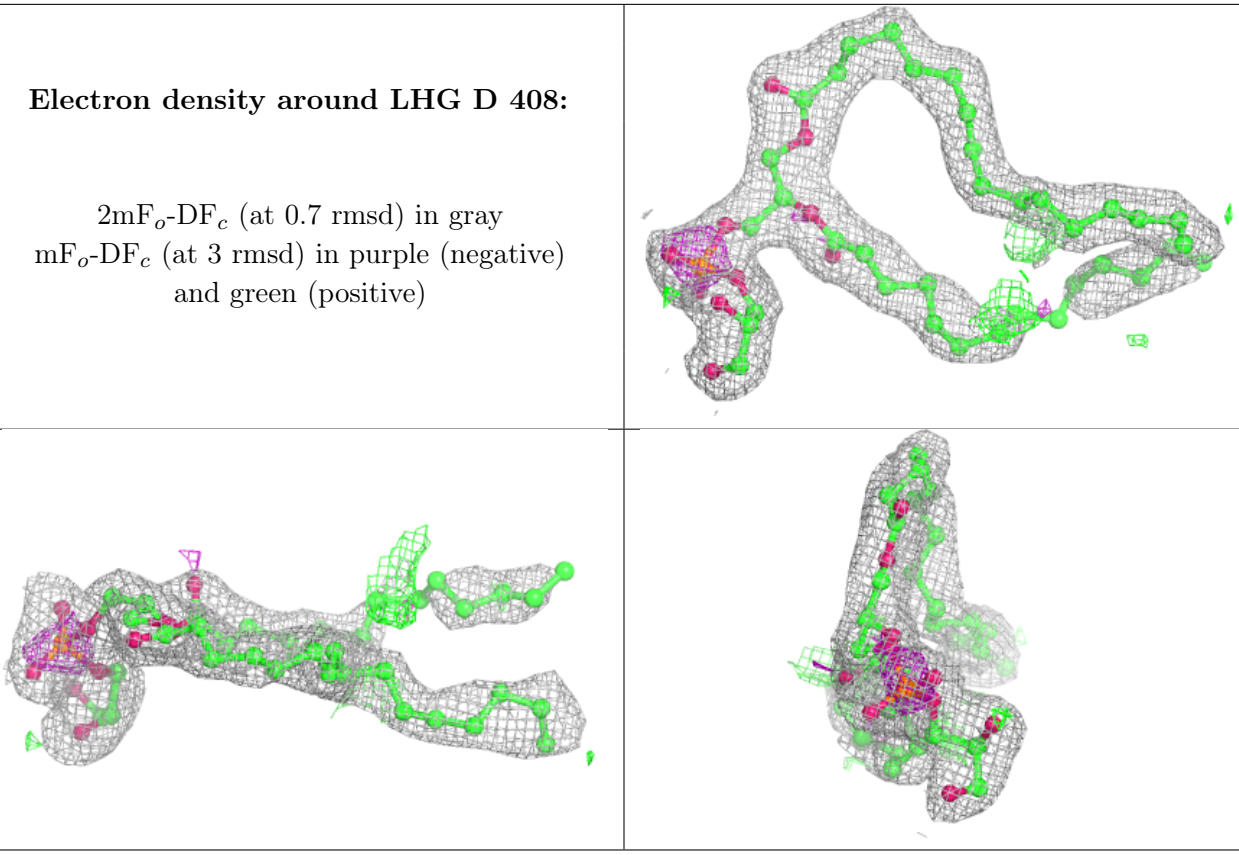
Electron density around BCR A 611:

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



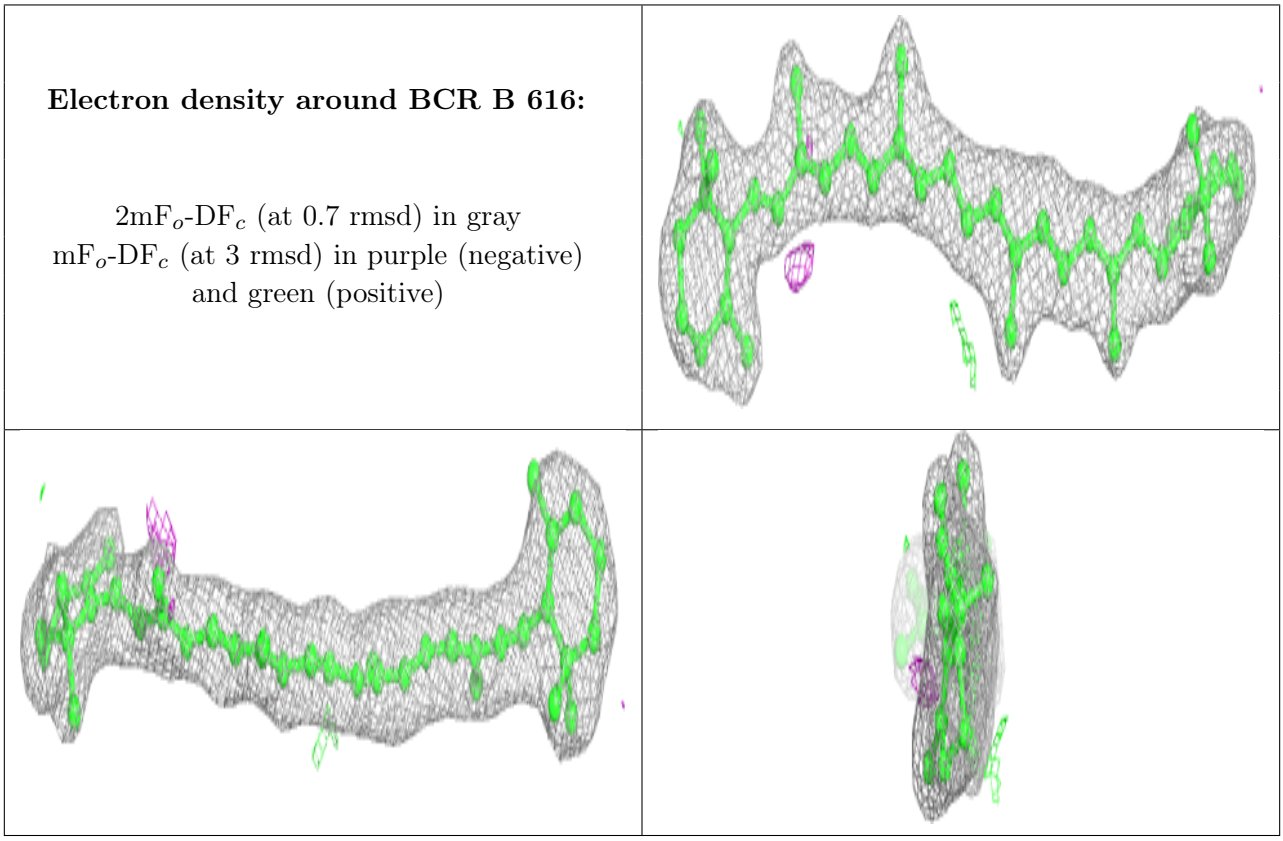
Electron density around LHG D 408:

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



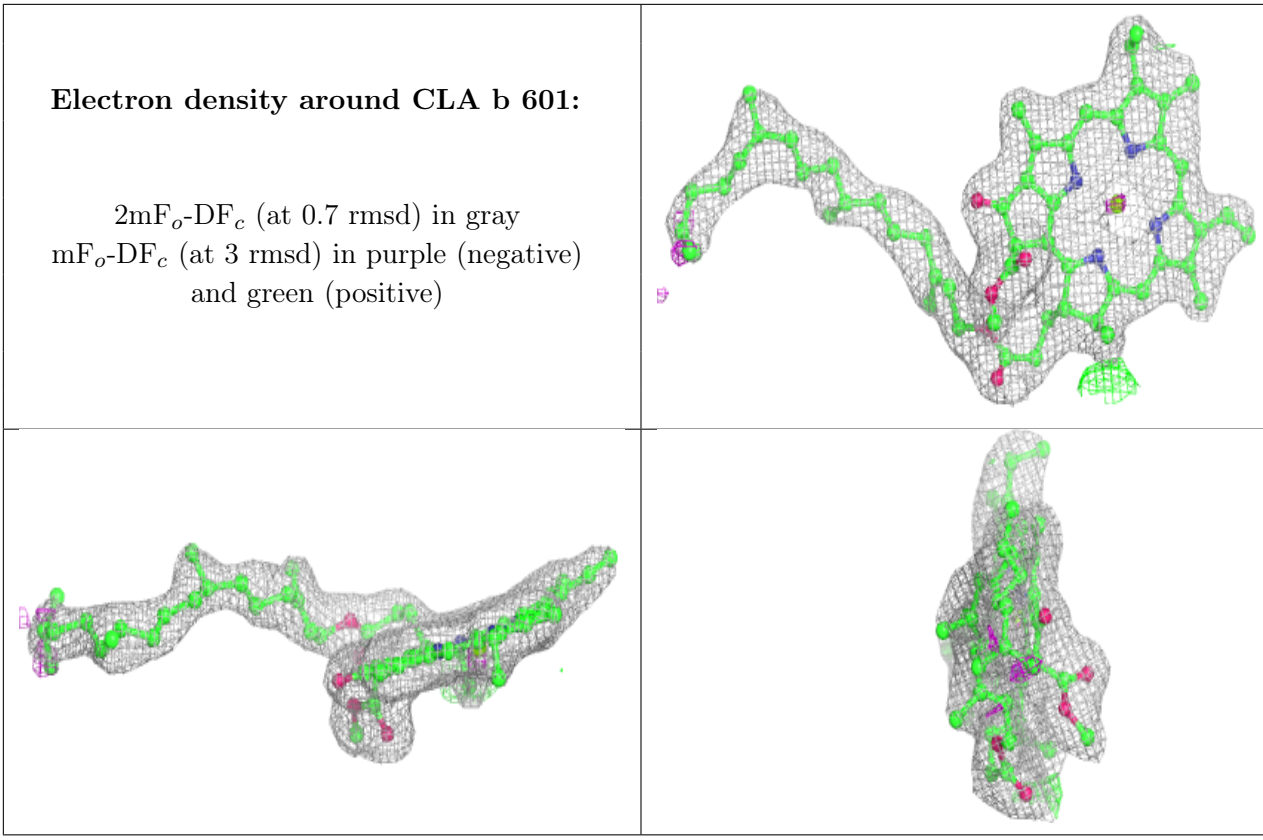
Electron density around BCR B 616:

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



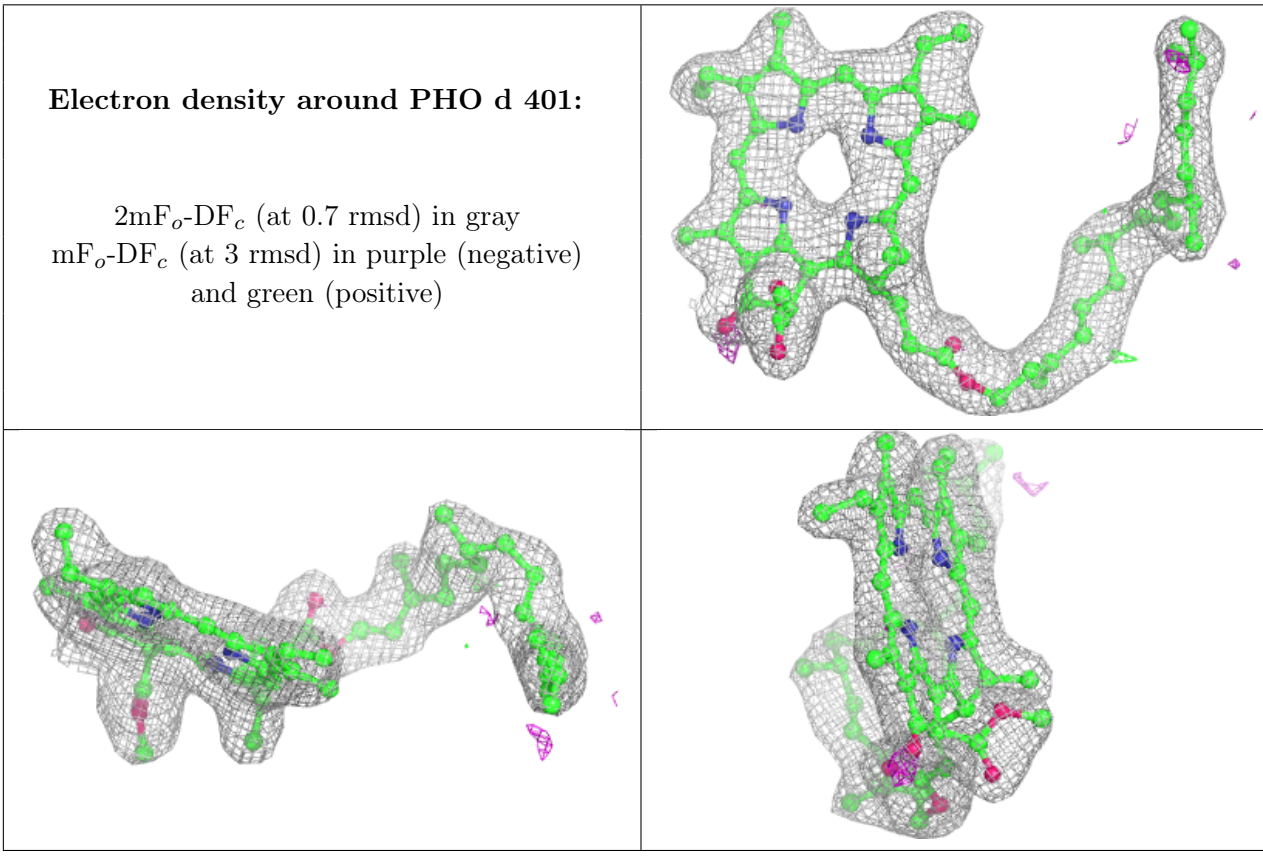
Electron density around CLA b 601:

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



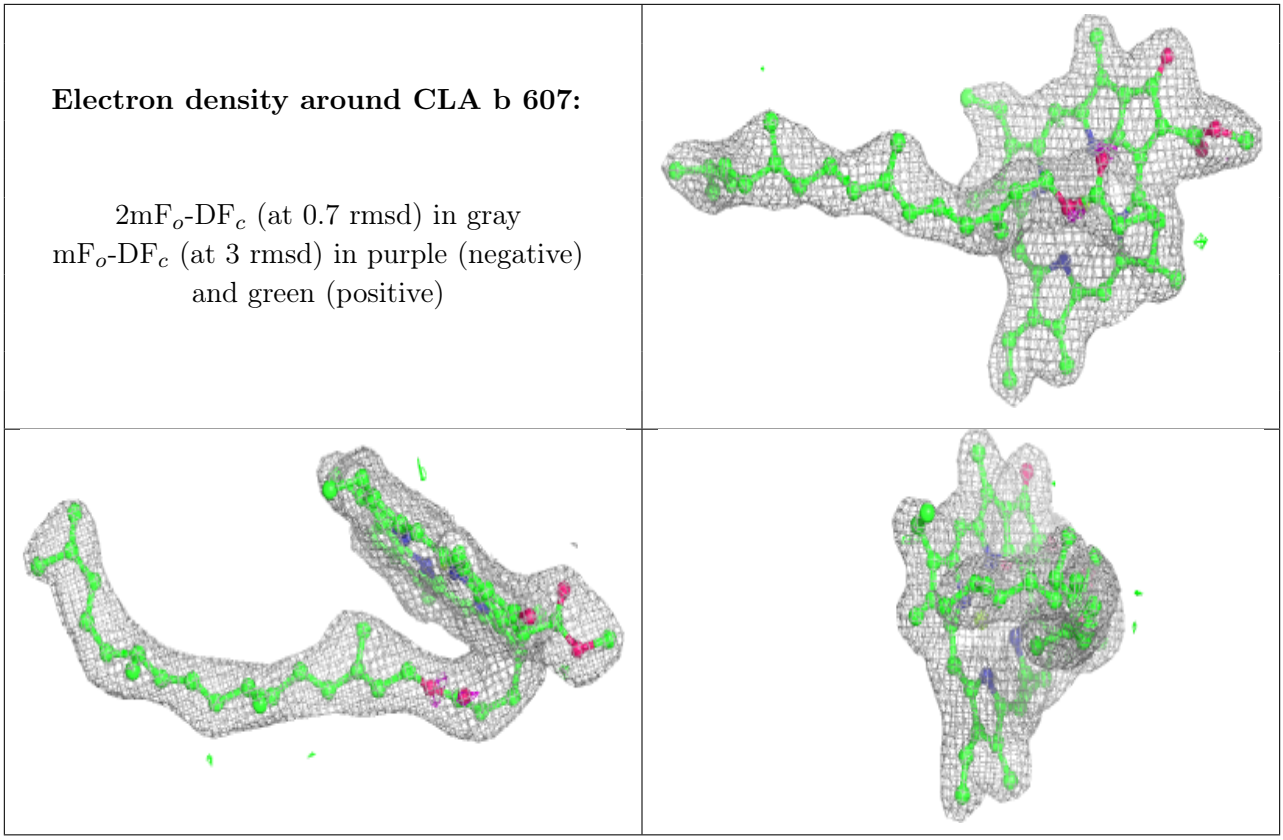
Electron density around PHO d 401:

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



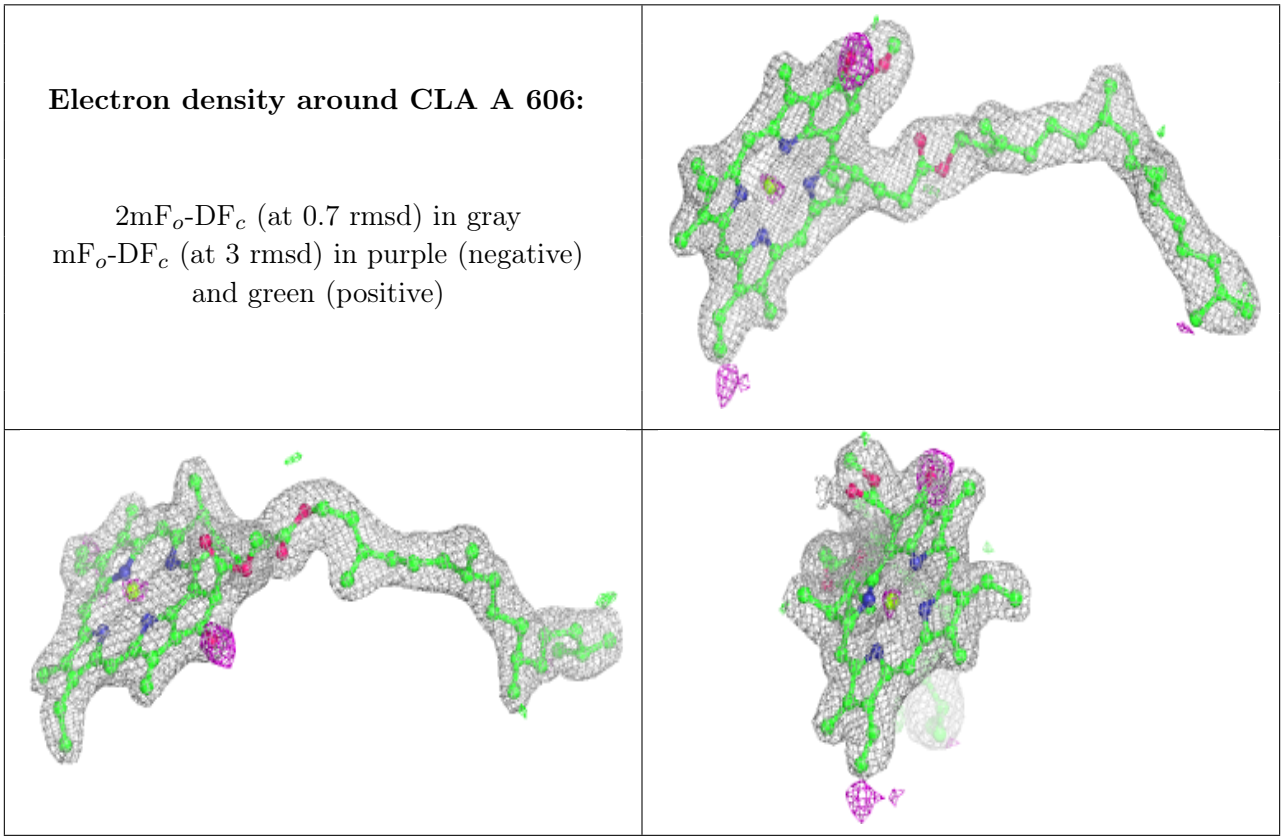
Electron density around CLA b 607:

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



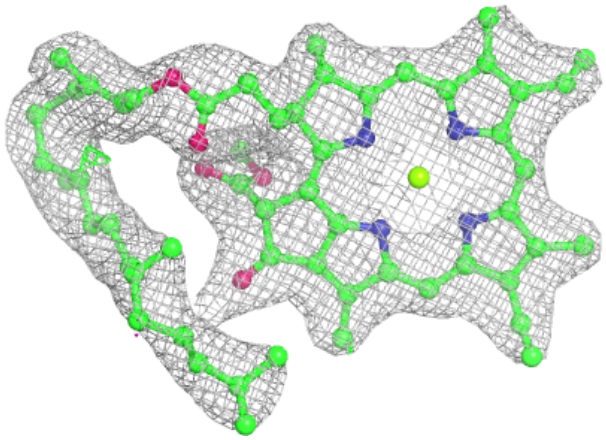
Electron density around CLA A 606:

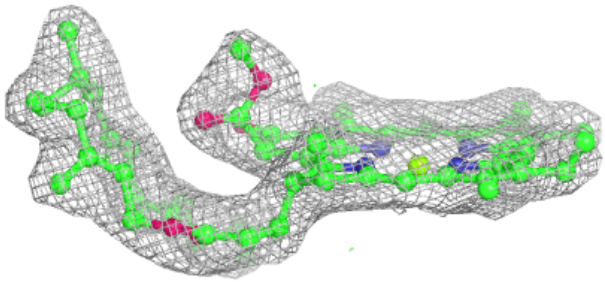
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

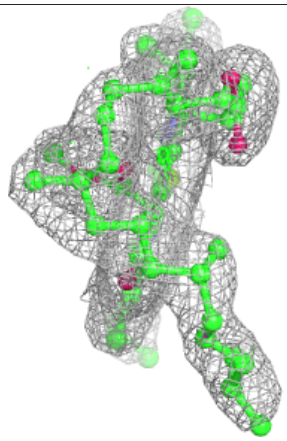


Electron density around CLA b 609:

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

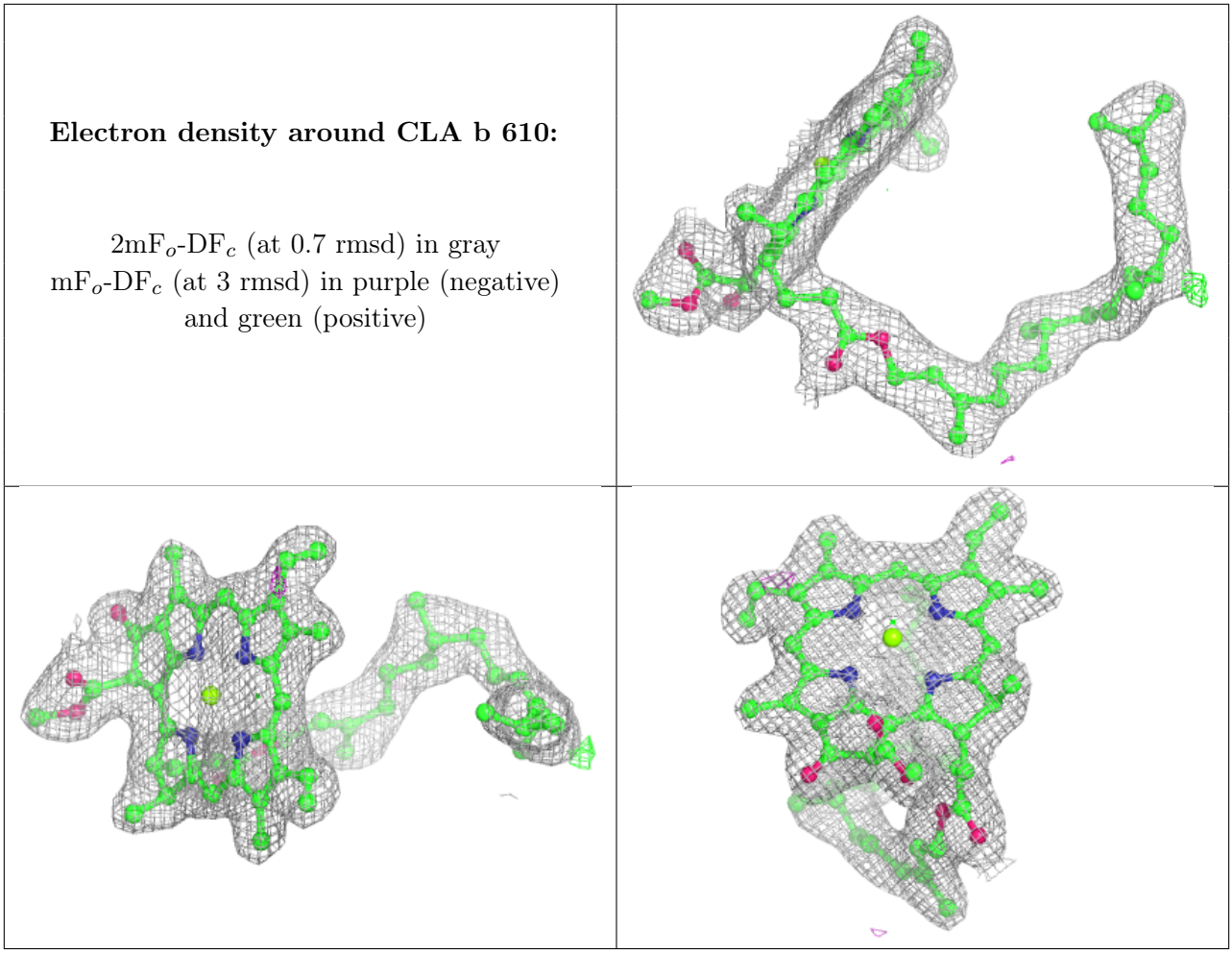






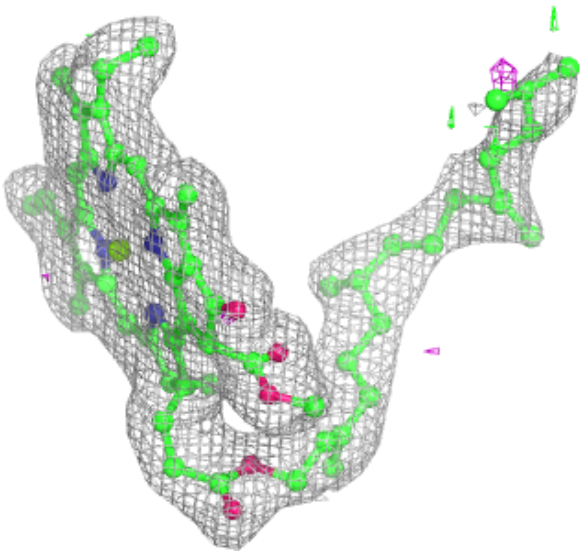
Electron density around CLA b 610:

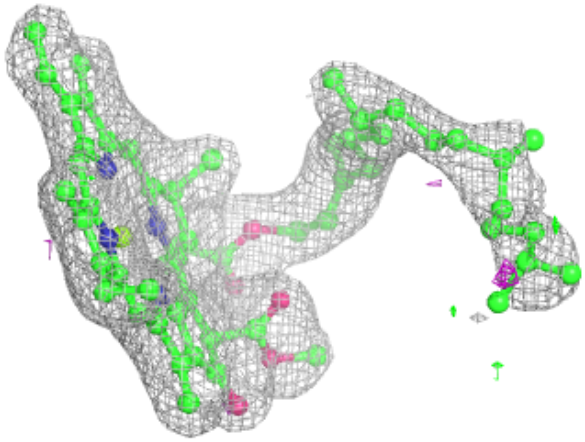
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

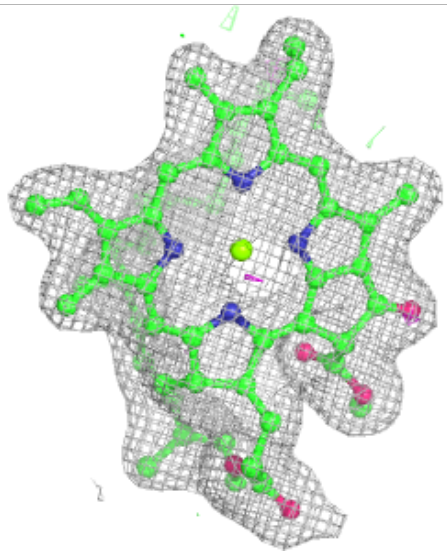


Electron density around CLA b 612:

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

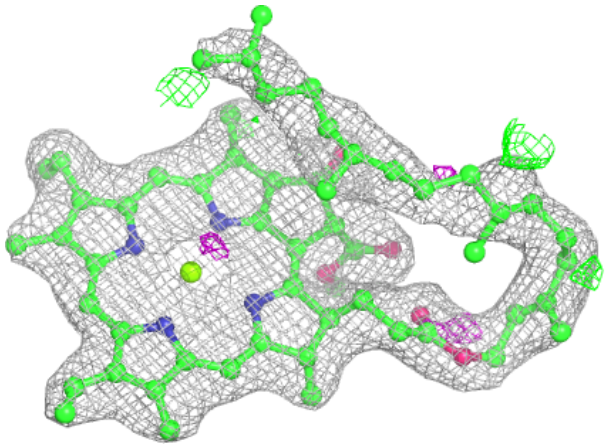


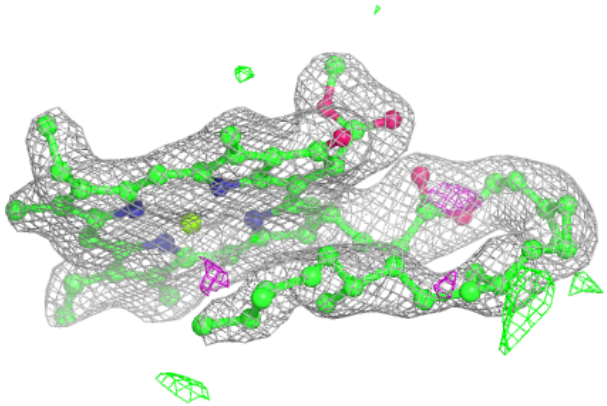


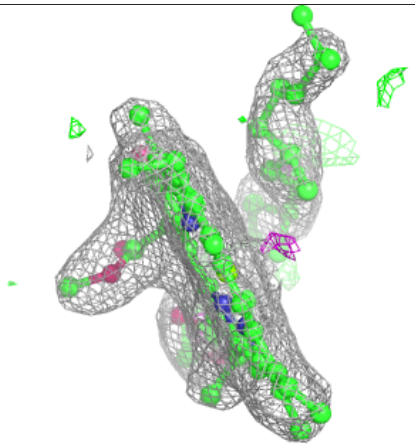


Electron density around CLA C 509:

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

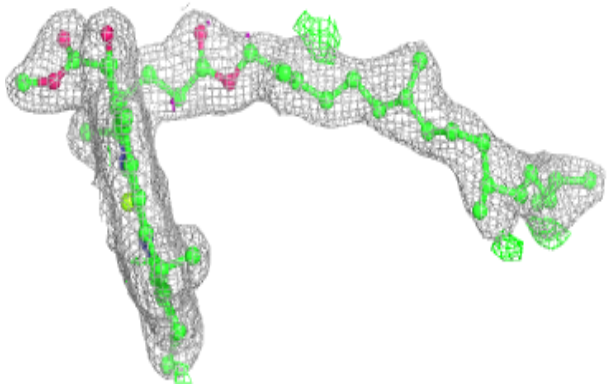


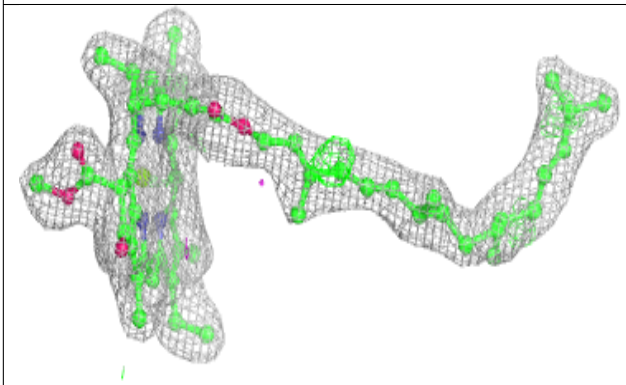


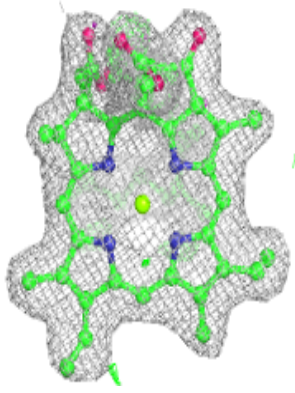


Electron density around CLA B 604:

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

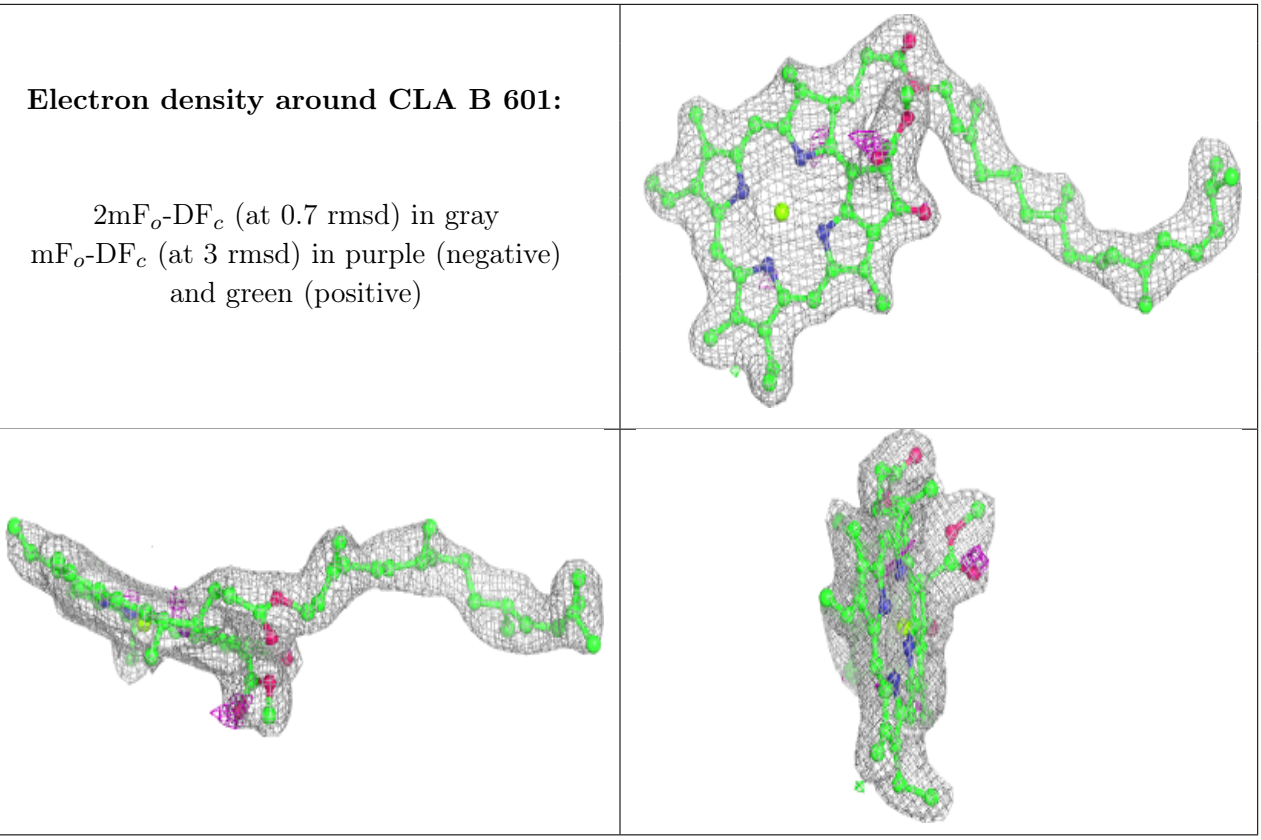






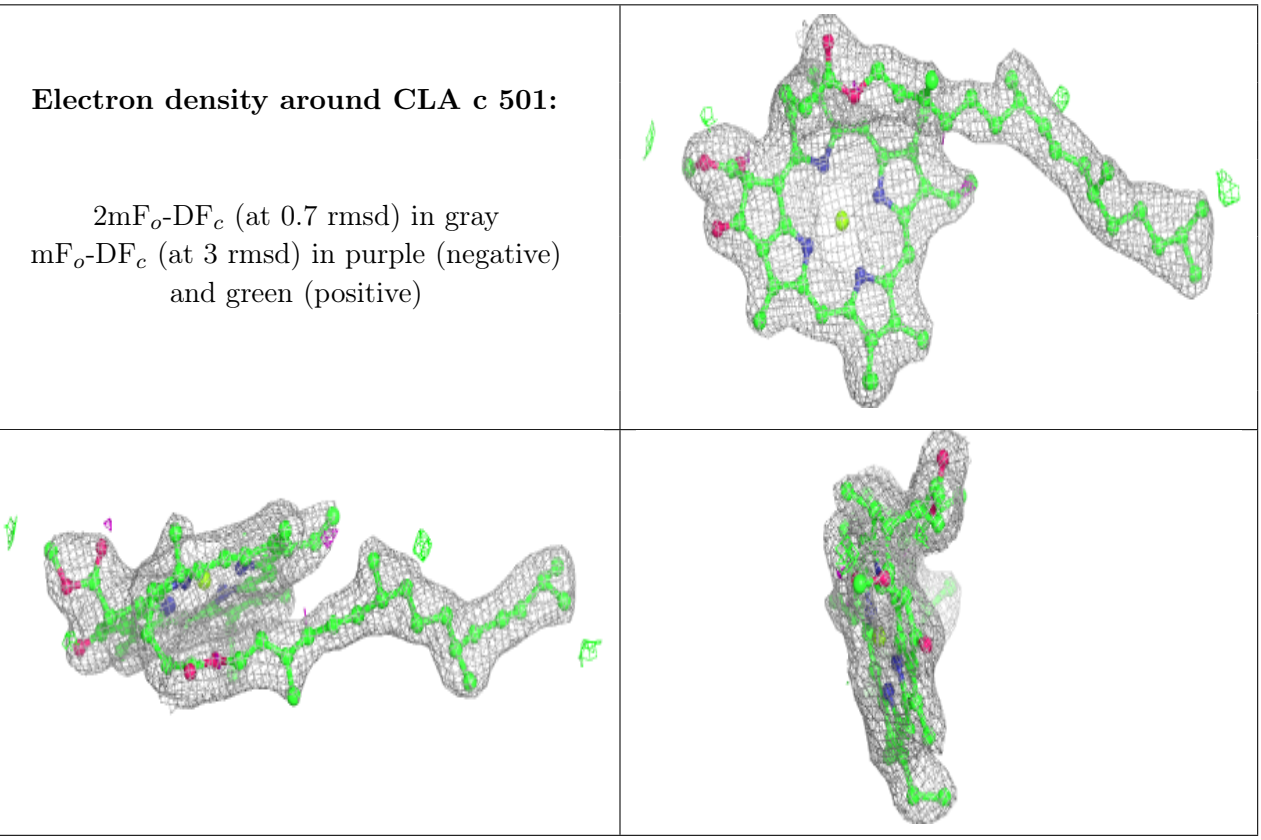
Electron density around CLA B 601:

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



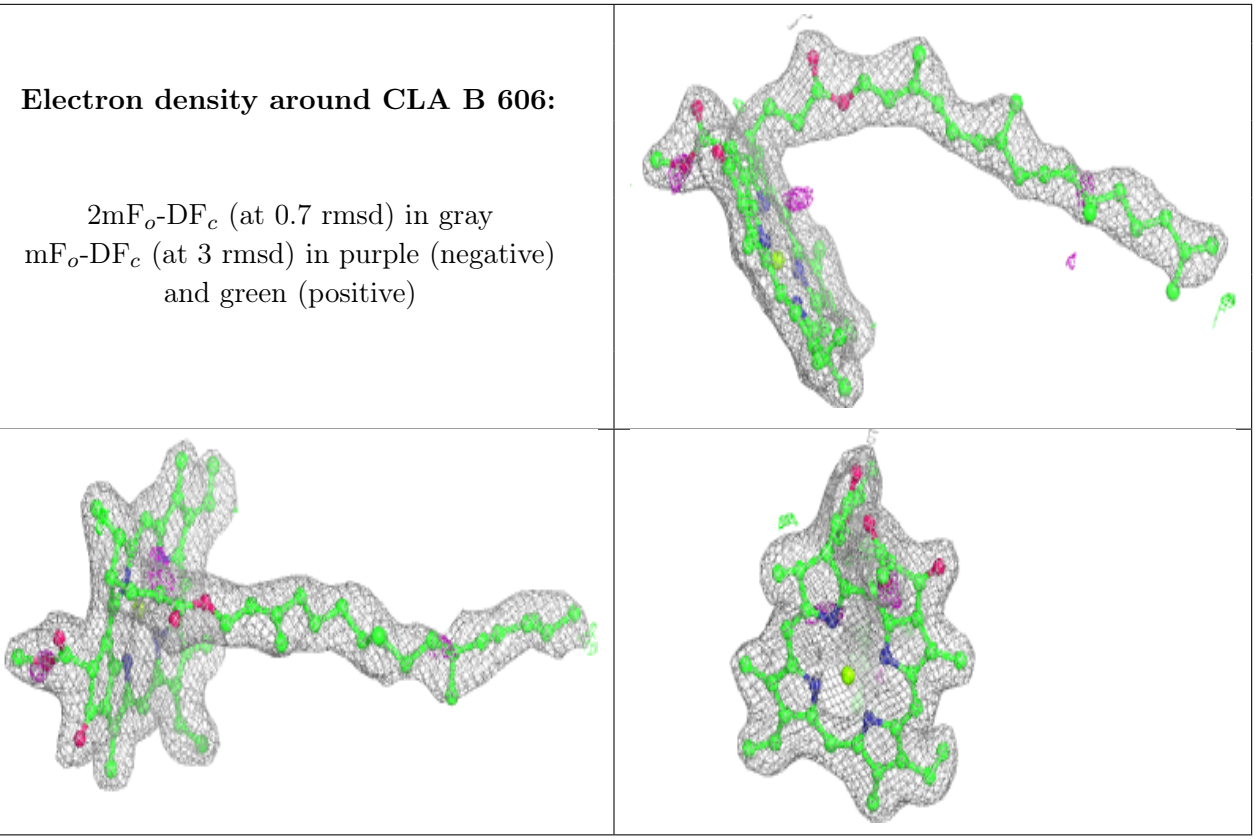
Electron density around CLA c 501:

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



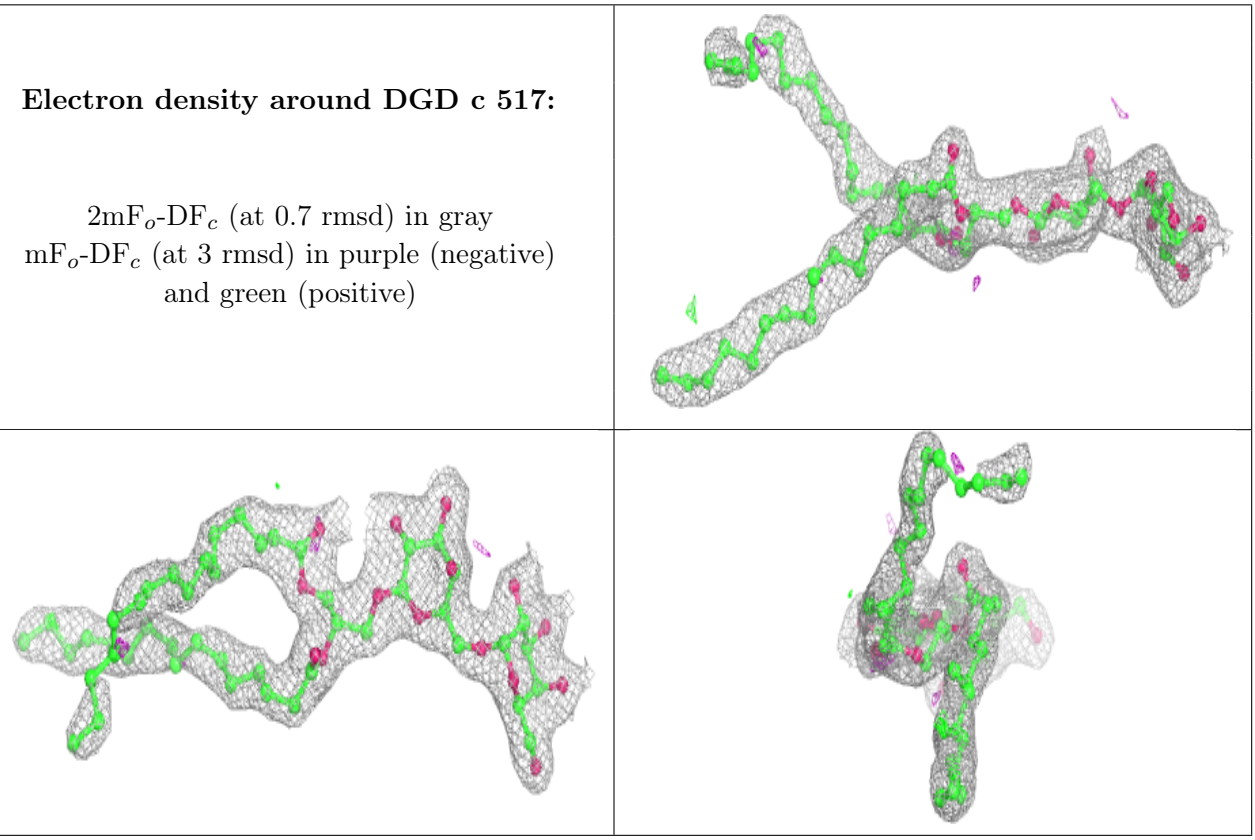
Electron density around CLA B 606:

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



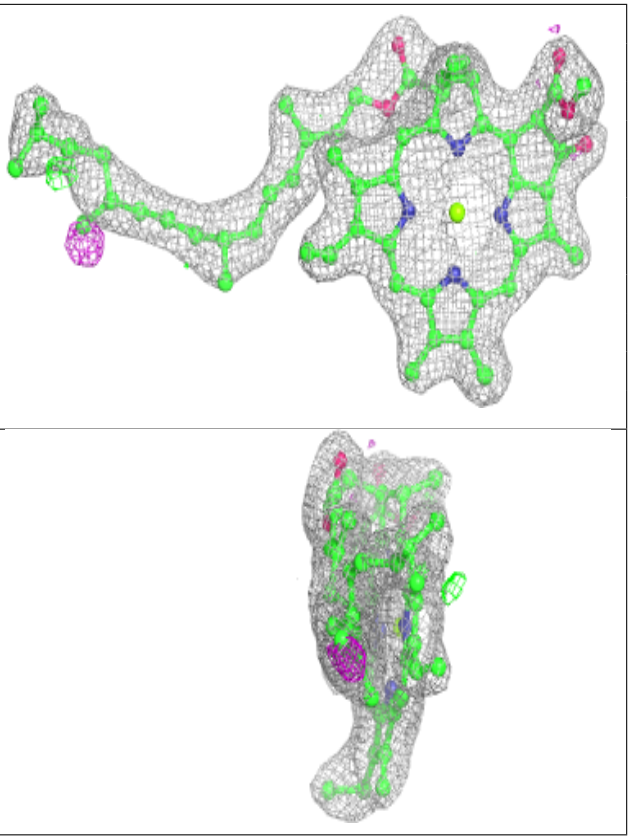
Electron density around DGD c 517:

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



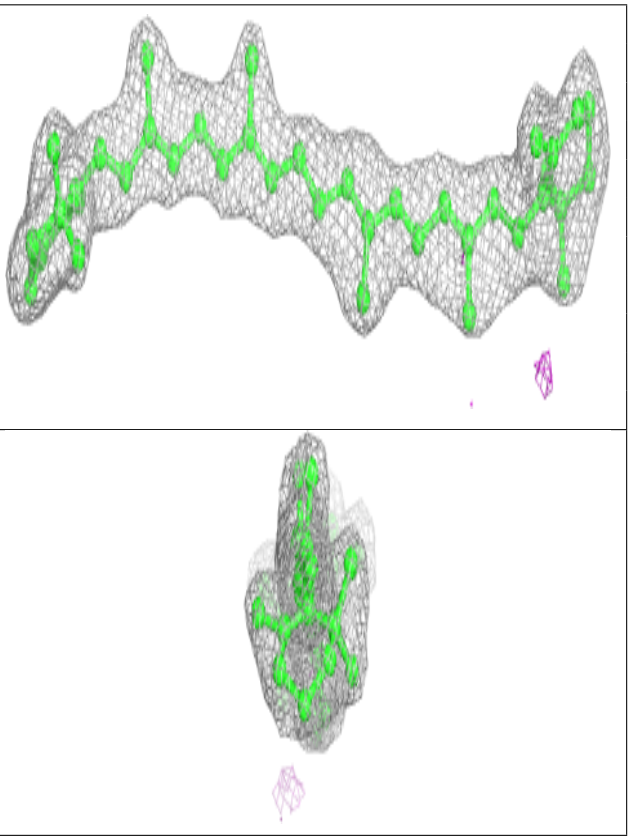
Electron density around CLA B 602:

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



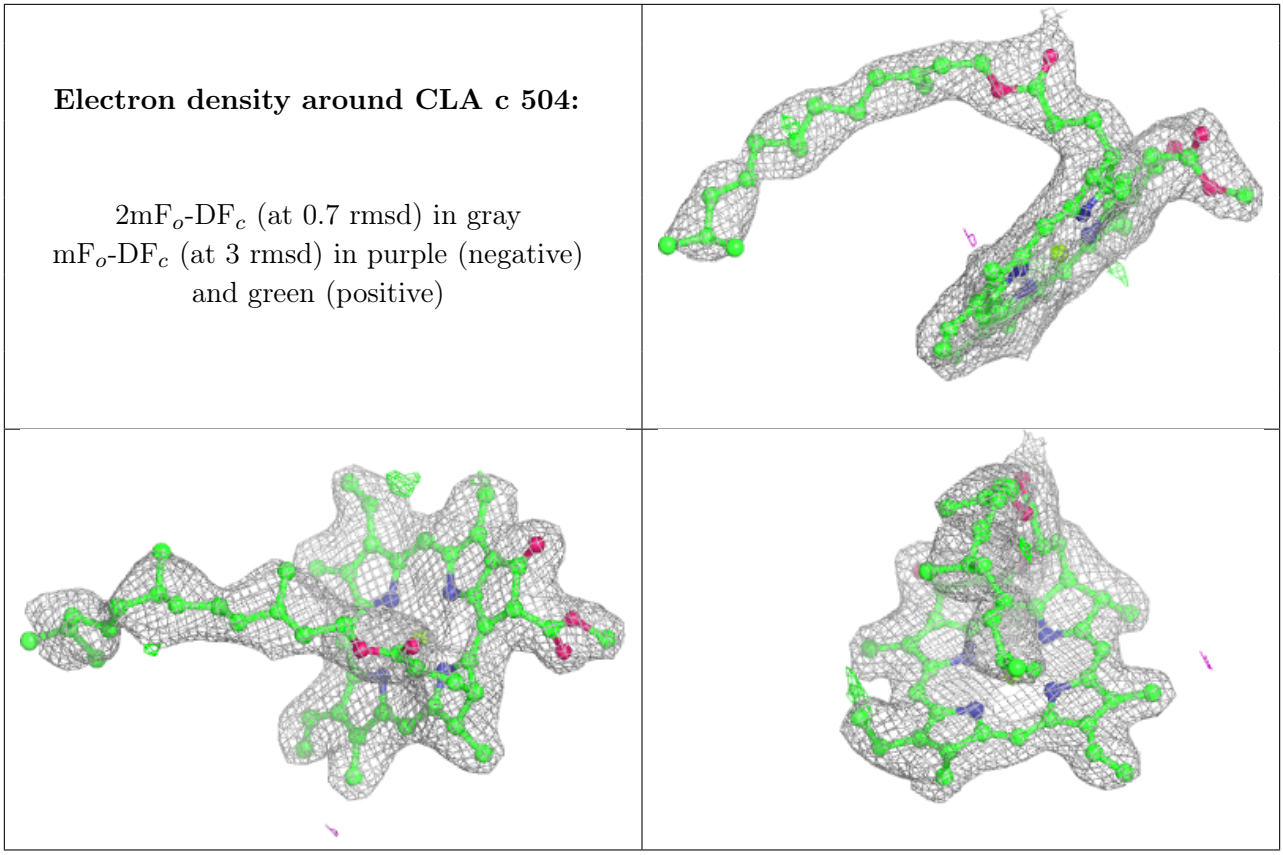
Electron density around BCR a 611:

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



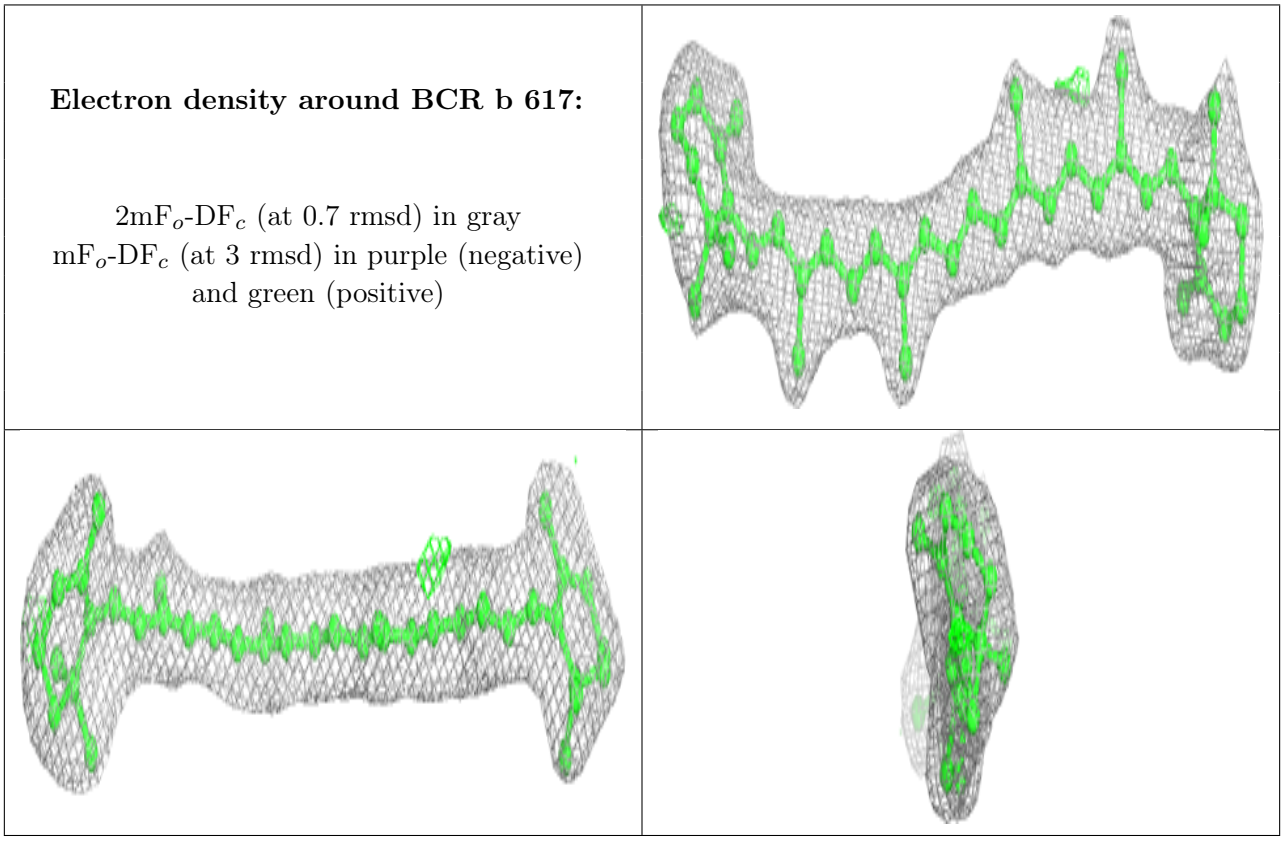
Electron density around CLA c 504:

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



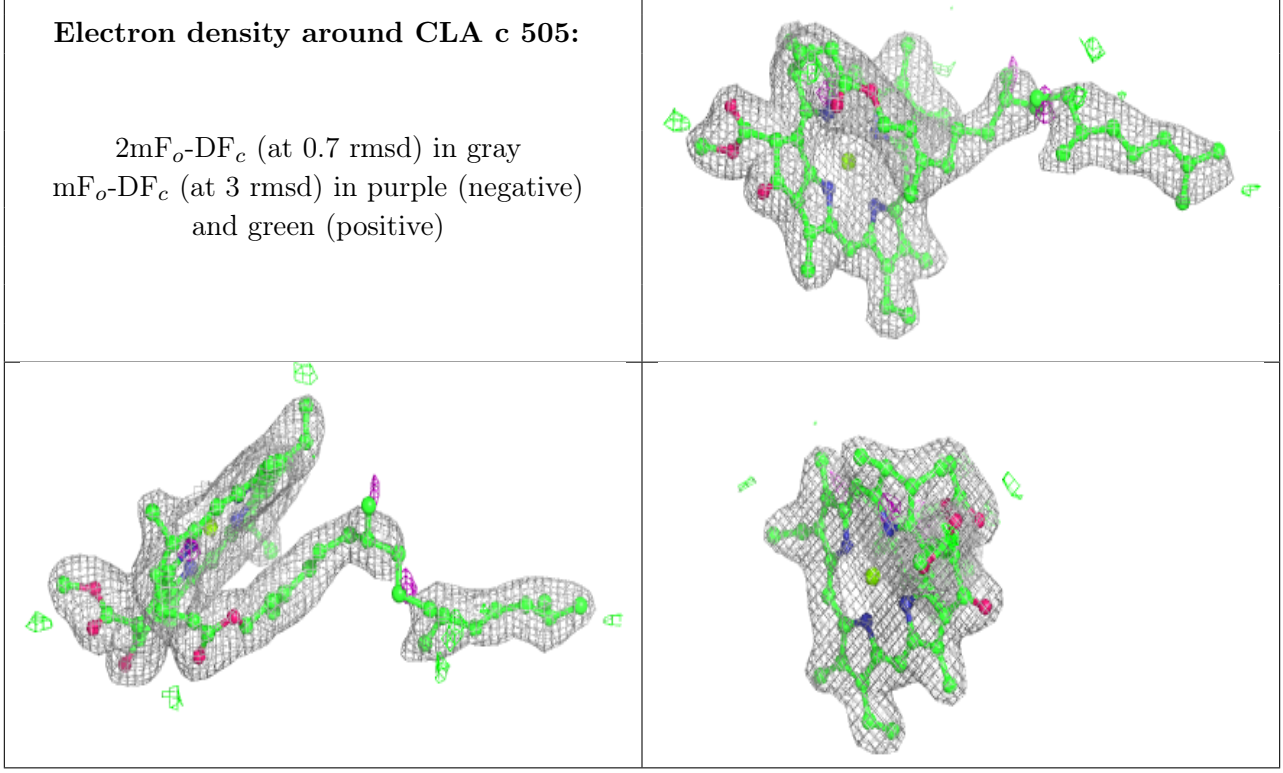
Electron density around BCR b 617:

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



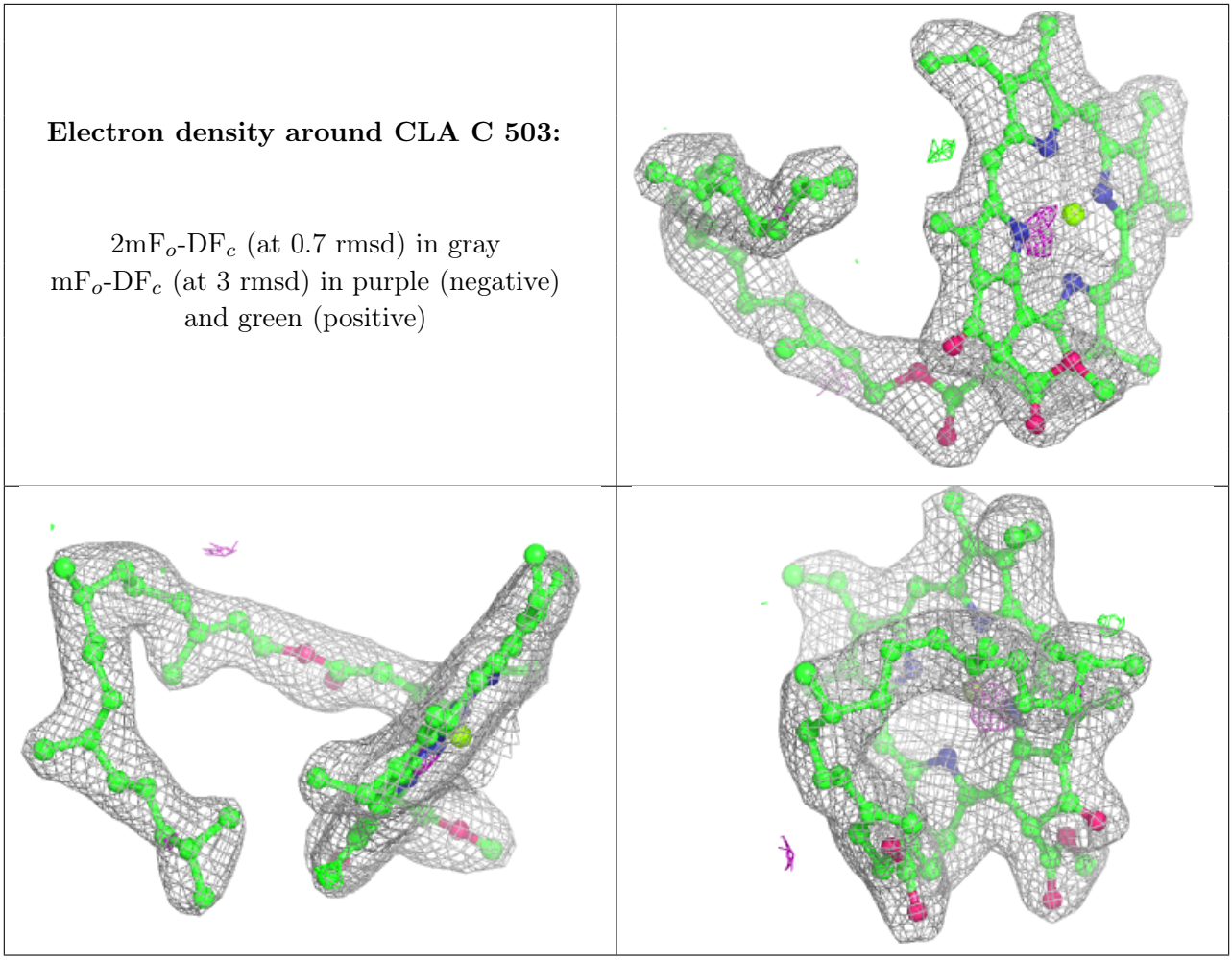
Electron density around CLA c 505:

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



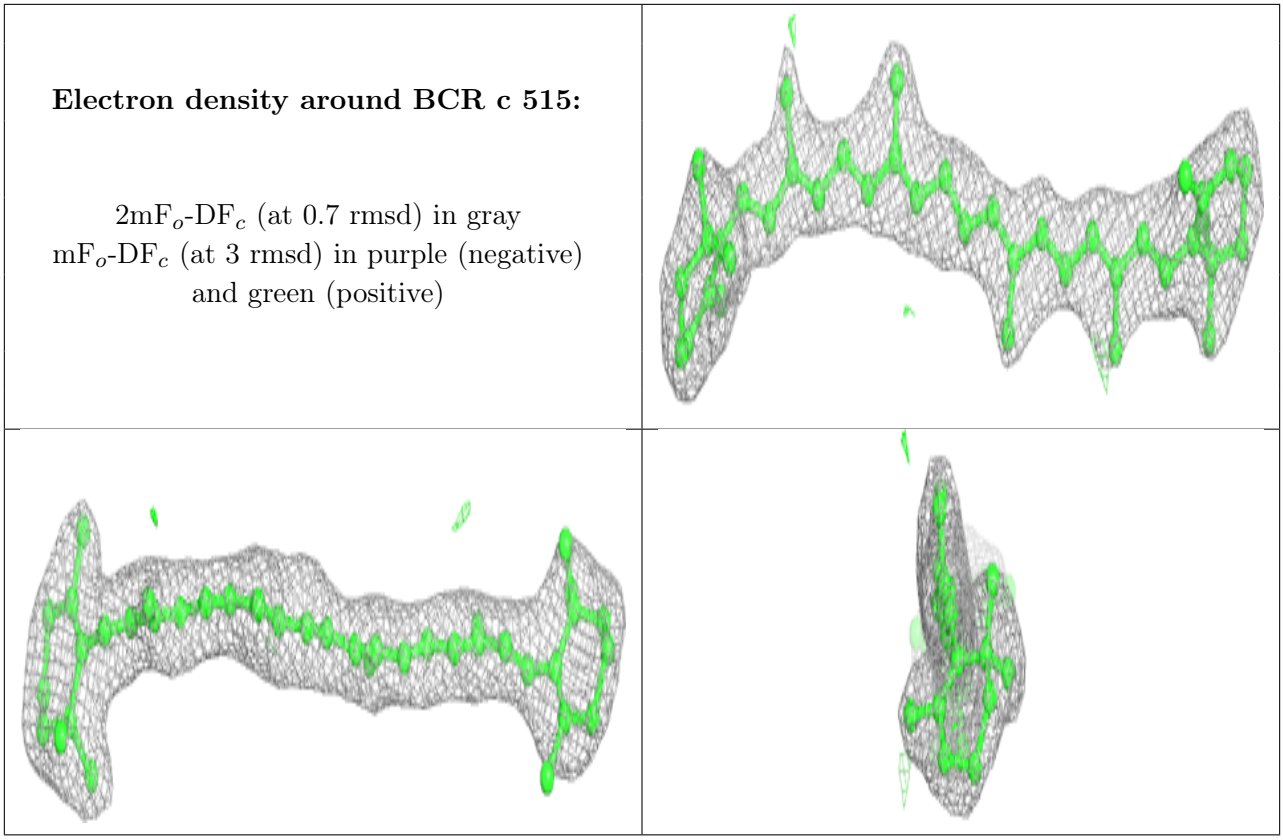
Electron density around CLA C 503:

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



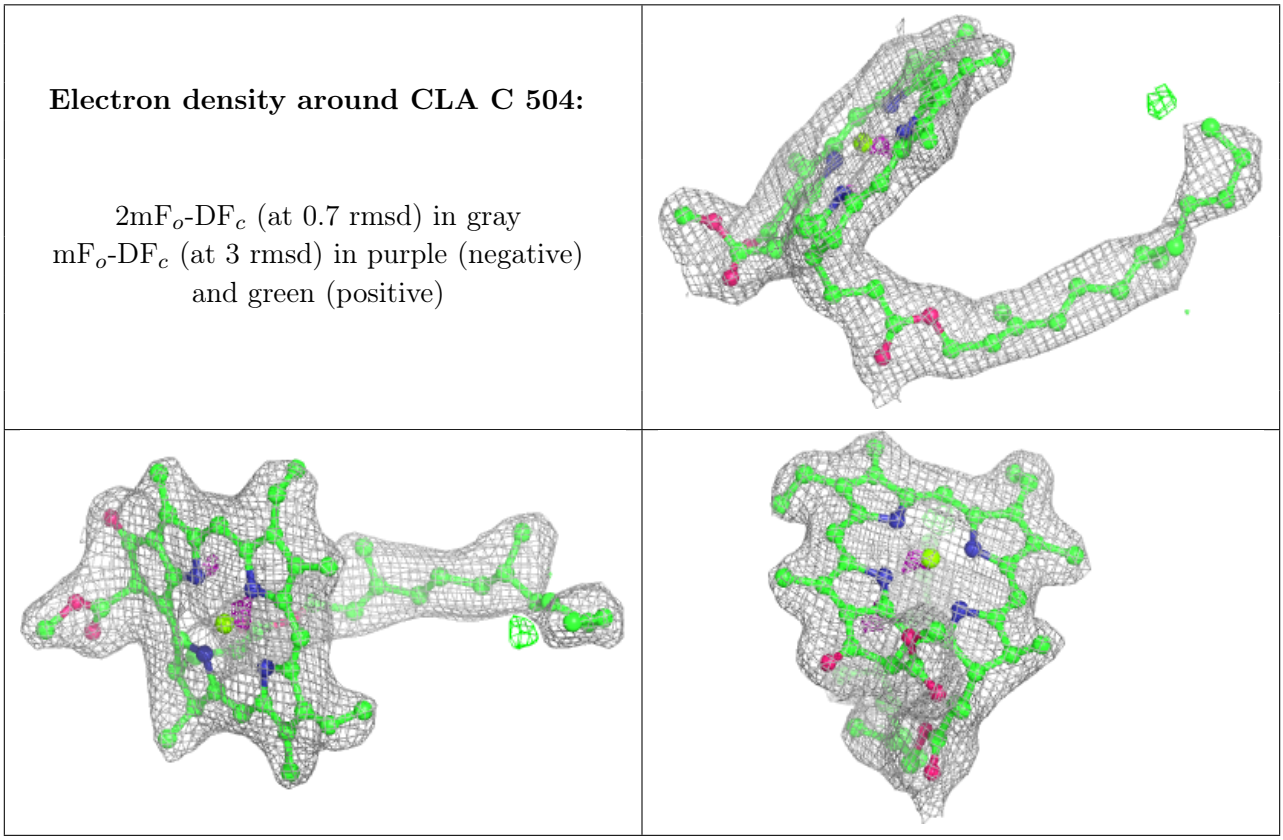
Electron density around BCR c 515:

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



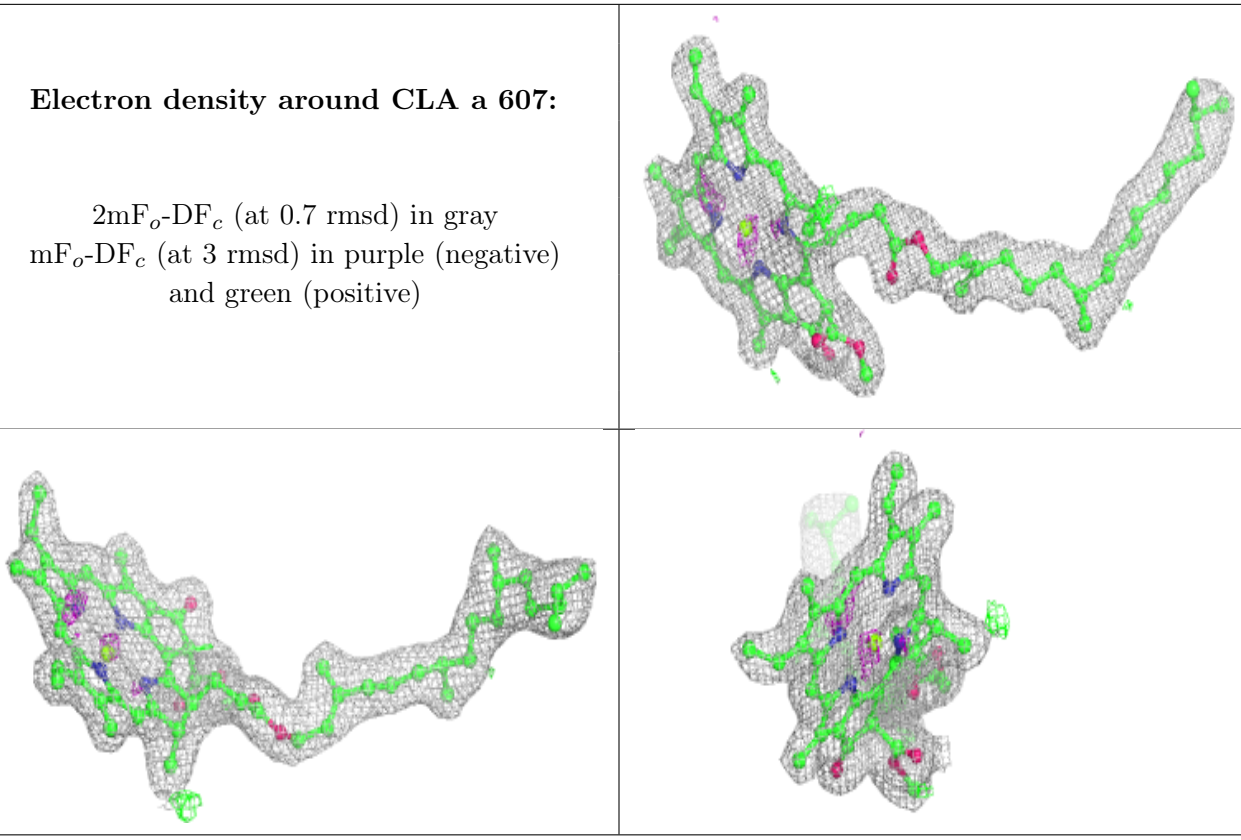
Electron density around CLA C 504:

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



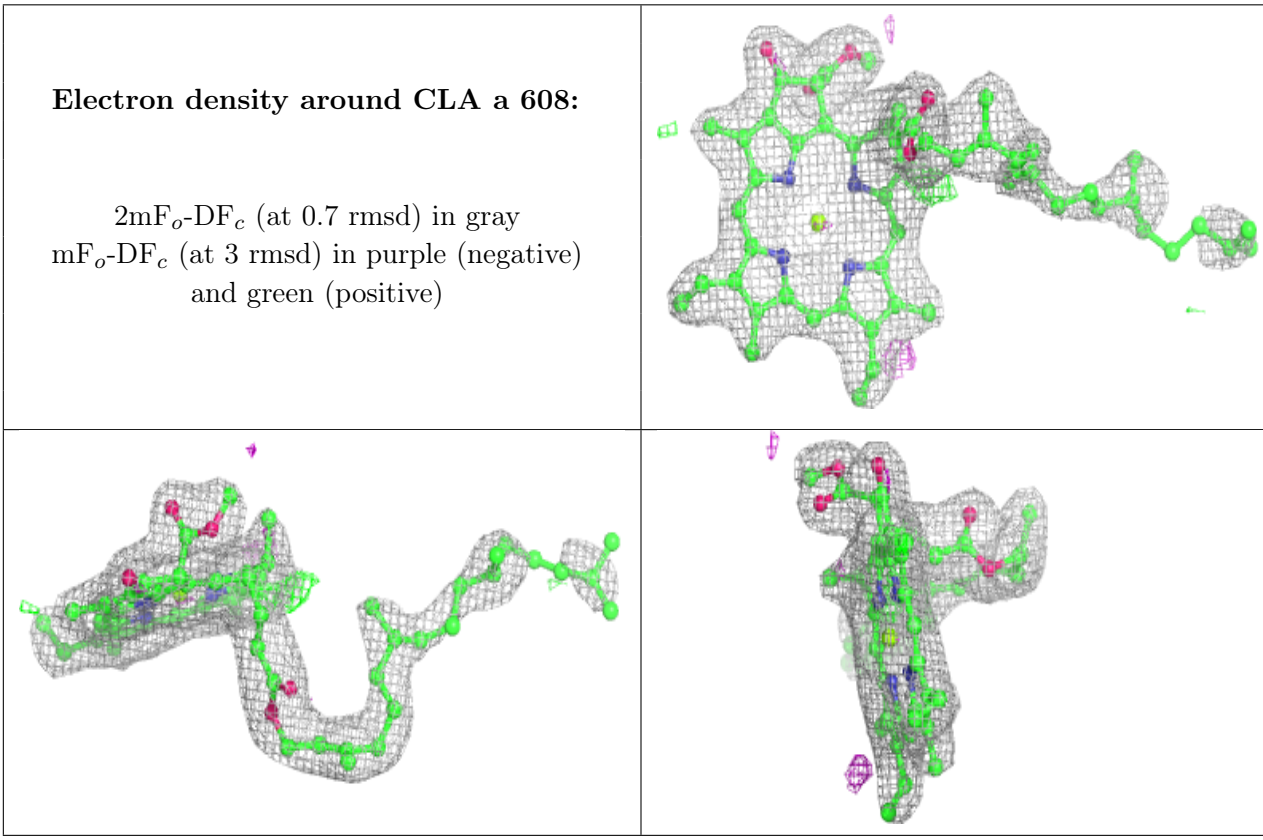
Electron density around CLA a 607:

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



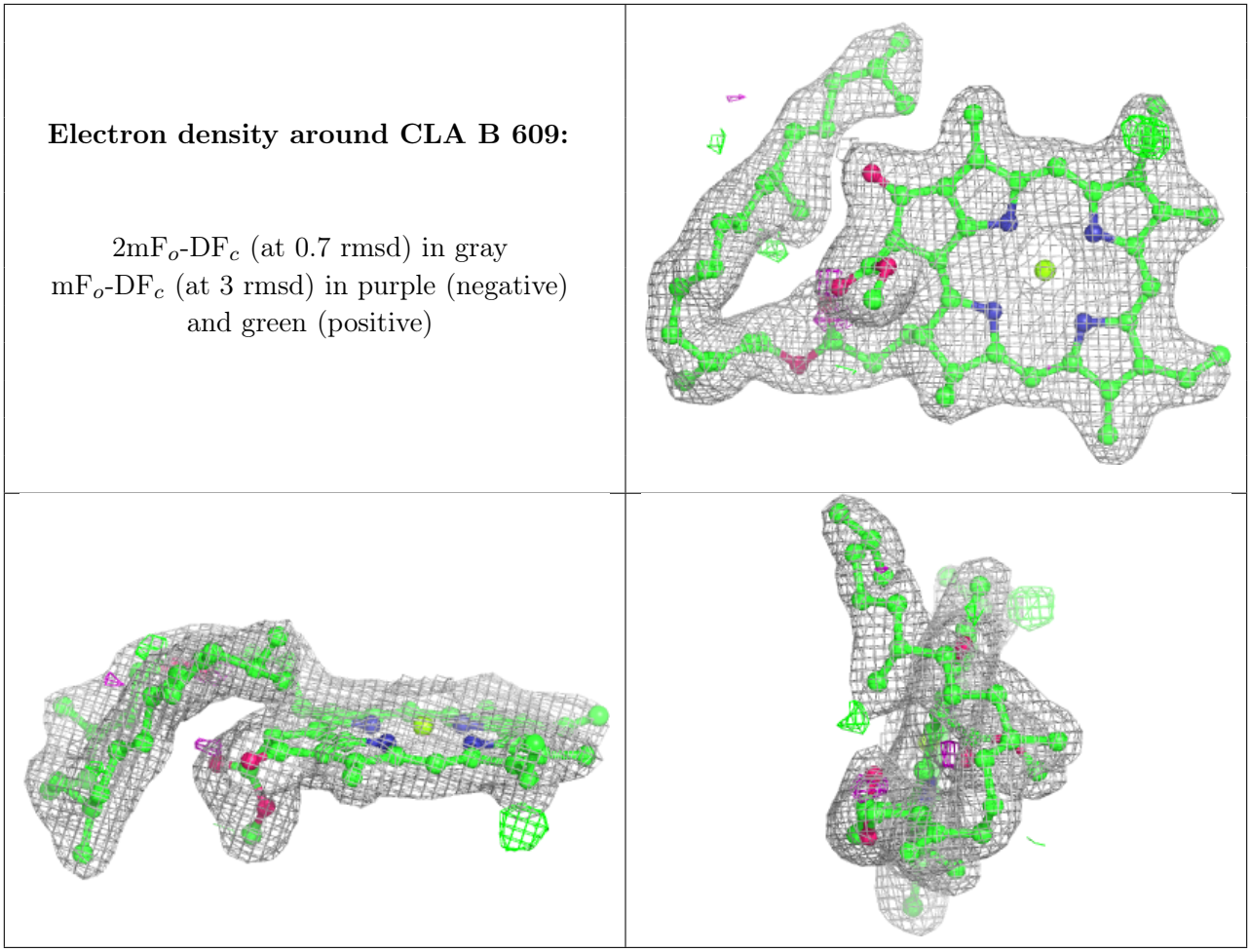
Electron density around CLA a 608:

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



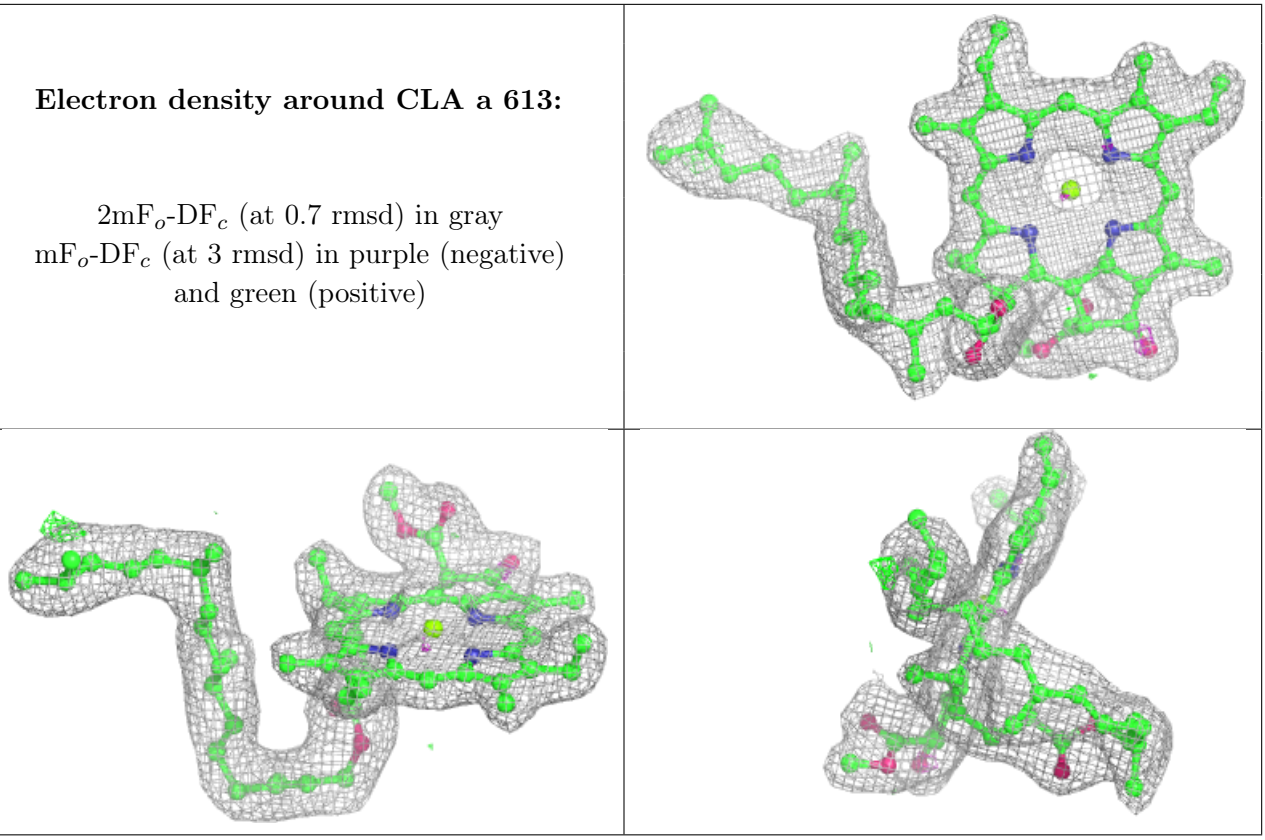
Electron density around CLA B 609:

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



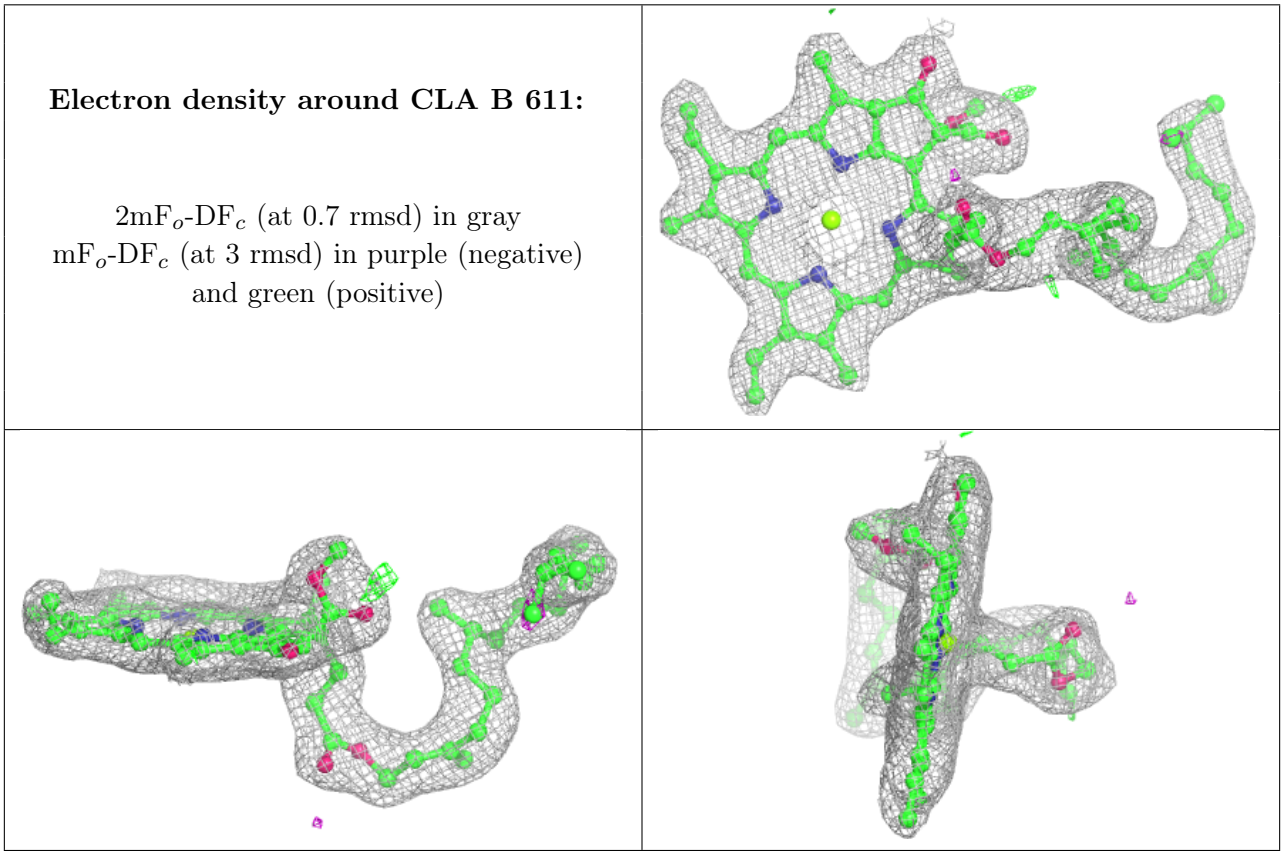
Electron density around CLA a 613:

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



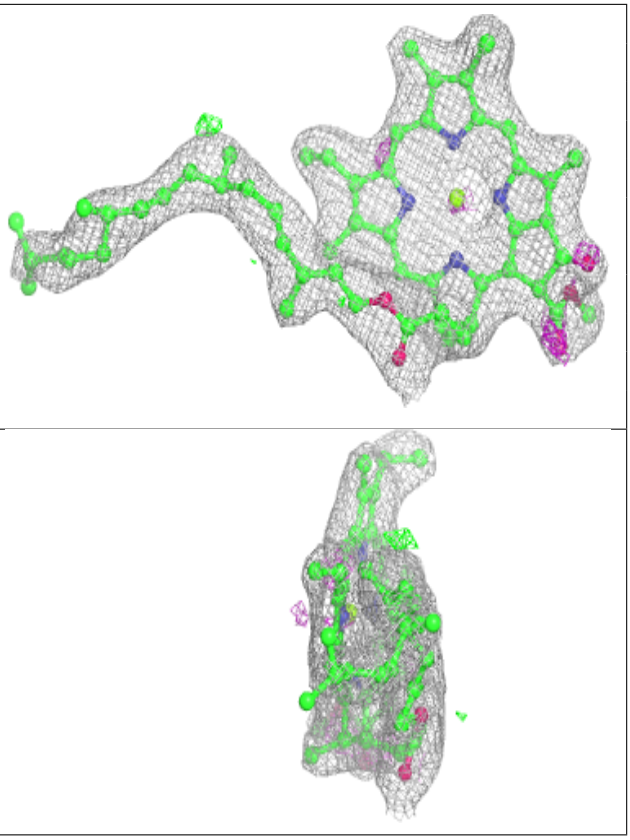
Electron density around CLA B 611:

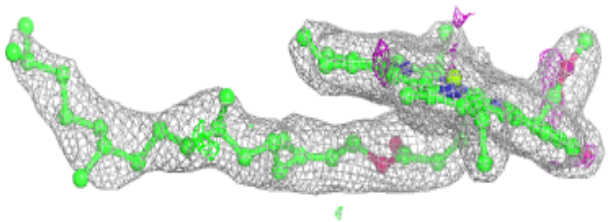
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 602:

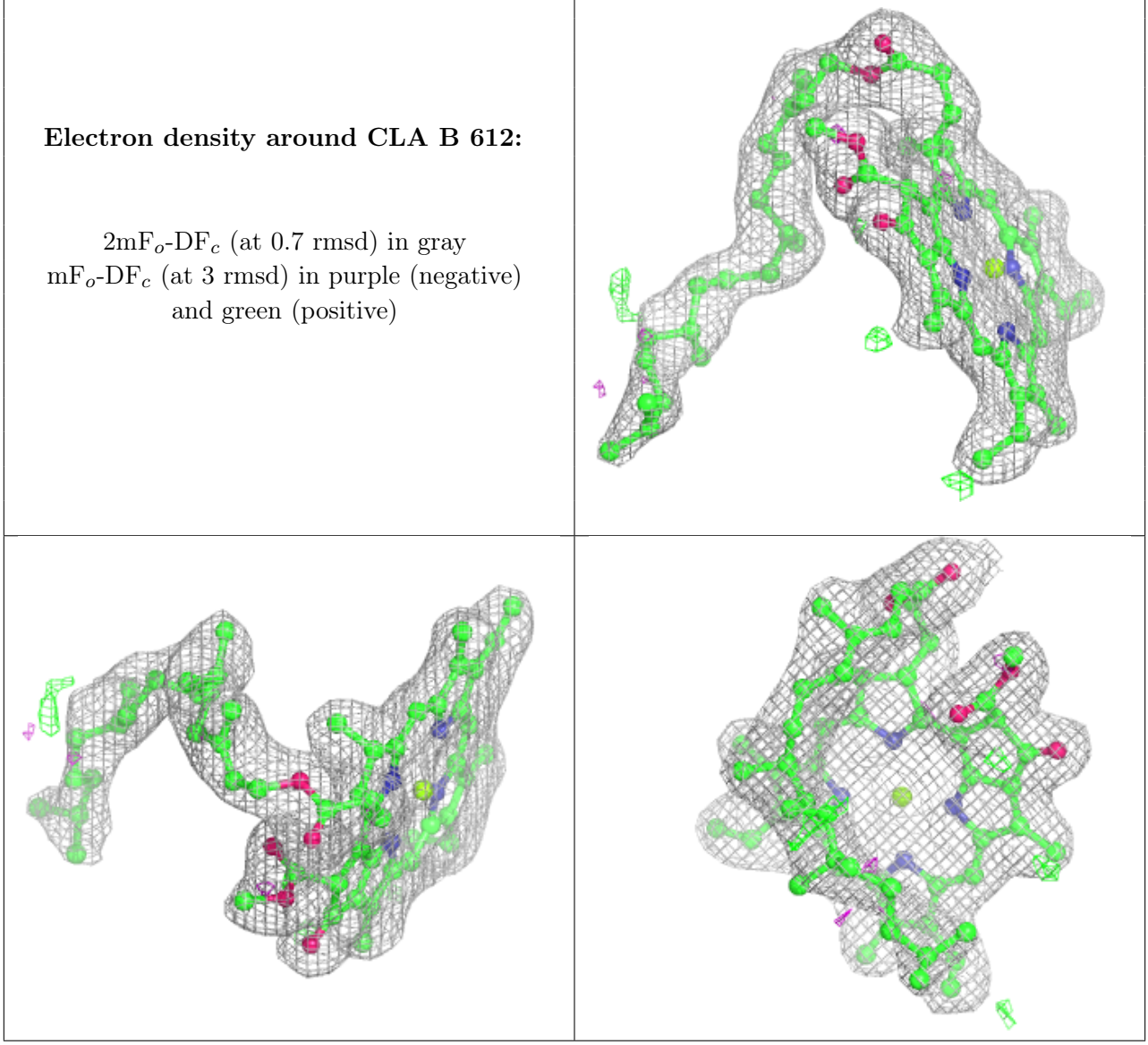
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





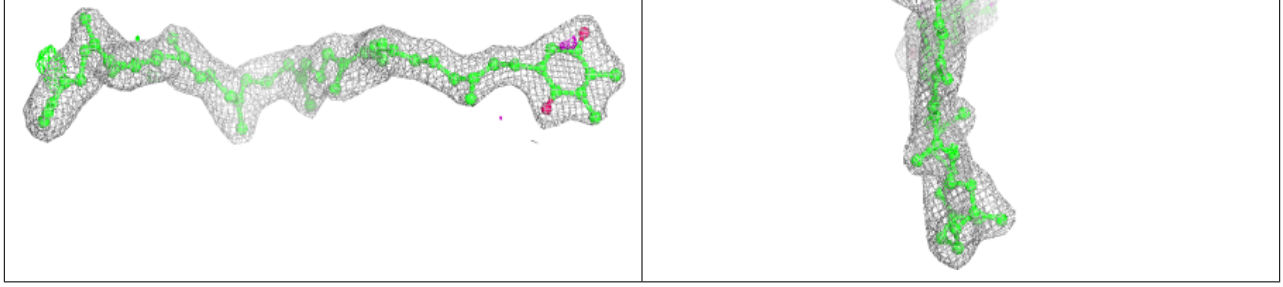
Electron density around CLA B 612:

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



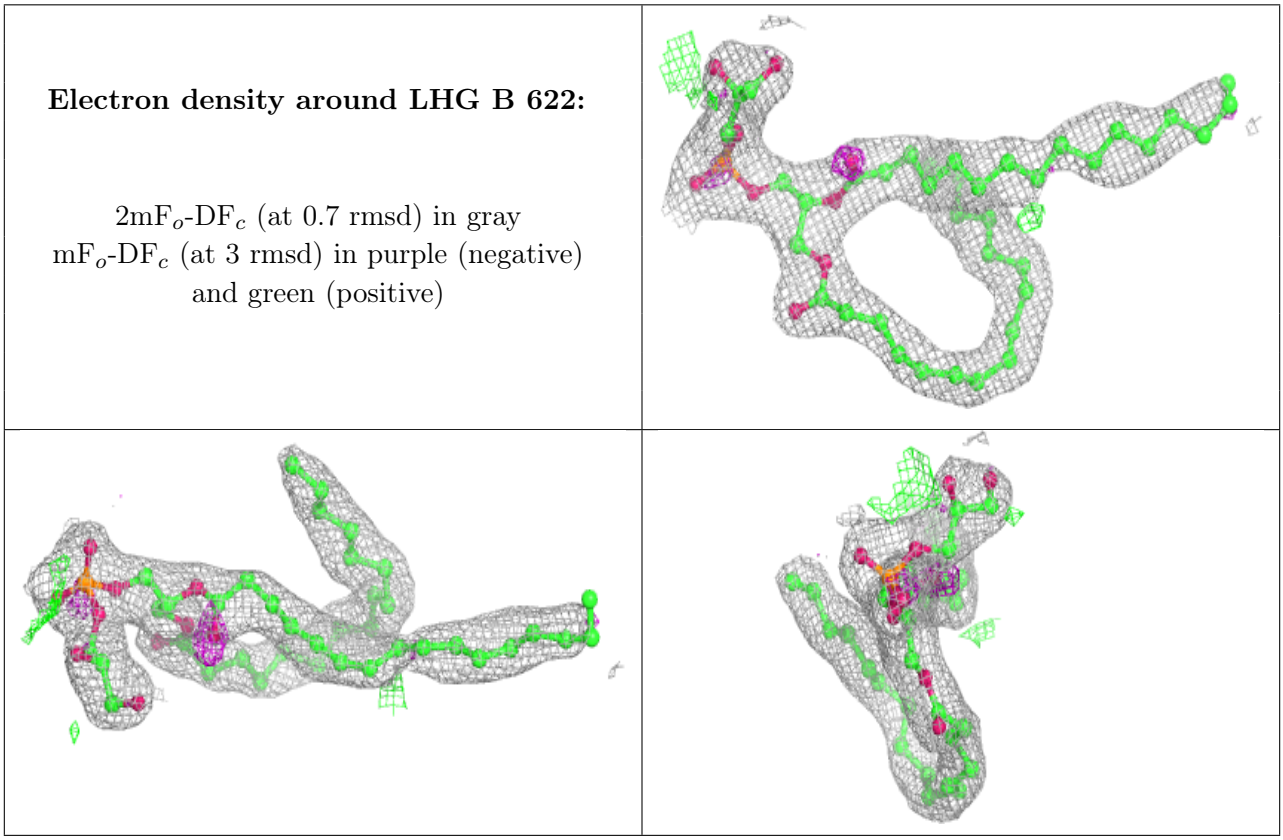
Electron density around PL9 d 405:

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



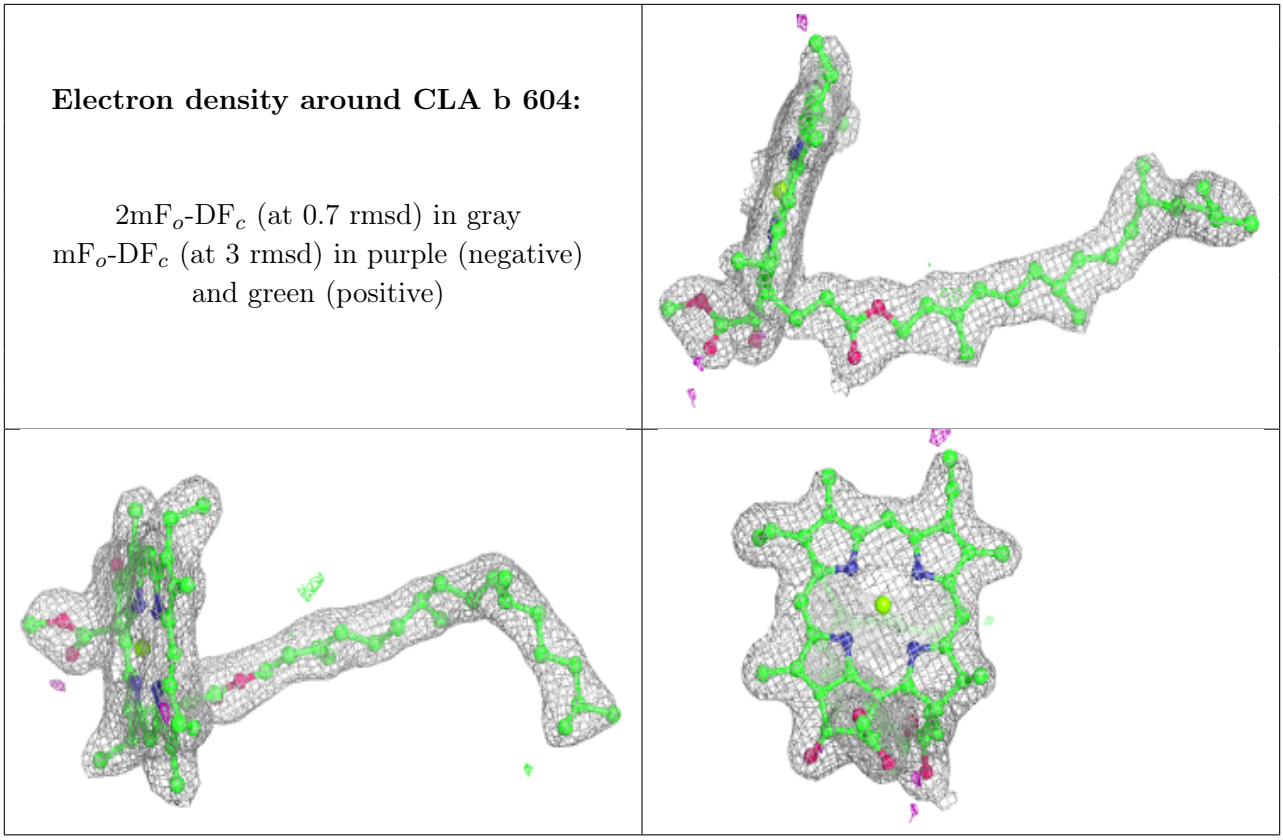
Electron density around LHG B 622:

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



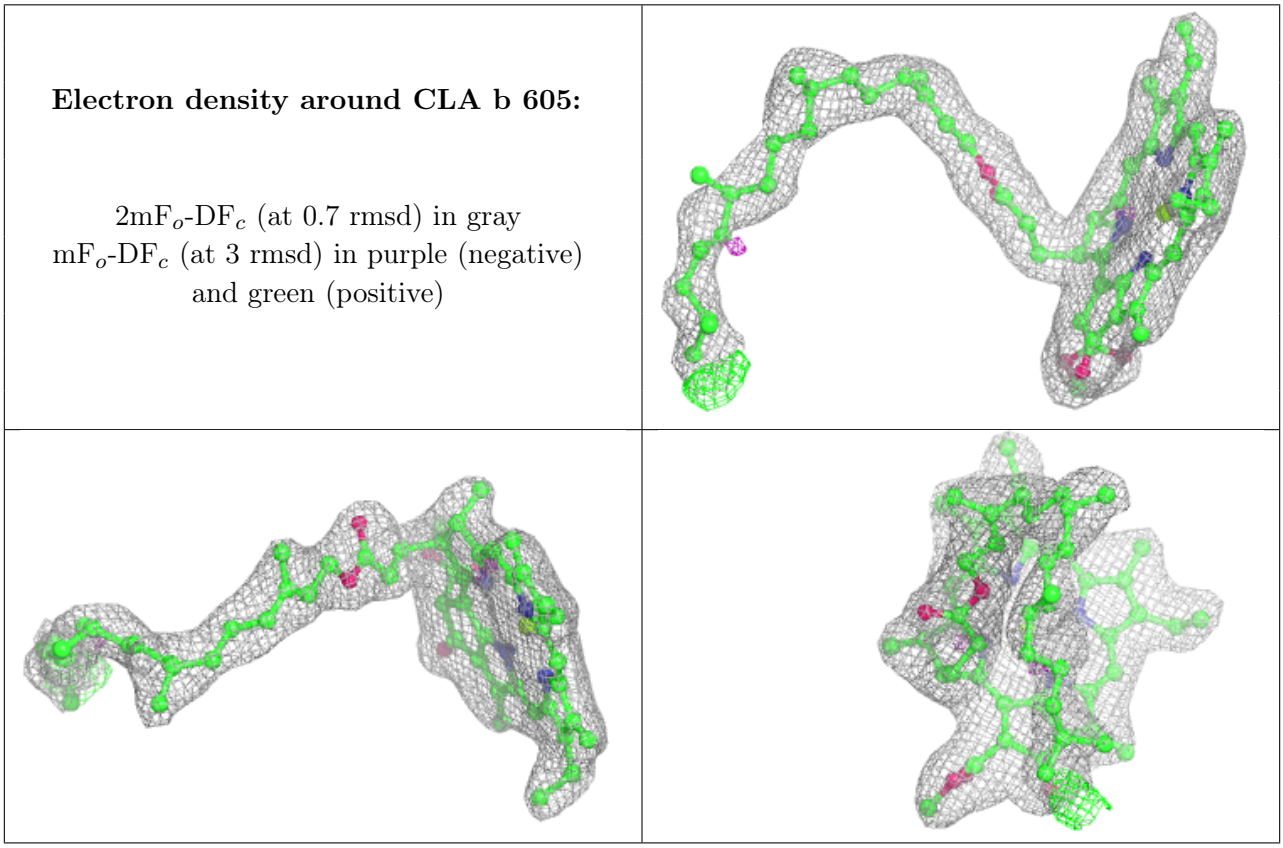
Electron density around CLA b 604:

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



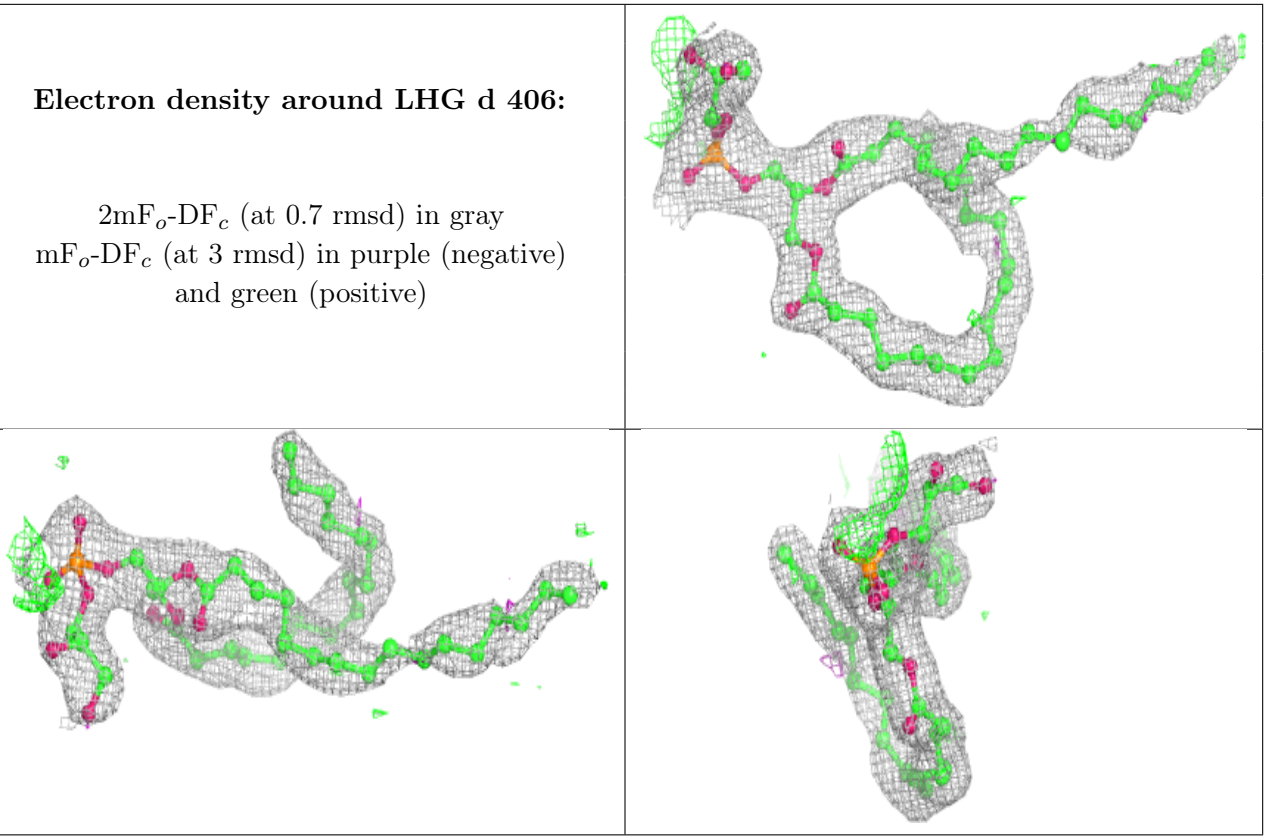
Electron density around CLA b 605:

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



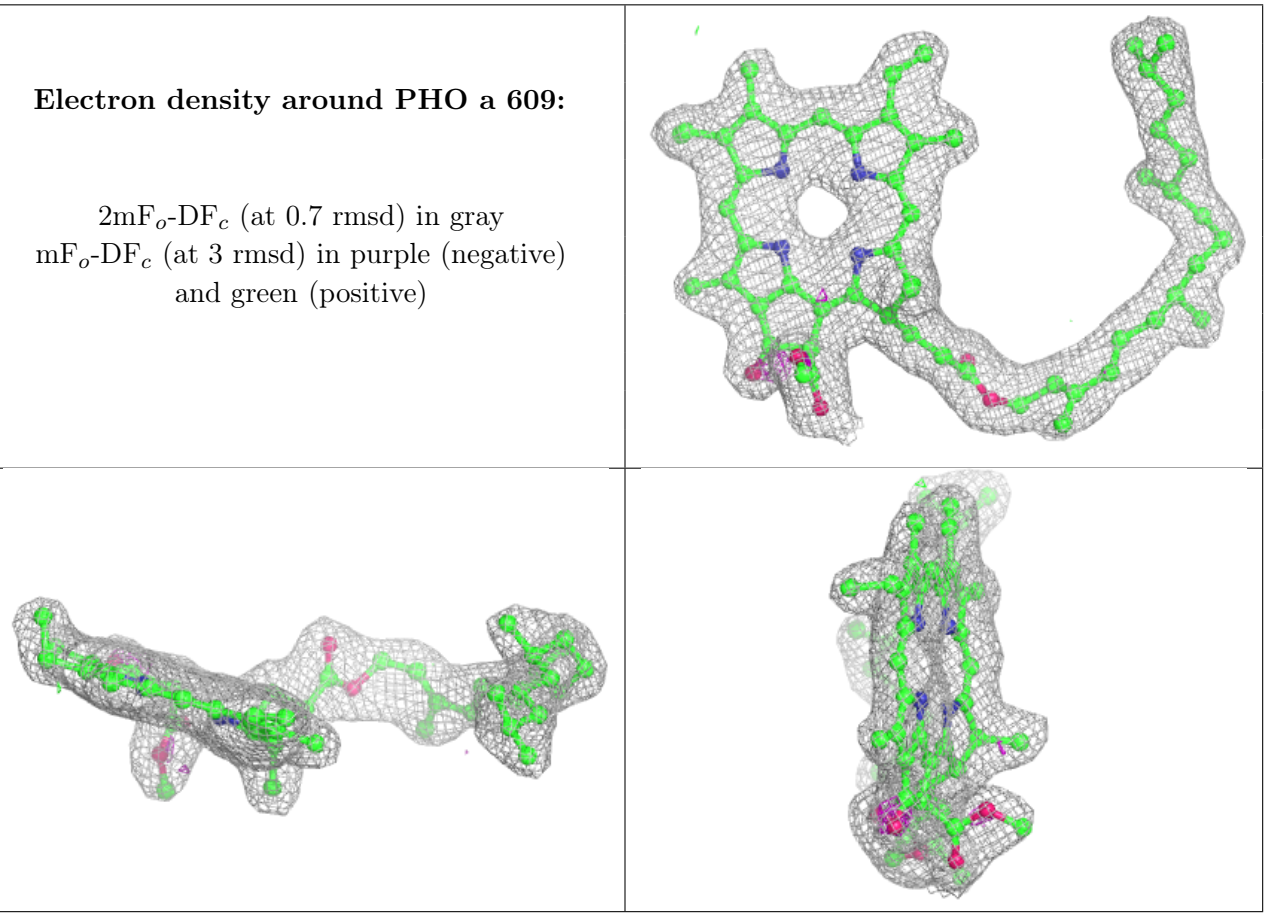
Electron density around LHG d 406:

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



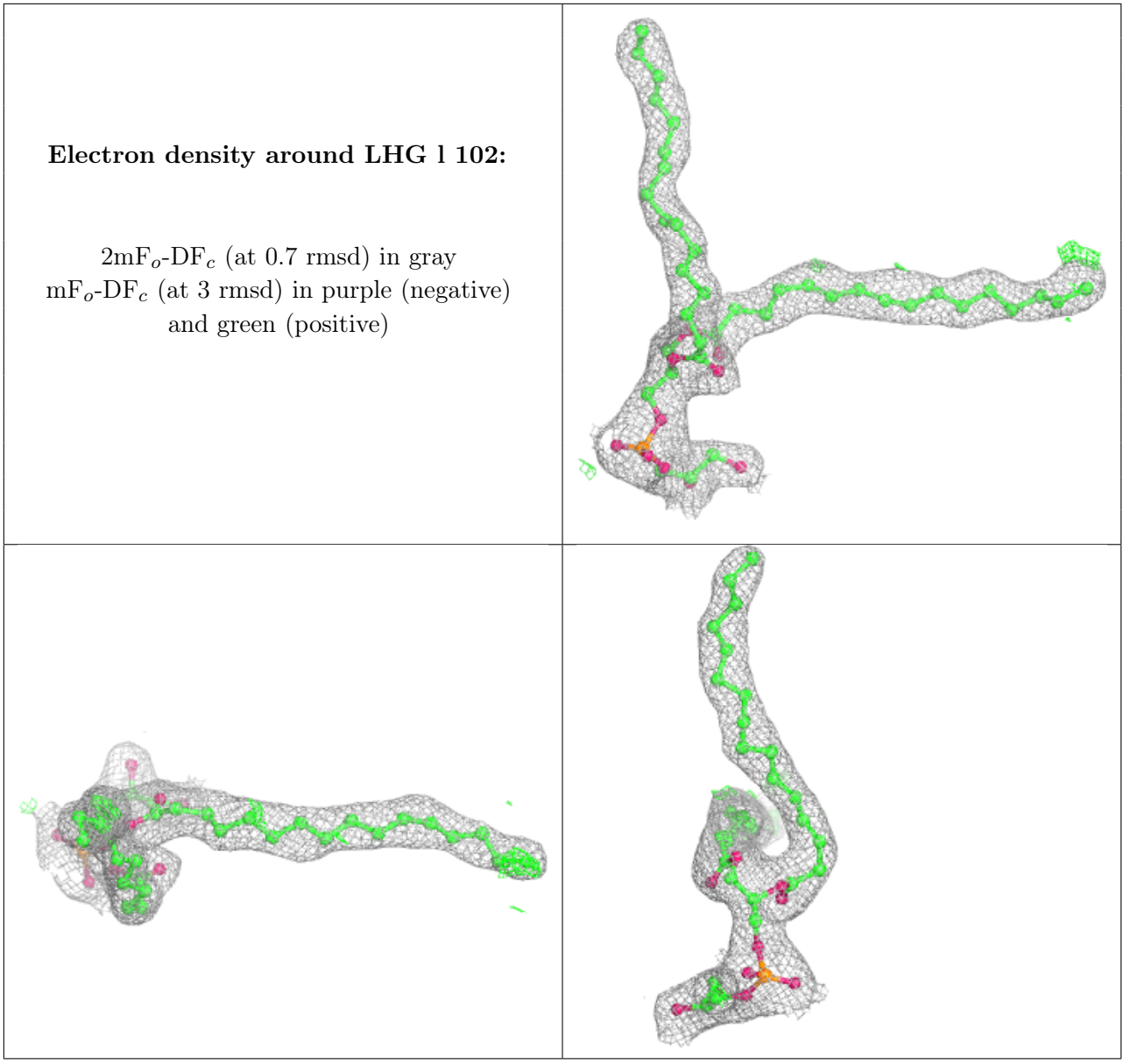
Electron density around PHO a 609:

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



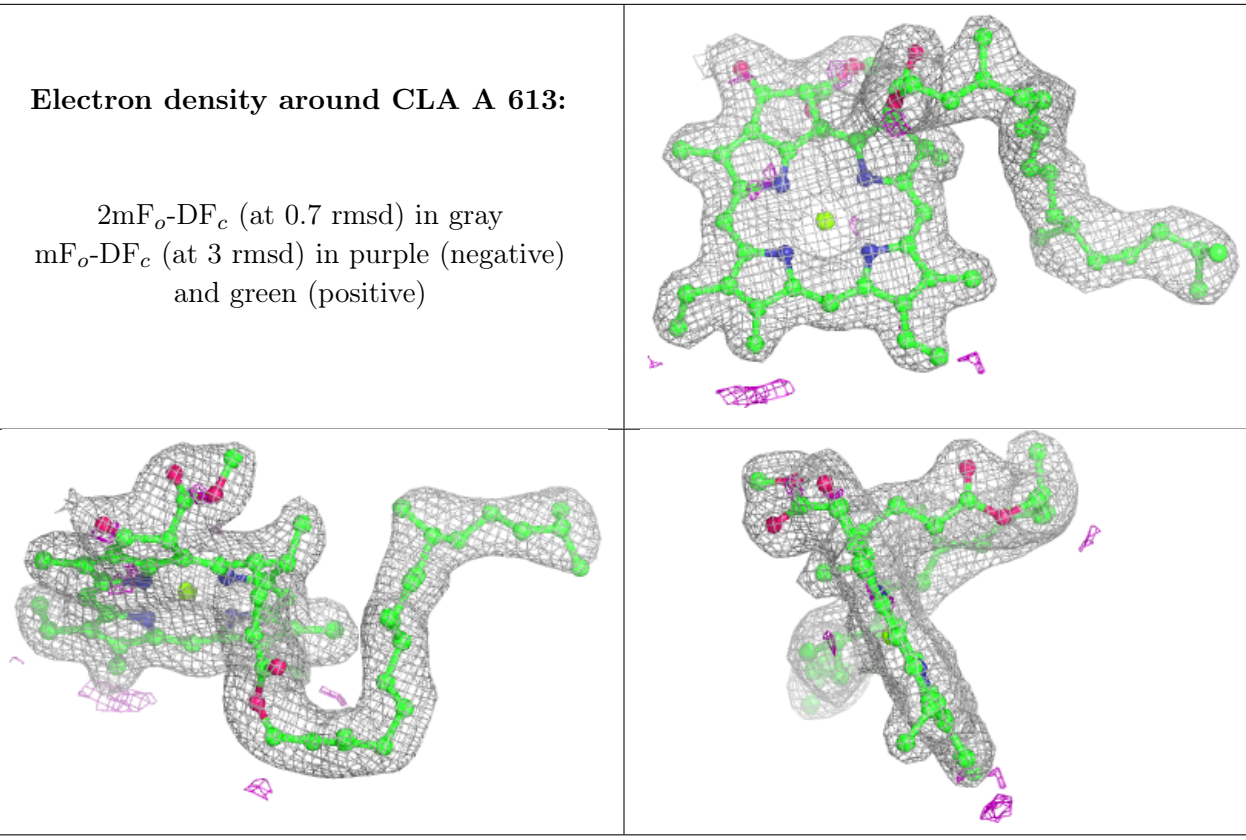
Electron density around LHG l 102:

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



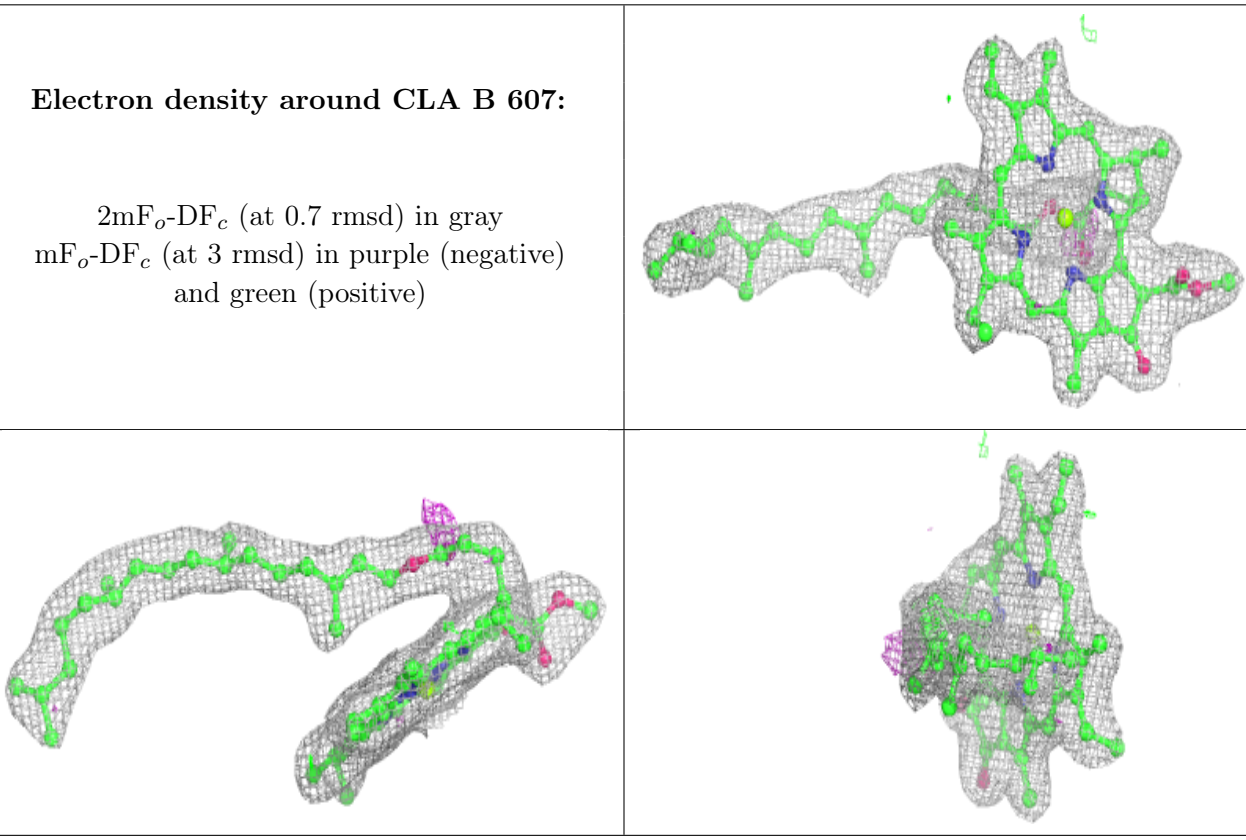
Electron density around CLA A 613:

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



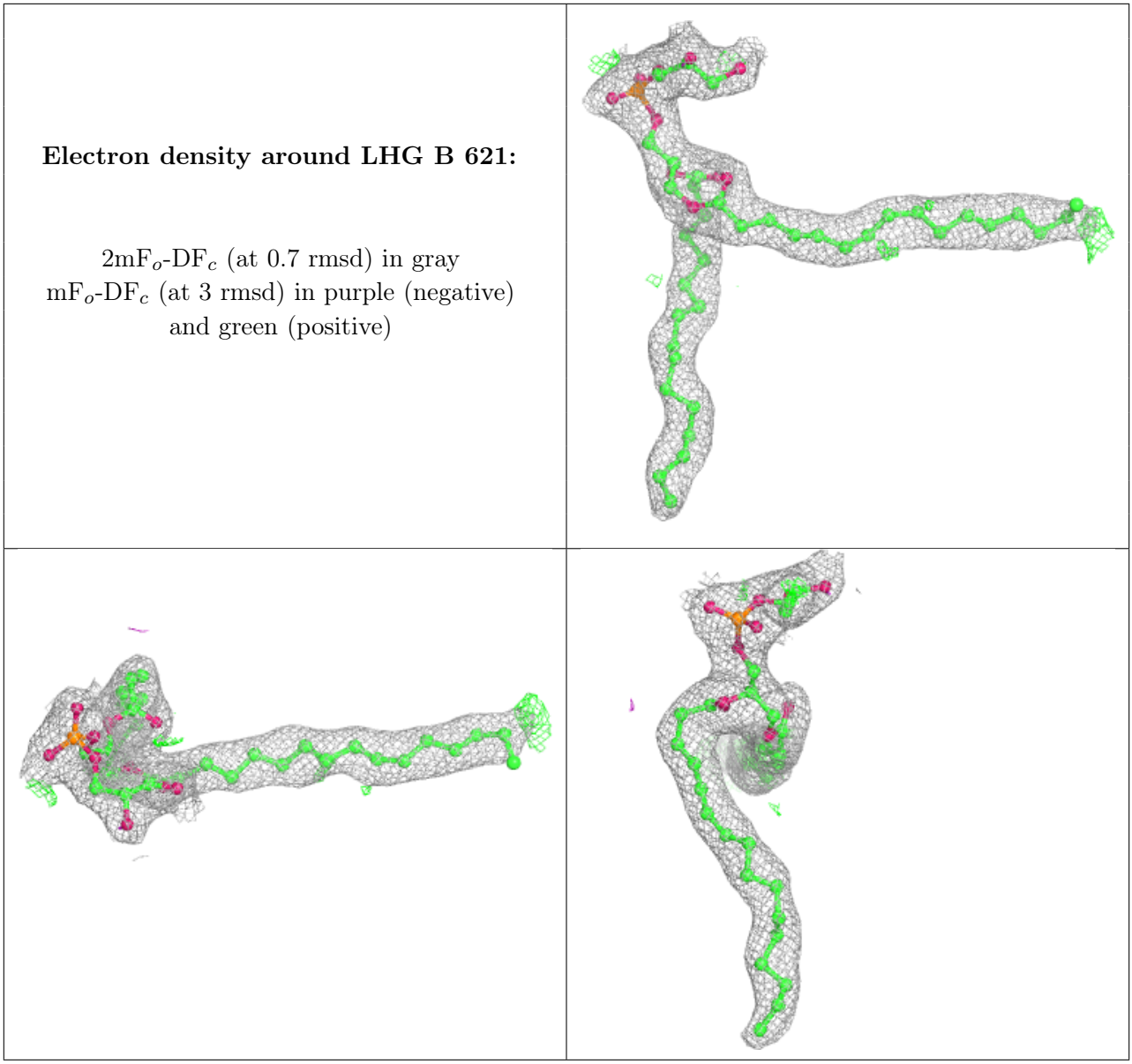
Electron density around CLA B 607:

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



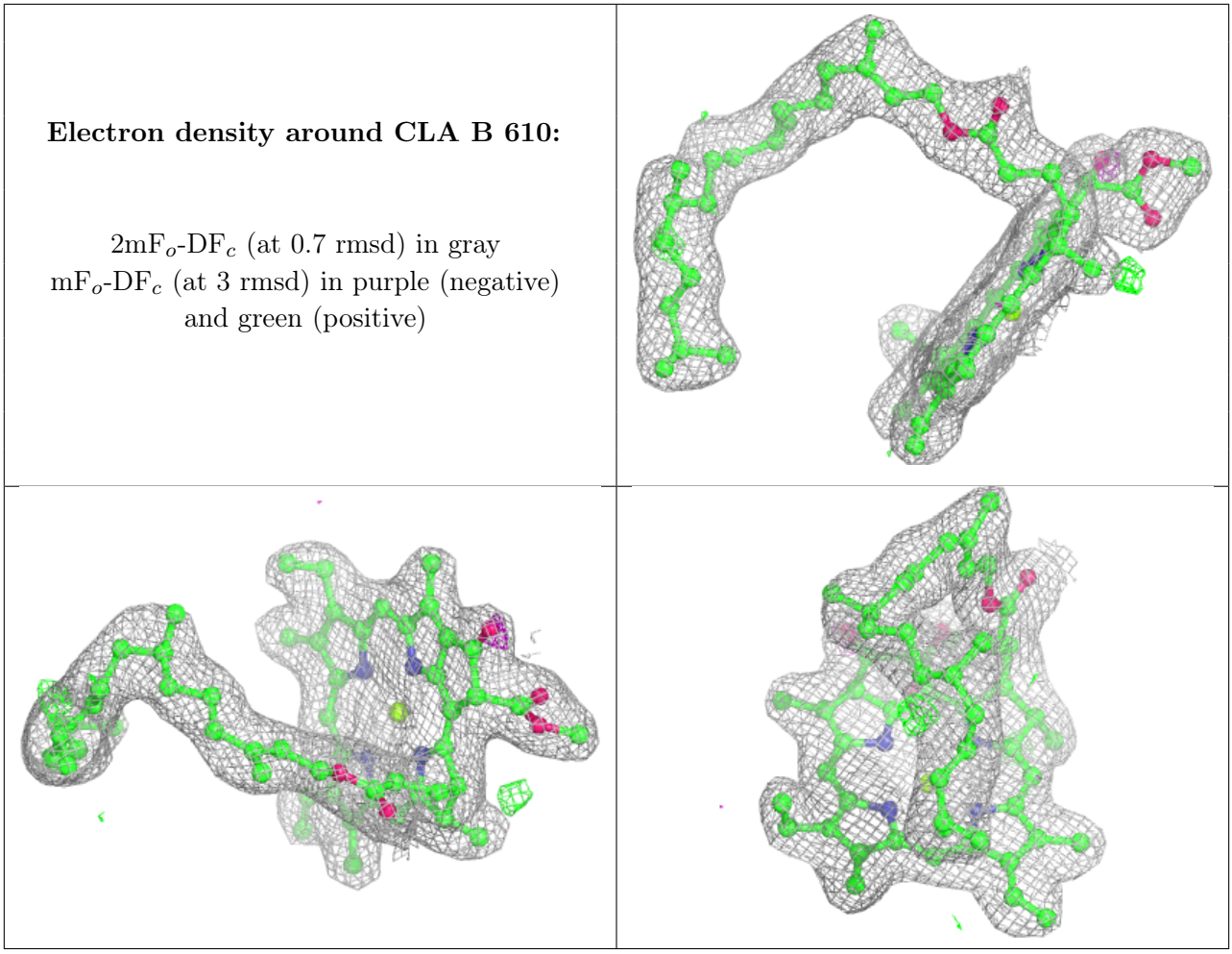
Electron density around LHG B 621:

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



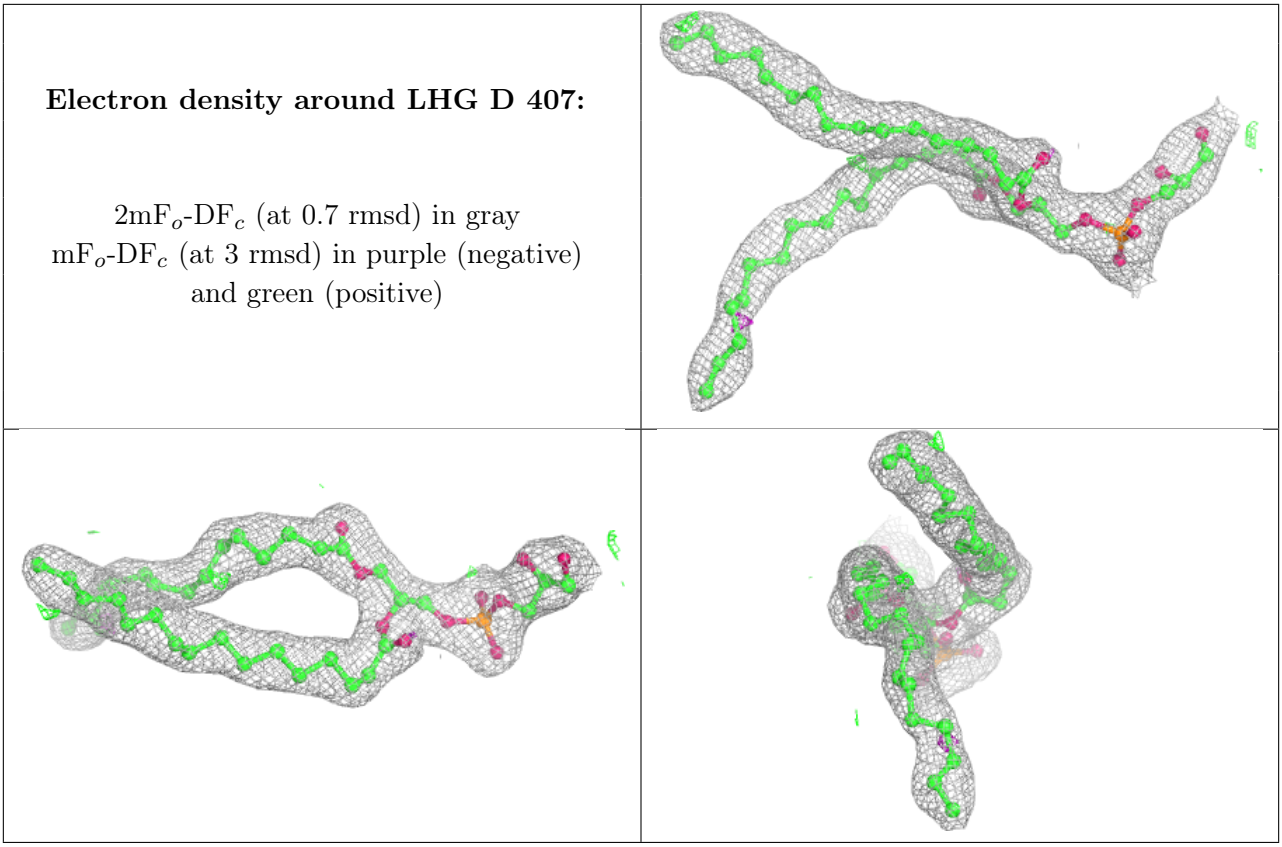
Electron density around CLA B 610:

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



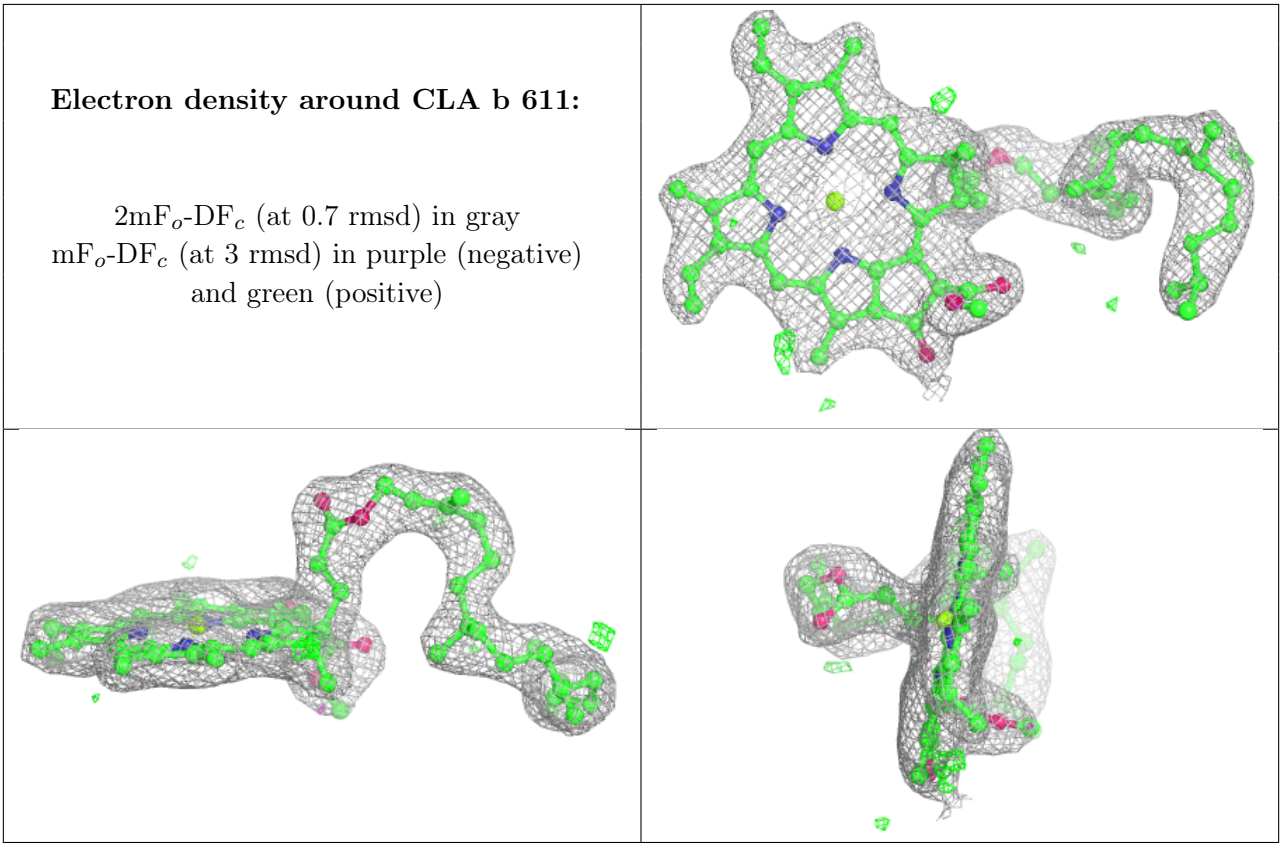
Electron density around LHG D 407:

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



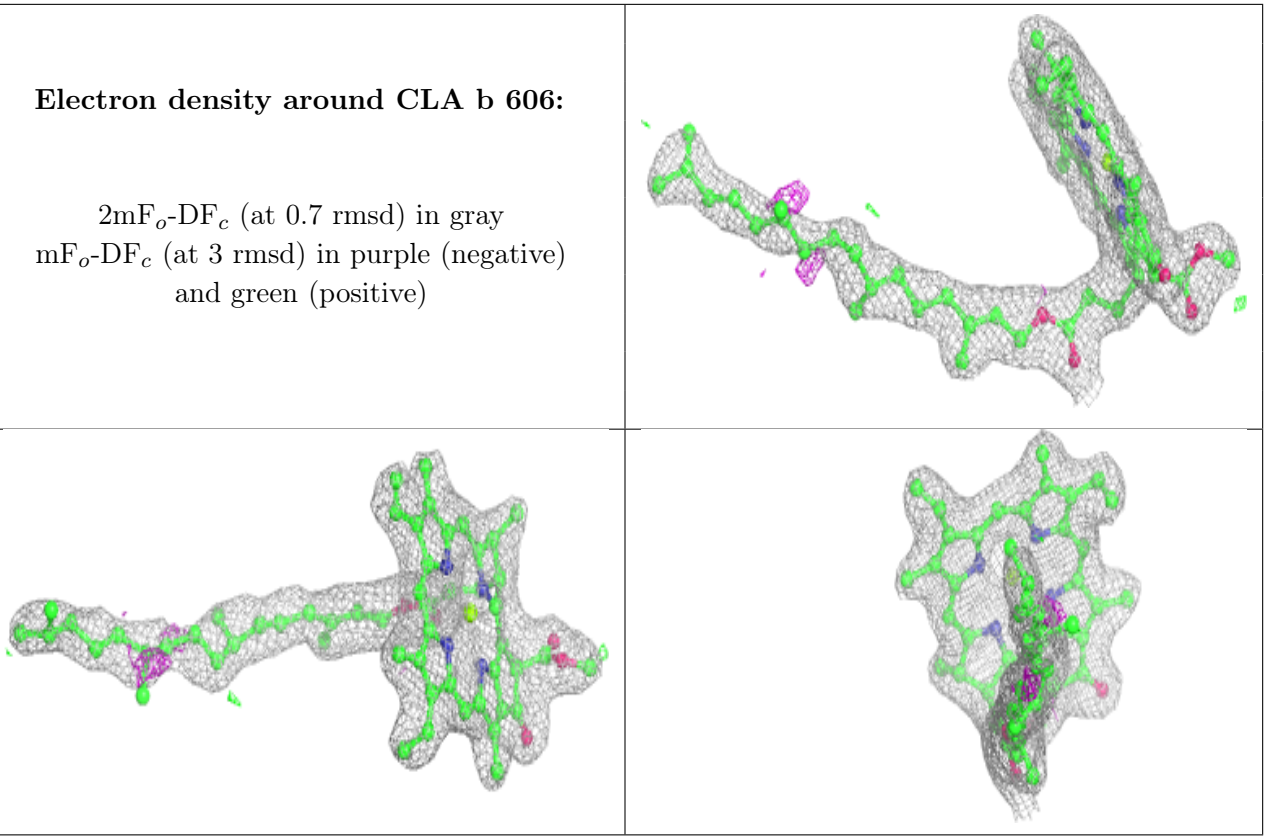
Electron density around CLA b 611:

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



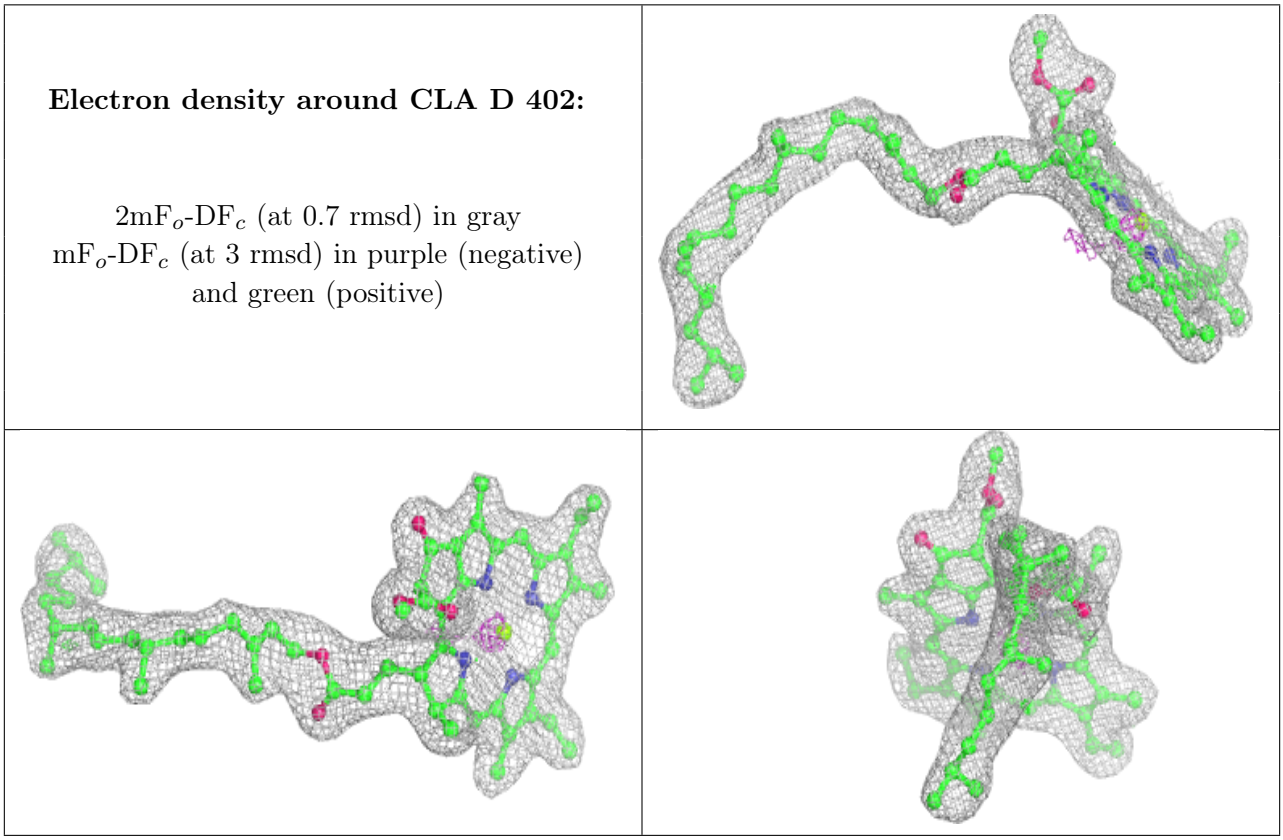
Electron density around CLA b 606:

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



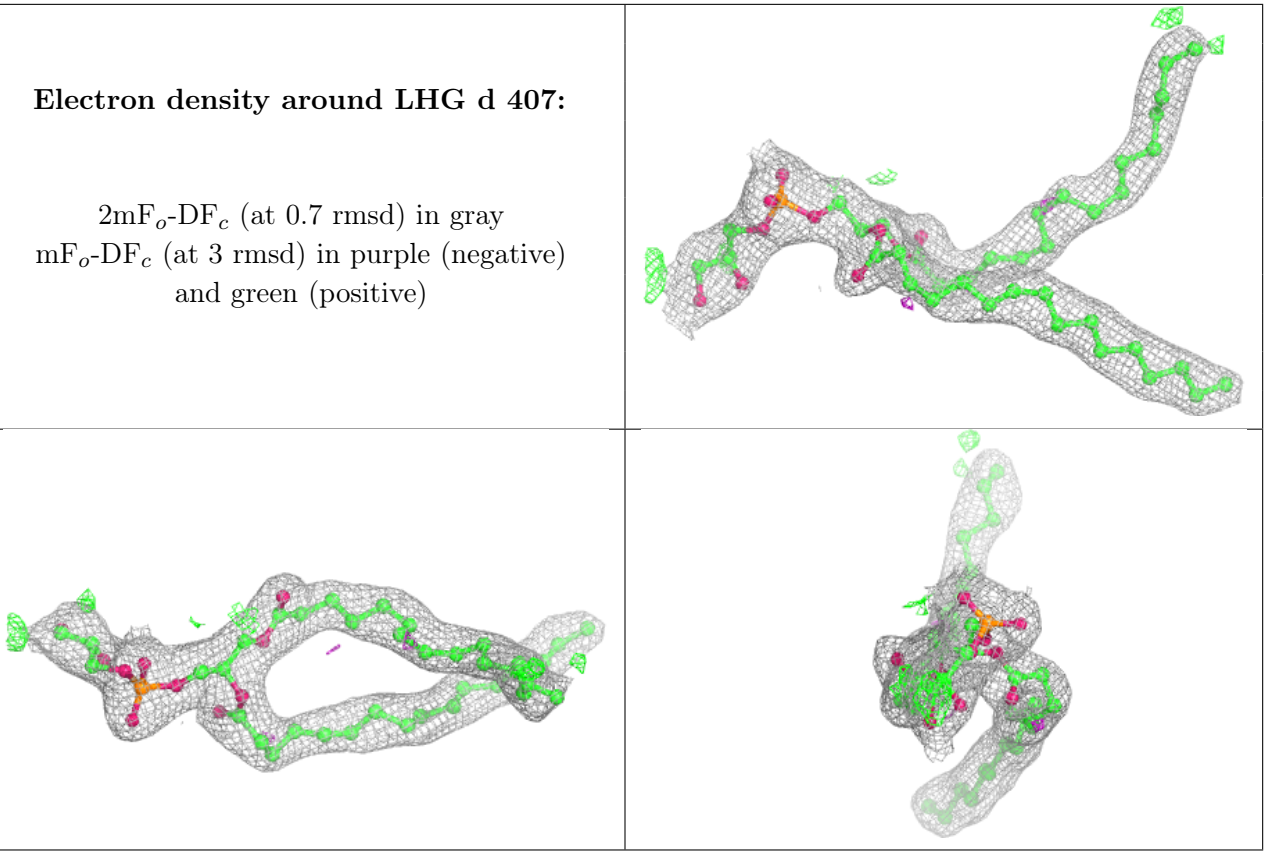
Electron density around CLA D 402:

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



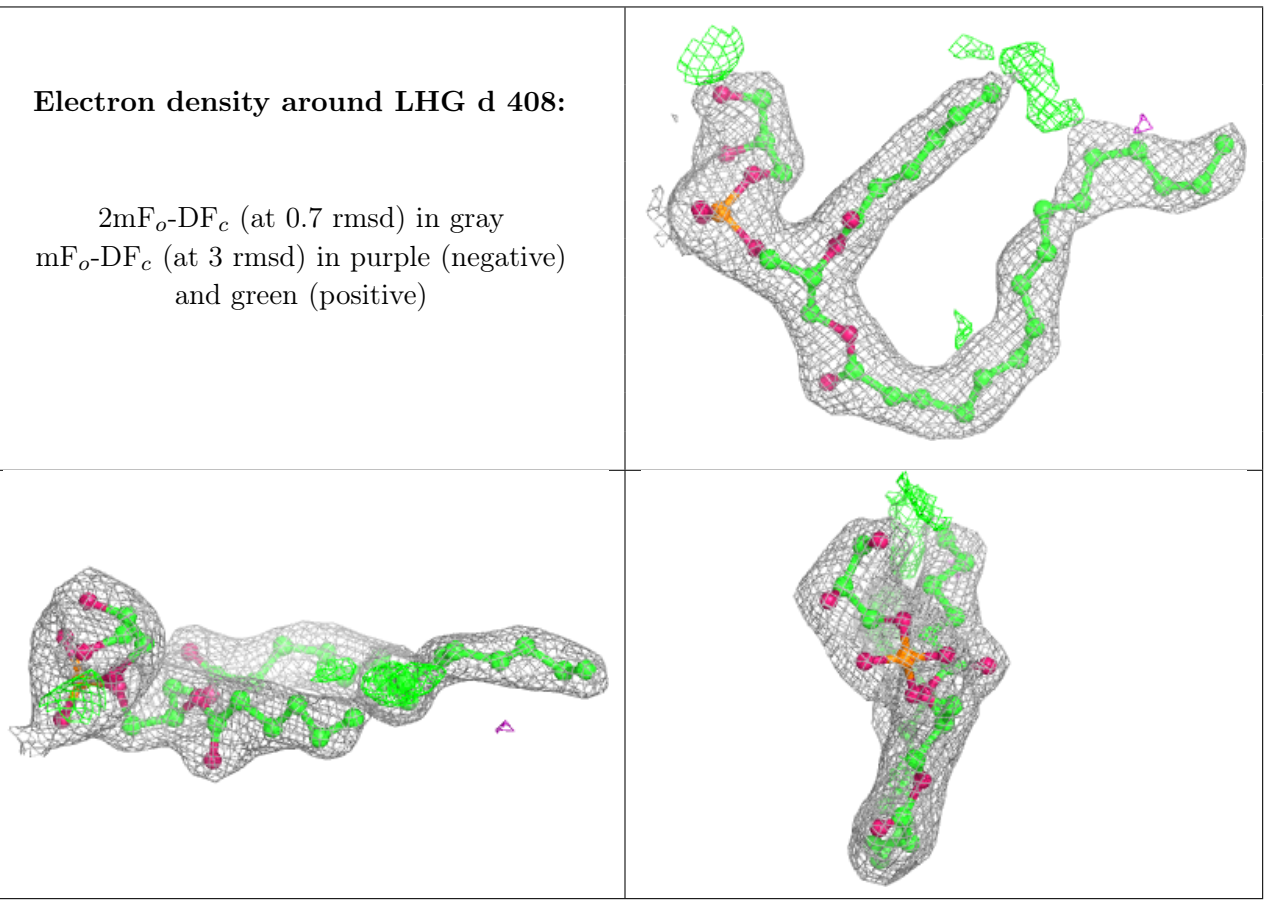
Electron density around LHG d 407:

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



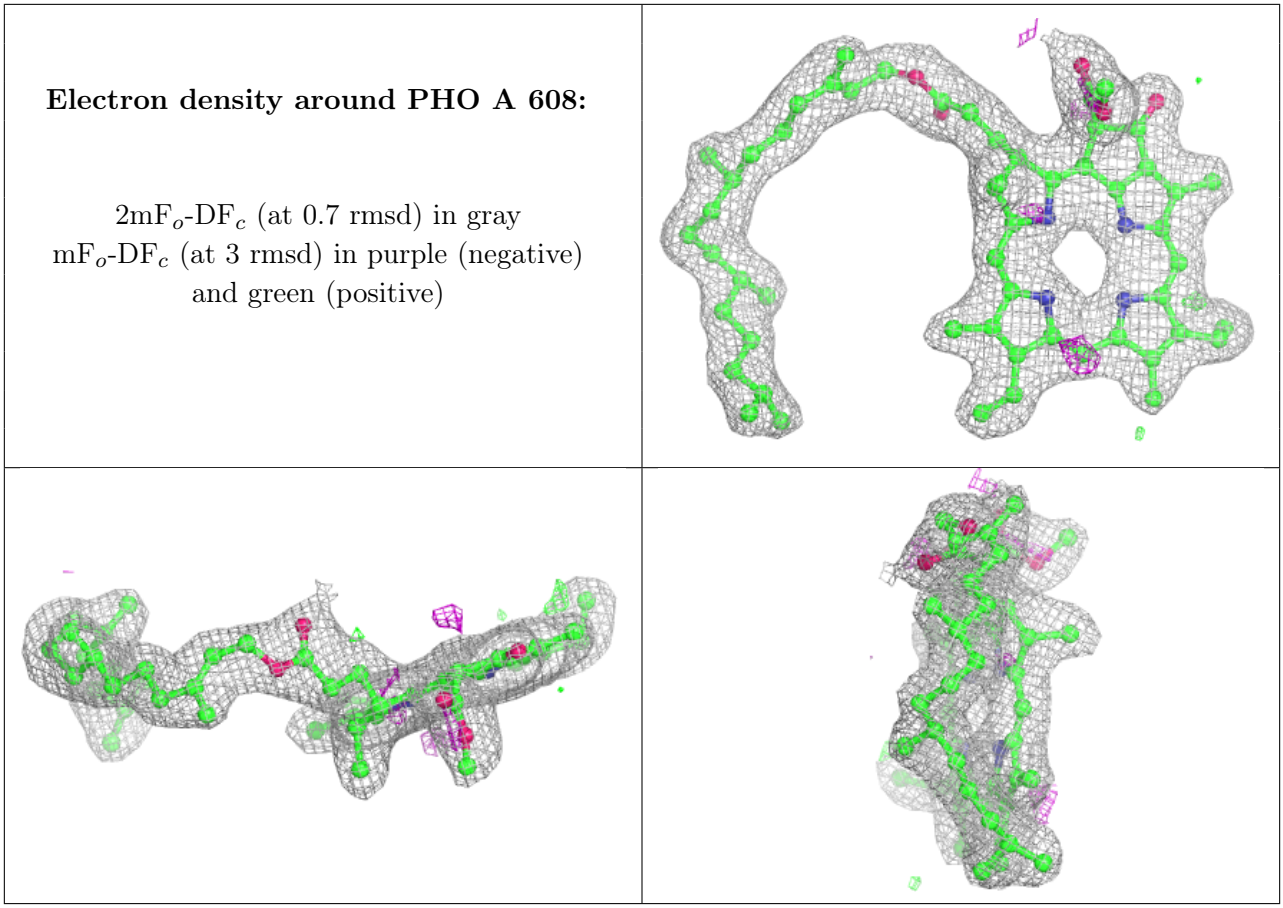
Electron density around LHG d 408:

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



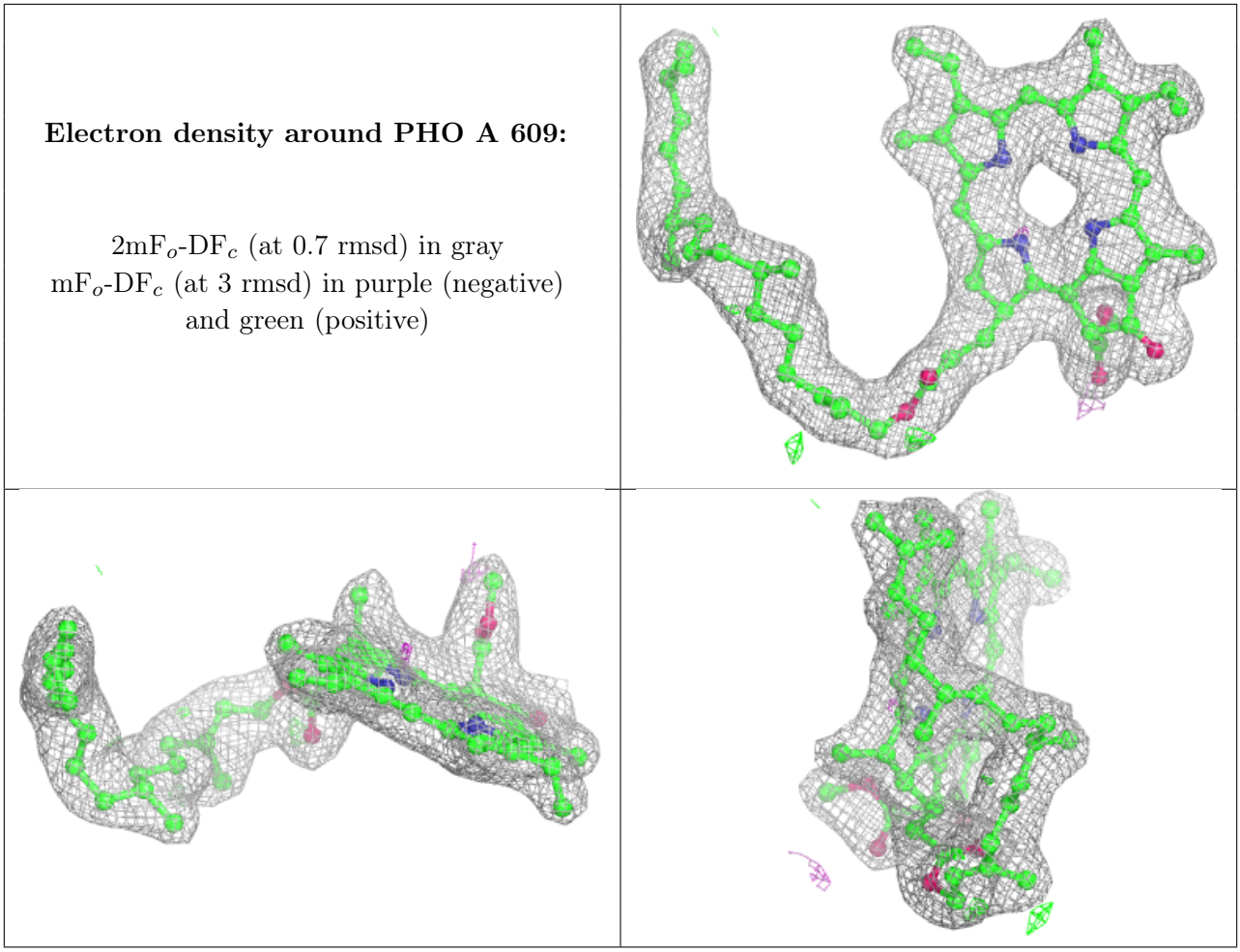
Electron density around PHO A 608:

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



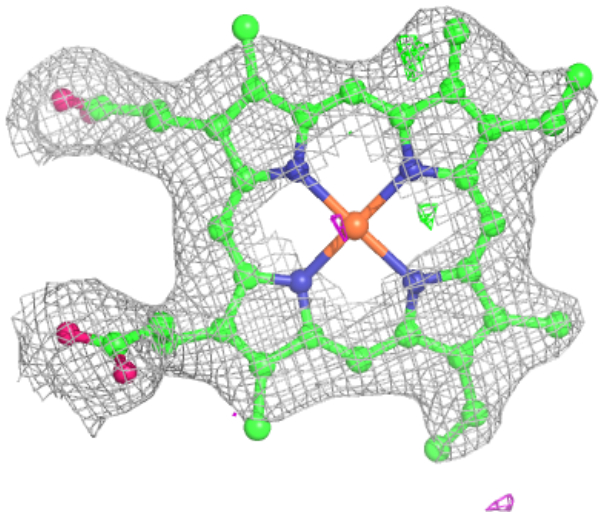
Electron density around PHO A 609:

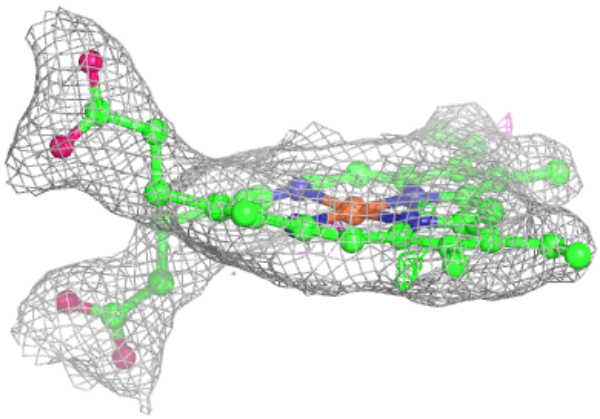
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

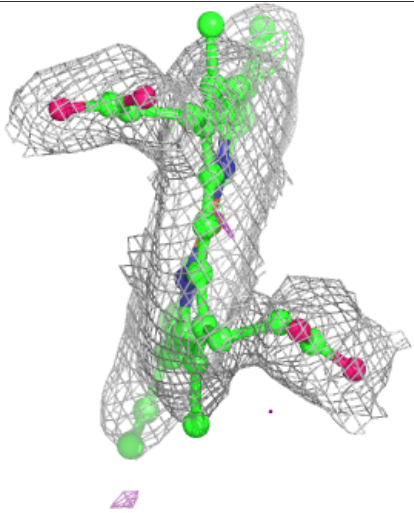


Electron density around HEM F 101:

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

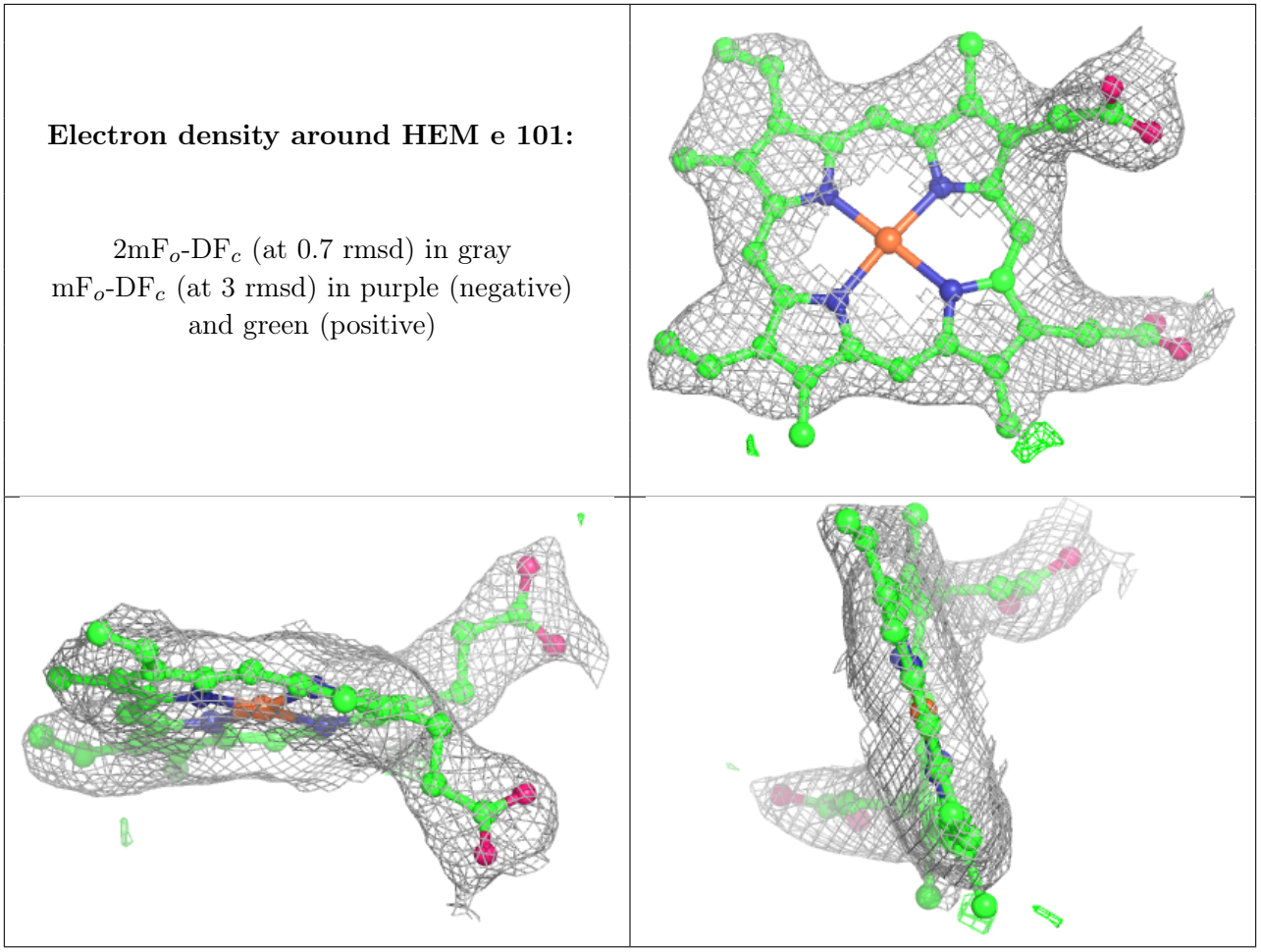






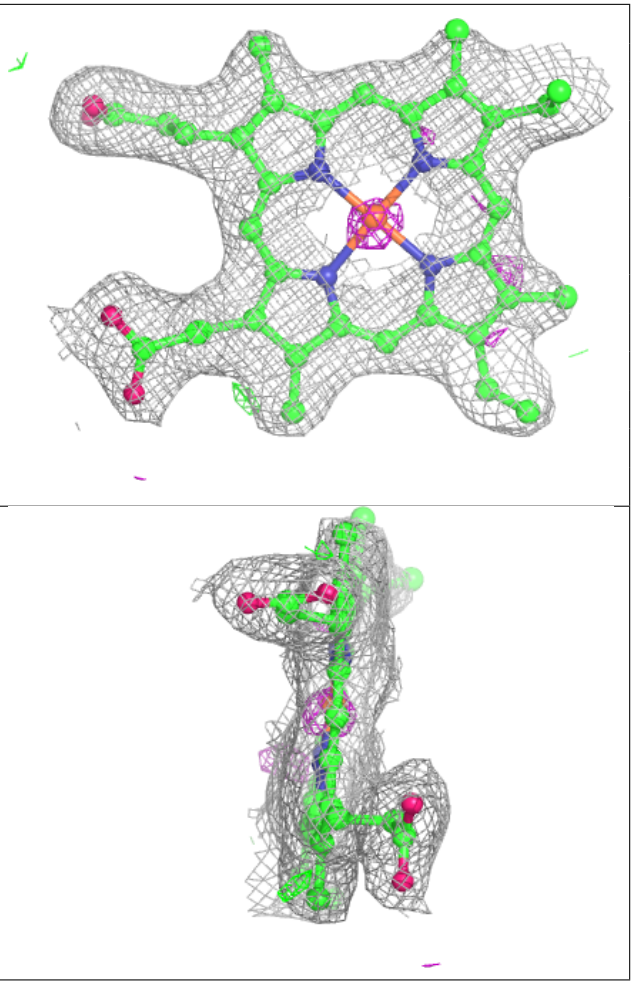
Electron density around HEM e 101:

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



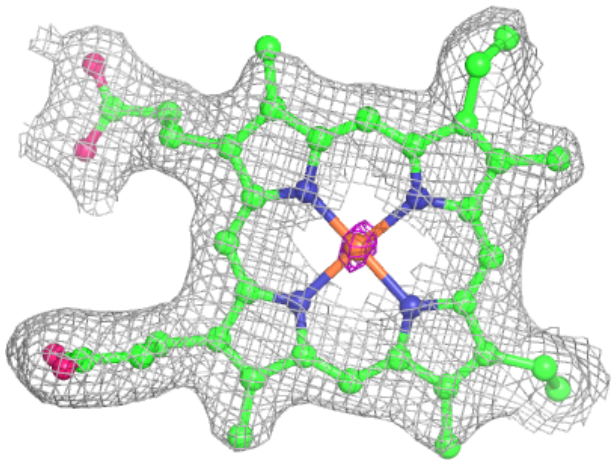
Electron density around HEC V 201:

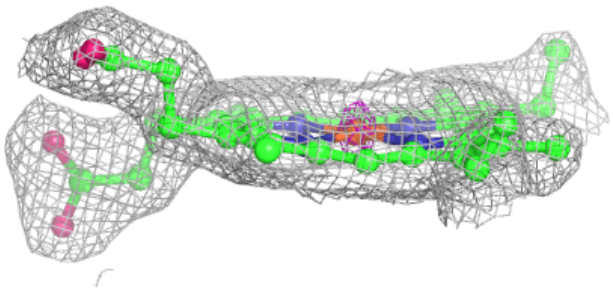
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC v 201:

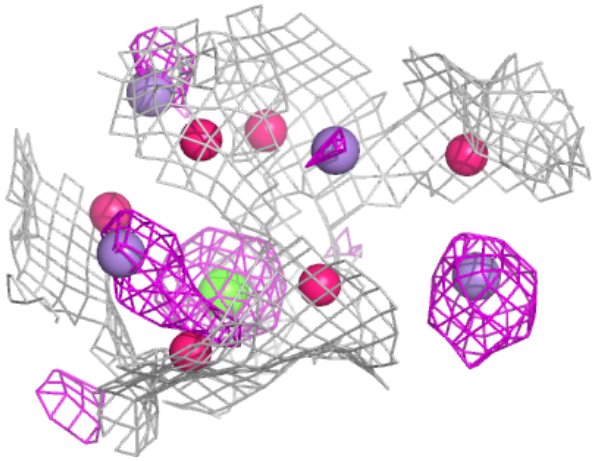
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

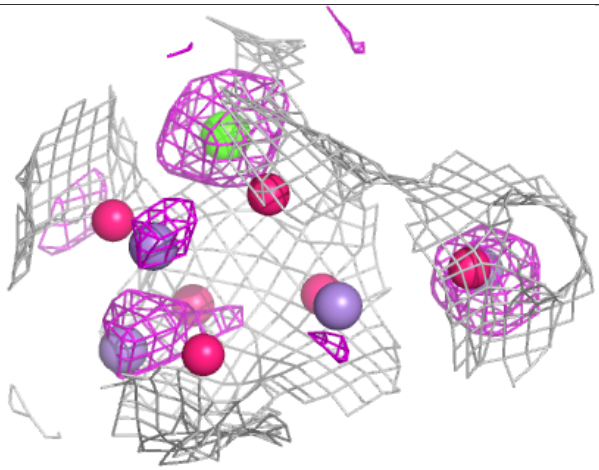


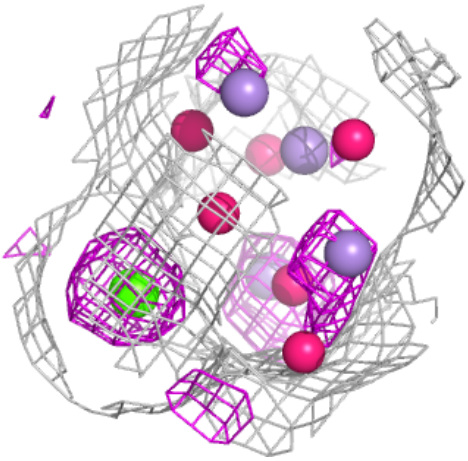


Electron density around OEY A 601 (B):

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

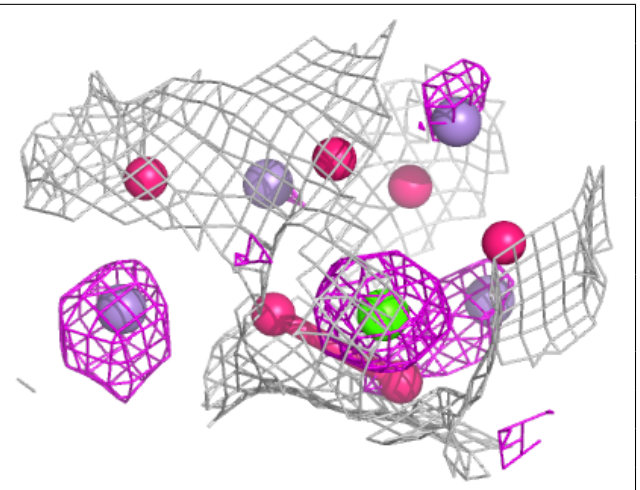


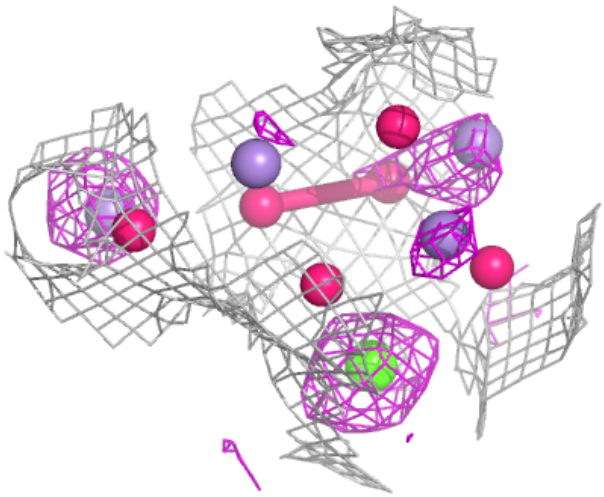


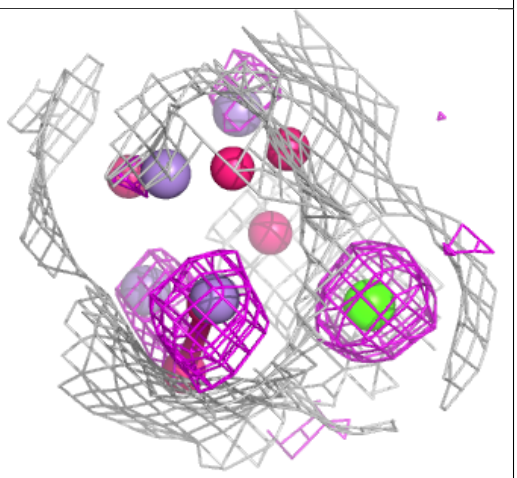


Electron density around OEY A 601 (C):

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

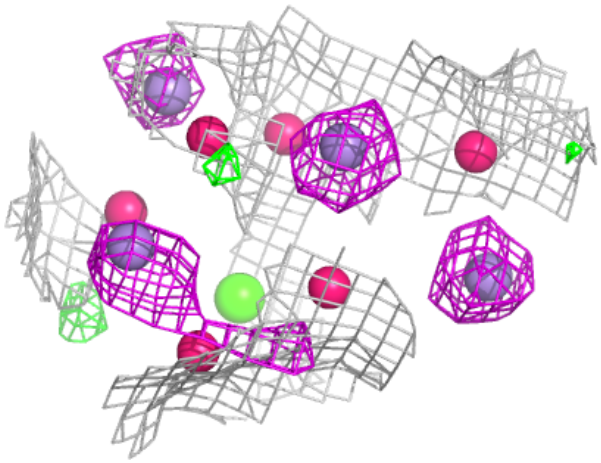


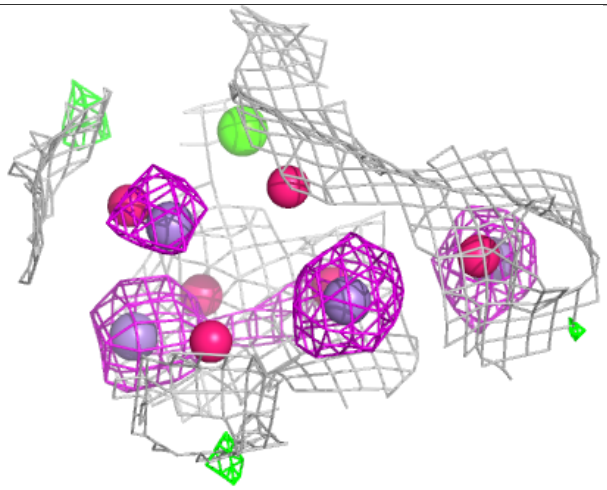


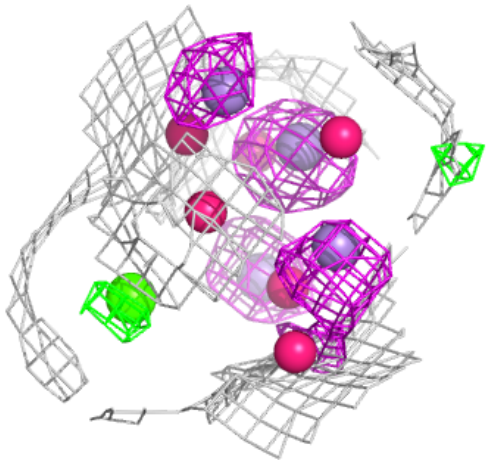


Electron density around OEY a 601 (B):

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

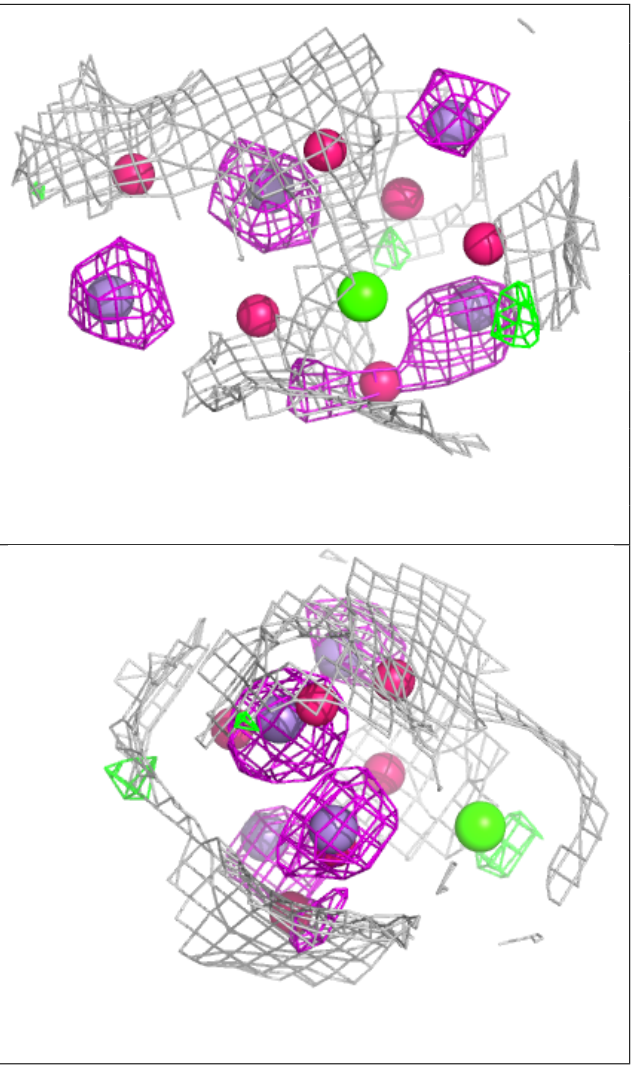


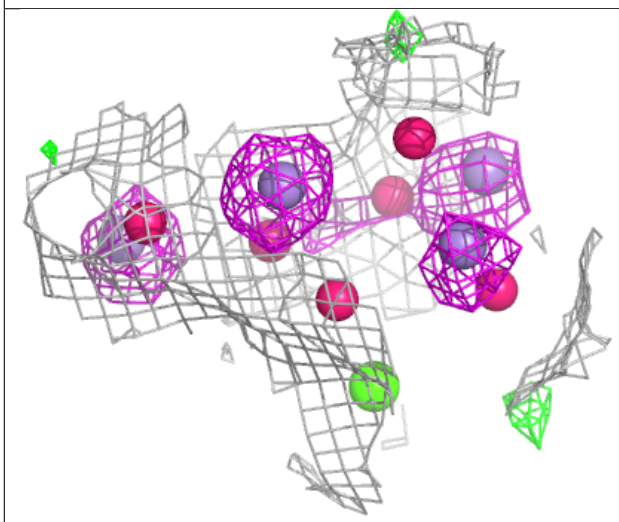




Electron density around OEY a 601 (C):

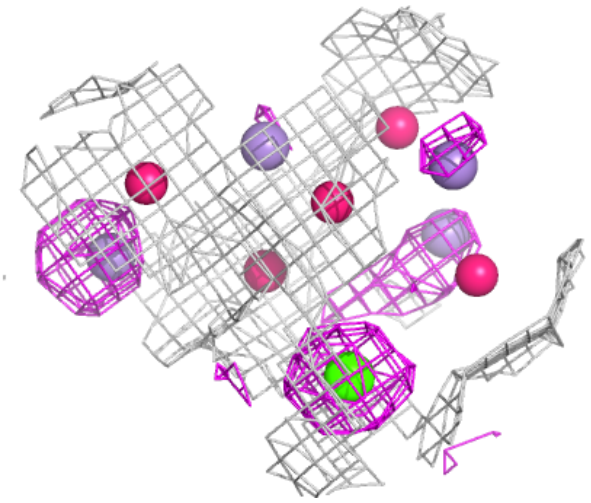
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

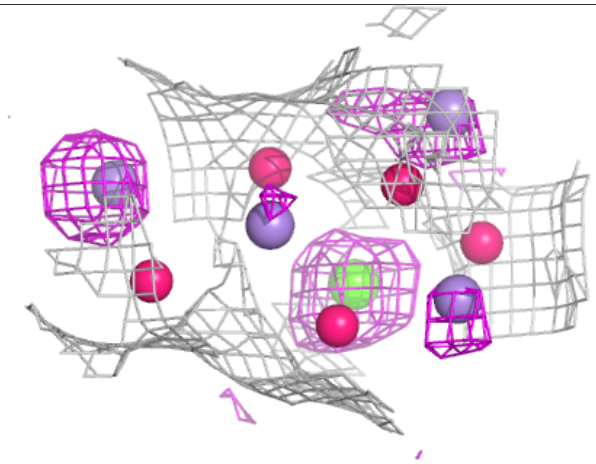


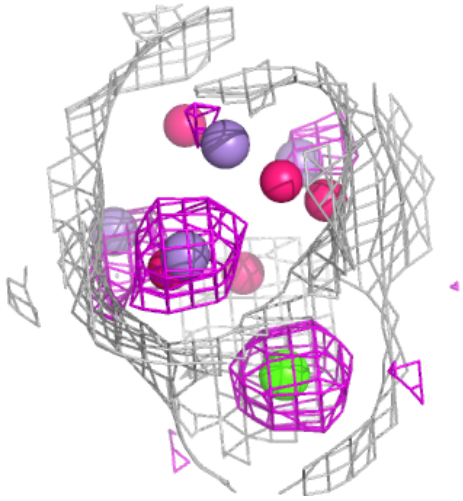


Electron density around OEX A 602 (A):

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

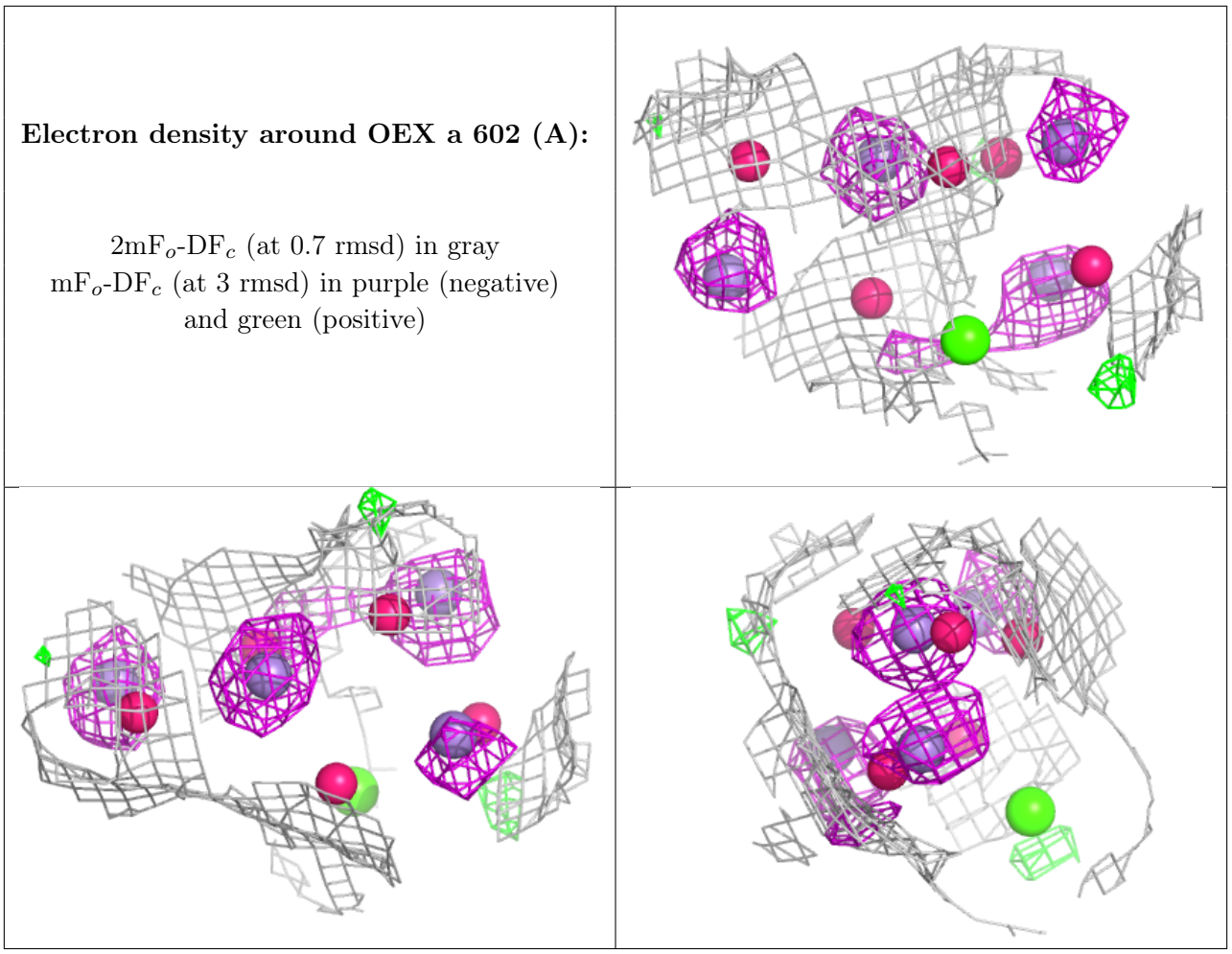






Electron density around OEX a 602 (A):

$2mF_o$-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.