Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2023 – 02:03 PM EDT

PDB ID	:	8F4I
Title	:	RT XFEL structure of Photosystem II 2000 microseconds after the third illumination at 2.00 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	:	2.00 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 ⓘ 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 ⓘ) were used in the production of this report:

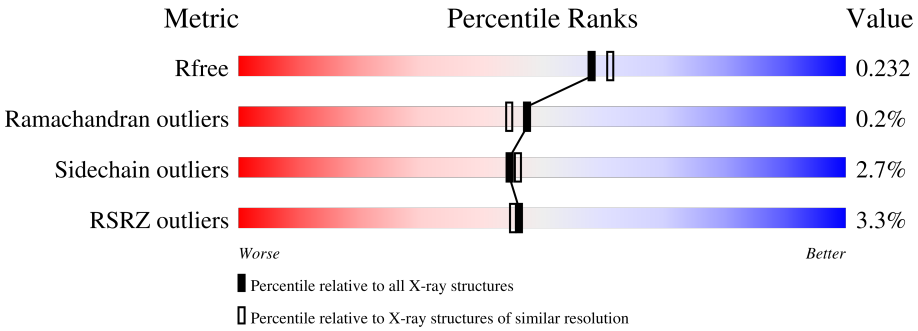
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35

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 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

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

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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

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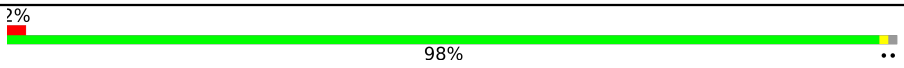
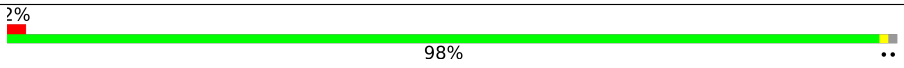
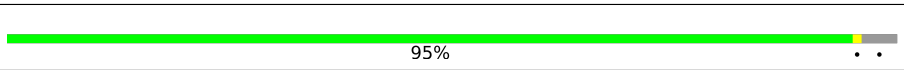
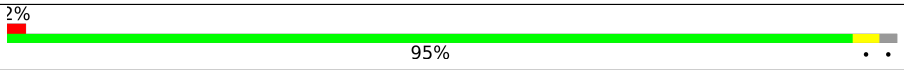
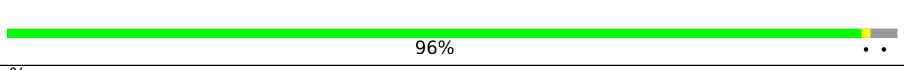
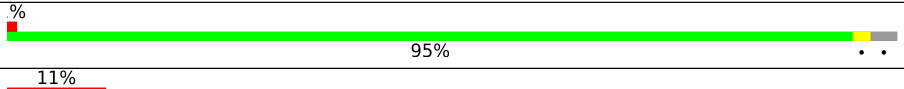
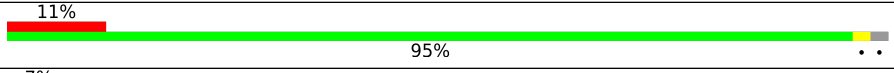
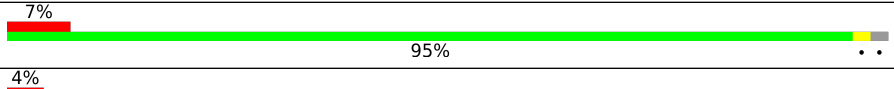
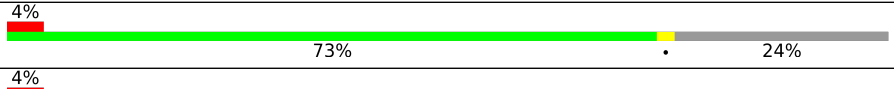
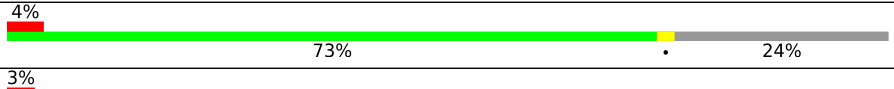
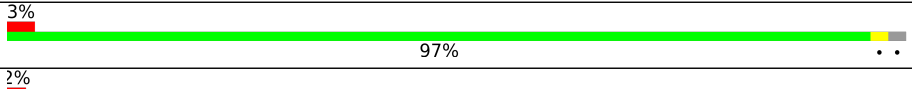
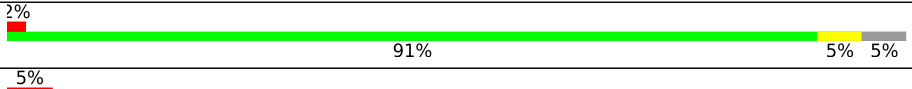
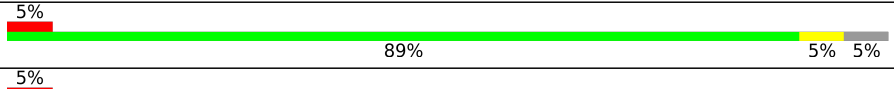
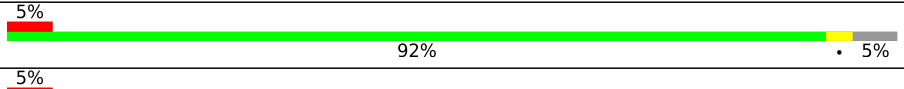
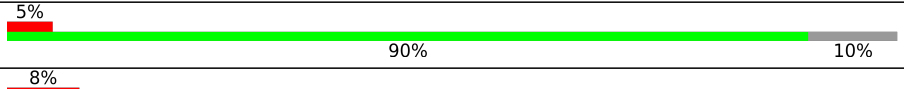
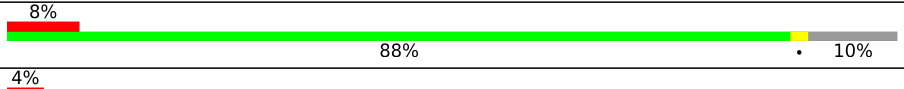
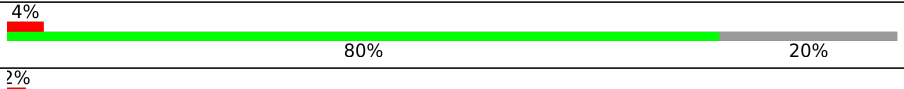
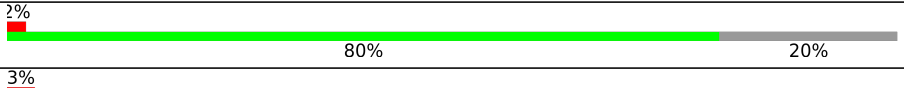
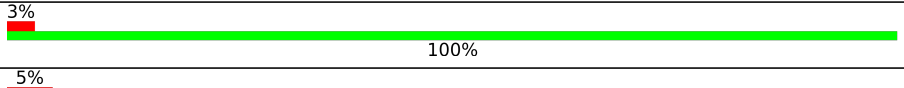
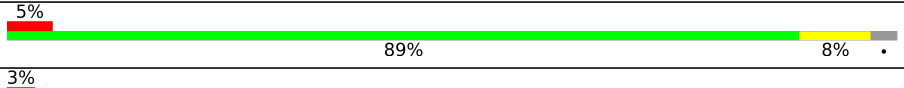
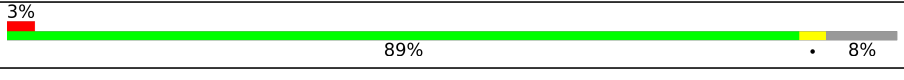
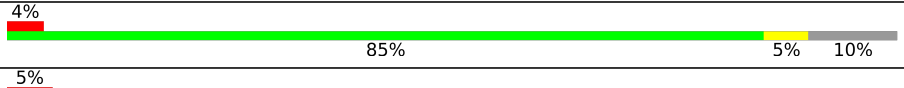
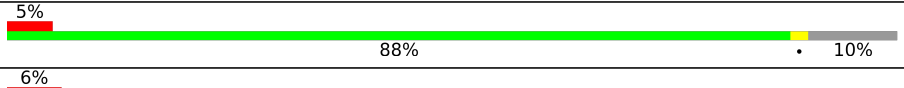
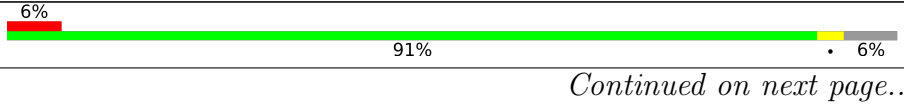
Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	t	32	9% 91% 6%
15	U	134	% 70% 28%
15	u	134	% 71% 28%
16	V	163	82% 16%
16	v	163	2% 82% 16%
17	Y	46	13% 57% 41%
17	y	46	9% 57% 9% 35%
18	X	41	7% 90% 7%
18	x	41	12% 93% 5%
19	Z	62	21% 90% 10%
19	z	62	15% 94% 6%
20	R	41	17% 71% 10% 17%
20	r	41	32% 66% 10% 24%

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	609	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	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	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	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	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	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 54640 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	k	37	Total C N O 293 204 43 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 C N O S 304 202 48 53 1	0	0	0
11	l	36	Total C N O 296 197 47 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 C N O S 256 171 37 47 1	0	0	0
12	m	32	Total C N O S 251 168 36 46 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 C N O S 1870 1168 313 385 4	0	1	0
13	o	244	Total C N O S 1874 1170 317 383 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 C N O S 258 181 36 39 2	0	0	0
14	t	30	Total C N O S 256 180 36 38 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 C N O 774 491 129 154	0	0	0
15	u	97	Total C N O 774 491 129 154	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			

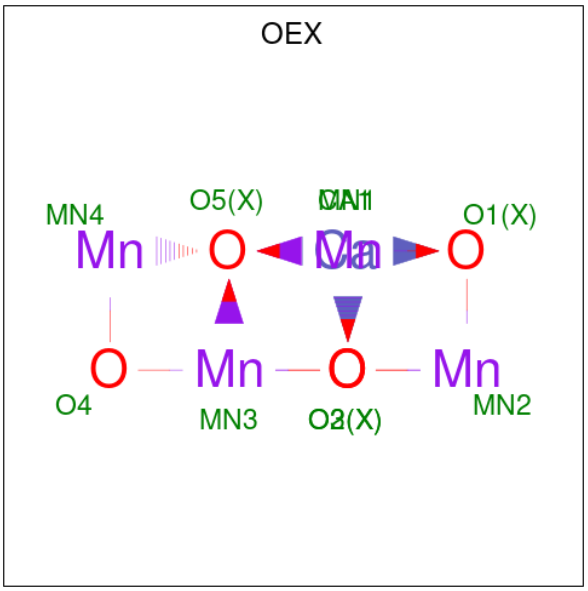
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

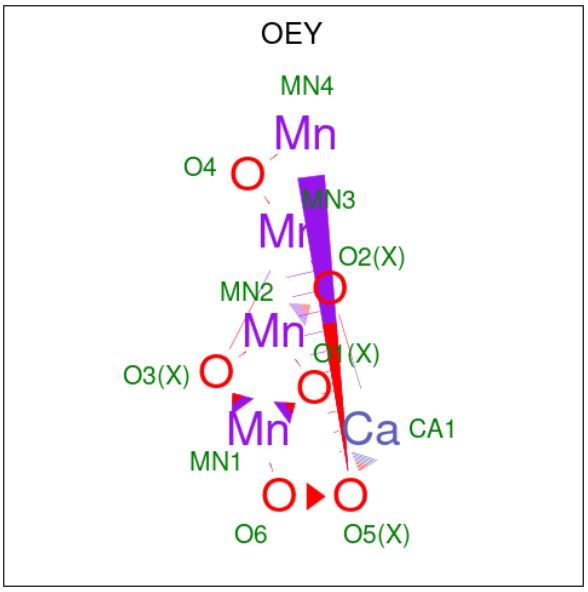
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

- Molecule 21 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 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
22	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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

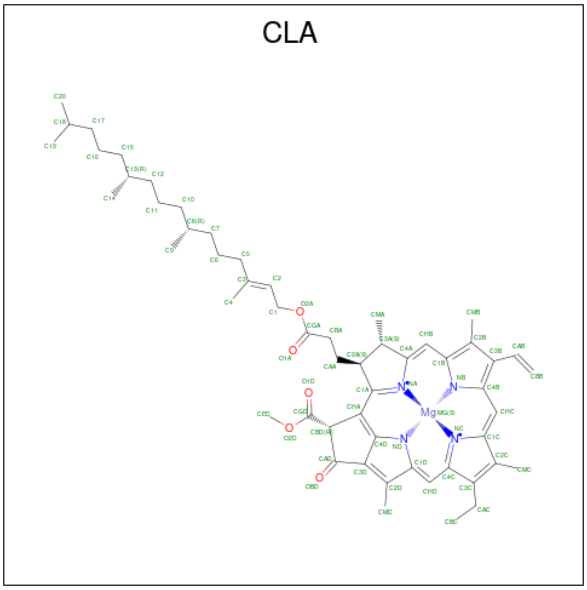
- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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		

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C Mg N O 59 49 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	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	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

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

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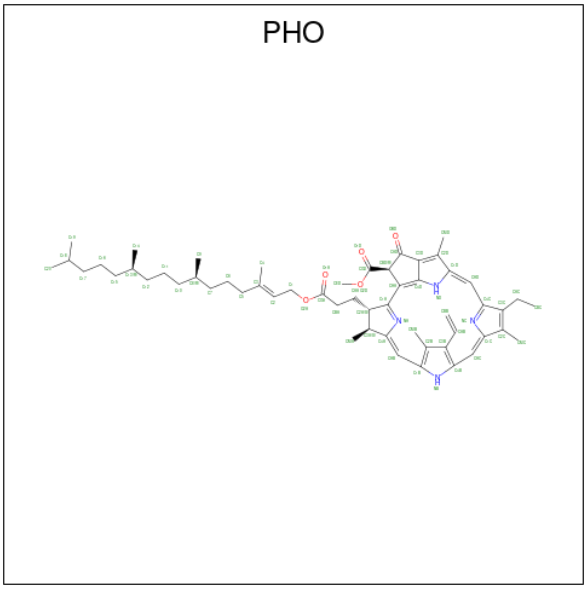
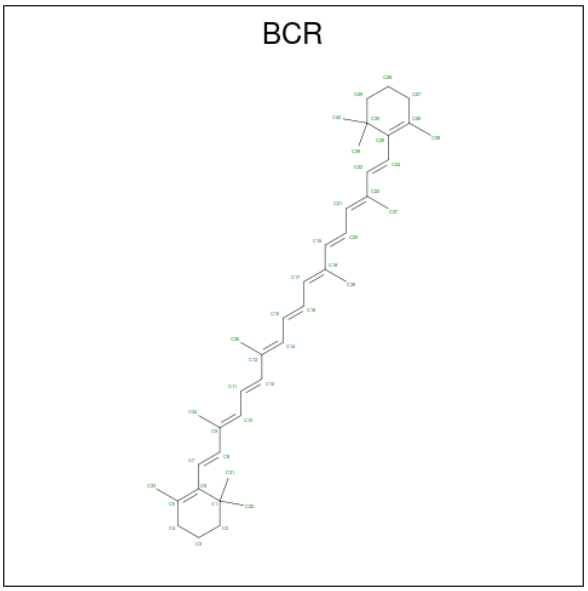
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	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	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0

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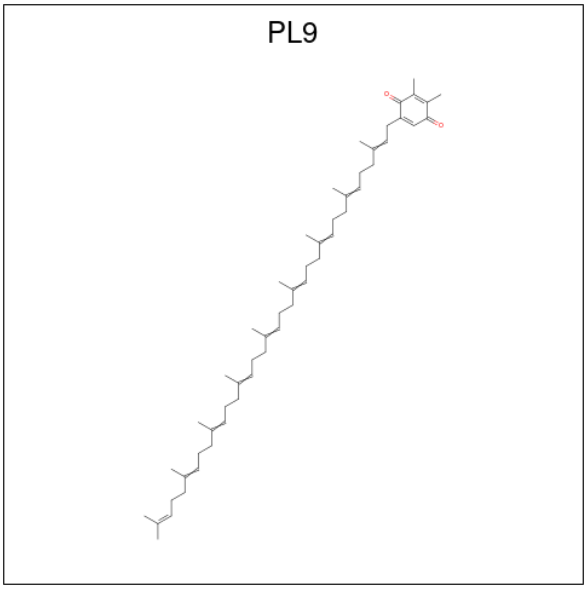
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0
27	x	1	Total C 40 40	0	0

- 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

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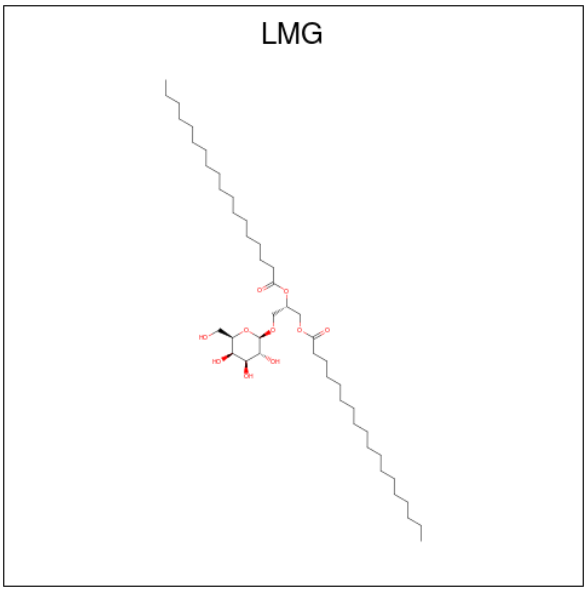
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	a	1	Total C O 55 53 2	0	0
28	d	1	Total C O 55 53 2	0	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 48 38 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	B	1	Total C O 28 24 4	0	0
29	C	1	Total C O 48 38 10	0	0
29	D	1	Total C O 51 41 10	0	0
29	D	1	Total C O 33 27 6	0	0
29	b	1	Total C O 55 45 10	0	0
29	c	1	Total C O 37 27 10	0	0
29	c	1	Total C O 48 38 10	0	0

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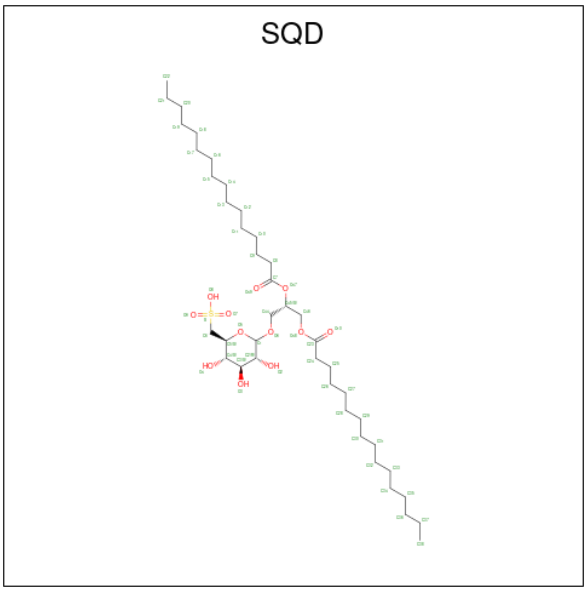
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C O 49 39 10	0	0
29	d	1	Total C O 23 21 2	0	0
29	d	1	Total C O 44 34 10	0	0
29	m	1	Total C O 51 41 10	0	0

- Molecule 30 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
30	A	1	Total C O S 52 39 12 1	0	0
30	A	1	Total C O 39 35 4	0	0
30	B	1	Total C O S 54 41 12 1	0	0
30	D	1	Total C O S 36 25 10 1	0	0
30	a	1	Total C O S 54 41 12 1	0	0
30	a	1	Total C O 36 31 5	0	0
30	b	1	Total C O S 49 36 12 1	0	0

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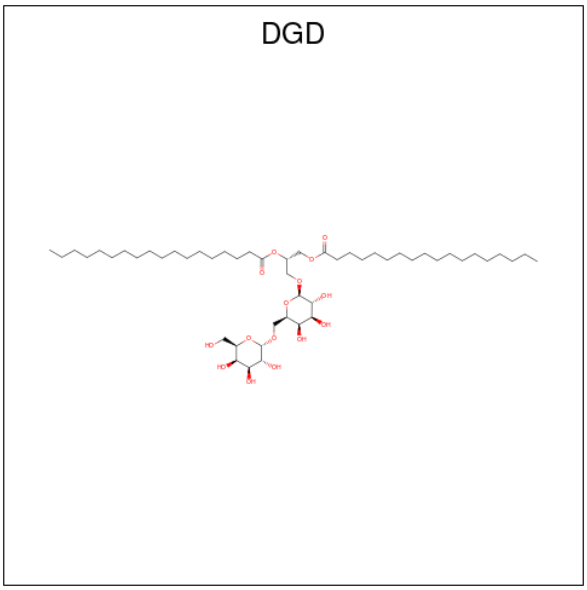
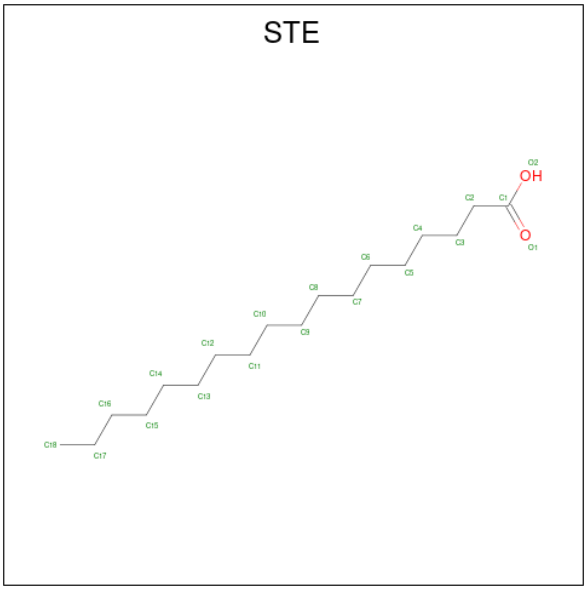
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: $C_{18}H_{36}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C O 17 15 2	0	0
32	B	1	Total C O 14 12 2	0	0
32	B	1	Total C O 12 10 2	0	0
32	B	1	Total C O 18 16 2	0	0
32	B	1	Total C O 12 10 2	0	0
32	B	1	Total C 16 16	0	0
32	C	1	Total C O 12 10 2	0	0
32	C	1	Total C O 12 10 2	0	0
32	C	1	Total C 16 16	0	0
32	E	1	Total C O 12 10 2	0	0
32	H	1	Total C 18 18	0	0
32	I	1	Total C 15 15	0	0
32	J	1	Total C O 12 10 2	0	0

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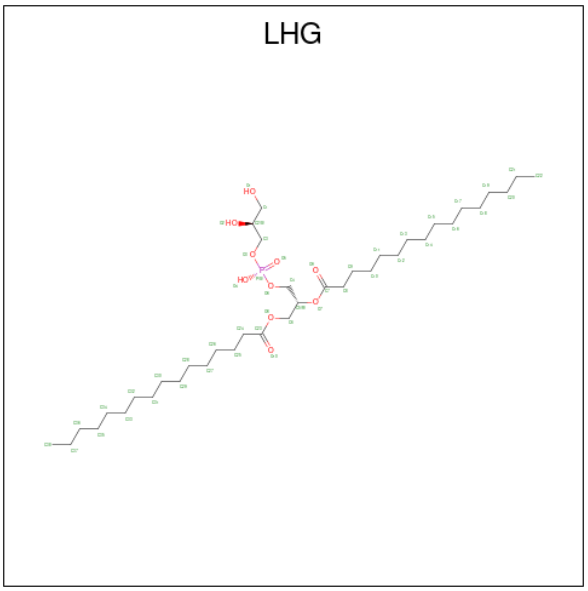
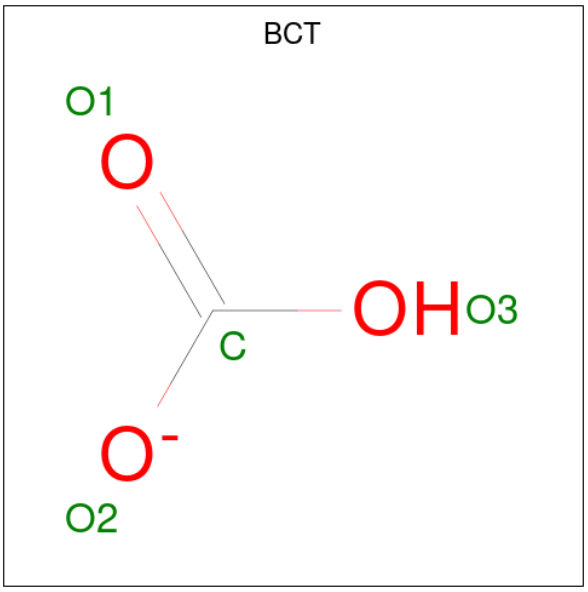
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	M	1	Total C O 15 13 2	0	0
32	M	1	Total C 10 10	0	0
32	T	1	Total C 16 16	0	0
32	T	1	Total C 15 15	0	0
32	X	1	Total C O 20 18 2	0	0
32	a	1	Total C O 12 10 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C O 16 14 2	0	0
32	b	1	Total C O 20 18 2	0	0
32	b	1	Total C 10 10	0	0
32	c	1	Total C O 20 18 2	0	0
32	c	1	Total C O 12 10 2	0	0
32	d	1	Total C O 17 15 2	0	0
32	d	1	Total C O 20 18 2	0	0
32	j	1	Total C O 12 10 2	0	0
32	l	1	Total C 18 18	0	0
32	m	1	Total C O 12 10 2	0	0
32	t	1	Total C 10 10	0	0

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



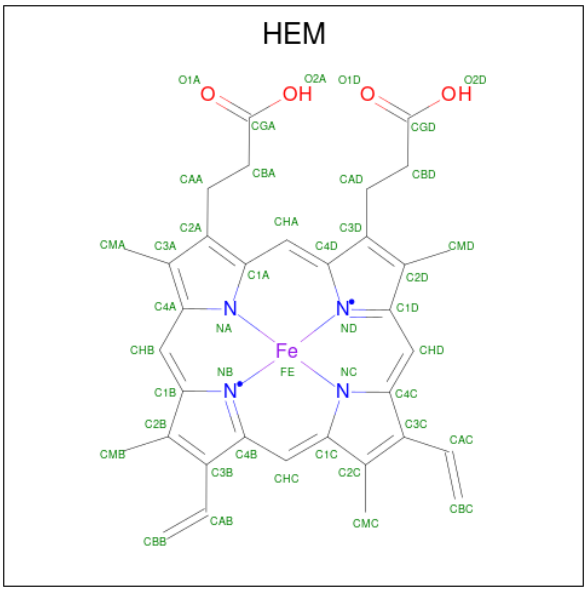
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	D	1	Total	C	O	P	0	0
			47	36	10	1		
33	D	1	Total	C	O	P	0	0
			49	38	10	1		
33	E	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			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	d	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		

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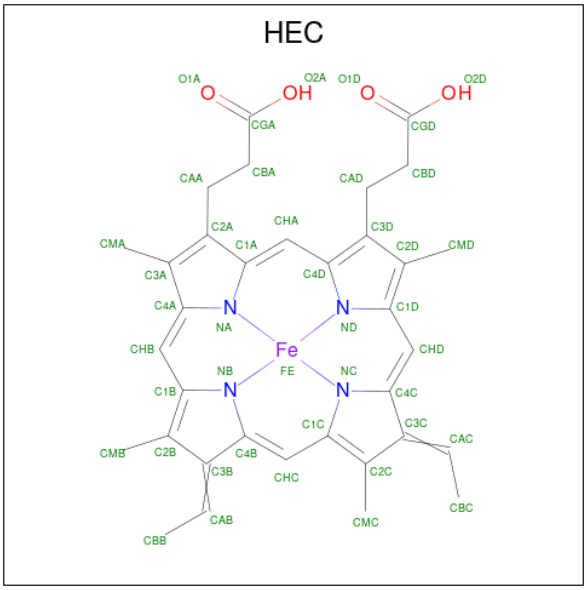
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	144	Total	O	0	4
			152	152		
37	B	218	Total	O	0	0
			218	218		
37	C	183	Total	O	0	0
			183	183		
37	D	124	Total	O	0	0
			124	124		
37	E	37	Total	O	0	0
			37	37		
37	F	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	30	Total O 30 30	0	0
37	I	8	Total O 8 8	0	0
37	J	8	Total O 8 8	0	0
37	K	6	Total O 6 6	0	0
37	L	10	Total O 10 10	0	0
37	M	6	Total O 6 6	0	0
37	O	97	Total O 97 97	0	0
37	T	15	Total O 15 15	0	0
37	U	47	Total O 47 47	0	0
37	V	67	Total O 67 67	0	0
37	Y	2	Total O 2 2	0	0
37	X	8	Total O 8 8	0	0
37	Z	9	Total O 9 9	0	0
37	R	5	Total O 5 5	0	0
37	a	133	Total O 141 141	0	4
37	b	221	Total O 221 221	0	0
37	c	182	Total O 182 182	0	0
37	d	123	Total O 123 123	0	0
37	e	24	Total O 24 24	0	0
37	f	10	Total O 10 10	0	0
37	h	19	Total O 19 19	0	0

Continued on next page...

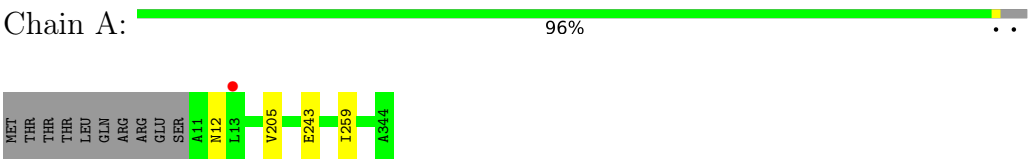
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	i	9	Total O 9 9	0	0
37	j	10	Total O 10 10	0	0
37	k	3	Total O 3 3	0	0
37	l	7	Total O 7 7	0	0
37	m	9	Total O 9 9	0	0
37	o	88	Total O 88 88	0	0
37	t	9	Total O 9 9	0	0
37	u	61	Total O 61 61	0	0
37	v	68	Total O 68 68	0	0
37	y	3	Total O 3 3	0	0
37	x	5	Total O 5 5	0	0
37	z	7	Total O 7 7	0	0

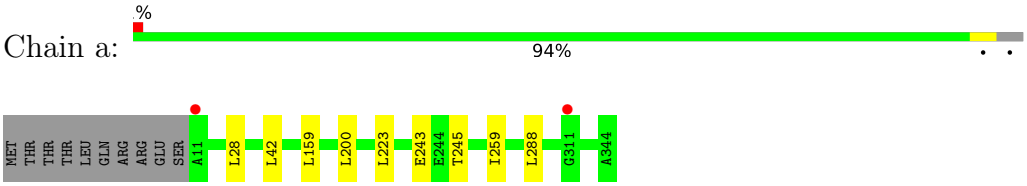
3 Residue-property plots (i)

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.

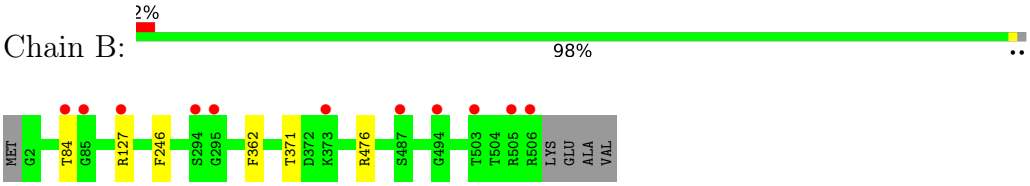
• Molecule 1: Photosystem II protein D1 1



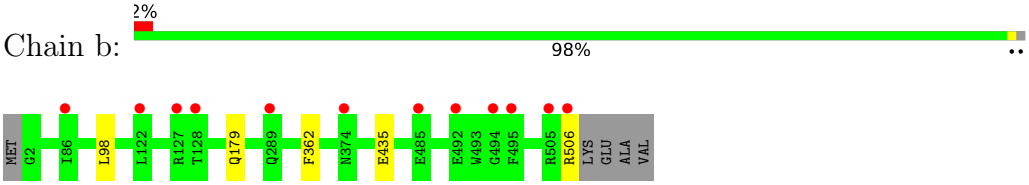
• Molecule 1: Photosystem II protein D1 1



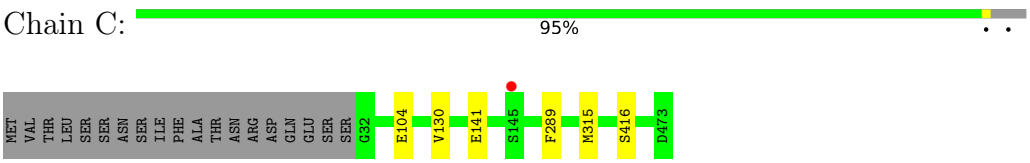
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

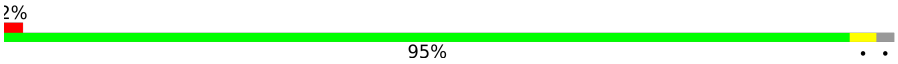


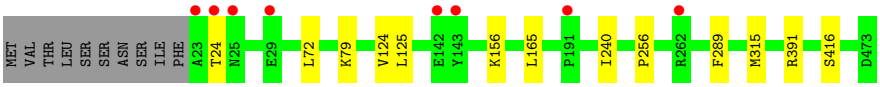
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

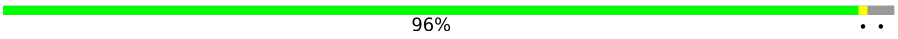
Chain c:

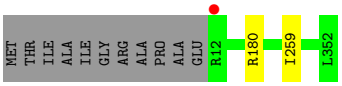




• Molecule 4: Photosystem II D2 protein

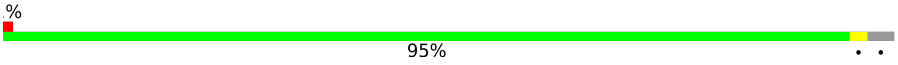
Chain D:

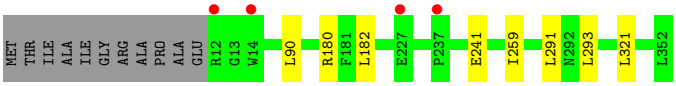




• Molecule 4: Photosystem II D2 protein

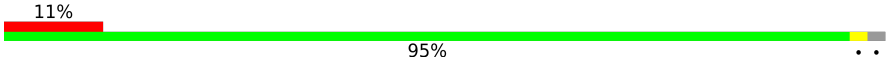
Chain d:





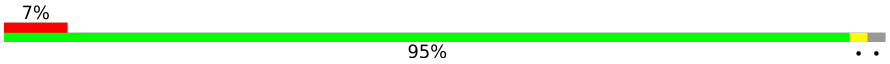
• Molecule 5: Cytochrome b559 subunit alpha

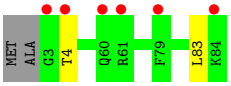
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

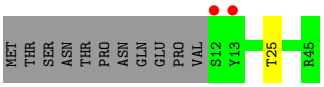
Chain e:





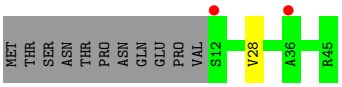
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



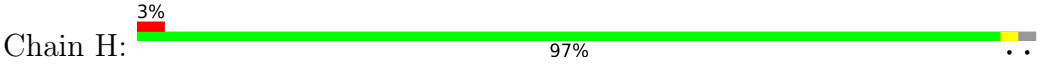
• Molecule 6: Cytochrome b559 subunit beta

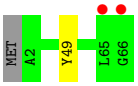
Chain f:



• Molecule 7: Photosystem II reaction center protein H

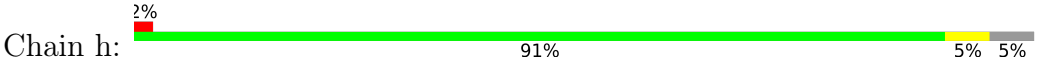
Chain H:

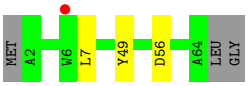




• Molecule 7: Photosystem II reaction center protein H

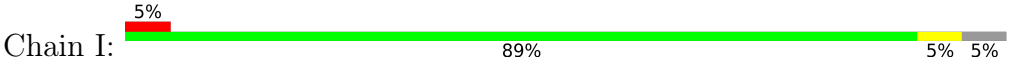
Chain h:

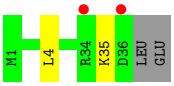




• Molecule 8: Photosystem II reaction center protein I

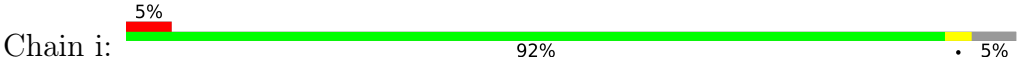
Chain I:

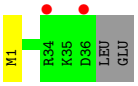




• Molecule 8: Photosystem II reaction center protein I

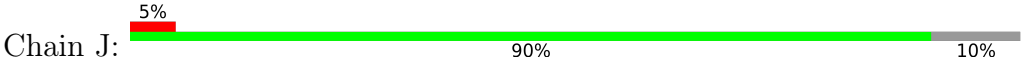
Chain i:

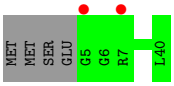




• Molecule 9: Photosystem II reaction center protein J

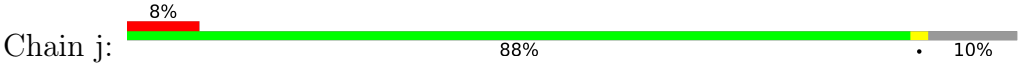
Chain J:

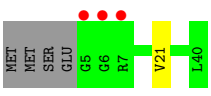




• Molecule 9: Photosystem II reaction center protein J

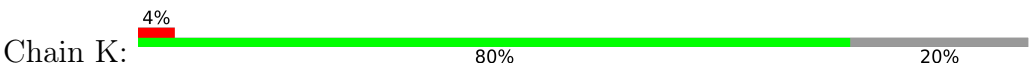
Chain j:

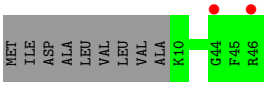




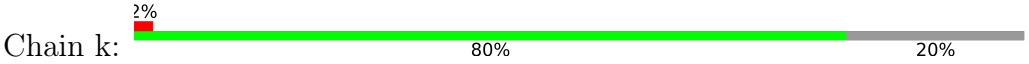
• Molecule 10: Photosystem II reaction center protein K

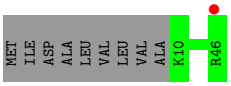
Chain K:





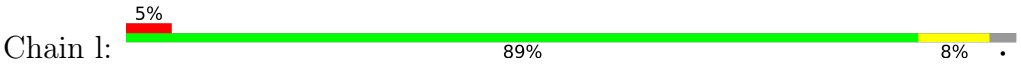
• Molecule 10: Photosystem II reaction center protein K



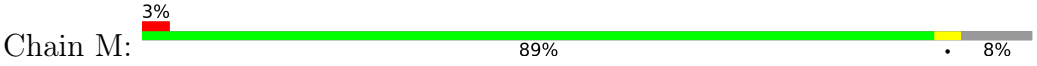


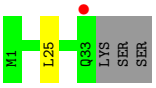
• Molecule 11: Photosystem II reaction center protein L

• Molecule 11: Photosystem II reaction center protein L

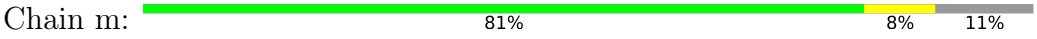


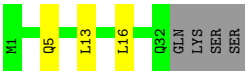
• Molecule 12: Photosystem II reaction center protein M



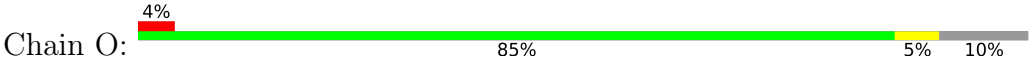


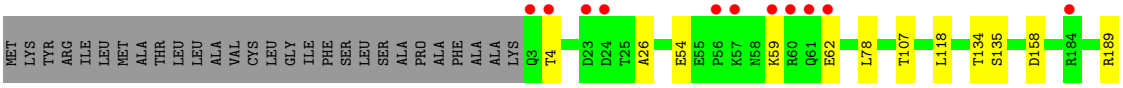
• Molecule 12: Photosystem II reaction center protein M



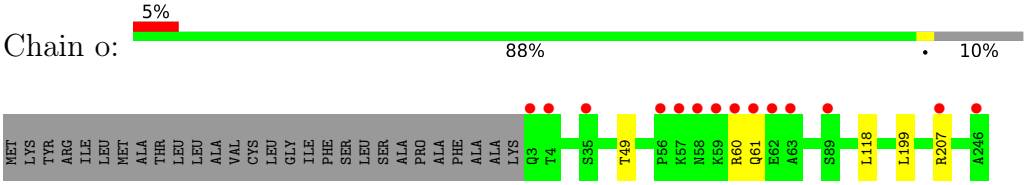


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

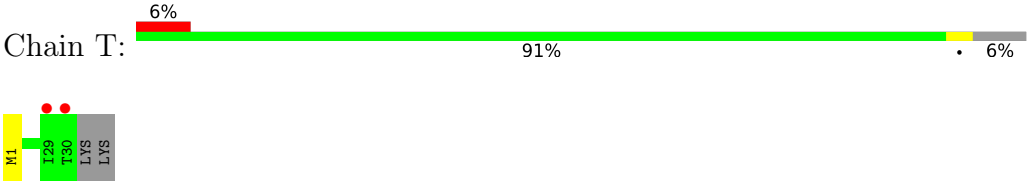




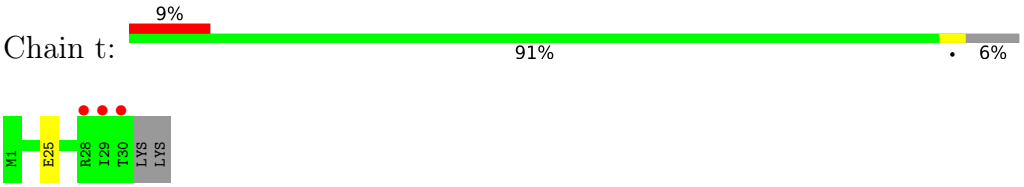
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



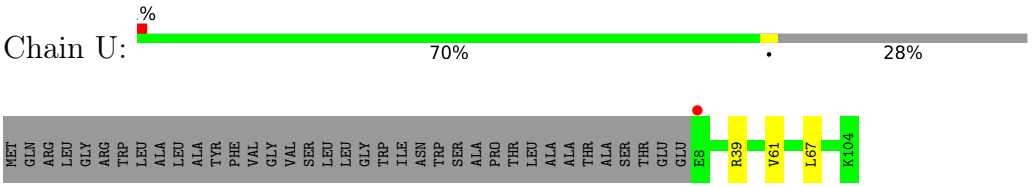
• Molecule 14: Photosystem II reaction center protein T



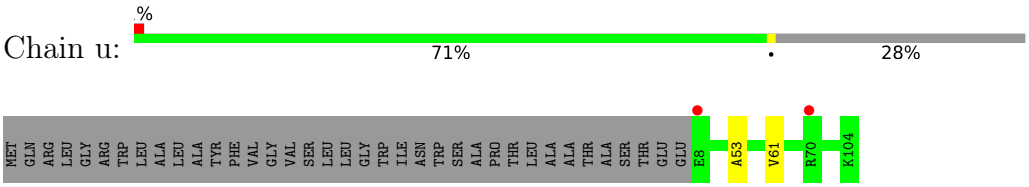
• Molecule 14: Photosystem II reaction center protein T



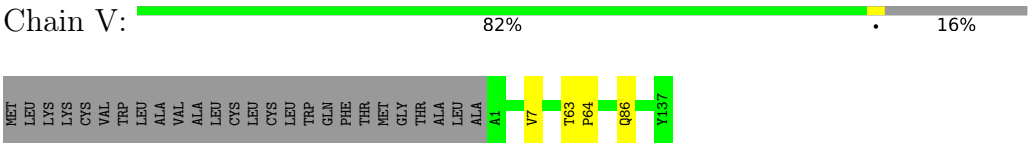
• Molecule 15: Photosystem II 12 kDa extrinsic protein



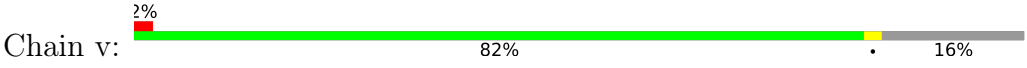
• Molecule 15: Photosystem II 12 kDa extrinsic protein

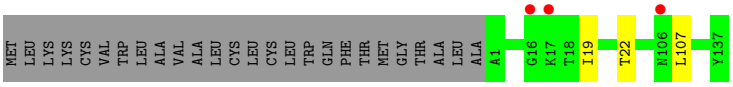


• Molecule 16: Cytochrome c-550

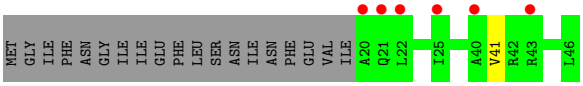


• Molecule 16: Cytochrome c-550

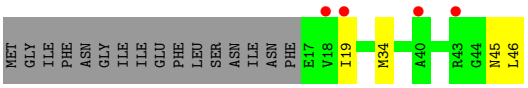




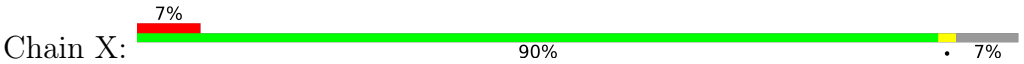
• Molecule 17: Photosystem II reaction center protein Ycf12

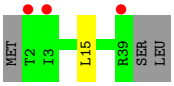


• Molecule 17: Photosystem II reaction center protein Ycf12

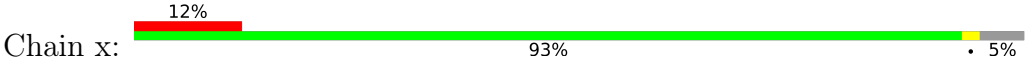


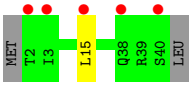
• Molecule 18: Photosystem II reaction center X protein



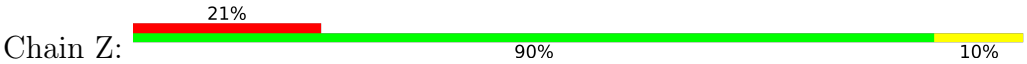


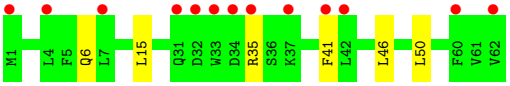
• Molecule 18: Photosystem II reaction center X protein



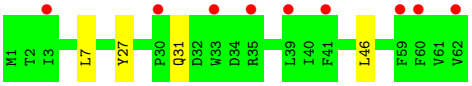


• Molecule 19: Photosystem II reaction center protein Z



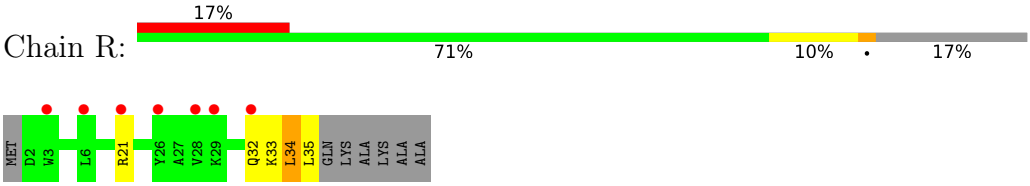


• Molecule 19: Photosystem II reaction center protein Z



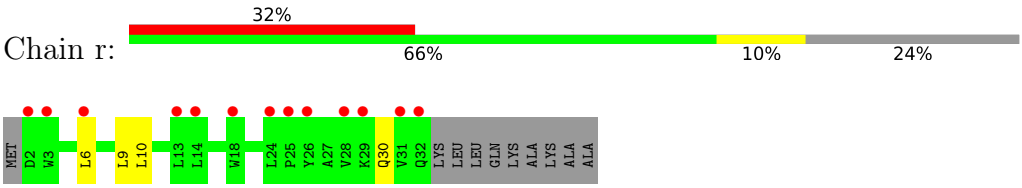
• Molecule 20: Photosystem II protein Y

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	117.31Å 222.59Å 308.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.72 – 2.00 19.72 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.72-2.00) 87.8 (19.72-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.47 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.232 0.186 , 0.232	Depositor DCC
R_{free} test set	4797 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	54640	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: SQD, LHG, CL, DGD, PL9, BCR, FE2, OEX, STE, OEY, PHO, LMG, CLA, HEC, HEM, FME, BCT

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	0.42	0/3717	0.57	0/5060
1	a	0.39	0/3714	0.56	0/5056
2	B	0.40	0/4155	0.57	0/5661
2	b	0.40	0/4118	0.57	0/5611
3	C	0.39	0/3711	0.55	0/5051
3	c	0.38	0/3791	0.55	0/5158
4	D	0.42	0/2838	0.58	0/3862
4	d	0.41	0/2847	0.57	0/3874
5	E	0.35	0/688	0.53	0/940
5	e	0.32	0/683	0.53	0/932
6	F	0.37	0/284	0.49	0/387
6	f	0.31	0/284	0.53	0/387
7	H	0.39	0/523	0.54	0/713
7	h	0.38	0/511	0.56	0/697
8	I	0.41	0/293	0.60	0/396
8	i	0.40	0/293	0.54	0/396
9	J	0.36	0/263	0.56	0/356
9	j	0.32	0/263	0.53	0/356
10	K	0.34	0/303	0.49	0/416
10	k	0.33	0/303	0.52	0/416
11	L	0.38	0/311	0.56	0/422
11	l	0.42	0/303	0.61	0/412
12	M	0.34	0/249	0.51	0/341
12	m	0.42	0/244	0.52	0/334
13	O	0.37	0/1904	0.63	1/2585 (0.0%)
13	o	0.38	0/1905	0.62	0/2583
14	T	0.45	0/257	0.59	0/349
14	t	0.40	0/255	0.52	0/346
15	U	0.36	0/785	0.56	0/1064
15	u	0.35	0/785	0.58	0/1064
16	V	0.36	0/1085	0.56	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.34	0/1085	0.55	0/1473
17	Y	0.30	0/197	0.52	0/264
17	y	0.28	0/219	0.50	0/294
18	X	0.32	0/284	0.48	0/384
18	x	0.30	0/289	0.43	0/391
19	Z	0.31	0/490	0.47	0/669
19	z	0.28	0/488	0.42	0/666
20	R	0.31	0/277	0.60	1/380 (0.3%)
20	r	0.30	0/252	0.49	0/347
All	All	0.38	0/45246	0.56	2/61566 (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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	R	34	LEU	CA-CB-CG	6.33	129.85	115.30
13	O	158	ASP	CB-CG-OD1	5.40	123.16	118.30

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%)	455 (99%)	2 (0%)	1 (0%)	47	44
1	a	458/344 (133%)	452 (99%)	5 (1%)	1 (0%)	47	44
2	B	507/510 (99%)	500 (99%)	7 (1%)	0	100	100
2	b	503/510 (99%)	492 (98%)	11 (2%)	0	100	100
3	C	461/461 (100%)	453 (98%)	7 (2%)	1 (0%)	47	44
3	c	471/461 (102%)	462 (98%)	8 (2%)	1 (0%)	47	44
4	D	341/352 (97%)	329 (96%)	12 (4%)	0	100	100
4	d	342/352 (97%)	332 (97%)	10 (3%)	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%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	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%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	232 (96%)	7 (3%)	4 (2%)	9	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	242/272 (89%)	230 (95%)	11 (4%)	1 (0%)	34 30
14	T	28/32 (88%)	28 (100%)	0	0	100 100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100 100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100 100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	14 8
16	V	135/163 (83%)	131 (97%)	3 (2%)	1 (1%)	22 16
16	v	135/163 (83%)	129 (96%)	6 (4%)	0	100 100
17	Y	25/46 (54%)	25 (100%)	0	0	100 100
17	y	28/46 (61%)	27 (96%)	1 (4%)	0	100 100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100 100
18	x	37/41 (90%)	37 (100%)	0	0	100 100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100 100
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100 100
20	R	32/41 (78%)	30 (94%)	2 (6%)	0	100 100
20	r	29/41 (71%)	28 (97%)	0	1 (3%)	3 1
All	All	5534/5700 (97%)	5398 (98%)	124 (2%)	12 (0%)	47 44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	V	64	PRO
3	C	416	SER
3	c	416	SER
15	u	53	ALA
13	O	59	LYS
13	O	62	GLU
13	O	134	THR
13	O	26	ALA
13	o	61	GLN
20	r	30	GLN
1	A	259	ILE
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%)	371 (99%)	3 (1%)	81	86
1	a	373/280 (133%)	363 (97%)	10 (3%)	44	46
2	B	407/407 (100%)	401 (98%)	6 (2%)	65	69
2	b	402/407 (99%)	397 (99%)	5 (1%)	71	76
3	C	361/362 (100%)	356 (99%)	5 (1%)	67	72
3	c	370/362 (102%)	357 (96%)	13 (4%)	36	35
4	D	278/283 (98%)	276 (99%)	2 (1%)	84	88
4	d	279/283 (99%)	271 (97%)	8 (3%)	42	43
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	27
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	44
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	34
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	34
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	50 (94%)	3 (6%)	20	16
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	13
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	27
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	34
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	3
13	O	206/228 (90%)	198 (96%)	8 (4%)	32	30
13	o	207/228 (91%)	202 (98%)	5 (2%)	49	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	T	26/28 (93%)	26 (100%)	0	100 100
14	t	25/28 (89%)	24 (96%)	1 (4%)	31 29
15	U	84/112 (75%)	81 (96%)	3 (4%)	35 34
15	u	84/112 (75%)	83 (99%)	1 (1%)	71 76
16	V	117/138 (85%)	115 (98%)	2 (2%)	60 65
16	v	117/138 (85%)	114 (97%)	3 (3%)	46 48
17	Y	19/37 (51%)	18 (95%)	1 (5%)	22 18
17	y	22/37 (60%)	18 (82%)	4 (18%)	1 1
18	X	31/34 (91%)	30 (97%)	1 (3%)	39 38
18	x	31/34 (91%)	30 (97%)	1 (3%)	39 38
19	Z	52/52 (100%)	46 (88%)	6 (12%)	5 3
19	z	51/52 (98%)	47 (92%)	4 (8%)	12 8
20	R	28/33 (85%)	23 (82%)	5 (18%)	2 1
20	r	25/33 (76%)	22 (88%)	3 (12%)	5 2
All	All	4572/4654 (98%)	4451 (97%)	121 (3%)	44 48

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	205	VAL
1	A	243	GLU
2	B	84	THR
2	B	127	ARG
2	B	246	PHE
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
4	D	259	ILE
5	E	4	THR
5	E	22[A]	ILE

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Mol	Chain	Res	Type
5	E	22[B]	ILE
6	F	25	THR
7	H	49	TYR
8	I	4	LEU
8	I	35	LYS
12	M	25	LEU
13	O	4	THR
13	O	54	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	189	ARG
13	O	214	THR
15	U	39	ARG
15	U	61	VAL
15	U	67	LEU
16	V	7	VAL
16	V	86	GLN
17	Y	41	VAL
18	X	15	LEU
19	Z	6	GLN
19	Z	15	LEU
19	Z	35	ARG
19	Z	41	PHE
19	Z	46	LEU
19	Z	50	LEU
20	R	21	ARG
20	R	32	GLN
20	R	33	LYS
20	R	34	LEU
20	R	35	LEU
1	a	28	LEU
1	a	42	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	243	GLU
1	a	245	THR
1	a	288	LEU

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Mol	Chain	Res	Type
2	b	98	LEU
2	b	179	GLN
2	b	362	PHE
2	b	435	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	79	LYS
3	c	124	VAL
3	c	125	LEU
3	c	156	LYS
3	c	165	LEU
3	c	240	ILE
3	c	256	PRO
3	c	289	PHE
3	c	315	MET
3	c	391[A]	ARG
3	c	391[B]	ARG
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	4	THR
5	e	83	LEU
6	f	28	VAL
7	h	7	LEU
7	h	49	TYR
7	h	56	ASP
9	j	21	VAL
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	5	GLN
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	60	ARG
13	o	118	LEU

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Mol	Chain	Res	Type
13	o	199	LEU
13	o	207	ARG
14	t	25	GLU
15	u	61	VAL
16	v	19	ILE
16	v	22	THR
16	v	107	LEU
17	y	19	ILE
17	y	34	MET
17	y	45	ASN
17	y	46	LEU
18	x	15	LEU
19	z	7	LEU
19	z	27	TYR
19	z	31	GLN
19	z	46	LEU
20	r	6	LEU
20	r	9	LEU
20	r	10	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	325	ASN
3	C	311	GLN
5	E	74	GLN
12	M	32	GLN
13	O	36	GLN
13	O	82	GLN
13	O	88	ASN
16	V	86	GLN
20	R	32	GLN
1	a	19	ASN
1	a	234	ASN
2	b	179	GLN
2	b	409	GLN
2	b	490	GLN
3	c	28	GLN
3	c	311	GLN
5	e	60	GLN
5	e	82	GLN
12	m	5	GLN

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Mol	Chain	Res	Type
18	x	33	GLN
19	z	31	GLN
20	r	30	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	1.01	0	7,9,11	1.11	0
8	FME	I	1	8	8,9,10	0.99	0	7,9,11	1.07	0
12	FME	m	1	12	8,9,10	0.95	0	7,9,11	0.62	0
14	FME	T	1	14	8,9,10	1.16	1 (12%)	7,9,11	1.05	0
8	FME	i	1	8	8,9,10	1.03	0	7,9,11	1.14	1 (14%)
14	FME	t	1	14	8,9,10	0.97	0	7,9,11	1.07	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
12	FME	M	1	12	-	5/7/9/11	-
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	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	1	FME	CA-N	-2.13	1.43	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	CA-N-CN	-2.39	119.14	122.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 190 ligands modelled in this entry, 6 are monoatomic - 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	$\#\|Z\|>2$
25	CLA	c	513	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	9 (11%)
29	LMG	m	101	-	51,51,55	0.74	0	59,59,63	1.40	9 (15%)
29	LMG	c	520	-	48,48,55	0.91	3 (6%)	56,56,63	1.29	6 (10%)
25	CLA	b	610	37	65,73,73	1.50	10 (15%)	76,113,113	1.53	11 (14%)
31	DGD	C	519	-	63,63,67	0.82	1 (1%)	77,77,81	1.36	6 (7%)
25	CLA	b	613	-	65,73,73	1.54	8 (12%)	76,113,113	1.50	11 (14%)
25	CLA	B	602	-	65,73,73	1.52	6 (9%)	76,113,113	1.52	12 (15%)
25	CLA	c	510	-	65,73,73	1.61	6 (9%)	76,113,113	1.39	6 (7%)
31	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.30	7 (9%)
25	CLA	b	608	-	65,73,73	1.64	7 (10%)	76,113,113	1.56	12 (15%)
26	PHO	D	402	-	51,69,69	0.95	4 (7%)	47,99,99	1.34	7 (14%)
25	CLA	B	616	-	60,68,73	1.67	6 (10%)	70,107,113	1.54	9 (12%)
25	CLA	b	607	37	65,73,73	1.52	7 (10%)	76,113,113	1.29	7 (9%)
32	STE	B	628	-	11,11,19	0.76	0	11,11,19	1.17	1 (9%)
25	CLA	C	509	-	65,73,73	1.54	8 (12%)	76,113,113	1.43	7 (9%)
25	CLA	a	606	-	65,73,73	1.57	8 (12%)	76,113,113	1.28	8 (10%)
32	STE	l	102	-	17,17,19	0.29	0	16,16,19	0.96	0
27	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	6 (10%)
25	CLA	C	505	-	65,73,73	1.57	6 (9%)	76,113,113	1.53	10 (13%)
25	CLA	B	607	37	65,73,73	1.59	7 (10%)	76,113,113	1.28	4 (5%)
25	CLA	b	612	-	65,73,73	1.48	8 (12%)	76,113,113	1.46	12 (15%)
27	BCR	d	405	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	7 (12%)
25	CLA	B	608	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	6 (7%)
27	BCR	b	619	-	41,41,41	0.95	2 (4%)	56,56,56	1.14	2 (3%)
32	STE	b	624	-	19,19,19	0.62	0	19,19,19	1.10	1 (5%)
25	CLA	b	611	-	65,73,73	1.58	6 (9%)	76,113,113	1.49	10 (13%)
33	LHG	d	407	-	48,48,48	0.68	1 (2%)	51,54,54	1.22	6 (11%)
22	OEY	a	602[A]	1,37,3	0,16,16	-	-	-		
27	BCR	B	619	-	41,41,41	0.97	2 (4%)	56,56,56	1.24	4 (7%)
25	CLA	c	507	37	65,73,73	1.57	9 (13%)	76,113,113	1.43	10 (13%)
30	SQD	A	614	-	51,52,54	1.56	8 (15%)	60,63,65	1.95	12 (20%)
33	LHG	D	412	-	48,48,48	0.77	1 (2%)	51,54,54	1.30	6 (11%)
25	CLA	c	508	-	64,72,73	1.48	6 (9%)	74,111,113	1.36	8 (10%)
25	CLA	c	512	-	65,73,73	1.50	6 (9%)	76,113,113	1.43	9 (11%)
21	OEX	a	601[C]	1,37,3	0,15,15	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	611	-	65,73,73	1.53	5 (7%)	76,113,113	1.40	7 (9%)
25	CLA	b	602	-	65,73,73	1.38	6 (9%)	76,113,113	1.42	9 (11%)
28	PL9	a	611	-	55,55,55	0.79	2 (3%)	68,69,69	1.61	11 (16%)
25	CLA	a	612	37	65,73,73	1.58	7 (10%)	76,113,113	1.48	11 (14%)
31	DGD	A	616	-	67,67,67	0.97	4 (5%)	81,81,81	1.32	12 (14%)
27	BCR	B	617	-	41,41,41	0.97	2 (4%)	56,56,56	1.17	7 (12%)
32	STE	a	617	-	11,11,19	0.79	0	11,11,19	1.00	0
25	CLA	A	612	37	65,73,73	1.51	6 (9%)	76,113,113	1.35	8 (10%)
27	BCR	x	101	-	41,41,41	0.94	1 (2%)	56,56,56	1.25	7 (12%)
32	STE	B	627	-	17,17,19	0.63	0	17,17,19	1.21	1 (5%)
25	CLA	c	501	-	65,73,73	1.53	6 (9%)	76,113,113	1.48	9 (11%)
29	LMG	d	410	-	44,44,55	0.82	2 (4%)	52,52,63	1.29	7 (13%)
26	PHO	A	608	-	51,69,69	0.89	2 (3%)	47,99,99	1.24	5 (10%)
27	BCR	A	610	-	41,41,41	0.94	2 (4%)	56,56,56	1.19	3 (5%)
25	CLA	B	601	37	65,73,73	1.62	7 (10%)	76,113,113	1.45	9 (11%)
25	CLA	A	609	-	54,62,73	1.60	7 (12%)	62,99,113	1.59	10 (16%)
30	SQD	f	101	-	40,41,54	1.65	7 (17%)	49,52,65	1.75	11 (22%)
35	HEM	F	101	5,6	41,50,50	1.50	5 (12%)	45,82,82	1.31	5 (11%)
29	LMG	D	407	-	51,51,55	0.80	3 (5%)	59,59,63	1.37	7 (11%)
32	STE	J	101	-	11,11,19	0.72	0	11,11,19	1.14	0
25	CLA	B	614	-	65,73,73	1.62	6 (9%)	76,113,113	1.39	8 (10%)
32	STE	c	521	-	11,11,19	0.75	0	11,11,19	1.08	0
33	LHG	d	408	-	38,38,48	0.79	1 (2%)	41,44,54	1.17	3 (7%)
29	LMG	A	613	-	48,48,55	0.75	0	56,56,63	1.36	5 (8%)
31	DGD	H	102	-	63,63,67	1.05	5 (7%)	77,77,81	1.38	10 (12%)
27	BCR	k	103	-	41,41,41	1.02	2 (4%)	56,56,56	1.12	4 (7%)
32	STE	C	523	-	15,15,19	0.33	0	14,14,19	0.86	0
25	CLA	D	404	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	9 (11%)
25	CLA	C	501	-	65,73,73	1.60	8 (12%)	76,113,113	1.42	10 (13%)
25	CLA	c	511	3	65,73,73	1.74	6 (9%)	76,113,113	1.54	5 (6%)
30	SQD	a	615	-	35,35,54	1.68	5 (14%)	37,37,65	1.45	5 (13%)
32	STE	b	625	-	9,9,19	0.30	0	8,8,19	0.78	0
29	LMG	c	518	-	37,37,55	0.94	2 (5%)	45,45,63	1.34	6 (13%)
29	LMG	C	520	-	48,48,55	0.74	2 (4%)	56,56,63	1.38	7 (12%)
25	CLA	b	605	-	65,73,73	1.56	5 (7%)	76,113,113	1.36	7 (9%)
32	STE	b	621	-	19,19,19	0.58	0	19,19,19	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	c	505	-	65,73,73	1.43	7 (10%)	76,113,113	1.31	9 (11%)
25	CLA	B	613	-	65,73,73	1.64	8 (12%)	76,113,113	1.41	7 (9%)
34	BCT	d	401	23	2,3,3	1.24	0	2,3,3	3.14	1 (50%)
25	CLA	b	609	-	65,73,73	1.57	8 (12%)	76,113,113	1.47	9 (11%)
27	BCR	a	610	-	41,41,41	0.95	2 (4%)	56,56,56	1.14	2 (3%)
27	BCR	k	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.05	3 (5%)
25	CLA	a	609	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	9 (11%)
29	LMG	B	620	-	51,51,55	0.81	1 (1%)	59,59,63	1.37	7 (11%)
25	CLA	B	609	-	65,73,73	1.61	8 (12%)	76,113,113	1.46	9 (11%)
25	CLA	b	614	-	65,73,73	1.58	6 (9%)	76,113,113	1.39	10 (13%)
33	LHG	E	101	-	48,48,48	0.73	2 (4%)	51,54,54	1.21	6 (11%)
25	CLA	B	610	37	65,73,73	1.44	7 (10%)	76,113,113	1.36	7 (9%)
36	HEC	V	201	16	32,50,50	2.02	3 (9%)	24,82,82	2.24	7 (29%)
25	CLA	C	506	-	65,73,73	1.64	7 (10%)	76,113,113	1.34	10 (13%)
33	LHG	B	623	-	48,48,48	0.73	1 (2%)	51,54,54	1.15	3 (5%)
29	LMG	b	622	-	55,55,55	0.71	2 (3%)	63,63,63	1.35	10 (15%)
34	BCT	D	401	23	2,3,3	1.24	0	2,3,3	3.18	1 (50%)
21	OEX	A	601[B]	1,37,3	0,15,15	-	-	-		
25	CLA	B	615	-	65,73,73	1.71	8 (12%)	76,113,113	1.37	9 (11%)
27	BCR	b	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	5 (8%)
33	LHG	l	101	-	48,48,48	0.60	0	51,54,54	1.16	6 (11%)
28	PL9	D	406	-	55,55,55	0.98	2 (3%)	68,69,69	1.58	13 (19%)
33	LHG	a	613	-	48,48,48	0.74	2 (4%)	51,54,54	1.29	7 (13%)
25	CLA	B	605	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	8 (10%)
30	SQD	a	614	-	53,54,54	1.57	8 (15%)	62,65,65	1.80	11 (17%)
25	CLA	C	503	-	65,73,73	1.78	8 (12%)	76,113,113	1.52	7 (9%)
25	CLA	d	403	-	65,73,73	1.47	7 (10%)	76,113,113	1.44	10 (13%)
25	CLA	a	607	37	65,73,73	1.59	8 (12%)	76,113,113	1.34	9 (11%)
31	DGD	C	518	-	63,63,67	1.07	4 (6%)	77,77,81	1.36	11 (14%)
32	STE	B	629	-	15,15,19	0.34	0	14,14,19	0.80	0
25	CLA	C	504	37	59,67,73	1.49	6 (10%)	68,105,113	1.37	8 (11%)
32	STE	I	101	-	14,14,19	0.35	0	13,13,19	0.82	0
25	CLA	B	606	-	65,73,73	1.67	7 (10%)	76,113,113	1.50	8 (10%)
25	CLA	C	513	-	65,73,73	1.57	7 (10%)	76,113,113	1.53	8 (10%)
25	CLA	d	404	-	65,73,73	1.49	6 (9%)	76,113,113	1.28	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	DGD	h	101	-	63,63,67	0.93	4 (6%)	77,77,81	1.41	13 (16%)
26	PHO	a	608	-	51,69,69	0.93	2 (3%)	47,99,99	1.28	7 (14%)
25	CLA	D	403	-	65,73,73	1.33	4 (6%)	76,113,113	1.34	11 (14%)
30	SQD	A	615	-	38,38,54	1.72	5 (13%)	40,40,65	1.21	2 (5%)
36	HEC	v	201	16	32,50,50	2.18	4 (12%)	24,82,82	1.85	6 (25%)
22	OEY	A	602[A]	1,37,3	0,16,16	-	-	-		
25	CLA	c	503	-	65,73,73	1.49	9 (13%)	76,113,113	1.47	10 (13%)
33	LHG	e	102	-	41,41,48	0.72	1 (2%)	44,47,54	1.27	6 (13%)
29	LMG	D	411	-	31,31,55	0.63	1 (3%)	33,33,63	1.24	2 (6%)
25	CLA	B	604	-	65,73,73	1.60	6 (9%)	76,113,113	1.59	12 (15%)
33	LHG	D	410	-	46,46,48	0.94	2 (4%)	49,52,54	1.28	5 (10%)
32	STE	T	103	-	14,14,19	0.35	0	13,13,19	0.82	0
32	STE	C	522	-	11,11,19	0.67	0	11,11,19	1.22	1 (9%)
27	BCR	k	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.30	10 (17%)
25	CLA	b	604	-	65,73,73	1.41	6 (9%)	76,113,113	1.54	12 (15%)
25	CLA	c	504	37	60,68,73	1.63	6 (10%)	70,107,113	1.42	9 (12%)
25	CLA	c	502	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	10 (13%)
32	STE	m	102	-	11,11,19	0.69	0	11,11,19	1.42	2 (18%)
31	DGD	C	517	-	63,63,67	1.00	5 (7%)	77,77,81	1.37	8 (10%)
32	STE	B	621	-	16,16,19	0.68	0	16,16,19	1.07	0
29	LMG	c	522	-	49,49,55	0.88	4 (8%)	57,57,63	1.27	6 (10%)
30	SQD	D	408	-	35,36,54	1.49	5 (14%)	42,45,65	1.65	9 (21%)
27	BCR	C	515	-	41,41,41	1.03	2 (4%)	56,56,56	1.16	4 (7%)
31	DGD	c	515	-	63,63,67	0.95	3 (4%)	77,77,81	1.43	11 (14%)
29	LMG	d	409	-	21,21,55	0.52	1 (4%)	20,20,63	1.25	2 (10%)
21	OEX	A	601[C]	1,37,3	0,15,15	-	-	-		
32	STE	X	101	-	19,19,19	0.56	0	19,19,19	1.16	0
32	STE	d	412	-	19,19,19	0.54	0	19,19,19	1.23	1 (5%)
27	BCR	C	516	-	41,41,41	1.01	2 (4%)	56,56,56	1.07	3 (5%)
25	CLA	c	506	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	6 (7%)
27	BCR	B	618	-	41,41,41	1.00	2 (4%)	56,56,56	1.18	5 (8%)
32	STE	B	625	-	13,13,19	0.68	0	13,13,19	1.26	2 (15%)
25	CLA	C	510	-	65,73,73	1.44	7 (10%)	76,113,113	1.50	9 (11%)
25	CLA	C	511	3	65,73,73	1.60	7 (10%)	76,113,113	1.55	9 (11%)
25	CLA	b	615	-	65,73,73	1.64	7 (10%)	76,113,113	1.35	10 (13%)
27	BCR	b	617	-	41,41,41	0.93	2 (4%)	56,56,56	1.27	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	STE	M	102	-	9,9,19	0.33	0	8,8,19	0.85	0
27	BCR	T	101	-	41,41,41	0.93	2 (4%)	56,56,56	1.23	7 (12%)
27	BCR	C	514	-	41,41,41	0.99	2 (4%)	56,56,56	1.21	7 (12%)
32	STE	B	626	-	11,11,19	0.77	0	11,11,19	1.11	0
32	STE	M	101	-	14,14,19	0.71	0	14,14,19	1.03	0
25	CLA	b	601	37	65,73,73	1.60	8 (12%)	76,113,113	1.49	8 (10%)
29	LMG	B	622	-	26,26,55	0.68	2 (7%)	26,26,63	1.27	3 (11%)
32	STE	d	411	-	16,16,19	0.53	0	16,16,19	1.34	2 (12%)
25	CLA	C	507	37	65,73,73	1.45	6 (9%)	76,113,113	1.52	9 (11%)
25	CLA	b	606	-	65,73,73	1.68	7 (10%)	76,113,113	1.57	5 (6%)
27	BCR	t	101	-	41,41,41	0.99	2 (4%)	56,56,56	1.36	7 (12%)
31	DGD	a	616	-	43,43,67	0.70	1 (2%)	45,45,81	1.37	7 (15%)
25	CLA	B	603	-	65,73,73	1.42	7 (10%)	76,113,113	1.42	11 (14%)
25	CLA	b	603	-	65,73,73	1.45	7 (10%)	76,113,113	1.55	9 (11%)
26	PHO	d	402	-	51,69,69	0.98	1 (1%)	47,99,99	1.36	7 (14%)
32	STE	E	102	-	11,11,19	0.74	0	11,11,19	1.13	1 (9%)
25	CLA	C	508	-	65,73,73	1.49	6 (9%)	76,113,113	1.57	8 (10%)
25	CLA	C	512	-	65,73,73	1.51	7 (10%)	76,113,113	1.40	10 (13%)
27	BCR	D	405	-	41,41,41	1.04	3 (7%)	56,56,56	1.17	4 (7%)
21	OEX	a	601[B]	1,37,3	0,15,15	-	-	-		
35	HEM	e	101	5,6	41,50,50	1.47	4 (9%)	45,82,82	1.65	10 (22%)
30	SQD	B	624	-	53,54,54	1.55	10 (18%)	62,65,65	1.72	10 (16%)
32	STE	T	102	-	15,15,19	0.33	0	14,14,19	0.91	0
27	BCR	K	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.10	3 (5%)
25	CLA	A	607	37	65,73,73	1.46	6 (9%)	76,113,113	1.34	10 (13%)
25	CLA	A	606	-	65,73,73	1.44	7 (10%)	76,113,113	1.38	8 (10%)
25	CLA	C	502	-	65,73,73	1.58	6 (9%)	76,113,113	1.28	7 (9%)
28	PL9	A	611	-	55,55,55	0.64	0	68,69,69	1.56	10 (14%)
32	STE	b	623	-	15,15,19	0.70	0	15,15,19	0.99	0
32	STE	j	101	-	11,11,19	0.71	0	11,11,19	1.24	2 (18%)
25	CLA	B	612	-	65,73,73	1.42	4 (6%)	76,113,113	1.50	11 (14%)
30	SQD	b	620	-	48,49,54	1.59	10 (20%)	57,60,65	1.75	10 (17%)
32	STE	H	103	-	17,17,19	0.35	0	16,16,19	0.76	0
25	CLA	c	509	-	65,73,73	1.41	5 (7%)	76,113,113	1.54	9 (11%)
32	STE	t	102	-	9,9,19	0.36	0	8,8,19	0.72	0
27	BCR	H	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	DGD	c	516	-	63,63,67	1.02	7 (11%)	77,77,81	1.32	9 (11%)
32	STE	c	519	-	19,19,19	0.60	0	19,19,19	1.00	0
33	LHG	D	409	-	48,48,48	0.72	2 (4%)	51,54,54	1.24	7 (13%)
25	CLA	b	616	-	60,68,73	1.57	6 (10%)	70,107,113	1.47	8 (11%)
28	PL9	d	406	-	55,55,55	1.02	3 (5%)	68,69,69	1.66	11 (16%)
32	STE	C	521	-	11,11,19	0.65	0	11,11,19	1.61	2 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	513	-	1/1/15/20	10/37/115/115	-
29	LMG	m	101	-	-	18/46/66/70	0/1/1/1
29	LMG	c	520	-	-	23/43/63/70	0/1/1/1
25	CLA	b	610	37	1/1/15/20	4/37/115/115	-
31	DGD	C	519	-	-	16/51/91/95	0/2/2/2
25	CLA	b	613	-	1/1/15/20	7/37/115/115	-
25	CLA	B	602	-	1/1/15/20	5/37/115/115	-
25	CLA	c	510	-	1/1/15/20	9/37/115/115	-
31	DGD	c	517	-	-	17/51/91/95	0/2/2/2
25	CLA	b	608	-	1/1/15/20	4/37/115/115	-
26	PHO	D	402	-	-	2/37/103/103	0/5/6/6
25	CLA	B	616	-	1/1/14/20	11/31/109/115	-
25	CLA	b	607	37	1/1/15/20	14/37/115/115	-
32	STE	B	628	-	-	5/9/9/17	-
25	CLA	C	509	-	1/1/15/20	12/37/115/115	-
25	CLA	a	606	-	1/1/15/20	4/37/115/115	-
32	STE	l	102	-	-	6/15/15/17	-
27	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CLA	C	505	-	1/1/15/20	13/37/115/115	-
25	CLA	B	607	37	1/1/15/20	10/37/115/115	-
25	CLA	b	612	-	1/1/15/20	7/37/115/115	-
27	BCR	d	405	-	-	5/29/63/63	0/2/2/2
25	CLA	B	608	-	-	2/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	b	619	-	-	2/29/63/63	0/2/2/2
32	STE	b	624	-	-	8/17/17/17	-
25	CLA	b	611	-	1/1/15/20	10/37/115/115	-
33	LHG	d	407	-	-	18/53/53/53	-
27	BCR	B	619	-	-	6/29/63/63	0/2/2/2
25	CLA	c	507	37	1/1/15/20	7/37/115/115	-
30	SQD	A	614	-	-	20/47/67/69	0/1/1/1
33	LHG	D	412	-	-	14/53/53/53	-
25	CLA	c	508	-	-	6/36/114/115	-
25	CLA	c	512	-	1/1/15/20	19/37/115/115	-
25	CLA	B	611	-	1/1/15/20	2/37/115/115	-
28	PL9	a	611	-	-	21/53/73/73	0/1/1/1
25	CLA	b	602	-	1/1/15/20	4/37/115/115	-
25	CLA	a	612	37	1/1/15/20	2/37/115/115	-
31	DGD	A	616	-	-	25/55/95/95	0/2/2/2
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
32	STE	a	617	-	-	4/9/9/17	-
25	CLA	A	612	37	-	6/37/115/115	-
27	BCR	x	101	-	-	7/29/63/63	0/2/2/2
32	STE	B	627	-	-	8/15/15/17	-
25	CLA	c	501	-	1/1/15/20	3/37/115/115	-
29	LMG	d	410	-	-	9/39/59/70	0/1/1/1
26	PHO	A	608	-	-	4/37/103/103	0/5/6/6
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
25	CLA	B	601	37	1/1/15/20	14/37/115/115	-
25	CLA	A	609	-	1/1/12/20	4/24/102/115	-
30	SQD	f	101	-	-	17/36/56/69	0/1/1/1
35	HEM	F	101	5,6	-	2/12/54/54	-
29	LMG	D	407	-	-	15/46/66/70	0/1/1/1
32	STE	J	101	-	-	5/9/9/17	-
25	CLA	B	614	-	1/1/15/20	13/37/115/115	-
32	STE	c	521	-	-	6/9/9/17	-
33	LHG	d	408	-	-	13/43/43/53	-
29	LMG	A	613	-	-	18/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	H	102	-	-	19/51/91/95	0/2/2/2
27	BCR	k	103	-	-	5/29/63/63	0/2/2/2
32	STE	C	523	-	-	2/13/13/17	-
25	CLA	D	404	-	-	8/37/115/115	-
25	CLA	C	501	-	1/1/15/20	4/37/115/115	-
25	CLA	c	511	3	1/1/15/20	6/37/115/115	-
30	SQD	a	615	-	-	16/37/37/69	-
32	STE	b	625	-	-	3/7/7/17	-
29	LMG	c	518	-	-	10/31/51/70	0/1/1/1
29	LMG	C	520	-	-	18/43/63/70	0/1/1/1
25	CLA	b	605	-	1/1/15/20	10/37/115/115	-
32	STE	b	621	-	-	13/17/17/17	-
25	CLA	c	505	-	1/1/15/20	10/37/115/115	-
25	CLA	B	613	-	1/1/15/20	6/37/115/115	-
25	CLA	b	609	-	-	7/37/115/115	-
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
25	CLA	a	609	-	1/1/15/20	8/37/115/115	-
29	LMG	B	620	-	-	25/46/66/70	0/1/1/1
25	CLA	B	609	-	-	3/37/115/115	-
25	CLA	b	614	-	1/1/15/20	13/37/115/115	-
33	LHG	E	101	-	-	18/53/53/53	-
25	CLA	B	610	37	1/1/15/20	7/37/115/115	-
36	HEC	V	201	16	-	2/10/54/54	-
25	CLA	C	506	-	1/1/15/20	12/37/115/115	-
33	LHG	B	623	-	-	25/53/53/53	-
29	LMG	b	622	-	-	27/50/70/70	0/1/1/1
25	CLA	B	615	-	1/1/15/20	9/37/115/115	-
27	BCR	b	618	-	-	3/29/63/63	0/2/2/2
33	LHG	l	101	-	-	19/53/53/53	-
28	PL9	D	406	-	-	6/53/73/73	0/1/1/1
33	LHG	a	613	-	-	21/53/53/53	-
25	CLA	B	605	-	1/1/15/20	8/37/115/115	-
30	SQD	a	614	-	-	21/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	403	-	1/1/15/20	4/37/115/115	-
25	CLA	C	503	-	-	5/37/115/115	-
25	CLA	a	607	37	1/1/15/20	9/37/115/115	-
31	DGD	C	518	-	-	20/51/91/95	0/2/2/2
32	STE	B	629	-	-	7/13/13/17	-
25	CLA	C	504	37	1/1/13/20	9/30/108/115	-
32	STE	I	101	-	-	4/12/12/17	-
25	CLA	B	606	-	1/1/15/20	15/37/115/115	-
25	CLA	C	513	-	1/1/15/20	13/37/115/115	-
25	CLA	d	404	-	1/1/15/20	9/37/115/115	-
31	DGD	h	101	-	-	16/51/91/95	0/2/2/2
26	PHO	a	608	-	-	2/37/103/103	0/5/6/6
25	CLA	D	403	-	1/1/15/20	8/37/115/115	-
30	SQD	A	615	-	-	17/39/39/69	-
36	HEC	v	201	16	-	2/10/54/54	-
25	CLA	c	503	-	1/1/15/20	7/37/115/115	-
33	LHG	e	102	-	-	27/46/46/53	-
29	LMG	D	411	-	-	16/33/33/70	-
25	CLA	B	604	-	1/1/15/20	10/37/115/115	-
33	LHG	D	410	-	-	23/51/51/53	-
32	STE	T	103	-	-	9/12/12/17	-
32	STE	C	522	-	-	4/9/9/17	-
27	BCR	k	101	-	-	10/29/63/63	0/2/2/2
25	CLA	b	604	-	1/1/15/20	11/37/115/115	-
25	CLA	c	504	37	1/1/14/20	8/31/109/115	-
25	CLA	c	502	-	-	4/37/115/115	-
32	STE	m	102	-	-	3/9/9/17	-
31	DGD	C	517	-	-	21/51/91/95	0/2/2/2
32	STE	B	621	-	-	6/14/14/17	-
29	LMG	c	522	-	-	26/44/64/70	0/1/1/1
30	SQD	D	408	-	-	13/28/48/69	0/1/1/1
27	BCR	C	515	-	-	5/29/63/63	0/2/2/2
31	DGD	c	515	-	-	29/51/91/95	0/2/2/2
29	LMG	d	409	-	-	7/17/17/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	X	101	-	-	10/17/17/17	-
32	STE	d	412	-	-	9/17/17/17	-
27	BCR	C	516	-	-	8/29/63/63	0/2/2/2
25	CLA	c	506	-	1/1/15/20	15/37/115/115	-
27	BCR	B	618	-	-	4/29/63/63	0/2/2/2
32	STE	B	625	-	-	3/11/11/17	-
25	CLA	C	510	-	1/1/15/20	6/37/115/115	-
25	CLA	C	511	3	1/1/15/20	6/37/115/115	-
25	CLA	b	615	-	1/1/15/20	11/37/115/115	-
27	BCR	b	617	-	-	3/29/63/63	0/2/2/2
32	STE	M	102	-	-	2/7/7/17	-
27	BCR	T	101	-	-	8/29/63/63	0/2/2/2
27	BCR	C	514	-	-	1/29/63/63	0/2/2/2
32	STE	B	626	-	-	6/9/9/17	-
32	STE	M	101	-	-	7/12/12/17	-
25	CLA	b	601	37	1/1/15/20	15/37/115/115	-
29	LMG	B	622	-	-	10/22/22/70	-
32	STE	d	411	-	-	8/14/14/17	-
25	CLA	C	507	37	1/1/15/20	8/37/115/115	-
25	CLA	b	606	-	1/1/15/20	12/37/115/115	-
27	BCR	t	101	-	-	5/29/63/63	0/2/2/2
31	DGD	a	616	-	-	30/45/45/95	-
25	CLA	B	603	-	1/1/15/20	9/37/115/115	-
25	CLA	b	603	-	1/1/15/20	10/37/115/115	-
26	PHO	d	402	-	-	4/37/103/103	0/5/6/6
32	STE	E	102	-	-	4/9/9/17	-
25	CLA	C	508	-	1/1/15/20	8/37/115/115	-
25	CLA	C	512	-	1/1/15/20	12/37/115/115	-
27	BCR	D	405	-	-	5/29/63/63	0/2/2/2
35	HEM	e	101	5,6	-	5/12/54/54	-
30	SQD	B	624	-	-	23/49/69/69	0/1/1/1
32	STE	T	102	-	-	8/13/13/17	-
27	BCR	K	101	-	-	6/29/63/63	0/2/2/2
25	CLA	A	607	37	-	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	A	606	-	1/1/15/20	5/37/115/115	-
25	CLA	C	502	-	-	8/37/115/115	-
28	PL9	A	611	-	-	28/53/73/73	0/1/1/1
32	STE	b	623	-	-	6/13/13/17	-
32	STE	j	101	-	-	5/9/9/17	-
25	CLA	B	612	-	1/1/15/20	10/37/115/115	-
30	SQD	b	620	-	-	23/44/64/69	0/1/1/1
32	STE	H	103	-	-	10/15/15/17	-
25	CLA	c	509	-	1/1/15/20	14/37/115/115	-
32	STE	t	102	-	-	3/7/7/17	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
31	DGD	c	516	-	-	17/51/91/95	0/2/2/2
32	STE	c	519	-	-	9/17/17/17	-
33	LHG	D	409	-	-	19/53/53/53	-
25	CLA	b	616	-	1/1/14/20	5/31/109/115	-
28	PL9	d	406	-	-	8/53/73/73	0/1/1/1
32	STE	C	521	-	-	3/9/9/17	-

All (678) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	504	CLA	C4B-NB	8.71	1.43	1.35
25	B	614	CLA	C4B-NB	8.20	1.42	1.35
25	b	614	CLA	C4B-NB	8.20	1.42	1.35
25	b	605	CLA	C4B-NB	8.16	1.42	1.35
25	B	615	CLA	C4B-NB	8.14	1.42	1.35
25	C	502	CLA	C4B-NB	7.87	1.42	1.35
25	B	609	CLA	C4B-NB	7.86	1.42	1.35
25	c	511	CLA	C4B-NB	7.85	1.42	1.35
25	B	601	CLA	C4B-NB	7.78	1.42	1.35
25	C	505	CLA	C4B-NB	7.71	1.42	1.35
25	b	607	CLA	C4B-NB	7.66	1.42	1.35
25	b	601	CLA	C4B-NB	7.66	1.42	1.35
25	c	507	CLA	C4B-NB	7.62	1.42	1.35
25	b	606	CLA	C4B-NB	7.58	1.42	1.35
25	C	511	CLA	C4B-NB	7.58	1.42	1.35
25	B	613	CLA	C4B-NB	7.56	1.42	1.35
25	a	607	CLA	C4B-NB	7.54	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	503	CLA	C4B-NB	7.48	1.41	1.35
25	B	607	CLA	C4B-NB	7.46	1.41	1.35
25	C	501	CLA	C4B-NB	7.44	1.41	1.35
25	b	613	CLA	C4B-NB	7.44	1.41	1.35
25	d	403	CLA	C4B-NB	7.44	1.41	1.35
25	B	608	CLA	C4B-NB	7.41	1.41	1.35
25	B	612	CLA	C4B-NB	7.38	1.41	1.35
25	a	609	CLA	C4B-NB	7.36	1.41	1.35
25	b	608	CLA	C4B-NB	7.36	1.41	1.35
25	B	606	CLA	C4B-NB	7.35	1.41	1.35
25	C	506	CLA	C4B-NB	7.34	1.41	1.35
25	C	507	CLA	C4B-NB	7.33	1.41	1.35
25	C	512	CLA	C4B-NB	7.31	1.41	1.35
25	d	404	CLA	C4B-NB	7.30	1.41	1.35
25	C	509	CLA	C4B-NB	7.28	1.41	1.35
25	c	505	CLA	C4B-NB	7.27	1.41	1.35
25	B	602	CLA	C4B-NB	7.26	1.41	1.35
25	C	504	CLA	C4B-NB	7.25	1.41	1.35
25	b	609	CLA	C4B-NB	7.21	1.41	1.35
25	b	615	CLA	C4B-NB	7.20	1.41	1.35
25	B	606	CLA	MG-NA	7.19	2.23	2.06
25	b	603	CLA	C4B-NB	7.19	1.41	1.35
25	B	611	CLA	C4B-NB	7.17	1.41	1.35
25	c	511	CLA	MG-NA	7.17	2.23	2.06
25	b	612	CLA	C4B-NB	7.16	1.41	1.35
25	b	616	CLA	C4B-NB	7.16	1.41	1.35
25	c	512	CLA	C4B-NB	7.15	1.41	1.35
25	C	513	CLA	C4B-NB	7.13	1.41	1.35
25	c	501	CLA	C4B-NB	7.12	1.41	1.35
25	b	604	CLA	C4B-NB	7.12	1.41	1.35
25	B	616	CLA	C4B-NB	7.05	1.41	1.35
25	A	607	CLA	C4B-NB	7.03	1.41	1.35
25	b	610	CLA	C4B-NB	7.01	1.41	1.35
25	C	508	CLA	C4B-NB	7.01	1.41	1.35
25	c	506	CLA	C4B-NB	6.99	1.41	1.35
25	c	510	CLA	C4B-NB	6.98	1.41	1.35
25	a	606	CLA	C4B-NB	6.93	1.41	1.35
25	c	509	CLA	C4B-NB	6.91	1.41	1.35
25	C	510	CLA	C4B-NB	6.90	1.41	1.35
25	b	611	CLA	C4B-NB	6.84	1.41	1.35
25	a	612	CLA	C4B-NB	6.83	1.41	1.35
25	c	503	CLA	C4B-NB	6.76	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	604	CLA	C4B-NB	6.76	1.41	1.35
25	A	609	CLA	C4B-NB	6.62	1.41	1.35
25	b	602	CLA	C4B-NB	6.59	1.41	1.35
25	c	513	CLA	C4B-NB	6.55	1.41	1.35
25	c	508	CLA	C4B-NB	6.55	1.41	1.35
25	D	404	CLA	C4B-NB	6.54	1.41	1.35
25	c	502	CLA	C4B-NB	6.47	1.41	1.35
36	v	201	HEC	C2B-C3B	-6.39	1.34	1.40
25	b	615	CLA	MG-NA	6.33	2.21	2.06
25	B	605	CLA	C4B-NB	6.29	1.40	1.35
25	A	606	CLA	C4B-NB	6.28	1.40	1.35
25	B	610	CLA	C4B-NB	6.28	1.40	1.35
25	B	603	CLA	C4B-NB	6.26	1.40	1.35
25	b	606	CLA	MG-NA	6.22	2.21	2.06
25	B	616	CLA	MG-NA	6.15	2.20	2.06
36	V	201	HEC	C2B-C3B	-6.12	1.34	1.40
25	b	611	CLA	MG-NA	6.09	2.20	2.06
25	C	503	CLA	MG-NC	5.94	2.20	2.06
25	D	403	CLA	C4B-NB	5.92	1.40	1.35
25	A	612	CLA	C4B-NB	5.81	1.40	1.35
25	b	608	CLA	MG-NA	5.71	2.19	2.06
25	B	615	CLA	MG-NA	5.57	2.19	2.06
36	v	201	HEC	C3C-C2C	-5.55	1.35	1.40
30	A	615	SQD	O47-C45	-5.41	1.37	1.47
36	v	201	HEC	C3D-C2D	5.31	1.53	1.37
36	V	201	HEC	C3C-C2C	-5.24	1.35	1.40
30	a	614	SQD	O48-C23	5.23	1.48	1.33
25	c	510	CLA	MG-NA	5.12	2.18	2.06
25	a	612	CLA	MG-NA	5.08	2.18	2.06
25	C	511	CLA	MG-NA	5.07	2.18	2.06
35	F	101	HEM	C3C-C2C	-5.05	1.33	1.40
36	V	201	HEC	C3D-C2D	5.04	1.52	1.37
25	b	613	CLA	MG-NA	4.97	2.18	2.06
30	a	615	SQD	O48-C23	4.96	1.47	1.33
25	B	604	CLA	MG-NA	4.94	2.18	2.06
25	b	601	CLA	MG-NA	4.93	2.18	2.06
30	A	615	SQD	O48-C23	4.83	1.47	1.33
25	B	613	CLA	MG-ND	-4.80	1.96	2.05
25	B	607	CLA	MG-NC	4.72	2.17	2.06
25	C	506	CLA	MG-NA	4.72	2.17	2.06
30	B	624	SQD	O48-C23	4.71	1.47	1.33
30	D	408	SQD	O48-C23	4.68	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	404	CLA	C1D-ND	4.68	1.43	1.37
25	B	601	CLA	C1D-ND	4.65	1.43	1.37
30	b	620	SQD	O48-C23	4.64	1.46	1.33
30	f	101	SQD	O48-C23	4.62	1.46	1.33
25	A	609	CLA	C1D-ND	4.62	1.43	1.37
25	B	611	CLA	MG-NA	4.59	2.17	2.06
30	A	614	SQD	O48-C23	4.55	1.46	1.33
25	B	607	CLA	C1D-ND	4.48	1.43	1.37
25	C	501	CLA	MG-NA	4.46	2.16	2.06
25	a	612	CLA	C1D-ND	4.39	1.43	1.37
25	A	612	CLA	C1D-ND	4.35	1.43	1.37
25	A	612	CLA	MG-NA	4.33	2.16	2.06
25	B	616	CLA	C1D-ND	4.30	1.43	1.37
25	c	507	CLA	MG-NA	4.28	2.16	2.06
25	B	602	CLA	MG-NA	4.28	2.16	2.06
25	B	602	CLA	C1D-ND	4.25	1.43	1.37
25	C	501	CLA	C1D-ND	4.24	1.43	1.37
25	C	513	CLA	MG-ND	4.23	2.14	2.05
25	B	609	CLA	MG-NA	4.21	2.16	2.06
25	C	503	CLA	C1D-ND	4.20	1.42	1.37
25	c	510	CLA	C1D-ND	4.18	1.42	1.37
25	C	505	CLA	MG-NA	4.18	2.16	2.06
25	B	614	CLA	C1D-ND	4.17	1.42	1.37
25	B	614	CLA	MG-NA	4.10	2.16	2.06
25	b	610	CLA	C1D-ND	4.10	1.42	1.37
25	B	613	CLA	C4D-ND	-4.07	1.32	1.37
25	C	506	CLA	C1D-ND	4.07	1.42	1.37
25	b	614	CLA	C1D-ND	4.00	1.42	1.37
25	c	509	CLA	C1D-ND	4.00	1.42	1.37
25	b	609	CLA	MG-NA	3.99	2.15	2.06
25	C	503	CLA	MG-NA	3.96	2.15	2.06
25	C	509	CLA	MG-NA	3.96	2.15	2.06
25	b	606	CLA	C1D-ND	3.96	1.42	1.37
25	a	609	CLA	C1D-ND	3.93	1.42	1.37
25	a	606	CLA	MG-NA	3.90	2.15	2.06
25	b	609	CLA	C1D-ND	3.88	1.42	1.37
25	B	611	CLA	C1D-ND	3.88	1.42	1.37
25	B	604	CLA	C1D-ND	3.88	1.42	1.37
25	c	508	CLA	C4D-ND	-3.87	1.32	1.37
25	B	605	CLA	C1D-ND	3.84	1.42	1.37
25	C	502	CLA	MG-NA	3.83	2.15	2.06
25	a	606	CLA	C4D-ND	-3.83	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	C1D-ND	3.82	1.42	1.37
25	A	609	CLA	C4D-ND	-3.82	1.32	1.37
33	D	410	LHG	P-O6	3.82	1.74	1.59
25	b	616	CLA	C1D-ND	3.81	1.42	1.37
30	a	615	SQD	O47-C7	3.79	1.45	1.34
25	c	512	CLA	C1D-ND	3.79	1.42	1.37
25	d	403	CLA	C1D-ND	3.78	1.42	1.37
25	B	604	CLA	MG-NC	3.78	2.15	2.06
25	A	607	CLA	C4D-ND	-3.77	1.32	1.37
25	c	501	CLA	MG-ND	-3.75	1.98	2.05
25	B	613	CLA	C1D-ND	3.75	1.42	1.37
25	B	609	CLA	C1D-ND	3.75	1.42	1.37
25	a	606	CLA	C1D-ND	3.74	1.42	1.37
25	c	508	CLA	C1D-ND	3.73	1.42	1.37
25	A	606	CLA	C1D-ND	3.73	1.42	1.37
25	C	505	CLA	CHC-C1C	3.71	1.44	1.35
35	e	101	HEM	C3C-C2C	-3.71	1.35	1.40
25	a	607	CLA	C1D-ND	3.69	1.42	1.37
27	c	514	BCR	C1-C6	-3.69	1.48	1.53
25	b	612	CLA	C1D-ND	3.68	1.42	1.37
35	e	101	HEM	C3C-CAC	3.67	1.55	1.47
27	C	515	BCR	C1-C6	-3.67	1.48	1.53
25	C	511	CLA	C1D-ND	3.67	1.42	1.37
25	C	507	CLA	C1D-ND	3.66	1.42	1.37
25	B	601	CLA	MG-NC	3.66	2.15	2.06
25	b	611	CLA	C1D-ND	3.65	1.42	1.37
25	C	506	CLA	CHC-C1C	3.64	1.44	1.35
25	C	509	CLA	C1D-ND	3.64	1.42	1.37
25	B	615	CLA	C1D-ND	3.63	1.42	1.37
25	C	508	CLA	C4D-ND	-3.63	1.32	1.37
30	A	614	SQD	O47-C45	-3.62	1.37	1.46
25	B	606	CLA	C1D-ND	3.61	1.42	1.37
25	b	615	CLA	C1D-ND	3.61	1.42	1.37
25	B	605	CLA	MG-NC	3.60	2.14	2.06
25	d	404	CLA	MG-NC	3.59	2.14	2.06
25	B	615	CLA	CHC-C1C	3.58	1.44	1.35
25	a	607	CLA	CHC-C1C	3.58	1.44	1.35
25	B	612	CLA	C4D-ND	-3.57	1.32	1.37
25	b	608	CLA	C1D-ND	3.57	1.42	1.37
25	c	501	CLA	C1D-ND	3.57	1.42	1.37
25	c	503	CLA	C1D-ND	3.57	1.42	1.37
25	c	513	CLA	C1D-ND	3.57	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	614	SQD	O47-C7	3.55	1.44	1.34
25	A	612	CLA	MG-ND	-3.54	1.98	2.05
30	f	101	SQD	O47-C7	3.54	1.44	1.34
25	c	510	CLA	CHC-C1C	3.53	1.44	1.35
30	B	624	SQD	O47-C7	3.52	1.44	1.34
25	c	508	CLA	MG-NC	3.51	2.14	2.06
25	b	605	CLA	C4D-ND	-3.51	1.32	1.37
25	c	512	CLA	CHC-C1C	3.50	1.43	1.35
25	B	605	CLA	C4D-ND	-3.50	1.32	1.37
25	b	605	CLA	MG-NA	3.50	2.14	2.06
25	C	505	CLA	C1D-ND	3.50	1.42	1.37
25	b	614	CLA	CHC-C1C	3.50	1.43	1.35
25	c	502	CLA	C1D-ND	3.49	1.42	1.37
25	B	610	CLA	C1D-ND	3.49	1.42	1.37
25	B	612	CLA	C1D-ND	3.48	1.42	1.37
25	C	502	CLA	C1D-ND	3.48	1.42	1.37
25	C	505	CLA	MG-ND	-3.46	1.98	2.05
25	c	503	CLA	MG-NA	3.46	2.14	2.06
25	b	607	CLA	C1D-ND	3.45	1.42	1.37
25	c	504	CLA	C4D-ND	-3.45	1.33	1.37
25	c	505	CLA	C4D-ND	-3.45	1.33	1.37
27	b	618	BCR	C30-C25	-3.45	1.49	1.53
25	c	511	CLA	C1D-ND	3.45	1.42	1.37
25	B	613	CLA	MG-NA	3.44	2.14	2.06
25	B	612	CLA	CHC-C1C	3.44	1.43	1.35
25	c	501	CLA	C4D-ND	-3.44	1.33	1.37
25	b	601	CLA	C1D-ND	3.44	1.42	1.37
25	b	605	CLA	C1D-ND	3.44	1.42	1.37
25	b	612	CLA	C4D-ND	-3.44	1.33	1.37
25	C	512	CLA	MG-NA	3.43	2.14	2.06
25	b	608	CLA	CHC-C1C	3.43	1.43	1.35
25	b	607	CLA	MG-NA	3.42	2.14	2.06
25	C	504	CLA	C1D-ND	3.42	1.42	1.37
25	C	509	CLA	CHC-C1C	3.40	1.43	1.35
25	a	607	CLA	C4D-ND	-3.40	1.33	1.37
25	b	605	CLA	CHC-C1C	3.39	1.43	1.35
25	c	508	CLA	CHC-C1C	3.38	1.43	1.35
25	b	616	CLA	C4D-ND	-3.38	1.33	1.37
31	C	517	DGD	O2G-C2G	-3.38	1.38	1.46
25	C	503	CLA	C4D-ND	-3.35	1.33	1.37
25	C	510	CLA	C1D-ND	3.35	1.41	1.37
30	b	620	SQD	O47-C7	3.35	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	CHC-C1C	3.34	1.43	1.35
25	A	612	CLA	CHC-C1C	3.34	1.43	1.35
35	F	101	HEM	C3C-CAC	3.34	1.54	1.47
28	d	406	PL9	C6-C1	-3.33	1.42	1.48
25	C	506	CLA	MG-ND	-3.33	1.99	2.05
25	b	601	CLA	CHC-C1C	3.33	1.43	1.35
30	b	620	SQD	O5-C1	3.32	1.50	1.41
30	A	615	SQD	O47-C7	3.32	1.43	1.34
25	C	502	CLA	C4D-ND	-3.32	1.33	1.37
25	D	403	CLA	CHC-C1C	3.31	1.43	1.35
25	C	503	CLA	MG-ND	3.31	2.12	2.05
27	B	618	BCR	C30-C25	-3.30	1.49	1.53
25	C	512	CLA	CHC-C1C	3.30	1.43	1.35
25	b	615	CLA	CHC-C1C	3.30	1.43	1.35
25	c	506	CLA	CHC-C1C	3.30	1.43	1.35
25	B	613	CLA	CHC-C1C	3.29	1.43	1.35
25	b	611	CLA	CHC-C1C	3.29	1.43	1.35
25	D	403	CLA	C4D-ND	-3.29	1.33	1.37
25	c	502	CLA	MG-ND	3.28	2.12	2.05
25	b	612	CLA	CHC-C1C	3.28	1.43	1.35
25	C	508	CLA	CHC-C1C	3.27	1.43	1.35
25	C	511	CLA	CHC-C1C	3.27	1.43	1.35
25	d	403	CLA	MG-NC	3.26	2.14	2.06
25	A	606	CLA	C4D-ND	-3.26	1.33	1.37
25	C	513	CLA	C4D-ND	-3.26	1.33	1.37
25	B	603	CLA	C4D-ND	-3.25	1.33	1.37
25	b	602	CLA	C1D-ND	3.25	1.41	1.37
27	k	102	BCR	C1-C6	-3.24	1.49	1.53
30	a	615	SQD	C24-C23	3.24	1.60	1.50
25	B	608	CLA	C1D-ND	3.23	1.41	1.37
27	D	405	BCR	C1-C6	-3.23	1.49	1.53
25	B	610	CLA	CHC-C1C	3.23	1.43	1.35
25	c	502	CLA	C4D-ND	-3.22	1.33	1.37
31	C	517	DGD	C4E-C3E	3.22	1.60	1.52
30	f	101	SQD	O47-C45	-3.22	1.38	1.46
25	C	504	CLA	CHC-C1C	3.22	1.43	1.35
25	C	508	CLA	C1D-ND	3.22	1.41	1.37
30	a	614	SQD	O47-C45	-3.21	1.38	1.46
25	b	609	CLA	CHC-C1C	3.21	1.43	1.35
25	c	507	CLA	C1D-ND	3.20	1.41	1.37
25	B	614	CLA	C4D-ND	-3.20	1.33	1.37
30	A	614	SQD	O5-C1	3.20	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	C4D-ND	-3.20	1.33	1.37
25	c	501	CLA	CHC-C1C	3.20	1.43	1.35
25	c	503	CLA	CHC-C1C	3.19	1.43	1.35
25	C	506	CLA	C4D-ND	-3.18	1.33	1.37
30	A	614	SQD	C24-C23	3.18	1.60	1.50
25	C	512	CLA	C1D-ND	3.18	1.41	1.37
27	c	514	BCR	C30-C25	-3.18	1.49	1.53
27	K	101	BCR	C30-C25	-3.17	1.49	1.53
25	c	511	CLA	CHC-C1C	3.17	1.43	1.35
25	b	610	CLA	C4D-ND	-3.17	1.33	1.37
27	H	101	BCR	C30-C25	-3.17	1.49	1.53
30	B	624	SQD	O47-C45	-3.16	1.38	1.46
25	b	603	CLA	C4D-ND	-3.16	1.33	1.37
25	c	506	CLA	C1D-ND	3.16	1.41	1.37
25	c	513	CLA	MG-ND	-3.15	1.99	2.05
30	a	614	SQD	C24-C23	3.15	1.59	1.50
30	B	624	SQD	O5-C1	3.14	1.49	1.41
30	A	615	SQD	C24-C23	3.14	1.59	1.50
25	C	513	CLA	MG-NC	3.14	2.13	2.06
25	c	505	CLA	CHC-C1C	3.14	1.43	1.35
25	b	604	CLA	C1D-ND	3.14	1.41	1.37
25	a	606	CLA	CHC-C1C	3.14	1.43	1.35
25	c	513	CLA	CHC-C1C	3.13	1.43	1.35
27	C	516	BCR	C1-C6	-3.13	1.49	1.53
25	B	611	CLA	CHC-C1C	3.13	1.43	1.35
31	c	515	DGD	C4D-C3D	3.13	1.60	1.52
25	A	607	CLA	CHC-C1C	3.13	1.43	1.35
25	c	504	CLA	C1D-ND	3.12	1.41	1.37
25	D	403	CLA	C1D-ND	3.12	1.41	1.37
25	b	603	CLA	C1D-ND	3.12	1.41	1.37
30	D	408	SQD	C24-C23	3.12	1.59	1.50
25	C	501	CLA	CHC-C1C	3.12	1.43	1.35
25	C	510	CLA	CHC-C1C	3.11	1.42	1.35
25	C	507	CLA	CHC-C1C	3.11	1.42	1.35
25	d	404	CLA	CHC-C1C	3.09	1.42	1.35
25	b	602	CLA	CHC-C1C	3.09	1.42	1.35
30	f	101	SQD	C24-C23	3.09	1.59	1.50
31	H	102	DGD	O5D-C1E	3.09	1.45	1.40
25	C	501	CLA	C4D-ND	-3.08	1.33	1.37
25	a	612	CLA	C4D-ND	-3.08	1.33	1.37
25	d	404	CLA	C1D-ND	3.08	1.41	1.37
25	b	613	CLA	C1D-ND	3.08	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	607	CLA	C1D-ND	3.08	1.41	1.37
25	b	616	CLA	CHC-C1C	3.07	1.42	1.35
25	c	502	CLA	CHC-C1C	3.07	1.42	1.35
25	B	608	CLA	C4D-ND	-3.07	1.33	1.37
25	B	609	CLA	CHC-C1C	3.06	1.42	1.35
25	B	603	CLA	C1D-ND	3.06	1.41	1.37
25	B	606	CLA	CHC-C1C	3.05	1.42	1.35
25	B	616	CLA	CHC-C1C	3.05	1.42	1.35
25	B	614	CLA	CHC-C1C	3.05	1.42	1.35
27	k	101	BCR	C30-C25	-3.05	1.49	1.53
25	C	510	CLA	C4D-ND	-3.04	1.33	1.37
25	B	603	CLA	CHC-C1C	3.04	1.42	1.35
25	C	503	CLA	CHC-C1C	3.04	1.42	1.35
25	c	504	CLA	CHC-C1C	3.04	1.42	1.35
27	b	618	BCR	C1-C6	-3.04	1.49	1.53
25	a	607	CLA	MG-ND	-3.02	1.99	2.05
30	A	614	SQD	O47-C7	3.02	1.42	1.34
33	D	412	LHG	O7-C5	-3.02	1.39	1.46
33	E	101	LHG	P-O6	3.00	1.71	1.59
25	c	513	CLA	C4D-ND	-3.00	1.33	1.37
25	c	513	CLA	MG-NA	3.00	2.13	2.06
25	c	507	CLA	C4D-ND	-2.99	1.33	1.37
27	k	102	BCR	C30-C25	-2.99	1.49	1.53
25	D	404	CLA	C4D-ND	-2.99	1.33	1.37
25	c	503	CLA	C4D-ND	-2.99	1.33	1.37
27	k	103	BCR	C1-C6	-2.98	1.49	1.53
25	C	512	CLA	C4D-ND	-2.98	1.33	1.37
27	k	101	BCR	C1-C6	-2.98	1.49	1.53
25	b	604	CLA	CHC-C1C	2.98	1.42	1.35
25	B	604	CLA	CHC-C1C	2.97	1.42	1.35
25	c	509	CLA	C4D-ND	-2.97	1.33	1.37
25	c	507	CLA	CHC-C1C	2.96	1.42	1.35
27	b	619	BCR	C1-C6	-2.95	1.49	1.53
30	f	101	SQD	O5-C1	2.94	1.49	1.41
25	B	601	CLA	CHC-C1C	2.93	1.42	1.35
27	d	405	BCR	C30-C25	-2.92	1.49	1.53
25	C	508	CLA	MG-NA	2.92	2.13	2.06
25	C	513	CLA	CHC-C1C	2.92	1.42	1.35
25	A	606	CLA	CHC-C1C	2.92	1.42	1.35
30	D	408	SQD	O5-C1	2.91	1.49	1.41
25	b	603	CLA	CHC-C1C	2.91	1.42	1.35
25	c	510	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	CLA	CHC-C1C	2.90	1.42	1.35
30	b	620	SQD	O47-C45	-2.90	1.39	1.46
25	b	614	CLA	C4D-ND	-2.90	1.33	1.37
27	a	610	BCR	C1-C6	-2.90	1.49	1.53
25	c	512	CLA	C4D-ND	-2.89	1.33	1.37
25	A	612	CLA	C4D-ND	-2.88	1.33	1.37
25	b	606	CLA	C4D-ND	-2.88	1.33	1.37
25	B	609	CLA	C4D-ND	-2.88	1.33	1.37
25	C	509	CLA	C4D-ND	-2.88	1.33	1.37
25	B	611	CLA	C4D-ND	-2.88	1.33	1.37
25	C	504	CLA	C4D-ND	-2.88	1.33	1.37
30	b	620	SQD	C24-C23	2.87	1.59	1.50
25	C	511	CLA	C4D-ND	-2.87	1.33	1.37
25	c	506	CLA	C4D-ND	-2.87	1.33	1.37
25	B	610	CLA	C3B-C2B	-2.86	1.36	1.40
29	D	407	LMG	C4-C5	2.86	1.59	1.53
25	d	403	CLA	CHC-C1C	2.86	1.42	1.35
25	a	607	CLA	MG-NC	2.86	2.13	2.06
25	B	607	CLA	CHC-C1C	2.86	1.42	1.35
30	a	615	SQD	O47-C45	-2.85	1.39	1.46
30	a	614	SQD	O5-C1	2.85	1.49	1.41
27	B	619	BCR	C1-C6	-2.85	1.49	1.53
35	F	101	HEM	CAB-C3B	2.85	1.55	1.47
27	C	514	BCR	C1-C6	-2.85	1.49	1.53
27	d	405	BCR	C1-C6	-2.84	1.49	1.53
25	b	609	CLA	C4D-ND	-2.84	1.33	1.37
25	B	601	CLA	MG-NA	2.83	2.13	2.06
25	c	509	CLA	CHC-C1C	2.82	1.42	1.35
25	B	610	CLA	C4D-ND	-2.82	1.33	1.37
25	b	604	CLA	C4D-ND	-2.82	1.33	1.37
25	a	609	CLA	C4D-ND	-2.81	1.33	1.37
25	B	602	CLA	CMB-C2B	-2.81	1.45	1.51
25	b	603	CLA	CMB-C2B	-2.81	1.45	1.51
25	b	607	CLA	CHC-C1C	2.80	1.42	1.35
25	b	608	CLA	C4D-ND	-2.80	1.33	1.37
25	c	505	CLA	C1D-ND	2.79	1.41	1.37
25	d	404	CLA	C4D-ND	-2.76	1.33	1.37
25	c	511	CLA	C4D-ND	-2.75	1.33	1.37
25	B	609	CLA	MG-ND	2.74	2.11	2.05
33	d	408	LHG	O7-C5	-2.74	1.39	1.46
27	B	617	BCR	C1-C6	-2.73	1.50	1.53
33	D	409	LHG	O7-C5	-2.73	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	MG-NA	2.73	2.12	2.06
25	b	607	CLA	C4D-ND	-2.73	1.33	1.37
25	a	606	CLA	MG-NC	2.73	2.12	2.06
25	A	606	CLA	MG-NC	2.72	2.12	2.06
25	A	607	CLA	MG-NA	2.72	2.12	2.06
25	B	605	CLA	CHC-C1C	2.72	1.41	1.35
27	K	101	BCR	C1-C6	-2.72	1.50	1.53
25	b	613	CLA	C4D-ND	-2.71	1.34	1.37
25	a	612	CLA	CHC-C1C	2.70	1.41	1.35
31	C	518	DGD	C1G-C2G	2.69	1.59	1.50
25	B	603	CLA	MG-NA	2.69	2.12	2.06
25	b	606	CLA	CHC-C1C	2.68	1.41	1.35
27	C	514	BCR	C30-C25	-2.67	1.50	1.53
25	B	616	CLA	C4D-ND	-2.67	1.34	1.37
25	c	501	CLA	MG-NC	2.66	2.12	2.06
25	b	602	CLA	C4D-ND	-2.66	1.34	1.37
25	B	607	CLA	C4D-ND	-2.65	1.34	1.37
25	b	609	CLA	MG-ND	2.65	2.11	2.05
33	D	410	LHG	O3-C3	-2.65	1.34	1.44
27	B	617	BCR	C30-C25	-2.65	1.50	1.53
27	D	405	BCR	C30-C25	-2.65	1.50	1.53
25	B	602	CLA	CHC-C1C	2.64	1.41	1.35
27	b	617	BCR	C1-C6	-2.64	1.50	1.53
25	B	608	CLA	CHC-C1C	2.64	1.41	1.35
27	C	516	BCR	C30-C25	-2.64	1.50	1.53
28	a	611	PL9	C7-C3	-2.64	1.48	1.51
25	C	505	CLA	C4D-ND	-2.64	1.34	1.37
26	d	402	PHO	CAC-C3C	-2.62	1.47	1.52
27	k	103	BCR	C30-C25	-2.62	1.50	1.53
31	C	518	DGD	C4D-C3D	2.62	1.59	1.52
25	a	609	CLA	MG-ND	-2.61	2.00	2.05
35	e	101	HEM	CAB-C3B	2.61	1.54	1.47
33	B	623	LHG	O7-C5	-2.61	1.40	1.46
33	a	613	LHG	C24-C23	2.61	1.58	1.50
30	B	624	SQD	C24-C23	2.61	1.58	1.50
25	b	614	CLA	MG-NA	2.60	2.12	2.06
25	b	613	CLA	CHC-C1C	2.60	1.41	1.35
30	A	615	SQD	C46-C45	2.58	1.56	1.50
25	c	506	CLA	MG-NA	2.58	2.12	2.06
25	A	609	CLA	CMB-C2B	-2.58	1.46	1.51
31	H	102	DGD	C4D-C5D	2.58	1.58	1.53
27	T	101	BCR	C30-C25	-2.57	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	605	CLA	MG-ND	-2.56	2.00	2.05
27	t	101	BCR	C1-C6	-2.56	1.50	1.53
25	b	610	CLA	CHC-C1C	2.55	1.41	1.35
25	b	606	CLA	CMB-C2B	-2.55	1.46	1.51
31	h	101	DGD	C4D-C3D	2.55	1.58	1.52
27	a	610	BCR	C30-C25	-2.53	1.50	1.53
25	d	403	CLA	C4D-ND	-2.53	1.34	1.37
25	b	612	CLA	CMB-C2B	-2.53	1.46	1.51
25	b	601	CLA	C4D-ND	-2.53	1.34	1.37
25	a	606	CLA	MG-ND	-2.52	2.00	2.05
28	a	611	PL9	C53-C6	-2.52	1.45	1.50
25	b	615	CLA	C4D-ND	-2.52	1.34	1.37
29	c	520	LMG	C4-C3	2.51	1.58	1.52
25	C	510	CLA	MG-NA	2.51	2.12	2.06
27	A	610	BCR	C1-C6	-2.51	1.50	1.53
31	A	616	DGD	C4D-C3D	2.50	1.58	1.52
26	a	608	PHO	CAC-C3C	-2.50	1.47	1.52
25	B	607	CLA	CMB-C2B	-2.50	1.46	1.51
25	D	404	CLA	CHC-C1C	2.49	1.41	1.35
25	b	603	CLA	CMC-C2C	-2.49	1.45	1.50
25	B	606	CLA	C4D-ND	-2.49	1.34	1.37
27	t	101	BCR	C30-C25	-2.48	1.50	1.53
25	b	611	CLA	C4D-ND	-2.48	1.34	1.37
27	x	101	BCR	C30-C25	-2.48	1.50	1.53
25	C	504	CLA	MG-NA	2.48	2.12	2.06
31	A	616	DGD	C4D-C5D	2.47	1.58	1.53
29	c	520	LMG	C3-C2	2.46	1.58	1.52
25	c	503	CLA	MG-NC	2.46	2.12	2.06
27	B	618	BCR	C1-C6	-2.46	1.50	1.53
25	C	512	CLA	CMB-C2B	-2.46	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.45	1.46	1.51
25	C	507	CLA	C4D-ND	-2.44	1.34	1.37
25	a	609	CLA	CHC-C1C	2.44	1.41	1.35
25	A	606	CLA	MG-NA	2.43	2.12	2.06
25	A	607	CLA	CMB-C2B	-2.42	1.46	1.51
25	C	502	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	610	CLA	MG-NC	2.41	2.12	2.06
25	B	601	CLA	CMB-C2B	-2.41	1.46	1.51
25	D	404	CLA	MG-NC	2.41	2.12	2.06
29	B	622	LMG	O8-C28	2.40	1.38	1.30
25	b	608	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	613	LHG	P-O6	2.39	1.69	1.59
31	c	517	DGD	O2G-C2G	-2.38	1.40	1.46
31	c	516	DGD	C1G-C2G	2.37	1.58	1.50
29	c	522	LMG	C4-C5	2.37	1.58	1.53
25	c	504	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.36	1.46	1.51
30	f	101	SQD	O7-S	2.36	1.52	1.45
25	b	609	CLA	CMB-C2B	-2.35	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.35	1.46	1.51
28	d	406	PL9	C53-C6	-2.34	1.45	1.50
26	D	402	PHO	CAC-C3C	-2.34	1.48	1.52
31	C	518	DGD	O3D-C3D	-2.34	1.37	1.43
30	b	620	SQD	O9-S	2.34	1.51	1.45
25	c	506	CLA	MG-ND	-2.33	2.01	2.05
25	c	511	CLA	CMB-C2B	-2.33	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.33	1.46	1.51
25	B	604	CLA	C4D-ND	-2.33	1.34	1.37
31	c	516	DGD	C3E-C2E	2.33	1.58	1.52
25	C	510	CLA	CMB-C2B	-2.33	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.33	1.46	1.51
30	a	614	SQD	O7-S	2.32	1.51	1.45
25	b	610	CLA	CMB-C2B	-2.32	1.46	1.51
29	D	407	LMG	C7-C8	2.32	1.57	1.50
31	H	102	DGD	C4E-C5E	2.32	1.57	1.53
29	b	622	LMG	C3-C2	2.32	1.58	1.52
27	C	515	BCR	C30-C25	-2.31	1.50	1.53
25	b	607	CLA	MG-NC	2.31	2.11	2.06
31	A	616	DGD	C1E-C2E	2.31	1.59	1.52
25	c	512	CLA	C1D-C2D	2.31	1.49	1.45
25	b	610	CLA	CMD-C2D	-2.31	1.45	1.50
25	c	507	CLA	C3B-CAB	-2.31	1.43	1.47
25	c	510	CLA	CMB-C2B	-2.30	1.46	1.51
25	b	616	CLA	MG-NC	2.30	2.11	2.06
25	a	612	CLA	CMB-C2B	-2.30	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.29	1.46	1.51
25	b	606	CLA	MG-ND	2.29	2.10	2.05
31	c	517	DGD	C4D-C5D	2.29	1.57	1.53
25	a	606	CLA	CMB-C2B	-2.29	1.46	1.51
31	H	102	DGD	O2G-C2G	-2.29	1.40	1.46
30	b	620	SQD	O5-C5	2.29	1.49	1.44
25	B	610	CLA	MG-NA	2.28	2.11	2.06
25	b	616	CLA	CMB-C2B	-2.28	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	608	CLA	CMB-C2B	-2.27	1.46	1.51
25	A	609	CLA	C3D-C4D	2.27	1.49	1.44
25	a	609	CLA	CMB-C2B	-2.27	1.46	1.51
25	b	603	CLA	CMD-C2D	-2.26	1.46	1.50
25	C	504	CLA	CMB-C2B	-2.26	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.26	1.46	1.51
30	B	624	SQD	O9-S	2.26	1.51	1.45
28	d	406	PL9	C3-C4	-2.25	1.45	1.49
31	c	516	DGD	O5D-C1E	2.25	1.44	1.40
25	B	601	CLA	C4D-ND	-2.25	1.34	1.37
25	c	505	CLA	CMB-C2B	-2.25	1.47	1.51
25	c	505	CLA	MG-NA	2.25	2.11	2.06
31	h	101	DGD	C1E-C2E	2.25	1.59	1.52
30	b	620	SQD	C6-S	2.24	1.85	1.77
25	B	603	CLA	CMB-C2B	-2.24	1.47	1.51
25	C	511	CLA	C1B-NB	2.24	1.37	1.35
25	C	501	CLA	CMB-C2B	-2.24	1.47	1.51
33	e	102	LHG	P-O6	2.24	1.68	1.59
31	a	616	DGD	O1G-C1A	2.24	1.39	1.33
27	T	101	BCR	C1-C6	-2.24	1.50	1.53
29	d	410	LMG	O7-C8	-2.24	1.41	1.46
29	c	522	LMG	C3-C2	2.24	1.58	1.52
27	B	619	BCR	C30-C25	-2.24	1.50	1.53
25	a	607	CLA	CMB-C2B	-2.24	1.47	1.51
25	C	501	CLA	C3B-C2B	-2.23	1.37	1.40
25	C	509	CLA	CMB-C2B	-2.23	1.47	1.51
25	b	607	CLA	CMB-C2B	-2.23	1.47	1.51
26	D	402	PHO	CMD-C2D	-2.23	1.46	1.51
31	h	101	DGD	C4D-C5D	2.23	1.57	1.53
29	C	520	LMG	O7-C8	-2.23	1.41	1.46
25	c	507	CLA	C3B-C2B	-2.22	1.37	1.40
25	b	613	CLA	CMB-C2B	-2.22	1.47	1.51
31	C	518	DGD	O5D-C6D	-2.22	1.39	1.43
25	B	608	CLA	MG-NA	2.22	2.11	2.06
25	A	606	CLA	MG-ND	-2.22	2.01	2.05
25	D	404	CLA	CMD-C2D	-2.21	1.46	1.50
35	F	101	HEM	CMD-C2D	2.21	1.55	1.50
30	a	614	SQD	C6-S	2.21	1.85	1.77
25	d	403	CLA	CMD-C2D	-2.21	1.46	1.50
25	B	602	CLA	C4D-ND	-2.21	1.34	1.37
25	c	503	CLA	CMD-C2D	-2.20	1.46	1.50
31	c	515	DGD	O1G-C1G	-2.20	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	615	CLA	CMB-C2B	-2.20	1.47	1.51
25	C	501	CLA	C1D-C2D	2.19	1.49	1.45
28	D	406	PL9	C7-C3	-2.19	1.49	1.51
25	b	608	CLA	CMD-C2D	-2.19	1.46	1.50
31	C	517	DGD	C6D-C5D	2.19	1.58	1.51
29	B	620	LMG	C4-C5	2.18	1.57	1.53
25	b	604	CLA	MG-NA	2.18	2.11	2.06
25	C	513	CLA	CMB-C2B	-2.17	1.47	1.51
30	B	624	SQD	O7-S	2.17	1.51	1.45
25	C	508	CLA	C1D-C2D	2.17	1.49	1.45
25	b	615	CLA	C3B-C2B	-2.17	1.37	1.40
25	B	609	CLA	C1D-C2D	2.17	1.49	1.45
25	D	404	CLA	CMB-C2B	-2.17	1.47	1.51
26	D	402	PHO	CMB-C2B	-2.17	1.46	1.51
25	C	510	CLA	CMD-C2D	-2.16	1.46	1.50
31	A	616	DGD	O1G-C1G	-2.16	1.40	1.45
26	A	608	PHO	CAC-C3C	-2.16	1.48	1.52
25	b	602	CLA	CMD-C2D	-2.16	1.46	1.50
29	c	522	LMG	C1-C2	2.15	1.58	1.52
29	c	518	LMG	C4-C5	2.15	1.57	1.53
25	C	509	CLA	O2D-CGD	2.15	1.38	1.33
29	C	520	LMG	C4-C5	2.14	1.57	1.53
25	b	609	CLA	C1D-C2D	2.14	1.49	1.45
25	C	503	CLA	CMB-C2B	-2.14	1.47	1.51
25	a	607	CLA	C3B-CAB	-2.14	1.43	1.47
30	a	614	SQD	C46-C45	2.14	1.57	1.50
28	D	406	PL9	C3-C4	-2.13	1.46	1.49
31	C	517	DGD	C3D-C2D	2.13	1.57	1.52
35	F	101	HEM	CMB-C2B	2.13	1.55	1.50
25	b	611	CLA	C1D-C2D	2.13	1.49	1.45
29	c	520	LMG	C1-C2	2.13	1.58	1.52
25	d	404	CLA	CMB-C2B	-2.12	1.47	1.51
25	C	509	CLA	CMD-C2D	-2.12	1.46	1.50
25	b	602	CLA	MG-NA	2.12	2.11	2.06
33	d	407	LHG	O8-C6	-2.12	1.40	1.45
35	e	101	HEM	C3B-C2B	-2.11	1.33	1.37
25	B	615	CLA	C1D-C2D	2.11	1.49	1.45
25	b	612	CLA	CMC-C2C	-2.11	1.46	1.50
31	h	101	DGD	C4E-C5E	2.11	1.57	1.53
25	a	609	CLA	CMC-C2C	-2.11	1.46	1.50
25	C	507	CLA	CMD-C2D	-2.10	1.46	1.50
29	b	622	LMG	C4-C3	2.10	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	610	BCR	C33-C5	-2.10	1.47	1.50
30	B	624	SQD	C44-C45	2.10	1.57	1.50
25	c	505	CLA	C3C-C2C	2.10	1.41	1.36
25	b	612	CLA	MG-ND	-2.10	2.01	2.05
29	c	518	LMG	C4-C3	2.10	1.57	1.52
25	B	607	CLA	CMD-C2D	-2.10	1.46	1.50
29	B	622	LMG	O7-C10	2.10	1.37	1.30
25	B	615	CLA	C3B-CAB	-2.10	1.43	1.47
30	D	408	SQD	C6-S	2.10	1.85	1.77
31	c	516	DGD	C4D-C3D	2.09	1.57	1.52
25	B	606	CLA	C3B-CAB	-2.09	1.43	1.47
25	c	503	CLA	CMB-C2B	-2.09	1.47	1.51
26	a	608	PHO	O2D-CGD	2.09	1.38	1.33
31	C	517	DGD	C3G-C2G	2.08	1.57	1.50
25	c	503	CLA	CMC-C2C	-2.08	1.46	1.50
25	c	508	CLA	C3C-C2C	2.08	1.41	1.36
25	c	502	CLA	CMB-C2B	-2.08	1.47	1.51
27	b	617	BCR	C30-C25	-2.08	1.50	1.53
30	B	624	SQD	C8-C7	2.08	1.56	1.50
27	b	619	BCR	C30-C25	-2.08	1.50	1.53
25	a	609	CLA	C4B-CHC	-2.08	1.35	1.41
25	b	604	CLA	CMB-C2B	-2.07	1.47	1.51
31	C	519	DGD	O1G-C1G	-2.07	1.40	1.45
30	A	614	SQD	C8-C7	2.07	1.56	1.50
30	A	614	SQD	C6-S	2.07	1.84	1.77
33	D	409	LHG	P-O6	2.07	1.67	1.59
30	f	101	SQD	O9-S	2.07	1.51	1.45
36	v	201	HEC	C1D-ND	2.06	1.40	1.36
25	b	601	CLA	C1B-NB	2.06	1.37	1.35
31	c	516	DGD	O3D-C3D	-2.06	1.38	1.43
30	D	408	SQD	O9-S	2.06	1.51	1.45
31	c	516	DGD	O3E-C3E	-2.06	1.38	1.43
25	B	613	CLA	CMD-C2D	-2.06	1.46	1.50
29	D	411	LMG	C9-C8	2.06	1.57	1.50
30	b	620	SQD	O7-S	2.06	1.51	1.45
25	b	610	CLA	C4B-CHC	-2.06	1.35	1.41
25	c	506	CLA	CMB-C2B	-2.06	1.47	1.51
25	c	502	CLA	MG-NA	2.06	2.11	2.06
31	c	516	DGD	C6E-C5E	2.05	1.58	1.51
25	c	504	CLA	O2D-CGD	2.05	1.38	1.33
30	a	615	SQD	C44-C45	2.05	1.56	1.51
29	d	409	LMG	O7-C10	2.05	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	CLA	CMC-C2C	-2.05	1.46	1.50
29	c	522	LMG	O7-C8	-2.05	1.41	1.46
25	B	606	CLA	C3B-C2B	-2.05	1.37	1.40
30	B	624	SQD	O5-C5	2.05	1.49	1.44
25	c	507	CLA	C3D-C4D	2.04	1.48	1.44
31	c	515	DGD	C4E-C3E	2.04	1.57	1.52
25	B	616	CLA	C4B-CHC	-2.04	1.35	1.41
25	b	613	CLA	CMD-C2D	-2.03	1.46	1.50
25	B	613	CLA	C3B-CAB	-2.03	1.43	1.47
25	B	609	CLA	C3D-C4D	2.03	1.48	1.44
26	D	402	PHO	O2D-CGD	2.03	1.38	1.33
29	D	407	LMG	O7-C8	-2.03	1.41	1.46
25	A	609	CLA	C4B-CHC	-2.03	1.35	1.41
27	D	405	BCR	C38-C26	-2.03	1.47	1.50
29	d	410	LMG	C7-C8	2.03	1.56	1.50
25	B	603	CLA	CMD-C2D	-2.03	1.46	1.50
25	b	612	CLA	MG-NA	2.02	2.11	2.06
30	A	614	SQD	O9-S	2.02	1.51	1.45
25	b	614	CLA	CMB-C2B	-2.02	1.47	1.51
26	A	608	PHO	CMD-C2D	-2.02	1.46	1.51
33	E	101	LHG	O7-C5	-2.02	1.41	1.46
25	b	610	CLA	C3B-C2B	-2.02	1.37	1.40
25	b	601	CLA	CMB-C2B	-2.02	1.47	1.51
31	H	102	DGD	C1E-C2E	2.01	1.58	1.52
30	b	620	SQD	C46-C45	2.01	1.56	1.50
25	d	403	CLA	CMB-C2B	-2.01	1.47	1.51
25	C	506	CLA	C3B-C2B	-2.01	1.37	1.40
25	b	613	CLA	C3B-C2B	-2.01	1.37	1.40
25	C	512	CLA	CMD-C2D	-2.01	1.46	1.50
25	a	612	CLA	C3D-C4D	2.01	1.48	1.44
25	b	610	CLA	C3B-CAB	-2.00	1.43	1.47

All (1143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	C4A-NA-C1A	8.86	110.69	106.71
25	b	606	CLA	C4A-NA-C1A	8.78	110.66	106.71
25	B	604	CLA	C4A-NA-C1A	8.55	110.55	106.71
25	B	606	CLA	C4A-NA-C1A	8.29	110.43	106.71
25	C	511	CLA	C4A-NA-C1A	8.29	110.43	106.71
25	C	513	CLA	C4A-NA-C1A	8.15	110.37	106.71
25	C	507	CLA	C4A-NA-C1A	8.04	110.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	503	CLA	C4A-NA-C1A	7.71	110.17	106.71
25	C	505	CLA	C4A-NA-C1A	7.39	110.03	106.71
25	b	601	CLA	C4A-NA-C1A	7.35	110.01	106.71
25	C	510	CLA	C4A-NA-C1A	7.29	109.98	106.71
25	c	507	CLA	C4A-NA-C1A	7.25	109.96	106.71
25	c	509	CLA	C4A-NA-C1A	7.12	109.91	106.71
25	B	601	CLA	C4A-NA-C1A	7.08	109.89	106.71
25	B	609	CLA	C4A-NA-C1A	7.00	109.85	106.71
25	B	605	CLA	C4A-NA-C1A	6.93	109.82	106.71
25	c	503	CLA	C4A-NA-C1A	6.83	109.78	106.71
25	C	501	CLA	C4A-NA-C1A	6.82	109.77	106.71
25	C	508	CLA	C4A-NA-C1A	6.82	109.77	106.71
25	b	604	CLA	C4A-NA-C1A	6.79	109.76	106.71
25	B	611	CLA	C4A-NA-C1A	6.72	109.73	106.71
25	c	510	CLA	C4A-NA-C1A	6.68	109.71	106.71
28	a	611	PL9	C7-C3-C4	6.62	122.26	116.88
25	c	501	CLA	C4A-NA-C1A	6.57	109.66	106.71
25	B	616	CLA	C4A-NA-C1A	6.56	109.65	106.71
25	c	506	CLA	C4A-NA-C1A	6.54	109.65	106.71
30	a	614	SQD	O6-C1-C2	6.54	118.51	108.30
25	C	509	CLA	C4A-NA-C1A	6.38	109.57	106.71
25	b	613	CLA	C4A-NA-C1A	6.21	109.50	106.71
25	A	606	CLA	C4A-NA-C1A	6.18	109.48	106.71
25	B	608	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	b	602	CLA	C4A-NA-C1A	6.06	109.43	106.71
25	b	611	CLA	C4A-NA-C1A	6.04	109.42	106.71
28	d	406	PL9	C7-C3-C4	6.04	121.79	116.88
25	D	404	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	b	615	CLA	C4A-NA-C1A	6.03	109.42	106.71
28	A	611	PL9	C7-C3-C4	6.03	121.78	116.88
25	B	615	CLA	C4A-NA-C1A	5.92	109.37	106.71
25	A	609	CLA	C4A-NA-C1A	5.87	109.35	106.71
25	A	612	CLA	C4A-NA-C1A	5.80	109.31	106.71
30	A	614	SQD	O6-C1-C2	5.80	117.35	108.30
25	b	610	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	d	403	CLA	C4A-NA-C1A	5.70	109.27	106.71
30	a	614	SQD	C1-O5-C5	-5.69	102.52	113.69
25	B	614	CLA	C4A-NA-C1A	5.63	109.24	106.71
30	A	614	SQD	C1-O5-C5	-5.47	102.96	113.69
25	b	616	CLA	C4A-NA-C1A	5.45	109.16	106.71
36	V	201	HEC	CBD-CAD-C3D	-5.44	103.33	112.62
25	C	504	CLA	C4A-NA-C1A	5.41	109.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	506	CLA	C4A-NA-C1A	5.37	109.12	106.71
25	b	608	CLA	C4A-NA-C1A	5.25	109.06	106.71
25	b	608	CLA	CMB-C2B-C1B	-5.23	120.42	128.46
25	b	605	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	b	609	CLA	CMB-C2B-C1B	-5.18	120.51	128.46
25	B	607	CLA	C4A-NA-C1A	5.15	109.02	106.71
25	b	607	CLA	C4A-NA-C1A	5.14	109.02	106.71
25	c	513	CLA	C4A-NA-C1A	5.10	109.00	106.71
25	B	613	CLA	C1-C2-C3	-5.09	117.24	126.04
25	a	612	CLA	C4A-NA-C1A	5.07	108.99	106.71
25	b	609	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	b	612	CLA	CMB-C2B-C1B	-5.06	120.69	128.46
25	a	607	CLA	C4A-NA-C1A	5.05	108.98	106.71
25	c	502	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	c	504	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	B	612	CLA	C4A-NA-C1A	5.01	108.96	106.71
30	a	615	SQD	O47-C7-C8	4.99	122.26	111.50
25	B	602	CLA	C4A-NA-C1A	4.94	108.93	106.71
25	A	607	CLA	C4A-NA-C1A	4.93	108.92	106.71
25	c	505	CLA	C4A-NA-C1A	4.89	108.90	106.71
25	c	512	CLA	C4A-NA-C1A	4.88	108.90	106.71
25	B	613	CLA	C4A-NA-C1A	4.84	108.88	106.71
25	B	608	CLA	CMB-C2B-C1B	-4.83	121.05	128.46
30	b	620	SQD	O6-C1-C2	4.79	115.78	108.30
25	b	614	CLA	C4A-NA-C1A	4.78	108.85	106.71
25	c	513	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
25	b	603	CLA	C4A-NA-C1A	4.74	108.84	106.71
30	b	620	SQD	O7-S-C6	4.69	112.51	106.94
25	C	502	CLA	C4A-NA-C1A	4.68	108.81	106.71
25	c	504	CLA	CMB-C2B-C1B	-4.67	121.28	128.46
28	D	406	PL9	C7-C3-C4	4.63	120.64	116.88
25	C	512	CLA	C4A-NA-C1A	4.63	108.79	106.71
25	B	607	CLA	CMB-C2B-C1B	-4.61	121.37	128.46
25	B	603	CLA	C4A-NA-C1A	4.58	108.76	106.71
28	a	611	PL9	C7-C3-C2	-4.57	117.30	123.30
25	b	603	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
25	C	508	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
30	A	614	SQD	C1-C2-C3	-4.52	100.59	110.00
25	B	602	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
30	A	614	SQD	O7-S-C6	4.51	112.30	106.94
30	f	101	SQD	O7-S-C6	4.48	112.26	106.94
25	a	612	CLA	CMB-C2B-C1B	-4.46	121.60	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	616	CLA	CMB-C2B-C1B	-4.46	121.60	128.46
25	C	510	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
25	a	606	CLA	C4A-NA-C1A	4.43	108.70	106.71
25	B	612	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
25	c	508	CLA	C4A-NA-C1A	4.42	108.69	106.71
30	B	624	SQD	O47-C7-C8	4.41	121.00	111.50
35	e	101	HEM	CBA-CAA-C2A	-4.40	105.11	112.62
25	D	403	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
25	C	509	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
30	B	624	SQD	C3-C4-C5	4.35	118.00	110.24
31	H	102	DGD	O3G-C3G-C2G	-4.35	100.41	110.90
30	f	101	SQD	O6-C1-C2	4.34	115.07	108.30
30	b	620	SQD	O5-C5-C4	4.31	117.52	109.69
25	a	609	CLA	O2D-CGD-O1D	-4.30	115.43	123.84
25	b	609	CLA	CMB-C2B-C3B	4.29	132.71	124.68
25	d	404	CLA	C4A-NA-C1A	4.27	108.63	106.71
30	B	624	SQD	O6-C1-C2	4.26	114.95	108.30
33	D	410	LHG	O4-P-O5	4.26	133.28	112.24
25	c	512	CLA	C1-C2-C3	-4.25	118.70	126.04
34	D	401	BCT	O2-C-O1	4.24	130.53	119.55
25	b	608	CLA	CMB-C2B-C3B	4.23	132.60	124.68
25	b	606	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
25	b	612	CLA	CMB-C2B-C3B	4.21	132.56	124.68
25	b	606	CLA	O2D-CGD-O1D	-4.21	115.61	123.84
25	c	501	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
33	e	102	LHG	O4-P-O5	4.18	132.91	112.24
25	b	603	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
36	v	201	HEC	CBD-CAD-C3D	-4.17	105.50	112.62
25	c	510	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
25	B	612	CLA	CMB-C2B-C3B	4.16	132.47	124.68
25	C	505	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
36	V	201	HEC	CMC-C2C-C1C	-4.15	122.09	128.46
30	D	408	SQD	O9-S-C6	4.13	111.85	106.94
26	D	402	PHO	C1-C2-C3	-4.13	118.91	126.04
30	A	614	SQD	O47-C7-C8	4.12	120.38	111.50
31	C	519	DGD	O3G-C3G-C2G	-4.12	100.96	110.90
25	c	513	CLA	CMB-C2B-C3B	4.10	132.35	124.68
25	D	404	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
33	B	623	LHG	O4-P-O5	4.09	132.46	112.24
33	l	101	LHG	O4-P-O5	4.06	132.31	112.24
25	b	604	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
34	d	401	BCT	O2-C-O1	4.05	130.05	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	407	LHG	O4-P-O5	4.05	132.26	112.24
25	b	607	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
25	B	603	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
31	C	518	DGD	O3G-C3G-C2G	-4.03	101.18	110.90
33	E	101	LHG	O4-P-O5	4.02	132.10	112.24
33	a	613	LHG	O4-P-O5	4.01	132.06	112.24
36	V	201	HEC	CMB-C2B-C1B	-4.00	122.31	128.46
25	a	606	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
25	B	613	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
36	v	201	HEC	CMC-C2C-C1C	-3.98	122.34	128.46
28	d	406	PL9	C7-C8-C9	-3.98	120.17	126.79
25	b	616	CLA	CMB-C2B-C3B	3.97	132.11	124.68
25	A	612	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
25	B	616	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
33	d	408	LHG	O4-P-O5	3.94	131.73	112.24
25	A	609	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
25	C	508	CLA	CHD-C1D-ND	-3.93	120.84	124.45
25	B	608	CLA	CMB-C2B-C3B	3.93	132.03	124.68
30	f	101	SQD	O9-S-O7	-3.91	100.42	113.95
25	C	508	CLA	CMB-C2B-C3B	3.91	131.99	124.68
28	d	406	PL9	C7-C3-C2	-3.91	118.16	123.30
25	b	613	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
33	D	412	LHG	O4-P-O5	3.90	131.51	112.24
25	B	601	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
25	B	610	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
25	C	509	CLA	CMB-C2B-C3B	3.88	131.94	124.68
25	B	607	CLA	CMB-C2B-C3B	3.88	131.94	124.68
25	b	603	CLA	CMB-C2B-C3B	3.87	131.92	124.68
25	d	404	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
33	D	409	LHG	O4-P-O5	3.85	131.26	112.24
25	B	609	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	b	611	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	C	506	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
32	C	521	STE	C3-C2-C1	-3.78	104.94	114.47
25	B	614	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
31	C	517	DGD	O3G-C3G-C2G	-3.77	101.81	110.90
25	D	403	CLA	CMB-C2B-C3B	3.76	131.72	124.68
31	c	515	DGD	O3G-C3G-C2G	-3.75	101.84	110.90
35	e	101	HEM	CBD-CAD-C3D	-3.75	102.20	112.63
30	f	101	SQD	O9-S-C6	3.75	111.40	106.94
25	a	607	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
25	c	501	CLA	O2D-CGD-O1D	-3.75	116.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	611	CLA	CMB-C2B-C3B	3.74	131.67	124.68
25	a	609	CLA	O2D-CGD-CBD	3.73	117.90	111.27
25	c	509	CLA	O2A-CGA-O1A	-3.73	114.17	123.59
32	d	412	STE	C3-C2-C1	-3.73	105.07	114.47
25	B	614	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
30	B	624	SQD	C1-O5-C5	-3.73	106.38	113.69
25	A	612	CLA	CMB-C2B-C3B	3.72	131.63	124.68
25	b	601	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
25	c	505	CLA	CMB-C2B-C1B	-3.71	122.75	128.46
25	C	513	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
25	d	403	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
25	c	501	CLA	CMB-C2B-C3B	3.70	131.60	124.68
25	B	602	CLA	CMB-C2B-C3B	3.70	131.60	124.68
25	b	613	CLA	C1-C2-C3	-3.70	119.64	126.04
25	a	609	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	b	617	BCR	C2-C1-C6	3.69	116.16	110.48
25	c	504	CLA	CMB-C2B-C3B	3.68	131.57	124.68
30	D	408	SQD	O8-S-C6	3.68	111.60	105.74
25	c	502	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
25	D	404	CLA	CMB-C2B-C3B	3.66	131.52	124.68
25	B	603	CLA	CMB-C2B-C3B	3.66	131.52	124.68
25	C	511	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
25	C	510	CLA	CMB-C2B-C3B	3.64	131.49	124.68
25	b	602	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	B	612	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
30	a	614	SQD	O47-C7-C8	3.62	119.30	111.50
30	D	408	SQD	C1-O5-C5	-3.62	106.59	113.69
25	A	609	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
36	V	201	HEC	CMC-C2C-C3C	3.59	130.04	125.82
25	C	505	CLA	CMB-C2B-C3B	3.58	131.38	124.68
25	b	612	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
25	C	512	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	c	511	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	c	502	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
25	b	604	CLA	CMB-C2B-C3B	3.56	131.34	124.68
25	B	613	CLA	CMB-C2B-C3B	3.56	131.34	124.68
25	C	502	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	a	612	CLA	CMB-C2B-C3B	3.55	131.31	124.68
25	C	507	CLA	CHB-C4A-NA	3.55	129.42	124.51
25	a	609	CLA	C4A-NA-C1A	3.54	108.30	106.71
25	B	610	CLA	C4A-NA-C1A	3.54	108.30	106.71
25	A	606	CLA	CMB-C2B-C1B	-3.54	123.03	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	616	CLA	CMB-C2B-C3B	3.53	131.29	124.68
30	A	614	SQD	O8-S-C6	3.53	111.37	105.74
28	A	611	PL9	C7-C3-C2	-3.53	118.66	123.30
27	D	405	BCR	C7-C8-C9	-3.53	120.91	126.23
25	b	614	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
30	A	614	SQD	O9-S-O7	-3.52	101.78	113.95
36	v	201	HEC	CBA-CAA-C2A	-3.51	106.68	112.60
25	A	607	CLA	C1-C2-C3	-3.51	119.97	126.04
25	C	513	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
25	b	610	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
25	B	602	CLA	O2D-CGD-CBD	3.50	117.48	111.27
25	d	403	CLA	O2D-CGD-O1D	-3.49	117.00	123.84
33	a	613	LHG	O8-C23-C24	3.49	122.86	111.91
31	C	519	DGD	O6D-C1D-O3G	-3.49	101.71	109.97
25	B	602	CLA	O2D-CGD-O1D	-3.47	117.04	123.84
30	B	624	SQD	O7-S-C6	3.47	111.07	106.94
31	a	616	DGD	O3G-C3G-C2G	-3.47	102.57	111.78
25	a	606	CLA	CMB-C2B-C3B	3.47	131.17	124.68
25	c	506	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
29	b	622	LMG	C1-O6-C5	-3.47	106.89	113.69
27	B	619	BCR	C2-C1-C6	3.46	115.81	110.48
26	A	608	PHO	CMB-C2B-C3B	3.46	131.15	124.68
25	b	610	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
25	b	611	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
26	d	402	PHO	C1-C2-C3	-3.42	120.12	126.04
25	B	604	CLA	C2D-C1D-ND	-3.42	107.59	110.10
25	c	508	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
30	f	101	SQD	O47-C7-C8	3.41	120.31	110.80
25	d	404	CLA	CMB-C2B-C3B	3.41	131.06	124.68
25	c	509	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
25	c	507	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
25	C	508	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
29	m	101	LMG	O1-C1-C2	-3.40	103.00	108.30
28	d	406	PL9	C22-C23-C24	-3.40	119.48	127.66
30	a	614	SQD	O9-S-C6	3.39	110.97	106.94
25	b	601	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
25	B	606	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
25	b	605	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
30	B	624	SQD	O5-C5-C4	3.38	115.83	109.69
25	c	510	CLA	CMB-C2B-C3B	3.37	130.99	124.68
36	V	201	HEC	C1D-C2D-C3D	-3.36	104.66	107.00
29	C	520	LMG	O1-C7-C8	-3.36	102.80	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	607	CLA	CMB-C2B-C3B	3.35	130.95	124.68
30	A	615	SQD	O47-C7-C8	3.34	118.71	111.50
25	a	609	CLA	CMB-C2B-C3B	3.34	130.93	124.68
25	b	602	CLA	CHB-C4A-NA	3.34	129.12	124.51
31	A	616	DGD	C3G-C2G-C1G	-3.33	103.91	111.79
25	A	609	CLA	CMB-C2B-C3B	3.33	130.90	124.68
25	C	512	CLA	CHB-C4A-NA	3.32	129.11	124.51
36	V	201	HEC	CMB-C2B-C3B	3.32	129.73	125.82
25	A	606	CLA	CMB-C2B-C3B	3.32	130.88	124.68
27	x	101	BCR	C2-C1-C6	3.31	115.58	110.48
25	B	614	CLA	C1-C2-C3	-3.31	120.32	126.04
25	B	611	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	b	607	CLA	CMB-C2B-C3B	3.30	130.86	124.68
25	B	615	CLA	CHD-C1D-ND	-3.30	121.42	124.45
28	D	406	PL9	C7-C8-C9	-3.29	121.31	126.79
30	a	615	SQD	O48-C23-C24	3.29	122.23	111.91
25	b	616	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	b	606	CLA	O2D-CGD-CBD	3.29	117.11	111.27
25	d	403	CLA	CMB-C2B-C3B	3.29	130.82	124.68
27	b	617	BCR	C15-C14-C13	-3.28	122.63	127.31
25	A	607	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
25	B	610	CLA	CHB-C4A-NA	3.27	129.03	124.51
25	C	506	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
25	b	602	CLA	CMB-C2B-C3B	3.25	130.77	124.68
25	b	611	CLA	O2D-CGD-CBD	3.25	117.05	111.27
26	d	402	PHO	CMC-C2C-C3C	3.25	131.06	124.94
26	D	402	PHO	O2D-CGD-O1D	-3.24	117.49	123.84
25	c	502	CLA	CHD-C1D-ND	-3.24	121.48	124.45
25	b	603	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
25	c	502	CLA	CMB-C2B-C3B	3.23	130.72	124.68
25	B	610	CLA	CHD-C1D-ND	-3.23	121.49	124.45
25	b	601	CLA	CHB-C4A-NA	3.23	128.98	124.51
25	c	508	CLA	CMB-C2B-C3B	3.22	130.71	124.68
25	C	503	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
31	h	101	DGD	O3G-C3G-C2G	-3.22	103.13	110.90
25	C	504	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
25	B	609	CLA	CMB-C2B-C3B	3.22	130.69	124.68
25	C	501	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
31	C	517	DGD	CDB-CCB-CBB	-3.21	98.15	114.42
25	b	606	CLA	CMB-C2B-C3B	3.21	130.68	124.68
25	c	505	CLA	CMB-C2B-C3B	3.20	130.66	124.68
25	C	510	CLA	O2D-CGD-O1D	-3.19	117.59	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	402	PHO	CMB-C2B-C3B	3.18	130.64	124.68
25	B	610	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
28	A	611	PL9	C40-C39-C41	3.18	120.62	115.27
30	A	614	SQD	O5-C1-C2	-3.18	103.62	110.35
31	c	517	DGD	O3G-C3G-C2G	-3.17	103.24	110.90
28	D	406	PL9	C7-C3-C2	-3.17	119.14	123.30
25	C	505	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
25	b	613	CLA	CMB-C2B-C3B	3.15	130.58	124.68
25	C	513	CLA	CMB-C2B-C3B	3.15	130.57	124.68
30	b	620	SQD	C1-C2-C3	-3.15	103.44	110.00
25	B	602	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
29	D	407	LMG	O1-C1-C2	-3.15	103.39	108.30
28	a	611	PL9	C22-C23-C24	-3.15	120.09	127.66
25	A	609	CLA	O2D-CGD-CBD	3.14	116.85	111.27
25	c	512	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	c	509	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
27	t	101	BCR	C15-C16-C17	-3.13	117.05	123.47
25	C	503	CLA	C7-C6-C5	-3.13	104.86	113.36
26	a	608	PHO	CMB-C2B-C3B	3.13	130.53	124.68
25	c	512	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
30	a	614	SQD	O8-S-C6	3.12	110.71	105.74
30	A	614	SQD	O9-S-C6	3.11	110.63	106.94
25	c	503	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
31	C	517	DGD	O5D-C6D-C5D	-3.11	103.30	109.05
30	B	624	SQD	O9-S-O7	-3.11	103.20	113.95
30	B	624	SQD	O48-C23-C24	3.10	121.64	111.91
25	C	512	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
25	B	612	CLA	CHB-C4A-NA	3.09	128.79	124.51
25	B	608	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
28	d	406	PL9	C40-C39-C41	3.08	120.45	115.27
25	b	601	CLA	CMB-C2B-C3B	3.08	130.44	124.68
26	a	608	PHO	CMC-C2C-C3C	3.07	130.73	124.94
28	D	406	PL9	C40-C39-C41	3.07	120.44	115.27
30	A	615	SQD	O48-C23-C24	3.07	121.53	111.91
25	c	508	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	b	603	CLA	CHD-C1D-ND	-3.06	121.64	124.45
25	c	508	CLA	CHB-C4A-NA	3.05	128.74	124.51
25	B	612	CLA	CHD-C1D-ND	-3.05	121.65	124.45
25	A	609	CLA	CHB-C4A-NA	3.05	128.73	124.51
31	C	519	DGD	O3E-C3E-C2E	-3.05	103.30	110.35
25	b	612	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
31	c	515	DGD	C3G-C2G-C1G	-3.04	104.60	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	507	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	B	616	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
35	F	101	HEM	CBD-CAD-C3D	-3.04	104.19	112.63
25	a	612	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	A	606	CLA	CHB-C4A-NA	3.03	128.71	124.51
25	C	506	CLA	CMB-C2B-C3B	3.03	130.35	124.68
25	A	607	CLA	CMB-C2B-C3B	3.03	130.35	124.68
28	D	406	PL9	C37-C38-C39	-3.03	120.36	127.66
25	c	509	CLA	CHB-C4A-NA	3.02	128.69	124.51
25	b	614	CLA	CHD-C1D-ND	-3.02	121.68	124.45
25	B	610	CLA	O2A-CGA-O1A	-3.01	115.99	123.59
25	b	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
27	B	617	BCR	C2-C1-C6	3.01	115.11	110.48
29	d	410	LMG	O6-C1-O1	-3.01	102.86	109.97
25	c	506	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	b	615	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
25	C	511	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	C	504	CLA	CHD-C1D-ND	-3.00	121.70	124.45
25	B	611	CLA	CMB-C2B-C3B	2.99	130.28	124.68
26	D	402	PHO	CMB-C2B-C3B	2.99	130.28	124.68
35	F	101	HEM	CBA-CAA-C2A	-2.99	107.51	112.62
30	a	614	SQD	O48-C23-C24	2.99	121.30	111.91
25	D	403	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
30	b	620	SQD	C3-C4-C5	2.99	115.58	110.24
31	c	516	DGD	O3G-C3G-C2G	-2.99	103.68	110.90
25	B	614	CLA	CMB-C2B-C3B	2.98	130.26	124.68
25	b	605	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
25	a	612	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	c	504	CLA	O2A-CGA-O1A	-2.98	116.08	123.59
25	C	502	CLA	CHD-C1D-ND	-2.97	121.73	124.45
30	b	620	SQD	O9-S-O7	-2.96	103.70	113.95
30	a	614	SQD	C1-C2-C3	-2.96	103.83	110.00
25	b	614	CLA	CMB-C2B-C3B	2.95	130.20	124.68
25	b	607	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
25	c	504	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
30	D	408	SQD	O9-S-O7	-2.95	103.75	113.95
25	b	604	CLA	C1-C2-C3	-2.94	120.95	126.04
25	b	612	CLA	C11-C12-C13	-2.94	106.41	115.92
26	A	608	PHO	O2D-CGD-O1D	-2.94	118.09	123.84
25	d	403	CLA	CHB-C4A-NA	2.94	128.57	124.51
30	b	620	SQD	O8-S-C6	2.93	110.41	105.74
25	D	404	CLA	C1B-CHB-C4A	-2.93	124.32	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	602	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	C	503	CLA	CMB-C2B-C3B	2.92	130.14	124.68
25	B	603	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
33	D	412	LHG	O8-C23-C24	2.91	121.03	111.91
31	c	517	DGD	CDB-CCB-CBB	-2.91	99.67	114.42
25	b	601	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	c	516	DGD	O6D-C1D-O3G	-2.90	103.09	109.97
25	D	403	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	b	611	CLA	CHD-C1D-ND	-2.90	121.79	124.45
31	h	101	DGD	CDB-CCB-CBB	-2.90	99.71	114.42
30	a	614	SQD	O7-S-C6	2.90	110.38	106.94
30	a	614	SQD	O9-S-O7	-2.90	103.92	113.95
25	B	601	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
25	b	604	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	c	509	CLA	CMB-C2B-C3B	2.89	130.09	124.68
25	B	609	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
26	d	402	PHO	O1D-CGD-CBD	2.89	129.55	124.74
25	B	615	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
27	k	102	BCR	C33-C5-C6	-2.89	121.29	124.53
27	t	101	BCR	C7-C8-C9	-2.88	121.88	126.23
30	b	620	SQD	O48-C23-C24	2.88	120.94	111.91
27	B	619	BCR	C3-C4-C5	-2.88	108.94	114.08
25	C	501	CLA	O2D-CGD-CBD	2.87	116.37	111.27
25	C	512	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	b	610	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
25	B	615	CLA	CHB-C4A-NA	2.87	128.47	124.51
25	C	509	CLA	CED-O2D-CGD	2.86	122.42	115.94
27	a	610	BCR	C27-C26-C25	2.86	126.89	122.73
30	f	101	SQD	O5-C5-C4	2.86	114.89	109.69
30	b	620	SQD	O47-C7-C8	2.85	117.65	111.50
28	A	611	PL9	C22-C23-C24	-2.85	120.80	127.66
25	C	512	CLA	C1-C2-C3	-2.85	121.12	126.04
31	C	517	DGD	O6D-C1D-O3G	-2.84	103.25	109.97
31	C	519	DGD	CDB-CCB-CBB	-2.84	100.02	114.42
25	b	610	CLA	C1-C2-C3	-2.83	121.14	126.04
27	c	514	BCR	C27-C26-C25	2.83	126.84	122.73
25	c	507	CLA	CMB-C2B-C3B	2.83	129.97	124.68
25	b	616	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
25	B	604	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	a	609	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
25	c	505	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	b	610	CLA	O2A-CGA-O1A	-2.82	116.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	604	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
35	e	101	HEM	CHC-C4B-C3B	2.82	128.88	124.57
25	a	607	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	d	403	CLA	O2A-CGA-O1A	-2.82	116.48	123.59
28	D	406	PL9	C42-C43-C44	-2.81	120.88	127.66
27	b	618	BCR	C15-C14-C13	-2.81	123.30	127.31
27	T	101	BCR	C33-C5-C6	-2.81	121.37	124.53
25	C	501	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
25	C	502	CLA	CMB-C2B-C3B	2.81	129.93	124.68
25	c	502	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
27	T	101	BCR	C27-C26-C25	2.80	126.80	122.73
25	C	503	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	c	520	LMG	O6-C1-O1	-2.80	103.34	109.97
27	t	101	BCR	C11-C10-C9	-2.80	123.31	127.31
27	k	103	BCR	C11-C10-C9	-2.80	123.32	127.31
25	b	610	CLA	CHB-C4A-NA	2.79	128.38	124.51
25	c	512	CLA	CHD-C1D-ND	-2.79	121.89	124.45
29	A	613	LMG	O6-C1-O1	-2.79	103.37	109.97
26	A	608	PHO	CMC-C2C-C3C	2.78	130.19	124.94
31	h	101	DGD	C1D-C2D-C3D	-2.78	104.20	110.00
31	a	616	DGD	CDB-CCB-CBB	-2.78	100.31	114.42
25	a	609	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	b	610	CLA	CMB-C2B-C3B	2.78	129.88	124.68
25	c	512	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	A	609	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
25	c	503	CLA	CMB-C2B-C3B	2.78	129.87	124.68
25	C	502	CLA	O2A-CGA-O1A	-2.77	116.59	123.59
33	e	102	LHG	O8-C23-C24	2.77	120.61	111.91
25	C	512	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	c	512	CLA	CMB-C2B-C3B	2.76	129.85	124.68
25	B	605	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
25	c	502	CLA	C1-C2-C3	-2.76	121.27	126.04
33	d	407	LHG	O8-C23-C24	2.76	120.56	111.91
25	c	513	CLA	CHB-C4A-NA	2.76	128.32	124.51
25	c	511	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	c	508	CLA	O2D-CGD-CBD	2.75	116.16	111.27
25	c	506	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	C	507	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
28	a	611	PL9	C40-C39-C41	2.75	119.89	115.27
25	d	403	CLA	O2D-CGD-CBD	2.74	116.14	111.27
25	B	606	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
27	t	101	BCR	C33-C5-C6	-2.74	121.45	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	616	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	b	614	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	b	616	CLA	CHD-C1D-ND	-2.74	121.94	124.45
33	D	409	LHG	O8-C23-C24	2.73	120.49	111.91
36	v	201	HEC	CMC-C2C-C3C	2.73	129.03	125.82
25	B	615	CLA	C6-C7-C8	-2.73	107.11	115.92
30	B	624	SQD	O8-S-C6	2.72	110.08	105.74
27	k	101	BCR	C7-C8-C9	-2.72	122.12	126.23
25	b	615	CLA	CHD-C1D-ND	-2.72	121.96	124.45
25	C	511	CLA	O2A-CGA-O1A	-2.71	116.74	123.59
31	c	515	DGD	O6D-C1D-O3G	-2.71	103.55	109.97
25	b	612	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
31	A	616	DGD	CDB-CCB-CBB	-2.71	100.66	114.42
25	c	513	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
27	k	101	BCR	C27-C26-C25	2.71	126.67	122.73
30	D	408	SQD	O48-C23-C24	2.70	120.39	111.91
27	d	405	BCR	C27-C26-C25	2.70	126.66	122.73
30	B	624	SQD	C4-C3-C2	2.70	115.53	110.82
31	C	518	DGD	CDB-CCB-CBB	-2.70	100.72	114.42
25	b	612	CLA	C4A-NA-C1A	2.70	107.92	106.71
31	A	616	DGD	O3G-C3G-C2G	-2.69	104.40	110.90
25	B	609	CLA	CHD-C1D-ND	-2.69	121.98	124.45
29	b	622	LMG	O2-C2-C1	-2.69	103.52	110.05
27	b	617	BCR	C35-C13-C14	-2.68	119.16	122.92
27	A	610	BCR	C15-C16-C17	-2.68	117.97	123.47
25	a	606	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
25	A	612	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
27	B	618	BCR	C15-C14-C13	-2.67	123.50	127.31
27	C	514	BCR	C15-C14-C13	-2.67	123.50	127.31
25	c	509	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
33	a	613	LHG	O8-C23-O10	-2.67	116.86	123.59
25	B	603	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
30	D	408	SQD	O6-C1-C2	2.67	112.47	108.30
25	B	605	CLA	CMB-C2B-C3B	2.66	129.66	124.68
28	D	406	PL9	C12-C13-C14	-2.66	121.25	127.66
25	B	611	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
25	B	614	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	b	614	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	b	608	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
25	C	510	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
25	b	614	CLA	C1-C2-C3	-2.65	121.45	126.04
25	D	403	CLA	C4A-NA-C1A	2.65	107.90	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	412	LHG	C11-C10-C9	-2.65	100.97	114.42
25	C	501	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
25	B	604	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
27	H	101	BCR	C27-C26-C25	2.65	126.58	122.73
25	c	507	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	B	604	CLA	CHB-C4A-NA	2.65	128.17	124.51
27	B	617	BCR	C27-C26-C25	2.65	126.57	122.73
27	k	101	BCR	C2-C1-C6	2.64	114.55	110.48
27	c	514	BCR	C15-C16-C17	-2.64	118.07	123.47
25	d	404	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	C	507	CLA	CMB-C2B-C3B	2.64	129.61	124.68
25	b	608	CLA	C2D-C1D-ND	-2.63	108.16	110.10
27	C	514	BCR	C2-C1-C6	2.63	114.53	110.48
35	e	101	HEM	C3B-C2B-C1B	2.63	108.44	106.49
25	C	510	CLA	O2D-CGD-CBD	2.63	115.95	111.27
25	C	511	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
25	c	504	CLA	CHD-C1D-ND	-2.63	122.04	124.45
25	C	509	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	c	503	CLA	C1-C2-C3	-2.63	121.50	126.04
25	B	603	CLA	CHD-C1D-ND	-2.63	122.04	124.45
32	d	411	STE	C3-C2-C1	-2.63	107.85	114.47
25	b	608	CLA	CHB-C4A-NA	2.63	128.14	124.51
31	c	515	DGD	C3D-C4D-C5D	-2.62	105.56	110.24
25	B	612	CLA	C1-C2-C3	-2.62	121.51	126.04
29	m	101	LMG	C6-C5-C4	-2.62	106.87	113.00
25	b	612	CLA	C1-C2-C3	-2.62	121.52	126.04
31	C	518	DGD	O5D-C6D-C5D	-2.62	104.20	109.05
25	b	605	CLA	C1-C2-C3	-2.62	121.52	126.04
25	b	601	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
33	E	101	LHG	O8-C23-C24	2.61	120.11	111.91
25	b	603	CLA	C4-C3-C5	2.61	119.66	115.27
27	H	101	BCR	C16-C15-C14	-2.61	118.13	123.47
31	H	102	DGD	O6D-C1D-O3G	-2.61	103.80	109.97
29	D	407	LMG	O6-C1-O1	-2.60	103.81	109.97
25	b	603	CLA	O2D-CGD-CBD	2.60	115.90	111.27
25	C	513	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
31	C	518	DGD	C3E-C4E-C5E	-2.60	105.60	110.24
28	d	406	PL9	C35-C34-C36	2.60	119.65	115.27
25	C	513	CLA	CHB-C4A-NA	2.60	128.11	124.51
29	D	411	LMG	O1-C7-C8	-2.60	104.89	111.78
25	c	510	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	f	101	SQD	O48-C23-C24	2.60	120.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	515	DGD	O5D-C6D-C5D	-2.60	104.24	109.05
31	H	102	DGD	CDB-CCB-CBB	-2.60	101.24	114.42
25	B	612	CLA	O2A-CGA-O1A	-2.59	117.04	123.59
25	B	606	CLA	O2D-CGD-CBD	2.59	115.88	111.27
27	d	405	BCR	C11-C10-C9	-2.59	123.61	127.31
25	b	616	CLA	CHB-C4A-NA	2.59	128.10	124.51
27	C	514	BCR	C15-C16-C17	-2.59	118.16	123.47
25	B	603	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
25	c	507	CLA	CHD-C1D-ND	-2.59	122.07	124.45
25	a	612	CLA	O2D-CGD-CBD	2.59	115.87	111.27
33	D	409	LHG	C20-C19-C18	-2.59	101.28	114.42
27	k	101	BCR	C15-C16-C17	-2.59	118.17	123.47
27	C	516	BCR	C27-C26-C25	2.59	126.48	122.73
25	b	609	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	A	609	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	a	612	CLA	CHD-C1D-ND	-2.58	122.08	124.45
28	d	406	PL9	C37-C38-C39	-2.58	121.45	127.66
29	A	613	LMG	C40-C39-C38	-2.58	101.33	114.42
31	c	516	DGD	CDB-CCB-CBB	-2.57	101.36	114.42
29	m	101	LMG	O3-C3-C2	-2.57	104.40	110.35
25	c	507	CLA	CHB-C4A-NA	2.57	128.07	124.51
28	d	406	PL9	C12-C13-C14	-2.57	121.48	127.66
30	D	408	SQD	O5-C5-C4	2.57	114.35	109.69
25	D	404	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	C	506	CLA	CHB-C4A-NA	2.56	128.05	124.51
33	D	410	LHG	C11-C10-C9	-2.56	101.42	114.42
29	c	518	LMG	O2-C2-C1	-2.56	103.83	110.05
25	C	504	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
25	B	601	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
25	c	503	CLA	C7-C6-C5	-2.56	106.41	113.36
28	A	611	PL9	C36-C34-C33	-2.56	115.94	121.12
27	c	514	BCR	C35-C13-C14	-2.56	119.34	122.92
25	b	608	CLA	CHD-C1D-ND	-2.55	122.11	124.45
36	v	201	HEC	C1D-C2D-C3D	-2.55	105.22	107.00
25	b	613	CLA	C2A-C1A-CHA	2.55	128.31	123.86
25	b	609	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
25	C	510	CLA	CHB-C4A-NA	2.54	128.03	124.51
33	D	412	LHG	C20-C19-C18	-2.54	101.51	114.42
27	c	514	BCR	C33-C5-C6	-2.54	121.67	124.53
25	b	613	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	C	501	CLA	CHD-C1D-ND	-2.54	122.12	124.45
27	d	405	BCR	C38-C26-C25	-2.54	121.67	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	607	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
25	c	513	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
25	D	403	CLA	O2D-CGD-CBD	2.54	115.78	111.27
25	C	503	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
27	B	619	BCR	C29-C30-C25	2.54	114.39	110.48
25	B	602	CLA	C1-C2-C3	-2.53	121.67	126.04
25	a	607	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
27	k	101	BCR	C3-C4-C5	-2.53	109.56	114.08
27	H	101	BCR	C11-C10-C9	-2.53	123.70	127.31
27	x	101	BCR	C35-C13-C14	-2.53	119.38	122.92
28	D	406	PL9	C27-C28-C29	-2.53	121.58	127.66
25	B	612	CLA	C11-C12-C13	-2.52	107.76	115.92
25	d	404	CLA	CHD-C1D-ND	-2.52	122.14	124.45
25	A	612	CLA	CHB-C4A-NA	2.52	128.00	124.51
27	C	515	BCR	C15-C16-C17	-2.52	118.31	123.47
25	A	606	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
25	C	506	CLA	C1-C2-C3	-2.52	121.69	126.04
31	C	518	DGD	O6D-C1D-O3G	-2.52	104.02	109.97
27	A	610	BCR	C2-C1-C6	2.52	114.35	110.48
25	B	612	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
25	B	604	CLA	CMB-C2B-C1B	-2.51	124.60	128.46
25	a	607	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
25	c	503	CLA	CHD-C1D-ND	-2.51	122.15	124.45
25	b	615	CLA	CHB-C4A-NA	2.51	127.98	124.51
29	A	613	LMG	C38-C37-C36	-2.51	101.69	114.42
31	c	517	DGD	O6D-C1D-O3G	-2.51	104.03	109.97
29	B	620	LMG	C40-C39-C38	-2.51	101.69	114.42
31	c	515	DGD	O3E-C3E-C2E	-2.51	104.55	110.35
25	b	609	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	C	505	CLA	CHB-C4A-NA	2.51	127.98	124.51
30	b	620	SQD	O9-S-C6	2.50	109.91	106.94
25	c	508	CLA	CHD-C1D-ND	-2.50	122.16	124.45
30	D	408	SQD	C1-C2-C3	-2.50	104.79	110.00
27	C	514	BCR	C24-C23-C22	-2.50	122.46	126.23
26	D	402	PHO	CMC-C2C-C3C	2.50	129.65	124.94
30	a	615	SQD	C46-C45-C44	-2.50	105.96	111.80
29	c	518	LMG	O6-C1-O1	-2.50	104.06	109.97
30	f	101	SQD	O5-C1-C2	-2.50	105.07	110.35
27	k	103	BCR	C27-C26-C25	2.49	126.35	122.73
27	C	515	BCR	C15-C14-C13	-2.49	123.75	127.31
35	F	101	HEM	CHC-C4B-NB	2.49	127.14	124.43
25	C	511	CLA	CHB-C4A-NA	2.49	127.95	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	612	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
25	A	612	CLA	O2D-CGD-CBD	2.49	115.69	111.27
27	t	101	BCR	C27-C26-C25	2.49	126.34	122.73
31	c	515	DGD	CDB-CCB-CBB	-2.49	101.80	114.42
33	a	613	LHG	C11-C10-C9	-2.49	101.80	114.42
29	C	520	LMG	O6-C1-O1	-2.49	104.09	109.97
26	d	402	PHO	CMA-C3A-C4A	-2.48	108.94	114.38
29	c	522	LMG	C38-C37-C36	-2.48	101.83	114.42
25	C	512	CLA	C6-C5-C3	-2.48	106.96	113.45
29	b	622	LMG	O1-C7-C8	-2.48	104.93	110.90
25	B	611	CLA	O2D-CGD-CBD	2.47	115.67	111.27
25	C	511	CLA	CHD-C1D-ND	-2.47	122.18	124.45
27	k	103	BCR	C16-C15-C14	-2.47	118.41	123.47
31	C	518	DGD	O2D-C2D-C1D	-2.47	104.05	110.05
33	d	408	LHG	O8-C23-C24	2.47	119.65	111.91
25	B	602	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
33	D	410	LHG	O8-C23-C24	2.46	119.64	111.91
25	c	504	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
25	c	511	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
31	c	516	DGD	C1D-C2D-C3D	-2.46	104.87	110.00
25	C	509	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
25	b	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
28	D	406	PL9	C22-C23-C24	-2.46	121.74	127.66
25	b	611	CLA	C1-C2-C3	-2.46	121.79	126.04
33	l	101	LHG	O8-C23-C24	2.45	119.61	111.91
32	B	627	STE	C3-C2-C1	-2.45	108.29	114.47
31	A	616	DGD	C1D-C2D-C3D	-2.45	104.89	110.00
25	B	605	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
27	D	405	BCR	C27-C26-C25	2.45	126.29	122.73
25	a	606	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
31	c	515	DGD	O3G-C1D-C2D	-2.45	104.48	108.30
25	A	607	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
25	B	604	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
27	C	514	BCR	C27-C26-C25	2.44	126.27	122.73
33	D	412	LHG	C18-C17-C16	-2.44	102.04	114.42
25	c	513	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
25	b	611	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
25	B	603	CLA	CHD-C4C-NC	2.44	128.04	124.20
32	m	102	STE	O2-C1-C2	2.44	121.86	114.03
25	b	614	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	d	404	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
25	B	601	CLA	CMB-C2B-C3B	2.43	129.23	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	409	LMG	C38-C37-C36	-2.43	102.07	114.42
25	C	508	CLA	CHD-C1D-C2D	2.43	130.58	125.48
25	D	404	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	B	602	CLA	CAC-C3C-C4C	2.43	127.96	124.81
29	A	613	LMG	O8-C28-O10	-2.43	117.46	123.59
28	a	611	PL9	O2-C1-C2	-2.43	116.22	121.78
29	C	520	LMG	C40-C39-C38	-2.43	102.10	114.42
25	c	512	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
25	B	601	CLA	CAA-CBA-CGA	-2.43	106.17	113.25
27	C	515	BCR	C27-C26-C25	2.43	126.25	122.73
25	b	601	CLA	O2D-CGD-CBD	2.42	115.58	111.27
35	e	101	HEM	C1B-NB-C4B	2.42	107.58	105.07
25	B	609	CLA	C7-C6-C5	-2.42	106.78	113.36
27	k	101	BCR	C15-C14-C13	-2.42	123.85	127.31
25	c	508	CLA	C1-C2-C3	-2.42	121.85	126.04
25	a	607	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
27	k	102	BCR	C27-C26-C25	2.42	126.25	122.73
32	m	102	STE	C3-C2-C1	-2.42	108.37	114.47
29	d	409	LMG	C40-C39-C38	-2.42	102.15	114.42
25	B	616	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
26	a	608	PHO	O2A-CGA-O1A	-2.42	117.49	123.59
29	d	410	LMG	C40-C39-C38	-2.42	102.16	114.42
25	b	607	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
26	D	402	PHO	O1D-CGD-CBD	2.42	128.76	124.74
25	b	613	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
27	x	101	BCR	C11-C10-C9	-2.41	123.86	127.31
25	C	512	CLA	O2D-CGD-CBD	2.41	115.56	111.27
29	c	518	LMG	C40-C39-C38	-2.41	102.18	114.42
29	B	620	LMG	C38-C37-C36	-2.41	102.19	114.42
31	A	616	DGD	C4E-C3E-C2E	-2.41	106.61	110.82
28	a	611	PL9	C37-C38-C39	-2.41	121.86	127.66
30	f	101	SQD	C1-O5-C5	-2.41	108.96	113.69
29	c	522	LMG	C40-C39-C38	-2.41	102.21	114.42
25	b	607	CLA	C1-O2A-CGA	2.41	122.76	116.44
25	b	614	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
29	b	622	LMG	O1-C1-C2	-2.40	104.55	108.30
25	b	611	CLA	CHB-C4A-NA	2.40	127.83	124.51
27	c	514	BCR	C7-C8-C9	-2.40	122.60	126.23
26	a	608	PHO	OBD-CAD-CBD	-2.40	122.30	125.82
25	B	616	CLA	C1-C2-C3	-2.40	121.89	126.04
28	A	611	PL9	O2-C1-C2	-2.40	116.28	121.78
31	h	101	DGD	O6E-C5E-C4E	2.40	114.05	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	603	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
27	a	610	BCR	C33-C5-C6	-2.40	121.84	124.53
33	d	407	LHG	C11-C10-C9	-2.40	102.26	114.42
25	C	501	CLA	CHB-C4A-NA	2.40	127.82	124.51
25	b	615	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
27	C	516	BCR	C33-C5-C6	-2.39	121.84	124.53
28	D	406	PL9	C32-C33-C34	-2.39	121.90	127.66
35	e	101	HEM	CAB-C3B-C2B	-2.39	120.72	128.60
30	a	614	SQD	C44-O6-C1	-2.39	109.07	113.74
25	c	505	CLA	C1-C2-C3	-2.39	121.91	126.04
25	b	610	CLA	O1D-CGD-CBD	2.39	129.38	124.48
25	B	601	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
33	E	101	LHG	C11-C10-C9	-2.39	102.29	114.42
25	C	510	CLA	C11-C12-C13	-2.39	108.20	115.92
27	A	610	BCR	C27-C26-C25	2.39	126.20	122.73
27	x	101	BCR	C27-C26-C25	2.38	126.19	122.73
33	d	407	LHG	C18-C17-C16	-2.38	102.33	114.42
25	a	606	CLA	CHB-C4A-NA	2.38	127.80	124.51
27	b	619	BCR	C29-C30-C25	2.38	114.14	110.48
27	b	618	BCR	C27-C26-C25	2.37	126.18	122.73
29	c	520	LMG	C40-C39-C38	-2.37	102.37	114.42
25	b	613	CLA	CHA-C1A-NA	-2.37	120.96	126.40
25	B	606	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
31	h	101	DGD	CBB-CAB-C9B	-2.37	102.40	114.42
25	B	604	CLA	O2A-C1-C2	2.37	114.86	108.64
32	d	411	STE	O2-C1-C2	2.37	121.63	114.03
27	b	618	BCR	C11-C10-C9	-2.36	123.94	127.31
25	c	501	CLA	CHD-C1D-ND	-2.36	122.28	124.45
29	B	620	LMG	C1-O6-C5	-2.36	109.05	113.69
25	C	512	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
29	d	410	LMG	O2-C2-C1	-2.36	104.31	110.05
28	a	611	PL9	O2-C1-C6	2.36	124.68	120.59
28	A	611	PL9	C20-C19-C21	2.36	119.24	115.27
30	A	614	SQD	O48-C23-C24	2.36	119.32	111.91
33	D	409	LHG	C27-C26-C25	-2.36	102.45	114.42
29	m	101	LMG	O1-C7-C8	-2.36	105.21	110.90
29	C	520	LMG	C1-O6-C5	-2.36	109.06	113.69
31	A	616	DGD	O5D-C6D-C5D	-2.36	104.69	109.05
25	C	505	CLA	C1-C2-C3	-2.35	121.97	126.04
30	a	615	SQD	C9-C8-C7	-2.35	105.07	113.62
27	B	618	BCR	C2-C1-C6	2.35	114.10	110.48
25	B	604	CLA	CMB-C2B-C3B	2.35	129.07	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	404	CLA	C2D-C1D-ND	-2.35	108.37	110.10
25	c	507	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
31	a	616	DGD	C8B-C7B-C6B	-2.35	102.50	114.42
28	d	406	PL9	C36-C34-C33	-2.35	116.37	121.12
25	b	608	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
25	c	503	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	c	513	CLA	CHD-C1D-ND	-2.34	122.30	124.45
27	B	617	BCR	C3-C4-C5	-2.34	109.90	114.08
30	A	614	SQD	O47-C7-O49	-2.34	118.05	123.70
25	A	609	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
25	C	507	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	c	503	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
25	b	605	CLA	CMB-C2B-C3B	2.33	129.04	124.68
26	A	608	PHO	O2D-CGD-CBD	2.33	113.95	111.00
25	c	501	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
33	e	102	LHG	C11-C10-C9	-2.33	102.61	114.42
33	E	101	LHG	C20-C19-C18	-2.32	102.63	114.42
33	e	102	LHG	C20-C19-C18	-2.32	102.63	114.42
25	D	403	CLA	CED-O2D-CGD	2.32	121.19	115.94
29	m	101	LMG	C38-C37-C36	-2.32	102.64	114.42
25	c	510	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
27	b	619	BCR	C27-C26-C25	2.32	126.10	122.73
31	H	102	DGD	O1G-C1A-O1A	-2.32	117.74	123.59
25	b	605	CLA	CHD-C1D-ND	-2.32	122.32	124.45
31	C	517	DGD	CBB-CAB-C9B	-2.32	102.66	114.42
25	c	509	CLA	O1D-CGD-CBD	2.32	129.22	124.48
25	c	507	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
25	b	616	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
27	C	514	BCR	C33-C5-C6	-2.32	121.93	124.53
29	m	101	LMG	C40-C39-C38	-2.31	102.68	114.42
26	a	608	PHO	C1-C2-C3	-2.31	122.04	126.04
35	e	101	HEM	C4D-ND-C1D	2.31	107.46	105.07
25	c	507	CLA	C2A-C1A-CHA	2.31	127.90	123.86
25	b	604	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	B	610	CLA	O2D-CGD-CBD	2.31	115.37	111.27
25	A	607	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
35	e	101	HEM	C4B-CHC-C1C	2.31	125.61	122.56
25	B	616	CLA	CHD-C1D-ND	-2.31	122.33	124.45
25	B	613	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
25	B	601	CLA	O1D-CGD-CBD	2.30	129.20	124.48
33	l	101	LHG	C11-C10-C9	-2.30	102.73	114.42
25	C	503	CLA	O2A-C1-C2	-2.30	102.59	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	617	BCR	C27-C26-C25	2.30	126.07	122.73
28	a	611	PL9	C20-C19-C21	2.30	119.14	115.27
25	c	503	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
25	d	403	CLA	C4-C3-C5	2.30	119.14	115.27
25	A	609	CLA	CHD-C4C-NC	2.30	127.82	124.20
25	B	615	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
25	D	404	CLA	O2D-CGD-CBD	2.30	115.35	111.27
25	D	403	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
29	B	620	LMG	O2-C2-C1	-2.29	104.48	110.05
27	b	617	BCR	C29-C30-C25	2.29	114.01	110.48
25	b	604	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	C	510	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	b	605	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
25	D	404	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
33	B	623	LHG	C20-C19-C18	-2.28	102.84	114.42
25	C	502	CLA	CHA-C1A-NA	-2.28	121.17	126.40
25	C	513	CLA	CHD-C1D-ND	-2.28	122.36	124.45
27	k	103	BCR	C33-C5-C6	-2.28	121.97	124.53
27	k	102	BCR	C24-C23-C22	-2.28	122.79	126.23
30	f	101	SQD	O8-S-C6	2.28	109.37	105.74
25	C	504	CLA	CMB-C2B-C3B	2.28	128.94	124.68
33	E	101	LHG	C27-C26-C25	-2.28	102.86	114.42
25	B	603	CLA	C2D-C1D-ND	-2.28	108.42	110.10
27	B	618	BCR	C27-C26-C25	2.28	126.03	122.73
31	c	515	DGD	CBB-CAB-C9B	-2.27	102.88	114.42
25	d	403	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
33	D	409	LHG	O8-C23-O10	-2.27	117.86	123.59
25	c	509	CLA	CHD-C1D-ND	-2.27	122.37	124.45
25	B	615	CLA	CMB-C2B-C3B	2.27	128.92	124.68
26	d	402	PHO	O2D-CGD-O1D	-2.27	119.40	123.84
27	B	617	BCR	C11-C10-C9	-2.27	124.07	127.31
25	c	501	CLA	C1-C2-C3	-2.27	122.12	126.04
31	a	616	DGD	CFB-CEB-CDB	-2.27	102.92	114.42
32	j	101	STE	O2-C1-C2	2.27	121.31	114.03
25	c	503	CLA	C11-C12-C13	-2.26	108.60	115.92
29	c	522	LMG	O6-C1-O1	-2.26	104.61	109.97
25	a	607	CLA	O2D-CGD-CBD	2.26	115.29	111.27
28	A	611	PL9	C27-C28-C29	-2.26	122.21	127.66
25	B	601	CLA	C2A-C1A-CHA	2.26	127.82	123.86
31	A	616	DGD	O6D-C1D-O3G	-2.26	104.62	109.97
25	b	610	CLA	CHD-C1D-ND	-2.26	122.38	124.45
36	v	201	HEC	CMB-C2B-C1B	-2.26	124.99	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	513	CLA	C2D-C1D-ND	-2.26	108.44	110.10
25	b	602	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
27	B	618	BCR	C35-C13-C14	-2.26	119.76	122.92
25	b	607	CLA	CHB-C4A-NA	2.25	127.63	124.51
27	H	101	BCR	C2-C1-C6	2.25	113.95	110.48
29	c	520	LMG	O3-C3-C2	-2.25	105.14	110.35
25	C	507	CLA	CHD-C1D-ND	-2.25	122.38	124.45
25	C	506	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
28	a	611	PL9	C7-C8-C9	-2.25	123.04	126.79
31	A	616	DGD	C3E-C4E-C5E	-2.25	106.22	110.24
25	B	614	CLA	O2D-CGD-CBD	2.25	115.27	111.27
31	a	616	DGD	C5B-C4B-C3B	-2.25	103.00	114.42
29	D	407	LMG	O2-C2-C1	-2.25	104.58	110.05
31	A	616	DGD	O2D-C2D-C1D	-2.25	104.58	110.05
29	B	622	LMG	C38-C37-C36	-2.25	103.02	114.42
25	B	605	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
25	c	505	CLA	CHD-C1D-ND	-2.24	122.39	124.45
31	h	101	DGD	O6E-C5E-C6E	-2.24	100.86	106.44
33	D	410	LHG	C27-C26-C25	-2.24	103.04	114.42
25	b	611	CLA	C7-C6-C5	-2.24	107.27	113.36
25	b	615	CLA	CMB-C2B-C3B	2.24	128.87	124.68
31	C	519	DGD	CBB-CAB-C9B	-2.24	103.06	114.42
29	c	518	LMG	O1-C7-C8	-2.24	105.50	110.90
31	c	517	DGD	C8B-C7B-C6B	-2.24	103.07	114.42
29	b	622	LMG	C40-C39-C38	-2.24	103.07	114.42
25	c	506	CLA	CHD-C1D-ND	-2.23	122.40	124.45
26	a	608	PHO	O2D-CGD-O1D	-2.23	119.47	123.84
29	D	411	LMG	O7-C10-O9	-2.23	118.31	123.70
32	B	628	STE	O2-C1-C2	2.23	121.19	114.03
28	A	611	PL9	O2-C1-C6	2.23	124.45	120.59
25	B	607	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
25	b	609	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
27	B	617	BCR	C38-C26-C27	-2.23	109.33	113.62
25	B	613	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	B	611	CLA	CHD-C1D-ND	-2.23	122.41	124.45
25	B	605	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	a	606	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
28	D	406	PL9	C36-C34-C33	-2.23	116.61	121.12
25	C	505	CLA	C2D-C1D-ND	-2.22	108.47	110.10
32	E	102	STE	O2-C1-C2	2.22	121.17	114.03
32	b	624	STE	C3-C2-C1	-2.22	108.87	114.47
27	k	101	BCR	C11-C10-C9	-2.22	124.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	612	CLA	CHD-C1D-ND	-2.22	122.41	124.45
35	F	101	HEM	C4B-CHC-C1C	2.22	125.48	122.56
29	m	101	LMG	O7-C10-O9	-2.22	118.35	123.70
25	D	403	CLA	C4-C3-C5	2.21	119.00	115.27
31	h	101	DGD	C7B-C6B-C5B	-2.21	103.20	114.42
25	C	504	CLA	CHB-C4A-NA	2.21	127.57	124.51
27	t	101	BCR	C15-C14-C13	-2.21	124.16	127.31
29	C	520	LMG	C38-C37-C36	-2.21	103.22	114.42
25	b	615	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
33	d	407	LHG	C20-C19-C18	-2.20	103.24	114.42
29	m	101	LMG	O6-C1-O1	-2.20	104.76	109.97
27	T	101	BCR	C35-C13-C14	-2.20	119.84	122.92
33	D	410	LHG	C18-C17-C16	-2.20	103.25	114.42
25	b	604	CLA	C6-C7-C8	-2.20	108.81	115.92
29	b	622	LMG	C8-O7-C10	2.20	123.20	117.79
25	D	403	CLA	CHD-C1D-ND	-2.19	122.44	124.45
31	h	101	DGD	O6D-C1D-O3G	-2.19	104.79	109.97
25	C	502	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
29	C	520	LMG	O3-C3-C2	-2.18	105.30	110.35
25	C	501	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
31	c	516	DGD	C5B-C4B-C3B	-2.18	103.36	114.42
27	k	101	BCR	C24-C23-C22	-2.18	122.94	126.23
25	B	609	CLA	C1-C2-C3	-2.18	122.28	126.04
25	b	615	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
25	B	613	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
25	C	504	CLA	CHD-C4C-NC	2.18	127.63	124.20
29	c	518	LMG	C38-C37-C36	-2.18	103.38	114.42
25	B	606	CLA	CHD-C1D-ND	-2.18	122.45	124.45
27	B	617	BCR	C33-C5-C6	-2.17	122.09	124.53
31	C	518	DGD	C1D-C2D-C3D	-2.17	105.47	110.00
32	B	625	STE	C3-C2-C1	-2.17	109.00	114.47
33	D	409	LHG	C18-C17-C16	-2.17	103.41	114.42
29	C	520	LMG	O8-C28-O10	-2.17	118.12	123.59
31	C	517	DGD	CAB-C9B-C8B	-2.17	103.41	114.42
26	D	402	PHO	O2D-CGD-CBD	2.17	113.74	111.00
25	A	606	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
25	b	613	CLA	O2D-CGD-CBD	2.17	115.12	111.27
29	d	410	LMG	O1-C7-C8	-2.17	105.67	110.90
31	c	517	DGD	CBB-CAB-C9B	-2.17	103.43	114.42
25	C	506	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
25	b	609	CLA	C3C-C4C-NC	-2.16	108.14	110.57
31	C	517	DGD	C6B-C5B-C4B	-2.16	103.44	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	506	CLA	O1D-CGD-CBD	2.16	128.91	124.48
25	a	609	CLA	CMD-C2D-C3D	2.16	132.59	127.61
29	d	410	LMG	C38-C37-C36	-2.16	103.46	114.42
25	B	608	CLA	O2D-CGD-CBD	2.16	115.10	111.27
29	b	622	LMG	C42-C41-C40	-2.16	103.47	114.42
25	B	606	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
31	A	616	DGD	CBB-CAB-C9B	-2.16	103.48	114.42
33	E	101	LHG	C18-C17-C16	-2.16	103.48	114.42
27	C	515	BCR	C35-C13-C14	-2.16	119.90	122.92
27	T	101	BCR	C38-C26-C27	-2.15	109.48	113.62
25	b	613	CLA	C7-C6-C5	-2.15	107.51	113.36
25	C	501	CLA	CMB-C2B-C3B	2.15	128.71	124.68
33	e	102	LHG	C18-C17-C16	-2.15	103.50	114.42
25	A	607	CLA	O2D-CGD-CBD	2.15	115.09	111.27
27	d	405	BCR	C1-C6-C5	-2.15	119.58	122.61
25	D	403	CLA	CHB-C4A-NA	2.15	127.48	124.51
31	C	518	DGD	CAB-C9B-C8B	-2.15	103.52	114.42
25	b	610	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
27	B	618	BCR	C3-C4-C5	-2.15	110.24	114.08
31	c	517	DGD	CAB-C9B-C8B	-2.15	103.52	114.42
25	c	506	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
25	B	604	CLA	O2D-CGD-CBD	2.15	115.08	111.27
31	c	515	DGD	O1G-C1A-C2A	-2.14	105.18	111.91
25	c	504	CLA	O2D-CGD-CBD	2.14	115.08	111.27
25	c	510	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
30	A	614	SQD	O6-C44-C45	-2.14	105.73	110.90
29	B	620	LMG	O7-C10-O9	-2.14	118.53	123.70
27	H	101	BCR	C16-C17-C18	-2.14	124.26	127.31
25	A	607	CLA	C1D-ND-C4D	2.14	107.86	106.33
29	d	410	LMG	O3-C3-C2	-2.14	105.40	110.35
25	a	609	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
31	C	517	DGD	C3D-C4D-C5D	-2.14	106.42	110.24
29	D	407	LMG	O3-C3-C2	-2.14	105.41	110.35
25	b	604	CLA	O2D-CGD-CBD	2.14	115.06	111.27
25	C	504	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
27	k	101	BCR	C38-C26-C25	-2.13	122.13	124.53
29	c	522	LMG	C1-O6-C5	-2.13	109.50	113.69
26	A	608	PHO	C1-C2-C3	-2.13	122.36	126.04
28	d	406	PL9	O2-C1-C2	-2.13	116.89	121.78
25	B	602	CLA	CHD-C1D-ND	-2.13	122.50	124.45
25	c	502	CLA	CHB-C4A-NA	2.13	127.46	124.51
26	a	608	PHO	CMA-C3A-C4A	-2.13	109.71	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	409	LHG	C11-C10-C9	-2.13	103.62	114.42
27	x	101	BCR	C34-C9-C10	-2.13	119.94	122.92
27	d	405	BCR	C30-C25-C26	-2.13	119.62	122.61
25	B	606	CLA	CMB-C2B-C3B	2.13	128.66	124.68
25	b	604	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
29	c	522	LMG	O7-C10-O9	-2.13	118.56	123.70
28	a	611	PL9	C35-C34-C36	2.12	118.84	115.27
30	f	101	SQD	C1-C2-C3	-2.12	105.58	110.00
25	a	612	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
27	b	617	BCR	C33-C5-C6	-2.12	122.15	124.53
27	b	618	BCR	C8-C7-C6	-2.12	121.25	127.20
31	A	616	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
31	H	102	DGD	CBB-CAB-C9B	-2.12	103.67	114.42
29	D	407	LMG	C40-C39-C38	-2.12	103.67	114.42
27	k	101	BCR	C33-C5-C6	-2.12	122.15	124.53
31	H	102	DGD	O6E-C5E-C4E	2.12	113.54	109.69
25	c	504	CLA	CHB-C4A-NA	2.12	127.44	124.51
29	D	407	LMG	C38-C37-C36	-2.12	103.68	114.42
25	b	612	CLA	O2D-CGD-CBD	2.12	115.03	111.27
25	c	511	CLA	CHD-C1D-ND	-2.12	122.51	124.45
31	c	516	DGD	C8B-C7B-C6B	-2.11	103.69	114.42
25	b	602	CLA	O2D-CGD-CBD	2.11	115.02	111.27
32	C	521	STE	O2-C1-C2	2.11	120.81	114.03
31	C	518	DGD	CBB-CAB-C9B	-2.11	103.71	114.42
25	A	606	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
25	A	606	CLA	CHD-C1D-ND	-2.11	122.52	124.45
31	H	102	DGD	C8B-C7B-C6B	-2.11	103.72	114.42
29	m	101	LMG	C9-C8-C7	-2.11	106.80	111.79
35	F	101	HEM	C4D-ND-C1D	2.11	107.25	105.07
25	c	505	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	C	505	CLA	O1D-CGD-CBD	2.11	128.79	124.48
29	c	520	LMG	C38-C37-C36	-2.11	103.74	114.42
30	a	614	SQD	O5-C1-C2	-2.10	105.89	110.35
29	A	613	LMG	O1-C7-C8	-2.10	105.82	110.90
25	C	507	CLA	C2A-C1A-CHA	2.10	127.53	123.86
33	l	101	LHG	C18-C17-C16	-2.10	103.76	114.42
25	C	505	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	b	602	CLA	CHD-C1D-ND	-2.10	122.53	124.45
31	h	101	DGD	C6D-C5D-C4D	2.10	116.47	112.09
33	l	101	LHG	C20-C19-C18	-2.09	103.79	114.42
25	B	608	CLA	CHB-C4A-NA	2.09	127.41	124.51
33	d	407	LHG	O8-C23-O10	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	615	CLA	CHD-C4C-NC	2.09	127.50	124.20
27	D	405	BCR	C38-C26-C25	-2.09	122.18	124.53
27	K	101	BCR	C24-C23-C22	-2.09	123.07	126.23
25	a	606	CLA	C7-C6-C5	-2.09	107.68	113.36
25	b	614	CLA	O2A-C1-C2	-2.09	103.14	108.64
25	b	608	CLA	CHD-C4C-NC	2.09	127.50	124.20
25	B	609	CLA	C16-C15-C13	-2.09	109.16	115.92
27	d	405	BCR	C33-C5-C6	-2.09	122.18	124.53
32	j	101	STE	C3-C2-C1	-2.09	109.21	114.47
28	D	406	PL9	O2-C1-C2	-2.09	117.00	121.78
25	B	604	CLA	CHA-C4D-ND	2.09	136.86	132.50
25	A	607	CLA	CHB-C4A-NA	2.08	127.39	124.51
30	D	408	SQD	C3-C4-C5	2.08	113.95	110.24
27	d	405	BCR	C37-C22-C21	-2.08	120.01	122.92
31	c	516	DGD	C3E-C4E-C5E	-2.08	106.53	110.24
25	C	511	CLA	C1-C2-C3	-2.08	122.45	126.04
29	B	620	LMG	O1-C7-C8	-2.08	105.88	110.90
25	a	612	CLA	C2D-C1D-ND	-2.08	108.57	110.10
32	B	625	STE	O2-C1-C2	2.08	120.70	114.03
25	b	604	CLA	C11-C12-C13	-2.08	109.21	115.92
31	H	102	DGD	C1E-O6E-C5E	2.08	117.76	113.69
25	C	508	CLA	C2D-C1D-ND	-2.07	108.58	110.10
31	C	518	DGD	C5B-C4B-C3B	-2.07	103.89	114.42
27	b	618	BCR	C30-C25-C26	-2.07	119.69	122.61
25	a	607	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	b	602	CLA	C1-C2-C3	-2.07	122.46	126.04
31	c	516	DGD	O2D-C2D-C1D	-2.07	105.01	110.05
25	C	501	CLA	C2D-C1D-ND	-2.07	108.58	110.10
31	a	616	DGD	C1G-C2G-C3G	-2.07	106.95	111.80
25	a	612	CLA	CHB-C4A-NA	2.07	127.38	124.51
31	h	101	DGD	O3E-C3E-C2E	-2.07	105.56	110.35
25	B	602	CLA	CHA-C4D-ND	2.07	136.83	132.50
25	C	508	CLA	O2D-CGD-CBD	2.07	114.94	111.27
25	b	615	CLA	CHA-C4D-ND	2.07	136.83	132.50
33	D	412	LHG	C15-C14-C13	-2.07	103.93	114.42
25	b	608	CLA	O2D-CGD-CBD	2.07	114.94	111.27
27	T	101	BCR	C2-C1-C6	2.07	113.66	110.48
25	c	501	CLA	O2D-CGD-CBD	2.06	114.94	111.27
25	B	614	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
31	c	515	DGD	C1D-C2D-C3D	-2.06	105.70	110.00
33	e	102	LHG	C27-C26-C25	-2.06	103.97	114.42
33	d	408	LHG	C27-C26-C25	-2.06	103.97	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	609	CLA	CED-O2D-CGD	2.06	120.59	115.94
27	t	101	BCR	C38-C26-C27	-2.06	109.66	113.62
27	c	514	BCR	C2-C1-C6	2.06	113.65	110.48
31	h	101	DGD	C1E-O6E-C5E	2.05	117.72	113.69
25	C	509	CLA	CHD-C1D-ND	-2.05	122.57	124.45
29	c	520	LMG	C42-C41-C40	-2.05	104.00	114.42
27	x	101	BCR	C3-C4-C5	-2.05	110.41	114.08
29	c	520	LMG	C9-C8-C7	-2.05	106.93	111.79
25	B	605	CLA	C16-C15-C13	-2.05	109.28	115.92
32	C	522	STE	O2-C1-C2	2.05	120.62	114.03
31	h	101	DGD	O5D-C1E-C2E	2.05	111.50	108.30
26	D	402	PHO	CBA-CAA-C2A	-2.05	107.82	113.81
29	c	518	LMG	O8-C28-O10	-2.05	118.42	123.59
31	c	516	DGD	CBB-CAB-C9B	-2.05	104.03	114.42
31	A	616	DGD	C7A-C6A-C5A	-2.05	104.03	114.42
25	B	603	CLA	C3C-C4C-NC	-2.05	108.28	110.57
33	a	613	LHG	C20-C19-C18	-2.05	104.04	114.42
25	C	507	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
25	b	613	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
33	B	623	LHG	C27-C26-C25	-2.04	104.05	114.42
29	B	620	LMG	C22-C21-C20	-2.04	104.06	114.42
29	B	622	LMG	O7-C10-O9	-2.04	118.21	123.30
36	V	201	HEC	CAD-CBD-CGD	-2.04	108.04	113.76
33	a	613	LHG	O8-C6-C5	-2.04	102.50	108.43
31	H	102	DGD	C1D-C2D-C3D	-2.04	105.75	110.00
28	d	406	PL9	C42-C43-C44	-2.04	122.75	127.66
26	d	402	PHO	C1A-C2A-C3A	-2.04	100.90	102.84
25	C	506	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	C	505	CLA	C16-C15-C13	-2.04	109.33	115.92
25	B	603	CLA	O2D-CGD-CBD	2.04	114.89	111.27
25	B	611	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
31	C	518	DGD	C3D-C4D-C5D	-2.03	106.61	110.24
33	a	613	LHG	C18-C17-C16	-2.03	104.10	114.42
35	e	101	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
31	C	519	DGD	CAB-C9B-C8B	-2.03	104.10	114.42
29	D	407	LMG	O1-C7-C8	-2.03	105.99	110.90
25	d	404	CLA	CHA-C1A-NA	-2.03	121.74	126.40
27	D	405	BCR	C33-C5-C6	-2.03	122.25	124.53
25	a	612	CLA	C3C-C4C-NC	-2.03	108.29	110.57
25	c	505	CLA	O2D-CGD-CBD	2.03	114.88	111.27
25	c	512	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
28	a	611	PL9	C31-C32-C33	-2.03	105.21	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	514	BCR	C35-C13-C14	-2.03	120.08	122.92
27	H	101	BCR	C35-C13-C12	2.03	121.27	118.08
25	B	615	CLA	C3C-C4C-NC	-2.02	108.30	110.57
29	c	522	LMG	O8-C28-O10	-2.02	118.48	123.59
25	B	604	CLA	C3C-C4C-NC	-2.02	108.30	110.57
25	B	609	CLA	CHB-C4A-NA	2.02	127.31	124.51
25	c	505	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
35	e	101	HEM	CMC-C2C-C3C	2.02	128.46	124.68
27	B	617	BCR	C15-C16-C17	-2.02	119.34	123.47
28	A	611	PL9	C31-C32-C33	-2.02	105.25	111.88
25	c	502	CLA	O1D-CGD-CBD	2.02	128.61	124.48
25	C	511	CLA	CHD-C4C-NC	2.02	127.38	124.20
25	c	507	CLA	CHA-C1A-NA	-2.02	121.78	126.40
27	T	101	BCR	C31-C1-C6	2.02	113.57	110.30
25	C	513	CLA	O1D-CGD-CBD	2.02	128.61	124.48
27	K	101	BCR	C27-C26-C25	2.02	125.66	122.73
25	B	615	CLA	C16-C15-C13	-2.02	109.40	115.92
25	c	502	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
25	c	501	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
27	K	101	BCR	C15-C14-C13	-2.01	124.44	127.31
28	D	406	PL9	C35-C34-C36	2.01	118.66	115.27
29	d	410	LMG	C6-C5-C4	-2.01	108.29	113.00
25	b	608	CLA	CHD-C1D-C2D	2.01	129.70	125.48
25	A	612	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
25	B	612	CLA	O2D-CGD-CBD	2.01	114.84	111.27
30	a	615	SQD	O49-C7-C8	-2.01	115.89	123.73
27	T	101	BCR	C1-C6-C5	-2.01	119.78	122.61
25	b	612	CLA	C16-C15-C13	-2.01	109.43	115.92
29	b	622	LMG	C24-C23-C22	-2.01	104.23	114.42
31	H	102	DGD	CAB-C9B-C8B	-2.01	104.23	114.42
31	a	616	DGD	CBB-CAB-C9B	-2.01	104.23	114.42
25	B	605	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
29	b	622	LMG	C3-C4-C5	-2.01	106.66	110.24
33	l	101	LHG	C27-C26-C25	-2.01	104.24	114.42
27	x	101	BCR	C16-C15-C14	-2.00	119.37	123.47
29	b	622	LMG	O5-C6-C5	-2.00	104.41	111.29
31	h	101	DGD	CAB-C9B-C8B	-2.00	104.25	114.42
25	d	403	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
31	c	517	DGD	O5D-C6D-C5D	-2.00	105.34	109.05
27	B	619	BCR	C34-C9-C10	-2.00	120.12	122.92
29	B	622	LMG	C30-C29-C28	-2.00	109.42	114.47
25	b	608	CLA	O2A-C1-C2	-2.00	103.37	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	516	BCR	C8-C7-C6	-2.00	121.58	127.20
25	B	616	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (60) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
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	403	CLA	ND
25	d	404	CLA	ND

All (1750) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	612	CLA	CHA-CBD-CGD-O2D
25	A	612	CLA	C14-C13-C15-C16
25	B	601	CLA	C1A-C2A-CAA-CBA
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	C4-C3-C5-C6
25	C	502	CLA	C14-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	a	607	CLA	CHA-CBD-CGD-O1D
25	a	607	CLA	CHA-CBD-CGD-O2D
25	a	612	CLA	CHA-CBD-CGD-O1D
25	a	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	b	601	CLA	C1A-C2A-CAA-CBA
25	b	603	CLA	C2-C3-C5-C6
25	b	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	C14-C13-C15-C16
25	b	614	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O1D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	C2-C3-C5-C6
25	b	614	CLA	C4-C3-C5-C6
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	C2-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
25	c	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	512	CLA	C6-C7-C8-C9
27	B	617	BCR	C1-C6-C7-C8
27	B	619	BCR	C11-C12-C13-C35
27	B	619	BCR	C37-C22-C23-C24
27	C	515	BCR	C7-C8-C9-C34
27	C	515	BCR	C11-C12-C13-C14
27	C	515	BCR	C11-C12-C13-C35
27	C	516	BCR	C5-C6-C7-C8
27	C	516	BCR	C7-C8-C9-C34
27	C	516	BCR	C20-C21-C22-C37
27	C	516	BCR	C37-C22-C23-C24
27	D	405	BCR	C37-C22-C23-C24
27	K	101	BCR	C37-C22-C23-C24
27	b	619	BCR	C37-C22-C23-C24
27	d	405	BCR	C20-C21-C22-C37
27	d	405	BCR	C37-C22-C23-C24
27	d	405	BCR	C22-C23-C24-C25
27	k	101	BCR	C23-C24-C25-C30
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C7-C8-C9-C34
27	t	101	BCR	C7-C8-C9-C34
27	x	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C22-C23-C24-C25
28	A	611	PL9	C22-C23-C24-C26
28	A	611	PL9	C35-C34-C36-C37
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C37-C38-C39-C41
28	A	611	PL9	C38-C39-C41-C42
28	A	611	PL9	C40-C39-C41-C42
28	D	406	PL9	C32-C33-C34-C36
28	D	406	PL9	C47-C48-C49-C51
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C23-C24-C26-C27
28	a	611	PL9	C32-C33-C34-C35
28	a	611	PL9	C32-C33-C34-C36
28	a	611	PL9	C33-C34-C36-C37
28	a	611	PL9	C35-C34-C36-C37
28	d	406	PL9	C32-C33-C34-C35
28	d	406	PL9	C32-C33-C34-C36
28	d	406	PL9	C38-C39-C41-C42
28	d	406	PL9	C42-C43-C44-C46
29	A	613	LMG	O6-C1-O1-C7
29	A	613	LMG	O9-C10-O7-C8
29	D	411	LMG	C11-C10-O7-C8
29	b	622	LMG	C2-C1-O1-C7
29	b	622	LMG	O6-C1-O1-C7
29	c	522	LMG	O6-C1-O1-C7
30	B	624	SQD	C2-C1-O6-C44
30	B	624	SQD	O5-C1-O6-C44
30	B	624	SQD	O6-C44-C45-O47
30	B	624	SQD	O49-C7-O47-C45
30	B	624	SQD	C8-C7-O47-C45
30	D	408	SQD	C45-C44-O6-C1
30	a	614	SQD	O6-C44-C45-O47
30	a	615	SQD	O47-C45-C46-O48
30	a	615	SQD	O49-C7-O47-C45
30	f	101	SQD	C2-C1-O6-C44
30	f	101	SQD	O5-C1-O6-C44
30	f	101	SQD	C8-C7-O47-C45
31	A	616	DGD	C2B-C1B-O2G-C2G
31	A	616	DGD	O1B-C1B-O2G-C2G
31	A	616	DGD	O2G-C2G-C3G-O3G
31	a	616	DGD	C2B-C1B-O2G-C2G
33	B	623	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
33	B	623	LHG	C4-O6-P-O4
33	B	623	LHG	C4-O6-P-O5
33	D	409	LHG	C3-O3-P-O5
33	D	409	LHG	C4-O6-P-O4
33	D	410	LHG	C3-O3-P-O5
33	D	412	LHG	C3-O3-P-O4
33	a	613	LHG	O1-C1-C2-C3
33	a	613	LHG	C3-O3-P-O4
33	a	613	LHG	C3-O3-P-O5
33	d	407	LHG	C4-O6-P-O4
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	O10-C23-O8-C6
33	e	102	LHG	C24-C23-O8-C6
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
25	b	601	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	CBD-CGD-O2D-CED
29	c	522	LMG	O10-C28-O8-C9
30	b	620	SQD	O10-C23-O48-C46
30	f	101	SQD	O10-C23-O48-C46
25	B	601	CLA	O1D-CGD-O2D-CED
29	c	520	LMG	C29-C28-O8-C9
30	b	620	SQD	C24-C23-O48-C46
28	D	406	PL9	C47-C48-C49-C50
28	a	611	PL9	C47-C48-C49-C51
25	c	513	CLA	CBD-CGD-O2D-CED
29	B	620	LMG	O10-C28-O8-C9
29	c	520	LMG	O10-C28-O8-C9
33	E	101	LHG	O10-C23-O8-C6
25	C	511	CLA	CBD-CGD-O2D-CED
25	c	501	CLA	CBD-CGD-O2D-CED
29	D	411	LMG	O9-C10-O7-C8
29	c	520	LMG	O9-C10-O7-C8
30	f	101	SQD	O49-C7-O47-C45
31	a	616	DGD	O1B-C1B-O2G-C2G
25	A	609	CLA	C3-C5-C6-C7
25	b	614	CLA	C3-C5-C6-C7
25	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	c	522	LMG	C29-C28-O8-C9
30	f	101	SQD	C24-C23-O48-C46
33	E	101	LHG	C24-C23-O8-C6
29	A	613	LMG	C11-C10-O7-C8
29	c	520	LMG	C11-C10-O7-C8
30	a	615	SQD	C8-C7-O47-C45
25	C	504	CLA	C4-C3-C5-C6
25	C	513	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	c	513	CLA	C4-C3-C5-C6
29	c	520	LMG	C4-C5-C6-O5
25	B	614	CLA	C2-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
28	A	611	PL9	C23-C24-C26-C27
25	C	509	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	C	513	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	B	616	CLA	CBA-CGA-O2A-C1
28	a	611	PL9	C47-C48-C49-C50
28	a	611	PL9	C42-C43-C44-C45
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C42-C43-C44-C46
25	B	616	CLA	O1A-CGA-O2A-C1
30	a	615	SQD	O10-C23-O48-C46
25	C	501	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
33	D	409	LHG	O2-C2-C3-O3
33	d	407	LHG	O2-C2-C3-O3
29	B	620	LMG	C29-C28-O8-C9
29	c	518	LMG	C11-C10-O7-C8
25	C	513	CLA	O1A-CGA-O2A-C1
29	C	520	LMG	C11-C10-O7-C8
30	b	620	SQD	C8-C7-O47-C45
26	d	402	PHO	CBD-CGD-O2D-CED
30	A	614	SQD	C30-C31-C32-C33
33	E	101	LHG	C32-C33-C34-C35
32	C	521	STE	C4-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	a	615	SQD	C24-C23-O48-C46
29	b	622	LMG	O6-C5-C6-O5
29	c	520	LMG	O6-C5-C6-O5
32	b	621	STE	C2-C3-C4-C5
31	c	517	DGD	O1A-C1A-O1G-C1G
33	d	408	LHG	C24-C25-C26-C27
28	A	611	PL9	C45-C44-C46-C47
25	C	504	CLA	C2-C3-C5-C6
28	A	611	PL9	C33-C34-C36-C37
28	A	611	PL9	C43-C44-C46-C47
25	B	606	CLA	C2A-CAA-CBA-CGA
32	H	103	STE	C14-C15-C16-C17
31	h	101	DGD	O6E-C5E-C6E-O5E
30	b	620	SQD	O5-C1-O6-C44
28	A	611	PL9	C34-C36-C37-C38
28	D	406	PL9	C44-C46-C47-C48
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C34-C36-C37-C38
30	B	624	SQD	C34-C35-C36-C37
33	D	409	LHG	C1-C2-C3-O3
30	b	620	SQD	O49-C7-O47-C45
32	B	629	STE	C11-C12-C13-C14
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	CBA-CGA-O2A-C1
25	c	506	CLA	CBA-CGA-O2A-C1
30	D	408	SQD	C24-C23-O48-C46
30	a	614	SQD	C11-C12-C13-C14
25	C	513	CLA	C15-C16-C17-C18
31	A	616	DGD	O6E-C5E-C6E-O5E
33	d	407	LHG	C32-C33-C34-C35
25	B	610	CLA	C15-C16-C17-C18
25	a	607	CLA	C13-C15-C16-C17
25	b	603	CLA	C13-C15-C16-C17
25	b	607	CLA	C5-C6-C7-C8
33	D	410	LHG	O2-C2-C3-O3
33	e	102	LHG	O2-C2-C3-O3
29	c	522	LMG	C2-C1-O1-C7
25	c	506	CLA	O1A-CGA-O2A-C1
31	a	616	DGD	O1A-C1A-O1G-C1G
31	A	616	DGD	C4E-C5E-C6E-O5E
25	b	605	CLA	C2-C3-C5-C6
25	c	513	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	606	CLA	C11-C10-C8-C9
25	B	607	CLA	C14-C13-C15-C16
25	B	610	CLA	C14-C13-C15-C16
25	B	616	CLA	C11-C10-C8-C9
25	C	503	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C10-C8-C9
25	b	605	CLA	C11-C10-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	c	509	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	511	CLA	C14-C13-C15-C16
27	B	618	BCR	C7-C8-C9-C34
27	b	618	BCR	C7-C8-C9-C34
27	c	514	BCR	C7-C8-C9-C34
27	D	405	BCR	C21-C22-C23-C24
31	h	101	DGD	C4E-C5E-C6E-O5E
30	A	614	SQD	C23-C24-C25-C26
32	b	621	STE	C1-C2-C3-C4
30	D	408	SQD	O10-C23-O48-C46
25	B	601	CLA	C5-C6-C7-C8
25	B	606	CLA	C13-C15-C16-C17
25	c	509	CLA	C10-C11-C12-C13
25	B	601	CLA	C13-C15-C16-C17
25	B	606	CLA	C8-C10-C11-C12
25	C	506	CLA	C8-C10-C11-C12
25	C	509	CLA	C10-C11-C12-C13
25	D	404	CLA	C13-C15-C16-C17
29	B	620	LMG	C10-C11-C12-C13
29	D	411	LMG	C10-C11-C12-C13
31	a	616	DGD	C1A-C2A-C3A-C4A
31	a	616	DGD	C1B-C2B-C3B-C4B
32	B	626	STE	C1-C2-C3-C4
32	d	412	STE	C1-C2-C3-C4
33	l	101	LHG	C23-C24-C25-C26
32	b	624	STE	C2-C3-C4-C5
29	B	620	LMG	O6-C5-C6-O5
25	A	607	CLA	C10-C11-C12-C13
25	B	613	CLA	C8-C10-C11-C12
25	C	502	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	C	503	CLA	C5-C6-C7-C8
25	C	505	CLA	C15-C16-C17-C18
25	b	601	CLA	C13-C15-C16-C17
25	b	605	CLA	C5-C6-C7-C8
25	b	614	CLA	C13-C15-C16-C17
25	b	615	CLA	C5-C6-C7-C8
25	c	510	CLA	C10-C11-C12-C13
28	A	611	PL9	C47-C48-C49-C51
33	e	102	LHG	O1-C1-C2-O2
29	d	410	LMG	C28-C29-C30-C31
30	f	101	SQD	C23-C24-C25-C26
32	b	623	STE	C1-C2-C3-C4
33	D	412	LHG	C23-C24-C25-C26
33	E	101	LHG	C23-C24-C25-C26
33	e	102	LHG	C7-C8-C9-C10
25	B	603	CLA	C8-C10-C11-C12
25	B	615	CLA	C5-C6-C7-C8
25	c	509	CLA	C5-C6-C7-C8
31	a	616	DGD	C2A-C1A-O1G-C1G
33	e	102	LHG	C26-C27-C28-C29
31	c	515	DGD	O6E-C5E-C6E-O5E
30	b	620	SQD	C12-C13-C14-C15
25	B	601	CLA	C15-C16-C17-C18
25	a	606	CLA	C15-C16-C17-C18
25	b	615	CLA	C10-C11-C12-C13
29	D	407	LMG	C10-C11-C12-C13
30	A	614	SQD	C7-C8-C9-C10
25	C	512	CLA	C13-C15-C16-C17
25	c	509	CLA	C13-C15-C16-C17
25	c	510	CLA	C5-C6-C7-C8
25	c	512	CLA	C13-C15-C16-C17
25	B	606	CLA	C12-C13-C15-C16
25	C	509	CLA	C11-C10-C8-C7
25	D	403	CLA	C12-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C10
25	b	606	CLA	C6-C7-C8-C10
25	b	614	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C12-C13-C15
25	c	506	CLA	C11-C12-C13-C15
25	B	601	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	B	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C5-C6-C7-C8
25	C	505	CLA	C5-C6-C7-C8
25	b	607	CLA	C10-C11-C12-C13
25	b	611	CLA	C13-C15-C16-C17
25	c	510	CLA	C15-C16-C17-C18
28	A	611	PL9	C29-C31-C32-C33
31	c	516	DGD	C1A-C2A-C3A-C4A
27	B	619	BCR	C10-C11-C12-C13
27	k	101	BCR	C18-C19-C20-C21
33	a	613	LHG	O2-C2-C3-O3
25	b	602	CLA	C13-C15-C16-C17
25	b	609	CLA	C15-C16-C17-C18
25	b	616	CLA	C5-C6-C7-C8
31	c	517	DGD	C2A-C1A-O1G-C1G
30	b	620	SQD	C10-C11-C12-C13
25	B	604	CLA	C10-C11-C12-C13
25	B	611	CLA	C8-C10-C11-C12
25	C	510	CLA	C8-C10-C11-C12
25	a	607	CLA	C8-C10-C11-C12
25	a	609	CLA	C5-C6-C7-C8
25	b	607	CLA	C8-C10-C11-C12
25	c	503	CLA	C5-C6-C7-C8
25	c	506	CLA	C13-C15-C16-C17
25	C	509	CLA	C13-C15-C16-C17
25	C	512	CLA	C10-C11-C12-C13
25	b	601	CLA	C8-C10-C11-C12
25	b	601	CLA	C10-C11-C12-C13
25	b	614	CLA	C8-C10-C11-C12
25	c	507	CLA	C5-C6-C7-C8
25	c	510	CLA	C8-C10-C11-C12
25	c	513	CLA	C13-C15-C16-C17
33	D	409	LHG	C3-O3-P-O6
33	D	410	LHG	C3-O3-P-O6
33	a	613	LHG	C3-O3-P-O6
33	d	407	LHG	C4-O6-P-O3
25	b	601	CLA	C3-C5-C6-C7
25	B	614	CLA	C13-C15-C16-C17
33	B	623	LHG	C23-C24-C25-C26
25	C	511	CLA	O1D-CGD-O2D-CED
33	a	613	LHG	C1-C2-C3-O3
29	C	520	LMG	O9-C10-O7-C8
33	e	102	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C4-C3-C5-C6
28	A	611	PL9	C25-C24-C26-C27
28	d	406	PL9	C40-C39-C41-C42
25	b	614	CLA	C5-C6-C7-C8
25	b	601	CLA	C16-C17-C18-C19
25	C	509	CLA	O1D-CGD-O2D-CED
33	E	101	LHG	C27-C28-C29-C30
25	c	503	CLA	C8-C10-C11-C12
29	m	101	LMG	C10-C11-C12-C13
29	c	522	LMG	C13-C14-C15-C16
32	H	103	STE	C7-C8-C9-C10
32	b	621	STE	C7-C8-C9-C10
33	B	623	LHG	C17-C18-C19-C20
33	D	409	LHG	C11-C10-C9-C8
25	c	511	CLA	C15-C16-C17-C18
27	C	516	BCR	C16-C17-C18-C36
27	D	405	BCR	C20-C21-C22-C37
27	T	101	BCR	C35-C13-C14-C15
27	T	101	BCR	C16-C17-C18-C36
27	c	514	BCR	C35-C13-C14-C15
27	k	101	BCR	C11-C10-C9-C34
27	k	101	BCR	C35-C13-C14-C15
29	A	613	LMG	C16-C17-C18-C19
29	D	407	LMG	C39-C40-C41-C42
29	b	622	LMG	C35-C36-C37-C38
29	c	520	LMG	C33-C34-C35-C36
30	A	615	SQD	C28-C29-C30-C31
31	A	616	DGD	C6B-C7B-C8B-C9B
31	a	616	DGD	CBA-CCA-CDA-CEA
31	c	515	DGD	C4B-C5B-C6B-C7B
31	c	517	DGD	CBA-CCA-CDA-CEA
31	h	101	DGD	C3B-C4B-C5B-C6B
32	B	625	STE	C6-C7-C8-C9
32	B	628	STE	C2-C3-C4-C5
32	H	103	STE	C5-C6-C7-C8
32	H	103	STE	C12-C13-C14-C15
32	T	103	STE	C11-C12-C13-C14
32	b	623	STE	C5-C6-C7-C8
32	d	411	STE	C11-C10-C9-C8
33	D	410	LHG	C11-C12-C13-C14
33	D	410	LHG	C29-C30-C31-C32
33	E	101	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
33	a	613	LHG	C32-C33-C34-C35
25	b	607	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C20
25	c	504	CLA	C11-C12-C13-C14
29	C	520	LMG	C17-C18-C19-C20
29	b	622	LMG	C41-C42-C43-C44
30	B	624	SQD	C17-C18-C19-C20
31	H	102	DGD	C5B-C6B-C7B-C8B
32	C	522	STE	C3-C4-C5-C6
32	I	101	STE	C11-C10-C9-C8
32	X	101	STE	C14-C15-C16-C17
33	D	409	LHG	C12-C13-C14-C15
33	D	410	LHG	C9-C10-C11-C12
33	a	613	LHG	C15-C16-C17-C18
33	e	102	LHG	C14-C15-C16-C17
29	D	411	LMG	C9-C8-O7-C10
30	b	620	SQD	C46-C45-O47-C7
30	A	614	SQD	C11-C12-C13-C14
30	D	408	SQD	C25-C26-C27-C28
31	c	515	DGD	C6A-C7A-C8A-C9A
31	h	101	DGD	CBA-CCA-CDA-CEA
32	B	629	STE	C11-C10-C9-C8
32	T	102	STE	C5-C6-C7-C8
32	c	519	STE	C9-C10-C11-C12
32	d	412	STE	C4-C5-C6-C7
33	E	101	LHG	C16-C17-C18-C19
33	a	613	LHG	C10-C11-C12-C13
25	c	501	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1A-CGA-O2A-C1
30	a	614	SQD	C24-C25-C26-C27
31	a	616	DGD	C8B-C9B-CAB-CBB
31	c	515	DGD	C3B-C4B-C5B-C6B
31	c	515	DGD	C8B-C9B-CAB-CBB
31	c	516	DGD	C6A-C7A-C8A-C9A
31	c	517	DGD	C4A-C5A-C6A-C7A
32	B	628	STE	C3-C4-C5-C6
32	H	103	STE	C11-C10-C9-C8
32	T	102	STE	C4-C5-C6-C7
32	c	521	STE	C2-C3-C4-C5
32	d	411	STE	C9-C10-C11-C12
29	b	622	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	d	409	LMG	C33-C34-C35-C36
29	d	410	LMG	C38-C39-C40-C41
30	D	408	SQD	C30-C31-C32-C33
27	B	619	BCR	C12-C13-C14-C15
27	C	515	BCR	C11-C10-C9-C8
27	K	101	BCR	C11-C10-C9-C8
27	T	101	BCR	C12-C13-C14-C15
27	T	101	BCR	C16-C17-C18-C19
27	k	102	BCR	C20-C21-C22-C23
27	x	101	BCR	C11-C10-C9-C8
27	x	101	BCR	C16-C17-C18-C19
31	C	518	DGD	C2E-C1E-O5D-C6D
29	c	522	LMG	C12-C13-C14-C15
29	d	409	LMG	C32-C33-C34-C35
31	A	616	DGD	C4B-C5B-C6B-C7B
31	A	616	DGD	C5B-C6B-C7B-C8B
31	a	616	DGD	C4A-C5A-C6A-C7A
32	B	625	STE	C11-C10-C9-C8
32	H	103	STE	C6-C7-C8-C9
33	D	410	LHG	C25-C26-C27-C28
25	C	513	CLA	C10-C11-C12-C13
25	B	603	CLA	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C20
25	C	506	CLA	C4-C3-C5-C6
25	c	510	CLA	C4-C3-C5-C6
31	c	516	DGD	CCA-CDA-CEA-CFA
32	B	625	STE	C3-C4-C5-C6
32	T	102	STE	C6-C7-C8-C9
32	c	519	STE	C2-C3-C4-C5
25	C	508	CLA	C11-C10-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	D	404	CLA	C6-C7-C8-C9
25	a	609	CLA	C6-C7-C8-C9
25	b	603	CLA	C6-C7-C8-C9
25	b	605	CLA	C11-C12-C13-C14
25	b	611	CLA	C14-C13-C15-C16
29	A	613	LMG	C34-C35-C36-C37
30	A	614	SQD	C11-C10-C9-C8
30	a	614	SQD	C32-C33-C34-C35
30	a	615	SQD	C30-C31-C32-C33
30	f	101	SQD	C29-C30-C31-C32
30	f	101	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	A	616	DGD	CBA-CCA-CDA-CEA
31	A	616	DGD	CCB-CDB-CEB-CFB
31	C	519	DGD	C7B-C8B-C9B-CAB
31	a	616	DGD	C8A-C9A-CAA-CBA
31	c	517	DGD	C5A-C6A-C7A-C8A
32	H	103	STE	C13-C14-C15-C16
32	b	624	STE	C12-C13-C14-C15
32	c	521	STE	C4-C5-C6-C7
32	l	102	STE	C13-C14-C15-C16
33	B	623	LHG	C16-C17-C18-C19
33	D	409	LHG	C32-C33-C34-C35
33	D	409	LHG	C33-C34-C35-C36
33	D	410	LHG	C32-C33-C34-C35
33	E	101	LHG	C18-C19-C20-C21
33	a	613	LHG	C29-C30-C31-C32
25	C	504	CLA	C8-C10-C11-C12
29	C	520	LMG	C31-C32-C33-C34
29	d	409	LMG	C35-C36-C37-C38
29	m	101	LMG	C17-C18-C19-C20
30	b	620	SQD	C26-C27-C28-C29
31	c	515	DGD	C5B-C6B-C7B-C8B
32	B	627	STE	C5-C6-C7-C8
32	T	102	STE	C7-C8-C9-C10
32	T	103	STE	C12-C13-C14-C15
32	d	411	STE	C6-C7-C8-C9
32	d	412	STE	C7-C8-C9-C10
33	D	409	LHG	C30-C31-C32-C33
33	e	102	LHG	C27-C28-C29-C30
33	d	408	LHG	O1-C1-C2-C3
25	B	603	CLA	C13-C15-C16-C17
25	C	506	CLA	C13-C15-C16-C17
25	b	606	CLA	C15-C16-C17-C18
29	C	520	LMG	C14-C15-C16-C17
29	b	622	LMG	C16-C17-C18-C19
29	c	520	LMG	C30-C31-C32-C33
29	c	522	LMG	C38-C39-C40-C41
30	A	614	SQD	C27-C28-C29-C30
31	c	515	DGD	C3A-C4A-C5A-C6A
31	c	517	DGD	C7B-C8B-C9B-CAB
31	h	101	DGD	C6B-C7B-C8B-C9B
32	C	521	STE	C5-C6-C7-C8
32	X	101	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	X	101	STE	C12-C13-C14-C15
32	b	624	STE	C3-C4-C5-C6
32	l	102	STE	C9-C10-C11-C12
33	B	623	LHG	C13-C14-C15-C16
33	a	613	LHG	C7-C8-C9-C10
25	C	512	CLA	O1D-CGD-O2D-CED
29	A	613	LMG	C35-C36-C37-C38
29	B	620	LMG	C35-C36-C37-C38
29	C	520	LMG	C13-C14-C15-C16
30	A	614	SQD	C16-C17-C18-C19
30	B	624	SQD	C11-C12-C13-C14
30	B	624	SQD	C32-C33-C34-C35
30	b	620	SQD	C9-C10-C11-C12
31	C	518	DGD	C8B-C9B-CAB-CBB
31	C	519	DGD	C5A-C6A-C7A-C8A
31	a	616	DGD	CDA-CEA-CFA-CGA
31	c	516	DGD	C7B-C8B-C9B-CAB
31	h	101	DGD	C5A-C6A-C7A-C8A
32	J	101	STE	C4-C5-C6-C7
32	J	101	STE	C6-C7-C8-C9
32	X	101	STE	C11-C12-C13-C14
32	b	625	STE	C3-C4-C5-C6
32	d	412	STE	C3-C4-C5-C6
32	d	412	STE	C12-C13-C14-C15
32	j	101	STE	C5-C6-C7-C8
33	B	623	LHG	C27-C28-C29-C30
33	D	410	LHG	C24-C25-C26-C27
33	D	412	LHG	C28-C29-C30-C31
33	d	408	LHG	C27-C28-C29-C30
33	d	408	LHG	C32-C33-C34-C35
33	l	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C17-C18-C19-C20
33	l	101	LHG	C27-C28-C29-C30
25	B	601	CLA	C16-C17-C18-C19
25	B	601	CLA	C16-C17-C18-C20
25	B	606	CLA	C16-C17-C18-C19
25	B	616	CLA	C11-C12-C13-C15
25	a	606	CLA	C16-C17-C18-C19
25	b	607	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C19
25	c	512	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C16-C17-C18-C20
31	C	518	DGD	O6E-C1E-O5D-C6D
25	B	615	CLA	C15-C16-C17-C18
25	b	608	CLA	C13-C15-C16-C17
29	m	101	LMG	C32-C33-C34-C35
30	a	614	SQD	C12-C13-C14-C15
30	a	614	SQD	C30-C31-C32-C33
31	H	102	DGD	CBA-CCA-CDA-CEA
32	B	629	STE	C6-C7-C8-C9
32	C	521	STE	C6-C7-C8-C9
32	C	522	STE	C5-C6-C7-C8
33	B	623	LHG	C30-C31-C32-C33
33	D	409	LHG	C15-C16-C17-C18
33	D	410	LHG	C33-C34-C35-C36
33	l	101	LHG	C9-C10-C11-C12
29	A	613	LMG	C38-C39-C40-C41
29	c	520	LMG	C14-C15-C16-C17
31	H	102	DGD	CBB-CCB-CDB-CEB
31	a	616	DGD	CEB-CFB-CGB-CHB
32	b	625	STE	C2-C3-C4-C5
32	l	102	STE	C4-C5-C6-C7
31	A	616	DGD	C1B-C2B-C3B-C4B
33	e	102	LHG	C23-C24-C25-C26
29	d	410	LMG	C14-C15-C16-C17
32	B	629	STE	C5-C6-C7-C8
33	D	412	LHG	C29-C30-C31-C32
25	B	605	CLA	C3-C5-C6-C7
29	D	407	LMG	O6-C5-C6-O5
29	D	407	LMG	C37-C38-C39-C40
29	b	622	LMG	C34-C35-C36-C37
31	C	519	DGD	CBA-CCA-CDA-CEA
32	j	101	STE	C2-C3-C4-C5
25	C	501	CLA	O1D-CGD-O2D-CED
25	b	601	CLA	C3A-C2A-CAA-CBA
25	b	615	CLA	C15-C16-C17-C18
29	D	411	LMG	C14-C15-C16-C17
29	c	522	LMG	C37-C38-C39-C40
30	A	614	SQD	C34-C35-C36-C37
31	H	102	DGD	C9A-CAA-CBA-CCA
31	a	616	DGD	C3A-C4A-C5A-C6A
31	c	517	DGD	C6A-C7A-C8A-C9A
32	b	621	STE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	a	613	LHG	C28-C29-C30-C31
33	d	407	LHG	C29-C30-C31-C32
25	B	603	CLA	C16-C17-C18-C19
25	B	606	CLA	C16-C17-C18-C20
25	B	616	CLA	C11-C12-C13-C14
25	a	606	CLA	C16-C17-C18-C20
30	f	101	SQD	C25-C26-C27-C28
31	H	102	DGD	C3A-C4A-C5A-C6A
33	e	102	LHG	C18-C19-C20-C21
25	C	513	CLA	C8-C10-C11-C12
29	A	613	LMG	O6-C5-C6-O5
30	b	620	SQD	C24-C25-C26-C27
32	X	101	STE	C10-C11-C12-C13
29	b	622	LMG	C4-C5-C6-O5
25	C	505	CLA	C2-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
32	d	412	STE	C5-C6-C7-C8
33	a	613	LHG	O1-C1-C2-O2
29	B	622	LMG	C13-C14-C15-C16
29	c	520	LMG	C31-C32-C33-C34
30	A	614	SQD	C14-C15-C16-C17
32	T	103	STE	C11-C10-C9-C8
33	d	407	LHG	C34-C35-C36-C37
29	c	520	LMG	C10-C11-C12-C13
25	B	615	CLA	C16-C17-C18-C20
25	c	503	CLA	C16-C17-C18-C19
29	D	407	LMG	C17-C18-C19-C20
30	A	614	SQD	C28-C29-C30-C31
30	a	615	SQD	C11-C10-C9-C8
33	D	412	LHG	C25-C26-C27-C28
29	A	613	LMG	C17-C18-C19-C20
29	d	409	LMG	C37-C38-C39-C40
30	a	614	SQD	C14-C15-C16-C17
31	C	519	DGD	C3A-C4A-C5A-C6A
31	c	515	DGD	C9B-CAB-CBB-CCB
33	E	101	LHG	C33-C34-C35-C36
30	b	620	SQD	C23-C24-C25-C26
31	c	515	DGD	C1A-C2A-C3A-C4A
30	a	614	SQD	C10-C11-C12-C13
31	C	517	DGD	C5B-C6B-C7B-C8B
32	c	519	STE	C4-C5-C6-C7
32	c	519	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	b	622	LMG	O9-C10-O7-C8
28	A	611	PL9	C12-C13-C14-C16
29	B	620	LMG	C12-C13-C14-C15
29	B	620	LMG	C37-C38-C39-C40
29	m	101	LMG	C14-C15-C16-C17
31	c	515	DGD	CAB-CBB-CCB-CDB
31	h	101	DGD	C5B-C6B-C7B-C8B
32	X	101	STE	C6-C7-C8-C9
33	B	623	LHG	C9-C10-C11-C12
33	E	101	LHG	C9-C10-C11-C12
25	c	504	CLA	C8-C10-C11-C12
29	d	410	LMG	C36-C37-C38-C39
30	A	614	SQD	C24-C25-C26-C27
30	b	620	SQD	C11-C10-C9-C8
31	c	515	DGD	C2A-C3A-C4A-C5A
31	h	101	DGD	C6A-C7A-C8A-C9A
33	D	410	LHG	C30-C31-C32-C33
25	c	504	CLA	C11-C12-C13-C15
27	C	516	BCR	C1-C6-C7-C8
27	D	405	BCR	C23-C24-C25-C26
27	D	405	BCR	C23-C24-C25-C30
27	b	617	BCR	C1-C6-C7-C8
27	b	617	BCR	C5-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C26
27	k	102	BCR	C1-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
30	A	615	SQD	C10-C11-C12-C13
32	M	101	STE	C11-C10-C9-C8
32	b	621	STE	C14-C15-C16-C17
30	B	624	SQD	C24-C23-O48-C46
25	B	607	CLA	C13-C15-C16-C17
30	a	614	SQD	C27-C28-C29-C30
31	a	616	DGD	C3B-C4B-C5B-C6B
29	b	622	LMG	C10-C11-C12-C13
29	B	622	LMG	C14-C15-C16-C17
25	C	506	CLA	C15-C16-C17-C18
29	c	520	LMG	C39-C40-C41-C42
29	c	522	LMG	C18-C19-C20-C21
30	a	614	SQD	C28-C29-C30-C31
25	C	505	CLA	C4-C3-C5-C6
28	a	611	PL9	C40-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
25	A	607	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C12-C13-C15
25	B	611	CLA	C11-C10-C8-C7
25	C	503	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C10-C8-C7
25	C	510	CLA	C6-C7-C8-C10
25	a	609	CLA	C6-C7-C8-C10
25	b	605	CLA	C11-C12-C13-C15
25	b	606	CLA	C11-C10-C8-C7
25	b	611	CLA	C12-C13-C15-C16
25	b	612	CLA	C12-C13-C15-C16
29	B	620	LMG	C16-C17-C18-C19
29	B	620	LMG	C32-C33-C34-C35
29	D	407	LMG	C30-C31-C32-C33
29	c	520	LMG	C11-C12-C13-C14
32	H	103	STE	C4-C5-C6-C7
25	B	616	CLA	C8-C10-C11-C12
27	k	101	BCR	C13-C14-C15-C16
30	D	408	SQD	C23-C24-C25-C26
32	B	621	STE	C1-C2-C3-C4
31	C	518	DGD	C4A-C5A-C6A-C7A
33	d	408	LHG	C26-C27-C28-C29
25	B	602	CLA	C13-C15-C16-C17
25	B	613	CLA	C5-C6-C7-C8
29	b	622	LMG	C19-C20-C21-C22
31	c	515	DGD	CCB-CDB-CEB-CFB
32	H	103	STE	C3-C4-C5-C6
32	X	101	STE	C9-C10-C11-C12
32	b	625	STE	C4-C5-C6-C7
26	d	402	PHO	O1D-CGD-O2D-CED
29	c	518	LMG	C36-C37-C38-C39
30	A	615	SQD	C9-C10-C11-C12
29	c	522	LMG	C28-C29-C30-C31
29	m	101	LMG	C28-C29-C30-C31
28	d	406	PL9	C42-C43-C44-C45
25	A	609	CLA	C5-C6-C7-C8
31	H	102	DGD	CCA-CDA-CEA-CFA
32	T	103	STE	C14-C15-C16-C17
25	B	610	CLA	C16-C17-C18-C20
25	C	502	CLA	C16-C17-C18-C19
28	a	611	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C32-C33-C34-C35
29	D	407	LMG	C36-C37-C38-C39
29	d	409	LMG	C31-C32-C33-C34
30	D	408	SQD	C34-C35-C36-C37
29	D	411	LMG	C28-C29-C30-C31
33	e	102	LHG	C8-C7-O7-C5
27	T	101	BCR	C18-C19-C20-C21
27	d	405	BCR	C18-C19-C20-C21
29	b	622	LMG	C15-C16-C17-C18
30	a	614	SQD	C9-C10-C11-C12
32	b	624	STE	C14-C15-C16-C17
29	D	411	LMG	C31-C32-C33-C34
29	b	622	LMG	C29-C30-C31-C32
29	B	620	LMG	C29-C30-C31-C32
32	B	628	STE	C5-C6-C7-C8
33	a	613	LHG	C16-C17-C18-C19
29	d	410	LMG	O6-C5-C6-O5
29	C	520	LMG	C37-C38-C39-C40
32	T	103	STE	C10-C11-C12-C13
33	E	101	LHG	C34-C35-C36-C37
29	D	407	LMG	C15-C16-C17-C18
29	c	518	LMG	C39-C40-C41-C42
32	M	101	STE	C7-C8-C9-C10
33	D	410	LHG	C10-C11-C12-C13
33	d	407	LHG	C11-C12-C13-C14
25	C	513	CLA	C5-C6-C7-C8
28	d	406	PL9	C45-C44-C46-C47
28	D	406	PL9	C4-C3-C7-C8
31	C	517	DGD	C9B-CAB-CBB-CCB
31	c	517	DGD	C8B-C9B-CAB-CBB
25	A	607	CLA	C6-C7-C8-C9
25	B	602	CLA	C11-C12-C13-C14
25	B	604	CLA	C11-C12-C13-C14
25	B	606	CLA	C14-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C14
25	C	504	CLA	C11-C10-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C9
25	b	601	CLA	C11-C12-C13-C14
25	b	612	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	506	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C12-C13-C14
31	A	616	DGD	C2B-C3B-C4B-C5B
29	c	520	LMG	C41-C42-C43-C44
29	c	522	LMG	C29-C30-C31-C32
33	D	409	LHG	C25-C26-C27-C28
27	B	619	BCR	C7-C8-C9-C34
29	m	101	LMG	C11-C12-C13-C14
32	E	102	STE	C4-C5-C6-C7
33	D	410	LHG	C11-C10-C9-C8
27	k	102	BCR	C21-C22-C23-C24
30	B	624	SQD	O10-C23-O48-C46
25	a	609	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	B	615	CLA	C16-C17-C18-C19
29	c	522	LMG	O9-C10-O7-C8
30	B	624	SQD	C9-C10-C11-C12
30	D	408	SQD	C31-C32-C33-C34
32	B	628	STE	C6-C7-C8-C9
32	T	102	STE	C13-C14-C15-C16
33	a	613	LHG	C30-C31-C32-C33
33	l	101	LHG	C13-C14-C15-C16
31	h	101	DGD	CBB-CCB-CDB-CEB
32	B	627	STE	C6-C7-C8-C9
33	D	409	LHG	C16-C17-C18-C19
32	c	519	STE	C1-C2-C3-C4
25	B	601	CLA	C8-C10-C11-C12
25	B	602	CLA	C8-C10-C11-C12
25	c	511	CLA	C13-C15-C16-C17
25	d	404	CLA	C10-C11-C12-C13
29	C	520	LMG	C38-C39-C40-C41
30	A	614	SQD	C26-C27-C28-C29
30	a	614	SQD	C17-C18-C19-C20
31	C	519	DGD	CBB-CCB-CDB-CEB
32	T	103	STE	C6-C7-C8-C9
29	B	622	LMG	C29-C30-C31-C32
29	c	518	LMG	C35-C36-C37-C38
33	E	101	LHG	C30-C31-C32-C33
31	C	517	DGD	C2B-C3B-C4B-C5B
31	a	616	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
32	a	617	STE	C4-C5-C6-C7
33	D	409	LHG	C13-C14-C15-C16
29	c	520	LMG	C28-C29-C30-C31
29	D	407	LMG	C38-C39-C40-C41
32	b	623	STE	C10-C11-C12-C13
32	l	102	STE	C10-C11-C12-C13
33	d	407	LHG	C1-C2-C3-O3
29	c	520	LMG	C34-C35-C36-C37
31	C	519	DGD	C4B-C5B-C6B-C7B
31	c	515	DGD	CBB-CCB-CDB-CEB
33	d	408	LHG	C33-C34-C35-C36
29	B	620	LMG	C19-C20-C21-C22
29	B	620	LMG	C33-C34-C35-C36
30	D	408	SQD	C29-C30-C31-C32
32	B	627	STE	C4-C5-C6-C7
32	m	102	STE	C6-C7-C8-C9
29	b	622	LMG	O1-C7-C8-C9
29	c	520	LMG	O1-C7-C8-C9
30	a	614	SQD	O6-C44-C45-C46
30	a	615	SQD	C44-C45-C46-O48
32	l	102	STE	C1-C2-C3-C4
29	C	520	LMG	C30-C31-C32-C33
31	A	616	DGD	C2A-C3A-C4A-C5A
30	B	624	SQD	C45-C44-O6-C1
31	C	518	DGD	C5D-C6D-O5D-C1E
31	c	516	DGD	C5D-C6D-O5D-C1E
32	d	412	STE	C15-C16-C17-C18
25	B	614	CLA	C8-C10-C11-C12
29	b	622	LMG	C17-C18-C19-C20
30	B	624	SQD	C19-C20-C21-C22
32	J	101	STE	C7-C8-C9-C10
33	B	623	LHG	C32-C33-C34-C35
29	c	518	LMG	O6-C5-C6-O5
33	d	408	LHG	C23-C24-C25-C26
25	D	403	CLA	C15-C16-C17-C18
30	A	614	SQD	C32-C33-C34-C35
31	H	102	DGD	CDB-CEB-CFB-CGB
30	a	614	SQD	C19-C20-C21-C22
31	c	516	DGD	C3A-C4A-C5A-C6A
33	D	410	LHG	C31-C32-C33-C34
25	b	603	CLA	C8-C10-C11-C12
31	c	517	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
29	B	620	LMG	C17-C18-C19-C20
29	c	522	LMG	C34-C35-C36-C37
30	A	615	SQD	C11-C12-C13-C14
32	l	102	STE	C14-C15-C16-C17
29	b	622	LMG	C11-C10-O7-C8
31	c	516	DGD	CDA-CEA-CFA-CGA
27	b	618	BCR	C35-C13-C14-C15
27	b	619	BCR	C20-C21-C22-C37
25	b	611	CLA	C4-C3-C5-C6
31	A	616	DGD	CEB-CFB-CGB-CHB
31	C	518	DGD	C6A-C7A-C8A-C9A
32	B	627	STE	C13-C14-C15-C16
25	c	510	CLA	C2-C3-C5-C6
28	d	406	PL9	C43-C44-C46-C47
29	A	613	LMG	C29-C28-O8-C9
31	C	517	DGD	O6E-C5E-C6E-O5E
32	B	629	STE	C3-C4-C5-C6
25	b	606	CLA	C10-C11-C12-C13
25	c	505	CLA	C15-C16-C17-C18
33	l	101	LHG	C30-C31-C32-C33
25	a	609	CLA	C10-C11-C12-C13
25	c	506	CLA	C2-C1-O2A-CGA
30	A	614	SQD	C17-C18-C19-C20
29	D	411	LMG	C36-C37-C38-C39
30	b	620	SQD	C19-C20-C21-C22
32	d	411	STE	C2-C3-C4-C5
33	d	407	LHG	C12-C13-C14-C15
33	e	102	LHG	C11-C10-C9-C8
29	B	620	LMG	C20-C21-C22-C23
30	A	614	SQD	C13-C14-C15-C16
32	m	102	STE	C5-C6-C7-C8
33	D	412	LHG	C19-C20-C21-C22
25	C	502	CLA	C16-C17-C18-C20
29	B	622	LMG	C33-C34-C35-C36
29	m	101	LMG	C38-C39-C40-C41
30	A	614	SQD	C35-C36-C37-C38
31	C	518	DGD	C6B-C7B-C8B-C9B
32	a	617	STE	C2-C3-C4-C5
29	c	522	LMG	C39-C40-C41-C42
33	e	102	LHG	C13-C14-C15-C16
27	B	619	BCR	C11-C10-C9-C8
31	c	516	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
29	c	520	LMG	O7-C8-C9-O8
31	c	515	DGD	O6D-C5D-C6D-O5D
31	a	616	DGD	C5A-C6A-C7A-C8A
32	B	621	STE	C12-C13-C14-C15
32	B	627	STE	C2-C3-C4-C5
28	A	611	PL9	C15-C14-C16-C17
28	A	611	PL9	C17-C18-C19-C20
25	A	607	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C10-C8-C7
25	B	604	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C10-C8-C7
25	B	615	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	C	504	CLA	C11-C10-C8-C7
25	C	506	CLA	C12-C13-C15-C16
25	C	510	CLA	C11-C10-C8-C7
25	C	512	CLA	C6-C7-C8-C10
25	a	607	CLA	C11-C10-C8-C7
25	b	601	CLA	C11-C12-C13-C15
25	b	604	CLA	C12-C13-C15-C16
25	b	607	CLA	C6-C7-C8-C10
25	b	611	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
25	c	505	CLA	C6-C7-C8-C10
25	c	506	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C10-C8-C7
25	d	403	CLA	C11-C12-C13-C15
25	d	404	CLA	C12-C13-C15-C16
29	d	410	LMG	C32-C33-C34-C35
31	C	518	DGD	CDB-CEB-CFB-CGB
25	A	607	CLA	C11-C10-C8-C9
25	A	607	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C10-C8-C9
25	B	604	CLA	C11-C10-C8-C9
25	B	605	CLA	C11-C10-C8-C9
25	B	616	CLA	C6-C7-C8-C9
25	C	505	CLA	C6-C7-C8-C9
25	C	505	CLA	C11-C10-C8-C9
25	D	403	CLA	C14-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	615	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	505	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	c	513	CLA	C11-C12-C13-C14
25	d	404	CLA	C6-C7-C8-C9
25	d	404	CLA	C14-C13-C15-C16
29	B	622	LMG	C37-C38-C39-C40
31	a	616	DGD	CBB-CCB-CDB-CEB
33	a	613	LHG	C17-C18-C19-C20
29	D	407	LMG	C20-C21-C22-C23
32	b	624	STE	C9-C10-C11-C12
32	t	102	STE	C5-C6-C7-C8
29	c	522	LMG	C40-C41-C42-C43
27	k	101	BCR	C7-C8-C9-C10
30	A	615	SQD	C14-C15-C16-C17
25	C	512	CLA	C8-C10-C11-C12
25	c	503	CLA	C10-C11-C12-C13
31	h	101	DGD	C2B-C3B-C4B-C5B
32	T	103	STE	C9-C10-C11-C12
25	C	513	CLA	C13-C15-C16-C17
31	a	616	DGD	CEA-CFA-CGA-CHA
31	h	101	DGD	C4A-C5A-C6A-C7A
25	C	505	CLA	C10-C11-C12-C13
33	e	102	LHG	O6-C4-C5-C6
28	A	611	PL9	C19-C21-C22-C23
28	a	611	PL9	C19-C21-C22-C23
32	B	629	STE	C4-C5-C6-C7
29	D	411	LMG	C15-C16-C17-C18
32	M	101	STE	C10-C11-C12-C13
25	B	608	CLA	C15-C16-C17-C18
26	d	402	PHO	C5-C6-C7-C8
25	c	509	CLA	CAA-CBA-CGA-O2A
25	A	609	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
28	a	611	PL9	C38-C39-C41-C42
25	B	612	CLA	C10-C11-C12-C13
29	D	407	LMG	C12-C13-C14-C15
30	b	620	SQD	C18-C19-C20-C21
31	C	517	DGD	CCB-CDB-CEB-CFB
33	D	410	LHG	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C20
32	m	102	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	D	412	LHG	C27-C28-C29-C30
25	c	503	CLA	C15-C16-C17-C18
25	c	506	CLA	C8-C10-C11-C12
29	c	518	LMG	C38-C39-C40-C41
33	E	101	LHG	C25-C26-C27-C28
29	B	620	LMG	C4-C5-C6-O5
25	C	507	CLA	C5-C6-C7-C8
32	X	101	STE	C4-C5-C6-C7
33	B	623	LHG	C19-C20-C21-C22
29	D	411	LMG	C7-C8-C9-O8
29	c	520	LMG	C7-C8-C9-O8
31	A	616	DGD	O1G-C1G-C2G-C3G
31	A	616	DGD	C1G-C2G-C3G-O3G
31	c	515	DGD	O1G-C1G-C2G-C3G
33	E	101	LHG	C4-C5-C6-O8
29	B	620	LMG	C31-C32-C33-C34
31	C	517	DGD	C4A-C5A-C6A-C7A
31	c	517	DGD	C3B-C4B-C5B-C6B
28	A	611	PL9	C32-C33-C34-C36
29	b	622	LMG	C13-C14-C15-C16
29	d	409	LMG	C39-C40-C41-C42
31	H	102	DGD	C4A-C5A-C6A-C7A
33	d	407	LHG	C14-C15-C16-C17
31	C	519	DGD	CCB-CDB-CEB-CFB
25	c	510	CLA	C3-C5-C6-C7
31	C	517	DGD	C1B-C2B-C3B-C4B
29	d	410	LMG	C13-C14-C15-C16
25	b	616	CLA	C4-C3-C5-C6
25	B	612	CLA	C16-C17-C18-C20
25	c	506	CLA	C2-C3-C5-C6
29	d	409	LMG	C34-C35-C36-C37
30	b	620	SQD	C28-C29-C30-C31
33	D	409	LHG	C4-O6-P-O3
31	H	102	DGD	C1B-C2B-C3B-C4B
31	A	616	DGD	C7B-C8B-C9B-CAB
32	b	624	STE	C4-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
31	c	517	DGD	C3A-C4A-C5A-C6A
33	e	102	LHG	O6-C4-C5-O7
28	D	406	PL9	C32-C33-C34-C35
25	B	614	CLA	C16-C17-C18-C20
25	b	615	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C15-C16-C17-C18
25	A	606	CLA	C2C-C3C-CAC-CBC
29	m	101	LMG	C31-C32-C33-C34
33	B	623	LHG	C18-C19-C20-C21
32	T	102	STE	C11-C10-C9-C8
29	A	613	LMG	O1-C7-C8-O7
29	B	620	LMG	O7-C8-C9-O8
29	b	622	LMG	O1-C7-C8-O7
29	c	520	LMG	O1-C7-C8-O7
30	f	101	SQD	O6-C44-C45-O47
33	E	101	LHG	O7-C5-C6-O8
29	A	613	LMG	C29-C30-C31-C32
29	c	522	LMG	C15-C16-C17-C18
30	B	624	SQD	C13-C14-C15-C16
25	B	610	CLA	C16-C17-C18-C19
25	b	601	CLA	C16-C17-C18-C20
31	c	516	DGD	O6E-C1E-O5D-C6D
28	A	611	PL9	C44-C46-C47-C48
28	a	611	PL9	C44-C46-C47-C48
31	C	518	DGD	CDA-CEA-CFA-CGA
32	t	102	STE	C6-C7-C8-C9
31	C	517	DGD	C6A-C7A-C8A-C9A
31	C	519	DGD	C6A-C7A-C8A-C9A
31	H	102	DGD	C3B-C4B-C5B-C6B
25	B	615	CLA	C13-C15-C16-C17
25	B	603	CLA	C11-C12-C13-C14
25	B	604	CLA	C14-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C14
25	C	507	CLA	C11-C12-C13-C14
25	a	607	CLA	C11-C10-C8-C9
25	a	609	CLA	C14-C13-C15-C16
25	b	604	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
30	A	615	SQD	C12-C13-C14-C15
32	T	102	STE	C10-C11-C12-C13
32	T	103	STE	C15-C16-C17-C18
30	A	614	SQD	C10-C11-C12-C13
31	C	518	DGD	C2A-C3A-C4A-C5A
25	A	607	CLA	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C19
25	B	612	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	A	610	BCR	C23-C24-C25-C26
27	A	610	BCR	C23-C24-C25-C30
27	B	617	BCR	C5-C6-C7-C8
27	H	101	BCR	C23-C24-C25-C26
27	H	101	BCR	C23-C24-C25-C30
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	k	103	BCR	C5-C6-C7-C8
27	x	101	BCR	C23-C24-C25-C26
27	x	101	BCR	C23-C24-C25-C30
33	D	410	LHG	C26-C27-C28-C29
33	e	102	LHG	C28-C29-C30-C31
32	T	103	STE	C4-C5-C6-C7
27	C	516	BCR	C21-C22-C23-C24
27	c	514	BCR	C7-C8-C9-C10
27	t	101	BCR	C7-C8-C9-C10
30	a	615	SQD	C12-C13-C14-C15
29	C	520	LMG	C12-C13-C14-C15
25	D	404	CLA	C16-C17-C18-C19
29	c	518	LMG	C28-C29-C30-C31
32	B	621	STE	C11-C12-C13-C14
30	A	615	SQD	C18-C19-C20-C21
31	C	518	DGD	C8A-C9A-CAA-CBA
29	m	101	LMG	C37-C38-C39-C40
33	B	623	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
31	C	517	DGD	C4B-C5B-C6B-C7B
32	M	102	STE	C5-C6-C7-C8
32	j	101	STE	C3-C4-C5-C6
33	E	101	LHG	C12-C13-C14-C15
25	A	607	CLA	C11-C12-C13-C15
25	A	612	CLA	C12-C13-C15-C16
25	B	606	CLA	C11-C12-C13-C15
25	B	610	CLA	C12-C13-C15-C16
25	B	616	CLA	C11-C10-C8-C7
25	C	502	CLA	C12-C13-C15-C16
25	C	505	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	507	CLA	C11-C10-C8-C7
25	C	509	CLA	C12-C13-C15-C16
25	C	513	CLA	C6-C7-C8-C10
25	D	404	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	a	607	CLA	C12-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C15
25	b	606	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C12-C13-C15
25	b	611	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C10-C8-C7
25	c	505	CLA	C11-C10-C8-C7
25	c	511	CLA	C12-C13-C15-C16
25	c	512	CLA	C6-C7-C8-C10
25	c	513	CLA	C11-C12-C13-C15
25	d	404	CLA	C11-C12-C13-C15
25	C	506	CLA	C3-C5-C6-C7
29	m	101	LMG	O10-C28-O8-C9
31	C	519	DGD	CAB-CBB-CCB-CDB
31	H	102	DGD	C6B-C7B-C8B-C9B
25	b	611	CLA	C10-C11-C12-C13
25	c	512	CLA	C2A-CAA-CBA-CGA
30	f	101	SQD	C27-C28-C29-C30
27	A	610	BCR	C11-C10-C9-C34
27	K	101	BCR	C11-C10-C9-C34
27	T	101	BCR	C11-C10-C9-C34
27	b	617	BCR	C16-C17-C18-C36
27	x	101	BCR	C16-C17-C18-C36
31	c	515	DGD	C8A-C9A-CAA-CBA
31	C	517	DGD	C5A-C6A-C7A-C8A
31	C	517	DGD	CAB-CBB-CCB-CDB
25	b	613	CLA	C16-C17-C18-C19
25	a	609	CLA	C13-C15-C16-C17
25	c	509	CLA	C15-C16-C17-C18
31	C	519	DGD	C4A-C5A-C6A-C7A
33	d	407	LHG	C33-C34-C35-C36
31	H	102	DGD	C6A-C7A-C8A-C9A
32	b	623	STE	C11-C12-C13-C14
25	C	507	CLA	C10-C11-C12-C13
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	510	CLA	CAD-CBD-CGD-O2D
25	D	404	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
29	b	622	LMG	C9-C8-O7-C10
32	t	102	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
25	c	509	CLA	C8-C10-C11-C12
25	c	513	CLA	C5-C6-C7-C8
31	C	518	DGD	O6D-C1D-O3G-C3G
25	b	611	CLA	C2-C3-C5-C6
33	D	410	LHG	C7-C8-C9-C10
29	B	620	LMG	C7-C8-C9-O8
30	B	624	SQD	O6-C44-C45-C46
31	a	616	DGD	O1G-C1G-C2G-C3G
30	A	615	SQD	C30-C31-C32-C33
33	B	623	LHG	O6-C4-C5-O7
33	l	101	LHG	O6-C4-C5-O7
31	C	517	DGD	CCA-CDA-CEA-CFA
31	c	515	DGD	C7A-C8A-C9A-CAA
35	e	101	HEM	C4B-C3B-CAB-CBB
27	x	101	BCR	C14-C15-C16-C17
25	A	607	CLA	C13-C15-C16-C17
30	b	620	SQD	C17-C18-C19-C20
25	D	404	CLA	C16-C17-C18-C20
25	A	612	CLA	CHA-CBD-CGD-O1D
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
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	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	b	604	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O2D
33	B	623	LHG	O10-C23-O8-C6
29	D	411	LMG	O7-C8-C9-O8
31	A	616	DGD	O1G-C1G-C2G-O2G
29	c	518	LMG	C31-C32-C33-C34
29	B	620	LMG	C39-C40-C41-C42
32	C	522	STE	C4-C5-C6-C7
33	D	409	LHG	O1-C1-C2-O2
30	B	624	SQD	C30-C31-C32-C33
31	a	616	DGD	C6A-C7A-C8A-C9A
29	B	620	LMG	C14-C15-C16-C17
29	c	522	LMG	C32-C33-C34-C35
30	f	101	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	C	518	DGD	C5B-C6B-C7B-C8B
32	X	101	STE	C11-C10-C9-C8
32	c	519	STE	C3-C4-C5-C6
28	A	611	PL9	C4-C3-C7-C8
28	a	611	PL9	C4-C3-C7-C8
25	B	603	CLA	C14-C13-C15-C16
25	C	508	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C14
29	A	613	LMG	C14-C15-C16-C17
29	B	620	LMG	C13-C14-C15-C16
31	C	517	DGD	C2A-C3A-C4A-C5A
31	a	616	DGD	CCA-CDA-CEA-CFA
33	B	623	LHG	C12-C13-C14-C15
29	A	613	LMG	C28-C29-C30-C31
31	C	518	DGD	C1A-C2A-C3A-C4A
29	c	522	LMG	C11-C12-C13-C14
32	B	626	STE	C4-C5-C6-C7
32	I	101	STE	C5-C6-C7-C8
25	B	603	CLA	C10-C11-C12-C13
33	D	412	LHG	C11-C10-C9-C8
32	T	102	STE	C11-C12-C13-C14
25	C	505	CLA	C13-C15-C16-C17
25	c	512	CLA	C1A-C2A-CAA-CBA
25	A	607	CLA	C16-C17-C18-C19
25	B	614	CLA	C15-C16-C17-C18
31	c	515	DGD	C4D-C5D-C6D-O5D
31	H	102	DGD	C7A-C8A-C9A-CAA
33	D	412	LHG	C32-C33-C34-C35
33	d	408	LHG	C30-C31-C32-C33
25	C	509	CLA	C2-C1-O2A-CGA
29	c	522	LMG	C31-C32-C33-C34
30	B	624	SQD	C25-C26-C27-C28
30	D	408	SQD	C27-C28-C29-C30
31	H	102	DGD	C2B-C3B-C4B-C5B
33	a	613	LHG	C27-C28-C29-C30
25	B	605	CLA	C15-C16-C17-C18
33	e	102	LHG	C3-O3-P-O6
29	b	622	LMG	C18-C19-C20-C21
33	D	409	LHG	C28-C29-C30-C31
33	d	407	LHG	C28-C29-C30-C31
33	D	409	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
33	d	407	LHG	C4-O6-P-O5
33	e	102	LHG	C3-O3-P-O4
31	H	102	DGD	CDA-CEA-CFA-CGA
33	l	101	LHG	C29-C30-C31-C32
29	m	101	LMG	C29-C28-O8-C9
31	H	102	DGD	C7B-C8B-C9B-CAB
28	A	611	PL9	C47-C48-C49-C50
29	c	522	LMG	C20-C21-C22-C23
25	b	609	CLA	C13-C15-C16-C17
25	c	505	CLA	C16-C17-C18-C19
31	c	516	DGD	C9B-CAB-CBB-CCB
25	B	601	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
31	C	518	DGD	CAA-CBA-CCA-CDA
25	b	615	CLA	C8-C10-C11-C12
29	c	520	LMG	C36-C37-C38-C39
32	E	102	STE	C3-C4-C5-C6
25	b	607	CLA	CBA-CGA-O2A-C1
33	D	410	LHG	C1-C2-C3-O3
31	c	517	DGD	CCB-CDB-CEB-CFB
25	B	603	CLA	C12-C13-C15-C16
25	B	606	CLA	C6-C7-C8-C10
25	B	606	CLA	C11-C10-C8-C7
25	B	615	CLA	C6-C7-C8-C10
25	C	508	CLA	C11-C12-C13-C15
25	C	512	CLA	C11-C10-C8-C7
25	D	404	CLA	C11-C12-C13-C15
25	a	609	CLA	C12-C13-C15-C16
25	b	603	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
31	c	517	DGD	C4B-C5B-C6B-C7B
32	M	101	STE	C3-C4-C5-C6
25	b	602	CLA	C8-C10-C11-C12
32	M	101	STE	C6-C7-C8-C9
32	c	521	STE	C6-C7-C8-C9
30	a	615	SQD	C15-C16-C17-C18
32	M	102	STE	C1-C2-C3-C4
25	b	603	CLA	C16-C17-C18-C20
30	A	615	SQD	C32-C33-C34-C35
31	A	616	DGD	CFB-CGB-CHB-CIB

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Mol	Chain	Res	Type	Atoms
31	C	517	DGD	C8B-C9B-CAB-CBB
31	c	516	DGD	C9A-CAA-CBA-CCA
29	b	622	LMG	C28-C29-C30-C31
29	c	522	LMG	O1-C7-C8-C9
30	b	620	SQD	C11-C12-C13-C14
32	J	101	STE	C3-C4-C5-C6
32	b	624	STE	C11-C12-C13-C14
33	B	623	LHG	C15-C16-C17-C18
31	c	515	DGD	O1G-C1G-C2G-O2G
33	B	623	LHG	C31-C32-C33-C34
25	C	508	CLA	C5-C6-C7-C8
30	a	614	SQD	C26-C27-C28-C29
25	b	607	CLA	O1A-CGA-O2A-C1
32	I	101	STE	C1-C2-C3-C4
33	d	408	LHG	C2-C3-O3-P
30	A	614	SQD	C24-C23-O48-C46
29	D	407	LMG	C35-C36-C37-C38
29	b	622	LMG	C38-C39-C40-C41
32	b	623	STE	C11-C10-C9-C8
29	A	613	LMG	C32-C33-C34-C35
25	b	612	CLA	C13-C15-C16-C17
25	B	605	CLA	C6-C7-C8-C9
25	D	404	CLA	C11-C12-C13-C14
25	a	607	CLA	C14-C13-C15-C16
25	b	601	CLA	C11-C10-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	607	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C12-C13-C14
25	c	505	CLA	C6-C7-C8-C9
25	c	505	CLA	C14-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C14
30	A	614	SQD	O10-C23-O48-C46
31	c	516	DGD	C8B-C9B-CAB-CBB
32	E	102	STE	C5-C6-C7-C8
33	d	407	LHG	C25-C26-C27-C28
33	d	408	LHG	C25-C26-C27-C28
33	l	101	LHG	C15-C16-C17-C18
25	C	504	CLA	C11-C12-C13-C14
33	l	101	LHG	C33-C34-C35-C36
33	d	408	LHG	O1-C1-C2-O2
30	a	615	SQD	C11-C12-C13-C14
25	B	614	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C16-C17-C18-C20
32	B	626	STE	C2-C3-C4-C5
32	J	101	STE	C2-C3-C4-C5
32	c	519	STE	C11-C10-C9-C8
33	B	623	LHG	C10-C11-C12-C13
30	a	615	SQD	C10-C11-C12-C13
31	C	519	DGD	C2B-C3B-C4B-C5B
31	c	515	DGD	C9A-CAA-CBA-CCA
33	D	412	LHG	C18-C19-C20-C21
25	A	606	CLA	C16-C17-C18-C20
31	H	102	DGD	C4B-C5B-C6B-C7B
33	B	623	LHG	C26-C27-C28-C29
33	B	623	LHG	C33-C34-C35-C36
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	608	CLA	C13-C15-C16-C17
26	a	608	PHO	C8-C10-C11-C12
33	B	623	LHG	C24-C25-C26-C27
31	c	517	DGD	C1B-C2B-C3B-C4B
25	C	509	CLA	C3-C5-C6-C7
31	H	102	DGD	CAB-CBB-CCB-CDB
25	C	501	CLA	C2A-CAA-CBA-CGA
25	b	605	CLA	C10-C11-C12-C13
25	C	506	CLA	C2-C1-O2A-CGA
30	a	614	SQD	C23-C24-C25-C26
25	a	607	CLA	C15-C16-C17-C18
29	D	411	LMG	C11-C12-C13-C14
30	A	615	SQD	C24-C25-C26-C27
31	a	616	DGD	CAA-CBA-CCA-CDA
31	a	616	DGD	C5B-C6B-C7B-C8B
33	E	101	LHG	C2-C3-O3-P
31	C	517	DGD	O1A-C1A-O1G-C1G
33	D	410	LHG	C27-C28-C29-C30
33	d	407	LHG	C15-C16-C17-C18
30	B	624	SQD	C23-C24-C25-C26
25	b	609	CLA	C4-C3-C5-C6
27	B	618	BCR	C23-C24-C25-C30
27	k	103	BCR	C1-C6-C7-C8
25	A	609	CLA	C2-C3-C5-C6
29	c	518	LMG	C29-C28-O8-C9
30	D	408	SQD	O48-C23-C24-C25
25	c	513	CLA	C2A-CAA-CBA-CGA
27	K	101	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
25	D	403	CLA	C2C-C3C-CAC-CBC
31	C	517	DGD	O1G-C1G-C2G-O2G
31	a	616	DGD	O1G-C1G-C2G-O2G
25	A	606	CLA	C4C-C3C-CAC-CBC
31	C	519	DGD	C3B-C4B-C5B-C6B
33	d	407	LHG	C3-O3-P-O6
31	C	519	DGD	C7A-C8A-C9A-CAA
32	B	621	STE	C2-C3-C4-C5
33	a	613	LHG	C25-C26-C27-C28
31	A	616	DGD	O6D-C5D-C6D-O5D
29	D	411	LMG	C37-C38-C39-C40
29	m	101	LMG	C30-C31-C32-C33
31	C	518	DGD	C2B-C3B-C4B-C5B
29	C	520	LMG	O1-C7-C8-C9
29	D	411	LMG	C29-C30-C31-C32
31	c	516	DGD	C8A-C9A-CAA-CBA
25	C	505	CLA	C12-C13-C15-C16
25	b	613	CLA	C11-C10-C8-C7
25	c	509	CLA	C11-C12-C13-C15
25	c	512	CLA	C12-C13-C15-C16
25	d	404	CLA	C6-C7-C8-C10
31	c	515	DGD	O1G-C1A-C2A-C3A
31	h	101	DGD	O2G-C1B-C2B-C3B
25	B	606	CLA	C11-C12-C13-C14
25	C	509	CLA	C14-C13-C15-C16
25	b	610	CLA	C16-C17-C18-C20
30	A	615	SQD	O49-C7-O47-C45
29	D	407	LMG	C11-C12-C13-C14
33	l	101	LHG	C34-C35-C36-C37
29	c	520	LMG	C38-C39-C40-C41
33	a	613	LHG	C26-C27-C28-C29
31	a	616	DGD	CFB-CGB-CHB-CIB
33	E	101	LHG	C19-C20-C21-C22
29	D	411	LMG	C16-C17-C18-C19
33	D	412	LHG	C24-C23-O8-C6
25	b	604	CLA	C5-C6-C7-C8
33	e	102	LHG	C24-C25-C26-C27
25	b	603	CLA	C16-C17-C18-C19
25	c	510	CLA	CBA-CGA-O2A-C1
29	C	520	LMG	C29-C28-O8-C9
31	c	515	DGD	O1A-C1A-O1G-C1G
31	A	616	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
33	a	613	LHG	C19-C20-C21-C22
28	A	611	PL9	C39-C41-C42-C43
30	f	101	SQD	C24-C25-C26-C27
31	c	515	DGD	C4A-C5A-C6A-C7A
31	h	101	DGD	CAB-CBB-CCB-CDB
29	B	622	LMG	C31-C32-C33-C34
27	k	101	BCR	C10-C11-C12-C13
25	c	510	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	C16-C17-C18-C20
31	C	517	DGD	C3A-C4A-C5A-C6A
31	a	616	DGD	CFA-CGA-CHA-CIA
25	b	609	CLA	C2-C3-C5-C6
25	b	610	CLA	C8-C10-C11-C12
25	c	506	CLA	C15-C16-C17-C18
32	b	621	STE	C11-C12-C13-C14
25	B	613	CLA	C2-C1-O2A-CGA
25	D	403	CLA	C2-C1-O2A-CGA
25	b	611	CLA	C8-C10-C11-C12
32	b	621	STE	C11-C10-C9-C8
28	a	611	PL9	C37-C38-C39-C40
32	M	101	STE	O2-C1-C2-C3
25	c	501	CLA	C2A-CAA-CBA-CGA
31	a	616	DGD	C7B-C8B-C9B-CAB
25	B	601	CLA	C3A-C2A-CAA-CBA
29	B	622	LMG	O7-C10-C11-C12
33	e	102	LHG	C19-C20-C21-C22
31	C	519	DGD	C2A-C3A-C4A-C5A
25	c	509	CLA	CAA-CBA-CGA-O1A
29	C	520	LMG	C18-C19-C20-C21
32	M	101	STE	O1-C1-C2-C3
29	m	101	LMG	C13-C14-C15-C16
33	D	410	LHG	C14-C15-C16-C17
32	b	621	STE	C9-C10-C11-C12
25	b	616	CLA	C11-C10-C8-C9
25	c	512	CLA	C11-C12-C13-C14
32	B	628	STE	C4-C5-C6-C7
36	V	201	HEC	CAD-CBD-CGD-O2D
29	c	522	LMG	C36-C37-C38-C39
31	C	517	DGD	O6D-C5D-C6D-O5D
31	C	519	DGD	O6D-C5D-C6D-O5D
29	B	622	LMG	O9-C10-C11-C12
32	c	519	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	F	101	HEM	CAD-CBD-CGD-O2D
32	B	626	STE	C5-C6-C7-C8
25	C	511	CLA	C16-C17-C18-C19
26	a	608	PHO	O2A-C1-C2-C3
31	A	616	DGD	CDB-CEB-CFB-CGB
33	l	101	LHG	C31-C32-C33-C34
32	a	617	STE	C6-C7-C8-C9
36	v	201	HEC	CAD-CBD-CGD-O1D
29	A	613	LMG	C9-C8-O7-C10
31	a	616	DGD	C1G-C2G-O2G-C1B
25	c	503	CLA	C1A-C2A-CAA-CBA
32	H	103	STE	C1-C2-C3-C4
25	b	606	CLA	C16-C17-C18-C19
25	b	605	CLA	C11-C10-C8-C7
32	B	621	STE	C6-C7-C8-C9
32	b	621	STE	O1-C1-C2-C3
29	b	622	LMG	C32-C33-C34-C35
32	c	519	STE	O2-C1-C2-C3
35	F	101	HEM	CAD-CBD-CGD-O1D
25	C	509	CLA	C8-C10-C11-C12
29	B	622	LMG	C32-C33-C34-C35
25	c	505	CLA	C5-C6-C7-C8
32	a	617	STE	C7-C8-C9-C10
32	c	521	STE	C1-C2-C3-C4
36	V	201	HEC	CAD-CBD-CGD-O1D
29	C	520	LMG	C15-C16-C17-C18
29	B	620	LMG	O9-C10-O7-C8
25	C	506	CLA	O1D-CGD-O2D-CED
29	D	407	LMG	C14-C15-C16-C17
33	D	412	LHG	C24-C25-C26-C27
25	B	605	CLA	C8-C10-C11-C12
32	C	522	STE	C1-C2-C3-C4
31	h	101	DGD	CDA-CEA-CFA-CGA
29	c	522	LMG	C17-C18-C19-C20
32	b	621	STE	C12-C13-C14-C15
25	C	506	CLA	CBD-CGD-O2D-CED
32	j	101	STE	C1-C2-C3-C4
31	C	518	DGD	C2D-C1D-O3G-C3G
36	v	201	HEC	CAD-CBD-CGD-O2D
30	A	615	SQD	C19-C20-C21-C22
30	a	614	SQD	O47-C45-C46-O48
30	b	620	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
31	c	516	DGD	O1G-C1G-C2G-O2G
25	b	608	CLA	CBA-CGA-O2A-C1
31	h	101	DGD	O1B-C1B-C2B-C3B
25	b	616	CLA	C10-C11-C12-C13
30	a	614	SQD	O10-C23-O48-C46
30	b	620	SQD	C29-C30-C31-C32
31	c	516	DGD	CBB-CCB-CDB-CEB
32	B	626	STE	O2-C1-C2-C3
32	d	411	STE	C3-C4-C5-C6
29	d	410	LMG	C34-C35-C36-C37
25	A	606	CLA	C2-C1-O2A-CGA
25	c	507	CLA	C6-C7-C8-C9
25	c	511	CLA	C6-C7-C8-C9
32	b	621	STE	O2-C1-C2-C3
31	H	102	DGD	O2G-C1B-C2B-C3B
31	h	101	DGD	CDB-CEB-CFB-CGB
25	A	606	CLA	C15-C16-C17-C18
25	B	614	CLA	C2A-CAA-CBA-CGA
25	b	615	CLA	C16-C17-C18-C20
27	A	610	BCR	C1-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	C	514	BCR	C1-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C30
27	C	516	BCR	C23-C24-C25-C30
27	K	101	BCR	C23-C24-C25-C30
27	a	610	BCR	C1-C6-C7-C8
27	a	610	BCR	C5-C6-C7-C8
27	c	514	BCR	C1-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C30
27	k	103	BCR	C23-C24-C25-C30
31	C	517	DGD	O1G-C1A-C2A-C3A
31	C	518	DGD	C3B-C4B-C5B-C6B
31	C	519	DGD	C5B-C6B-C7B-C8B
33	D	412	LHG	C10-C11-C12-C13
25	b	608	CLA	O1A-CGA-O2A-C1
25	c	508	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
25	b	616	CLA	C2-C3-C5-C6
31	C	518	DGD	C2G-C3G-O3G-C1D
32	b	624	STE	C5-C6-C7-C8
25	C	501	CLA	C16-C17-C18-C20
30	a	614	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
31	A	616	DGD	C6A-C7A-C8A-C9A
25	b	613	CLA	C13-C15-C16-C17
29	D	411	LMG	C33-C34-C35-C36
29	m	101	LMG	C40-C41-C42-C43
32	d	412	STE	C14-C15-C16-C17
30	a	614	SQD	C24-C23-O48-C46
25	D	403	CLA	C3-C5-C6-C7
32	d	411	STE	O2-C1-C2-C3
30	B	624	SQD	C33-C34-C35-C36
25	c	505	CLA	C12-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C10
28	A	611	PL9	C13-C14-C16-C17
29	d	410	LMG	C30-C31-C32-C33
32	b	623	STE	C2-C3-C4-C5
30	a	615	SQD	O6-C44-C45-O47
33	B	623	LHG	C14-C15-C16-C17
32	I	101	STE	C2-C3-C4-C5
30	a	615	SQD	C17-C18-C19-C20
31	c	517	DGD	CCA-CDA-CEA-CFA
25	B	612	CLA	C13-C15-C16-C17
30	a	615	SQD	O48-C23-C24-C25
30	D	408	SQD	C24-C25-C26-C27
29	C	520	LMG	C36-C37-C38-C39
25	b	608	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C19
32	B	626	STE	O1-C1-C2-C3
32	B	627	STE	O2-C1-C2-C3
25	a	606	CLA	C2C-C3C-CAC-CBC
27	B	618	BCR	C20-C21-C22-C37
27	k	103	BCR	C20-C21-C22-C37
27	t	101	BCR	C20-C21-C22-C37
32	b	621	STE	C5-C6-C7-C8
25	B	612	CLA	CAA-CBA-CGA-O2A
25	C	507	CLA	C4-C3-C5-C6
28	A	611	PL9	C30-C29-C31-C32
25	B	607	CLA	C8-C10-C11-C12
31	c	515	DGD	CAA-CBA-CCA-CDA
30	f	101	SQD	O48-C23-C24-C25
30	B	624	SQD	C29-C30-C31-C32
25	B	607	CLA	C11-C10-C8-C9
25	B	614	CLA	C11-C12-C13-C14
25	B	615	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	b	603	CLA	C11-C12-C13-C14
25	b	607	CLA	C11-C10-C8-C9
25	b	607	CLA	C14-C13-C15-C16
35	e	101	HEM	CAD-CBD-CGD-O1D
29	c	518	LMG	C34-C35-C36-C37
33	D	410	LHG	C15-C16-C17-C18
25	c	512	CLA	C3A-C2A-CAA-CBA
33	e	102	LHG	O8-C23-C24-C25
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	609	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
25	C	512	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	612	CLA	CAD-CBD-CGD-O2D
25	c	512	CLA	CAD-CBD-CGD-O2D
29	c	522	LMG	C9-C8-O7-C10
32	C	523	STE	C3-C4-C5-C6
25	C	505	CLA	C8-C10-C11-C12
25	c	509	CLA	C3-C5-C6-C7
33	l	101	LHG	C18-C19-C20-C21
31	C	517	DGD	C4D-C5D-C6D-O5D
32	d	411	STE	O1-C1-C2-C3
25	c	508	CLA	C2-C3-C5-C6
25	c	512	CLA	C2-C3-C5-C6
29	A	613	LMG	O1-C7-C8-C9
29	A	613	LMG	C7-C8-C9-O8
29	B	620	LMG	O1-C7-C8-C9
30	f	101	SQD	O6-C44-C45-C46
33	e	102	LHG	C4-C5-C6-O8
25	B	612	CLA	CBA-CGA-O2A-C1
35	e	101	HEM	CAD-CBD-CGD-O2D
25	d	404	CLA	C5-C6-C7-C8
25	B	604	CLA	O2A-C1-C2-C3
25	b	601	CLA	O2A-C1-C2-C3
26	A	608	PHO	O2A-C1-C2-C3
29	C	520	LMG	C39-C40-C41-C42
31	c	516	DGD	C5B-C6B-C7B-C8B
25	b	614	CLA	C2A-CAA-CBA-CGA
27	k	102	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	c	517	DGD	CDB-CEB-CFB-CGB
32	B	627	STE	O1-C1-C2-C3
30	B	624	SQD	C12-C13-C14-C15
30	a	614	SQD	C15-C16-C17-C18
31	c	515	DGD	O1B-C1B-O2G-C2G
25	A	607	CLA	CHA-CBD-CGD-O1D
25	A	607	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	CHA-CBD-CGD-O2D
25	B	612	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
32	B	629	STE	C7-C8-C9-C10
32	d	411	STE	C12-C13-C14-C15
29	m	101	LMG	C20-C21-C22-C23
29	c	522	LMG	O1-C7-C8-O7
33	a	613	LHG	C11-C12-C13-C14
25	b	610	CLA	C15-C16-C17-C18
33	l	101	LHG	C32-C33-C34-C35
31	C	518	DGD	C9B-CAB-CBB-CCB
26	A	608	PHO	CHA-CBD-CGD-O2D
26	D	402	PHO	CHA-CBD-CGD-O1D
26	D	402	PHO	CHA-CBD-CGD-O2D
30	A	615	SQD	C8-C7-O47-C45
25	b	613	CLA	CAA-CBA-CGA-O2A
32	d	412	STE	C2-C3-C4-C5
25	B	601	CLA	C4-C3-C5-C6
29	B	620	LMG	C28-C29-C30-C31
25	B	607	CLA	C12-C13-C15-C16
25	C	512	CLA	C16-C17-C18-C20
31	c	515	DGD	C4E-C5E-C6E-O5E
31	c	517	DGD	C7A-C8A-C9A-CAA
33	d	408	LHG	C29-C30-C31-C32
25	C	505	CLA	C14-C13-C15-C16
25	C	511	CLA	C6-C7-C8-C9
27	T	101	BCR	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
35	e	101	HEM	CAA-CBA-CGA-O2A
25	b	613	CLA	C16-C17-C18-C20
29	b	622	LMG	C36-C37-C38-C39
32	B	627	STE	C12-C13-C14-C15
32	C	523	STE	C12-C13-C14-C15
29	b	622	LMG	O9-C10-C11-C12
33	e	102	LHG	C16-C17-C18-C19
25	B	602	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C1A-C2A-CAA-CBA
33	D	412	LHG	C1-C2-C3-O3
31	c	515	DGD	O1B-C1B-C2B-C3B
29	B	620	LMG	C15-C16-C17-C18
33	d	407	LHG	C11-C10-C9-C8
31	c	515	DGD	C1G-C2G-C3G-O3G
32	B	621	STE	C10-C11-C12-C13
25	B	610	CLA	C2A-CAA-CBA-CGA
29	b	622	LMG	C39-C40-C41-C42
29	m	101	LMG	C12-C13-C14-C15
25	d	404	CLA	C16-C17-C18-C19
25	B	612	CLA	CAA-CBA-CGA-O1A
30	f	101	SQD	O10-C23-C24-C25
33	D	409	LHG	C4-O6-P-O5
33	d	407	LHG	C3-O3-P-O5
25	b	604	CLA	C16-C17-C18-C19
25	A	607	CLA	C2C-C3C-CAC-CBC
30	D	408	SQD	C32-C33-C34-C35
29	m	101	LMG	O9-C10-C11-C12
30	a	615	SQD	O10-C23-C24-C25
33	D	410	LHG	O10-C23-C24-C25
30	b	620	SQD	O47-C7-C8-C9
27	A	610	BCR	C5-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C26
27	b	618	BCR	C23-C24-C25-C30
27	d	405	BCR	C23-C24-C25-C30
27	k	102	BCR	C23-C24-C25-C26
25	A	612	CLA	C4C-C3C-CAC-CBC
25	c	507	CLA	C8-C10-C11-C12
31	C	517	DGD	O1B-C1B-C2B-C3B
31	c	516	DGD	O1B-C1B-C2B-C3B
29	c	520	LMG	C29-C30-C31-C32
25	c	502	CLA	C16-C17-C18-C19
33	B	623	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	c	522	LMG	C4-C5-C6-O5
32	b	621	STE	C4-C5-C6-C7
32	j	101	STE	C4-C5-C6-C7
25	b	612	CLA	CAA-CBA-CGA-O2A
29	C	520	LMG	O7-C10-C11-C12
31	a	616	DGD	O2G-C1B-C2B-C3B
31	A	616	DGD	C8B-C9B-CAB-CBB
25	B	613	CLA	C4-C3-C5-C6
27	k	103	BCR	C19-C20-C21-C22
25	c	508	CLA	C10-C11-C12-C13
30	b	620	SQD	C13-C14-C15-C16
25	A	607	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	607	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O1D
29	B	622	LMG	C28-C29-C30-C31
25	B	605	CLA	C14-C13-C15-C16
25	B	613	CLA	C6-C7-C8-C9
32	X	101	STE	C3-C4-C5-C6
26	A	608	PHO	C8-C10-C11-C12
30	B	624	SQD	C14-C15-C16-C17
33	D	410	LHG	O8-C23-C24-C25
25	B	612	CLA	O1D-CGD-O2D-CED
33	e	102	LHG	O10-C23-C24-C25
31	a	616	DGD	O1G-C1A-C2A-C3A
25	b	612	CLA	C10-C11-C12-C13
32	c	521	STE	O1-C1-C2-C3
30	A	615	SQD	C25-C26-C27-C28
30	A	615	SQD	C16-C17-C18-C19
25	b	613	CLA	C4-C3-C5-C6
28	a	611	PL9	C25-C24-C26-C27
25	B	607	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	c	509	CLA	C6-C7-C8-C10
26	d	402	PHO	C3A-C2A-CAA-CBA
28	A	611	PL9	C18-C19-C21-C22
25	b	613	CLA	CAA-CBA-CGA-O1A
29	D	407	LMG	O9-C10-C11-C12

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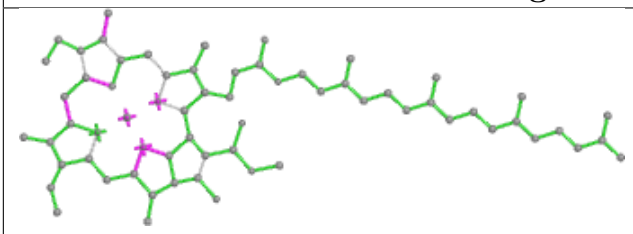
Mol	Chain	Res	Type	Atoms
35	e	101	HEM	CAA-CBA-CGA-O1A
30	A	615	SQD	O47-C7-C8-C9
30	A	615	SQD	O48-C23-C24-C25
27	T	101	BCR	C17-C18-C19-C20
31	c	515	DGD	O2G-C1B-C2B-C3B
25	A	612	CLA	C13-C15-C16-C17
30	A	614	SQD	C15-C16-C17-C18
31	A	616	DGD	C5A-C6A-C7A-C8A
25	b	612	CLA	CAA-CBA-CGA-O1A
29	m	101	LMG	O7-C10-C11-C12
25	c	509	CLA	C2A-CAA-CBA-CGA
30	b	620	SQD	O49-C7-C8-C9
32	E	102	STE	O1-C1-C2-C3
32	c	521	STE	O2-C1-C2-C3

There are no ring outliers.

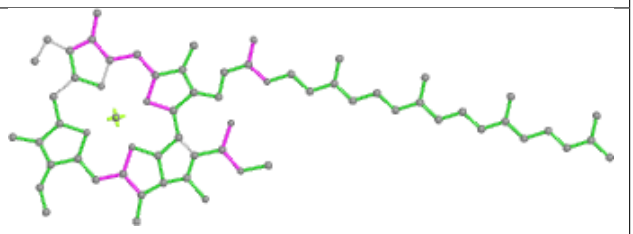
No monomer is involved in short contacts.

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

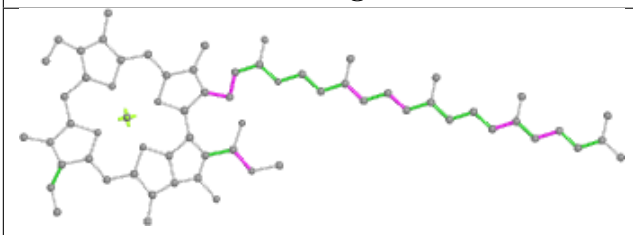
Ligand CLA c 513



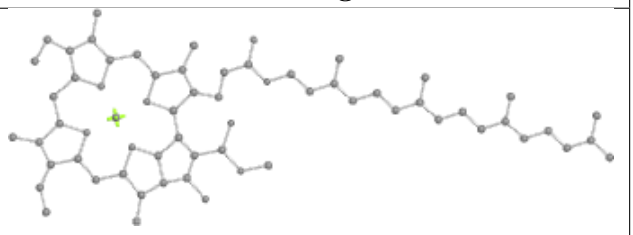
Bond lengths



Bond angles

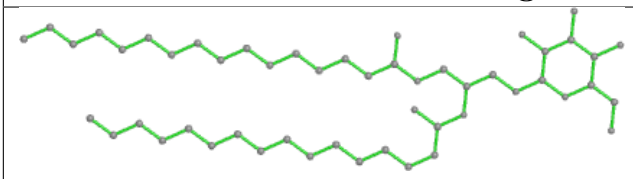


Torsions

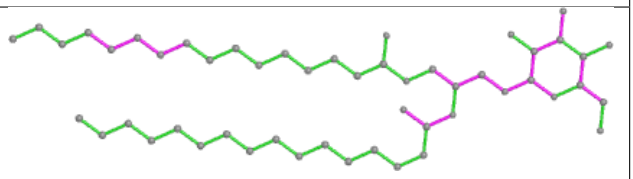


Rings

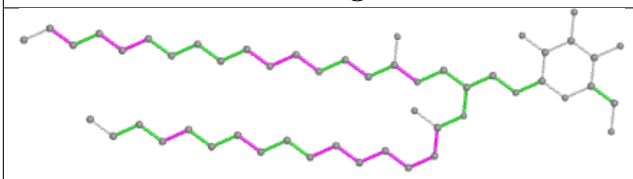
Ligand LMG m 101



Bond lengths



Bond angles



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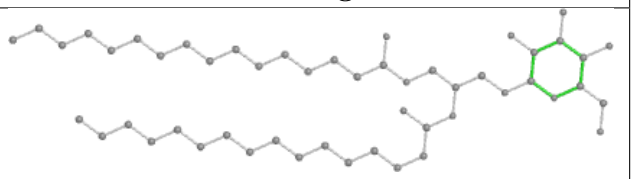
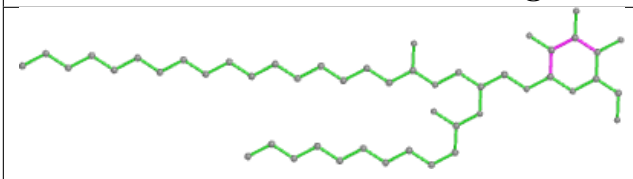
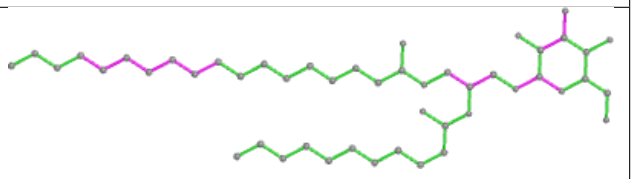


Rings

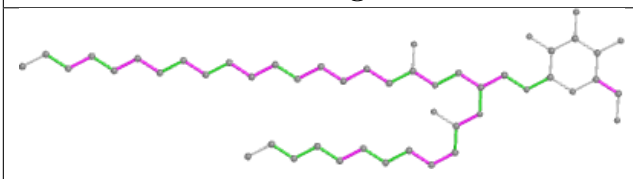
Ligand LMG c 520



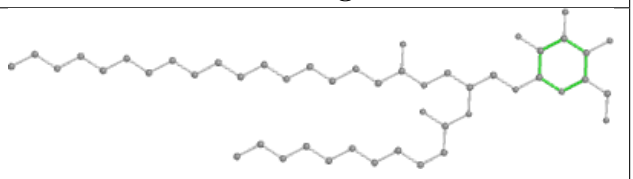
Bond lengths



Bond angles

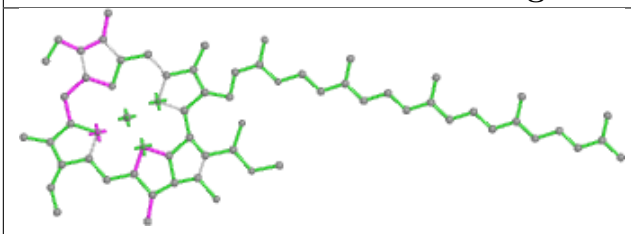


Torsions

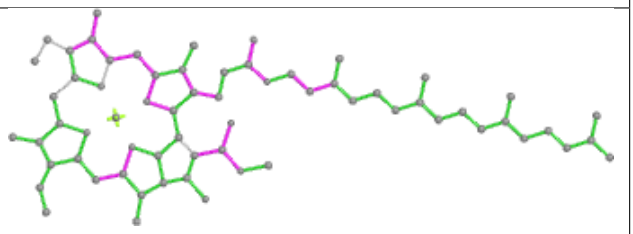


Rings

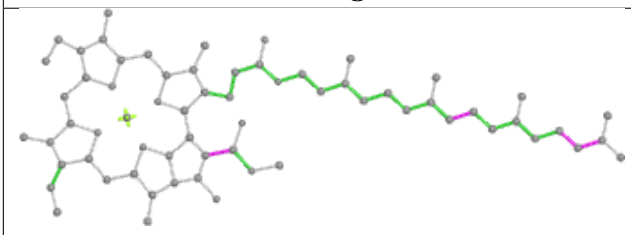
Ligand CLA b 610



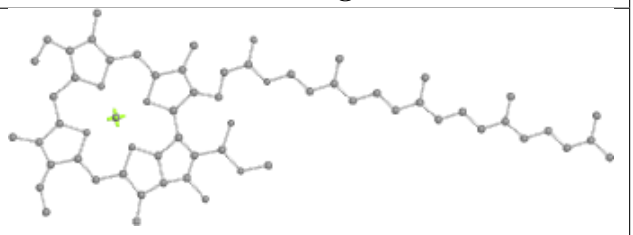
Bond lengths



Bond angles

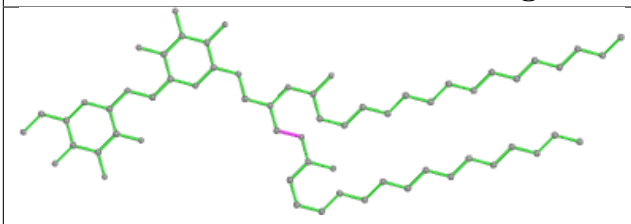


Torsions

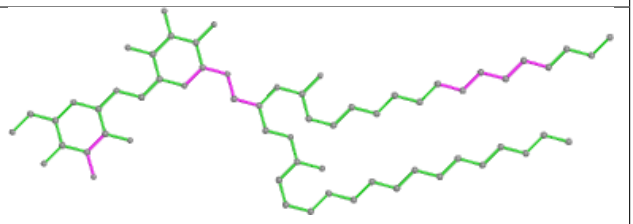


Rings

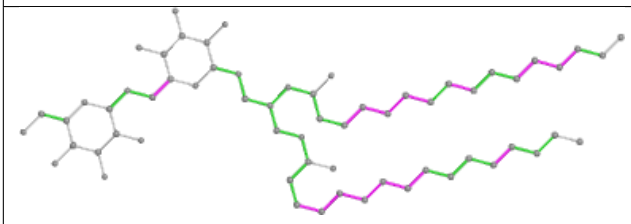
Ligand DGD C 519



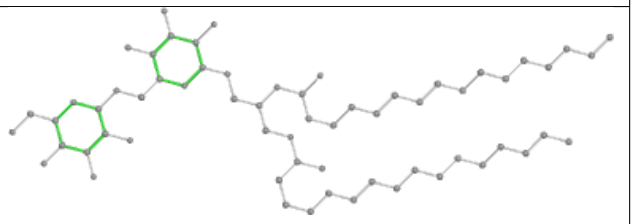
Bond lengths



Bond angles

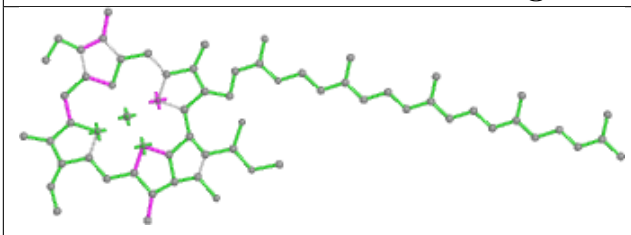


Torsions

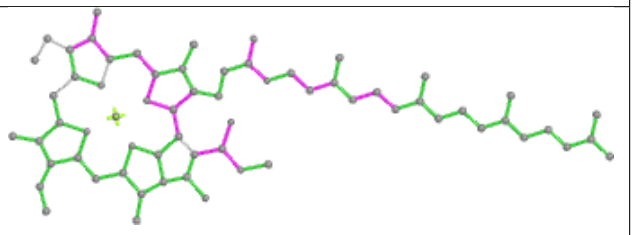


Rings

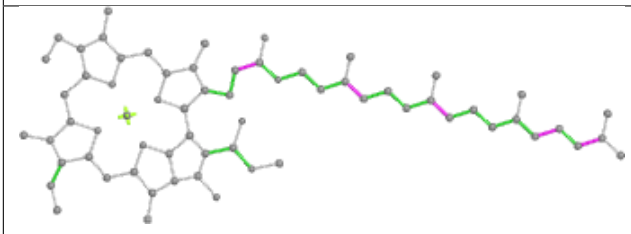
Ligand CLA b 613



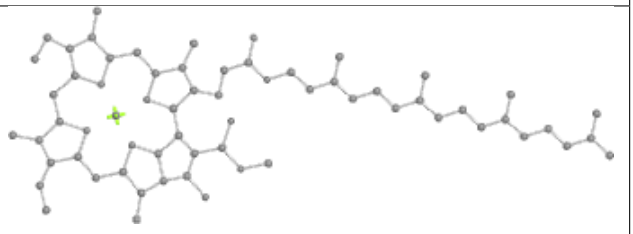
Bond lengths



Bond angles

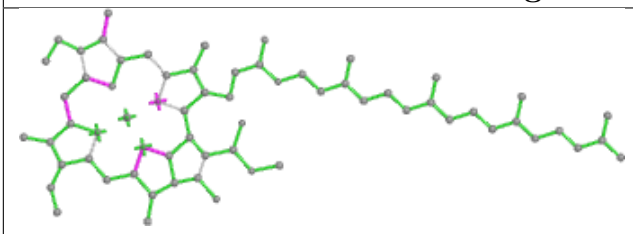


Torsions

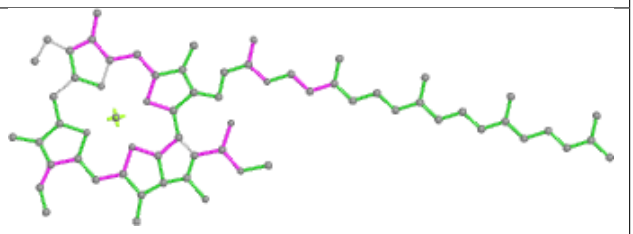


Rings

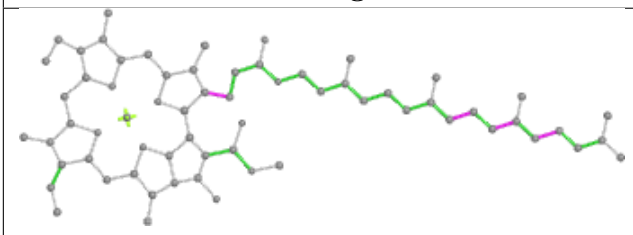
Ligand CLA B 602



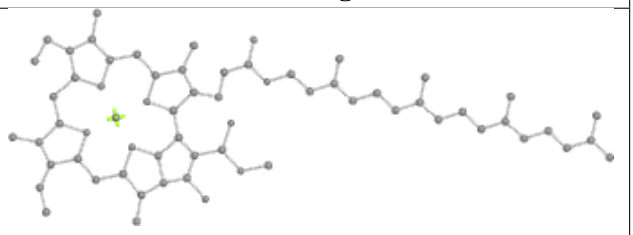
Bond lengths



Bond angles

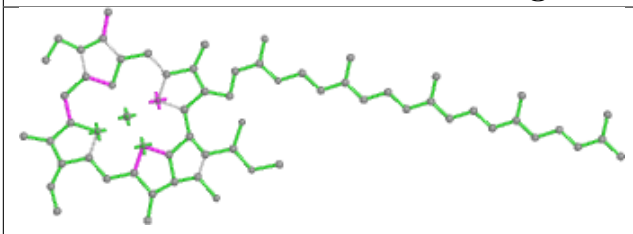


Torsions



Rings

Ligand CLA c 510



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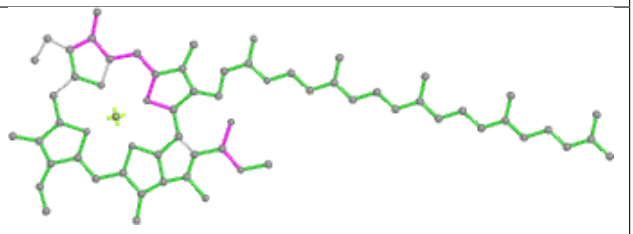
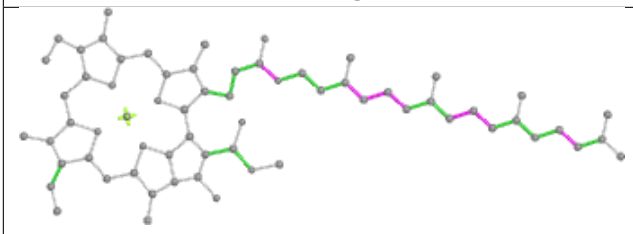


Bond angles



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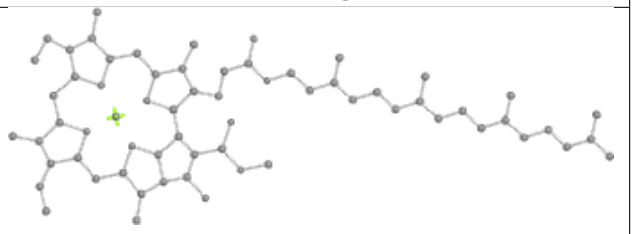
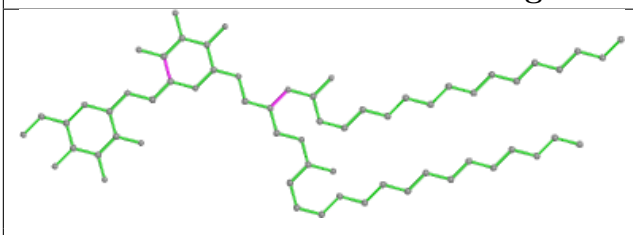


Rings

Ligand DGD c 517



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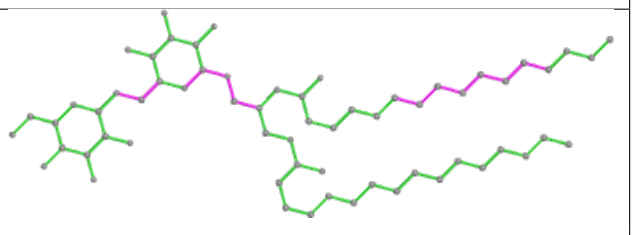
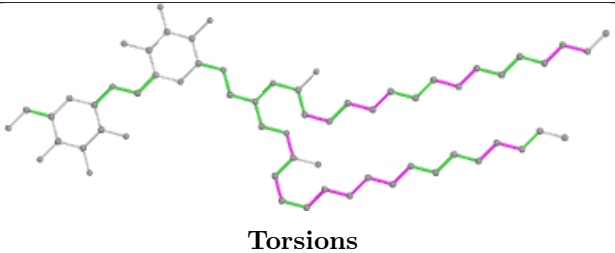


Bond angles



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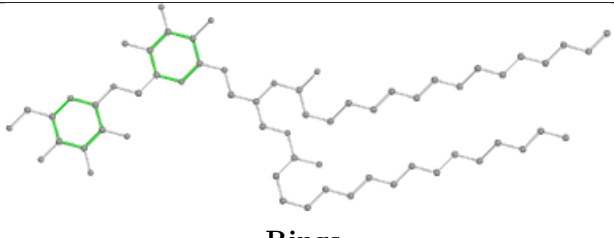
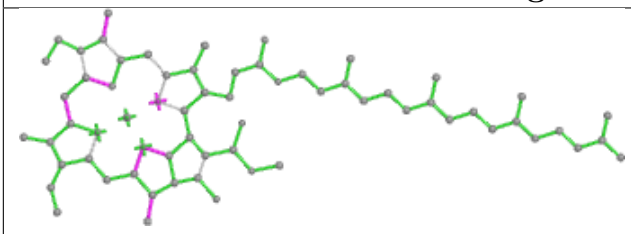
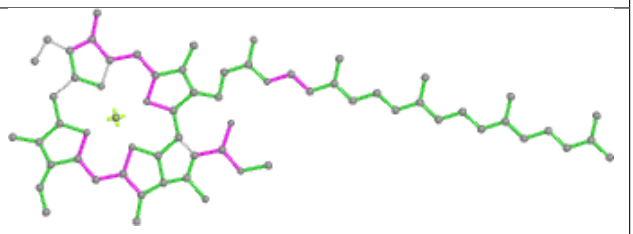


Rings

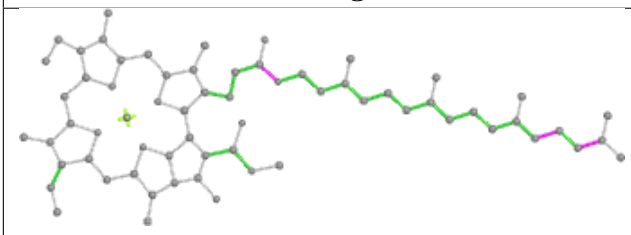
Ligand CLA b 608



Bond lengths



Bond angles



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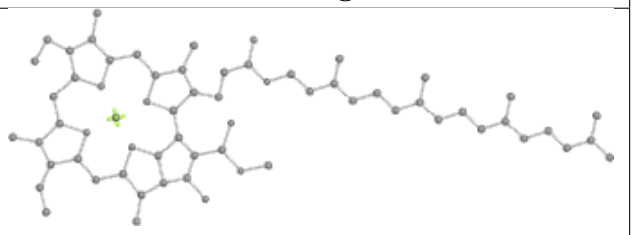
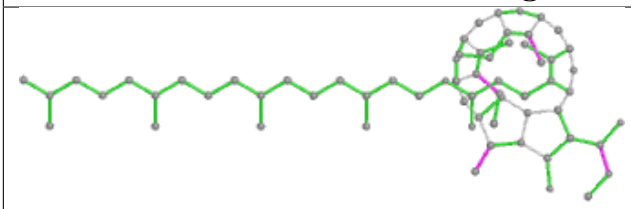
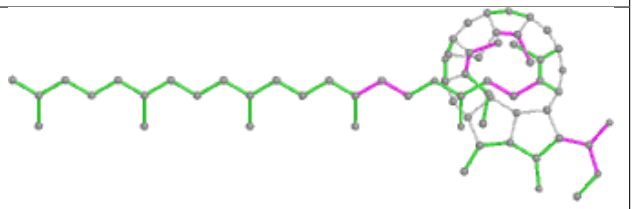


Rings

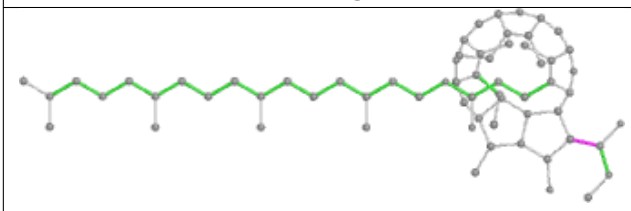
Ligand PHO D 402



Bond lengths



Bond angles



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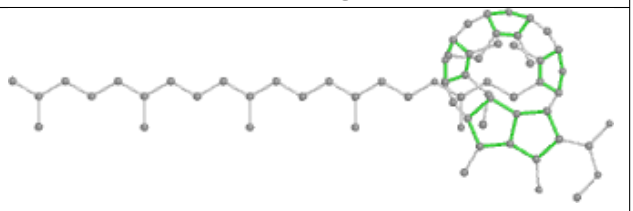
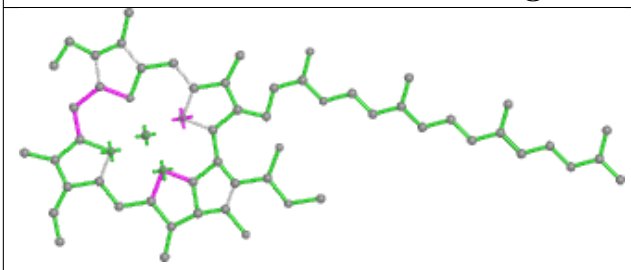


Rings

Ligand CLA B 616



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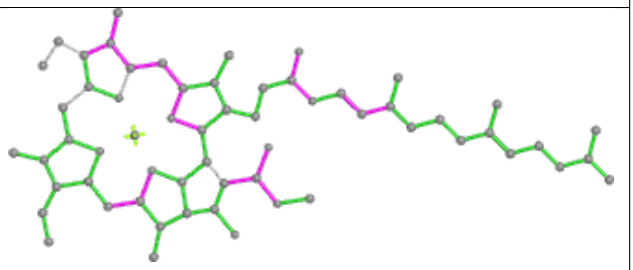
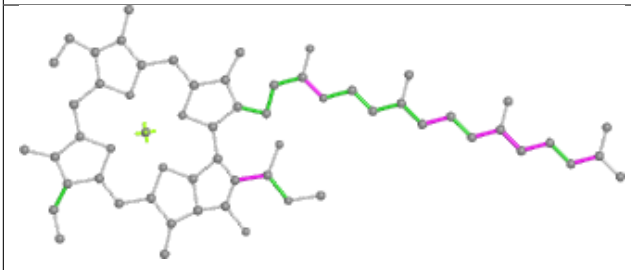
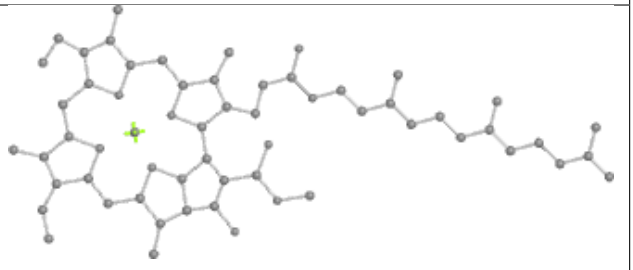


Bond angles

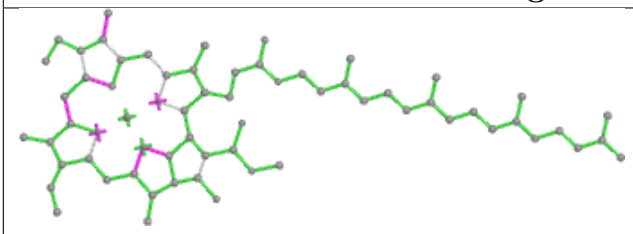


Torsions



Rings

Ligand CLA b 607



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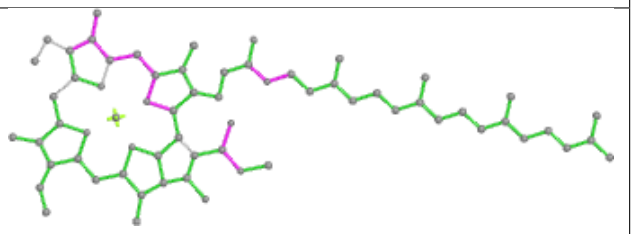
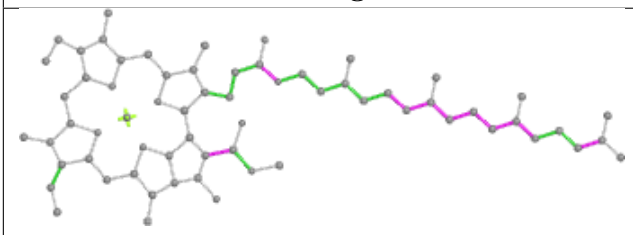
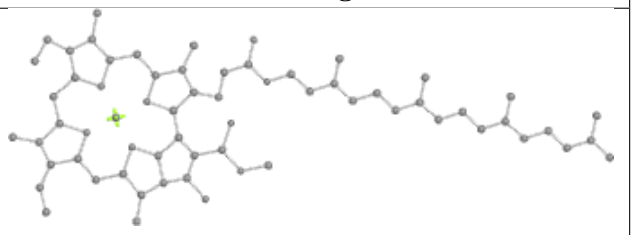


Bond angles

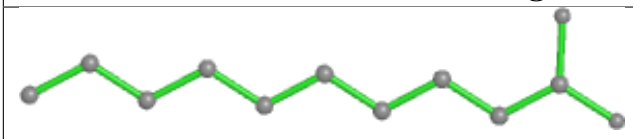


Torsions



Rings

Ligand STE B 628



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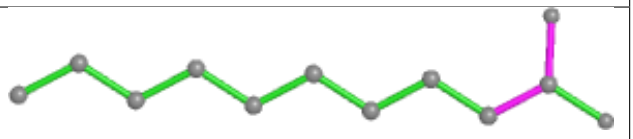
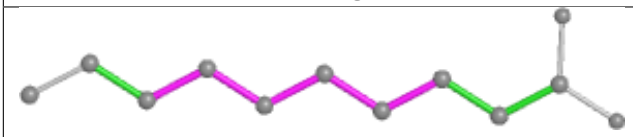


Bond angles



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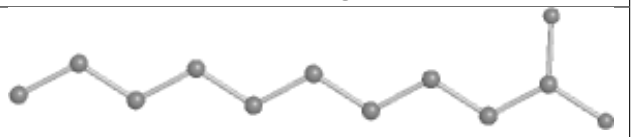
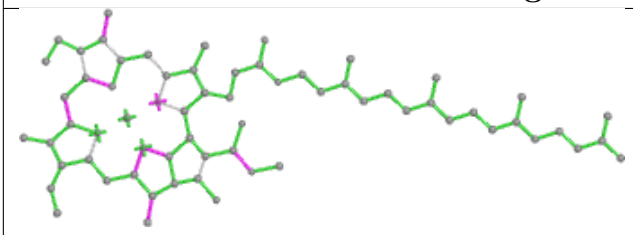


Rings

Ligand CLA C 509



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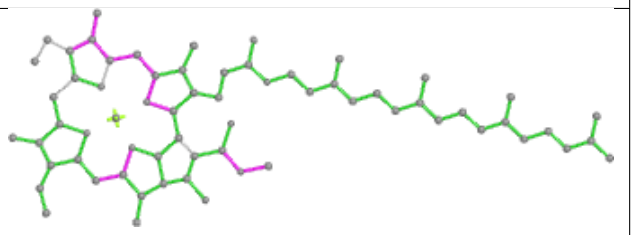
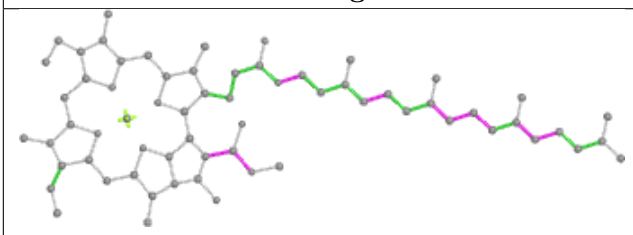
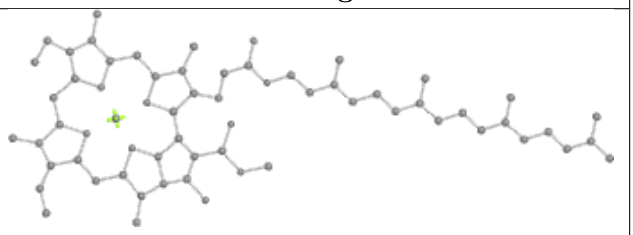


Bond angles

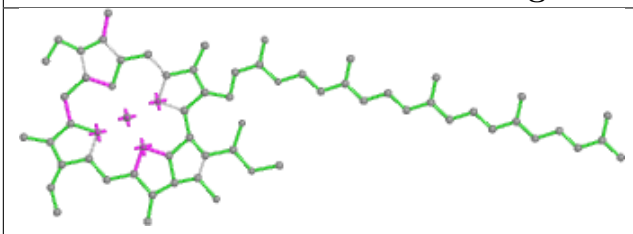


Torsions



Rings

Ligand CLA a 606



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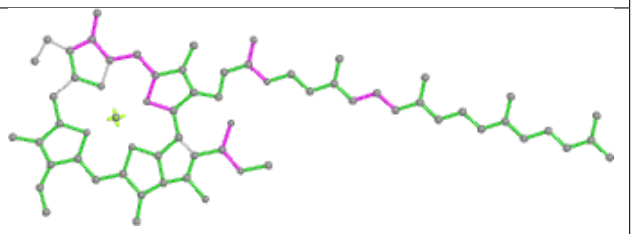
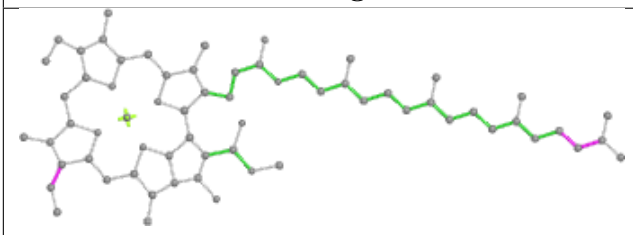


Bond angles



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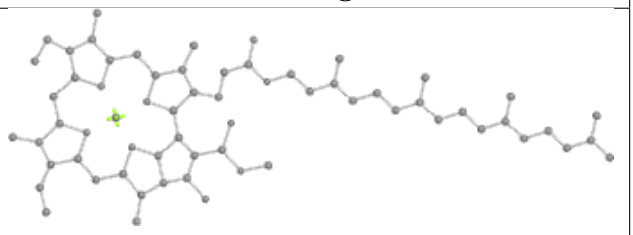
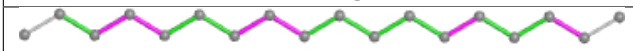


Rings

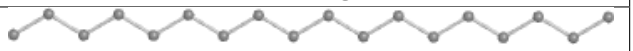
Ligand STE l 102

Bond lengths

Bond angles

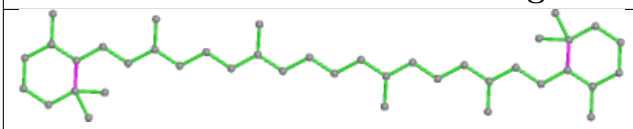


Torsions

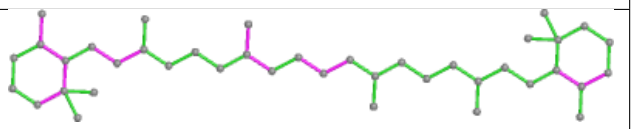


Rings

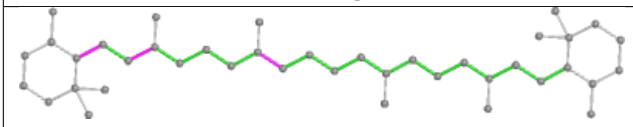
Ligand BCR c 514



Bond lengths



Bond angles



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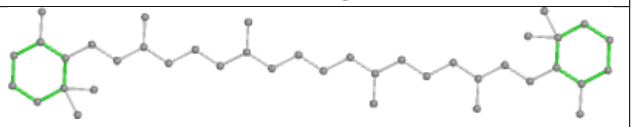
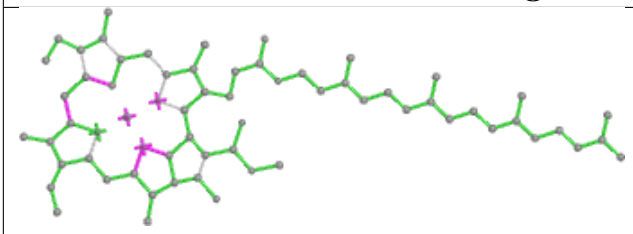


Rings

Ligand CLA C 505



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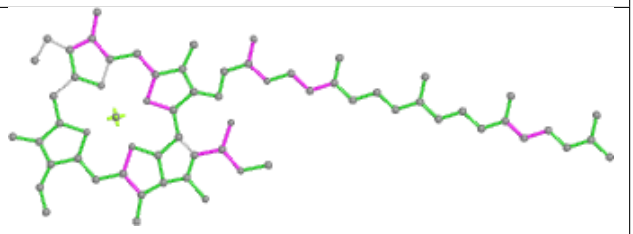
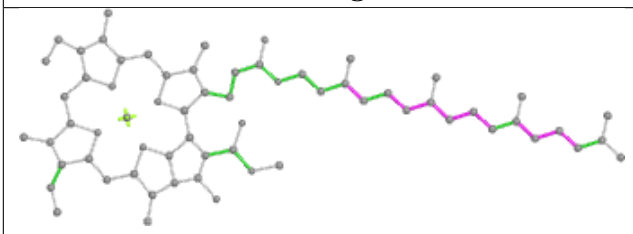


Bond angles



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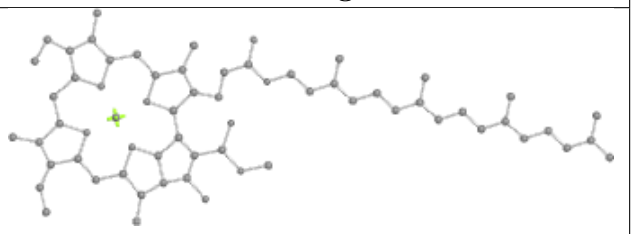
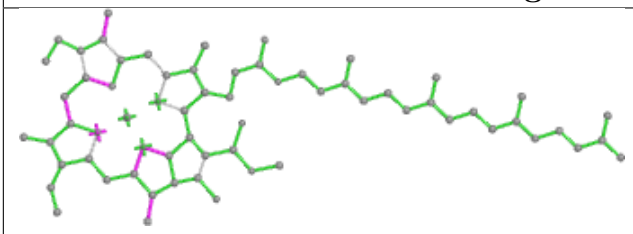
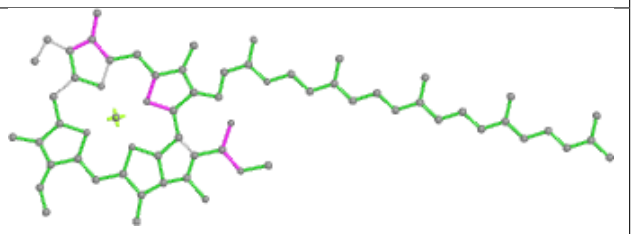


Rings

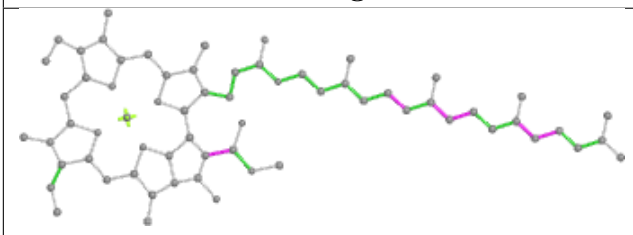
Ligand CLA B 607



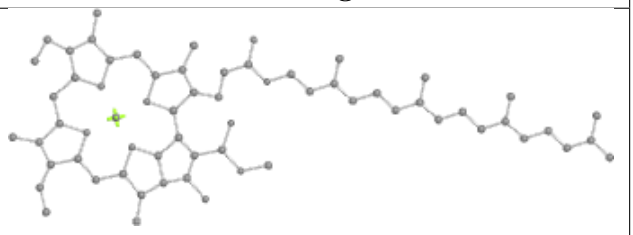
Bond lengths



Bond angles

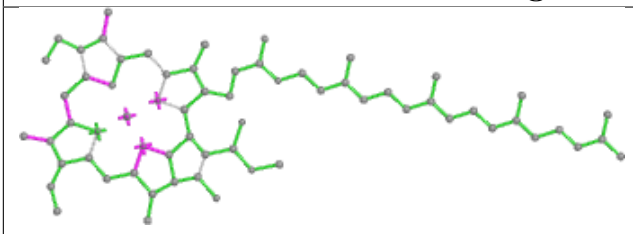


Torsions

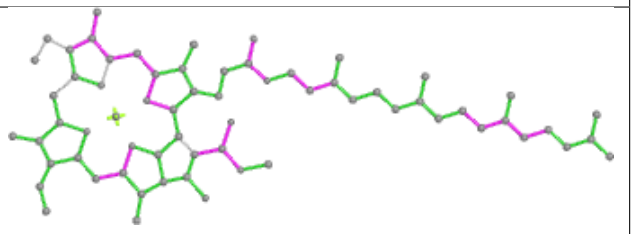


Rings

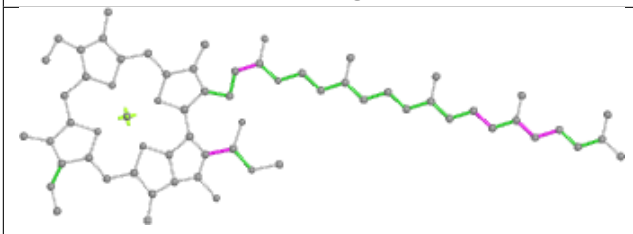
Ligand CLA b 612



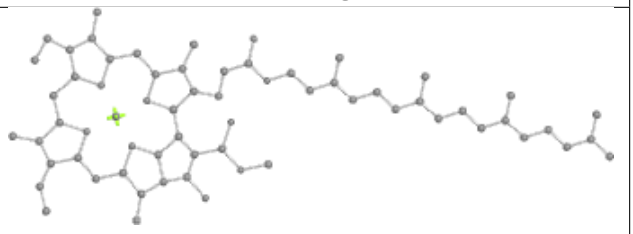
Bond lengths



Bond angles

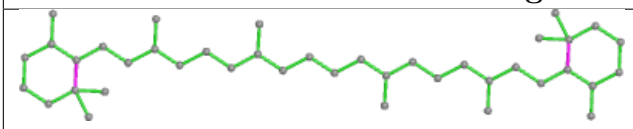


Torsions

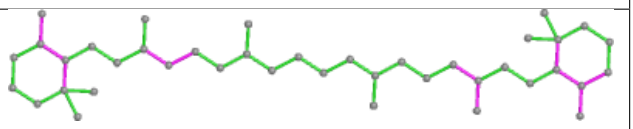


Rings

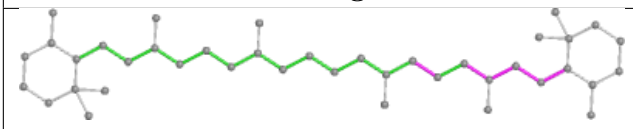
Ligand BCR d 405



Bond lengths



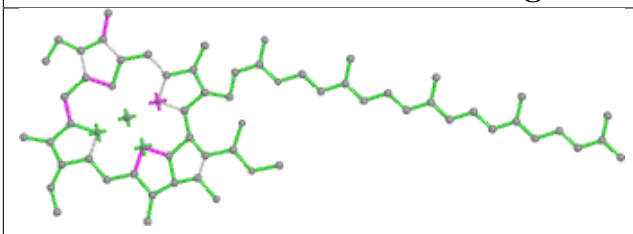
Bond angles



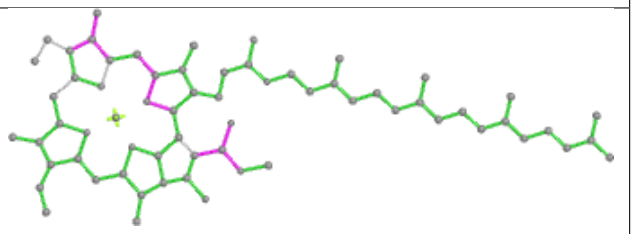
Torsions

Rings

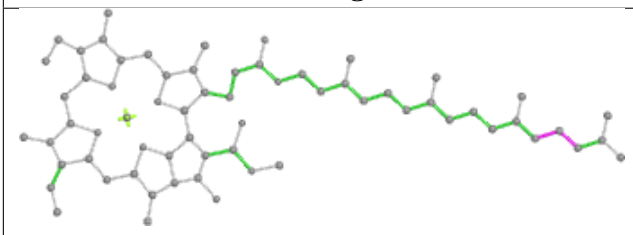
Ligand CLA B 608



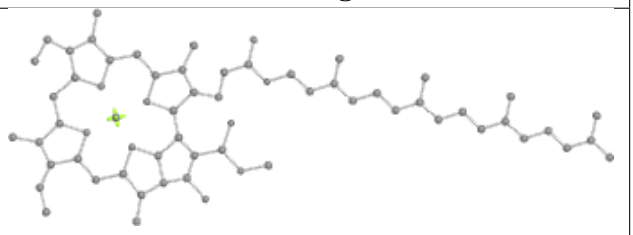
Bond lengths



Bond angles

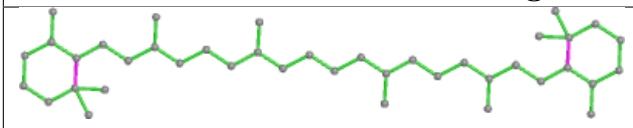


Torsions

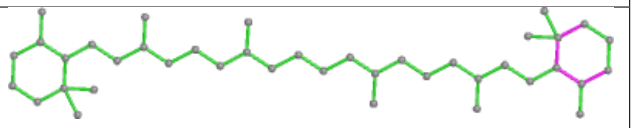


Rings

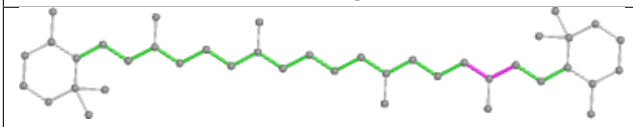
Ligand BCR b 619



Bond lengths



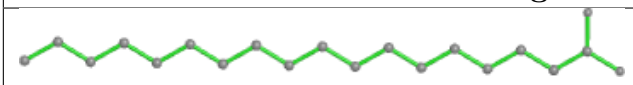
Bond angles



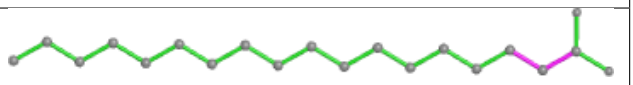
Torsions

Rings

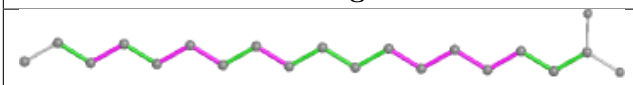
Ligand STE b 624



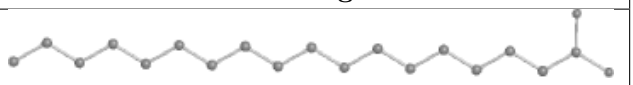
Bond lengths



Bond angles

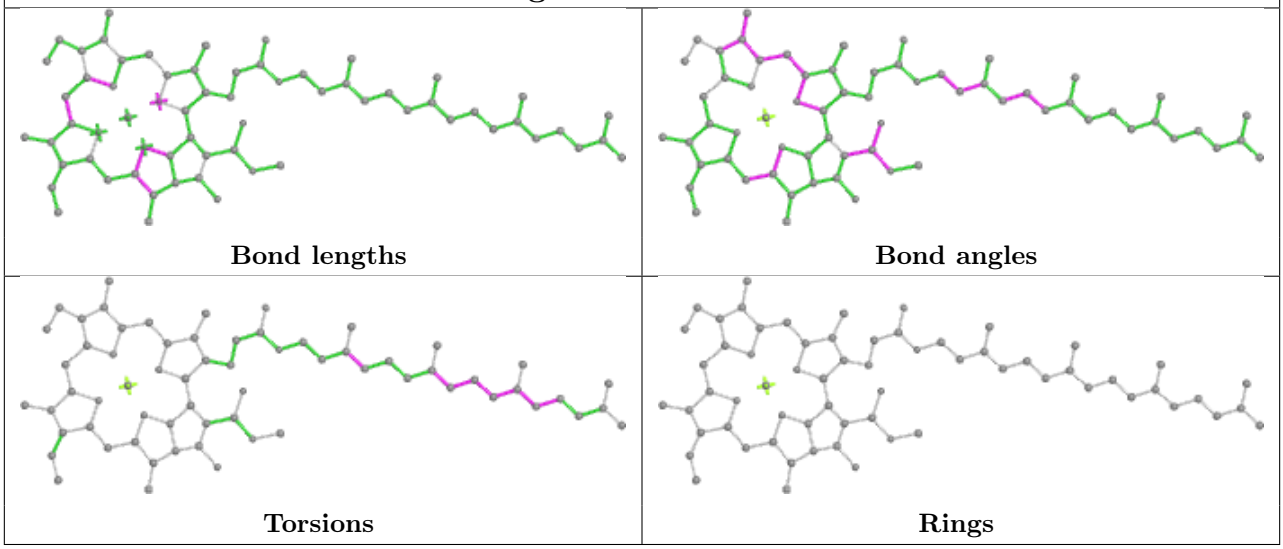


Torsions

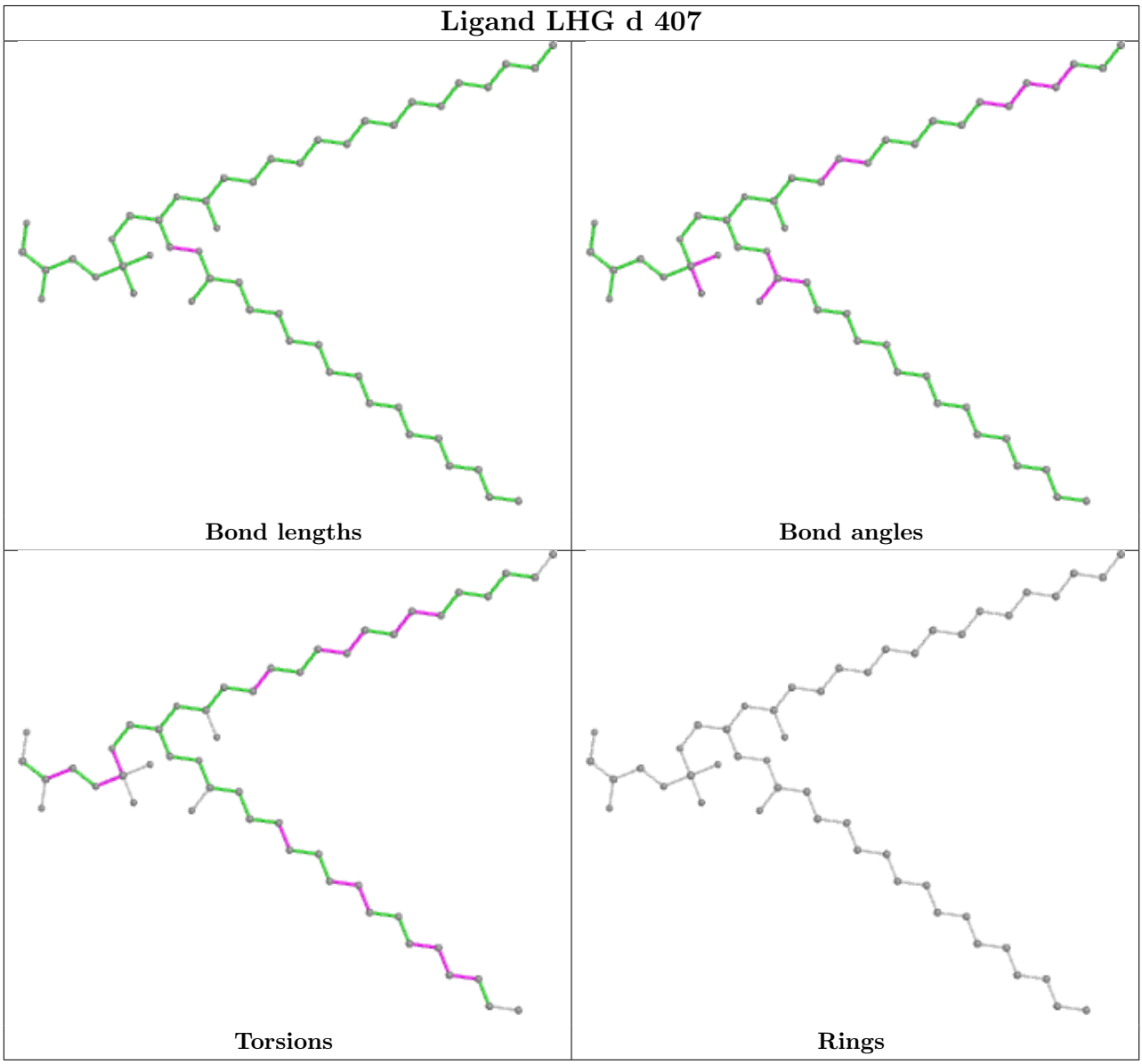


Rings

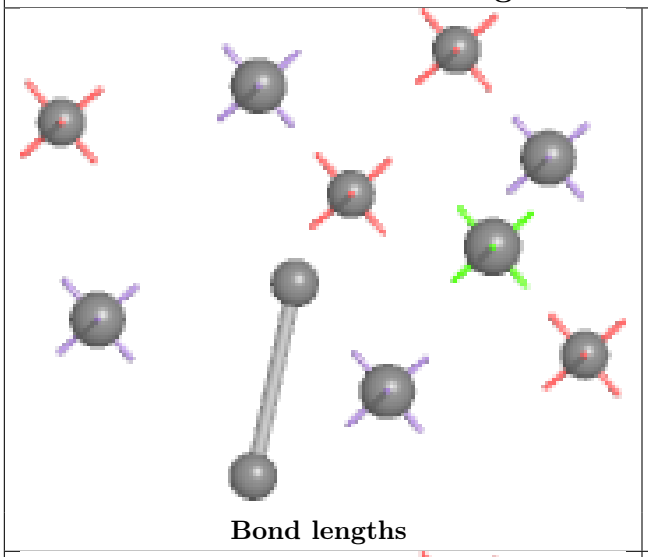
Ligand CLA b 611



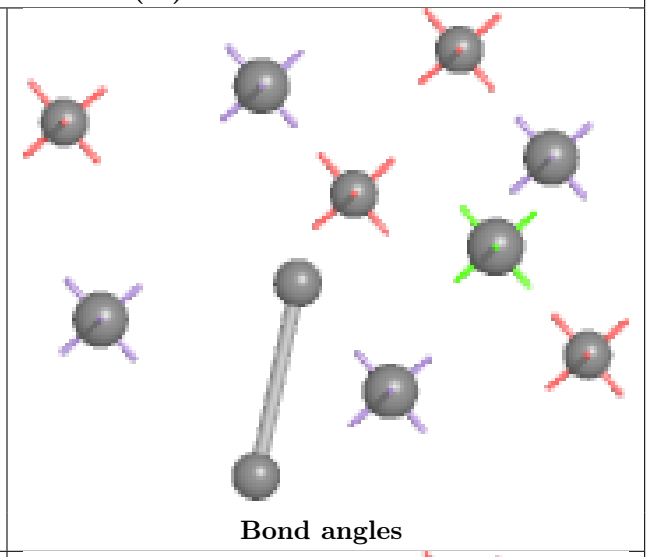
Ligand LHG d 407



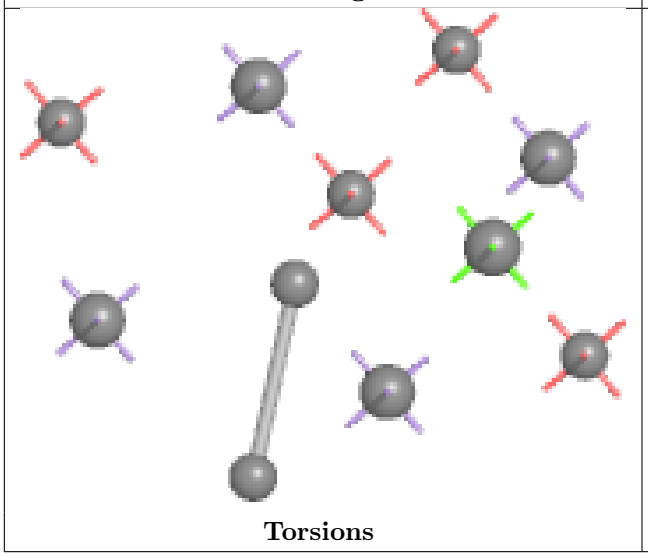
Ligand OEY a 602 (A)



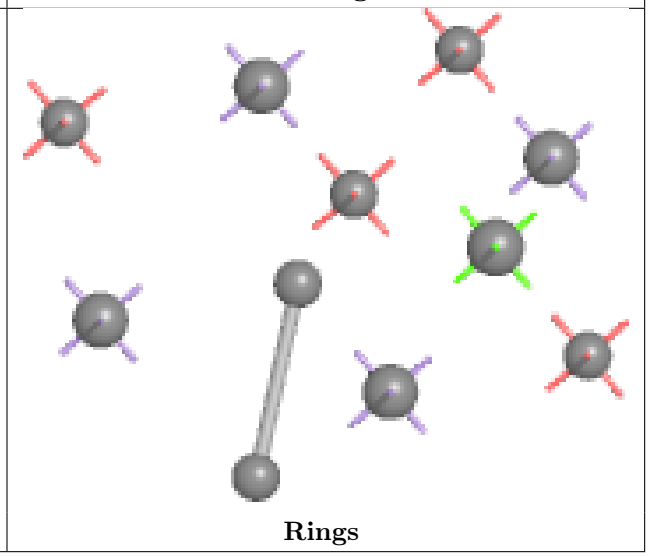
Bond lengths



Bond angles



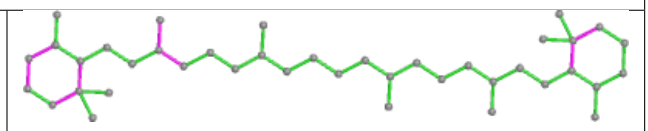
Torsions



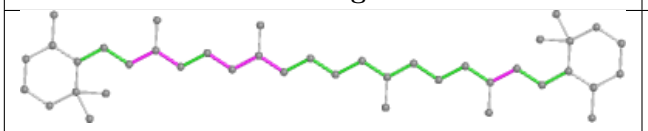
Rings

Ligand BCR B 619

Bond lengths



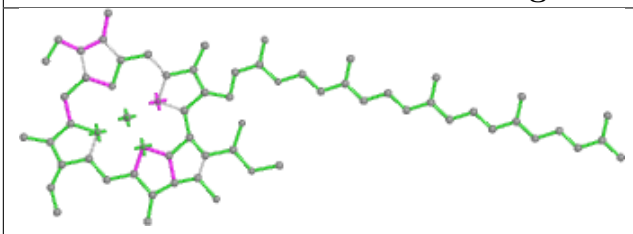
Bond angles



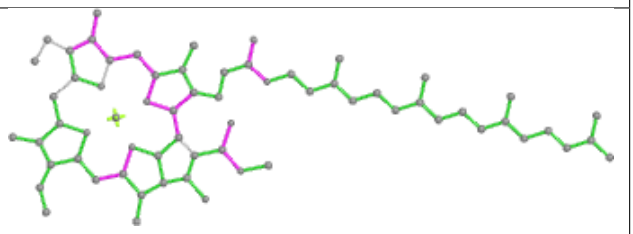
Torsions

Rings

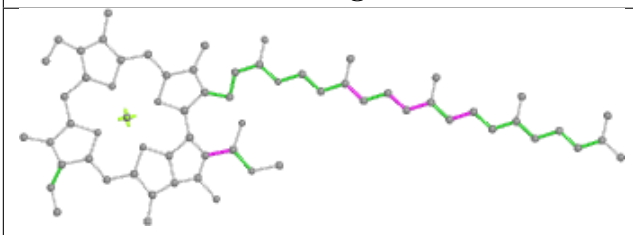
Ligand CLA c 507



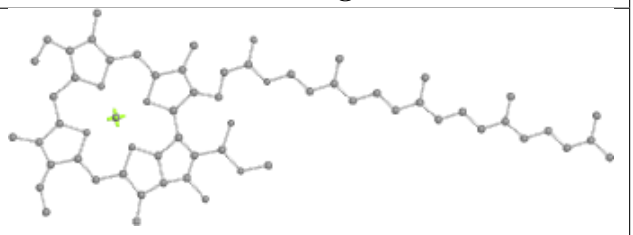
Bond lengths



Bond angles

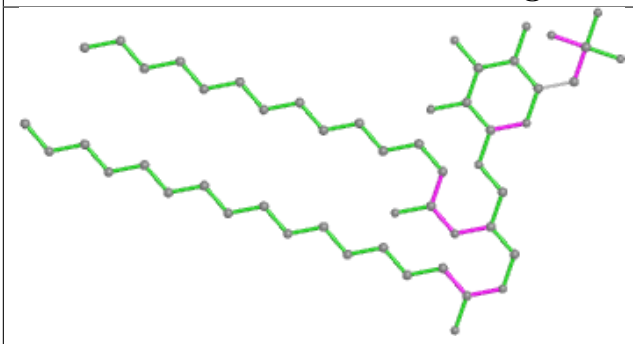


Torsions

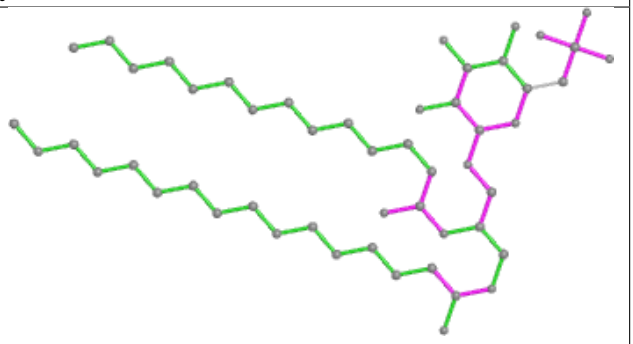


Rings

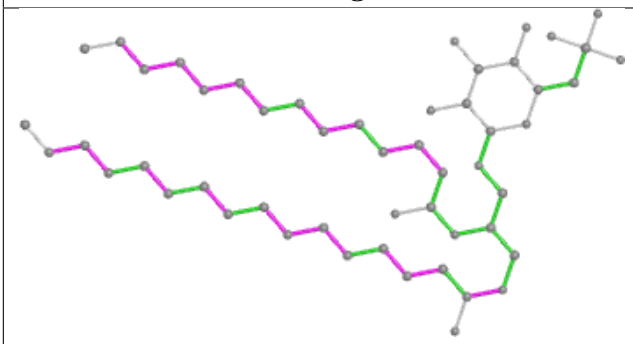
Ligand SQD A 614



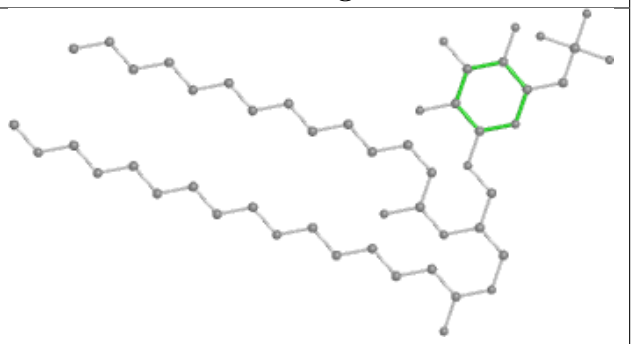
Bond lengths



Bond angles

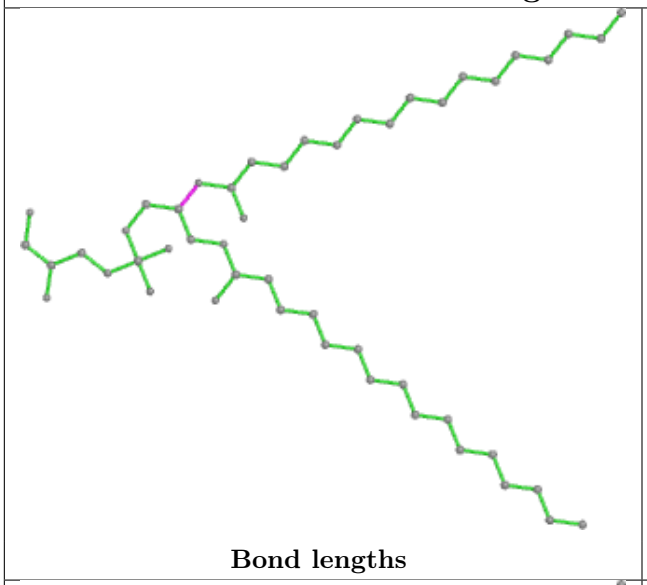


Torsions

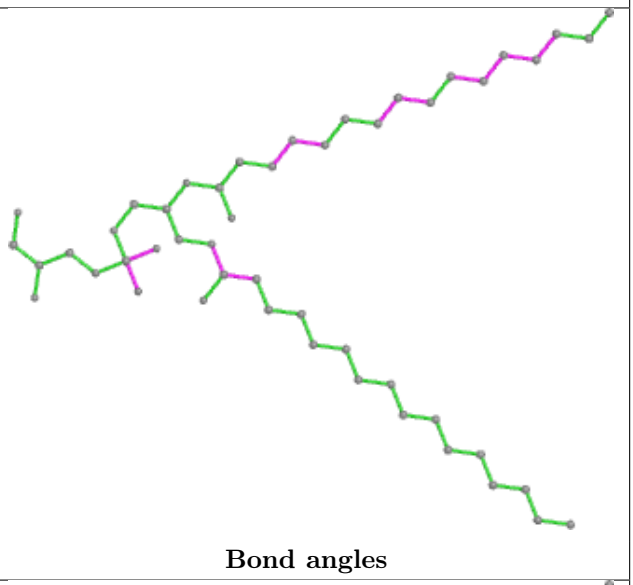


Rings

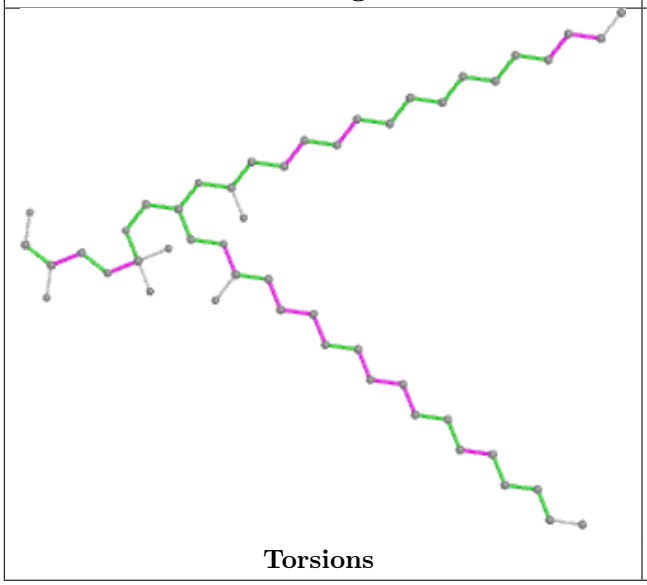
Ligand LHG D 412



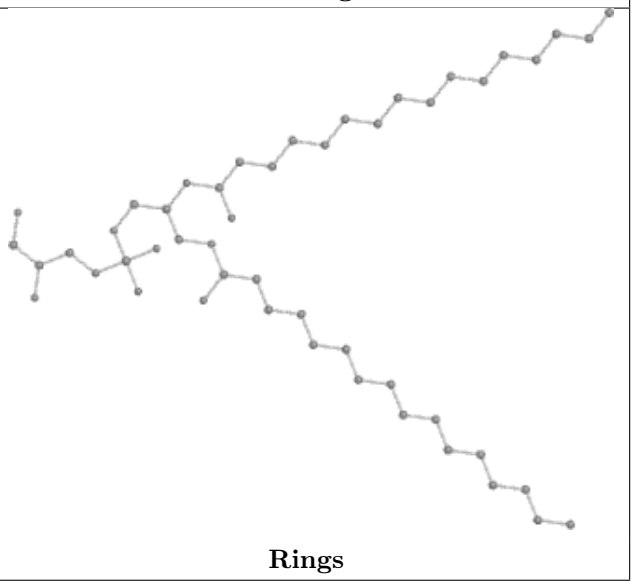
Bond lengths



Bond angles

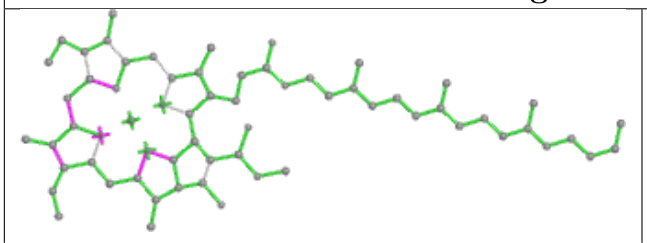


Torsions

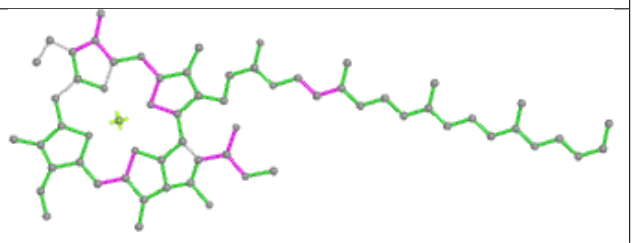


Rings

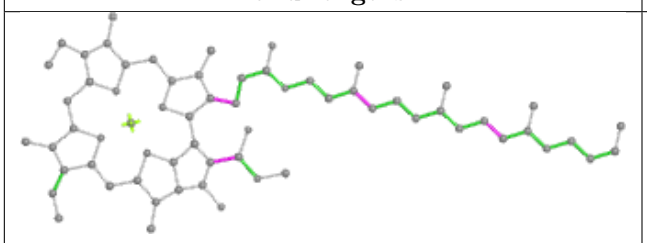
Ligand CLA c 508



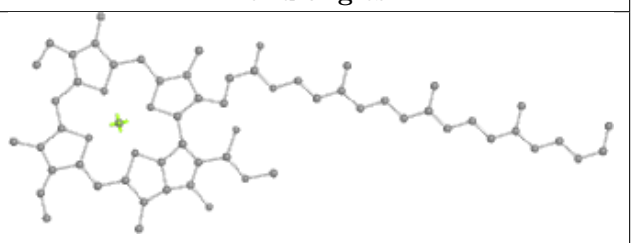
Bond lengths



Bond angles

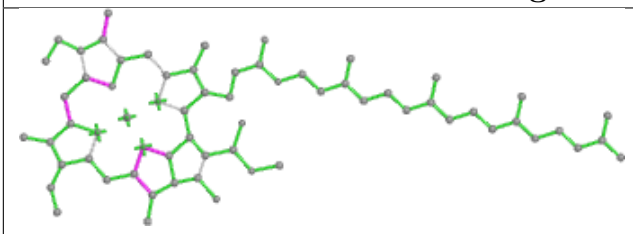


Torsions

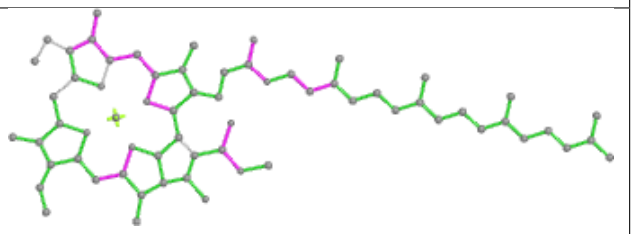


Rings

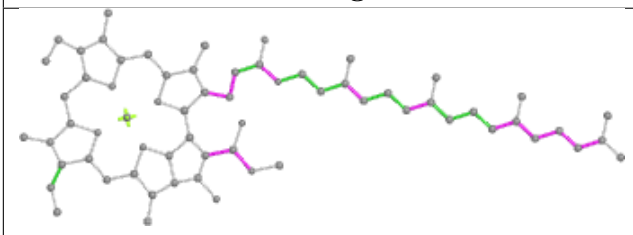
Ligand CLA c 512



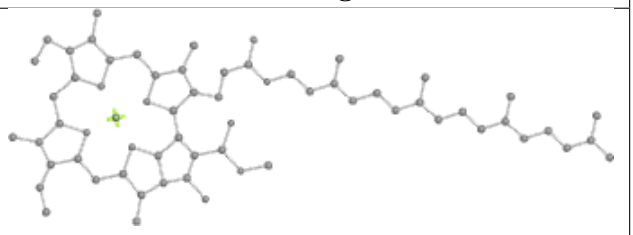
Bond lengths



Bond angles

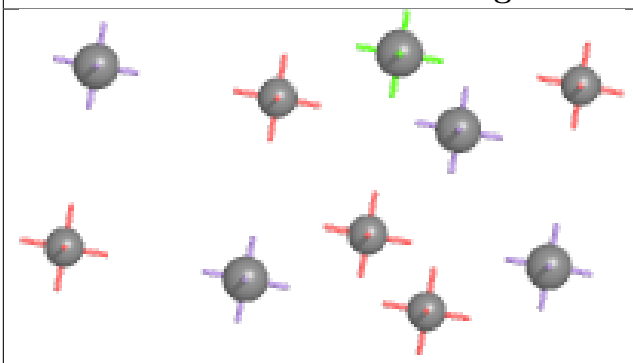


Torsions

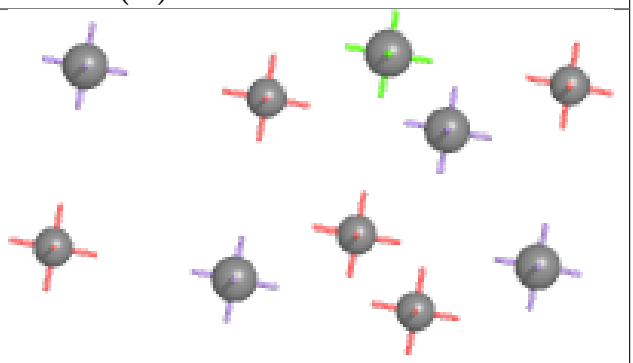


Rings

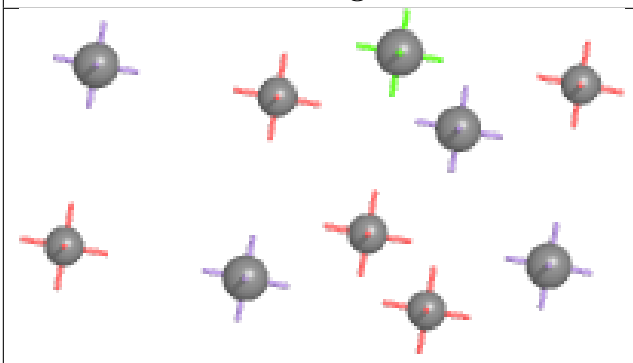
Ligand OEX a 601 (C)



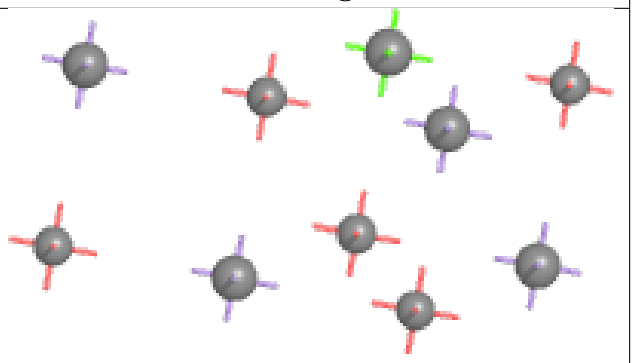
Bond lengths



Bond angles

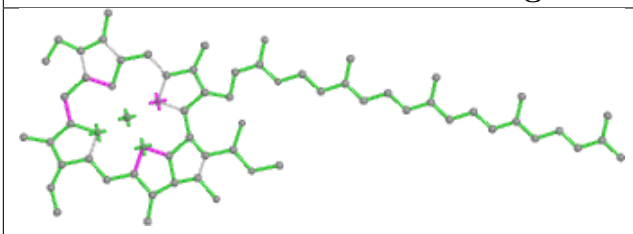


Torsions

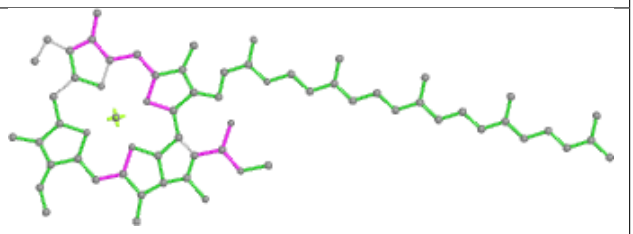


Rings

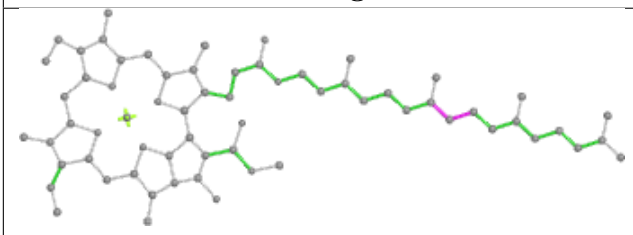
Ligand CLA B 611



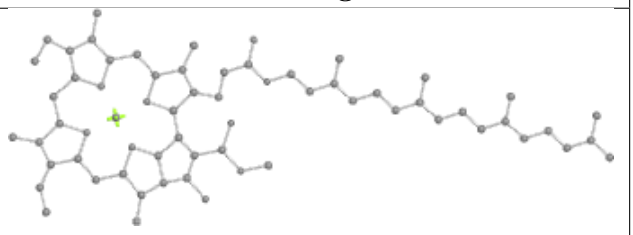
Bond lengths



Bond angles

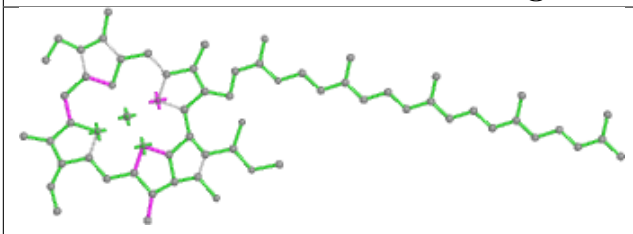


Torsions

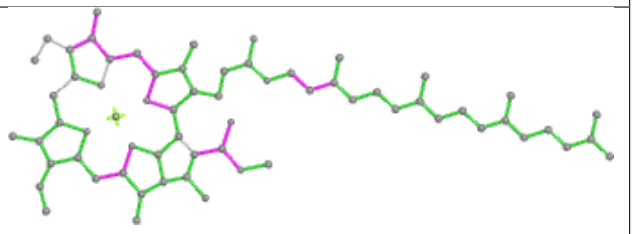


Rings

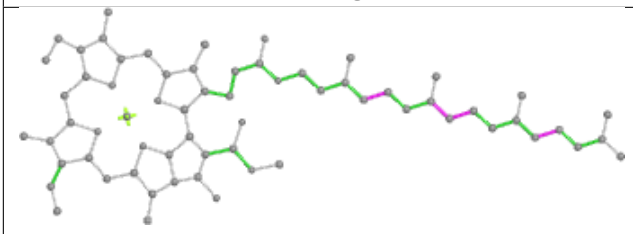
Ligand CLA b 602



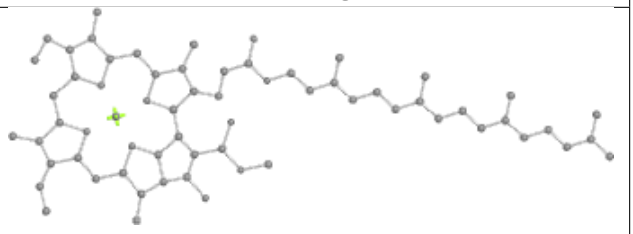
Bond lengths



Bond angles

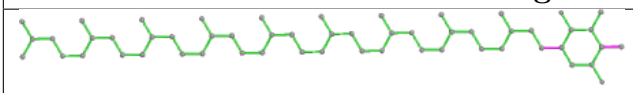


Torsions



Rings

Ligand PL9 a 611



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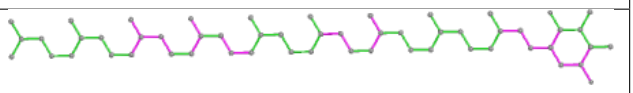
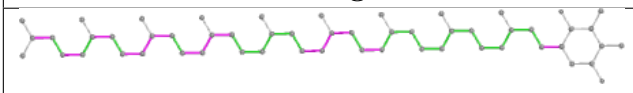
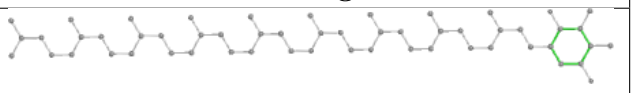


Bond angles

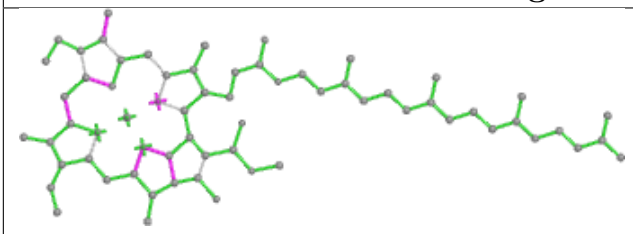


Torsions



Rings

Ligand CLA a 612



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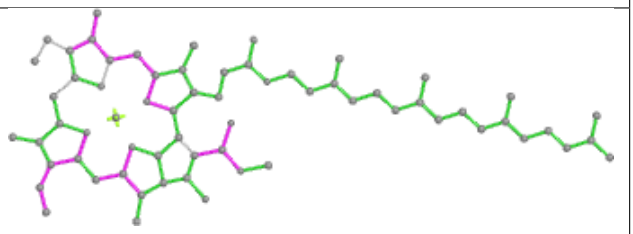
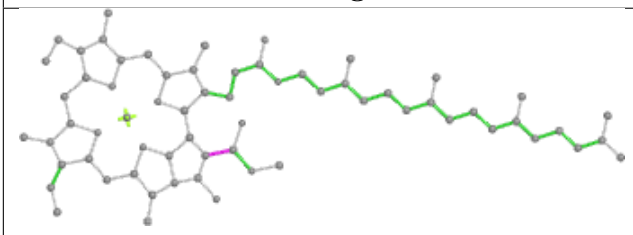
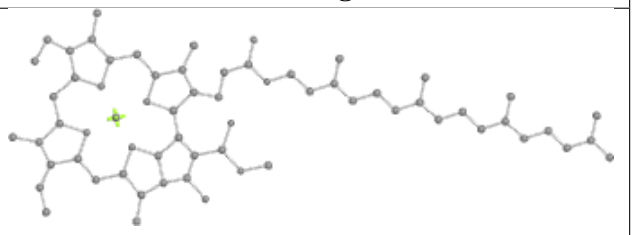


Bond angles

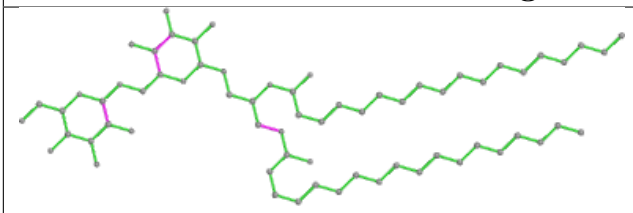


Torsions



Rings

Ligand DGD A 616



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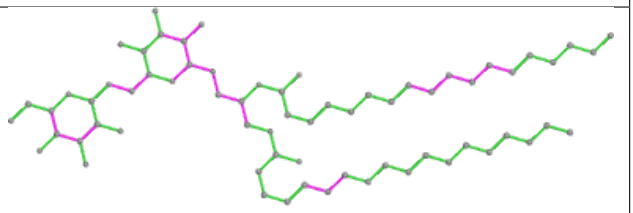
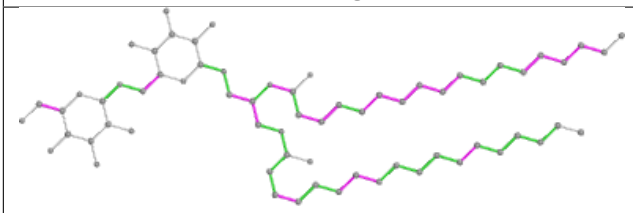


Bond angles



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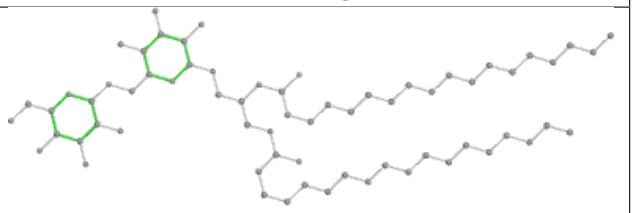
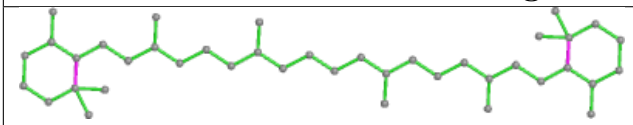


Rings

Ligand BCR B 617



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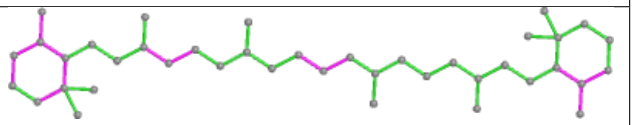
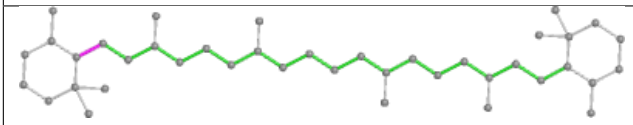


Bond angles



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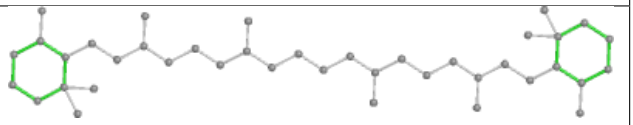
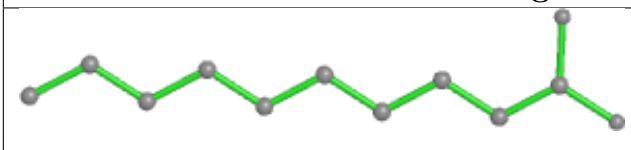


Rings

Ligand STE a 617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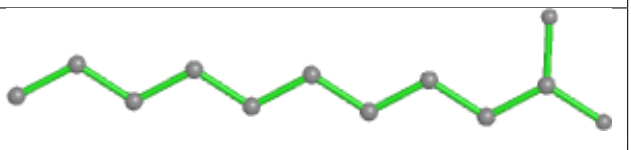
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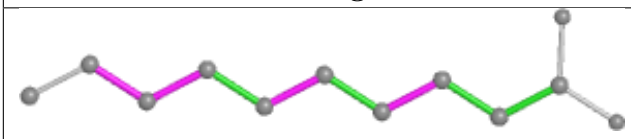
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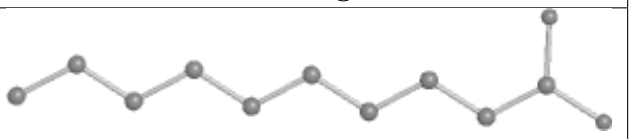
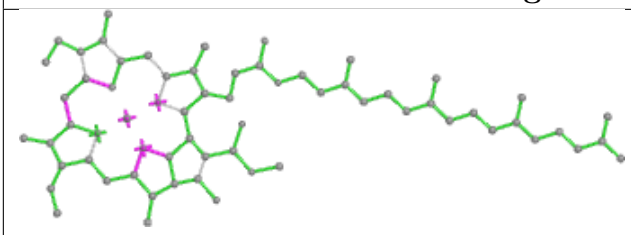

Rings

Ligand CLA A 612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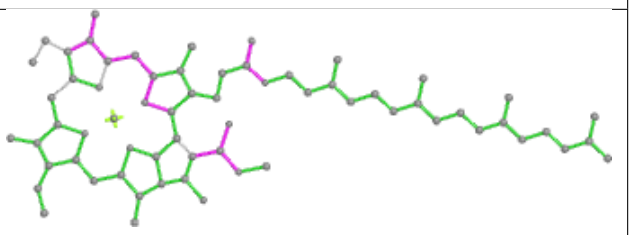
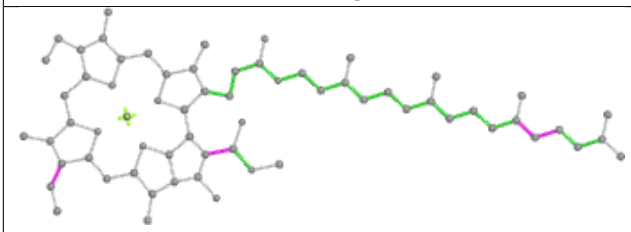

Bond angles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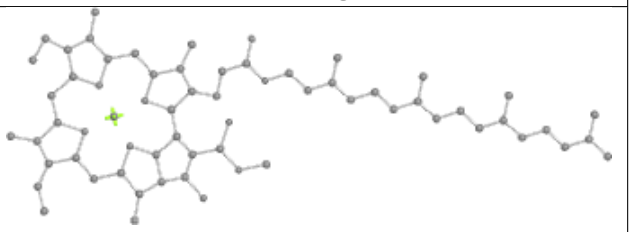
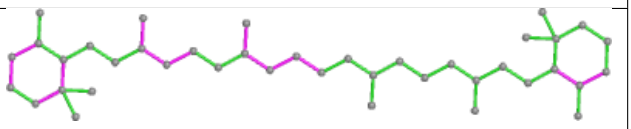
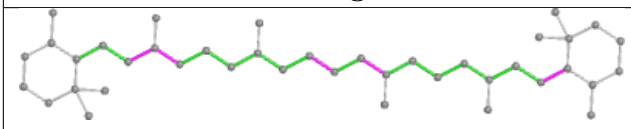

Rings

Ligand BCR x 101


Bond lengths


Bond angles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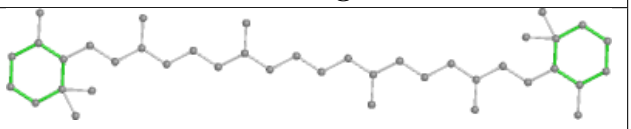
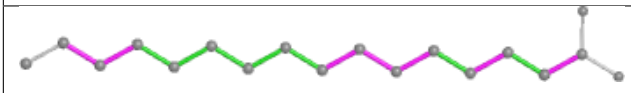

Rings

Ligand STE B 627


Bond lengths


Bond angles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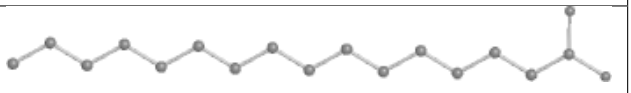
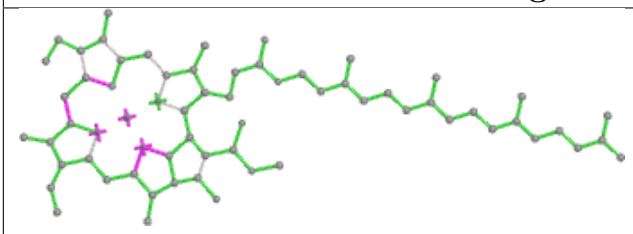
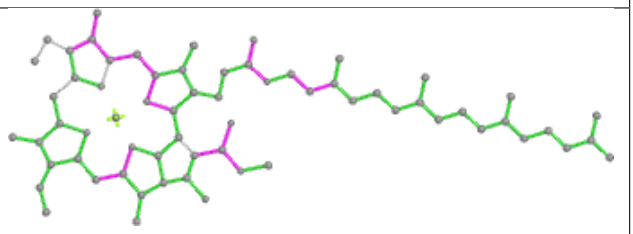

Rings

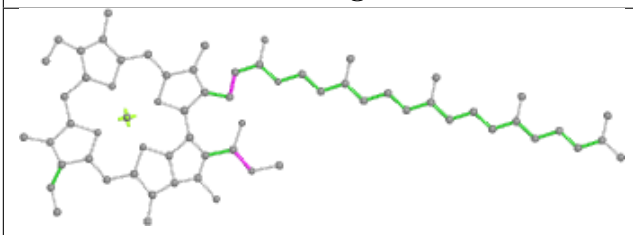
Ligand CLA c 501



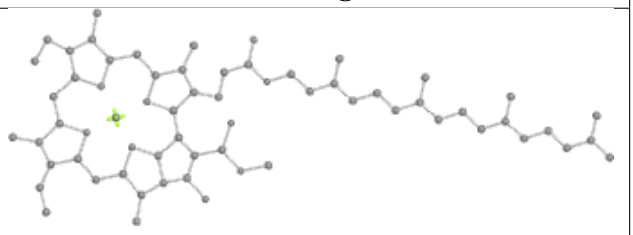
Bond lengths



Bond angles

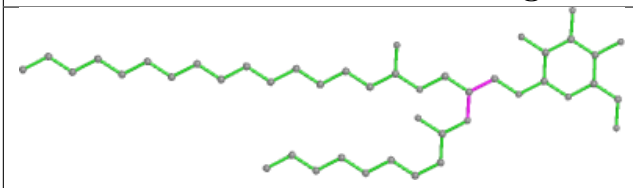


Torsions

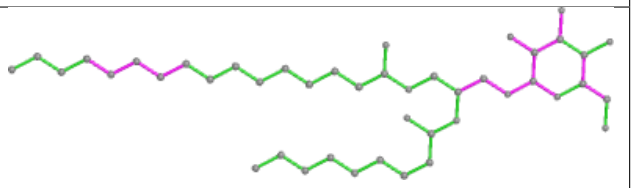


Rings

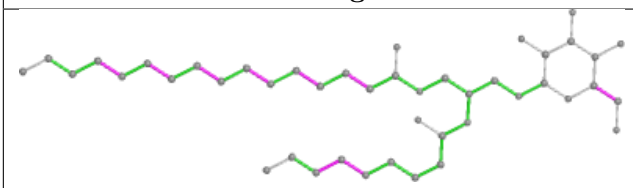
Ligand LMG d 410



Bond lengths



Bond angles



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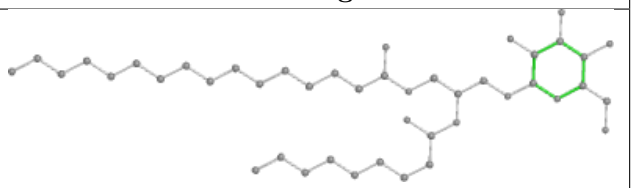
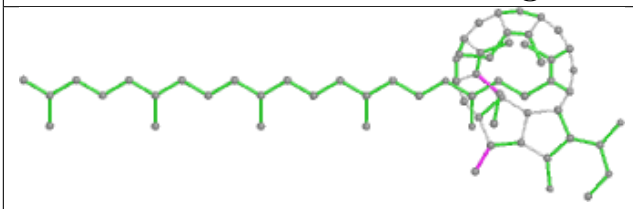


Rings

Ligand PHO A 608



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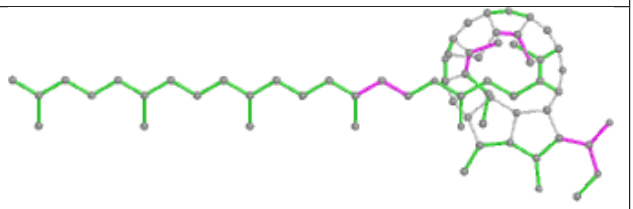
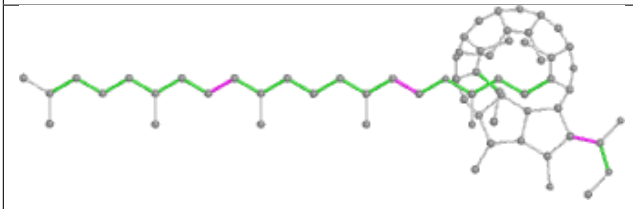
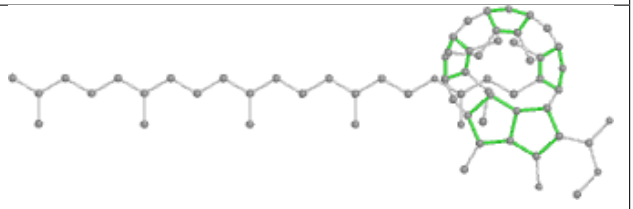


Bond angles

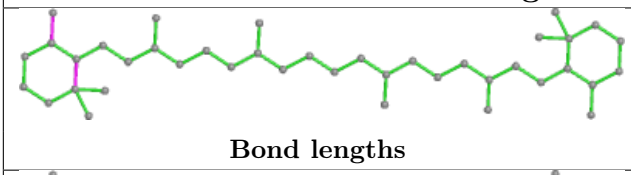


Torsions



Rings

Ligand BCR A 610



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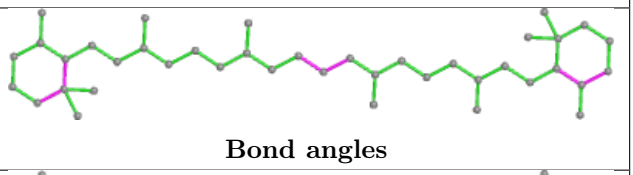
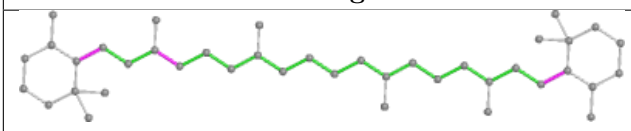


Bond angles



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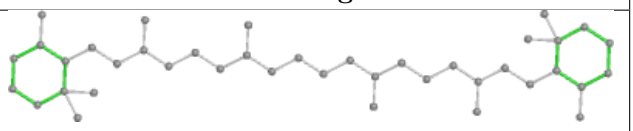
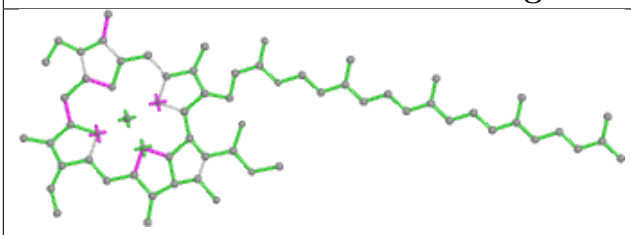
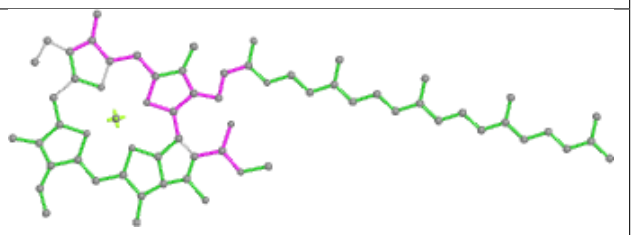


Rings

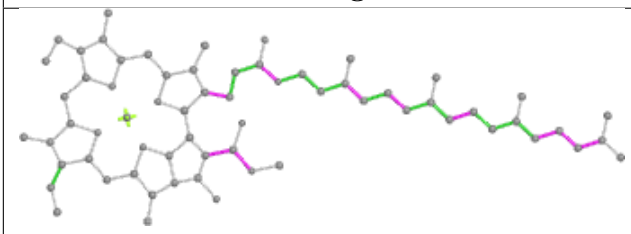
Ligand CLA B 601



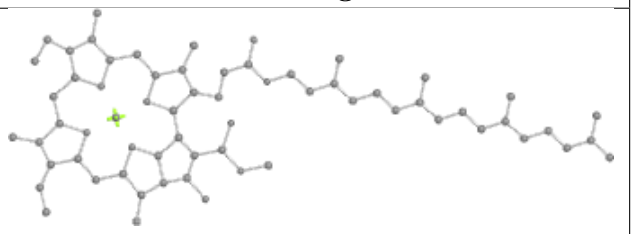
Bond lengths



Bond angles

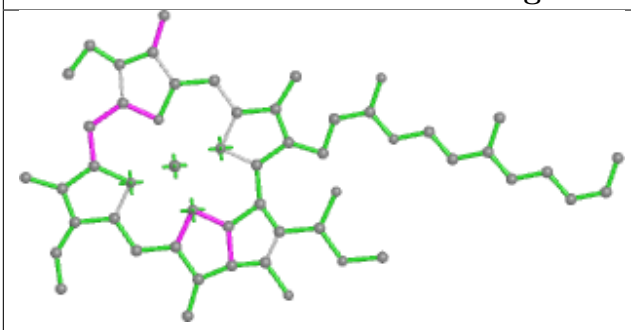


Torsions

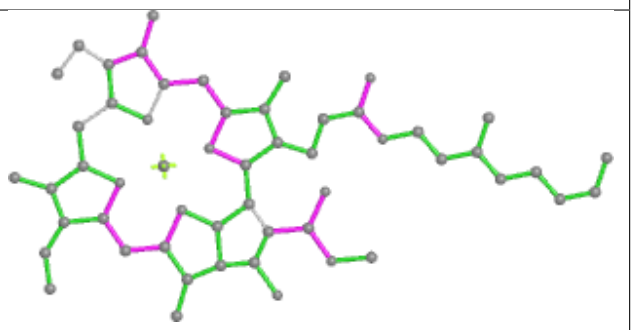


Rings

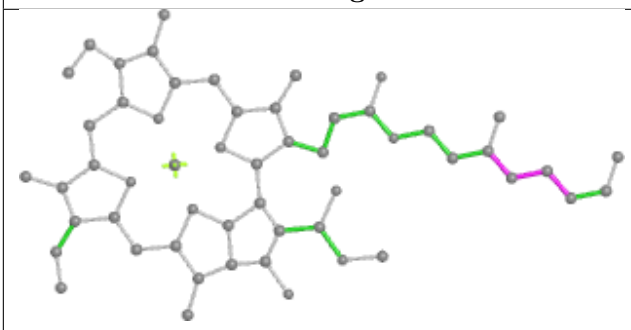
Ligand CLA A 609



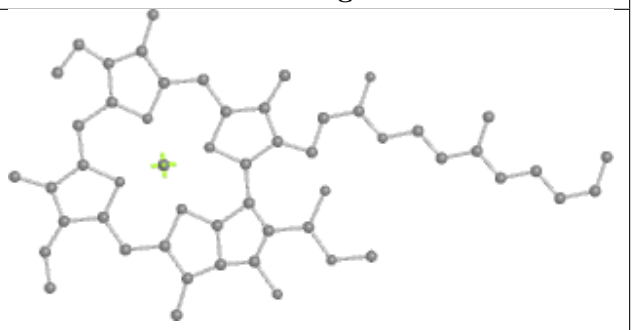
Bond lengths



Bond angles

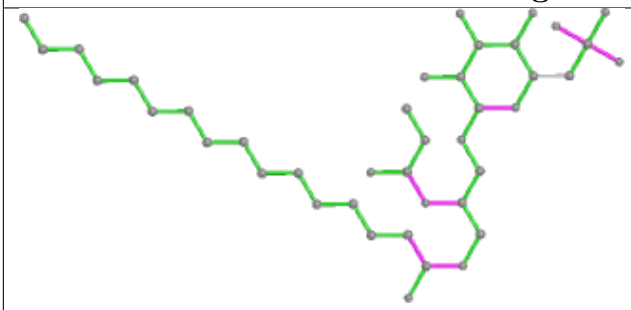


Torsions

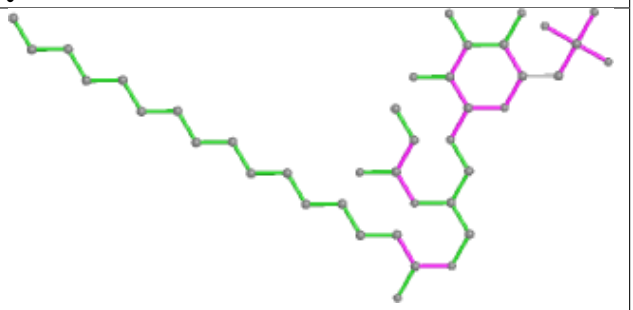


Rings

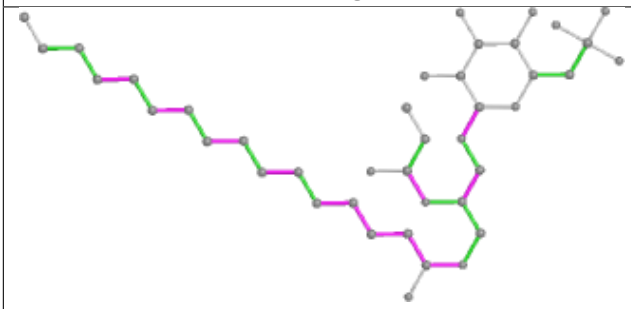
Ligand SQD f 101



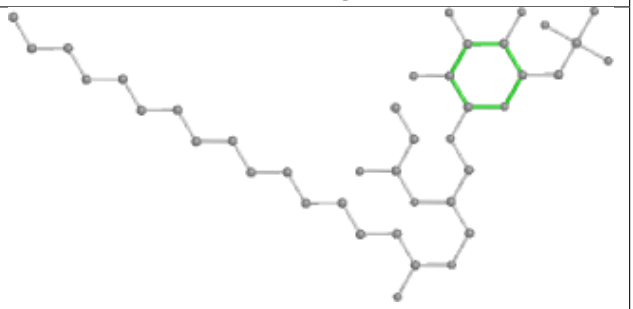
Bond lengths



Bond angles

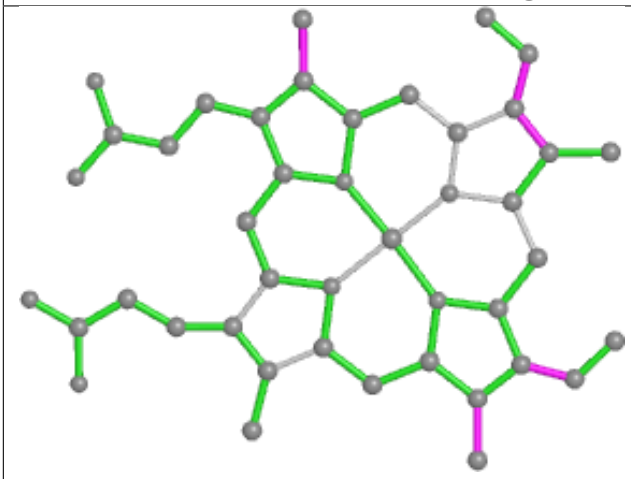


Torsions

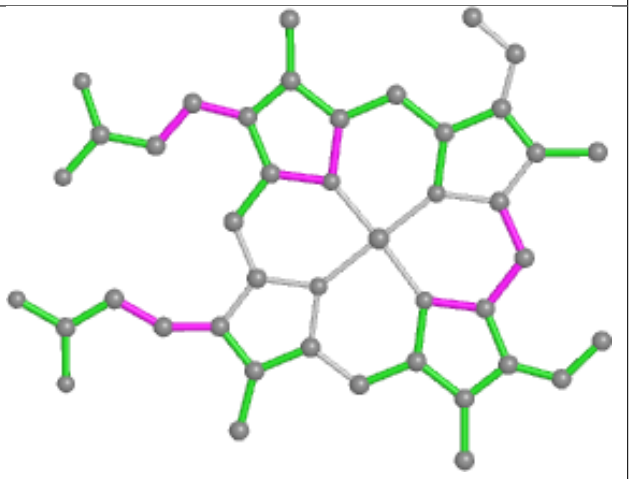


Rings

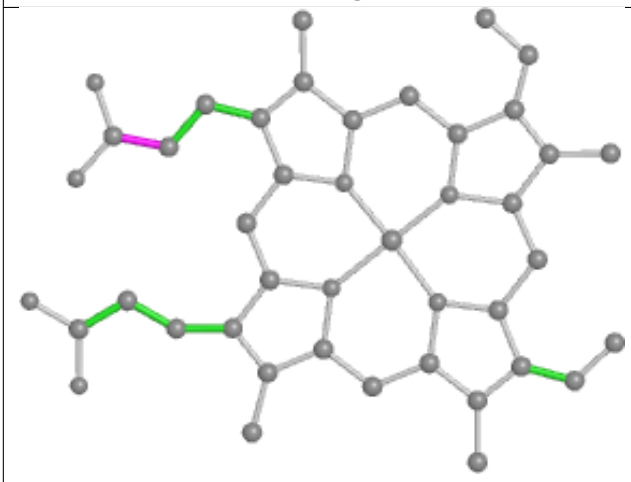
Ligand HEM F 101



Bond lengths



Bond angles



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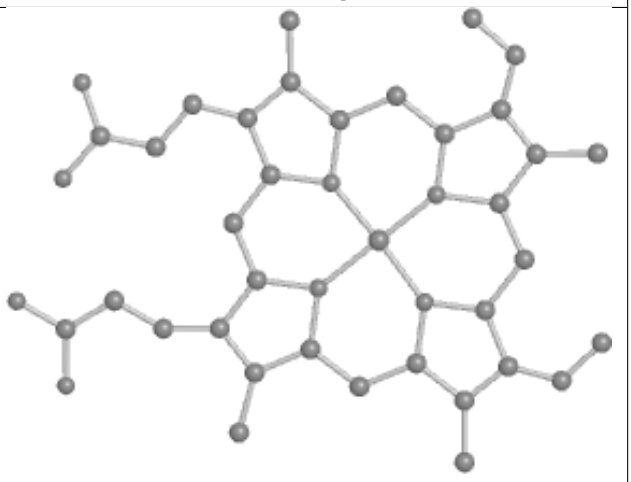
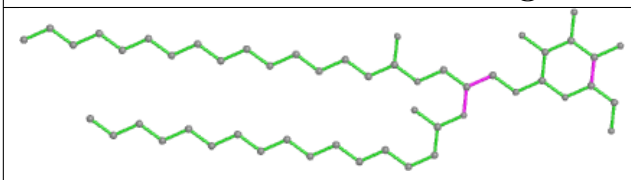
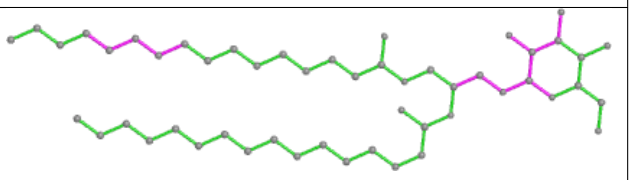


Rings

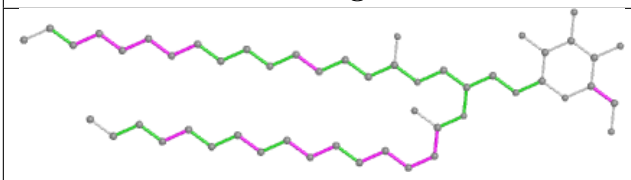
Ligand LMG D 407



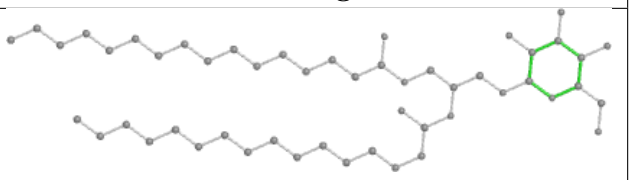
Bond lengths



Bond angles

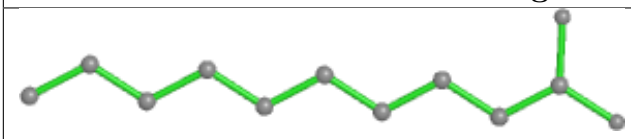


Torsions



Rings

Ligand STE J 101



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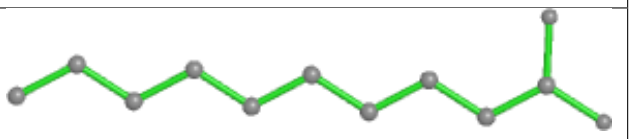
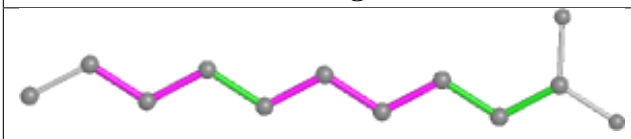
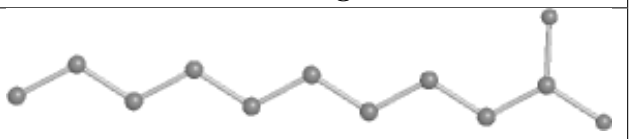


Bond angles

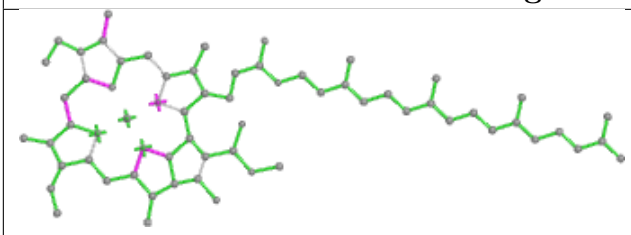


Torsions

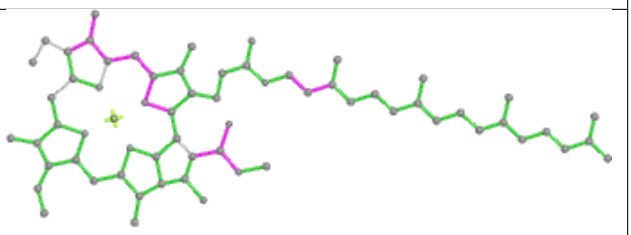


Rings

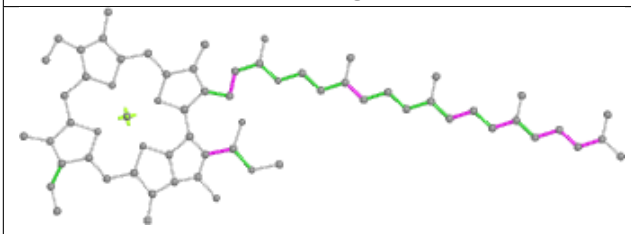
Ligand CLA B 614



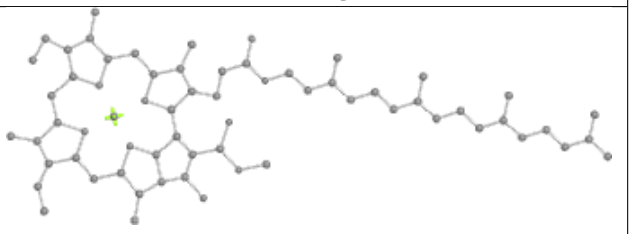
Bond lengths



Bond angles

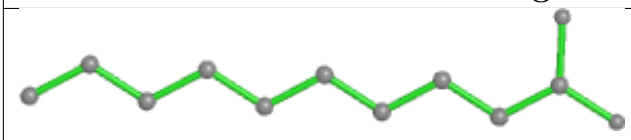


Torsions

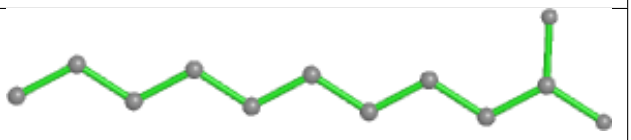


Rings

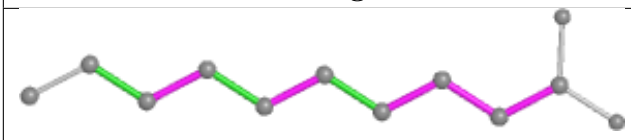
Ligand STE c 521



Bond lengths



Bond angles



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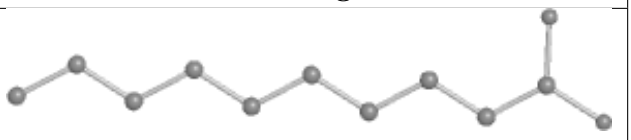
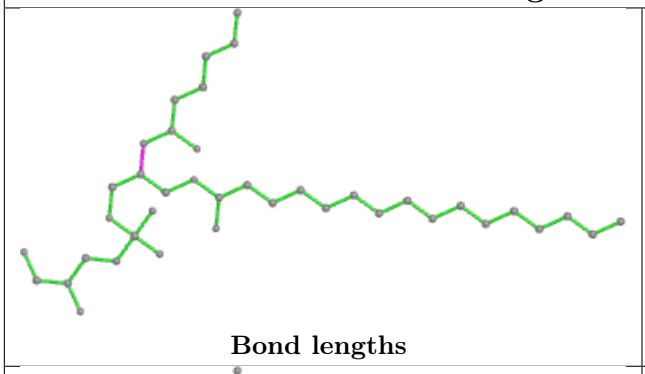
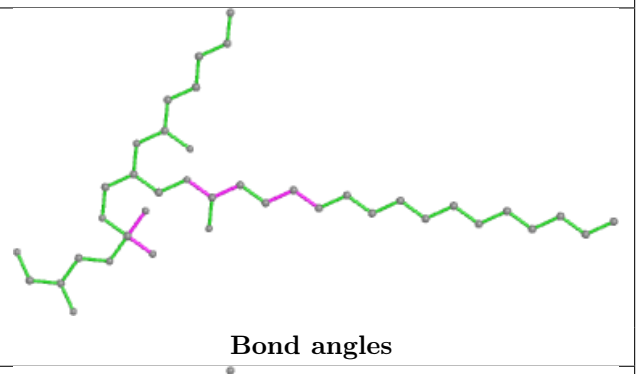


Rings

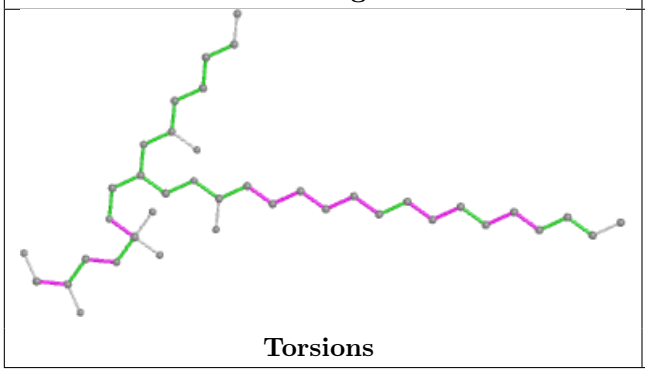
Ligand LHG d 408



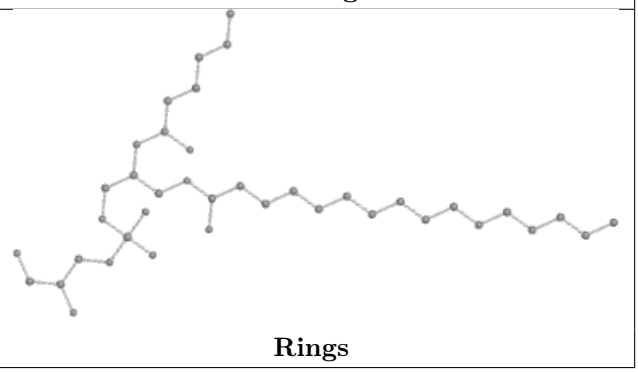
Bond lengths



Bond angles

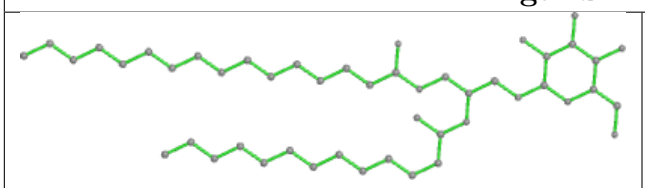


Torsions

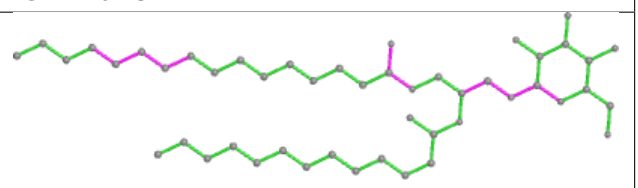


Rings

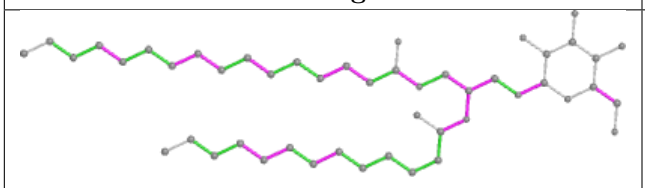
Ligand LMG A 613



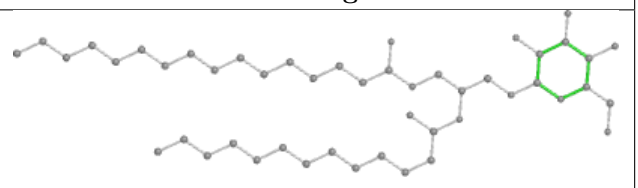
Bond lengths



Bond angles

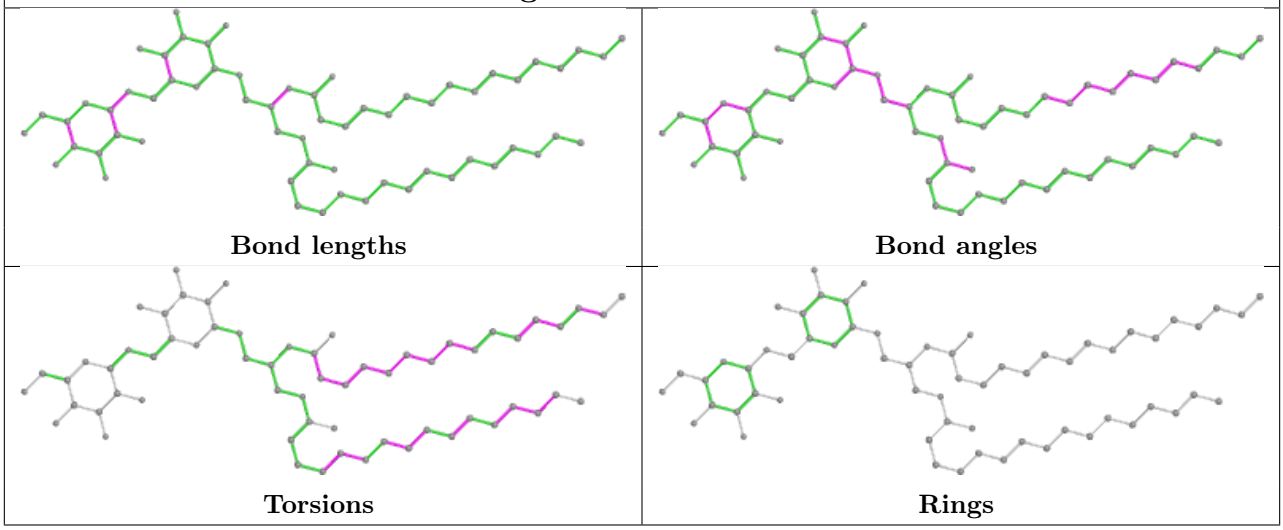


Torsions

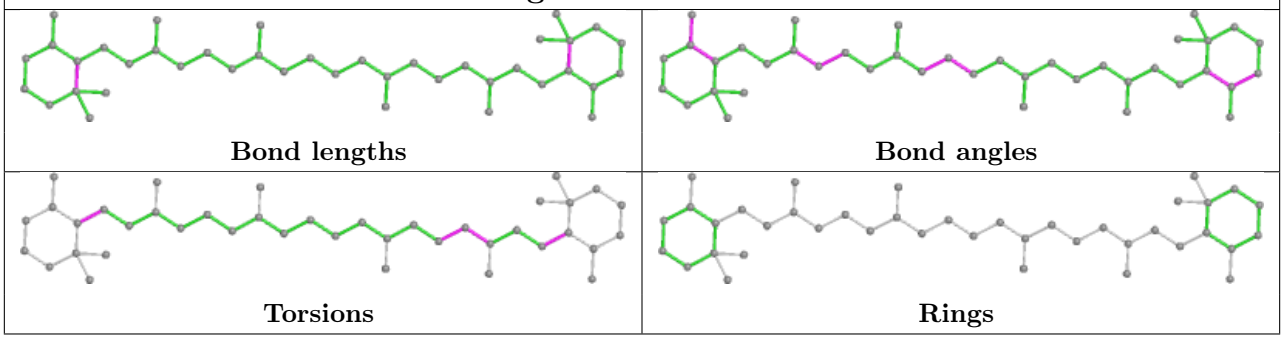


Rings

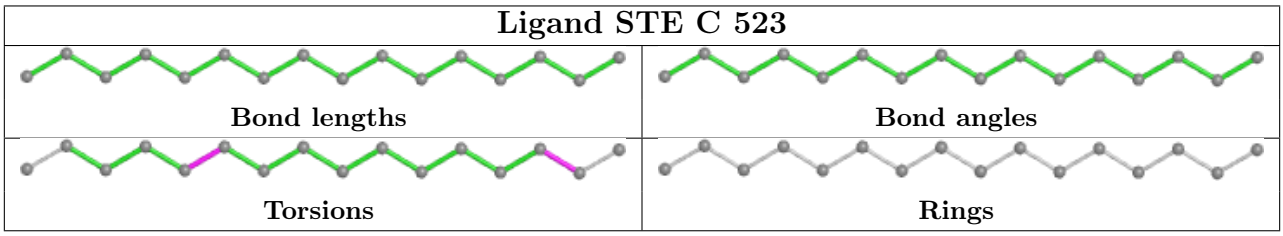
Ligand DGD H 102



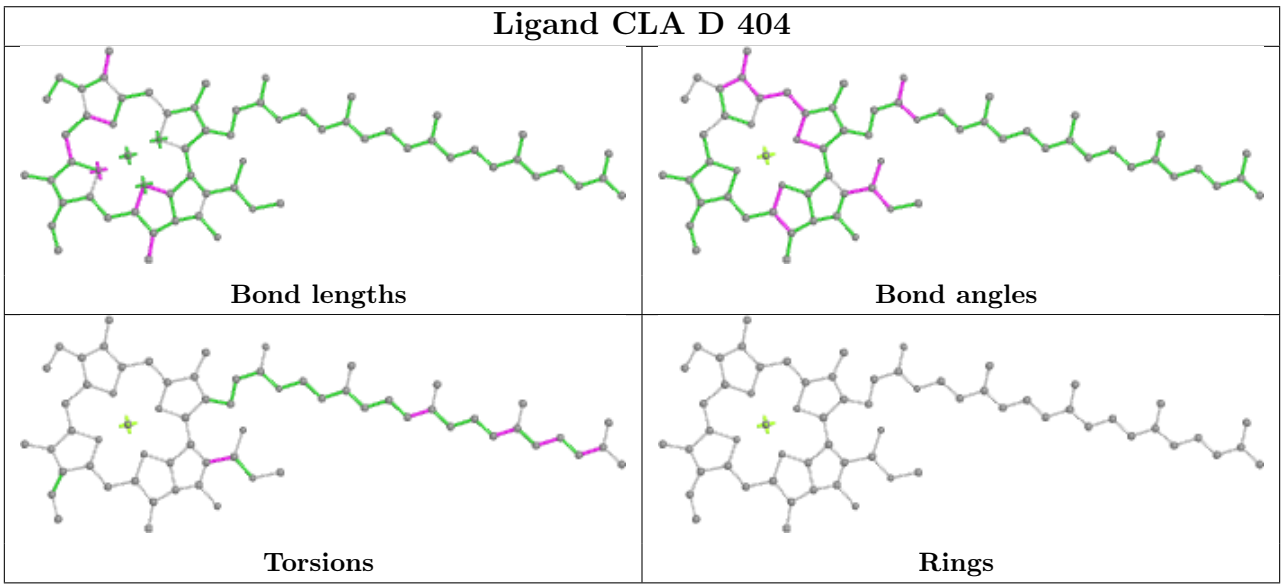
Ligand BCR k 103



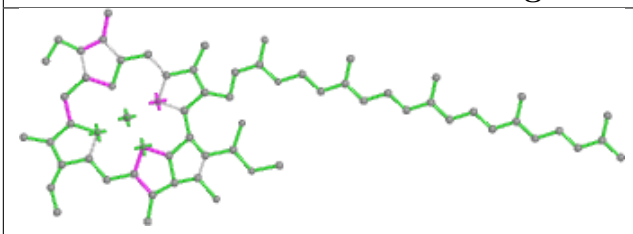
Ligand STE C 523



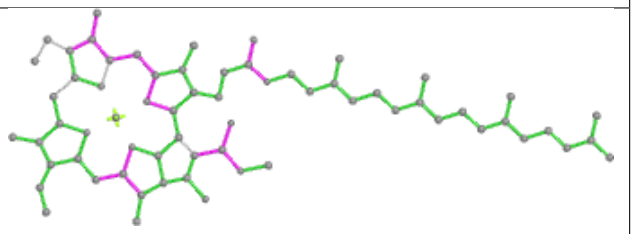
Ligand CLA D 404



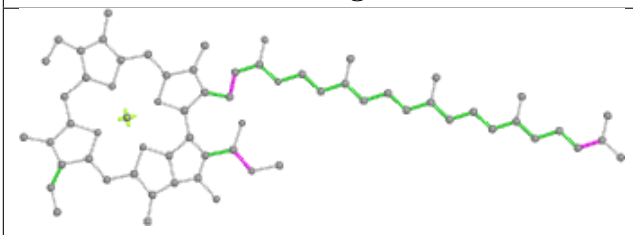
Ligand CLA C 501



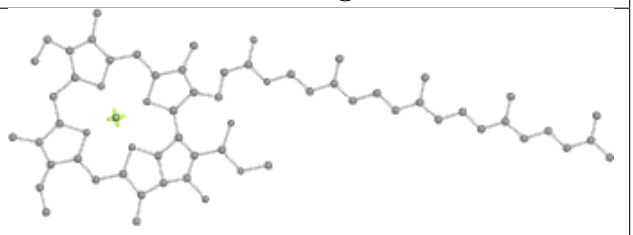
Bond lengths



Bond angles

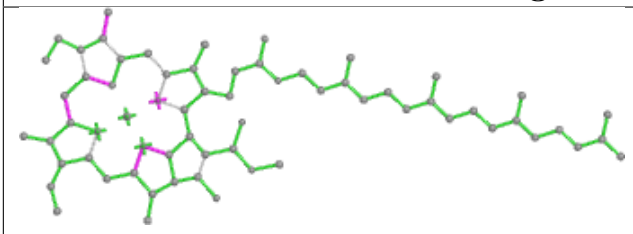


Torsions

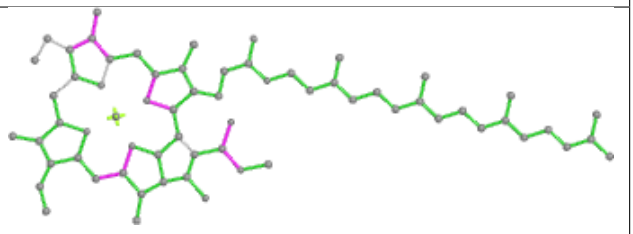


Rings

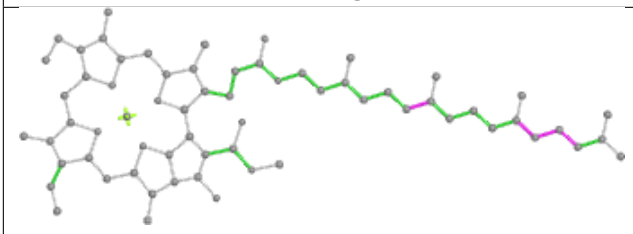
Ligand CLA c 511



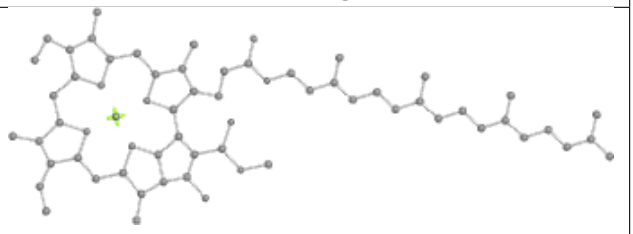
Bond lengths



Bond angles

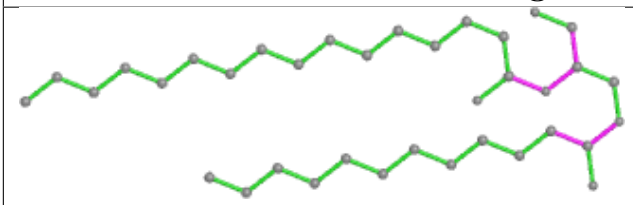


Torsions

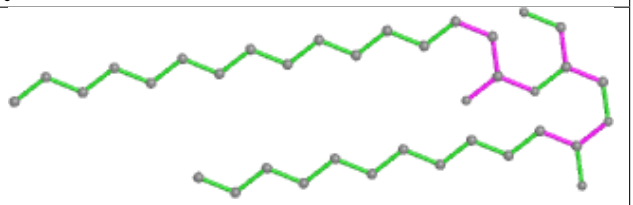


Rings

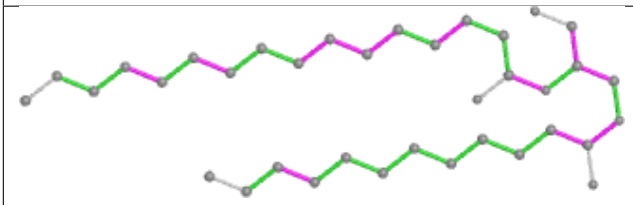
Ligand SQD a 615



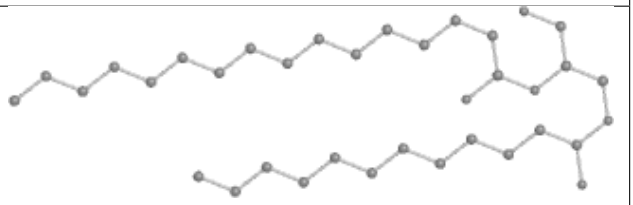
Bond lengths



Bond angles

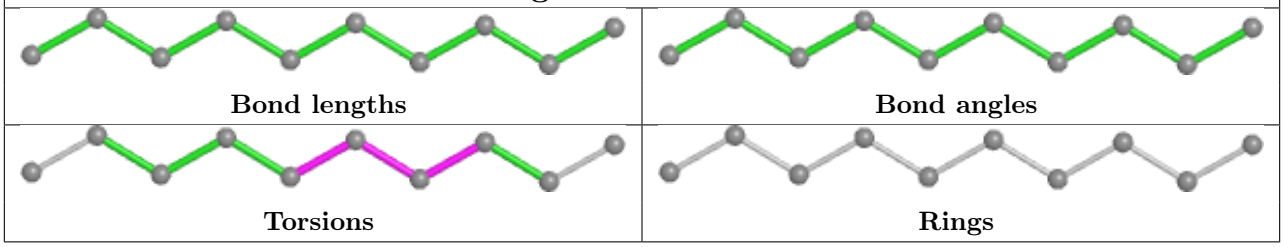


Torsions

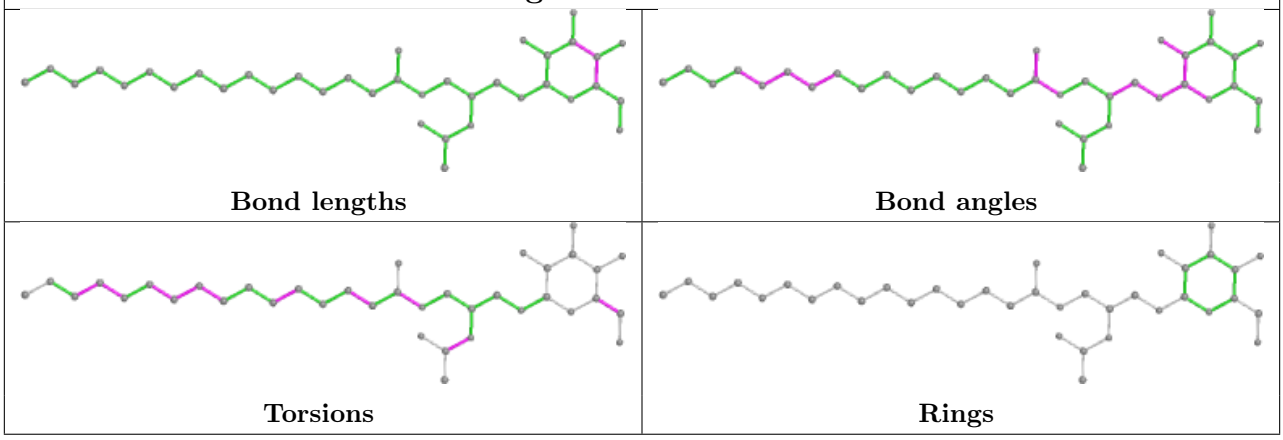


Rings

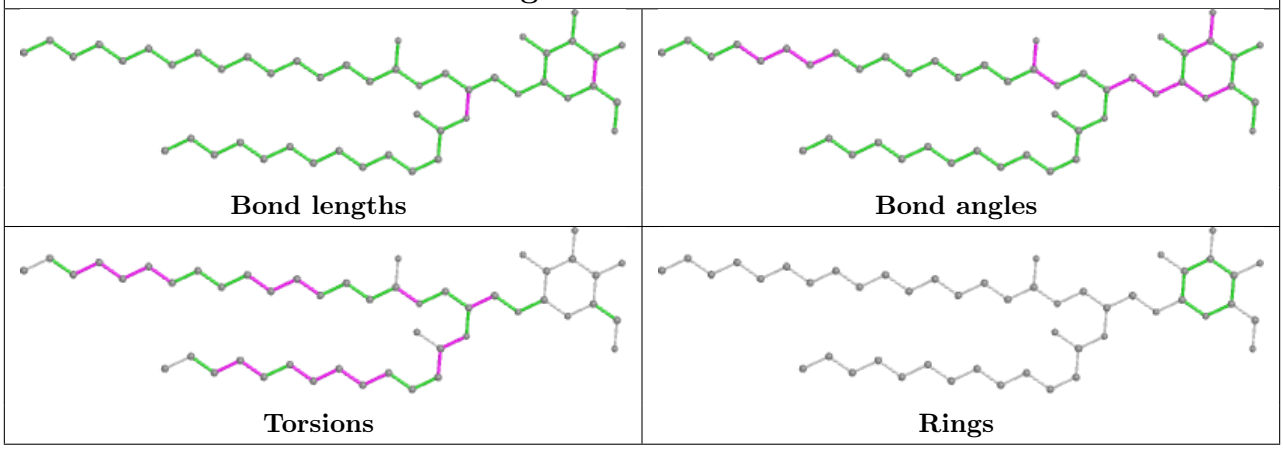
Ligand STE b 625



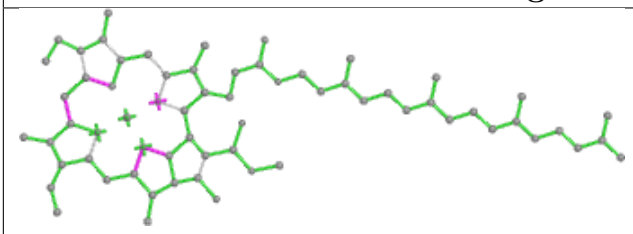
Ligand LMG c 518



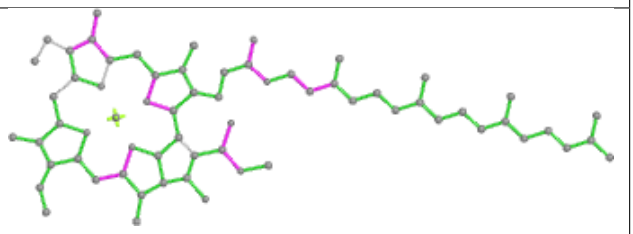
Ligand LMG C 520



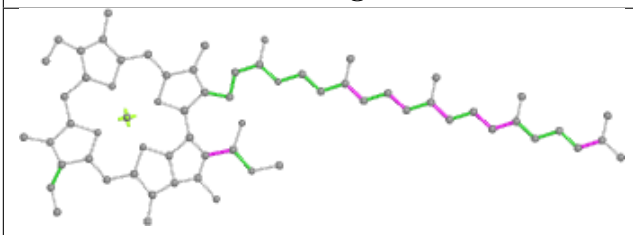
Ligand CLA b 605



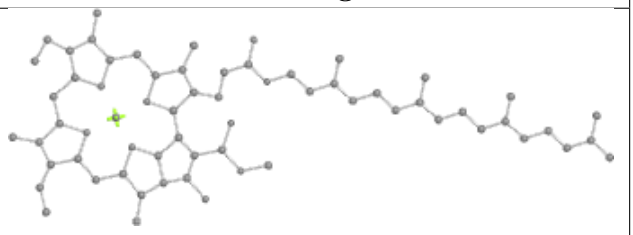
Bond lengths



Bond angles

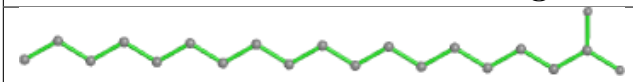


Torsions

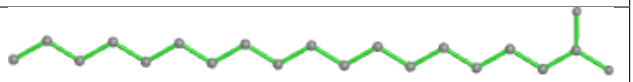


Rings

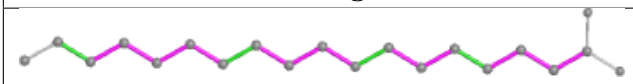
Ligand STE b 621



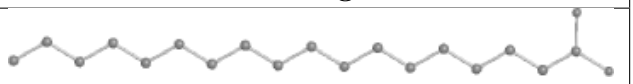
Bond lengths



Bond angles

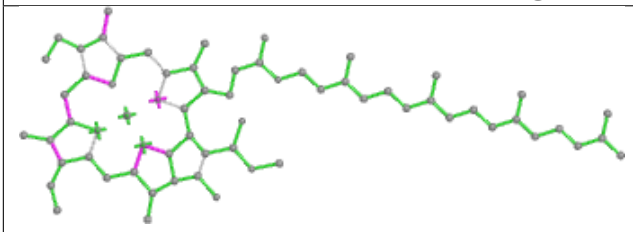


Torsions

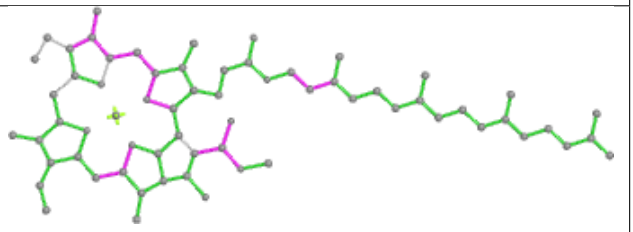


Rings

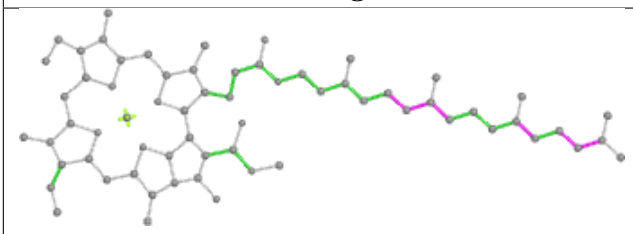
Ligand CLA c 505



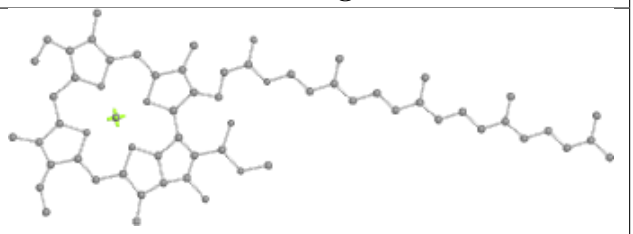
Bond lengths



Bond angles

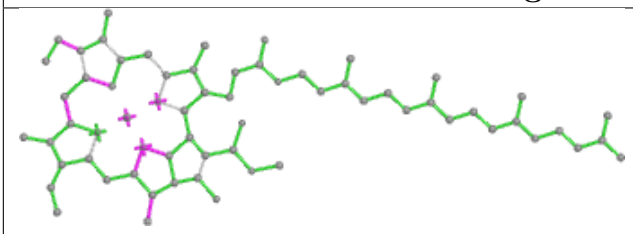


Torsions

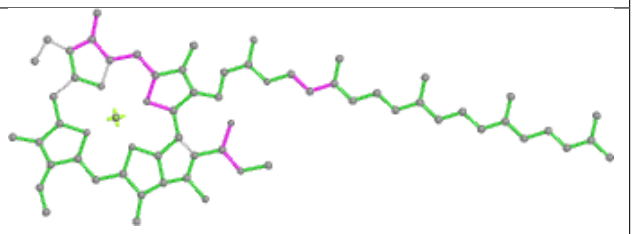


Rings

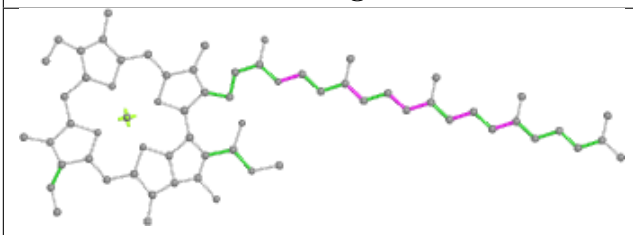
Ligand CLA B 613



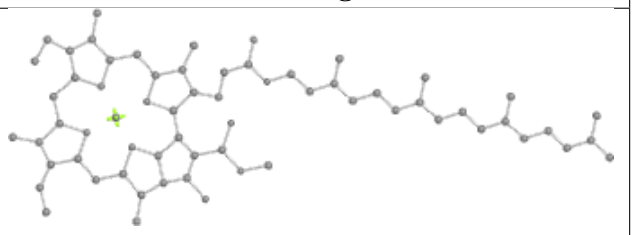
Bond lengths



Bond angles

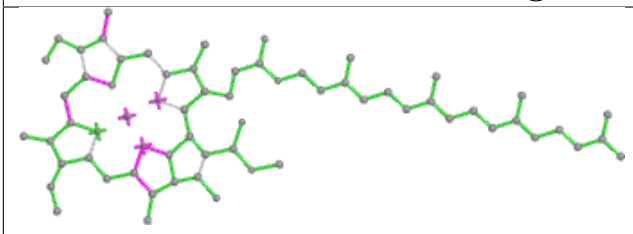


Torsions

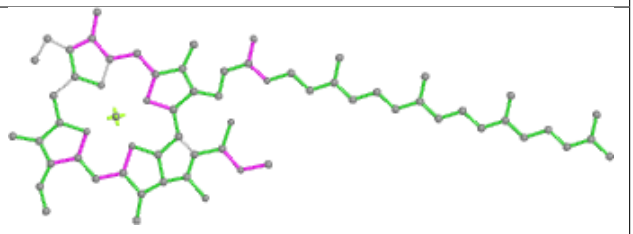


Rings

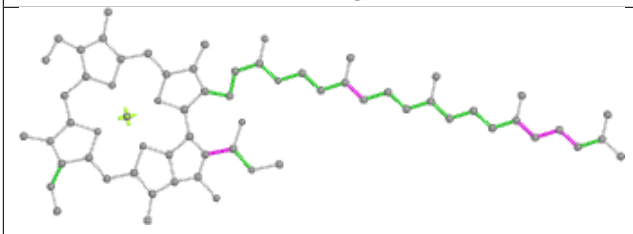
Ligand CLA b 609



Bond lengths



Bond angles



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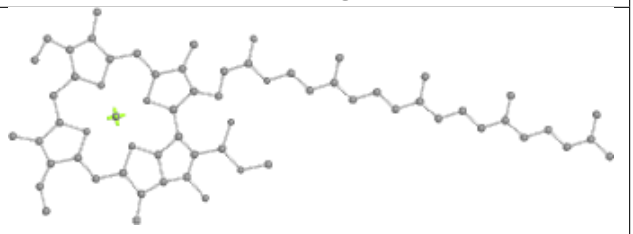
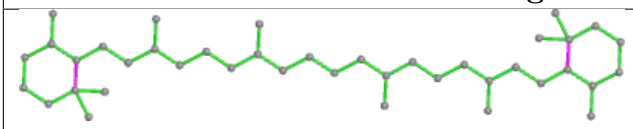
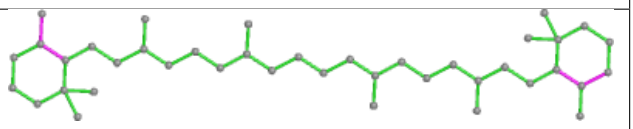


Rings

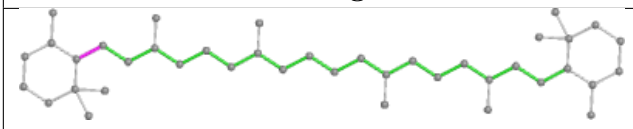
Ligand BCR a 610



Bond lengths



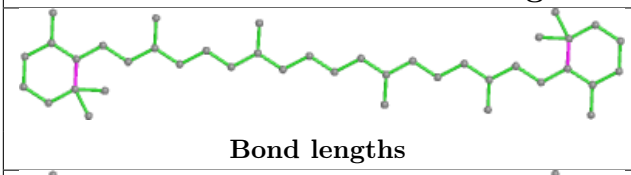
Bond angles



Torsions

Rings

Ligand BCR k 102



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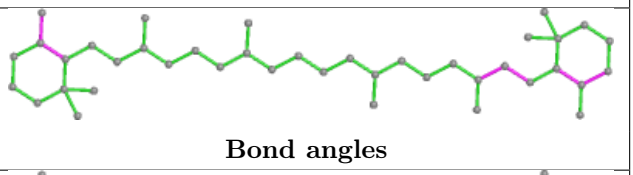
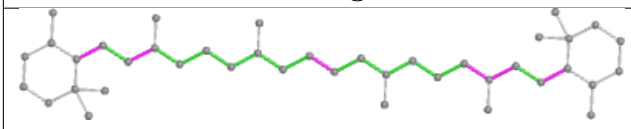


Bond angles



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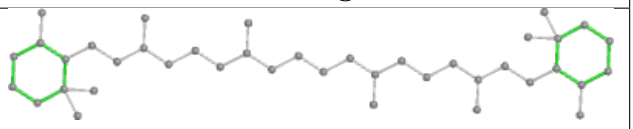
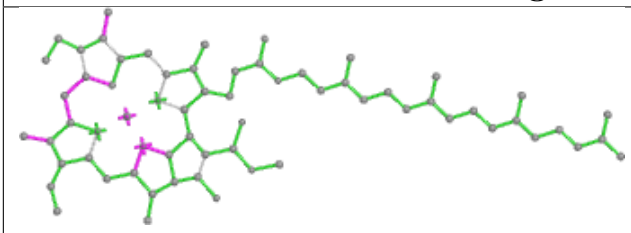


Rings

Ligand CLA a 609



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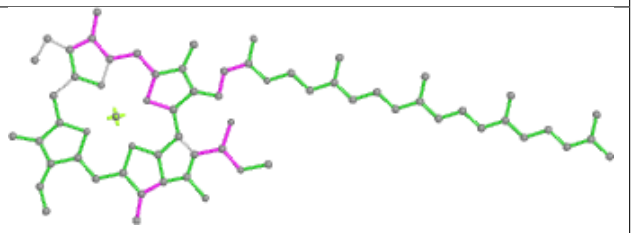
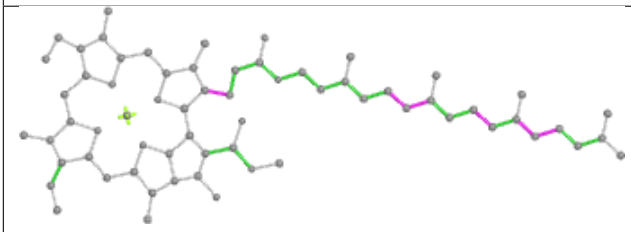


Bond angles



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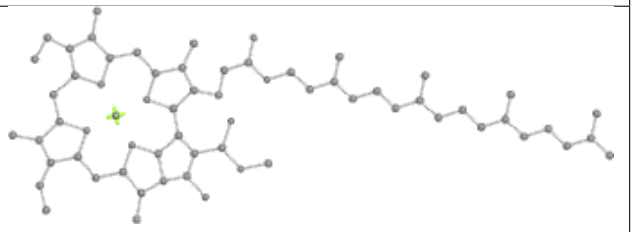
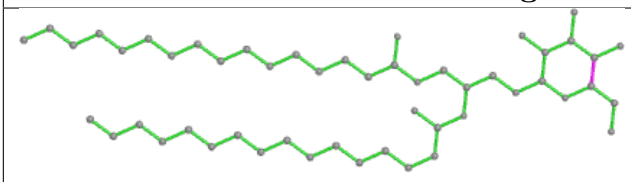


Rings

Ligand LMG B 620



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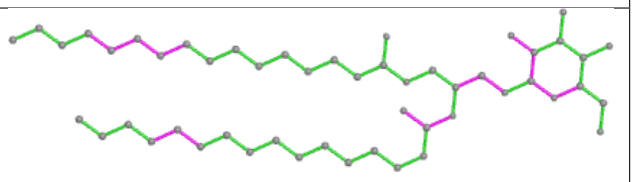
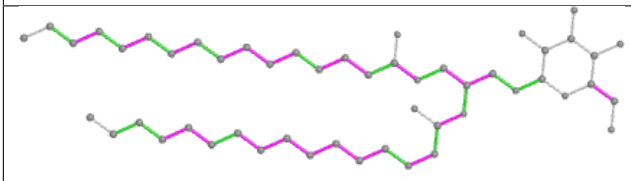


Bond angles



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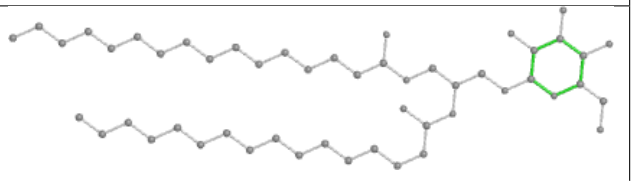
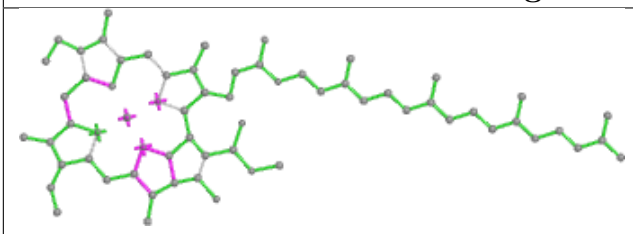
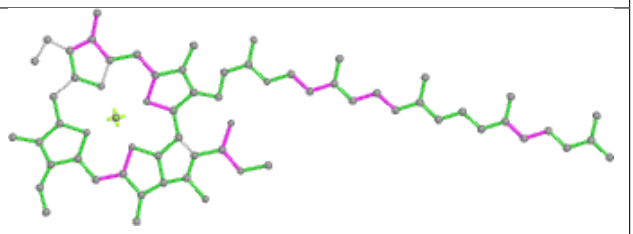


Rings

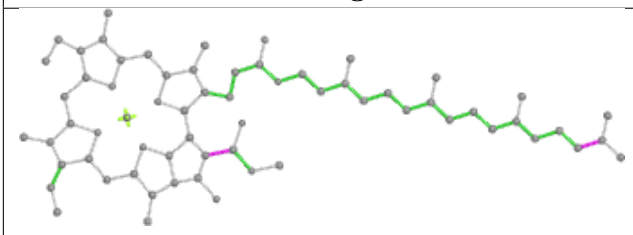
Ligand CLA B 609



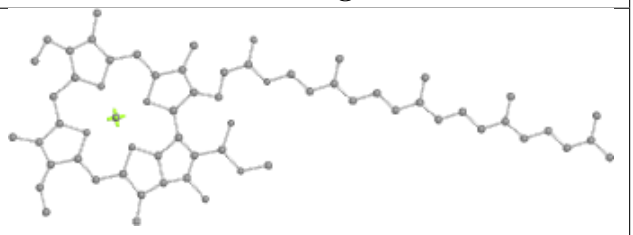
Bond lengths



Bond angles

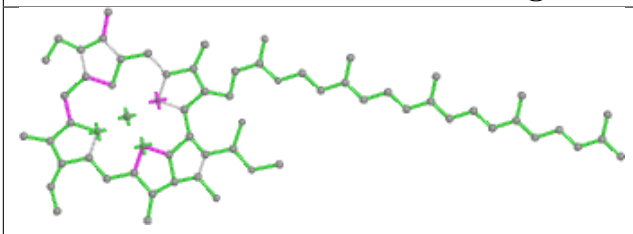


Torsions



Rings

Ligand CLA b 614



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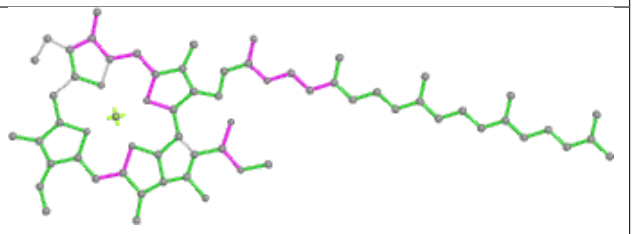
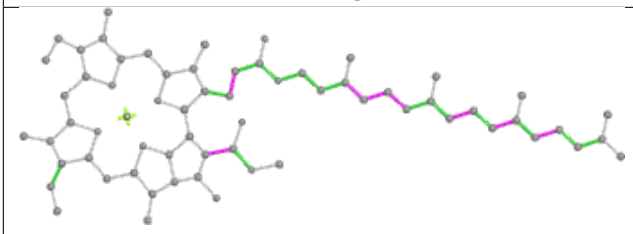
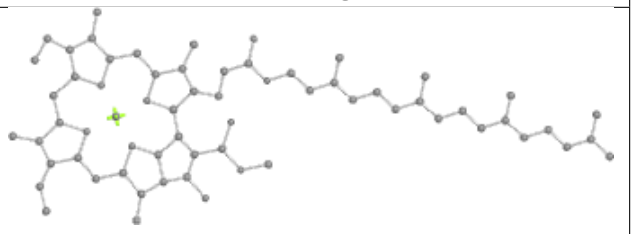


Bond angles

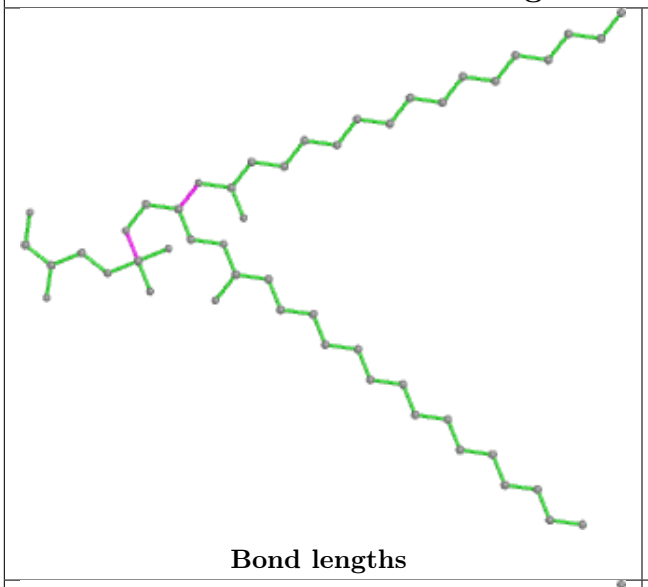


Torsions

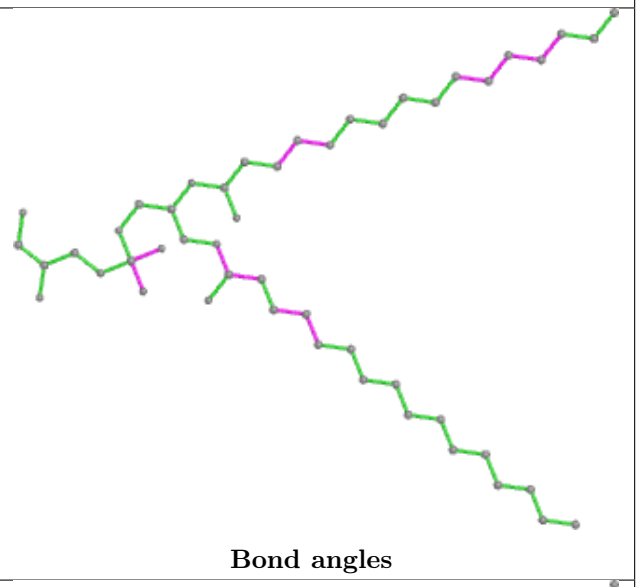


Rings

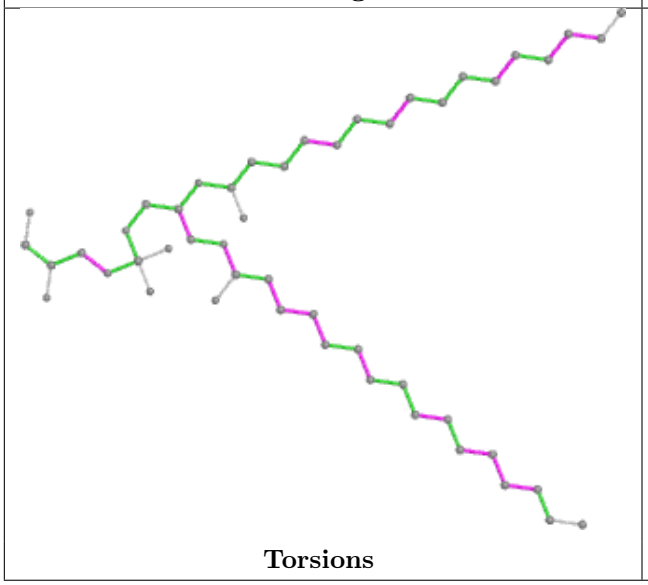
Ligand LHG E 101



Bond lengths



Bond angles



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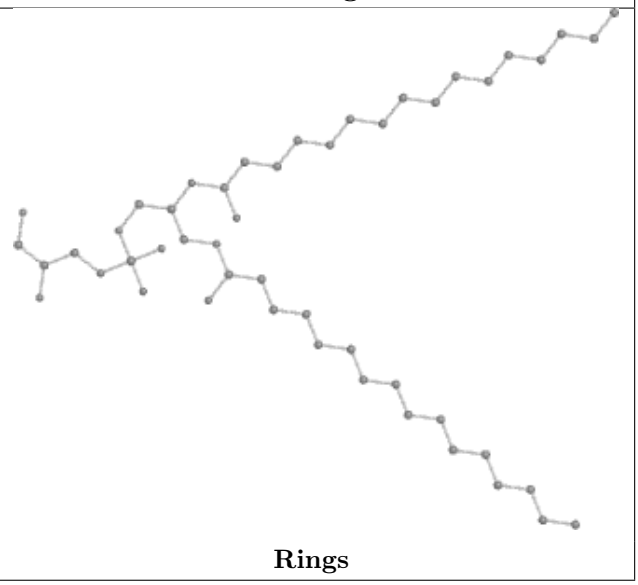
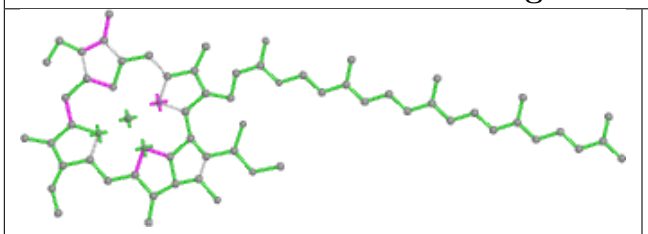


Rings

Ligand CLA B 610



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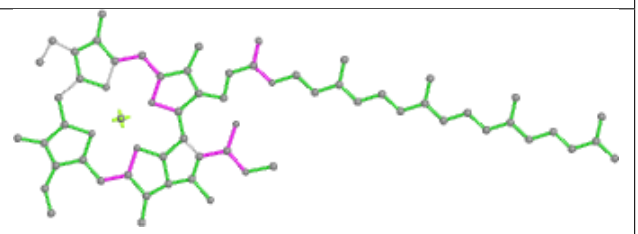
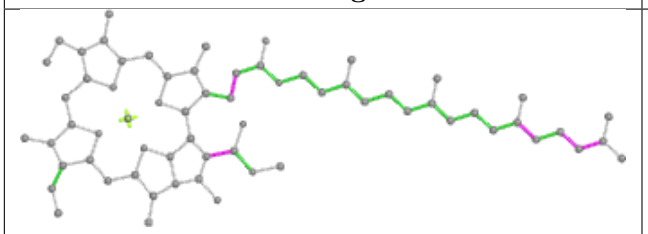
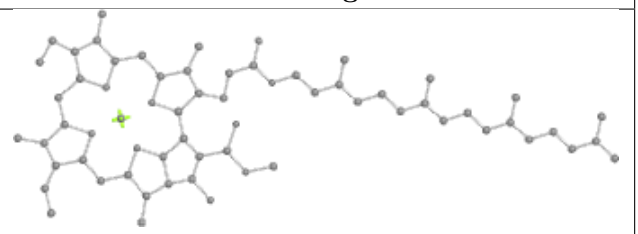


Bond angles

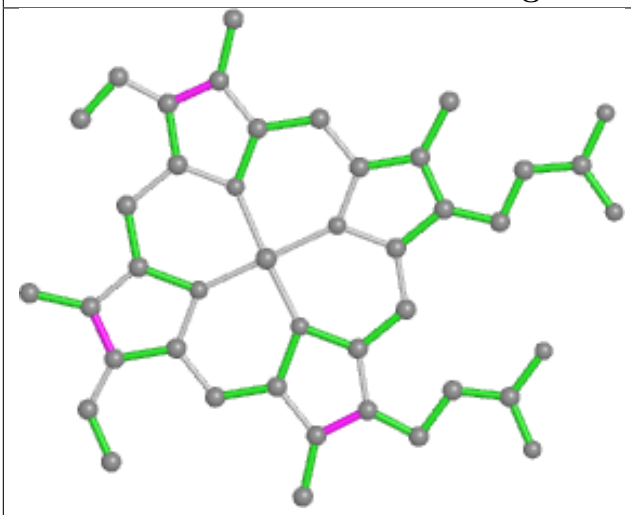


Torsions



Rings

Ligand HEC V 201



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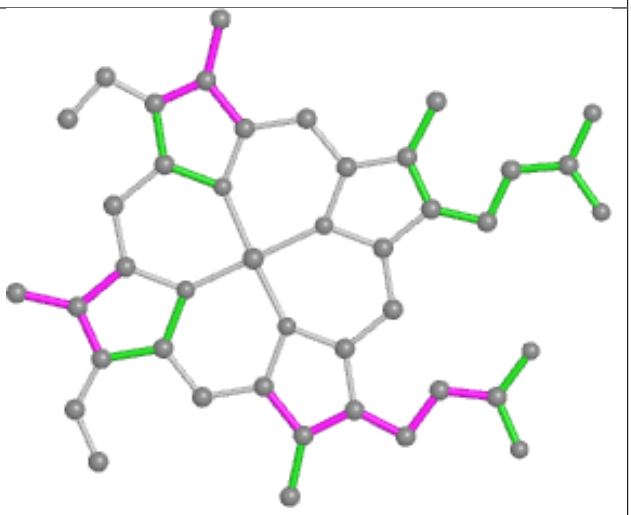
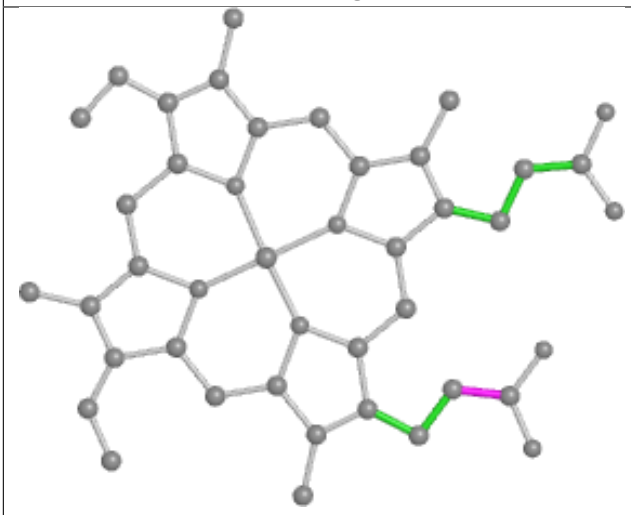


Bond angles



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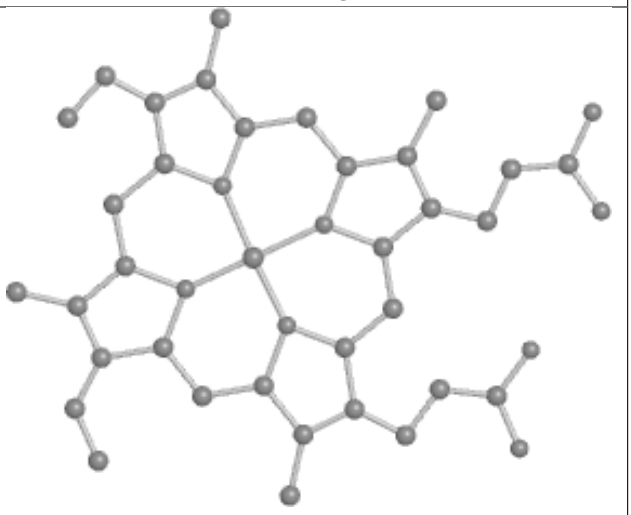
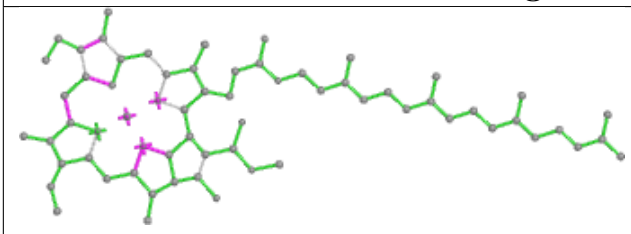


Rings

Ligand CLA C 506



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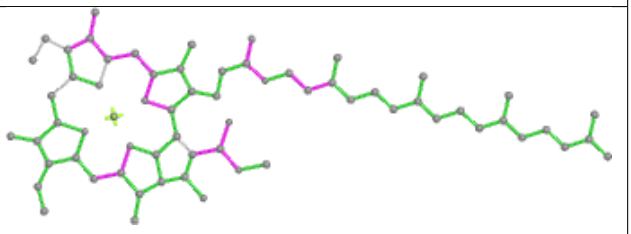
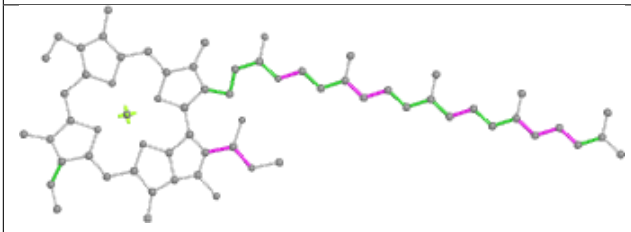
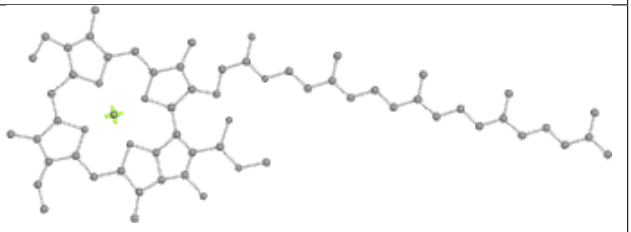


Bond angles

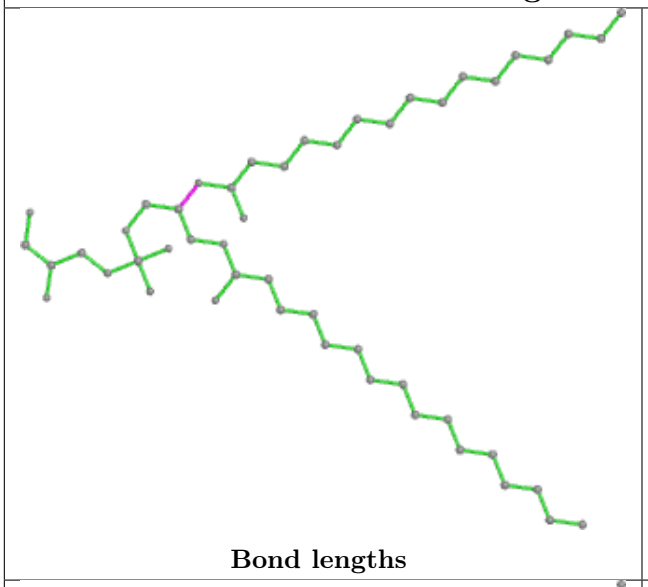


Torsions



Rings

Ligand LHG B 623



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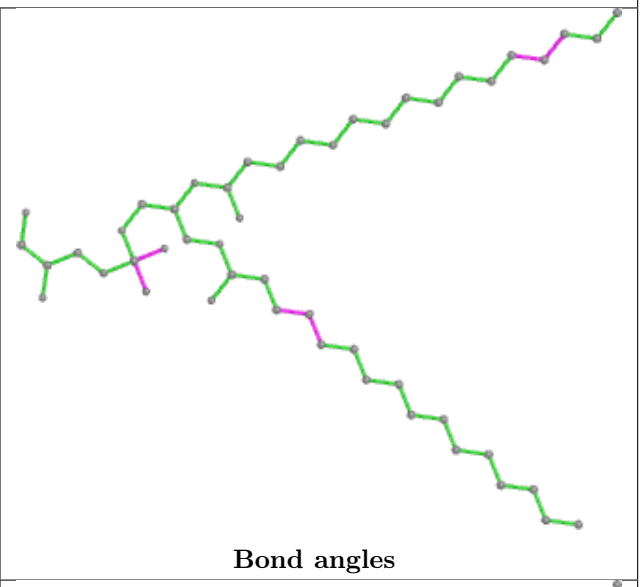
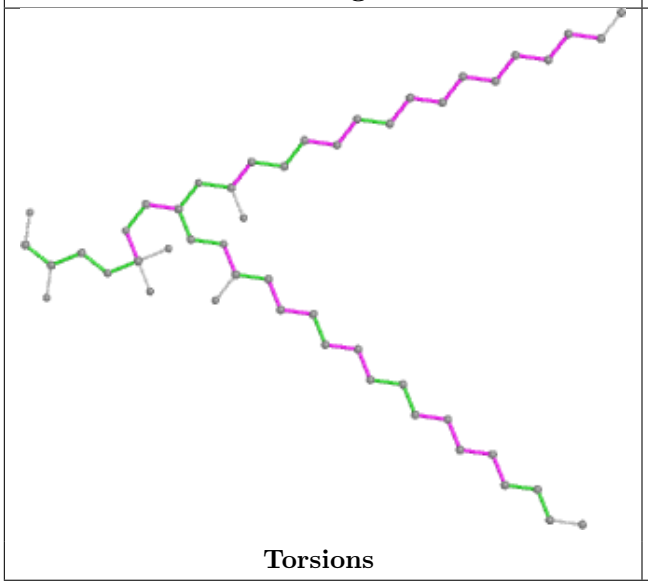


Bond angles



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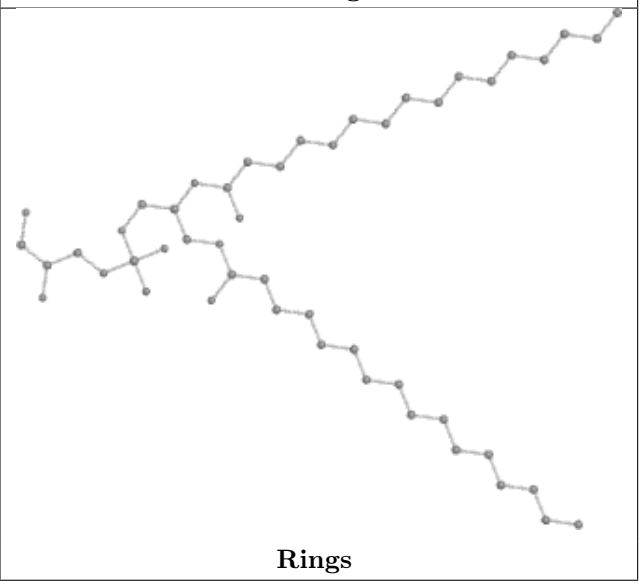
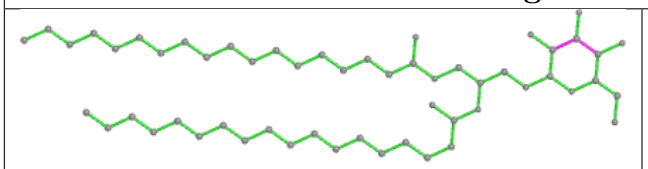
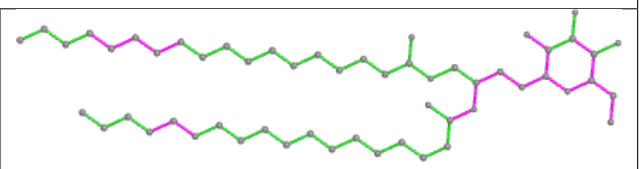


Rings

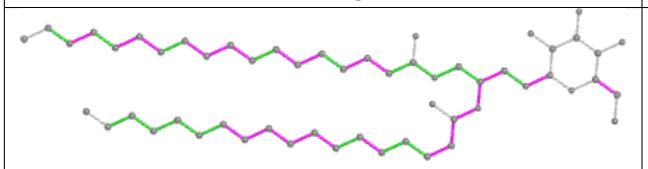
Ligand LMG b 622



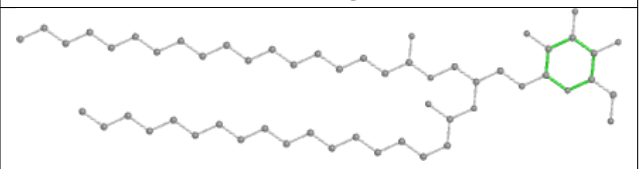
Bond lengths



Bond angles

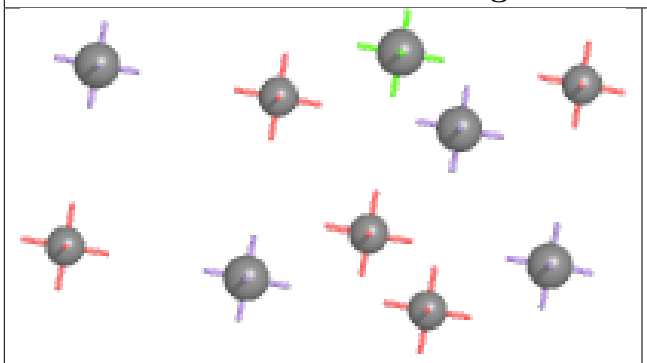


Torsions

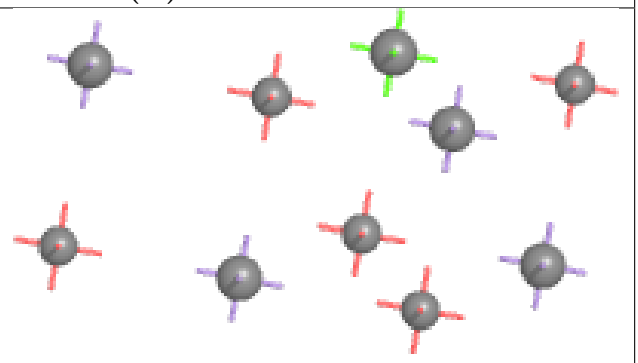


Rings

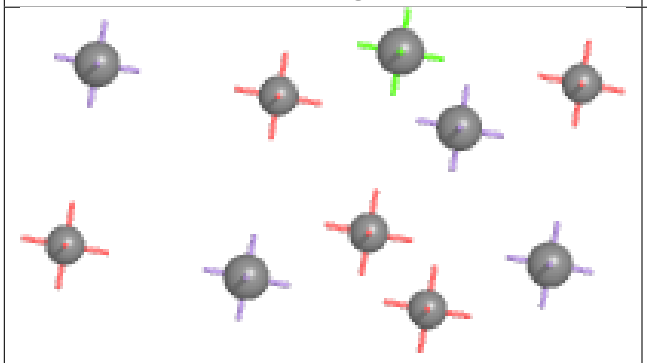
Ligand OEX A 601 (B)



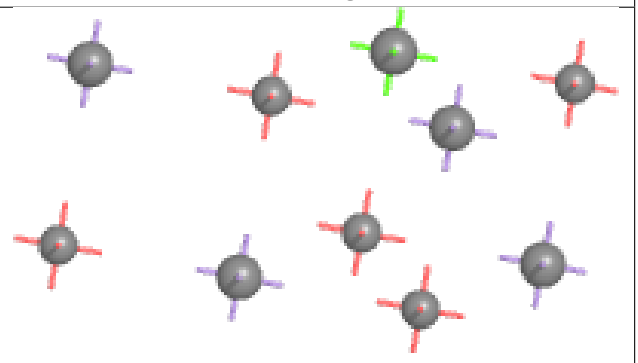
Bond lengths



Bond angles

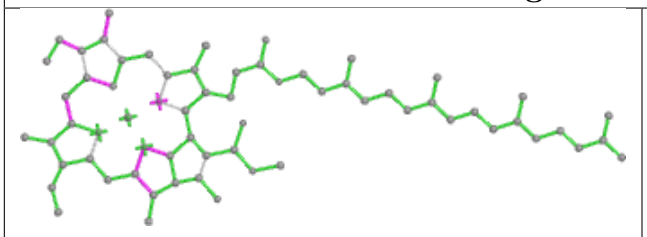


Torsions

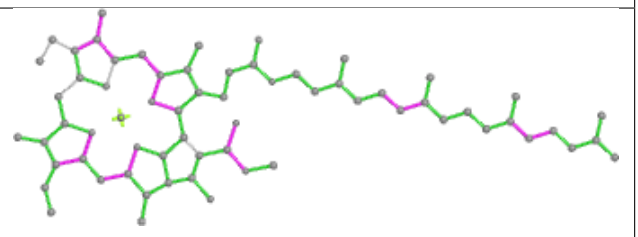


Rings

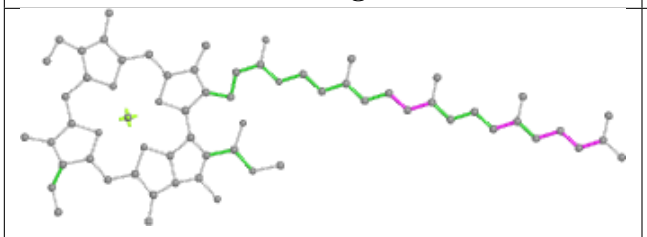
Ligand CLA B 615



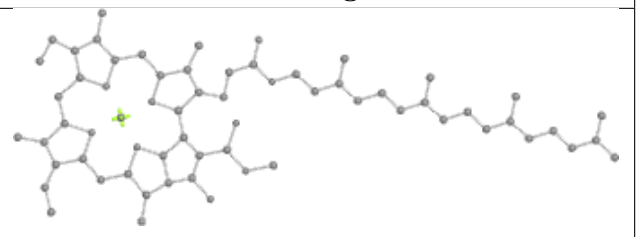
Bond lengths



Bond angles

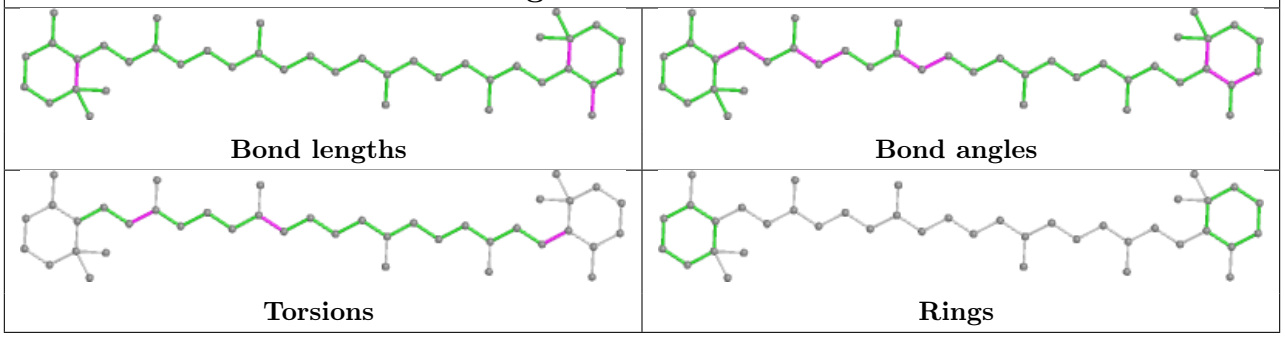


Torsions

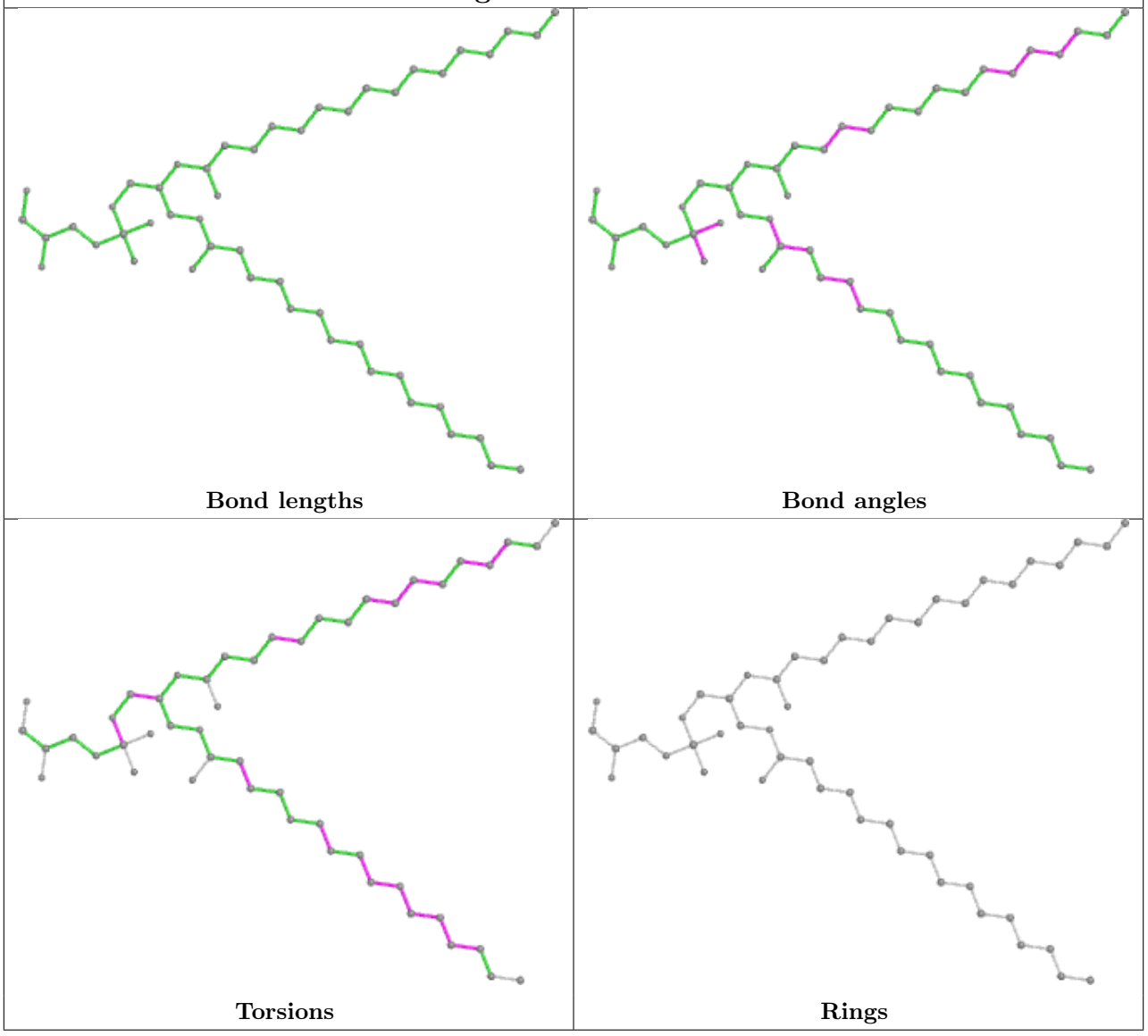


Rings

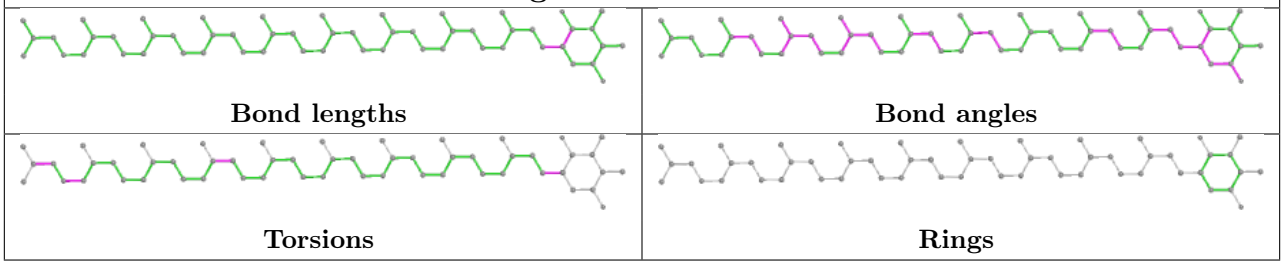
Ligand BCR b 618



Ligand LHG l 101



Ligand PL9 D 406



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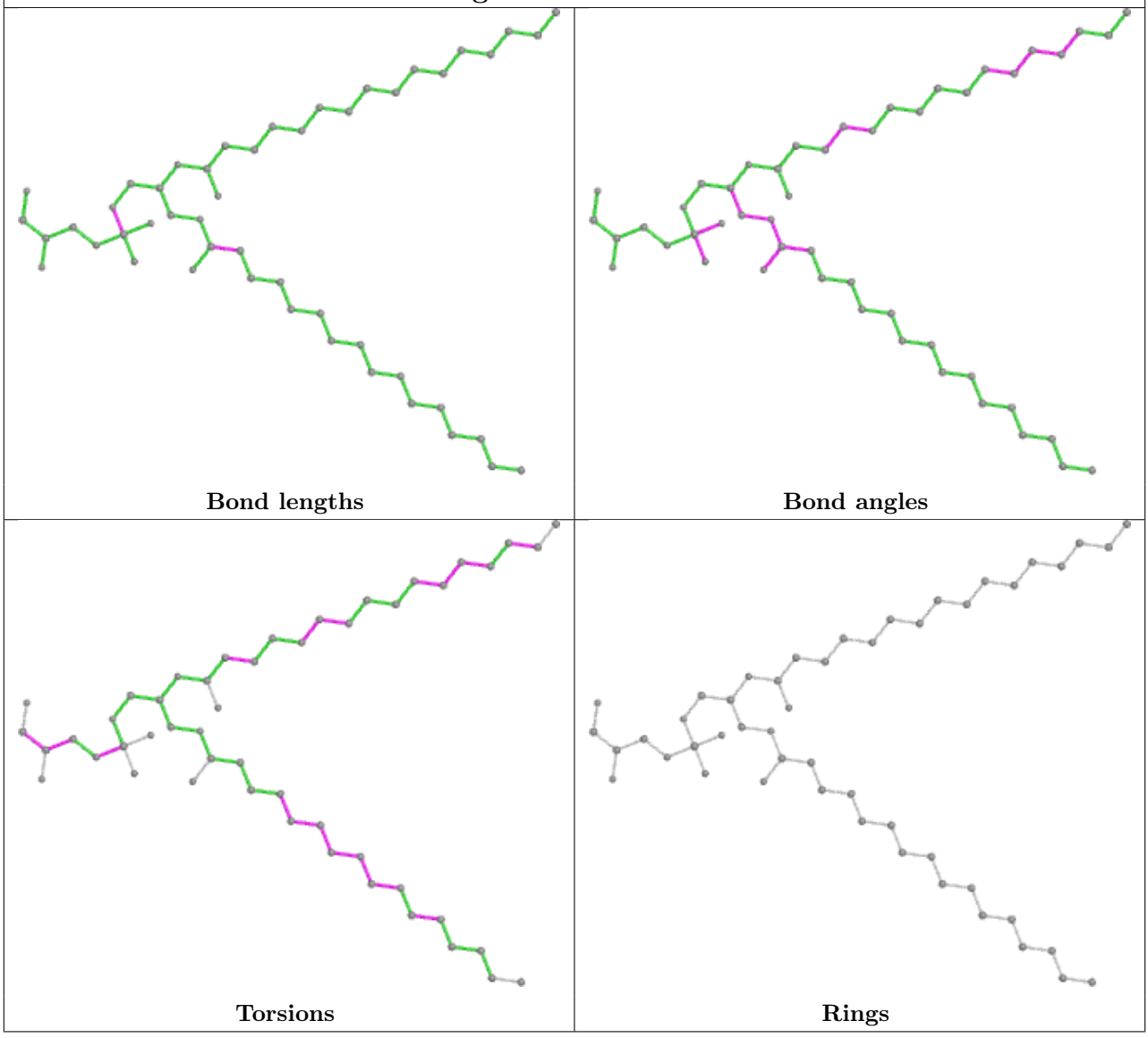
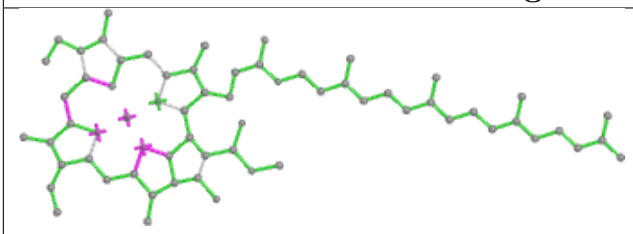
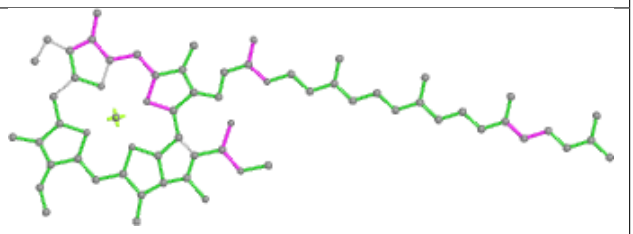


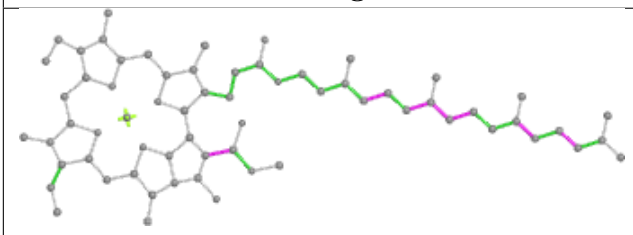
Ligand CLA B 605



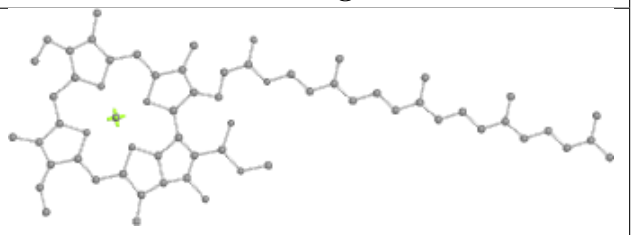
Bond lengths



Bond angles

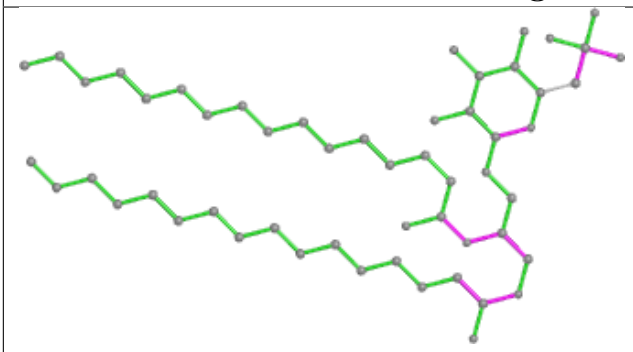


Torsions

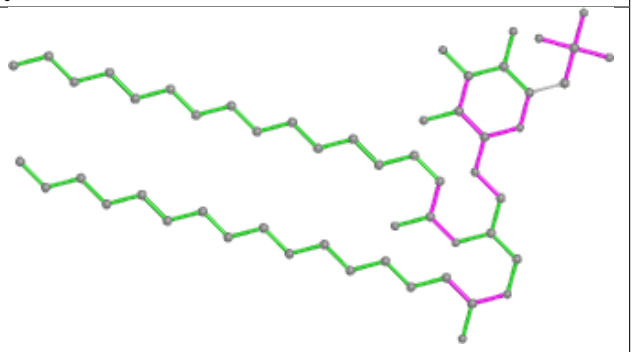


Rings

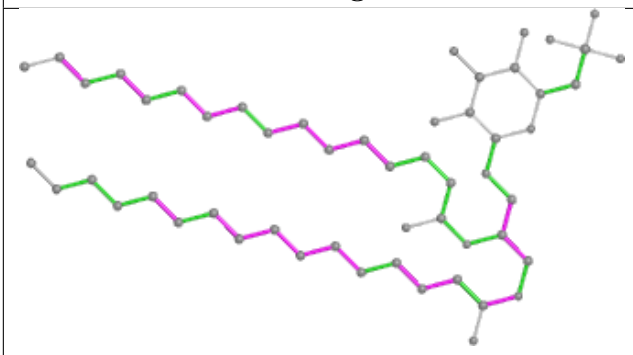
Ligand SQD a 614



Bond lengths



Bond angles



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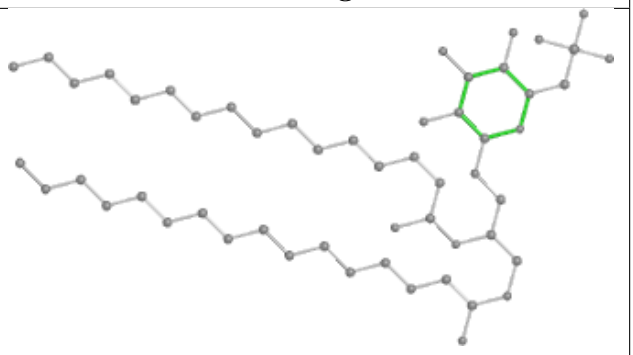
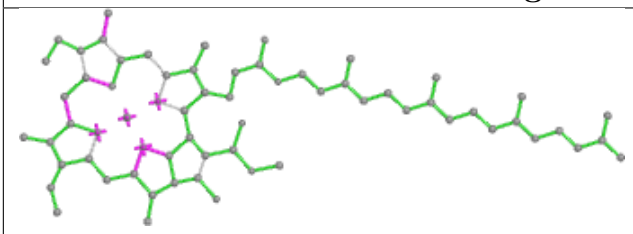
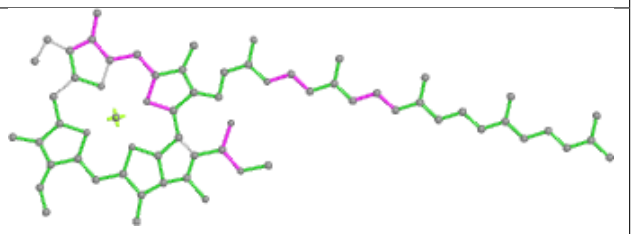


Rings

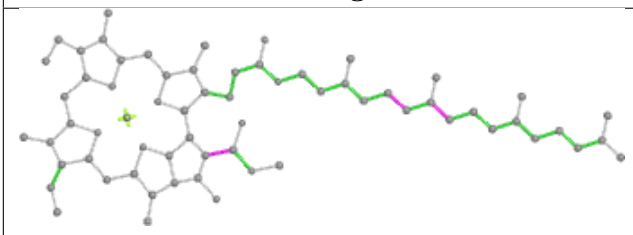
Ligand CLA C 503



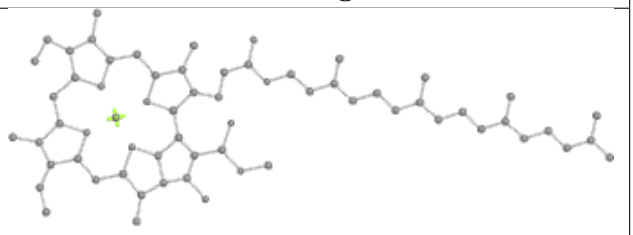
Bond lengths



Bond angles

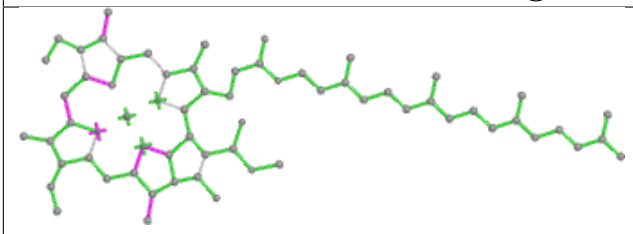


Torsions

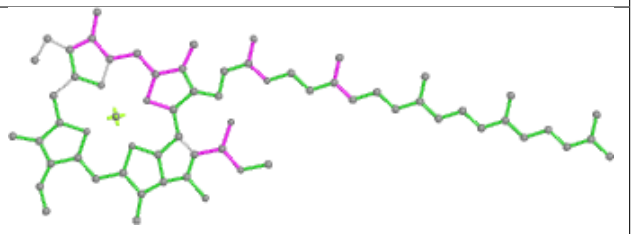


Rings

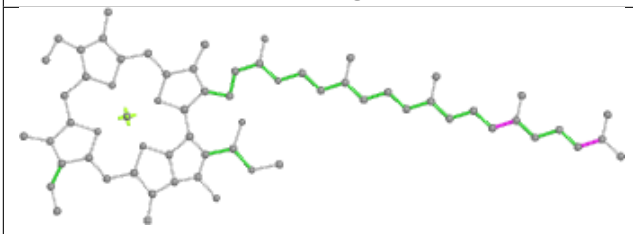
Ligand CLA d 403



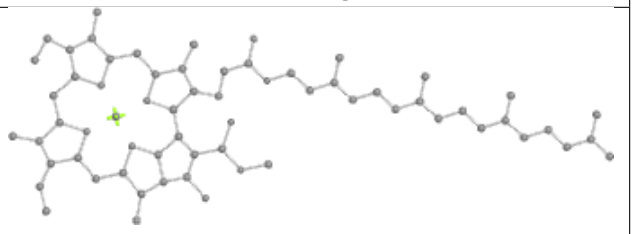
Bond lengths



Bond angles

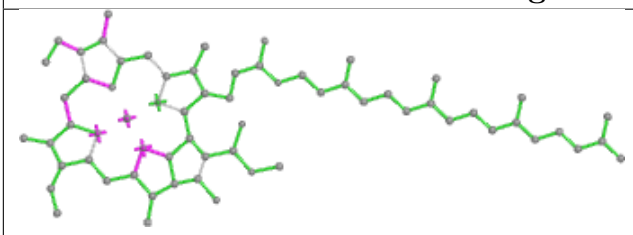


Torsions

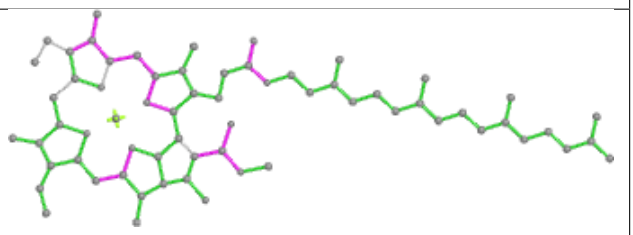


Rings

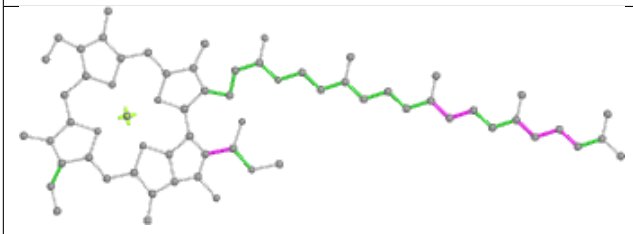
Ligand CLA a 607



Bond lengths



Bond angles



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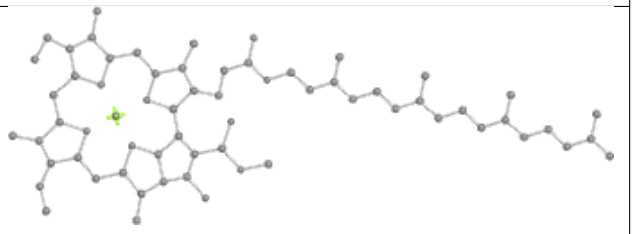
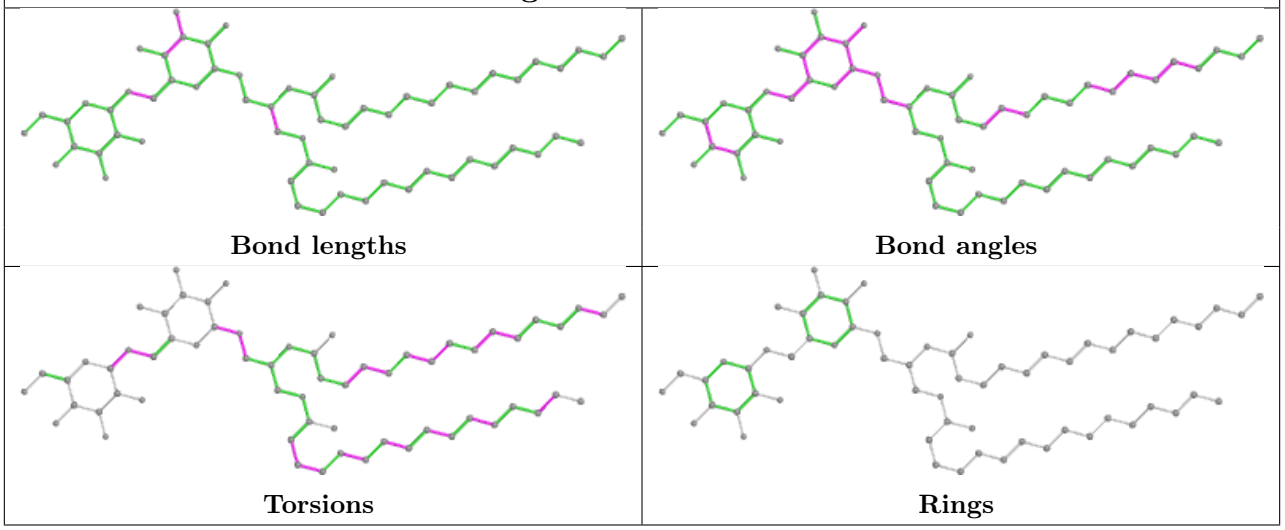
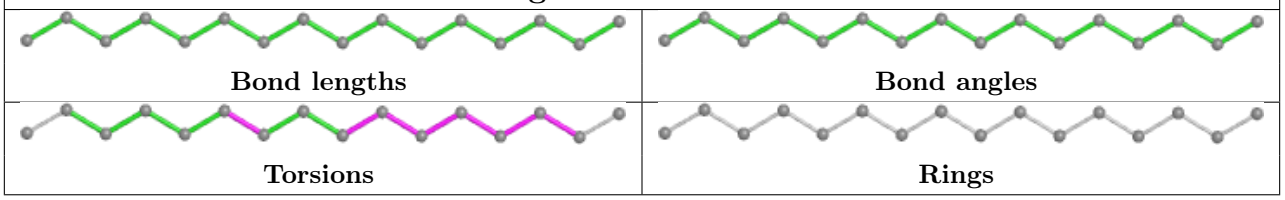


Rings

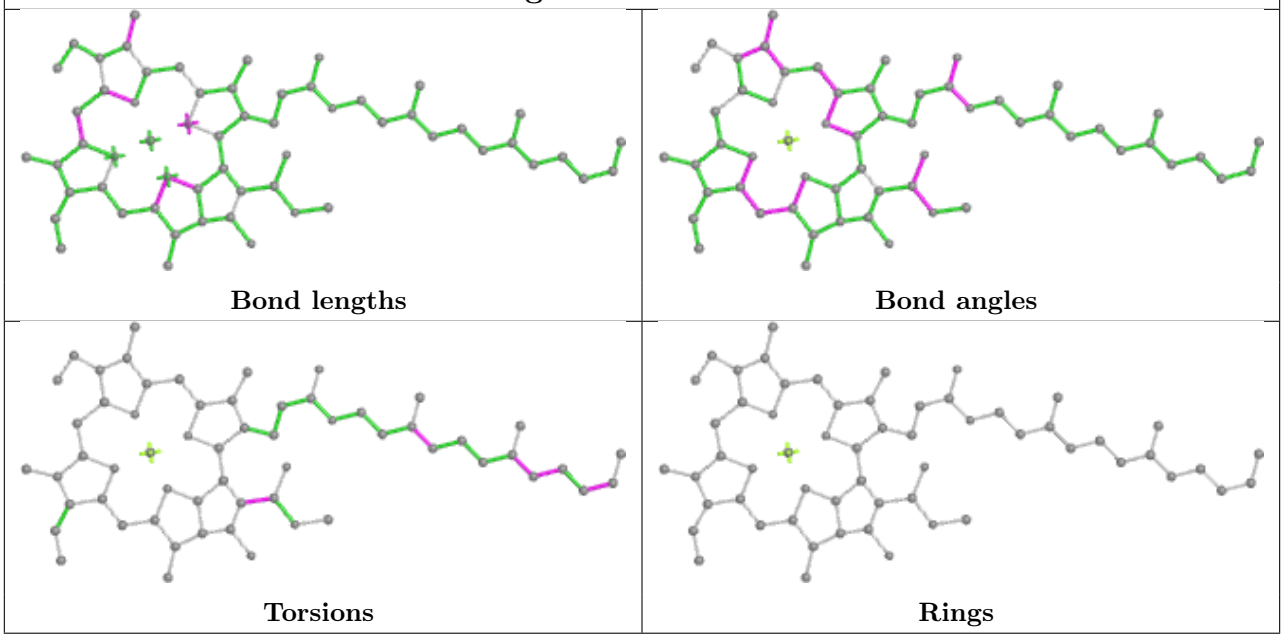
Ligand DGD C 518



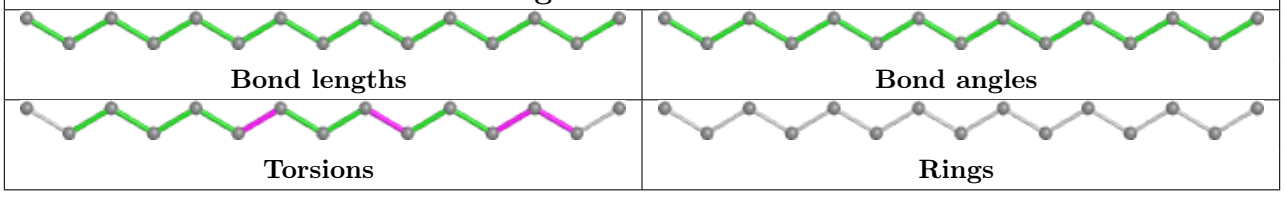
Ligand STE B 629



Ligand CLA C 504



Ligand STE I 101



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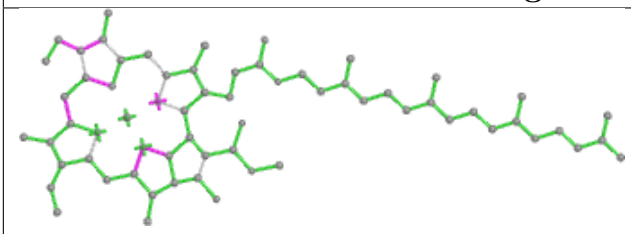
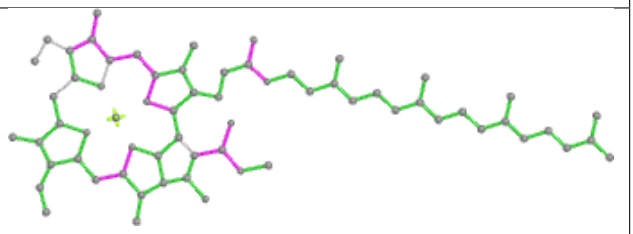
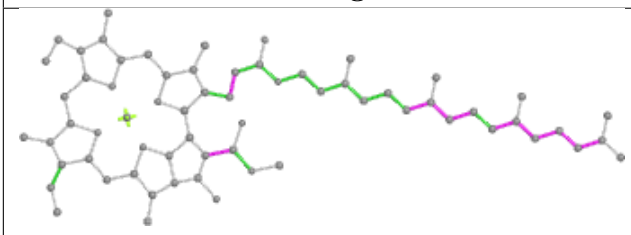


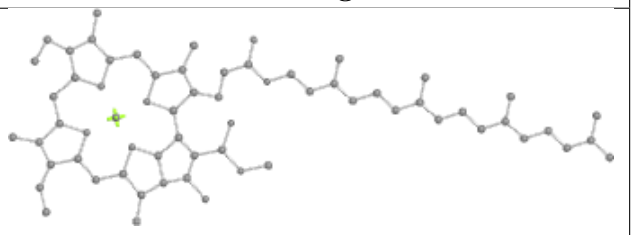
Bond lengths



Bond angles

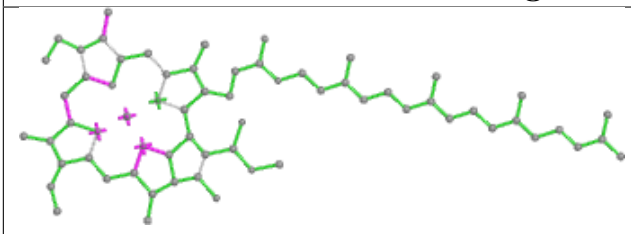


Torsions

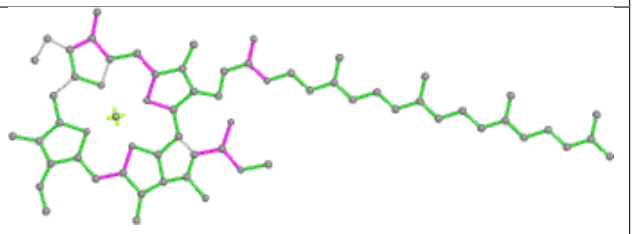


Rings

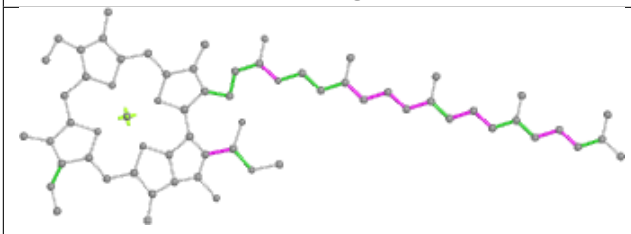
Ligand CLA C 513



Bond lengths



Bond angles



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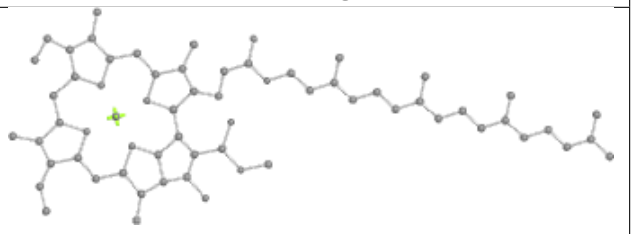
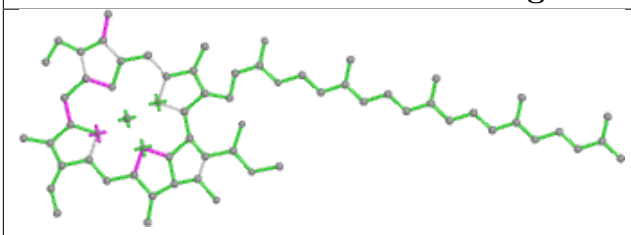
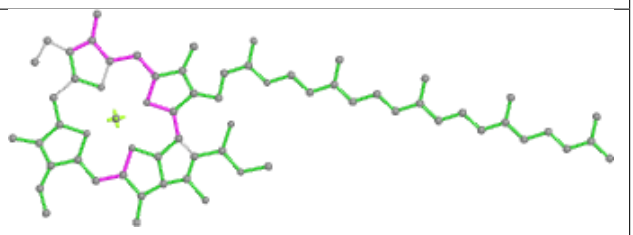


Rings

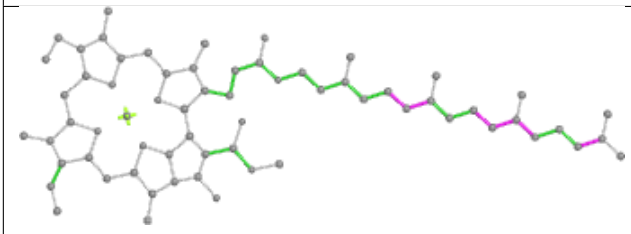
Ligand CLA d 404



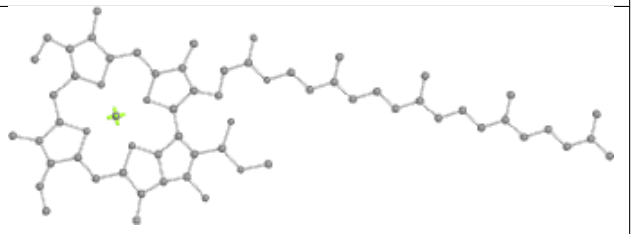
Bond lengths



Bond angles

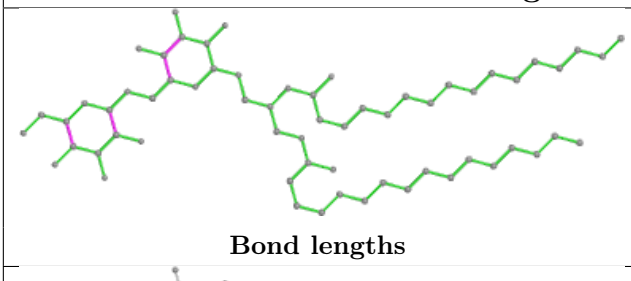


Torsions

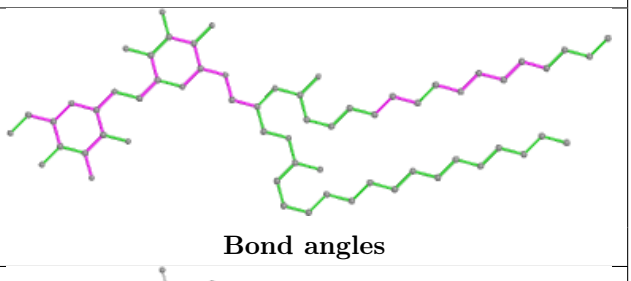


Rings

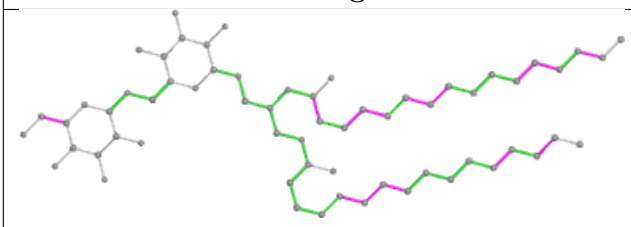
Ligand DGD h 101



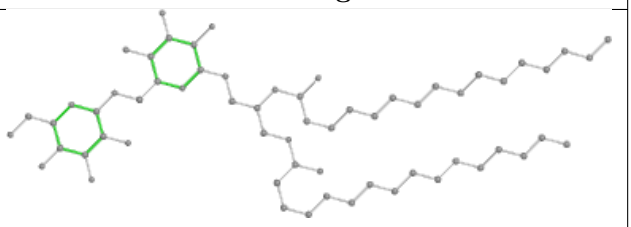
Bond lengths



Bond angles

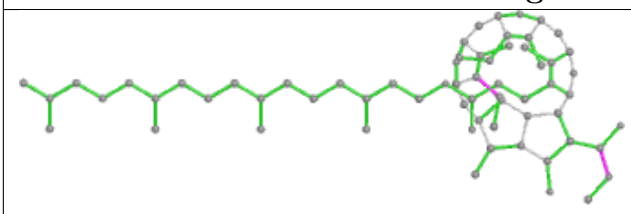


Torsions

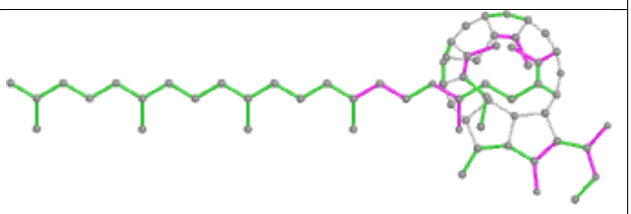


Rings

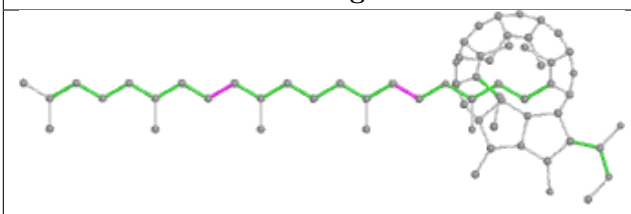
Ligand PHO a 608



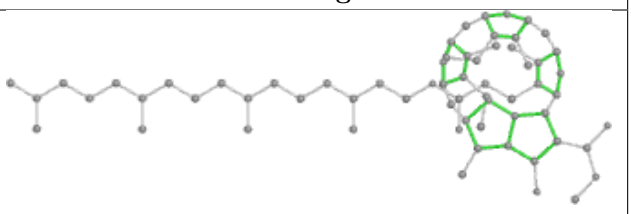
Bond lengths



Bond angles

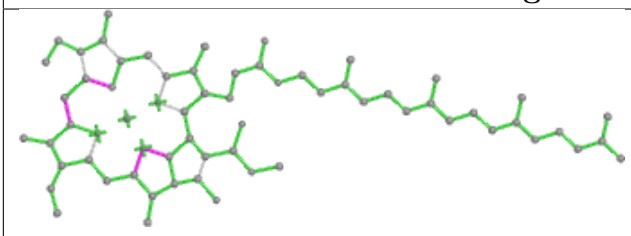


Torsions

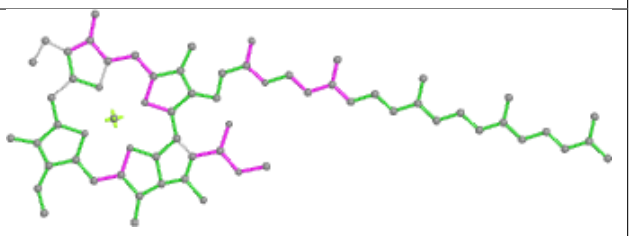


Rings

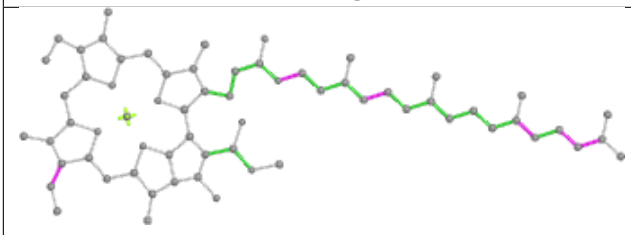
Ligand CLA D 403



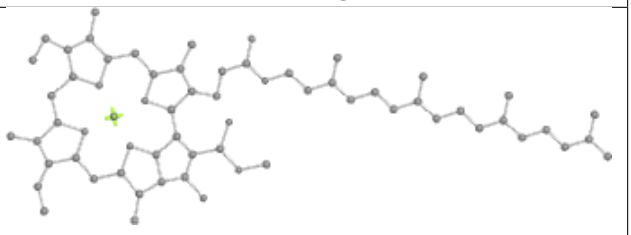
Bond lengths



Bond angles

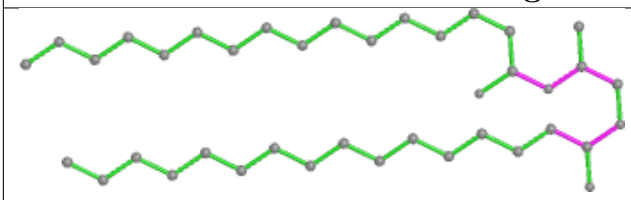


Torsions

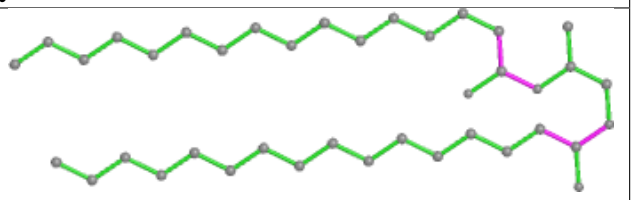


Rings

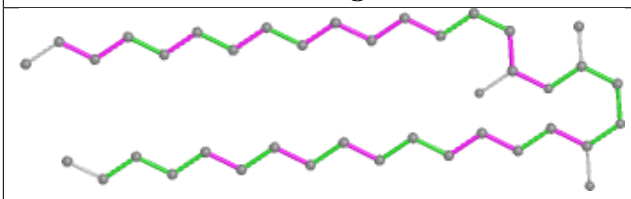
Ligand SQD A 615



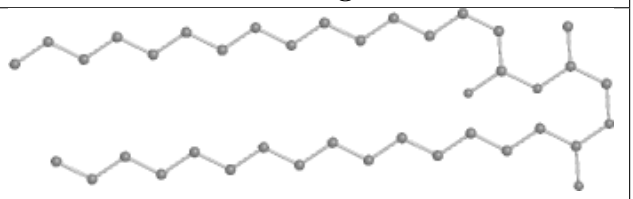
Bond lengths



Bond angles

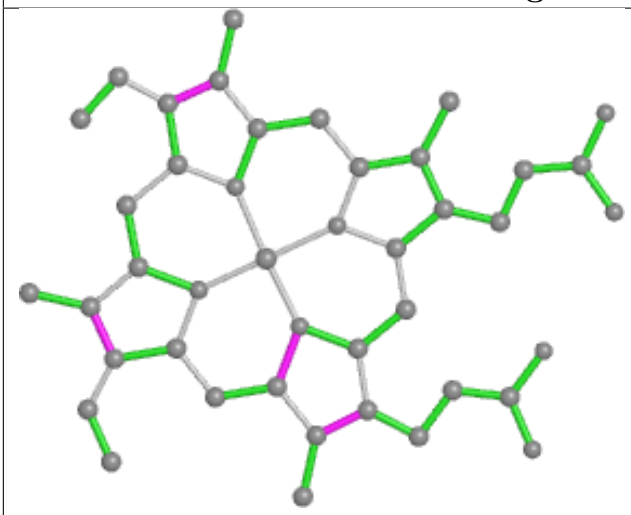


Torsions

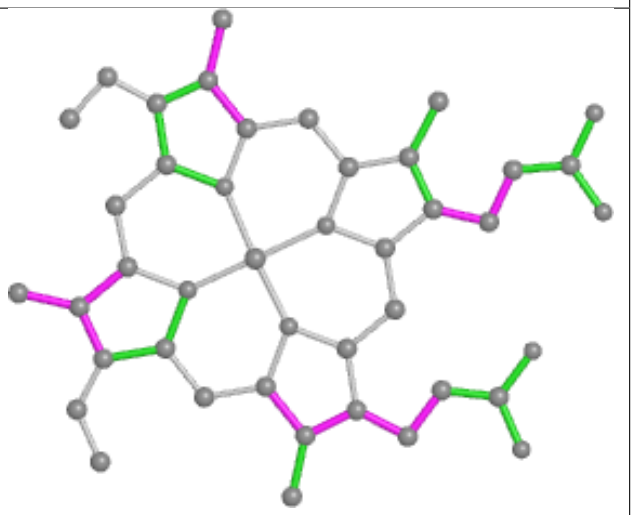


Rings

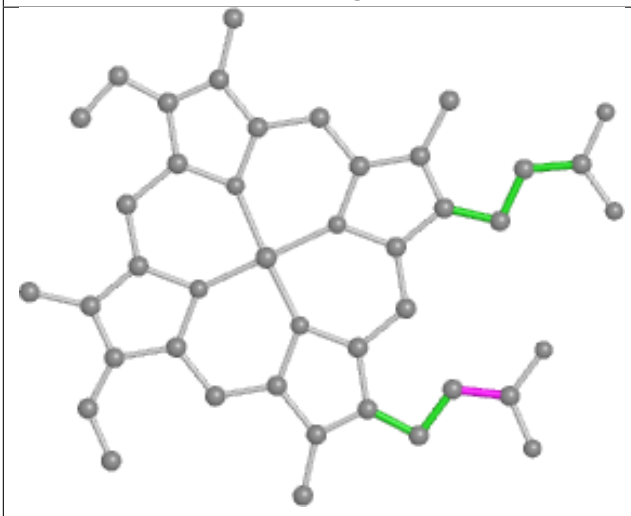
Ligand HEC v 201



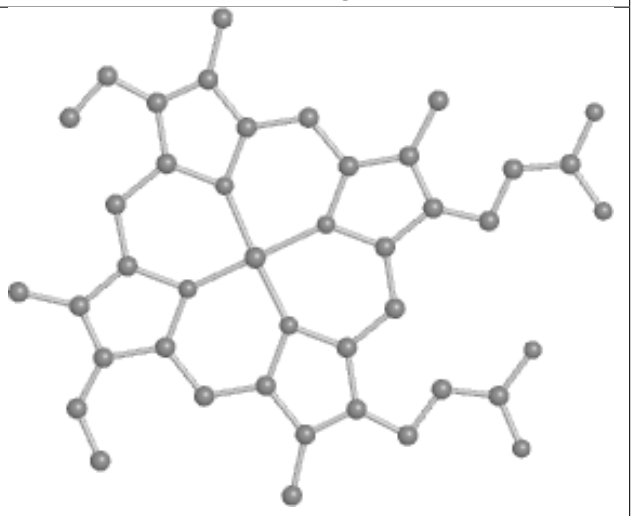
Bond lengths



Bond angles

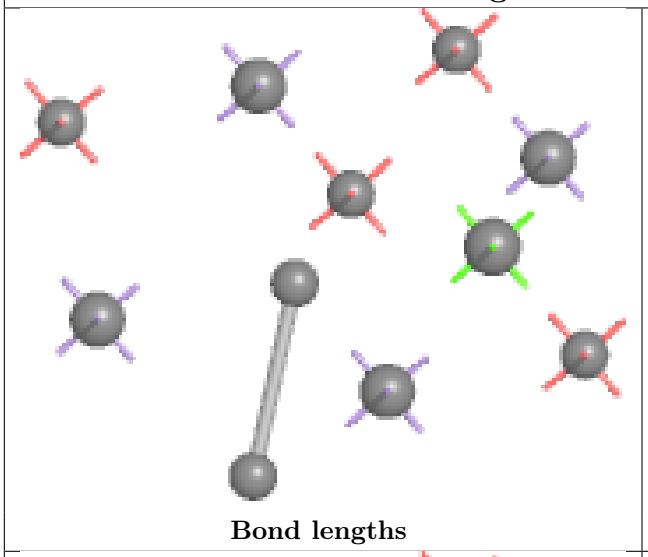


Torsions

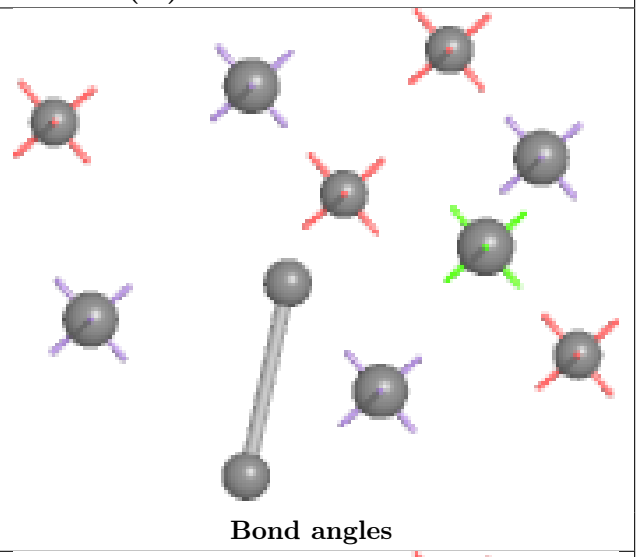


Rings

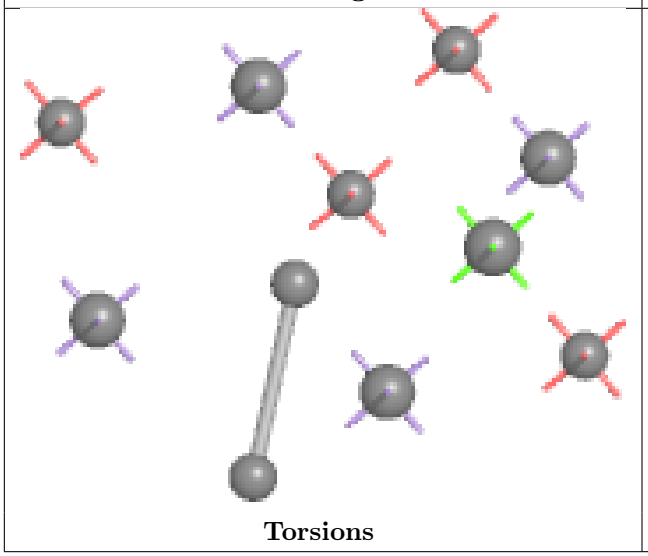
Ligand OEY A 602 (A)



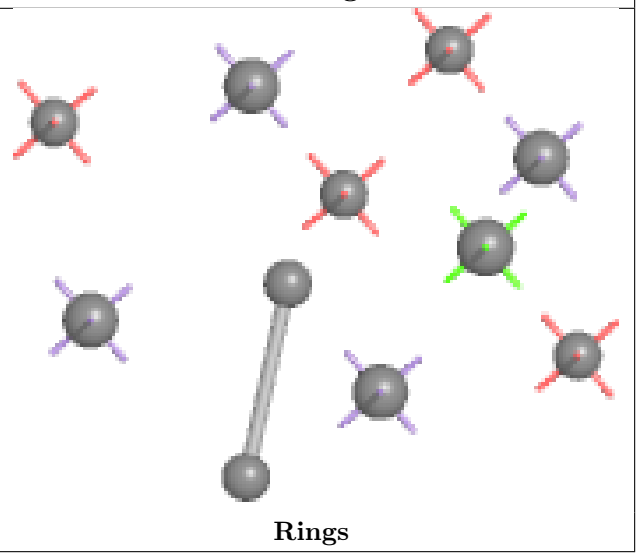
Bond lengths



Bond angles

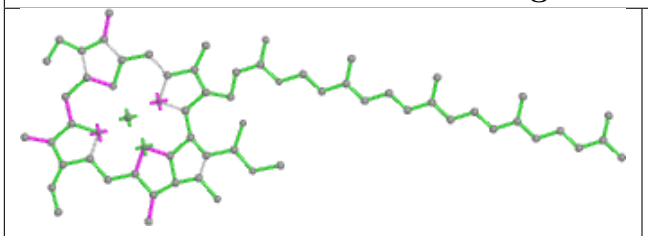


Torsions

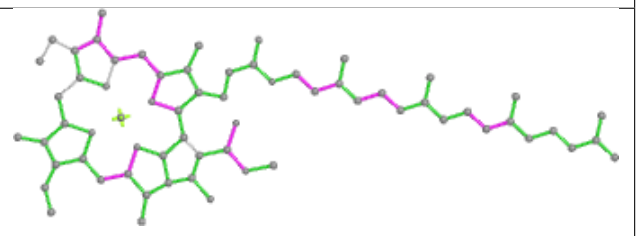


Rings

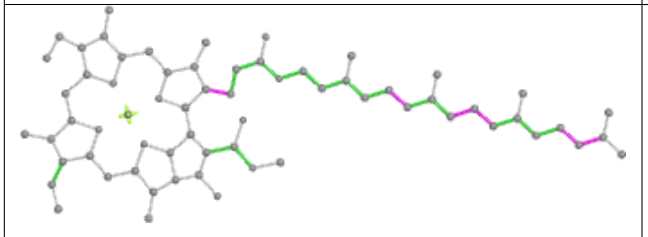
Ligand CLA c 503



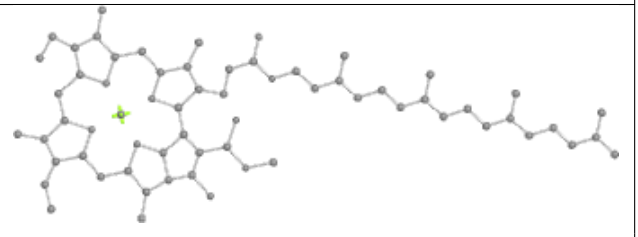
Bond lengths



Bond angles

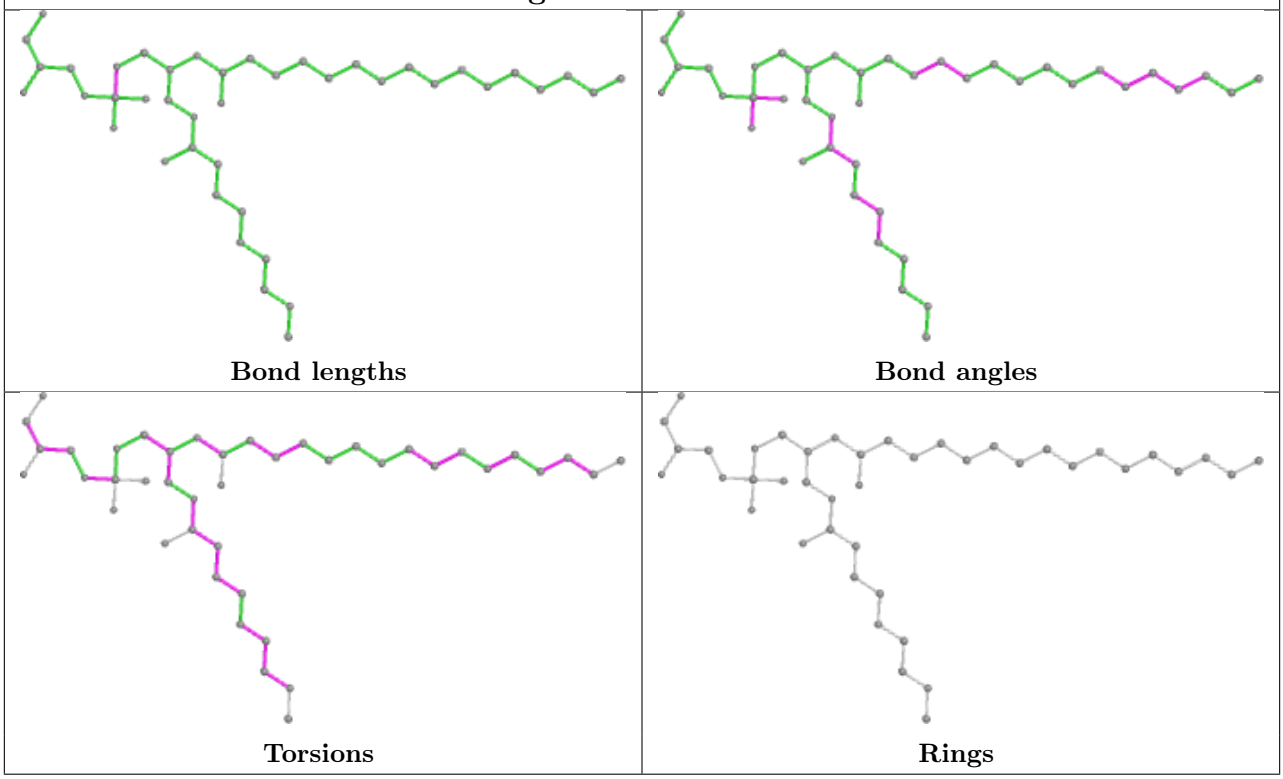


Torsions

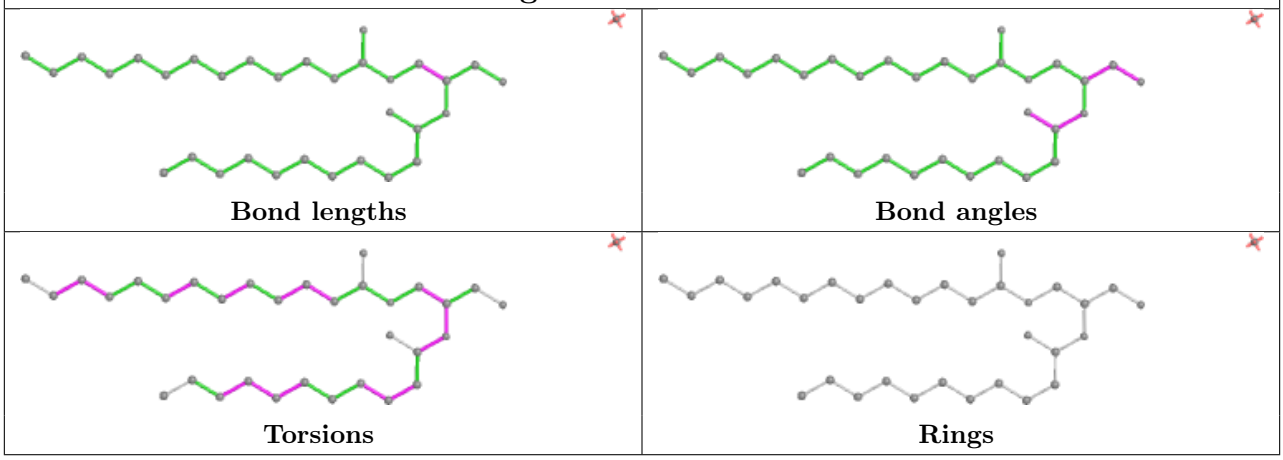


Rings

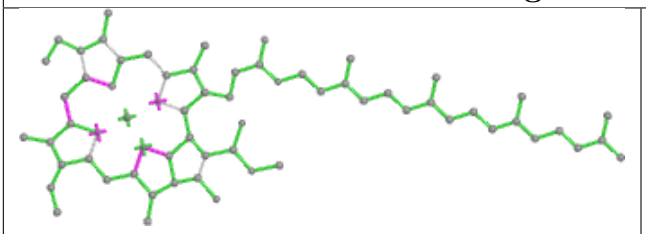
Ligand LHG e 102



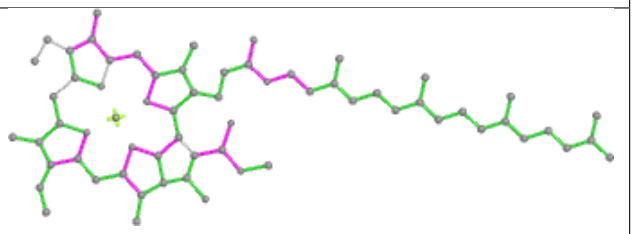
Ligand LMG D 411



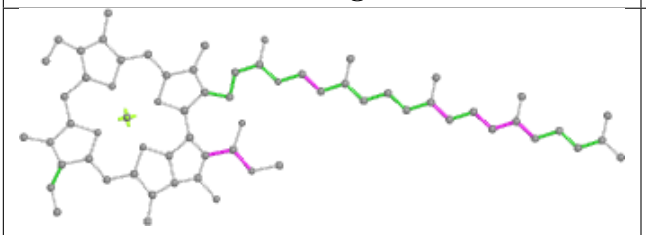
Ligand CLA B 604



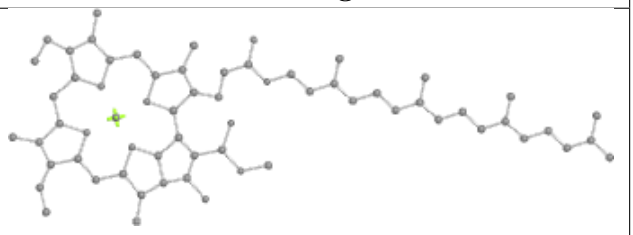
Bond lengths



Bond angles

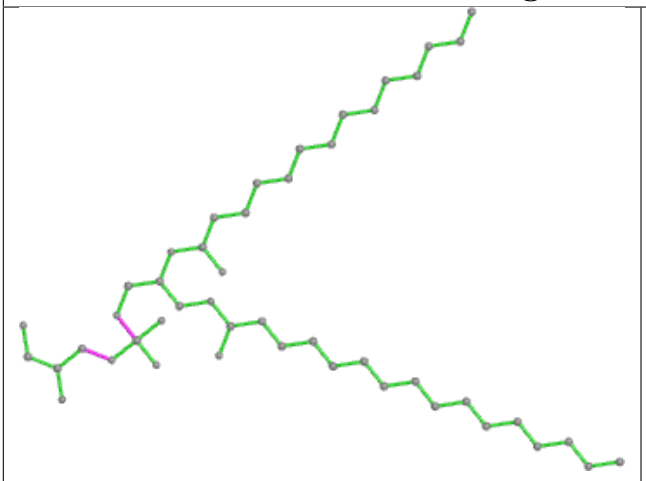


Torsions

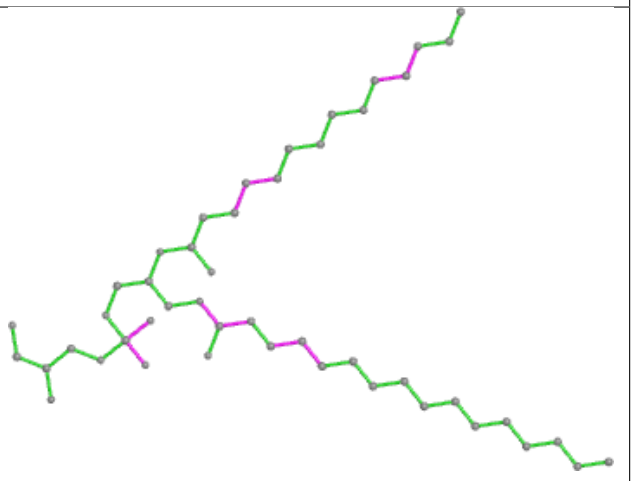


Rings

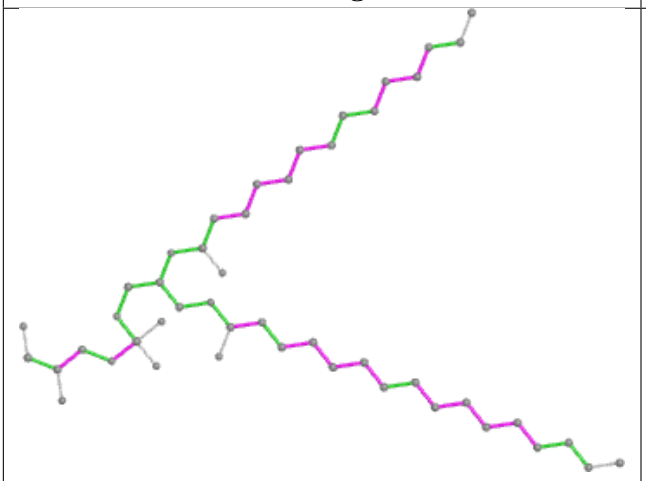
Ligand LHG D 410



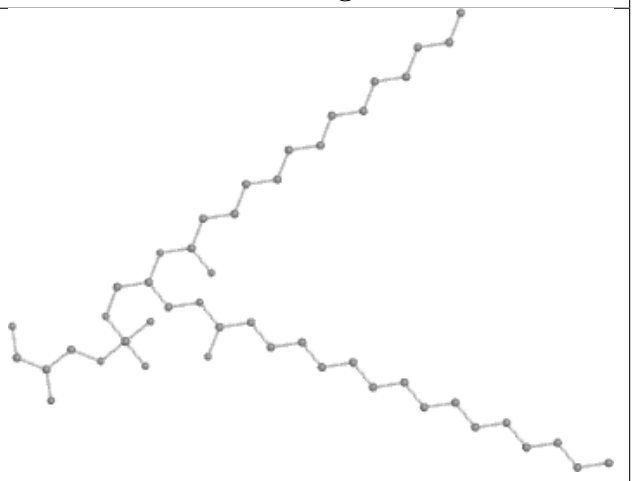
Bond lengths



Bond angles

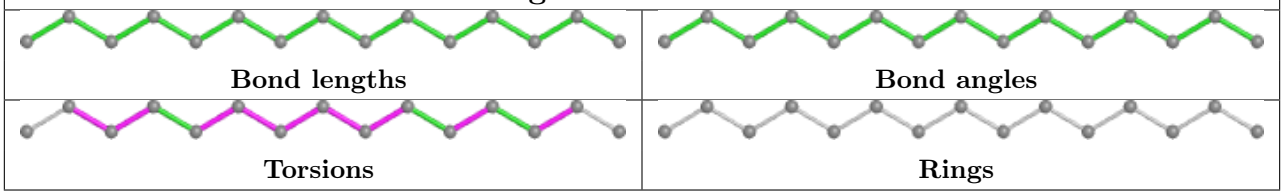


Torsions

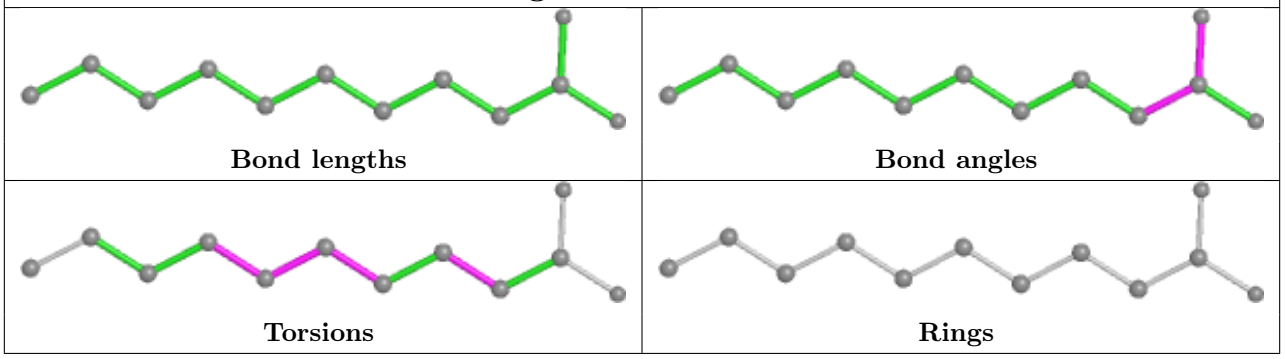


Rings

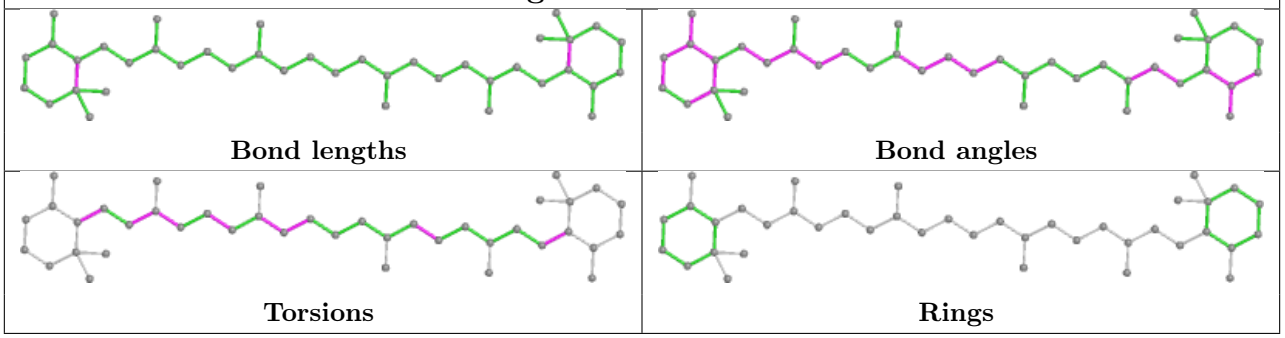
Ligand STE T 103



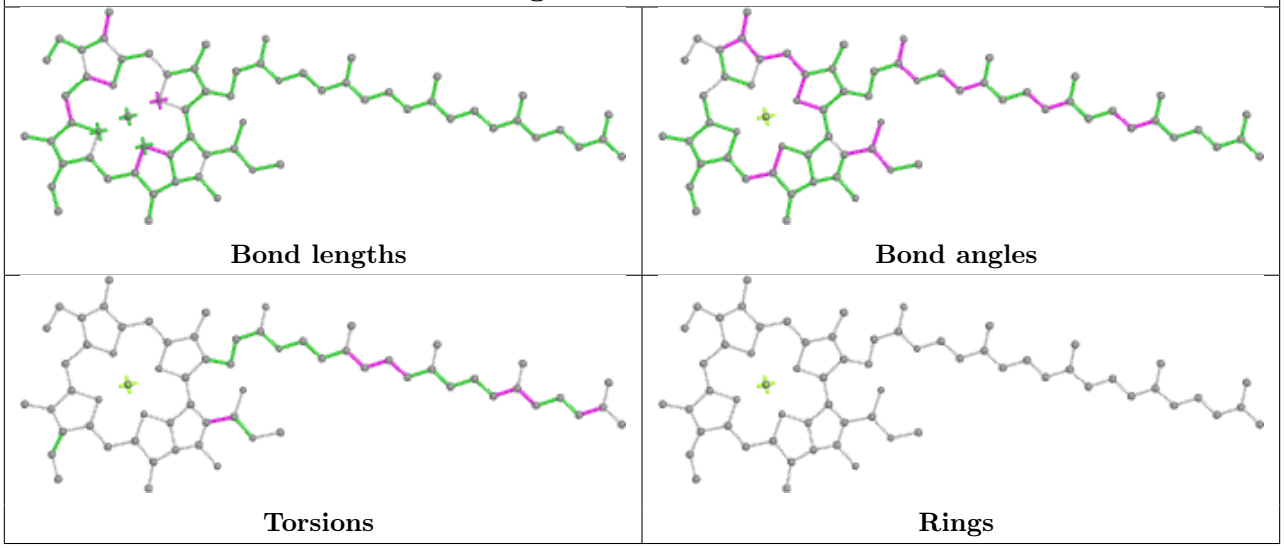
Ligand STE C 522



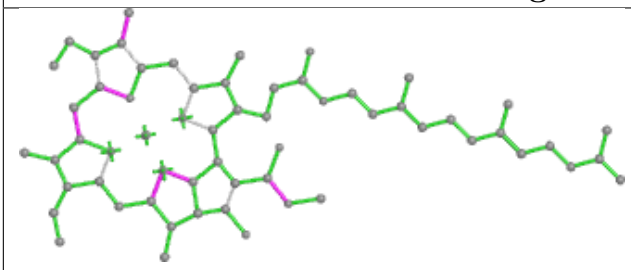
Ligand BCR k 101



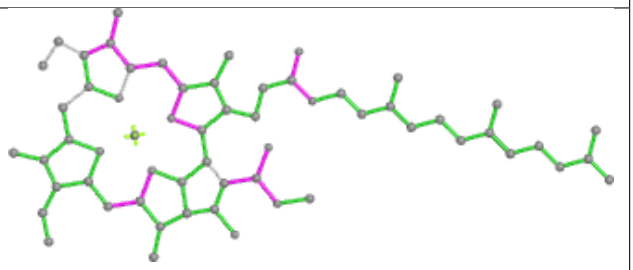
Ligand CLA b 604



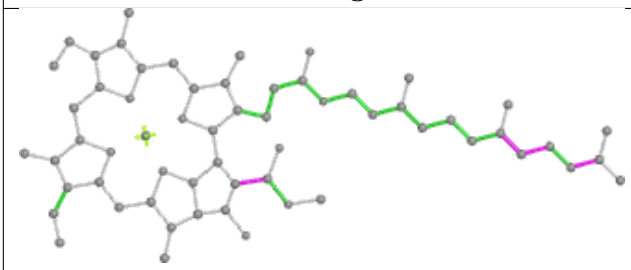
Ligand CLA c 504



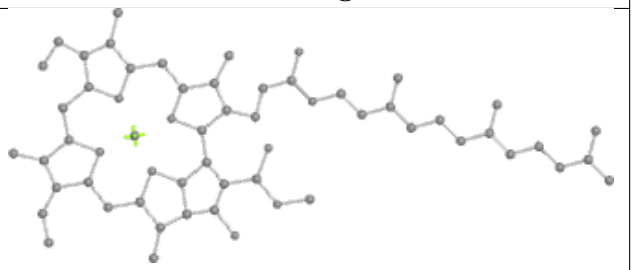
Bond lengths



Bond angles

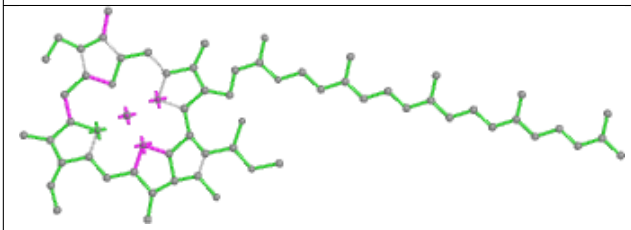


Torsions



Rings

Ligand CLA c 502



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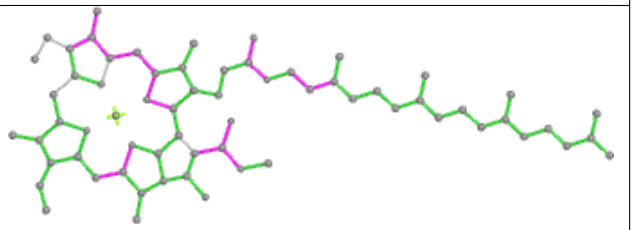
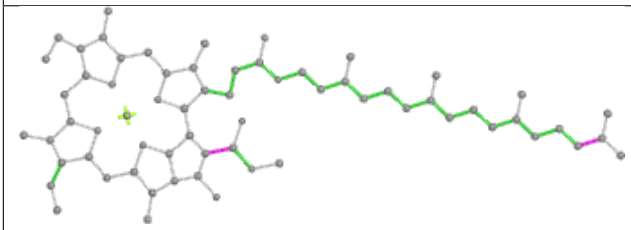
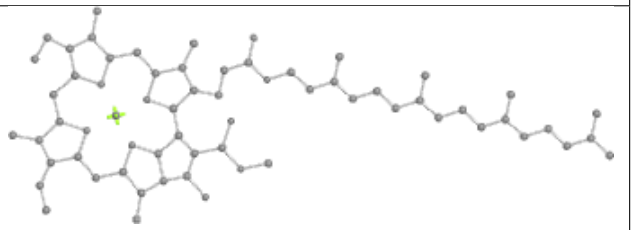


Bond angles

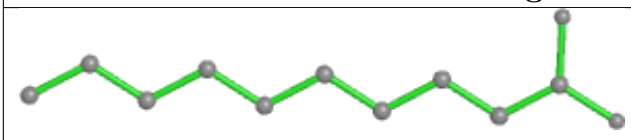


Torsions

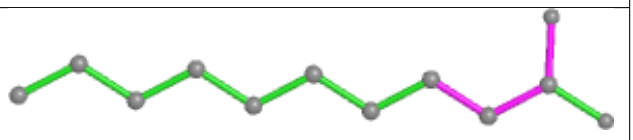


Rings

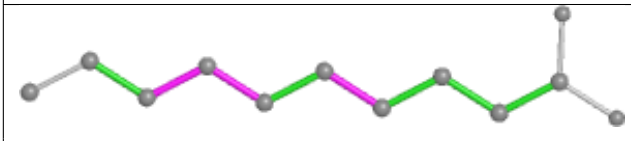
Ligand STE m 102



Bond lengths



Bond angles



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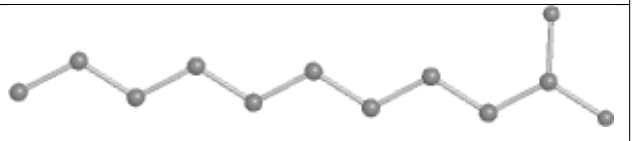
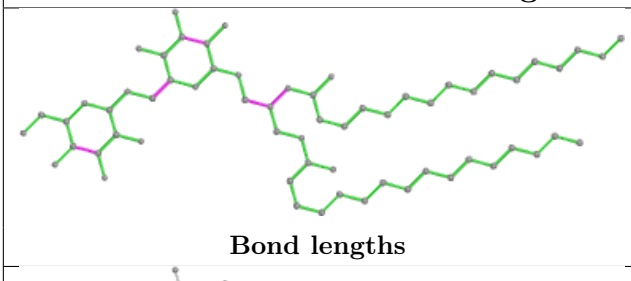
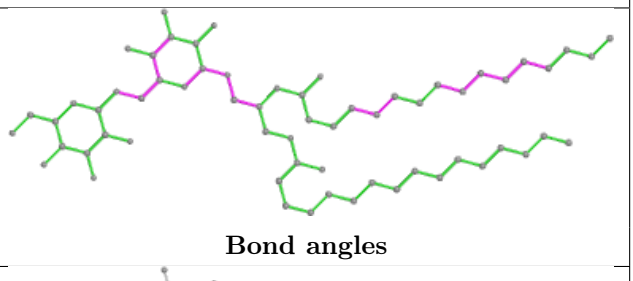


Rings

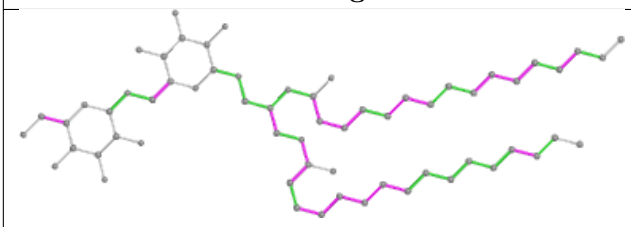
Ligand DGD C 517



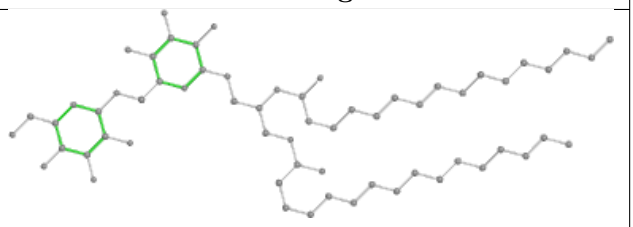
Bond lengths



Bond angles

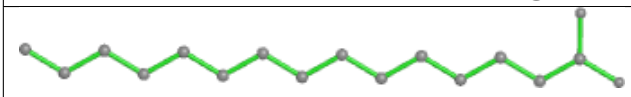


Torsions

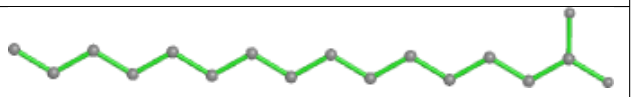


Rings

Ligand STE B 621

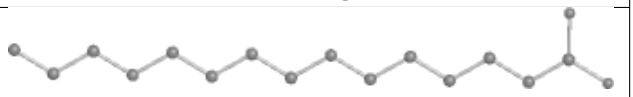


Bond lengths



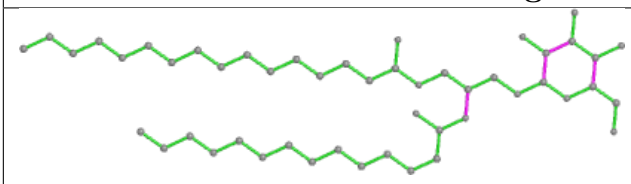
Bond angles

Torsions

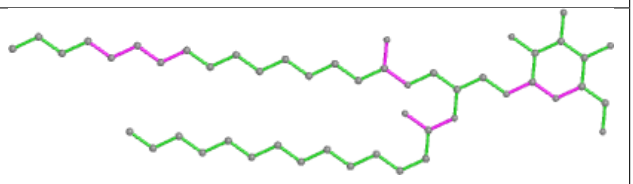


Rings

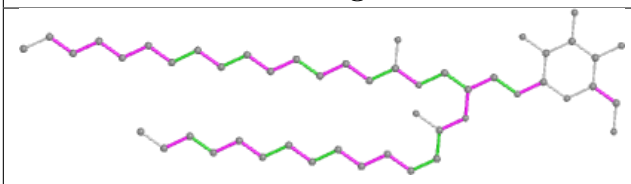
Ligand LMG c 522



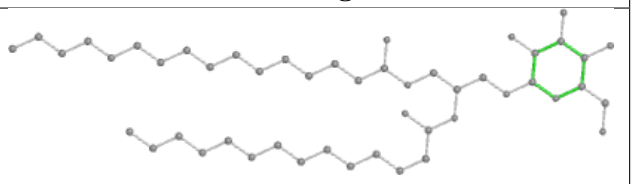
Bond lengths



Bond angles

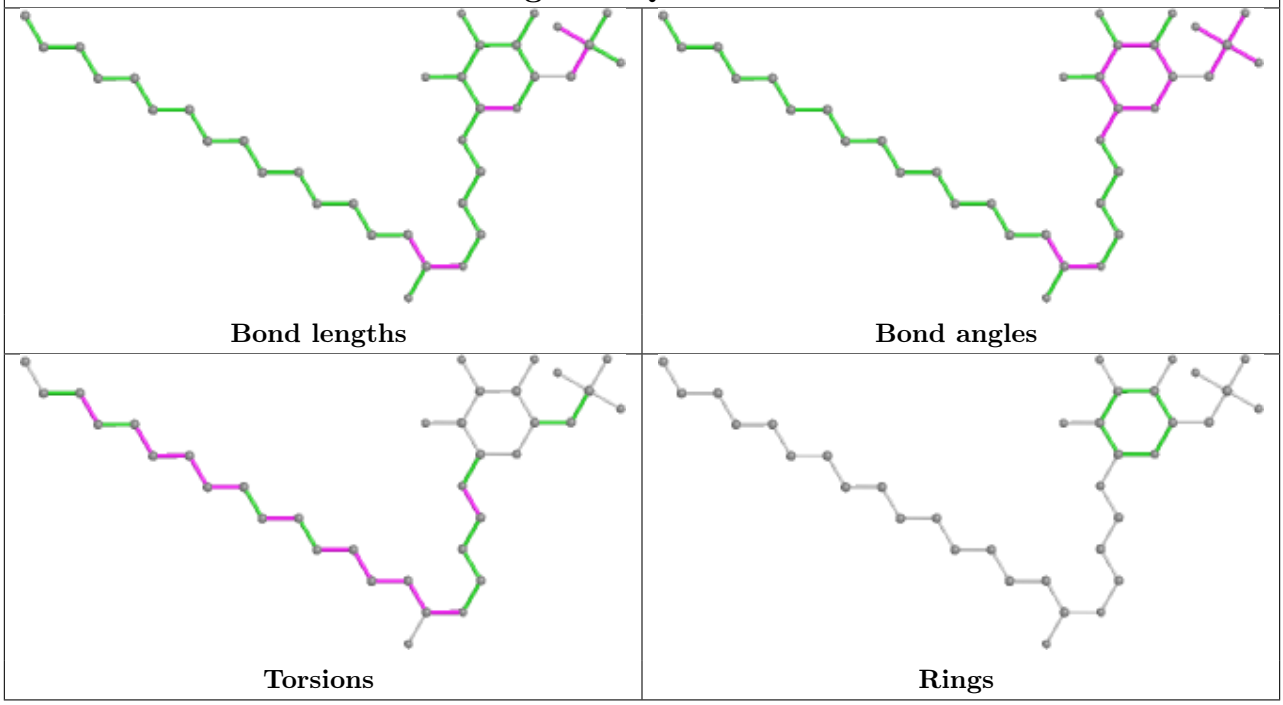


Torsions

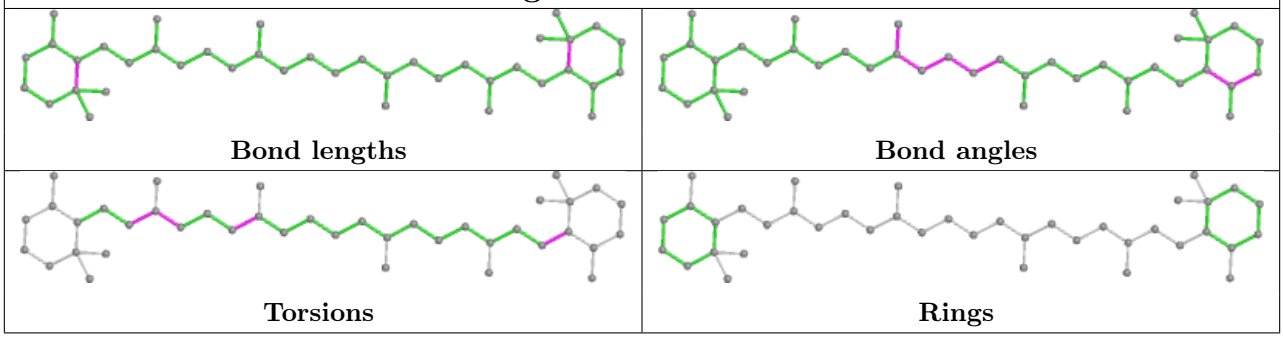


Rings

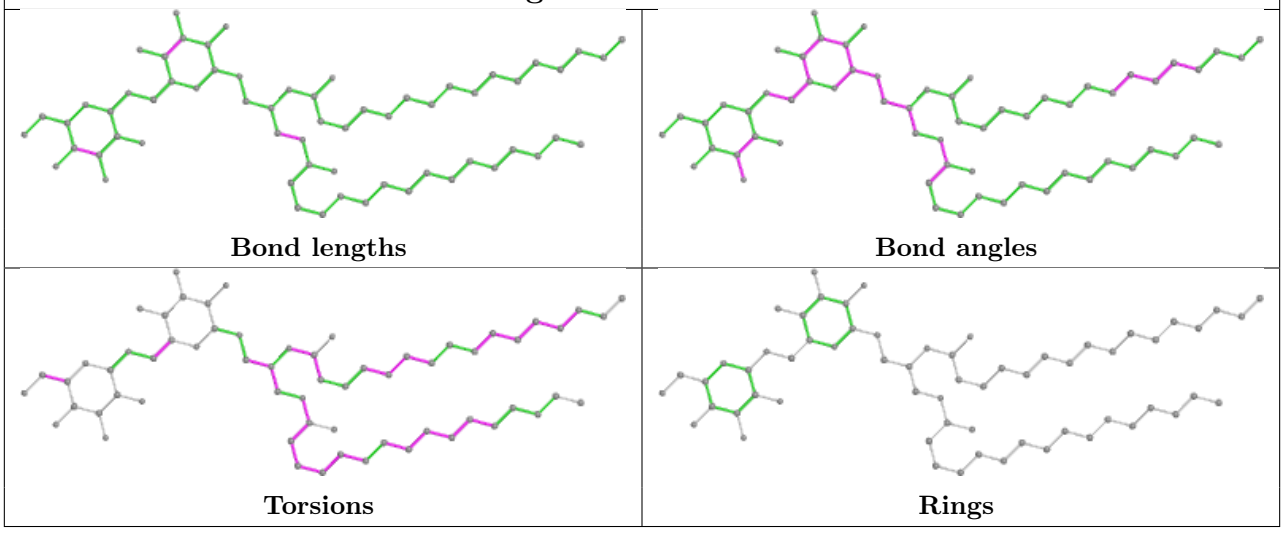
Ligand SQD D 408



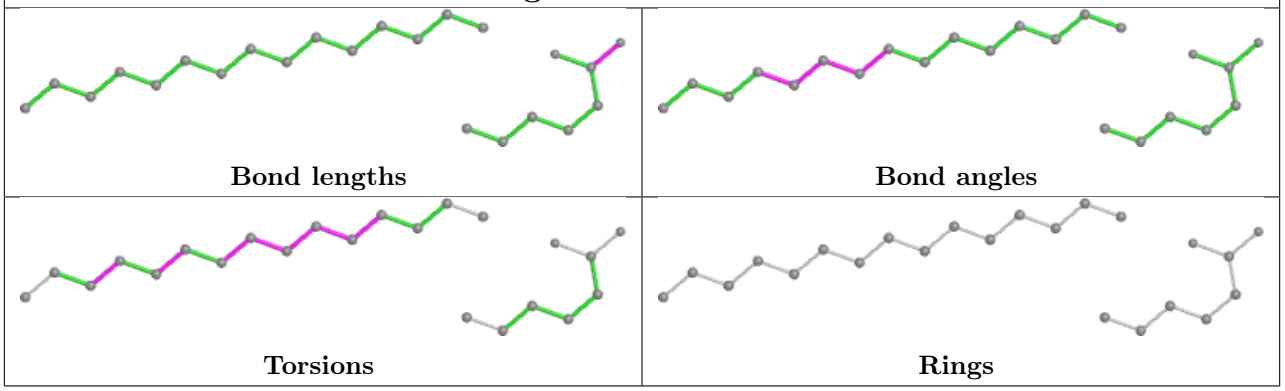
Ligand BCR C 515



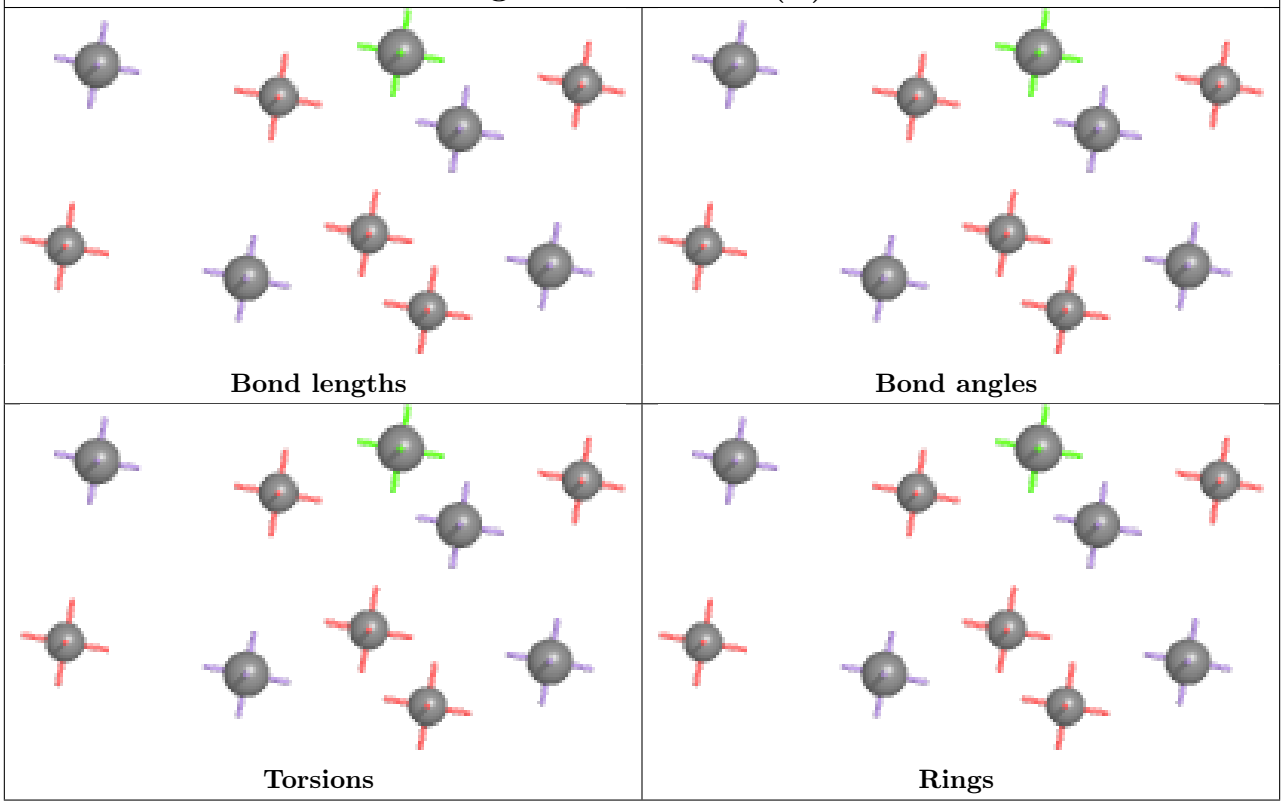
Ligand DGD c 515



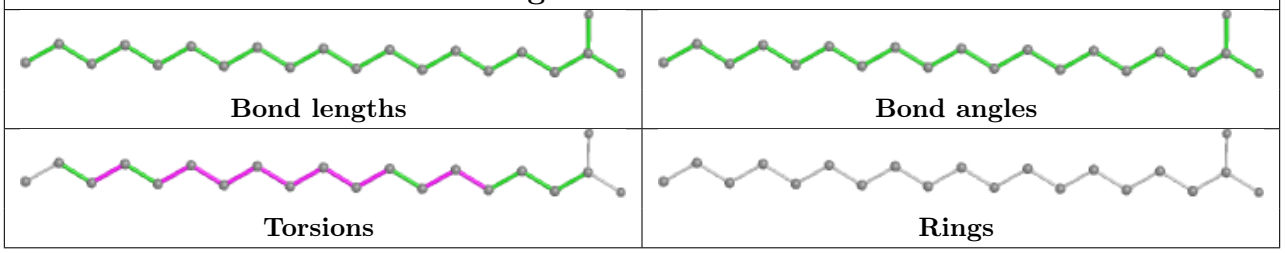
Ligand LMG d 409



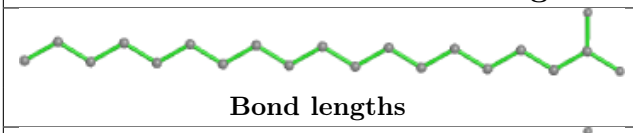
Ligand OEX A 601 (C)

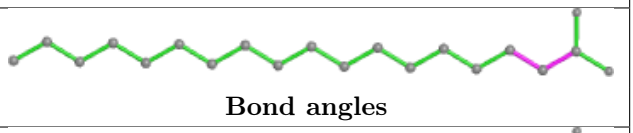


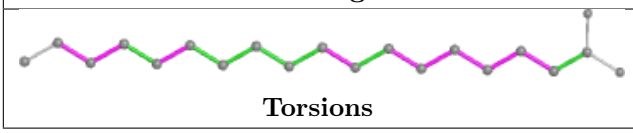
Ligand STE X 101

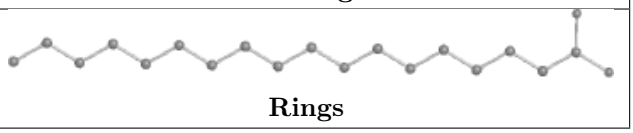


Ligand STE d 412

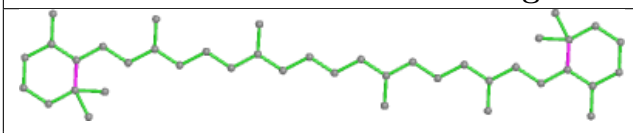

Bond lengths

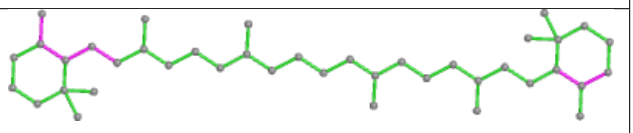

Bond angles

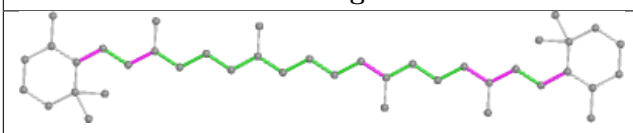

Torsions


Rings

Ligand BCR C 516


Bond lengths


Bond angles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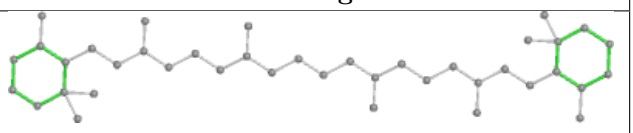
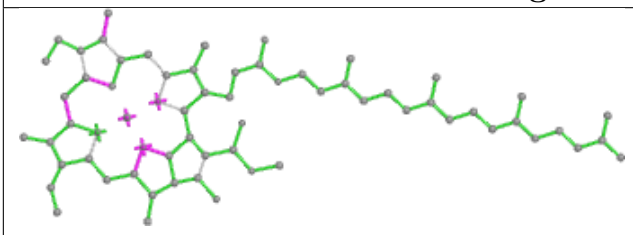
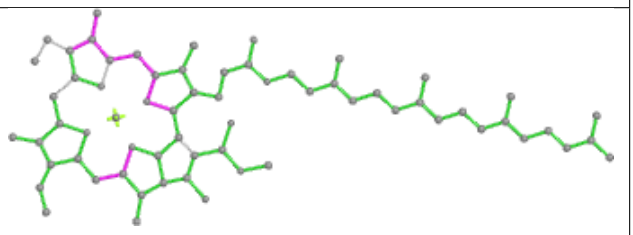
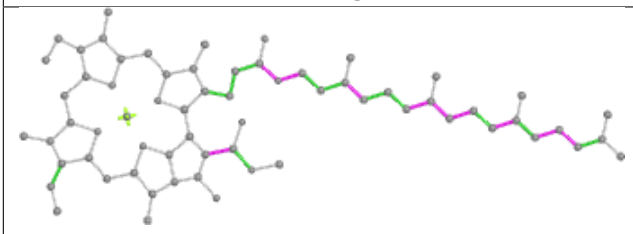

Rings

Ligand CLA c 506


Bond lengths


Bond angles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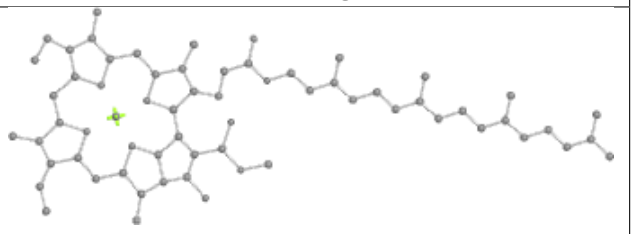
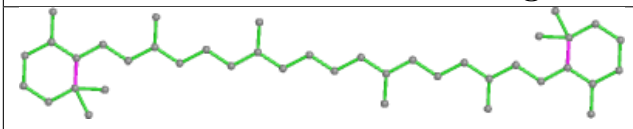
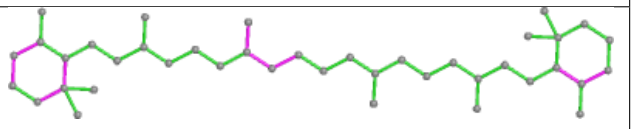
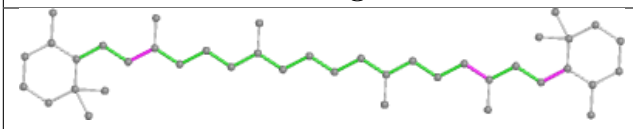
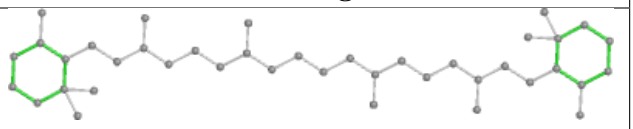

Rings

Ligand BCR B 618

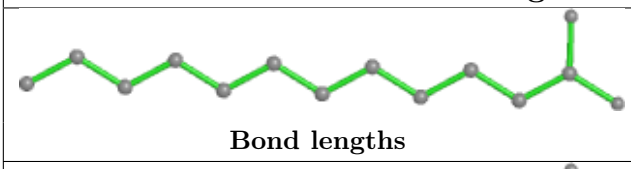

Bond lengths


Bond angles

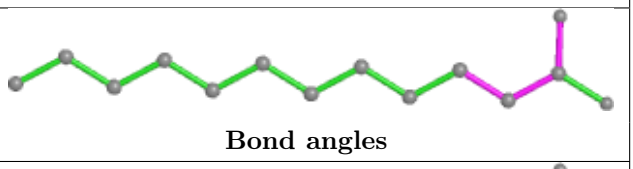

Torsions


Rings

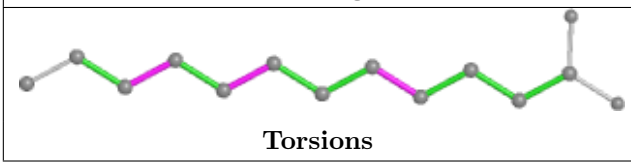
Ligand STE B 625



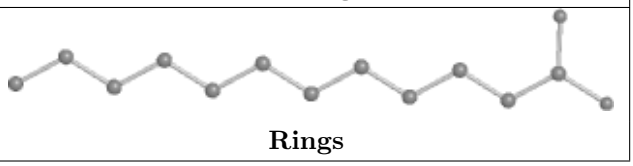
Bond lengths



Bond angles

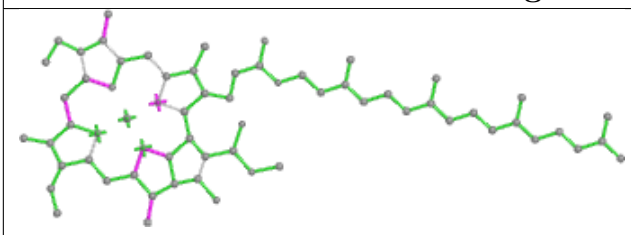


Torsions

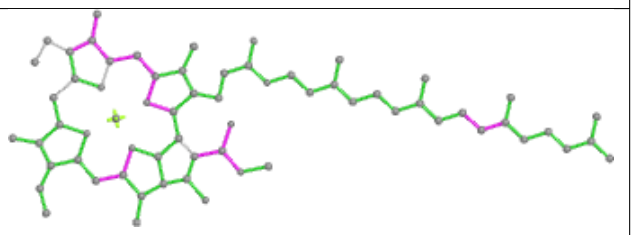


Rings

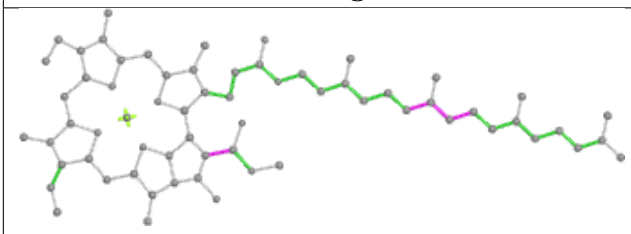
Ligand CLA C 510



Bond lengths



Bond angles



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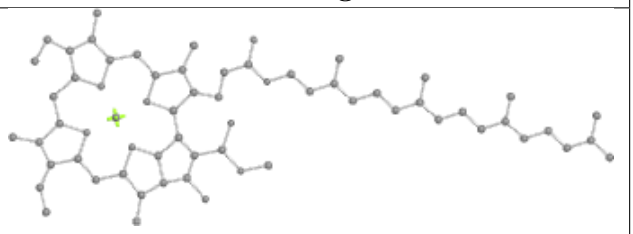
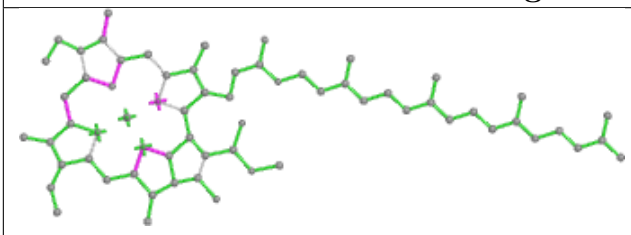
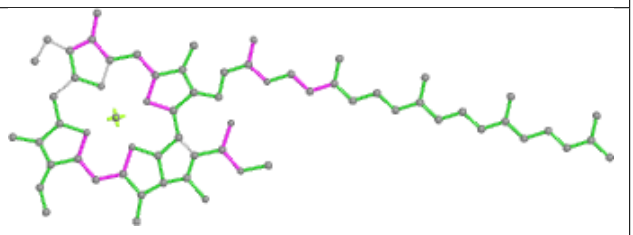


Rings

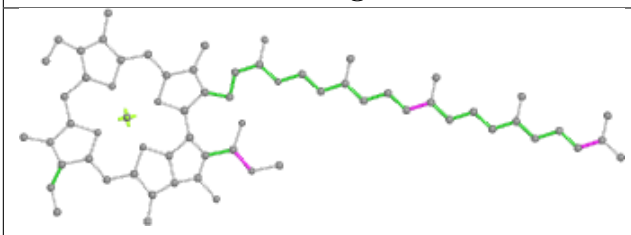
Ligand CLA C 511



Bond lengths



Bond angles



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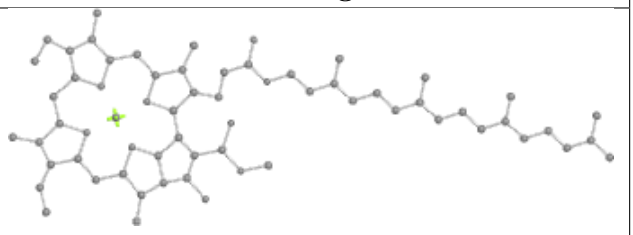
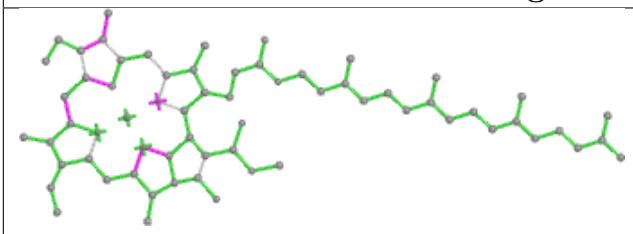
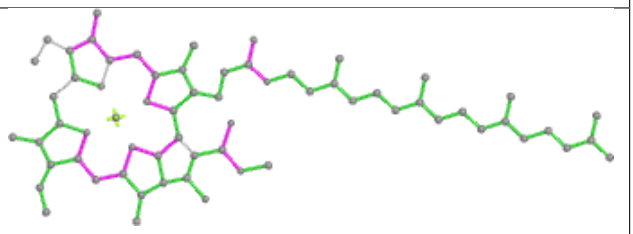
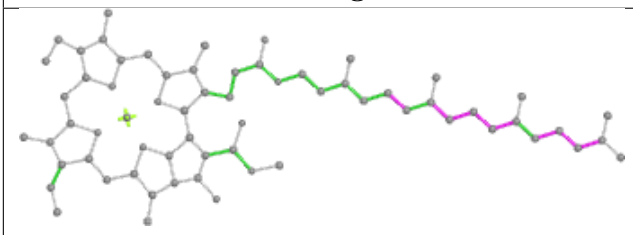


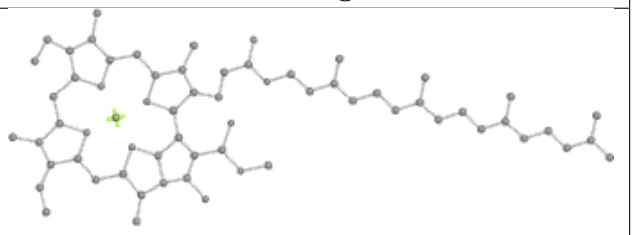
Rings

Ligand CLA b 615

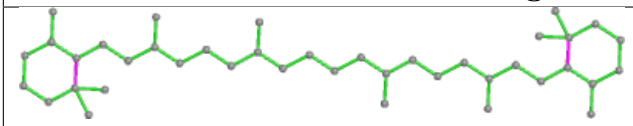

Bond lengths

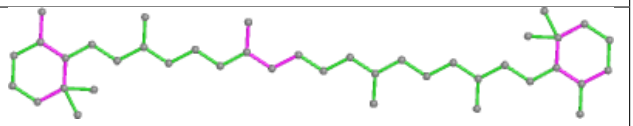

Bond angles

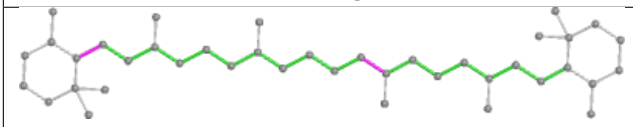

Torsions


Rings

Ligand BCR b 617


Bond lengths

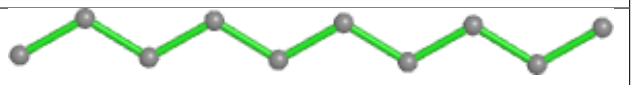

Bond angles

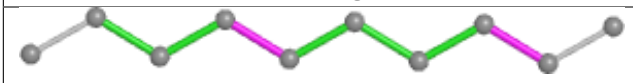

Torsions

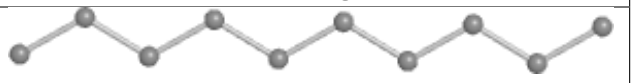

Rings

Ligand STE M 102

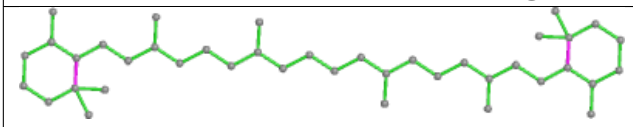

Bond lengths

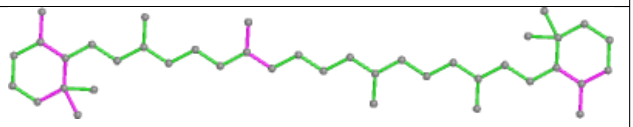

Bond angles

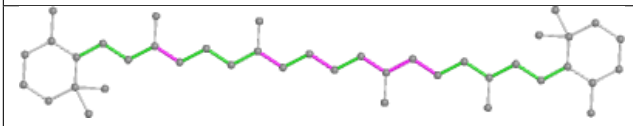

Torsions

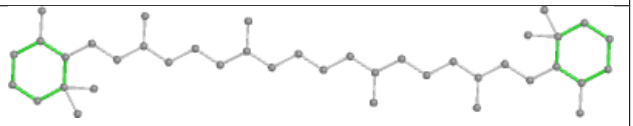

Rings

Ligand BCR T 101

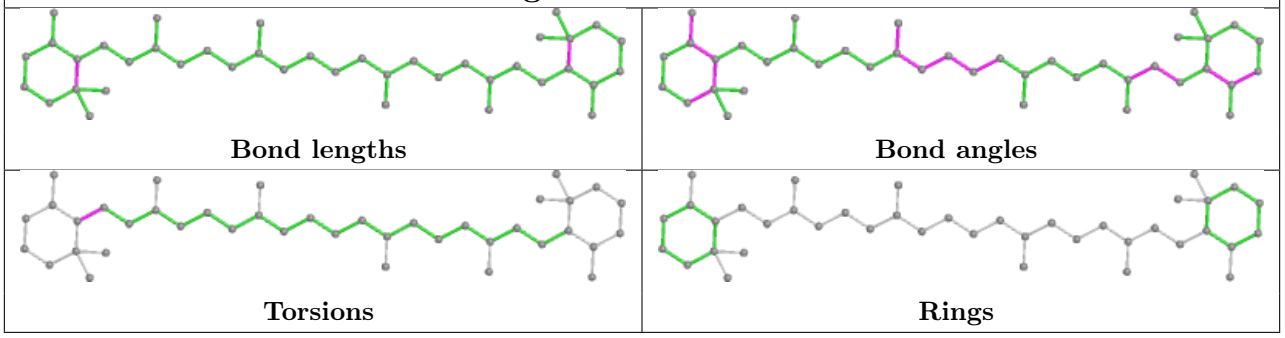

Bond lengths


Bond angles

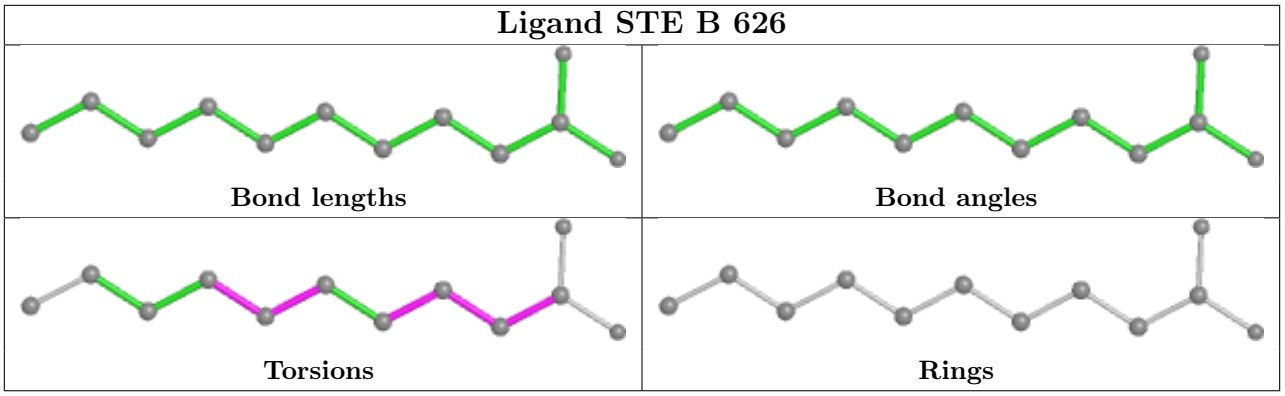

Torsions


Rings

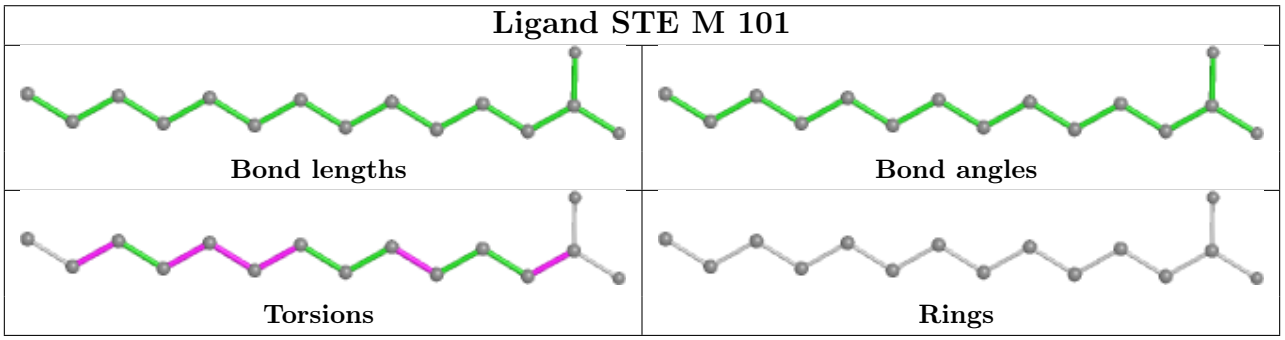
Ligand BCR C 514



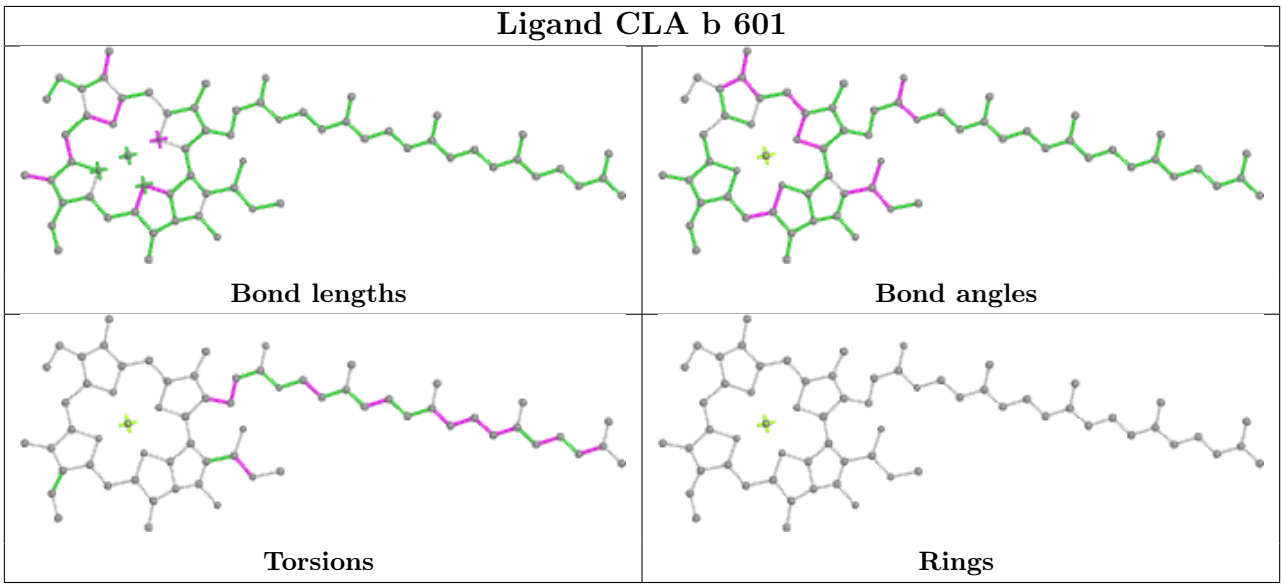
Ligand STE B 626



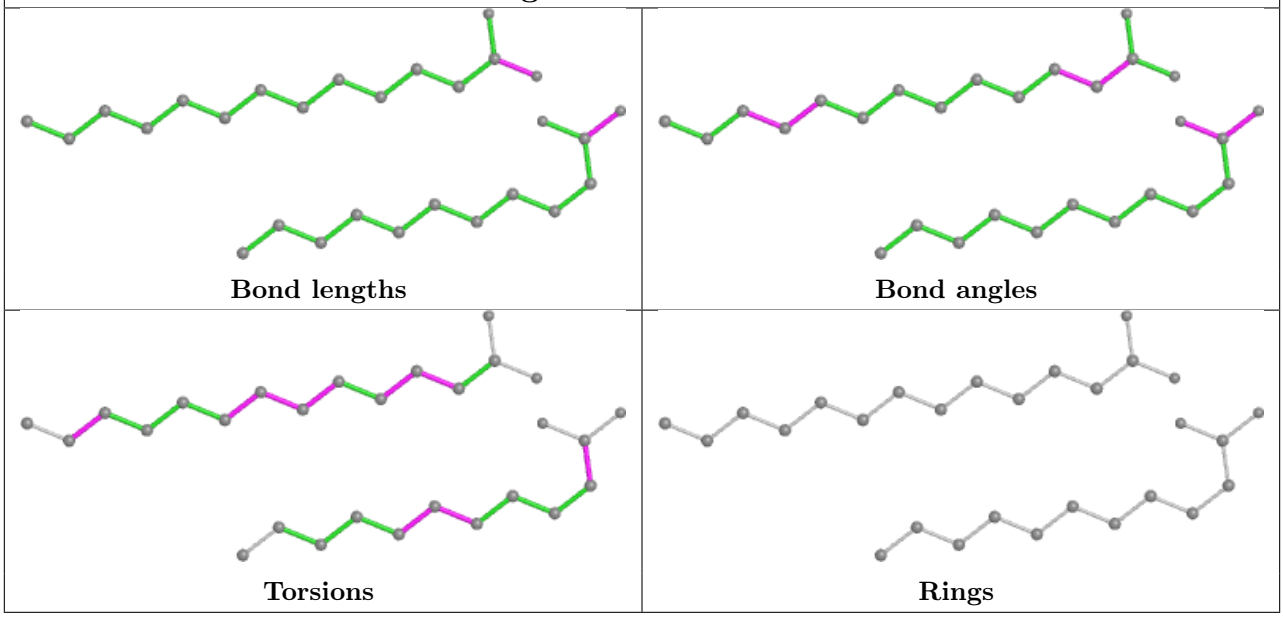
Ligand STE M 101



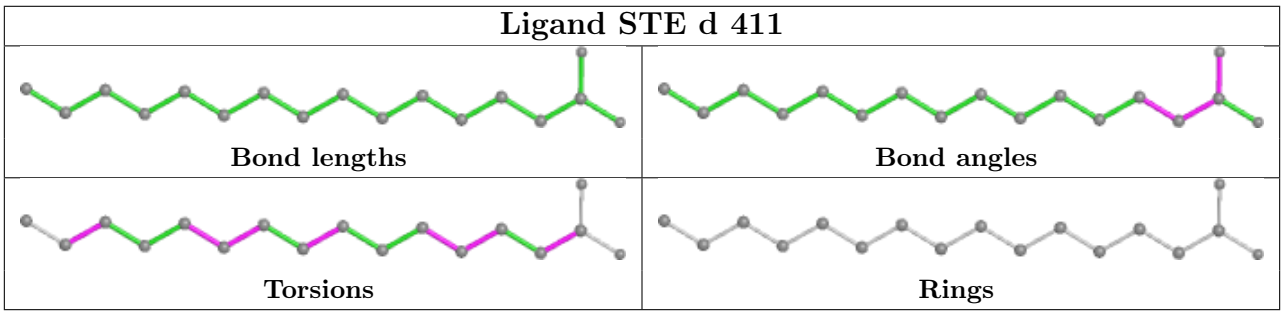
Ligand CLA b 601



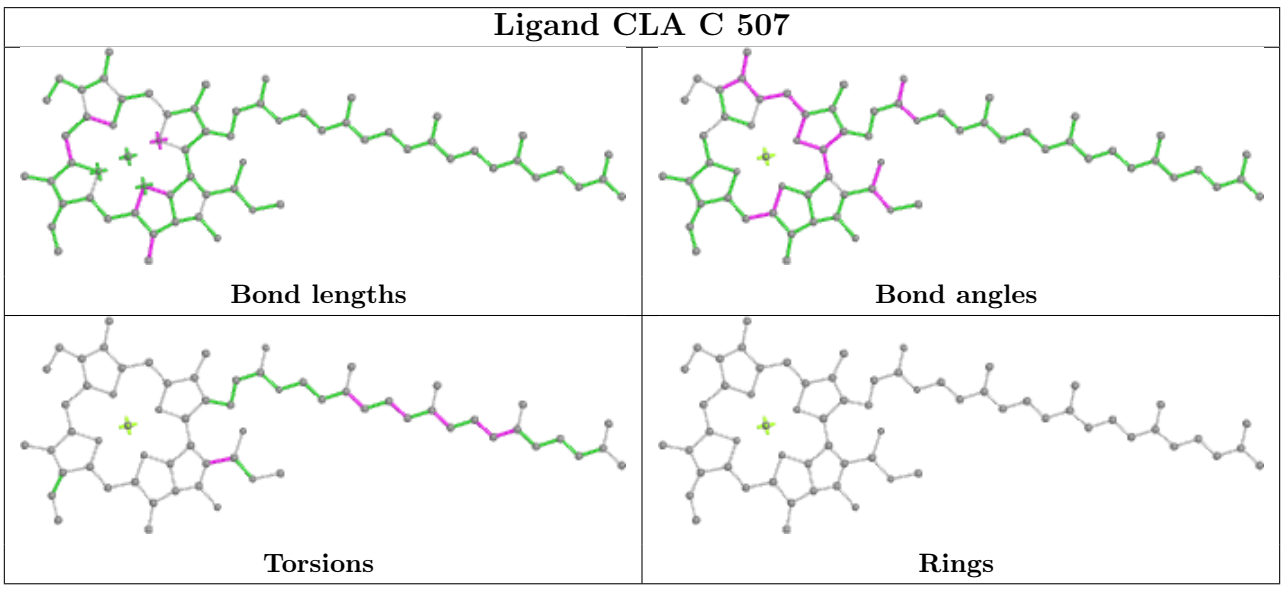
Ligand LMG B 622



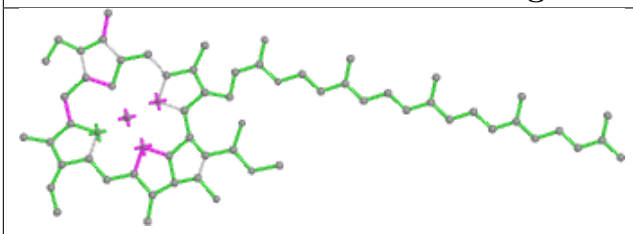
Ligand STE d 411



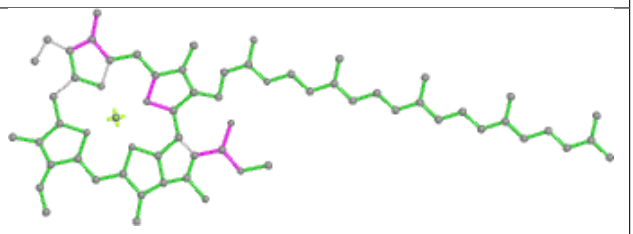
Ligand CLA C 507



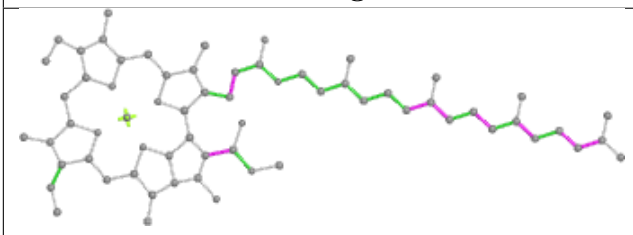
Ligand CLA b 606



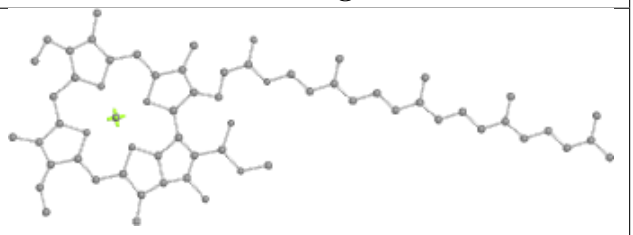
Bond lengths



Bond angles

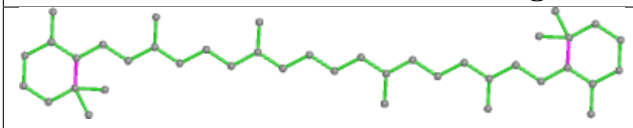


Torsions

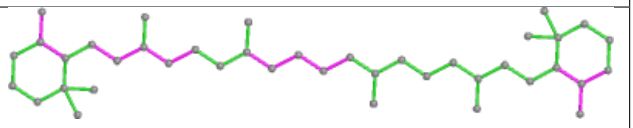


Rings

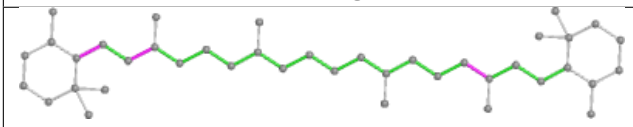
Ligand BCR t 101



Bond lengths



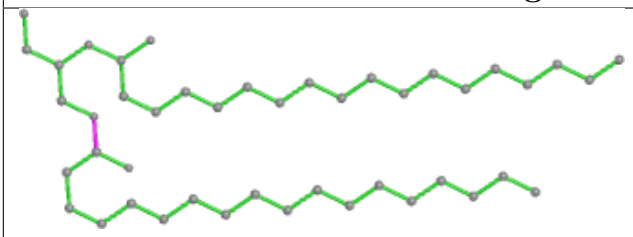
Bond angles



Torsions

Rings

Ligand DGD a 616



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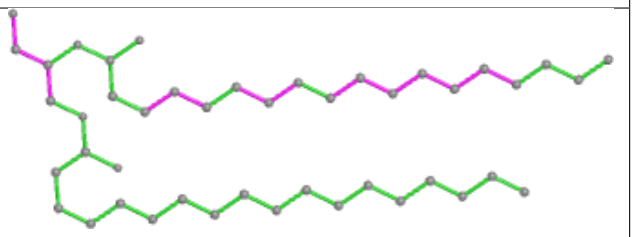

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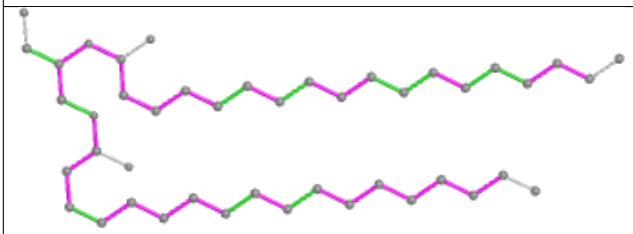
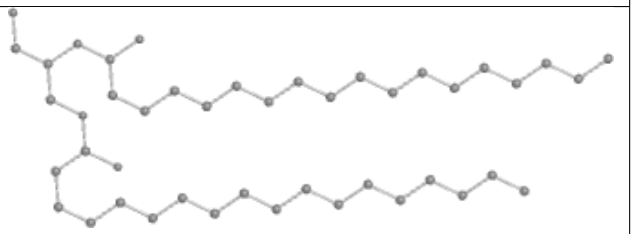
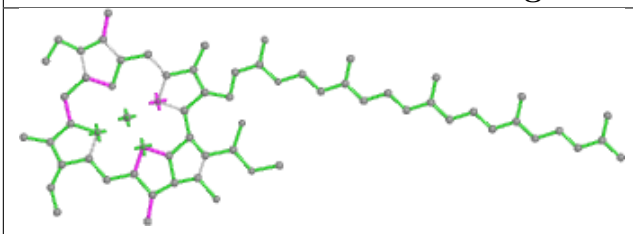


Torsions



Rings

Ligand CLA B 603



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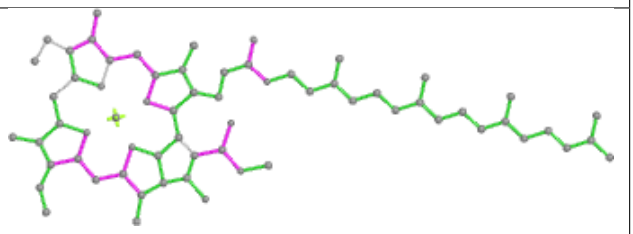

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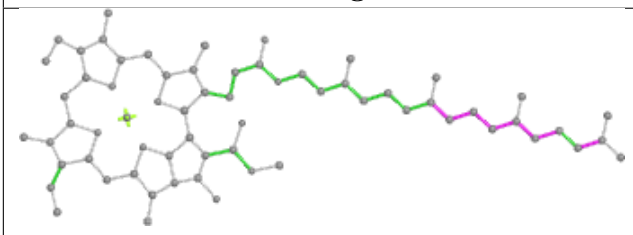

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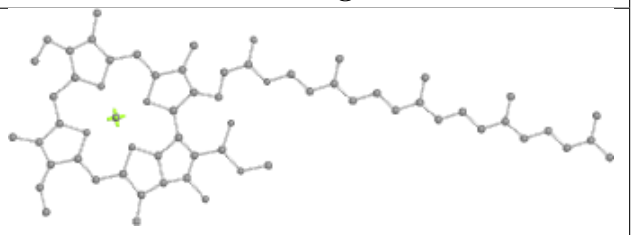
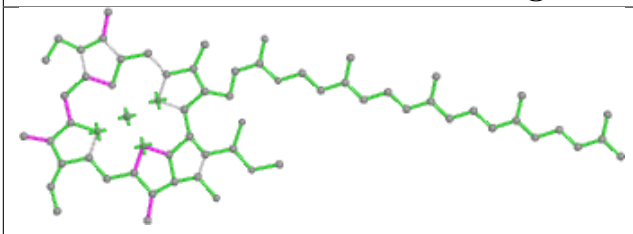


Rings

Ligand CLA b 603



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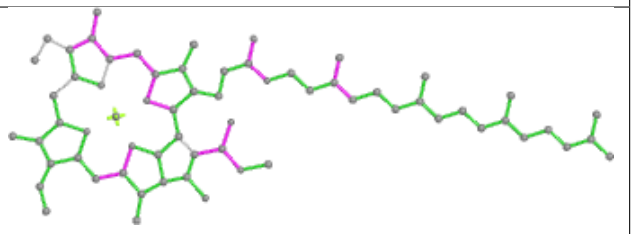

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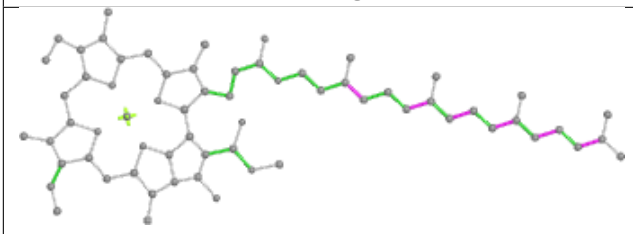

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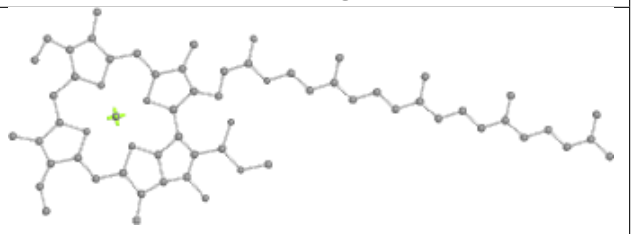
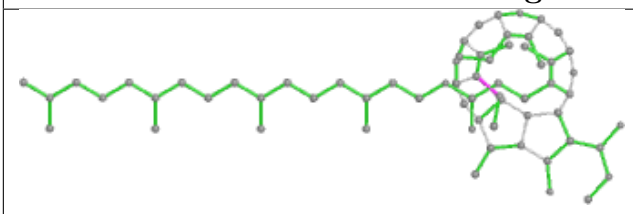


Rings

Ligand PHO d 402



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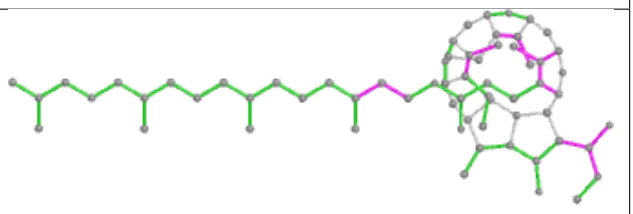
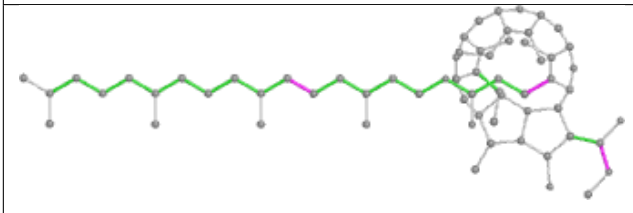


Bond angles



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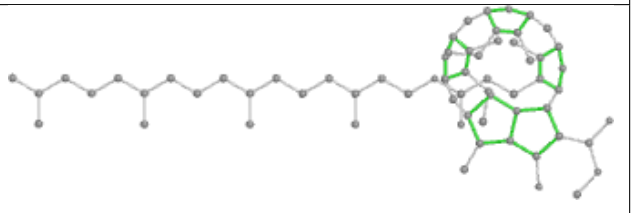
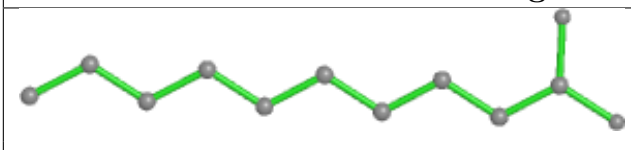


Rings

Ligand STE E 102



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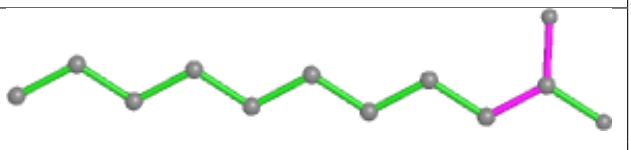
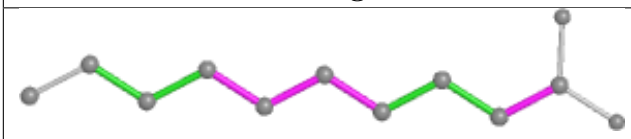


Bond angles



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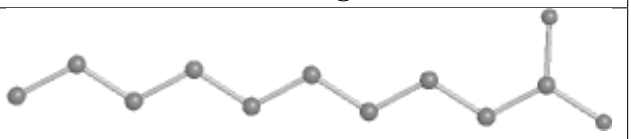
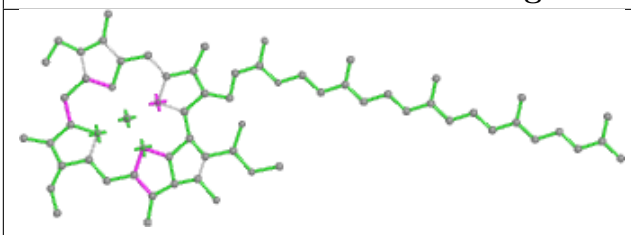


Rings

Ligand CLA C 508



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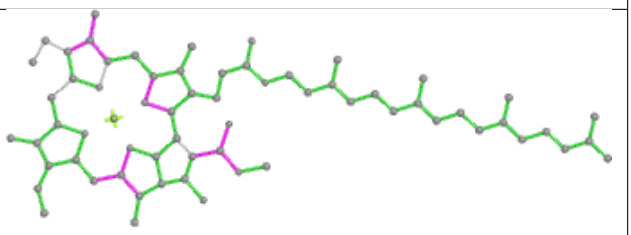
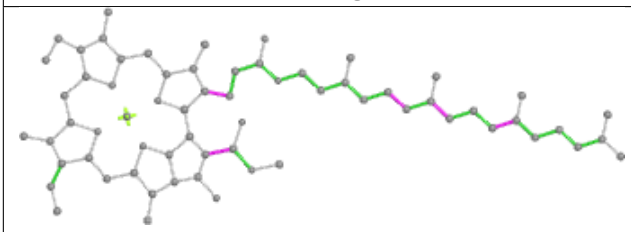


Bond angles



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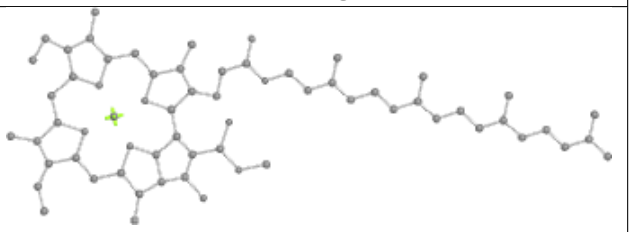
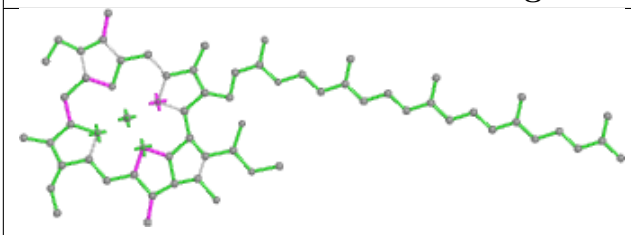


Rings

Ligand CLA C 512



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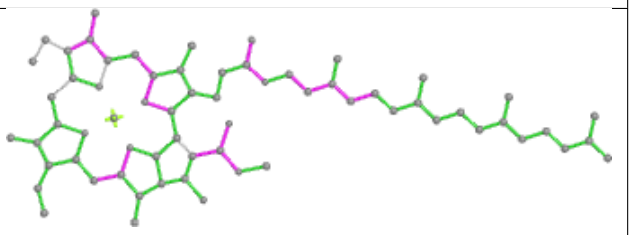
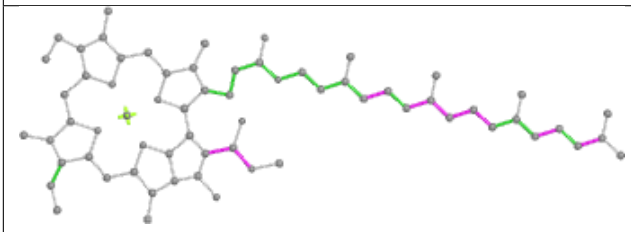


Bond angles



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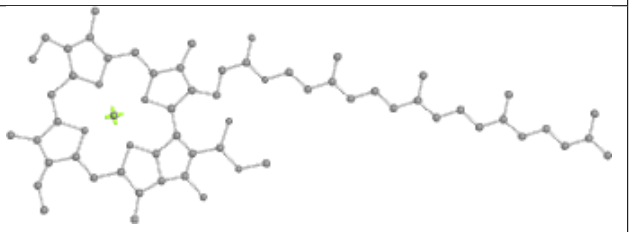
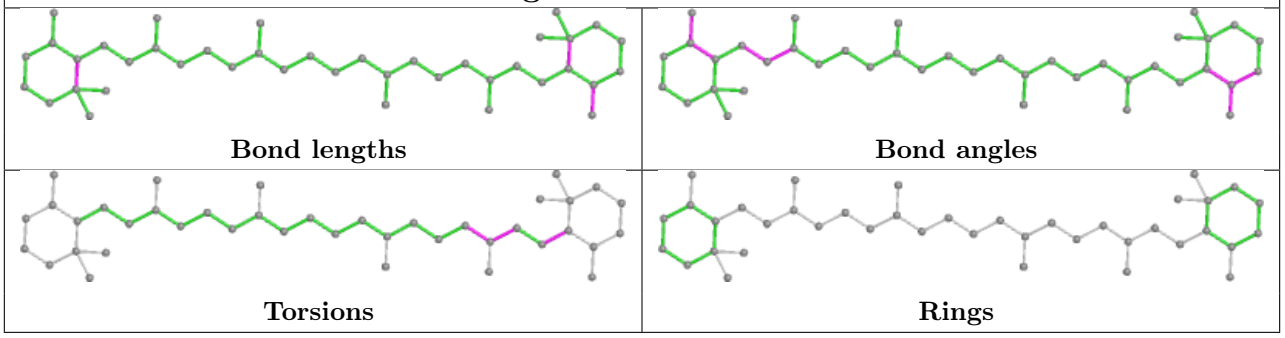
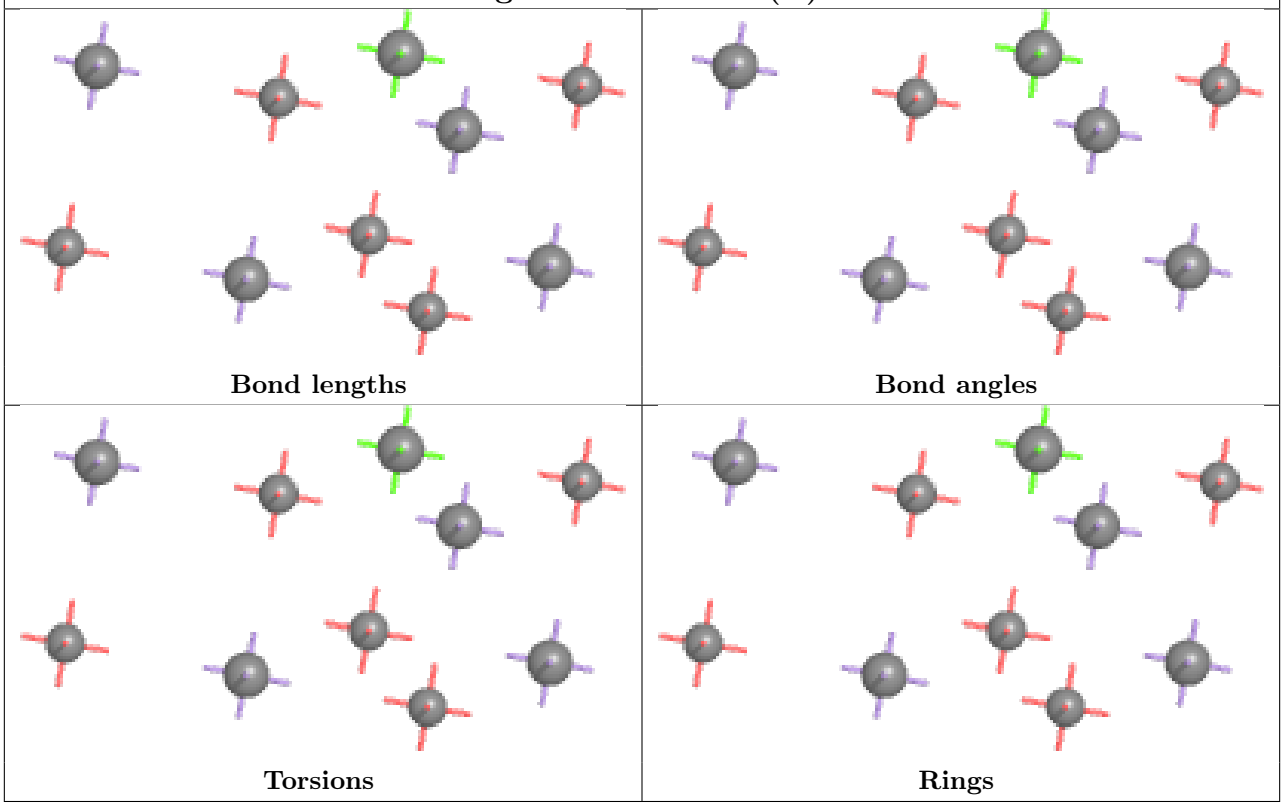


Rings

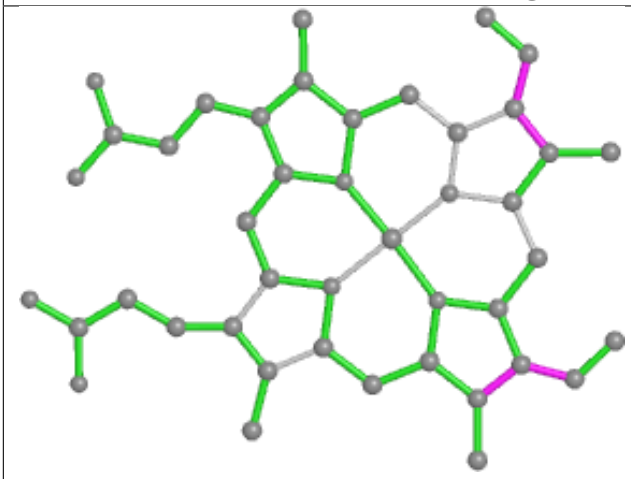
Ligand BCR D 405



Ligand OEX a 601 (B)



Ligand HEM e 101



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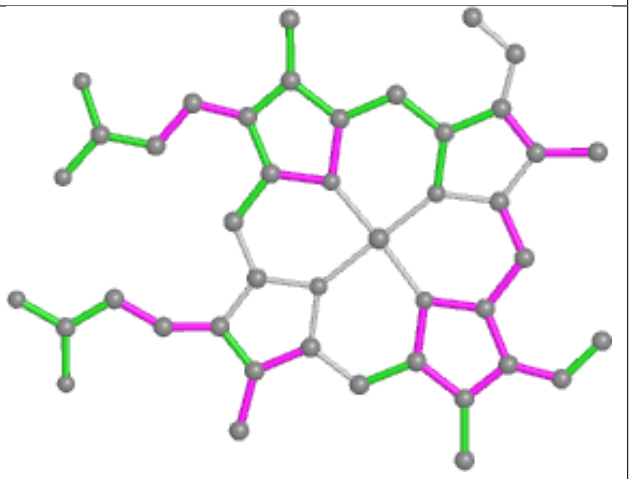
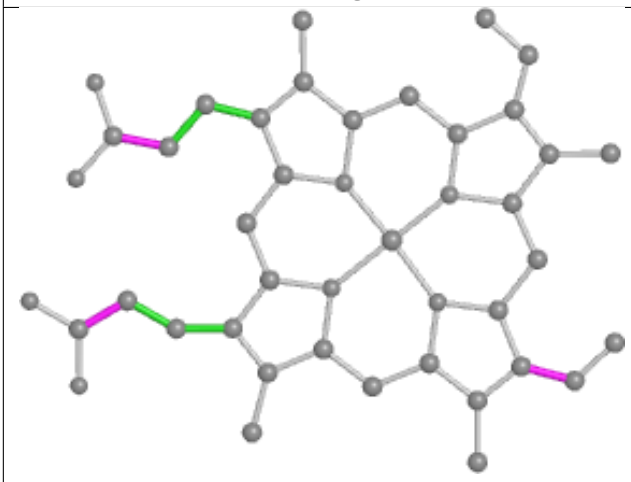


Bond angles



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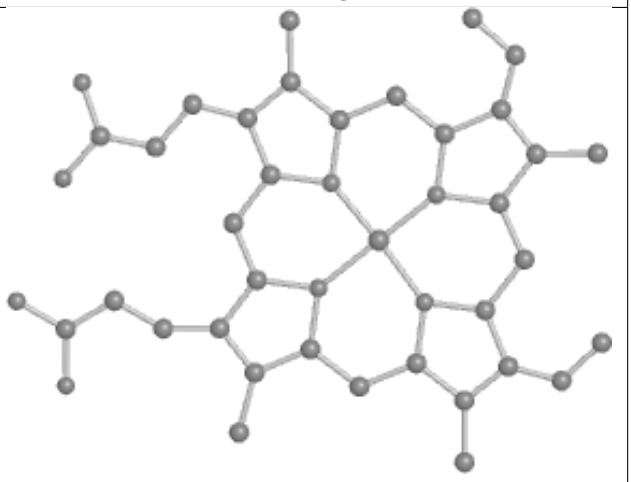
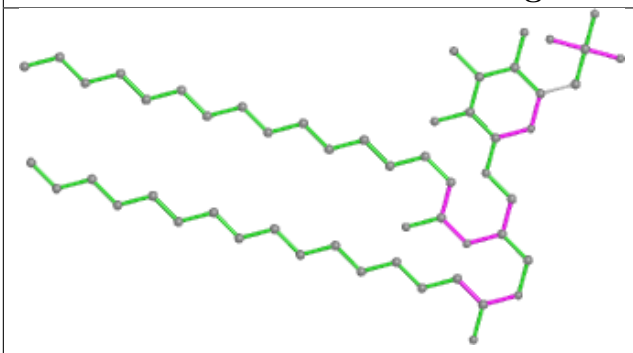


Rings

Ligand SQD B 624



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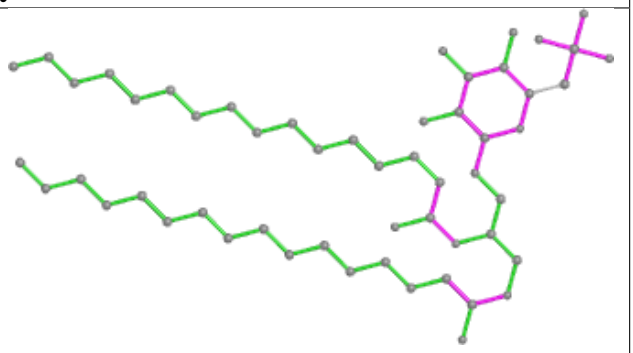
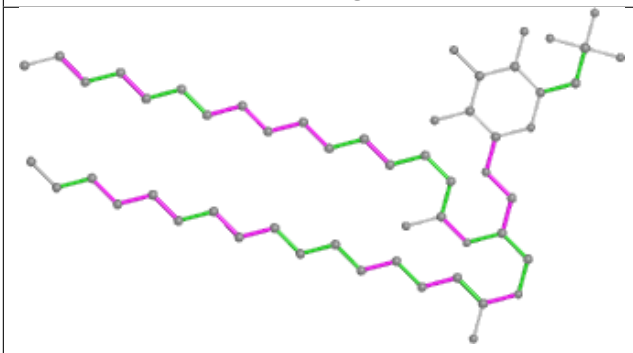


Bond angles



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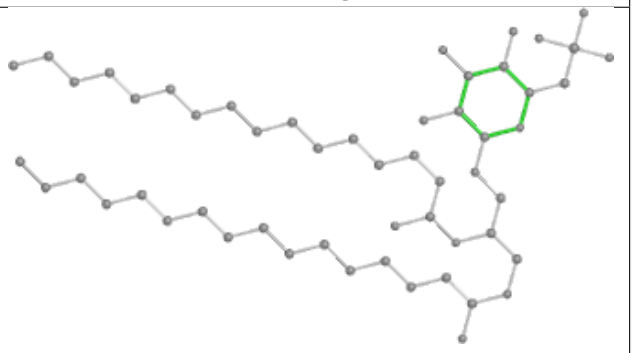
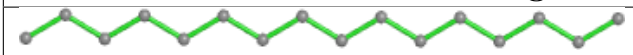


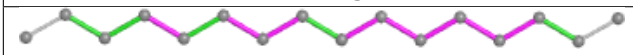
Rings

Ligand STE T 102



Bond lengths

Bond angles



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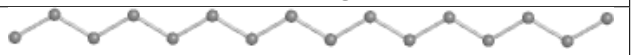
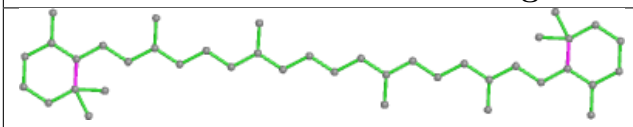


Rings

Ligand BCR K 101



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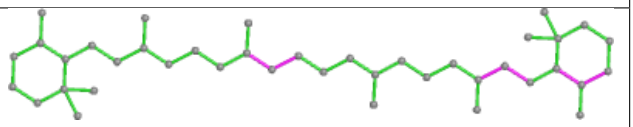
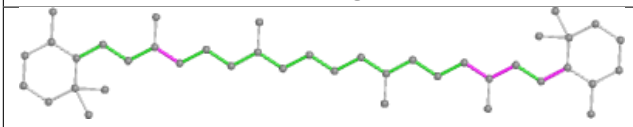


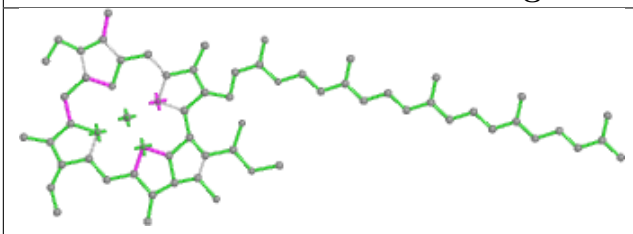
Bond angles



Torsions

Rings

Ligand CLA A 607



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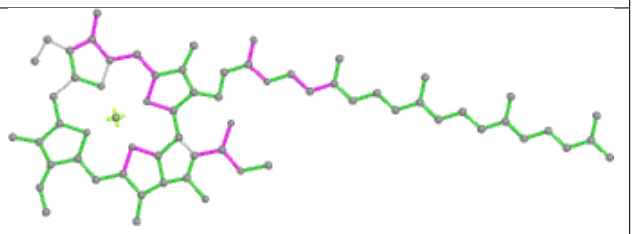
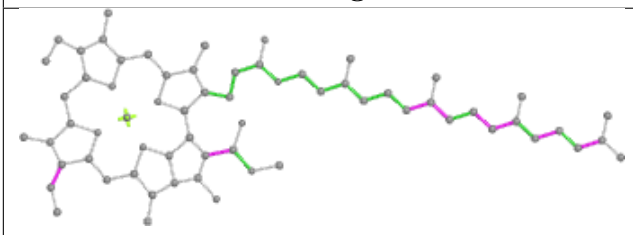
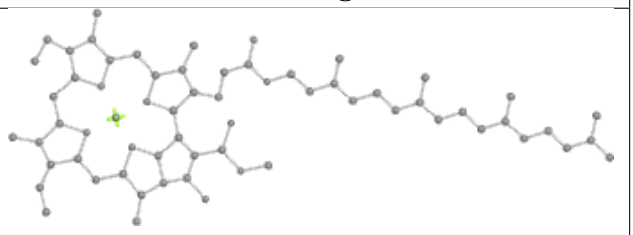


Bond angles

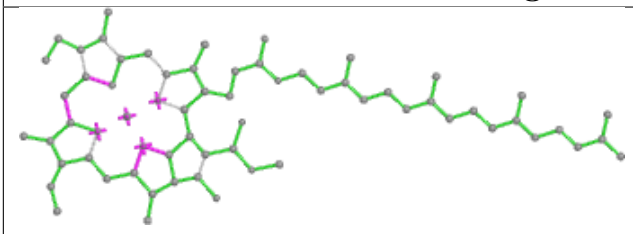


Torsions



Rings

Ligand CLA A 606



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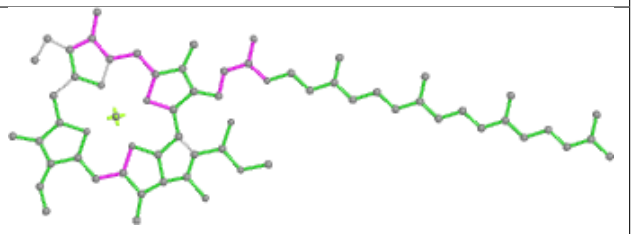
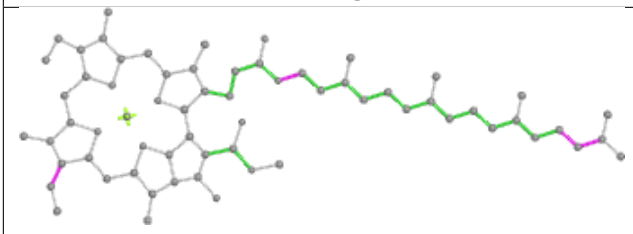
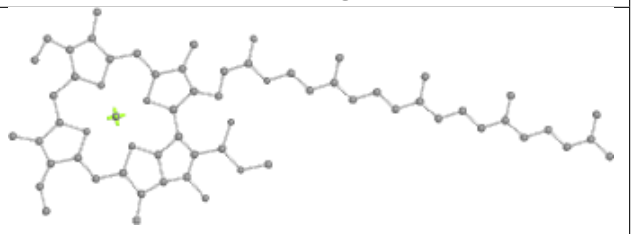


Bond angles

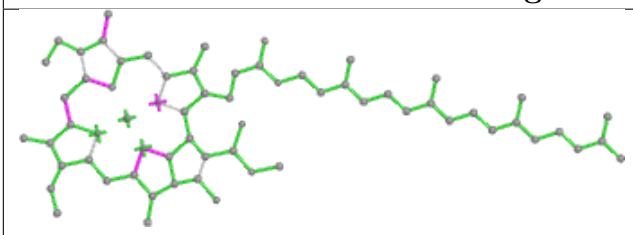


Torsions

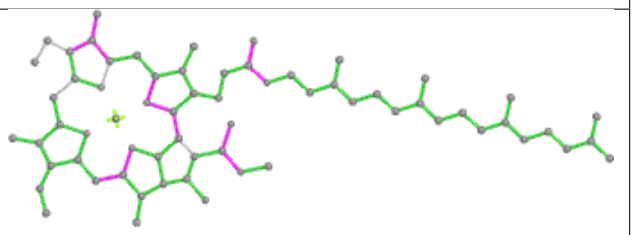


Rings

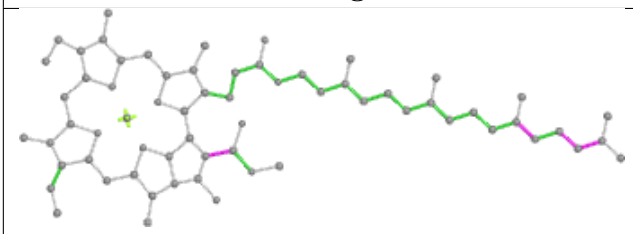
Ligand CLA C 502



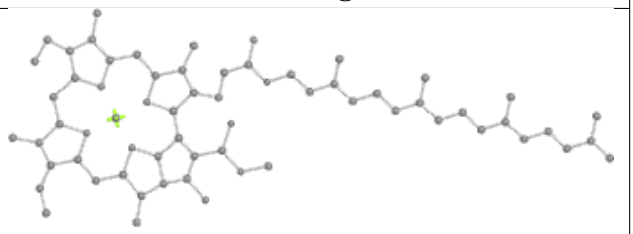
Bond lengths



Bond angles

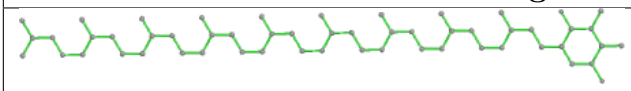


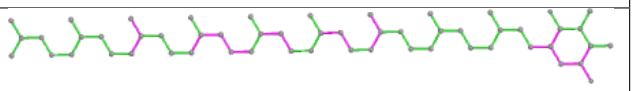
Torsions

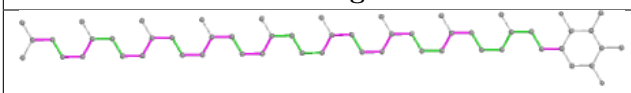


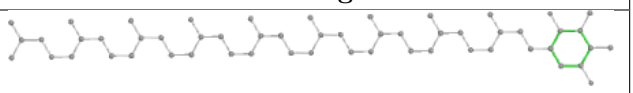
Rings

Ligand PL9 A 611

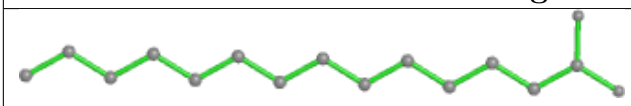

Bond lengths

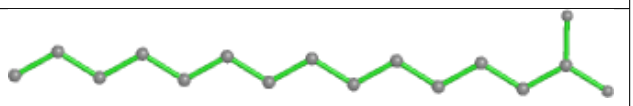

Bond angles

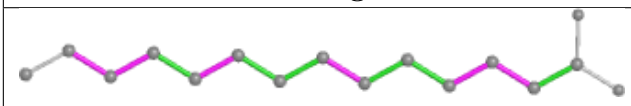

Torsions

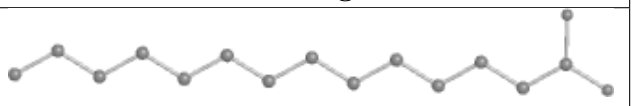

Rings

Ligand STE b 623

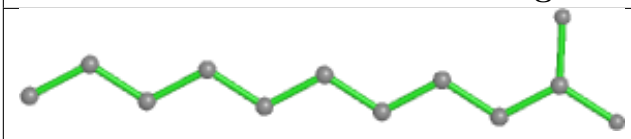

Bond lengths

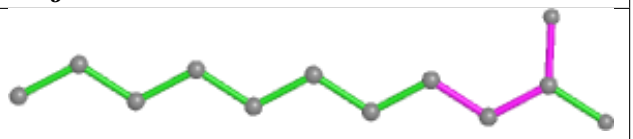

Bond angles

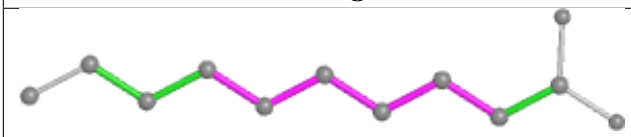

Torsions

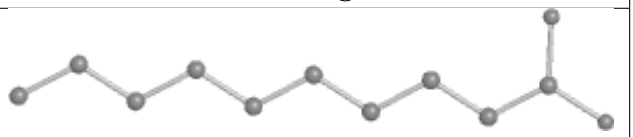

Rings

Ligand STE j 101

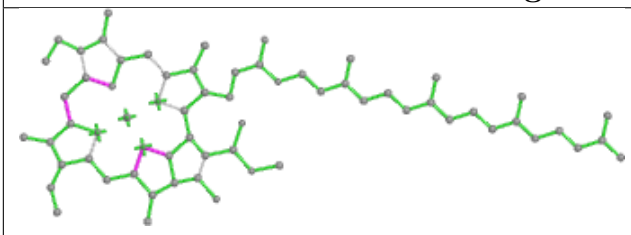

Bond lengths

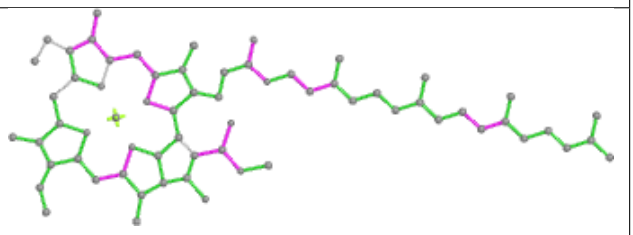

Bond angles

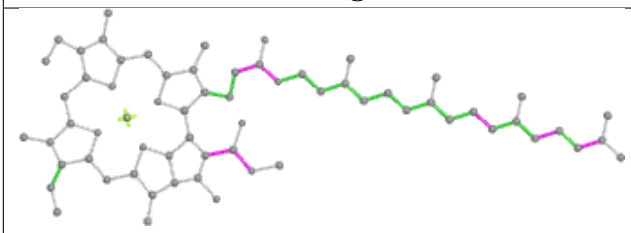

Torsions

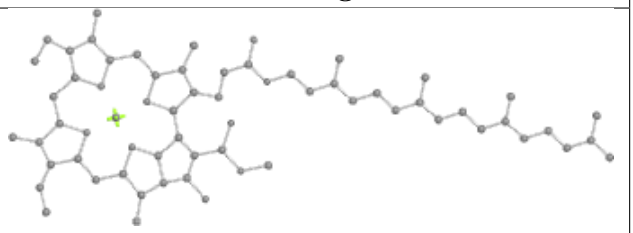

Rings

Ligand CLA B 612

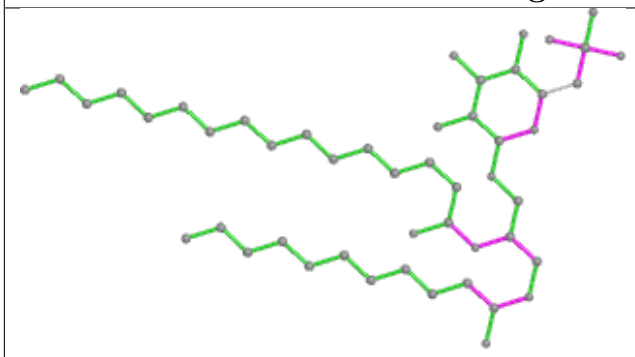

Bond lengths


Bond angles

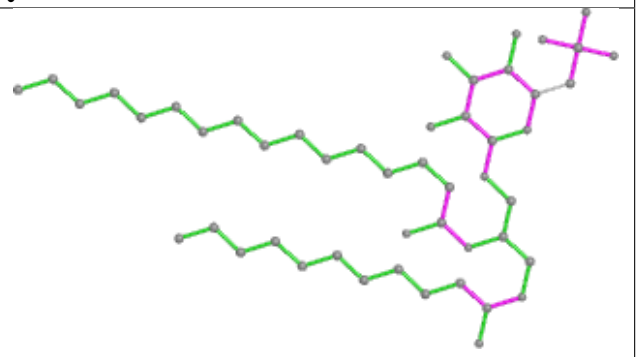

Torsions


Rings

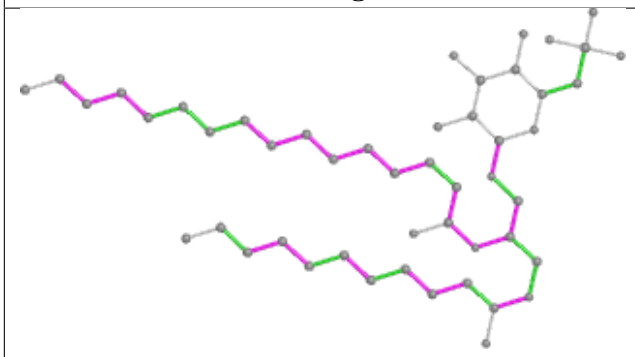
Ligand SQD b 620



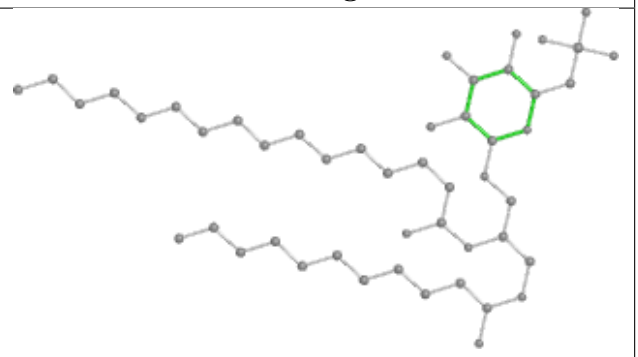
Bond lengths



Bond angles



Torsions

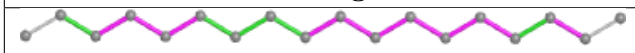


Rings

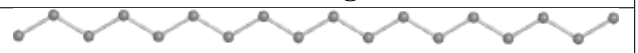
Ligand STE H 103

Bond lengths

Bond angles

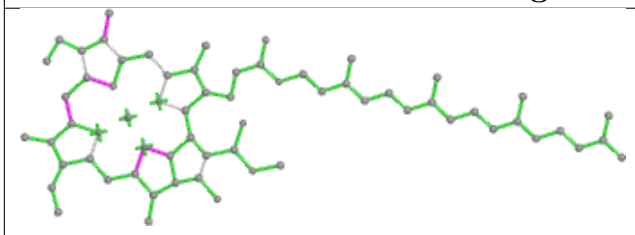


Torsions

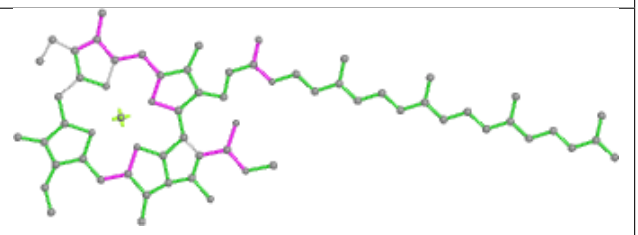


Rings

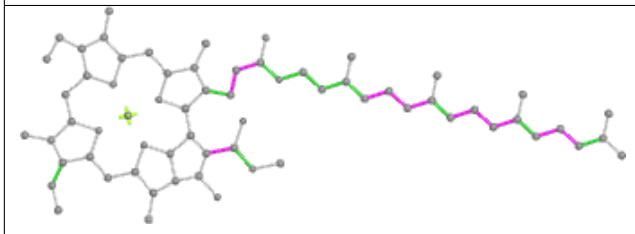
Ligand CLA c 509



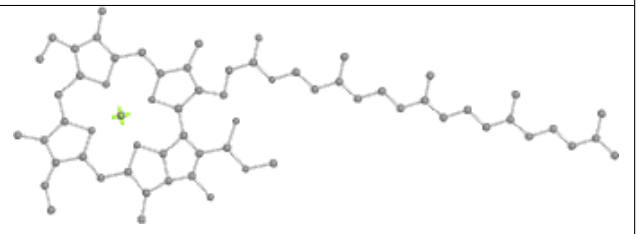
Bond lengths



Bond angles

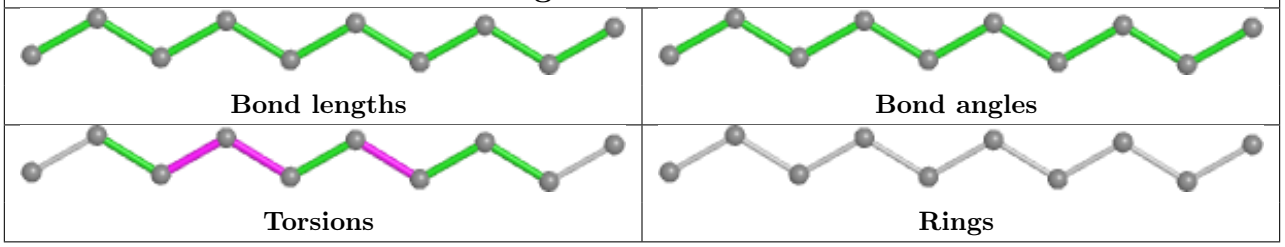


Torsions

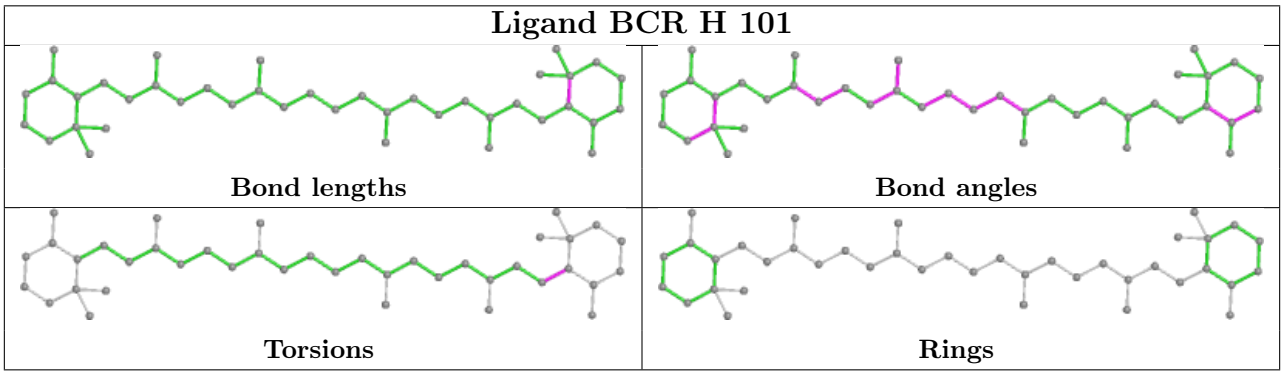


Rings

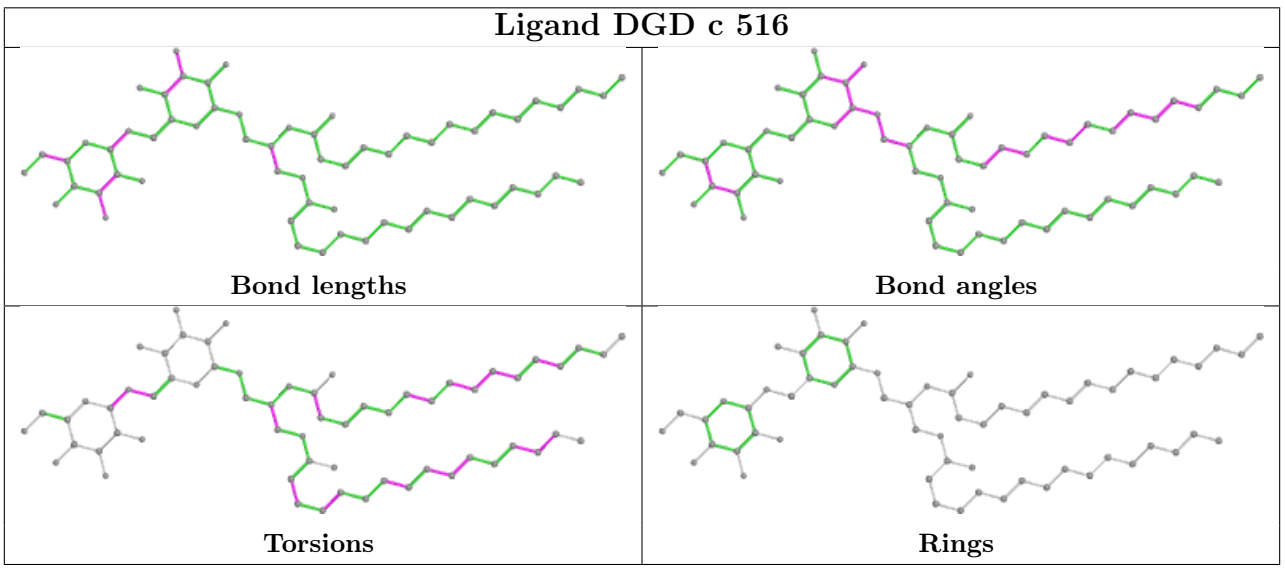
Ligand STE t 102



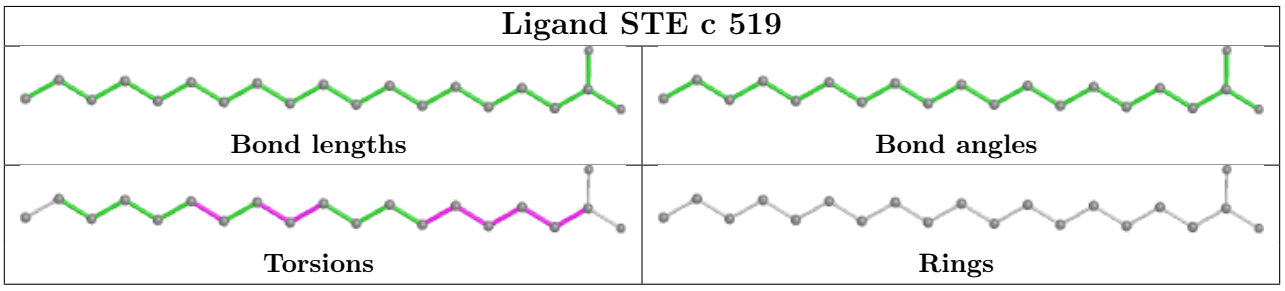
Ligand BCR H 101



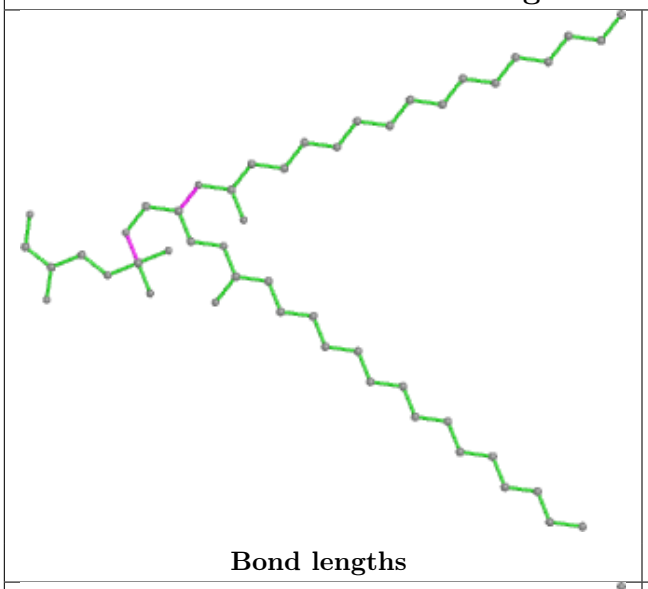
Ligand DGD c 516



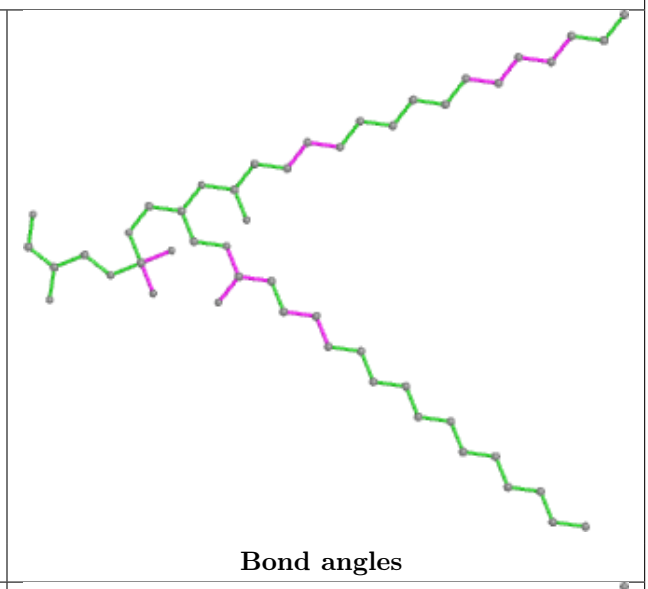
Ligand STE c 519



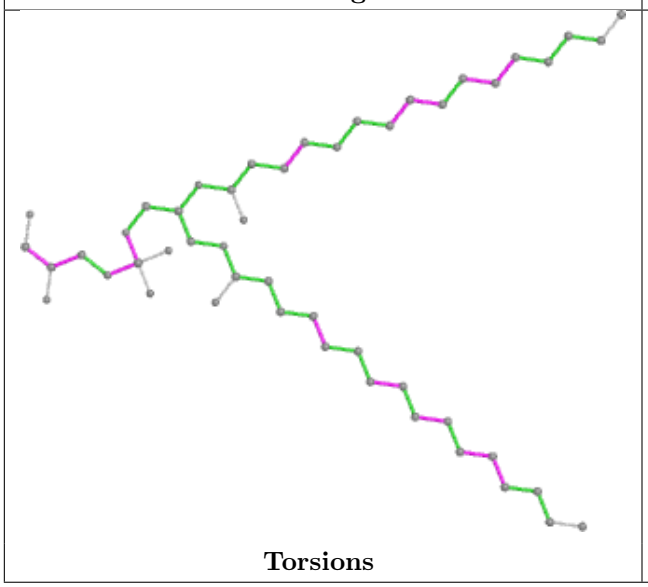
Ligand LHG D 409



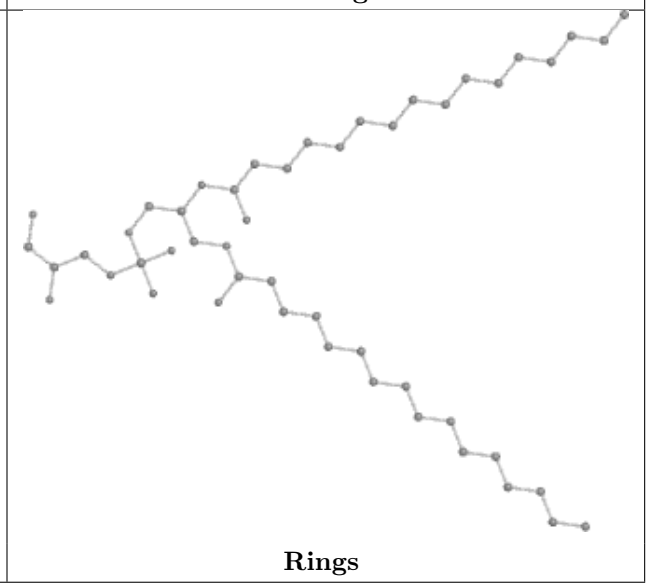
Bond lengths



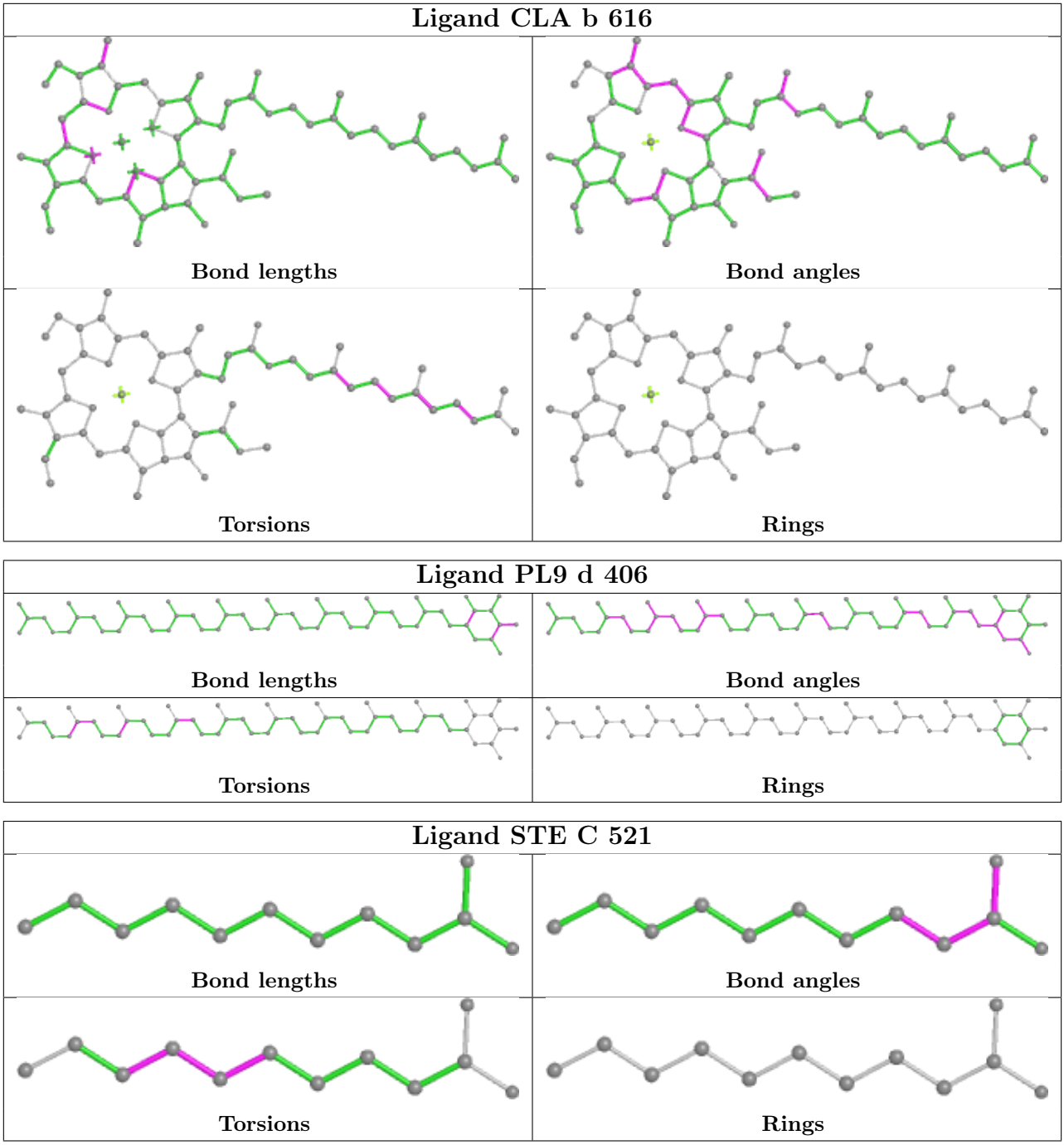
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.46	1 (0%)	94	93	21, 27, 45, 71	0
1	a	334/344 (97%)	-0.44	2 (0%)	89	88	22, 29, 52, 74	0
2	B	505/510 (99%)	-0.33	11 (2%)	62	60	23, 31, 58, 85	0
2	b	505/510 (99%)	-0.27	12 (2%)	59	57	24, 35, 64, 100	0
3	C	442/461 (95%)	-0.40	1 (0%)	95	94	24, 34, 49, 66	0
3	c	451/461 (97%)	-0.30	8 (1%)	68	66	25, 37, 57, 93	0
4	D	341/352 (96%)	-0.48	1 (0%)	94	93	21, 29, 44, 74	0
4	d	341/352 (96%)	-0.37	4 (1%)	79	78	24, 32, 54, 76	0
5	E	82/84 (97%)	0.34	9 (10%)	5	5	32, 48, 70, 85	0
5	e	82/84 (97%)	0.28	6 (7%)	15	14	38, 55, 72, 85	0
6	F	34/45 (75%)	-0.08	2 (5%)	22	21	34, 41, 58, 81	0
6	f	34/45 (75%)	0.15	2 (5%)	22	21	38, 48, 72, 79	0
7	H	65/66 (98%)	-0.15	2 (3%)	49	48	33, 40, 54, 64	0
7	h	63/66 (95%)	0.03	1 (1%)	72	70	37, 48, 59, 63	0
8	I	35/38 (92%)	-0.25	2 (5%)	23	23	31, 38, 62, 78	0
8	i	35/38 (92%)	-0.19	2 (5%)	23	23	31, 38, 66, 76	0
9	J	36/40 (90%)	-0.05	2 (5%)	24	23	33, 47, 68, 84	0
9	j	36/40 (90%)	0.37	3 (8%)	11	10	37, 50, 82, 86	0
10	K	37/46 (80%)	-0.08	2 (5%)	25	24	40, 47, 62, 69	0
10	k	37/46 (80%)	-0.10	1 (2%)	54	53	43, 51, 64, 76	0
11	L	37/37 (100%)	-0.28	1 (2%)	54	53	23, 28, 60, 62	0
11	l	36/37 (97%)	-0.25	2 (5%)	24	23	25, 29, 61, 78	0
12	M	32/36 (88%)	-0.25	1 (3%)	49	48	26, 32, 55, 63	0
12	m	31/36 (86%)	-0.24	0	100	100	27, 32, 51, 61	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	0.06	11 (4%) 33 32	23, 40, 78, 122	0
13	o	244/272 (89%)	-0.04	14 (5%) 23 23	25, 39, 73, 108	0
14	T	29/32 (90%)	-0.32	2 (6%) 16 16	25, 30, 52, 64	0
14	t	29/32 (90%)	-0.22	3 (10%) 6 6	26, 30, 62, 79	0
15	U	97/134 (72%)	-0.13	1 (1%) 82 81	30, 40, 66, 83	0
15	u	97/134 (72%)	-0.17	2 (2%) 63 62	28, 38, 52, 78	0
16	V	137/163 (84%)	-0.38	0 100 100	28, 38, 53, 68	0
16	v	137/163 (84%)	-0.13	3 (2%) 62 60	32, 44, 63, 78	0
17	Y	27/46 (58%)	0.96	6 (22%) 0 0	47, 63, 77, 83	0
17	y	30/46 (65%)	0.62	4 (13%) 3 2	55, 64, 75, 92	0
18	X	38/41 (92%)	0.08	3 (7%) 12 11	41, 48, 66, 71	0
18	x	39/41 (95%)	0.40	5 (12%) 3 3	46, 56, 79, 93	0
19	Z	62/62 (100%)	0.84	13 (20%) 1 0	52, 63, 100, 109	0
19	z	62/62 (100%)	0.64	9 (14%) 2 2	54, 65, 106, 112	0
20	R	34/41 (82%)	1.13	7 (20%) 1 0	56, 63, 72, 78	0
20	r	31/41 (75%)	1.62	13 (41%) 0 0	66, 77, 93, 94	0
All	All	5302/5700 (93%)	-0.20	174 (3%) 46 45	21, 36, 67, 122	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	60	ARG	9.6
13	O	59	LYS	8.2
13	O	3	GLN	7.8
6	F	12	SER	7.1
13	O	62	GLU	6.4
19	z	33	TRP	6.0
19	Z	33	TRP	5.9
5	E	3	GLY	5.9
9	j	6	GLY	5.9
2	b	495	PHE	5.9
13	o	60	ARG	5.8
13	o	3	GLN	5.6
13	o	4	THR	5.6
18	X	2	THR	5.3
2	b	86	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
14	t	30	THR	5.2
13	o	58	ASN	5.2
3	c	23	ALA	5.1
19	Z	4	LEU	5.0
13	O	56	PRO	4.9
20	R	32	GLN	4.9
3	c	24	THR	4.8
20	r	26	TYR	4.8
20	r	28	VAL	4.7
20	R	3	TRP	4.7
13	O	61	GLN	4.6
9	j	5	GLY	4.6
19	Z	62	VAL	4.4
6	F	13	TYR	4.4
13	O	4	THR	4.4
20	r	3	TRP	4.2
19	Z	35	ARG	4.1
2	b	127	ARG	3.9
20	R	6	LEU	3.8
19	z	60	PHE	3.8
2	B	127	ARG	3.7
5	e	61	ARG	3.7
18	X	39	ARG	3.7
15	U	8	GLU	3.7
17	Y	22	LEU	3.7
20	r	32	GLN	3.6
13	o	207	ARG	3.6
19	z	35	ARG	3.6
13	o	56	PRO	3.6
2	b	128	THR	3.5
7	H	66	GLY	3.5
14	T	30	THR	3.5
7	H	65	LEU	3.5
9	J	7	ARG	3.5
13	o	246	ALA	3.4
11	l	2	GLU	3.4
13	o	62	GLU	3.4
18	x	2	THR	3.4
19	Z	42	LEU	3.4
6	f	12	SER	3.4
4	d	227[A]	GLU	3.4
19	Z	1	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	13	LEU	3.4
4	D	12	ARG	3.3
16	v	16	GLY	3.3
17	Y	21	GLN	3.3
5	E	4	THR	3.3
19	Z	32	ASP	3.3
17	Y	40	ALA	3.3
1	a	11	ALA	3.2
5	e	79	PHE	3.2
13	o	89	SER	3.2
4	d	237	PRO	3.2
17	Y	43	ARG	3.1
13	o	61	GLN	3.1
20	r	18	TRP	3.1
2	B	506	ARG	3.0
5	e	84	LYS	3.0
17	Y	25	ILE	3.0
5	E	83	LEU	3.0
20	r	29	LYS	2.9
18	x	38	GLN	2.9
9	j	7	ARG	2.9
2	B	85	GLY	2.8
20	R	21	ARG	2.8
18	X	3	ILE	2.8
19	Z	41	PHE	2.8
8	i	34	ARG	2.8
19	z	41	PHE	2.8
19	z	59	PHE	2.8
5	E	82	GLN	2.8
2	b	505	ARG	2.8
10	k	46	ARG	2.8
20	r	2	ASP	2.7
2	b	506	ARG	2.7
19	Z	7	LEU	2.7
2	b	374	ASN	2.7
2	b	485	GLU	2.7
14	t	29	ILE	2.7
17	y	43	ARG	2.7
11	L	3	PRO	2.7
9	J	5	GLY	2.7
2	B	294	SER	2.7
2	b	494	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
19	Z	60	PHE	2.7
13	O	23	ASP	2.6
19	z	3	ILE	2.6
20	r	25	PRO	2.6
4	d	12	ARG	2.6
17	Y	20	ALA	2.6
7	h	6	TRP	2.6
13	o	35	SER	2.6
3	c	262	ARG	2.6
8	I	36	ASP	2.6
20	R	26	TYR	2.6
17	y	19	ILE	2.6
20	r	14	LEU	2.6
5	E	84	LYS	2.5
19	z	30	PRO	2.5
5	E	61	ARG	2.5
20	R	28	VAL	2.5
20	r	31	VAL	2.5
5	E	81	GLU	2.5
11	l	3	PRO	2.4
2	B	487	SER	2.4
20	r	24	LEU	2.4
2	B	505	ARG	2.4
12	M	33	GLN	2.3
8	I	34	ARG	2.3
13	O	24	ASP	2.3
17	y	40	ALA	2.3
5	E	5	THR	2.3
16	v	106	ASN	2.3
17	y	18	VAL	2.3
19	z	62	VAL	2.3
20	r	13	LEU	2.3
13	o	57	LYS	2.3
3	C	145	SER	2.3
3	c	143	TYR	2.2
19	Z	31	GLN	2.2
13	o	59	LYS	2.2
18	x	3	ILE	2.2
19	Z	34	ASP	2.2
5	e	4	THR	2.2
16	v	17	LYS	2.2
20	R	29	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	c	142	GLU	2.2
3	c	191	PRO	2.2
15	u	70	ARG	2.2
19	z	39	LEU	2.2
20	r	6	LEU	2.2
3	c	25	ASN	2.2
2	B	84	THR	2.2
1	a	311	GLY	2.2
18	x	15	LEU	2.2
3	c	29	GLU	2.2
4	d	14	TRP	2.1
19	Z	37	LYS	2.1
2	B	295	GLY	2.1
6	f	36	ALA	2.1
10	K	44	GLY	2.1
2	B	503	THR	2.1
10	K	46	ARG	2.1
14	t	28	ARG	2.1
15	u	8	GLU	2.1
18	x	40	SER	2.1
2	B	373	LYS	2.1
5	e	60	GLN	2.1
2	b	492	GLU	2.1
2	b	122	LEU	2.1
13	O	184	ARG	2.1
5	E	79	PHE	2.1
14	T	29	ILE	2.0
13	o	63	ALA	2.0
2	B	494	GLY	2.0
2	b	289	GLN	2.0
13	O	57	LYS	2.0
5	e	3	GLY	2.0
8	i	36	ASP	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
12	FME	M	1	10/11	0.88	0.18	36,47,61,62	0
14	FME	t	1	10/11	0.91	0.10	30,33,53,58	0
14	FME	T	1	10/11	0.92	0.13	30,35,53,62	0
12	FME	m	1	10/11	0.93	0.15	31,46,60,64	0
8	FME	I	1	10/11	0.95	0.10	38,44,53,54	0
8	FME	i	1	10/11	0.96	0.14	41,46,49,50	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
32	STE	H	103	18/20	0.69	0.24	55,61,68,71	0
32	STE	b	624	20/20	0.69	0.24	42,54,64,65	0
32	STE	B	621	17/20	0.70	0.21	33,44,61,62	0
33	LHG	E	101	49/49	0.70	0.27	42,70,88,94	0
32	STE	B	628	12/20	0.72	0.25	50,58,67,68	0
32	STE	a	617	12/20	0.72	0.26	55,60,65,66	0
32	STE	B	627	18/20	0.74	0.21	40,49,70,74	0
29	LMG	D	411	33/55	0.74	0.17	38,52,70,74	0
29	LMG	c	520	48/55	0.75	0.24	50,63,77,80	0
32	STE	b	623	16/20	0.75	0.16	53,56,72,73	0
32	STE	B	629	16/20	0.75	0.22	42,55,68,70	0
29	LMG	d	409	23/55	0.75	0.21	44,59,65,67	0
30	SQD	a	615	36/54	0.77	0.16	38,53,64,68	0
32	STE	X	101	20/20	0.77	0.28	35,47,61,70	0
29	LMG	b	622	55/55	0.78	0.26	47,60,69,72	0
31	DGD	a	616	44/66	0.78	0.16	39,50,65,71	0
32	STE	T	103	15/20	0.79	0.20	44,50,65,66	0
28	PL9	a	611	55/55	0.79	0.25	40,60,76,79	0
32	STE	b	621	20/20	0.80	0.20	36,46,66,70	0
32	STE	c	519	20/20	0.80	0.15	39,48,73,74	0
32	STE	c	521	12/20	0.80	0.29	51,62,67,72	0
32	STE	J	101	12/20	0.80	0.15	45,52,57,59	0
32	STE	E	102	12/20	0.81	0.18	58,65,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LHG	e	102	42/49	0.81	0.30	55,75,89,97	0
29	LMG	c	522	49/55	0.83	0.17	38,50,69,76	0
32	STE	C	521	12/20	0.83	0.16	38,42,54,55	0
29	LMG	A	613	48/55	0.83	0.17	38,53,64,69	0
30	SQD	B	624	54/54	0.83	0.17	37,54,77,83	0
25	CLA	b	601	65/65	0.83	0.19	43,60,76,81	0
32	STE	B	626	12/20	0.84	0.17	43,50,55,57	0
28	PL9	A	611	55/55	0.84	0.26	37,57,70,73	0
32	STE	l	102	18/20	0.85	0.18	33,43,60,63	0
31	DGD	A	616	66/66	0.85	0.17	46,55,64,69	0
32	STE	j	101	12/20	0.85	0.15	45,53,57,60	0
30	SQD	A	615	39/54	0.86	0.16	42,51,72,78	0
32	STE	I	101	15/20	0.86	0.15	41,50,61,61	0
29	LMG	B	622	28/55	0.86	0.14	39,49,57,63	0
25	CLA	c	512	65/65	0.86	0.16	42,51,72,74	0
29	LMG	B	620	51/55	0.86	0.14	31,47,57,60	0
32	STE	B	625	14/20	0.87	0.12	39,43,52,55	0
25	CLA	C	513	65/65	0.87	0.17	41,49,71,74	0
25	CLA	c	513	65/65	0.87	0.18	42,52,83,86	0
32	STE	T	102	16/20	0.87	0.13	37,44,53,55	0
30	SQD	b	620	49/54	0.87	0.17	35,51,73,77	0
25	CLA	C	512	65/65	0.87	0.17	38,45,70,82	0
32	STE	t	102	10/20	0.87	0.14	44,55,62,65	0
29	LMG	D	407	51/55	0.87	0.17	28,44,67,69	0
25	CLA	b	616	60/65	0.87	0.15	26,37,78,82	0
27	BCR	d	405	40/40	0.88	0.16	38,46,72,72	0
32	STE	M	101	15/20	0.88	0.15	34,43,54,57	0
29	LMG	c	518	37/55	0.88	0.17	40,55,66,66	0
27	BCR	D	405	40/40	0.88	0.13	31,39,67,71	0
32	STE	d	411	17/20	0.89	0.13	45,50,60,61	0
32	STE	d	412	20/20	0.89	0.17	41,53,59,60	0
29	LMG	m	101	51/55	0.89	0.13	37,48,58,60	0
30	SQD	f	101	41/54	0.89	0.17	57,70,83,85	0
32	STE	m	102	12/20	0.89	0.14	48,54,60,63	0
25	CLA	B	601	65/65	0.89	0.16	37,53,73,86	0
29	LMG	C	520	48/55	0.89	0.17	39,57,65,70	0
27	BCR	k	101	40/40	0.89	0.14	41,51,55,57	0
25	CLA	B	616	60/65	0.90	0.15	24,32,71,76	0
31	DGD	H	102	62/66	0.90	0.13	29,40,49,53	0
32	STE	C	522	12/20	0.90	0.14	45,52,60,61	0
25	CLA	c	506	65/65	0.90	0.14	32,40,77,79	0
29	LMG	d	410	44/55	0.90	0.15	36,44,65,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	BCR	K	101	40/40	0.91	0.15	35,42,55,57	0
25	CLA	C	506	65/65	0.91	0.12	29,37,61,65	0
25	CLA	D	404	65/65	0.91	0.15	26,32,76,85	0
31	DGD	h	101	62/66	0.91	0.12	31,43,49,55	0
32	STE	C	523	16/20	0.91	0.11	37,47,54,55	0
30	SQD	D	408	36/54	0.91	0.16	43,61,66,70	0
27	BCR	x	101	40/40	0.91	0.13	38,48,62,64	0
27	BCR	C	516	40/40	0.91	0.11	39,48,55,57	0
25	CLA	a	609	65/65	0.91	0.16	21,28,62,66	0
31	DGD	c	516	62/66	0.92	0.10	32,44,69,73	0
25	CLA	d	404	65/65	0.92	0.14	30,40,72,76	0
30	SQD	a	614	54/54	0.92	0.16	38,54,66,69	0
31	DGD	C	518	62/66	0.92	0.12	30,41,77,86	0
32	STE	M	102	10/20	0.92	0.13	42,45,48,49	0
32	STE	b	625	10/20	0.92	0.14	46,52,56,61	0
27	BCR	k	102	40/40	0.92	0.11	41,51,56,62	0
27	BCR	k	103	40/40	0.92	0.15	41,47,54,57	0
27	BCR	A	610	40/40	0.93	0.11	23,31,39,40	0
27	BCR	C	514	40/40	0.93	0.12	41,49,54,55	0
25	CLA	b	606	65/65	0.93	0.12	28,34,61,68	0
25	CLA	c	508	64/65	0.93	0.11	30,38,71,85	0
27	BCR	H	101	40/40	0.93	0.11	33,43,55,57	0
25	CLA	b	609	65/65	0.93	0.14	28,40,55,65	0
27	BCR	b	618	40/40	0.93	0.11	25,36,46,47	0
27	BCR	c	514	40/40	0.93	0.12	26,40,50,52	0
30	SQD	A	614	52/54	0.93	0.14	31,46,68,75	0
25	CLA	b	614	65/65	0.93	0.12	22,33,56,66	0
25	CLA	B	606	65/65	0.93	0.11	25,32,55,63	0
25	CLA	A	609	54/65	0.94	0.13	20,25,57,61	0
31	DGD	c	515	62/66	0.94	0.11	23,35,57,67	0
25	CLA	b	610	65/65	0.94	0.12	24,33,40,42	0
31	DGD	c	517	62/66	0.94	0.12	27,42,64,68	0
27	BCR	B	619	40/40	0.94	0.10	28,37,49,52	0
25	CLA	B	609	65/65	0.94	0.12	24,33,44,49	0
25	CLA	b	615	65/65	0.94	0.12	26,35,47,53	0
28	PL9	d	406	55/55	0.94	0.10	24,30,35,39	0
25	CLA	A	607	65/65	0.94	0.10	22,29,78,81	0
25	CLA	c	502	65/65	0.94	0.10	28,34,45,49	0
25	CLA	c	503	65/65	0.94	0.10	34,38,44,50	0
27	BCR	b	617	40/40	0.94	0.10	28,36,44,47	0
25	CLA	a	607	65/65	0.94	0.11	27,33,71,74	0
27	BCR	b	619	40/40	0.94	0.11	30,41,55,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	B	604	65/65	0.94	0.11	21,26,56,61	0
31	DGD	C	517	62/66	0.94	0.11	23,34,67,72	0
25	CLA	C	508	65/65	0.94	0.12	27,33,74,81	0
33	LHG	D	412	49/49	0.94	0.12	30,38,56,56	0
31	DGD	C	519	62/66	0.94	0.11	29,37,65,68	0
25	CLA	C	511	65/65	0.94	0.11	33,42,51,54	0
25	CLA	c	505	65/65	0.95	0.10	31,35,55,65	0
25	CLA	B	610	65/65	0.95	0.10	21,27,35,37	0
25	CLA	c	507	65/65	0.95	0.12	26,36,48,51	0
25	CLA	b	602	65/65	0.95	0.11	29,36,50,53	0
25	CLA	c	509	65/65	0.95	0.10	32,38,51,56	0
25	CLA	c	510	65/65	0.95	0.10	29,39,50,54	0
25	CLA	c	511	65/65	0.95	0.11	37,46,56,62	0
25	CLA	b	604	65/65	0.95	0.12	22,28,59,72	0
25	CLA	C	510	65/65	0.95	0.09	30,38,48,51	0
25	CLA	d	403	65/65	0.95	0.10	22,28,49,54	0
25	CLA	b	608	65/65	0.95	0.09	30,36,49,55	0
26	PHO	d	402	64/64	0.95	0.10	27,35,40,43	0
25	CLA	B	614	65/65	0.95	0.11	22,32,55,63	0
27	BCR	B	617	40/40	0.95	0.10	27,34,42,44	0
27	BCR	B	618	40/40	0.95	0.08	24,35,42,45	0
25	CLA	B	607	65/65	0.95	0.11	19,27,52,54	0
25	CLA	b	612	65/65	0.95	0.09	23,29,41,48	0
27	BCR	C	515	40/40	0.95	0.10	28,37,45,50	0
25	CLA	C	502	65/65	0.95	0.09	27,32,44,48	0
25	CLA	C	505	65/65	0.95	0.10	25,34,51,60	0
25	CLA	a	606	65/65	0.95	0.10	18,26,37,46	0
25	CLA	c	501	65/65	0.95	0.10	28,35,42,47	0
33	LHG	D	410	47/49	0.95	0.12	27,39,70,76	0
27	BCR	T	101	40/40	0.95	0.08	28,33,43,46	0
25	CLA	B	602	65/65	0.95	0.11	24,32,46,50	0
33	LHG	a	613	49/49	0.95	0.10	34,44,57,62	0
25	CLA	C	507	65/65	0.95	0.12	25,33,46,48	0
33	LHG	l	101	49/49	0.95	0.10	29,39,46,54	0
34	BCT	d	401	4/4	0.95	0.13	32,38,41,47	0
28	PL9	D	406	55/55	0.96	0.09	22,28,37,38	0
25	CLA	B	603	65/65	0.96	0.10	20,28,50,52	0
25	CLA	C	501	65/65	0.96	0.10	26,32,41,47	0
25	CLA	B	608	65/65	0.96	0.10	22,29,47,54	0
25	CLA	C	503	65/65	0.96	0.09	30,37,41,49	0
25	CLA	C	504	59/65	0.96	0.09	28,34,60,63	0
25	CLA	a	612	65/65	0.96	0.08	21,27,39,44	0

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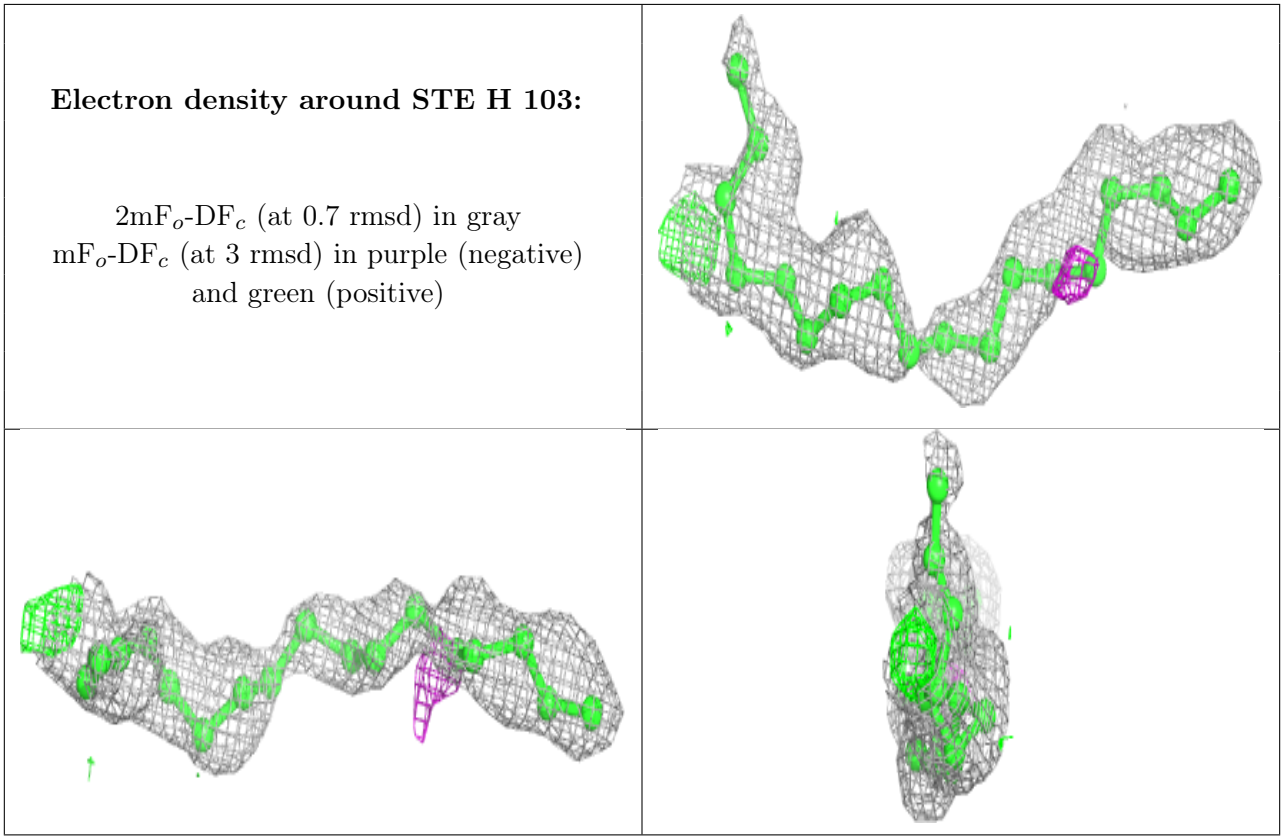
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	c	504	60/65	0.96	0.09	28,38,64,66	0
25	CLA	A	606	65/65	0.96	0.09	18,24,39,43	0
25	CLA	B	605	65/65	0.96	0.11	20,27,37,41	0
25	CLA	b	603	65/65	0.96	0.10	23,30,55,63	0
25	CLA	B	611	65/65	0.96	0.10	19,26,40,44	0
27	BCR	a	610	40/40	0.96	0.08	23,31,40,42	0
25	CLA	b	605	65/65	0.96	0.09	22,29,39,45	0
25	CLA	B	612	65/65	0.96	0.09	20,27,36,41	0
25	CLA	b	607	65/65	0.96	0.10	23,30,56,61	0
25	CLA	C	509	65/65	0.96	0.10	26,35,50,54	0
33	LHG	B	623	49/49	0.96	0.12	27,35,44,51	0
33	LHG	D	409	49/49	0.96	0.11	26,34,42,46	0
25	CLA	B	613	65/65	0.96	0.10	19,25,55,64	0
25	CLA	A	612	65/65	0.96	0.10	18,24,38,48	0
25	CLA	B	615	65/65	0.96	0.09	23,30,48,58	0
26	PHO	D	402	64/64	0.96	0.09	22,29,34,39	0
33	LHG	d	407	49/49	0.96	0.11	29,37,46,53	0
33	LHG	d	408	39/49	0.96	0.10	31,39,57,58	0
27	BCR	t	101	40/40	0.96	0.08	26,33,44,47	0
26	PHO	a	608	64/64	0.96	0.09	19,27,32,40	0
25	CLA	b	613	65/65	0.96	0.09	21,28,59,61	0
35	HEM	F	101	43/43	0.96	0.14	39,44,53,58	0
35	HEM	e	101	43/43	0.96	0.13	45,53,66,78	0
34	BCT	D	401	4/4	0.97	0.13	29,29,31,34	0
26	PHO	A	608	64/64	0.97	0.08	20,25,30,35	0
25	CLA	D	403	65/65	0.97	0.09	18,24,44,52	0
25	CLA	b	611	65/65	0.97	0.09	23,29,44,50	0
36	HEC	V	201	43/43	0.97	0.12	24,29,37,44	0
36	HEC	v	201	43/43	0.98	0.11	27,33,36,41	0
24	CL	A	605	1/1	0.99	0.04	27,27,27,27	0
24	CL	a	604	1/1	0.99	0.08	26,26,26,26	0
21	OEX	A	601[B]	10/10	0.99	0.10	24,28,32,32	10
21	OEX	A	601[C]	10/10	0.99	0.10	18,22,26,27	10
21	OEX	a	601[B]	10/10	0.99	0.08	25,29,31,31	10
21	OEX	a	601[C]	10/10	0.99	0.08	17,24,26,28	10
22	OEY	A	602[A]	11/11	0.99	0.09	25,28,31,31	11
22	OEY	a	602[A]	11/11	0.99	0.08	27,29,33,33	11
23	FE2	a	603	1/1	0.99	0.05	33,33,33,33	0
24	CL	A	604	1/1	0.99	0.04	27,27,27,27	0
23	FE2	A	603	1/1	1.00	0.02	26,26,26,26	0
24	CL	a	605	1/1	1.00	0.08	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.

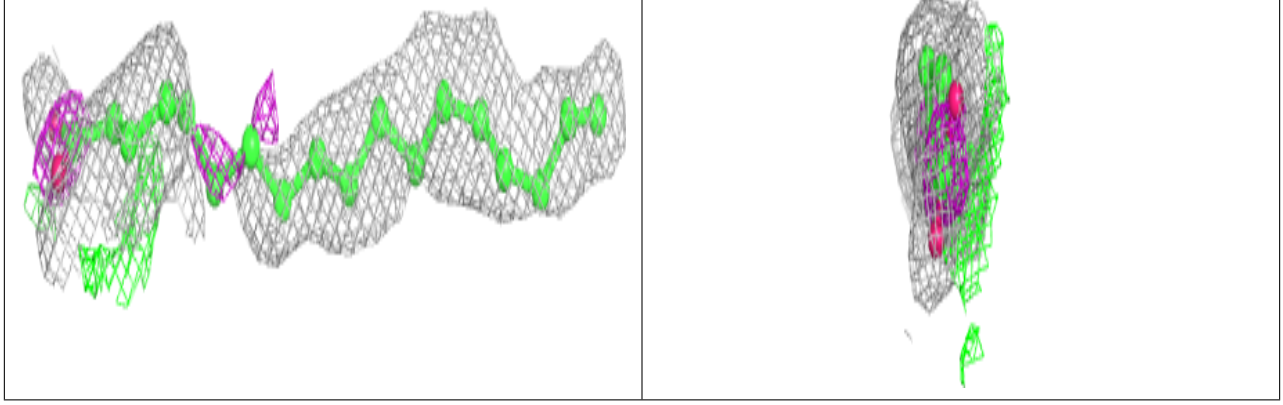
Electron density around STE H 103:

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



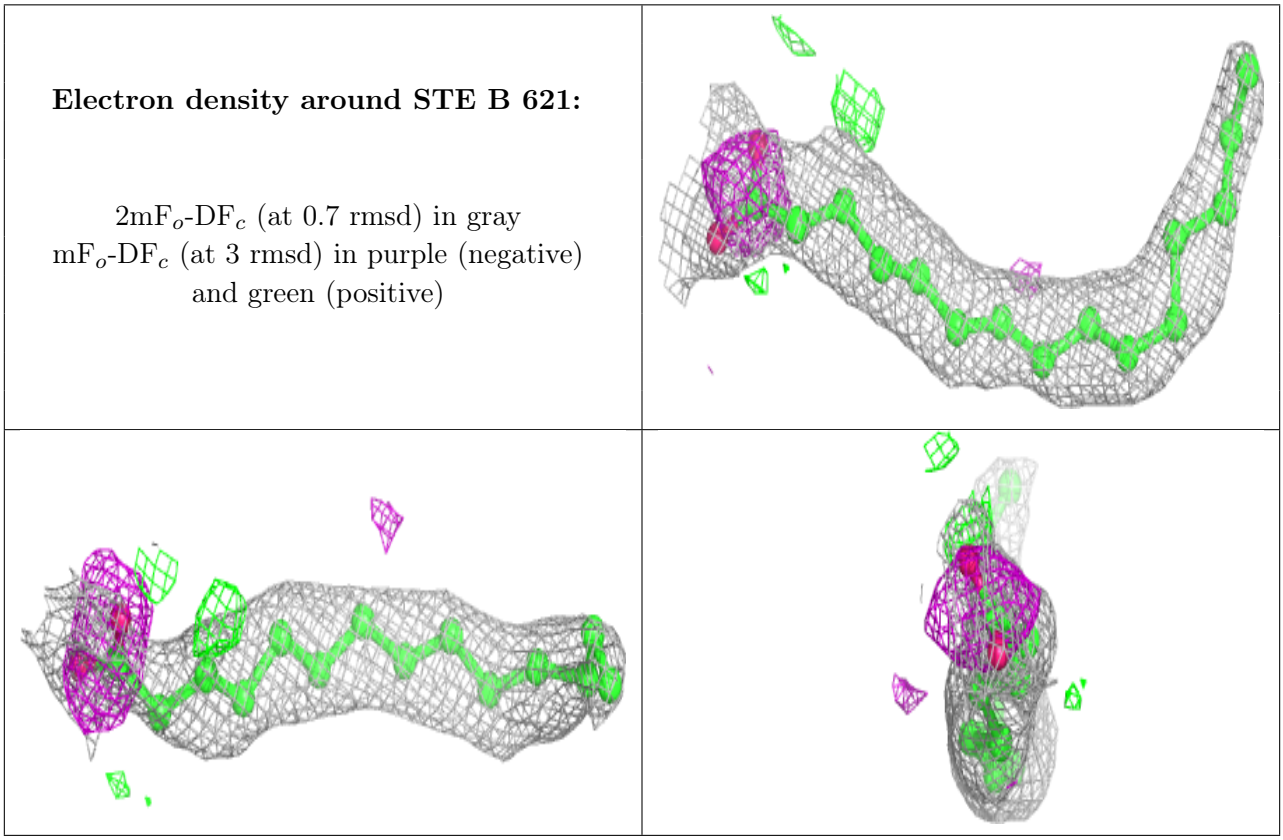
Electron density around STE b 624:

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



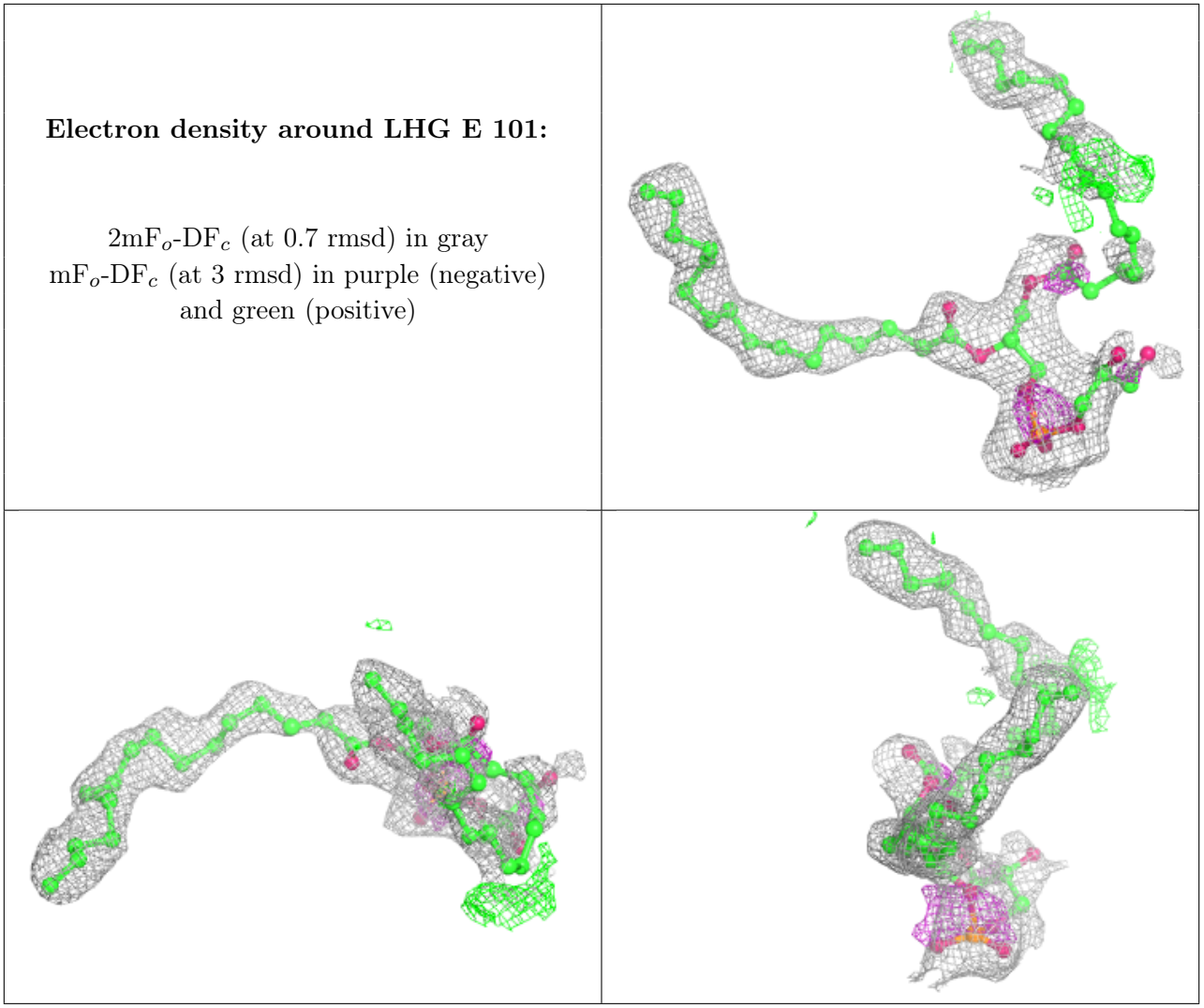
Electron density around STE B 621:

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



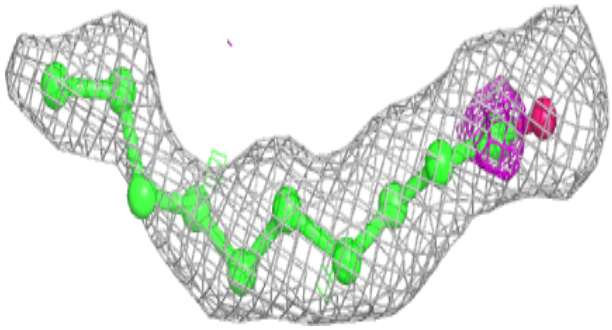
Electron density around LHG E 101:

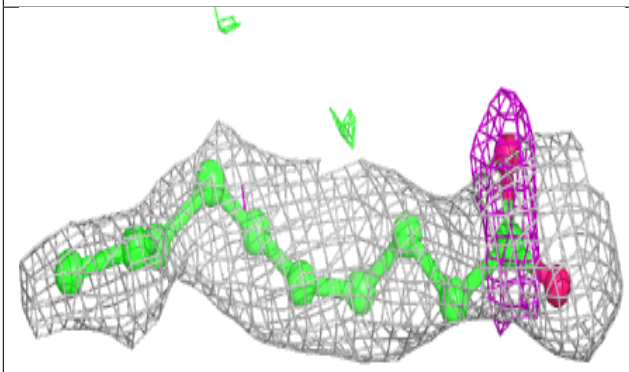
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

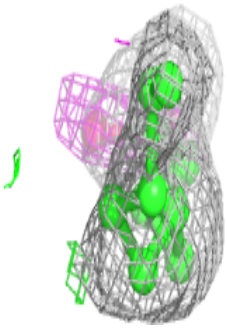


Electron density around STE B 628:

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

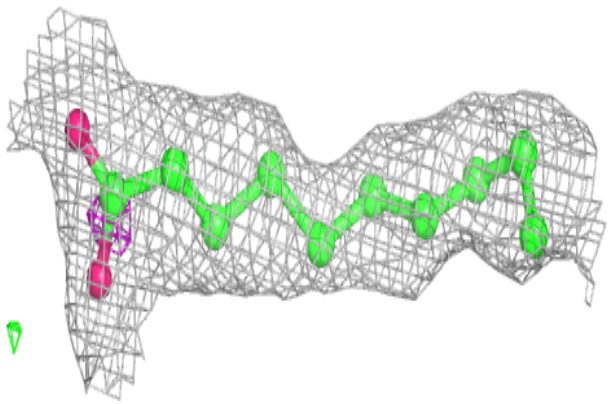


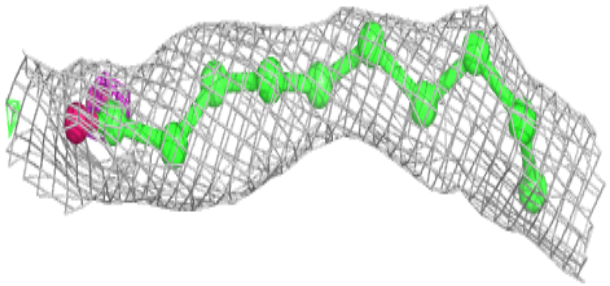


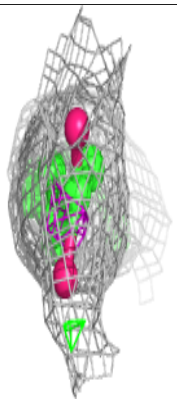


Electron density around STE a 617:

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

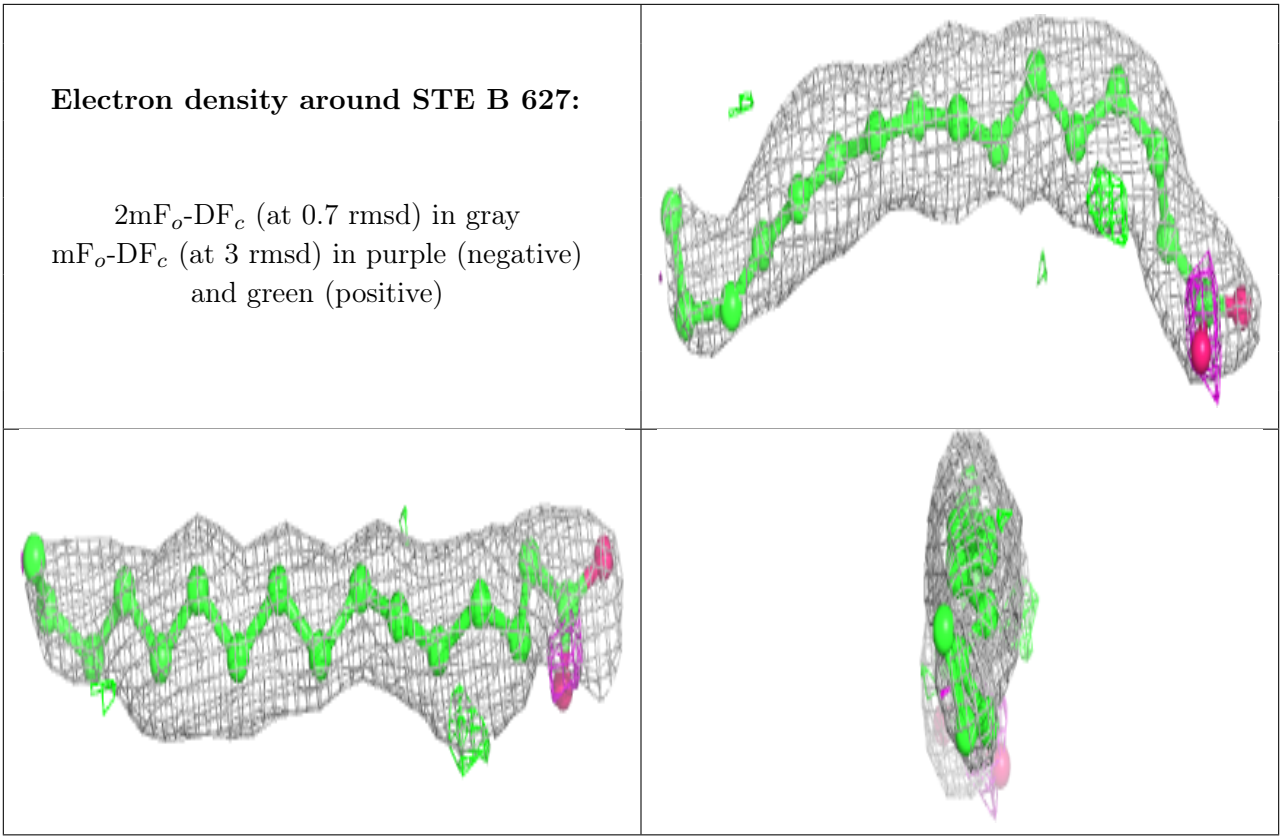






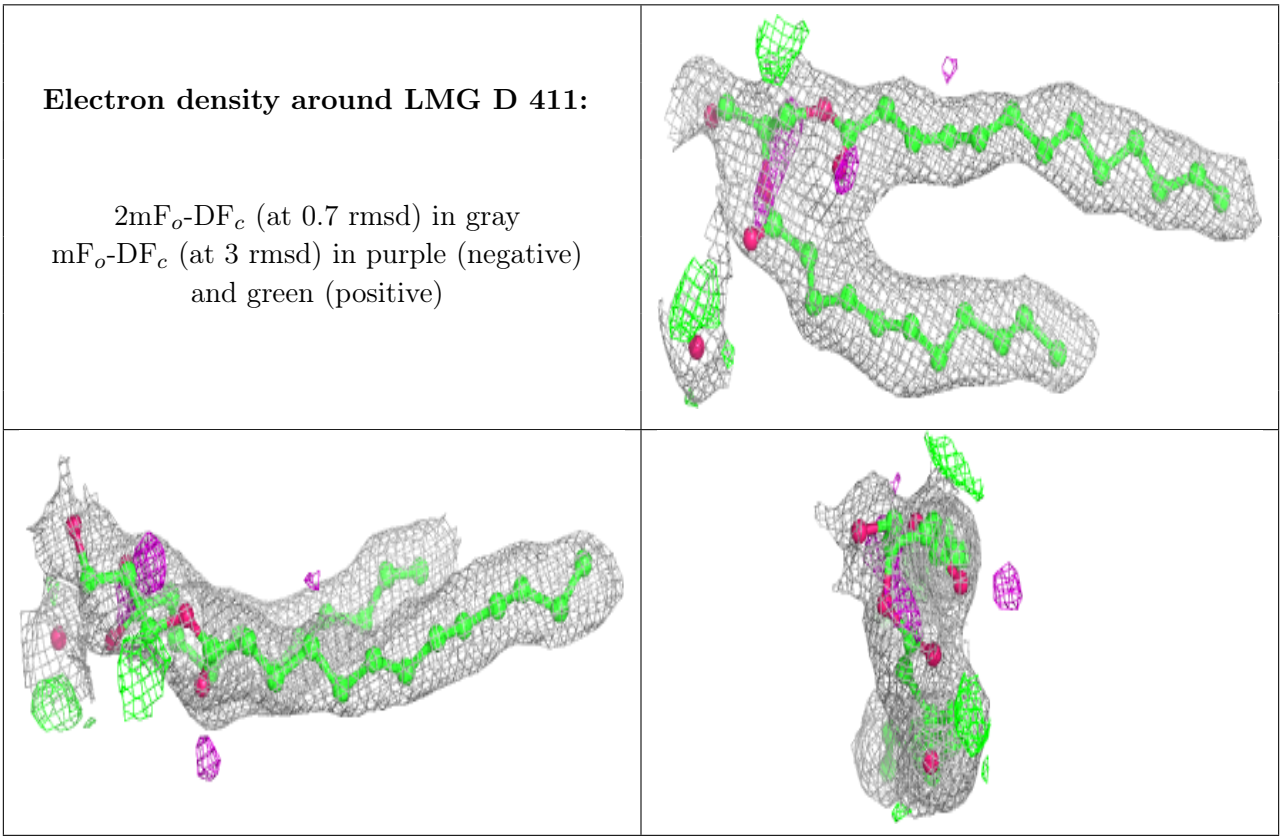
Electron density around STE B 627:

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



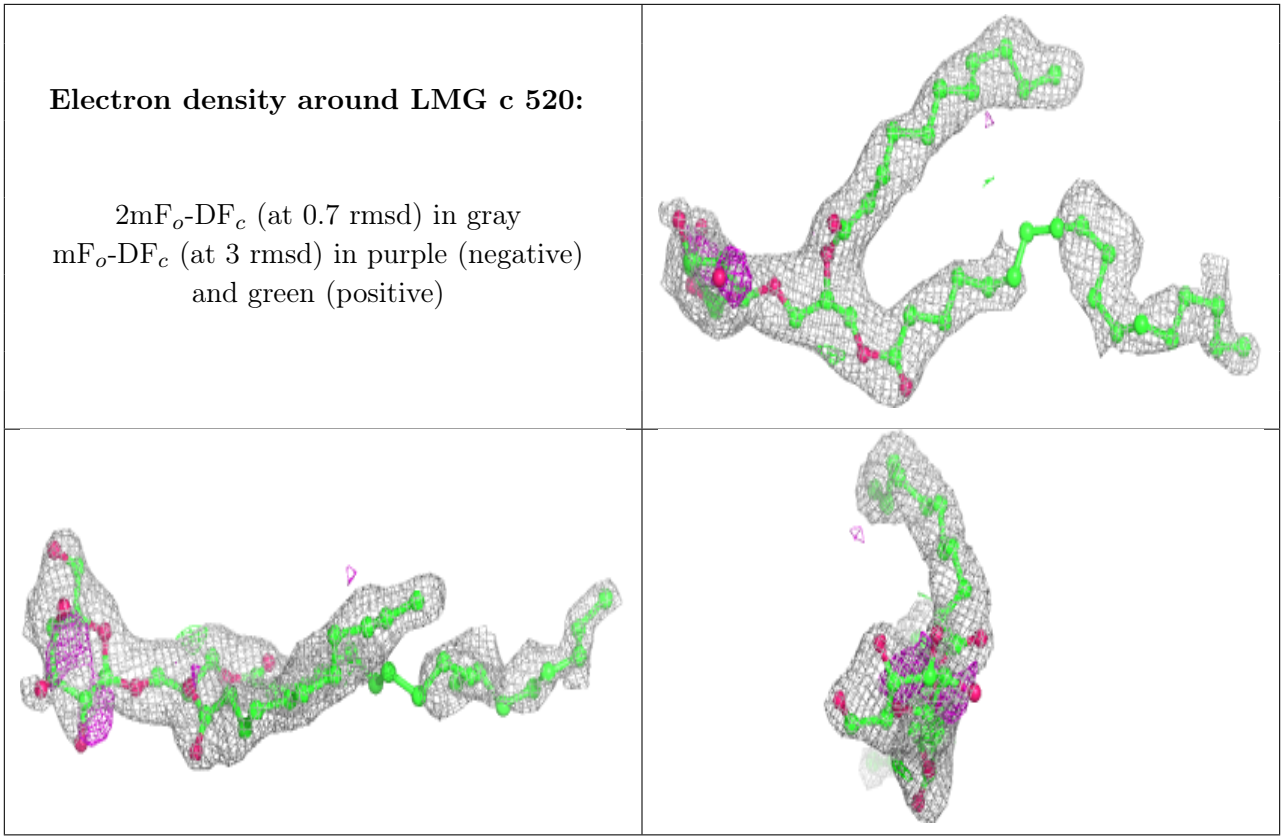
Electron density around LMG D 411:

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



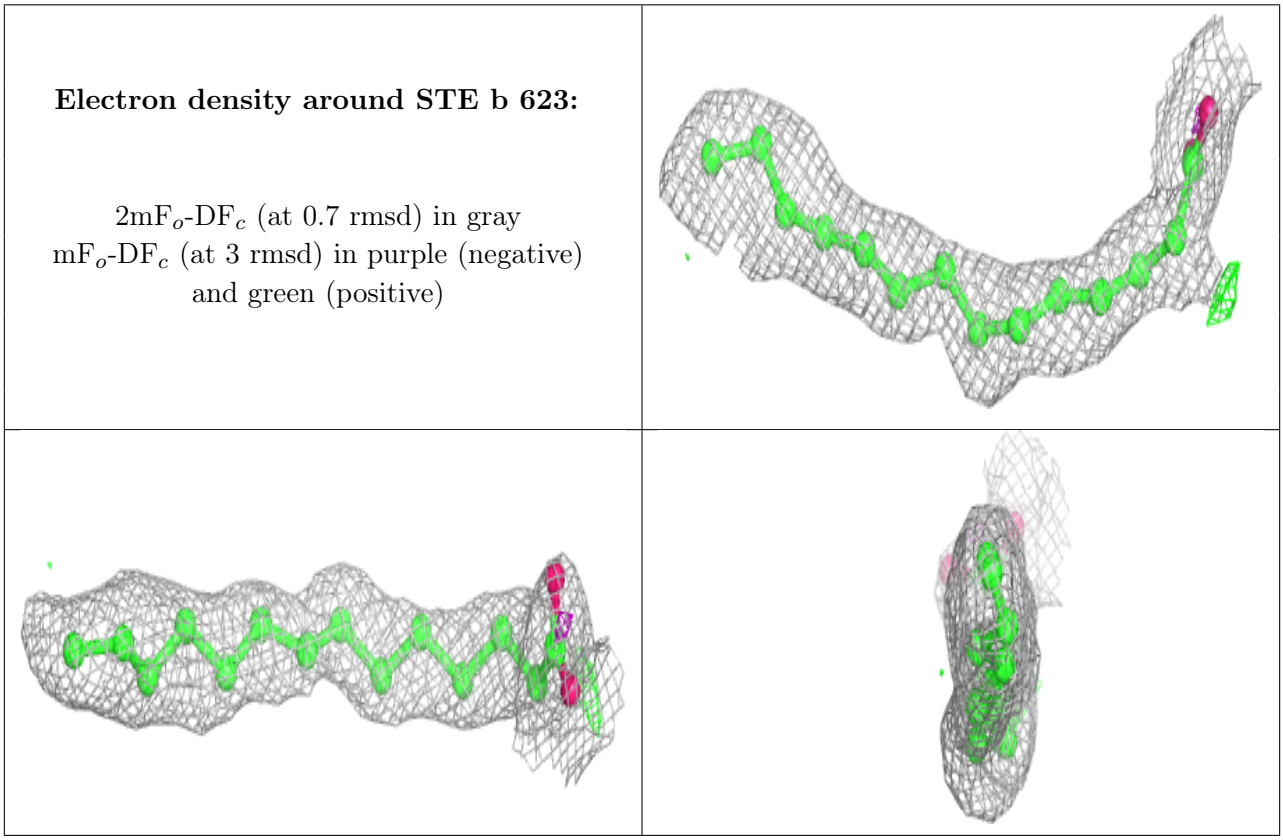
Electron density around LMG c 520:

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



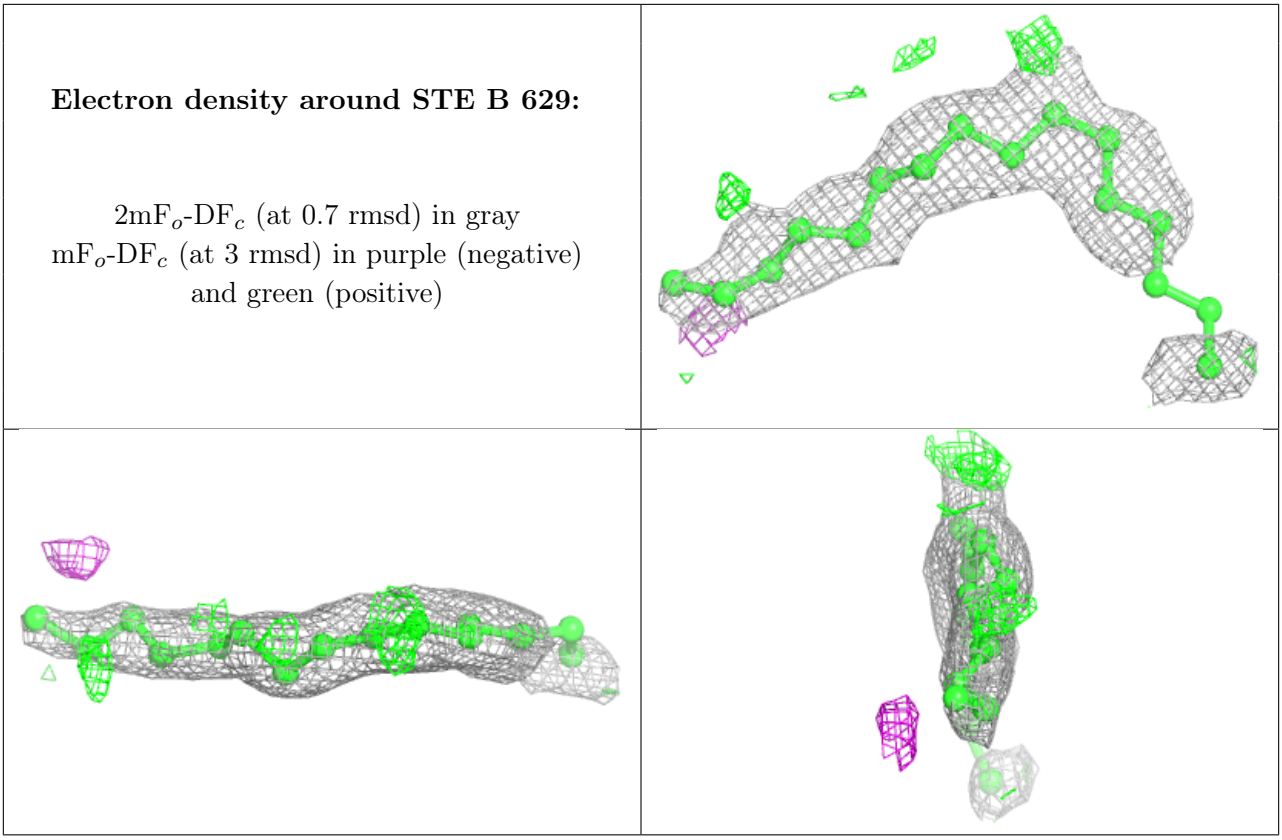
Electron density around STE b 623:

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



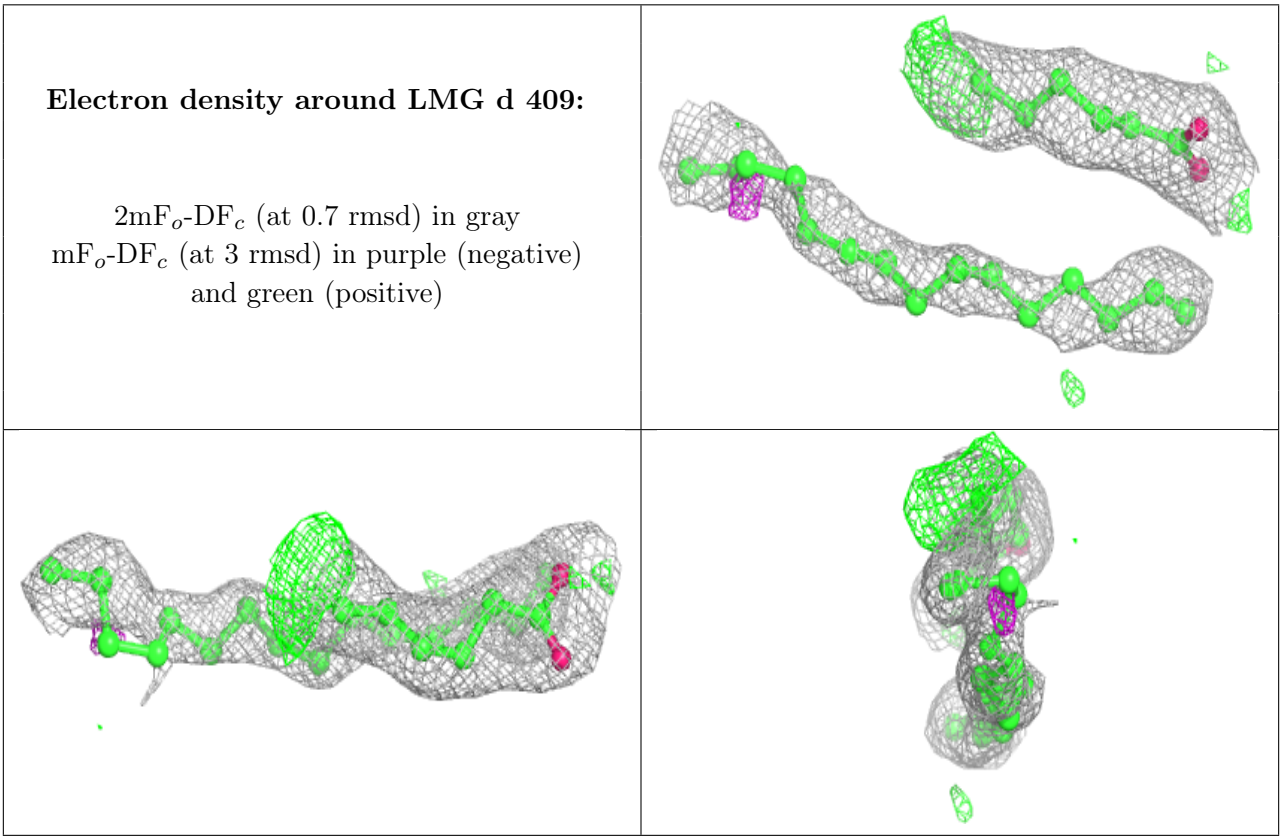
Electron density around STE B 629:

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



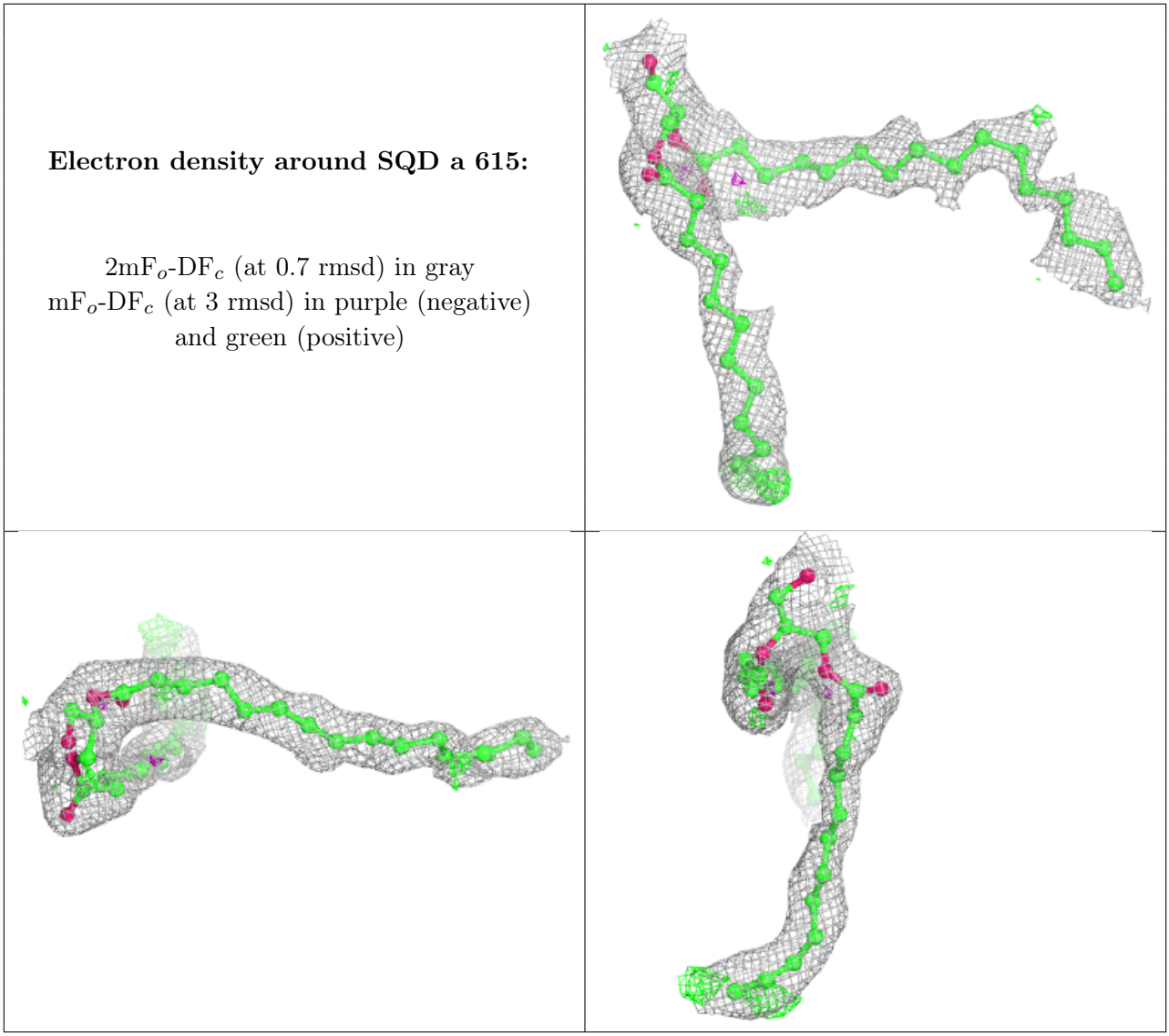
Electron density around LMG d 409:

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



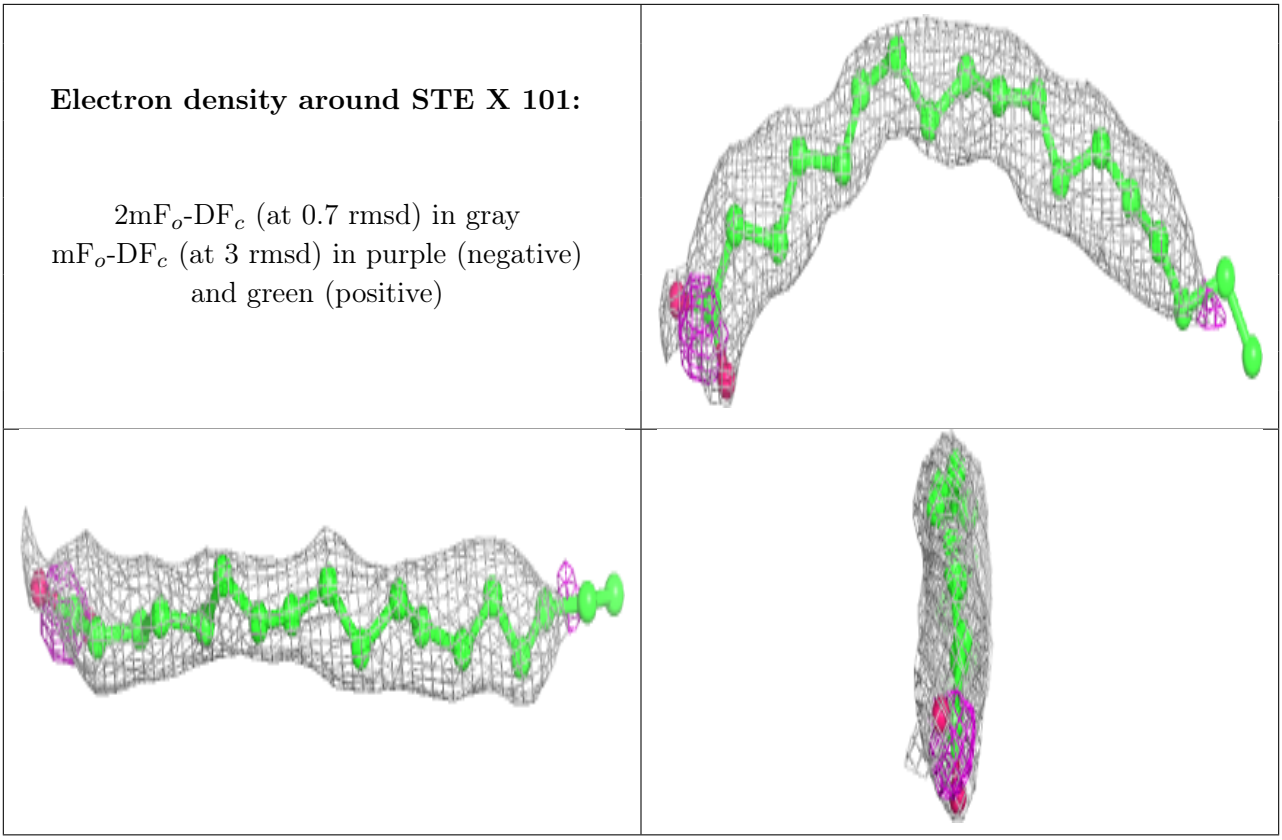
Electron density around SQD a 615:

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



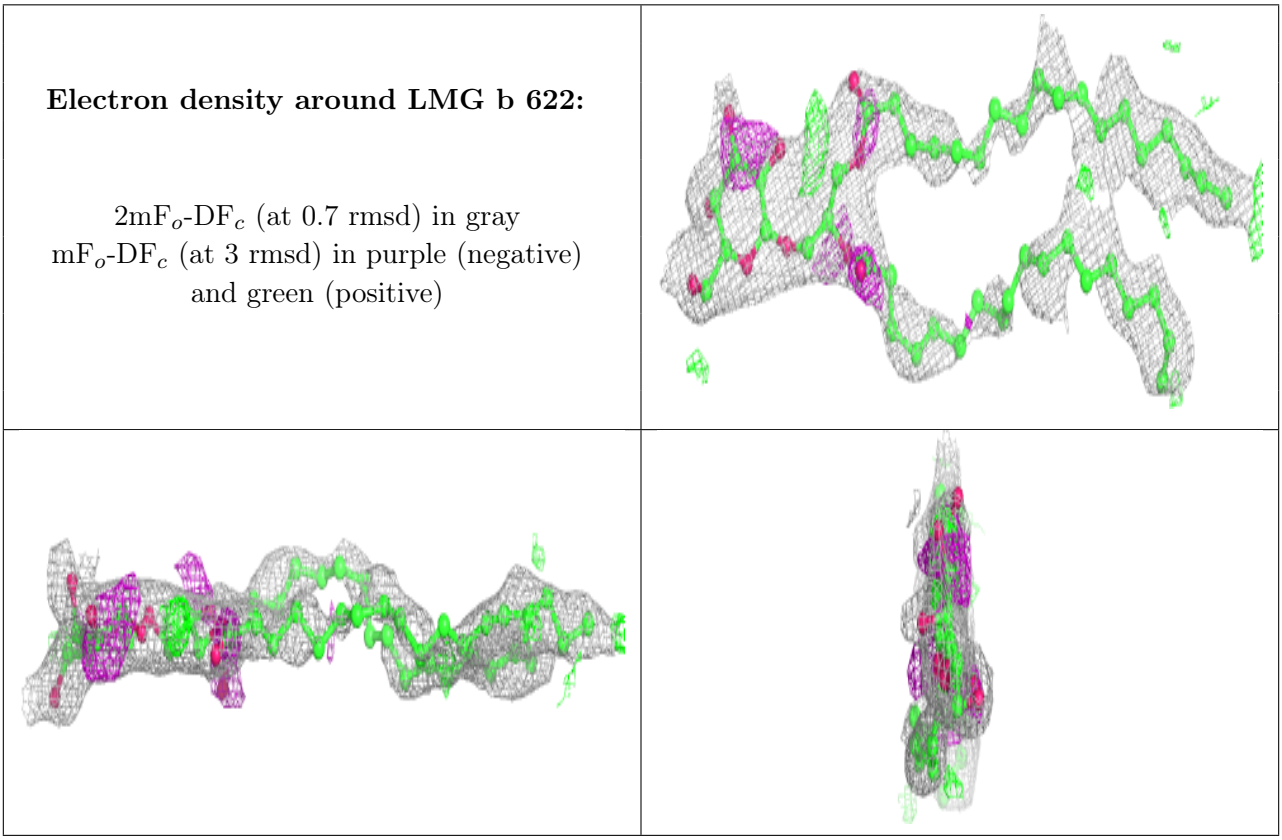
Electron density around STE X 101:

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



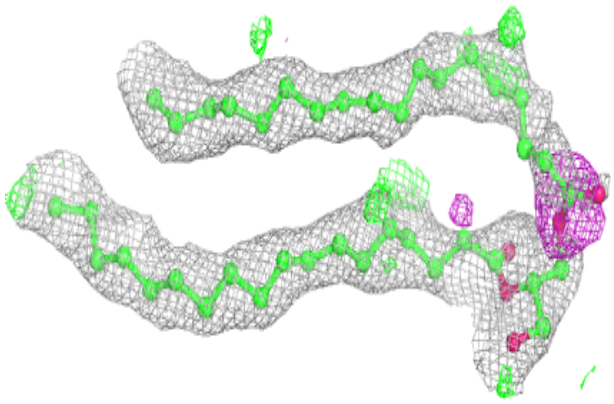
Electron density around LMG b 622:

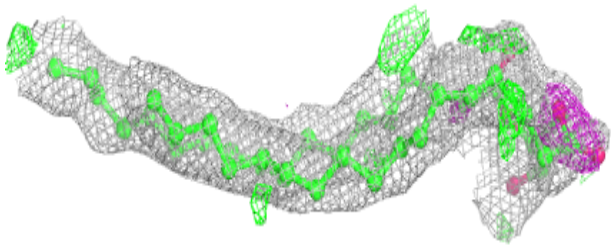
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

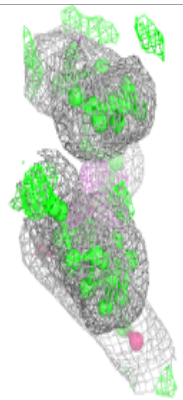


Electron density around DGD a 616:

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

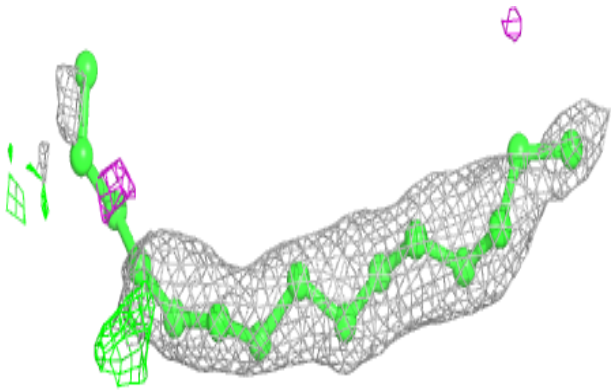


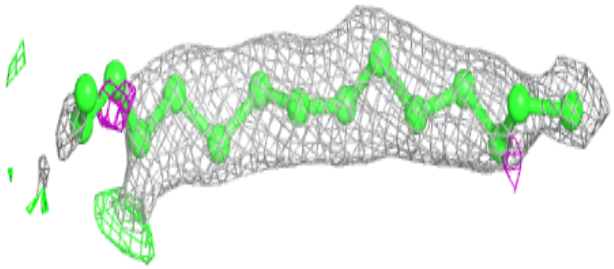


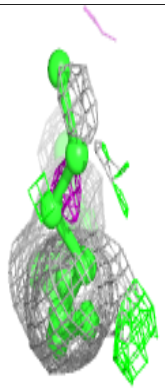


Electron density around STE T 103:

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

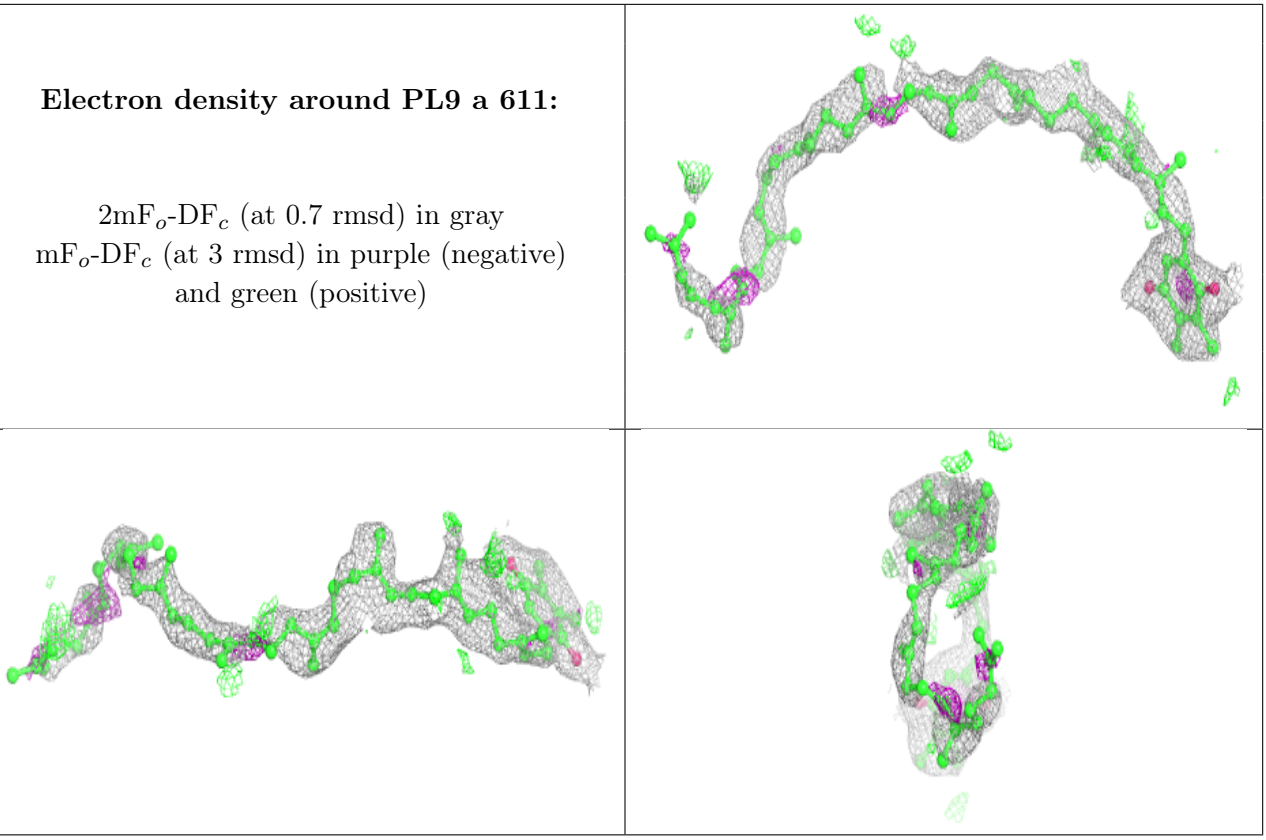






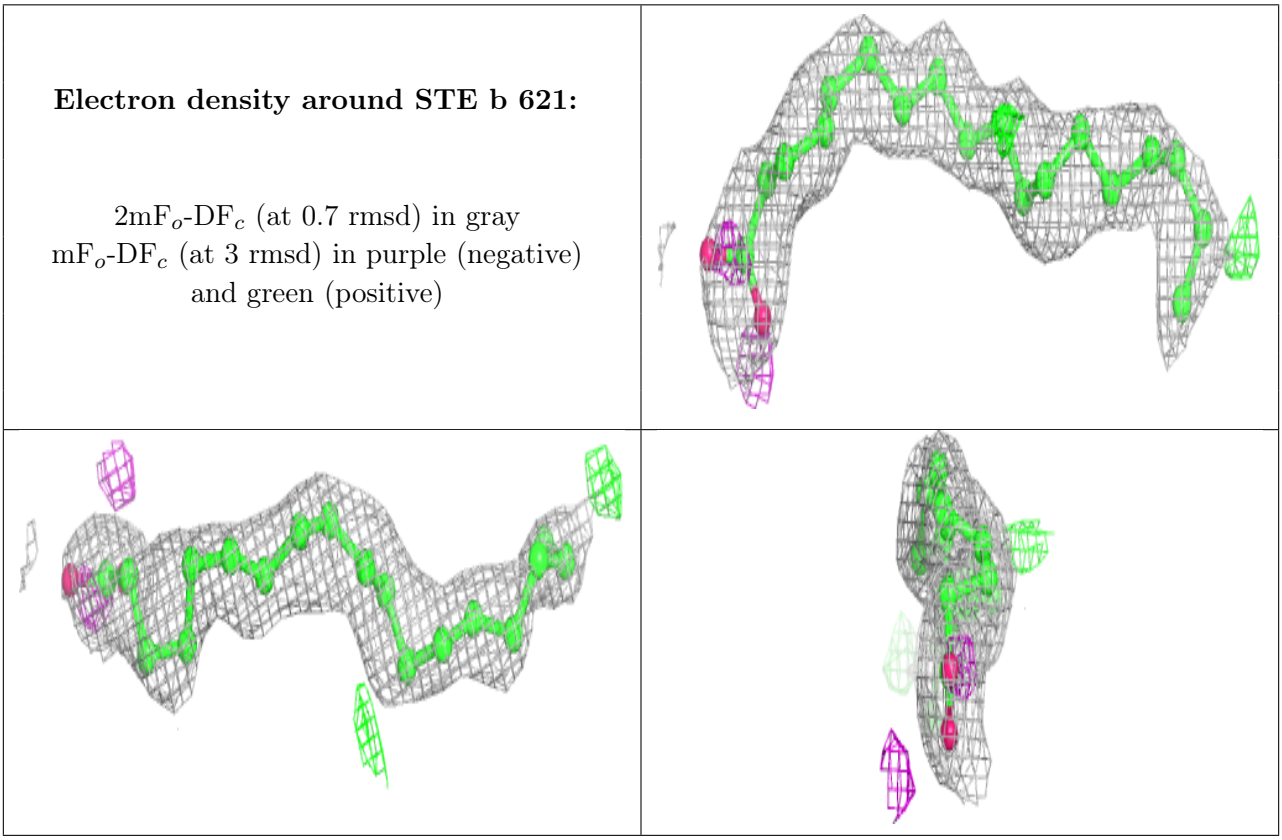
Electron density around PL9 a 611:

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



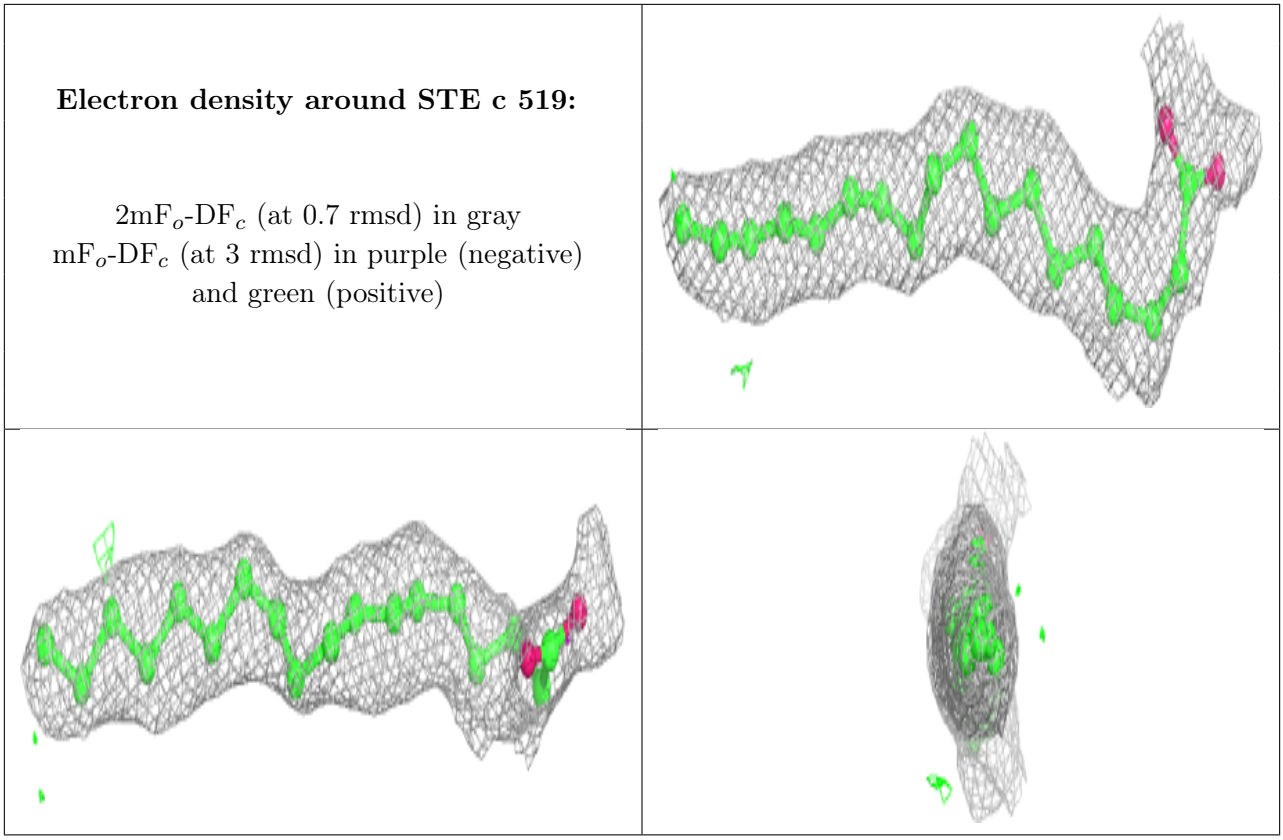
Electron density around STE b 621:

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



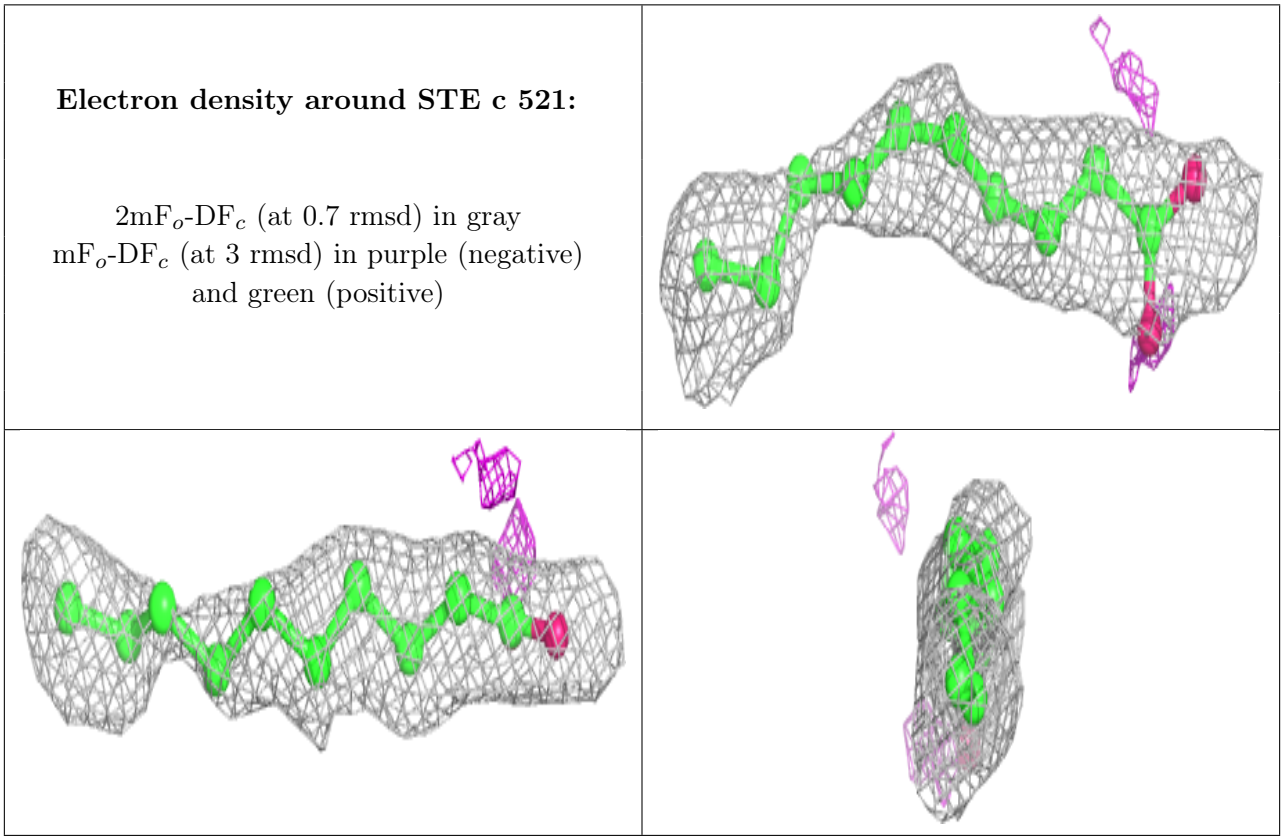
Electron density around STE c 519:

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



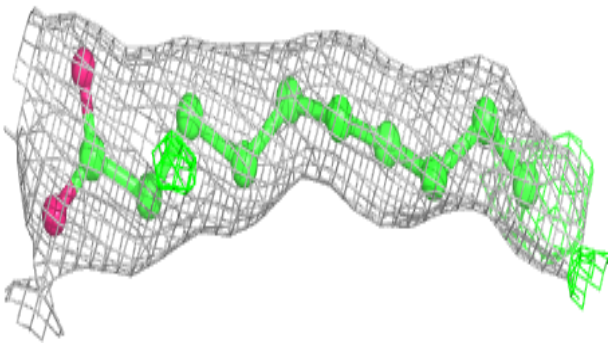
Electron density around STE c 521:

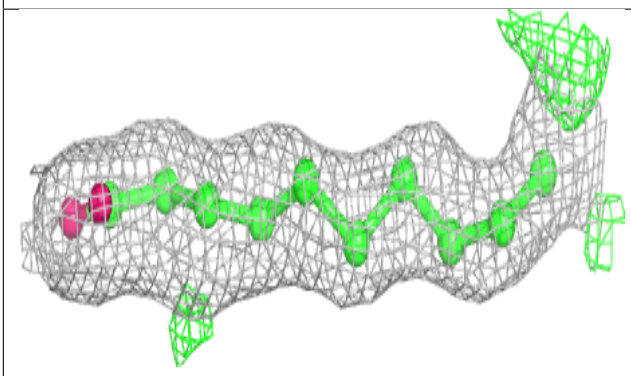
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

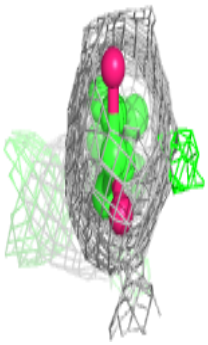


Electron density around STE J 101:

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

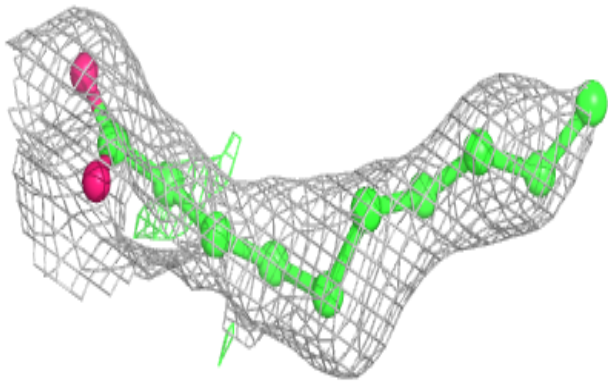


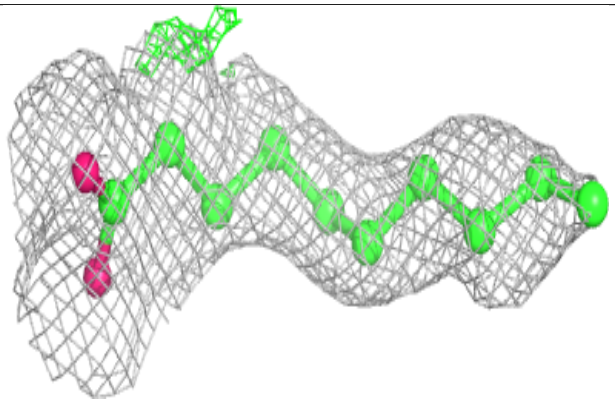


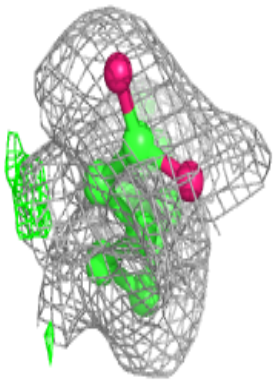


Electron density around STE E 102:

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

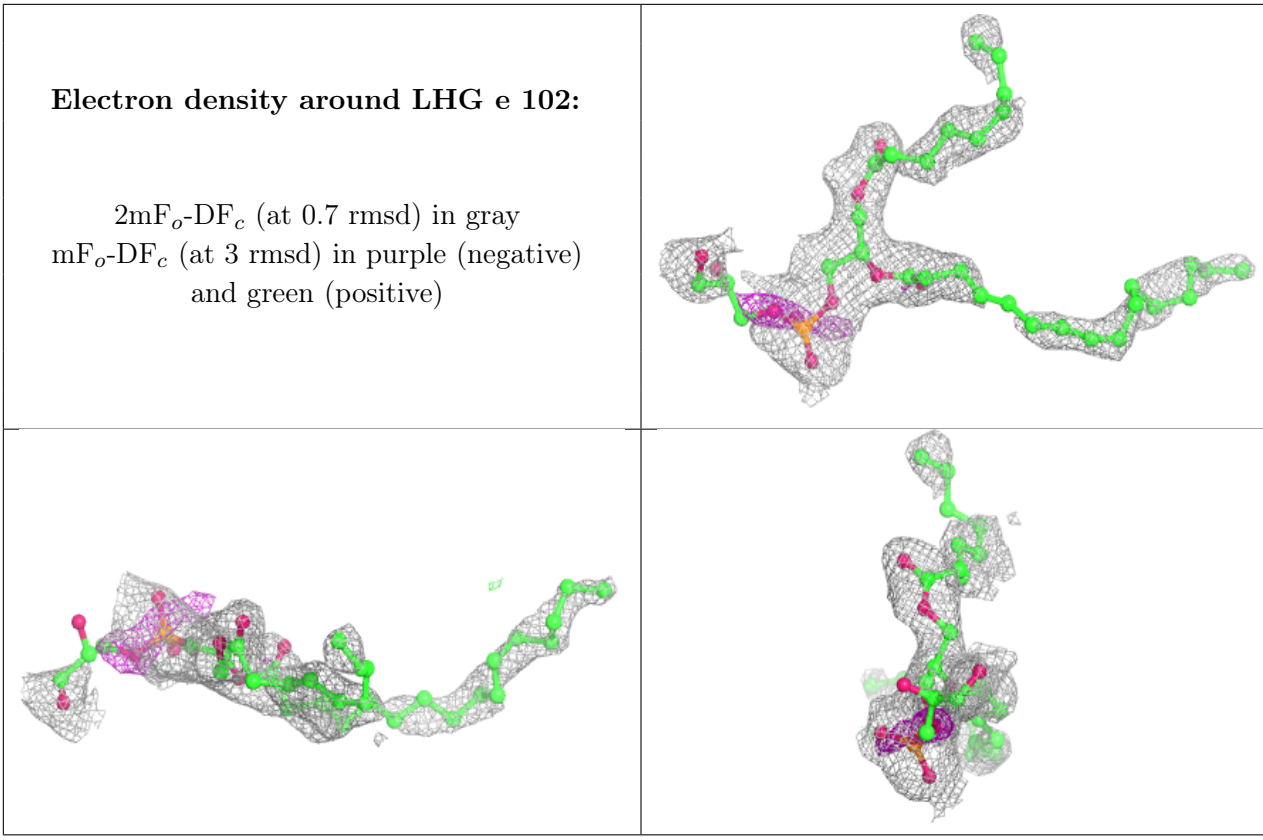






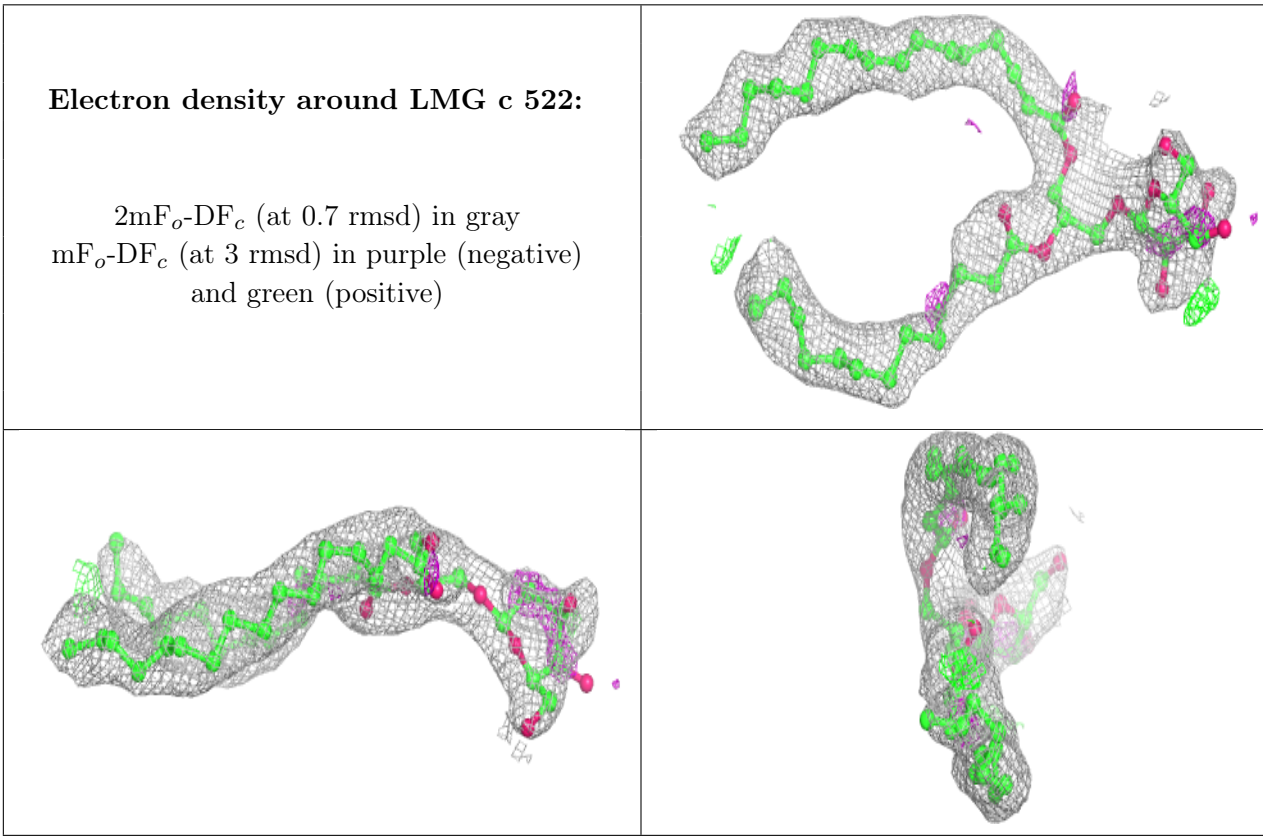
Electron density around LHG e 102:

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



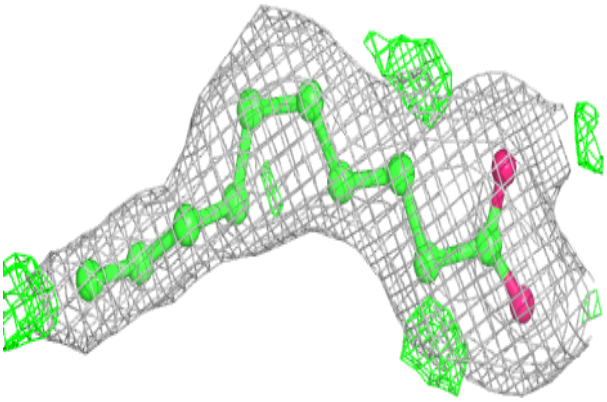
Electron density around LMG c 522:

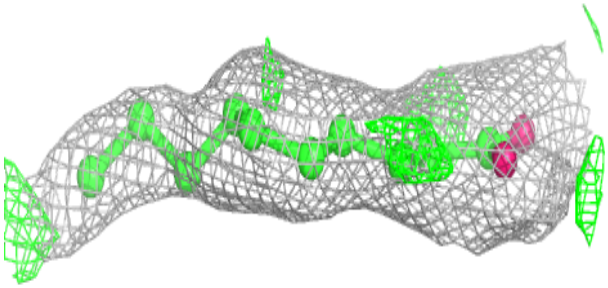
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

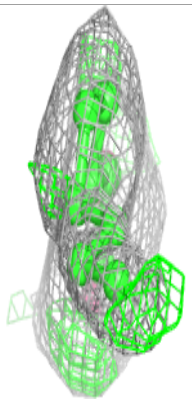


Electron density around STE C 521:

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

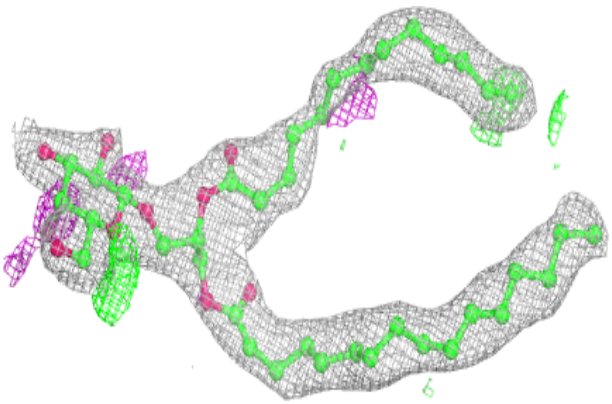


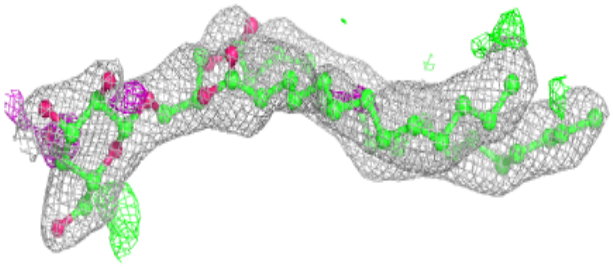


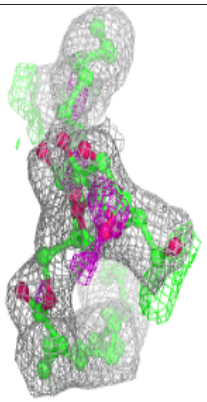


Electron density around LMG A 613:

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

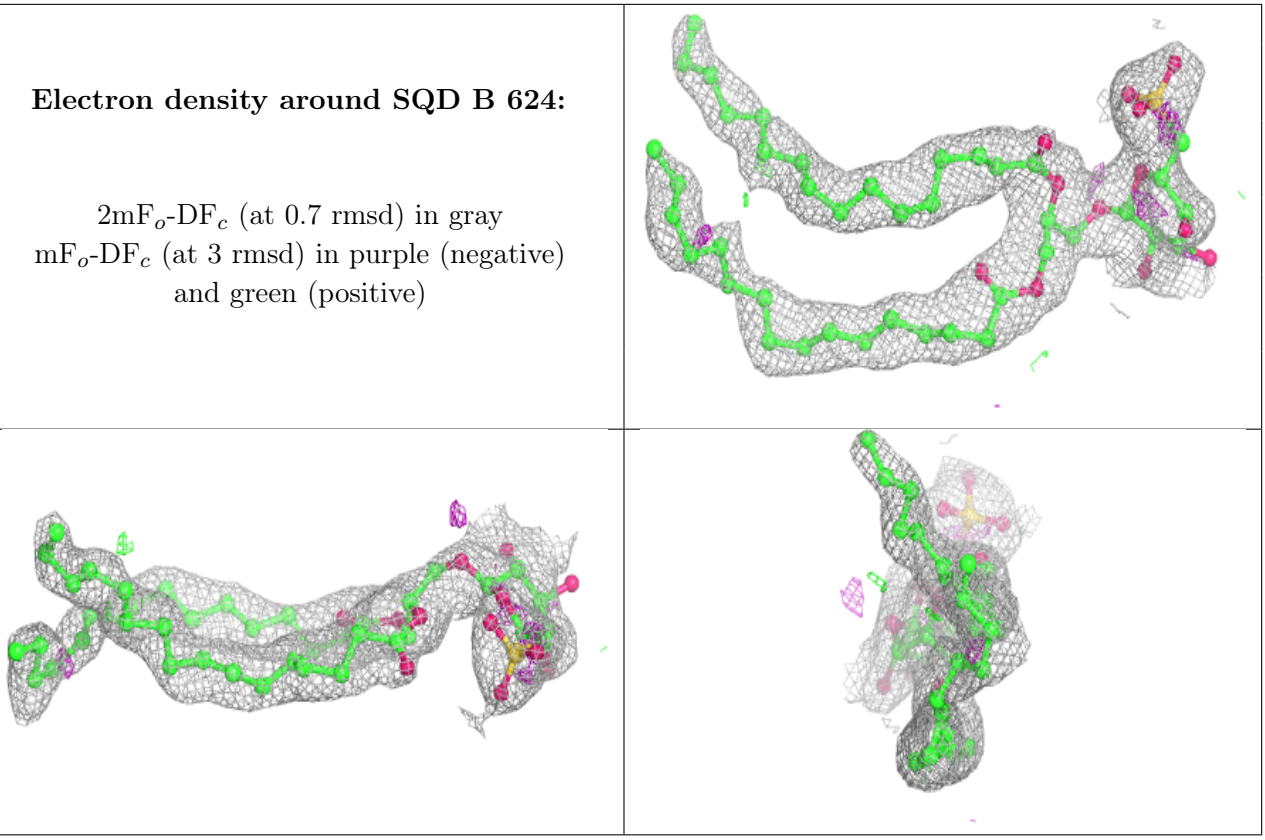






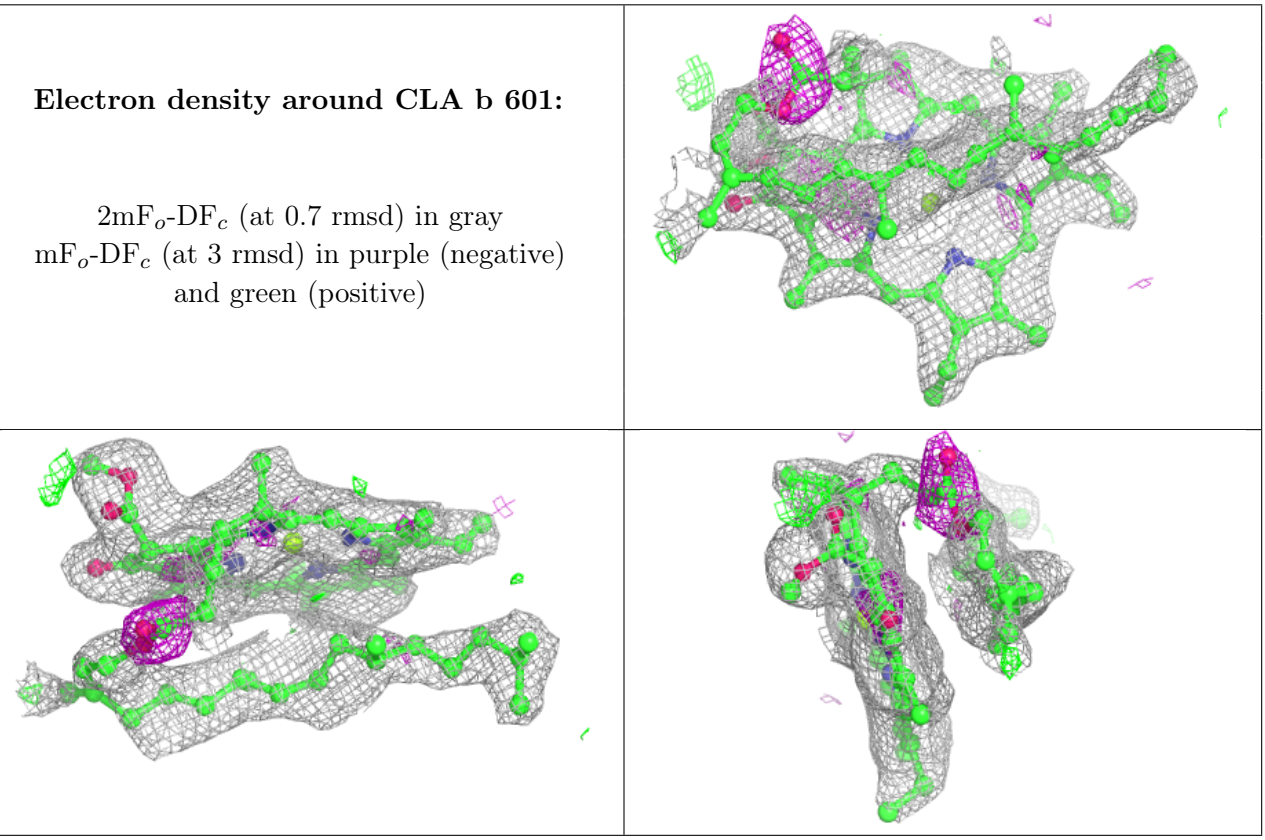
Electron density around SQD B 624:

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



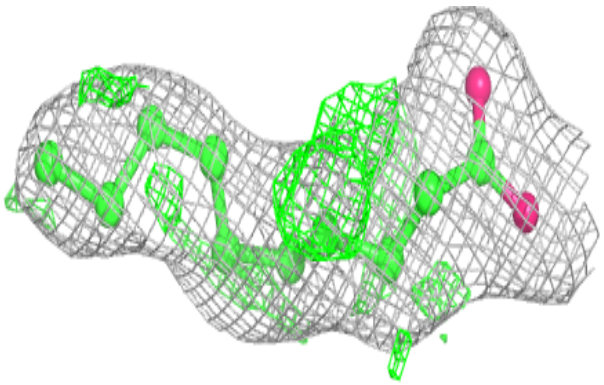
Electron density around CLA b 601:

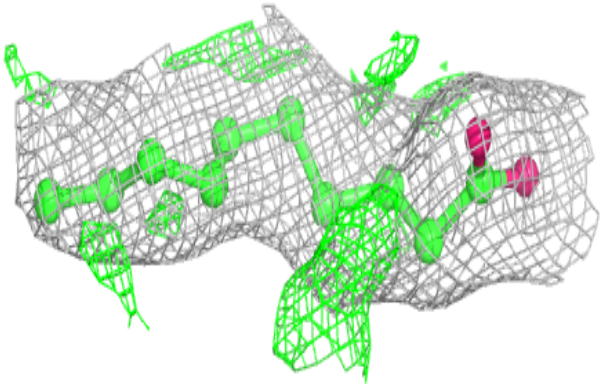
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

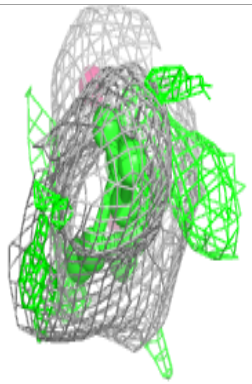


Electron density around STE B 626:

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

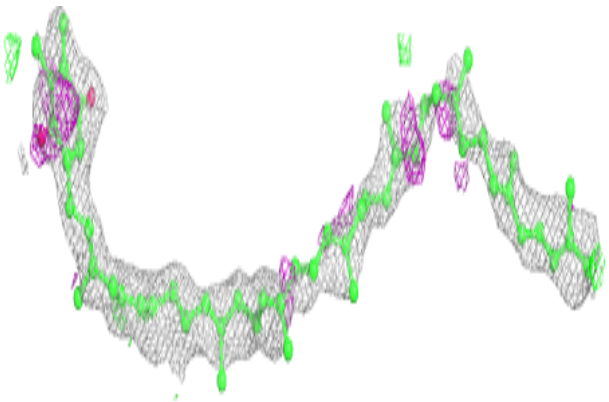


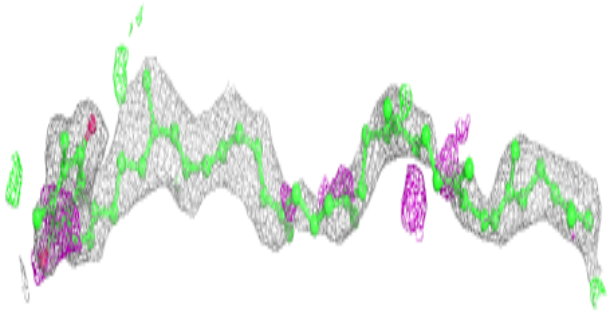


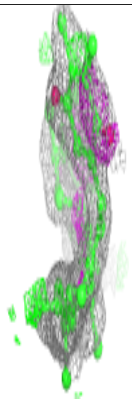


Electron density around PL9 A 611:

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

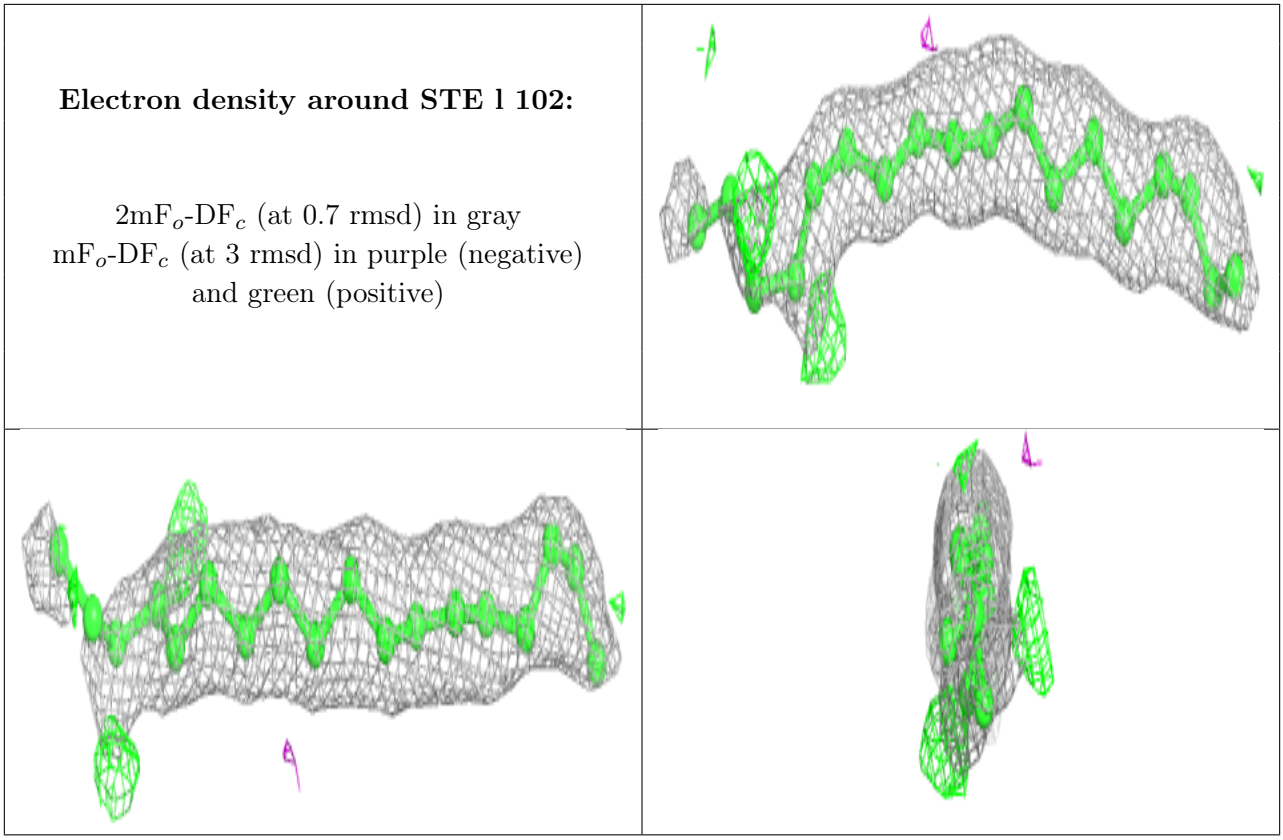






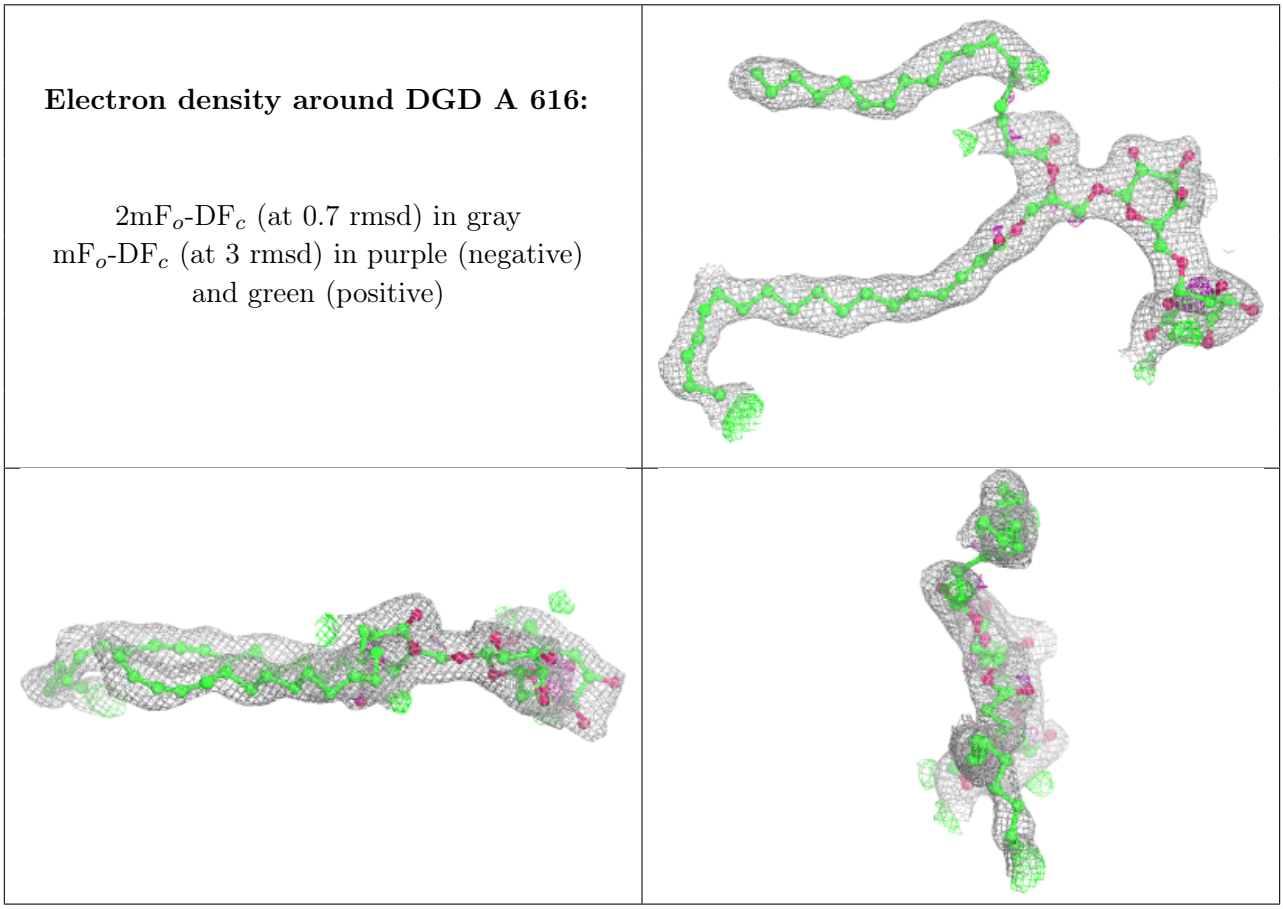
Electron density around STE l 102:

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



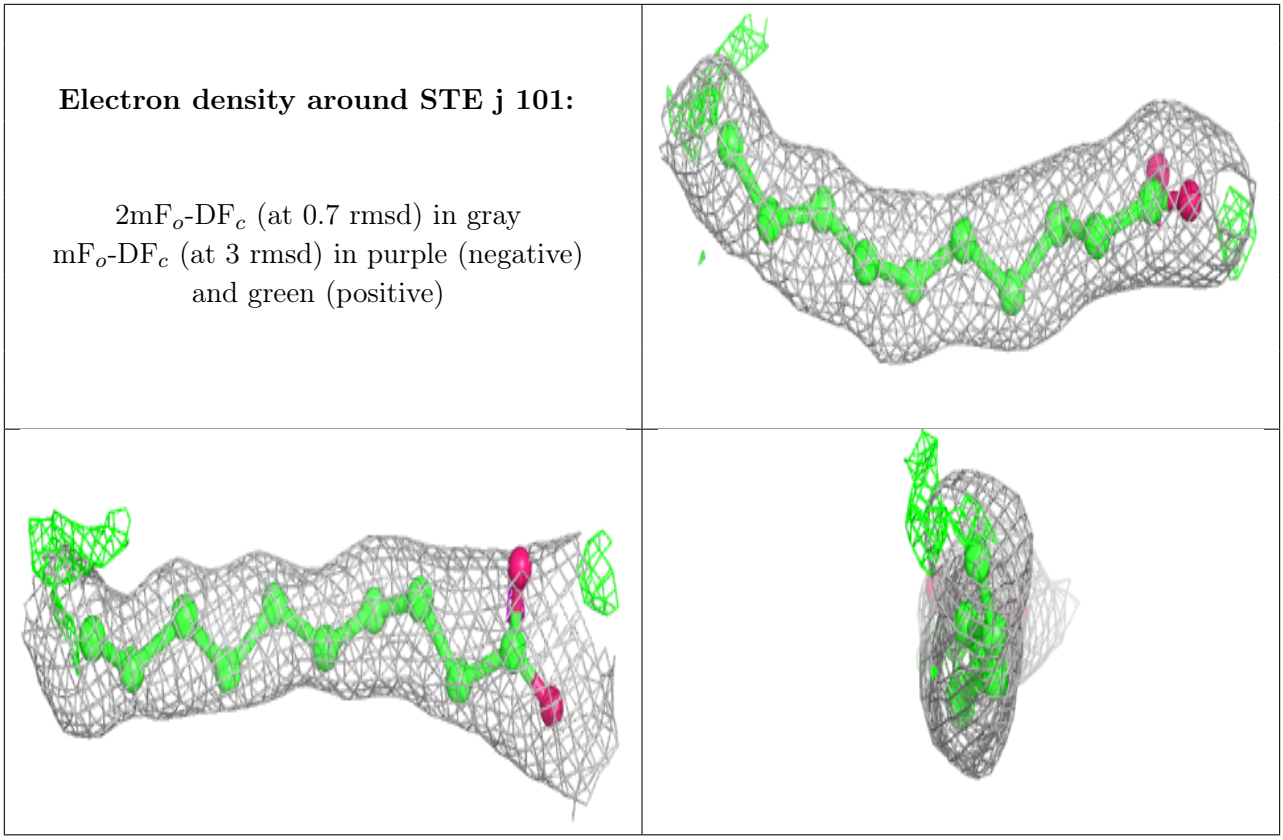
Electron density around DGD A 616:

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



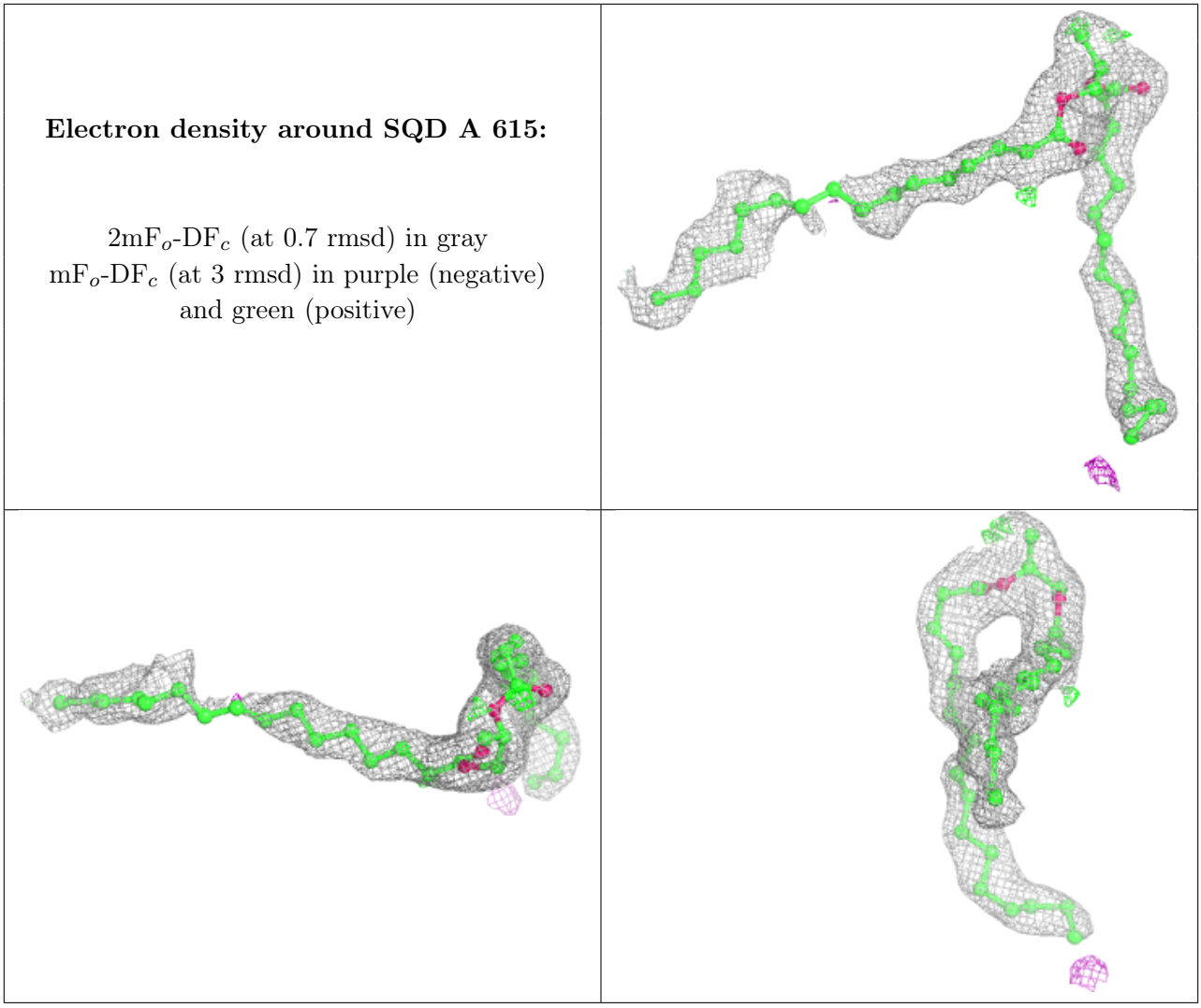
Electron density around STE j 101:

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



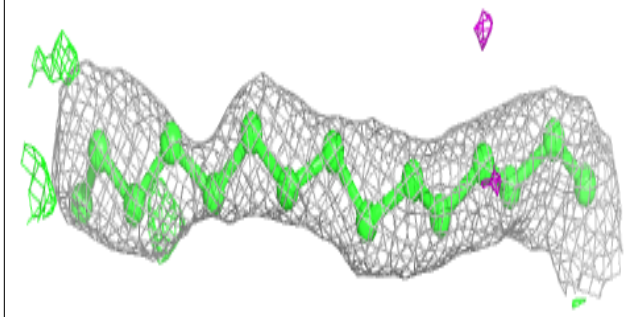
Electron density around SQD A 615:

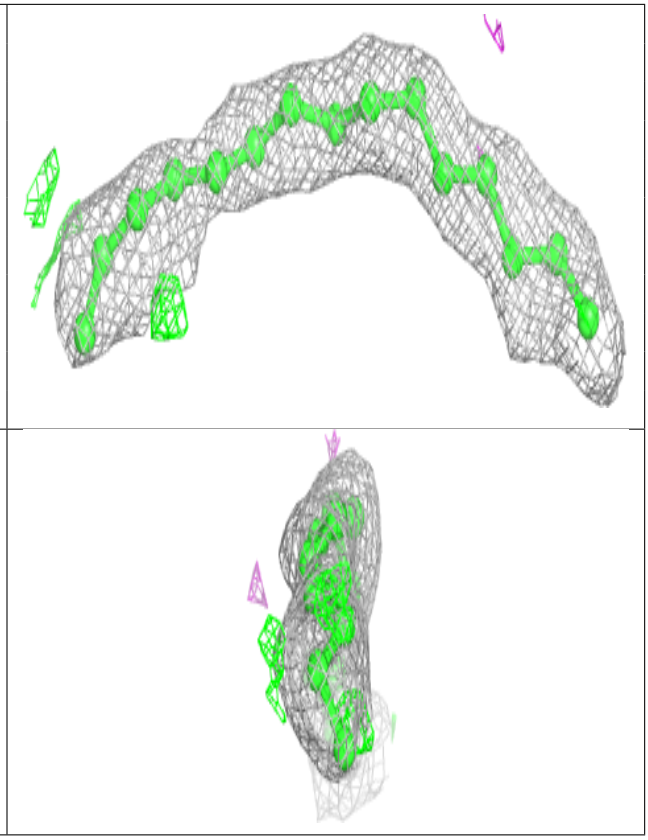
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around STE I 101:

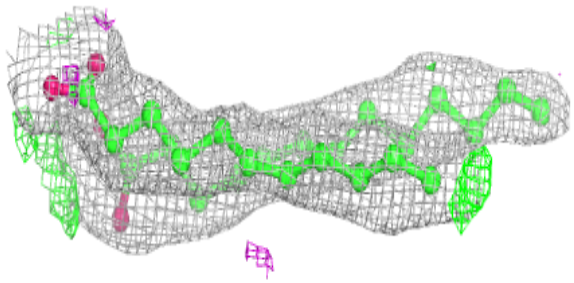
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

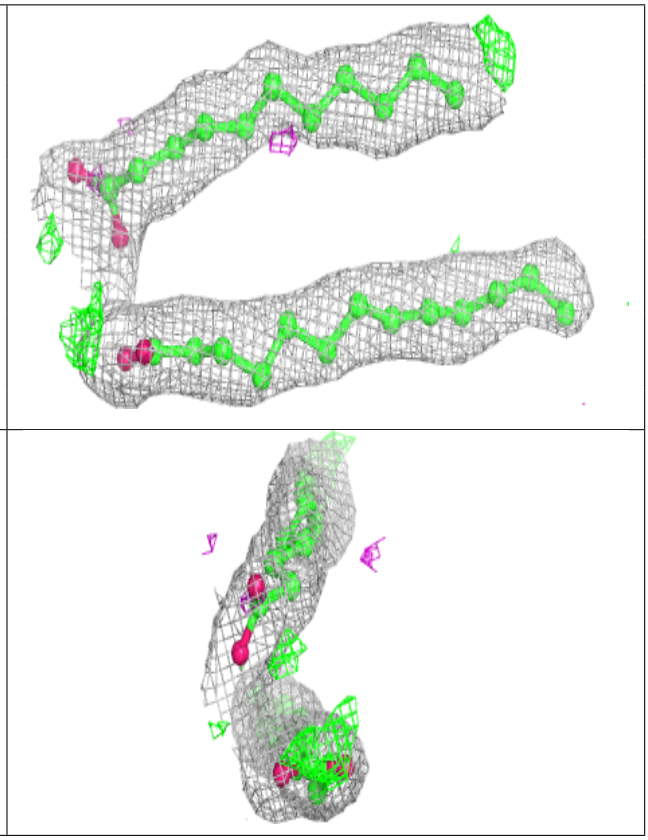




Electron density around LMG B 622:

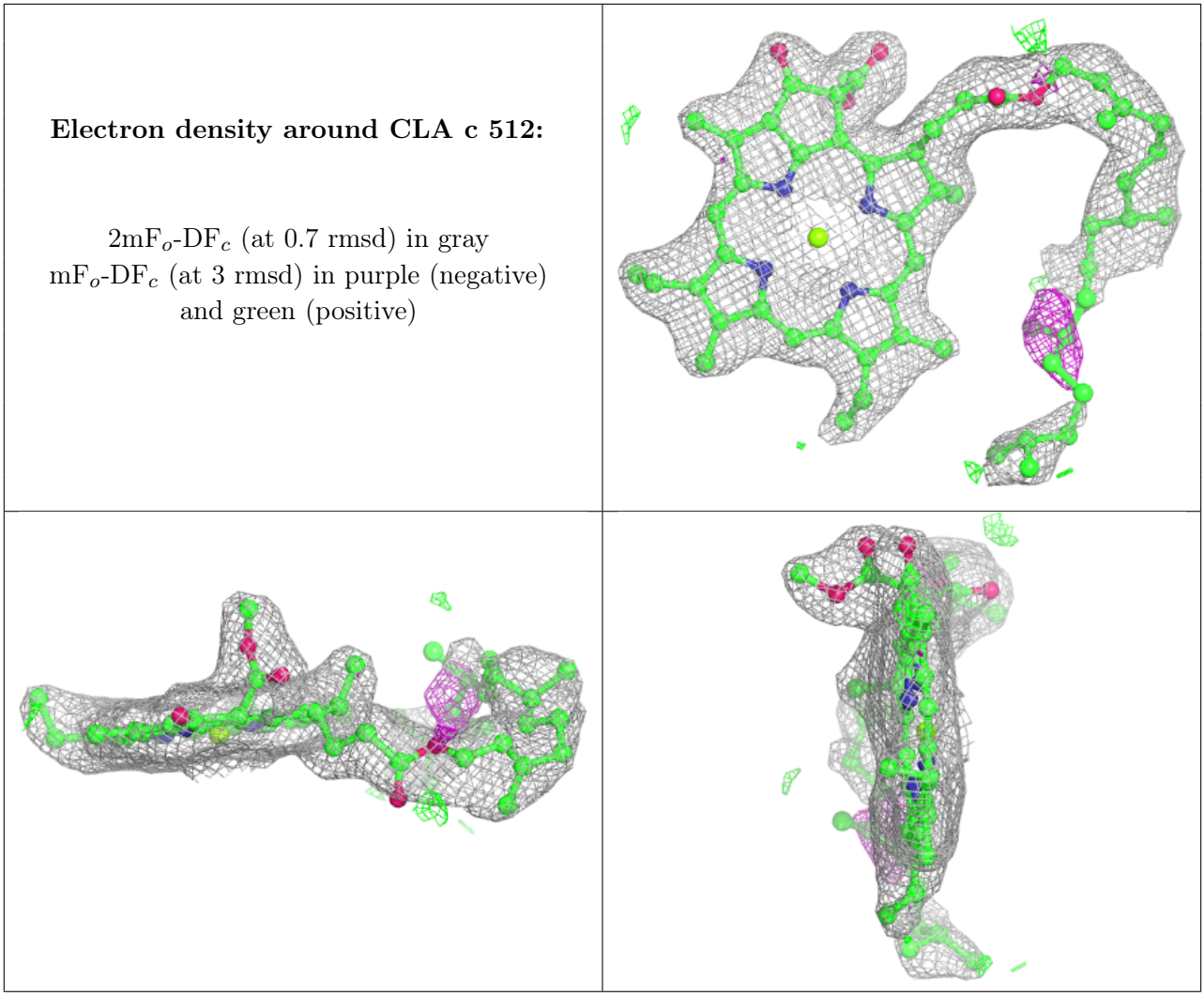
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





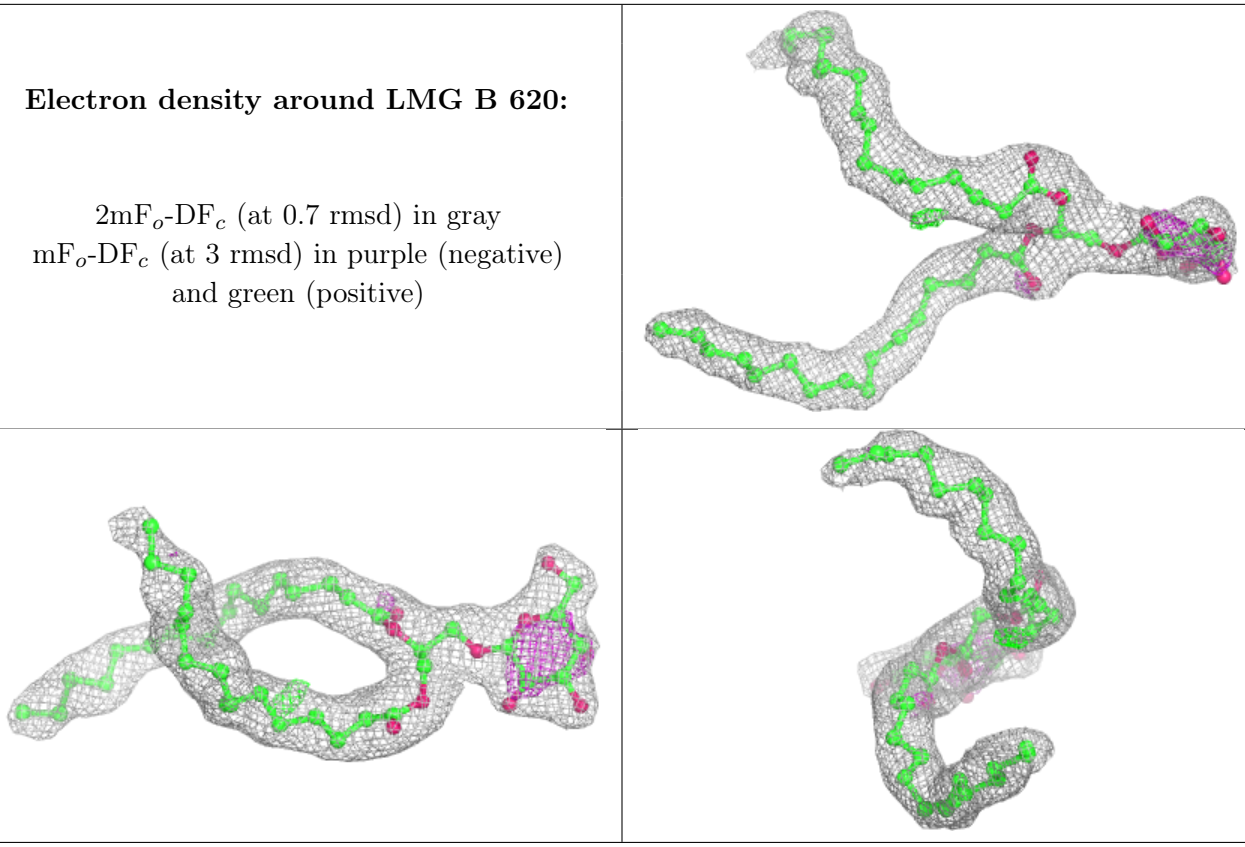
Electron density around CLA c 512:

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



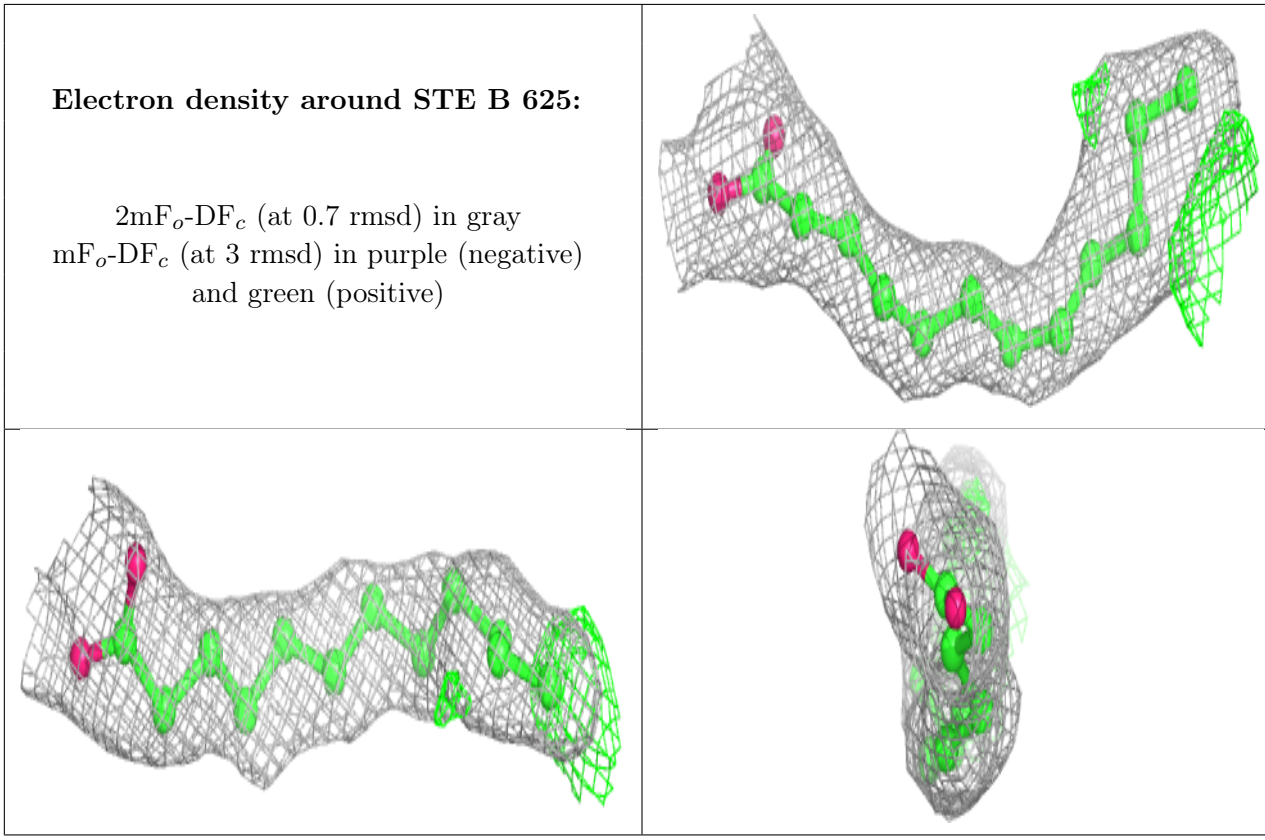
Electron density around LMG B 620:

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



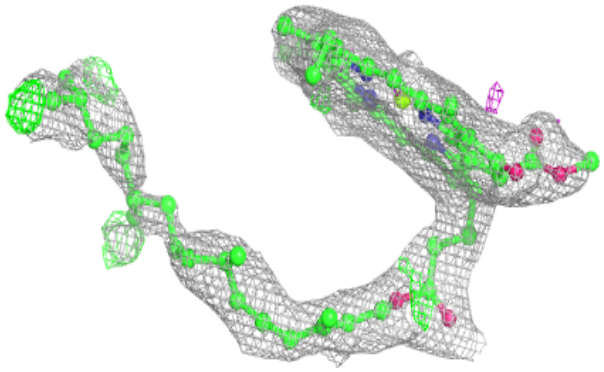
Electron density around STE B 625:

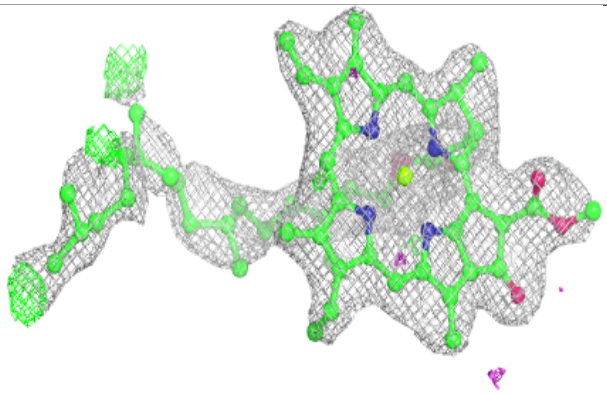
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

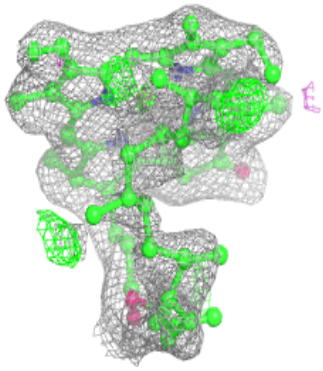


Electron density around CLA C 513:

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

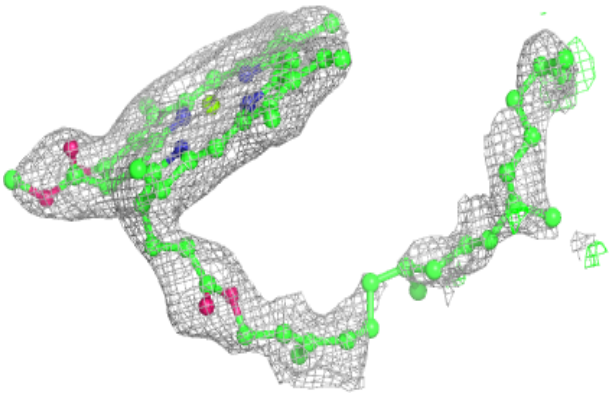


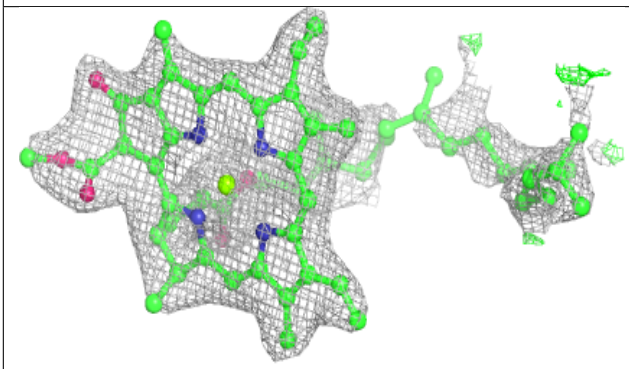


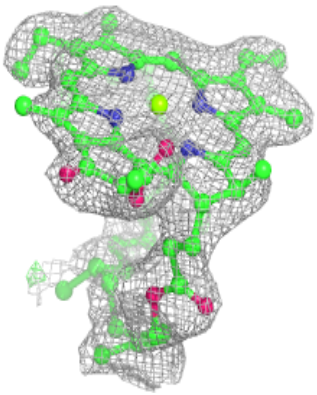


Electron density around CLA c 513:

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

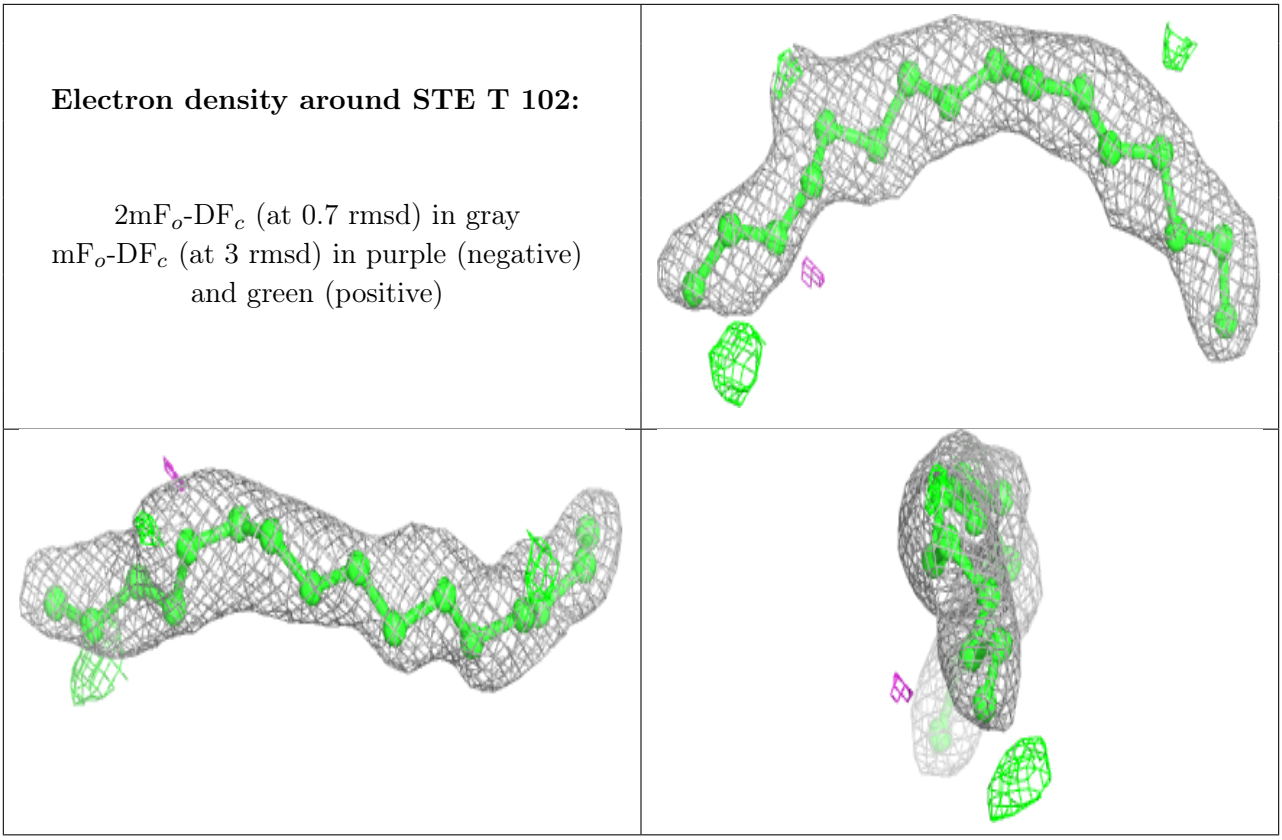






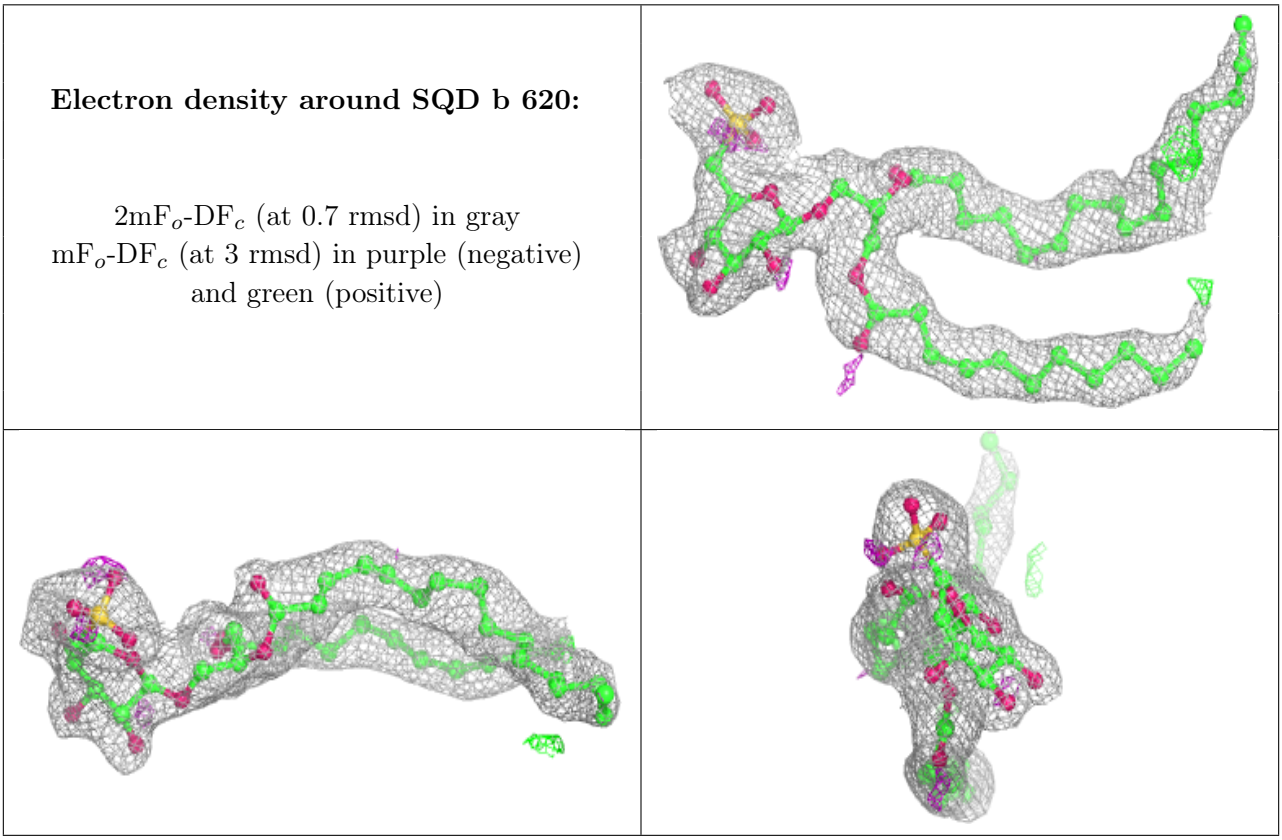
Electron density around STE T 102:

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



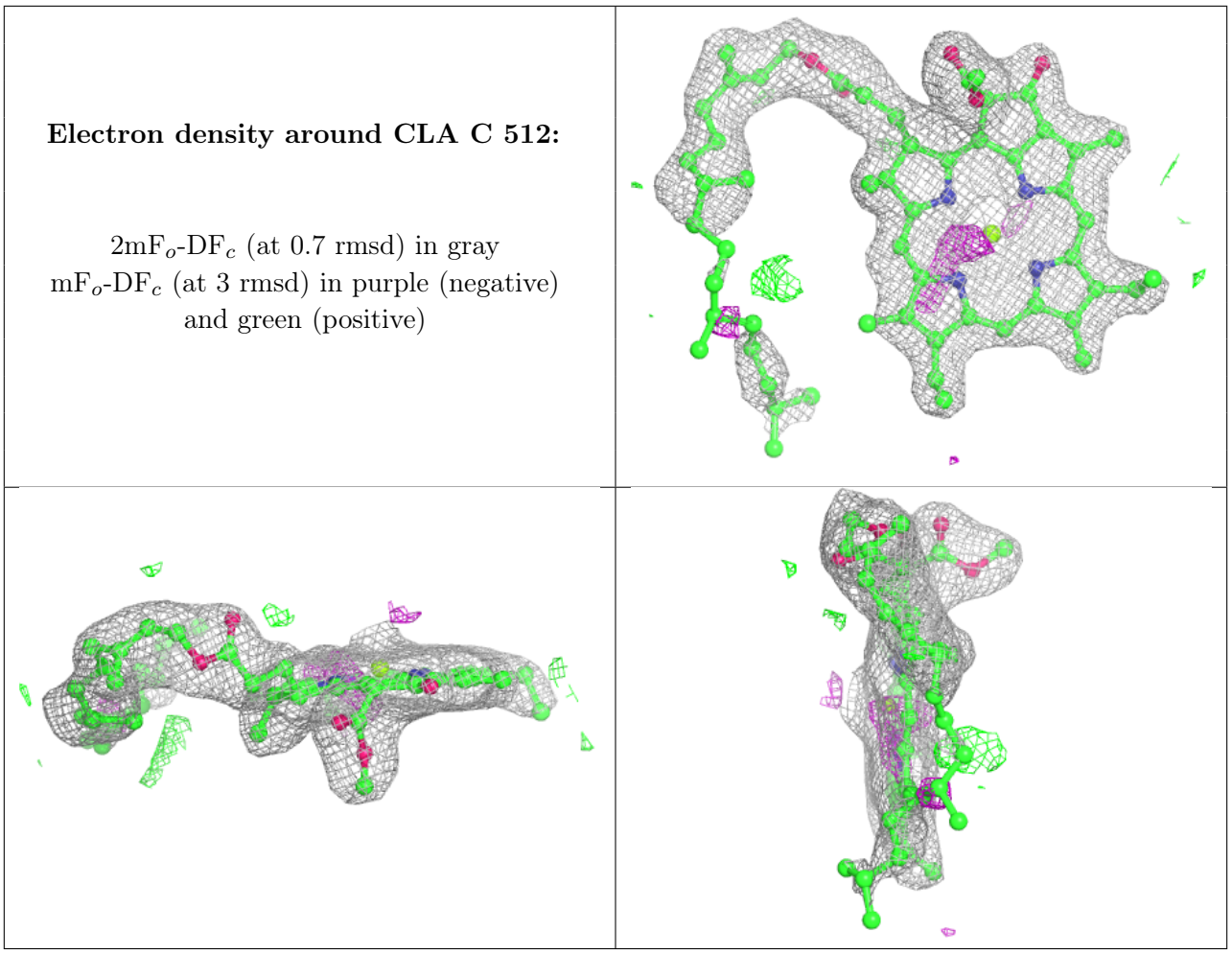
Electron density around SQD b 620:

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



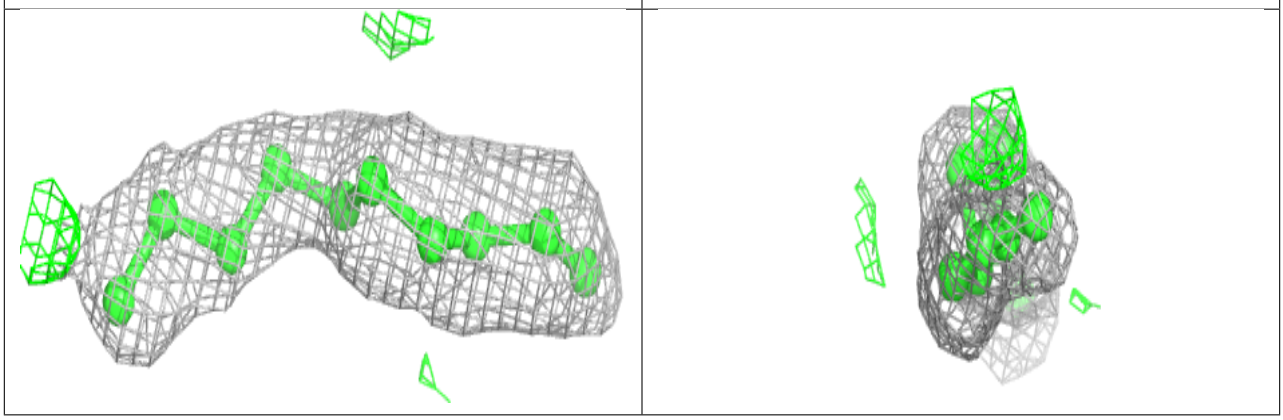
Electron density around CLA C 512:

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



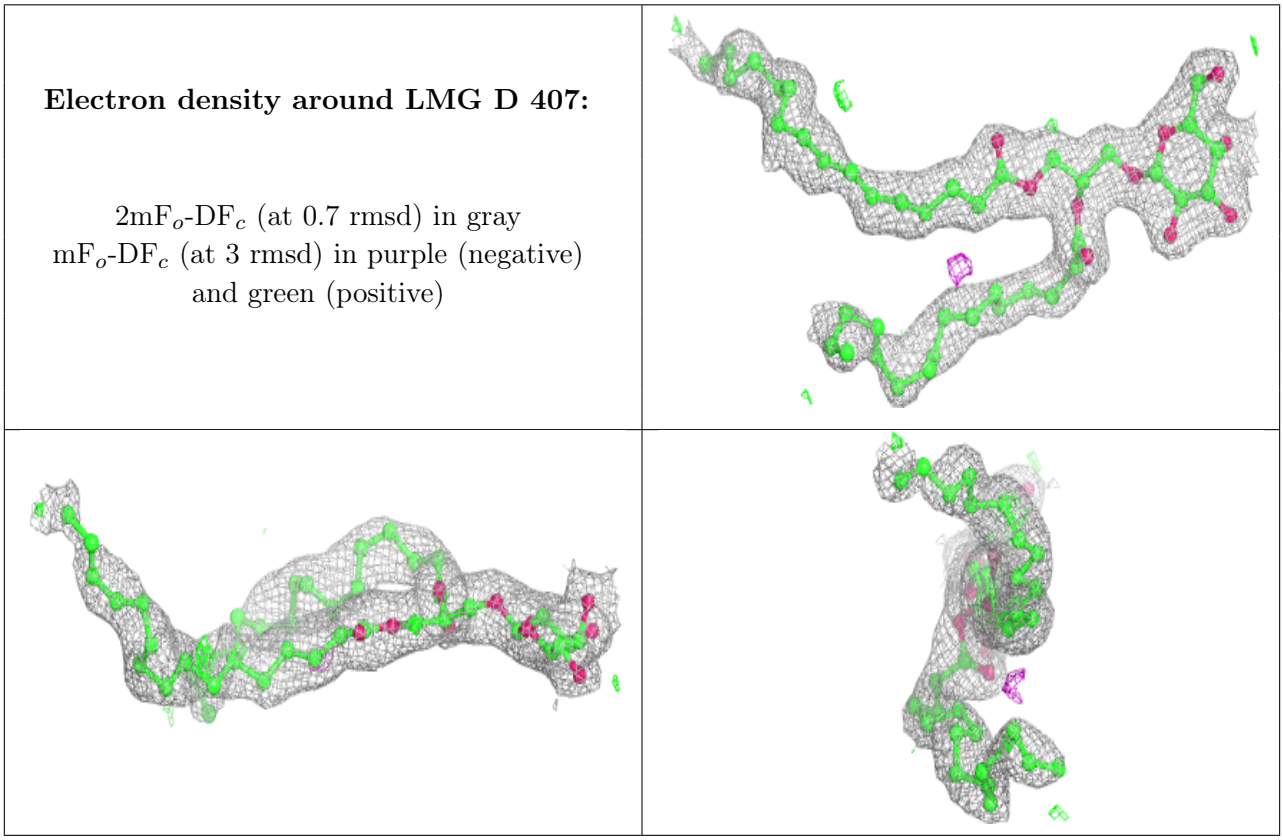
Electron density around STE t 102:

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



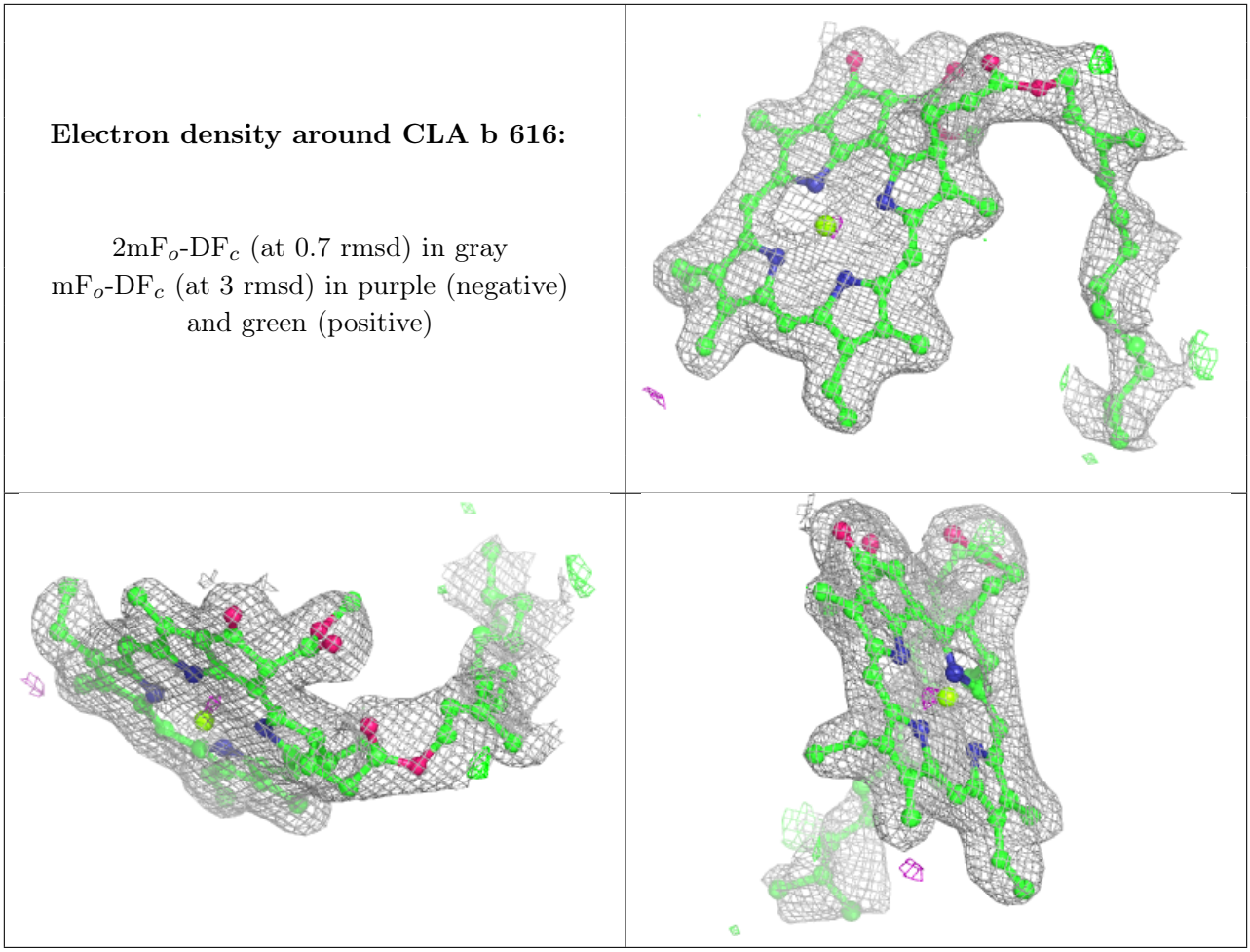
Electron density around LMG D 407:

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



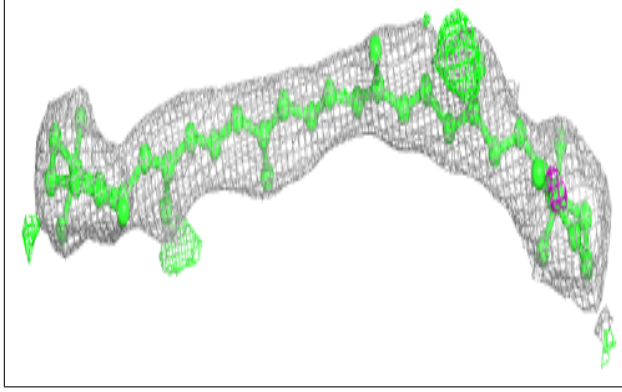
Electron density around CLA b 616:

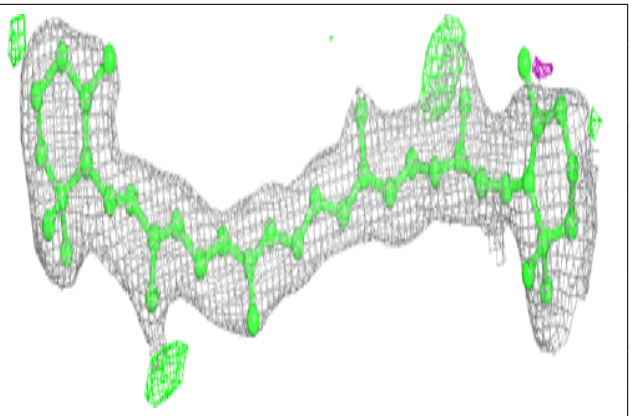
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

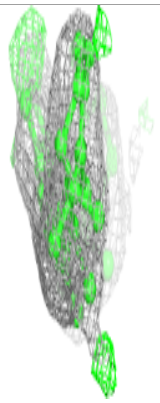


Electron density around BCR d 405:

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

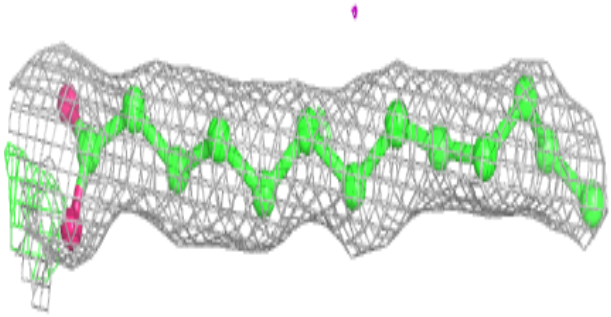


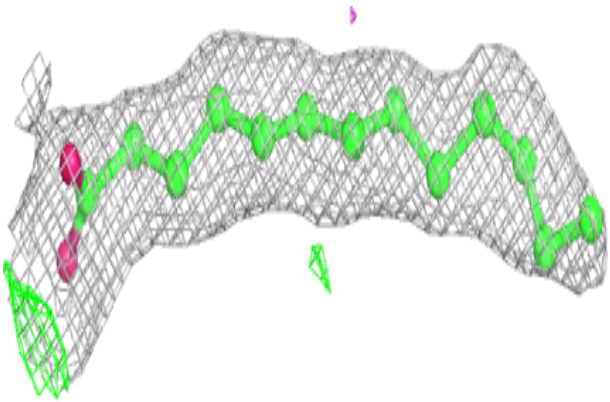


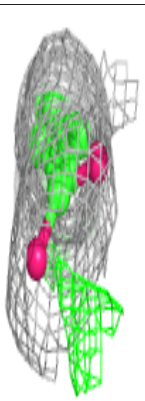


Electron density around STE M 101:

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

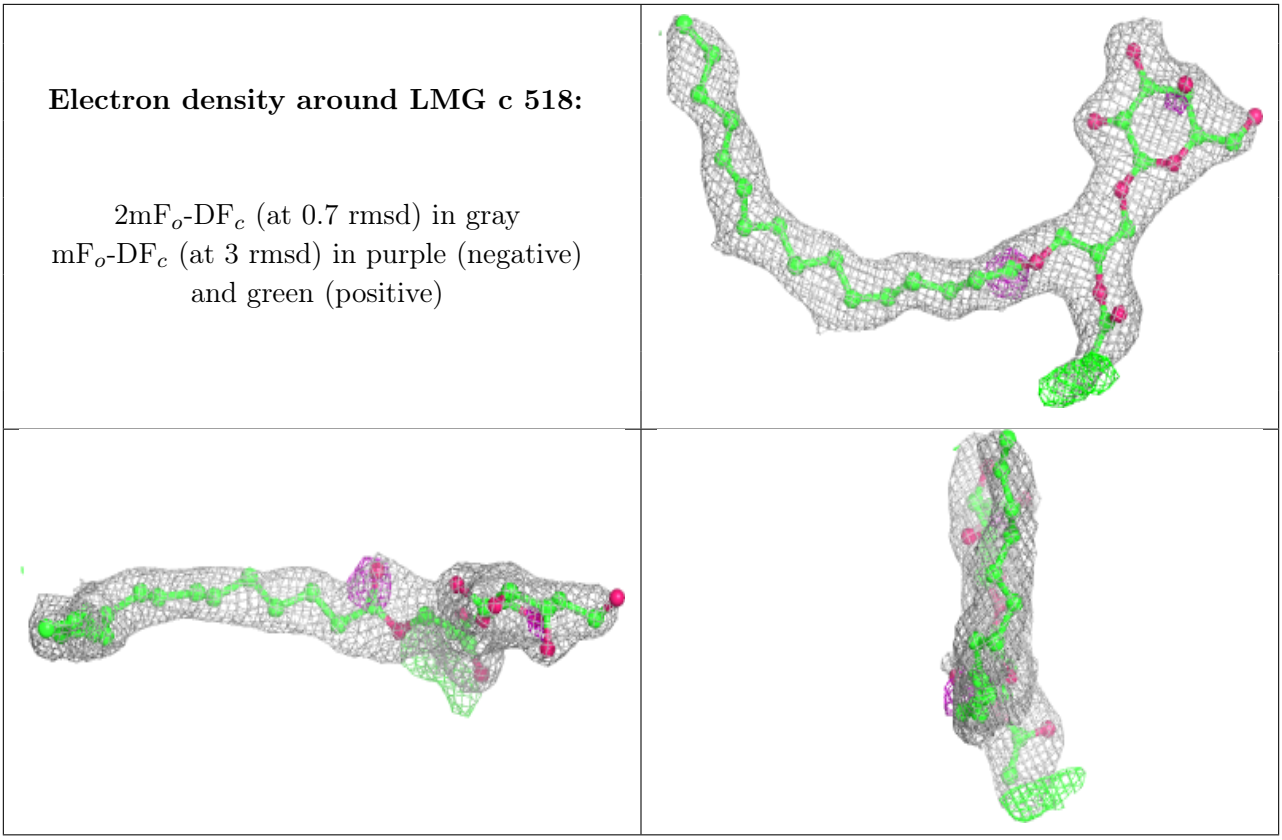






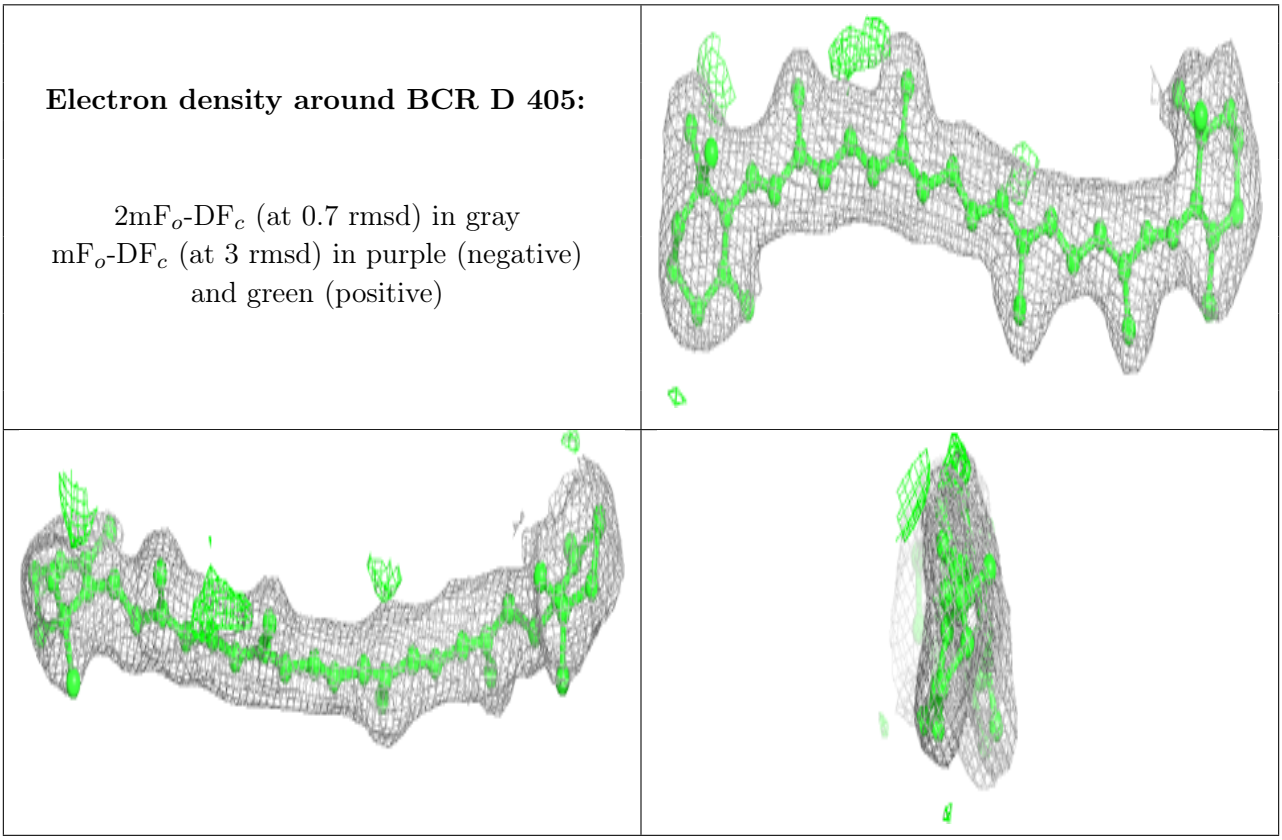
Electron density around LMG c 518:

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



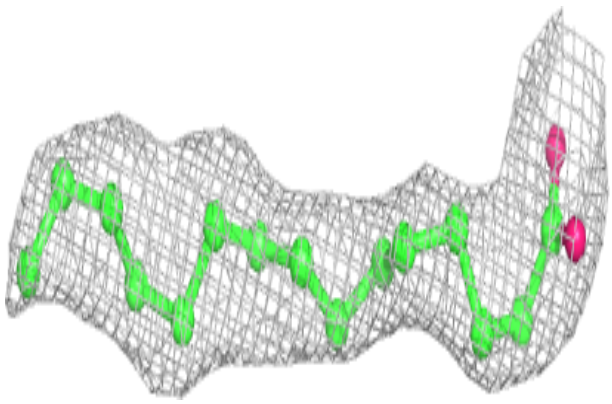
Electron density around BCR D 405:

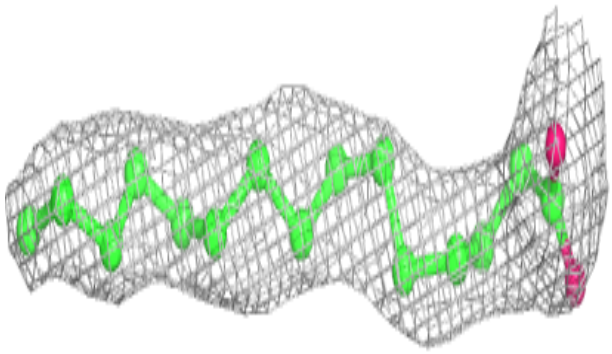
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

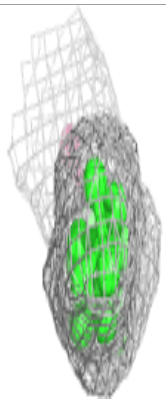


Electron density around STE d 411:

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

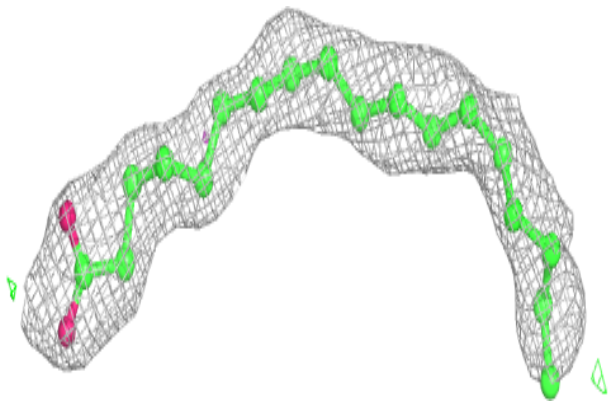


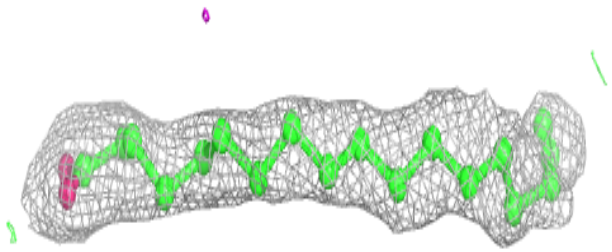


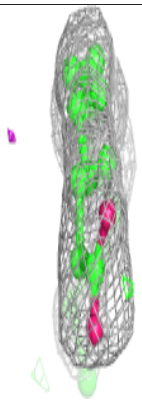


Electron density around STE d 412:

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

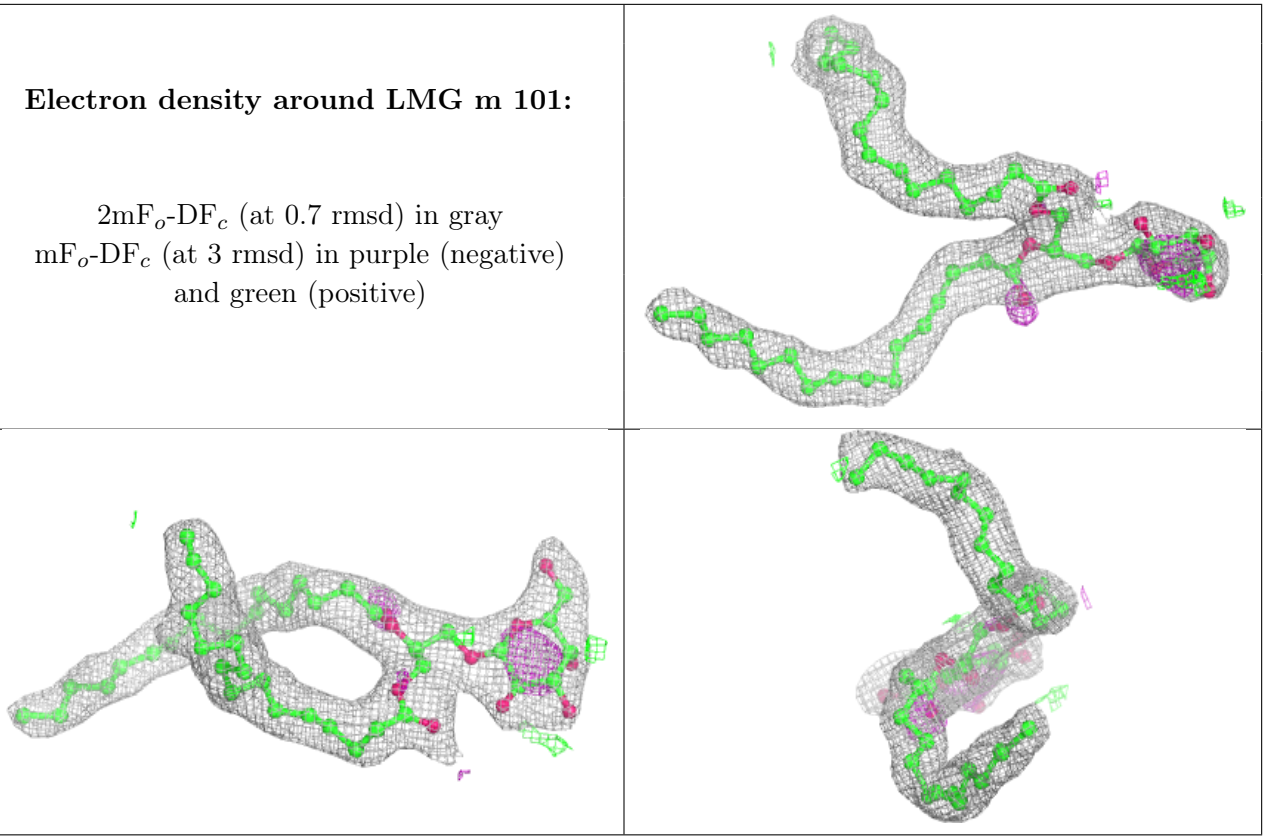






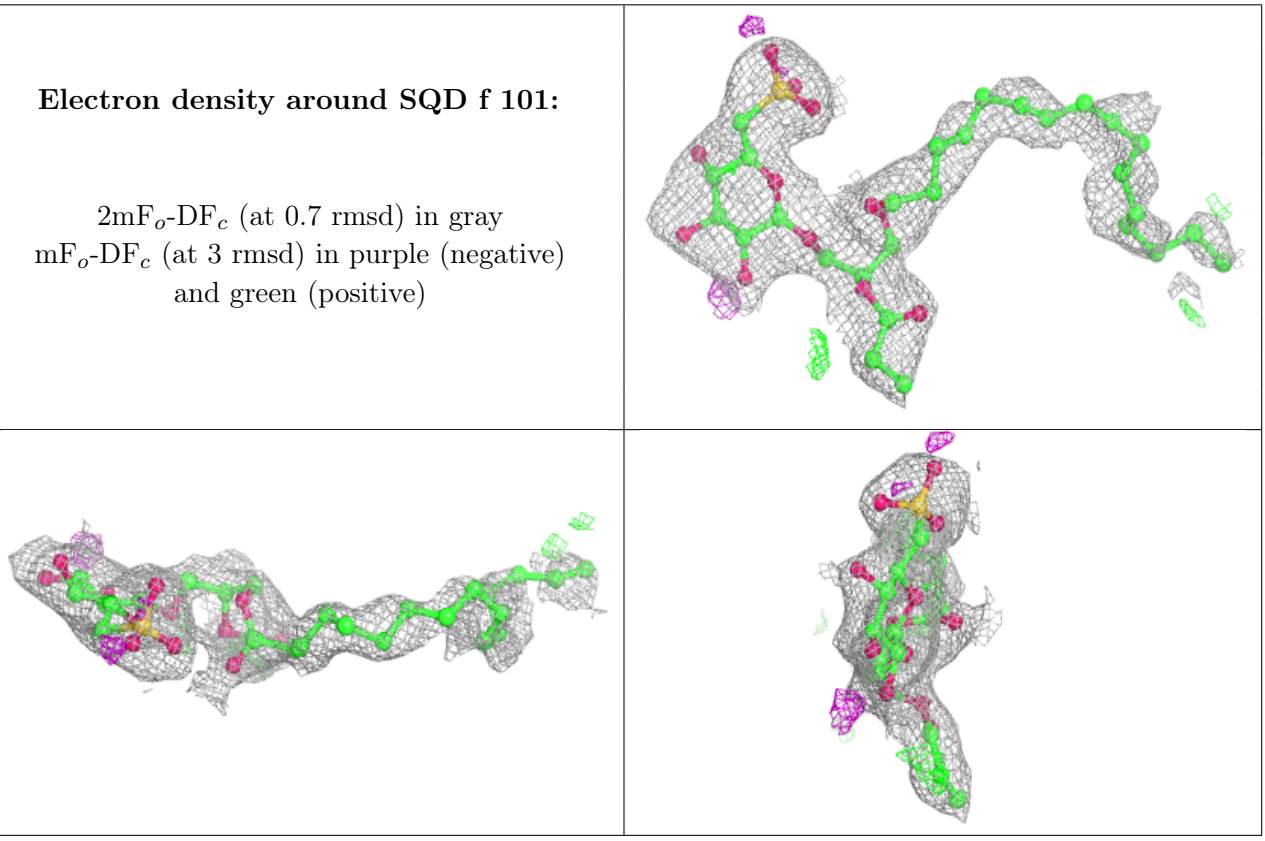
Electron density around LMG m 101:

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



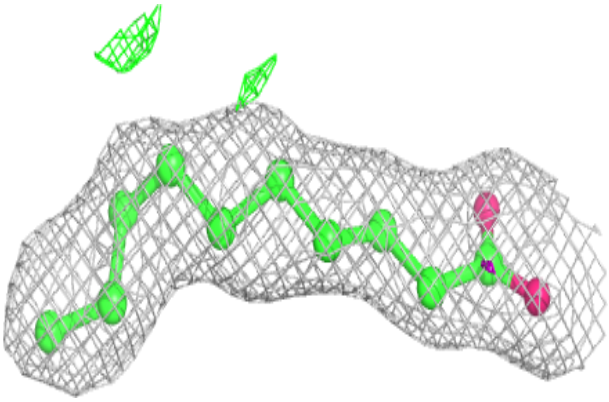
Electron density around SQD f 101:

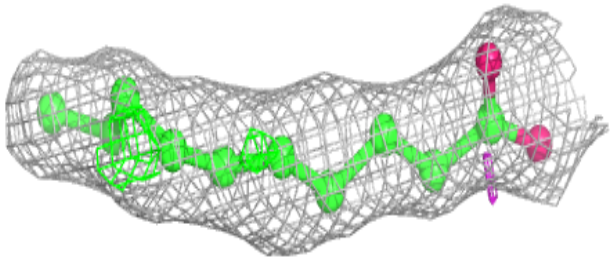
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

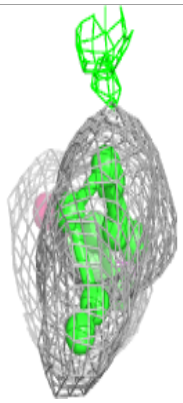


Electron density around STE m 102:

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

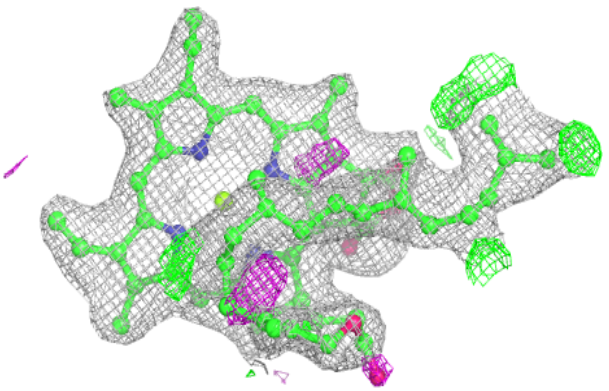


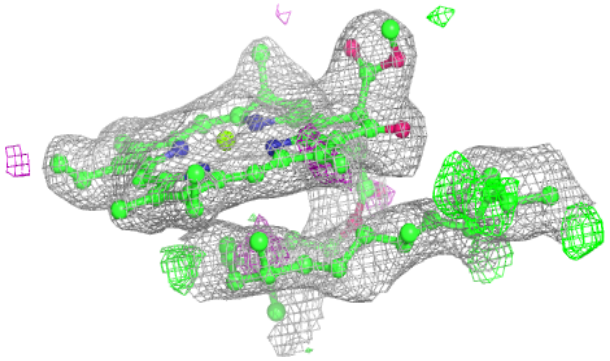


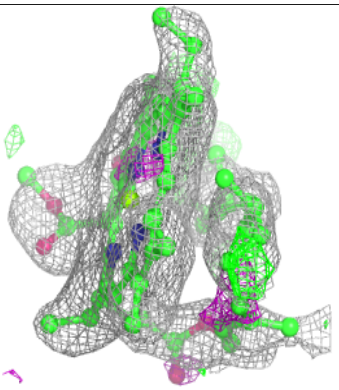


Electron density around CLA B 601:

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

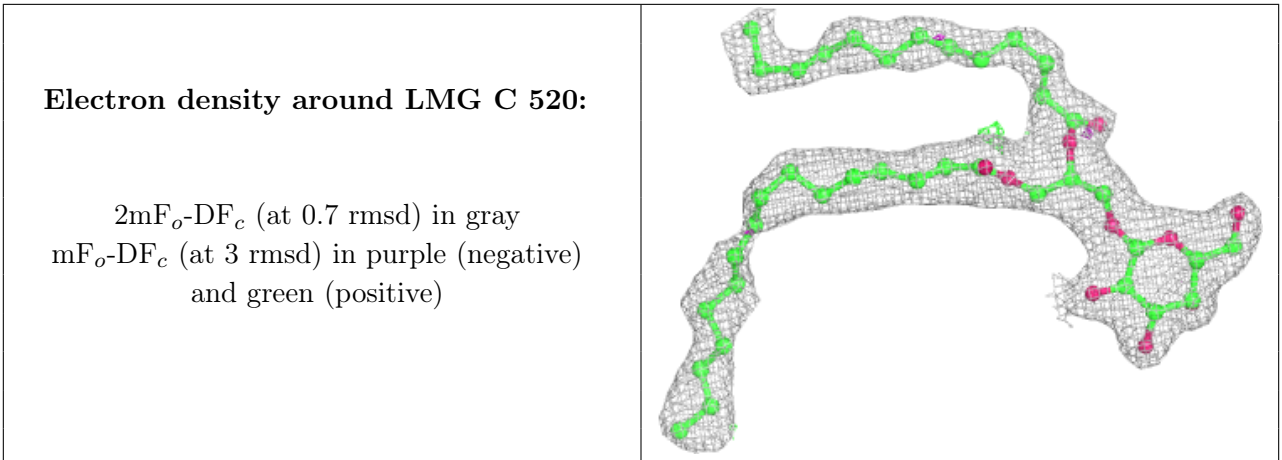


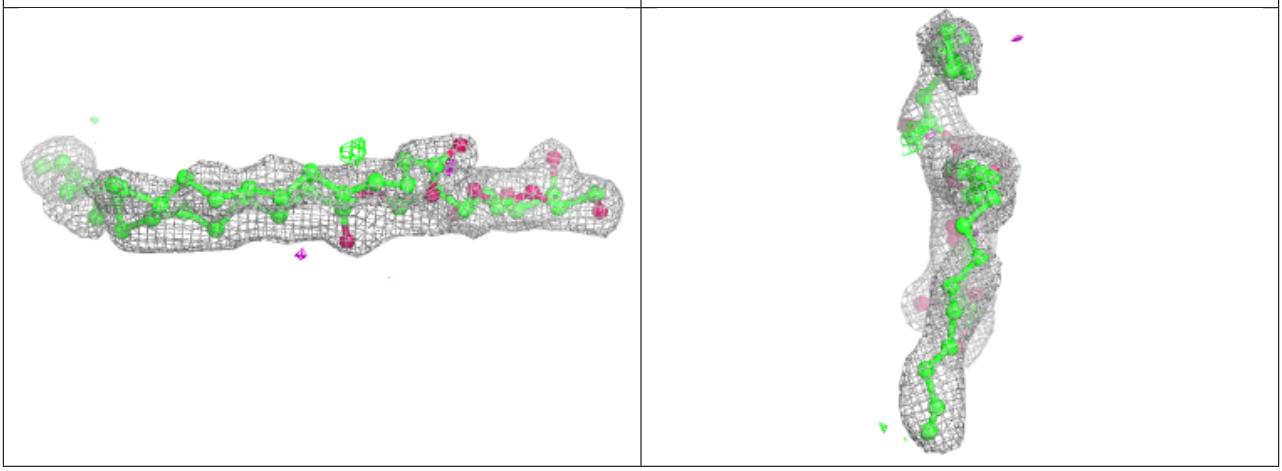




Electron density around LMG C 520:

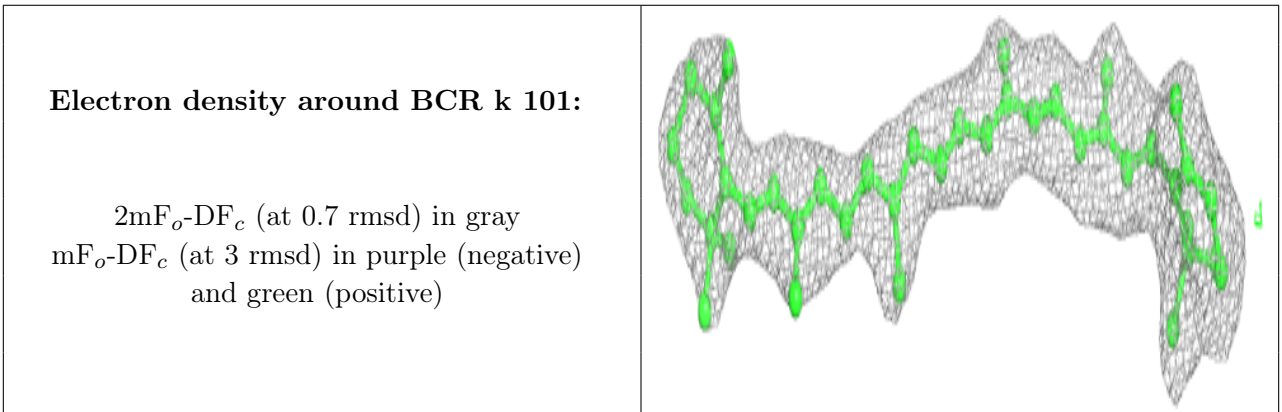
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

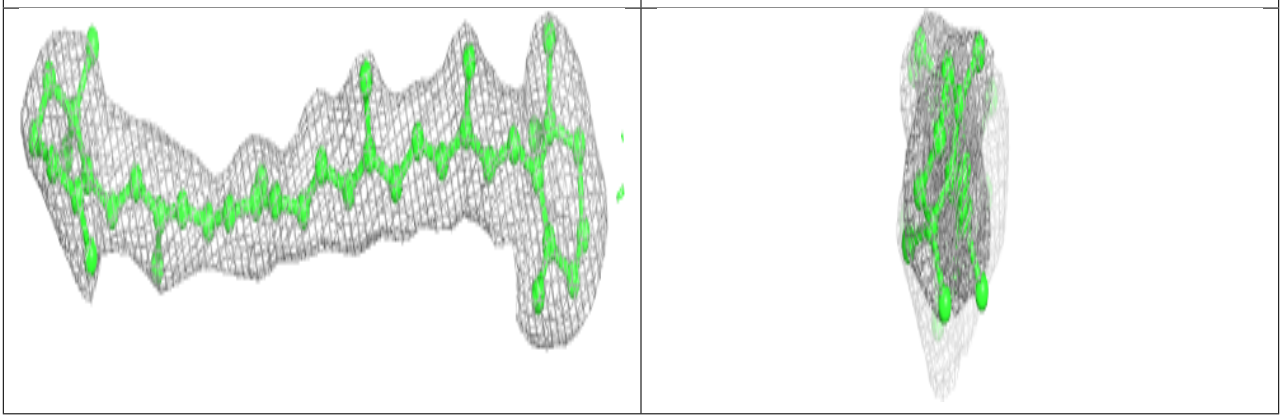




Electron density around BCR k 101:

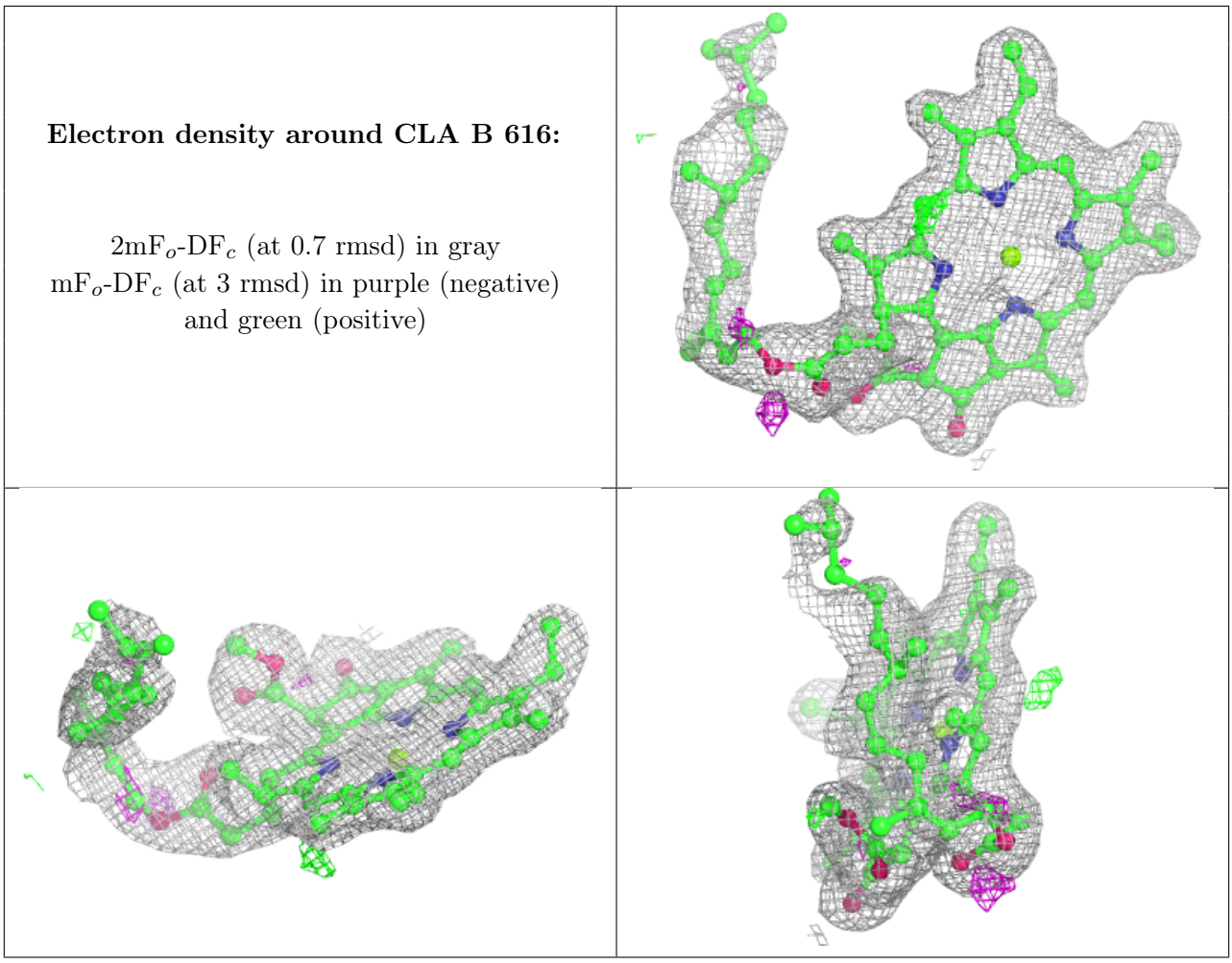
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





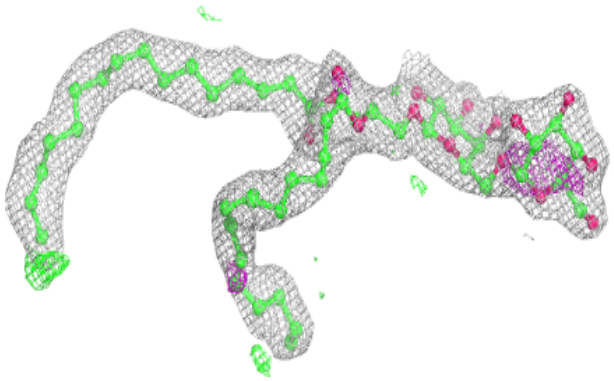
Electron density around CLA B 616:

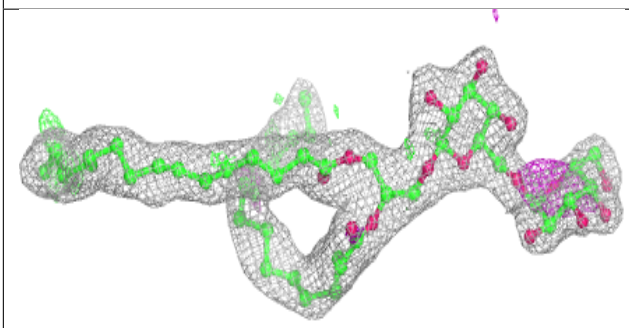
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

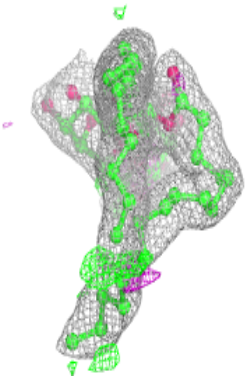


Electron density around DGD H 102:

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

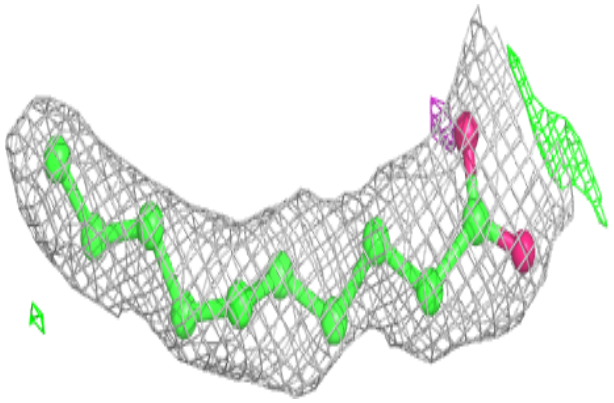


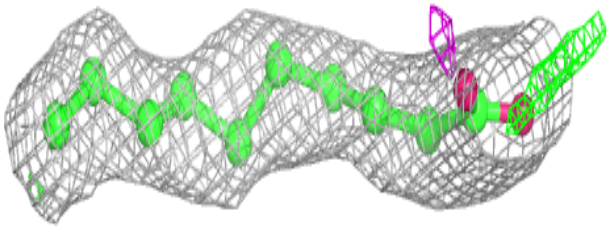


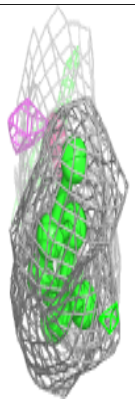


Electron density around STE C 522:

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

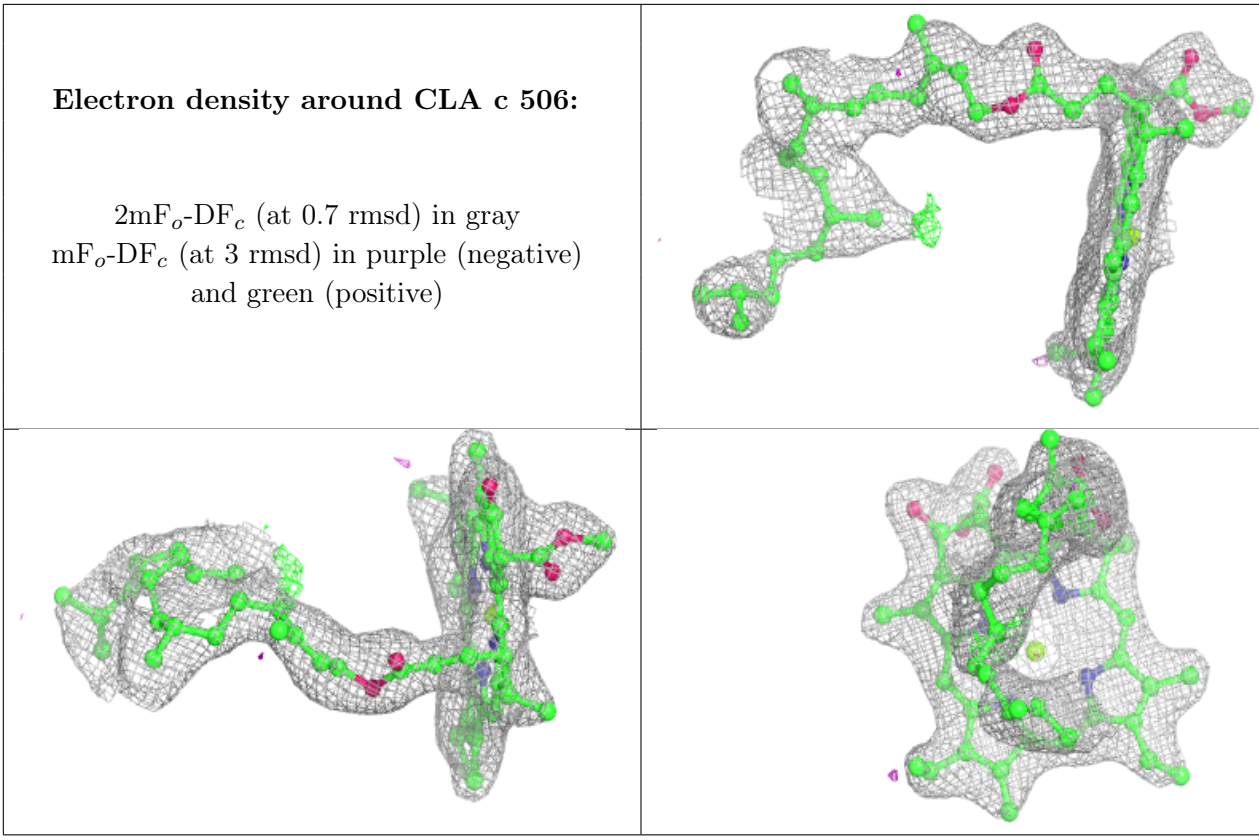






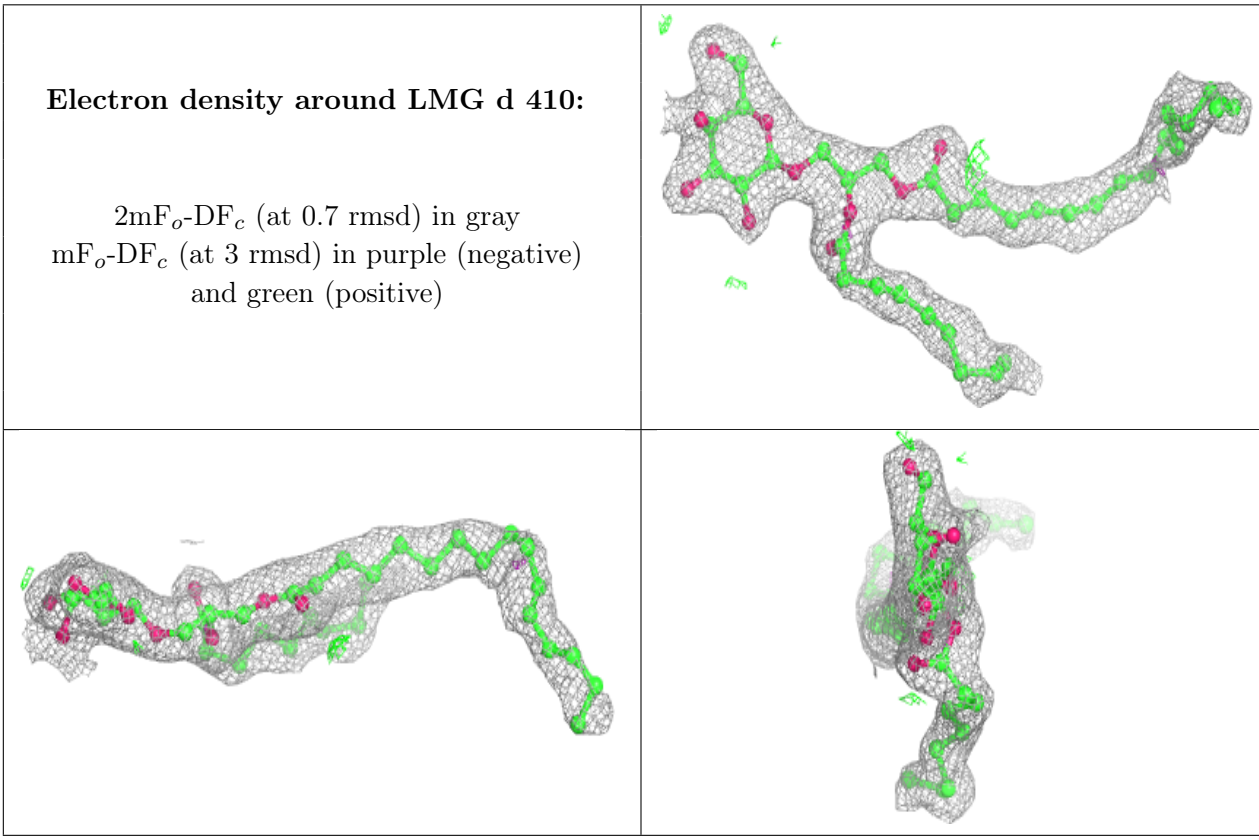
Electron density around CLA c 506:

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



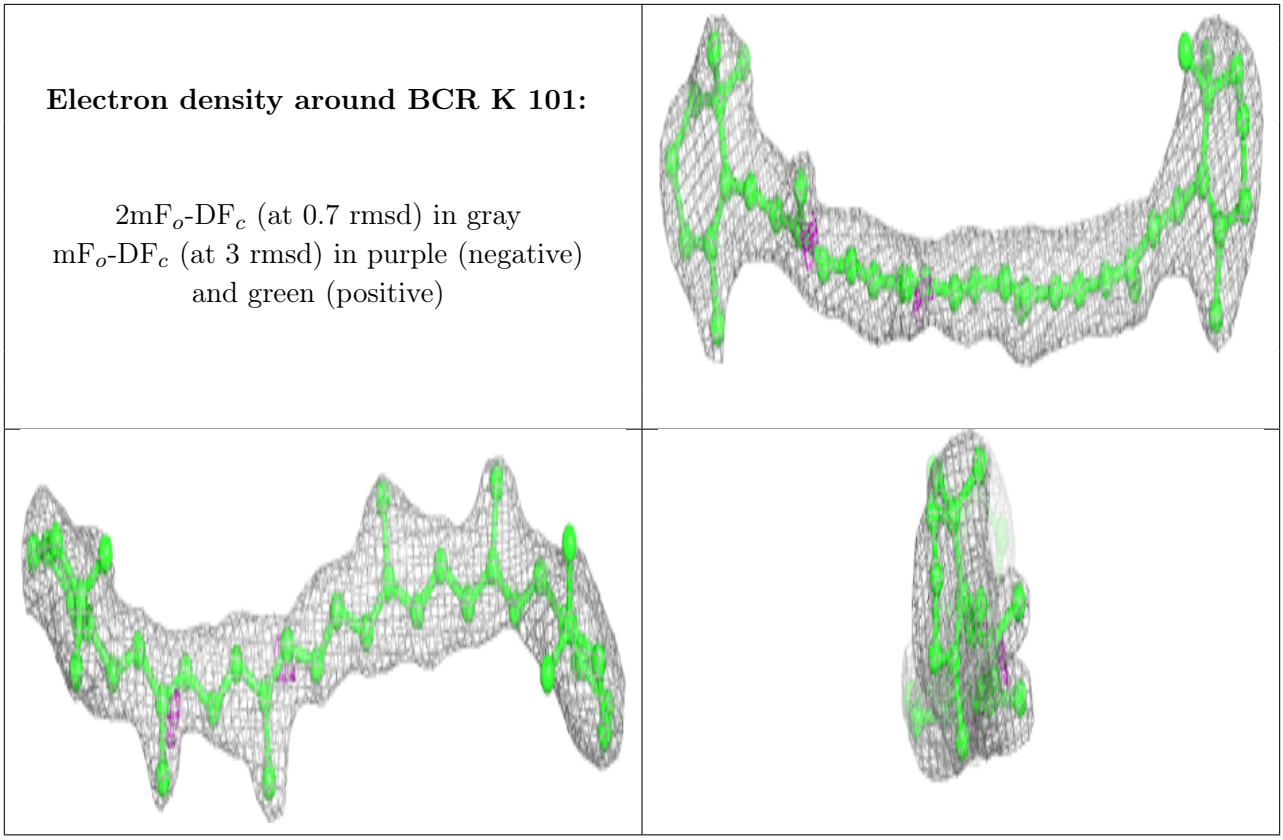
Electron density around LMG d 410:

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



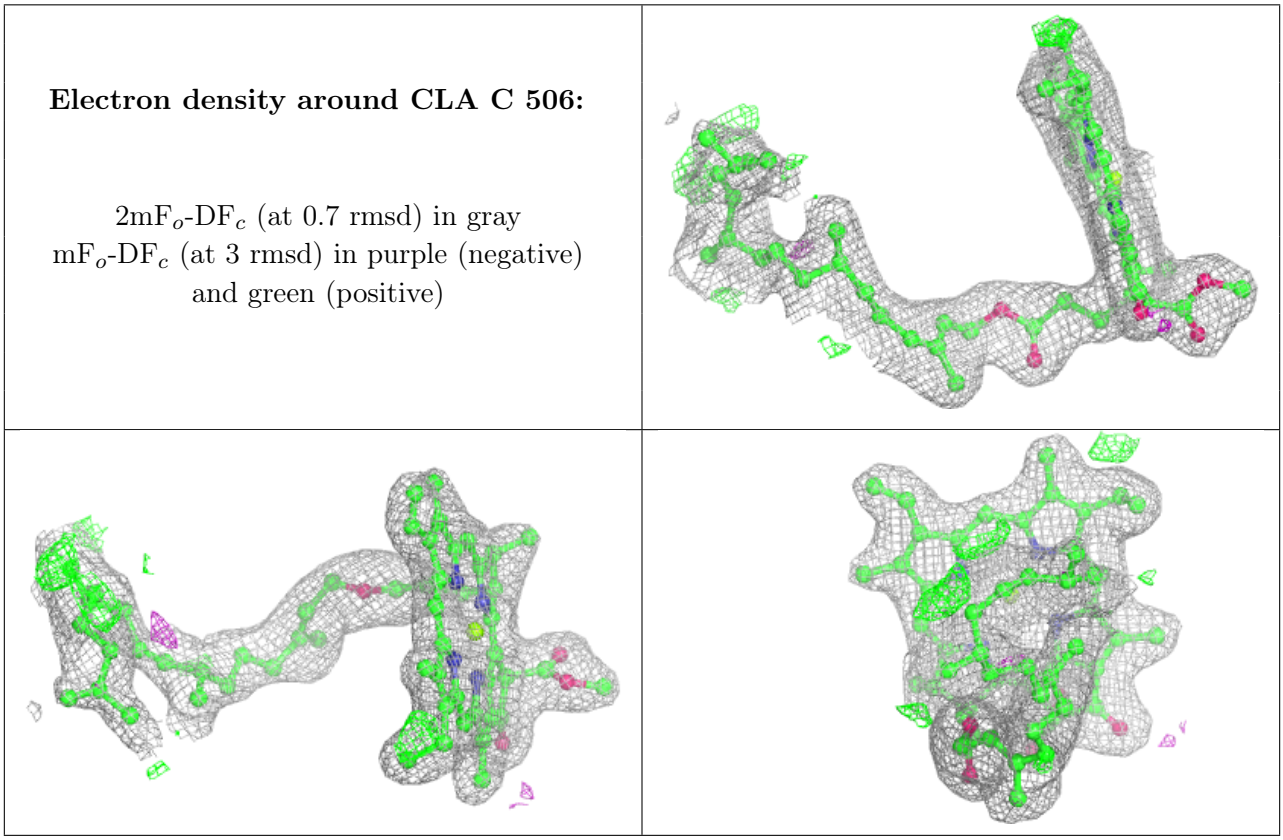
Electron density around BCR K 101:

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



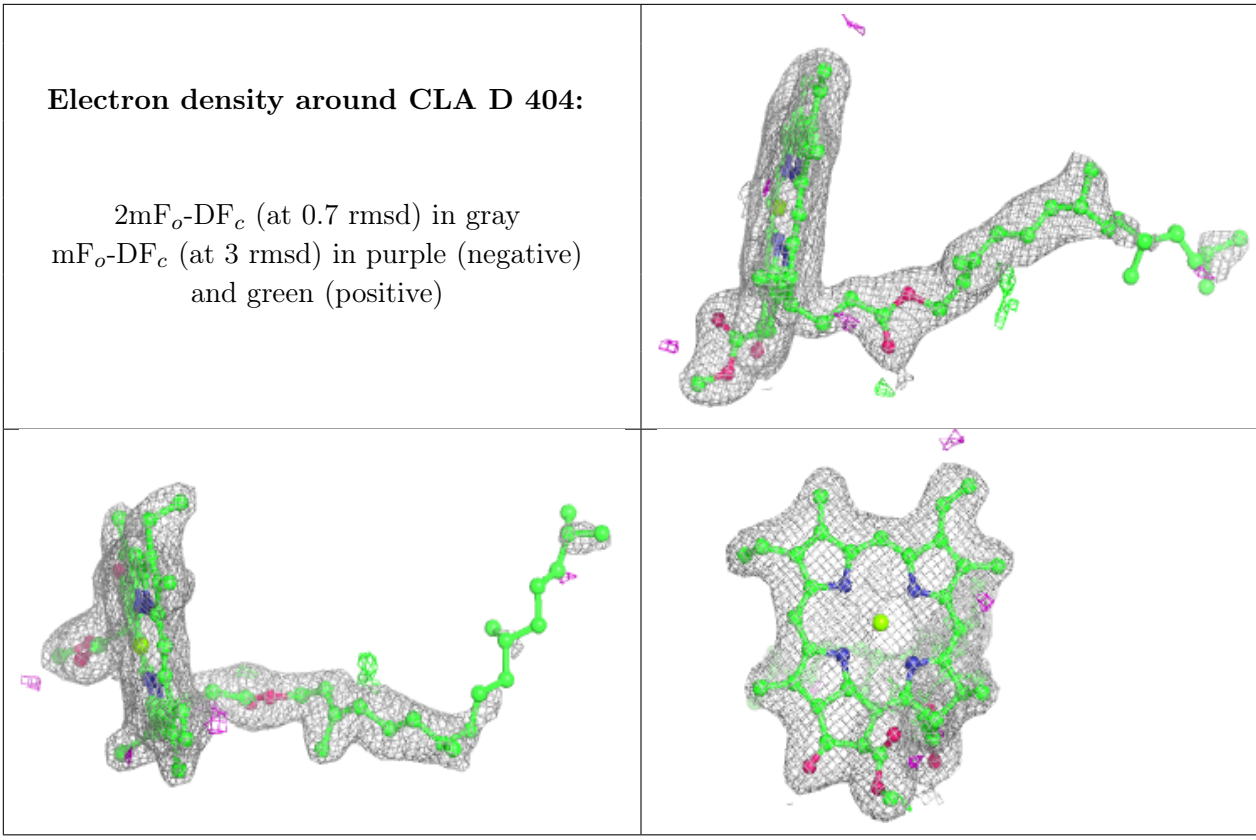
Electron density around CLA C 506:

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



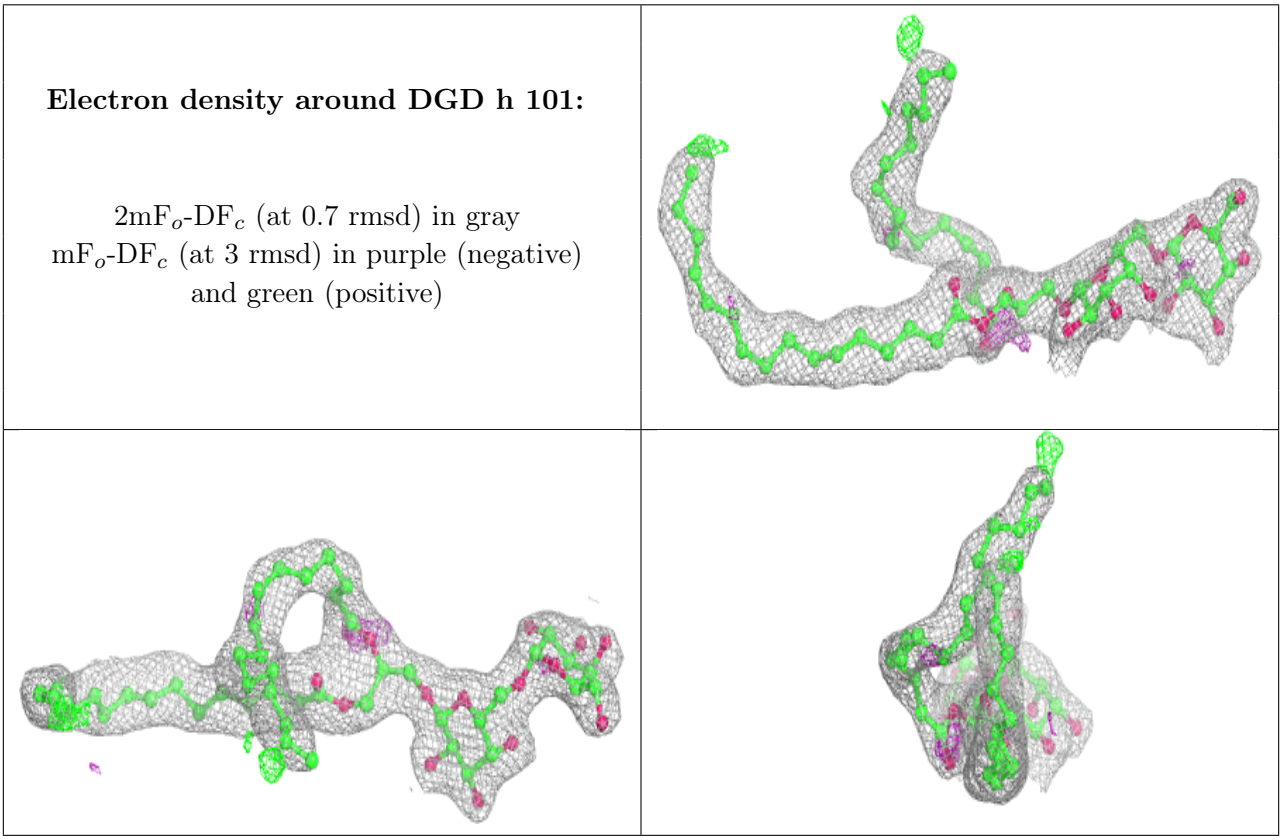
Electron density around CLA D 404:

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



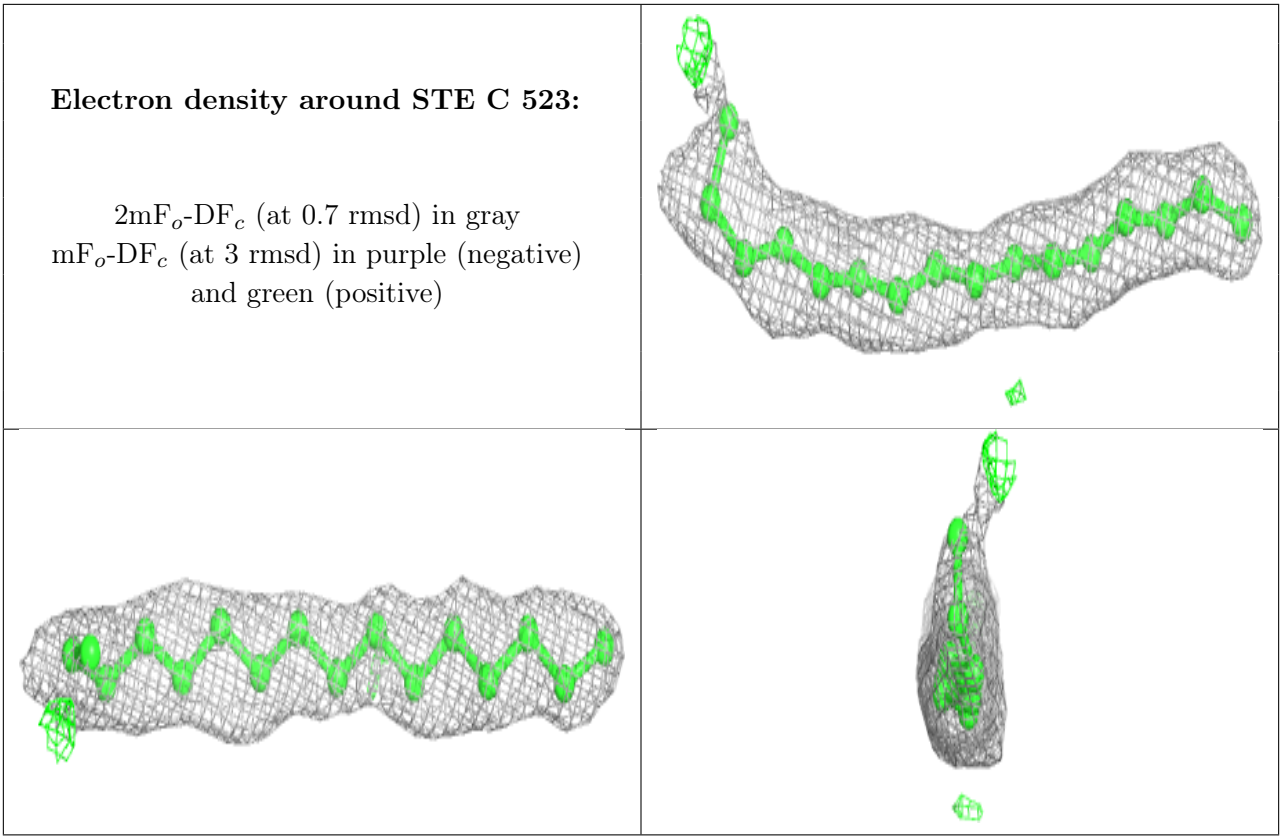
Electron density around DGD h 101:

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



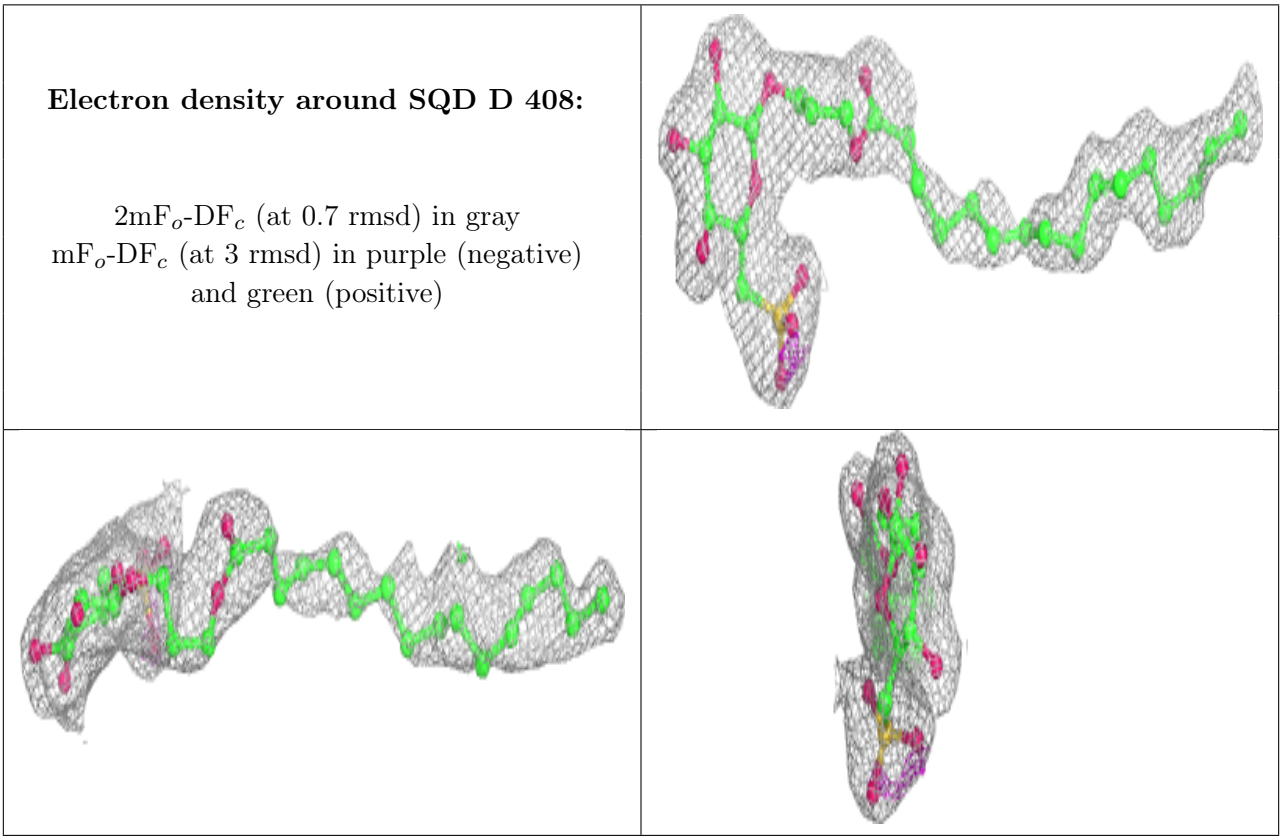
Electron density around STE C 523:

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



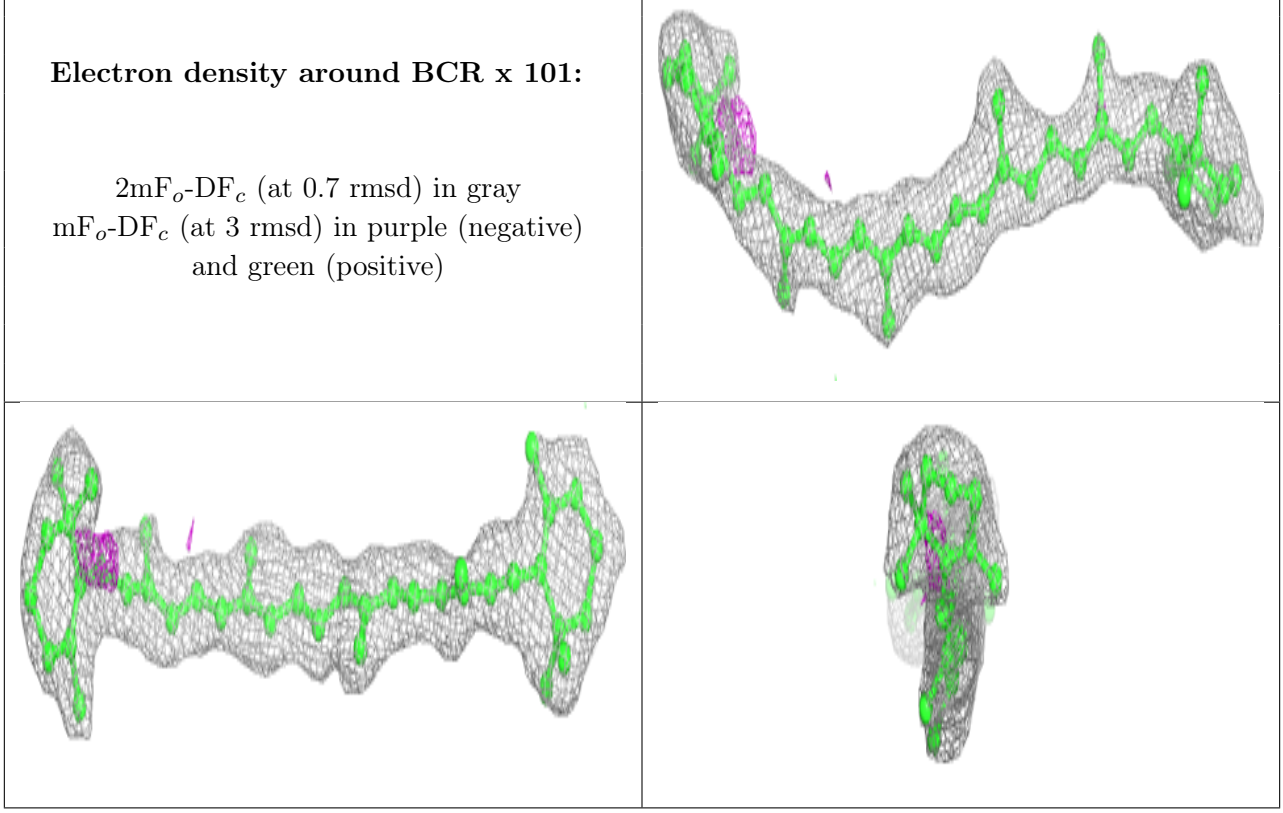
Electron density around SQD D 408:

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



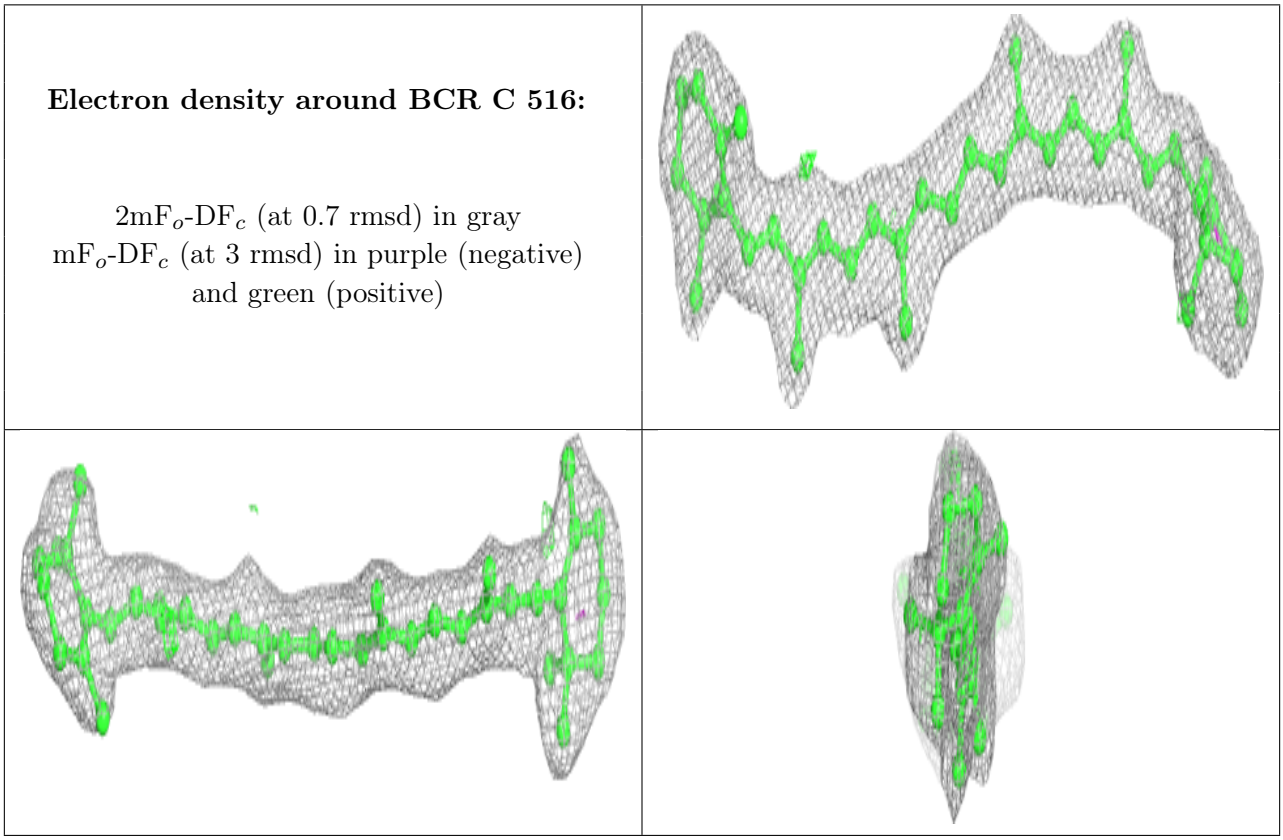
Electron density around BCR x 101:

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



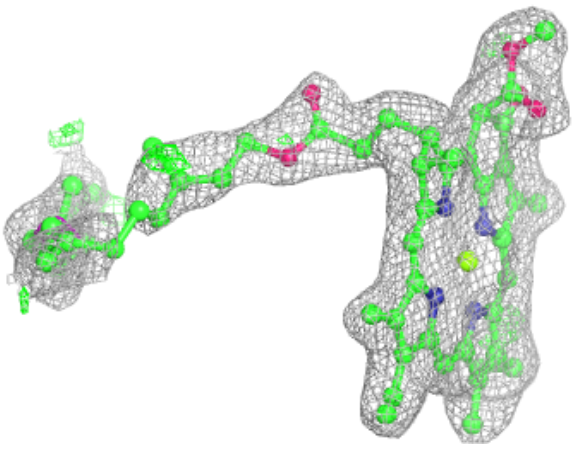
Electron density around BCR C 516:

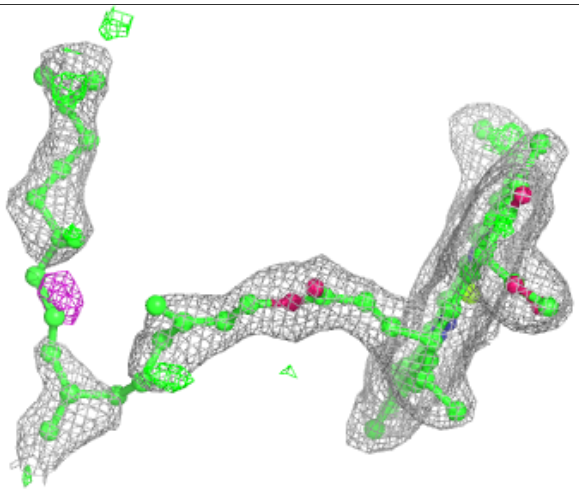
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

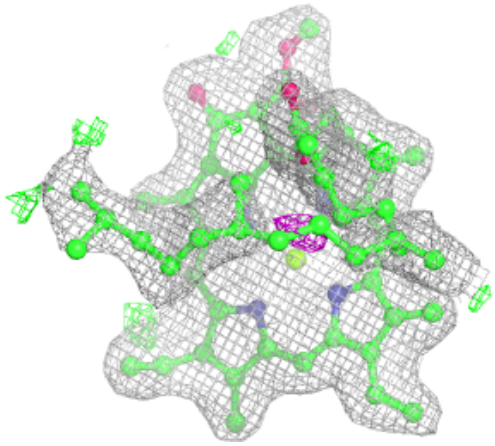


Electron density around CLA a 609:

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

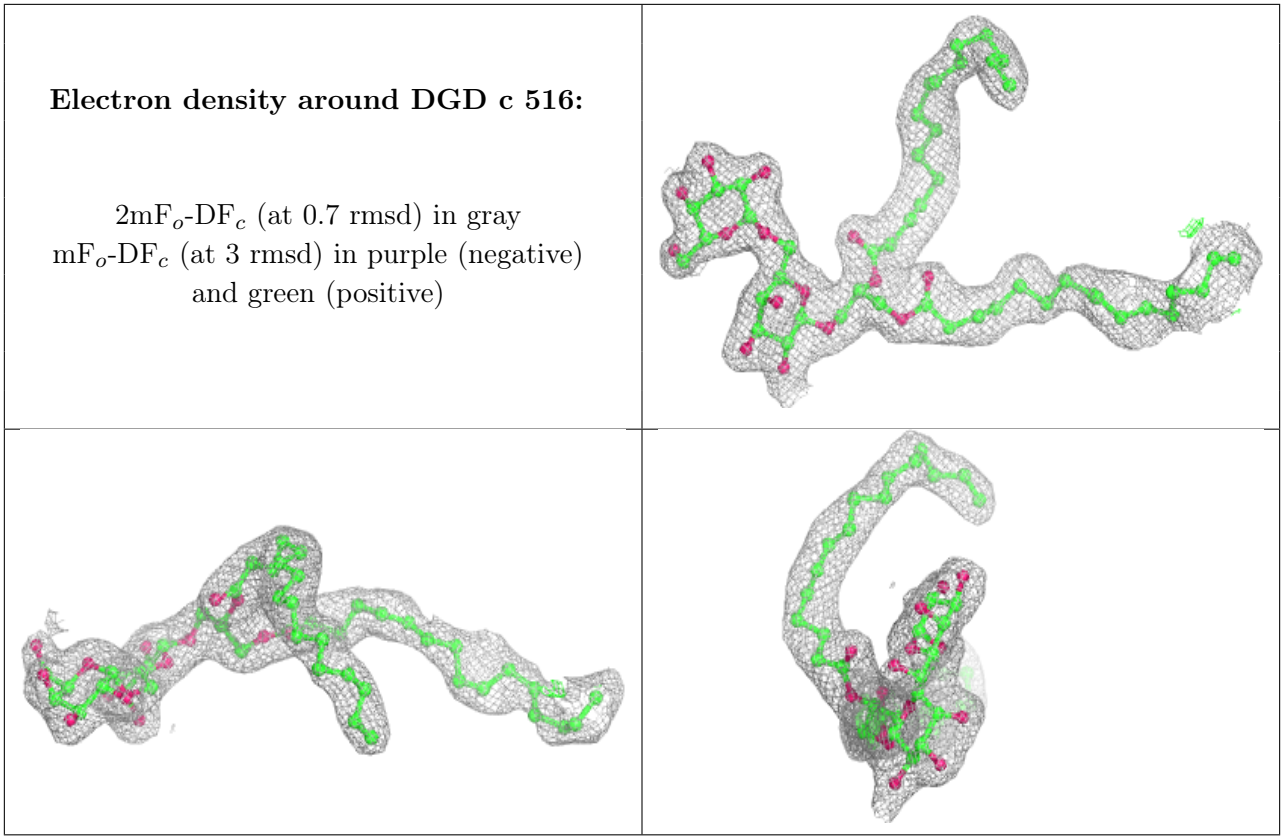






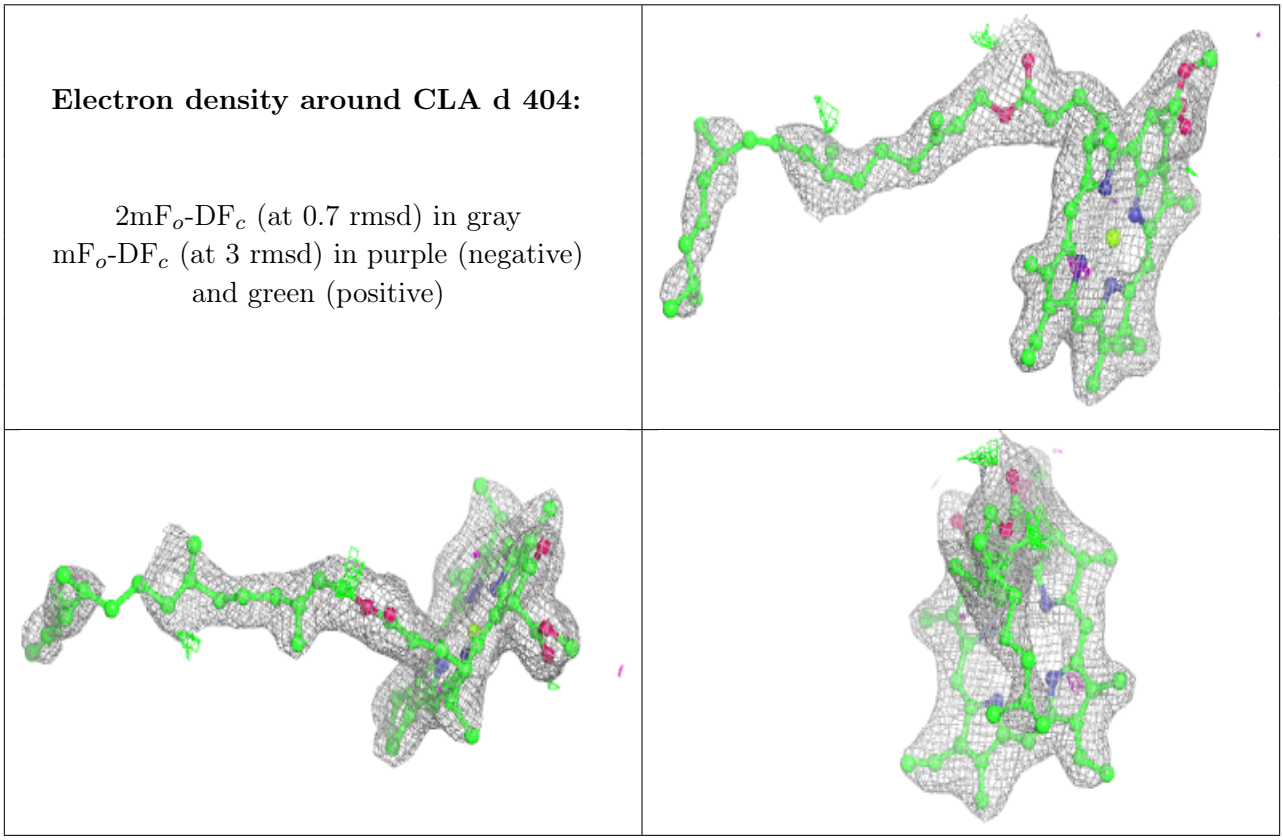
Electron density around DGD c 516:

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



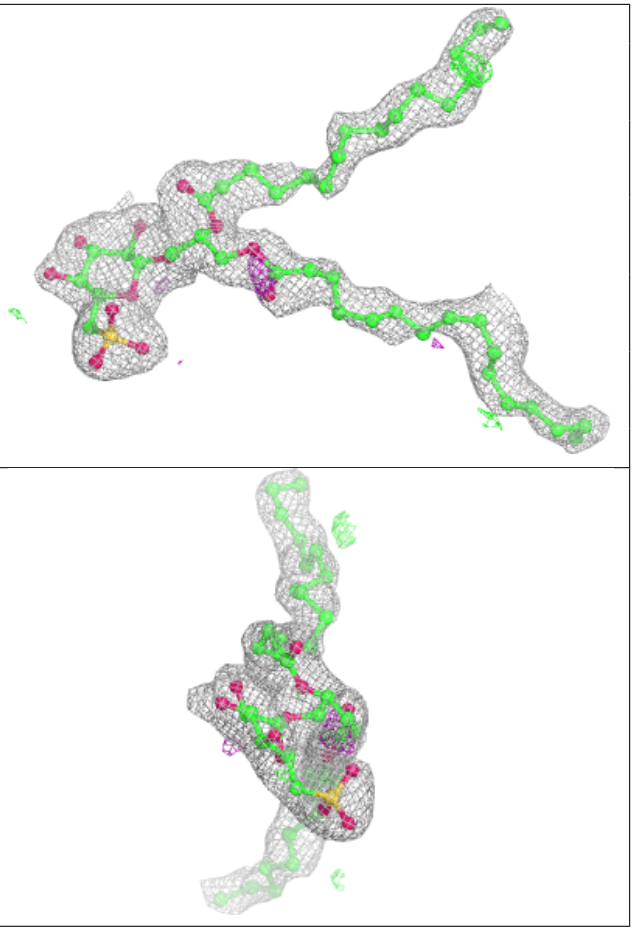
Electron density around CLA d 404:

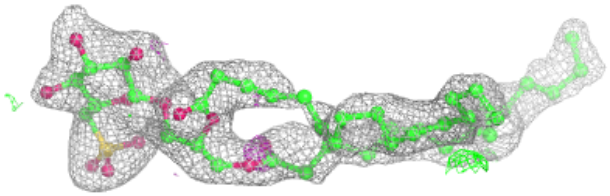
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD a 614:

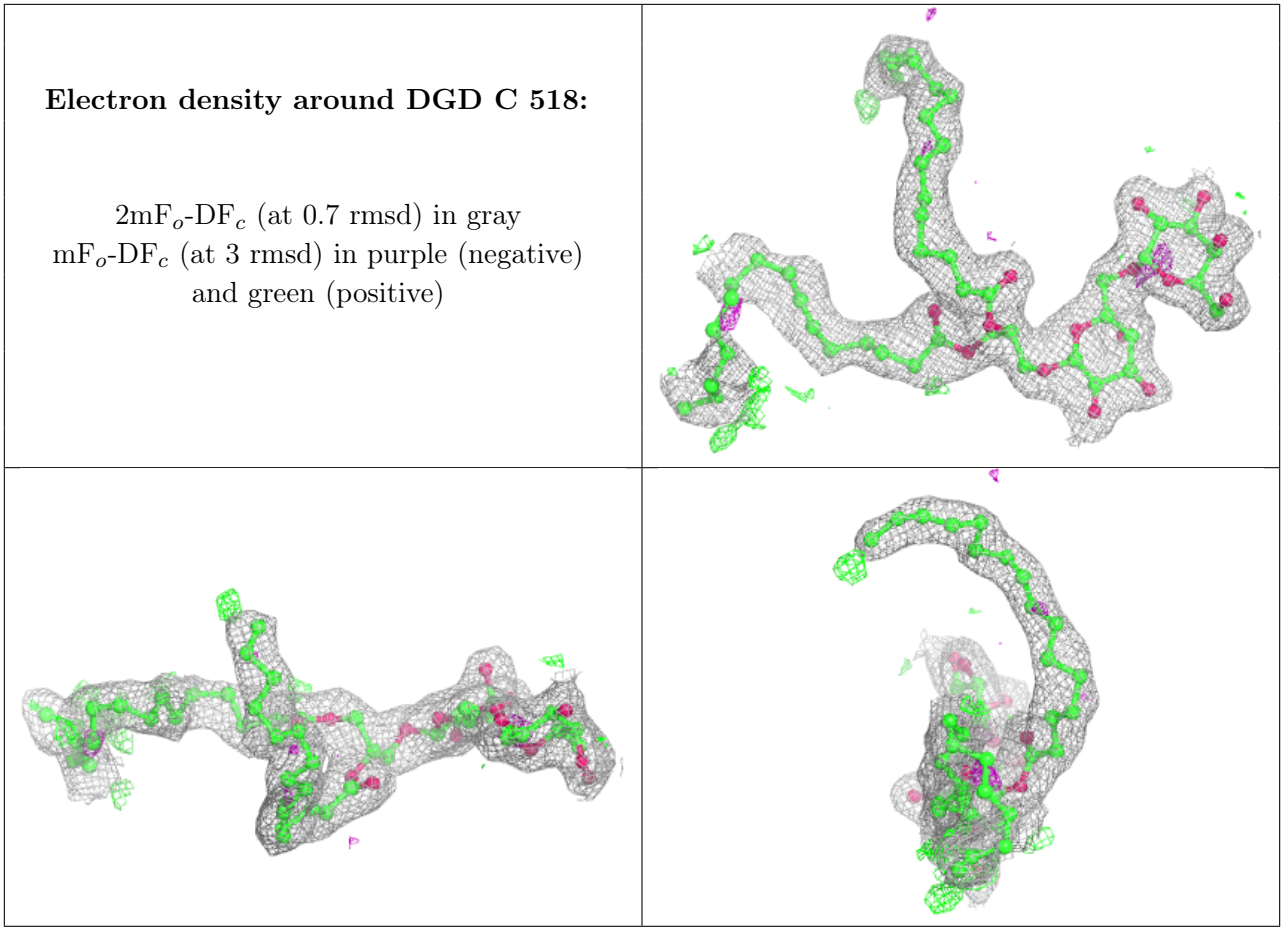
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





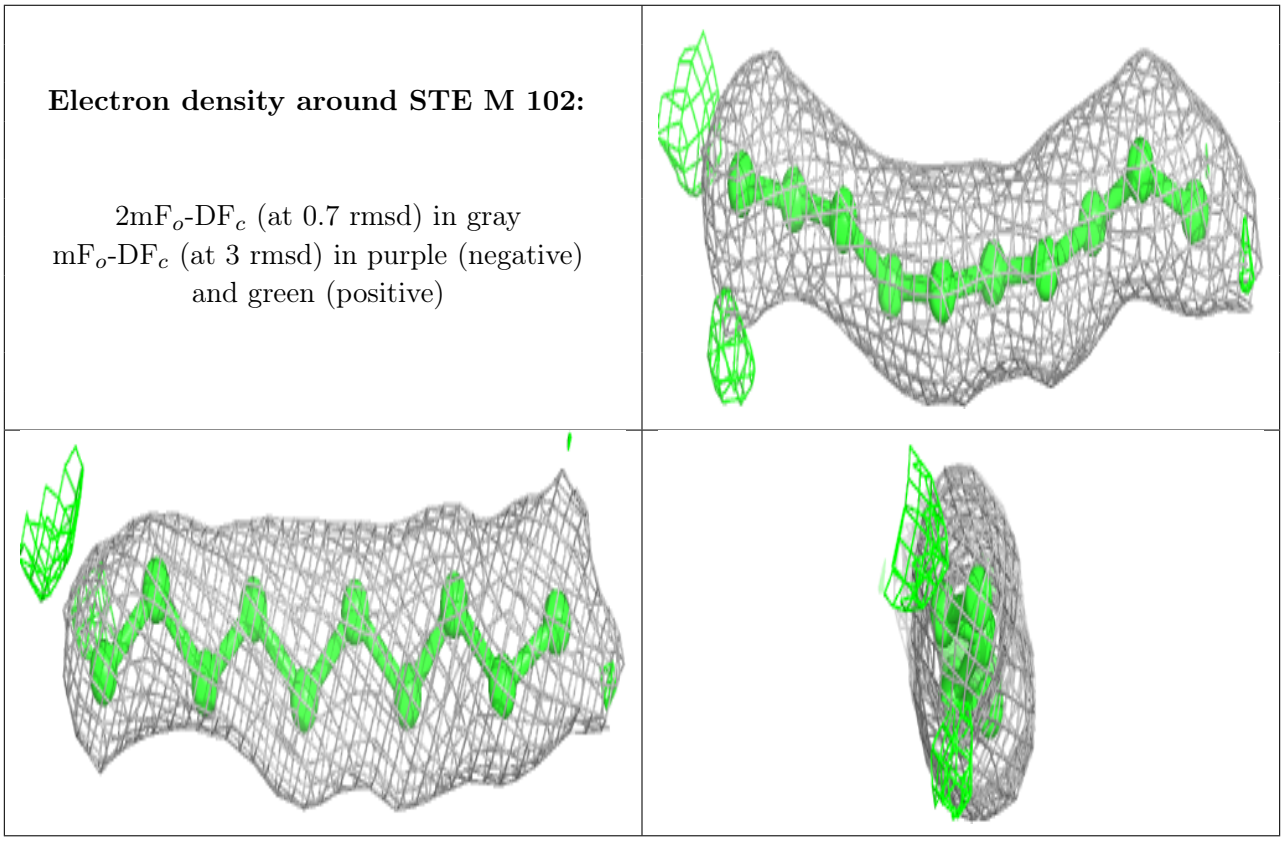
Electron density around DGD C 518:

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



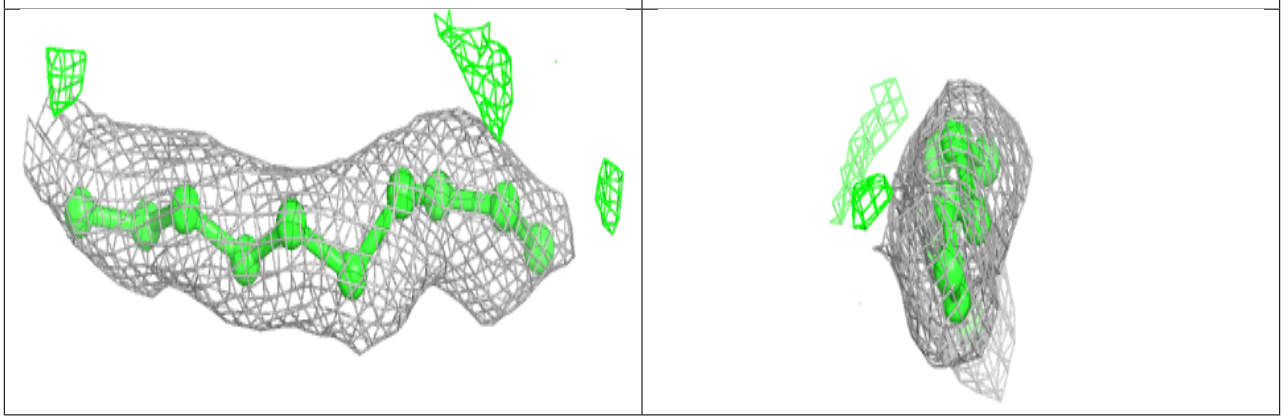
Electron density around STE M 102:

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



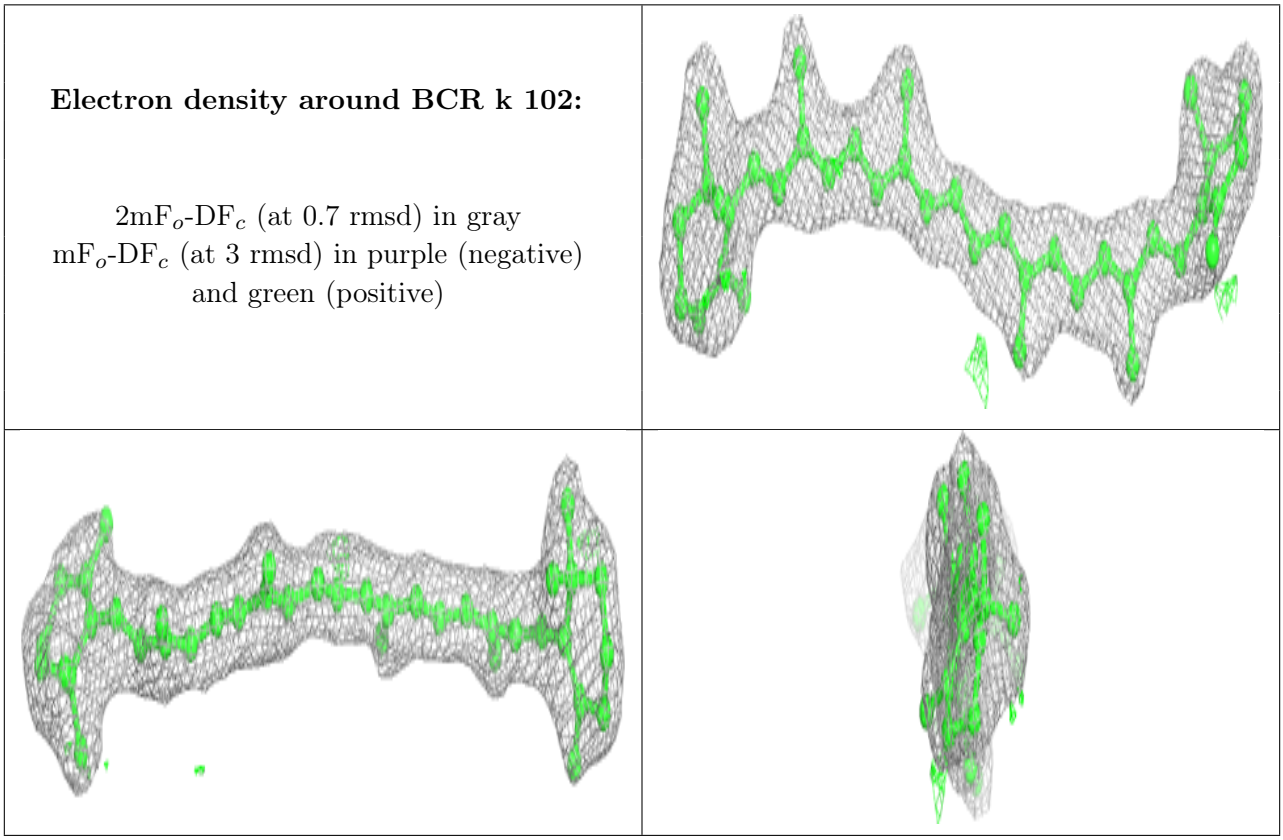
Electron density around STE b 625:

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



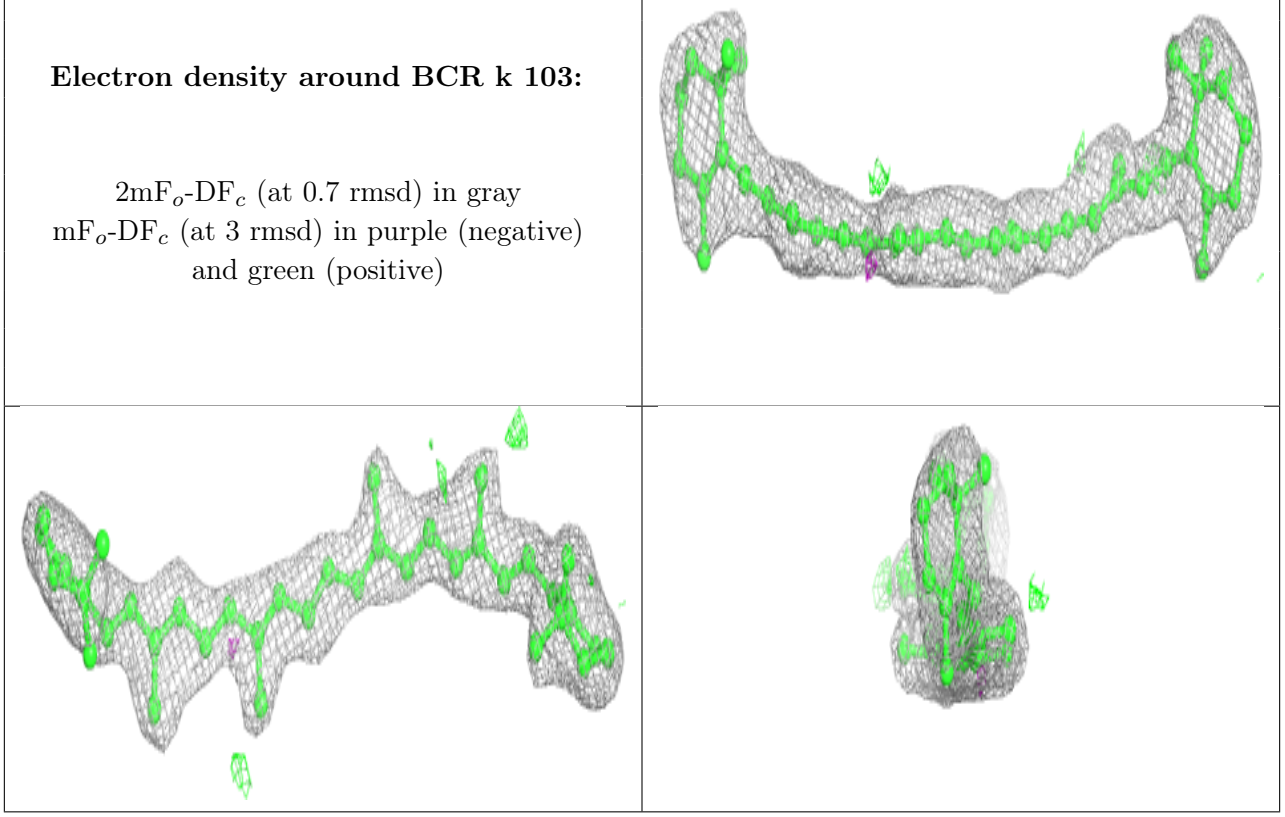
Electron density around BCR k 102:

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



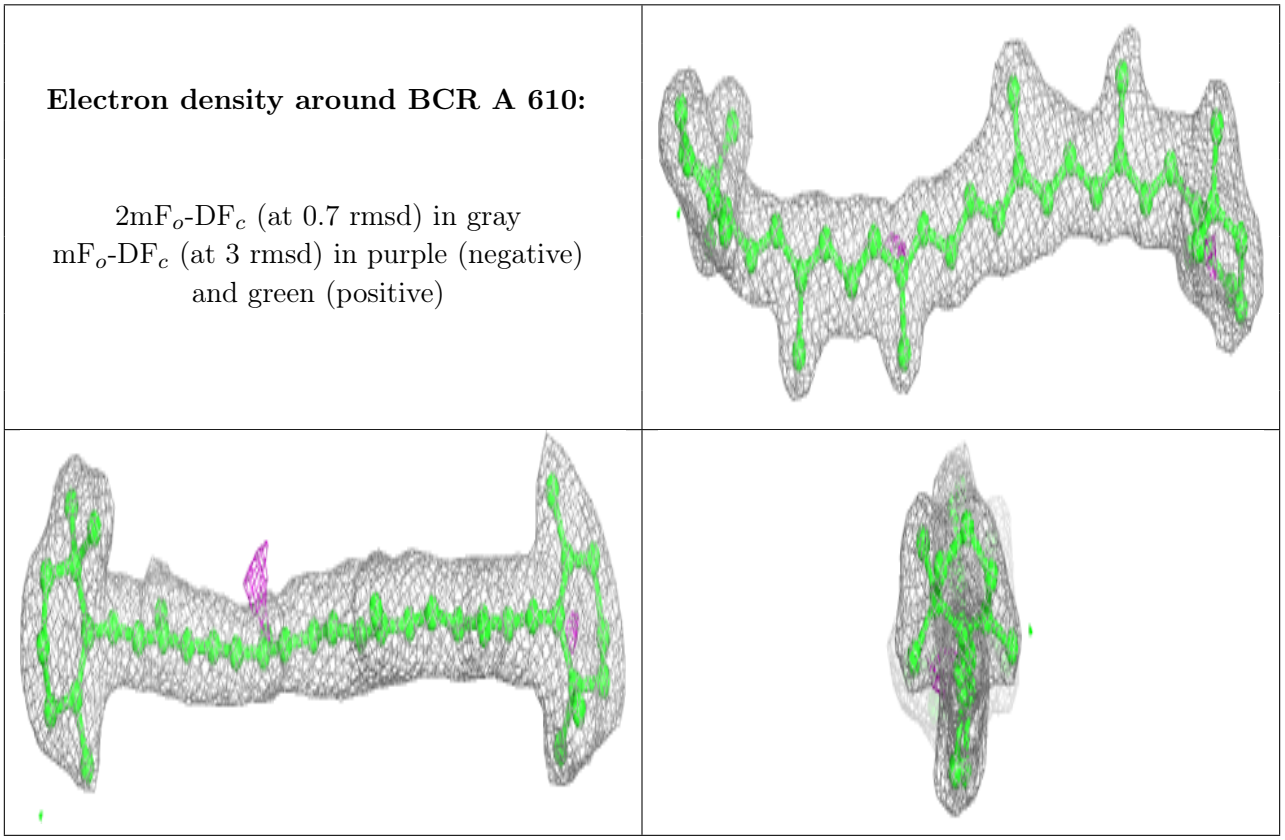
Electron density around BCR k 103:

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



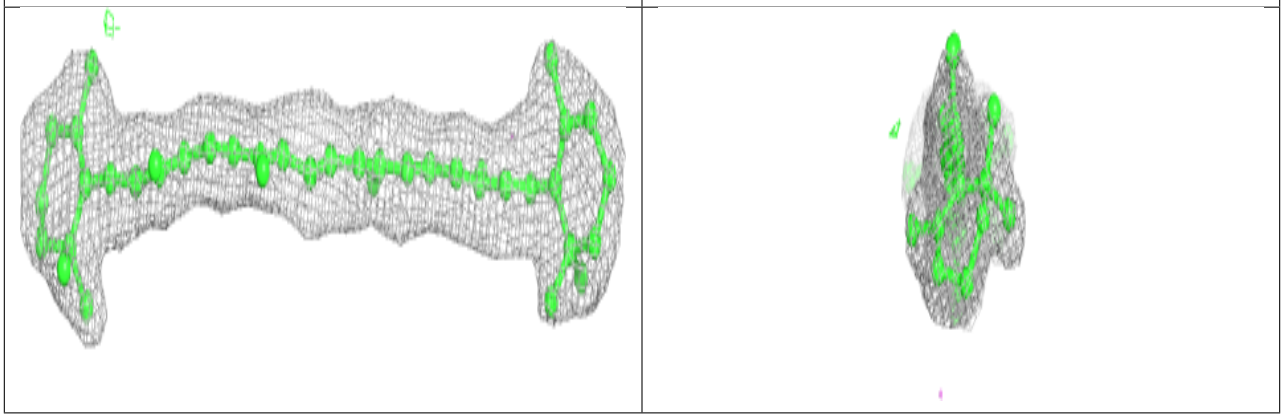
Electron density around BCR A 610:

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



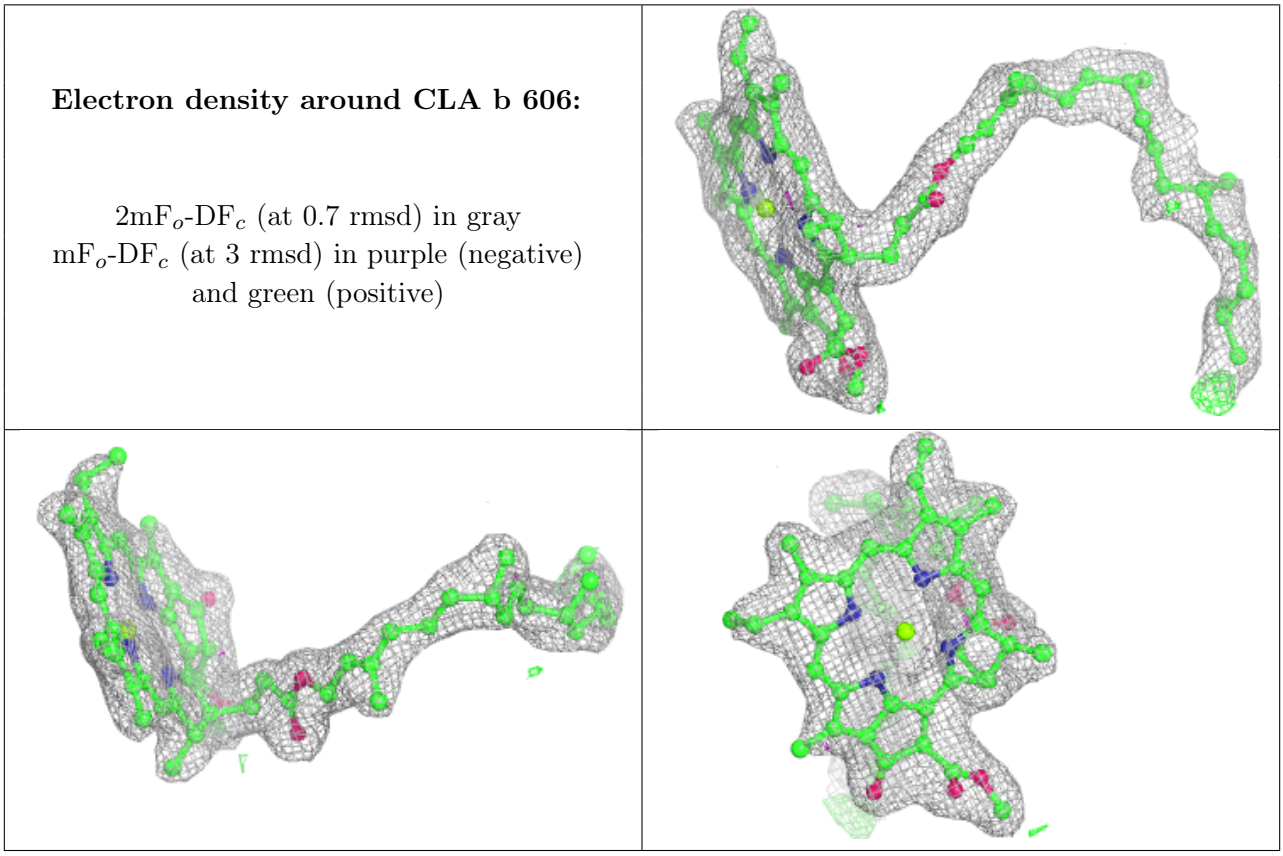
Electron density around BCR C 514:

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



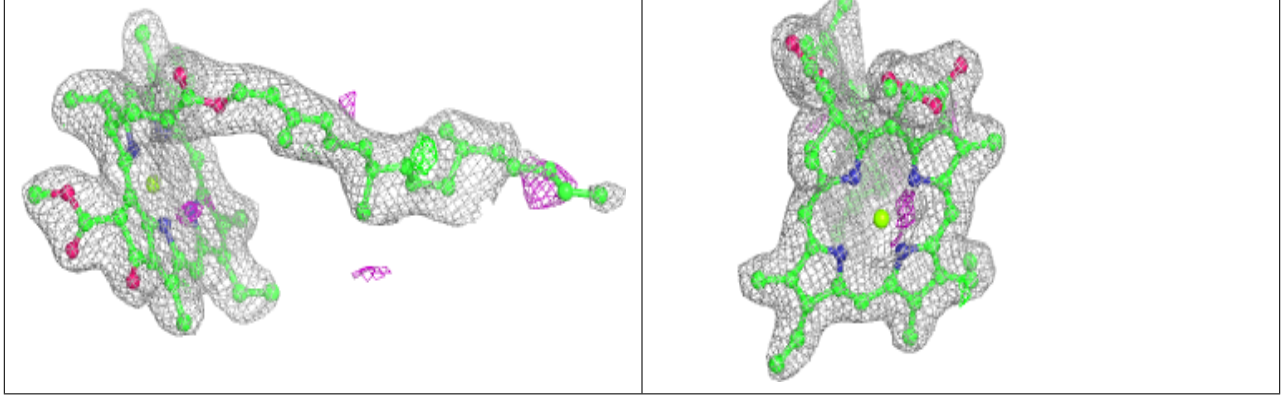
Electron density around CLA b 606:

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



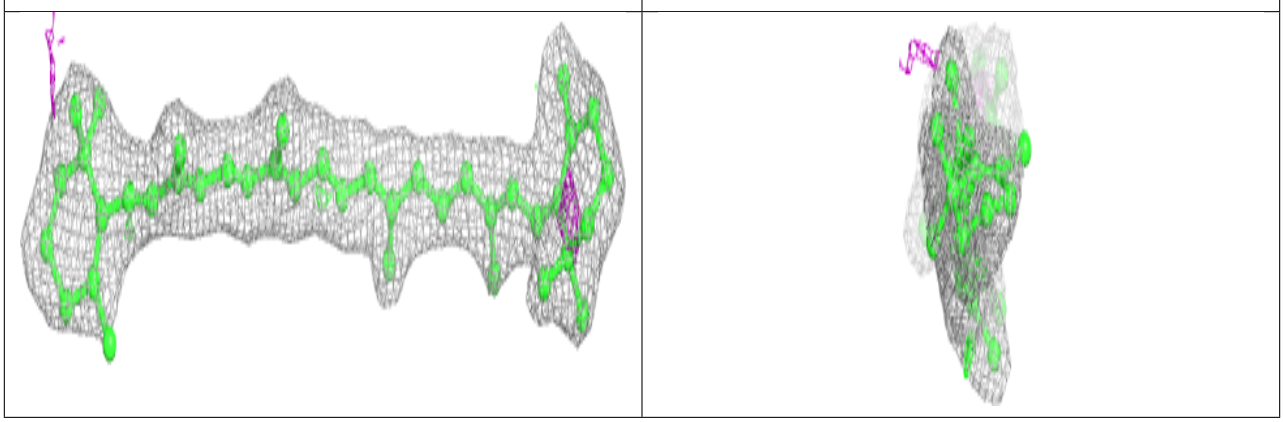
Electron density around CLA c 508:

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



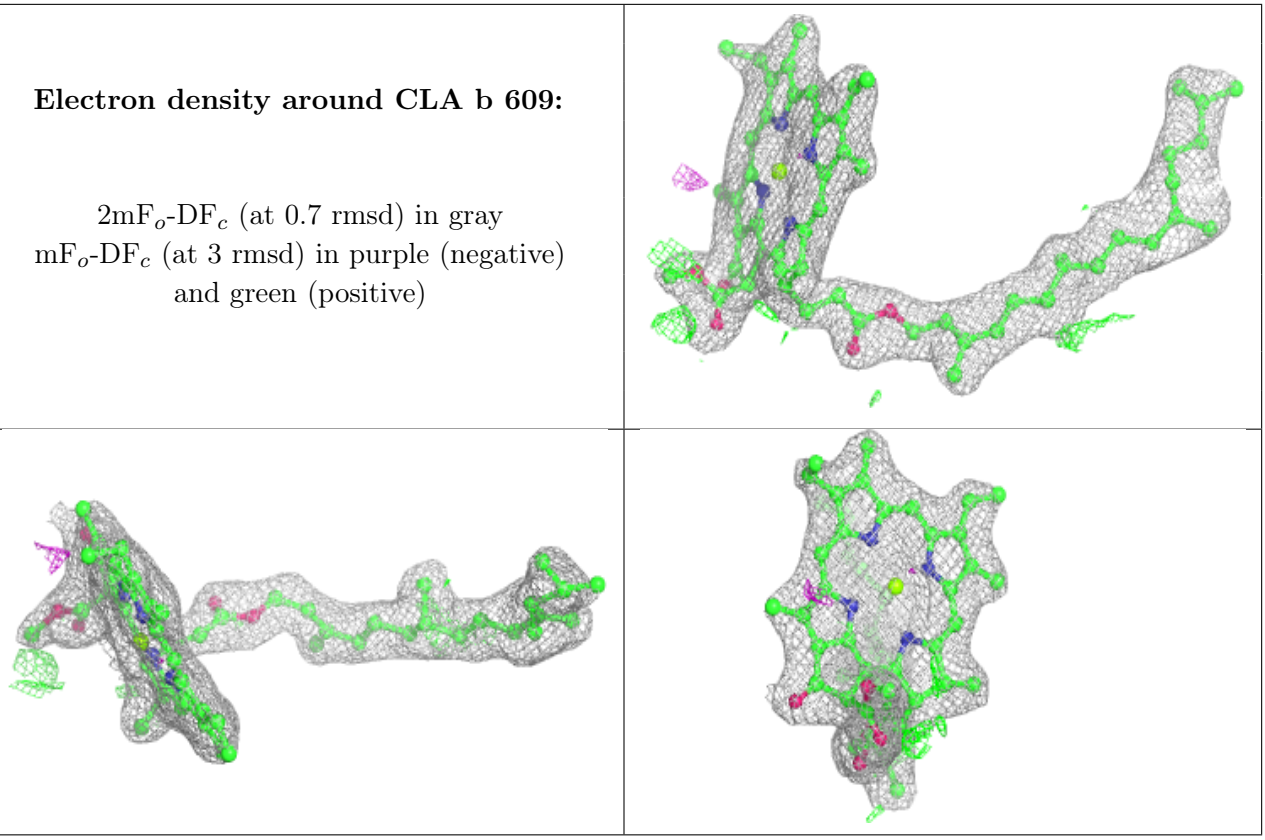
Electron density around BCR H 101:

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



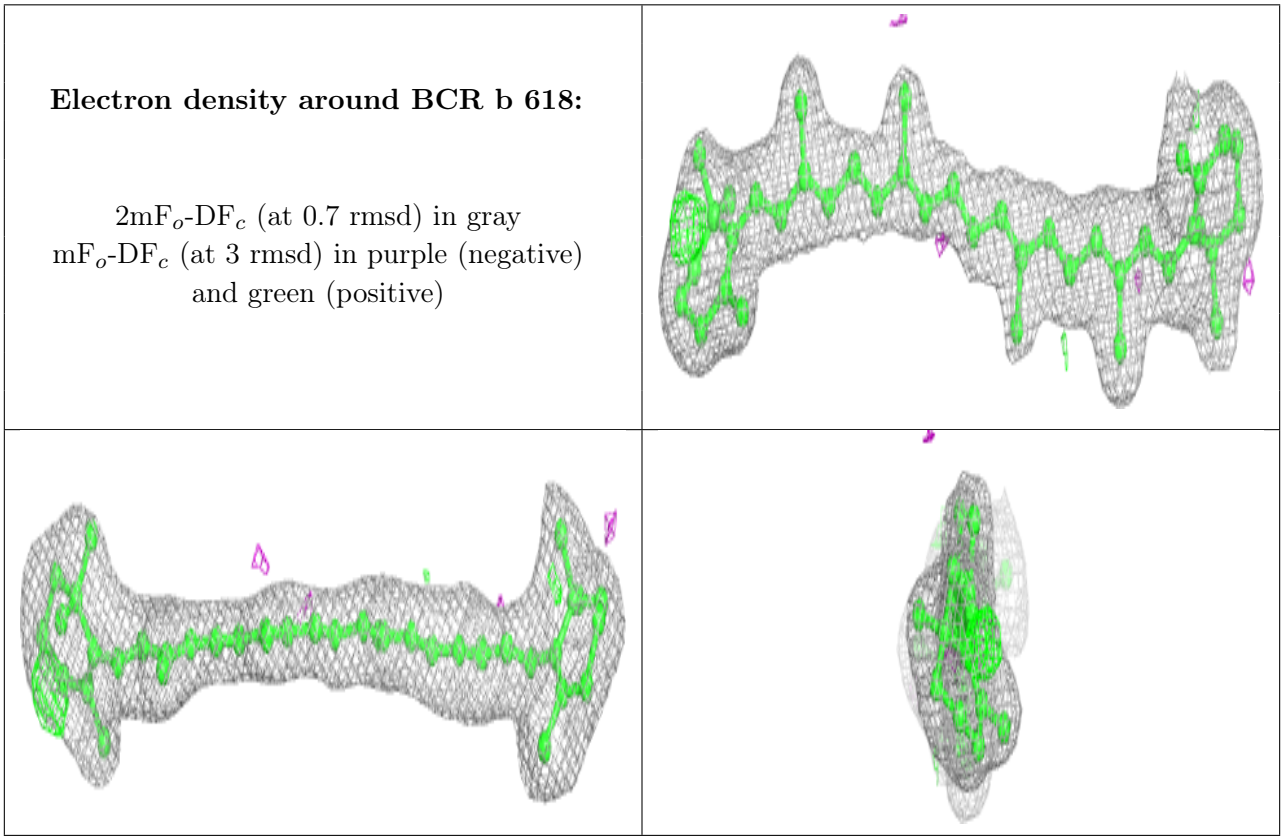
Electron density around CLA b 609:

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



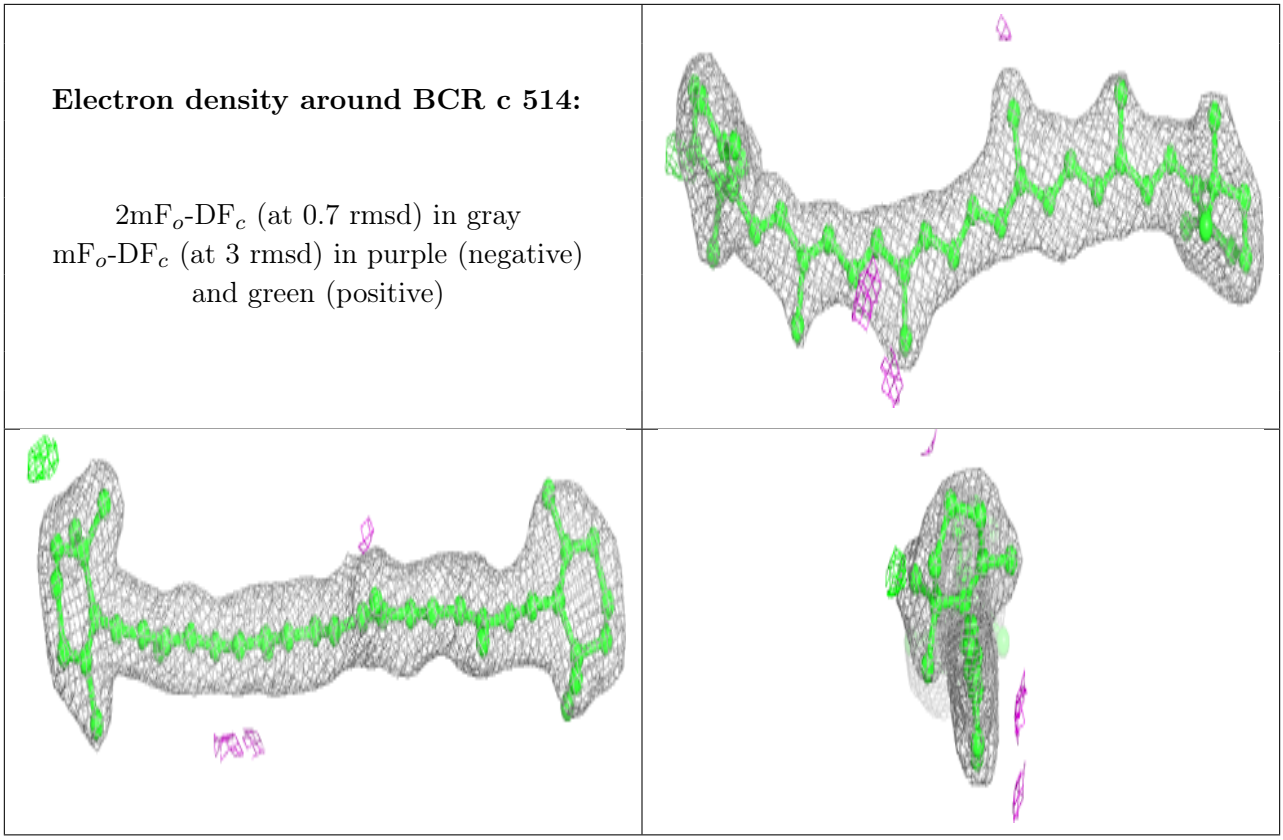
Electron density around BCR b 618:

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



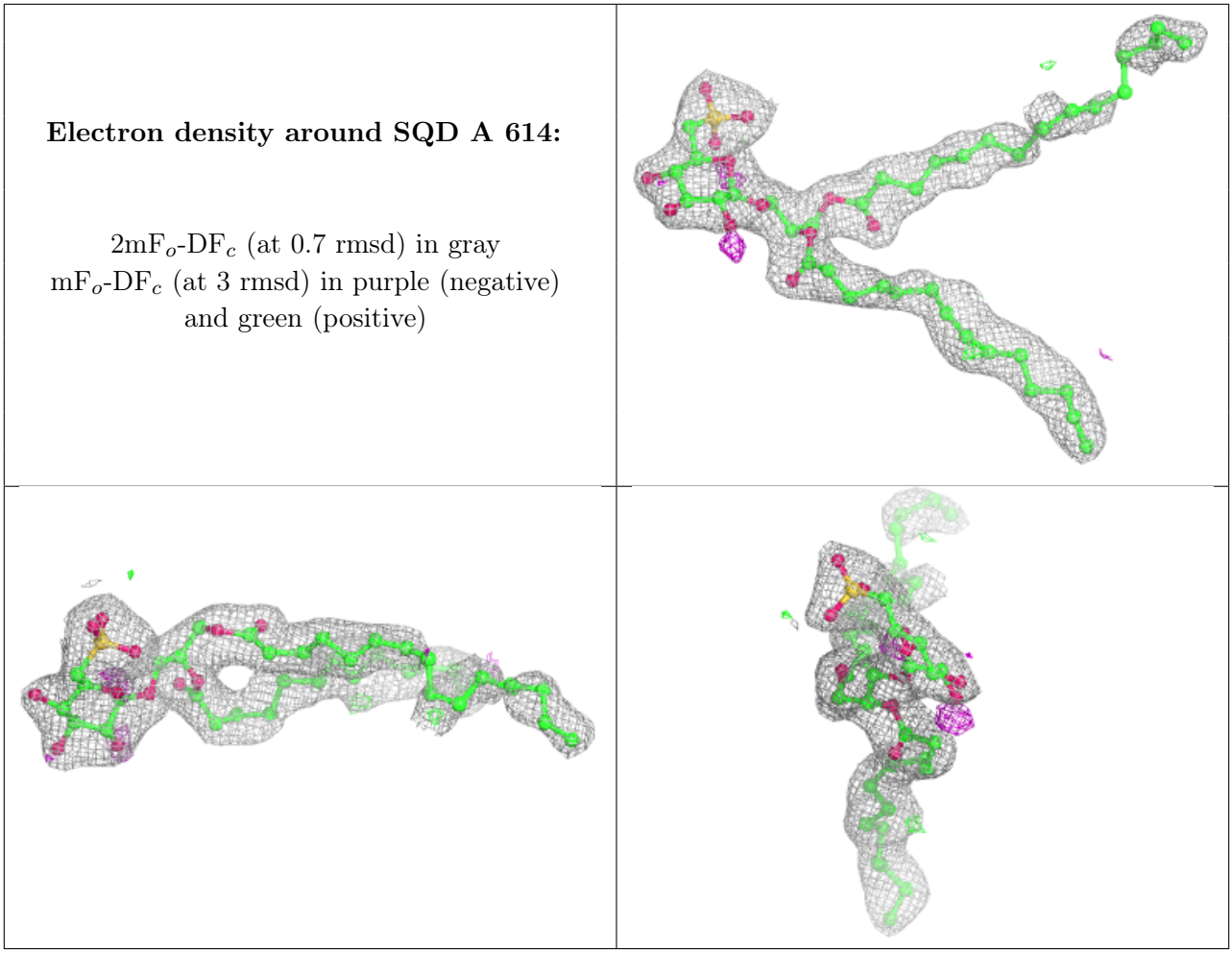
Electron density around BCR c 514:

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



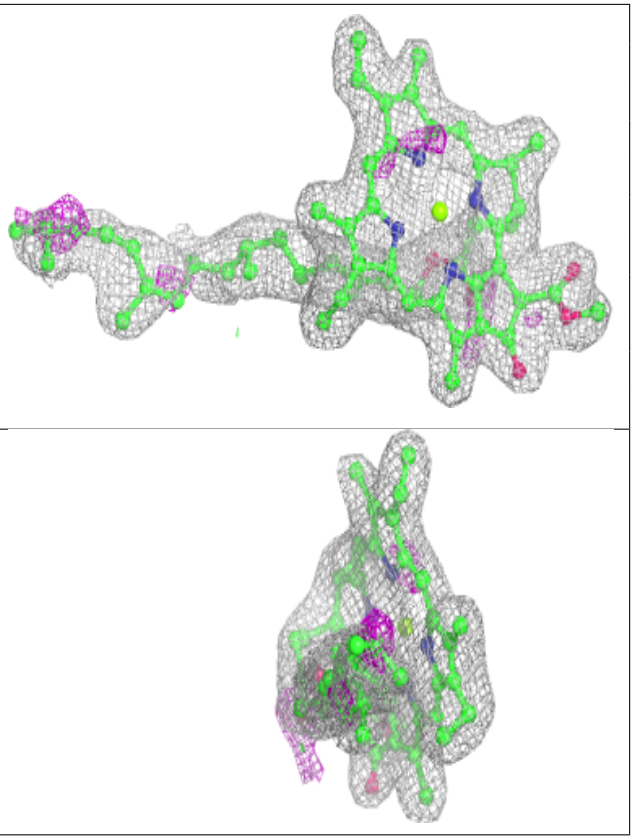
Electron density around SQD A 614:

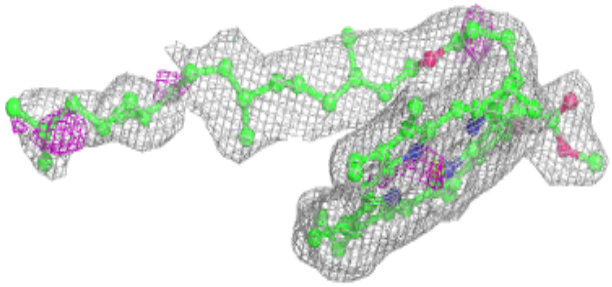
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 614:

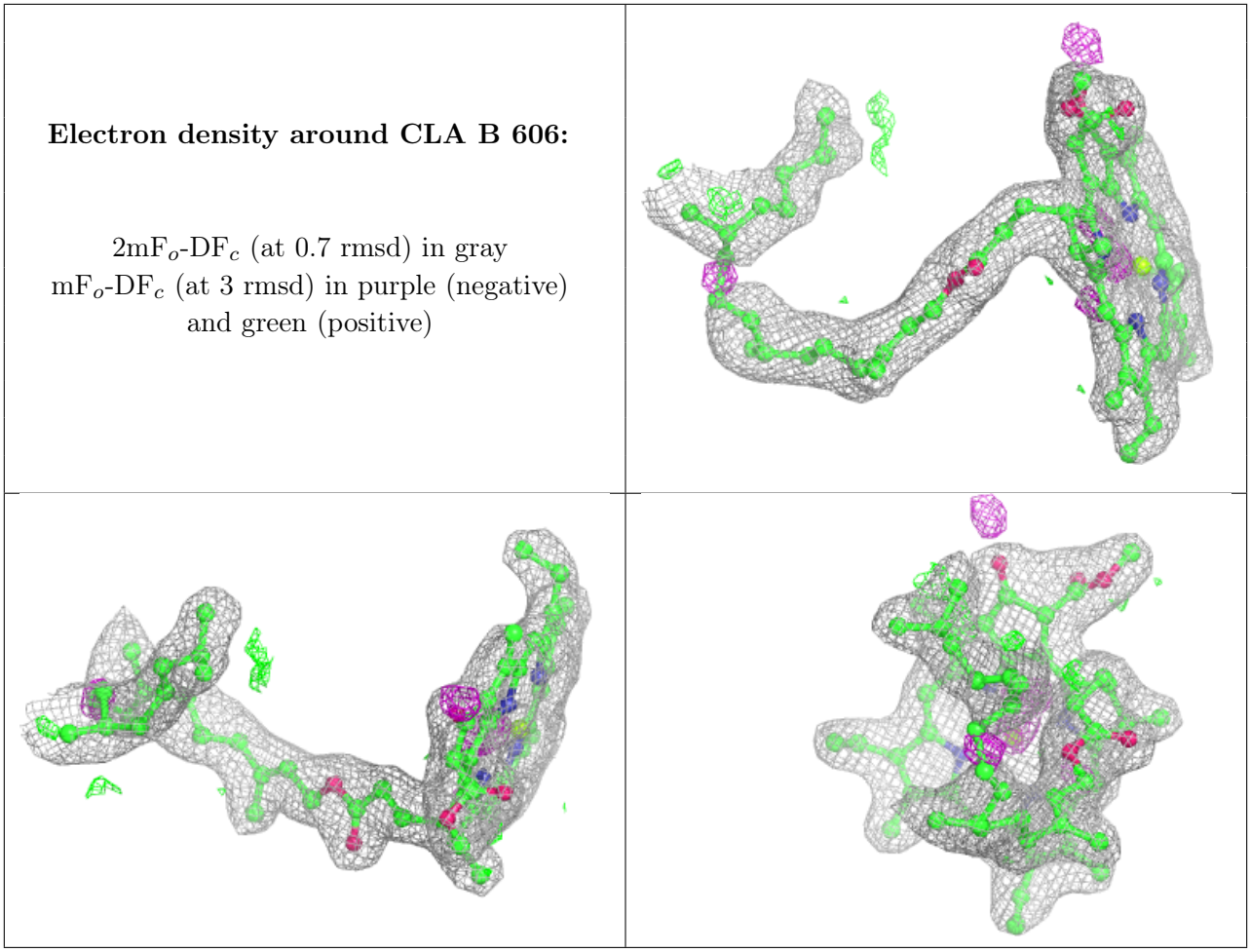
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





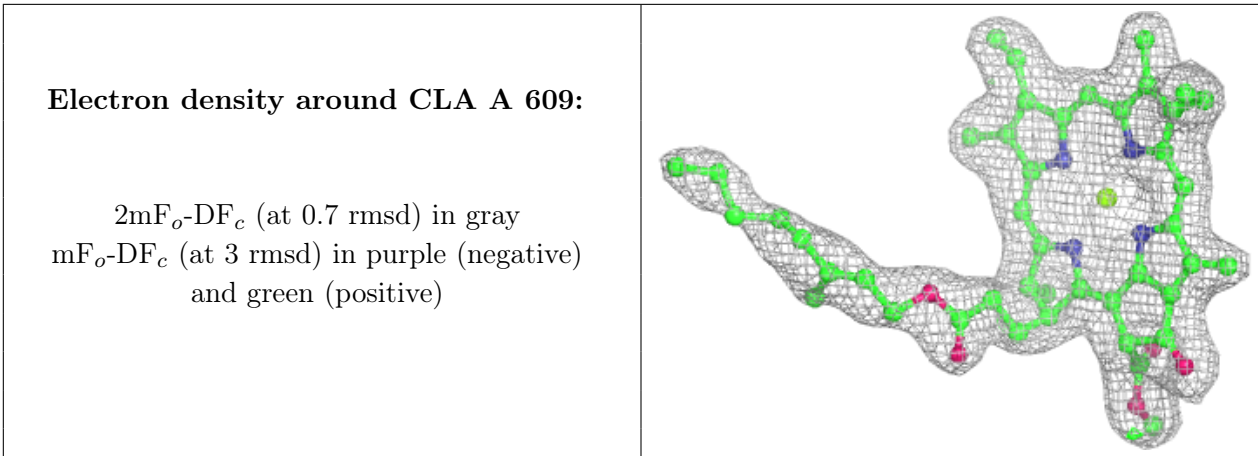
Electron density around CLA B 606:

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



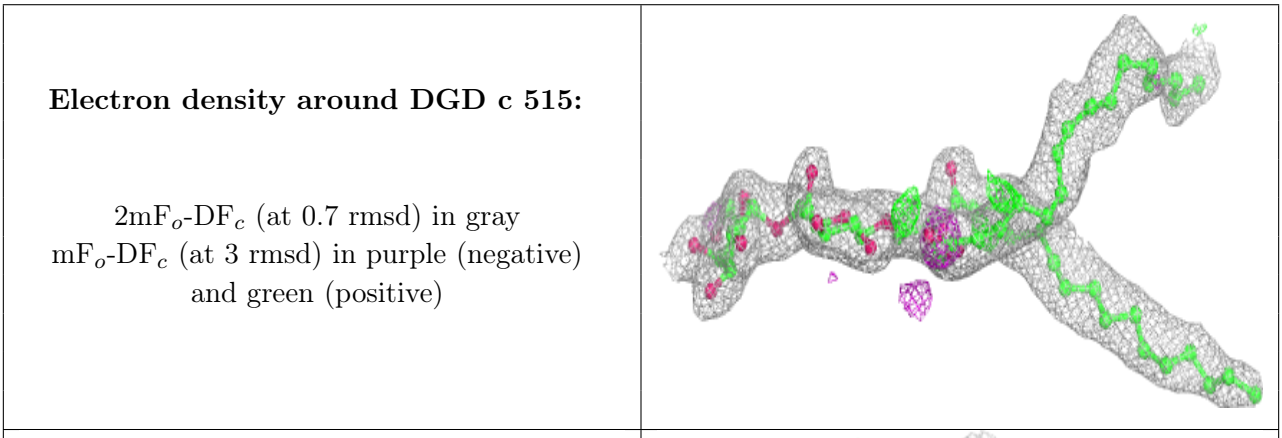
Electron density around CLA A 609:

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



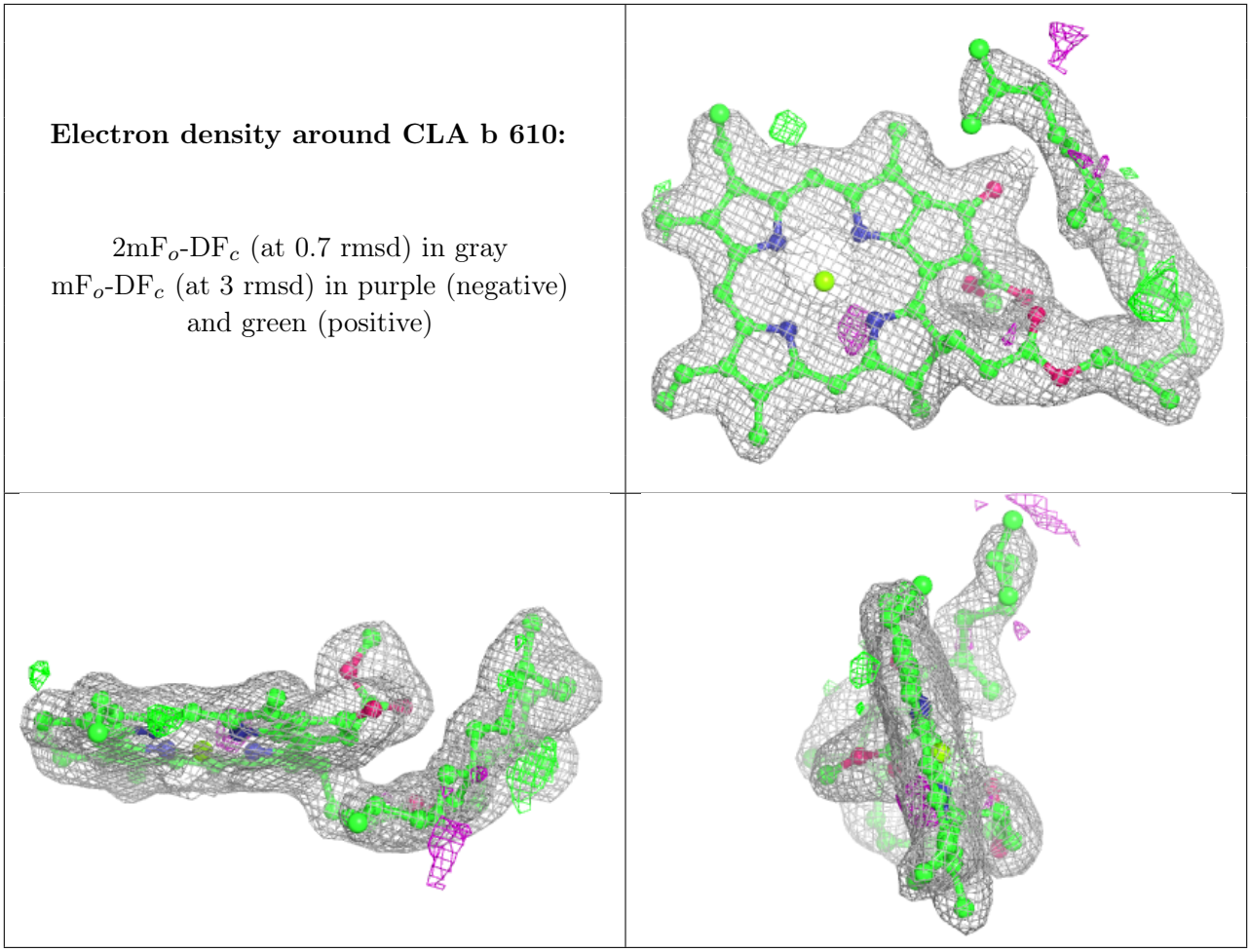
Electron density around DGD c 515:

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



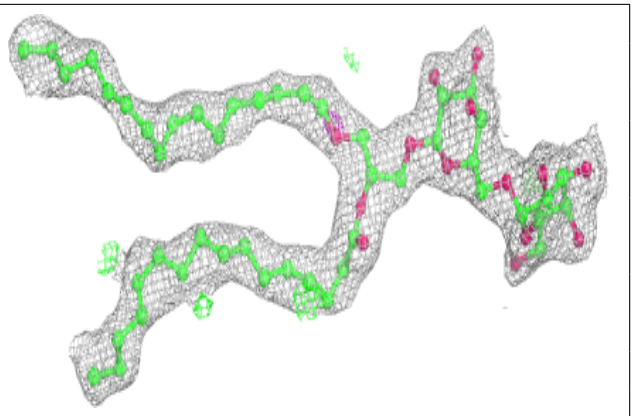
Electron density around CLA b 610:

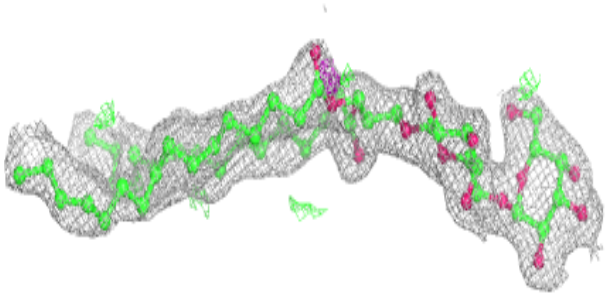
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

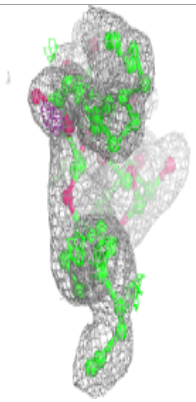


Electron density around DGD c 517:

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

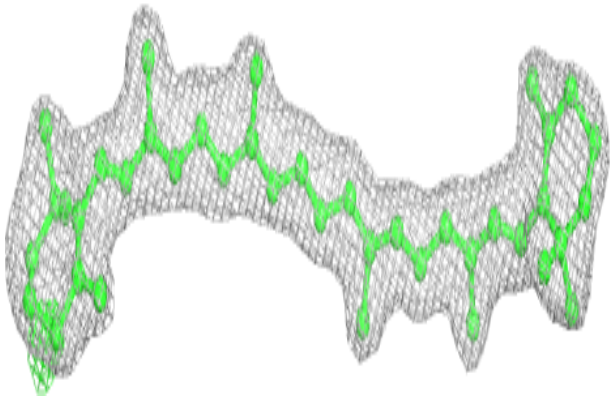


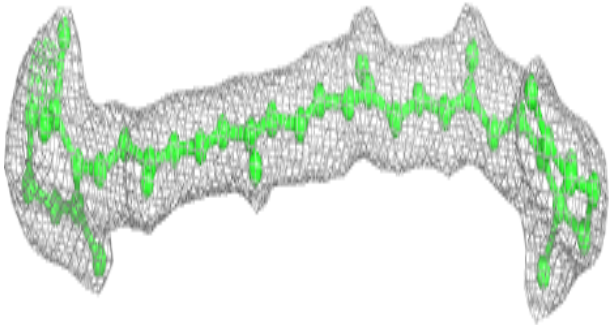


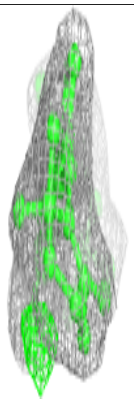


Electron density around BCR B 619:

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

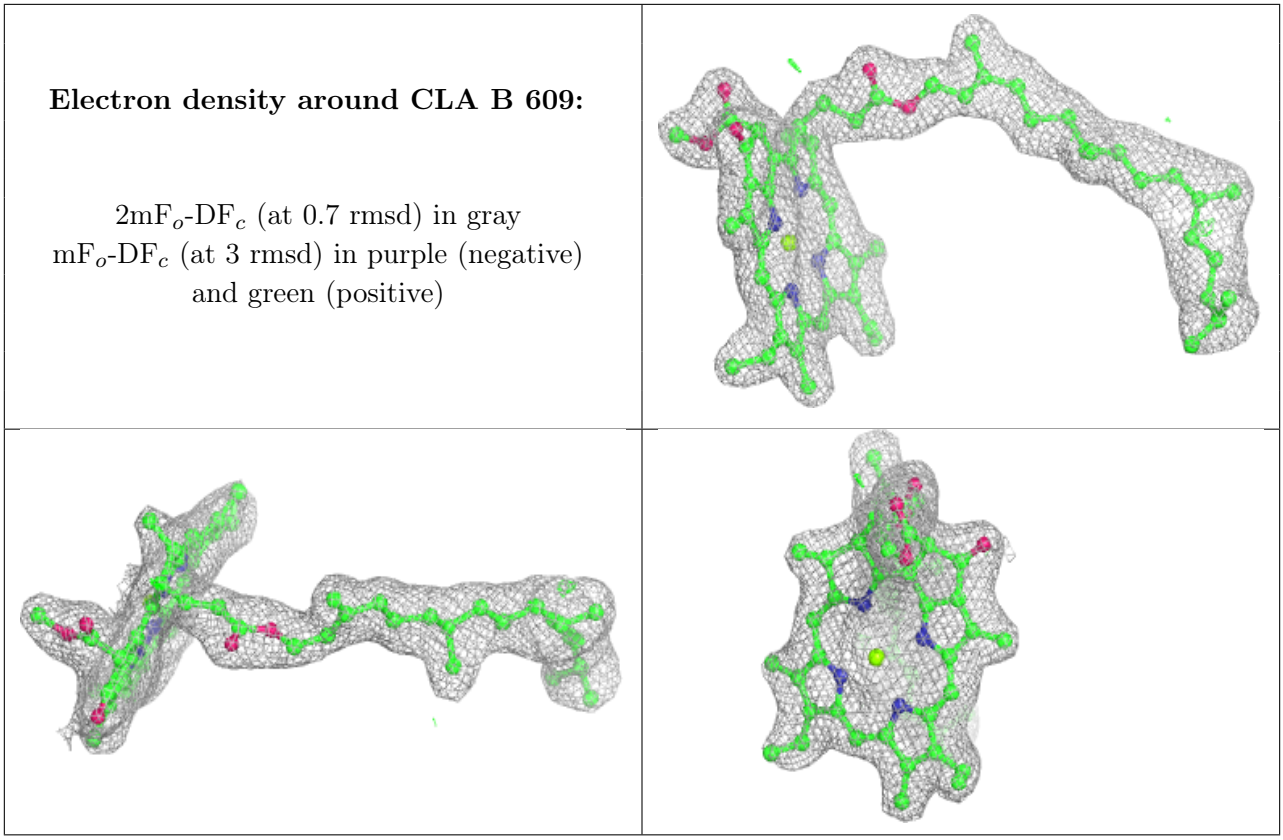






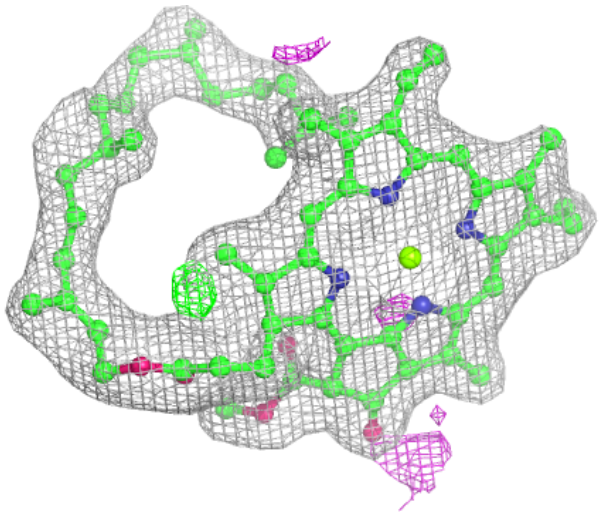
Electron density around CLA B 609:

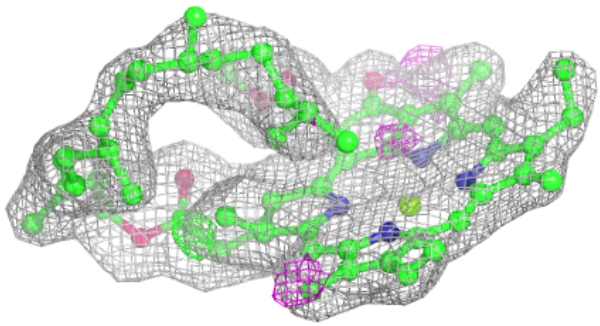
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

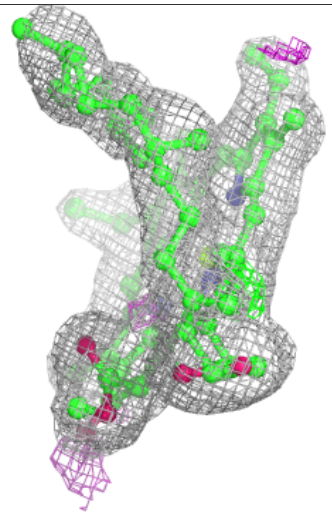


Electron density around CLA b 615:

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

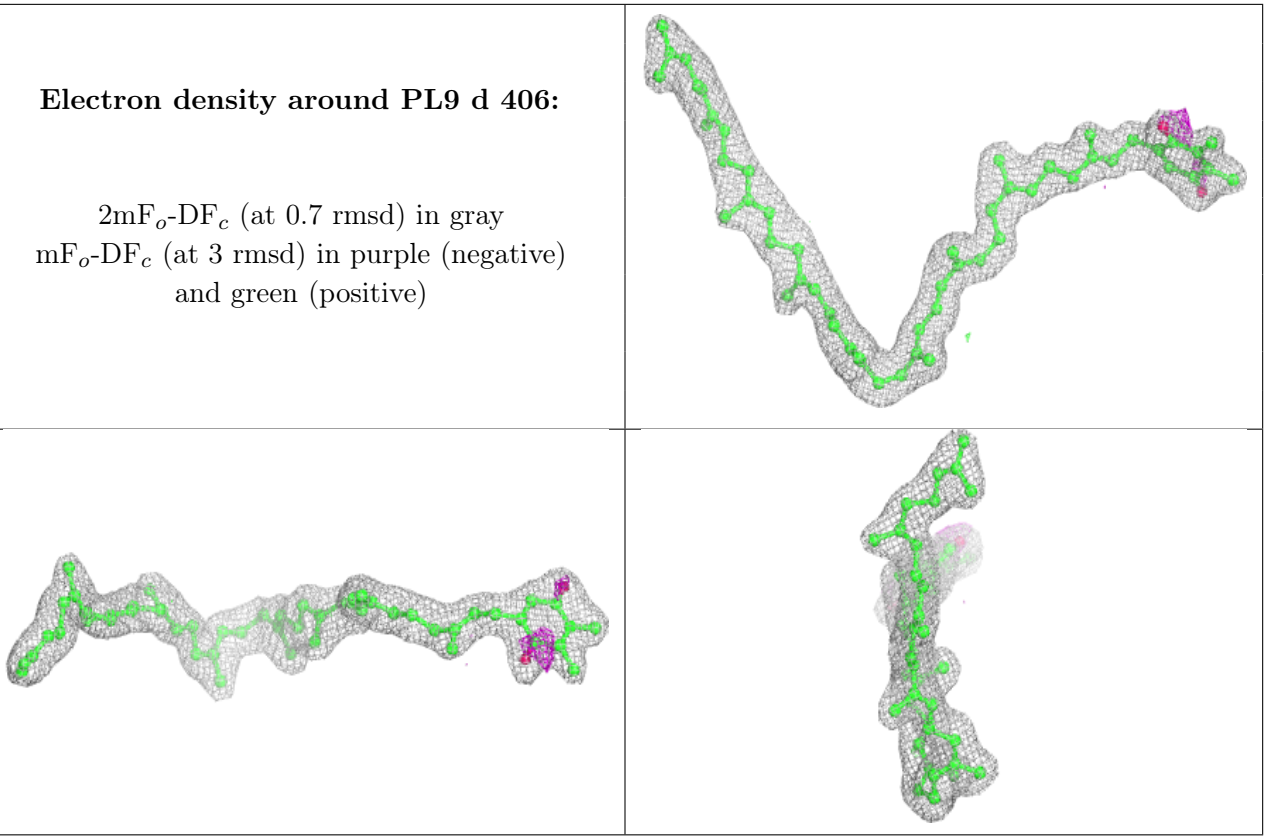






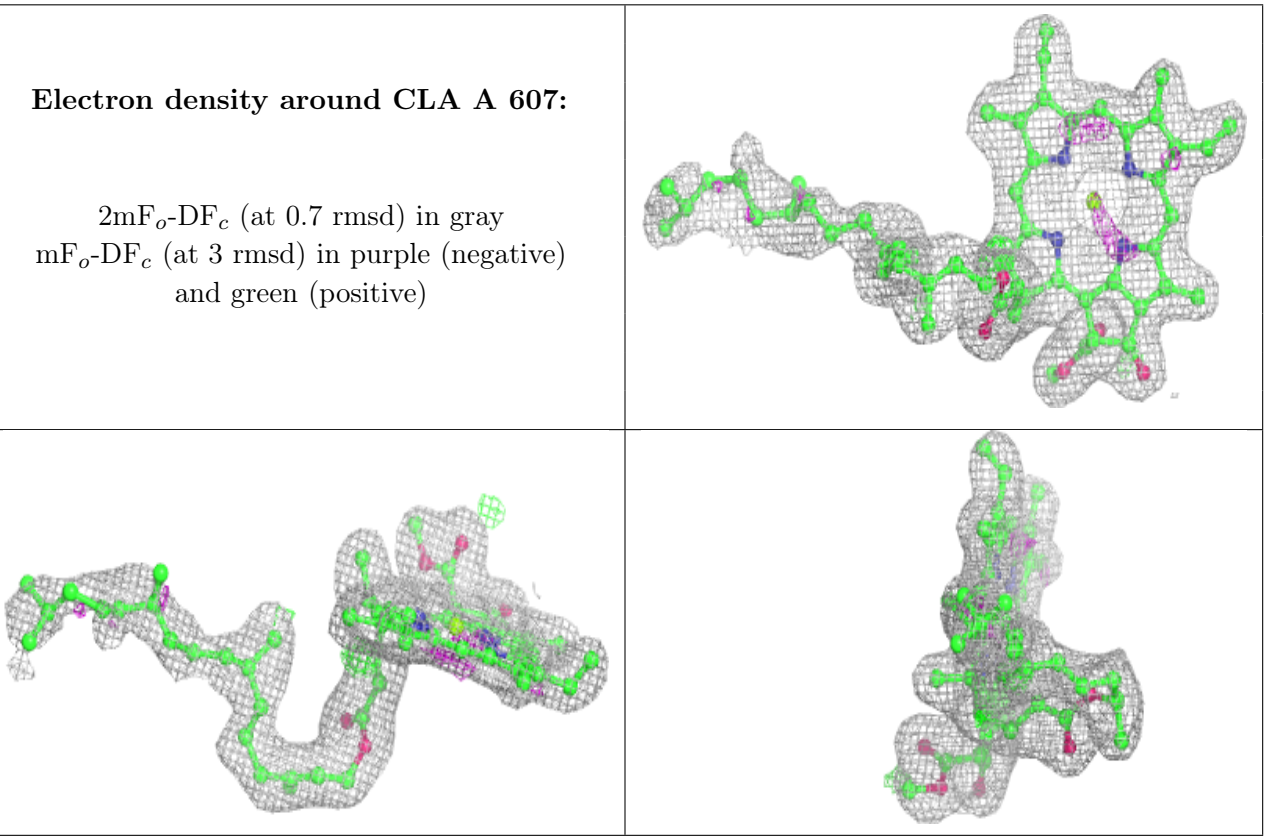
Electron density around PL9 d 406:

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



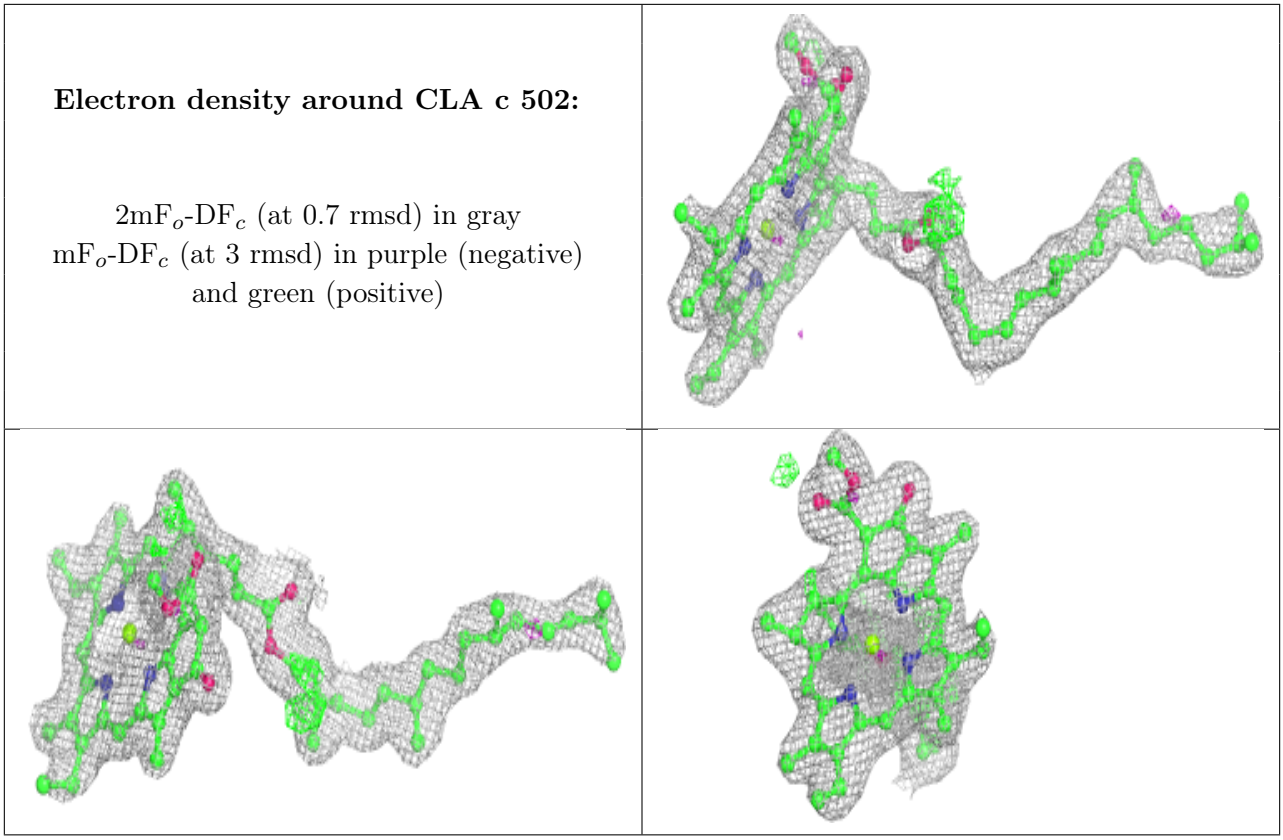
Electron density around CLA A 607:

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



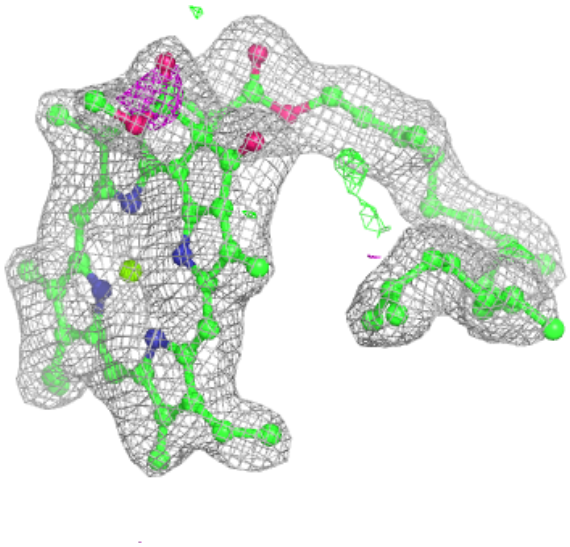
Electron density around CLA c 502:

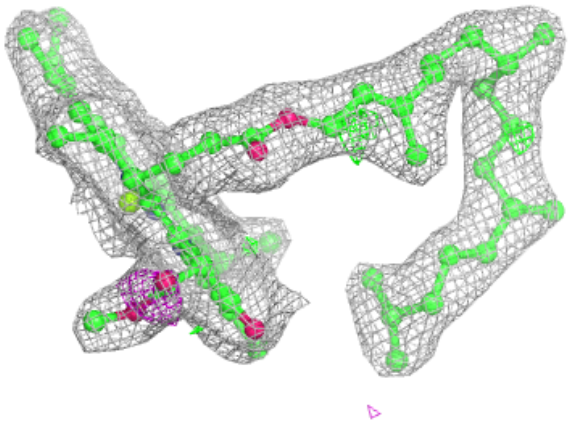
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

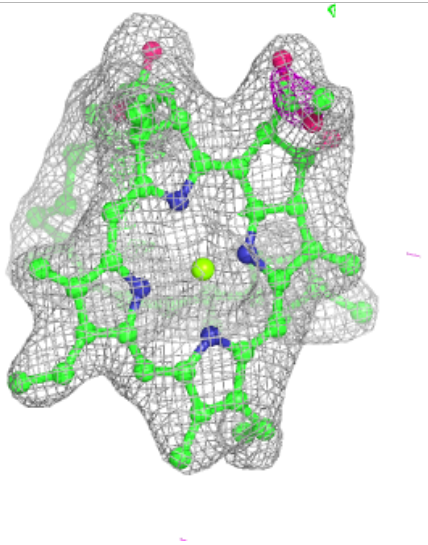


Electron density around CLA c 503:

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

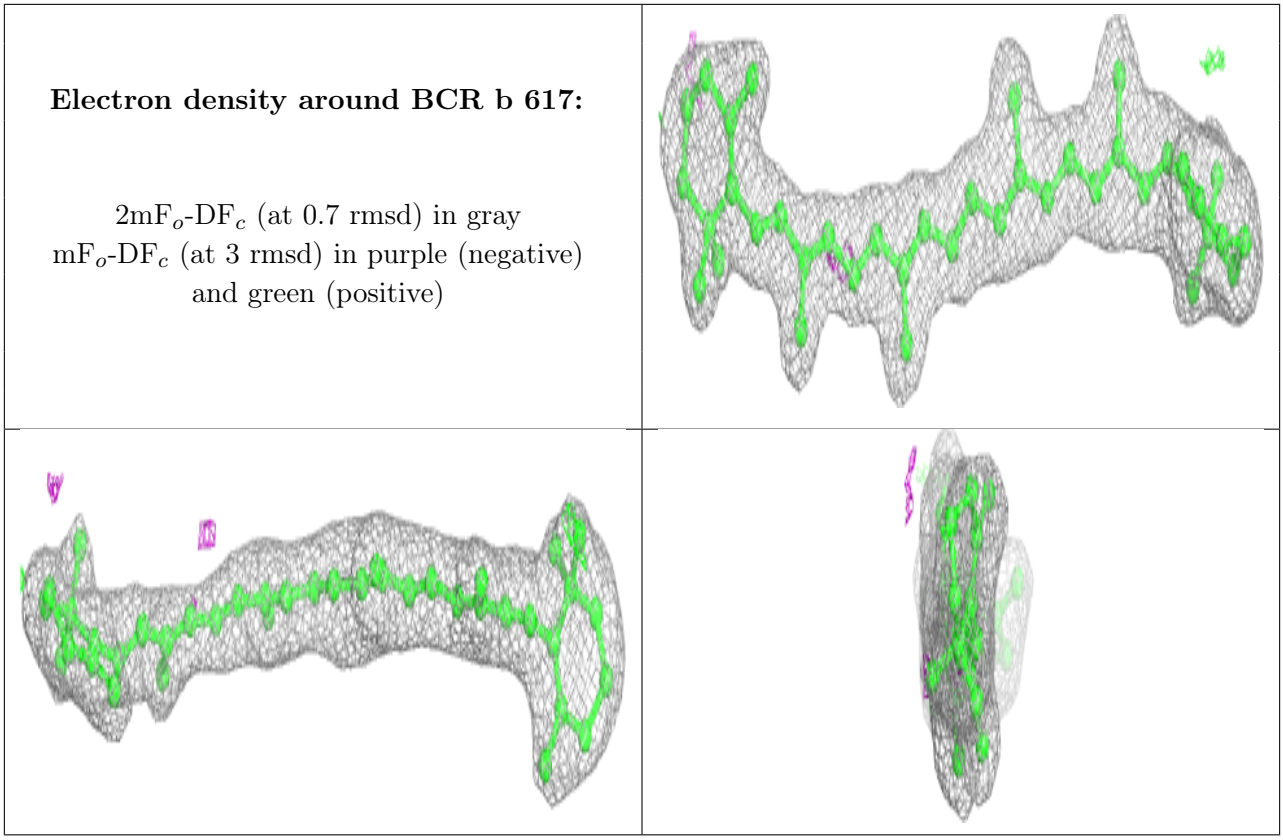






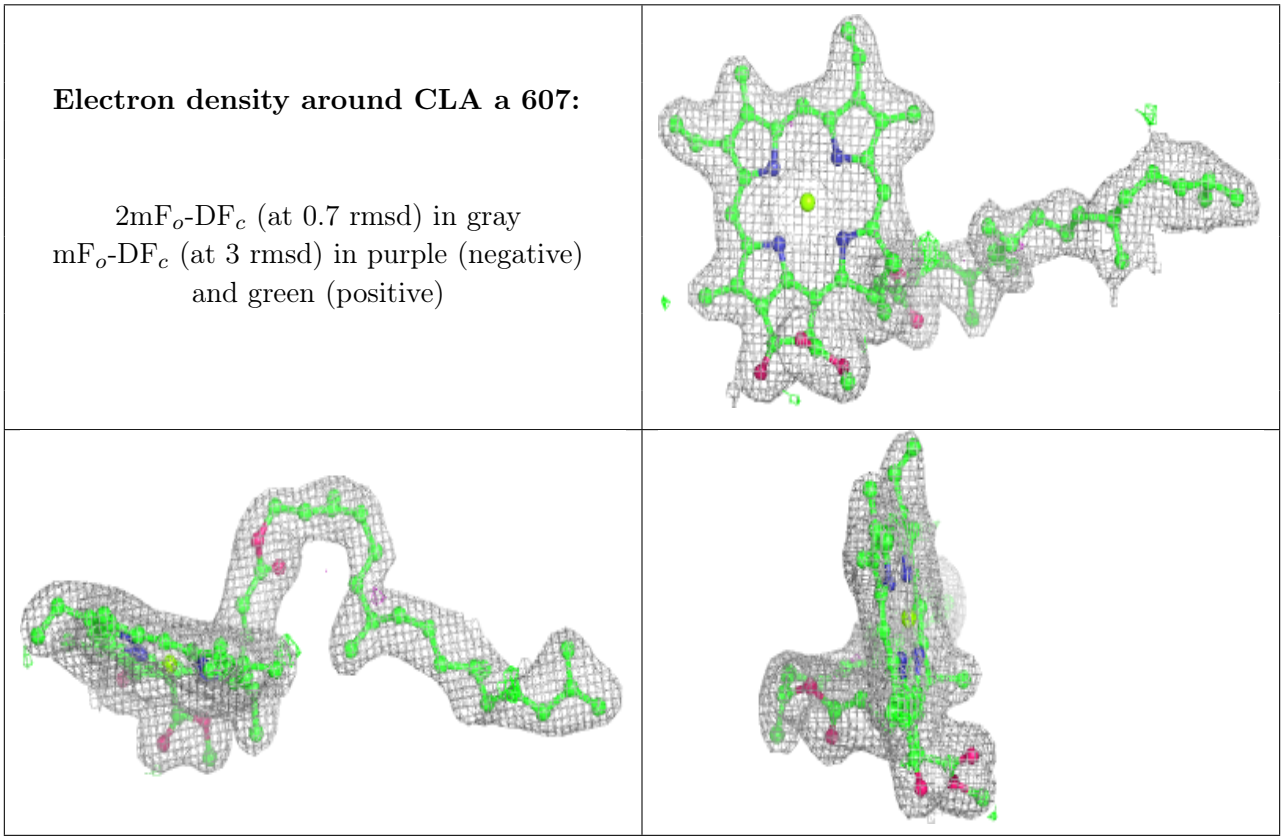
Electron density around BCR b 617:

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



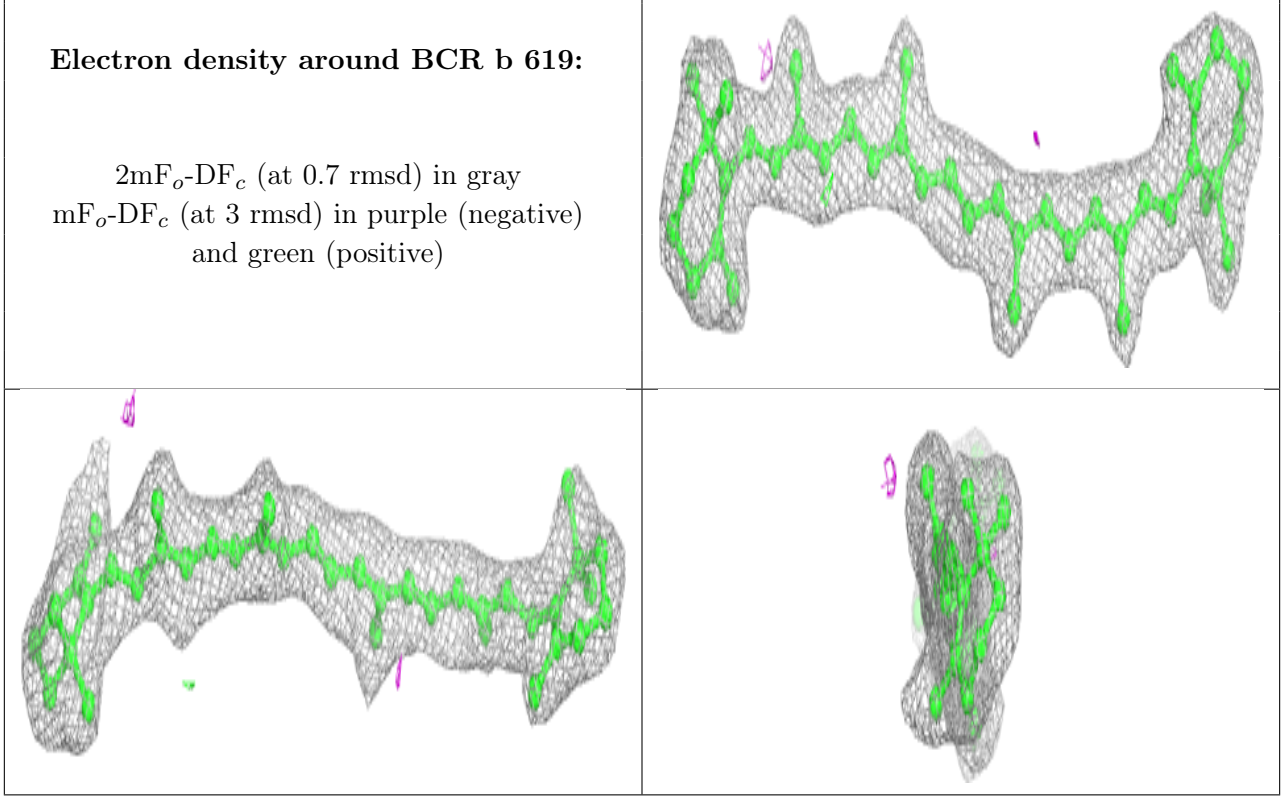
Electron density around CLA a 607:

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



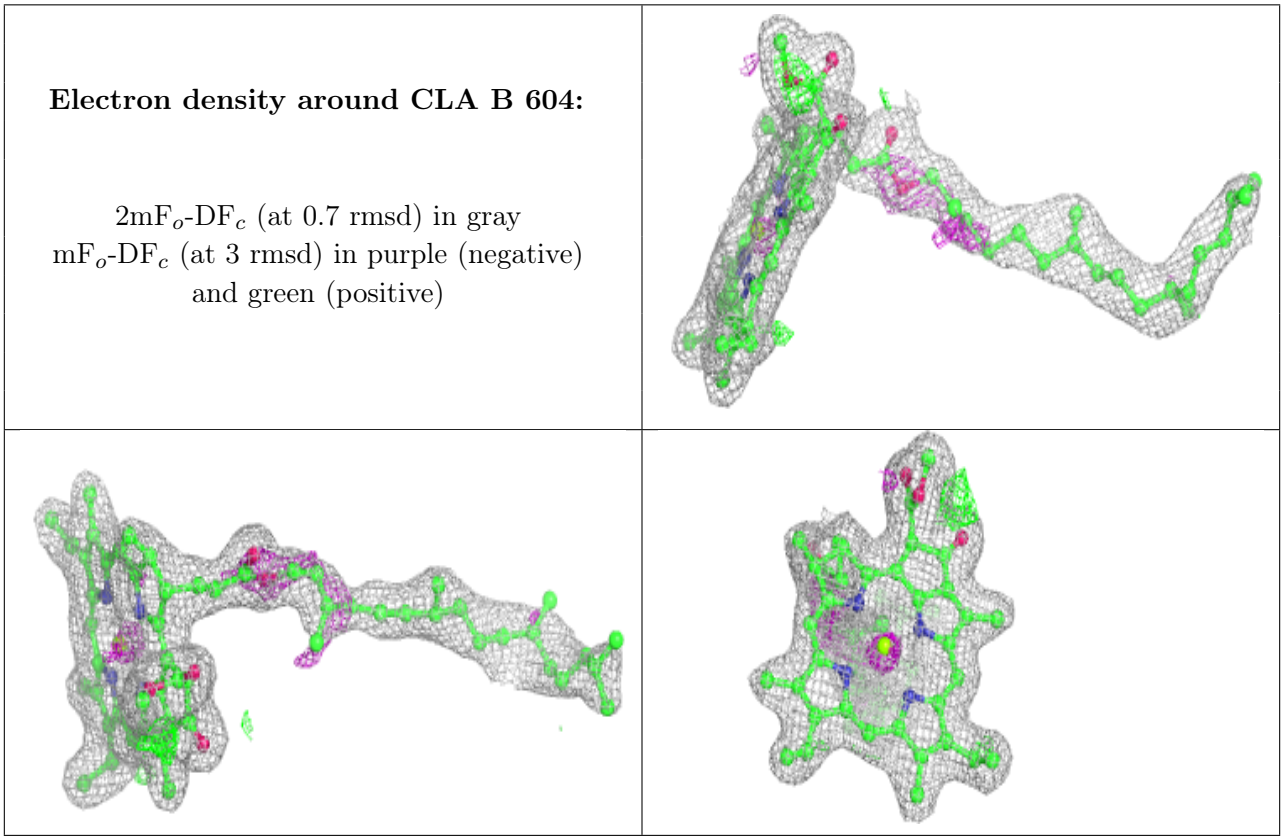
Electron density around BCR b 619:

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



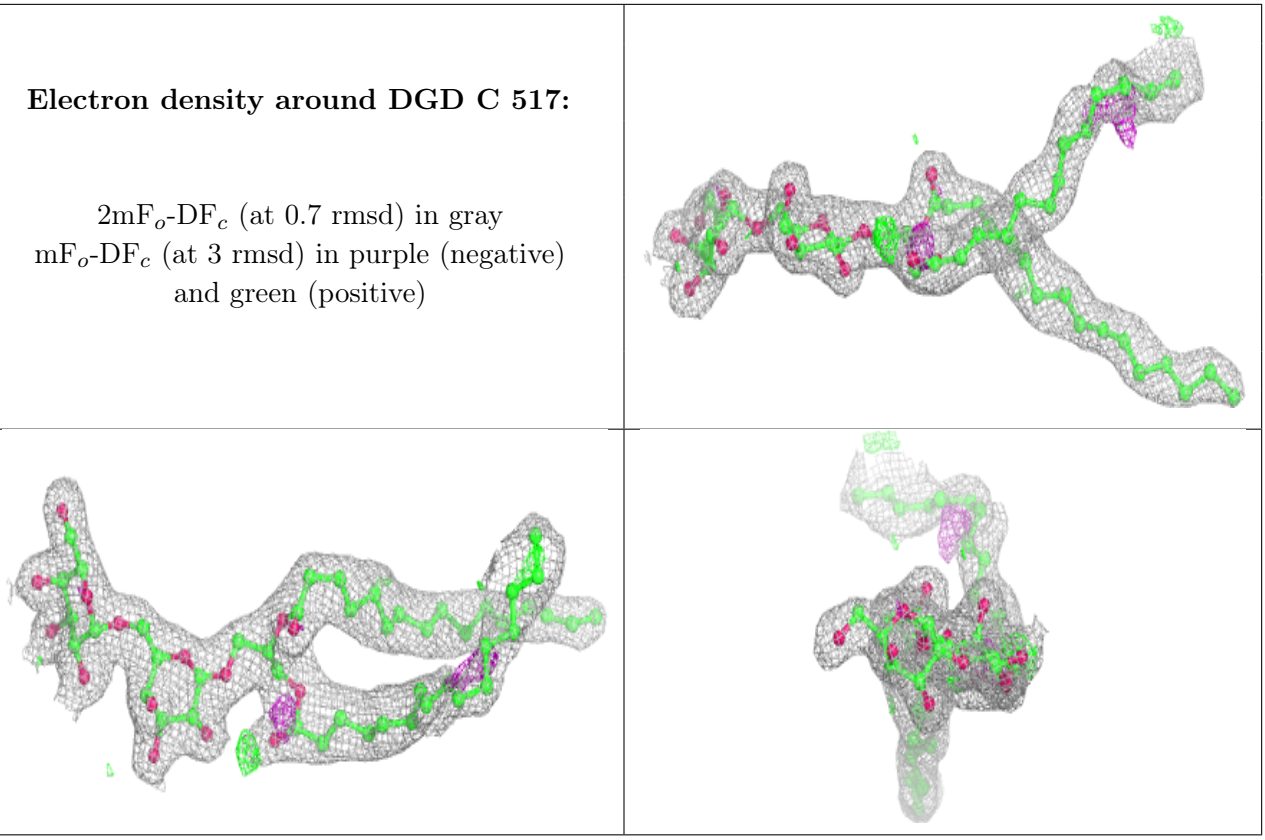
Electron density around CLA B 604:

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



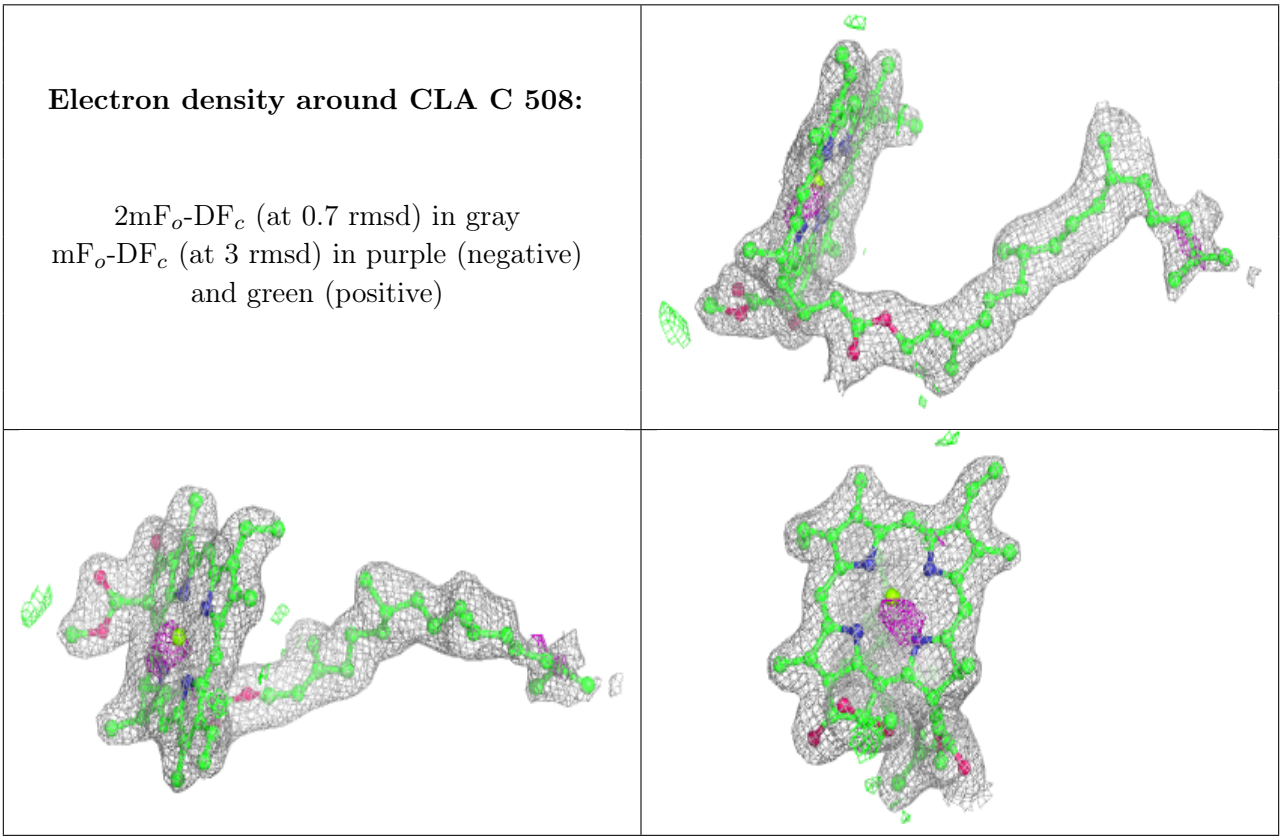
Electron density around DGD C 517:

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



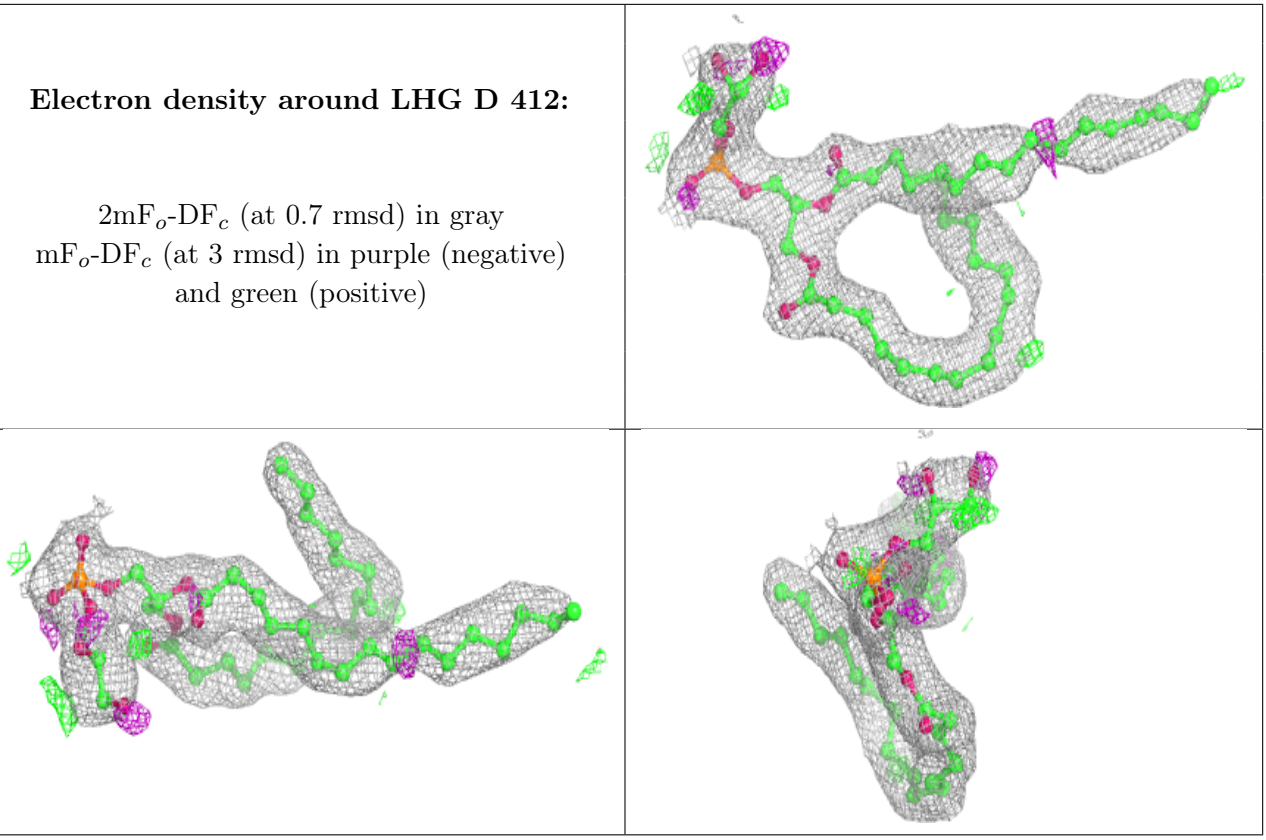
Electron density around CLA C 508:

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



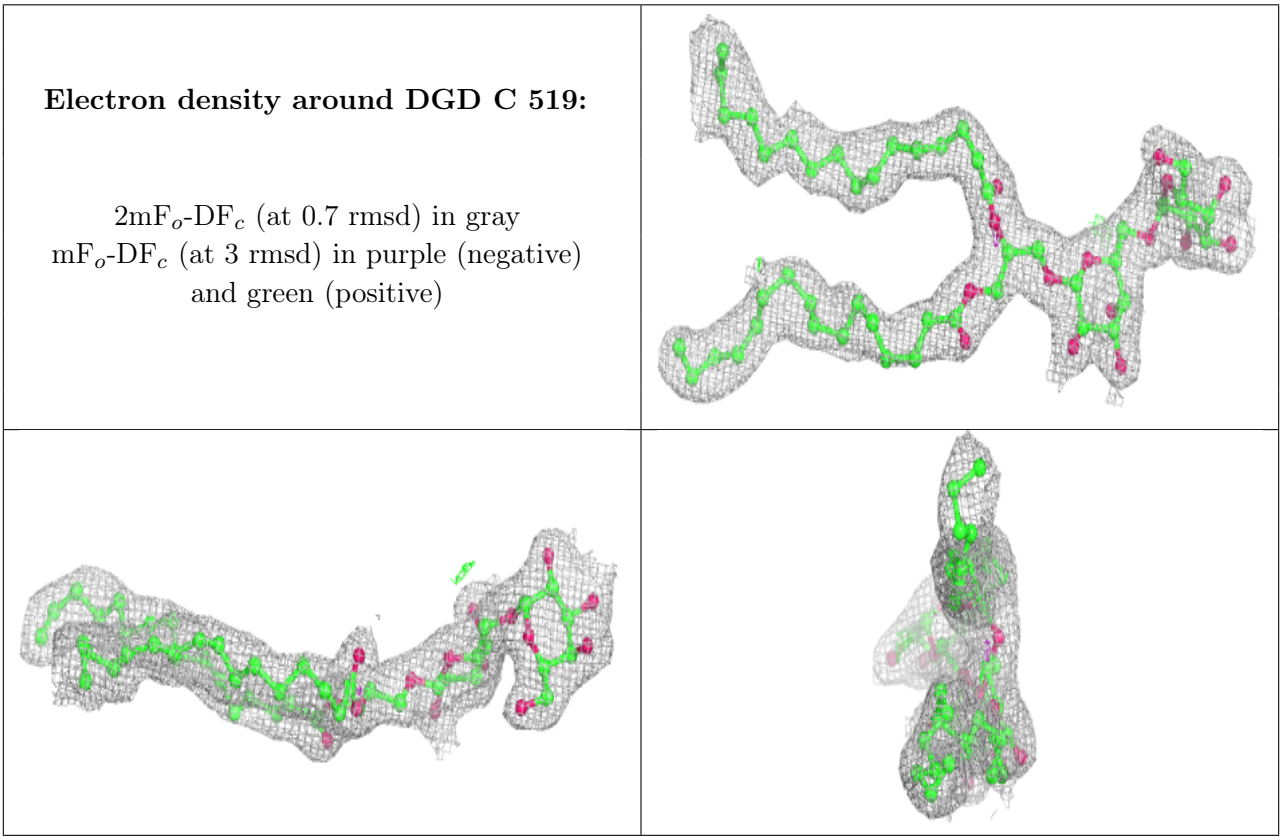
Electron density around LHG D 412:

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



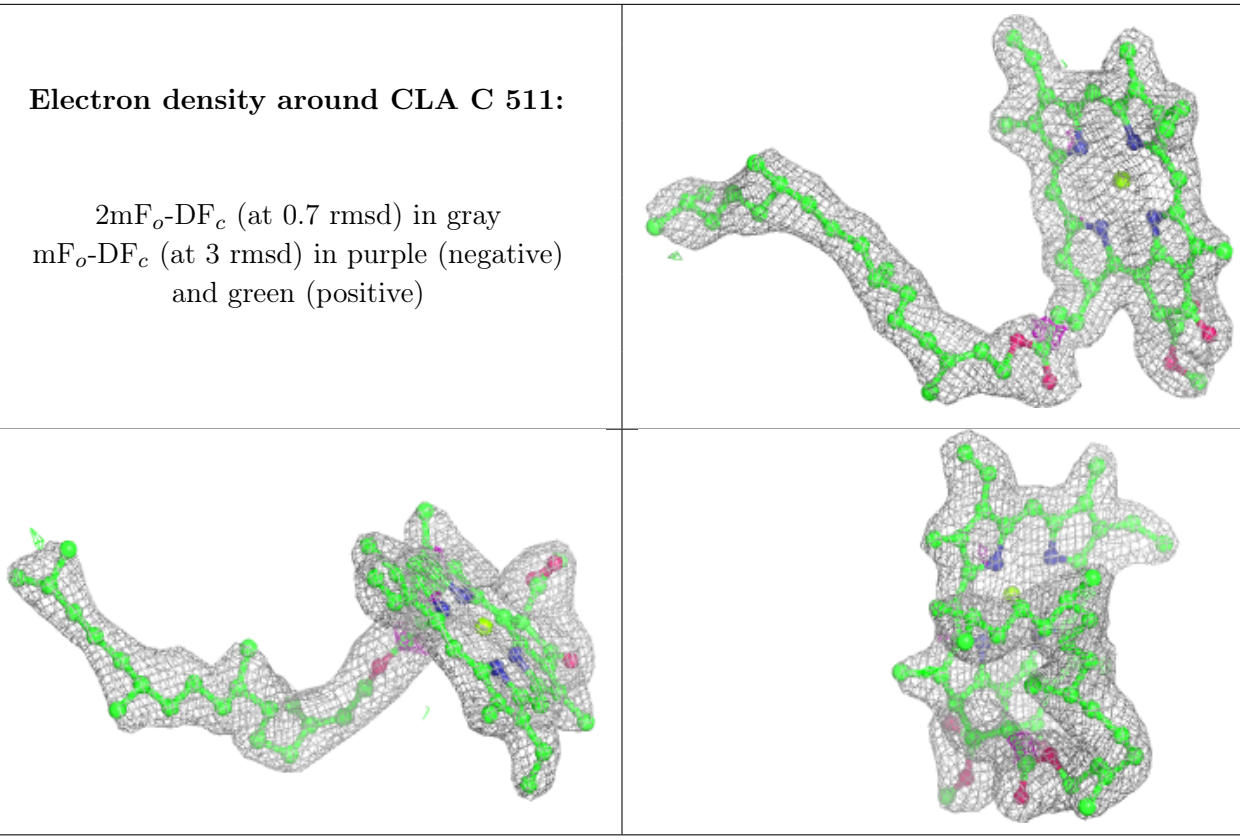
Electron density around DGD C 519:

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



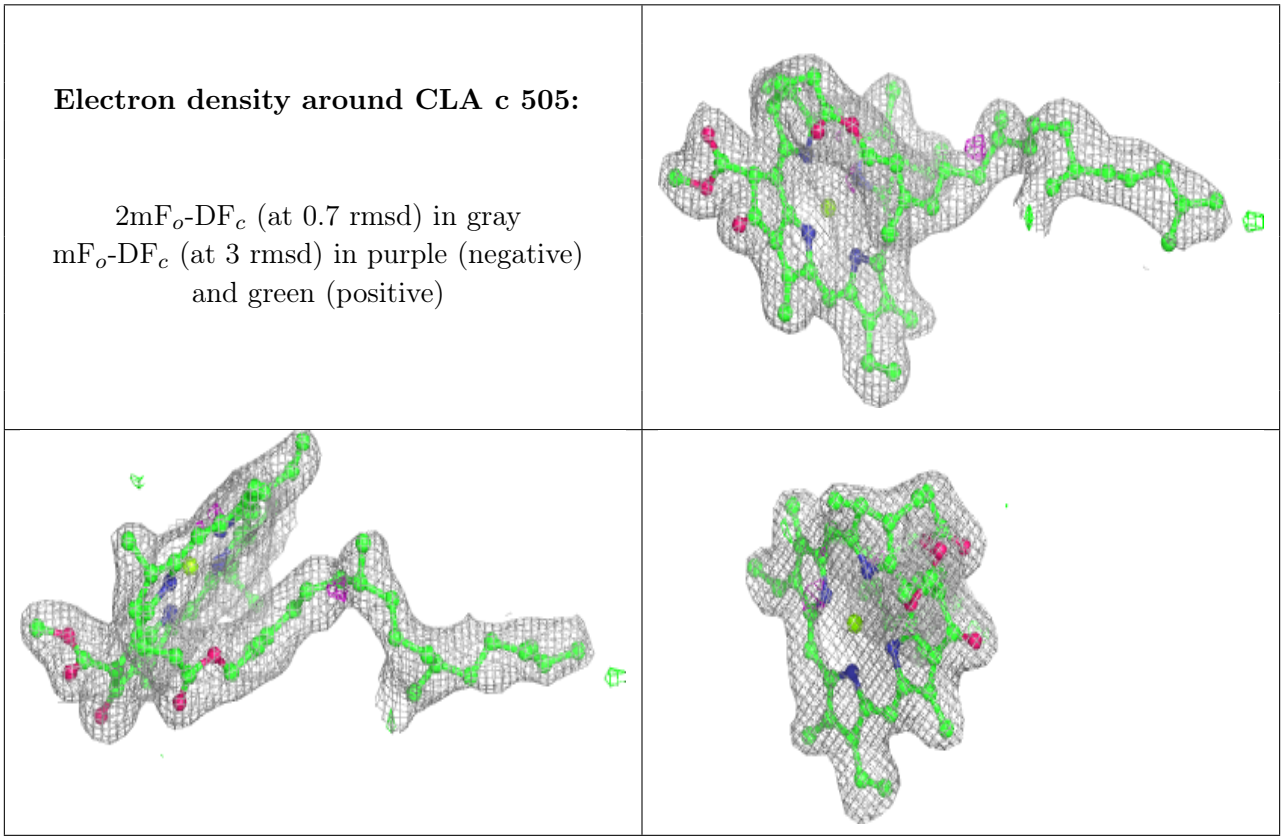
Electron density around CLA C 511:

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



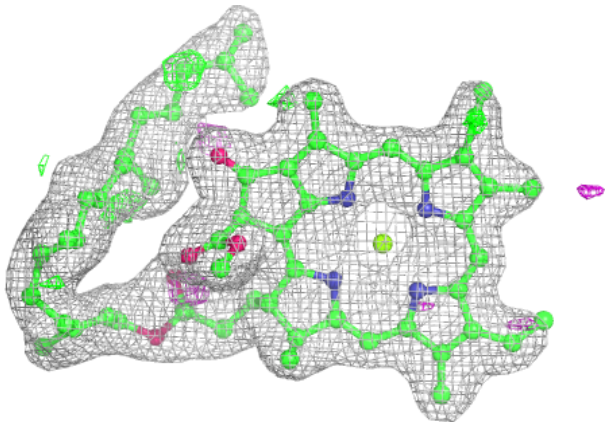
Electron density around CLA c 505:

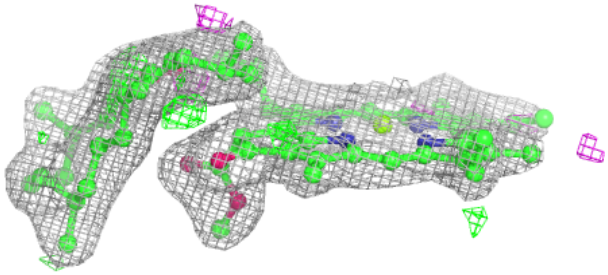
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

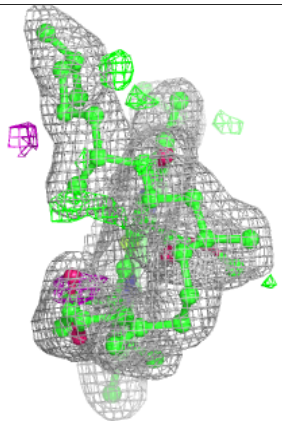


Electron density around CLA B 610:

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

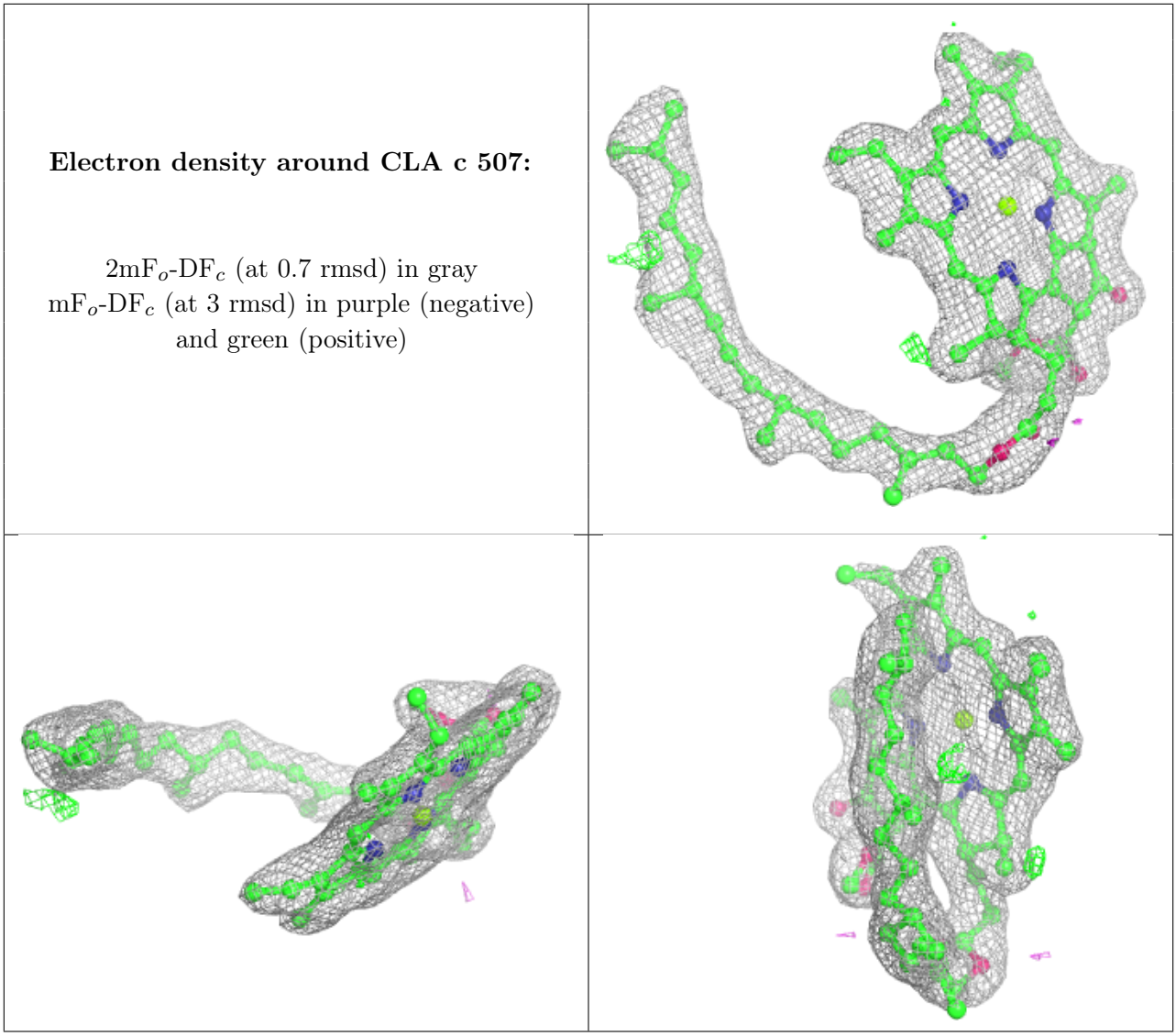






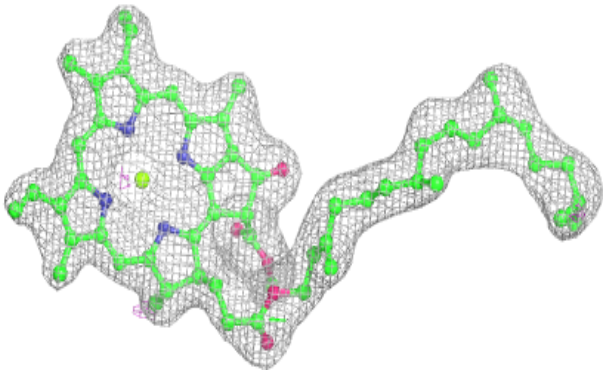
Electron density around CLA c 507:

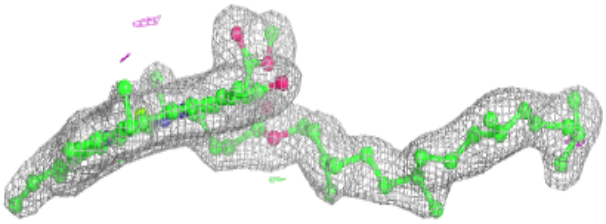
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

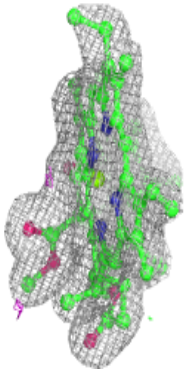


Electron density around CLA b 602:

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

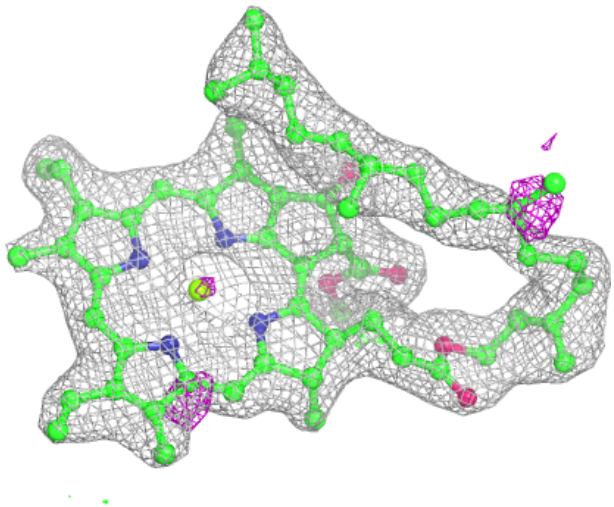


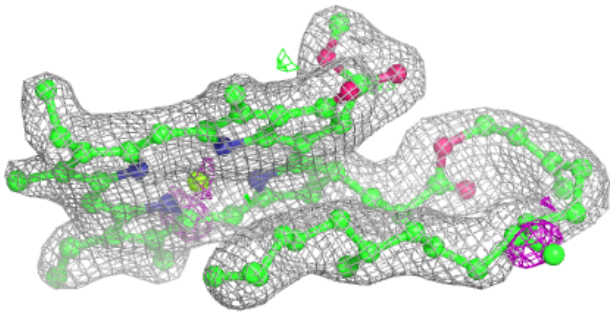


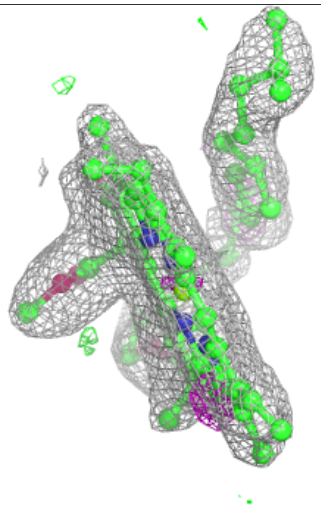


Electron density around CLA c 509:

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

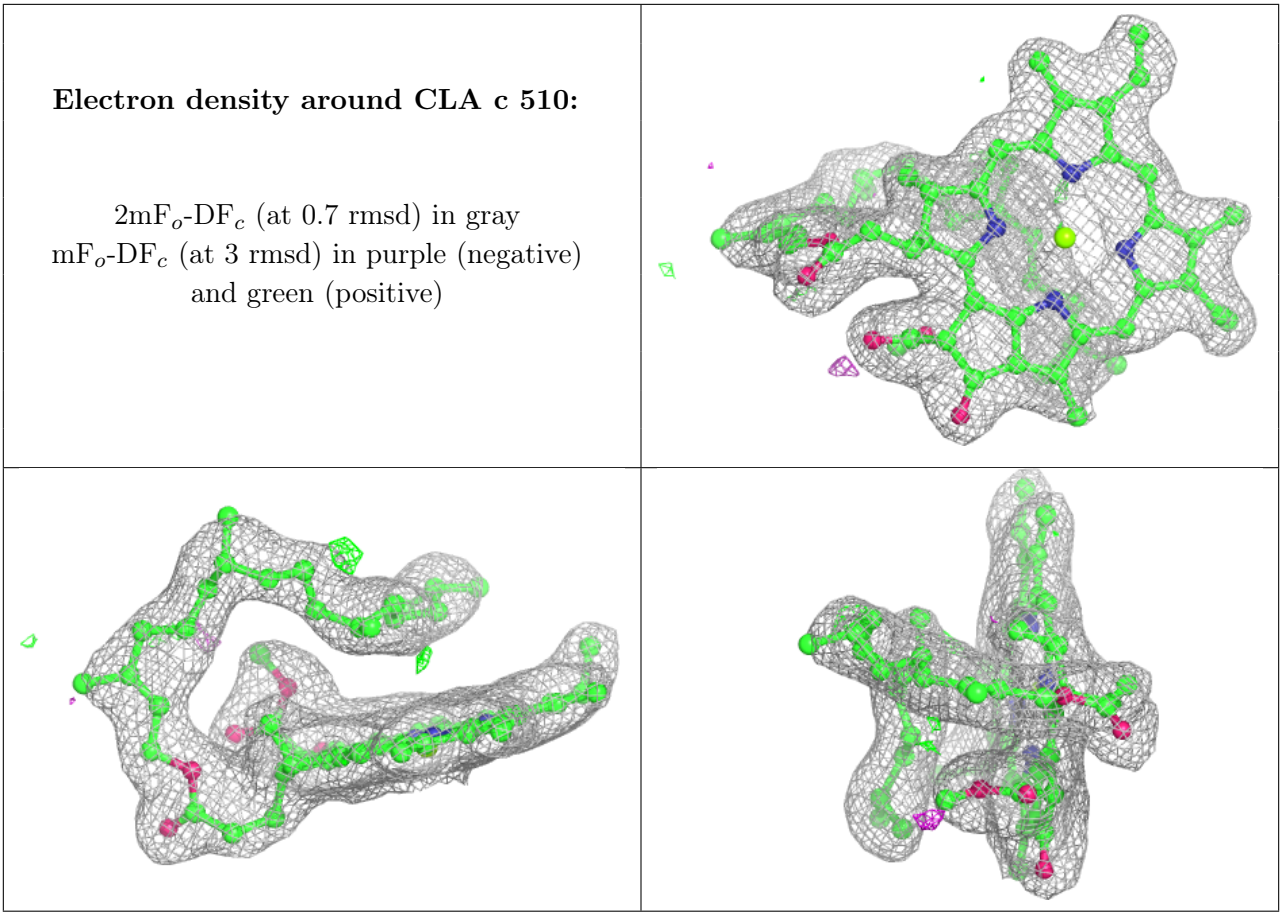






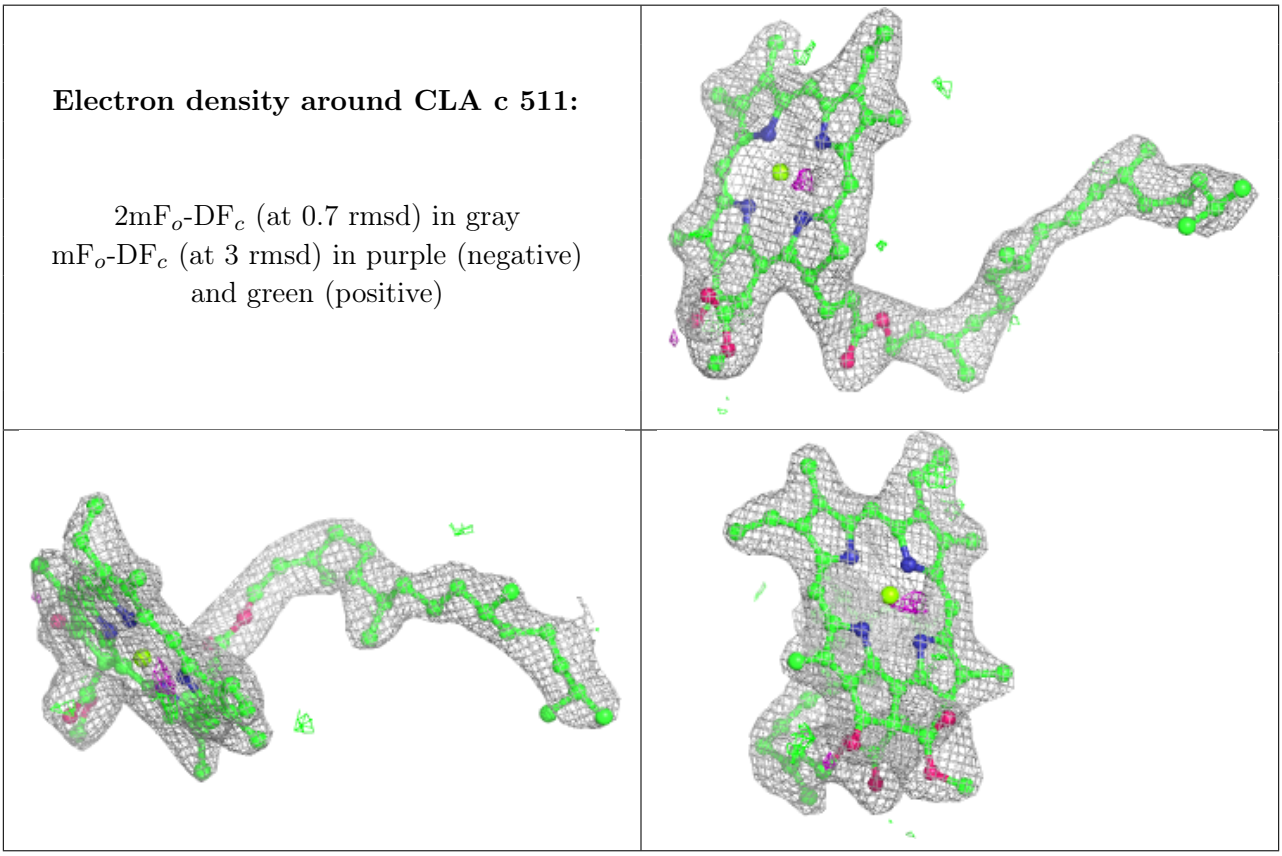
Electron density around CLA c 510:

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



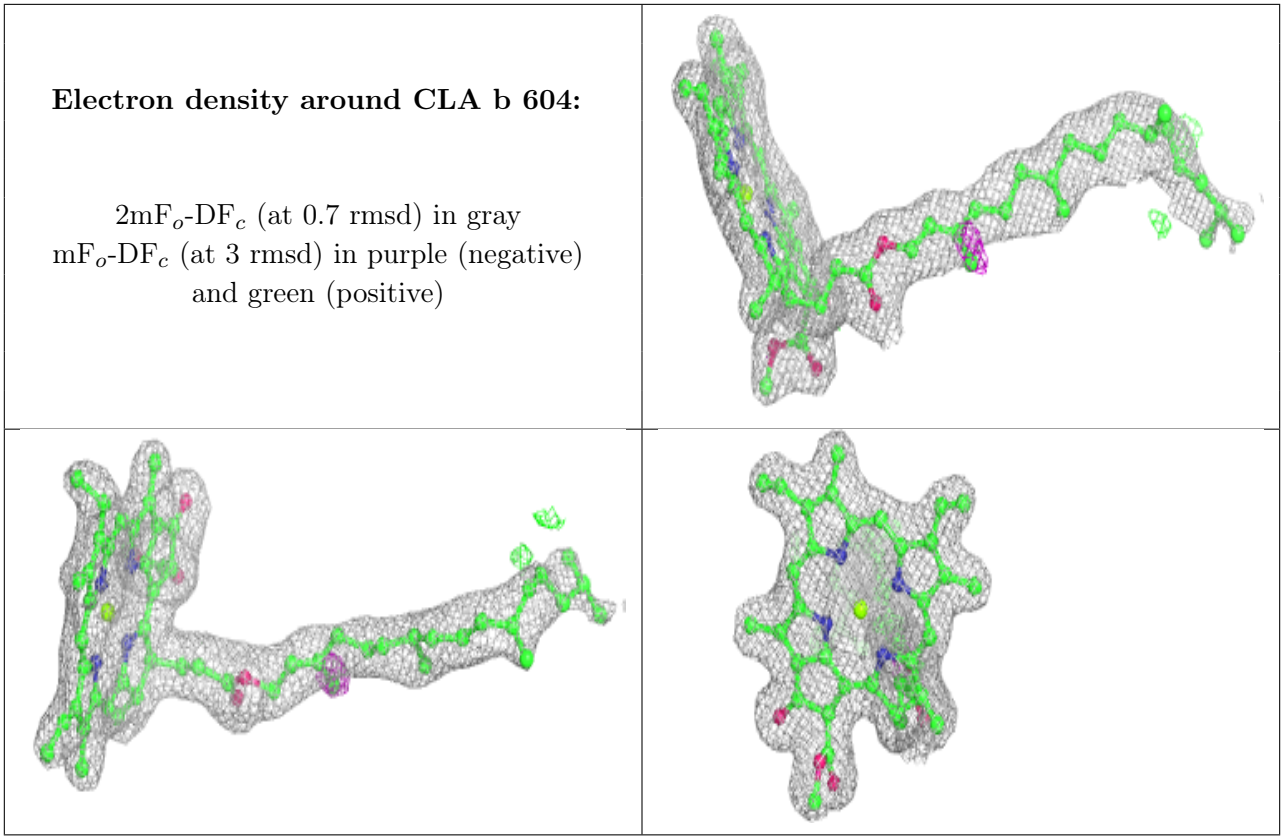
Electron density around CLA c 511:

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



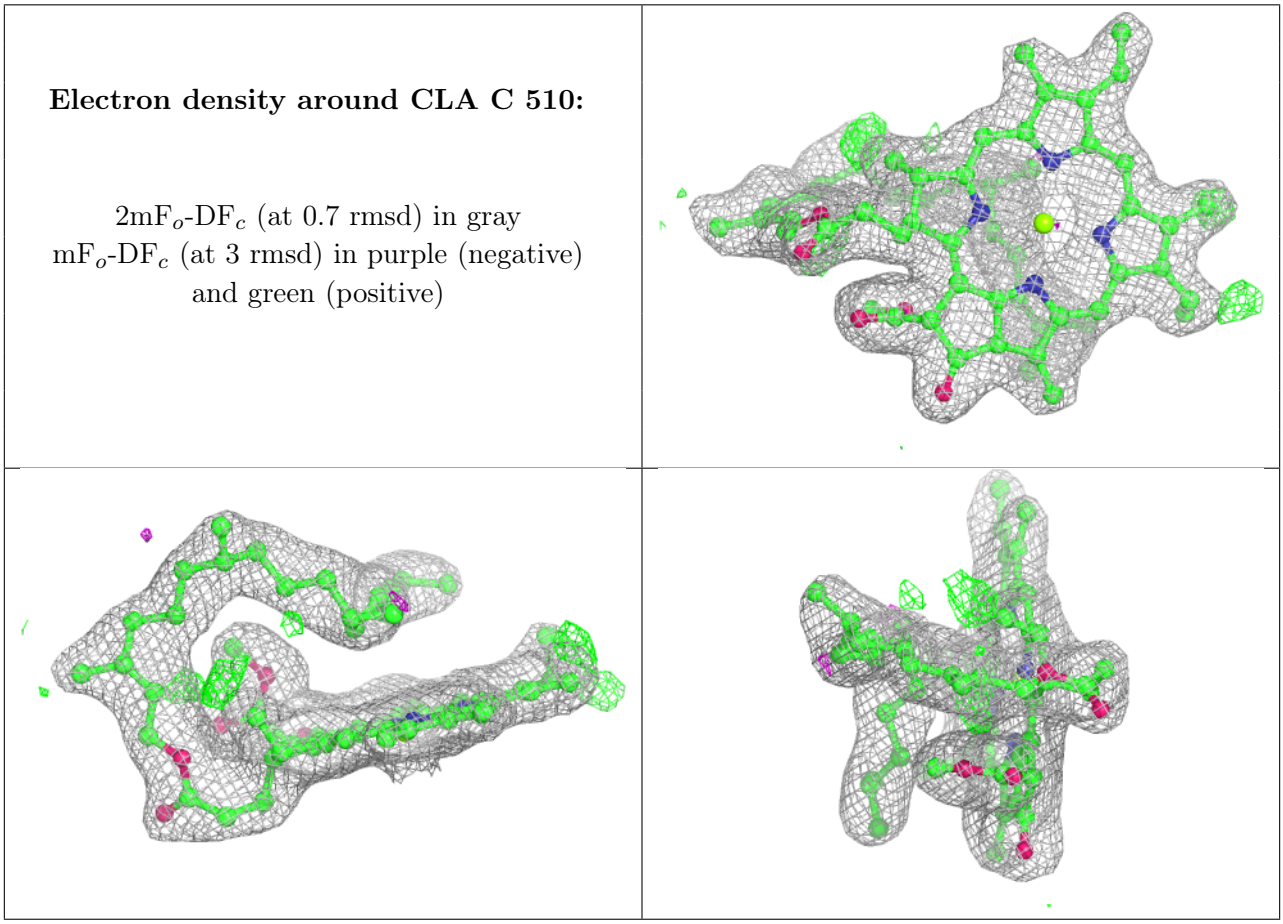
Electron density around CLA b 604:

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



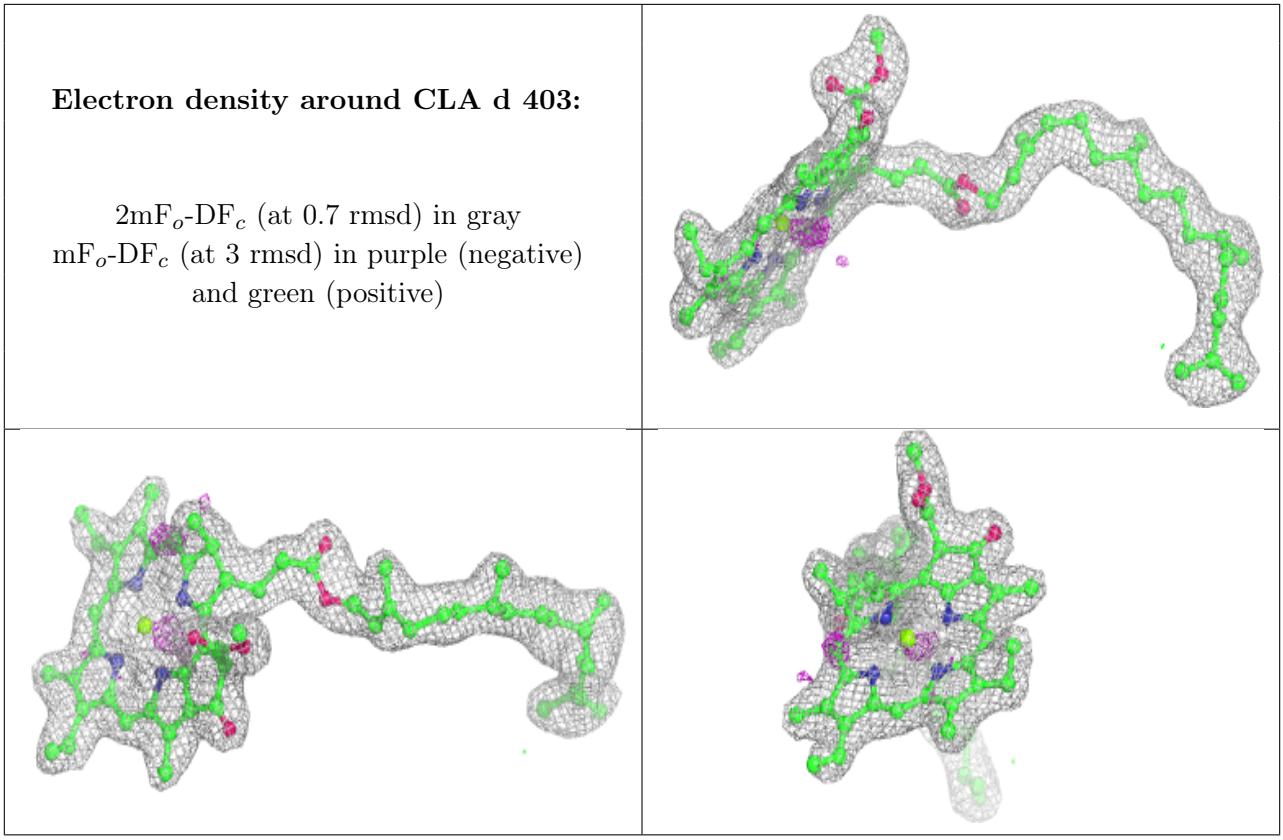
Electron density around CLA C 510:

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



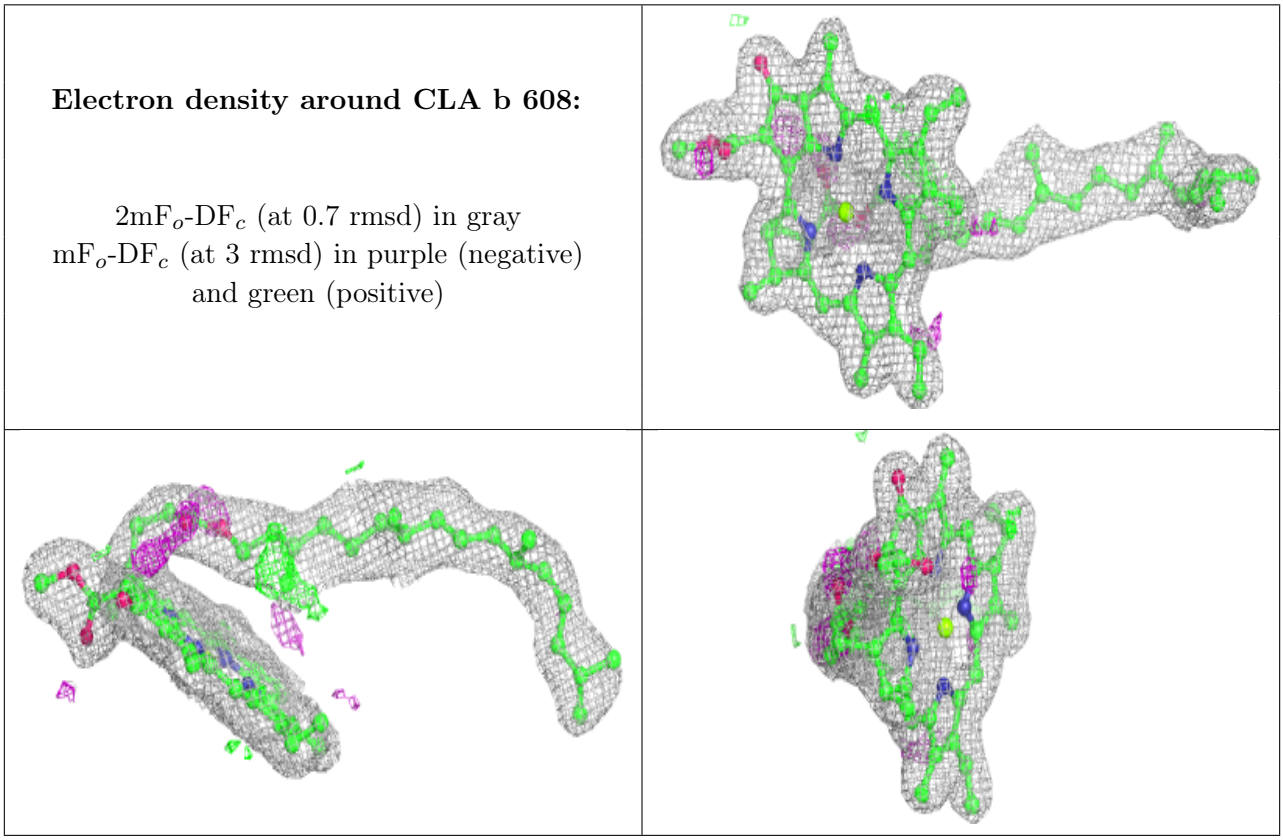
Electron density around CLA d 403:

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



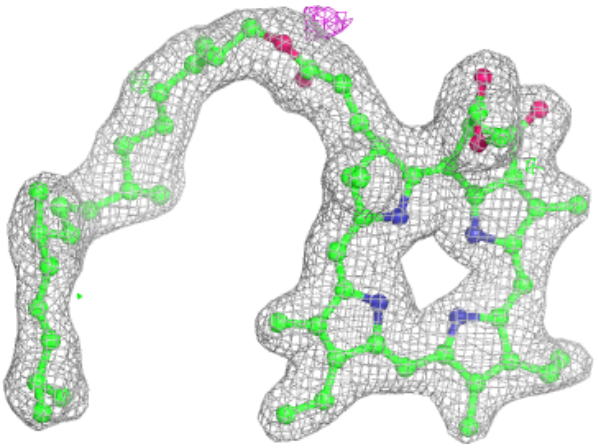
Electron density around CLA b 608:

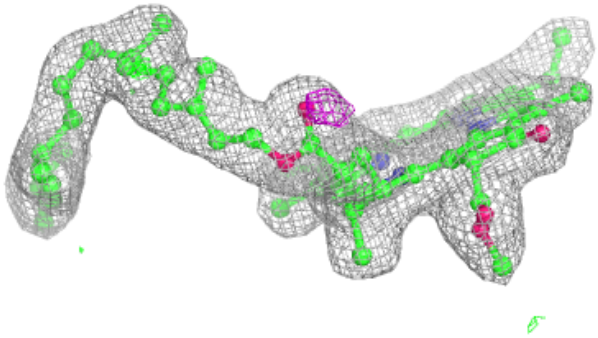
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO d 402:

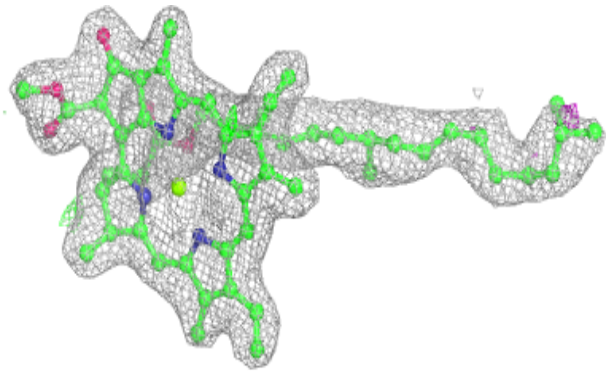
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

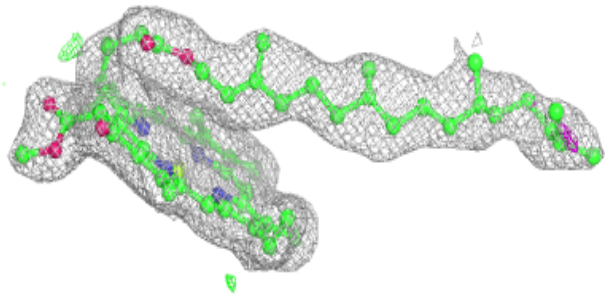


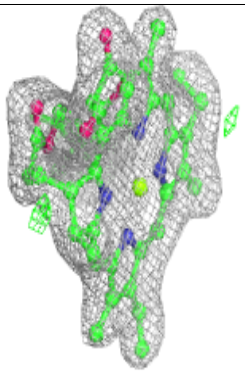


Electron density around CLA B 614:

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

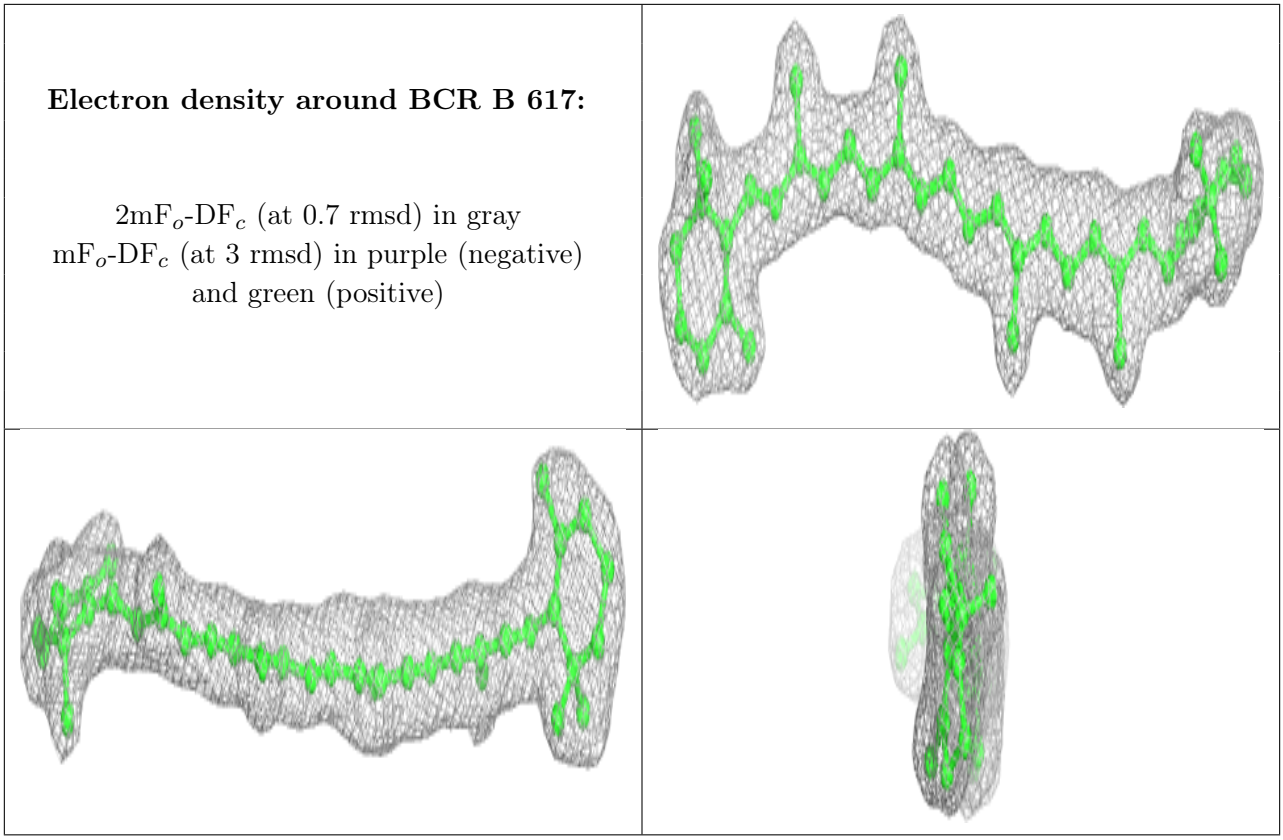






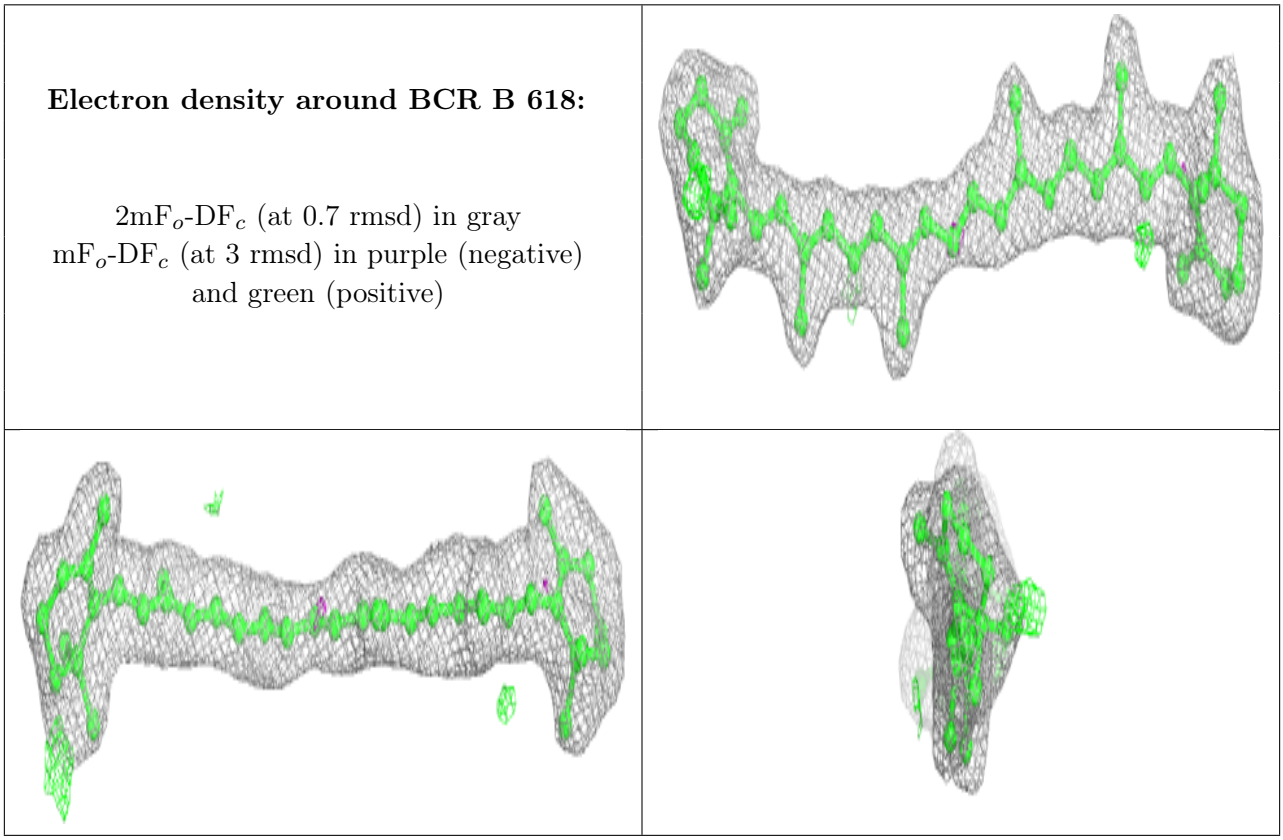
Electron density around BCR B 617:

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



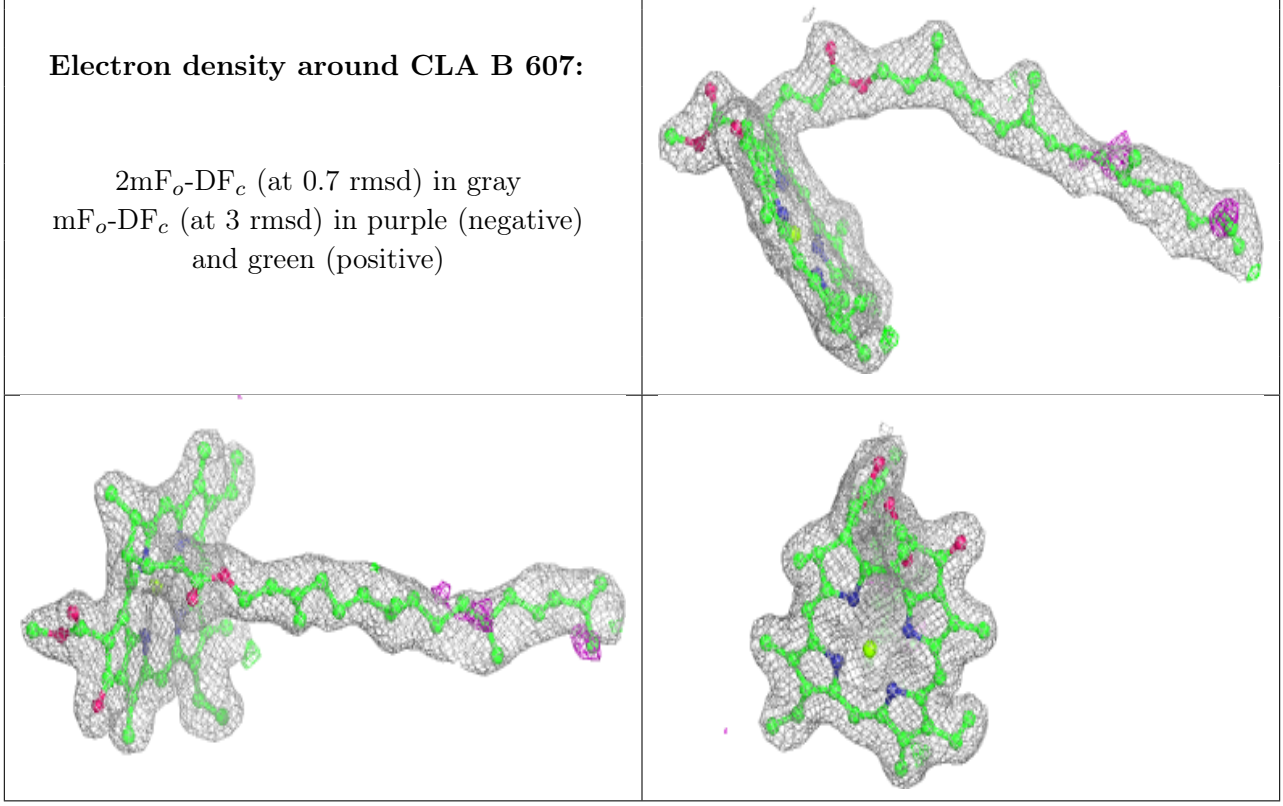
Electron density around BCR B 618:

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



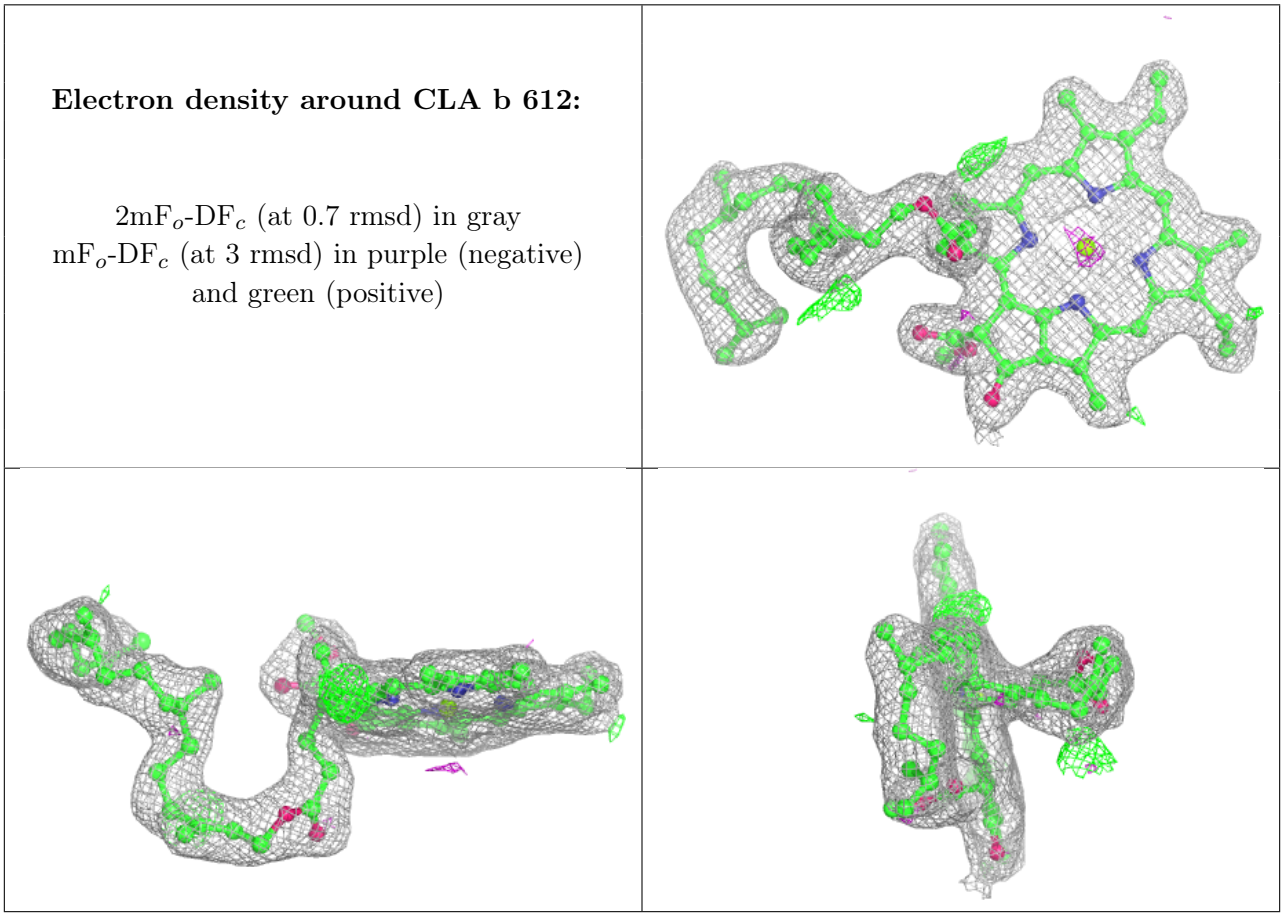
Electron density around CLA B 607:

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



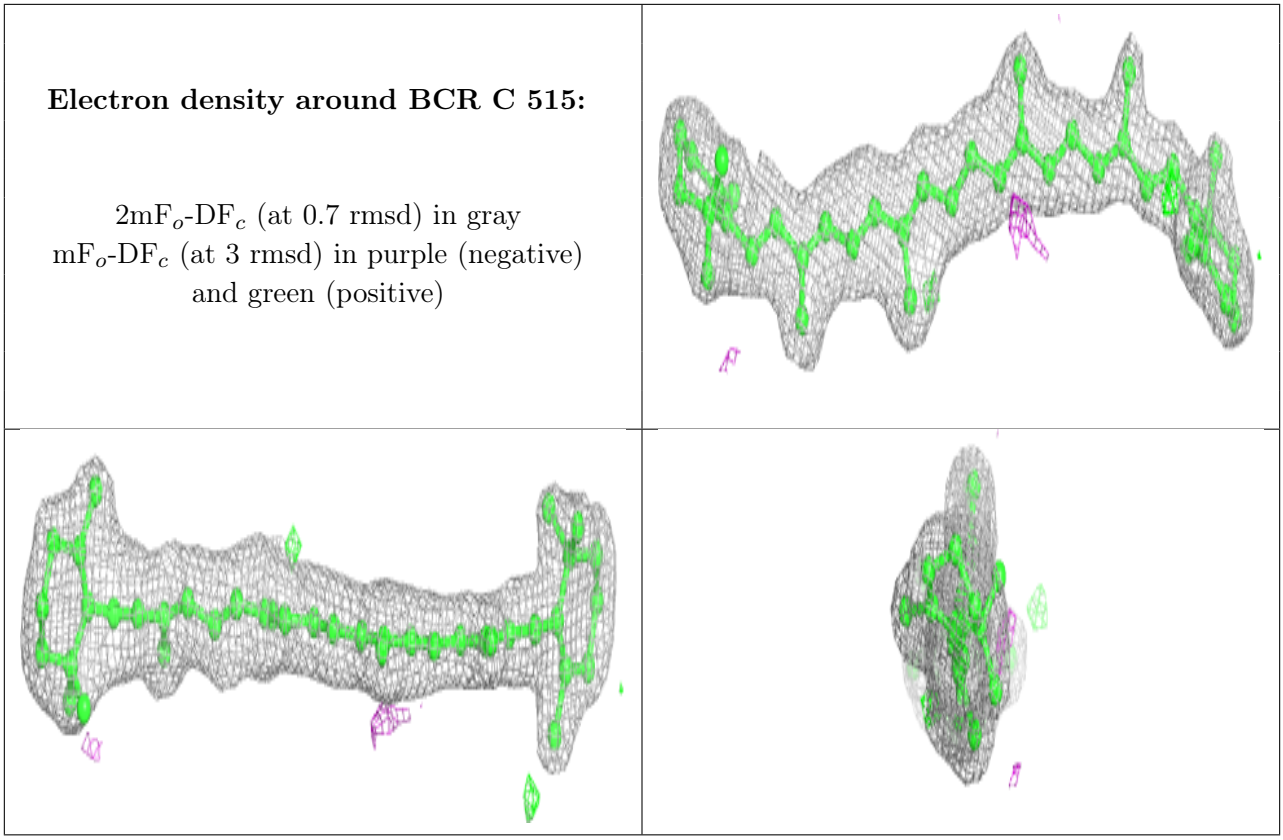
Electron density around CLA b 612:

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



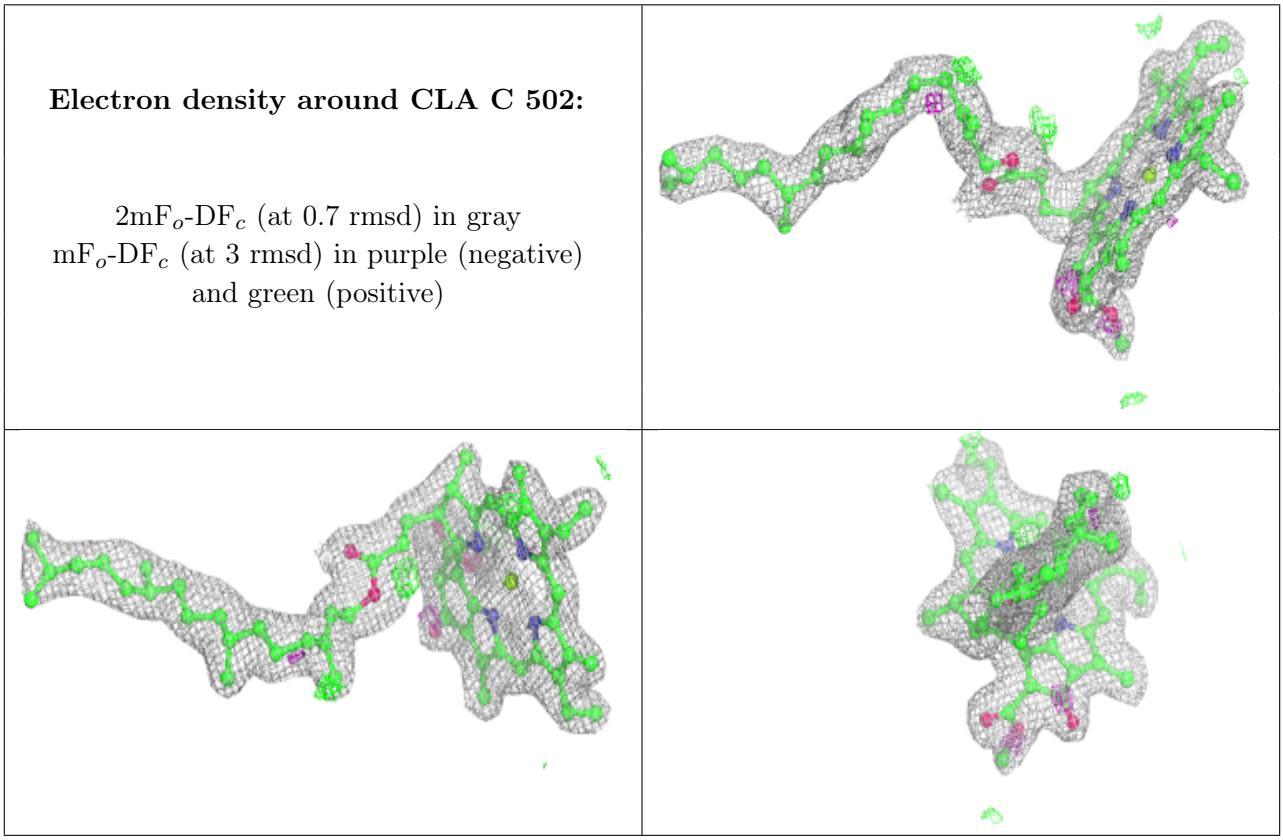
Electron density around BCR C 515:

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



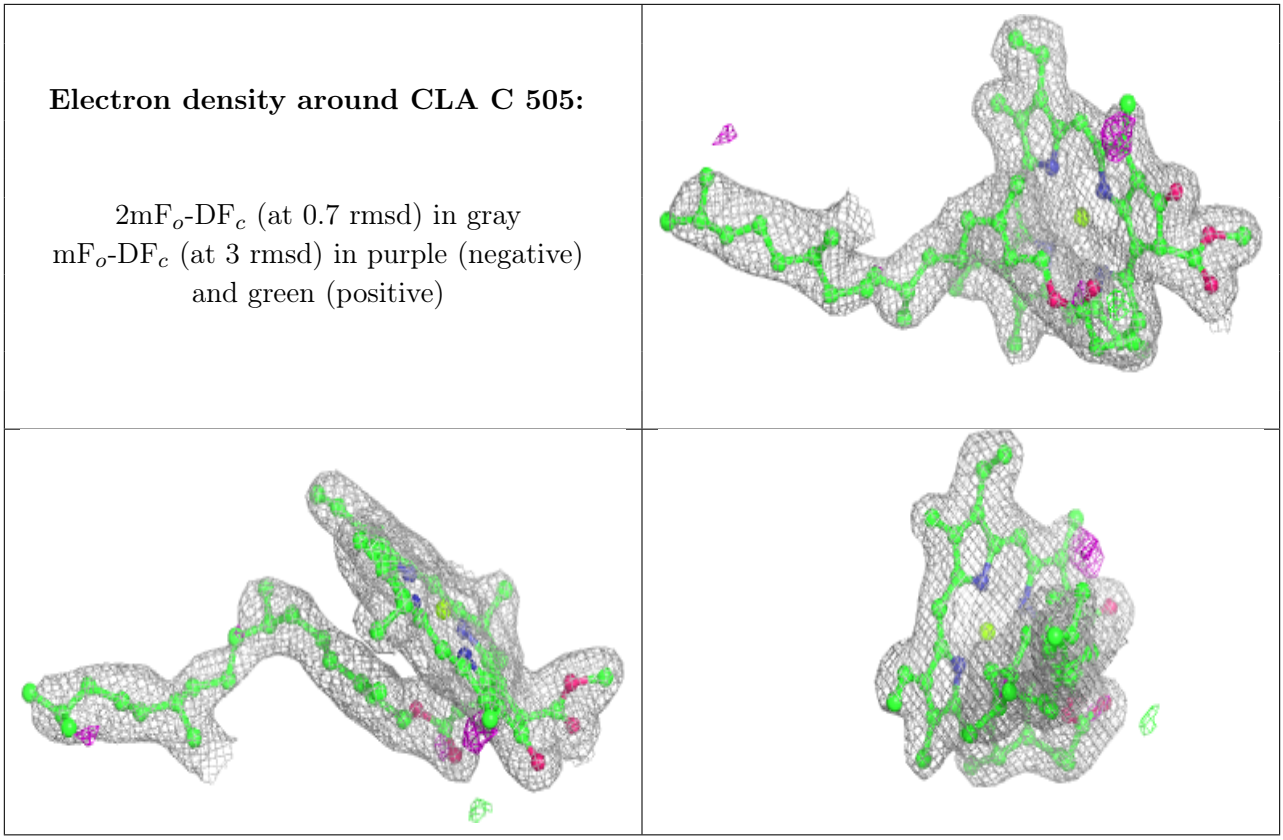
Electron density around CLA C 502:

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



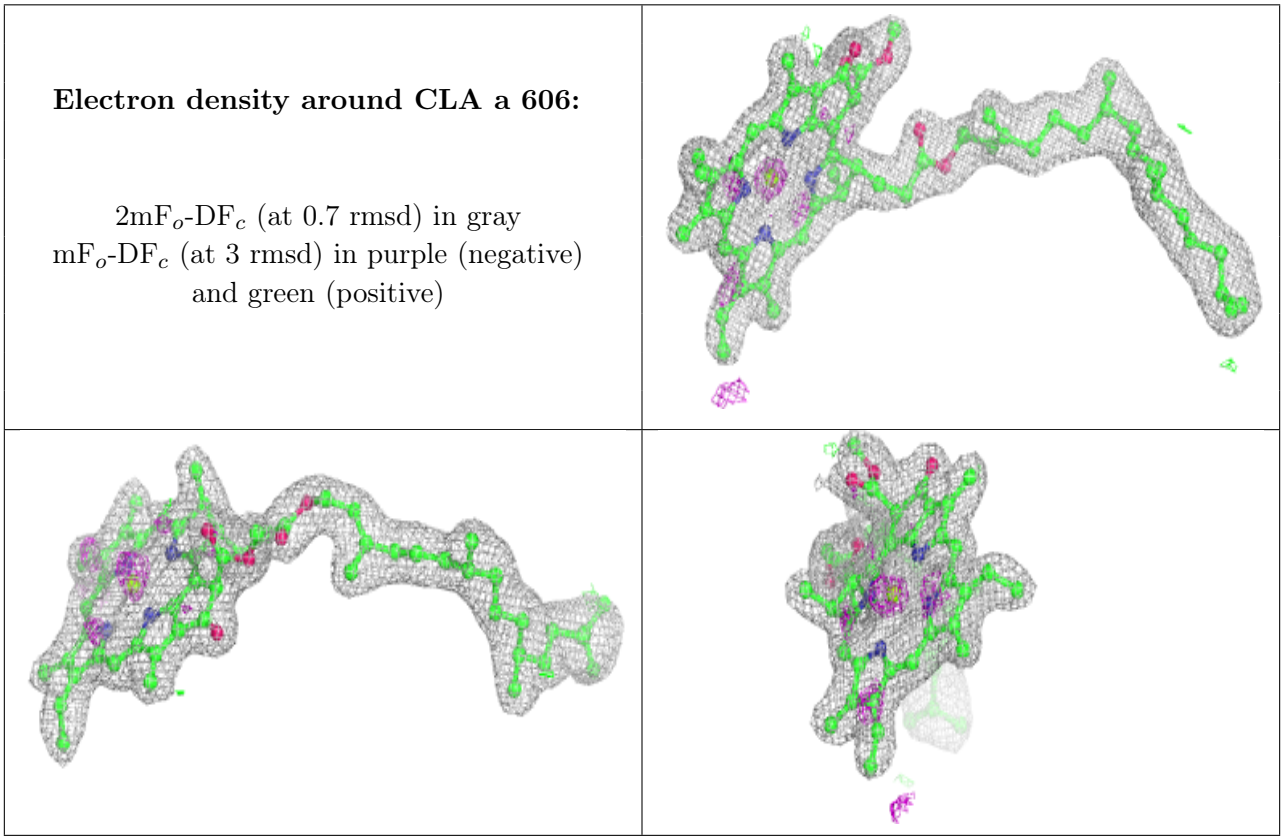
Electron density around CLA C 505:

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



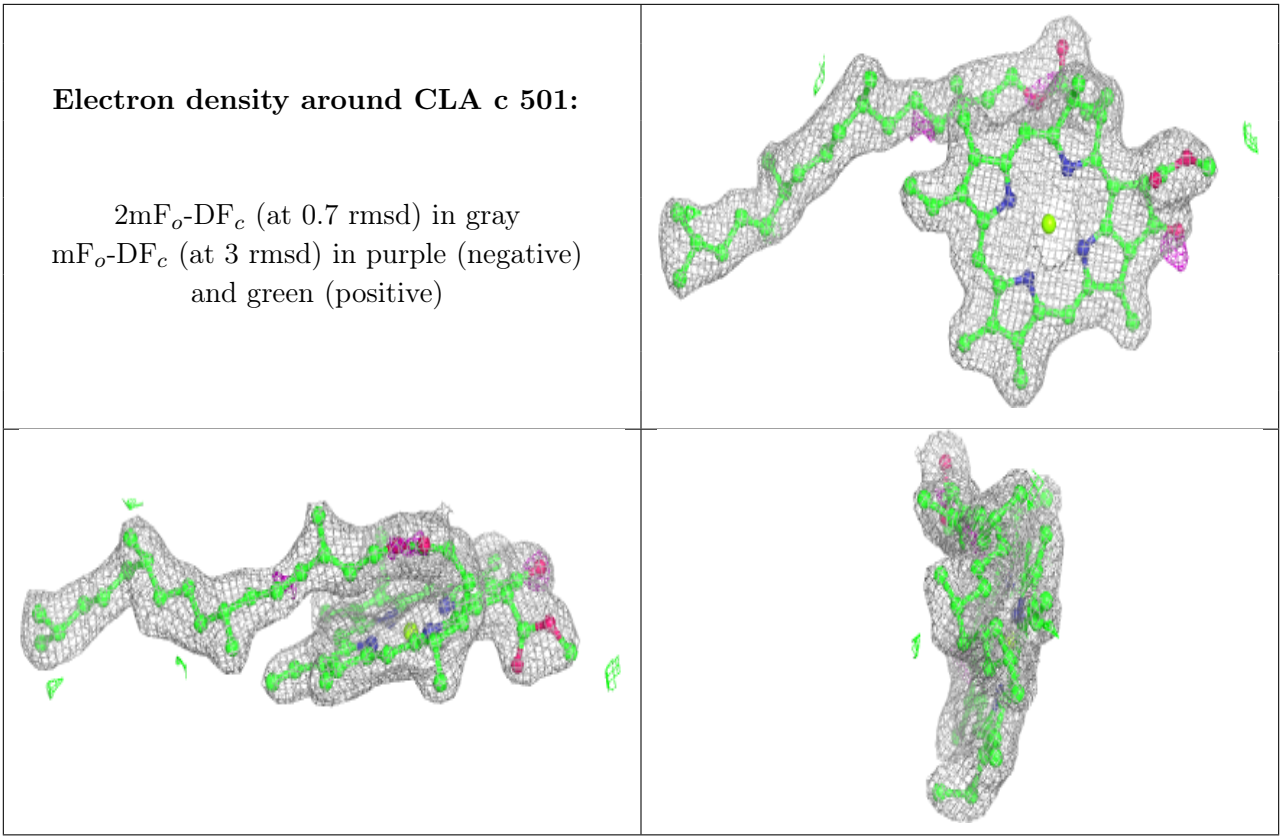
Electron density around CLA a 606:

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



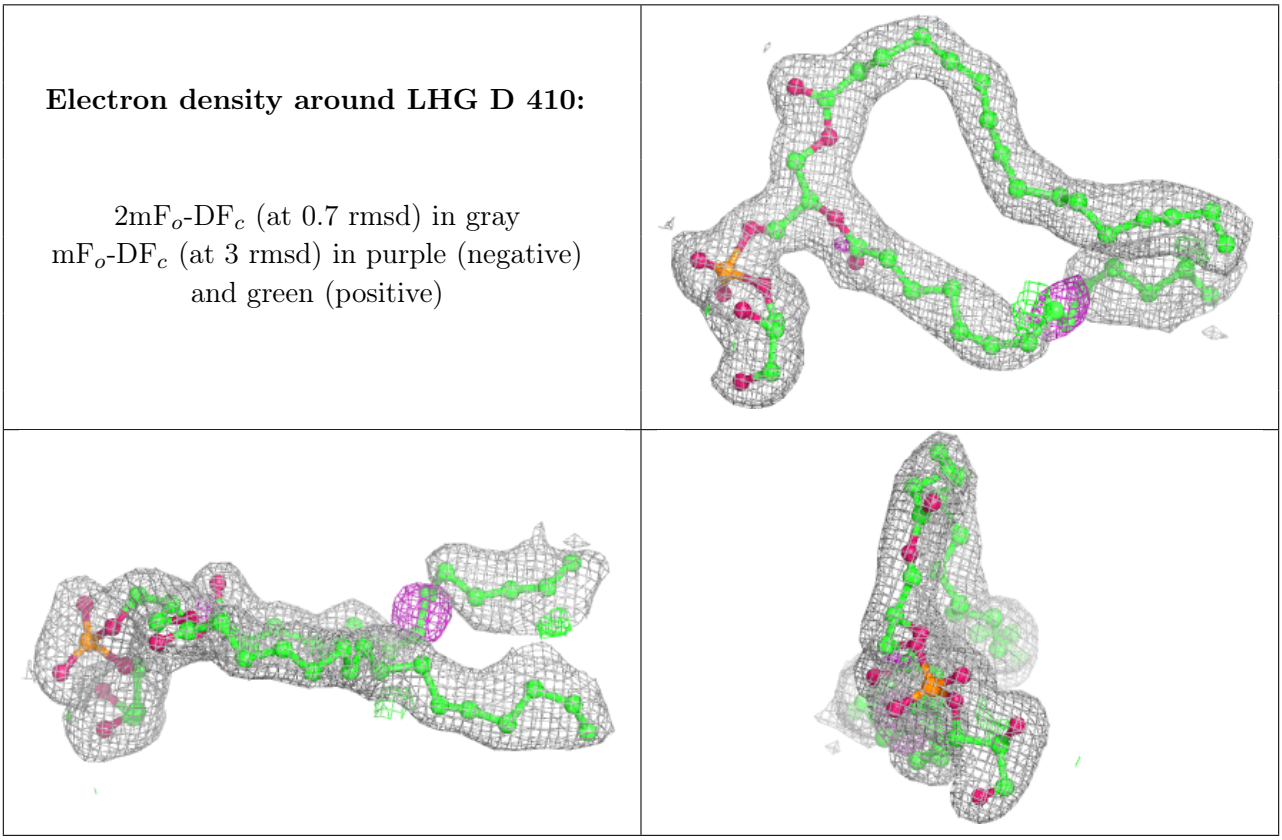
Electron density around CLA c 501:

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



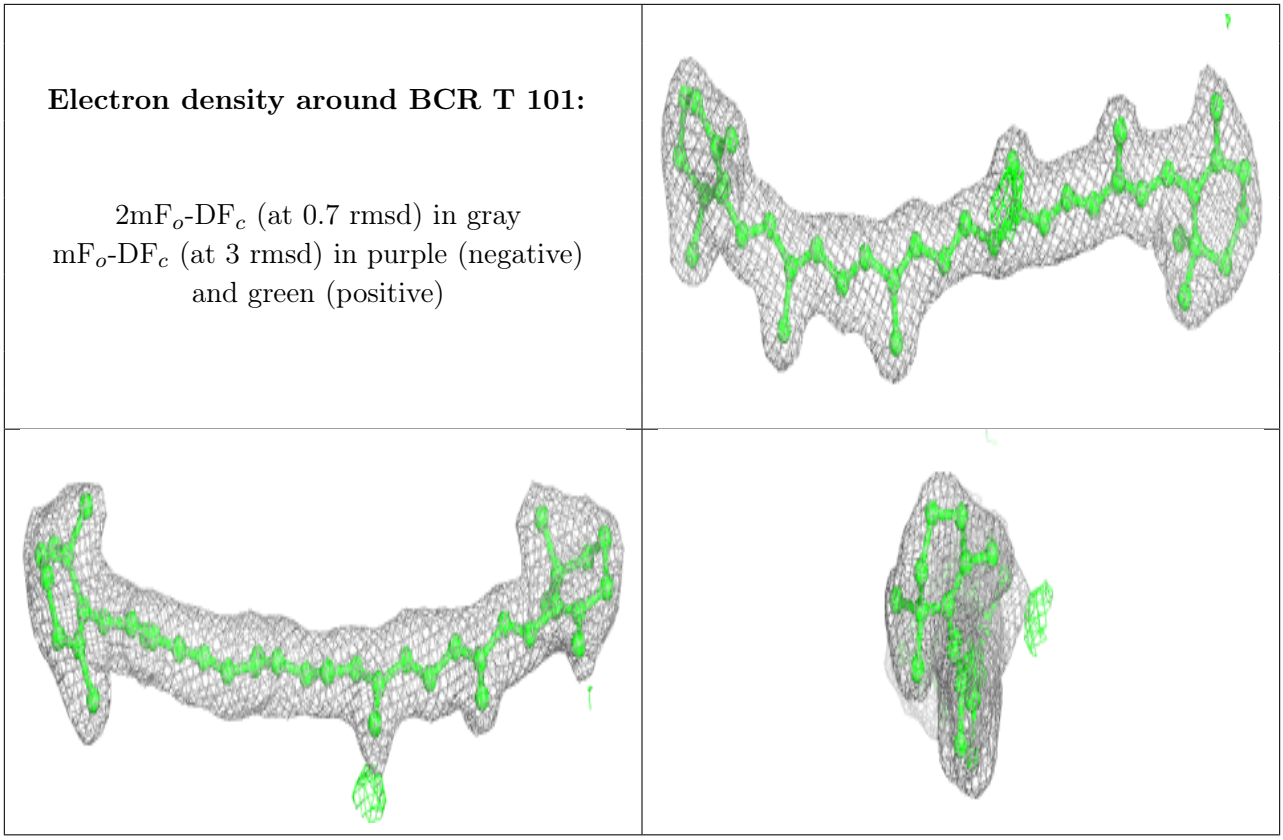
Electron density around LHG D 410:

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



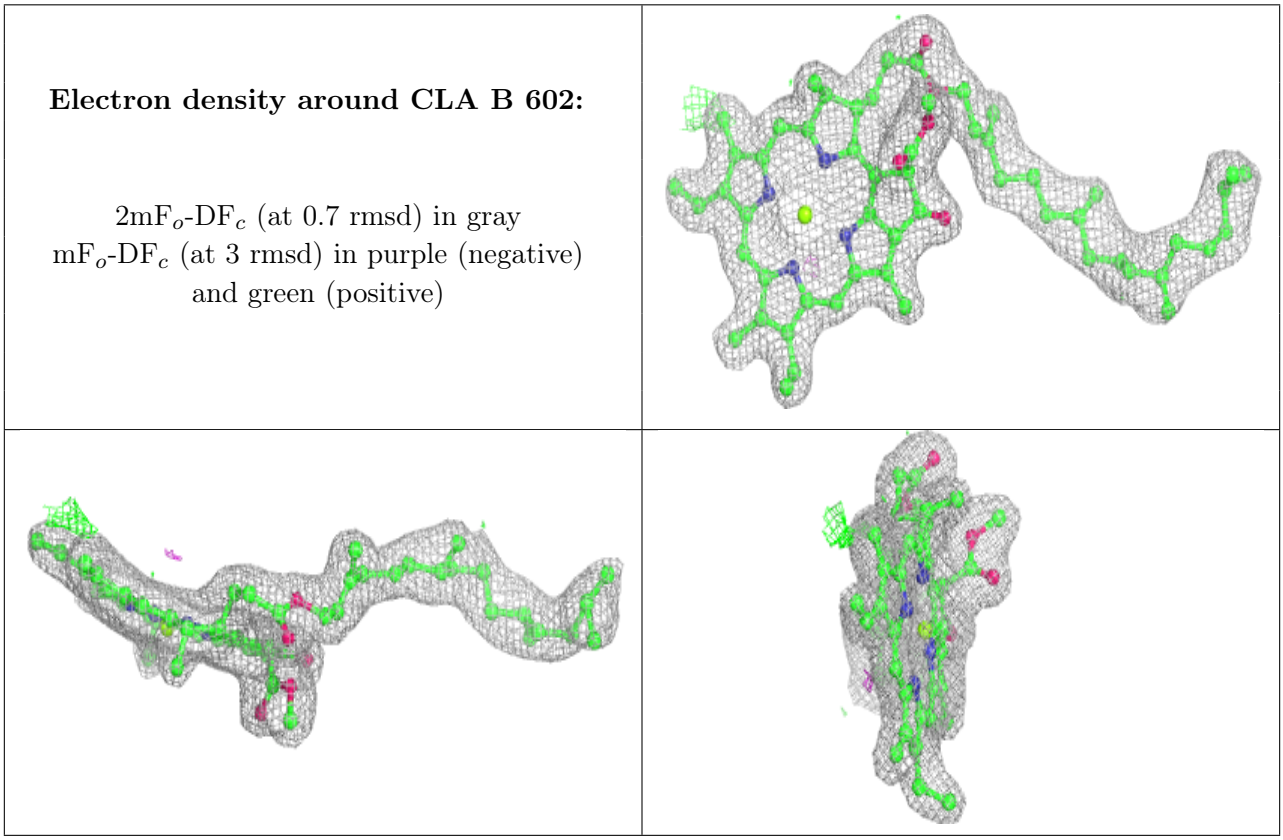
Electron density around BCR T 101:

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



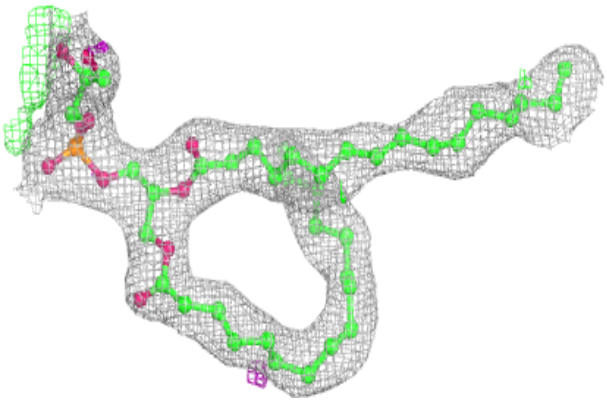
Electron density around CLA B 602:

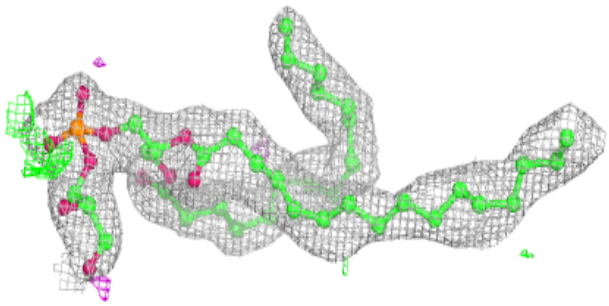
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

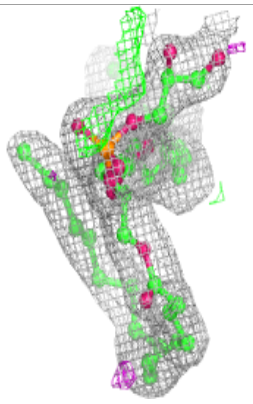


Electron density around LHG a 613:

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

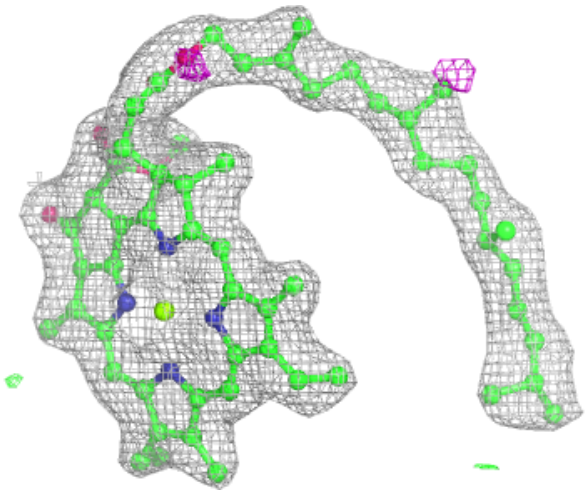


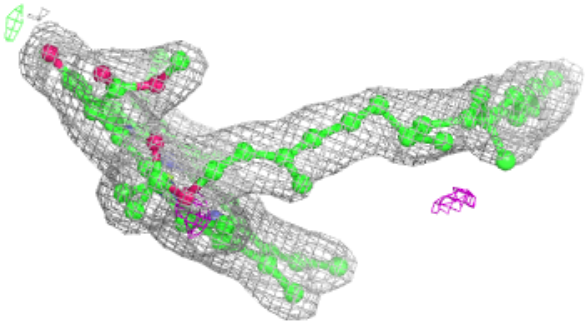


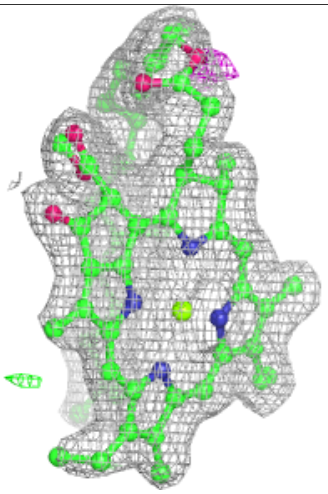


Electron density around CLA C 507:

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

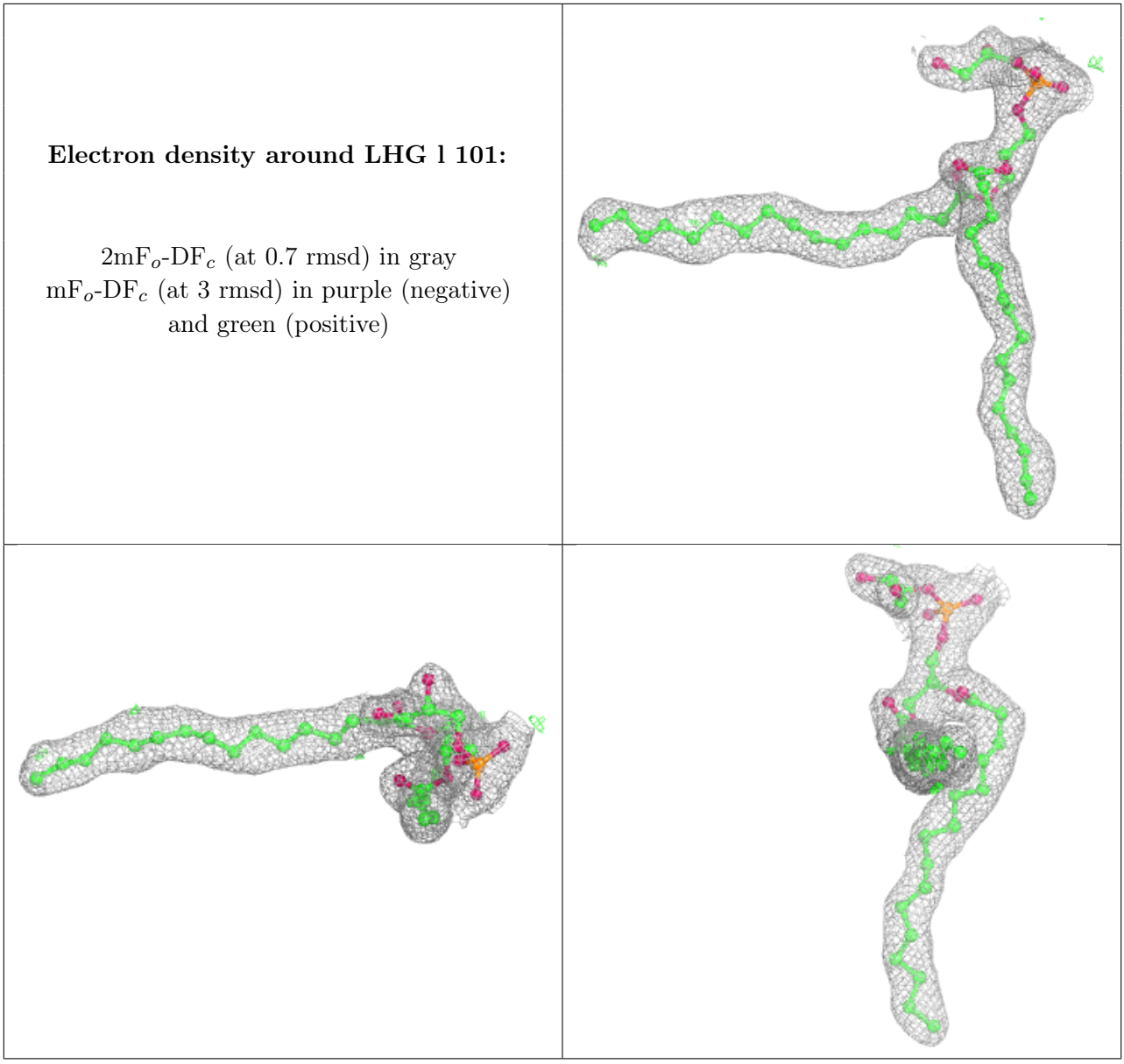






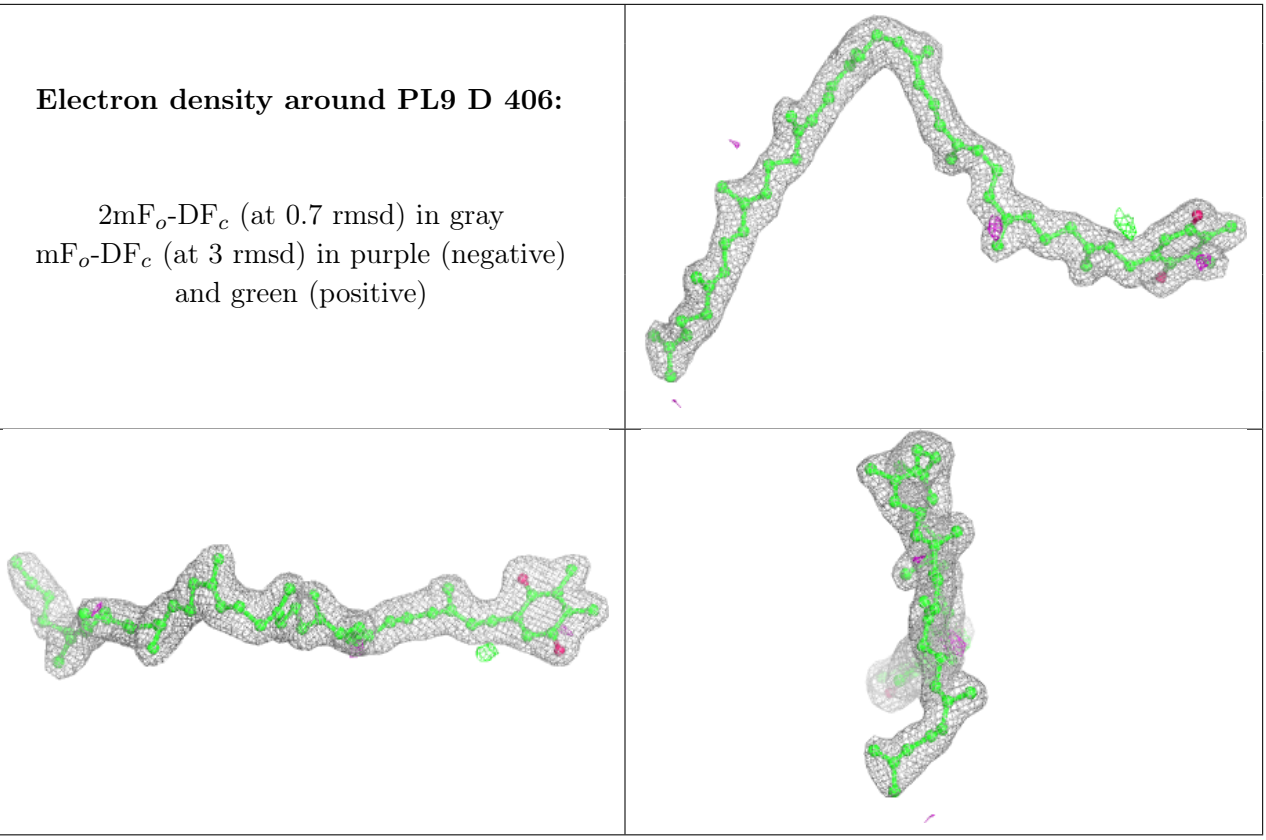
Electron density around LHG l 101:

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



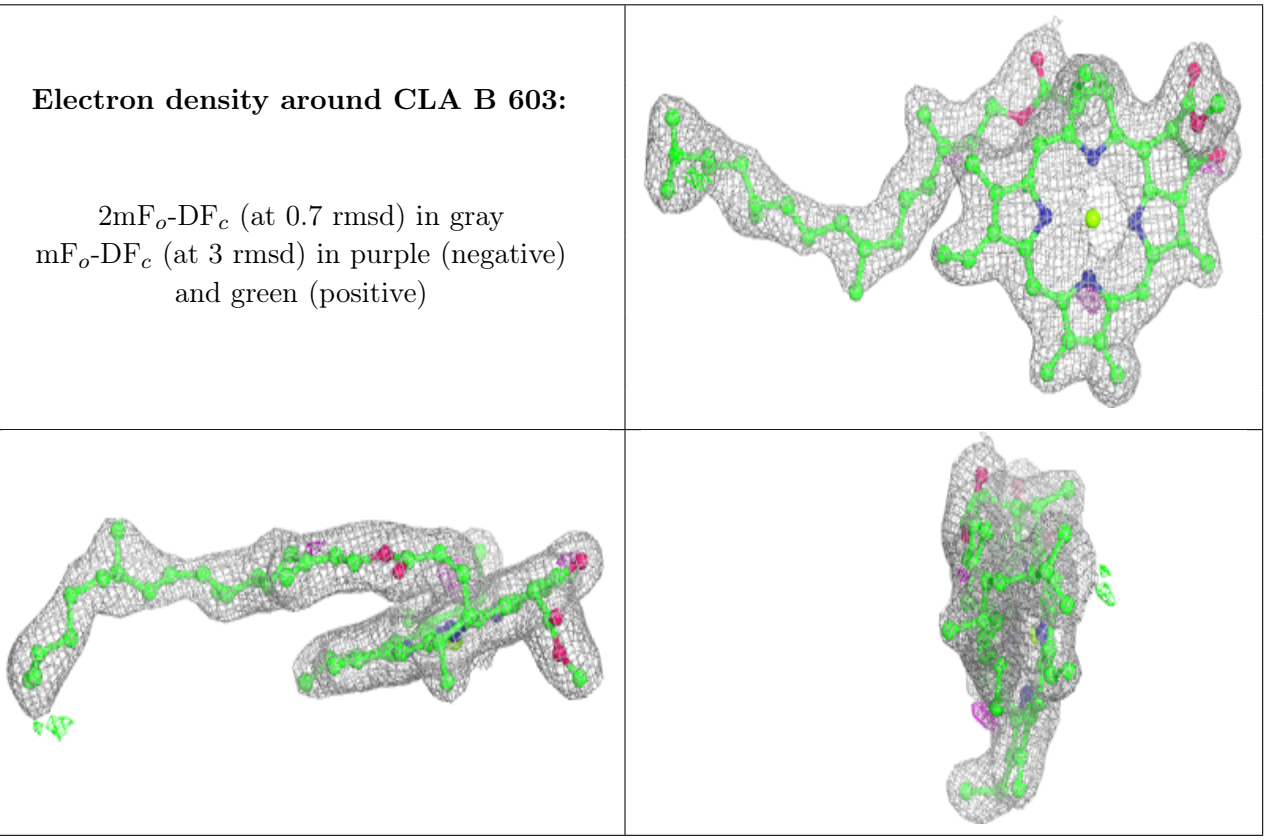
Electron density around PL9 D 406:

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



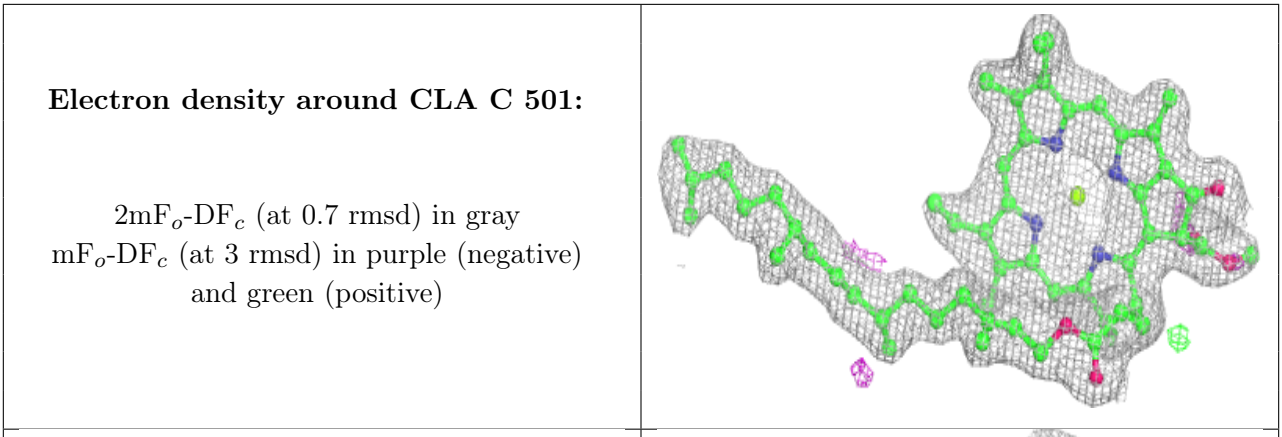
Electron density around CLA B 603:

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



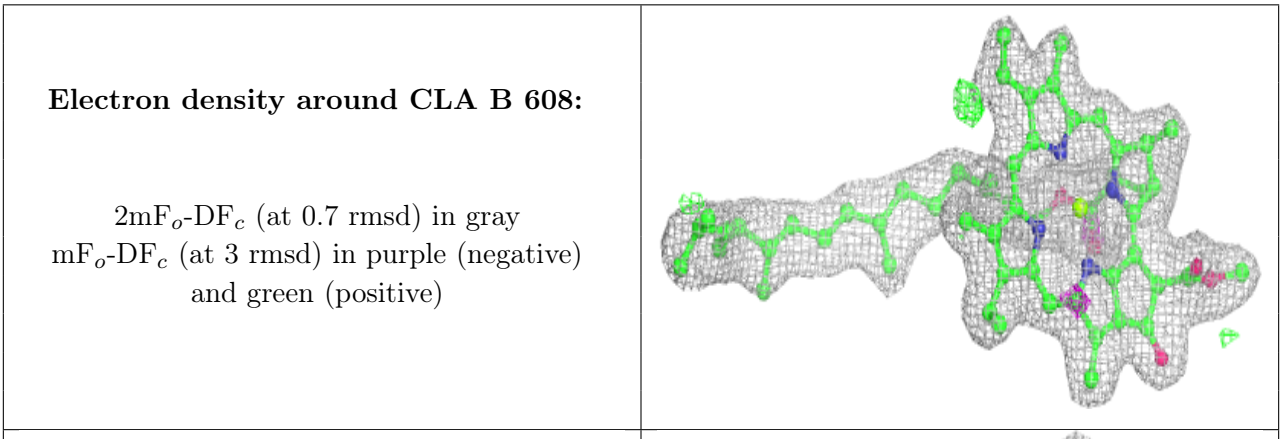
Electron density around CLA C 501:

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



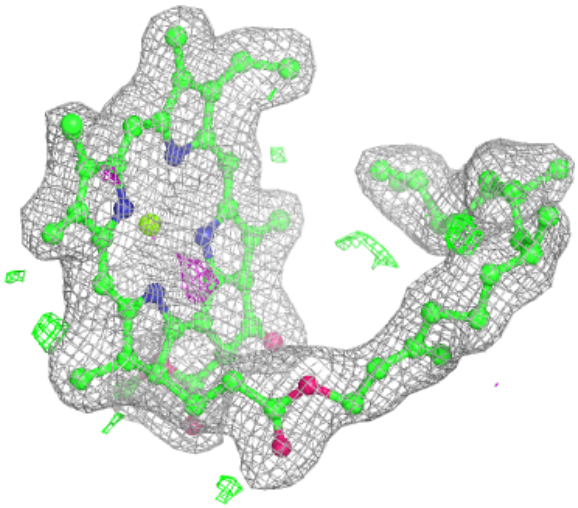
Electron density around CLA B 608:

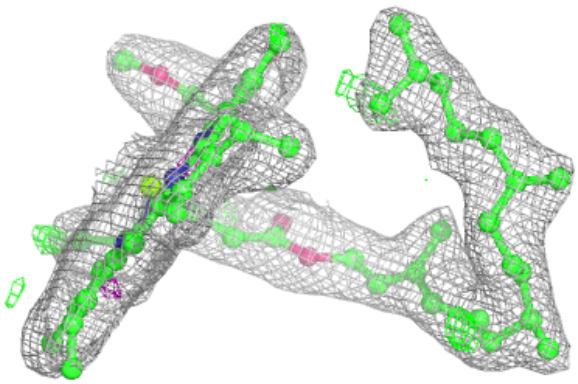
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

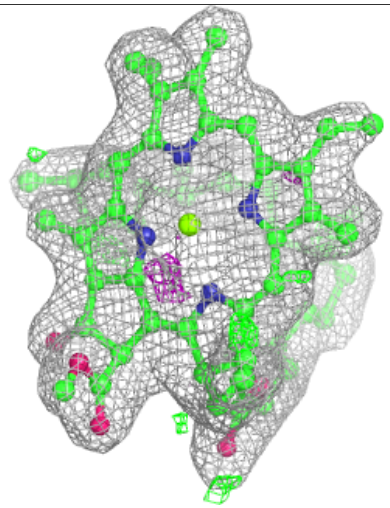


Electron density around CLA C 503:

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

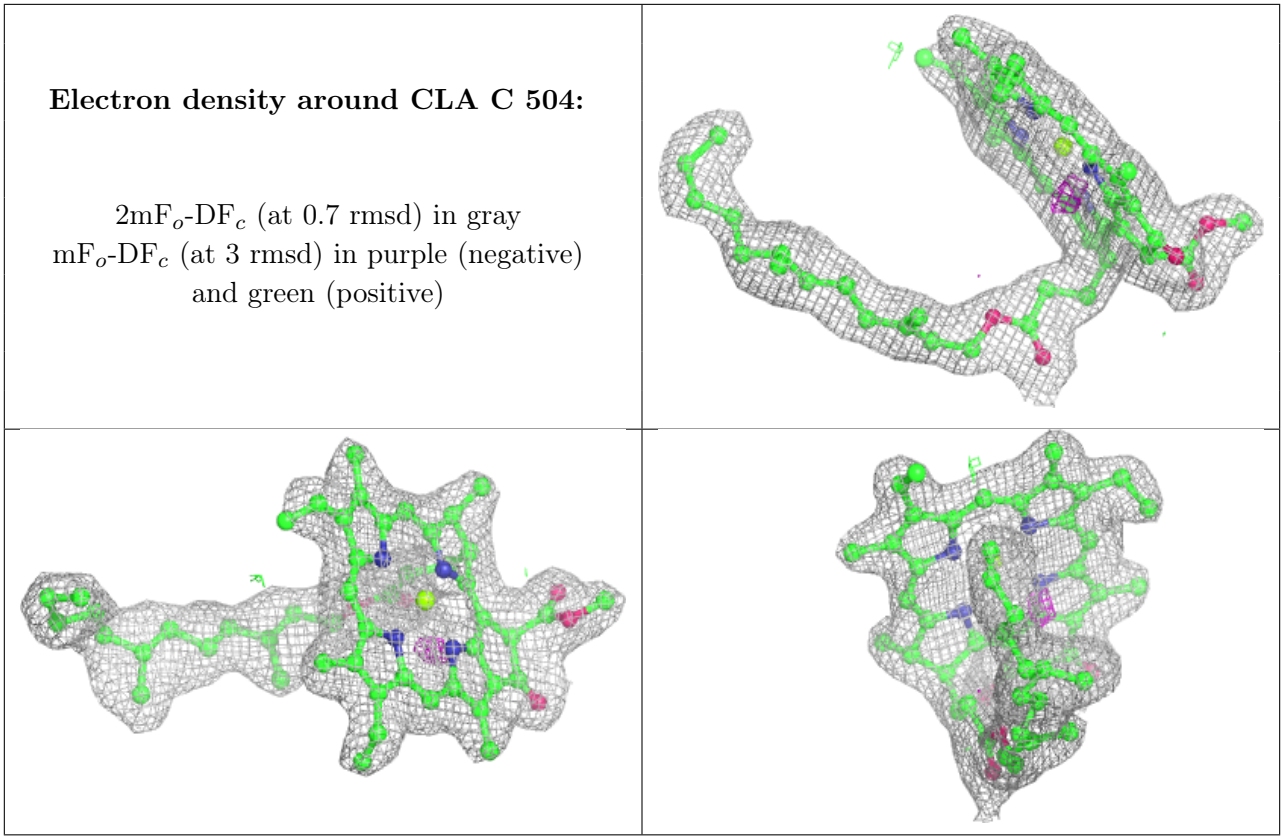






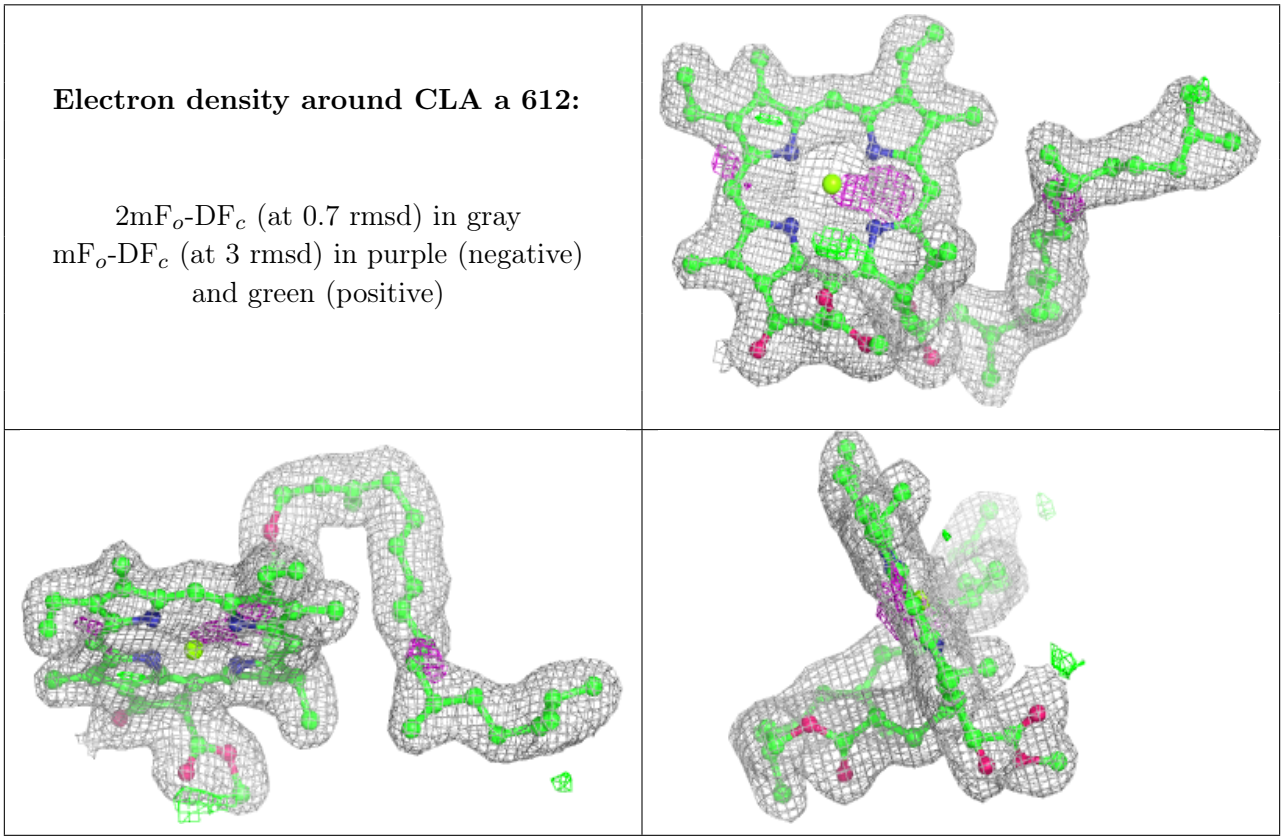
Electron density around CLA C 504:

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



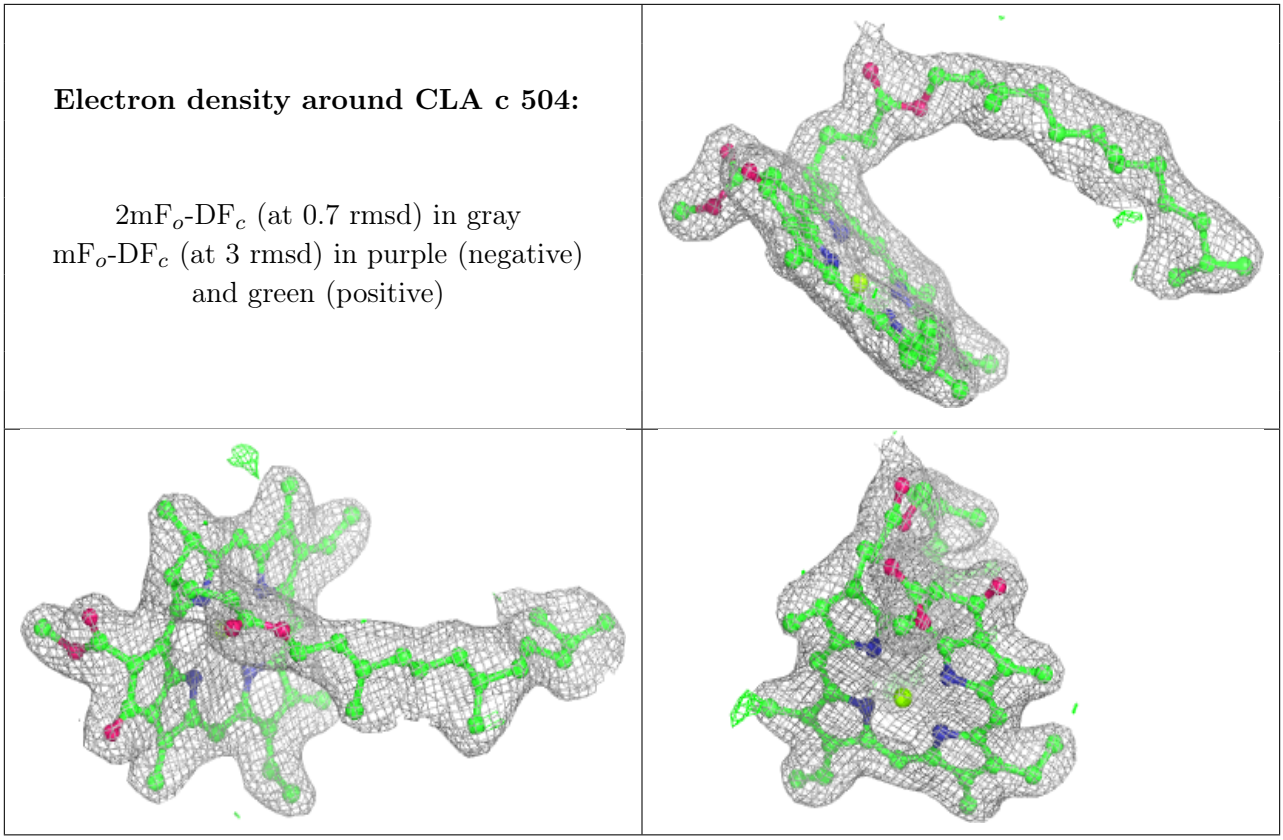
Electron density around CLA a 612:

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



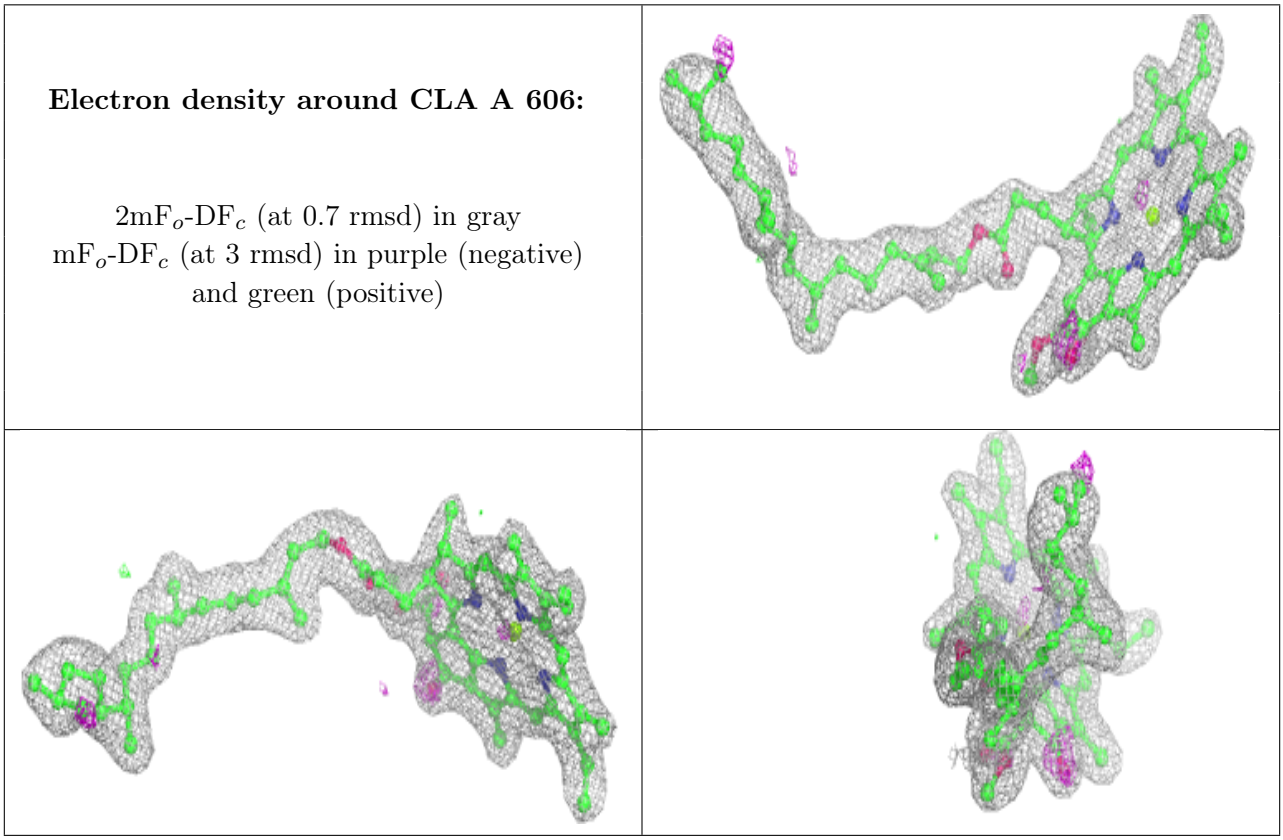
Electron density around CLA c 504:

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



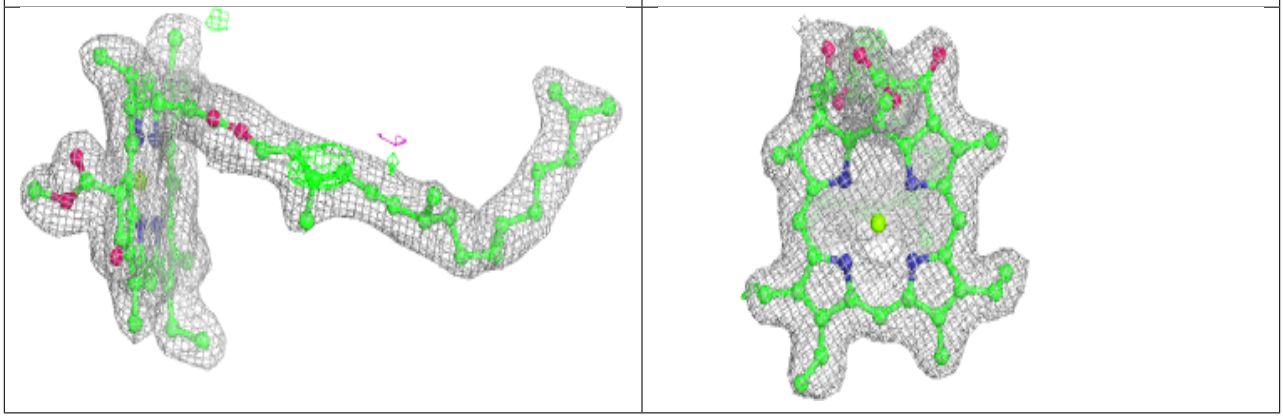
Electron density around CLA A 606:

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



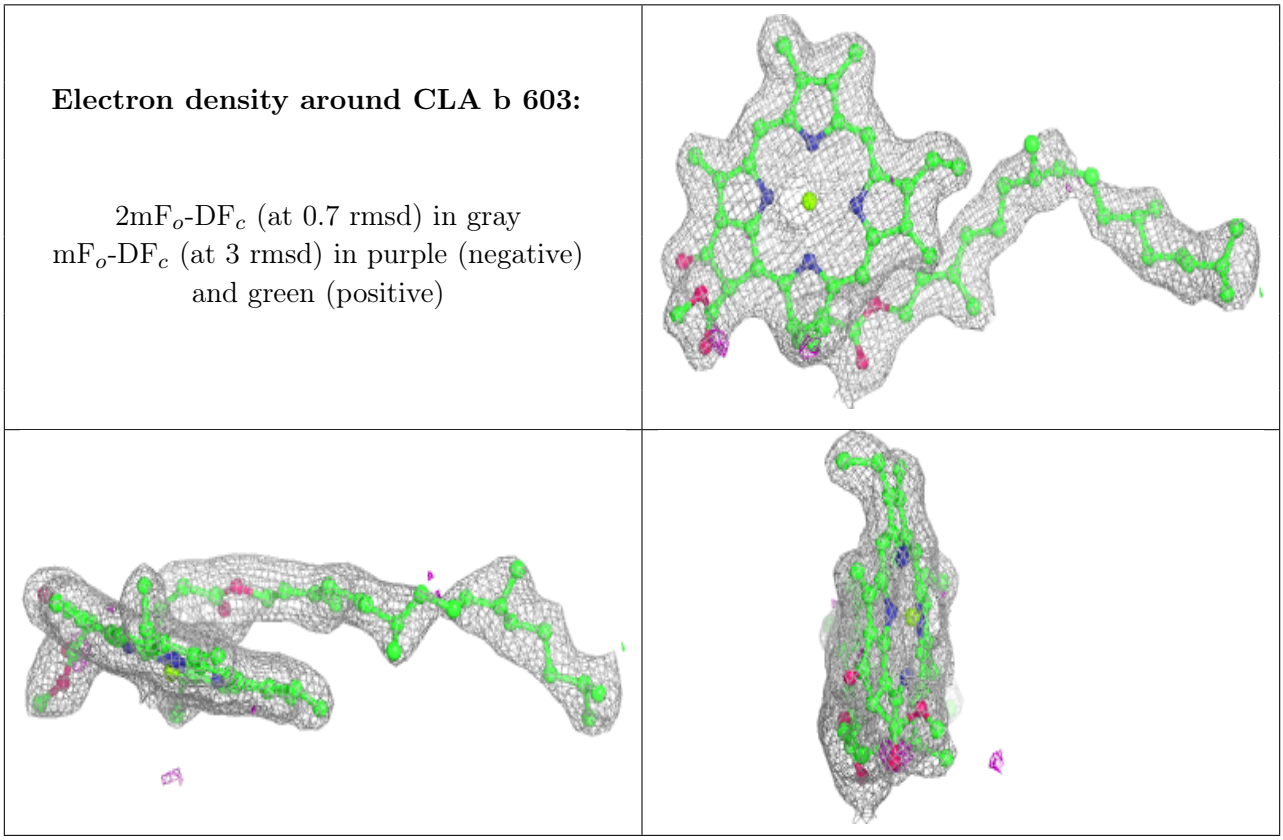
Electron density around CLA B 605:

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



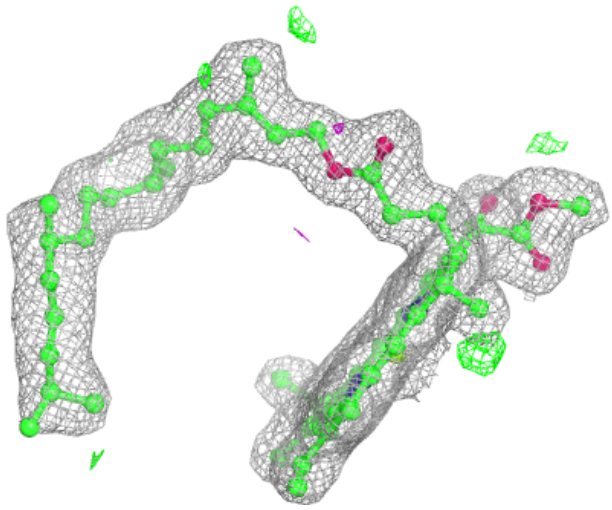
Electron density around CLA b 603:

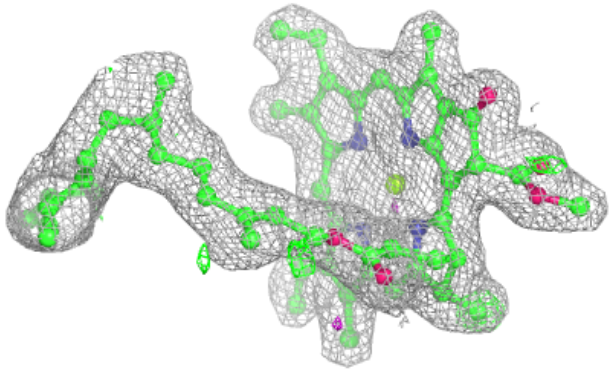
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

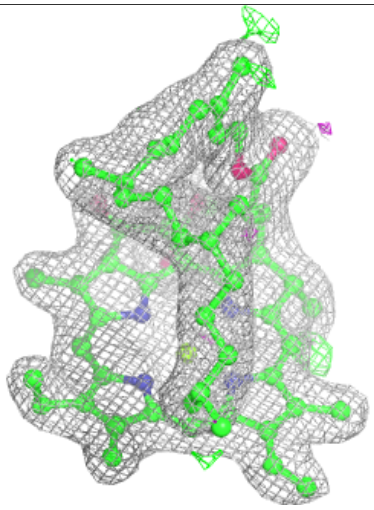


Electron density around CLA B 611:

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

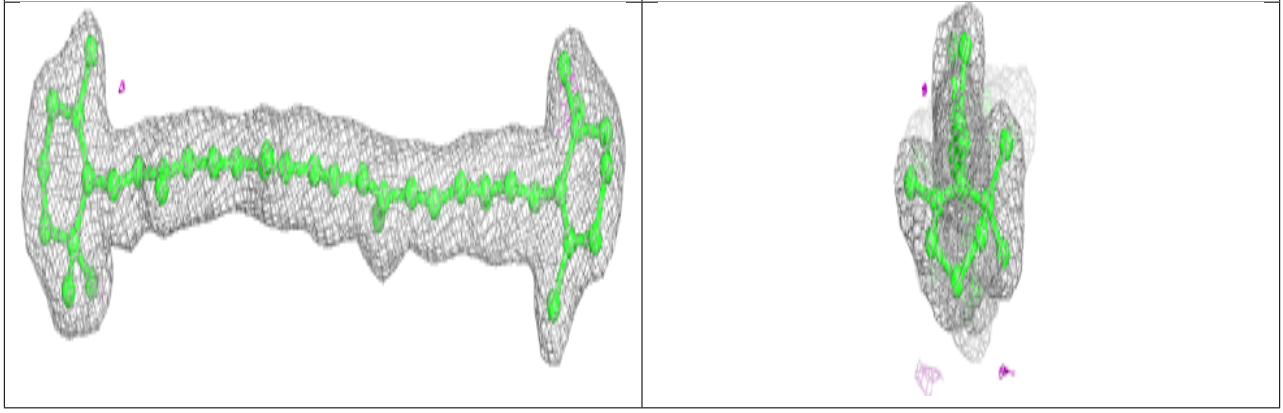






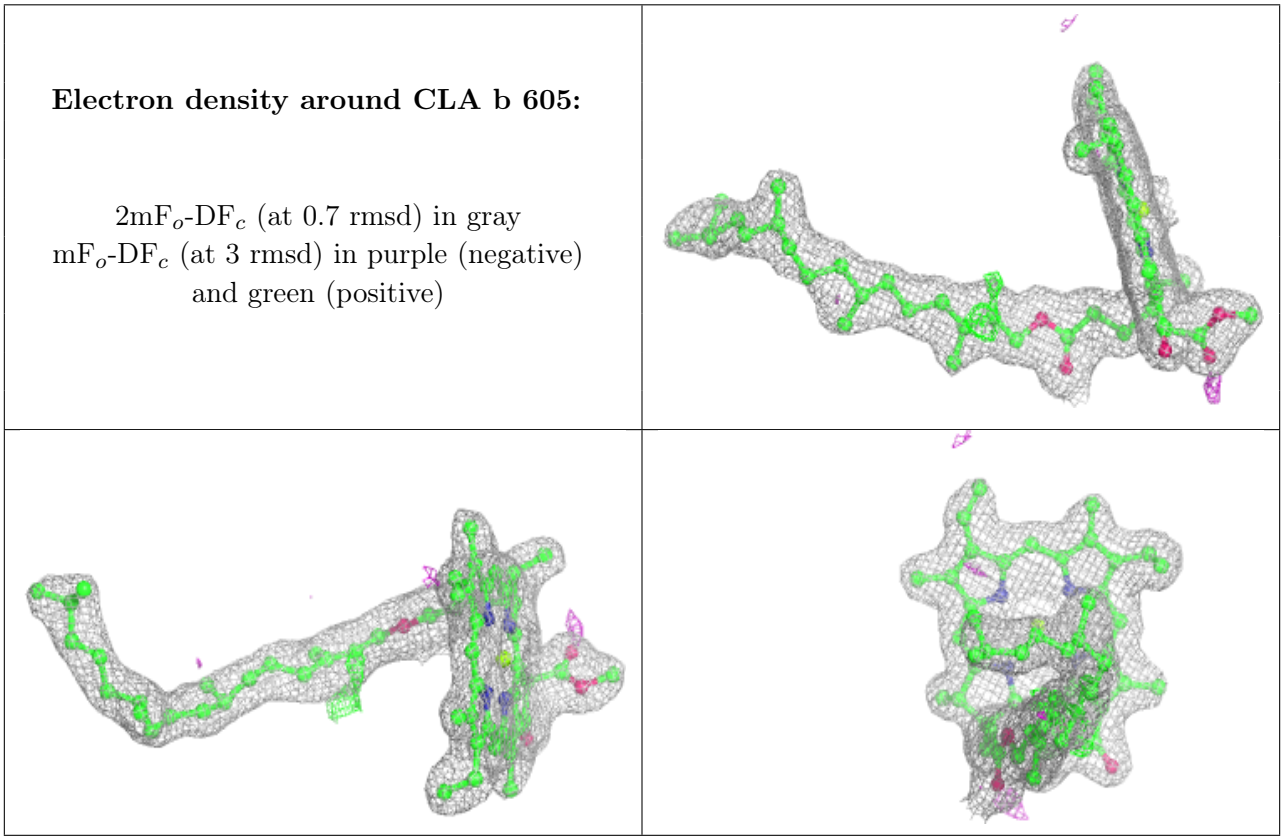
Electron density around BCR a 610:

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



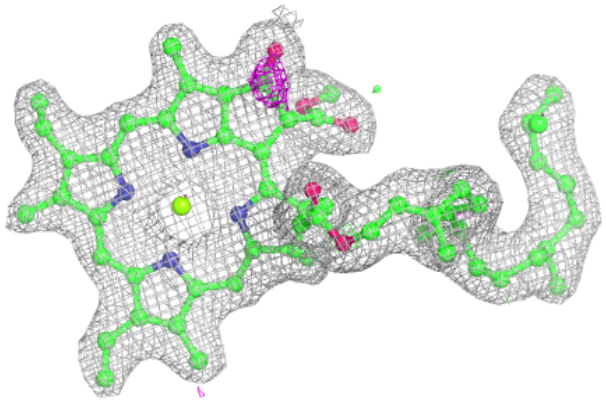
Electron density around CLA b 605:

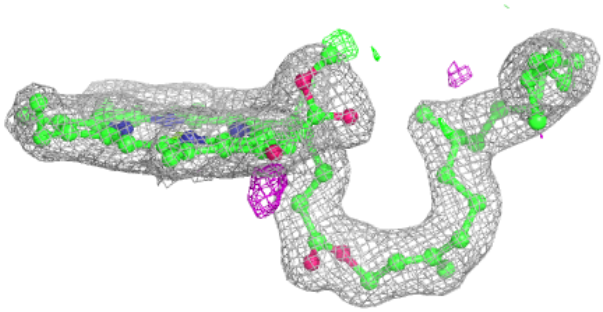
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

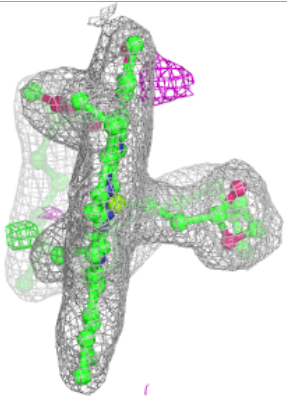


Electron density around CLA B 612:

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

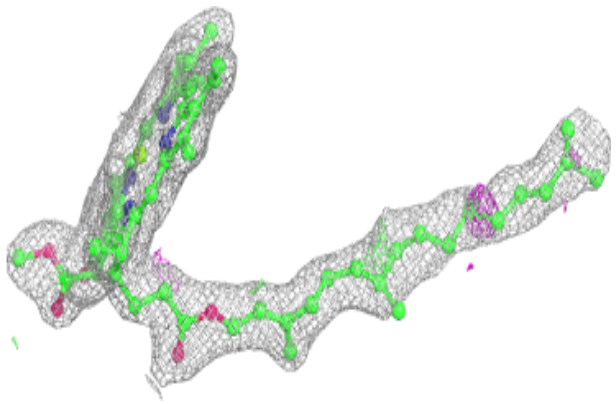


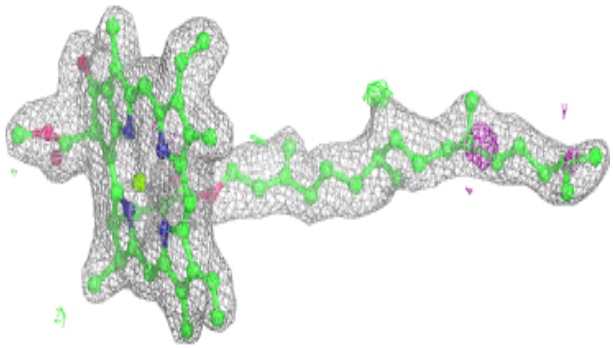


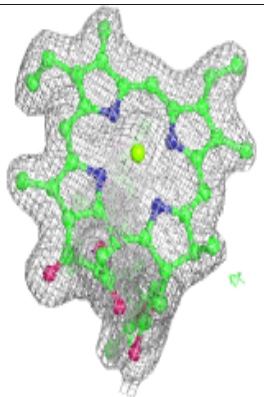


Electron density around CLA b 607:

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

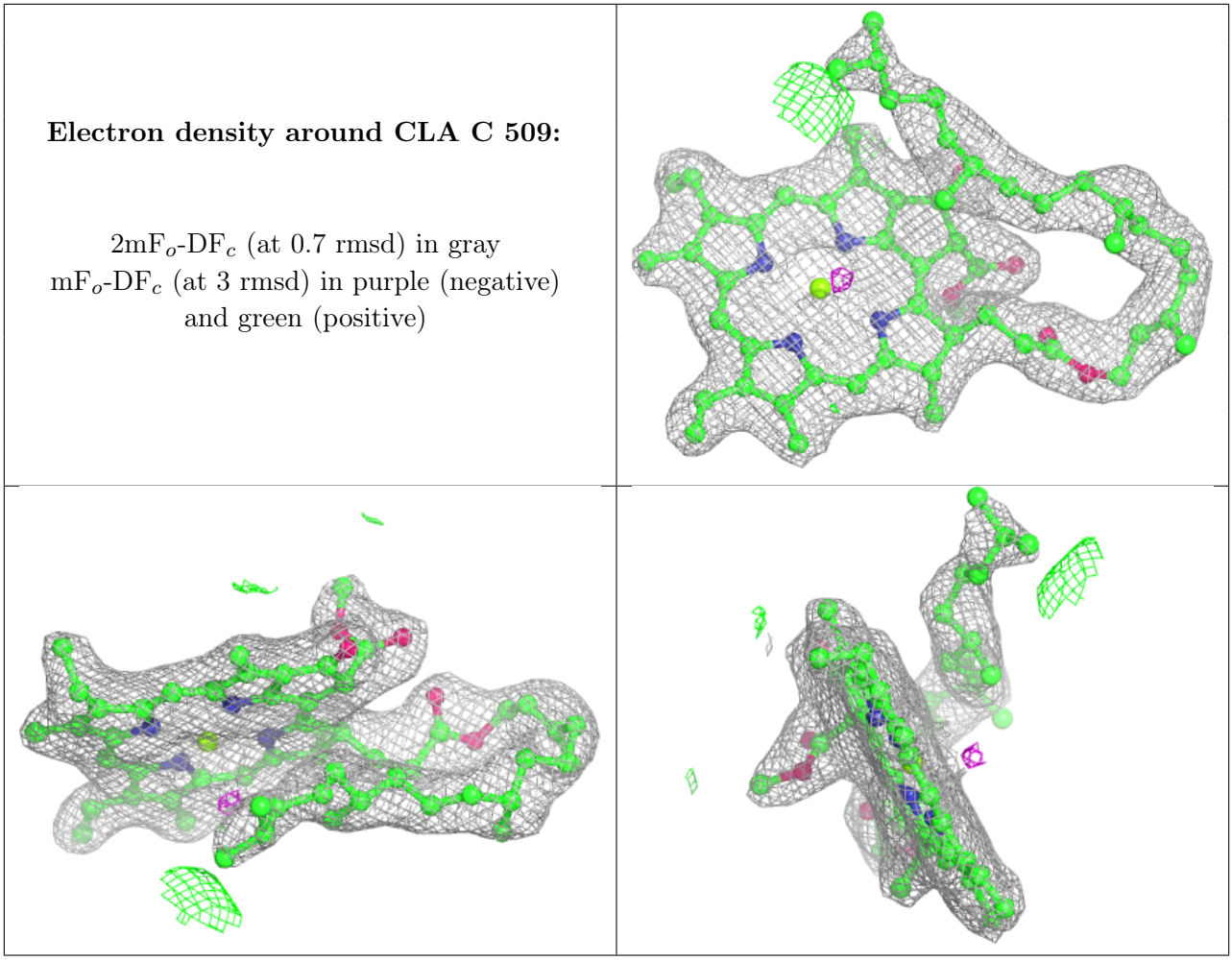






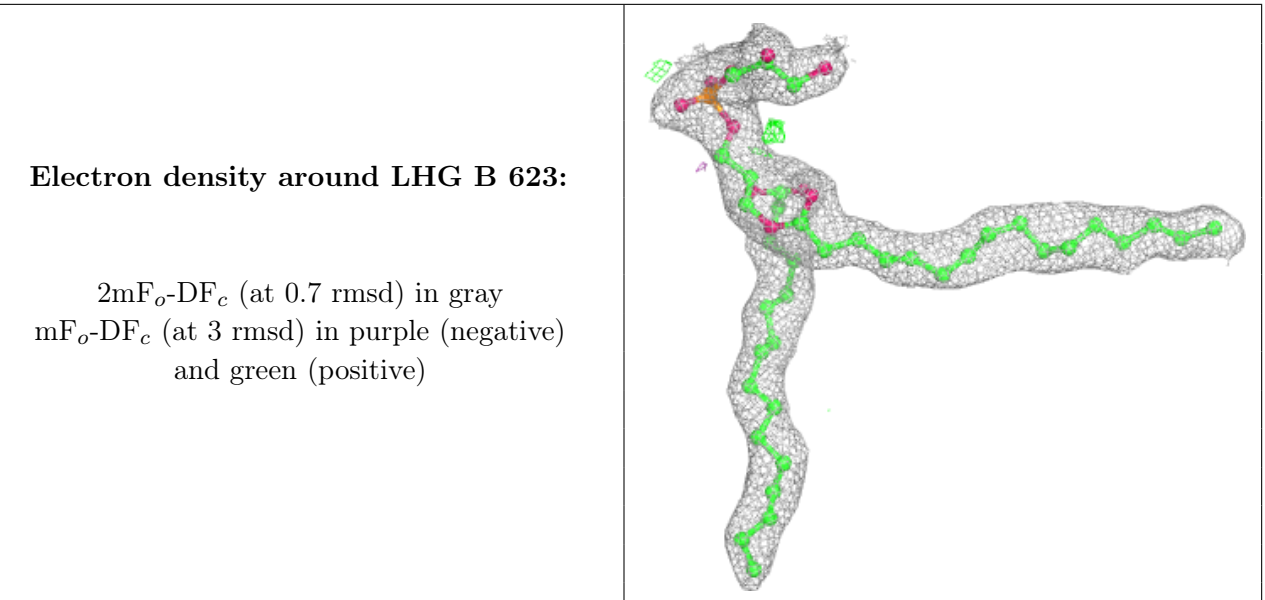
Electron density around CLA C 509:

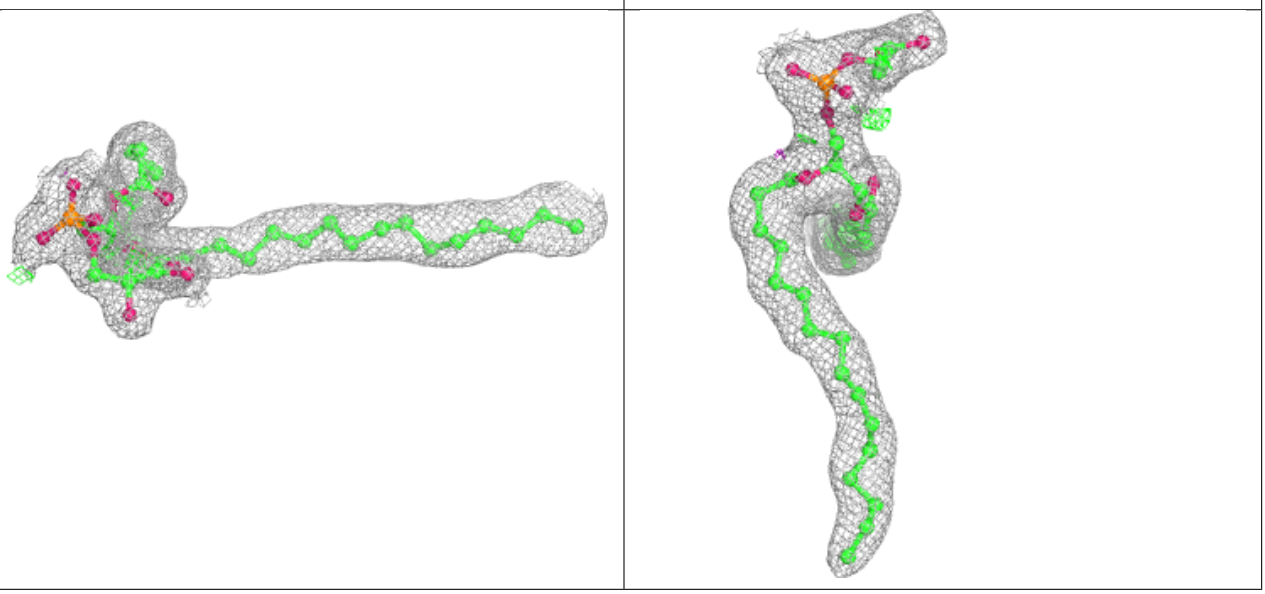
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG B 623:

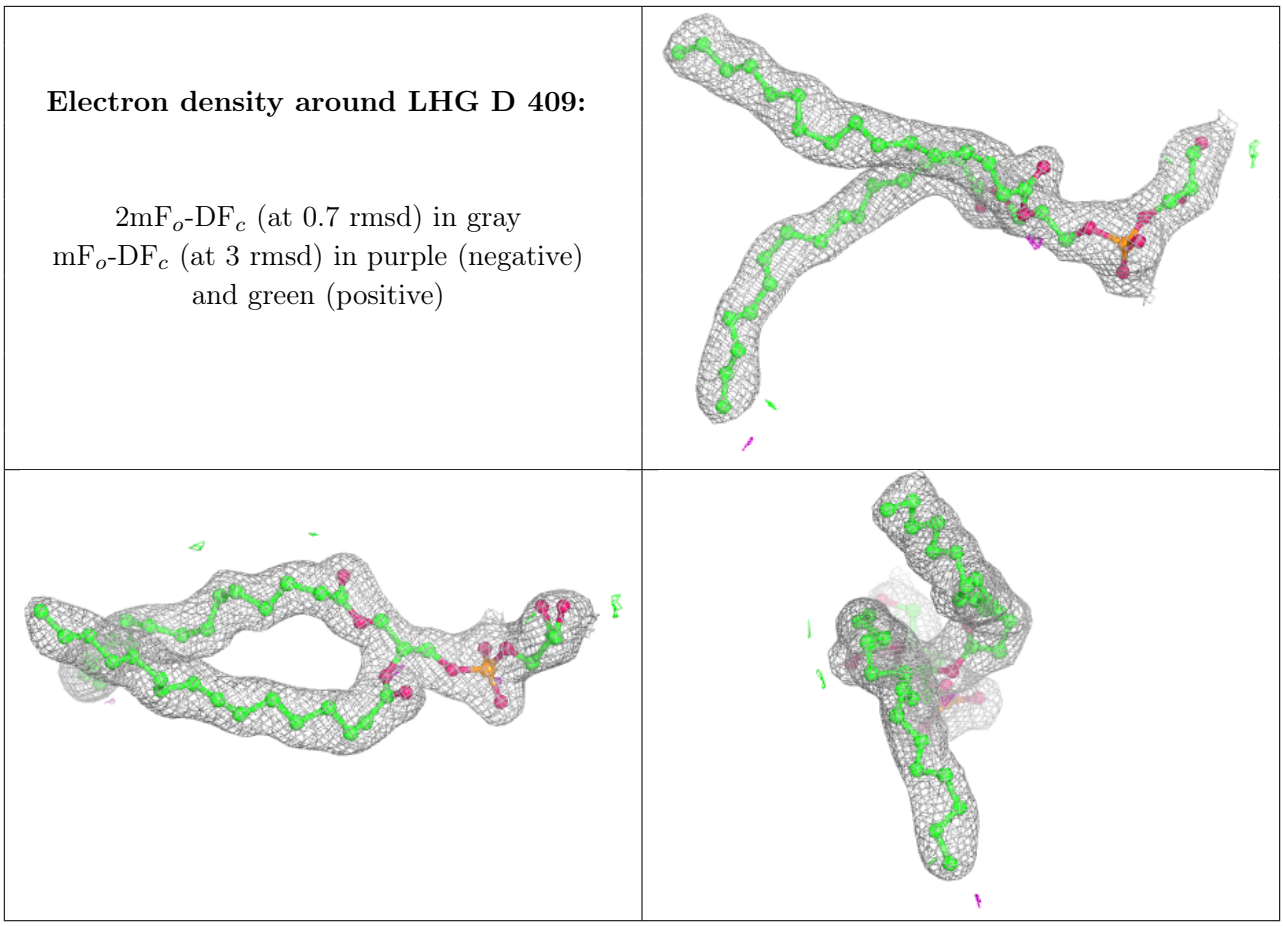
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





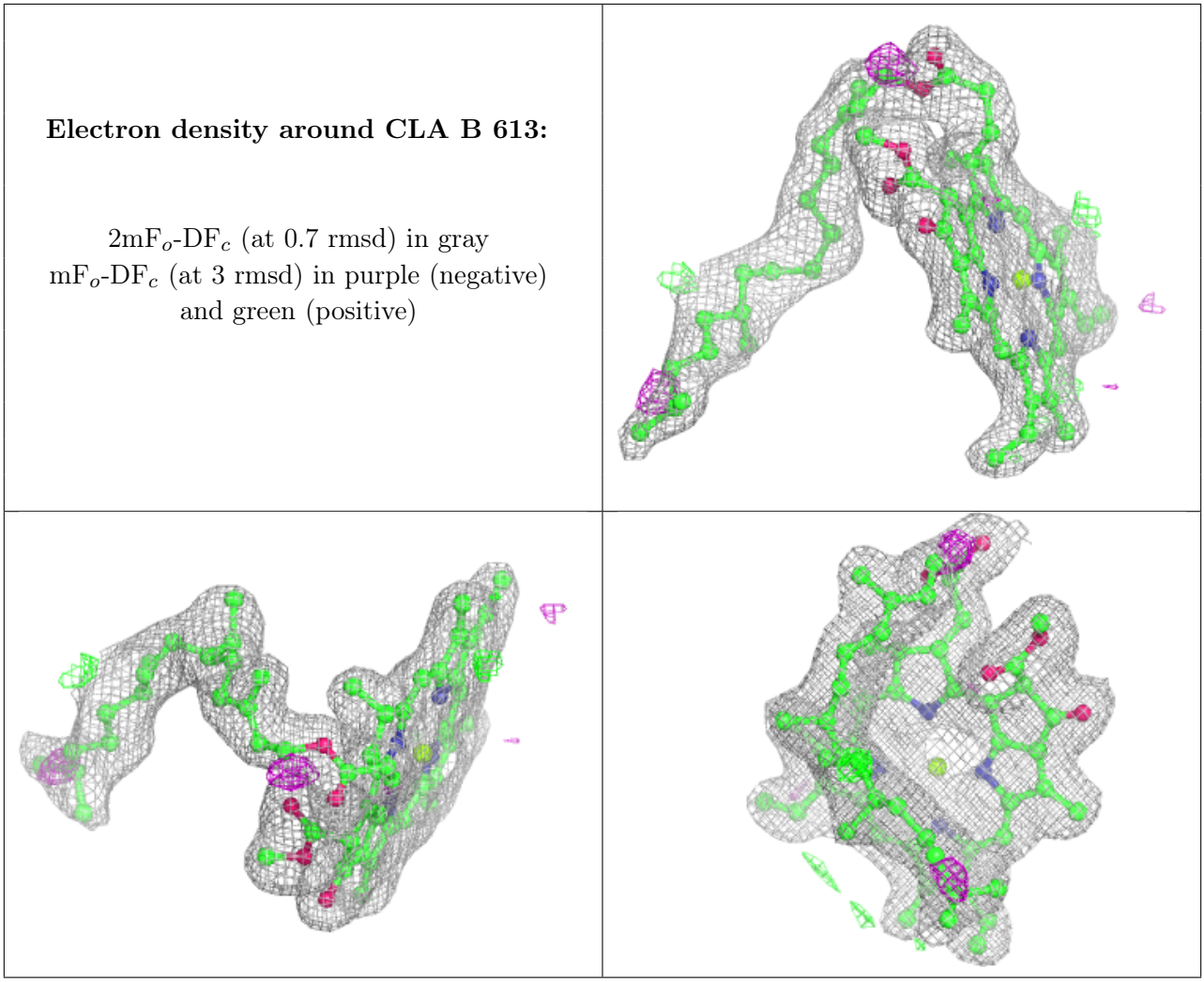
Electron density around LHG D 409:

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



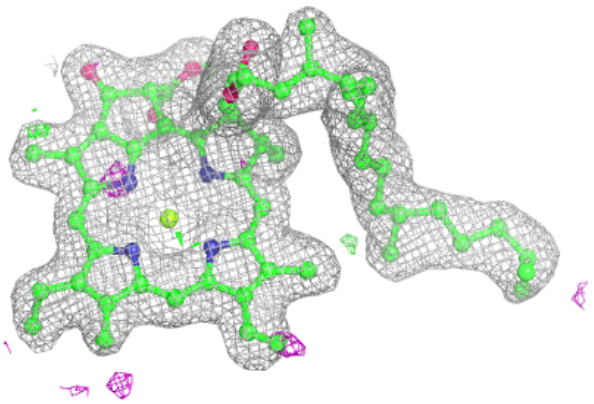
Electron density around CLA B 613:

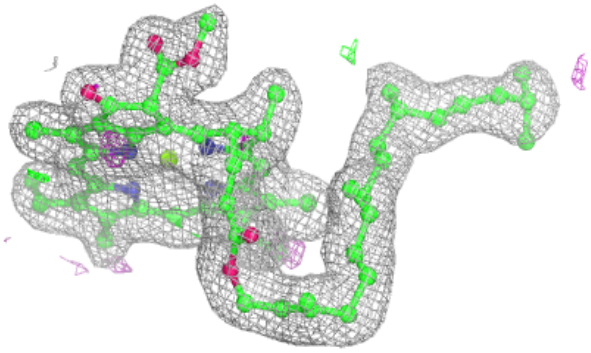
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

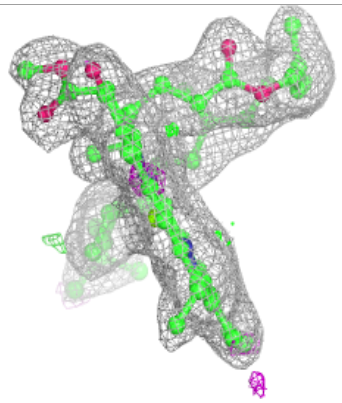


Electron density around CLA A 612:

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

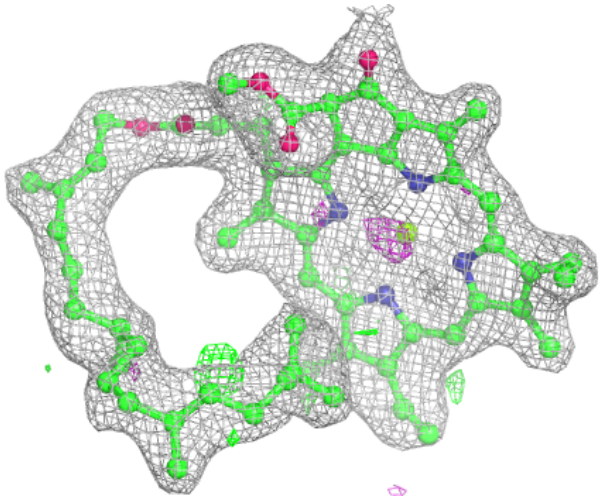


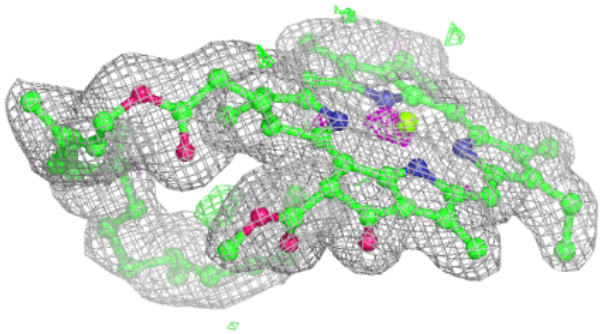


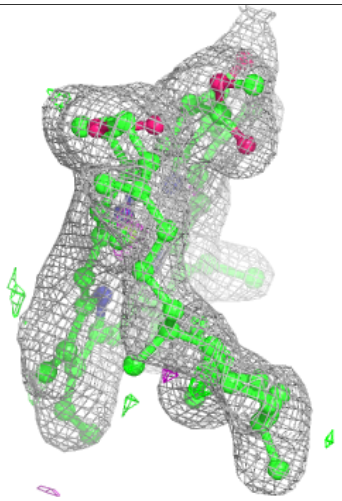


Electron density around CLA B 615:

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

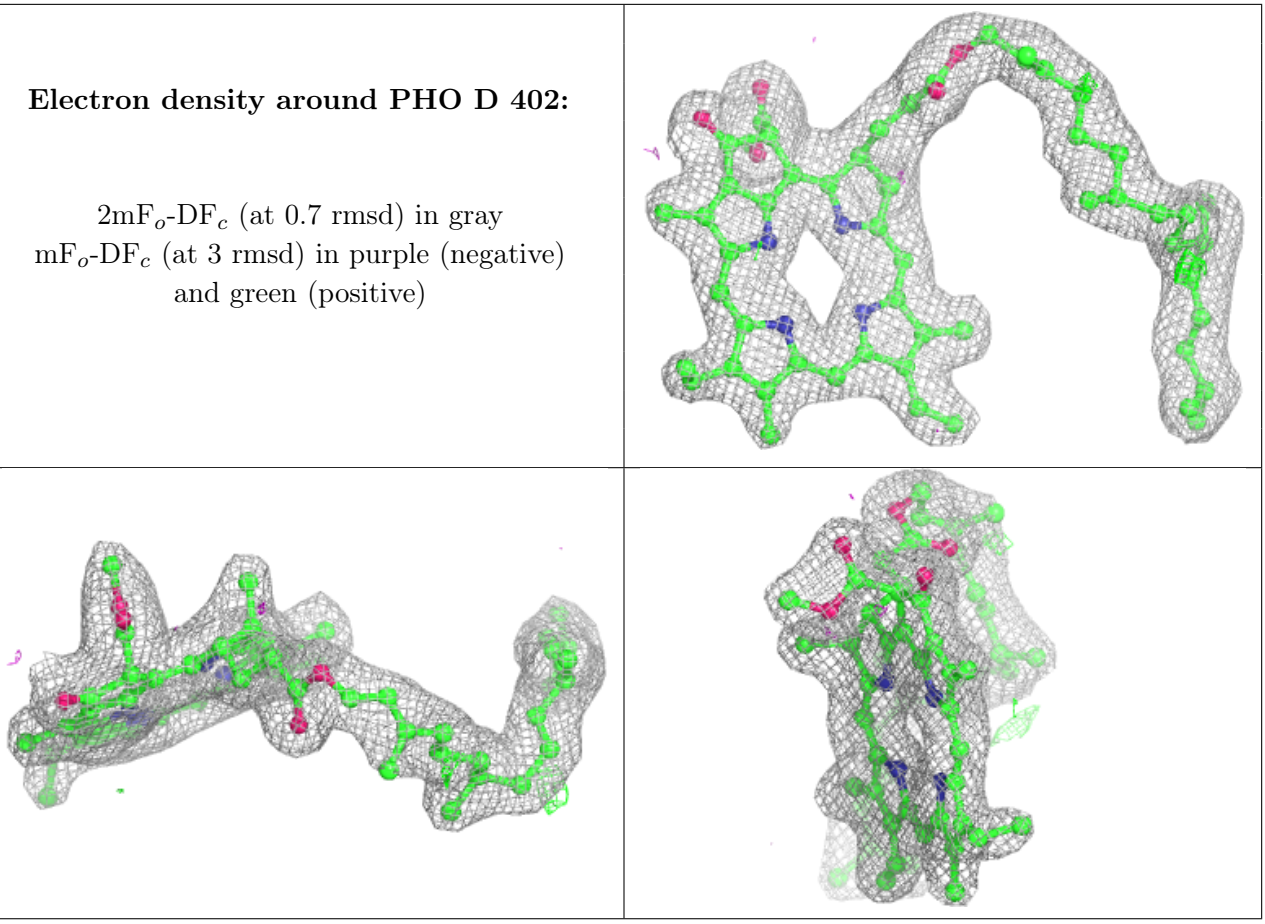






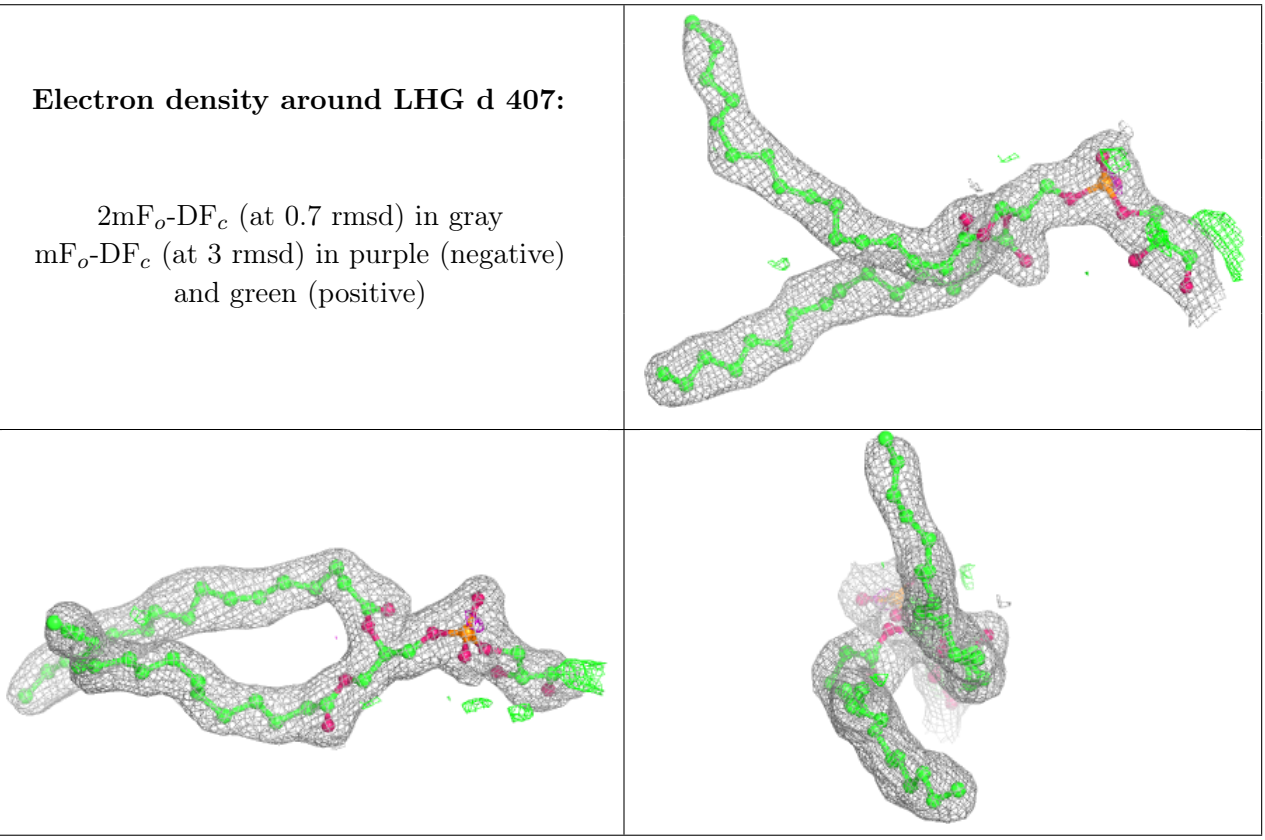
Electron density around PHO D 402:

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



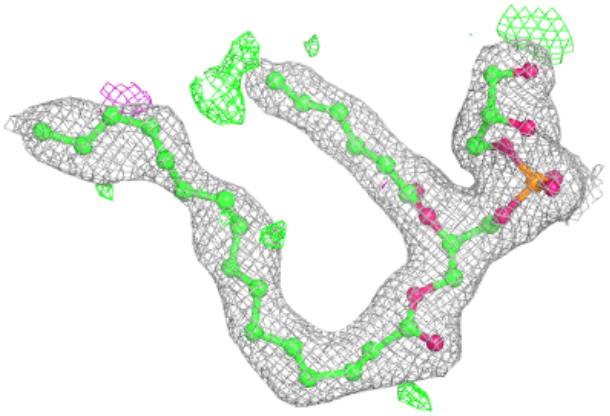
Electron density around LHG d 407:

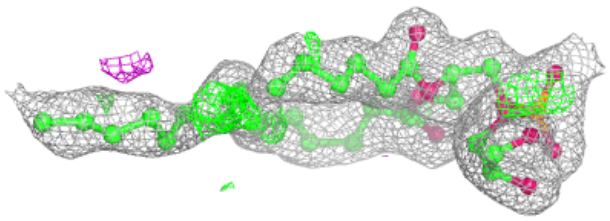
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

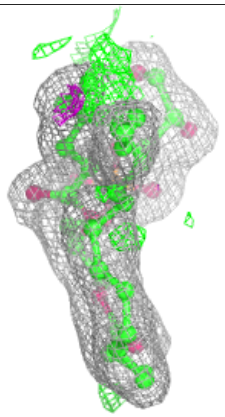


Electron density around LHG d 408:

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

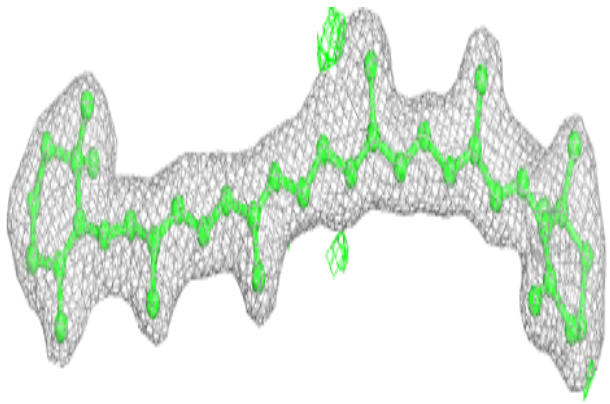


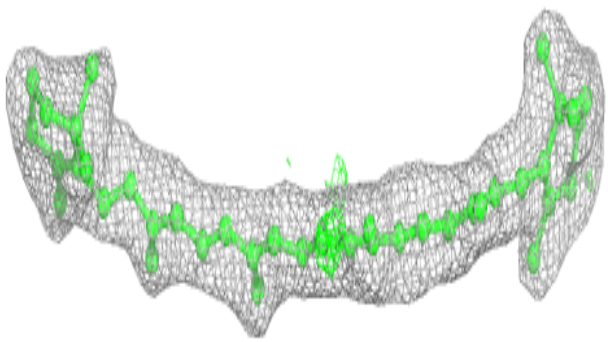


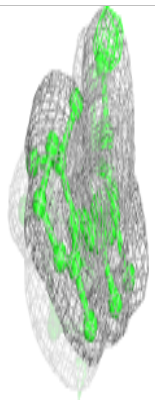


Electron density around BCR t 101:

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

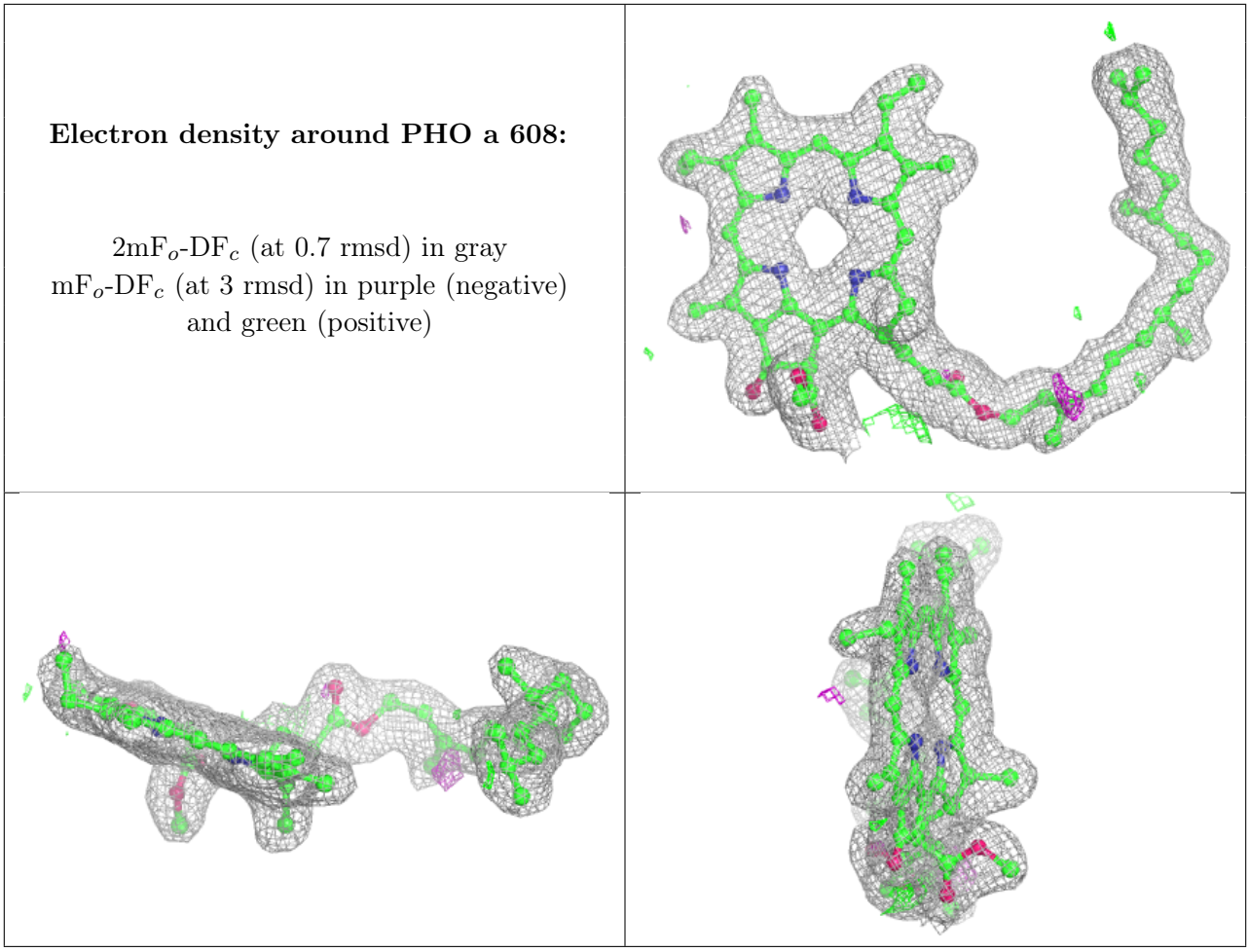






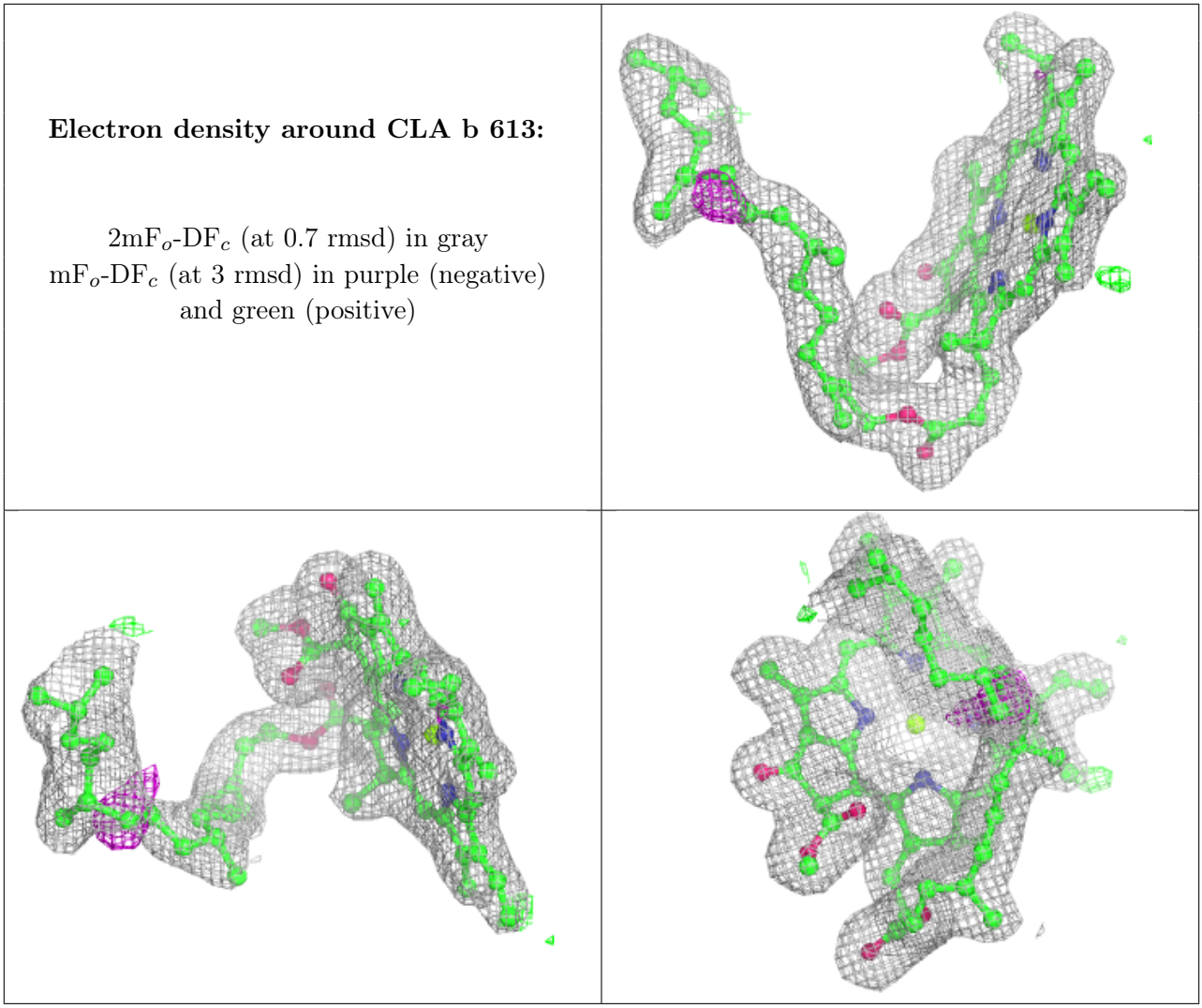
Electron density around PHO a 608:

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



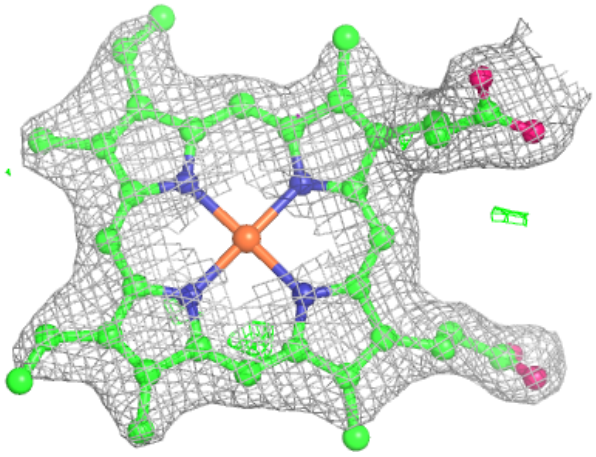
Electron density around CLA b 613:

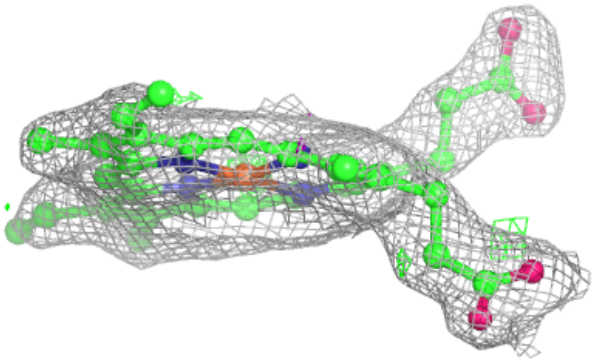
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

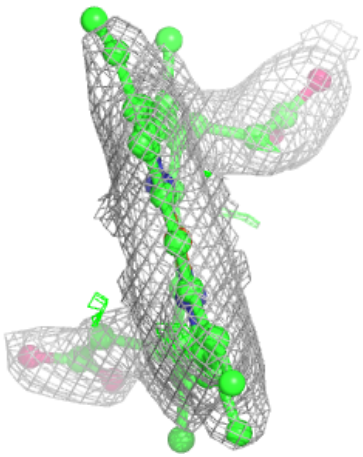


Electron density around HEM F 101:

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

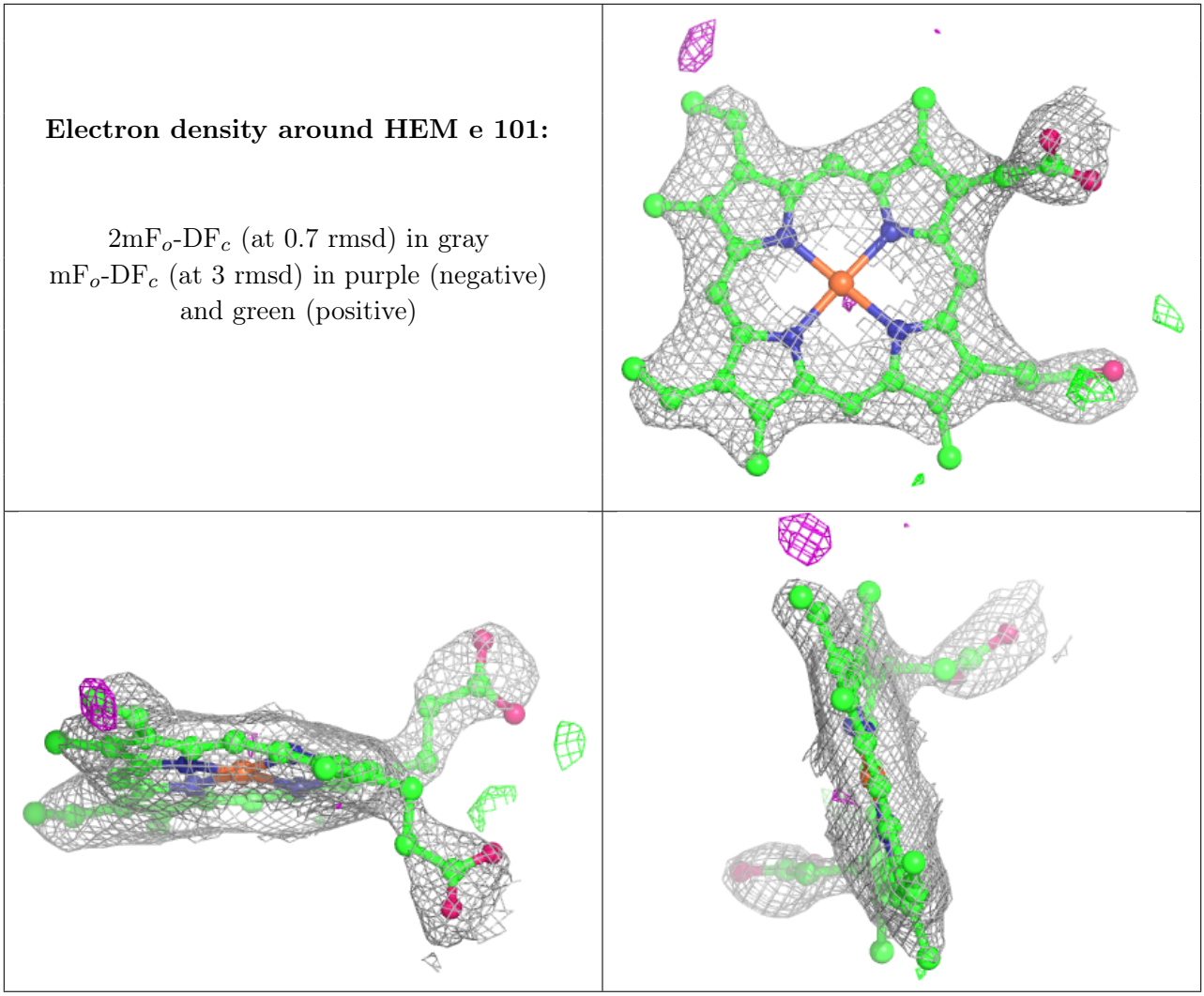






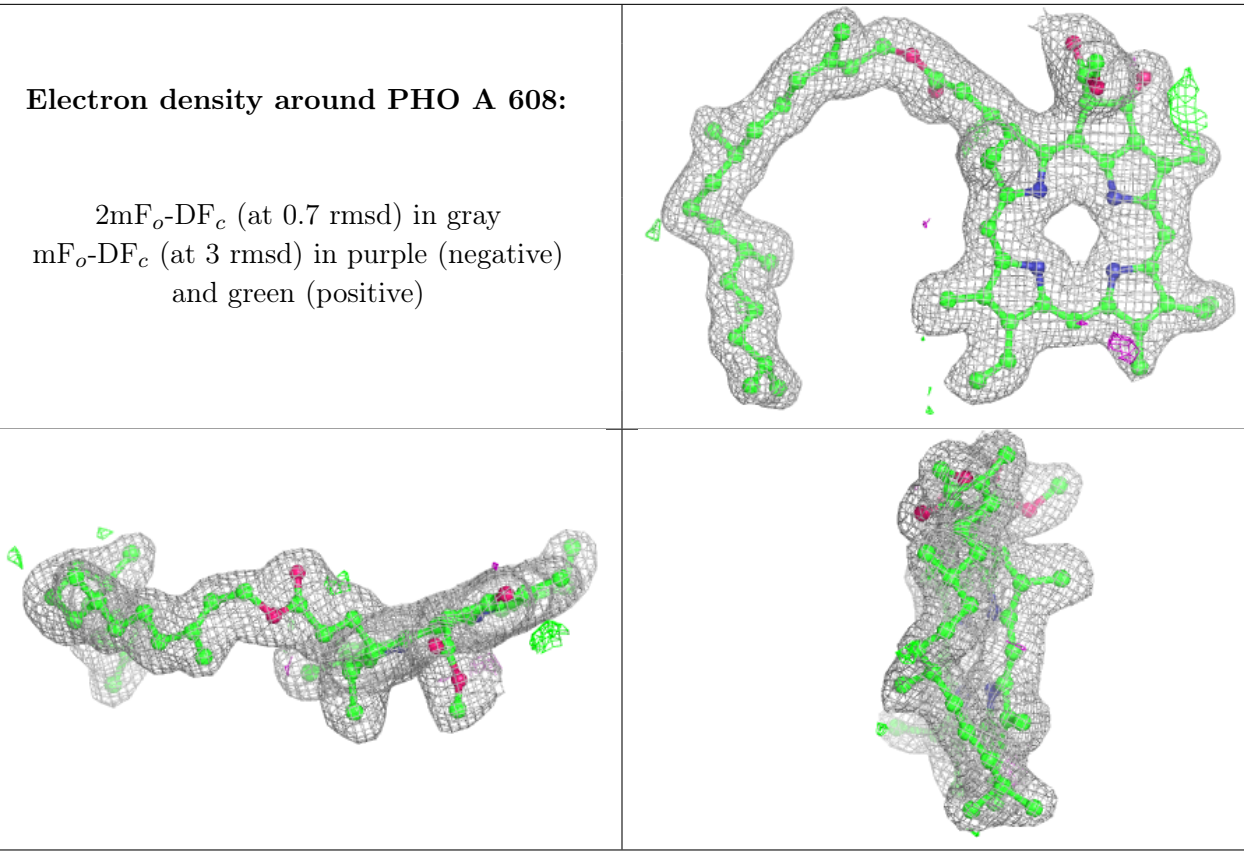
Electron density around HEM e 101:

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



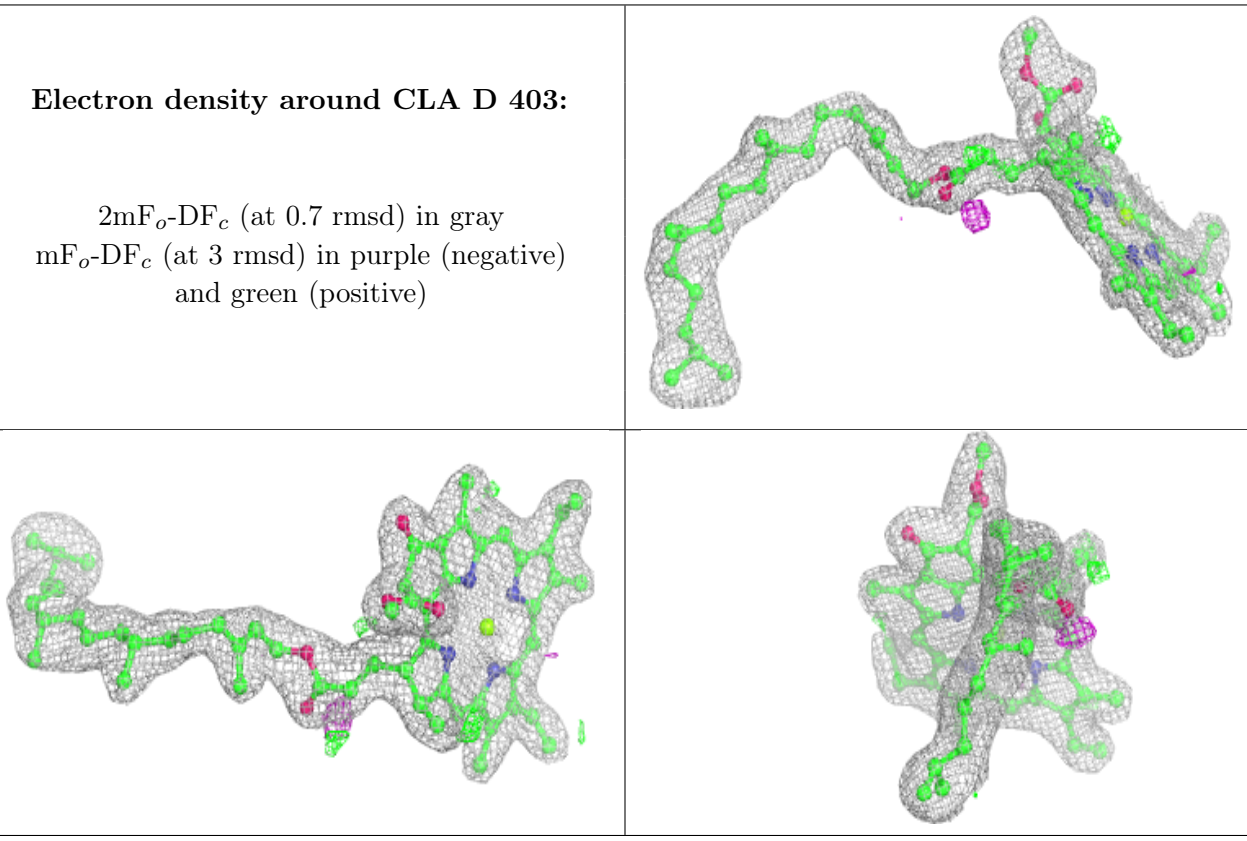
Electron density around PHO A 608:

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



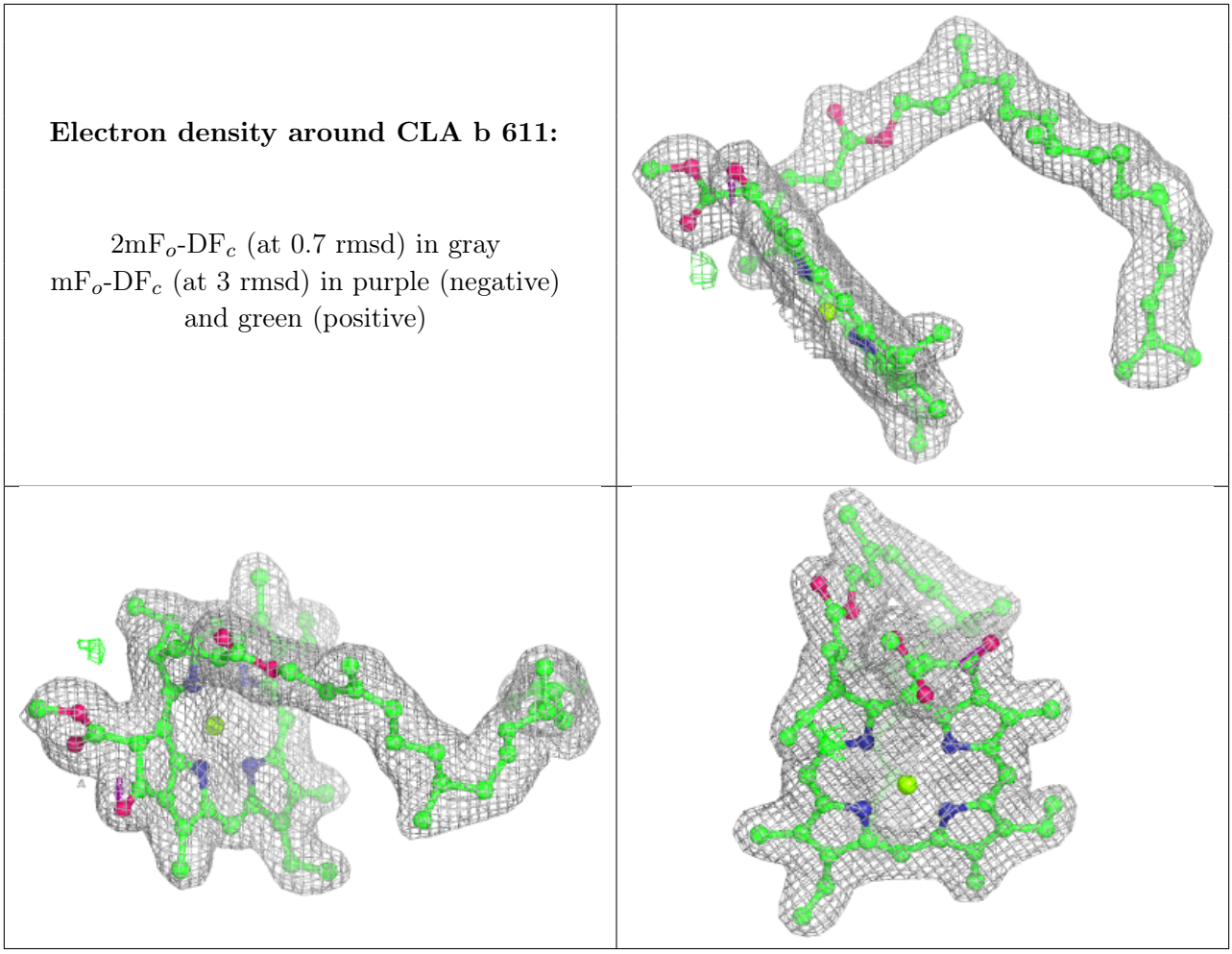
Electron density around CLA D 403:

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



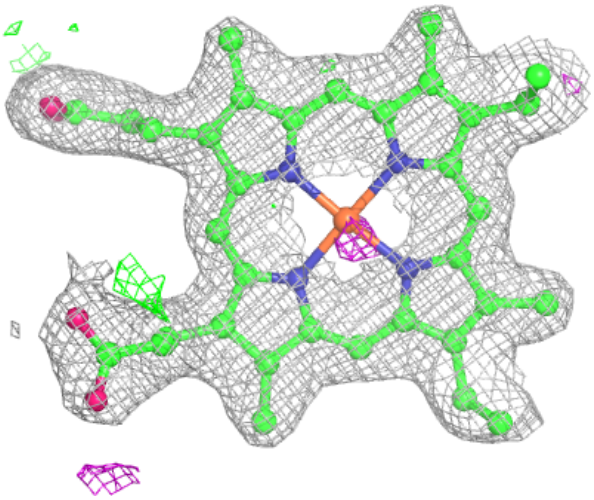
Electron density around CLA b 611:

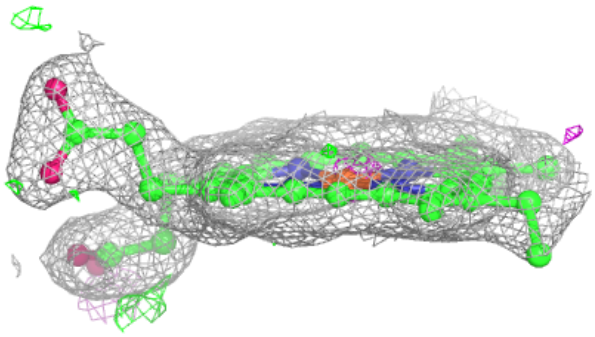
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

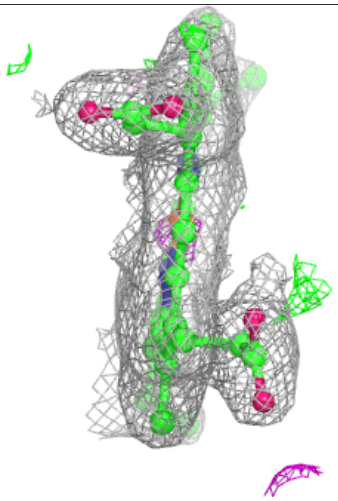


Electron density around HEC V 201:

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

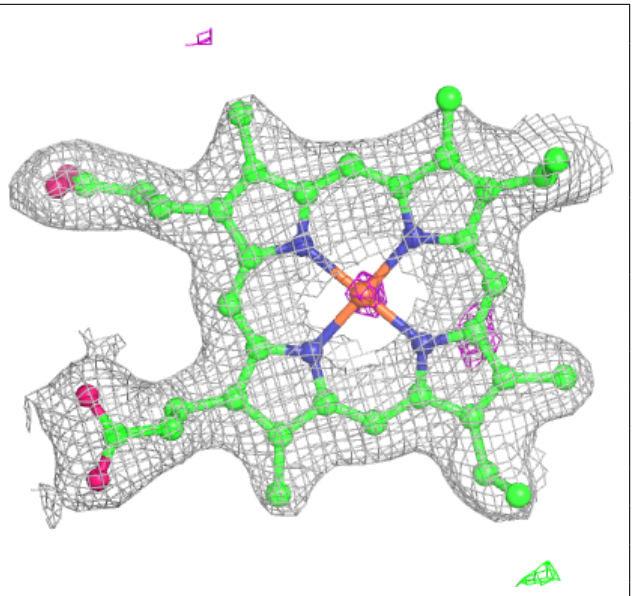


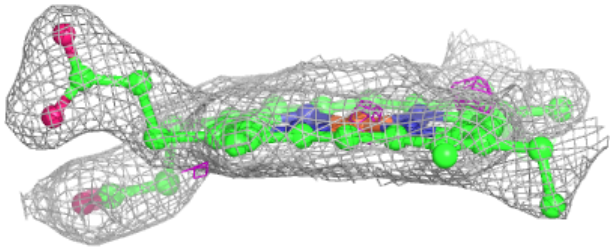




Electron density around HEC v 201:

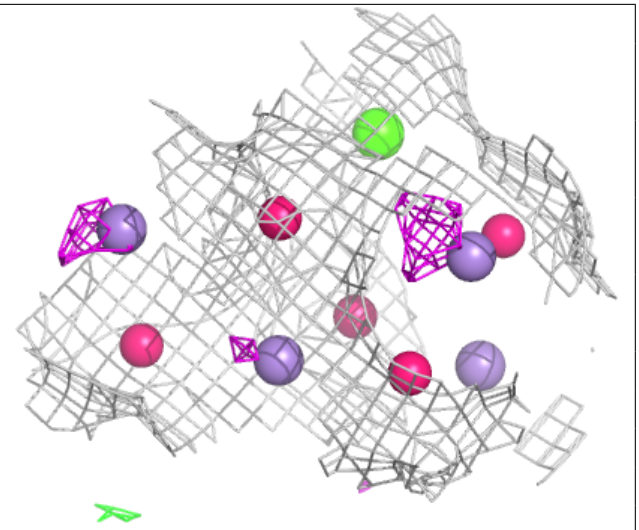
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

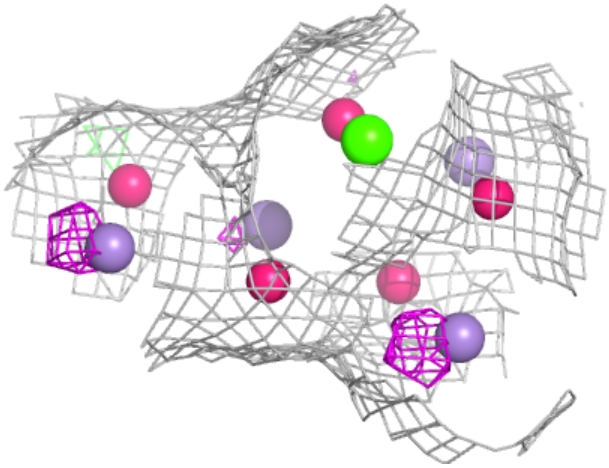


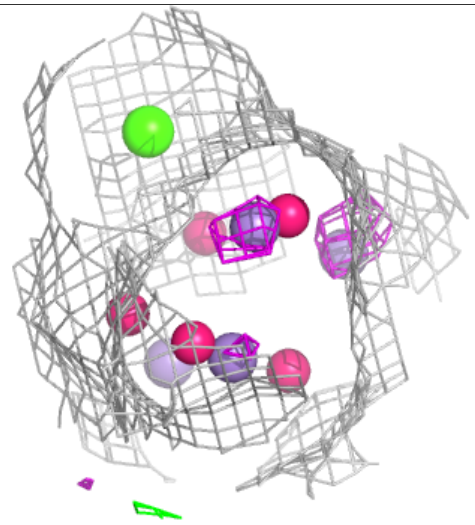


Electron density around OEX A 601 (B):

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

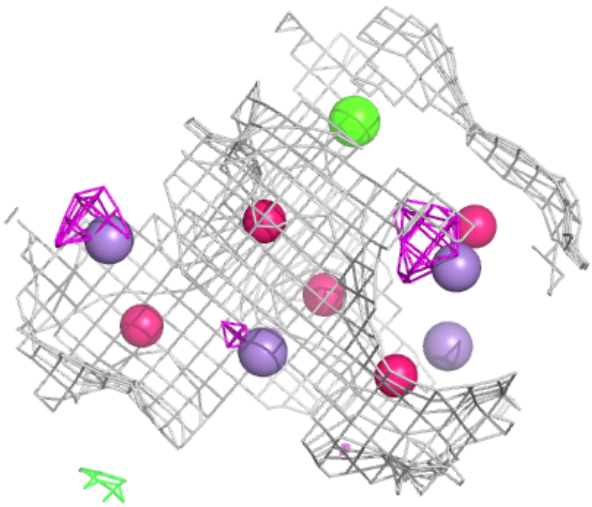


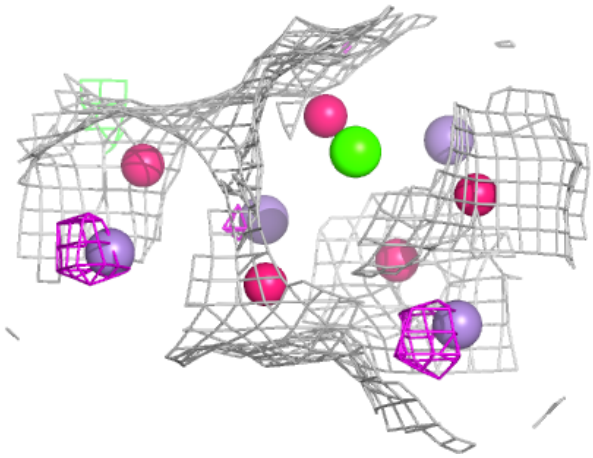


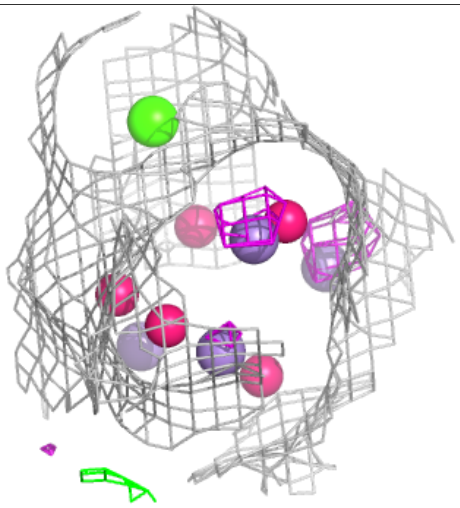


Electron density around OEX A 601 (C):

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

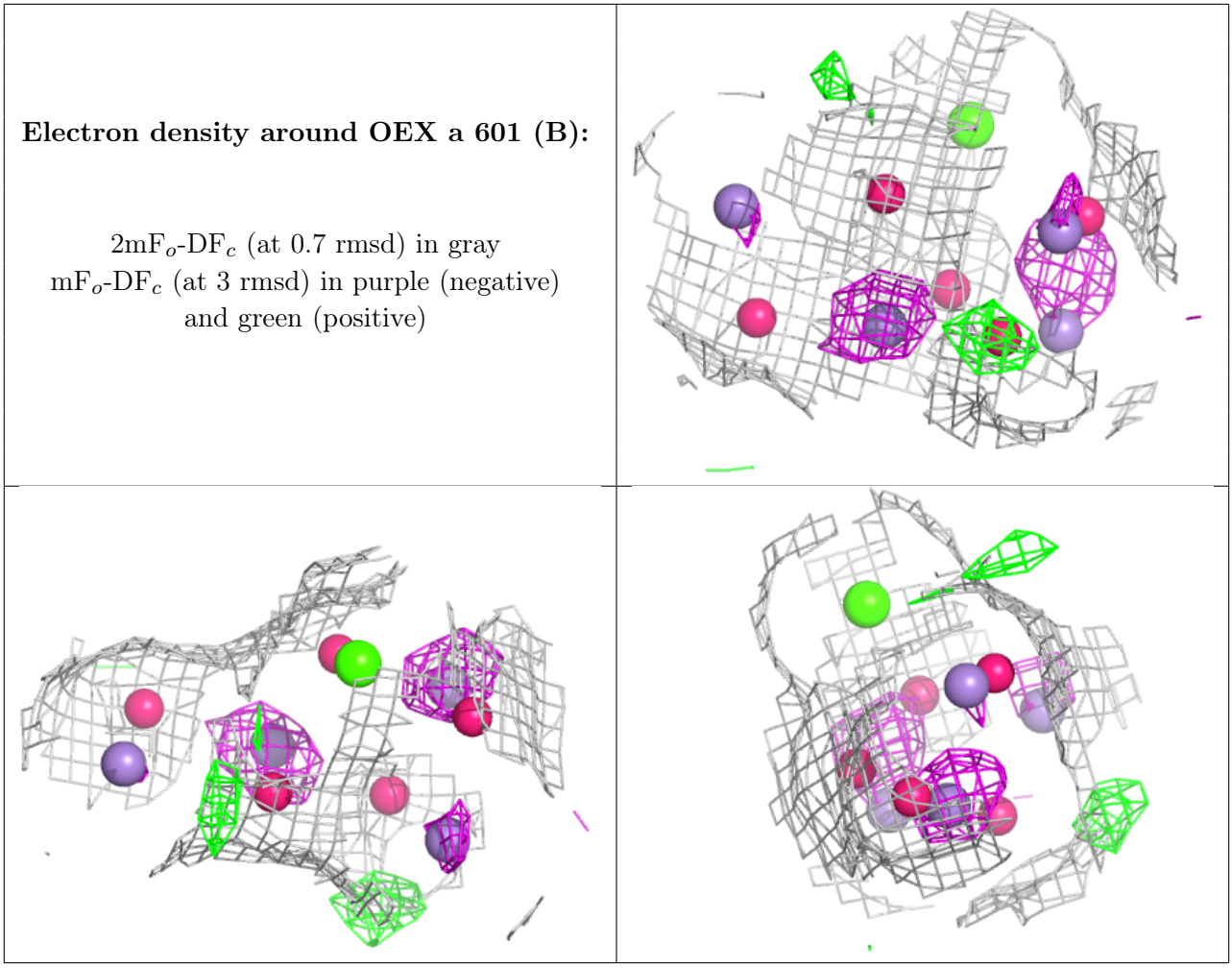






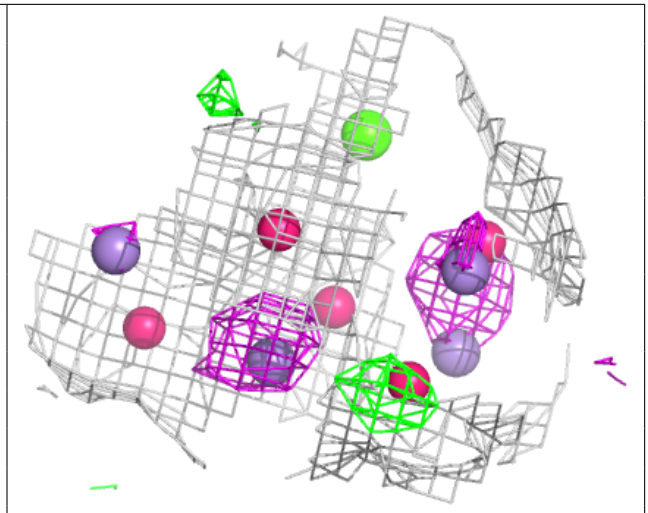
Electron density around OEX a 601 (B):

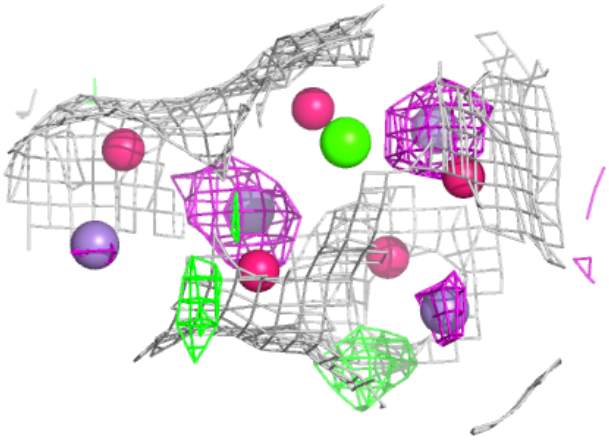
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

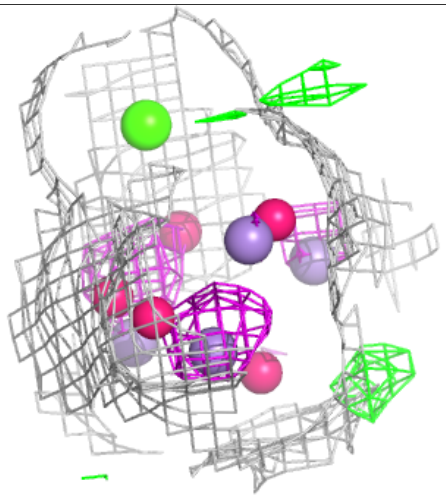


Electron density around OEX a 601 (C):

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

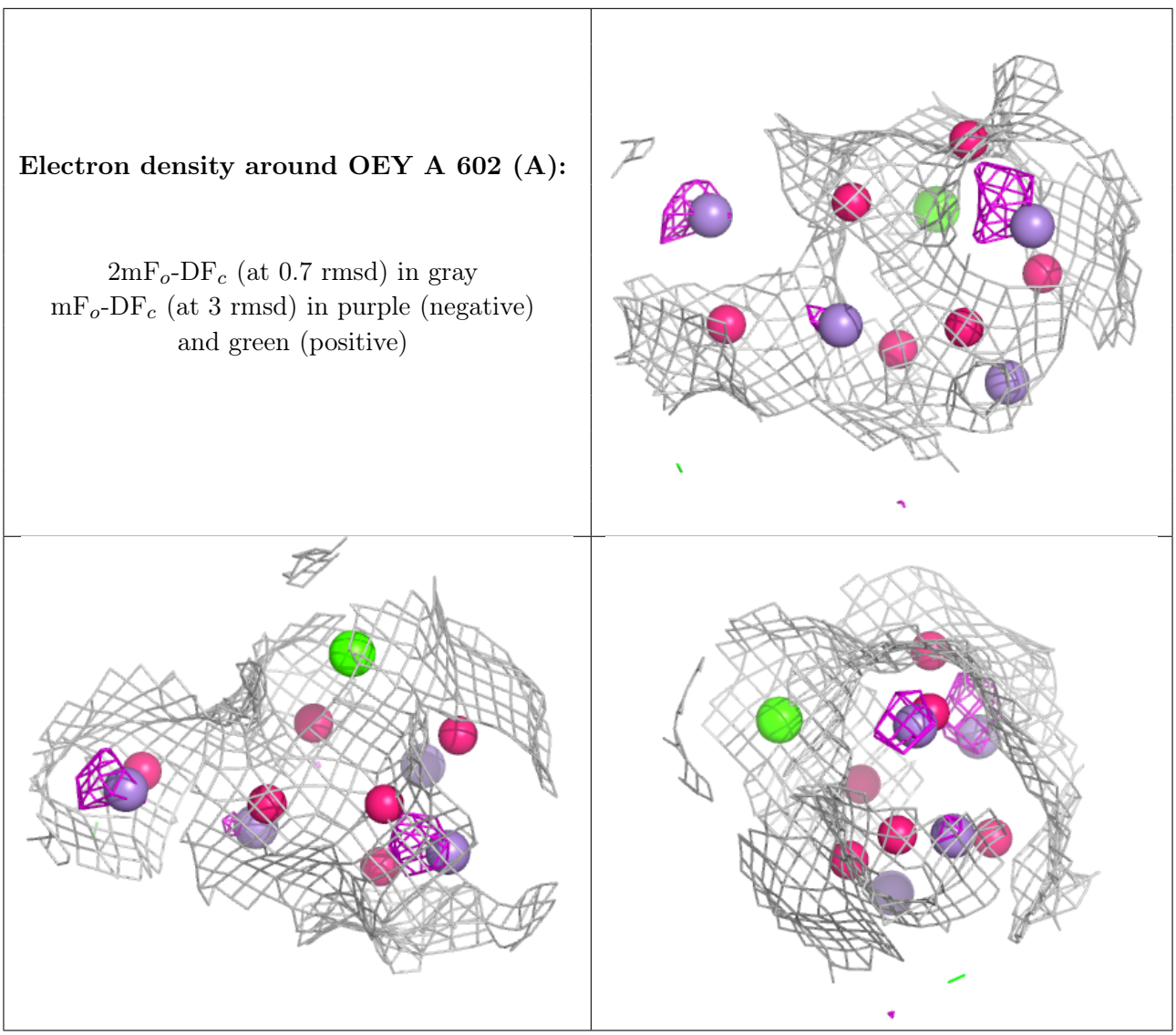






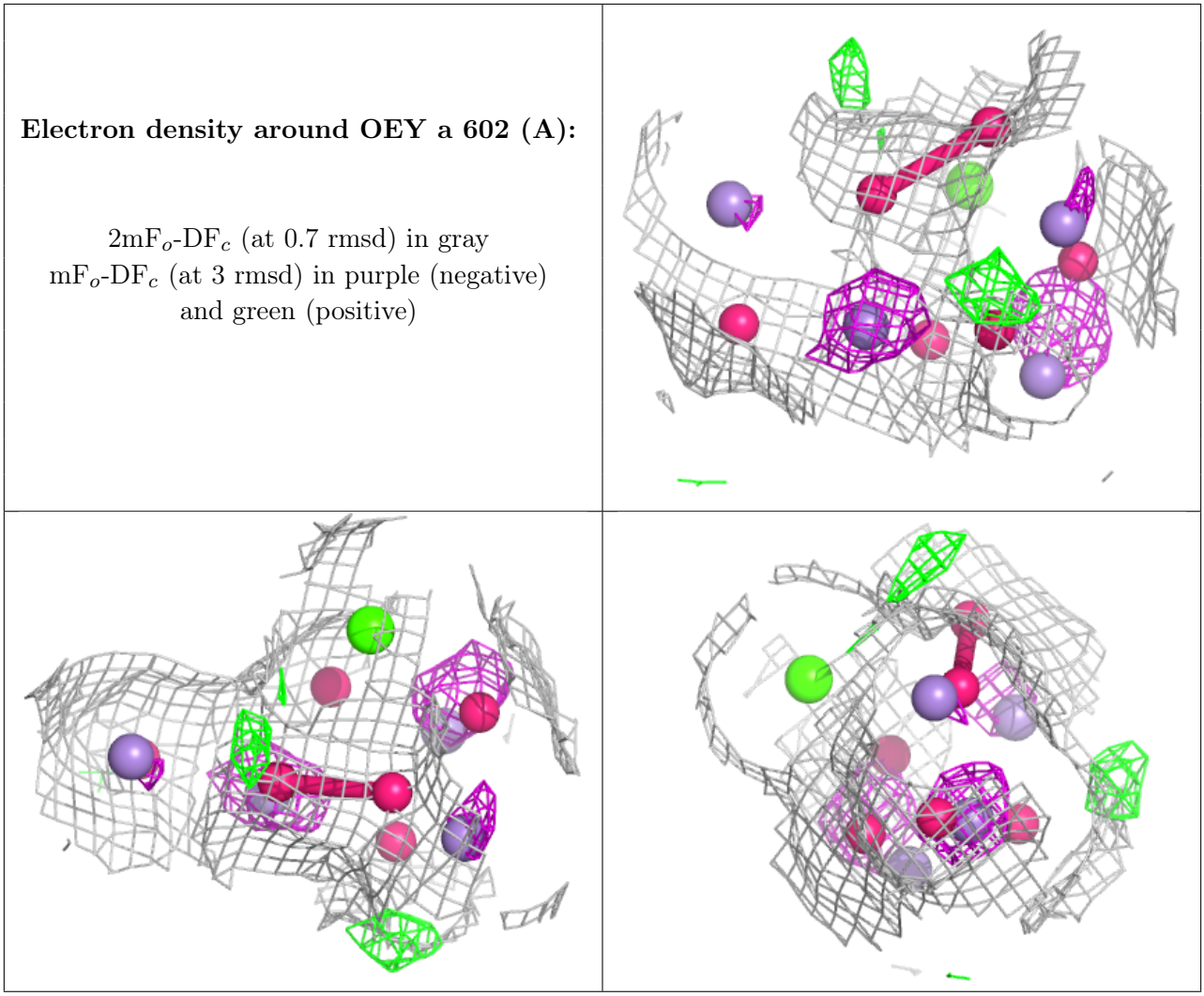
Electron density around OEY A 602 (A):

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



Electron density around OEY 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.