Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 11:48 AM EST

PDB ID	:	8EZ5
Title	:	RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution
Authors	:	Bhowmick, A.; Hussein, R.; Bogacz, I.; Simon, P.S.; Ibrahim, M.; Chatterjee, R.; Doyle, M.D.; Cheah, M.H.; Fransson, T.; Chernev, P.; Kim, I.-S.; Makita, H.; Dasgupta, M.; Kaminsky, C.J.; Zhang, M.; Gatcke, J.; Haupt, S.; Nangca, I.I.; Keable, S.M.; Aydin, O.; Tono, K.; Owada, S.; Gee, L.B.; Fuller, F.D.; Batyuk, A.; Alonso-Mori, R.; Holton, J.M.; Paley, D.W.; Moriarty, N.W.; Mamedov, F.; Adams, P.D.; Brewster, A.S.; Dobbek, H.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yano, J.; Yachandra, V.K.
Deposited on	:	2022-10-31
Resolution	:	2.09 Å(reported)

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

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

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

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

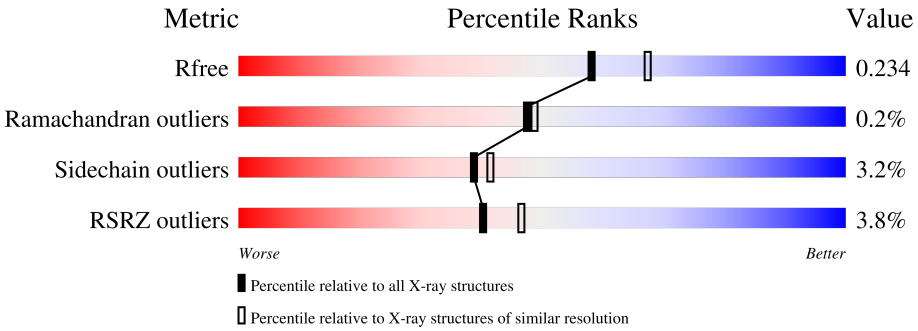
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

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

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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)	:	2.36

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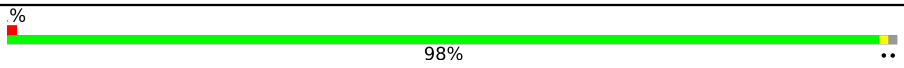
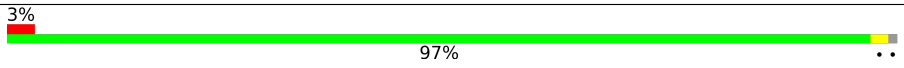
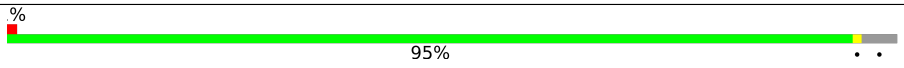
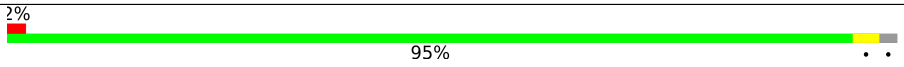
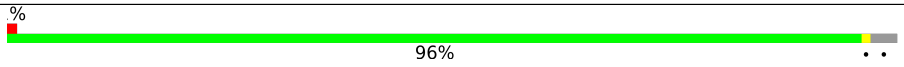
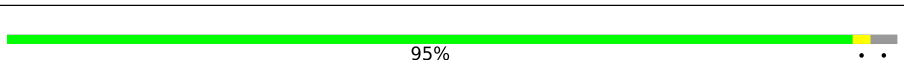
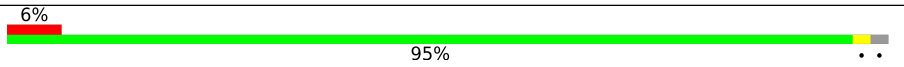
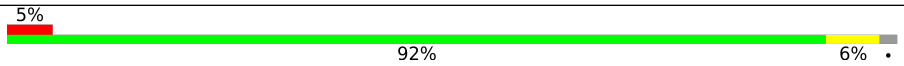
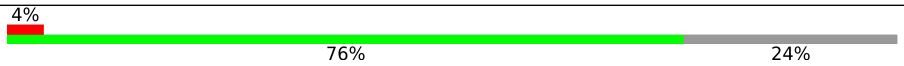
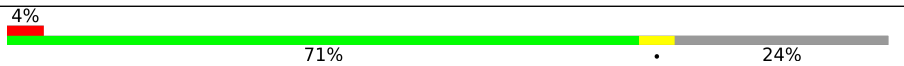
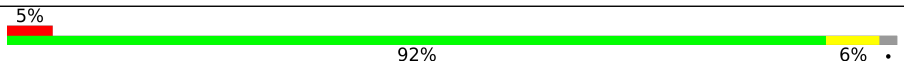
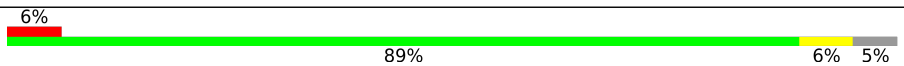
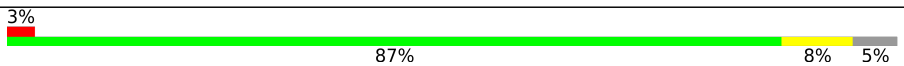
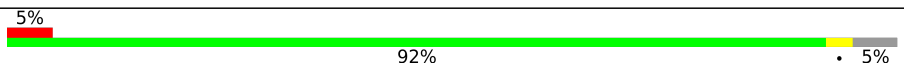
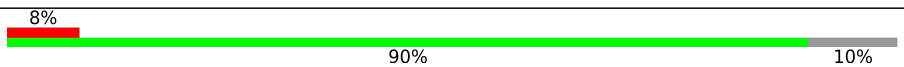
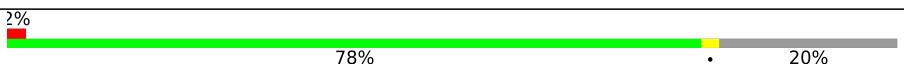
Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
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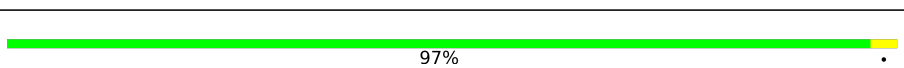
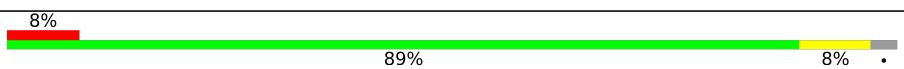
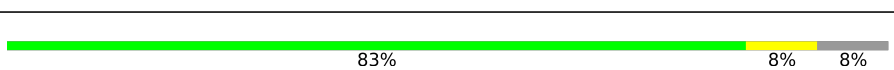
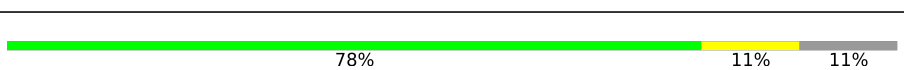
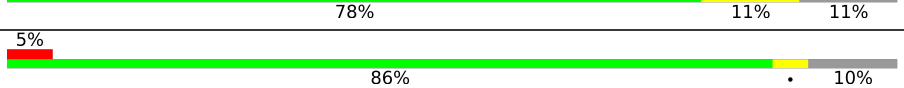
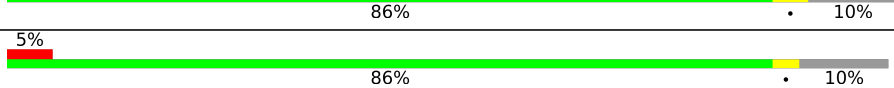
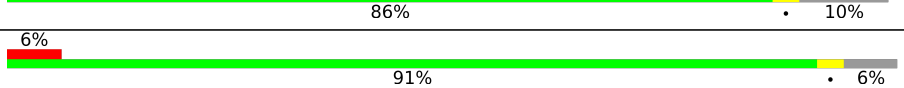
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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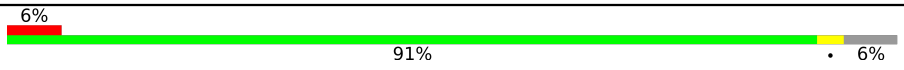
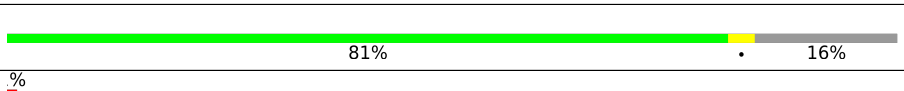
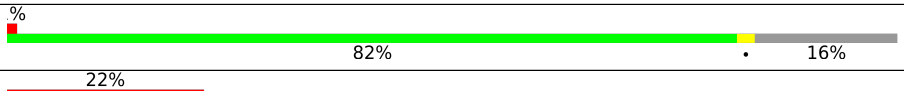
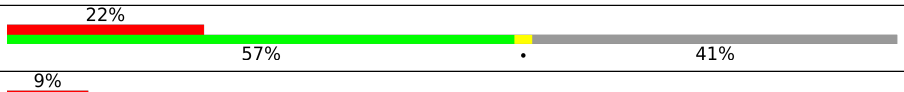
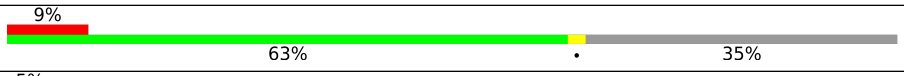
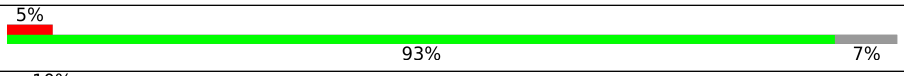
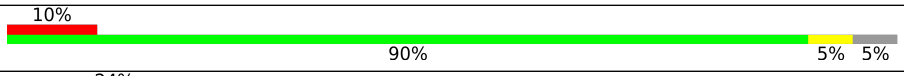
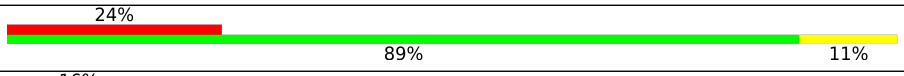
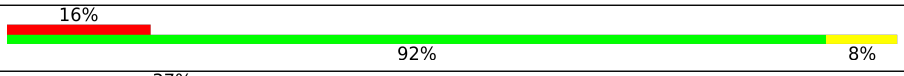
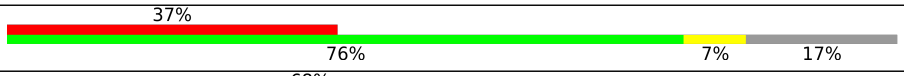
Mol	Chain	Length	Quality of chain
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	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	D	404	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	601	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 53041 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
			3113	2030	513	551	19			
1	a	334	Total	C	N	O	S	0	64	0
			3110	2027	513	551	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	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
			3509	2302	586	607	14			
3	c	451	Total	C	N	O	S	0	12	0
			3583	2343	602	624	14			

- 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
			2731	1809	446	464	12			
4	d	341	Total	C	N	O	S	0	3	0
			2737	1813	446	466	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			

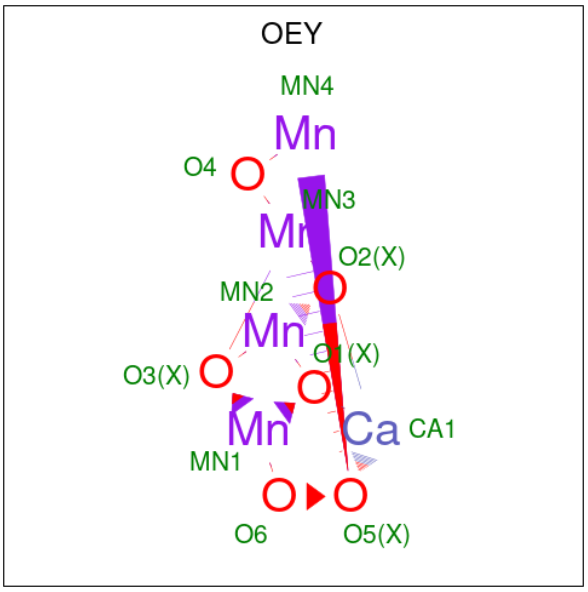
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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.

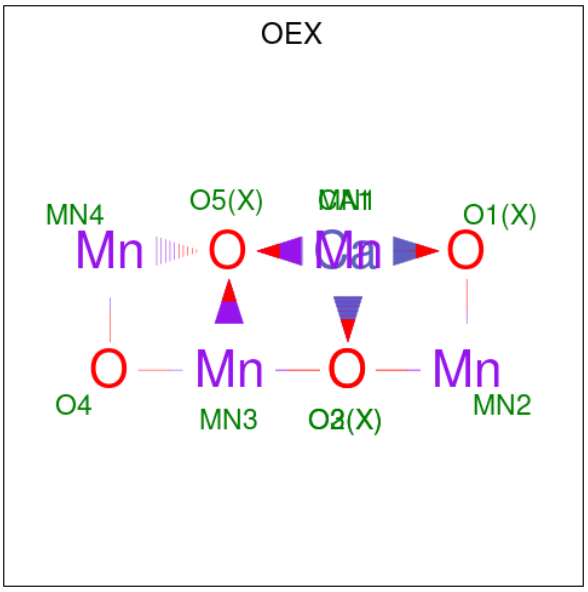
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			271	184	47	40			
20	r	31	Total	C	N	O	0	0	0
			246	166	43	37			

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



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

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



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

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

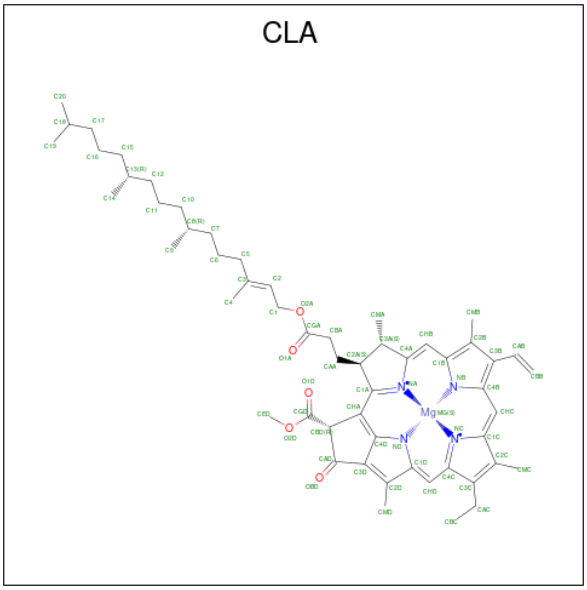
- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

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

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



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

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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	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
25	C	1	Total 59	C 49	Mg 1	N 4	O 5	0	0

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

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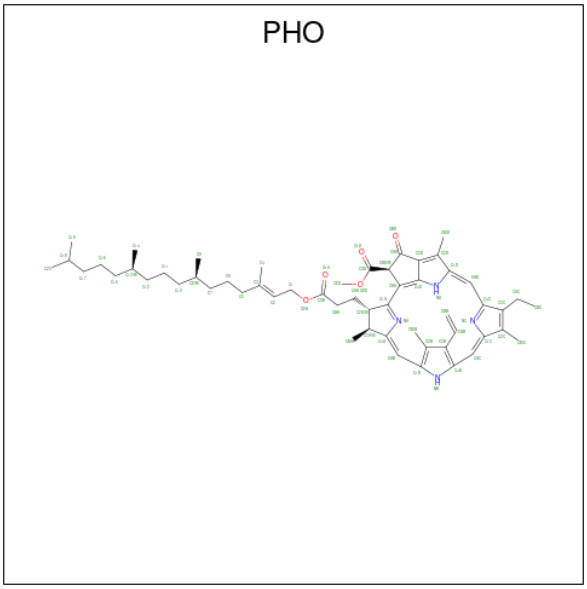
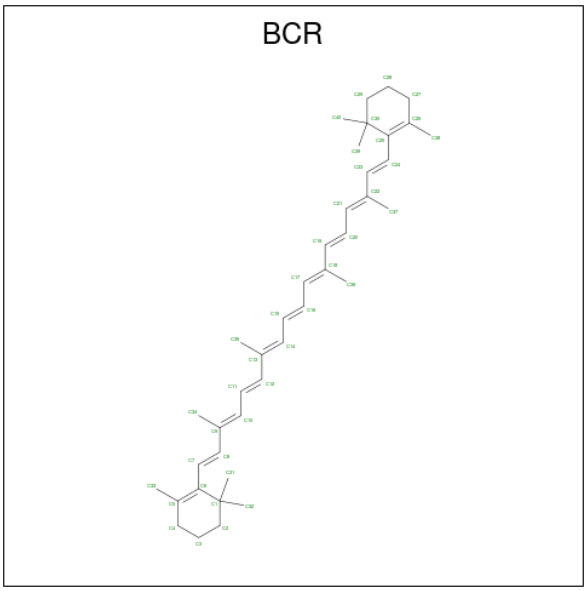
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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



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

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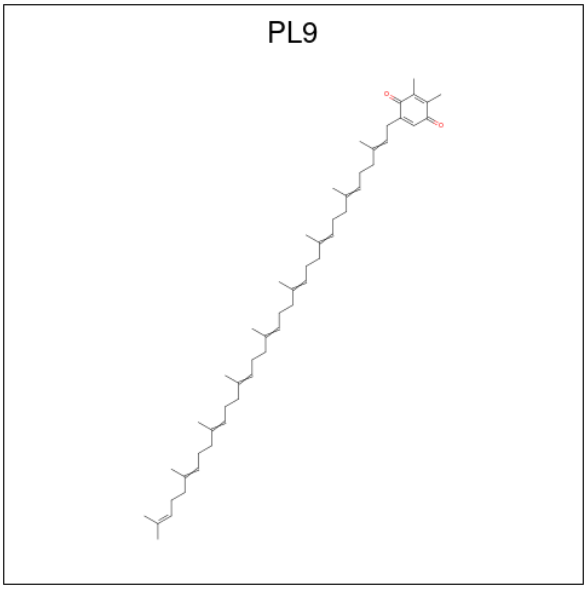
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0
27	t	1	Total C 40 40	0	0
27	x	1	Total C 40 40	0	0

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



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

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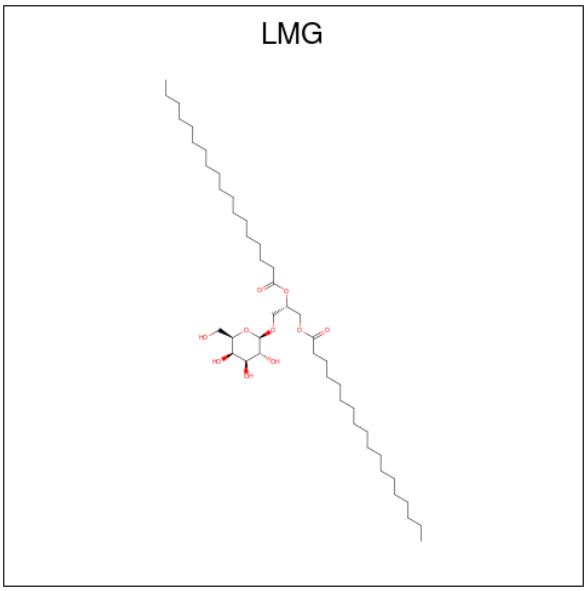
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	a	1	Total C O 55 53 2	0	0
28	d	1	Total C O 55 53 2	0	0

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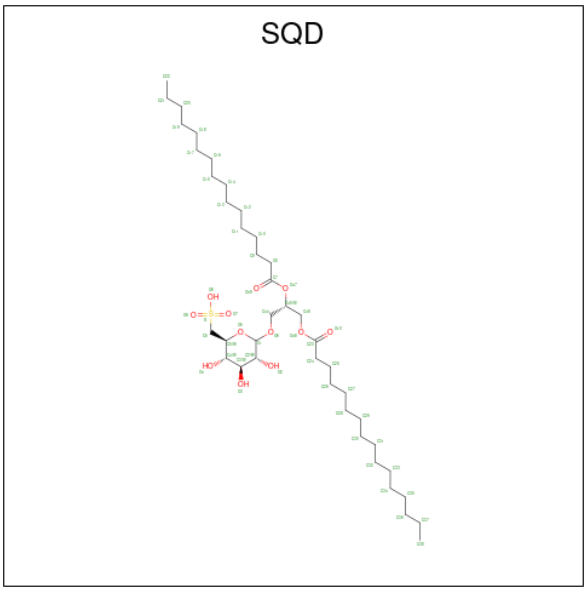
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	c	1	Total C O 49 39 10	0	0
29	d	1	Total C O 23 21 2	0	0
29	d	1	Total C O 44 34 10	0	0
29	m	1	Total C O 51 41 10	0	0

- 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	F	1	Total C O S 36 25 10 1	0	0
30	L	1	Total C O S 49 36 12 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

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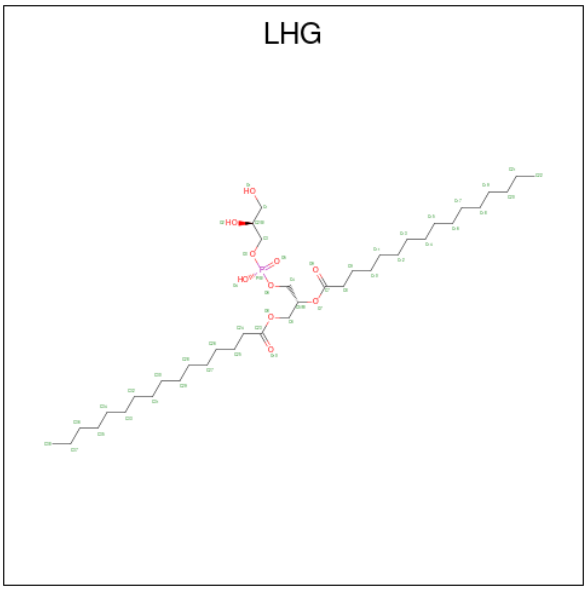
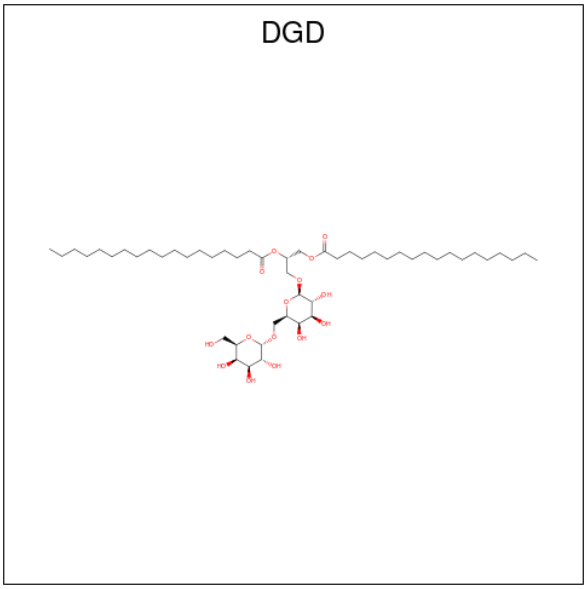
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	f	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



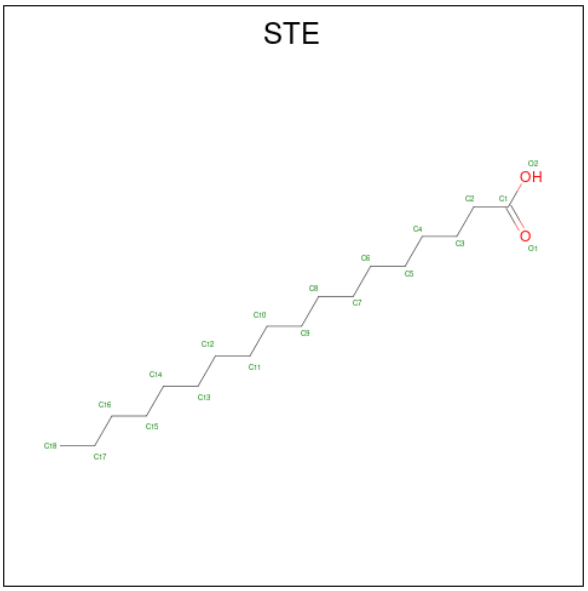
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			47	36	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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



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

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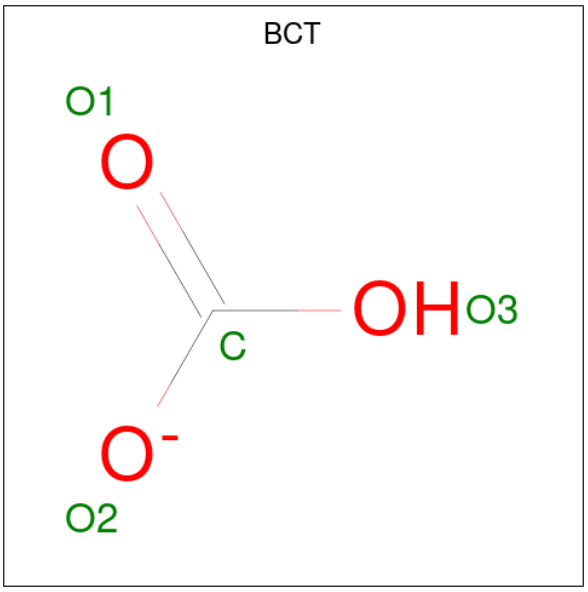
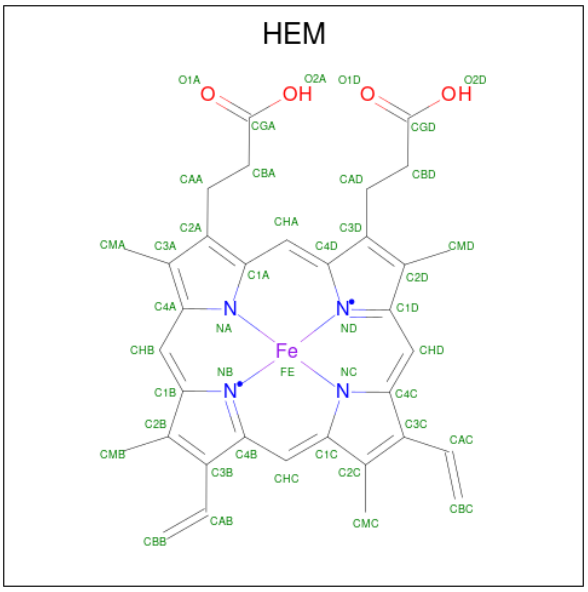
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	M	1	Total C 10 10	0	0
33	T	1	Total C 16 16	0	0
33	T	1	Total C 15 15	0	0
33	a	1	Total C 10 10	0	0
33	a	1	Total C O 12 10 2	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C O 20 18 2	0	0
33	b	1	Total C 10 10	0	0
33	c	1	Total C O 20 18 2	0	0
33	c	1	Total C O 12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

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



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

- 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	E	1	Total C Fe N O 43 34 1 4 4	0	0

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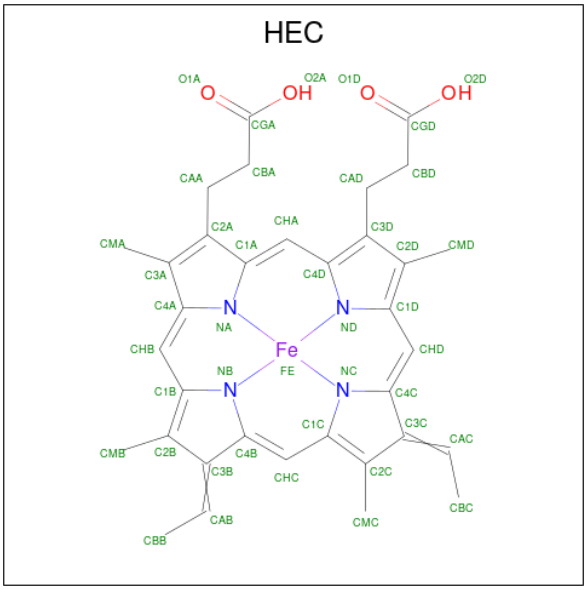
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	119	Total	O	0	4
			123	123		
37	B	197	Total	O	0	0
			197	197		
37	C	142	Total	O	0	0
			142	142		
37	D	106	Total	O	0	0
			106	106		
37	E	29	Total	O	0	0
			29	29		
37	F	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	27	Total O 27 27	0	0
37	I	13	Total O 13 13	0	0
37	J	12	Total O 12 12	0	0
37	K	2	Total O 2 2	0	0
37	L	9	Total O 9 9	0	0
37	M	5	Total O 5 5	0	0
37	O	73	Total O 73 73	0	0
37	T	9	Total O 9 9	0	0
37	U	29	Total O 29 29	0	0
37	V	51	Total O 51 51	0	0
37	Y	1	Total O 1 1	0	0
37	X	8	Total O 8 8	0	0
37	Z	3	Total O 3 3	0	0
37	R	6	Total O 6 6	0	0
37	a	100	Total O 104 104	0	4
37	b	163	Total O 163 163	0	0
37	c	160	Total O 160 160	0	0
37	d	95	Total O 95 95	0	0
37	e	13	Total O 13 13	0	0
37	f	3	Total O 3 3	0	0
37	h	20	Total O 20 20	0	0

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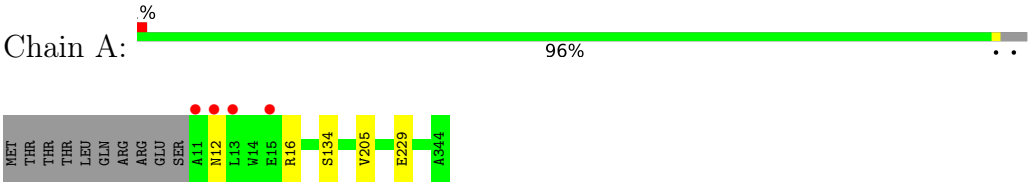
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	i	17	Total O 17 17	0	0
37	j	5	Total O 5 5	0	0
37	k	1	Total O 1 1	0	0
37	l	12	Total O 12 12	0	0
37	m	8	Total O 8 8	0	0
37	o	72	Total O 72 72	0	0
37	t	6	Total O 6 6	0	0
37	u	50	Total O 50 50	0	0
37	v	42	Total O 42 42	0	0
37	x	5	Total O 5 5	0	0
37	z	3	Total O 3 3	0	0
37	r	7	Total O 7 7	0	0

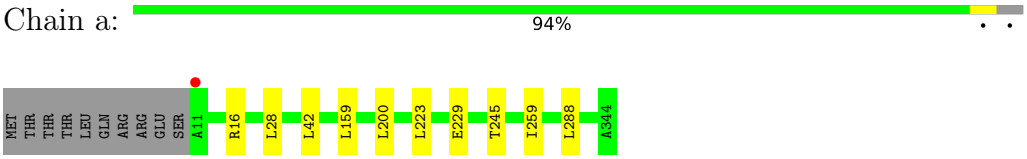
3 Residue-property plots (i)

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.

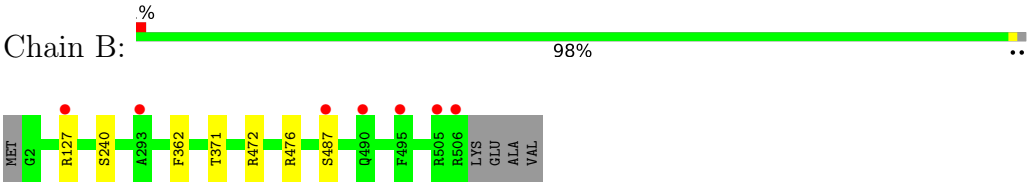
• Molecule 1: Photosystem II protein D1 1



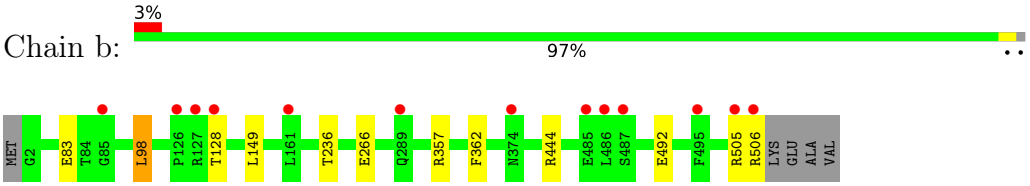
• Molecule 1: Photosystem II protein D1 1



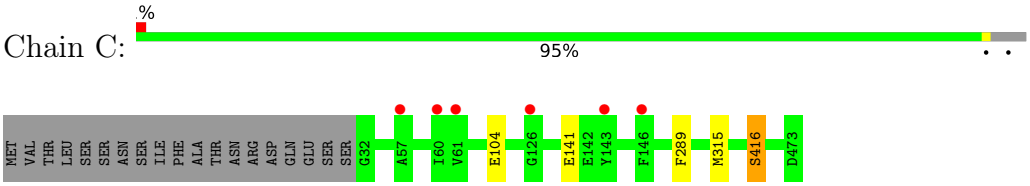
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

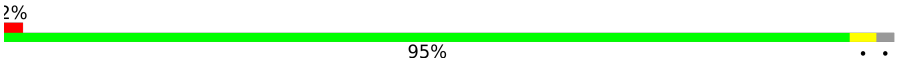


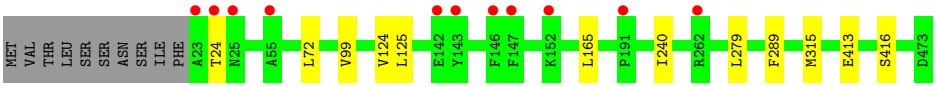
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

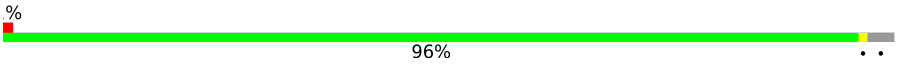
Chain c:

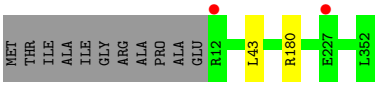




• Molecule 4: Photosystem II D2 protein

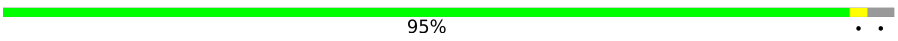
Chain D:





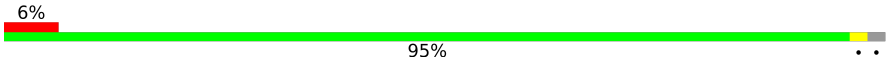
• Molecule 4: Photosystem II D2 protein

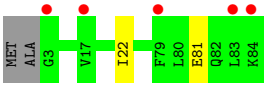
Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

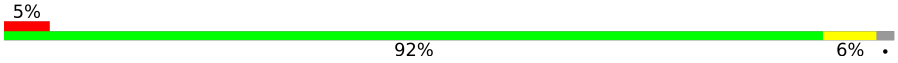
Chain E:

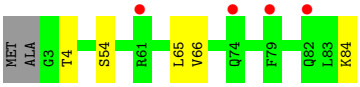




• Molecule 5: Cytochrome b559 subunit alpha

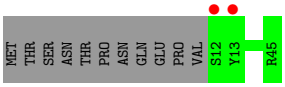
Chain e:





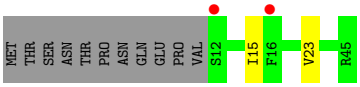
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



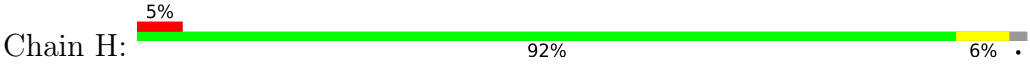
• Molecule 6: Cytochrome b559 subunit beta

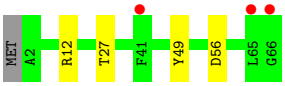
Chain f:



• Molecule 7: Photosystem II reaction center protein H

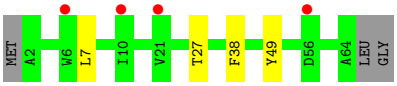
Chain H:





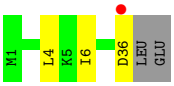
• Molecule 7: Photosystem II reaction center protein H

Chain h:



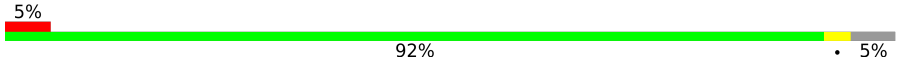
• Molecule 8: Photosystem II reaction center protein I

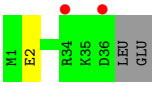
Chain I:



• Molecule 8: Photosystem II reaction center protein I

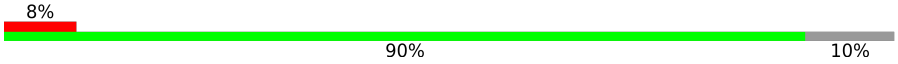
Chain i:

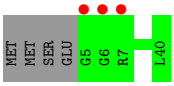




• Molecule 9: Photosystem II reaction center protein J

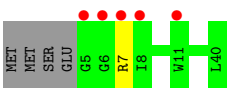
Chain J:





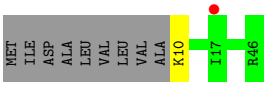
• Molecule 9: Photosystem II reaction center protein J

Chain j:



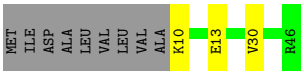
• Molecule 10: Photosystem II reaction center protein K

Chain K:



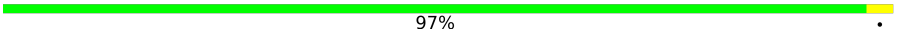
• Molecule 10: Photosystem II reaction center protein K

Chain k:



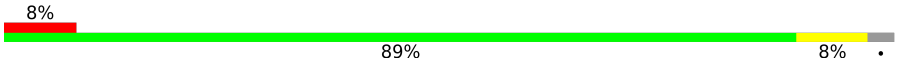
• Molecule 11: Photosystem II reaction center protein L

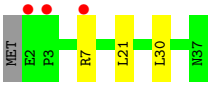
Chain L:



• Molecule 11: Photosystem II reaction center protein L

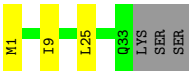
Chain l:





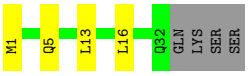
• Molecule 12: Photosystem II reaction center protein M

Chain M:



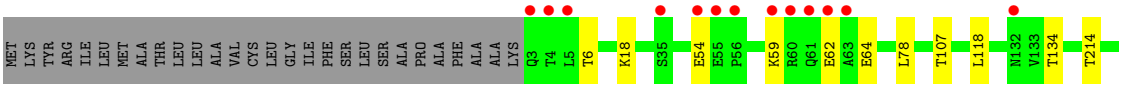
• Molecule 12: Photosystem II reaction center protein M

Chain m:



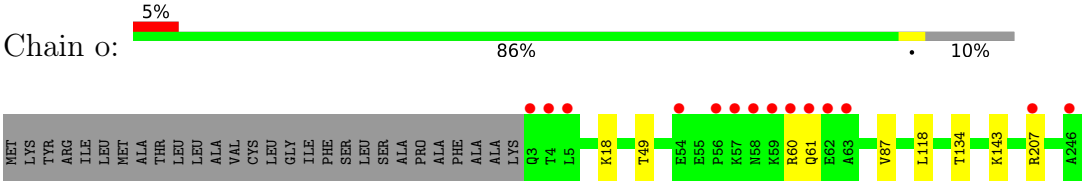
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



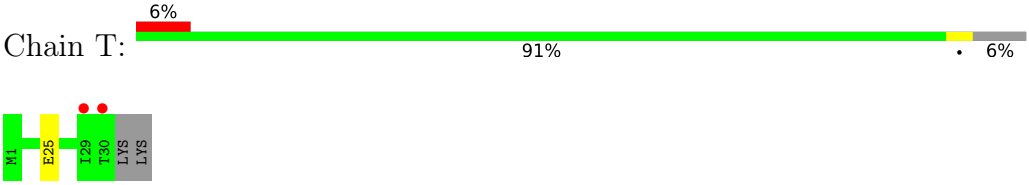
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



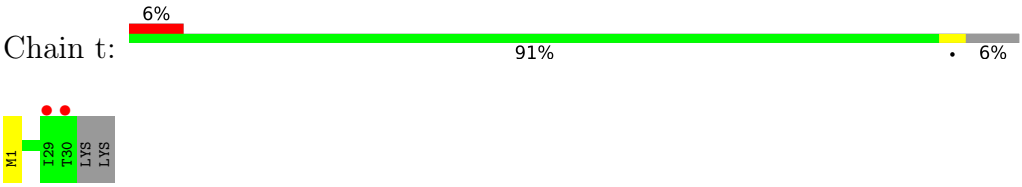
• Molecule 14: Photosystem II reaction center protein T

Chain T:



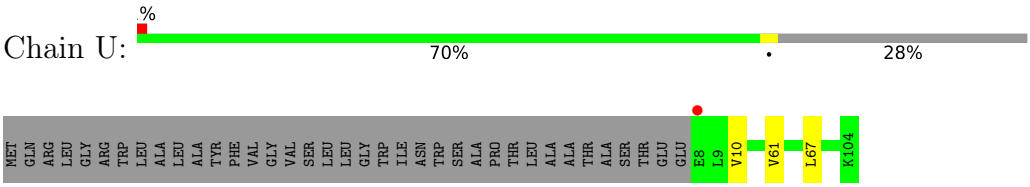
• Molecule 14: Photosystem II reaction center protein T

Chain t:



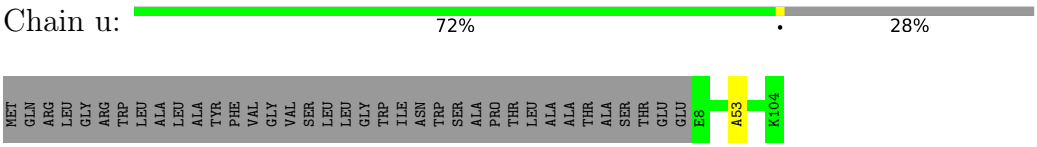
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



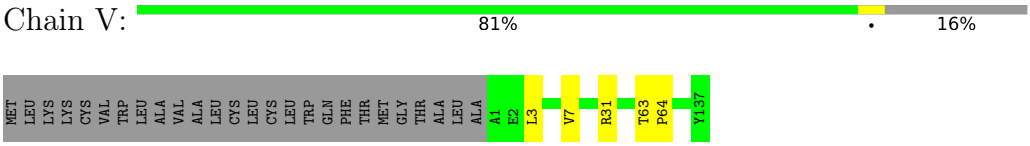
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



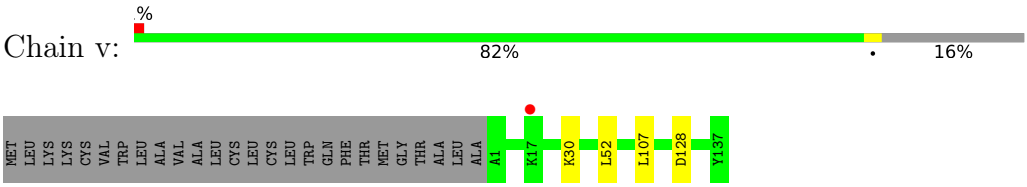
• Molecule 16: Cytochrome c-550

Chain V:



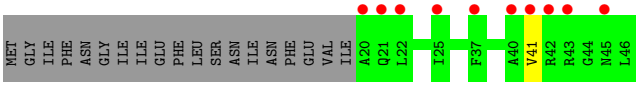
• Molecule 16: Cytochrome c-550

Chain v:



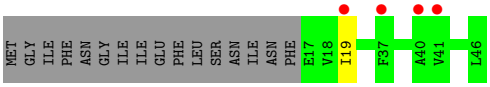
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



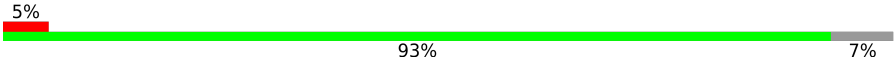
• Molecule 17: Photosystem II reaction center protein Ycf12

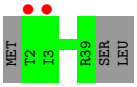
Chain y:



• Molecule 18: Photosystem II reaction center X protein

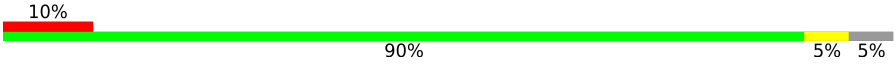
Chain X:

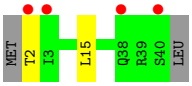




• Molecule 18: Photosystem II reaction center X protein

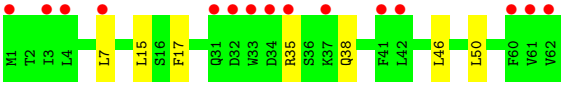
Chain x:





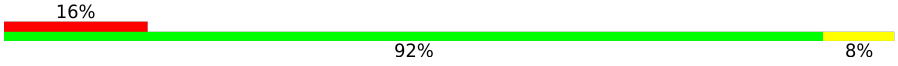
• Molecule 19: Photosystem II reaction center protein Z

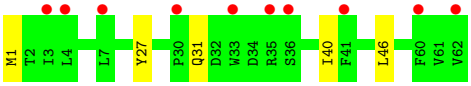
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

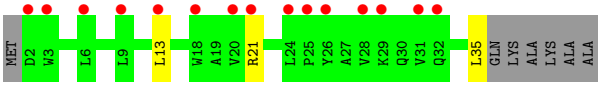
Chain z:





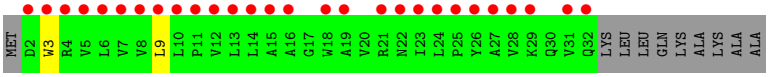
• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.65-2.09) 85.3 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.186 , 0.234 0.186 , 0.234	Depositor DCC
R_{free} test set	4165 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	53041	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: FME, OEX, PHO, FE2, BCT, LHG, STE, CL, DGD, SQD, BCR, PL9, CLA, LMG, HEM, OEY, HEC

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	0.43	0/3212	0.58	0/4376
1	a	0.42	0/3209	0.58	0/4372
2	B	0.40	0/4155	0.58	0/5661
2	b	0.39	0/4118	0.58	1/5611 (0.0%)
3	C	0.40	0/3625	0.55	0/4935
3	c	0.38	0/3705	0.54	0/5042
4	D	0.43	0/2825	0.57	0/3847
4	d	0.40	0/2834	0.58	0/3859
5	E	0.36	0/688	0.51	0/940
5	e	0.33	0/683	0.52	0/932
6	F	0.34	0/284	0.45	0/387
6	f	0.33	0/284	0.55	0/387
7	H	0.42	0/523	0.57	0/713
7	h	0.40	0/511	0.58	0/697
8	I	0.36	0/293	0.55	0/396
8	i	0.42	0/293	0.56	0/396
9	J	0.38	0/263	0.54	0/356
9	j	0.33	0/263	0.53	0/356
10	K	0.38	0/303	0.52	0/416
10	k	0.36	0/303	0.57	0/416
11	L	0.36	0/311	0.59	0/422
11	l	0.40	0/303	0.62	0/412
12	M	0.39	0/249	0.51	0/341
12	m	0.44	0/244	0.53	0/334
13	O	0.38	0/1904	0.63	0/2585
13	o	0.39	0/1905	0.62	0/2583
14	T	0.46	0/257	0.57	0/349
14	t	0.46	0/255	0.57	0/346
15	U	0.36	0/785	0.58	0/1064
15	u	0.37	0/785	0.59	0/1064
16	V	0.37	0/1085	0.59	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
16	v	0.35	0/1085	0.55	0/1473
17	Y	0.31	0/197	0.54	0/264
17	y	0.29	0/219	0.47	0/294
18	X	0.37	0/284	0.51	0/384
18	x	0.31	0/289	0.44	0/391
19	Z	0.32	0/490	0.49	0/669
19	z	0.30	0/488	0.42	0/666
20	R	0.36	0/277	0.58	0/380
20	r	0.31	0/252	0.51	0/347
All	All	0.39	0/44038	0.57	1/59936 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	98	LEU	CA-CB-CG	6.16	129.46	115.30

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	395/344 (115%)	387 (98%)	8 (2%)	0	100	100
1	a	395/344 (115%)	386 (98%)	8 (2%)	1 (0%)	41	41
2	B	507/510 (99%)	499 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	47	49
3	c	461/461 (100%)	449 (97%)	11 (2%)	1 (0%)	47	49
4	D	340/352 (97%)	332 (98%)	8 (2%)	0	100	100
4	d	341/352 (97%)	331 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	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%)	59 (94%)	3 (5%)	1 (2%)	9	5
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%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	229 (94%)	11 (4%)	3 (1%)	13	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	242/272 (89%)	231 (96%)	10 (4%)	1 (0%)	34 32
14	T	28/32 (88%)	28 (100%)	0	0	100 100
14	t	28/32 (88%)	28 (100%)	0	0	100 100
15	U	95/134 (71%)	92 (97%)	3 (3%)	0	100 100
15	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	14 9
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22 18
16	v	135/163 (83%)	132 (98%)	3 (2%)	0	100 100
17	Y	25/46 (54%)	24 (96%)	1 (4%)	0	100 100
17	y	28/46 (61%)	26 (93%)	2 (7%)	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%)	58 (97%)	2 (3%)	0	100 100
20	R	32/41 (78%)	32 (100%)	0	0	100 100
20	r	29/41 (71%)	29 (100%)	0	0	100 100
All	All	5386/5700 (94%)	5235 (97%)	141 (3%)	10 (0%)	47 49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
16	V	64	PRO
3	c	416	SER
13	O	59	LYS
13	o	61	GLN
15	u	53	ALA
13	O	62	GLU
13	O	134	THR
1	a	259	ILE
7	H	12	ARG

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	322/280 (115%)	317 (98%)	5 (2%)	62 69
1	a	321/280 (115%)	311 (97%)	10 (3%)	40 43
2	B	407/407 (100%)	400 (98%)	7 (2%)	60 67
2	b	402/407 (99%)	390 (97%)	12 (3%)	41 44
3	C	353/362 (98%)	348 (99%)	5 (1%)	67 73
3	c	362/362 (100%)	350 (97%)	12 (3%)	38 40
4	D	277/283 (98%)	275 (99%)	2 (1%)	84 88
4	d	278/283 (98%)	272 (98%)	6 (2%)	52 57
5	E	72/73 (99%)	69 (96%)	3 (4%)	30 30
5	e	71/73 (97%)	66 (93%)	5 (7%)	15 12
6	F	28/39 (72%)	28 (100%)	0	100 100
6	f	28/39 (72%)	26 (93%)	2 (7%)	14 11
7	H	54/55 (98%)	51 (94%)	3 (6%)	21 18
7	h	53/55 (96%)	49 (92%)	4 (8%)	13 10
8	I	32/34 (94%)	29 (91%)	3 (9%)	8 5
8	i	32/34 (94%)	31 (97%)	1 (3%)	40 43
9	J	24/28 (86%)	24 (100%)	0	100 100
9	j	24/28 (86%)	23 (96%)	1 (4%)	30 30
10	K	30/37 (81%)	29 (97%)	1 (3%)	38 40
10	k	30/37 (81%)	27 (90%)	3 (10%)	7 5
11	L	35/35 (100%)	34 (97%)	1 (3%)	42 46
11	l	34/35 (97%)	31 (91%)	3 (9%)	10 6
12	M	28/32 (88%)	26 (93%)	2 (7%)	14 11
12	m	28/32 (88%)	25 (89%)	3 (11%)	6 3
13	O	206/228 (90%)	198 (96%)	8 (4%)	32 33
13	o	207/228 (91%)	199 (96%)	8 (4%)	32 33
14	T	26/28 (93%)	25 (96%)	1 (4%)	33 34
14	t	25/28 (89%)	25 (100%)	0	100 100
15	U	84/112 (75%)	81 (96%)	3 (4%)	35 36
15	u	84/112 (75%)	84 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	V	117/138 (85%)	114 (97%)	3 (3%)	46 50
16	v	117/138 (85%)	113 (97%)	4 (3%)	37 39
17	Y	19/37 (51%)	18 (95%)	1 (5%)	22 20
17	y	22/37 (60%)	21 (96%)	1 (4%)	27 27
18	X	31/34 (91%)	31 (100%)	0	100 100
18	x	31/34 (91%)	29 (94%)	2 (6%)	17 14
19	Z	52/52 (100%)	45 (86%)	7 (14%)	4 2
19	z	51/52 (98%)	46 (90%)	5 (10%)	8 5
20	R	28/33 (85%)	25 (89%)	3 (11%)	6 3
20	r	25/33 (76%)	23 (92%)	2 (8%)	12 8
All	All	4450/4654 (96%)	4308 (97%)	142 (3%)	39 41

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	ARG
1	A	134	SER
1	A	205	VAL
1	A	229	GLU
2	B	127	ARG
2	B	240	SER
2	B	362	PHE
2	B	371	THR
2	B	472	ARG
2	B	476	ARG
2	B	487	SER
3	C	104	GLU
3	C	141	GLU
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	43	LEU
4	D	180	ARG
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
7	H	27	THR

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Mol	Chain	Res	Type
7	H	49	TYR
7	H	56	ASP
8	I	4	LEU
8	I	6	ILE
8	I	36	ASP
10	K	10	LYS
11	L	10	VAL
12	M	9	ILE
12	M	25	LEU
13	O	6	THR
13	O	18	LYS
13	O	54	GLU
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
14	T	25	GLU
15	U	10	VAL
15	U	61	VAL
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	31	ARG
17	Y	41	VAL
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	35	ARG
19	Z	38	GLN
19	Z	46	LEU
19	Z	50	LEU
20	R	13	LEU
20	R	21	ARG
20	R	35	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU

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Mol	Chain	Res	Type
1	a	229	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	266	GLU
2	b	357	ARG
2	b	362	PHE
2	b	444	ARG
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU
4	d	321	LEU
5	e	4	THR
5	e	54	SER
5	e	65	LEU
5	e	66	VAL
5	e	84	LYS
6	f	15	ILE
6	f	23	VAL
7	h	7	LEU
7	h	27	THR

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Mol	Chain	Res	Type
7	h	38	PHE
7	h	49	TYR
8	i	2	GLU
9	j	7	ARG
10	k	10	LYS
10	k	13	GLU
10	k	30	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	18	LYS
13	o	49	THR
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	134	THR
13	o	143	LYS
13	o	207	ARG
16	v	30	LYS
16	v	52	LEU
16	v	107	LEU
16	v	128	ASP
17	y	19	ILE
18	x	2	THR
18	x	15	LEU
19	z	1	MET
19	z	27	TYR
19	z	31	GLN
19	z	40	ILE
19	z	46	LEU
20	r	3	TRP
20	r	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	61	HIS
7	H	59	ASN
13	O	36	GLN

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Mol	Chain	Res	Type
13	O	88	ASN
13	O	231	HIS
16	V	86	GLN
19	Z	38	GLN
1	a	19	ASN
1	a	234	ASN
2	b	490	GLN
5	e	60	GLN
12	m	5	GLN
13	o	61	GLN
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	0.99	1 (12%)	7,9,11	1.12	0
8	FME	I	1	8	8,9,10	0.97	0	7,9,11	0.90	0
8	FME	i	1	8	8,9,10	1.00	0	7,9,11	0.82	0
14	FME	T	1	14	8,9,10	1.07	0	7,9,11	1.01	0
14	FME	t	1	14	8,9,10	1.19	1 (12%)	7,9,11	0.58	0
12	FME	m	1	12	8,9,10	1.05	1 (12%)	7,9,11	0.88	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	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.36	1.43	1.46
12	m	1	FME	CA-N	-2.23	1.43	1.46
12	M	1	FME	CA-N	-2.07	1.43	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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	B	606	-	65,73,73	1.62	8 (12%)	76,113,113	1.44	10 (13%)
25	CLA	b	612	-	65,73,73	1.42	8 (12%)	76,113,113	1.44	10 (13%)
33	STE	E	102	-	11,11,19	0.78	0	11,11,19	1.01	0
27	BCR	a	610	-	41,41,41	0.96	2 (4%)	56,56,56	1.26	6 (10%)
31	LHG	l	101	-	48,48,48	0.66	1 (2%)	51,54,54	1.18	6 (11%)
33	STE	H	103	-	17,17,19	0.39	0	16,16,19	0.73	0
32	DGD	c	517	-	63,63,67	0.97	3 (4%)	77,77,81	1.35	7 (9%)
25	CLA	C	505	-	65,73,73	1.62	6 (9%)	76,113,113	1.32	6 (7%)
29	LMG	C	518	-	48,48,55	0.82	1 (2%)	56,56,63	1.37	9 (16%)
25	CLA	A	606	-	65,73,73	1.45	6 (9%)	76,113,113	1.37	11 (14%)
27	BCR	b	617	-	41,41,41	0.96	2 (4%)	56,56,56	1.28	7 (12%)
33	STE	B	625	-	11,11,19	0.72	0	11,11,19	1.21	1 (9%)
36	HEC	v	201	16	32,50,50	2.13	3 (9%)	24,82,82	1.55	4 (16%)
25	CLA	B	611	-	65,73,73	1.42	6 (9%)	76,113,113	1.47	9 (11%)
33	STE	M	103	-	9,9,19	0.38	0	8,8,19	0.72	0
32	DGD	A	617	-	67,67,67	1.09	8 (11%)	81,81,81	1.42	15 (18%)
33	STE	I	101	-	14,14,19	0.42	0	13,13,19	0.63	0
25	CLA	B	602	-	65,73,73	1.56	6 (9%)	76,113,113	1.55	10 (13%)
25	CLA	D	404	-	65,73,73	1.56	7 (10%)	76,113,113	1.39	9 (11%)
25	CLA	C	508	-	65,73,73	1.61	8 (12%)	76,113,113	1.49	8 (10%)
25	CLA	B	615	-	65,73,73	1.71	7 (10%)	76,113,113	1.40	8 (10%)
33	STE	x	102	-	19,19,19	0.64	0	19,19,19	0.91	1 (5%)
29	LMG	d	411	-	44,44,55	0.94	2 (4%)	52,52,63	1.33	6 (11%)
29	LMG	c	524	-	49,49,55	0.84	2 (4%)	57,57,63	1.27	4 (7%)
33	STE	D	413	-	19,19,19	0.59	0	19,19,19	1.15	0
25	CLA	b	602	-	65,73,73	1.40	4 (6%)	76,113,113	1.49	10 (13%)
25	CLA	a	608	37	65,73,73	1.53	7 (10%)	76,113,113	1.45	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	b	621	-	55,55,55	0.85	2 (3%)	63,63,63	1.33	8 (12%)
25	CLA	b	613	-	65,73,73	1.70	8 (12%)	76,113,113	1.47	12 (15%)
27	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
33	STE	a	616	-	9,9,19	0.44	0	8,8,19	0.61	0
32	DGD	c	519	-	63,63,67	0.95	3 (4%)	77,77,81	1.41	8 (10%)
25	CLA	b	610	37	65,73,73	1.45	8 (12%)	76,113,113	1.45	12 (15%)
25	CLA	c	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.56	7 (9%)
25	CLA	B	610	37	65,73,73	1.49	6 (9%)	76,113,113	1.52	12 (15%)
33	STE	b	623	-	9,9,19	0.38	0	8,8,19	0.66	0
29	LMG	c	520	-	37,37,55	0.85	0	45,45,63	1.37	7 (15%)
25	CLA	B	603	-	65,73,73	1.50	9 (13%)	76,113,113	1.38	13 (17%)
22	OEX	a	602[A]	3,1,37	0,15,15	-	-	-		
27	BCR	c	516	-	41,41,41	1.00	2 (4%)	56,56,56	1.14	6 (10%)
27	BCR	D	406	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	5 (8%)
32	DGD	c	518	-	63,63,67	1.03	4 (6%)	77,77,81	1.40	9 (11%)
25	CLA	b	609	-	65,73,73	1.58	8 (12%)	76,113,113	1.35	9 (11%)
27	BCR	K	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.40	8 (14%)
25	CLA	c	505	-	65,73,73	1.45	5 (7%)	76,113,113	1.30	7 (9%)
26	PHO	D	402	-	51,69,69	0.97	4 (7%)	47,99,99	1.44	6 (12%)
25	CLA	c	502	-	65,73,73	1.48	7 (10%)	76,113,113	1.46	10 (13%)
25	CLA	d	403	-	65,73,73	1.46	7 (10%)	76,113,113	1.30	6 (7%)
33	STE	C	519	-	11,11,19	0.59	0	11,11,19	1.49	3 (27%)
33	STE	d	413	-	16,16,19	0.62	0	16,16,19	1.13	1 (6%)
25	CLA	c	508	-	64,72,73	1.56	9 (14%)	74,111,113	1.43	9 (12%)
25	CLA	C	513	-	65,73,73	1.52	7 (10%)	76,113,113	1.49	7 (9%)
33	STE	c	523	-	11,11,19	0.68	0	11,11,19	1.36	1 (9%)
25	CLA	b	611	-	65,73,73	1.51	7 (10%)	76,113,113	1.56	10 (13%)
35	HEM	f	101	5,6	41,50,50	1.47	6 (14%)	45,82,82	1.52	9 (20%)
25	CLA	B	609	-	65,73,73	1.46	6 (9%)	76,113,113	1.31	7 (9%)
27	BCR	C	514	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	6 (10%)
33	STE	d	412	-	15,15,19	0.72	0	15,15,19	0.99	0
29	LMG	D	411	-	31,31,55	0.73	1 (3%)	33,33,63	1.15	2 (6%)
21	OEY	A	601[B]	3,1,37	0,16,16	-	-	-		
25	CLA	B	613	-	65,73,73	1.50	7 (10%)	76,113,113	1.52	10 (13%)
25	CLA	A	609	-	54,62,73	1.60	8 (14%)	62,99,113	1.56	8 (12%)
25	CLA	C	503	-	65,73,73	1.81	8 (12%)	76,113,113	1.58	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	B	612	-	65,73,73	1.38	6 (9%)	76,113,113	1.52	12 (15%)
27	BCR	c	515	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	7 (12%)
31	LHG	e	101	-	41,41,48	0.76	1 (2%)	44,47,54	1.27	5 (11%)
33	STE	T	102	-	15,15,19	0.39	0	14,14,19	0.73	0
29	LMG	c	522	-	48,48,55	0.88	3 (6%)	56,56,63	1.33	9 (16%)
25	CLA	C	501	-	65,73,73	1.56	6 (9%)	76,113,113	1.48	10 (13%)
25	CLA	D	405	-	65,73,73	1.52	8 (12%)	76,113,113	1.51	7 (9%)
25	CLA	b	614	-	65,73,73	1.65	8 (12%)	76,113,113	1.29	9 (11%)
25	CLA	c	510	-	65,73,73	1.52	9 (13%)	76,113,113	1.52	10 (13%)
29	LMG	D	408	-	51,51,55	0.90	3 (5%)	59,59,63	1.34	7 (11%)
33	STE	t	102	-	13,13,19	0.65	0	13,13,19	1.16	1 (7%)
30	SQD	L	101	-	48,49,54	1.61	9 (18%)	57,60,65	2.00	13 (22%)
33	STE	B	620	-	16,16,19	0.63	0	16,16,19	1.15	0
30	SQD	A	613	-	51,52,54	1.56	6 (11%)	60,63,65	1.91	12 (20%)
25	CLA	b	615	-	65,73,73	1.55	9 (13%)	76,113,113	1.37	9 (11%)
31	LHG	D	410	-	46,46,48	0.78	1 (2%)	49,52,54	1.20	5 (10%)
34	BCT	a	606	23	2,3,3	1.12	0	2,3,3	2.02	1 (50%)
25	CLA	b	608	-	65,73,73	1.52	8 (12%)	76,113,113	1.52	13 (17%)
26	PHO	d	401	-	51,69,69	0.93	2 (3%)	47,99,99	1.25	6 (12%)
33	STE	l	102	-	17,17,19	0.33	0	16,16,19	0.96	0
27	BCR	B	618	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	8 (14%)
25	CLA	C	507	37	65,73,73	1.47	8 (12%)	76,113,113	1.58	10 (13%)
25	CLA	C	504	37	59,67,73	1.61	6 (10%)	68,105,113	1.37	7 (10%)
25	CLA	d	404	-	65,73,73	1.53	7 (10%)	76,113,113	1.35	6 (7%)
29	LMG	m	101	-	51,51,55	0.86	3 (5%)	59,59,63	1.47	9 (15%)
31	LHG	d	409	-	38,38,48	0.76	1 (2%)	41,44,54	1.12	2 (4%)
33	STE	T	103	-	14,14,19	0.31	0	13,13,19	0.96	0
33	STE	M	102	-	14,14,19	0.67	0	14,14,19	1.22	1 (7%)
25	CLA	B	601	37	65,73,73	1.67	9 (13%)	76,113,113	1.41	8 (10%)
29	LMG	A	612	-	48,48,55	0.78	2 (4%)	56,56,63	1.33	6 (10%)
33	STE	B	623	-	11,11,19	0.73	0	11,11,19	1.07	0
26	PHO	d	402	-	51,69,69	0.97	3 (5%)	47,99,99	1.47	7 (14%)
32	DGD	C	516	-	63,63,67	1.11	6 (9%)	77,77,81	1.43	13 (16%)
32	DGD	h	101	-	63,63,67	1.00	4 (6%)	77,77,81	1.47	11 (14%)
25	CLA	C	510	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	10 (13%)
31	LHG	d	408	-	48,48,48	0.60	1 (2%)	51,54,54	1.25	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PL9	D	407	-	55,55,55	0.91	2 (3%)	68,69,69	1.53	12 (17%)
31	LHG	d	407	-	48,48,48	0.79	2 (4%)	51,54,54	1.34	6 (11%)
33	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.24	0
27	BCR	b	619	-	41,41,41	1.03	2 (4%)	56,56,56	1.25	4 (7%)
27	BCR	Y	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.17	4 (7%)
32	DGD	C	517	-	63,63,67	0.93	2 (3%)	77,77,81	1.34	8 (10%)
25	CLA	B	608	-	65,73,73	1.59	9 (13%)	76,113,113	1.60	7 (9%)
25	CLA	C	511	3	65,73,73	1.55	6 (9%)	76,113,113	1.45	7 (9%)
27	BCR	t	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.33	7 (12%)
22	OEX	A	602[A]	3,1,37	0,15,15	-	-	-		
25	CLA	c	504	37	60,68,73	1.63	8 (13%)	70,107,113	1.49	7 (10%)
27	BCR	b	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	6 (10%)
27	BCR	d	405	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	7 (12%)
25	CLA	C	512	-	65,73,73	1.57	9 (13%)	76,113,113	1.42	11 (14%)
27	BCR	K	102	-	41,41,41	1.02	2 (4%)	56,56,56	1.13	3 (5%)
30	SQD	F	101	-	35,36,54	1.60	6 (17%)	42,45,65	1.99	13 (30%)
25	CLA	B	616	-	60,68,73	1.57	8 (13%)	70,107,113	1.59	9 (12%)
32	DGD	C	515	-	63,63,67	1.04	6 (9%)	77,77,81	1.41	11 (14%)
25	CLA	c	501	-	65,73,73	1.50	7 (10%)	76,113,113	1.47	8 (10%)
29	LMG	d	410	-	21,21,55	0.48	0	20,20,63	1.18	2 (10%)
25	CLA	C	506	-	65,73,73	1.52	8 (12%)	76,113,113	1.41	9 (11%)
25	CLA	C	502	-	65,73,73	1.51	9 (13%)	76,113,113	1.34	8 (10%)
30	SQD	f	102	-	40,41,54	1.68	8 (20%)	49,52,65	1.75	12 (24%)
33	STE	m	102	-	11,11,19	0.68	0	11,11,19	1.41	1 (9%)
25	CLA	c	511	3	65,73,73	1.68	6 (9%)	76,113,113	1.62	7 (9%)
26	PHO	A	608	-	51,69,69	0.97	3 (5%)	47,99,99	1.28	5 (10%)
27	BCR	x	101	-	41,41,41	0.96	2 (4%)	56,56,56	1.20	6 (10%)
25	CLA	c	509	-	65,73,73	1.55	7 (10%)	76,113,113	1.70	11 (14%)
25	CLA	c	513	-	65,73,73	1.57	7 (10%)	76,113,113	1.40	9 (11%)
31	LHG	A	614	-	48,48,48	0.70	1 (2%)	51,54,54	1.20	7 (13%)
31	LHG	D	412	-	48,48,48	0.88	2 (4%)	51,54,54	1.35	6 (11%)
29	LMG	B	621	-	26,26,55	0.58	0	26,26,63	1.36	2 (7%)
33	STE	B	624	-	17,17,19	0.62	0	17,17,19	1.04	0
25	CLA	a	607	-	65,73,73	1.76	9 (13%)	76,113,113	1.37	9 (11%)
25	CLA	b	616	-	60,68,73	1.45	7 (11%)	70,107,113	1.59	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PL9	A	611	-	55,55,55	0.95	1 (1%)	68,69,69	1.44	10 (14%)
25	CLA	B	607	37	65,73,73	1.52	9 (13%)	76,113,113	1.42	6 (7%)
33	STE	C	521	-	15,15,19	0.44	0	14,14,19	0.60	0
25	CLA	c	512	-	65,73,73	1.57	8 (12%)	76,113,113	1.43	9 (11%)
25	CLA	C	509	-	65,73,73	1.56	7 (10%)	76,113,113	1.50	7 (9%)
27	BCR	H	101	-	41,41,41	0.96	2 (4%)	56,56,56	1.24	5 (8%)
25	CLA	a	609	-	65,73,73	1.51	9 (13%)	76,113,113	1.26	9 (11%)
25	CLA	B	604	-	65,73,73	1.57	9 (13%)	76,113,113	1.73	11 (14%)
33	STE	c	521	-	19,19,19	0.67	0	19,19,19	0.93	0
25	CLA	A	607	37	65,73,73	1.53	7 (10%)	76,113,113	1.30	10 (13%)
30	SQD	a	613	-	53,54,54	1.50	9 (16%)	62,65,65	1.99	11 (17%)
32	DGD	a	615	-	43,43,67	0.76	2 (4%)	45,45,81	1.46	8 (17%)
33	STE	B	626	-	15,15,19	0.37	0	14,14,19	0.81	0
25	CLA	B	614	-	65,73,73	1.67	8 (12%)	76,113,113	1.27	7 (9%)
25	CLA	b	606	-	65,73,73	1.61	8 (12%)	76,113,113	1.67	9 (11%)
35	HEM	E	101	5,6	41,50,50	1.50	4 (9%)	45,82,82	1.30	4 (8%)
30	SQD	A	616	-	38,38,54	1.73	5 (13%)	40,40,65	1.28	2 (5%)
25	CLA	D	403	37	65,73,73	1.52	6 (9%)	76,113,113	1.19	8 (10%)
25	CLA	b	604	-	65,73,73	1.56	6 (9%)	76,113,113	1.70	10 (13%)
33	STE	a	617	-	11,11,19	0.78	0	11,11,19	1.08	1 (9%)
33	STE	j	101	-	11,11,19	0.68	0	11,11,19	1.40	2 (18%)
25	CLA	b	605	-	65,73,73	1.46	5 (7%)	76,113,113	1.44	13 (17%)
25	CLA	c	507	37	65,73,73	1.60	8 (12%)	76,113,113	1.33	8 (10%)
27	BCR	B	619	-	41,41,41	0.98	1 (2%)	56,56,56	1.31	6 (10%)
25	CLA	a	612	37	65,73,73	1.54	6 (9%)	76,113,113	1.45	9 (11%)
25	CLA	b	601	37	65,73,73	1.63	8 (12%)	76,113,113	1.51	7 (9%)
29	LMG	M	101	-	51,51,55	0.86	1 (1%)	59,59,63	1.39	6 (10%)
21	OEY	a	601[B]	3,1,37	0,16,16	-	-	-		
33	STE	b	622	-	19,19,19	0.67	0	19,19,19	0.96	1 (5%)
32	DGD	H	102	-	63,63,67	1.07	5 (7%)	77,77,81	1.40	8 (10%)
33	STE	C	520	-	11,11,19	0.69	0	11,11,19	1.42	2 (18%)
27	BCR	k	101	-	41,41,41	1.03	3 (7%)	56,56,56	1.05	2 (3%)
27	BCR	B	617	-	41,41,41	1.01	3 (7%)	56,56,56	1.22	5 (8%)
28	PL9	d	406	-	55,55,55	1.02	4 (7%)	68,69,69	1.64	17 (25%)
36	HEC	V	201	16	32,50,50	1.98	3 (9%)	24,82,82	2.07	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LHG	A	615	-	48,48,48	0.74	3 (6%)	51,54,54	1.19	2 (3%)
34	BCT	D	401	23	2,3,3	1.03	0	2,3,3	1.95	1 (50%)
25	CLA	c	506	-	65,73,73	1.51	9 (13%)	76,113,113	1.45	6 (7%)
27	BCR	A	610	-	41,41,41	0.96	1 (2%)	56,56,56	1.37	11 (19%)
25	CLA	B	605	-	65,73,73	1.45	8 (12%)	76,113,113	1.33	8 (10%)
28	PL9	a	611	-	55,55,55	0.79	2 (3%)	68,69,69	1.53	15 (22%)
31	LHG	D	409	-	48,48,48	0.77	1 (2%)	51,54,54	1.30	7 (13%)
33	STE	b	620	-	19,19,19	0.62	0	19,19,19	0.98	0
30	SQD	a	614	-	35,35,54	1.69	7 (20%)	37,37,65	1.35	4 (10%)
25	CLA	b	607	37	65,73,73	1.49	8 (12%)	76,113,113	1.41	9 (11%)
27	BCR	T	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.17	5 (8%)
30	SQD	B	622	-	53,54,54	1.58	9 (16%)	62,65,65	1.56	8 (12%)
25	CLA	b	603	-	65,73,73	1.51	8 (12%)	76,113,113	1.55	11 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	606	-	1/1/15/20	14/37/115/115	-
25	CLA	b	612	-	1/1/15/20	5/37/115/115	-
33	STE	E	102	-	-	4/9/9/17	-
27	BCR	a	610	-	-	2/29/63/63	0/2/2/2
31	LHG	l	101	-	-	21/53/53/53	-
33	STE	H	103	-	-	6/15/15/17	-
32	DGD	c	517	-	-	29/51/91/95	0/2/2/2
25	CLA	C	505	-	1/1/15/20	18/37/115/115	-
29	LMG	C	518	-	-	20/43/63/70	0/1/1/1
25	CLA	A	606	-	1/1/15/20	7/37/115/115	-
27	BCR	b	617	-	-	5/29/63/63	0/2/2/2
33	STE	B	625	-	-	8/9/9/17	-
36	HEC	v	201	16	-	2/10/54/54	-
25	CLA	B	611	-	1/1/15/20	9/37/115/115	-
33	STE	M	103	-	-	3/7/7/17	-
32	DGD	A	617	-	-	28/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	I	101	-	-	6/12/12/17	-
25	CLA	B	602	-	1/1/15/20	8/37/115/115	-
25	CLA	D	404	-	1/1/15/20	6/37/115/115	-
25	CLA	C	508	-	-	11/37/115/115	-
25	CLA	B	615	-	1/1/15/20	8/37/115/115	-
33	STE	x	102	-	-	10/17/17/17	-
29	LMG	d	411	-	-	11/39/59/70	0/1/1/1
29	LMG	c	524	-	-	19/44/64/70	0/1/1/1
33	STE	D	413	-	-	9/17/17/17	-
25	CLA	b	602	-	-	13/37/115/115	-
25	CLA	a	608	37	-	14/37/115/115	-
29	LMG	b	621	-	-	27/50/70/70	0/1/1/1
25	CLA	b	613	-	1/1/15/20	9/37/115/115	-
27	BCR	c	514	-	-	10/29/63/63	0/2/2/2
33	STE	a	616	-	-	3/7/7/17	-
32	DGD	c	519	-	-	21/51/91/95	0/2/2/2
25	CLA	b	610	37	1/1/15/20	6/37/115/115	-
25	CLA	c	503	-	-	8/37/115/115	-
25	CLA	B	610	37	1/1/15/20	8/37/115/115	-
33	STE	b	623	-	-	5/7/7/17	-
29	LMG	c	520	-	-	10/31/51/70	0/1/1/1
25	CLA	B	603	-	1/1/15/20	12/37/115/115	-
27	BCR	c	516	-	-	7/29/63/63	0/2/2/2
27	BCR	D	406	-	-	6/29/63/63	0/2/2/2
32	DGD	c	518	-	-	24/51/91/95	0/2/2/2
25	CLA	b	609	-	1/1/15/20	9/37/115/115	-
27	BCR	K	101	-	-	7/29/63/63	0/2/2/2
25	CLA	c	505	-	1/1/15/20	11/37/115/115	-
26	PHO	D	402	-	-	3/37/103/103	0/5/6/6
25	CLA	c	502	-	1/1/15/20	11/37/115/115	-
25	CLA	d	403	-	1/1/15/20	6/37/115/115	-
33	STE	C	519	-	-	5/9/9/17	-
33	STE	d	413	-	-	10/14/14/17	-
25	CLA	c	508	-	-	5/36/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	513	-	1/1/15/20	16/37/115/115	-
33	STE	c	523	-	-	4/9/9/17	-
25	CLA	b	611	-	1/1/15/20	7/37/115/115	-
35	HEM	f	101	5,6	-	5/12/54/54	-
25	CLA	B	609	-	-	4/37/115/115	-
27	BCR	C	514	-	-	7/29/63/63	0/2/2/2
33	STE	d	412	-	-	6/13/13/17	-
29	LMG	D	411	-	-	20/33/33/70	-
25	CLA	B	613	-	1/1/15/20	14/37/115/115	-
25	CLA	A	609	-	1/1/12/20	3/24/102/115	-
25	CLA	C	503	-	1/1/15/20	7/37/115/115	-
25	CLA	B	612	-	1/1/15/20	11/37/115/115	-
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
31	LHG	e	101	-	-	22/46/46/53	-
33	STE	T	102	-	-	7/13/13/17	-
29	LMG	c	522	-	-	22/43/63/70	0/1/1/1
25	CLA	C	501	-	1/1/15/20	5/37/115/115	-
25	CLA	D	405	-	-	7/37/115/115	-
25	CLA	b	614	-	1/1/15/20	15/37/115/115	-
25	CLA	c	510	-	1/1/15/20	18/37/115/115	-
29	LMG	D	408	-	-	17/46/66/70	0/1/1/1
33	STE	t	102	-	-	5/11/11/17	-
30	SQD	L	101	-	-	17/44/64/69	0/1/1/1
33	STE	B	620	-	-	8/14/14/17	-
30	SQD	A	613	-	-	17/47/67/69	0/1/1/1
25	CLA	b	615	-	1/1/15/20	11/37/115/115	-
31	LHG	D	410	-	-	16/51/51/53	-
25	CLA	b	608	-	1/1/15/20	8/37/115/115	-
26	PHO	d	401	-	-	6/37/103/103	0/5/6/6
33	STE	l	102	-	-	9/15/15/17	-
27	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	C	507	37	1/1/15/20	4/37/115/115	-
25	CLA	C	504	37	1/1/13/20	8/30/108/115	-
25	CLA	d	404	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	m	101	-	-	12/46/66/70	0/1/1/1
31	LHG	d	409	-	-	11/43/43/53	-
33	STE	T	103	-	-	8/12/12/17	-
33	STE	M	102	-	-	5/12/12/17	-
25	CLA	B	601	37	1/1/15/20	16/37/115/115	-
29	LMG	A	612	-	-	23/43/63/70	0/1/1/1
33	STE	B	623	-	-	7/9/9/17	-
26	PHO	d	402	-	-	7/37/103/103	0/5/6/6
32	DGD	C	516	-	-	22/51/91/95	0/2/2/2
32	DGD	h	101	-	-	16/51/91/95	0/2/2/2
25	CLA	C	510	-	1/1/15/20	11/37/115/115	-
31	LHG	d	408	-	-	20/53/53/53	-
28	PL9	D	407	-	-	7/53/73/73	0/1/1/1
31	LHG	d	407	-	-	22/53/53/53	-
33	STE	J	101	-	-	2/9/9/17	-
27	BCR	b	619	-	-	3/29/63/63	0/2/2/2
27	BCR	Y	101	-	-	7/29/63/63	0/2/2/2
32	DGD	C	517	-	-	14/51/91/95	0/2/2/2
25	CLA	B	608	-	1/1/15/20	4/37/115/115	-
25	CLA	C	511	3	1/1/15/20	6/37/115/115	-
27	BCR	t	101	-	-	7/29/63/63	0/2/2/2
25	CLA	c	504	37	1/1/14/20	8/31/109/115	-
27	BCR	b	618	-	-	6/29/63/63	0/2/2/2
27	BCR	d	405	-	-	7/29/63/63	0/2/2/2
25	CLA	C	512	-	1/1/15/20	15/37/115/115	-
27	BCR	K	102	-	-	11/29/63/63	0/2/2/2
30	SQD	F	101	-	-	11/28/48/69	0/1/1/1
25	CLA	B	616	-	1/1/14/20	14/31/109/115	-
32	DGD	C	515	-	-	23/51/91/95	0/2/2/2
25	CLA	c	501	-	1/1/15/20	5/37/115/115	-
29	LMG	d	410	-	-	11/17/17/70	-
25	CLA	C	506	-	1/1/15/20	11/37/115/115	-
25	CLA	C	502	-	1/1/15/20	12/37/115/115	-
30	SQD	f	102	-	-	11/36/56/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	m	102	-	-	4/9/9/17	-
25	CLA	c	511	3	1/1/15/20	11/37/115/115	-
26	PHO	A	608	-	-	6/37/103/103	0/5/6/6
27	BCR	x	101	-	-	9/29/63/63	0/2/2/2
25	CLA	c	509	-	1/1/15/20	12/37/115/115	-
25	CLA	c	513	-	1/1/15/20	10/37/115/115	-
31	LHG	A	614	-	-	29/53/53/53	-
31	LHG	D	412	-	-	15/53/53/53	-
29	LMG	B	621	-	-	14/22/22/70	-
33	STE	B	624	-	-	9/15/15/17	-
25	CLA	a	607	-	1/1/15/20	4/37/115/115	-
25	CLA	b	616	-	1/1/14/20	7/31/109/115	-
28	PL9	A	611	-	-	25/53/73/73	0/1/1/1
25	CLA	B	607	37	1/1/15/20	13/37/115/115	-
33	STE	C	521	-	-	6/13/13/17	-
25	CLA	c	512	-	1/1/15/20	21/37/115/115	-
25	CLA	C	509	-	1/1/15/20	12/37/115/115	-
27	BCR	H	101	-	-	6/29/63/63	0/2/2/2
25	CLA	a	609	-	1/1/15/20	8/37/115/115	-
25	CLA	B	604	-	1/1/15/20	12/37/115/115	-
33	STE	c	521	-	-	8/17/17/17	-
25	CLA	A	607	37	-	11/37/115/115	-
30	SQD	a	613	-	-	25/49/69/69	0/1/1/1
32	DGD	a	615	-	-	28/45/45/95	-
33	STE	B	626	-	-	7/13/13/17	-
25	CLA	B	614	-	1/1/15/20	12/37/115/115	-
25	CLA	b	606	-	1/1/15/20	13/37/115/115	-
35	HEM	E	101	5,6	-	2/12/54/54	-
30	SQD	A	616	-	-	18/39/39/69	-
25	CLA	D	403	37	1/1/15/20	14/37/115/115	-
25	CLA	b	604	-	1/1/15/20	9/37/115/115	-
33	STE	a	617	-	-	4/9/9/17	-
33	STE	j	101	-	-	4/9/9/17	-
25	CLA	b	605	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	507	37	1/1/15/20	8/37/115/115	-
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	CLA	a	612	37	1/1/15/20	5/37/115/115	-
25	CLA	b	601	37	1/1/15/20	15/37/115/115	-
29	LMG	M	101	-	-	21/46/66/70	0/1/1/1
33	STE	b	622	-	-	8/17/17/17	-
32	DGD	H	102	-	-	18/51/91/95	0/2/2/2
33	STE	C	520	-	-	5/9/9/17	-
27	BCR	k	101	-	-	11/29/63/63	0/2/2/2
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
28	PL9	d	406	-	-	12/53/73/73	0/1/1/1
36	HEC	V	201	16	-	2/10/54/54	-
31	LHG	A	615	-	-	17/53/53/53	-
25	CLA	c	506	-	1/1/15/20	16/37/115/115	-
27	BCR	A	610	-	-	4/29/63/63	0/2/2/2
25	CLA	B	605	-	1/1/15/20	12/37/115/115	-
28	PL9	a	611	-	-	15/53/73/73	0/1/1/1
31	LHG	D	409	-	-	23/53/53/53	-
33	STE	b	620	-	-	9/17/17/17	-
30	SQD	a	614	-	-	18/37/37/69	-
25	CLA	b	607	37	1/1/15/20	17/37/115/115	-
27	BCR	T	101	-	-	8/29/63/63	0/2/2/2
30	SQD	B	622	-	-	26/49/69/69	0/1/1/1
25	CLA	b	603	-	1/1/15/20	4/37/115/115	-

All (734) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	C4B-NB	8.88	1.43	1.35
25	B	615	CLA	C4B-NB	8.55	1.42	1.35
25	b	604	CLA	C4B-NB	8.30	1.42	1.35
25	c	504	CLA	C4B-NB	8.23	1.42	1.35
25	B	602	CLA	C4B-NB	8.02	1.42	1.35
25	C	503	CLA	C4B-NB	7.91	1.42	1.35
25	C	504	CLA	C4B-NB	7.85	1.42	1.35
25	b	609	CLA	C4B-NB	7.83	1.42	1.35
25	B	614	CLA	C4B-NB	7.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	CLA	C4B-NB	7.75	1.42	1.35
25	c	513	CLA	C4B-NB	7.65	1.42	1.35
25	C	501	CLA	C4B-NB	7.64	1.42	1.35
25	c	511	CLA	C4B-NB	7.61	1.42	1.35
25	B	610	CLA	C4B-NB	7.61	1.42	1.35
25	a	607	CLA	C4B-NB	7.59	1.42	1.35
25	B	601	CLA	C4B-NB	7.57	1.42	1.35
25	c	509	CLA	C4B-NB	7.56	1.42	1.35
25	c	512	CLA	C4B-NB	7.55	1.41	1.35
25	d	404	CLA	C4B-NB	7.53	1.41	1.35
25	B	606	CLA	C4B-NB	7.49	1.41	1.35
25	C	513	CLA	C4B-NB	7.46	1.41	1.35
25	b	608	CLA	C4B-NB	7.43	1.41	1.35
25	D	403	CLA	C4B-NB	7.40	1.41	1.35
25	C	508	CLA	C4B-NB	7.38	1.41	1.35
25	b	605	CLA	C4B-NB	7.36	1.41	1.35
25	c	501	CLA	C4B-NB	7.33	1.41	1.35
25	c	508	CLA	C4B-NB	7.32	1.41	1.35
25	C	510	CLA	C4B-NB	7.28	1.41	1.35
25	c	505	CLA	C4B-NB	7.27	1.41	1.35
25	C	505	CLA	C4B-NB	7.25	1.41	1.35
25	B	608	CLA	C4B-NB	7.25	1.41	1.35
25	C	509	CLA	C4B-NB	7.21	1.41	1.35
25	c	507	CLA	C4B-NB	7.19	1.41	1.35
25	a	609	CLA	C4B-NB	7.17	1.41	1.35
25	b	603	CLA	C4B-NB	7.13	1.41	1.35
25	C	507	CLA	C4B-NB	7.11	1.41	1.35
25	C	511	CLA	C4B-NB	7.10	1.41	1.35
25	b	607	CLA	C4B-NB	7.07	1.41	1.35
25	c	502	CLA	C4B-NB	7.05	1.41	1.35
25	A	607	CLA	C4B-NB	7.05	1.41	1.35
25	b	615	CLA	C4B-NB	7.03	1.41	1.35
25	a	608	CLA	C4B-NB	7.01	1.41	1.35
25	B	613	CLA	C4B-NB	7.01	1.41	1.35
25	c	506	CLA	C4B-NB	7.00	1.41	1.35
25	C	506	CLA	C4B-NB	6.99	1.41	1.35
25	a	612	CLA	C4B-NB	6.96	1.41	1.35
25	c	503	CLA	C4B-NB	6.94	1.41	1.35
25	b	613	CLA	C4B-NB	6.92	1.41	1.35
25	B	611	CLA	C4B-NB	6.89	1.41	1.35
25	B	616	CLA	C4B-NB	6.89	1.41	1.35
25	D	405	CLA	C4B-NB	6.84	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	C4B-NB	6.82	1.41	1.35
25	b	613	CLA	MG-NA	6.80	2.22	2.06
25	B	609	CLA	C4B-NB	6.80	1.41	1.35
25	D	404	CLA	C4B-NB	6.75	1.41	1.35
25	B	605	CLA	C4B-NB	6.74	1.41	1.35
25	b	611	CLA	C4B-NB	6.68	1.41	1.35
25	C	502	CLA	C4B-NB	6.63	1.41	1.35
25	b	602	CLA	C4B-NB	6.61	1.41	1.35
25	A	606	CLA	C4B-NB	6.60	1.41	1.35
36	v	201	HEC	C2B-C3B	-6.57	1.33	1.40
25	A	609	CLA	C4B-NB	6.53	1.41	1.35
25	b	606	CLA	C4B-NB	6.49	1.41	1.35
25	b	616	CLA	C4B-NB	6.46	1.41	1.35
25	B	604	CLA	C4B-NB	6.37	1.40	1.35
25	b	610	CLA	C4B-NB	6.36	1.40	1.35
25	c	510	CLA	C4B-NB	6.34	1.40	1.35
25	B	612	CLA	C4B-NB	6.33	1.40	1.35
25	c	511	CLA	MG-NA	6.31	2.21	2.06
25	B	607	CLA	C4B-NB	6.17	1.40	1.35
36	V	201	HEC	C2B-C3B	-6.14	1.34	1.40
25	b	606	CLA	MG-NA	6.14	2.20	2.06
25	B	603	CLA	C4B-NB	6.11	1.40	1.35
25	C	503	CLA	MG-NA	6.01	2.20	2.06
25	C	505	CLA	MG-NA	6.00	2.20	2.06
25	d	403	CLA	C4B-NB	5.98	1.40	1.35
25	B	601	CLA	MG-NA	5.74	2.19	2.06
25	B	604	CLA	MG-NC	5.62	2.19	2.06
25	b	612	CLA	C4B-NB	5.60	1.40	1.35
25	B	615	CLA	MG-NA	5.46	2.19	2.06
36	v	201	HEC	C3D-C2D	5.30	1.53	1.37
25	D	404	CLA	MG-NA	5.28	2.18	2.06
30	A	616	SQD	O47-C45	-5.26	1.38	1.47
25	b	611	CLA	MG-NA	5.21	2.18	2.06
36	v	201	HEC	C3C-C2C	-5.05	1.35	1.40
25	C	508	CLA	MG-NA	5.05	2.18	2.06
35	E	101	HEM	C3C-C2C	-5.05	1.33	1.40
30	F	101	SQD	O48-C23	4.99	1.47	1.33
25	C	511	CLA	MG-NA	4.96	2.18	2.06
36	V	201	HEC	C3C-C2C	-4.82	1.35	1.40
30	B	622	SQD	O48-C23	4.82	1.47	1.33
30	L	101	SQD	O48-C23	4.78	1.47	1.33
36	V	201	HEC	C3D-C2D	4.78	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	614	SQD	O48-C23	4.75	1.47	1.33
30	A	613	SQD	O48-C23	4.75	1.47	1.33
30	A	616	SQD	O48-C23	4.74	1.47	1.33
25	a	612	CLA	MG-NA	4.72	2.17	2.06
30	f	102	SQD	O48-C23	4.70	1.47	1.33
25	B	614	CLA	MG-NA	4.70	2.17	2.06
25	c	507	CLA	MG-NA	4.69	2.17	2.06
25	b	615	CLA	MG-NA	4.66	2.17	2.06
25	a	607	CLA	C1D-ND	4.63	1.43	1.37
25	C	503	CLA	MG-ND	4.61	2.14	2.05
25	a	607	CLA	MG-NC	4.55	2.17	2.06
30	a	613	SQD	O48-C23	4.55	1.46	1.33
25	b	601	CLA	MG-NA	4.48	2.16	2.06
25	B	606	CLA	MG-NA	4.46	2.16	2.06
25	a	609	CLA	MG-ND	-4.42	1.97	2.05
25	d	403	CLA	C1D-ND	4.37	1.43	1.37
25	B	609	CLA	C1D-ND	4.30	1.43	1.37
25	B	607	CLA	C1D-ND	4.29	1.43	1.37
25	b	612	CLA	MG-ND	-4.24	1.97	2.05
25	a	608	CLA	C1D-ND	4.22	1.43	1.37
25	D	405	CLA	C1D-ND	4.20	1.42	1.37
25	b	613	CLA	C1D-ND	4.14	1.42	1.37
25	a	607	CLA	MG-ND	-4.13	1.97	2.05
25	c	510	CLA	C1D-ND	4.12	1.42	1.37
25	C	513	CLA	C1D-ND	4.12	1.42	1.37
25	C	506	CLA	C1D-ND	4.11	1.42	1.37
25	C	512	CLA	MG-ND	-4.06	1.97	2.05
25	B	601	CLA	C1D-ND	4.06	1.42	1.37
25	b	601	CLA	C1D-ND	4.03	1.42	1.37
25	B	614	CLA	C1D-ND	4.02	1.42	1.37
25	b	612	CLA	C1D-ND	3.97	1.42	1.37
25	c	501	CLA	C1D-ND	3.97	1.42	1.37
25	A	606	CLA	MG-NA	3.95	2.15	2.06
25	A	607	CLA	C1D-ND	3.95	1.42	1.37
25	b	603	CLA	C1D-ND	3.94	1.42	1.37
25	c	513	CLA	C1D-ND	3.94	1.42	1.37
25	A	609	CLA	C1D-ND	3.93	1.42	1.37
25	c	507	CLA	C1D-ND	3.91	1.42	1.37
25	D	404	CLA	C1D-ND	3.91	1.42	1.37
25	a	612	CLA	C1D-ND	3.91	1.42	1.37
30	B	622	SQD	O47-C7	3.89	1.45	1.34
25	c	506	CLA	C1D-ND	3.87	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	503	CLA	C1D-ND	3.86	1.42	1.37
25	b	614	CLA	C1D-ND	3.86	1.42	1.37
25	c	512	CLA	C1D-ND	3.86	1.42	1.37
25	C	512	CLA	MG-NA	3.86	2.15	2.06
25	B	616	CLA	MG-NA	3.83	2.15	2.06
25	C	509	CLA	C1D-ND	3.80	1.42	1.37
25	B	616	CLA	C1D-ND	3.80	1.42	1.37
25	a	607	CLA	MG-NA	3.79	2.15	2.06
25	B	608	CLA	MG-NA	3.78	2.15	2.06
25	B	608	CLA	C1D-ND	3.78	1.42	1.37
25	b	607	CLA	MG-NA	3.77	2.15	2.06
25	b	616	CLA	C1D-ND	3.77	1.42	1.37
25	C	501	CLA	C1D-ND	3.77	1.42	1.37
25	B	606	CLA	C1D-ND	3.76	1.42	1.37
25	c	502	CLA	C1D-ND	3.76	1.42	1.37
30	L	101	SQD	O47-C7	3.76	1.44	1.34
25	b	604	CLA	C4D-ND	-3.76	1.32	1.37
27	b	618	BCR	C30-C25	-3.74	1.48	1.53
25	b	606	CLA	C1D-ND	3.72	1.42	1.37
30	a	614	SQD	O47-C7	3.72	1.44	1.34
25	d	404	CLA	C1D-ND	3.72	1.42	1.37
25	B	613	CLA	MG-ND	-3.71	1.98	2.05
25	D	403	CLA	C1D-ND	3.71	1.42	1.37
25	B	602	CLA	C1D-ND	3.69	1.42	1.37
25	b	602	CLA	C1D-ND	3.68	1.42	1.37
25	C	504	CLA	C1D-ND	3.67	1.42	1.37
25	c	511	CLA	C1D-ND	3.66	1.42	1.37
25	B	611	CLA	C1D-ND	3.66	1.42	1.37
28	d	406	PL9	C3-C4	-3.66	1.43	1.49
25	c	503	CLA	C1D-ND	3.65	1.42	1.37
25	C	509	CLA	MG-NA	3.65	2.14	2.06
25	b	610	CLA	C1D-ND	3.64	1.42	1.37
25	b	608	CLA	C1D-ND	3.64	1.42	1.37
27	T	101	BCR	C1-C6	-3.63	1.48	1.53
25	B	608	CLA	MG-NC	3.63	2.14	2.06
25	c	509	CLA	C1D-ND	3.62	1.42	1.37
25	B	615	CLA	C1D-ND	3.62	1.42	1.37
25	c	508	CLA	MG-NC	3.62	2.14	2.06
25	C	508	CLA	C1D-ND	3.61	1.42	1.37
25	c	508	CLA	C4D-ND	-3.61	1.32	1.37
25	B	611	CLA	CHC-C1C	3.60	1.44	1.35
25	b	604	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	604	CLA	C1D-ND	3.60	1.42	1.37
27	B	618	BCR	C30-C25	-3.58	1.48	1.53
25	B	610	CLA	CHC-C1C	3.58	1.44	1.35
35	f	101	HEM	C3C-CAC	3.58	1.55	1.47
35	f	101	HEM	C3C-C2C	-3.57	1.35	1.40
29	D	408	LMG	C4-C5	3.55	1.60	1.53
30	f	102	SQD	O47-C7	3.55	1.44	1.34
25	B	613	CLA	C4D-ND	-3.55	1.32	1.37
25	b	608	CLA	CHC-C1C	3.54	1.44	1.35
25	B	603	CLA	C4D-ND	-3.54	1.32	1.37
25	c	512	CLA	MG-NA	3.53	2.14	2.06
30	A	616	SQD	O47-C7	3.53	1.44	1.34
27	C	514	BCR	C1-C6	-3.53	1.48	1.53
27	c	515	BCR	C1-C6	-3.51	1.48	1.53
31	D	412	LHG	O7-C5	-3.51	1.37	1.46
25	C	512	CLA	C1D-ND	3.50	1.42	1.37
25	b	605	CLA	C4D-ND	-3.48	1.32	1.37
25	c	504	CLA	CHC-C1C	3.47	1.43	1.35
25	c	508	CLA	C1D-ND	3.47	1.42	1.37
25	b	609	CLA	C1D-ND	3.46	1.42	1.37
25	c	511	CLA	CHC-C1C	3.45	1.43	1.35
25	b	607	CLA	C1D-ND	3.45	1.42	1.37
25	C	509	CLA	CHC-C1C	3.45	1.43	1.35
25	B	614	CLA	MG-ND	-3.44	1.99	2.05
28	A	611	PL9	C7-C3	-3.44	1.47	1.51
25	B	607	CLA	MG-NA	3.44	2.14	2.06
30	A	613	SQD	O47-C45	-3.44	1.38	1.46
25	a	608	CLA	CHC-C1C	3.43	1.43	1.35
25	C	511	CLA	C1D-ND	3.42	1.42	1.37
25	b	601	CLA	CHC-C1C	3.42	1.43	1.35
25	A	606	CLA	C1D-ND	3.42	1.42	1.37
25	c	505	CLA	CHC-C1C	3.42	1.43	1.35
25	C	504	CLA	CHC-C1C	3.41	1.43	1.35
25	B	606	CLA	CHC-C1C	3.41	1.43	1.35
25	b	611	CLA	C1D-ND	3.41	1.42	1.37
25	C	510	CLA	C1D-ND	3.40	1.42	1.37
25	C	507	CLA	C1D-ND	3.39	1.42	1.37
25	C	504	CLA	MG-NA	3.39	2.14	2.06
25	B	603	CLA	CHC-C1C	3.39	1.43	1.35
25	C	502	CLA	C1D-ND	3.37	1.41	1.37
27	c	514	BCR	C1-C6	-3.37	1.49	1.53
30	F	101	SQD	C24-C23	3.37	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	CLA	C4D-ND	-3.36	1.33	1.37
25	B	615	CLA	CHC-C1C	3.35	1.43	1.35
25	B	612	CLA	C4D-ND	-3.35	1.33	1.37
25	C	506	CLA	MG-ND	-3.34	1.99	2.05
32	C	516	DGD	C4D-C3D	3.34	1.60	1.52
30	a	614	SQD	C24-C23	3.34	1.60	1.50
25	C	505	CLA	CHC-C1C	3.34	1.43	1.35
25	B	602	CLA	CHC-C1C	3.33	1.43	1.35
25	b	602	CLA	C4D-ND	-3.33	1.33	1.37
25	c	503	CLA	C4D-ND	-3.33	1.33	1.37
30	a	613	SQD	O47-C45	-3.33	1.38	1.46
25	b	605	CLA	CHC-C1C	3.32	1.43	1.35
25	C	505	CLA	C1D-ND	3.32	1.41	1.37
25	C	510	CLA	CHC-C1C	3.32	1.43	1.35
25	B	612	CLA	C1D-ND	3.31	1.41	1.37
25	B	604	CLA	CHC-C1C	3.31	1.43	1.35
25	B	603	CLA	MG-NA	3.31	2.14	2.06
25	c	505	CLA	C4D-ND	-3.31	1.33	1.37
25	B	612	CLA	CHC-C1C	3.30	1.43	1.35
25	c	508	CLA	CHC-C1C	3.30	1.43	1.35
25	d	404	CLA	CHC-C1C	3.30	1.43	1.35
25	D	403	CLA	CHC-C1C	3.30	1.43	1.35
25	D	404	CLA	C4D-ND	-3.30	1.33	1.37
30	B	622	SQD	O5-C1	3.30	1.50	1.41
25	b	614	CLA	CHC-C1C	3.30	1.43	1.35
25	a	608	CLA	C4D-ND	-3.29	1.33	1.37
25	C	503	CLA	CHC-C1C	3.29	1.43	1.35
25	c	513	CLA	CHC-C1C	3.29	1.43	1.35
25	C	512	CLA	CHC-C1C	3.29	1.43	1.35
30	F	101	SQD	O5-C1	3.29	1.50	1.41
25	A	607	CLA	C4D-ND	-3.28	1.33	1.37
25	c	509	CLA	MG-ND	3.28	2.12	2.05
25	C	502	CLA	CHC-C1C	3.28	1.43	1.35
25	a	607	CLA	CHC-C1C	3.27	1.43	1.35
25	c	503	CLA	CHC-C1C	3.27	1.43	1.35
25	C	513	CLA	CHC-C1C	3.27	1.43	1.35
25	c	506	CLA	CHC-C1C	3.26	1.43	1.35
32	c	517	DGD	O2G-C2G	-3.26	1.38	1.46
25	C	501	CLA	MG-NA	3.25	2.14	2.06
25	b	604	CLA	CHC-C1C	3.25	1.43	1.35
25	b	615	CLA	C1D-ND	3.25	1.41	1.37
25	c	504	CLA	C4D-ND	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	609	CLA	MG-ND	-3.24	1.99	2.05
25	B	603	CLA	MG-ND	3.23	2.12	2.05
27	Y	101	BCR	C1-C6	-3.23	1.49	1.53
25	b	606	CLA	C4D-ND	-3.22	1.33	1.37
25	B	614	CLA	CHC-C1C	3.21	1.43	1.35
25	d	403	CLA	MG-NA	3.21	2.13	2.06
25	b	613	CLA	MG-ND	-3.21	1.99	2.05
25	C	508	CLA	CHC-C1C	3.21	1.43	1.35
25	b	616	CLA	C4D-ND	-3.21	1.33	1.37
25	B	605	CLA	CHC-C1C	3.21	1.43	1.35
25	c	512	CLA	CHC-C1C	3.20	1.43	1.35
25	B	605	CLA	C4D-ND	-3.20	1.33	1.37
30	f	102	SQD	C24-C23	3.19	1.60	1.50
25	C	508	CLA	C4D-ND	-3.19	1.33	1.37
25	b	605	CLA	C1D-ND	3.19	1.41	1.37
30	f	102	SQD	O47-C45	-3.19	1.38	1.46
25	B	614	CLA	C4D-ND	-3.19	1.33	1.37
28	D	407	PL9	C6-C1	-3.19	1.42	1.48
25	A	607	CLA	MG-NA	3.18	2.13	2.06
25	c	501	CLA	C4D-ND	-3.18	1.33	1.37
25	C	502	CLA	MG-ND	-3.18	1.99	2.05
25	C	503	CLA	C4D-ND	-3.17	1.33	1.37
25	C	507	CLA	CHC-C1C	3.17	1.43	1.35
25	A	607	CLA	CHC-C1C	3.17	1.43	1.35
25	B	613	CLA	C1D-ND	3.17	1.41	1.37
30	A	613	SQD	C24-C23	3.16	1.60	1.50
25	C	505	CLA	C4D-ND	-3.16	1.33	1.37
25	d	403	CLA	C4D-ND	-3.16	1.33	1.37
25	B	607	CLA	C4D-ND	-3.16	1.33	1.37
25	c	507	CLA	C4D-ND	-3.15	1.33	1.37
25	B	610	CLA	C1D-ND	3.15	1.41	1.37
25	c	502	CLA	C4D-ND	-3.14	1.33	1.37
25	d	403	CLA	CHC-C1C	3.13	1.43	1.35
27	d	405	BCR	C1-C6	-3.13	1.49	1.53
25	b	610	CLA	MG-NA	3.13	2.13	2.06
25	b	606	CLA	CHC-C1C	3.13	1.43	1.35
25	a	609	CLA	C1D-ND	3.13	1.41	1.37
25	B	607	CLA	CHC-C1C	3.12	1.43	1.35
25	c	501	CLA	CHC-C1C	3.12	1.43	1.35
25	C	506	CLA	CHC-C1C	3.12	1.43	1.35
35	E	101	HEM	C3C-CAC	3.12	1.54	1.47
27	d	405	BCR	C30-C25	-3.12	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	601	CLA	CHC-C1C	3.12	1.43	1.35
25	b	607	CLA	CHC-C1C	3.11	1.42	1.35
25	c	509	CLA	MG-NC	3.11	2.13	2.06
25	A	606	CLA	CHC-C1C	3.10	1.42	1.35
25	c	509	CLA	C4D-ND	-3.10	1.33	1.37
25	B	613	CLA	CHC-C1C	3.10	1.42	1.35
27	D	406	BCR	C1-C6	-3.10	1.49	1.53
25	b	602	CLA	CHC-C1C	3.10	1.42	1.35
25	c	506	CLA	C4D-ND	-3.09	1.33	1.37
25	c	510	CLA	CHC-C1C	3.09	1.42	1.35
25	b	608	CLA	MG-NA	3.09	2.13	2.06
27	D	406	BCR	C30-C25	-3.09	1.49	1.53
25	b	615	CLA	CHC-C1C	3.08	1.42	1.35
25	B	609	CLA	C4D-ND	-3.08	1.33	1.37
25	c	513	CLA	C4D-ND	-3.08	1.33	1.37
25	c	505	CLA	C1D-ND	3.08	1.41	1.37
25	c	503	CLA	MG-NA	3.07	2.13	2.06
25	C	502	CLA	C4D-ND	-3.07	1.33	1.37
25	C	501	CLA	C4D-ND	-3.06	1.33	1.37
30	f	102	SQD	O5-C1	3.06	1.49	1.41
30	B	622	SQD	O47-C45	-3.06	1.38	1.46
25	c	509	CLA	CHC-C1C	3.06	1.42	1.35
25	c	513	CLA	MG-NC	3.04	2.13	2.06
27	b	618	BCR	C1-C6	-3.04	1.49	1.53
30	A	613	SQD	O47-C7	3.04	1.42	1.34
27	c	514	BCR	C30-C25	-3.03	1.49	1.53
25	C	511	CLA	CHC-C1C	3.03	1.42	1.35
30	A	616	SQD	C24-C23	3.03	1.59	1.50
25	B	608	CLA	C4D-ND	-3.03	1.33	1.37
25	D	405	CLA	MG-NA	3.02	2.13	2.06
30	a	613	SQD	O47-C7	3.02	1.42	1.34
27	k	101	BCR	C1-C6	-3.02	1.49	1.53
30	L	101	SQD	O5-C1	3.01	1.49	1.41
32	A	617	DGD	O5D-C6D	-3.01	1.38	1.43
25	c	502	CLA	CHC-C1C	3.01	1.42	1.35
30	B	622	SQD	C24-C23	3.01	1.59	1.50
31	D	410	LHG	P-O6	3.00	1.71	1.59
25	C	501	CLA	CHC-C1C	3.00	1.42	1.35
30	a	613	SQD	C24-C23	3.00	1.59	1.50
27	B	617	BCR	C1-C6	-2.99	1.49	1.53
25	B	615	CLA	C4D-ND	-2.99	1.33	1.37
25	b	611	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	C4D-ND	-2.99	1.33	1.37
27	K	101	BCR	C30-C25	-2.99	1.49	1.53
25	D	403	CLA	C4D-ND	-2.98	1.33	1.37
25	b	603	CLA	MG-NA	2.98	2.13	2.06
25	b	610	CLA	C4D-ND	-2.98	1.33	1.37
25	c	504	CLA	C1D-ND	2.97	1.41	1.37
25	B	610	CLA	CMB-C2B	-2.97	1.45	1.51
25	C	509	CLA	C4D-ND	-2.96	1.33	1.37
25	b	609	CLA	C4D-ND	-2.96	1.33	1.37
26	d	402	PHO	CAC-C3C	-2.95	1.47	1.52
30	a	614	SQD	O47-C45	-2.95	1.39	1.46
25	B	605	CLA	C1D-ND	2.95	1.41	1.37
25	C	507	CLA	MG-ND	-2.94	1.99	2.05
25	B	604	CLA	C4D-ND	-2.94	1.33	1.37
25	B	616	CLA	CHC-C1C	2.92	1.42	1.35
25	c	506	CLA	MG-NC	2.92	2.13	2.06
25	D	404	CLA	CHC-C1C	2.92	1.42	1.35
25	b	616	CLA	CHC-C1C	2.92	1.42	1.35
35	E	101	HEM	CAB-C3B	2.91	1.55	1.47
25	B	602	CLA	C4D-ND	-2.91	1.33	1.37
25	c	504	CLA	MG-ND	-2.91	2.00	2.05
25	C	504	CLA	C4D-ND	-2.90	1.33	1.37
25	C	512	CLA	C4D-ND	-2.90	1.33	1.37
31	d	407	LHG	O7-C5	-2.90	1.39	1.46
27	B	619	BCR	C1-C6	-2.89	1.49	1.53
25	b	603	CLA	C4D-ND	-2.89	1.33	1.37
25	b	609	CLA	CMB-C2B	-2.88	1.45	1.51
30	L	101	SQD	O47-C45	-2.88	1.39	1.46
25	b	609	CLA	CHC-C1C	2.87	1.42	1.35
25	a	607	CLA	C4D-ND	-2.87	1.33	1.37
32	a	615	DGD	O1G-C1A	2.86	1.41	1.33
27	H	101	BCR	C30-C25	-2.86	1.49	1.53
25	c	511	CLA	C4D-ND	-2.85	1.33	1.37
25	C	513	CLA	C4D-ND	-2.85	1.33	1.37
32	H	102	DGD	O5D-C1E	2.85	1.45	1.40
32	c	519	DGD	C6D-C5D	2.85	1.60	1.51
25	a	609	CLA	CHC-C1C	2.85	1.42	1.35
32	C	515	DGD	O2G-C2G	-2.85	1.39	1.46
27	K	102	BCR	C30-C25	-2.85	1.49	1.53
27	b	619	BCR	C1-C6	-2.84	1.49	1.53
30	L	101	SQD	C24-C23	2.84	1.59	1.50
25	c	510	CLA	C4D-ND	-2.83	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	CHC-C1C	2.83	1.42	1.35
25	d	404	CLA	C4D-ND	-2.83	1.33	1.37
25	b	603	CLA	CHC-C1C	2.83	1.42	1.35
27	b	619	BCR	C30-C25	-2.82	1.49	1.53
25	c	510	CLA	MG-NC	2.82	2.13	2.06
25	C	510	CLA	MG-NA	2.82	2.13	2.06
25	C	507	CLA	MG-NA	2.81	2.13	2.06
25	B	606	CLA	C4D-ND	-2.80	1.33	1.37
25	B	609	CLA	CHC-C1C	2.80	1.42	1.35
25	D	405	CLA	CHC-C1C	2.80	1.42	1.35
25	B	611	CLA	C4D-ND	-2.80	1.33	1.37
30	A	613	SQD	O5-C1	2.79	1.49	1.41
27	c	516	BCR	C1-C6	-2.79	1.49	1.53
29	m	101	LMG	C4-C3	2.79	1.59	1.52
25	B	605	CLA	MG-NA	2.76	2.12	2.06
25	B	608	CLA	CHC-C1C	2.76	1.42	1.35
25	B	613	CLA	MG-NA	2.76	2.12	2.06
25	C	510	CLA	C4D-ND	-2.75	1.33	1.37
27	x	101	BCR	C30-C25	-2.75	1.50	1.53
27	K	101	BCR	C1-C6	-2.75	1.50	1.53
25	b	613	CLA	CMB-C2B	-2.75	1.45	1.51
25	C	513	CLA	MG-NA	2.75	2.12	2.06
25	A	609	CLA	CHC-C1C	2.74	1.42	1.35
25	B	607	CLA	C1B-NB	2.73	1.37	1.35
25	D	405	CLA	C4D-ND	-2.73	1.33	1.37
32	A	617	DGD	C1E-C2E	2.73	1.60	1.52
25	a	608	CLA	MG-ND	-2.72	2.00	2.05
25	b	612	CLA	CHC-C1C	2.72	1.41	1.35
27	k	101	BCR	C30-C25	-2.72	1.50	1.53
27	b	617	BCR	C1-C6	-2.71	1.50	1.53
25	b	615	CLA	CMB-C2B	-2.71	1.46	1.51
27	A	610	BCR	C1-C6	-2.71	1.50	1.53
25	b	612	CLA	C4D-ND	-2.71	1.34	1.37
25	a	609	CLA	C4D-ND	-2.70	1.34	1.37
25	d	403	CLA	CMB-C2B	-2.70	1.46	1.51
26	D	402	PHO	CAC-C3C	-2.70	1.47	1.52
25	a	612	CLA	CHC-C1C	2.69	1.41	1.35
25	c	510	CLA	CMB-C2B	-2.69	1.46	1.51
25	C	506	CLA	MG-NA	2.69	2.12	2.06
27	c	516	BCR	C30-C25	-2.68	1.50	1.53
25	a	607	CLA	CMB-C2B	-2.68	1.46	1.51
28	D	407	PL9	C52-C5	-2.68	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	607	CLA	C4D-ND	-2.66	1.34	1.37
32	h	101	DGD	C1E-C2E	2.66	1.60	1.52
25	a	612	CLA	C4D-ND	-2.66	1.34	1.37
25	C	502	CLA	MG-NA	2.66	2.12	2.06
29	c	524	LMG	C4-C5	2.66	1.58	1.53
27	c	515	BCR	C30-C25	-2.65	1.50	1.53
25	B	612	CLA	MG-NA	2.65	2.12	2.06
25	A	606	CLA	C4D-ND	-2.65	1.34	1.37
29	b	621	LMG	C3-C2	2.64	1.59	1.52
25	b	613	CLA	CHC-C1C	2.64	1.41	1.35
25	C	511	CLA	C4D-ND	-2.64	1.34	1.37
25	B	603	CLA	C1D-ND	2.63	1.41	1.37
29	d	411	LMG	C4-C5	2.63	1.58	1.53
25	c	512	CLA	C4D-ND	-2.63	1.34	1.37
25	B	601	CLA	CMB-C2B	-2.62	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.62	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.61	1.46	1.51
35	f	101	HEM	FE-NB	2.61	2.09	1.96
25	b	615	CLA	C4D-ND	-2.60	1.34	1.37
32	A	617	DGD	C3E-C2E	2.60	1.58	1.52
25	C	506	CLA	C4D-ND	-2.60	1.34	1.37
35	f	101	HEM	CAB-C3B	2.60	1.54	1.47
31	d	409	LHG	P-O6	2.59	1.69	1.59
31	D	412	LHG	C24-C23	2.59	1.58	1.50
25	D	405	CLA	MG-NC	2.59	2.12	2.06
27	Y	101	BCR	C30-C25	-2.58	1.50	1.53
32	h	101	DGD	O2G-C2G	-2.57	1.40	1.46
25	b	614	CLA	MG-ND	-2.57	2.00	2.05
27	K	102	BCR	C1-C6	-2.57	1.50	1.53
32	A	617	DGD	C4D-C5D	2.57	1.58	1.53
25	B	610	CLA	C3B-C2B	-2.57	1.36	1.40
25	c	510	CLA	MG-NA	2.57	2.12	2.06
30	A	616	SQD	C46-C45	2.56	1.56	1.50
25	B	610	CLA	C4D-ND	-2.56	1.34	1.37
25	c	513	CLA	MG-ND	-2.56	2.00	2.05
25	A	609	CLA	MG-ND	-2.55	2.00	2.05
25	B	606	CLA	C3B-C2B	-2.54	1.36	1.40
30	a	613	SQD	O5-C1	2.54	1.48	1.41
31	A	614	LHG	P-O6	2.54	1.69	1.59
25	b	608	CLA	C4D-ND	-2.53	1.34	1.37
25	c	510	CLA	MG-ND	-2.52	2.00	2.05
28	a	611	PL9	C53-C6	-2.52	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	CHC-C1C	2.52	1.41	1.35
32	C	516	DGD	C1E-C2E	2.52	1.59	1.52
25	a	608	CLA	CMB-C2B	-2.51	1.46	1.51
25	b	601	CLA	C4D-ND	-2.51	1.34	1.37
25	B	606	CLA	CMB-C2B	-2.51	1.46	1.51
27	a	610	BCR	C1-C6	-2.50	1.50	1.53
25	a	612	CLA	CMB-C2B	-2.50	1.46	1.51
25	c	501	CLA	CMB-C2B	-2.49	1.46	1.51
27	T	101	BCR	C30-C25	-2.49	1.50	1.53
31	D	409	LHG	P-O6	2.49	1.69	1.59
25	B	616	CLA	C4D-ND	-2.48	1.34	1.37
25	B	603	CLA	CMC-C2C	-2.48	1.45	1.50
32	C	515	DGD	C4D-C3D	2.47	1.58	1.52
32	A	617	DGD	C6E-C5E	2.46	1.60	1.51
25	D	405	CLA	CMB-C2B	-2.46	1.46	1.51
27	B	617	BCR	C30-C25	-2.46	1.50	1.53
32	H	102	DGD	O1G-C1G	-2.46	1.39	1.45
25	b	603	CLA	CMB-C2B	-2.46	1.46	1.51
25	C	507	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	608	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.44	1.46	1.51
31	e	101	LHG	P-O6	2.44	1.69	1.59
25	c	512	CLA	CMB-C2B	-2.44	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.44	1.46	1.51
32	C	516	DGD	C1G-C2G	2.44	1.58	1.50
32	c	518	DGD	C4D-C3D	2.43	1.58	1.52
25	d	404	CLA	CMB-C2B	-2.42	1.46	1.51
25	c	507	CLA	C3B-C2B	-2.42	1.37	1.40
25	c	513	CLA	CMB-C2B	-2.42	1.46	1.51
25	b	614	CLA	MG-NA	2.41	2.12	2.06
25	C	509	CLA	CMB-C2B	-2.41	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.41	1.46	1.51
25	C	508	CLA	C1B-NB	2.41	1.37	1.35
25	D	403	CLA	C1D-C2D	2.39	1.50	1.45
29	M	101	LMG	C4-C5	2.39	1.58	1.53
32	H	102	DGD	C4D-C5D	2.39	1.58	1.53
25	c	507	CLA	C3B-CAB	-2.39	1.43	1.47
25	b	616	CLA	CMB-C2B	-2.39	1.46	1.51
32	c	519	DGD	O2G-C2G	-2.39	1.40	1.46
29	D	411	LMG	C7-C8	2.39	1.57	1.51
25	b	615	CLA	MG-ND	-2.39	2.01	2.05
27	b	617	BCR	C30-C25	-2.38	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	CMB-C2B	-2.38	1.46	1.51
27	C	514	BCR	C30-C25	-2.38	1.50	1.53
25	c	510	CLA	CMD-C2D	-2.38	1.45	1.50
32	C	515	DGD	C4E-C3E	2.37	1.58	1.52
32	c	518	DGD	C3D-C2D	2.37	1.58	1.52
29	m	101	LMG	O7-C8	-2.37	1.40	1.46
25	b	604	CLA	CMB-C2B	-2.37	1.46	1.51
30	L	101	SQD	C6-S	2.37	1.86	1.77
25	b	612	CLA	CMB-C2B	-2.36	1.46	1.51
30	F	101	SQD	O5-C5	2.36	1.50	1.44
25	B	606	CLA	C3B-CAB	-2.36	1.43	1.47
25	C	501	CLA	CMB-C2B	-2.36	1.46	1.51
25	b	615	CLA	CMD-C2D	-2.36	1.45	1.50
25	c	506	CLA	MG-ND	-2.35	2.01	2.05
30	a	613	SQD	O7-S	2.35	1.52	1.45
25	b	608	CLA	CMB-C2B	-2.35	1.46	1.51
25	a	609	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.35	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.35	1.46	1.51
26	d	402	PHO	CMC-C2C	-2.34	1.46	1.51
30	B	622	SQD	O9-S	2.33	1.51	1.45
28	a	611	PL9	C7-C3	-2.33	1.48	1.51
30	A	613	SQD	O9-S	2.33	1.51	1.45
25	C	502	CLA	CMB-C2B	-2.33	1.46	1.51
25	b	601	CLA	CMB-C2B	-2.32	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.32	1.46	1.51
28	d	406	PL9	C46-C44	-2.32	1.46	1.51
25	D	405	CLA	CMC-C2C	-2.32	1.45	1.50
26	d	401	PHO	O2D-CGD	2.32	1.38	1.33
25	B	603	CLA	CMD-C2D	-2.32	1.45	1.50
25	b	611	CLA	C4D-ND	-2.31	1.34	1.37
27	t	101	BCR	C1-C6	-2.31	1.50	1.53
30	F	101	SQD	O7-S	2.31	1.51	1.45
26	A	608	PHO	CAC-C3C	-2.31	1.48	1.52
25	b	613	CLA	C4D-ND	-2.30	1.34	1.37
25	c	504	CLA	CMB-C2B	-2.30	1.46	1.51
25	B	616	CLA	MG-NC	2.30	2.11	2.06
25	c	503	CLA	CMB-C2B	-2.30	1.46	1.51
29	c	522	LMG	C3-C2	2.30	1.58	1.52
25	b	612	CLA	MG-NC	2.29	2.11	2.06
30	F	101	SQD	O9-S	2.29	1.51	1.45
25	b	607	CLA	CMD-C2D	-2.29	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	614	CLA	CMC-C2C	-2.29	1.45	1.50
25	D	404	CLA	CMB-C2B	-2.29	1.46	1.51
25	a	609	CLA	CMC-C2C	-2.28	1.46	1.50
29	c	522	LMG	C4-C3	2.28	1.58	1.52
25	b	604	CLA	MG-NC	2.28	2.11	2.06
31	A	615	LHG	O8-C23	2.28	1.40	1.33
25	B	608	CLA	C1D-C2D	2.27	1.49	1.45
32	c	517	DGD	C4D-C3D	2.27	1.58	1.52
28	d	406	PL9	C6-C1	-2.27	1.44	1.48
30	L	101	SQD	O9-S	2.27	1.51	1.45
25	D	404	CLA	CMD-C2D	-2.27	1.46	1.50
32	H	102	DGD	C1E-C2E	2.27	1.59	1.52
29	D	408	LMG	O2-C2	-2.26	1.37	1.43
25	b	610	CLA	CMB-C2B	-2.26	1.46	1.51
25	C	505	CLA	C1B-NB	2.26	1.37	1.35
25	B	604	CLA	MG-NA	2.26	2.11	2.06
25	B	616	CLA	CMC-C2C	-2.26	1.46	1.50
30	f	102	SQD	O9-S	2.26	1.51	1.45
25	B	601	CLA	CMC-C2C	-2.25	1.46	1.50
25	c	508	CLA	CMB-C2B	-2.25	1.47	1.51
25	B	604	CLA	CMB-C2B	-2.25	1.47	1.51
35	f	101	HEM	C3B-C2B	-2.25	1.32	1.37
25	c	512	CLA	C3B-C2B	-2.24	1.37	1.40
25	b	607	CLA	C3B-C2B	-2.24	1.37	1.40
25	B	609	CLA	CMD-C2D	-2.24	1.46	1.50
25	b	605	CLA	CMB-C2B	-2.24	1.47	1.51
25	b	609	CLA	MG-NA	2.24	2.11	2.06
25	C	503	CLA	CMB-C2B	-2.24	1.47	1.51
25	b	611	CLA	CMB-C2B	-2.24	1.47	1.51
25	B	615	CLA	CMB-C2B	-2.24	1.47	1.51
25	C	502	CLA	C3B-C2B	-2.24	1.37	1.40
29	A	612	LMG	C4-C5	2.23	1.57	1.53
25	b	610	CLA	C3B-C2B	-2.23	1.37	1.40
32	c	518	DGD	O6D-C5D	-2.23	1.38	1.44
29	b	621	LMG	C1-C2	2.23	1.58	1.52
25	b	611	CLA	CMD-C2D	-2.23	1.46	1.50
25	b	608	CLA	C3C-C2C	2.23	1.41	1.36
25	b	603	CLA	CMD-C2D	-2.22	1.46	1.50
32	h	101	DGD	C4D-C3D	2.22	1.58	1.52
27	B	618	BCR	C1-C6	-2.22	1.50	1.53
25	C	513	CLA	CMB-C2B	-2.22	1.47	1.51
28	d	406	PL9	C41-C39	-2.22	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	608	PHO	CMC-C2C	-2.22	1.46	1.51
25	B	601	CLA	C3B-C2B	-2.22	1.37	1.40
25	B	605	CLA	C3B-C2B	-2.22	1.37	1.40
25	B	608	CLA	CMD-C2D	-2.21	1.46	1.50
25	B	611	CLA	CMB-C2B	-2.21	1.47	1.51
26	D	402	PHO	CMC-C2C	-2.21	1.46	1.51
30	f	102	SQD	O5-C5	2.20	1.49	1.44
25	C	509	CLA	O2D-CGD	2.20	1.38	1.33
32	C	517	DGD	C6D-C5D	2.20	1.58	1.51
30	a	613	SQD	C6-S	2.19	1.85	1.77
25	c	508	CLA	MG-ND	2.19	2.10	2.05
30	B	622	SQD	O7-S	2.19	1.51	1.45
32	c	519	DGD	O1G-C1G	-2.19	1.40	1.45
25	c	504	CLA	CMD-C2D	-2.18	1.46	1.50
25	b	613	CLA	CMD-C2D	-2.18	1.46	1.50
30	B	622	SQD	C8-C7	2.18	1.57	1.50
25	c	503	CLA	CMC-C2C	-2.18	1.46	1.50
25	c	512	CLA	C1D-C2D	2.18	1.49	1.45
25	C	510	CLA	MG-NC	2.18	2.11	2.06
30	f	102	SQD	O7-S	2.17	1.51	1.45
29	c	524	LMG	C1-C2	2.17	1.58	1.52
32	c	517	DGD	C4D-C5D	2.16	1.57	1.53
25	B	613	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	616	CLA	CMC-C2C	-2.16	1.46	1.50
25	b	614	CLA	CMB-C2B	-2.16	1.47	1.51
29	c	522	LMG	C1-C2	2.16	1.58	1.52
25	C	513	CLA	CMC-C2C	-2.16	1.46	1.50
25	A	606	CLA	MG-ND	-2.15	2.01	2.05
25	b	606	CLA	C1B-NB	2.15	1.37	1.35
30	B	622	SQD	C6-S	2.15	1.85	1.77
25	C	508	CLA	CMB-C2B	-2.15	1.47	1.51
25	C	504	CLA	CMB-C2B	-2.14	1.47	1.51
25	c	506	CLA	CMB-C2B	-2.14	1.47	1.51
32	A	617	DGD	C4E-C5E	2.14	1.57	1.53
25	d	403	CLA	CMD-C2D	-2.14	1.46	1.50
25	d	404	CLA	MG-NA	2.14	2.11	2.06
25	c	502	CLA	CMD-C2D	-2.14	1.46	1.50
25	c	506	CLA	CMC-C2C	-2.14	1.46	1.50
25	C	503	CLA	MG-NC	2.14	2.11	2.06
26	D	402	PHO	CMB-C2B	-2.14	1.46	1.51
32	a	615	DGD	C1G-C2G	2.13	1.57	1.50
25	B	601	CLA	C4D-ND	-2.13	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	614	CLA	C3B-CAB	-2.12	1.43	1.47
29	D	408	LMG	C7-C8	2.12	1.57	1.50
25	D	403	CLA	MG-NC	2.12	2.11	2.06
25	B	611	CLA	CMD-C2D	-2.12	1.46	1.50
25	A	607	CLA	CMB-C2B	-2.11	1.47	1.51
32	C	516	DGD	O3D-C3D	-2.11	1.38	1.43
30	a	614	SQD	C46-C45	2.11	1.57	1.50
25	c	511	CLA	CMB-C2B	-2.11	1.47	1.51
25	B	616	CLA	CMB-C2B	-2.10	1.47	1.51
32	H	102	DGD	O2D-C2D	-2.10	1.38	1.43
25	C	508	CLA	C1D-C2D	2.10	1.49	1.45
29	d	411	LMG	O1-C7	-2.10	1.39	1.43
25	C	512	CLA	C1D-C2D	2.10	1.49	1.45
31	A	615	LHG	O7-C5	-2.09	1.41	1.46
26	d	401	PHO	CAC-C3C	-2.09	1.48	1.52
25	a	609	CLA	CMD-C2D	-2.09	1.46	1.50
29	A	612	LMG	C4-C3	2.09	1.57	1.52
32	C	516	DGD	C4D-C5D	2.09	1.57	1.53
25	A	607	CLA	C3B-C2B	-2.09	1.37	1.40
25	C	512	CLA	CMD-C2D	-2.09	1.46	1.50
25	A	609	CLA	MG-NA	-2.09	2.01	2.06
25	c	504	CLA	CMC-C2C	-2.08	1.46	1.50
26	d	402	PHO	CMD-C2D	-2.08	1.46	1.51
32	C	517	DGD	O1G-C1G	-2.08	1.40	1.45
30	L	101	SQD	O7-S	2.08	1.51	1.45
25	B	607	CLA	CMB-C2B	-2.08	1.47	1.51
27	x	101	BCR	C1-C6	-2.08	1.50	1.53
31	d	407	LHG	C24-C23	2.08	1.56	1.50
32	C	515	DGD	C3E-C2E	2.08	1.57	1.52
25	B	615	CLA	C3B-CAB	-2.08	1.43	1.47
25	b	615	CLA	C3B-C2B	-2.08	1.37	1.40
25	B	607	CLA	CMC-C2C	-2.08	1.46	1.50
32	c	518	DGD	O2G-C2G	-2.07	1.41	1.46
25	a	609	CLA	C4B-CHC	-2.07	1.35	1.41
25	c	508	CLA	CMD-C2D	-2.07	1.46	1.50
29	C	518	LMG	O7-C8	-2.07	1.41	1.46
26	D	402	PHO	CMD-C2D	-2.07	1.46	1.51
25	b	612	CLA	CMC-C2C	-2.07	1.46	1.50
25	B	605	CLA	CMB-C2B	-2.07	1.47	1.51
25	B	607	CLA	C3D-C4D	2.07	1.48	1.44
25	c	501	CLA	MG-NC	2.07	2.11	2.06
26	A	608	PHO	CMD-C2D	-2.06	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	O2G-C2G	-2.05	1.41	1.46
25	A	609	CLA	CMB-C2B	-2.05	1.47	1.51
30	L	101	SQD	C44-C45	2.05	1.57	1.50
27	a	610	BCR	C30-C25	-2.05	1.50	1.53
25	b	601	CLA	C3D-C4D	2.05	1.48	1.44
25	C	506	CLA	CMC-C2C	-2.05	1.46	1.50
30	a	614	SQD	C44-C45	2.05	1.56	1.51
27	B	617	BCR	C33-C5	-2.05	1.47	1.50
25	B	604	CLA	CMD-C2D	-2.05	1.46	1.50
29	m	101	LMG	O1-C7	-2.04	1.40	1.43
25	B	609	CLA	O2D-CGD	2.04	1.38	1.33
31	A	615	LHG	P-O6	2.04	1.67	1.59
27	k	101	BCR	C33-C5	-2.04	1.47	1.50
25	B	612	CLA	CMC-C2C	-2.04	1.46	1.50
32	A	617	DGD	C3G-C2G	2.04	1.57	1.50
25	C	510	CLA	CMB-C2B	-2.04	1.47	1.51
31	l	101	LHG	P-O6	2.04	1.67	1.59
27	H	101	BCR	C1-C6	-2.04	1.51	1.53
25	b	606	CLA	MG-ND	2.03	2.09	2.05
25	B	601	CLA	MG-ND	-2.03	2.01	2.05
32	C	515	DGD	O3E-C3E	-2.03	1.38	1.43
25	c	508	CLA	CMC-C2C	-2.03	1.46	1.50
25	b	609	CLA	CMD-C2D	-2.03	1.46	1.50
32	C	515	DGD	O2E-C2E	-2.03	1.38	1.43
25	C	506	CLA	CMB-C2B	-2.03	1.47	1.51
35	E	101	HEM	CMD-C2D	2.03	1.55	1.50
25	a	607	CLA	C3D-C4D	2.03	1.48	1.44
25	B	605	CLA	CMC-C2C	-2.02	1.46	1.50
25	B	604	CLA	C3C-C2C	2.02	1.41	1.36
25	A	609	CLA	CMD-C2D	-2.02	1.46	1.50
25	c	502	CLA	C4B-CHC	-2.02	1.35	1.41
30	a	614	SQD	C25-C24	2.02	1.59	1.52
25	b	616	CLA	CMD-C2D	-2.02	1.46	1.50
25	c	506	CLA	CMD-C2D	-2.02	1.46	1.50
35	f	101	HEM	CAA-C2A	2.02	1.55	1.52
32	h	101	DGD	O2E-C2E	-2.02	1.38	1.43
25	b	610	CLA	C3D-C4D	2.02	1.48	1.44
25	b	601	CLA	C1B-NB	2.02	1.37	1.35
30	a	613	SQD	O9-S	2.02	1.51	1.45
25	d	404	CLA	O2D-CGD	2.01	1.38	1.33
25	B	602	CLA	C1D-C2D	2.01	1.49	1.45
25	b	608	CLA	C1D-C2D	2.01	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	617	DGD	C4D-C3D	2.01	1.57	1.52
25	a	608	CLA	CMC-C2C	-2.01	1.46	1.50
31	d	408	LHG	O7-C5	-2.01	1.41	1.46
25	b	603	CLA	C3B-CAB	-2.01	1.43	1.47
25	b	606	CLA	CMB-C2B	-2.01	1.47	1.51
25	C	507	CLA	MG-NC	2.01	2.11	2.06
25	c	501	CLA	C1D-C2D	2.01	1.49	1.45
25	c	505	CLA	CMB-C2B	-2.00	1.47	1.51
30	a	613	SQD	C46-C45	2.00	1.56	1.50
25	C	507	CLA	C4D-ND	-2.00	1.34	1.37
25	C	502	CLA	C3D-C4D	2.00	1.48	1.44

All (1181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	511	CLA	C4A-NA-C1A	10.20	111.29	106.71
25	c	509	CLA	C4A-NA-C1A	9.60	111.02	106.71
25	c	503	CLA	C4A-NA-C1A	8.97	110.74	106.71
25	B	604	CLA	C4A-NA-C1A	8.95	110.73	106.71
25	b	601	CLA	C4A-NA-C1A	8.26	110.42	106.71
25	b	606	CLA	C4A-NA-C1A	8.17	110.38	106.71
25	C	513	CLA	C4A-NA-C1A	8.05	110.33	106.71
25	b	604	CLA	C4A-NA-C1A	7.88	110.25	106.71
25	C	507	CLA	C4A-NA-C1A	7.74	110.18	106.71
25	B	601	CLA	C4A-NA-C1A	7.62	110.13	106.71
25	C	503	CLA	C4A-NA-C1A	7.39	110.03	106.71
25	B	616	CLA	C4A-NA-C1A	7.37	110.02	106.71
25	B	607	CLA	C4A-NA-C1A	7.34	110.01	106.71
25	C	511	CLA	C4A-NA-C1A	7.21	109.95	106.71
25	B	615	CLA	C4A-NA-C1A	7.18	109.93	106.71
25	C	501	CLA	C4A-NA-C1A	7.18	109.93	106.71
25	C	508	CLA	C4A-NA-C1A	6.96	109.83	106.71
25	b	611	CLA	C4A-NA-C1A	6.93	109.82	106.71
30	L	101	SQD	O6-C1-C2	6.83	118.97	108.30
25	D	405	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	c	501	CLA	C4A-NA-C1A	6.70	109.72	106.71
25	c	506	CLA	C4A-NA-C1A	6.60	109.67	106.71
30	a	613	SQD	O6-C1-C2	6.53	118.50	108.30
25	c	510	CLA	C4A-NA-C1A	6.50	109.63	106.71
25	C	505	CLA	C4A-NA-C1A	6.49	109.62	106.71
30	a	613	SQD	C1-O5-C5	-6.27	101.38	113.69
25	B	608	CLA	C4A-NA-C1A	6.19	109.49	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	506	CLA	C4A-NA-C1A	6.17	109.48	106.71
25	c	508	CLA	C4A-NA-C1A	6.13	109.46	106.71
25	B	606	CLA	C4A-NA-C1A	6.01	109.41	106.71
25	c	512	CLA	C4A-NA-C1A	6.00	109.41	106.71
30	A	613	SQD	O6-C1-C2	5.95	117.59	108.30
25	c	507	CLA	C4A-NA-C1A	5.94	109.38	106.71
25	C	509	CLA	C4A-NA-C1A	5.92	109.37	106.71
25	b	615	CLA	C4A-NA-C1A	5.77	109.30	106.71
25	D	404	CLA	C4A-NA-C1A	5.74	109.29	106.71
25	b	607	CLA	C4A-NA-C1A	5.74	109.29	106.71
25	c	504	CLA	C4A-NA-C1A	5.67	109.25	106.71
25	c	505	CLA	C4A-NA-C1A	5.64	109.24	106.71
25	a	612	CLA	C4A-NA-C1A	5.64	109.24	106.71
25	B	609	CLA	C4A-NA-C1A	5.62	109.23	106.71
28	a	611	PL9	C7-C3-C4	5.60	121.43	116.88
25	b	608	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	C	512	CLA	C4A-NA-C1A	5.50	109.18	106.71
28	D	407	PL9	C7-C3-C4	5.49	121.34	116.88
25	b	616	CLA	C4A-NA-C1A	5.45	109.16	106.71
36	V	201	HEC	CBD-CAD-C3D	-5.43	103.35	112.62
30	F	101	SQD	O9-S-C6	5.42	113.39	106.94
25	c	502	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	b	616	CLA	CMB-C2B-C1B	-5.32	120.28	128.46
30	A	613	SQD	C1-O5-C5	-5.26	103.36	113.69
25	c	513	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	B	605	CLA	C4A-NA-C1A	5.22	109.06	106.71
25	C	510	CLA	C4A-NA-C1A	5.20	109.04	106.71
25	D	405	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
30	L	101	SQD	O7-S-C6	5.15	113.06	106.94
25	B	602	CLA	C4A-NA-C1A	5.14	109.02	106.71
25	c	504	CLA	CMB-C2B-C1B	-5.13	120.57	128.46
30	B	622	SQD	O7-S-C6	5.10	113.00	106.94
25	d	404	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
25	a	607	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	b	613	CLA	C4A-NA-C1A	5.01	108.96	106.71
25	B	608	CLA	CMB-C2B-C1B	-5.01	120.77	128.46
25	b	603	CLA	C4A-NA-C1A	5.00	108.95	106.71
25	b	604	CLA	C1-C2-C3	-4.96	117.46	126.04
25	B	602	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
25	B	613	CLA	C1-C2-C3	-4.90	117.57	126.04
25	A	609	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
30	f	102	SQD	O7-S-C6	4.77	112.61	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	611	PL9	C7-C3-C4	4.74	120.73	116.88
25	B	612	CLA	C4A-NA-C1A	4.71	108.83	106.71
25	a	608	CLA	C4A-NA-C1A	4.71	108.82	106.71
25	C	509	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
25	b	609	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
25	B	608	CLA	O2D-CGD-O1D	-4.67	114.71	123.84
25	c	513	CLA	CMB-C2B-C1B	-4.65	121.31	128.46
30	F	101	SQD	C1-O5-C5	-4.60	104.66	113.69
30	a	614	SQD	O47-C7-C8	4.58	121.38	111.50
25	B	610	CLA	C4A-NA-C1A	4.58	108.77	106.71
30	B	622	SQD	O47-C7-C8	4.58	121.37	111.50
25	b	616	CLA	CMB-C2B-C3B	4.58	133.24	124.68
30	A	613	SQD	C1-C2-C3	-4.54	100.54	110.00
25	c	510	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
25	B	614	CLA	C4A-NA-C1A	4.52	108.74	106.71
25	B	612	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
25	B	611	CLA	C4A-NA-C1A	4.47	108.72	106.71
25	d	404	CLA	CMB-C2B-C3B	4.47	133.04	124.68
25	B	613	CLA	CMB-C2B-C1B	-4.46	121.60	128.46
28	d	406	PL9	C7-C3-C4	4.45	120.50	116.88
25	d	403	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
25	b	613	CLA	CMB-C2B-C1B	-4.44	121.63	128.46
25	B	610	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
25	D	405	CLA	CMB-C2B-C3B	4.41	132.94	124.68
26	D	402	PHO	C1-C2-C3	-4.40	118.43	126.04
25	d	403	CLA	C4A-NA-C1A	4.39	108.68	106.71
25	b	608	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
30	a	613	SQD	O7-S-C6	4.36	112.12	106.94
31	A	615	LHG	O4-P-O5	4.35	133.76	112.24
25	C	510	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
25	A	609	CLA	CMB-C2B-C3B	4.35	132.81	124.68
25	B	602	CLA	CMB-C2B-C3B	4.35	132.81	124.68
25	b	606	CLA	O2D-CGD-O1D	-4.33	115.38	123.84
30	L	101	SQD	O47-C7-C8	4.33	120.82	111.50
27	K	101	BCR	C11-C10-C9	-4.32	121.14	127.31
25	B	612	CLA	CMB-C2B-C3B	4.30	132.73	124.68
25	b	605	CLA	C4A-NA-C1A	4.30	108.64	106.71
26	d	402	PHO	C1-C2-C3	-4.30	118.60	126.04
25	b	606	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
25	c	506	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
25	C	502	CLA	C4A-NA-C1A	4.27	108.63	106.71
30	A	613	SQD	O47-C7-C8	4.27	120.70	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	612	CLA	C4A-NA-C1A	4.26	108.62	106.71
25	b	603	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
25	b	603	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
25	c	504	CLA	CMB-C2B-C3B	4.23	132.60	124.68
25	C	504	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
25	c	501	CLA	O2D-CGD-O1D	-4.22	115.58	123.84
31	e	101	LHG	O4-P-O5	4.21	133.03	112.24
31	D	412	LHG	O4-P-O5	4.18	132.92	112.24
25	C	509	CLA	CMB-C2B-C3B	4.17	132.49	124.68
32	c	518	DGD	O3G-C3G-C2G	-4.17	100.83	110.90
25	B	611	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
25	C	504	CLA	C4A-NA-C1A	4.17	108.58	106.71
32	H	102	DGD	O3G-C3G-C2G	-4.17	100.85	110.90
25	B	604	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
31	A	614	LHG	O4-P-O5	4.15	132.76	112.24
32	a	615	DGD	O3G-C3G-C2G	-4.14	100.80	111.78
25	B	603	CLA	C4A-NA-C1A	4.13	108.56	106.71
25	C	508	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
31	d	408	LHG	O4-P-O5	4.12	132.61	112.24
31	D	409	LHG	O4-P-O5	4.12	132.59	112.24
25	b	602	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
30	A	613	SQD	O8-S-C6	4.11	112.28	105.74
25	B	613	CLA	C4A-NA-C1A	4.09	108.55	106.71
31	d	407	LHG	O4-P-O5	4.07	132.37	112.24
25	b	611	CLA	O2D-CGD-O1D	-4.06	115.90	123.84
25	a	607	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
25	b	605	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
25	A	606	CLA	C4A-NA-C1A	4.04	108.52	106.71
25	b	607	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
30	B	622	SQD	O9-S-O7	-4.03	100.00	113.95
36	V	201	HEC	CMC-C2C-C1C	-4.03	122.28	128.46
25	b	614	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
31	D	410	LHG	O4-P-O5	3.99	131.98	112.24
25	B	608	CLA	O2D-CGD-CBD	3.98	118.35	111.27
31	d	409	LHG	O4-P-O5	3.98	131.93	112.24
25	C	506	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
25	b	612	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
25	A	609	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
25	B	602	CLA	O2D-CGD-CBD	3.96	118.30	111.27
25	C	510	CLA	CMB-C2B-C3B	3.95	132.07	124.68
32	C	515	DGD	O3G-C3G-C2G	-3.95	101.36	110.90
25	A	607	CLA	C4A-NA-C1A	3.95	108.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	612	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
25	c	502	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
25	B	613	CLA	CMB-C2B-C3B	3.94	132.04	124.68
30	a	613	SQD	O47-C7-C8	3.94	119.98	111.50
25	B	608	CLA	CMB-C2B-C3B	3.93	132.03	124.68
32	h	101	DGD	O3G-C3G-C2G	-3.93	101.42	110.90
25	a	608	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	C	508	CLA	CHD-C1D-ND	-3.92	120.86	124.45
25	c	512	CLA	C1-C2-C3	-3.90	119.30	126.04
26	d	402	PHO	O1D-CGD-CBD	3.90	131.23	124.74
25	c	508	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
25	B	610	CLA	CHB-C4A-NA	3.89	129.90	124.51
25	b	602	CLA	CMB-C2B-C3B	3.88	131.93	124.68
28	a	611	PL9	C7-C3-C2	-3.87	118.20	123.30
26	d	402	PHO	O2D-CGD-O1D	-3.87	116.28	123.84
30	F	101	SQD	C44-O6-C1	3.87	120.25	113.84
32	c	519	DGD	O3G-C3G-C2G	-3.86	101.58	110.90
25	b	609	CLA	C4A-NA-C1A	3.86	108.44	106.71
30	a	613	SQD	C44-O6-C1	-3.85	106.22	113.74
31	l	101	LHG	O4-P-O5	3.84	131.23	112.24
25	B	607	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
25	B	611	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
25	c	509	CLA	O2A-CGA-O1A	-3.83	113.94	123.59
32	C	516	DGD	O3G-C3G-C2G	-3.82	101.69	110.90
25	c	513	CLA	CMB-C2B-C3B	3.81	131.81	124.68
25	C	507	CLA	O2D-CGD-O1D	-3.81	116.38	123.84
25	b	602	CLA	C4A-NA-C1A	3.81	108.42	106.71
25	b	603	CLA	CHD-C1D-ND	-3.80	120.96	124.45
25	B	616	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
30	A	616	SQD	O47-C7-C8	3.79	119.67	111.50
25	a	612	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
25	A	609	CLA	C4A-NA-C1A	3.77	108.40	106.71
25	C	511	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	a	609	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	b	616	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
25	c	510	CLA	CMB-C2B-C3B	3.76	131.72	124.68
25	B	605	CLA	CHD-C1D-ND	-3.76	121.00	124.45
30	a	613	SQD	O9-S-O7	-3.75	100.98	113.95
30	f	102	SQD	O9-S-O7	-3.74	100.99	113.95
25	b	610	CLA	C4A-NA-C1A	3.74	108.39	106.71
25	d	403	CLA	CMB-C2B-C3B	3.71	131.63	124.68
25	c	510	CLA	O2D-CGD-O1D	-3.70	116.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	503	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
30	L	101	SQD	O9-S-C6	3.68	111.32	106.94
25	C	513	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	b	603	CLA	CMB-C2B-C3B	3.66	131.53	124.68
25	C	501	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
30	A	613	SQD	O9-S-O7	-3.66	101.29	113.95
25	B	603	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
25	B	606	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
25	b	604	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
25	C	507	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
25	c	501	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	b	615	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
32	A	617	DGD	O3G-C3G-C2G	-3.62	102.17	110.90
25	b	602	CLA	CHB-C4A-NA	3.62	129.51	124.51
26	A	608	PHO	CMB-C2B-C3B	3.60	131.42	124.68
30	L	101	SQD	O48-C23-C24	3.60	123.20	111.91
25	B	602	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
25	b	608	CLA	CMB-C2B-C3B	3.59	131.39	124.68
25	b	611	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
25	b	613	CLA	CMB-C2B-C3B	3.57	131.37	124.68
25	b	614	CLA	C4A-NA-C1A	3.57	108.31	106.71
25	b	606	CLA	CMB-C2B-C3B	3.57	131.35	124.68
30	F	101	SQD	O5-C1-O6	3.56	118.41	109.97
27	b	617	BCR	C2-C1-C6	3.55	115.94	110.48
25	c	506	CLA	CMB-C2B-C3B	3.54	131.31	124.68
25	A	606	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
25	d	404	CLA	C4A-NA-C1A	3.54	108.30	106.71
25	c	509	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
25	B	607	CLA	CMB-C2B-C3B	3.54	131.29	124.68
25	b	609	CLA	CMB-C2B-C3B	3.52	131.27	124.68
25	B	604	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
25	b	616	CLA	CHD-C1D-ND	-3.52	121.22	124.45
32	C	516	DGD	O5D-C6D-C5D	-3.50	102.57	109.05
25	c	502	CLA	CHD-C1D-ND	-3.50	121.24	124.45
25	b	611	CLA	O2D-CGD-CBD	3.49	117.48	111.27
25	b	603	CLA	C1B-CHB-C4A	-3.49	123.20	130.12
25	C	505	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
25	b	605	CLA	CHD-C1D-ND	-3.48	121.25	124.45
25	B	612	CLA	O2D-CGD-O1D	-3.47	117.04	123.84
25	C	506	CLA	CMB-C2B-C3B	3.47	131.16	124.68
25	b	606	CLA	O2D-CGD-CBD	3.46	117.42	111.27
25	a	607	CLA	CMB-C2B-C3B	3.45	131.14	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	614	SQD	O48-C23-C24	3.45	122.75	111.91
32	C	517	DGD	O3G-C3G-C2G	-3.44	102.59	110.90
30	L	101	SQD	O9-S-O7	-3.44	102.05	113.95
25	b	604	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
25	B	611	CLA	O2D-CGD-CBD	3.43	117.37	111.27
25	D	403	CLA	CMB-C2B-C3B	3.43	131.10	124.68
30	B	622	SQD	O48-C23-C24	3.43	122.67	111.91
25	b	602	CLA	C1-C2-C3	-3.43	120.12	126.04
32	c	517	DGD	O3G-C3G-C2G	-3.43	102.63	110.90
32	A	617	DGD	C4E-C3E-C2E	-3.42	104.85	110.82
28	d	406	PL9	C40-C39-C41	3.42	121.02	115.27
30	f	102	SQD	O47-C7-C8	3.42	120.33	110.80
25	D	404	CLA	O2D-CGD-CBD	3.42	117.34	111.27
25	B	603	CLA	CMB-C2B-C3B	3.41	131.06	124.68
25	a	609	CLA	CMB-C2B-C3B	3.41	131.06	124.68
30	L	101	SQD	C1-C2-C3	-3.41	102.90	110.00
25	B	616	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
25	b	607	CLA	CMB-C2B-C3B	3.40	131.04	124.68
30	f	102	SQD	O5-C5-C4	3.39	115.85	109.69
36	V	201	HEC	CMC-C2C-C3C	3.39	129.80	125.82
25	B	604	CLA	CMB-C2B-C3B	3.39	131.02	124.68
36	V	201	HEC	C1D-C2D-C3D	-3.38	104.64	107.00
30	F	101	SQD	O9-S-O7	-3.37	102.27	113.95
25	b	612	CLA	CMB-C2B-C3B	3.37	130.99	124.68
32	H	102	DGD	C3E-C4E-C5E	-3.37	104.23	110.24
25	c	502	CLA	CMB-C2B-C3B	3.37	130.98	124.68
25	c	508	CLA	CMB-C2B-C3B	3.36	130.97	124.68
30	a	613	SQD	O8-S-C6	3.36	111.10	105.74
27	A	610	BCR	C11-C10-C9	-3.36	122.52	127.31
25	b	614	CLA	CHD-C1D-ND	-3.36	121.37	124.45
25	D	404	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
30	f	102	SQD	O6-C1-C2	3.35	113.53	108.30
30	L	101	SQD	O5-C5-C4	3.35	115.77	109.69
25	c	513	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
30	a	613	SQD	C1-C2-C3	-3.33	103.07	110.00
26	D	402	PHO	CMB-C2B-C3B	3.32	130.90	124.68
25	B	604	CLA	C2D-C1D-ND	-3.32	107.66	110.10
27	B	617	BCR	C2-C1-C6	3.32	115.59	110.48
25	B	609	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
25	b	610	CLA	C1-C2-C3	-3.31	120.31	126.04
25	C	509	CLA	CHD-C1D-ND	-3.31	121.41	124.45
27	K	101	BCR	C15-C16-C17	-3.30	116.71	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	614	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	B	613	CLA	CAC-C3C-C4C	3.30	129.09	124.81
25	B	601	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
25	b	602	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
25	b	610	CLA	CAC-C3C-C4C	3.29	129.08	124.81
25	D	403	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
25	c	507	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
25	C	508	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
25	B	610	CLA	O2A-CGA-O1A	-3.27	115.34	123.59
25	D	404	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
25	c	511	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
25	b	612	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
25	B	611	CLA	CMB-C2B-C3B	3.25	130.77	124.68
31	d	407	LHG	O8-C23-O10	-3.25	115.39	123.59
25	C	507	CLA	CMB-C2B-C3B	3.25	130.76	124.68
30	A	616	SQD	O48-C23-C24	3.25	122.10	111.91
25	b	601	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
25	C	508	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	c	515	BCR	C35-C13-C14	-3.23	118.39	122.92
35	f	101	HEM	CBA-CAA-C2A	-3.23	107.11	112.62
25	A	607	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
25	A	606	CLA	CMB-C2B-C3B	3.22	130.70	124.68
31	D	412	LHG	O8-C23-C24	3.22	122.02	111.91
25	B	615	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
25	b	601	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
25	b	605	CLA	CMB-C2B-C3B	3.22	130.70	124.68
25	a	608	CLA	CMB-C2B-C3B	3.21	130.69	124.68
25	C	512	CLA	CMB-C2B-C1B	-3.21	123.52	128.46
25	a	608	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
25	b	604	CLA	CHB-C4A-NA	3.21	128.95	124.51
30	A	613	SQD	O7-S-C6	3.20	110.74	106.94
26	A	608	PHO	O2D-CGD-CBD	3.19	115.04	111.00
25	a	609	CLA	C4A-NA-C1A	3.18	108.14	106.71
25	B	610	CLA	O2D-CGD-CBD	3.18	116.91	111.27
25	b	612	CLA	C1-C2-C3	-3.18	120.55	126.04
25	C	503	CLA	CMB-C2B-C3B	3.17	130.62	124.68
25	b	605	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
25	C	502	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
25	a	612	CLA	CMB-C2B-C3B	3.17	130.61	124.68
25	c	502	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
31	d	408	LHG	O8-C23-C24	3.17	121.85	111.91
25	A	609	CLA	C1B-CHB-C4A	-3.17	123.85	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	619	BCR	C2-C1-C6	3.16	115.35	110.48
29	m	101	LMG	O1-C7-C8	-3.15	103.29	110.90
30	F	101	SQD	O8-S-C6	3.15	110.76	105.74
25	C	513	CLA	CMB-C2B-C3B	3.15	130.57	124.68
36	v	201	HEC	CBD-CAD-C3D	-3.15	107.25	112.62
25	B	605	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
25	B	616	CLA	CMB-C2B-C3B	3.14	130.56	124.68
31	d	407	LHG	O8-C23-C24	3.14	121.76	111.91
25	c	512	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
25	b	610	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
25	C	510	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
30	A	613	SQD	O5-C1-C2	-3.12	103.75	110.35
25	C	503	CLA	CHD-C1D-ND	-3.12	121.59	124.45
25	c	511	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
29	c	522	LMG	O1-C1-C2	-3.10	103.46	108.30
25	C	507	CLA	CHB-C4A-NA	3.10	128.80	124.51
25	A	607	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
25	C	513	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
26	D	402	PHO	O2D-CGD-O1D	-3.09	117.79	123.84
25	c	505	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
30	F	101	SQD	O48-C23-C24	3.09	121.60	111.91
25	c	503	CLA	CHB-C4A-NA	3.09	128.78	124.51
25	B	610	CLA	C1-C2-C3	-3.08	120.72	126.04
25	b	601	CLA	CHB-C4A-NA	3.08	128.77	124.51
25	D	405	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
27	T	101	BCR	C7-C8-C9	-3.07	121.59	126.23
30	f	102	SQD	O9-S-C6	3.07	110.59	106.94
25	c	509	CLA	CMB-C2B-C3B	3.07	130.42	124.68
28	A	611	PL9	C7-C3-C2	-3.06	119.27	123.30
25	B	602	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	B	613	CLA	O2A-CGA-O1A	-3.06	115.88	123.59
25	b	610	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
25	c	512	CLA	CHD-C1D-ND	-3.06	121.64	124.45
26	A	608	PHO	O2D-CGD-O1D	-3.06	117.86	123.84
25	B	614	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
32	c	519	DGD	O6D-C1D-O3G	-3.06	102.74	109.97
25	a	608	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
35	E	101	HEM	CBD-CAD-C3D	-3.05	104.16	112.63
25	b	614	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	d	404	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
25	c	502	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
25	A	606	CLA	CHB-C4A-NA	3.04	128.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	611	CLA	CHD-C1D-ND	-3.04	121.66	124.45
25	A	606	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
29	M	101	LMG	C38-C37-C36	-3.03	99.04	114.42
25	C	504	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
29	d	411	LMG	O2-C2-C1	-3.03	102.69	110.05
25	a	612	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	C	504	CLA	CMB-C2B-C3B	3.03	130.34	124.68
25	b	610	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
25	c	505	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
25	C	512	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	a	612	CLA	O2D-CGD-CBD	3.02	116.63	111.27
25	C	512	CLA	CHB-C4A-NA	3.02	128.69	124.51
25	B	612	CLA	CHD-C1D-ND	-3.02	121.68	124.45
25	c	508	CLA	CHD-C1D-ND	-3.02	121.68	124.45
32	C	515	DGD	O6D-C1D-O3G	-3.01	102.84	109.97
26	d	401	PHO	CMB-C2B-C3B	3.01	130.31	124.68
25	b	613	CLA	C1-C2-C3	-3.01	120.84	126.04
35	f	101	HEM	C3B-C2B-C1B	3.01	108.72	106.49
32	C	516	DGD	O6D-C1D-O3G	-3.01	102.85	109.97
25	C	502	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	C	509	CLA	CHB-C4A-NA	3.00	128.66	124.51
29	D	408	LMG	O6-C1-O1	-3.00	102.87	109.97
25	c	509	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
25	b	613	CLA	O2D-CGD-CBD	2.99	116.58	111.27
25	b	602	CLA	CHD-C1D-ND	-2.99	121.70	124.45
29	C	518	LMG	O1-C7-C8	-2.99	103.68	110.90
25	D	403	CLA	CHD-C1D-ND	-2.99	121.71	124.45
25	D	403	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
25	b	602	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	B	604	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	C	513	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	B	614	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	A	609	CLA	CHD-C1D-ND	-2.98	121.72	124.45
25	B	609	CLA	CMB-C2B-C3B	2.98	130.25	124.68
33	C	520	STE	C3-C2-C1	-2.98	106.97	114.47
30	a	613	SQD	O48-C23-C24	2.98	121.24	111.91
25	b	603	CLA	O2D-CGD-CBD	2.97	116.55	111.27
25	b	607	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
28	d	406	PL9	C37-C38-C39	-2.96	120.52	127.66
25	B	603	CLA	CHD-C1D-ND	-2.96	121.73	124.45
25	b	613	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
32	c	518	DGD	O6D-C1D-O3G	-2.96	102.97	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	511	CLA	CMB-C2B-C3B	2.96	130.21	124.68
27	B	618	BCR	C24-C23-C22	-2.96	121.77	126.23
27	K	101	BCR	C15-C14-C13	-2.96	123.09	127.31
28	d	406	PL9	C36-C34-C33	-2.95	115.14	121.12
32	C	517	DGD	O6D-C1D-O3G	-2.95	102.98	109.97
25	b	609	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
32	A	617	DGD	O5D-C6D-C5D	-2.95	103.59	109.05
25	a	608	CLA	CHB-C4A-NA	2.95	128.59	124.51
27	B	619	BCR	C34-C9-C10	-2.95	118.79	122.92
25	b	604	CLA	CMB-C2B-C3B	2.93	130.17	124.68
25	b	608	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	b	610	CLA	CMB-C2B-C3B	2.93	130.16	124.68
25	A	607	CLA	CMB-C2B-C3B	2.92	130.15	124.68
25	B	606	CLA	CMB-C2B-C3B	2.92	130.14	124.68
25	C	511	CLA	CHB-C4A-NA	2.91	128.54	124.51
25	B	612	CLA	C11-C12-C13	-2.91	106.53	115.92
28	A	611	PL9	C36-C34-C33	-2.90	115.25	121.12
25	c	502	CLA	C1-C2-C3	-2.90	121.03	126.04
25	b	612	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	B	610	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
33	m	102	STE	O2-C1-C2	2.89	123.33	114.03
25	D	405	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
26	d	402	PHO	CMB-C2B-C3B	2.89	130.08	124.68
30	a	613	SQD	O9-S-C6	2.89	110.37	106.94
25	b	605	CLA	O2A-CGA-O1A	-2.89	116.31	123.59
25	b	610	CLA	CAA-CBA-CGA	-2.88	104.83	113.25
25	C	506	CLA	C1-C2-C3	-2.88	121.06	126.04
27	B	618	BCR	C15-C14-C13	-2.88	123.20	127.31
30	B	622	SQD	O8-S-C6	2.88	110.33	105.74
29	d	411	LMG	O6-C1-O1	-2.87	103.17	109.97
25	C	505	CLA	CMB-C2B-C3B	2.87	130.06	124.68
25	c	509	CLA	CHB-C4A-NA	2.87	128.49	124.51
33	j	101	STE	O2-C1-C2	2.87	123.24	114.03
25	b	607	CLA	CHB-C4A-NA	2.87	128.47	124.51
25	a	607	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
30	A	613	SQD	O9-S-C6	2.86	110.34	106.94
25	C	504	CLA	CHD-C1D-ND	-2.86	121.82	124.45
27	a	610	BCR	C2-C1-C6	2.86	114.89	110.48
25	c	504	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
32	H	102	DGD	O2D-C2D-C1D	-2.86	103.10	110.05
32	C	515	DGD	O5D-C6D-C5D	-2.85	103.77	109.05
25	a	609	CLA	CHB-C4A-NA	2.85	128.45	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	m	101	LMG	O3-C3-C2	-2.85	103.76	110.35
25	b	616	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
25	c	507	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
29	b	621	LMG	C3-C4-C5	-2.84	105.17	110.24
25	b	606	CLA	C1B-CHB-C4A	-2.84	124.48	130.12
27	D	406	BCR	C7-C8-C9	-2.84	121.94	126.23
32	c	519	DGD	CDB-CCB-CBB	-2.84	100.00	114.42
27	t	101	BCR	C15-C14-C13	-2.84	123.26	127.31
30	L	101	SQD	C3-C4-C5	2.83	115.30	110.24
25	d	403	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	C	514	BCR	C2-C1-C6	2.83	114.84	110.48
25	c	506	CLA	CHB-C4A-NA	2.83	128.43	124.51
25	b	610	CLA	CHD-C1D-ND	-2.83	121.85	124.45
25	B	610	CLA	CHD-C1D-ND	-2.83	121.85	124.45
25	b	602	CLA	O2D-CGD-CBD	2.83	116.29	111.27
30	B	622	SQD	O6-C1-C2	2.83	112.72	108.30
25	a	607	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
29	M	101	LMG	C1-C2-C3	-2.83	104.11	110.00
25	c	509	CLA	CHD-C1D-ND	-2.82	121.86	124.45
27	d	405	BCR	C27-C26-C25	2.82	126.83	122.73
28	d	406	PL9	C42-C43-C44	-2.82	120.86	127.66
25	c	501	CLA	CHD-C1D-ND	-2.82	121.86	124.45
25	c	501	CLA	CMB-C2B-C3B	2.82	129.95	124.68
25	C	512	CLA	CHD-C1D-ND	-2.82	121.87	124.45
25	C	503	CLA	C7-C6-C5	-2.82	105.71	113.36
27	d	405	BCR	C38-C26-C25	-2.81	121.37	124.53
32	H	102	DGD	CDB-CCB-CBB	-2.81	100.14	114.42
29	b	621	LMG	C1-O6-C5	-2.81	108.18	113.69
25	B	603	CLA	CHD-C4C-NC	2.81	128.62	124.20
26	d	402	PHO	CMC-C2C-C3C	2.80	130.23	124.94
29	c	522	LMG	C6-C5-C4	-2.80	106.44	113.00
25	B	612	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
30	f	102	SQD	C1-O5-C5	-2.80	108.19	113.69
27	C	514	BCR	C15-C16-C17	-2.80	117.74	123.47
27	c	515	BCR	C7-C8-C9	-2.80	122.00	126.23
25	A	606	CLA	C7-C6-C5	-2.80	105.76	113.36
25	C	511	CLA	CHD-C1D-ND	-2.80	121.89	124.45
32	A	617	DGD	CDB-CCB-CBB	-2.80	100.23	114.42
25	C	502	CLA	CMB-C2B-C3B	2.79	129.90	124.68
25	b	616	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	B	615	CLA	CHD-C1D-ND	-2.79	121.89	124.45
25	b	611	CLA	CHD-C1D-ND	-2.79	121.89	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	102	SQD	C1-C2-C3	-2.79	104.19	110.00
25	b	608	CLA	O2D-CGD-CBD	2.79	116.22	111.27
25	B	612	CLA	CHB-C4A-NA	2.78	128.36	124.51
32	c	517	DGD	O3G-C1D-C2D	-2.78	103.96	108.30
26	D	402	PHO	O1D-CGD-CBD	2.78	129.37	124.74
25	c	510	CLA	C2D-C1D-ND	-2.78	108.06	110.10
25	B	607	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
25	C	509	CLA	CED-O2D-CGD	2.78	122.22	115.94
32	a	615	DGD	CDB-CCB-CBB	-2.78	100.33	114.42
27	k	101	BCR	C33-C5-C6	-2.78	121.41	124.53
27	B	618	BCR	C3-C4-C5	-2.78	109.12	114.08
25	c	508	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	B	616	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	C	501	CLA	CMB-C2B-C3B	2.76	129.84	124.68
25	b	608	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	A	607	CLA	C1-C2-C3	-2.76	121.27	126.04
28	D	407	PL9	C7-C3-C2	-2.76	119.67	123.30
25	A	609	CLA	O2D-CGD-CBD	2.76	116.17	111.27
25	c	503	CLA	CHD-C1D-ND	-2.75	121.92	124.45
27	T	101	BCR	C27-C26-C25	2.75	126.73	122.73
25	b	601	CLA	CMB-C2B-C3B	2.75	129.82	124.68
27	c	514	BCR	C15-C14-C13	-2.75	123.39	127.31
33	c	523	STE	C3-C2-C1	-2.75	107.54	114.47
28	a	611	PL9	C7-C8-C9	-2.75	122.22	126.79
25	A	609	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	C	503	CLA	O2D-CGD-O1D	-2.73	118.49	123.84
28	D	407	PL9	C20-C19-C21	2.73	119.87	115.27
25	B	616	CLA	CAA-CBA-CGA	-2.73	105.28	113.25
32	c	517	DGD	CDB-CCB-CBB	-2.73	100.59	114.42
30	A	613	SQD	O48-C23-C24	2.72	120.46	111.91
28	d	406	PL9	C22-C23-C24	-2.72	121.10	127.66
25	B	606	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
28	D	407	PL9	C7-C8-C9	-2.72	122.26	126.79
27	Y	101	BCR	C27-C26-C25	2.72	126.68	122.73
25	c	501	CLA	O2D-CGD-CBD	2.71	116.09	111.27
34	a	606	BCT	O2-C-O1	-2.71	112.51	119.55
25	b	611	CLA	CMB-C2B-C3B	2.71	129.75	124.68
25	B	602	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
28	d	406	PL9	C7-C8-C9	-2.71	122.28	126.79
31	D	409	LHG	C18-C17-C16	-2.71	100.69	114.42
26	d	401	PHO	OBD-CAD-CBD	-2.70	121.86	125.82
25	c	508	CLA	CHB-C4A-NA	2.70	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	501	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
25	a	608	CLA	O2D-CGD-CBD	2.70	116.07	111.27
25	a	607	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
32	C	517	DGD	CDB-CCB-CBB	-2.70	100.72	114.42
25	b	606	CLA	CHB-C4A-NA	2.70	128.24	124.51
28	d	406	PL9	O1-C4-C3	-2.70	117.75	120.72
25	a	607	CLA	O1D-CGD-CBD	2.70	130.00	124.48
25	b	614	CLA	C1B-CHB-C4A	-2.70	124.78	130.12
28	D	407	PL9	C22-C23-C24	-2.70	121.17	127.66
25	B	611	CLA	C1-C2-C3	-2.69	121.39	126.04
25	b	615	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	c	503	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
27	Y	101	BCR	C33-C5-C6	-2.69	121.51	124.53
28	A	611	PL9	C22-C23-C24	-2.69	121.18	127.66
25	C	512	CLA	CMB-C2B-C3B	2.69	129.71	124.68
25	D	404	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
25	A	607	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
25	B	609	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
27	b	618	BCR	C8-C7-C6	-2.68	119.67	127.20
27	D	406	BCR	C3-C4-C5	-2.68	109.29	114.08
28	D	407	PL9	C12-C13-C14	-2.68	121.21	127.66
30	f	102	SQD	O5-C1-C2	-2.68	104.68	110.35
30	B	622	SQD	O9-S-C6	2.68	110.12	106.94
25	b	601	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	c	513	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
25	A	606	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
25	c	512	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	c	505	CLA	CMB-C2B-C3B	2.67	129.68	124.68
27	a	610	BCR	C24-C23-C22	-2.67	122.20	126.23
36	V	201	HEC	CMB-C2B-C1B	-2.67	124.36	128.46
30	a	613	SQD	C3-C4-C5	2.67	115.00	110.24
32	C	515	DGD	CDB-CCB-CBB	-2.67	100.88	114.42
32	C	516	DGD	CDB-CCB-CBB	-2.67	100.88	114.42
25	C	501	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
29	b	621	LMG	O7-C10-O9	-2.66	117.26	123.70
27	A	610	BCR	C27-C26-C25	2.66	126.60	122.73
35	f	101	HEM	CBD-CAD-C3D	-2.66	105.24	112.63
27	D	406	BCR	C2-C1-C6	2.65	114.57	110.48
32	h	101	DGD	O3E-C3E-C2E	-2.65	104.22	110.35
28	A	611	PL9	C20-C19-C21	2.65	119.73	115.27
25	B	614	CLA	CMB-C2B-C3B	2.65	129.63	124.68
25	c	508	CLA	C1-C2-C3	-2.65	121.46	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	511	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	B	611	CLA	CHB-C4A-NA	2.65	128.17	124.51
36	v	201	HEC	CMB-C2B-C1B	-2.65	124.39	128.46
27	c	514	BCR	C24-C23-C22	-2.65	122.24	126.23
25	D	403	CLA	C4A-NA-C1A	2.64	107.89	106.71
29	m	101	LMG	O6-C1-O1	-2.64	103.71	109.97
25	B	602	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
27	b	618	BCR	C15-C14-C13	-2.64	123.54	127.31
25	b	615	CLA	CHB-C4A-NA	2.64	128.16	124.51
25	b	612	CLA	O1D-CGD-CBD	2.63	129.88	124.48
27	b	619	BCR	C11-C10-C9	-2.63	123.55	127.31
32	h	101	DGD	CDB-CCB-CBB	-2.63	101.06	114.42
28	d	406	PL9	C7-C3-C2	-2.63	119.84	123.30
27	D	406	BCR	C27-C26-C25	2.63	126.55	122.73
25	C	507	CLA	O2D-CGD-CBD	2.63	115.94	111.27
29	b	621	LMG	O8-C28-O10	-2.63	116.95	123.59
29	m	101	LMG	O7-C10-O9	-2.63	117.35	123.70
25	b	615	CLA	CMB-C2B-C3B	2.63	129.59	124.68
25	b	613	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
27	B	617	BCR	C29-C30-C25	2.62	114.52	110.48
25	B	609	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	C	502	CLA	CHD-C1D-ND	-2.61	122.06	124.45
25	B	606	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
29	c	520	LMG	O6-C1-O1	-2.61	103.80	109.97
25	B	605	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
31	d	408	LHG	O8-C23-O10	-2.60	117.03	123.59
31	A	614	LHG	O8-C23-C24	2.60	120.06	111.91
25	B	615	CLA	CHB-C4A-NA	2.60	128.10	124.51
27	H	101	BCR	C27-C26-C25	2.60	126.50	122.73
25	b	613	CLA	C16-C15-C13	-2.60	107.53	115.92
25	c	502	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
32	A	617	DGD	C3G-C2G-C1G	-2.59	105.65	111.79
25	C	510	CLA	CHD-C1D-ND	-2.59	122.07	124.45
25	c	505	CLA	O2D-CGD-CBD	2.59	115.86	111.27
27	B	618	BCR	C35-C13-C14	-2.58	119.30	122.92
27	H	101	BCR	C35-C13-C14	-2.58	119.30	122.92
25	B	609	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
27	x	101	BCR	C2-C1-C6	2.58	114.45	110.48
27	c	515	BCR	C27-C26-C25	2.58	126.48	122.73
25	B	612	CLA	C1-C2-C3	-2.58	121.58	126.04
25	a	609	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
32	C	516	DGD	C1D-O6D-C5D	-2.58	108.63	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	v	201	HEC	CMC-C2C-C1C	-2.58	124.50	128.46
27	k	101	BCR	C27-C26-C25	2.57	126.47	122.73
32	h	101	DGD	C1D-C2D-C3D	-2.57	104.64	110.00
25	B	612	CLA	C16-C15-C13	-2.57	107.62	115.92
32	A	617	DGD	O6D-C1D-O3G	-2.56	103.90	109.97
26	d	401	PHO	O2A-CGA-O1A	-2.56	117.12	123.59
25	b	608	CLA	CHD-C1D-ND	-2.56	122.10	124.45
29	M	101	LMG	C1-O6-C5	-2.56	108.66	113.69
25	D	404	CLA	CMB-C2B-C3B	2.56	129.47	124.68
27	B	619	BCR	C29-C30-C25	2.56	114.42	110.48
27	c	514	BCR	C33-C5-C6	-2.56	121.66	124.53
25	c	506	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
27	c	516	BCR	C27-C26-C25	2.55	126.44	122.73
31	D	412	LHG	C18-C17-C16	-2.55	101.47	114.42
25	b	606	CLA	CHD-C1D-ND	-2.55	122.11	124.45
33	b	622	STE	C3-C2-C1	-2.55	108.04	114.47
32	c	517	DGD	O6D-C1D-O3G	-2.55	103.94	109.97
27	C	514	BCR	C15-C14-C13	-2.55	123.67	127.31
27	b	617	BCR	C33-C5-C6	-2.54	121.67	124.53
25	C	506	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
25	c	513	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	C	510	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
31	d	408	LHG	C20-C19-C18	-2.54	101.53	114.42
25	C	513	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	a	609	CLA	O2D-CGD-CBD	2.54	115.77	111.27
32	C	515	DGD	C6D-O5D-C1E	2.53	118.69	113.74
27	b	617	BCR	C3-C4-C5	-2.53	109.56	114.08
25	b	614	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
25	B	602	CLA	CHD-C1D-ND	-2.53	122.13	124.45
25	D	405	CLA	CHB-C4A-NA	2.52	128.00	124.51
29	M	101	LMG	C40-C39-C38	-2.52	101.61	114.42
31	l	101	LHG	C20-C19-C18	-2.52	101.61	114.42
25	a	608	CLA	CHD-C1D-ND	-2.52	122.14	124.45
28	d	406	PL9	C46-C47-C48	-2.52	103.59	111.88
32	a	615	DGD	C5B-C4B-C3B	-2.52	101.62	114.42
32	C	516	DGD	O2D-C2D-C1D	-2.52	103.92	110.05
30	F	101	SQD	O5-C5-C4	2.52	114.27	109.69
25	B	602	CLA	C16-C15-C13	-2.52	107.78	115.92
25	b	611	CLA	CHB-C4A-NA	2.52	127.99	124.51
27	K	102	BCR	C27-C26-C25	2.52	126.38	122.73
30	L	101	SQD	O8-S-C6	2.52	109.75	105.74
30	f	102	SQD	C3-C4-C5	2.51	114.72	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	615	CLA	O2D-CGD-CBD	2.51	115.73	111.27
25	b	610	CLA	CHB-C4A-NA	2.51	127.99	124.51
25	b	616	CLA	O2D-CGD-CBD	2.51	115.73	111.27
30	F	101	SQD	C46-C45-C44	-2.51	105.34	113.70
31	D	410	LHG	O8-C6-C5	-2.51	101.12	108.43
29	c	524	LMG	C1-O6-C5	-2.51	108.76	113.69
31	D	409	LHG	C11-C10-C9	-2.51	101.70	114.42
27	x	101	BCR	C27-C26-C25	2.51	126.37	122.73
28	a	611	PL9	C40-C39-C41	2.51	119.49	115.27
25	B	612	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
27	b	617	BCR	C27-C26-C25	2.50	126.36	122.73
27	H	101	BCR	C16-C15-C14	-2.50	118.35	123.47
30	f	102	SQD	O48-C23-C24	2.50	119.75	111.91
27	c	514	BCR	C15-C16-C17	-2.50	118.36	123.47
25	B	610	CLA	CMB-C2B-C1B	-2.50	124.63	128.46
25	b	605	CLA	O1D-CGD-CBD	2.49	129.59	124.48
32	C	515	DGD	C7B-C6B-C5B	-2.49	101.77	114.42
27	K	101	BCR	C24-C23-C22	-2.49	122.47	126.23
27	c	515	BCR	C15-C16-C17	-2.49	118.37	123.47
32	c	518	DGD	O2D-C2D-C1D	-2.49	104.00	110.05
33	M	102	STE	C3-C2-C1	-2.49	108.20	114.47
31	D	409	LHG	C27-C26-C25	-2.49	101.79	114.42
25	b	606	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
25	D	403	CLA	CHB-C4A-NA	2.48	127.95	124.51
25	C	508	CLA	O2D-CGD-CBD	2.48	115.68	111.27
31	e	101	LHG	O8-C23-C24	2.48	119.70	111.91
25	b	608	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
29	c	524	LMG	O6-C1-O1	-2.48	104.10	109.97
25	d	404	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
25	c	504	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	B	603	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	a	612	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	C	509	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
25	b	609	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
29	C	518	LMG	O2-C2-C1	-2.47	104.05	110.05
25	C	501	CLA	CHD-C1D-ND	-2.47	122.18	124.45
28	D	407	PL9	C37-C38-C39	-2.47	121.71	127.66
25	c	507	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
25	a	607	CLA	CHB-C4A-NA	2.47	127.92	124.51
32	c	518	DGD	CDB-CCB-CBB	-2.47	101.91	114.42
28	a	611	PL9	C22-C23-C24	-2.47	121.72	127.66
31	l	101	LHG	C11-C10-C9	-2.47	101.91	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	615	DGD	C1G-C2G-C3G	-2.46	106.03	111.80
30	L	101	SQD	O5-C1-C2	-2.46	105.13	110.35
27	H	101	BCR	C24-C23-C22	-2.46	122.51	126.23
26	D	402	PHO	CMC-C2C-C3C	2.46	129.59	124.94
27	a	610	BCR	C27-C26-C25	2.46	126.31	122.73
26	A	608	PHO	C1-C2-C3	-2.46	121.78	126.04
25	b	609	CLA	CHB-C4A-NA	2.46	127.92	124.51
29	m	101	LMG	O1-C1-C2	-2.46	104.46	108.30
27	b	618	BCR	C27-C26-C25	2.46	126.30	122.73
27	c	515	BCR	C2-C1-C6	2.46	114.26	110.48
25	c	505	CLA	CHB-C4A-NA	2.46	127.91	124.51
36	v	201	HEC	CBA-CAA-C2A	-2.46	108.47	112.60
25	a	612	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	c	512	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
32	C	517	DGD	C3G-C2G-C1G	-2.45	105.98	111.79
25	b	613	CLA	CHA-C1A-NA	-2.45	120.79	126.40
29	c	520	LMG	O8-C28-O10	-2.45	117.42	123.59
27	B	618	BCR	C2-C1-C6	2.45	114.25	110.48
31	D	409	LHG	O8-C23-C24	2.44	119.58	111.91
25	c	506	CLA	C1-O2A-CGA	2.44	122.86	116.44
31	D	409	LHG	C20-C19-C18	-2.44	102.02	114.42
29	c	520	LMG	C40-C39-C38	-2.44	102.04	114.42
29	C	518	LMG	O6-C1-O1	-2.44	104.20	109.97
25	C	512	CLA	CAA-CBA-CGA	-2.44	106.13	113.25
30	F	101	SQD	O5-C1-C2	-2.44	105.19	110.35
27	B	617	BCR	C3-C4-C5	-2.44	109.73	114.08
32	c	517	DGD	C3G-C2G-C1G	-2.43	106.03	111.79
25	B	613	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
25	b	615	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	d	404	CLA	CHD-C1D-ND	-2.43	122.22	124.45
31	e	101	LHG	C11-C10-C9	-2.43	102.08	114.42
26	D	402	PHO	C1B-NB-C4B	2.43	112.08	107.09
29	A	612	LMG	C40-C39-C38	-2.43	102.09	114.42
25	B	605	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
35	f	101	HEM	C1B-NB-C4B	2.43	107.58	105.07
25	c	501	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	B	614	CLA	CHB-C4A-NA	2.43	127.87	124.51
28	d	406	PL9	C50-C49-C48	-2.42	115.64	122.65
31	d	409	LHG	O8-C23-C24	2.42	119.51	111.91
25	A	606	CLA	C6-C5-C3	2.42	119.80	113.45
27	x	101	BCR	C15-C16-C17	-2.42	118.52	123.47
28	a	611	PL9	C36-C34-C33	-2.42	116.22	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	412	LHG	C11-C10-C9	-2.42	102.15	114.42
25	C	506	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
25	b	611	CLA	C2D-C1D-ND	-2.41	108.33	110.10
25	c	511	CLA	CMB-C2B-C3B	2.41	129.19	124.68
26	A	608	PHO	CMC-C2C-C3C	2.41	129.49	124.94
25	A	607	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
27	a	610	BCR	C11-C10-C9	-2.41	123.87	127.31
27	b	618	BCR	C35-C13-C14	-2.41	119.55	122.92
25	c	503	CLA	C11-C12-C13	-2.41	108.14	115.92
25	c	507	CLA	CMB-C2B-C3B	2.41	129.18	124.68
35	f	101	HEM	CHC-C4B-C3B	2.40	128.25	124.57
32	C	516	DGD	C1D-C2D-C3D	-2.40	104.99	110.00
29	d	410	LMG	O7-C10-O9	-2.40	117.31	123.30
31	d	408	LHG	C18-C17-C16	-2.40	102.23	114.42
25	C	506	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	b	607	CLA	C6-C7-C8	-2.40	108.16	115.92
29	A	612	LMG	O1-C7-C8	-2.40	105.11	110.90
33	C	519	STE	C3-C2-C1	-2.40	108.43	114.47
29	D	408	LMG	C38-C37-C36	-2.40	102.26	114.42
28	d	406	PL9	C27-C28-C29	-2.39	121.89	127.66
29	d	411	LMG	C40-C39-C38	-2.39	102.27	114.42
27	K	101	BCR	C7-C8-C9	-2.39	122.62	126.23
25	c	511	CLA	O2D-CGD-CBD	2.39	115.52	111.27
26	d	402	PHO	O2A-CGA-O1A	-2.39	117.56	123.59
27	B	619	BCR	C11-C10-C9	-2.39	123.90	127.31
30	L	101	SQD	C25-C24-C23	-2.39	104.93	113.62
25	b	615	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
25	B	603	CLA	O2D-CGD-CBD	2.39	115.51	111.27
29	m	101	LMG	C38-C37-C36	-2.39	102.30	114.42
25	C	512	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
28	A	611	PL9	C7-C8-C9	-2.38	122.82	126.79
29	C	518	LMG	O1-C1-C2	-2.38	104.58	108.30
25	B	605	CLA	O1D-CGD-CBD	2.38	129.36	124.48
27	A	610	BCR	C15-C14-C13	-2.38	123.91	127.31
25	A	607	CLA	CHD-C1D-ND	-2.38	122.27	124.45
25	b	609	CLA	CHD-C1D-ND	-2.38	122.27	124.45
27	K	101	BCR	C35-C13-C14	-2.38	119.59	122.92
32	h	101	DGD	O6D-C1D-O3G	-2.38	104.34	109.97
28	d	406	PL9	C20-C19-C21	2.38	119.27	115.27
33	C	519	STE	C4-C3-C2	-2.37	104.66	113.19
31	d	407	LHG	C11-C10-C9	-2.37	102.38	114.42
25	b	605	CLA	CHB-C4A-NA	2.37	127.79	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	617	DGD	O2D-C2D-C1D	-2.37	104.29	110.05
27	t	101	BCR	C35-C13-C14	-2.37	119.60	122.92
29	m	101	LMG	O8-C28-O10	-2.37	117.61	123.59
25	B	607	CLA	O2A-C1-C2	-2.37	102.41	108.64
25	b	609	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
25	b	603	CLA	CHB-C4A-NA	2.37	127.78	124.51
32	A	617	DGD	C3E-C4E-C5E	-2.37	106.02	110.24
25	b	610	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
25	B	604	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
27	d	405	BCR	C33-C5-C6	-2.36	121.88	124.53
27	b	617	BCR	C15-C14-C13	-2.36	123.94	127.31
27	t	101	BCR	C7-C8-C9	-2.36	122.67	126.23
28	a	611	PL9	O2-C1-C2	-2.36	116.38	121.78
29	c	520	LMG	C38-C37-C36	-2.36	102.46	114.42
25	b	605	CLA	O2A-C1-C2	-2.36	102.44	108.64
25	D	404	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
25	d	403	CLA	CHD-C1D-ND	-2.35	122.29	124.45
27	b	619	BCR	C15-C16-C17	-2.35	118.65	123.47
27	K	102	BCR	C3-C4-C5	-2.35	109.88	114.08
27	A	610	BCR	C15-C16-C17	-2.35	118.66	123.47
25	C	512	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
31	D	412	LHG	C20-C19-C18	-2.35	102.51	114.42
25	c	509	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
27	c	516	BCR	C33-C5-C6	-2.35	121.89	124.53
32	A	617	DGD	CBB-CAB-C9B	-2.35	102.52	114.42
27	d	405	BCR	C16-C15-C14	-2.35	118.67	123.47
25	c	511	CLA	CHB-C4A-NA	2.34	127.75	124.51
35	E	101	HEM	C4C-CHD-C1D	2.34	125.65	122.56
30	a	614	SQD	O48-C23-O10	-2.34	117.69	123.59
27	K	102	BCR	C2-C1-C6	2.34	114.08	110.48
32	h	101	DGD	C7B-C6B-C5B	-2.34	102.56	114.42
32	C	517	DGD	O3E-C3E-C2E	-2.34	104.95	110.35
32	a	615	DGD	CFB-CEB-CDB	-2.34	102.57	114.42
25	B	608	CLA	CHD-C1D-ND	-2.34	122.31	124.45
25	c	510	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
25	C	501	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
25	c	510	CLA	C1-C2-C3	-2.33	122.01	126.04
31	A	614	LHG	C11-C10-C9	-2.33	102.59	114.42
32	C	515	DGD	CAB-C9B-C8B	-2.33	102.60	114.42
25	B	610	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
25	A	607	CLA	O2D-CGD-CBD	2.33	115.41	111.27
25	b	604	CLA	O2A-CGA-O1A	-2.33	117.72	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	413	STE	O2-C1-C2	2.33	121.51	114.03
27	A	610	BCR	C33-C5-C6	-2.33	121.92	124.53
29	m	101	LMG	C40-C39-C38	-2.33	102.62	114.42
25	b	607	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
25	b	607	CLA	CHD-C1D-ND	-2.32	122.32	124.45
25	b	604	CLA	C11-C12-C13	-2.32	108.43	115.92
25	b	608	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
25	B	614	CLA	CHD-C1D-ND	-2.32	122.33	124.45
28	D	407	PL9	C36-C34-C33	-2.31	116.44	121.12
27	c	514	BCR	C27-C26-C25	2.31	126.09	122.73
25	C	507	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	d	401	PHO	C1-C2-C3	-2.31	122.05	126.04
25	b	608	CLA	C6-C7-C8	-2.31	108.46	115.92
27	c	516	BCR	C24-C23-C22	-2.31	122.75	126.23
29	c	522	LMG	O6-C1-O1	-2.31	104.51	109.97
25	b	613	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	D	403	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
25	c	504	CLA	CHD-C1D-ND	-2.30	122.34	124.45
25	C	504	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
25	c	504	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	A	607	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	B	601	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
29	D	408	LMG	O1-C7-C8	-2.30	105.36	110.90
27	B	619	BCR	C15-C16-C17	-2.30	118.77	123.47
25	B	604	CLA	C11-C10-C8	-2.29	108.50	115.92
31	l	101	LHG	O8-C23-C24	2.29	119.11	111.91
31	D	410	LHG	C27-C26-C25	-2.29	102.78	114.42
25	c	513	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
25	b	612	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
35	E	101	HEM	CBA-CAA-C2A	-2.29	108.71	112.62
25	c	513	CLA	C2D-C1D-ND	-2.29	108.42	110.10
29	D	408	LMG	C3-C4-C5	-2.29	106.16	110.24
25	B	606	CLA	O2D-CGD-CBD	2.29	115.33	111.27
25	c	510	CLA	CHB-C4A-NA	2.29	127.67	124.51
25	B	611	CLA	CHD-C4C-NC	2.28	127.80	124.20
25	b	604	CLA	C11-C10-C8	-2.28	108.55	115.92
27	b	618	BCR	C24-C23-C22	-2.28	122.79	126.23
25	b	604	CLA	C6-C7-C8	-2.28	108.56	115.92
25	C	512	CLA	O2D-CGD-CBD	2.28	115.31	111.27
25	D	404	CLA	CHB-C4A-NA	2.28	127.66	124.51
29	c	522	LMG	C40-C39-C38	-2.27	102.88	114.42
32	a	615	DGD	CAB-C9B-C8B	-2.27	102.88	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	610	BCR	C29-C30-C25	2.27	113.98	110.48
33	x	102	STE	C3-C2-C1	-2.27	108.74	114.47
25	C	502	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
35	f	101	HEM	CAB-C3B-C2B	-2.27	121.12	128.60
25	C	507	CLA	C2A-C1A-CHA	2.27	127.83	123.86
27	t	101	BCR	C33-C5-C6	-2.27	121.98	124.53
25	D	403	CLA	O2D-CGD-CBD	2.27	115.30	111.27
27	T	101	BCR	C33-C5-C6	-2.27	121.98	124.53
25	c	507	CLA	CHB-C4A-NA	2.27	127.65	124.51
29	b	621	LMG	O2-C2-C1	-2.27	104.54	110.05
25	c	512	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
27	c	516	BCR	C11-C10-C9	-2.26	124.08	127.31
30	B	622	SQD	C25-C24-C23	-2.26	105.39	113.62
25	b	605	CLA	CHD-C4C-NC	2.26	127.77	124.20
25	b	603	CLA	CHD-C1D-C2D	2.26	130.22	125.48
31	D	410	LHG	C11-C10-C9	-2.26	102.95	114.42
25	a	609	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
29	c	520	LMG	C6-C5-C4	-2.26	107.71	113.00
32	a	615	DGD	C7B-C6B-C5B	-2.26	102.96	114.42
31	D	412	LHG	O8-C23-O10	-2.26	117.89	123.59
25	C	507	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
27	c	514	BCR	C11-C10-C9	-2.25	124.09	127.31
25	C	506	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	b	614	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
32	H	102	DGD	C1D-C2D-C3D	-2.25	105.31	110.00
31	D	409	LHG	O8-C23-O10	-2.25	117.92	123.59
25	a	612	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
29	C	518	LMG	C6-C5-C4	-2.24	107.75	113.00
25	c	507	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
25	B	601	CLA	CMB-C2B-C1B	-2.24	125.02	128.46
25	c	502	CLA	CHB-C4A-NA	2.24	127.61	124.51
32	C	516	DGD	C6D-O5D-C1E	2.24	118.11	113.74
25	C	501	CLA	O2D-CGD-CBD	2.24	115.25	111.27
27	x	101	BCR	C3-C4-C5	-2.24	110.08	114.08
29	D	408	LMG	O1-C1-C2	-2.23	104.81	108.30
25	B	615	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
25	B	604	CLA	C1D-ND-C4D	2.23	107.92	106.33
28	A	611	PL9	C40-C39-C38	-2.23	117.95	123.68
32	c	519	DGD	C1D-C2D-C3D	-2.23	105.35	110.00
27	d	405	BCR	C30-C25-C26	-2.23	119.47	122.61
25	B	613	CLA	CHB-C4A-NA	2.23	127.60	124.51
25	a	608	CLA	O2A-CGA-O1A	-2.23	117.96	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b	621	LMG	O6-C5-C6	2.23	111.97	106.44
29	B	621	LMG	O7-C10-O9	-2.23	117.75	123.30
32	h	101	DGD	C5B-C4B-C3B	-2.23	103.13	114.42
31	e	101	LHG	C20-C19-C18	-2.23	103.13	114.42
25	B	605	CLA	CHB-C4A-NA	2.22	127.59	124.51
25	B	603	CLA	C2D-C1D-ND	-2.22	108.47	110.10
25	b	608	CLA	C1-C2-C3	-2.22	122.20	126.04
32	A	617	DGD	C5B-C4B-C3B	-2.22	103.15	114.42
25	c	507	CLA	CHA-C1A-NA	-2.22	121.31	126.40
31	A	615	LHG	C20-C19-C18	-2.22	103.16	114.42
32	H	102	DGD	C3G-C2G-C1G	-2.22	106.54	111.79
25	c	503	CLA	CMB-C2B-C3B	2.22	128.83	124.68
32	c	517	DGD	CBB-CAB-C9B	-2.22	103.17	114.42
32	C	516	DGD	CAB-C9B-C8B	-2.22	103.17	114.42
32	c	519	DGD	CBB-CAB-C9B	-2.21	103.18	114.42
32	H	102	DGD	CAB-C9B-C8B	-2.21	103.19	114.42
25	C	505	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
32	C	515	DGD	C5B-C4B-C3B	-2.21	103.19	114.42
25	B	604	CLA	C16-C15-C13	-2.21	108.77	115.92
25	B	606	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	b	603	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
28	A	611	PL9	C12-C13-C14	-2.21	122.34	127.66
25	C	510	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
28	D	407	PL9	C32-C33-C34	-2.21	122.34	127.66
32	A	617	DGD	C8B-C7B-C6B	-2.21	103.22	114.42
25	c	511	CLA	C2A-C1A-CHA	2.21	127.72	123.86
25	C	510	CLA	CHB-C4A-NA	2.21	127.56	124.51
30	f	102	SQD	O8-S-C6	2.21	109.25	105.74
32	h	101	DGD	CBB-CAB-C9B	-2.20	103.24	114.42
35	f	101	HEM	CMC-C2C-C3C	2.20	128.80	124.68
29	c	524	LMG	C9-C8-C7	-2.20	106.58	111.79
27	c	516	BCR	C2-C1-C6	2.20	113.87	110.48
32	c	519	DGD	CAB-C9B-C8B	-2.20	103.26	114.42
29	c	522	LMG	C38-C37-C36	-2.20	103.28	114.42
25	c	513	CLA	C1-C2-C3	-2.20	122.25	126.04
29	M	101	LMG	O3-C3-C2	-2.19	105.28	110.35
32	H	102	DGD	O6D-C1D-O3G	-2.19	104.78	109.97
35	f	101	HEM	C4D-ND-C1D	2.19	107.34	105.07
29	C	518	LMG	C38-C37-C36	-2.19	103.30	114.42
32	C	516	DGD	C3E-C4E-C5E	-2.19	106.34	110.24
27	B	617	BCR	C15-C14-C13	-2.19	124.19	127.31
27	t	101	BCR	C35-C13-C12	2.18	121.52	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	612	CLA	C11-C10-C8	-2.18	108.86	115.92
29	A	612	LMG	O6-C1-O1	-2.18	104.81	109.97
32	c	517	DGD	C5B-C4B-C3B	-2.18	103.35	114.42
25	C	512	CLA	C1-C2-C3	-2.18	122.27	126.04
25	B	605	CLA	CHD-C1D-C2D	2.18	130.05	125.48
25	C	513	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	b	610	CLA	O1D-CGD-CBD	2.18	128.94	124.48
31	A	614	LHG	C20-C19-C18	-2.18	103.37	114.42
32	h	101	DGD	C1D-O6D-C5D	-2.18	109.42	113.69
29	b	621	LMG	C40-C39-C38	-2.18	103.38	114.42
25	c	509	CLA	O2D-CGD-CBD	2.18	115.13	111.27
25	b	614	CLA	C1-C2-C3	-2.18	122.28	126.04
32	a	615	DGD	CBB-CAB-C9B	-2.18	103.38	114.42
25	b	601	CLA	O2D-CGD-CBD	2.17	115.13	111.27
33	a	617	STE	C3-C2-C1	-2.17	108.99	114.47
30	F	101	SQD	C3-C4-C5	2.17	114.12	110.24
27	b	618	BCR	C36-C18-C17	-2.17	119.88	122.92
29	A	612	LMG	C1-C2-C3	-2.17	105.47	110.00
29	A	612	LMG	C38-C37-C36	-2.17	103.40	114.42
29	c	522	LMG	O7-C10-O9	-2.17	118.45	123.70
27	B	619	BCR	C1-C6-C5	-2.17	119.56	122.61
32	A	617	DGD	O3G-C1D-C2D	-2.17	104.92	108.30
25	B	613	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	b	608	CLA	C11-C10-C8	-2.17	108.91	115.92
27	K	101	BCR	C27-C26-C25	2.17	125.88	122.73
27	x	101	BCR	C15-C14-C13	-2.17	124.22	127.31
34	D	401	BCT	O2-C-O1	-2.17	113.92	119.55
25	c	501	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
25	C	506	CLA	O1D-CGD-CBD	2.17	128.92	124.48
25	c	508	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
27	d	405	BCR	C24-C23-C22	-2.17	122.96	126.23
25	B	603	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
25	b	608	CLA	CHD-C4C-NC	2.16	127.61	124.20
25	B	610	CLA	CMB-C2B-C3B	2.16	128.73	124.68
25	c	512	CLA	CMB-C2B-C3B	2.16	128.73	124.68
25	c	508	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
29	d	411	LMG	C38-C37-C36	-2.16	103.46	114.42
28	d	406	PL9	C31-C32-C33	-2.16	104.79	111.88
29	C	518	LMG	C40-C39-C38	-2.16	103.47	114.42
25	b	614	CLA	CHB-C4A-NA	2.16	127.49	124.51
32	c	519	DGD	C8B-C7B-C6B	-2.16	103.48	114.42
27	C	514	BCR	C27-C26-C25	2.16	125.86	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	501	CLA	C2D-C1D-ND	-2.15	108.52	110.10
31	d	407	LHG	C20-C19-C18	-2.15	103.50	114.42
25	a	608	CLA	CAC-C3C-C4C	2.15	127.60	124.81
25	B	601	CLA	C4-C3-C5	2.15	118.88	115.27
32	C	517	DGD	O3G-C1D-C2D	-2.15	104.95	108.30
25	a	607	CLA	C4-C3-C5	2.15	118.88	115.27
29	c	520	LMG	O1-C7-C8	-2.14	105.72	110.90
25	B	603	CLA	CHB-C4A-NA	2.14	127.48	124.51
25	A	606	CLA	O1D-CGD-CBD	2.14	128.87	124.48
32	c	519	DGD	C6B-C5B-C4B	-2.14	103.54	114.42
27	b	617	BCR	C11-C10-C9	-2.14	124.26	127.31
25	b	605	CLA	CHD-C1D-C2D	2.14	129.96	125.48
25	b	615	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
29	D	408	LMG	O2-C2-C1	-2.13	104.86	110.05
25	B	607	CLA	CHB-C4A-NA	2.13	127.46	124.51
28	D	407	PL9	C27-C28-C29	-2.13	122.52	127.66
28	d	406	PL9	O2-C1-C2	-2.13	116.89	121.78
31	d	407	LHG	C5-O7-C7	-2.13	112.54	117.79
27	b	619	BCR	C29-C30-C25	2.13	113.76	110.48
25	b	603	CLA	C11-C12-C13	-2.13	109.03	115.92
25	b	611	CLA	CHC-C1C-NC	2.13	127.43	124.20
25	A	606	CLA	C11-C12-C13	-2.13	109.04	115.92
32	c	518	DGD	C5B-C4B-C3B	-2.13	103.62	114.42
29	c	524	LMG	O7-C10-O9	-2.13	118.56	123.70
25	b	607	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
32	C	516	DGD	C6D-C5D-C4D	2.13	116.53	112.09
32	A	617	DGD	CFB-CEB-CDB	-2.12	103.64	114.42
25	C	510	CLA	C16-C15-C13	-2.12	109.05	115.92
25	C	505	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
27	C	514	BCR	C33-C5-C6	-2.12	122.15	124.53
29	d	411	LMG	O1-C1-C2	-2.12	105.00	108.30
25	C	504	CLA	CHA-C1A-NA	-2.12	121.55	126.40
27	A	610	BCR	C2-C1-C6	2.12	113.74	110.48
27	B	618	BCR	C27-C26-C25	2.12	125.80	122.73
25	B	615	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
25	c	510	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
28	A	611	PL9	O1-C4-C3	-2.11	118.39	120.72
29	C	518	LMG	O7-C10-O9	-2.11	118.59	123.70
25	B	601	CLA	CHB-C4A-NA	2.11	127.44	124.51
29	C	518	LMG	O3-C3-C2	-2.11	105.47	110.35
29	m	101	LMG	O2-C2-C1	-2.11	104.93	110.05
30	L	101	SQD	C9-C8-C7	-2.11	105.96	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	515	DGD	O1G-C1A-C2A	-2.11	105.30	111.91
25	c	505	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
28	a	611	PL9	C11-C12-C13	-2.11	104.96	111.88
31	A	614	LHG	C18-C17-C16	-2.11	103.74	114.42
25	B	609	CLA	CAC-C3C-C4C	2.10	127.54	124.81
33	j	101	STE	C3-C2-C1	-2.10	109.17	114.47
30	a	614	SQD	C9-C8-C7	-2.10	105.98	113.62
26	d	401	PHO	CMA-C3A-C4A	-2.10	109.78	114.38
27	T	101	BCR	C38-C26-C27	-2.10	109.58	113.62
27	B	618	BCR	C38-C26-C25	-2.10	122.17	124.53
27	Y	101	BCR	C37-C22-C21	-2.10	119.98	122.92
27	t	101	BCR	C27-C26-C25	2.10	125.78	122.73
32	h	101	DGD	CAB-C9B-C8B	-2.10	103.78	114.42
25	b	613	CLA	CHA-C4D-ND	2.09	136.88	132.50
27	c	514	BCR	C2-C1-C6	2.09	113.70	110.48
25	B	616	CLA	O2D-CGD-CBD	2.09	114.99	111.27
25	B	606	CLA	CHD-C4C-NC	2.09	127.50	124.20
25	B	613	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
35	E	101	HEM	C4D-ND-C1D	2.09	107.23	105.07
25	B	603	CLA	C3C-C4C-NC	-2.09	108.23	110.57
29	M	101	LMG	O2-C2-C1	-2.09	104.97	110.05
25	C	508	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	C	505	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
32	A	617	DGD	CAB-C9B-C8B	-2.09	103.82	114.42
27	Y	101	BCR	C16-C15-C14	-2.09	119.20	123.47
31	l	101	LHG	C18-C17-C16	-2.09	103.83	114.42
29	d	411	LMG	C3-C4-C5	-2.09	106.52	110.24
25	c	510	CLA	O1D-CGD-CBD	2.08	128.75	124.48
28	a	611	PL9	C31-C32-C33	-2.08	105.04	111.88
25	C	502	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
29	c	522	LMG	O2-C2-C1	-2.08	104.99	110.05
29	c	522	LMG	C42-C41-C40	-2.08	103.86	114.42
25	C	510	CLA	O2D-CGD-CBD	2.08	114.96	111.27
25	b	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
25	d	403	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
29	c	522	LMG	O3-C3-C2	-2.08	105.55	110.35
26	d	402	PHO	C1B-NB-C4B	2.08	111.35	107.09
25	a	609	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
31	A	614	LHG	O8-C23-O10	-2.07	118.36	123.59
25	B	606	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	b	615	CLA	CHC-C1C-NC	2.07	127.35	124.20
27	B	618	BCR	C33-C5-C6	-2.07	122.20	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	t	101	BCR	C1-C6-C5	-2.07	119.69	122.61
29	D	411	LMG	C38-C37-C36	-2.07	103.91	114.42
28	a	611	PL9	C32-C33-C34	-2.07	122.67	127.66
32	C	515	DGD	O3E-C3E-C2E	-2.07	105.56	110.35
25	b	609	CLA	CHA-C1A-NA	-2.07	121.66	126.40
25	B	604	CLA	O2D-CGD-CBD	2.07	114.94	111.27
31	e	101	LHG	C18-C17-C16	-2.07	103.92	114.42
25	B	616	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	D	404	CLA	C11-C12-C13	-2.07	109.23	115.92
33	B	625	STE	O2-C1-C2	2.07	120.67	114.03
27	A	610	BCR	C16-C15-C14	-2.07	119.24	123.47
25	c	509	CLA	C1-O2A-CGA	-2.07	111.02	116.44
25	b	613	CLA	C2A-C1A-CHA	2.07	127.47	123.86
30	A	613	SQD	O5-C5-C4	2.07	113.45	109.69
29	A	612	LMG	O7-C10-O9	-2.07	118.71	123.70
28	D	407	PL9	C40-C39-C41	2.07	118.75	115.27
25	b	605	CLA	C7-C6-C5	-2.06	107.75	113.36
28	D	407	PL9	C42-C43-C44	-2.06	122.69	127.66
25	B	601	CLA	C2D-C1D-ND	-2.06	108.58	110.10
28	a	611	PL9	O2-C1-C6	2.06	124.16	120.59
25	B	603	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
28	d	406	PL9	O2-C1-C6	2.06	124.16	120.59
27	c	515	BCR	C8-C9-C10	2.06	122.10	118.94
32	C	516	DGD	O6E-C1E-O5D	-2.06	105.10	109.97
35	f	101	HEM	CHB-C1B-NB	2.06	126.92	124.38
27	A	610	BCR	C8-C7-C6	-2.06	121.43	127.20
32	C	517	DGD	CBB-CAB-C9B	-2.06	103.99	114.42
32	c	518	DGD	CBB-CAB-C9B	-2.06	103.99	114.42
30	F	101	SQD	C1-C2-C3	-2.06	105.72	110.00
32	C	516	DGD	C3D-C4D-C5D	-2.05	106.57	110.24
27	D	406	BCR	C30-C25-C26	-2.05	119.72	122.61
25	C	502	CLA	C16-C15-C13	-2.05	109.28	115.92
25	B	601	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	B	612	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	b	605	CLA	C1-C2-C3	-2.05	122.50	126.04
25	C	503	CLA	C4D-CHA-C1A	2.05	123.74	121.25
27	x	101	BCR	C35-C13-C14	-2.05	120.05	122.92
31	A	614	LHG	C27-C26-C25	-2.05	104.03	114.42
27	d	405	BCR	C11-C10-C9	-2.05	124.39	127.31
25	B	608	CLA	C11-C12-C13	-2.05	109.30	115.92
28	a	611	PL9	C20-C19-C21	2.05	118.72	115.27
29	b	621	LMG	C8-O7-C10	2.05	122.83	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	606	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	a	608	CLA	CHC-C1C-NC	2.05	127.31	124.20
30	A	613	SQD	O47-C7-O49	-2.05	118.76	123.70
25	a	609	CLA	CHA-C1A-NA	-2.05	121.71	126.40
32	C	515	DGD	CBB-CAB-C9B	-2.04	104.05	114.42
25	B	603	CLA	CHD-C1D-C2D	2.04	129.77	125.48
25	b	611	CLA	CHD-C1D-C2D	2.04	129.77	125.48
25	B	616	CLA	C2D-C1D-ND	-2.04	108.60	110.10
27	T	101	BCR	C15-C14-C13	-2.04	124.40	127.31
25	B	610	CLA	C4-C3-C5	2.04	118.70	115.27
25	B	606	CLA	CGD-CBD-CAD	-2.04	104.13	110.73
29	B	621	LMG	C38-C37-C36	-2.04	104.07	114.42
25	b	616	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	c	503	CLA	C7-C6-C5	-2.04	107.83	113.36
32	c	518	DGD	C1D-C2D-C3D	-2.04	105.76	110.00
27	B	617	BCR	C33-C5-C6	-2.03	122.24	124.53
33	C	519	STE	C6-C5-C4	-2.03	104.09	114.42
27	H	101	BCR	C2-C1-C6	2.03	113.61	110.48
32	h	101	DGD	O5D-C6D-C5D	-2.03	105.28	109.05
25	a	612	CLA	C2D-C1D-ND	-2.03	108.61	110.10
28	A	611	PL9	O2-C1-C2	-2.03	117.12	121.78
27	b	619	BCR	C27-C26-C25	2.03	125.68	122.73
32	c	518	DGD	C7B-C6B-C5B	-2.03	104.11	114.42
29	d	410	LMG	C38-C37-C36	-2.03	104.12	114.42
28	a	611	PL9	C35-C34-C36	2.03	118.68	115.27
25	c	502	CLA	CED-O2D-CGD	2.03	120.53	115.94
31	l	101	LHG	C27-C26-C25	-2.03	104.13	114.42
25	D	405	CLA	O2D-CGD-CBD	2.03	114.87	111.27
25	C	503	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
25	C	503	CLA	C1-C2-C3	2.03	129.55	126.04
27	A	610	BCR	C38-C26-C25	-2.03	122.25	124.53
28	a	611	PL9	O1-C4-C3	-2.03	118.49	120.72
25	c	509	CLA	C11-C10-C8	-2.03	109.37	115.92
27	A	610	BCR	C7-C8-C9	-2.03	123.17	126.23
29	D	408	LMG	O3-C3-C2	-2.02	105.67	110.35
32	A	617	DGD	C1D-C2D-C3D	-2.02	105.78	110.00
27	b	617	BCR	C29-C30-C25	2.02	113.59	110.48
33	t	102	STE	O2-C1-C2	2.02	120.53	114.03
25	C	503	CLA	O1D-CGD-CBD	2.02	128.62	124.48
31	d	408	LHG	C27-C26-C25	-2.02	104.17	114.42
25	C	501	CLA	C4-C3-C5	2.02	118.67	115.27
33	C	520	STE	O2-C1-C2	2.02	120.52	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	406	PL9	C32-C33-C34	-2.02	122.80	127.66
25	C	511	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
27	A	610	BCR	C37-C22-C21	-2.02	120.10	122.92
28	a	611	PL9	C27-C28-C29	-2.02	122.80	127.66
32	c	518	DGD	O6E-C1E-O5D	-2.01	105.21	109.97
32	C	517	DGD	C1D-C2D-C3D	-2.01	105.81	110.00
25	C	508	CLA	CHD-C1D-C2D	2.01	129.70	125.48
27	c	516	BCR	C38-C26-C25	-2.01	122.27	124.53
27	a	610	BCR	C39-C30-C25	-2.01	107.04	110.30
29	D	411	LMG	O7-C10-O9	-2.01	118.85	123.70
25	B	615	CLA	C6-C7-C8	-2.01	109.43	115.92
27	c	515	BCR	C33-C5-C6	-2.01	122.27	124.53
25	C	507	CLA	CHA-C1A-NA	-2.00	121.81	126.40
27	C	514	BCR	C35-C13-C14	-2.00	120.12	122.92
30	F	101	SQD	O7-S-C6	2.00	109.32	106.94
27	K	101	BCR	C34-C9-C10	-2.00	120.12	122.92
31	D	410	LHG	O8-C23-C24	2.00	118.19	111.91
25	c	512	CLA	C3C-C4C-NC	-2.00	108.33	110.57
29	c	520	LMG	O2-C2-C1	-2.00	105.19	110.05
26	d	401	PHO	CED-O2D-CGD	2.00	120.46	115.94

All (62) 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	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

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Mol	Chain	Res	Type	Atom
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	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
25	a	607	CLA	ND
25	a	609	CLA	ND
25	a	612	CLA	ND
25	b	601	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	c	501	CLA	ND
25	c	502	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

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Mol	Chain	Res	Type	Atom
25	d	403	CLA	ND
25	d	404	CLA	ND

All (1908) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	609	CLA	C2-C3-C5-C6
25	A	609	CLA	C4-C3-C5-C6
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	601	CLA	CAD-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	C11-C10-C8-C9
25	B	607	CLA	C2-C3-C5-C6
25	B	607	CLA	C4-C3-C5-C6
25	B	614	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	504	CLA	C4-C3-C5-C6
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	513	CLA	C12-C13-C15-C16
25	D	403	CLA	CHA-CBD-CGD-O1D
25	D	403	CLA	CHA-CBD-CGD-O2D
25	a	608	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	C2-C3-C5-C6
25	b	607	CLA	C4-C3-C5-C6
25	b	607	CLA	C11-C10-C8-C9
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	508	CLA	CHA-CBD-CGD-O1D
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	C6-C7-C8-C9
25	c	511	CLA	C14-C13-C15-C16
27	B	618	BCR	C20-C21-C22-C37
27	B	619	BCR	C7-C8-C9-C34
27	B	619	BCR	C37-C22-C23-C24
27	C	514	BCR	C20-C21-C22-C37
27	D	406	BCR	C37-C22-C23-C24
27	D	406	BCR	C22-C23-C24-C25
27	D	406	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	D	406	BCR	C23-C24-C25-C30
27	H	101	BCR	C11-C12-C13-C35
27	H	101	BCR	C23-C24-C25-C30
27	K	101	BCR	C7-C8-C9-C34
27	K	101	BCR	C37-C22-C23-C24
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C11-C12-C13-C35
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	T	101	BCR	C7-C8-C9-C10
27	T	101	BCR	C7-C8-C9-C34
27	Y	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C37-C22-C23-C24
27	b	617	BCR	C1-C6-C7-C8
27	b	617	BCR	C20-C21-C22-C37
27	b	618	BCR	C7-C8-C9-C34
27	b	619	BCR	C37-C22-C23-C24
27	d	405	BCR	C7-C8-C9-C34
27	d	405	BCR	C21-C22-C23-C24
27	d	405	BCR	C23-C24-C25-C30
27	k	101	BCR	C7-C8-C9-C34
27	k	101	BCR	C17-C18-C19-C20
27	k	101	BCR	C20-C21-C22-C37
27	t	101	BCR	C7-C8-C9-C34
28	A	611	PL9	C12-C13-C14-C15
28	A	611	PL9	C12-C13-C14-C16
28	A	611	PL9	C22-C23-C24-C25
28	A	611	PL9	C32-C33-C34-C36
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C40-C39-C41-C42
28	D	407	PL9	C32-C33-C34-C36
28	D	407	PL9	C47-C48-C49-C50
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C35-C34-C36-C37
28	a	611	PL9	C42-C43-C44-C46
28	a	611	PL9	C44-C46-C47-C48
28	d	406	PL9	C40-C39-C41-C42
28	d	406	PL9	C42-C43-C44-C46
28	d	406	PL9	C47-C48-C49-C51
29	A	612	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
29	A	612	LMG	O1-C7-C8-O7
29	A	612	LMG	O9-C10-O7-C8
29	A	612	LMG	C11-C10-O7-C8
29	c	524	LMG	O6-C1-O1-C7
30	A	616	SQD	C44-C45-C46-O48
30	B	622	SQD	C2-C1-O6-C44
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	C8-C7-O47-C45
30	B	622	SQD	O5-C5-C6-S
30	F	101	SQD	C45-C44-O6-C1
30	L	101	SQD	C8-C7-O47-C45
30	L	101	SQD	O10-C23-O48-C46
30	L	101	SQD	C24-C23-O48-C46
30	a	614	SQD	C8-C7-O47-C45
30	f	102	SQD	C2-C1-O6-C44
30	f	102	SQD	O5-C1-O6-C44
31	A	614	LHG	C3-O3-P-O5
31	A	614	LHG	O10-C23-O8-C6
31	A	615	LHG	C3-O3-P-O4
31	A	615	LHG	C4-O6-P-O4
31	D	409	LHG	C1-C2-C3-O3
31	D	409	LHG	O2-C2-C3-O3
31	D	409	LHG	C3-O3-P-O5
31	D	409	LHG	C4-O6-P-O4
31	D	412	LHG	O1-C1-C2-C3
31	D	412	LHG	C1-C2-C3-O3
31	D	412	LHG	C3-O3-P-O4
31	D	412	LHG	C3-O3-P-O5
31	D	412	LHG	C3-O3-P-O6
31	d	407	LHG	O1-C1-C2-O2
31	d	407	LHG	O1-C1-C2-C3
31	d	408	LHG	O1-C1-C2-C3
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C4-O6-P-O4
31	e	101	LHG	O1-C1-C2-O2
31	e	101	LHG	O1-C1-C2-C3
31	e	101	LHG	C3-O3-P-O4
31	e	101	LHG	O6-C4-C5-O7
31	e	101	LHG	O10-C23-O8-C6
31	l	101	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
32	A	617	DGD	O1B-C1B-O2G-C2G
25	b	601	CLA	CBD-CGD-O2D-CED
25	c	509	CLA	CBD-CGD-O2D-CED
25	c	510	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
26	d	402	PHO	CBD-CGD-O2D-CED
25	B	601	CLA	O1A-CGA-O2A-C1
30	F	101	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
25	B	601	CLA	CBA-CGA-O2A-C1
30	F	101	SQD	C24-C23-O48-C46
30	f	102	SQD	C24-C23-O48-C46
31	A	614	LHG	C24-C23-O8-C6
31	e	101	LHG	C24-C23-O8-C6
28	d	406	PL9	C47-C48-C49-C50
25	c	511	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED
25	b	601	CLA	O1D-CGD-O2D-CED
29	D	411	LMG	O9-C10-O7-C8
29	b	621	LMG	O9-C10-O7-C8
29	c	522	LMG	O9-C10-O7-C8
30	L	101	SQD	O49-C7-O47-C45
30	a	614	SQD	O49-C7-O47-C45
32	a	615	DGD	O1B-C1B-O2G-C2G
25	B	605	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
32	A	617	DGD	C2B-C1B-O2G-C2G
32	a	615	DGD	C2B-C1B-O2G-C2G
28	D	407	PL9	C47-C48-C49-C51
29	c	522	LMG	O6-C5-C6-O5
25	B	605	CLA	C4-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
28	A	611	PL9	C43-C44-C46-C47
28	d	406	PL9	C38-C39-C41-C42
25	B	603	CLA	CBD-CGD-O2D-CED
29	M	101	LMG	O10-C28-O8-C9
25	b	614	CLA	C3-C5-C6-C7
25	c	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	B	622	SQD	C24-C23-O48-C46
28	A	611	PL9	C27-C28-C29-C30
26	d	402	PHO	O1D-CGD-O2D-CED
28	A	611	PL9	C22-C23-C24-C26
28	A	611	PL9	C37-C38-C39-C41
29	c	524	LMG	O10-C28-O8-C9
30	B	622	SQD	O10-C23-O48-C46
25	c	509	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
25	b	606	CLA	C3-C5-C6-C7
30	a	614	SQD	C24-C23-O48-C46
32	c	519	DGD	O1A-C1A-O1G-C1G
29	C	518	LMG	C11-C10-O7-C8
29	b	621	LMG	C11-C10-O7-C8
25	B	610	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
29	b	621	LMG	O10-C28-O8-C9
30	L	101	SQD	C12-C13-C14-C15
31	D	412	LHG	C28-C29-C30-C31
31	d	409	LHG	C24-C25-C26-C27
29	c	524	LMG	C4-C5-C6-O5
25	C	513	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6
25	c	507	CLA	C4-C3-C5-C6
28	A	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C45-C44-C46-C47
29	c	522	LMG	C4-C5-C6-O5
25	B	614	CLA	C2-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	c	507	CLA	C2-C3-C5-C6
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C38-C39-C41-C42
28	a	611	PL9	C33-C34-C36-C37
25	D	404	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C2A-CAA-CBA-CGA
30	F	101	SQD	O5-C1-O6-C44
28	A	611	PL9	C34-C36-C37-C38
28	D	407	PL9	C44-C46-C47-C48
29	M	101	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
33	b	622	STE	C4-C5-C6-C7
25	c	510	CLA	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
30	a	614	SQD	O10-C23-O48-C46
29	D	411	LMG	C11-C10-O7-C8
25	B	604	CLA	C3-C5-C6-C7
25	C	509	CLA	C3-C5-C6-C7
25	C	513	CLA	C3-C5-C6-C7
25	a	609	CLA	CBA-CGA-O2A-C1
29	C	518	LMG	C29-C28-O8-C9
29	c	524	LMG	C29-C28-O8-C9
32	a	615	DGD	C2A-C1A-O1G-C1G
30	a	613	SQD	C11-C12-C13-C14
33	T	102	STE	C3-C4-C5-C6
30	A	616	SQD	C44-C45-O47-C7
29	c	524	LMG	O6-C5-C6-O5
32	A	617	DGD	C4E-C5E-C6E-O5E
25	B	611	CLA	C8-C10-C11-C12
25	C	510	CLA	C13-C15-C16-C17
25	b	615	CLA	C5-C6-C7-C8
31	D	412	LHG	O2-C2-C3-O3
29	c	524	LMG	C2-C1-O1-C7
29	c	522	LMG	O7-C8-C9-O8
30	a	613	SQD	O6-C44-C45-O47
32	a	615	DGD	O1A-C1A-O1G-C1G
25	A	607	CLA	C14-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C14
25	B	607	CLA	C14-C13-C15-C16
25	B	613	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16
25	C	503	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C10-C8-C9
25	C	512	CLA	C6-C7-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	C	513	CLA	C6-C7-C8-C9
25	a	608	CLA	C11-C12-C13-C14
25	b	601	CLA	C14-C13-C15-C16
25	b	606	CLA	C14-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C9
25	c	502	CLA	C6-C7-C8-C9
25	c	509	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	c	512	CLA	C6-C7-C8-C9
26	A	608	PHO	C14-C13-C15-C16
25	D	405	CLA	C10-C11-C12-C13
25	c	503	CLA	C5-C6-C7-C8
25	b	606	CLA	C2A-CAA-CBA-CGA
27	c	515	BCR	C7-C8-C9-C34
27	d	405	BCR	C37-C22-C23-C24
27	x	101	BCR	C7-C8-C9-C34
32	A	617	DGD	O6E-C5E-C6E-O5E
32	C	515	DGD	O6E-C5E-C6E-O5E
32	c	519	DGD	C8A-C9A-CAA-CBA
29	A	612	LMG	C4-C5-C6-O5
30	A	616	SQD	C7-C8-C9-C10
25	B	607	CLA	C10-C11-C12-C13
25	C	503	CLA	C5-C6-C7-C8
25	c	509	CLA	C10-C11-C12-C13
25	c	506	CLA	CBA-CGA-O2A-C1
25	B	607	CLA	C8-C10-C11-C12
25	C	506	CLA	C8-C10-C11-C12
25	C	506	CLA	C13-C15-C16-C17
25	C	509	CLA	C8-C10-C11-C12
25	C	513	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
25	c	506	CLA	C8-C10-C11-C12
25	c	510	CLA	C10-C11-C12-C13
29	D	411	LMG	C10-C11-C12-C13
29	b	621	LMG	C10-C11-C12-C13
30	A	613	SQD	C7-C8-C9-C10
32	H	102	DGD	C1A-C2A-C3A-C4A
32	c	518	DGD	C1B-C2B-C3B-C4B
25	B	603	CLA	C15-C16-C17-C18
25	B	607	CLA	C5-C6-C7-C8
25	C	509	CLA	C5-C6-C7-C8
25	a	609	CLA	C5-C6-C7-C8
25	b	614	CLA	C13-C15-C16-C17
25	c	503	CLA	C8-C10-C11-C12
25	c	506	CLA	C13-C15-C16-C17
28	d	406	PL9	C42-C43-C44-C45
25	a	609	CLA	O1A-CGA-O2A-C1
29	d	411	LMG	C28-C29-C30-C31
30	B	622	SQD	C23-C24-C25-C26
30	L	101	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	d	407	LHG	C7-C8-C9-C10
31	d	407	LHG	C23-C24-C25-C26
31	d	409	LHG	C23-C24-C25-C26
31	e	101	LHG	C23-C24-C25-C26
32	C	515	DGD	C1A-C2A-C3A-C4A
33	B	624	STE	C1-C2-C3-C4
33	E	102	STE	C1-C2-C3-C4
30	L	101	SQD	C11-C10-C9-C8
25	D	403	CLA	C15-C16-C17-C18
25	b	611	CLA	C8-C10-C11-C12
25	B	606	CLA	C13-C15-C16-C17
31	A	614	LHG	C7-C8-C9-C10
32	a	615	DGD	C1A-C2A-C3A-C4A
32	c	518	DGD	C1A-C2A-C3A-C4A
25	A	607	CLA	C12-C13-C15-C16
25	B	611	CLA	C12-C13-C15-C16
25	C	508	CLA	C12-C13-C15-C16
25	C	513	CLA	C11-C10-C8-C7
25	b	606	CLA	C11-C10-C8-C7
25	b	607	CLA	C11-C10-C8-C7
25	b	615	CLA	C11-C12-C13-C15
25	c	506	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1D-CGD-O2D-CED
25	B	613	CLA	C5-C6-C7-C8
25	b	601	CLA	C10-C11-C12-C13
25	c	510	CLA	C15-C16-C17-C18
29	C	518	LMG	O6-C1-O1-C7
32	C	516	DGD	O6E-C1E-O5D-C6D
25	B	613	CLA	C8-C10-C11-C12
28	A	611	PL9	C19-C21-C22-C23
28	A	611	PL9	C24-C26-C27-C28
28	d	406	PL9	C44-C46-C47-C48
33	B	620	STE	C1-C2-C3-C4
27	K	101	BCR	C10-C11-C12-C13
27	K	102	BCR	C18-C19-C20-C21
27	c	514	BCR	C18-C19-C20-C21
27	c	515	BCR	C18-C19-C20-C21
27	d	405	BCR	C10-C11-C12-C13
31	d	407	LHG	O2-C2-C3-O3
31	e	101	LHG	O2-C2-C3-O3
25	a	607	CLA	C15-C16-C17-C18
25	B	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	B	607	CLA	C13-C15-C16-C17
25	C	509	CLA	C10-C11-C12-C13
25	C	513	CLA	C5-C6-C7-C8
25	D	403	CLA	C13-C15-C16-C17
25	b	615	CLA	C15-C16-C17-C18
25	c	511	CLA	C15-C16-C17-C18
25	c	512	CLA	C13-C15-C16-C17
25	B	606	CLA	C10-C11-C12-C13
25	b	601	CLA	C13-C15-C16-C17
25	b	603	CLA	C13-C15-C16-C17
25	b	614	CLA	C8-C10-C11-C12
25	c	511	CLA	C13-C15-C16-C17
25	d	404	CLA	C8-C10-C11-C12
31	D	409	LHG	C3-O3-P-O6
31	d	407	LHG	C3-O3-P-O6
31	d	408	LHG	C3-O3-P-O6
31	e	101	LHG	C3-O3-P-O6
29	c	522	LMG	C10-C11-C12-C13
32	a	615	DGD	C1B-C2B-C3B-C4B
29	m	101	LMG	C29-C28-O8-C9
32	c	519	DGD	C2A-C1A-O1G-C1G
25	b	607	CLA	C8-C10-C11-C12
29	M	101	LMG	C28-C29-C30-C31
29	b	621	LMG	O6-C5-C6-O5
31	A	614	LHG	C1-C2-C3-O3
31	d	407	LHG	C1-C2-C3-O3
31	e	101	LHG	C1-C2-C3-O3
28	a	611	PL9	C32-C33-C34-C36
25	C	505	CLA	C10-C11-C12-C13
25	C	512	CLA	C13-C15-C16-C17
25	b	607	CLA	C10-C11-C12-C13
25	b	614	CLA	C16-C17-C18-C19
25	c	511	CLA	C16-C17-C18-C20
29	b	621	LMG	C29-C28-O8-C9
33	H	103	STE	C11-C12-C13-C14
33	l	102	STE	C3-C4-C5-C6
29	c	522	LMG	C11-C10-O7-C8
25	C	512	CLA	C8-C10-C11-C12
25	c	510	CLA	C8-C10-C11-C12
27	H	101	BCR	C20-C21-C22-C37
27	K	101	BCR	C16-C17-C18-C36
27	K	102	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
27	T	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C16-C17-C18-C36
27	b	617	BCR	C11-C10-C9-C34
27	b	618	BCR	C20-C21-C22-C37
27	b	619	BCR	C35-C13-C14-C15
27	b	619	BCR	C20-C21-C22-C37
27	c	514	BCR	C16-C17-C18-C36
27	k	101	BCR	C16-C17-C18-C36
27	t	101	BCR	C20-C21-C22-C37
29	A	612	LMG	C33-C34-C35-C36
29	C	518	LMG	C17-C18-C19-C20
29	D	408	LMG	C14-C15-C16-C17
29	D	411	LMG	C34-C35-C36-C37
29	M	101	LMG	C37-C38-C39-C40
29	c	522	LMG	C39-C40-C41-C42
29	d	410	LMG	C35-C36-C37-C38
29	m	101	LMG	C39-C40-C41-C42
30	F	101	SQD	C25-C26-C27-C28
30	a	614	SQD	C18-C19-C20-C21
31	D	409	LHG	C10-C11-C12-C13
31	d	408	LHG	C29-C30-C31-C32
31	e	101	LHG	C27-C28-C29-C30
32	C	515	DGD	C7B-C8B-C9B-CAB
32	a	615	DGD	C8B-C9B-CAB-CBB
32	c	517	DGD	C4B-C5B-C6B-C7B
32	h	101	DGD	C6B-C7B-C8B-C9B
33	B	625	STE	C5-C6-C7-C8
33	H	103	STE	C5-C6-C7-C8
33	I	101	STE	C10-C11-C12-C13
33	M	102	STE	C9-C10-C11-C12
33	d	413	STE	C10-C11-C12-C13
25	D	403	CLA	C16-C17-C18-C20
25	b	615	CLA	C16-C17-C18-C20
29	B	621	LMG	C33-C34-C35-C36
29	C	518	LMG	C13-C14-C15-C16
30	A	613	SQD	C16-C17-C18-C19
30	a	613	SQD	C17-C18-C19-C20
31	D	410	LHG	C29-C30-C31-C32
31	d	409	LHG	C26-C27-C28-C29
31	l	101	LHG	C32-C33-C34-C35
32	c	517	DGD	C7A-C8A-C9A-CAA
32	c	517	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
33	B	626	STE	C3-C4-C5-C6
33	d	413	STE	C11-C12-C13-C14
33	m	102	STE	C5-C6-C7-C8
33	x	102	STE	C2-C3-C4-C5
33	x	102	STE	C7-C8-C9-C10
30	L	101	SQD	C46-C45-O47-C7
29	C	518	LMG	C31-C32-C33-C34
31	D	410	LHG	C27-C28-C29-C30
32	c	517	DGD	C9B-CAB-CBB-CCB
32	c	518	DGD	C2A-C3A-C4A-C5A
33	C	520	STE	C3-C4-C5-C6
33	a	616	STE	C2-C3-C4-C5
33	b	622	STE	C14-C15-C16-C17
29	D	408	LMG	C36-C37-C38-C39
29	D	411	LMG	C14-C15-C16-C17
29	M	101	LMG	C14-C15-C16-C17
29	c	520	LMG	C31-C32-C33-C34
30	A	613	SQD	C11-C10-C9-C8
30	A	613	SQD	C10-C11-C12-C13
30	A	616	SQD	C18-C19-C20-C21
30	a	614	SQD	C10-C11-C12-C13
30	f	102	SQD	C29-C30-C31-C32
31	D	410	LHG	C25-C26-C27-C28
31	d	407	LHG	C18-C19-C20-C21
33	b	622	STE	C12-C13-C14-C15
33	x	102	STE	C12-C13-C14-C15
29	B	621	LMG	C32-C33-C34-C35
29	c	522	LMG	C16-C17-C18-C19
31	d	408	LHG	C32-C33-C34-C35
31	l	101	LHG	C24-C25-C26-C27
32	c	518	DGD	C8A-C9A-CAA-CBA
33	E	102	STE	C3-C4-C5-C6
31	A	614	LHG	C23-C24-C25-C26
27	C	514	BCR	C20-C21-C22-C23
27	K	101	BCR	C20-C21-C22-C23
27	b	618	BCR	C11-C10-C9-C8
27	c	514	BCR	C12-C13-C14-C15
27	c	514	BCR	C16-C17-C18-C19
27	k	101	BCR	C20-C21-C22-C23
27	x	101	BCR	C11-C10-C9-C8
27	x	101	BCR	C16-C17-C18-C19
29	A	612	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
29	C	518	LMG	C2-C1-O1-C7
32	C	516	DGD	C2E-C1E-O5D-C6D
32	c	518	DGD	C2E-C1E-O5D-C6D
25	c	512	CLA	CBA-CGA-O2A-C1
29	b	621	LMG	C11-C12-C13-C14
30	A	616	SQD	C28-C29-C30-C31
30	a	614	SQD	C14-C15-C16-C17
31	D	410	LHG	C34-C35-C36-C37
31	d	407	LHG	C32-C33-C34-C35
31	d	408	LHG	C34-C35-C36-C37
32	c	518	DGD	CCA-CDA-CEA-CFA
33	T	103	STE	C11-C10-C9-C8
33	a	617	STE	C4-C5-C6-C7
33	b	620	STE	C14-C15-C16-C17
25	C	510	CLA	C15-C16-C17-C18
25	B	602	CLA	C16-C17-C18-C19
25	a	608	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C19
25	b	609	CLA	C4-C3-C5-C6
29	d	410	LMG	C33-C34-C35-C36
30	B	622	SQD	C11-C12-C13-C14
31	A	615	LHG	C18-C19-C20-C21
31	l	101	LHG	C11-C12-C13-C14
32	C	516	DGD	C5A-C6A-C7A-C8A
32	H	102	DGD	C6A-C7A-C8A-C9A
32	c	519	DGD	CCA-CDA-CEA-CFA
33	B	620	STE	C9-C10-C11-C12
33	D	413	STE	C4-C5-C6-C7
33	t	102	STE	C11-C10-C9-C8
28	d	406	PL9	C33-C34-C36-C37
25	B	611	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C10-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	C	513	CLA	C14-C13-C15-C16
25	b	601	CLA	C6-C7-C8-C9
25	b	614	CLA	C6-C7-C8-C9
25	d	403	CLA	C6-C7-C8-C9
32	C	515	DGD	C1B-C2B-C3B-C4B
29	B	621	LMG	C31-C32-C33-C34
29	B	621	LMG	C34-C35-C36-C37
29	M	101	LMG	C33-C34-C35-C36
29	b	621	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
30	B	622	SQD	C18-C19-C20-C21
31	A	614	LHG	C17-C18-C19-C20
31	d	407	LHG	C11-C10-C9-C8
31	d	407	LHG	C16-C17-C18-C19
31	d	408	LHG	C12-C13-C14-C15
32	A	617	DGD	C2B-C3B-C4B-C5B
32	C	515	DGD	C9B-CAB-CBB-CCB
32	H	102	DGD	CAB-CBB-CCB-CDB
32	a	615	DGD	C6A-C7A-C8A-C9A
32	c	517	DGD	C4A-C5A-C6A-C7A
32	c	517	DGD	CCB-CDB-CEB-CFB
32	h	101	DGD	C3B-C4B-C5B-C6B
33	C	519	STE	C6-C7-C8-C9
33	d	413	STE	C2-C3-C4-C5
33	l	102	STE	C7-C8-C9-C10
25	c	512	CLA	C2A-CAA-CBA-CGA
27	K	102	BCR	C37-C22-C23-C24
31	D	410	LHG	C11-C12-C13-C14
32	H	102	DGD	C6B-C7B-C8B-C9B
33	d	413	STE	C5-C6-C7-C8
31	D	409	LHG	O1-C1-C2-C3
31	D	410	LHG	O1-C1-C2-C3
31	d	409	LHG	O1-C1-C2-C3
27	Y	101	BCR	C21-C22-C23-C24
27	b	617	BCR	C21-C22-C23-C24
27	k	101	BCR	C7-C8-C9-C10
32	c	517	DGD	O6E-C5E-C6E-O5E
25	C	505	CLA	C15-C16-C17-C18
25	d	404	CLA	C5-C6-C7-C8
29	D	408	LMG	C31-C32-C33-C34
29	b	621	LMG	C16-C17-C18-C19
29	c	522	LMG	C15-C16-C17-C18
32	c	517	DGD	C6B-C7B-C8B-C9B
33	c	521	STE	C9-C10-C11-C12
28	A	611	PL9	C27-C28-C29-C31
29	D	408	LMG	C10-C11-C12-C13
30	F	101	SQD	C23-C24-C25-C26
32	c	519	DGD	C1A-C2A-C3A-C4A
33	d	412	STE	C1-C2-C3-C4
33	d	413	STE	C1-C2-C3-C4
29	D	408	LMG	C15-C16-C17-C18
29	M	101	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	M	101	LMG	C15-C16-C17-C18
29	b	621	LMG	C40-C41-C42-C43
29	c	520	LMG	C38-C39-C40-C41
29	d	411	LMG	C39-C40-C41-C42
30	a	613	SQD	C26-C27-C28-C29
31	A	614	LHG	C15-C16-C17-C18
31	A	614	LHG	C25-C26-C27-C28
31	A	615	LHG	C27-C28-C29-C30
31	D	410	LHG	C9-C10-C11-C12
31	D	410	LHG	C33-C34-C35-C36
31	e	101	LHG	C11-C12-C13-C14
31	l	101	LHG	C33-C34-C35-C36
32	A	617	DGD	C2A-C3A-C4A-C5A
32	C	515	DGD	C4B-C5B-C6B-C7B
32	c	519	DGD	C9A-CAA-CBA-CCA
32	c	519	DGD	CBA-CCA-CDA-CEA
33	B	624	STE	C5-C6-C7-C8
33	B	624	STE	C12-C13-C14-C15
33	C	521	STE	C3-C4-C5-C6
33	D	413	STE	C7-C8-C9-C10
33	D	413	STE	C14-C15-C16-C17
33	J	101	STE	C3-C4-C5-C6
33	T	103	STE	C2-C3-C4-C5
33	b	620	STE	C2-C3-C4-C5
25	b	607	CLA	C16-C17-C18-C19
25	c	503	CLA	C16-C17-C18-C20
29	M	101	LMG	O6-C1-O1-C7
25	B	616	CLA	C5-C6-C7-C8
25	b	613	CLA	C13-C15-C16-C17
29	D	408	LMG	C17-C18-C19-C20
31	A	614	LHG	C13-C14-C15-C16
31	A	614	LHG	C29-C30-C31-C32
31	A	615	LHG	C12-C13-C14-C15
31	A	615	LHG	C17-C18-C19-C20
31	A	615	LHG	C32-C33-C34-C35
31	e	101	LHG	C17-C18-C19-C20
31	l	101	LHG	C16-C17-C18-C19
32	H	102	DGD	C8B-C9B-CAB-CBB
33	x	102	STE	C3-C4-C5-C6
25	B	603	CLA	O1D-CGD-O2D-CED
29	C	518	LMG	C30-C31-C32-C33
29	c	524	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	c	524	LMG	C33-C34-C35-C36
30	A	613	SQD	C12-C13-C14-C15
30	F	101	SQD	C26-C27-C28-C29
31	D	410	LHG	C15-C16-C17-C18
32	H	102	DGD	C5A-C6A-C7A-C8A
32	a	615	DGD	C5A-C6A-C7A-C8A
32	h	101	DGD	C5B-C6B-C7B-C8B
33	I	101	STE	C4-C5-C6-C7
33	c	523	STE	C5-C6-C7-C8
30	a	614	SQD	C11-C12-C13-C14
30	f	102	SQD	C24-C25-C26-C27
31	D	409	LHG	C17-C18-C19-C20
32	A	617	DGD	C8B-C9B-CAB-CBB
32	C	517	DGD	C8A-C9A-CAA-CBA
32	c	517	DGD	C5A-C6A-C7A-C8A
33	j	101	STE	C4-C5-C6-C7
33	m	102	STE	C6-C7-C8-C9
29	b	621	LMG	C12-C13-C14-C15
30	a	614	SQD	C11-C10-C9-C8
33	B	625	STE	C4-C5-C6-C7
33	B	626	STE	C4-C5-C6-C7
25	c	512	CLA	C3A-C2A-CAA-CBA
29	A	612	LMG	C35-C36-C37-C38
29	A	612	LMG	C38-C39-C40-C41
29	c	524	LMG	C12-C13-C14-C15
29	d	410	LMG	C32-C33-C34-C35
32	c	517	DGD	C3B-C4B-C5B-C6B
32	c	517	DGD	C5B-C6B-C7B-C8B
33	d	413	STE	C9-C10-C11-C12
33	x	102	STE	C4-C5-C6-C7
33	x	102	STE	C1-C2-C3-C4
25	B	602	CLA	C16-C17-C18-C20
25	b	604	CLA	C16-C17-C18-C20
25	c	506	CLA	C16-C17-C18-C20
29	c	522	LMG	C32-C33-C34-C35
29	m	101	LMG	C17-C18-C19-C20
30	A	616	SQD	C10-C11-C12-C13
30	a	613	SQD	C13-C14-C15-C16
31	A	614	LHG	C33-C34-C35-C36
32	C	516	DGD	C8B-C9B-CAB-CBB
32	c	517	DGD	C8B-C9B-CAB-CBB
25	C	505	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	D	408	LMG	C32-C33-C34-C35
29	M	101	LMG	C38-C39-C40-C41
29	d	410	LMG	C36-C37-C38-C39
31	D	409	LHG	C30-C31-C32-C33
31	d	409	LHG	C27-C28-C29-C30
32	C	516	DGD	C6A-C7A-C8A-C9A
33	x	102	STE	C5-C6-C7-C8
25	b	601	CLA	O2A-C1-C2-C3
27	D	406	BCR	C14-C15-C16-C17
27	K	101	BCR	C14-C15-C16-C17
25	C	505	CLA	C4-C3-C5-C6
28	D	407	PL9	C30-C29-C31-C32
28	d	406	PL9	C15-C14-C16-C17
25	C	505	CLA	C2-C3-C5-C6
26	A	608	PHO	C2-C3-C5-C6
28	d	406	PL9	C13-C14-C16-C17
31	A	614	LHG	C8-C7-O7-C5
30	A	616	SQD	C46-C45-O47-C7
31	A	615	LHG	C13-C14-C15-C16
31	d	408	LHG	C14-C15-C16-C17
32	C	517	DGD	C8B-C9B-CAB-CBB
31	D	412	LHG	O1-C1-C2-O2
31	d	408	LHG	O1-C1-C2-O2
32	C	516	DGD	C6B-C7B-C8B-C9B
32	a	615	DGD	CEB-CFB-CGB-CHB
32	c	519	DGD	C4A-C5A-C6A-C7A
33	B	620	STE	C6-C7-C8-C9
33	D	413	STE	C6-C7-C8-C9
33	T	103	STE	C3-C4-C5-C6
33	a	617	STE	C5-C6-C7-C8
33	c	521	STE	C11-C12-C13-C14
25	c	512	CLA	O1A-CGA-O2A-C1
25	B	601	CLA	C16-C17-C18-C20
25	B	612	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C19
25	b	607	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
31	d	407	LHG	C15-C16-C17-C18
32	A	617	DGD	CCA-CDA-CEA-CFA
31	e	101	LHG	C11-C10-C9-C8
32	C	516	DGD	CAA-CBA-CCA-CDA
32	C	517	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
33	b	620	STE	C6-C7-C8-C9
29	A	612	LMG	O6-C5-C6-O5
29	A	612	LMG	C12-C13-C14-C15
31	e	101	LHG	O9-C7-O7-C5
25	c	506	CLA	C2-C1-O2A-CGA
29	b	621	LMG	C18-C19-C20-C21
29	c	522	LMG	C30-C31-C32-C33
29	c	522	LMG	C35-C36-C37-C38
30	B	622	SQD	C33-C34-C35-C36
31	D	412	LHG	C26-C27-C28-C29
25	c	507	CLA	C8-C10-C11-C12
29	C	518	LMG	C14-C15-C16-C17
29	D	408	LMG	C39-C40-C41-C42
30	B	622	SQD	C13-C14-C15-C16
31	d	407	LHG	C27-C28-C29-C30
32	a	615	DGD	C6B-C7B-C8B-C9B
33	T	102	STE	C5-C6-C7-C8
25	c	503	CLA	C16-C17-C18-C19
27	H	101	BCR	C23-C24-C25-C26
27	K	102	BCR	C5-C6-C7-C8
27	Y	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	b	617	BCR	C5-C6-C7-C8
27	d	405	BCR	C23-C24-C25-C26
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	t	101	BCR	C1-C6-C7-C8
27	t	101	BCR	C5-C6-C7-C8
29	M	101	LMG	C35-C36-C37-C38
29	b	621	LMG	C13-C14-C15-C16
31	D	409	LHG	C28-C29-C30-C31
31	l	101	LHG	C14-C15-C16-C17
32	c	518	DGD	CCB-CDB-CEB-CFB
25	B	614	CLA	C13-C15-C16-C17
25	B	616	CLA	C8-C10-C11-C12
25	b	604	CLA	C15-C16-C17-C18
25	c	509	CLA	C13-C15-C16-C17
32	c	517	DGD	O6D-C5D-C6D-O5D
31	e	101	LHG	C8-C7-O7-C5
29	D	408	LMG	C12-C13-C14-C15
29	b	621	LMG	C23-C24-C25-C26
30	A	613	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
31	A	615	LHG	C11-C12-C13-C14
33	C	521	STE	C5-C6-C7-C8
33	c	521	STE	C2-C3-C4-C5
30	A	613	SQD	C23-C24-C25-C26
32	c	519	DGD	C1B-C2B-C3B-C4B
30	a	613	SQD	C34-C35-C36-C37
32	c	517	DGD	C8A-C9A-CAA-CBA
32	c	517	DGD	CCA-CDA-CEA-CFA
25	B	601	CLA	C15-C16-C17-C18
29	A	612	LMG	C16-C17-C18-C19
30	a	613	SQD	C15-C16-C17-C18
32	a	615	DGD	C4A-C5A-C6A-C7A
32	a	615	DGD	CEA-CFA-CGA-CHA
33	T	103	STE	C10-C11-C12-C13
33	t	102	STE	C2-C3-C4-C5
25	C	510	CLA	C4-C3-C5-C6
26	A	608	PHO	C4-C3-C5-C6
25	C	505	CLA	C11-C10-C8-C7
25	C	510	CLA	C2-C3-C5-C6
25	C	511	CLA	C6-C7-C8-C10
25	C	512	CLA	C6-C7-C8-C10
25	D	404	CLA	C12-C13-C15-C16
25	a	608	CLA	C6-C7-C8-C10
25	a	608	CLA	C12-C13-C15-C16
25	b	606	CLA	C12-C13-C15-C16
25	b	609	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
25	c	508	CLA	C11-C10-C8-C7
25	c	512	CLA	C11-C12-C13-C15
25	d	403	CLA	C6-C7-C8-C10
31	d	409	LHG	C31-C32-C33-C34
33	d	413	STE	C12-C13-C14-C15
25	b	601	CLA	C15-C16-C17-C18
25	b	603	CLA	C5-C6-C7-C8
25	b	608	CLA	C5-C6-C7-C8
25	C	508	CLA	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	C16-C17-C18-C19
29	c	524	LMG	C28-C29-C30-C31
33	B	625	STE	C1-C2-C3-C4
31	A	614	LHG	C18-C19-C20-C21
32	a	615	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
33	I	101	STE	C7-C8-C9-C10
29	b	621	LMG	C19-C20-C21-C22
29	c	520	LMG	C33-C34-C35-C36
29	d	410	LMG	C31-C32-C33-C34
29	d	410	LMG	C38-C39-C40-C41
31	D	409	LHG	C18-C19-C20-C21
31	D	410	LHG	C14-C15-C16-C17
33	D	413	STE	C13-C14-C15-C16
29	c	524	LMG	C18-C19-C20-C21
32	c	518	DGD	C4A-C5A-C6A-C7A
33	M	102	STE	C11-C10-C9-C8
33	d	412	STE	C6-C7-C8-C9
33	l	102	STE	C13-C14-C15-C16
25	D	404	CLA	O1D-CGD-O2D-CED
29	c	524	LMG	C35-C36-C37-C38
30	L	101	SQD	C29-C30-C31-C32
32	H	102	DGD	CCB-CDB-CEB-CFB
31	D	409	LHG	C29-C30-C31-C32
31	D	412	LHG	C12-C13-C14-C15
25	a	608	CLA	CBD-CGD-O2D-CED
25	a	608	CLA	C16-C17-C18-C19
30	L	101	SQD	O5-C1-O6-C44
32	c	518	DGD	O6D-C1D-O3G-C3G
32	c	518	DGD	O6E-C1E-O5D-C6D
25	C	505	CLA	C5-C6-C7-C8
25	c	505	CLA	C5-C6-C7-C8
29	c	522	LMG	C34-C35-C36-C37
32	a	615	DGD	C7B-C8B-C9B-CAB
32	c	519	DGD	C8B-C9B-CAB-CBB
30	A	616	SQD	C8-C7-O47-C45
27	C	514	BCR	C18-C19-C20-C21
30	L	101	SQD	C24-C25-C26-C27
31	A	614	LHG	C34-C35-C36-C37
32	a	615	DGD	C4B-C5B-C6B-C7B
25	a	609	CLA	C10-C11-C12-C13
25	b	614	CLA	C5-C6-C7-C8
31	A	615	LHG	C30-C31-C32-C33
32	C	515	DGD	CCB-CDB-CEB-CFB
32	h	101	DGD	CBA-CCA-CDA-CEA
33	B	620	STE	C11-C12-C13-C14
29	C	518	LMG	O9-C10-O7-C8
31	d	408	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
32	c	517	DGD	O1B-C1B-O2G-C2G
29	D	411	LMG	C35-C36-C37-C38
29	M	101	LMG	C2-C1-O1-C7
30	B	622	SQD	O6-C44-C45-O47
32	A	617	DGD	O2G-C2G-C3G-O3G
32	C	516	DGD	C9B-CAB-CBB-CCB
25	c	511	CLA	C16-C17-C18-C19
32	H	102	DGD	CBA-CCA-CDA-CEA
25	c	506	CLA	C5-C6-C7-C8
25	c	505	CLA	C4-C3-C5-C6
28	a	611	PL9	C20-C19-C21-C22
28	A	611	PL9	C4-C3-C7-C8
30	a	613	SQD	C19-C20-C21-C22
31	d	409	LHG	C33-C34-C35-C36
32	c	519	DGD	C2B-C3B-C4B-C5B
25	B	601	CLA	C11-C10-C8-C9
25	B	602	CLA	C11-C12-C13-C14
25	B	615	CLA	C11-C12-C13-C14
25	C	503	CLA	C14-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C9
25	C	507	CLA	C11-C10-C8-C9
25	C	513	CLA	C11-C10-C8-C9
25	a	608	CLA	C14-C13-C15-C16
25	b	608	CLA	C11-C12-C13-C14
25	c	504	CLA	C11-C10-C8-C9
25	c	508	CLA	C11-C10-C8-C9
25	c	512	CLA	C11-C12-C13-C14
31	A	614	LHG	C11-C10-C9-C8
33	c	521	STE	C10-C11-C12-C13
25	C	512	CLA	C3-C5-C6-C7
25	b	604	CLA	C3-C5-C6-C7
25	c	501	CLA	C2A-CAA-CBA-CGA
29	c	520	LMG	C36-C37-C38-C39
30	A	613	SQD	C14-C15-C16-C17
31	A	614	LHG	C32-C33-C34-C35
32	c	518	DGD	CAB-CBB-CCB-CDB
29	d	411	LMG	O6-C5-C6-O5
27	B	619	BCR	C11-C12-C13-C35
25	a	608	CLA	C13-C15-C16-C17
25	b	606	CLA	C10-C11-C12-C13
29	B	621	LMG	C16-C17-C18-C19
31	l	101	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
32	C	515	DGD	C8A-C9A-CAA-CBA
27	d	405	BCR	C7-C8-C9-C10
25	b	601	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	512	CLA	C1A-C2A-CAA-CBA
25	c	513	CLA	C1A-C2A-CAA-CBA
25	B	601	CLA	C16-C17-C18-C19
25	C	502	CLA	C16-C17-C18-C20
25	C	513	CLA	C16-C17-C18-C20
30	A	616	SQD	O49-C7-O47-C45
29	D	411	LMG	C16-C17-C18-C19
30	a	613	SQD	C12-C13-C14-C15
31	e	101	LHG	C16-C17-C18-C19
32	c	519	DGD	C5A-C6A-C7A-C8A
27	k	101	BCR	C19-C20-C21-C22
25	B	611	CLA	C13-C15-C16-C17
29	d	411	LMG	C37-C38-C39-C40
30	f	102	SQD	C28-C29-C30-C31
32	h	101	DGD	CAB-CBB-CCB-CDB
33	C	519	STE	C3-C4-C5-C6
25	B	610	CLA	O1D-CGD-O2D-CED
25	b	602	CLA	C15-C16-C17-C18
29	d	410	LMG	C39-C40-C41-C42
32	A	617	DGD	CEB-CFB-CGB-CHB
32	C	517	DGD	C2A-C3A-C4A-C5A
30	a	614	SQD	C15-C16-C17-C18
29	c	520	LMG	C39-C40-C41-C42
31	d	409	LHG	C30-C31-C32-C33
29	c	522	LMG	C11-C12-C13-C14
30	a	613	SQD	C30-C31-C32-C33
31	D	409	LHG	C11-C10-C9-C8
35	f	101	HEM	C2A-CAA-CBA-CGA
29	A	612	LMG	C14-C15-C16-C17
33	C	520	STE	C6-C7-C8-C9
25	C	503	CLA	C15-C16-C17-C18
29	C	518	LMG	C11-C12-C13-C14
29	b	621	LMG	C38-C39-C40-C41
30	A	616	SQD	C30-C31-C32-C33
30	L	101	SQD	C11-C12-C13-C14
33	C	521	STE	C7-C8-C9-C10
33	l	102	STE	C4-C5-C6-C7
25	C	504	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	C	515	DGD	C2A-C3A-C4A-C5A
25	C	501	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	C3-C5-C6-C7
29	A	612	LMG	O1-C7-C8-C9
29	C	518	LMG	O1-C7-C8-C9
29	M	101	LMG	O1-C7-C8-C9
29	M	101	LMG	C7-C8-C9-O8
30	A	613	SQD	O6-C44-C45-C46
30	B	622	SQD	O6-C44-C45-C46
30	a	613	SQD	O6-C44-C45-C46
31	A	614	LHG	C4-C5-C6-O8
32	A	617	DGD	C1G-C2G-C3G-O3G
33	B	624	STE	C7-C8-C9-C10
25	C	513	CLA	C8-C10-C11-C12
25	b	606	CLA	C15-C16-C17-C18
25	b	613	CLA	C10-C11-C12-C13
25	b	616	CLA	C10-C11-C12-C13
29	B	621	LMG	C37-C38-C39-C40
32	C	516	DGD	CDA-CEA-CFA-CGA
33	M	103	STE	C1-C2-C3-C4
32	c	518	DGD	C5D-C6D-O5D-C1E
29	m	101	LMG	C15-C16-C17-C18
29	m	101	LMG	C31-C32-C33-C34
30	A	613	SQD	C17-C18-C19-C20
32	A	617	DGD	C8A-C9A-CAA-CBA
33	B	624	STE	C3-C4-C5-C6
33	b	620	STE	C13-C14-C15-C16
25	B	605	CLA	C8-C10-C11-C12
25	B	615	CLA	C13-C15-C16-C17
29	D	408	LMG	C38-C39-C40-C41
29	D	411	LMG	C37-C38-C39-C40
31	A	614	LHG	C27-C28-C29-C30
29	C	518	LMG	C32-C33-C34-C35
32	C	515	DGD	C6B-C7B-C8B-C9B
32	c	517	DGD	CAB-CBB-CCB-CDB
33	B	620	STE	C7-C8-C9-C10
33	I	101	STE	C2-C3-C4-C5
31	D	409	LHG	O1-C1-C2-O2
30	A	616	SQD	C31-C32-C33-C34
31	A	615	LHG	C31-C32-C33-C34
31	d	408	LHG	C35-C36-C37-C38
31	l	101	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	C4E-C5E-C6E-O5E
30	L	101	SQD	C7-C8-C9-C10
25	A	606	CLA	C2C-C3C-CAC-CBC
29	b	621	LMG	C24-C25-C26-C27
30	f	102	SQD	C34-C35-C36-C37
32	A	617	DGD	C5B-C6B-C7B-C8B
27	c	514	BCR	C35-C13-C14-C15
27	c	515	BCR	C20-C21-C22-C37
32	h	101	DGD	O6E-C5E-C6E-O5E
30	L	101	SQD	C19-C20-C21-C22
32	c	519	DGD	CDA-CEA-CFA-CGA
33	B	626	STE	C6-C7-C8-C9
33	b	620	STE	C12-C13-C14-C15
32	c	518	DGD	O6E-C5E-C6E-O5E
30	A	616	SQD	C17-C18-C19-C20
32	a	615	DGD	CBA-CCA-CDA-CEA
25	B	605	CLA	C13-C15-C16-C17
25	B	612	CLA	C13-C15-C16-C17
25	C	509	CLA	C13-C15-C16-C17
32	C	517	DGD	CDA-CEA-CFA-CGA
33	B	620	STE	C4-C5-C6-C7
33	T	103	STE	C6-C7-C8-C9
29	A	612	LMG	C9-C8-O7-C10
29	D	408	LMG	O6-C5-C6-O5
25	b	615	CLA	C13-C15-C16-C17
25	c	503	CLA	C15-C16-C17-C18
25	C	506	CLA	C2-C1-O2A-CGA
28	d	406	PL9	C32-C33-C34-C36
32	A	617	DGD	CBB-CCB-CDB-CEB
29	d	411	LMG	C14-C15-C16-C17
29	d	411	LMG	C34-C35-C36-C37
29	m	101	LMG	C18-C19-C20-C21
33	B	624	STE	C13-C14-C15-C16
29	c	522	LMG	C29-C28-O8-C9
25	c	506	CLA	C16-C17-C18-C19
31	D	409	LHG	C25-C26-C27-C28
25	A	606	CLA	C13-C15-C16-C17
27	B	619	BCR	C11-C10-C9-C8
27	b	618	BCR	C20-C21-C22-C23
29	b	621	LMG	O1-C7-C8-O7
29	D	411	LMG	C33-C34-C35-C36
29	m	101	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	A	614	LHG	O9-C7-O7-C5
28	a	611	PL9	C47-C48-C49-C51
29	D	411	LMG	C32-C33-C34-C35
31	d	408	LHG	C11-C12-C13-C14
32	H	102	DGD	C7B-C8B-C9B-CAB
33	b	623	STE	C7-C8-C9-C10
28	A	611	PL9	C32-C33-C34-C35
33	D	413	STE	C12-C13-C14-C15
33	c	523	STE	C6-C7-C8-C9
25	b	613	CLA	C8-C10-C11-C12
25	A	607	CLA	C6-C7-C8-C10
25	B	601	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C12-C13-C15
25	B	604	CLA	C11-C10-C8-C7
25	B	604	CLA	C11-C12-C13-C15
25	B	604	CLA	C12-C13-C15-C16
25	B	607	CLA	C12-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C10
25	B	613	CLA	C12-C13-C15-C16
25	B	615	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	C	503	CLA	C12-C13-C15-C16
25	C	506	CLA	C6-C7-C8-C10
25	C	507	CLA	C11-C10-C8-C7
25	C	512	CLA	C11-C10-C8-C7
25	b	602	CLA	C6-C7-C8-C10
25	b	604	CLA	C12-C13-C15-C16
25	b	608	CLA	C11-C12-C13-C15
25	b	614	CLA	C11-C12-C13-C15
25	b	615	CLA	C11-C10-C8-C7
25	b	616	CLA	C11-C10-C8-C7
25	c	504	CLA	C11-C10-C8-C7
25	c	509	CLA	C6-C7-C8-C10
25	c	512	CLA	C11-C10-C8-C7
32	H	102	DGD	O2G-C1B-C2B-C3B
25	C	510	CLA	C3-C5-C6-C7
29	A	612	LMG	C17-C18-C19-C20
30	F	101	SQD	C30-C31-C32-C33
31	A	614	LHG	C24-C25-C26-C27
31	l	101	LHG	C17-C18-C19-C20
33	B	623	STE	C6-C7-C8-C9
33	C	521	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	j	101	STE	C5-C6-C7-C8
25	A	607	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C10-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	604	CLA	C14-C13-C15-C16
25	B	608	CLA	C6-C7-C8-C9
25	B	610	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	C	512	CLA	C11-C12-C13-C14
25	D	403	CLA	C11-C12-C13-C14
25	a	608	CLA	C6-C7-C8-C9
25	b	602	CLA	C6-C7-C8-C9
25	b	604	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C10-C8-C9
25	c	505	CLA	C11-C10-C8-C9
25	c	506	CLA	C11-C10-C8-C9
31	D	410	LHG	C30-C31-C32-C33
32	A	617	DGD	CFA-CGA-CHA-CIA
32	C	516	DGD	CCA-CDA-CEA-CFA
33	T	102	STE	C13-C14-C15-C16
31	d	407	LHG	C14-C15-C16-C17
32	a	615	DGD	CFA-CGA-CHA-CIA
25	c	502	CLA	CBD-CGD-O2D-CED
27	t	101	BCR	C11-C12-C13-C35
25	a	607	CLA	C16-C17-C18-C20
29	c	522	LMG	C13-C14-C15-C16
29	d	410	LMG	C37-C38-C39-C40
30	B	622	SQD	C29-C30-C31-C32
33	B	623	STE	C7-C8-C9-C10
33	b	623	STE	C4-C5-C6-C7
30	a	613	SQD	C31-C32-C33-C34
30	a	614	SQD	C31-C32-C33-C34
32	c	518	DGD	CBA-CCA-CDA-CEA
32	c	519	DGD	C2A-C3A-C4A-C5A
33	b	623	STE	C3-C4-C5-C6
25	c	502	CLA	C3-C5-C6-C7
25	B	606	CLA	C15-C16-C17-C18
25	C	508	CLA	C5-C6-C7-C8
31	D	412	LHG	C9-C10-C11-C12
33	B	625	STE	C3-C4-C5-C6
25	C	513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	B	620	STE	C11-C10-C9-C8
33	B	624	STE	C10-C11-C12-C13
25	C	508	CLA	C8-C10-C11-C12
25	b	608	CLA	C13-C15-C16-C17
31	e	101	LHG	O6-C4-C5-C6
28	a	611	PL9	C34-C36-C37-C38
30	B	622	SQD	C27-C28-C29-C30
33	a	617	STE	C2-C3-C4-C5
33	m	102	STE	C1-C2-C3-C4
32	c	519	DGD	C7B-C8B-C9B-CAB
25	c	502	CLA	C13-C15-C16-C17
25	B	616	CLA	C4-C3-C5-C6
28	A	611	PL9	C15-C14-C16-C17
31	D	410	LHG	C11-C10-C9-C8
30	a	613	SQD	C29-C30-C31-C32
31	d	407	LHG	C29-C30-C31-C32
32	a	615	DGD	CDA-CEA-CFA-CGA
33	C	519	STE	C2-C3-C4-C5
32	c	517	DGD	C4D-C5D-C6D-O5D
29	M	101	LMG	C17-C18-C19-C20
30	A	616	SQD	C33-C34-C35-C36
30	B	622	SQD	C19-C20-C21-C22
33	J	101	STE	C2-C3-C4-C5
25	B	605	CLA	C10-C11-C12-C13
32	C	515	DGD	O1G-C1A-C2A-C3A
29	D	411	LMG	C31-C32-C33-C34
31	e	101	LHG	C14-C15-C16-C17
32	A	617	DGD	CCB-CDB-CEB-CFB
32	C	516	DGD	C4B-C5B-C6B-C7B
32	c	519	DGD	C5B-C6B-C7B-C8B
33	H	103	STE	C13-C14-C15-C16
26	d	402	PHO	C3A-C2A-CAA-CBA
30	B	622	SQD	C9-C10-C11-C12
32	C	516	DGD	C4A-C5A-C6A-C7A
33	H	103	STE	C7-C8-C9-C10
33	T	102	STE	C10-C11-C12-C13
29	C	518	LMG	C15-C16-C17-C18
30	F	101	SQD	C33-C34-C35-C36
32	c	517	DGD	C6A-C7A-C8A-C9A
33	a	616	STE	C5-C6-C7-C8
30	A	616	SQD	C12-C13-C14-C15
25	D	405	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	b	621	LMG	O1-C7-C8-C9
29	c	522	LMG	C7-C8-C9-O8
30	a	613	SQD	C44-C45-C46-O48
30	a	614	SQD	C44-C45-C46-O48
29	b	621	LMG	C39-C40-C41-C42
31	e	101	LHG	C28-C29-C30-C31
32	A	617	DGD	C7B-C8B-C9B-CAB
29	A	612	LMG	C31-C32-C33-C34
30	A	613	SQD	C29-C30-C31-C32
31	l	101	LHG	C30-C31-C32-C33
32	H	102	DGD	C3A-C4A-C5A-C6A
32	h	101	DGD	CCA-CDA-CEA-CFA
25	B	613	CLA	C10-C11-C12-C13
25	C	505	CLA	C16-C17-C18-C19
25	a	607	CLA	C16-C17-C18-C19
25	c	502	CLA	O1D-CGD-O2D-CED
31	D	409	LHG	C32-C33-C34-C35
31	D	409	LHG	C4-O6-P-O3
33	C	520	STE	C1-C2-C3-C4
33	c	521	STE	C1-C2-C3-C4
25	b	601	CLA	C3-C5-C6-C7
29	c	520	LMG	C4-C5-C6-O5
25	B	615	CLA	C5-C6-C7-C8
33	M	102	STE	C4-C5-C6-C7
33	C	520	STE	C4-C5-C6-C7
33	D	413	STE	C11-C12-C13-C14
29	C	518	LMG	O10-C28-O8-C9
25	B	610	CLA	C16-C17-C18-C19
25	B	612	CLA	C16-C17-C18-C19
25	B	603	CLA	C10-C11-C12-C13
26	d	402	PHO	C5-C6-C7-C8
32	H	102	DGD	CDA-CEA-CFA-CGA
32	a	615	DGD	C9B-CAB-CBB-CCB
29	C	518	LMG	C40-C41-C42-C43
31	A	614	LHG	C9-C10-C11-C12
30	A	616	SQD	O47-C45-C46-O48
30	a	613	SQD	C27-C28-C29-C30
31	A	614	LHG	C14-C15-C16-C17
29	M	101	LMG	O7-C8-C9-O8
30	A	613	SQD	O6-C44-C45-O47
30	a	613	SQD	O47-C45-C46-O48
25	C	502	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	C	505	CLA	C16-C17-C18-C20
33	B	626	STE	C2-C3-C4-C5
32	C	516	DGD	O6D-C1D-O3G-C3G
32	c	517	DGD	O6E-C1E-O5D-C6D
25	a	612	CLA	CBD-CGD-O2D-CED
28	A	611	PL9	C29-C31-C32-C33
28	d	406	PL9	C34-C36-C37-C38
32	c	517	DGD	CDB-CEB-CFB-CGB
25	C	502	CLA	C3-C5-C6-C7
25	B	613	CLA	C2-C1-O2A-CGA
25	d	403	CLA	C2-C1-O2A-CGA
31	d	408	LHG	C15-C16-C17-C18
25	b	615	CLA	C10-C11-C12-C13
25	A	607	CLA	C11-C12-C13-C14
25	B	603	CLA	C11-C12-C13-C14
25	B	605	CLA	C6-C7-C8-C9
25	B	613	CLA	C14-C13-C15-C16
25	C	505	CLA	C14-C13-C15-C16
25	C	513	CLA	C11-C12-C13-C14
25	D	405	CLA	C6-C7-C8-C9
25	b	606	CLA	C11-C10-C8-C9
25	b	607	CLA	C14-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C14
25	b	616	CLA	C6-C7-C8-C9
25	c	510	CLA	C11-C12-C13-C14
33	I	101	STE	C12-C13-C14-C15
25	A	606	CLA	C15-C16-C17-C18
25	A	606	CLA	C4C-C3C-CAC-CBC
29	b	621	LMG	C22-C23-C24-C25
29	d	411	LMG	C36-C37-C38-C39
32	C	517	DGD	C3B-C4B-C5B-C6B
32	c	518	DGD	C7B-C8B-C9B-CAB
33	d	412	STE	C11-C10-C9-C8
33	m	102	STE	C4-C5-C6-C7
25	b	610	CLA	C2A-CAA-CBA-CGA
25	D	405	CLA	C16-C17-C18-C19
27	A	610	BCR	C1-C6-C7-C8
27	A	610	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C26
27	C	514	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
27	c	514	BCR	C5-C6-C7-C8
27	c	514	BCR	C23-C24-C25-C26
27	c	514	BCR	C23-C24-C25-C30
27	x	101	BCR	C23-C24-C25-C26
25	c	507	CLA	C5-C6-C7-C8
30	A	613	SQD	C32-C33-C34-C35
29	c	524	LMG	O8-C28-C29-C30
33	B	625	STE	C6-C7-C8-C9
27	D	406	BCR	C7-C8-C9-C10
27	T	101	BCR	C21-C22-C23-C24
25	C	512	CLA	C10-C11-C12-C13
25	b	602	CLA	C10-C11-C12-C13
25	b	607	CLA	C13-C15-C16-C17
25	A	609	CLA	C6-C7-C8-C9
30	L	101	SQD	C26-C27-C28-C29
29	M	101	LMG	C39-C40-C41-C42
30	A	613	SQD	C30-C31-C32-C33
30	a	613	SQD	C35-C36-C37-C38
32	c	519	DGD	C4B-C5B-C6B-C7B
33	B	626	STE	C9-C10-C11-C12
30	B	622	SQD	C35-C36-C37-C38
25	D	403	CLA	C16-C17-C18-C19
31	e	101	LHG	C7-C8-C9-C10
29	A	612	LMG	C40-C41-C42-C43
25	B	601	CLA	C5-C6-C7-C8
25	b	605	CLA	C8-C10-C11-C12
30	B	622	SQD	C16-C17-C18-C19
32	a	615	DGD	C8A-C9A-CAA-CBA
31	l	101	LHG	O6-C4-C5-C6
25	A	607	CLA	C11-C12-C13-C15
25	B	606	CLA	C11-C12-C13-C15
25	C	503	CLA	C11-C10-C8-C7
25	C	505	CLA	C12-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C12-C13-C15
25	C	513	CLA	C6-C7-C8-C10
25	D	403	CLA	C11-C12-C13-C15
25	D	405	CLA	C6-C7-C8-C10
25	a	609	CLA	C12-C13-C15-C16
25	b	603	CLA	C11-C12-C13-C15
25	b	607	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C12-C13-C15-C16
25	c	505	CLA	C6-C7-C8-C10
25	c	505	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C10-C8-C7
25	c	509	CLA	C11-C12-C13-C15
25	c	510	CLA	C6-C7-C8-C10
25	c	511	CLA	C12-C13-C15-C16
30	a	614	SQD	O6-C44-C45-O47
29	D	411	LMG	C15-C16-C17-C18
31	d	407	LHG	C31-C32-C33-C34
29	b	621	LMG	C14-C15-C16-C17
33	H	103	STE	C10-C11-C12-C13
27	T	101	BCR	C11-C10-C9-C34
27	a	610	BCR	C35-C13-C14-C15
27	c	515	BCR	C16-C17-C18-C36
27	t	101	BCR	C11-C10-C9-C34
27	x	101	BCR	C20-C21-C22-C37
29	D	408	LMG	C34-C35-C36-C37
25	B	616	CLA	CBD-CGD-O2D-CED
26	d	401	PHO	CBD-CGD-O2D-CED
25	B	607	CLA	C15-C16-C17-C18
32	C	516	DGD	C7B-C8B-C9B-CAB
25	c	511	CLA	C8-C10-C11-C12
25	c	501	CLA	CBD-CGD-O2D-CED
29	C	518	LMG	C18-C19-C20-C21
25	B	603	CLA	CAD-CBD-CGD-O2D
25	B	604	CLA	CAD-CBD-CGD-O2D
25	C	503	CLA	CAD-CBD-CGD-O2D
25	C	505	CLA	CAD-CBD-CGD-O2D
25	a	607	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
26	d	401	PHO	CAD-CBD-CGD-O2D
29	D	411	LMG	C9-C8-O7-C10
32	a	615	DGD	C1G-C2G-O2G-C1B
29	b	621	LMG	C31-C32-C33-C34
32	C	516	DGD	C3A-C4A-C5A-C6A
32	C	517	DGD	C2B-C3B-C4B-C5B
33	x	102	STE	C11-C10-C9-C8
29	b	621	LMG	C33-C34-C35-C36
32	a	615	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
25	B	612	CLA	CBA-CGA-O2A-C1
32	A	617	DGD	C2A-C1A-O1G-C1G
25	c	506	CLA	C4-C3-C5-C6
25	B	611	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C20
33	C	520	STE	C5-C6-C7-C8
25	c	509	CLA	C8-C10-C11-C12
26	D	402	PHO	C2C-C3C-CAC-CBC
29	D	411	LMG	C7-C8-C9-O8
29	c	524	LMG	C7-C8-C9-O8
31	l	101	LHG	O6-C4-C5-O7
25	b	601	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C16-C17-C18-C19
25	b	608	CLA	C16-C17-C18-C19
25	c	505	CLA	C16-C17-C18-C20
31	d	407	LHG	C17-C18-C19-C20
32	h	101	DGD	CAA-CBA-CCA-CDA
25	a	608	CLA	O1D-CGD-O2D-CED
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	CHA-CBD-CGD-O1D
25	a	608	CLA	CHA-CBD-CGD-O2D
25	b	607	CLA	CHA-CBD-CGD-O1D
25	b	607	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	510	CLA	CHA-CBD-CGD-O1D
32	A	617	DGD	C4A-C5A-C6A-C7A
32	a	615	DGD	CAB-CBB-CCB-CDB
32	C	516	DGD	C8A-C9A-CAA-CBA
32	c	519	DGD	C7A-C8A-C9A-CAA
27	H	101	BCR	C11-C10-C9-C8
29	C	518	LMG	O1-C7-C8-O7
29	M	101	LMG	O1-C7-C8-O7
29	c	524	LMG	O7-C8-C9-O8
32	C	515	DGD	O1G-C1G-C2G-O2G
32	c	517	DGD	O1G-C1G-C2G-O2G
25	C	511	CLA	O1D-CGD-O2D-CED
31	D	410	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	B	625	STE	C2-C3-C4-C5
25	B	606	CLA	C16-C17-C18-C19
31	d	409	LHG	O1-C1-C2-O2
25	B	616	CLA	O1D-CGD-O2D-CED
25	C	506	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
32	h	101	DGD	C9A-CAA-CBA-CCA
25	C	510	CLA	C11-C10-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	609	CLA	C14-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C9
25	C	505	CLA	O1D-CGD-O2D-CED
26	d	401	PHO	O1D-CGD-O2D-CED
29	A	612	LMG	C36-C37-C38-C39
31	A	615	LHG	C10-C11-C12-C13
32	C	517	DGD	O1A-C1A-O1G-C1G
25	B	603	CLA	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
25	D	405	CLA	C16-C17-C18-C20
31	l	101	LHG	C10-C11-C12-C13
32	a	615	DGD	CFB-CGB-CHB-CIB
25	B	602	CLA	C15-C16-C17-C18
33	a	617	STE	C7-C8-C9-C10
33	c	523	STE	C2-C3-C4-C5
29	M	101	LMG	O6-C5-C6-O5
29	m	101	LMG	C32-C33-C34-C35
25	B	604	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	C16-C17-C18-C19
32	C	517	DGD	C9A-CAA-CBA-CCA
32	h	101	DGD	CDB-CEB-CFB-CGB
33	d	412	STE	C9-C10-C11-C12
25	b	616	CLA	C2-C1-O2A-CGA
33	x	102	STE	C9-C10-C11-C12
32	c	517	DGD	C7B-C8B-C9B-CAB
25	C	508	CLA	O1D-CGD-O2D-CED
29	c	520	LMG	C35-C36-C37-C38
32	A	617	DGD	C7A-C8A-C9A-CAA
32	H	102	DGD	C4B-C5B-C6B-C7B
25	B	613	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	B	622	SQD	C15-C16-C17-C18
32	C	516	DGD	C3B-C4B-C5B-C6B
33	b	620	STE	C4-C5-C6-C7
31	D	409	LHG	C3-O3-P-O4
31	d	407	LHG	C3-O3-P-O5
29	m	101	LMG	C37-C38-C39-C40
25	C	511	CLA	CBA-CGA-O2A-C1
29	B	621	LMG	C11-C12-C13-C14
32	A	617	DGD	CDB-CEB-CFB-CGB
33	l	102	STE	C10-C11-C12-C13
25	c	509	CLA	CAA-CBA-CGA-O2A
31	D	412	LHG	C29-C30-C31-C32
31	d	407	LHG	C33-C34-C35-C36
33	d	412	STE	C3-C4-C5-C6
32	h	101	DGD	C2B-C3B-C4B-C5B
25	A	607	CLA	C16-C17-C18-C20
33	M	102	STE	C10-C11-C12-C13
25	B	609	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	b	607	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	510	CLA	CAD-CBD-CGD-O1D
33	M	103	STE	C6-C7-C8-C9
29	D	408	LMG	C30-C31-C32-C33
32	C	516	DGD	CBB-CCB-CDB-CEB
32	h	101	DGD	C1A-C2A-C3A-C4A
31	d	407	LHG	C25-C26-C27-C28
25	B	604	CLA	CBA-CGA-O2A-C1
25	D	404	CLA	C2C-C3C-CAC-CBC
25	B	610	CLA	C16-C17-C18-C20
25	C	501	CLA	C16-C17-C18-C20
25	B	611	CLA	C11-C10-C8-C7
25	B	613	CLA	C6-C7-C8-C10
25	B	613	CLA	C11-C12-C13-C15
25	B	614	CLA	C12-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C7
25	C	505	CLA	C6-C7-C8-C10
25	C	506	CLA	C12-C13-C15-C16
25	C	508	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C10-C8-C7
25	C	509	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	C11-C10-C8-C7
25	b	601	CLA	C12-C13-C15-C16
25	b	602	CLA	C11-C12-C13-C15
25	b	605	CLA	C12-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C15
25	b	608	CLA	C11-C10-C8-C7
25	c	502	CLA	C6-C7-C8-C10
25	c	512	CLA	C6-C7-C8-C10
25	c	512	CLA	C12-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C15
29	c	522	LMG	C31-C32-C33-C34
31	l	101	LHG	C25-C26-C27-C28
31	D	410	LHG	C12-C13-C14-C15
25	C	511	CLA	O1A-CGA-O2A-C1
31	A	614	LHG	O2-C2-C3-O3
25	B	605	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C19
25	b	612	CLA	C16-C17-C18-C20
33	d	413	STE	C6-C7-C8-C9
30	a	614	SQD	O47-C45-C46-O48
31	A	614	LHG	O7-C5-C6-O8
33	t	102	STE	C3-C4-C5-C6
32	a	615	DGD	C3B-C4B-C5B-C6B
33	b	622	STE	C2-C3-C4-C5
32	C	516	DGD	C2G-C3G-O3G-C1D
32	C	516	DGD	C5D-C6D-O5D-C1E
32	c	518	DGD	C2G-C3G-O3G-C1D
32	c	519	DGD	CAB-CBB-CCB-CDB
25	B	604	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	O1A-CGA-O2A-C1
25	B	614	CLA	C8-C10-C11-C12
32	h	101	DGD	C7A-C8A-C9A-CAA
25	B	606	CLA	C8-C10-C11-C12
25	B	606	CLA	C11-C12-C13-C14
25	B	607	CLA	C11-C10-C8-C9
25	B	616	CLA	C11-C10-C8-C9
25	C	502	CLA	C11-C12-C13-C14
25	C	510	CLA	C6-C7-C8-C9
25	a	609	CLA	C14-C13-C15-C16
25	b	603	CLA	C11-C12-C13-C14
25	c	510	CLA	C14-C13-C15-C16
31	D	409	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	D	412	LHG	C16-C17-C18-C19
33	b	620	STE	C3-C4-C5-C6
25	B	606	CLA	C16-C17-C18-C20
31	D	412	LHG	C27-C28-C29-C30
33	B	626	STE	C1-C2-C3-C4
28	A	611	PL9	C9-C11-C12-C13
25	B	616	CLA	O1A-CGA-O2A-C1
30	A	616	SQD	C19-C20-C21-C22
29	c	522	LMG	C41-C42-C43-C44
31	D	412	LHG	C19-C20-C21-C22
33	C	519	STE	C7-C8-C9-C10
33	B	623	STE	C4-C5-C6-C7
33	B	626	STE	C5-C6-C7-C8
31	d	409	LHG	C35-C36-C37-C38
25	b	615	CLA	C8-C10-C11-C12
27	K	102	BCR	C20-C21-C22-C37
32	C	515	DGD	C5B-C6B-C7B-C8B
29	D	411	LMG	C29-C30-C31-C32
33	E	102	STE	C4-C5-C6-C7
25	c	512	CLA	C2-C3-C5-C6
25	A	606	CLA	C16-C17-C18-C20
32	A	617	DGD	C5A-C6A-C7A-C8A
25	C	507	CLA	C5-C6-C7-C8
33	j	101	STE	C2-C3-C4-C5
25	c	513	CLA	C5-C6-C7-C8
29	b	621	LMG	C9-C8-O7-C10
33	l	102	STE	C1-C2-C3-C4
25	A	606	CLA	C2-C1-O2A-CGA
25	b	608	CLA	C2-C1-O2A-CGA
25	c	513	CLA	C2-C1-O2A-CGA
25	B	605	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C20
30	f	102	SQD	C35-C36-C37-C38
33	d	412	STE	C7-C8-C9-C10
30	a	614	SQD	C30-C31-C32-C33
30	a	613	SQD	C24-C23-O48-C46
25	C	505	CLA	O1A-CGA-O2A-C1
31	A	615	LHG	O10-C23-O8-C6
31	A	615	LHG	C14-C15-C16-C17
25	c	504	CLA	C8-C10-C11-C12
30	a	613	SQD	C24-C25-C26-C27
27	C	514	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	C	514	BCR	C5-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C26
27	k	101	BCR	C23-C24-C25-C30
27	x	101	BCR	C23-C24-C25-C30
28	A	611	PL9	C13-C14-C16-C17
30	L	101	SQD	C16-C17-C18-C19
30	a	613	SQD	C23-C24-C25-C26
30	B	622	SQD	C14-C15-C16-C17
25	C	510	CLA	C8-C10-C11-C12
27	c	514	BCR	C20-C21-C22-C23
25	b	610	CLA	C5-C6-C7-C8
26	d	402	PHO	CHA-CBD-CGD-O2D
32	C	517	DGD	C5B-C6B-C7B-C8B
33	B	623	STE	C5-C6-C7-C8
25	c	504	CLA	O1D-CGD-O2D-CED
28	a	611	PL9	C15-C14-C16-C17
32	H	102	DGD	C3B-C4B-C5B-C6B
33	x	102	STE	C15-C16-C17-C18
25	c	504	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	C13-C15-C16-C17
25	C	502	CLA	C11-C12-C13-C15
25	a	608	CLA	C11-C12-C13-C15
25	b	614	CLA	C6-C7-C8-C10
25	c	510	CLA	C11-C12-C13-C15
25	c	513	CLA	C6-C7-C8-C10
25	B	613	CLA	C6-C7-C8-C9
25	C	505	CLA	C6-C7-C8-C9
25	b	602	CLA	C11-C12-C13-C14
25	c	505	CLA	C6-C7-C8-C9
25	c	512	CLA	C11-C10-C8-C9
25	B	608	CLA	C16-C17-C18-C19
25	B	609	CLA	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C19
30	F	101	SQD	O6-C44-C45-C46
29	c	522	LMG	O10-C28-O8-C9
29	B	621	LMG	C15-C16-C17-C18
31	l	101	LHG	C29-C30-C31-C32
32	H	102	DGD	O6E-C5E-C6E-O5E
30	a	613	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
31	A	615	LHG	C19-C20-C21-C22
31	D	410	LHG	C2-C3-O3-P
31	d	409	LHG	C2-C3-O3-P
32	H	102	DGD	C9B-CAB-CBB-CCB
32	c	517	DGD	CBA-CCA-CDA-CEA
32	c	518	DGD	C8B-C9B-CAB-CBB
31	d	408	LHG	C1-C2-C3-O3
25	B	615	CLA	C16-C17-C18-C20
25	C	508	CLA	C16-C17-C18-C19
25	B	616	CLA	CBA-CGA-O2A-C1
35	E	101	HEM	CAD-CBD-CGD-O1D
25	C	505	CLA	CBA-CGA-O2A-C1
29	c	520	LMG	C29-C28-O8-C9
30	B	622	SQD	C34-C35-C36-C37
30	F	101	SQD	C27-C28-C29-C30
28	a	611	PL9	C19-C21-C22-C23
25	B	610	CLA	C15-C16-C17-C18
29	D	408	LMG	C13-C14-C15-C16
29	c	524	LMG	C13-C14-C15-C16
29	B	621	LMG	O7-C10-C11-C12
29	c	524	LMG	C38-C39-C40-C41
27	H	101	BCR	C10-C11-C12-C13
27	T	101	BCR	C18-C19-C20-C21
31	D	409	LHG	C15-C16-C17-C18
33	B	620	STE	C5-C6-C7-C8
31	d	408	LHG	C28-C29-C30-C31
25	D	404	CLA	C2-C1-O2A-CGA
33	T	103	STE	C5-C6-C7-C8
25	A	607	CLA	C16-C17-C18-C19
32	C	516	DGD	C2D-C1D-O3G-C3G
32	c	517	DGD	C2E-C1E-O5D-C6D
25	b	613	CLA	CBD-CGD-O2D-CED
32	A	617	DGD	CFB-CGB-CHB-CIB
25	B	603	CLA	C2A-CAA-CBA-CGA
25	C	501	CLA	C2A-CAA-CBA-CGA
30	a	613	SQD	C28-C29-C30-C31
32	c	518	DGD	CBB-CCB-CDB-CEB
33	c	521	STE	O2-C1-C2-C3
25	c	502	CLA	C16-C17-C18-C20
29	d	411	LMG	C11-C12-C13-C14
27	x	101	BCR	C15-C16-C17-C18
33	c	521	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	d	411	LMG	C10-C11-C12-C13
33	l	102	STE	C12-C13-C14-C15
28	a	611	PL9	C4-C3-C7-C8
25	B	603	CLA	C11-C10-C8-C9
25	C	501	CLA	C14-C13-C15-C16
25	C	507	CLA	C6-C7-C8-C9
25	b	605	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C12-C13-C14
25	c	512	CLA	C14-C13-C15-C16
25	d	403	CLA	C11-C12-C13-C14
35	f	101	HEM	CAD-CBD-CGD-O1D
25	b	609	CLA	C13-C15-C16-C17
33	b	620	STE	C5-C6-C7-C8
30	A	616	SQD	C34-C35-C36-C37
31	d	408	LHG	C33-C34-C35-C36
32	A	617	DGD	CEA-CFA-CGA-CHA
27	c	516	BCR	C20-C21-C22-C37
27	x	101	BCR	C35-C13-C14-C15
32	C	515	DGD	O1G-C1G-C2G-C3G
33	B	625	STE	O1-C1-C2-C3
29	d	411	LMG	C15-C16-C17-C18
32	C	516	DGD	CCB-CDB-CEB-CFB
25	B	616	CLA	O2A-C1-C2-C3
25	C	512	CLA	O2A-C1-C2-C3
26	d	401	PHO	O2A-C1-C2-C3
29	B	621	LMG	O9-C10-C11-C12
29	d	411	LMG	C30-C31-C32-C33
35	E	101	HEM	CAD-CBD-CGD-O2D
33	a	616	STE	C7-C8-C9-C10
25	A	607	CLA	C11-C10-C8-C7
25	B	615	CLA	C12-C13-C15-C16
25	B	616	CLA	C2-C3-C5-C6
25	D	403	CLA	C12-C13-C15-C16
25	b	606	CLA	C6-C7-C8-C10
25	c	501	CLA	C11-C12-C13-C15
25	c	507	CLA	C11-C10-C8-C7
33	b	622	STE	O1-C1-C2-C3
25	D	403	CLA	C2C-C3C-CAC-CBC
33	b	620	STE	C7-C8-C9-C10
27	a	610	BCR	C19-C20-C21-C22
27	c	516	BCR	C13-C14-C15-C16
31	A	615	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	M	103	STE	C4-C5-C6-C7
30	f	102	SQD	C32-C33-C34-C35
33	b	622	STE	O2-C1-C2-C3
33	E	102	STE	C7-C8-C9-C10
25	B	614	CLA	C2A-CAA-CBA-CGA
33	T	102	STE	C4-C5-C6-C7
29	d	410	LMG	O9-C10-C11-C12
29	M	101	LMG	C12-C13-C14-C15
33	t	102	STE	C6-C7-C8-C9
25	b	611	CLA	C10-C11-C12-C13
33	B	623	STE	O1-C1-C2-C3
31	l	101	LHG	C35-C36-C37-C38
30	a	614	SQD	C29-C30-C31-C32
32	C	515	DGD	C2B-C3B-C4B-C5B
29	d	410	LMG	C11-C12-C13-C14
25	B	612	CLA	C10-C11-C12-C13
29	B	621	LMG	C36-C37-C38-C39
29	A	612	LMG	C13-C14-C15-C16
27	t	101	BCR	C20-C21-C22-C23
27	x	101	BCR	C20-C21-C22-C23
32	c	518	DGD	C2D-C1D-O3G-C3G
29	D	411	LMG	O7-C8-C9-O8
30	f	102	SQD	O6-C44-C45-O47
33	H	103	STE	C6-C7-C8-C9
27	c	516	BCR	C19-C20-C21-C22
36	V	201	HEC	CAD-CBD-CGD-O2D
29	m	101	LMG	C33-C34-C35-C36
30	A	616	SQD	C11-C12-C13-C14
30	B	622	SQD	C28-C29-C30-C31
29	D	411	LMG	O1-C7-C8-C9
33	B	623	STE	O2-C1-C2-C3
29	C	518	LMG	C33-C34-C35-C36
33	b	622	STE	C5-C6-C7-C8
27	B	618	BCR	C18-C19-C20-C21
25	C	508	CLA	C14-C13-C15-C16
26	d	401	PHO	C14-C13-C15-C16
25	B	604	CLA	C2C-C3C-CAC-CBC
33	T	103	STE	C9-C10-C11-C12
26	d	402	PHO	C1A-C2A-CAA-CBA
29	M	101	LMG	C18-C19-C20-C21
25	D	403	CLA	C4C-C3C-CAC-CBC
27	A	610	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
27	B	617	BCR	C1-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C26
27	Y	101	BCR	C23-C24-C25-C30
27	b	618	BCR	C23-C24-C25-C30
27	c	516	BCR	C1-C6-C7-C8
27	c	516	BCR	C23-C24-C25-C30
29	C	518	LMG	C16-C17-C18-C19
32	c	517	DGD	O1G-C1G-C2G-C3G
25	b	602	CLA	CBD-CGD-O2D-CED
32	a	615	DGD	C2B-C3B-C4B-C5B
25	d	404	CLA	C4-C3-C5-C6
32	c	519	DGD	O6D-C5D-C6D-O5D
32	C	515	DGD	C5D-C6D-O5D-C1E
33	b	623	STE	C5-C6-C7-C8
32	h	101	DGD	O2G-C1B-C2B-C3B
25	B	603	CLA	C16-C17-C18-C19
25	d	404	CLA	C16-C17-C18-C19
25	B	610	CLA	C8-C10-C11-C12
25	c	512	CLA	C5-C6-C7-C8
29	d	410	LMG	O7-C10-C11-C12
32	C	515	DGD	C4D-C5D-C6D-O5D
29	B	621	LMG	C30-C31-C32-C33
31	D	409	LHG	C9-C10-C11-C12
33	b	623	STE	C1-C2-C3-C4
29	c	524	LMG	C11-C12-C13-C14
33	D	413	STE	O2-C1-C2-C3
29	b	621	LMG	O6-C1-O1-C7
32	C	515	DGD	O6E-C1E-O5D-C6D
33	t	102	STE	C4-C5-C6-C7
31	A	614	LHG	O6-C4-C5-C6
33	B	625	STE	O2-C1-C2-C3
26	A	608	PHO	C10-C11-C12-C13
31	D	409	LHG	C11-C12-C13-C14
33	l	102	STE	C15-C16-C17-C18
29	D	411	LMG	O1-C7-C8-O7
25	c	503	CLA	CBA-CGA-O2A-C1
30	a	613	SQD	C33-C34-C35-C36
25	b	612	CLA	C8-C10-C11-C12
25	b	613	CLA	CAA-CBA-CGA-O2A
30	L	101	SQD	C10-C11-C12-C13
26	d	402	PHO	C4C-C3C-CAC-CBC
33	l	102	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	B	613	CLA	CAA-CBA-CGA-O2A
30	a	613	SQD	O47-C7-C8-C9
32	C	515	DGD	CDB-CEB-CFB-CGB
33	b	622	STE	C6-C7-C8-C9
25	c	510	CLA	C4-C3-C5-C6
25	d	403	CLA	C4-C3-C5-C6
29	A	612	LMG	C39-C40-C41-C42
36	V	201	HEC	CAD-CBD-CGD-O1D
25	c	502	CLA	O1A-CGA-O2A-C1
33	C	521	STE	C6-C7-C8-C9
25	C	506	CLA	C16-C17-C18-C20
25	B	612	CLA	CAA-CBA-CGA-O2A
25	b	612	CLA	CAA-CBA-CGA-O2A
25	B	614	CLA	C6-C7-C8-C9
25	B	615	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	506	CLA	C14-C13-C15-C16
25	C	509	CLA	C14-C13-C15-C16
25	D	403	CLA	C14-C13-C15-C16
25	D	404	CLA	C14-C13-C15-C16
25	b	602	CLA	C11-C10-C8-C9
25	b	606	CLA	C6-C7-C8-C9
25	b	608	CLA	C11-C10-C8-C9
25	b	613	CLA	C11-C12-C13-C14
25	c	501	CLA	C11-C12-C13-C14
25	c	507	CLA	C11-C10-C8-C9
35	f	101	HEM	CAD-CBD-CGD-O2D
25	c	503	CLA	O1A-CGA-O2A-C1
29	D	411	LMG	O10-C28-O8-C9
32	C	515	DGD	O6D-C5D-C6D-O5D
25	B	605	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	B	616	CLA	CAD-CBD-CGD-O2D
25	C	512	CLA	CAD-CBD-CGD-O2D
25	b	601	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	b	612	CLA	CAD-CBD-CGD-O2D
25	c	503	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	c	512	CLA	CAD-CBD-CGD-O2D
29	c	520	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
31	D	410	LHG	C17-C18-C19-C20
25	A	607	CLA	C10-C11-C12-C13
25	b	609	CLA	C15-C16-C17-C18
33	D	413	STE	O1-C1-C2-C3
29	m	101	LMG	O8-C28-C29-C30
26	D	402	PHO	O1D-CGD-O2D-CED
25	c	501	CLA	O1D-CGD-O2D-CED
27	K	101	BCR	C22-C23-C24-C25
31	d	408	LHG	C31-C32-C33-C34
32	C	517	DGD	C3A-C4A-C5A-C6A
32	h	101	DGD	C7B-C8B-C9B-CAB
25	C	502	CLA	C4-C3-C5-C6
25	c	505	CLA	C16-C17-C18-C19
25	b	601	CLA	CAA-CBA-CGA-O2A
27	K	102	BCR	C17-C18-C19-C20
32	C	517	DGD	O6E-C5E-C6E-O5E
33	T	103	STE	C11-C12-C13-C14
29	A	612	LMG	C28-C29-C30-C31
29	A	612	LMG	C7-C8-C9-O8
32	A	617	DGD	O1G-C1G-C2G-C3G
36	v	201	HEC	CAD-CBD-CGD-O2D
32	c	518	DGD	CDA-CEA-CFA-CGA
25	B	601	CLA	O2A-C1-C2-C3
25	C	509	CLA	O2A-C1-C2-C3
25	D	405	CLA	O2A-C1-C2-C3
25	b	613	CLA	O2A-C1-C2-C3
26	D	402	PHO	CBD-CGD-O2D-CED
32	h	101	DGD	O1B-C1B-C2B-C3B
36	v	201	HEC	CAD-CBD-CGD-O1D
29	c	522	LMG	C42-C43-C44-C45
25	c	513	CLA	C16-C17-C18-C20
32	A	617	DGD	CBA-CCA-CDA-CEA
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	612	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	a	612	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	611	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	b	611	CLA	CHA-CBD-CGD-O2D
25	b	614	CLA	CHA-CBD-CGD-O1D
25	b	614	CLA	CHA-CBD-CGD-O2D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	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	510	CLA	CHA-CBD-CGD-O2D
32	c	518	DGD	C5B-C6B-C7B-C8B
25	B	609	CLA	C2-C3-C5-C6
25	c	510	CLA	C2-C3-C5-C6
32	a	615	DGD	C9A-CAA-CBA-CCA
25	c	513	CLA	C8-C10-C11-C12
31	A	614	LHG	O7-C7-C8-C9
33	B	623	STE	C3-C4-C5-C6
31	d	407	LHG	C26-C27-C28-C29
25	c	510	CLA	C5-C6-C7-C8
25	a	612	CLA	O1D-CGD-O2D-CED
26	A	608	PHO	CHA-CBD-CGD-O1D
26	d	401	PHO	CHA-CBD-CGD-O1D
25	c	502	CLA	CBA-CGA-O2A-C1
32	c	519	DGD	C9B-CAB-CBB-CCB
32	A	617	DGD	O2G-C1B-C2B-C3B
25	B	602	CLA	C12-C13-C15-C16
25	B	605	CLA	C11-C12-C13-C15
25	B	606	CLA	C11-C10-C8-C7
25	B	613	CLA	C2-C3-C5-C6
25	C	502	CLA	C2-C3-C5-C6
25	C	502	CLA	C6-C7-C8-C10
25	D	403	CLA	C6-C7-C8-C10
25	c	506	CLA	C11-C12-C13-C15
25	c	510	CLA	C12-C13-C15-C16
25	d	404	CLA	C11-C12-C13-C15
29	D	408	LMG	C18-C19-C20-C21
25	A	607	CLA	C11-C10-C8-C9
25	B	601	CLA	C11-C12-C13-C14
25	B	611	CLA	C14-C13-C15-C16
25	C	502	CLA	C6-C7-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	606	CLA	C11-C12-C13-C14
25	c	506	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	d	408	LHG	C7-C8-C9-C10
28	A	611	PL9	C44-C46-C47-C48
33	c	521	STE	C7-C8-C9-C10
35	f	101	HEM	CAA-CBA-CGA-O2A
30	B	622	SQD	C4-C5-C6-S
25	b	613	CLA	O1D-CGD-O2D-CED
33	j	101	STE	C7-C8-C9-C10
25	C	512	CLA	C2A-CAA-CBA-CGA
32	c	518	DGD	C5A-C6A-C7A-C8A
32	C	515	DGD	C4E-C5E-C6E-O5E
29	B	621	LMG	O8-C28-C29-C30
33	B	624	STE	C11-C12-C13-C14
31	l	101	LHG	O1-C1-C2-C3
27	K	102	BCR	C11-C12-C13-C14
32	C	517	DGD	O6D-C5D-C6D-O5D
29	D	411	LMG	C29-C28-O8-C9
25	b	604	CLA	C13-C15-C16-C17
25	b	610	CLA	C3-C5-C6-C7
25	B	602	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	b	601	CLA	CAA-CBA-CGA-O1A
25	b	612	CLA	CAA-CBA-CGA-O1A
33	d	413	STE	O1-C1-C2-C3
29	B	621	LMG	C29-C30-C31-C32
25	b	610	CLA	C10-C11-C12-C13
25	b	613	CLA	CAA-CBA-CGA-O1A
33	B	624	STE	C4-C5-C6-C7
32	c	517	DGD	C1G-C2G-C3G-O3G
31	A	615	LHG	O7-C7-C8-C9
33	I	101	STE	C11-C12-C13-C14
25	b	609	CLA	C16-C17-C18-C19
30	a	613	SQD	O49-C7-C8-C9
31	e	101	LHG	O10-C23-C24-C25
29	c	522	LMG	C36-C37-C38-C39
32	C	517	DGD	C6A-C7A-C8A-C9A
25	B	609	CLA	C4-C3-C5-C6
25	b	602	CLA	C8-C10-C11-C12
25	B	612	CLA	CAA-CBA-CGA-O1A
25	B	613	CLA	CAA-CBA-CGA-O1A
29	b	621	LMG	C2-C1-O1-C7
31	D	409	LHG	C4-O6-P-O5
25	B	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	A	617	DGD	O1B-C1B-C2B-C3B
27	A	610	BCR	C23-C24-C25-C26
27	B	617	BCR	C5-C6-C7-C8
27	b	618	BCR	C23-C24-C25-C26
27	c	516	BCR	C5-C6-C7-C8
27	c	516	BCR	C23-C24-C25-C26
25	C	510	CLA	C10-C11-C12-C13
31	A	614	LHG	O9-C7-C8-C9
32	c	517	DGD	O1B-C1B-C2B-C3B
29	m	101	LMG	O10-C28-O8-C9
32	C	515	DGD	O1B-C1B-C2B-C3B
30	A	613	SQD	C9-C10-C11-C12
33	T	102	STE	C1-C2-C3-C4
25	c	505	CLA	C15-C16-C17-C18
35	f	101	HEM	CAA-CBA-CGA-O1A
25	B	607	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	a	612	CLA	CAD-CBD-CGD-O1D
25	b	609	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CAD-CBD-CGD-O1D
29	D	408	LMG	C28-C29-C30-C31
31	d	407	LHG	O8-C23-C24-C25
25	B	606	CLA	C5-C6-C7-C8
25	b	610	CLA	C13-C15-C16-C17
25	A	606	CLA	C11-C10-C8-C9
25	B	611	CLA	C6-C7-C8-C9
25	B	612	CLA	C11-C10-C8-C9
25	D	403	CLA	C6-C7-C8-C9
25	a	609	CLA	C11-C10-C8-C9
29	c	524	LMG	C14-C15-C16-C17
32	H	102	DGD	C8A-C9A-CAA-CBA
30	A	613	SQD	O47-C7-C8-C9
29	D	408	LMG	C22-C23-C24-C25
33	C	521	STE	C11-C12-C13-C14
25	B	602	CLA	C2A-CAA-CBA-CGA
25	b	602	CLA	C2A-CAA-CBA-CGA
28	D	407	PL9	C46-C47-C48-C49
25	a	609	CLA	C15-C16-C17-C18
33	c	523	STE	O2-C1-C2-C3
31	A	614	LHG	C10-C11-C12-C13
25	B	601	CLA	C11-C12-C13-C15

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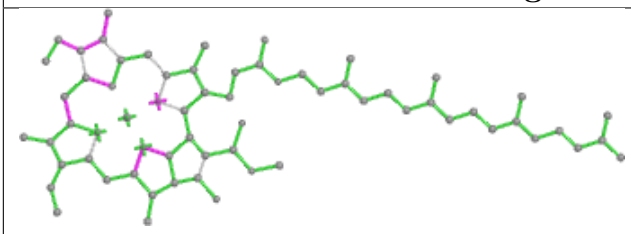
Mol	Chain	Res	Type	Atoms
25	a	612	CLA	C11-C12-C13-C15
25	b	602	CLA	C12-C13-C15-C16
25	c	506	CLA	C2-C3-C5-C6
25	c	506	CLA	C12-C13-C15-C16
28	a	611	PL9	C23-C24-C26-C27
33	C	519	STE	O2-C1-C2-C3
30	a	614	SQD	O48-C23-C24-C25
32	C	515	DGD	O2G-C1B-C2B-C3B
25	a	608	CLA	C3-C5-C6-C7
30	A	613	SQD	O49-C7-C8-C9
33	M	102	STE	O2-C1-C2-C3
33	d	413	STE	O2-C1-C2-C3
33	T	102	STE	C11-C10-C9-C8
30	B	622	SQD	O48-C23-C24-C25
32	c	517	DGD	O1G-C1A-C2A-C3A
25	b	605	CLA	C15-C16-C17-C18
30	a	614	SQD	O10-C23-C24-C25
32	c	518	DGD	O1B-C1B-C2B-C3B
29	c	520	LMG	O6-C5-C6-O5
31	d	408	LHG	O2-C2-C3-O3
25	b	604	CLA	C5-C6-C7-C8
25	c	512	CLA	C15-C16-C17-C18
28	D	407	PL9	C32-C33-C34-C35
32	c	518	DGD	O1A-C1A-C2A-C3A

There are no ring outliers.

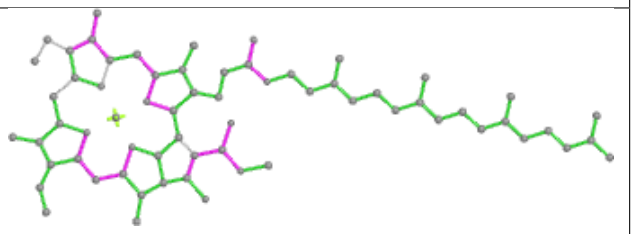
No monomer is involved in short contacts.

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

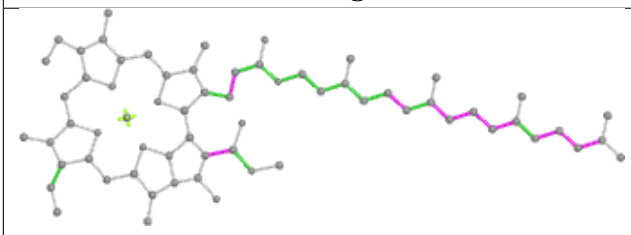
Ligand CLA B 606



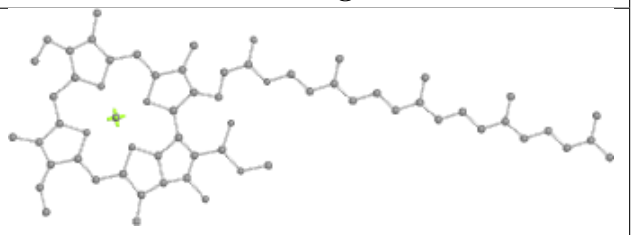
Bond lengths



Bond angles

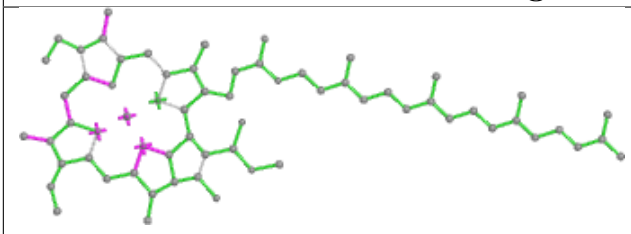


Torsions

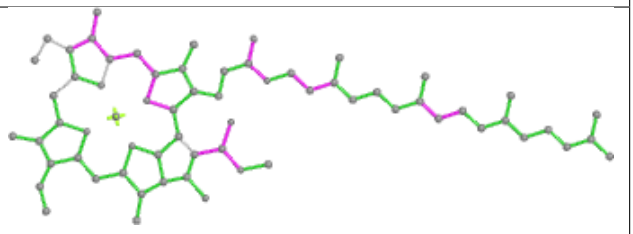


Rings

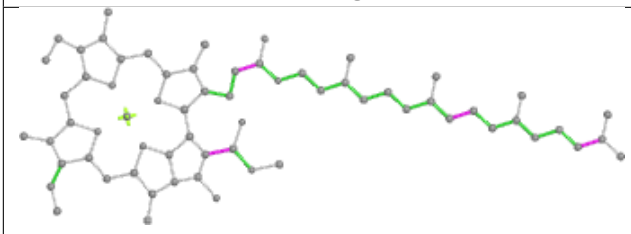
Ligand CLA b 612



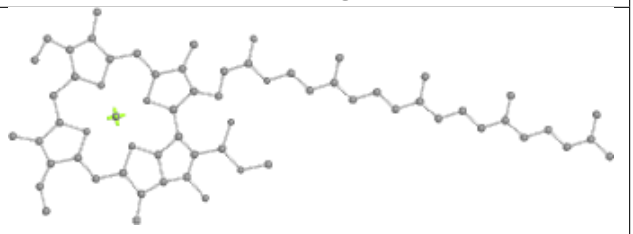
Bond lengths



Bond angles

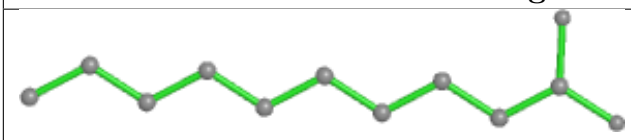


Torsions

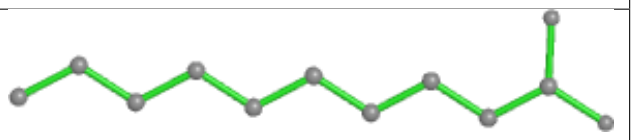


Rings

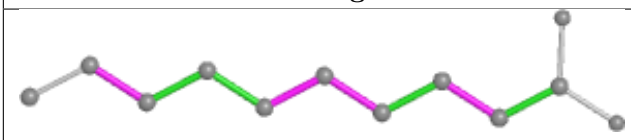
Ligand STE E 102



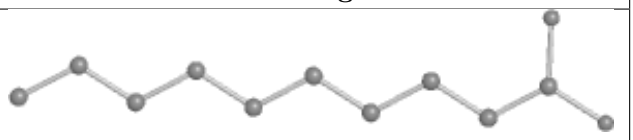
Bond lengths



Bond angles

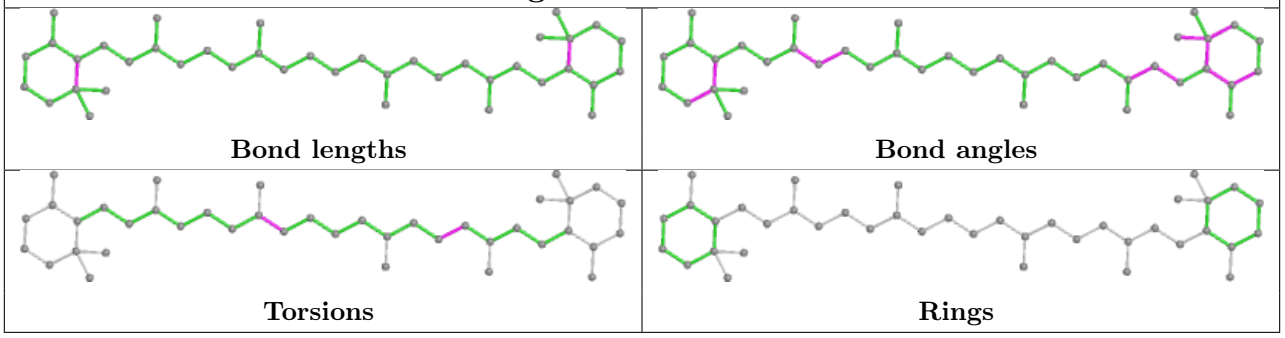


Torsions

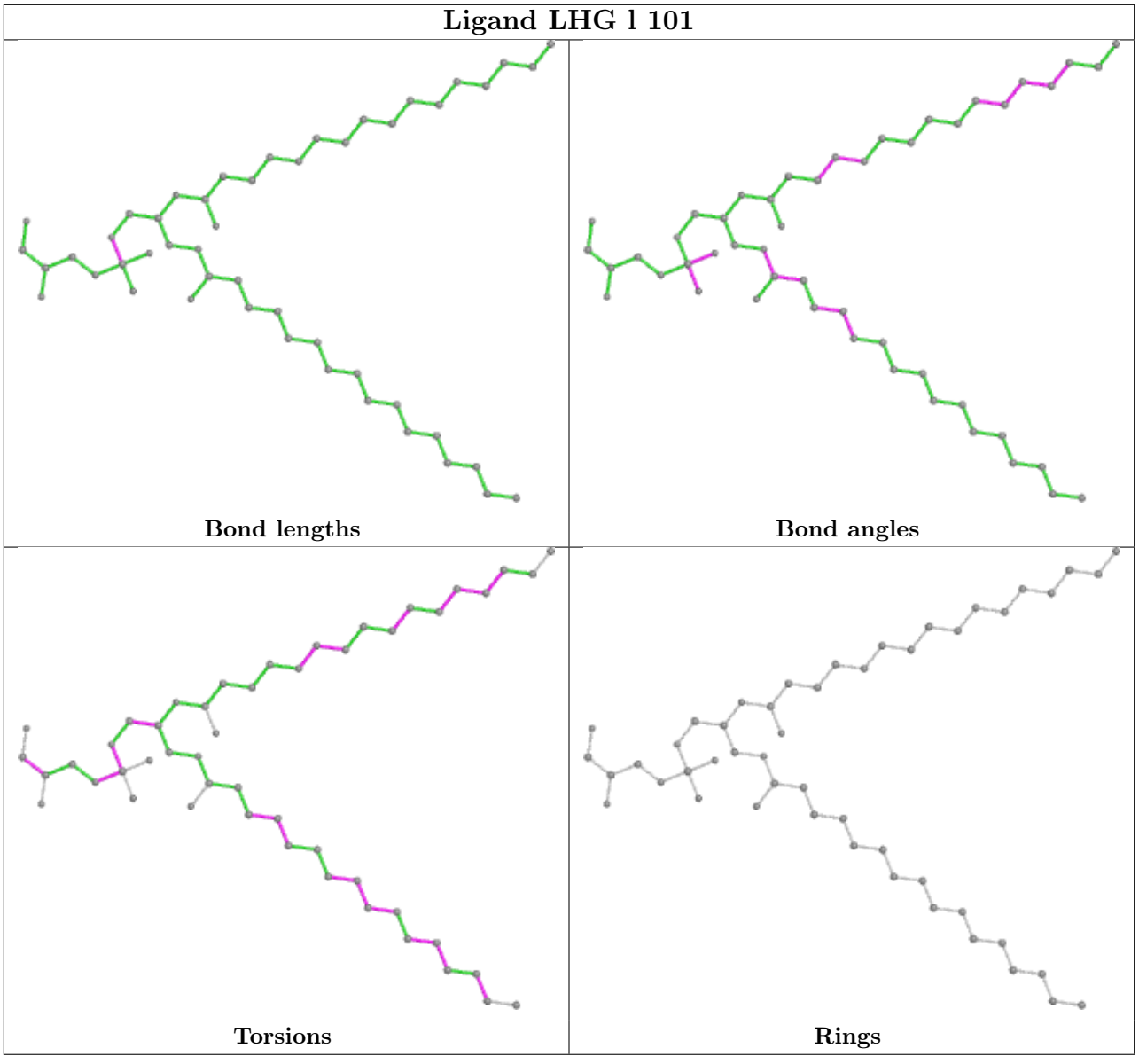


Rings

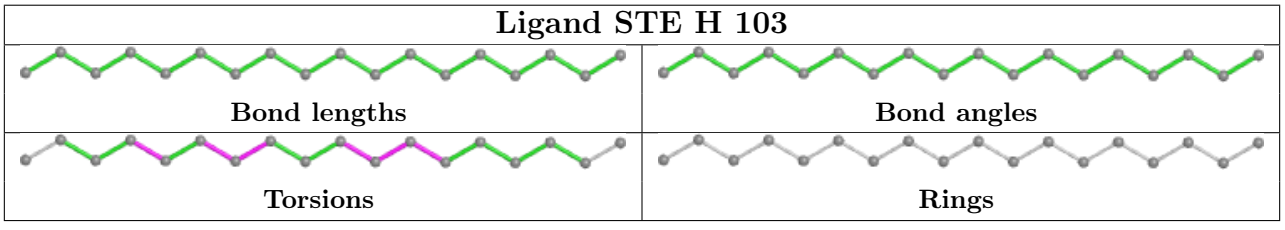
Ligand BCR a 610



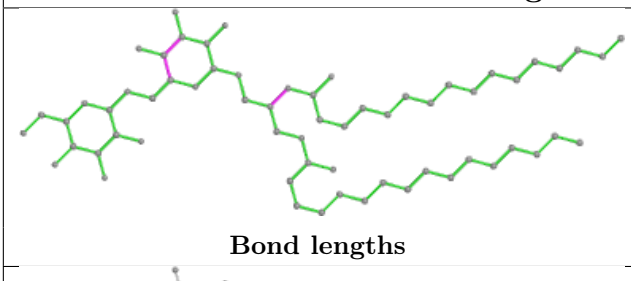
Ligand LHG l 101



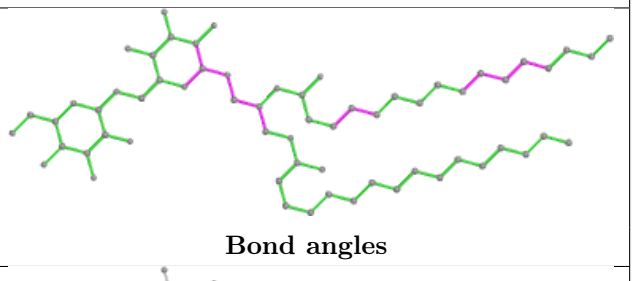
Ligand STE H 103



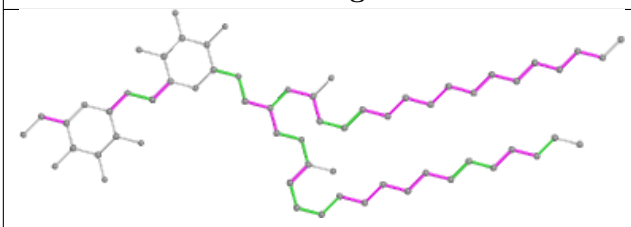
Ligand DGD c 517



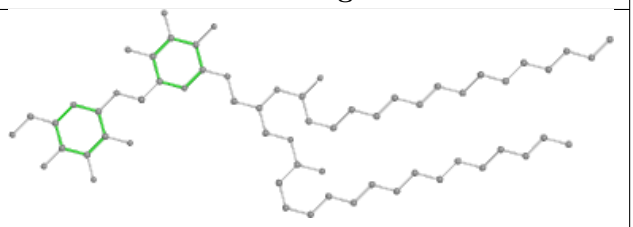
Bond lengths



Bond angles

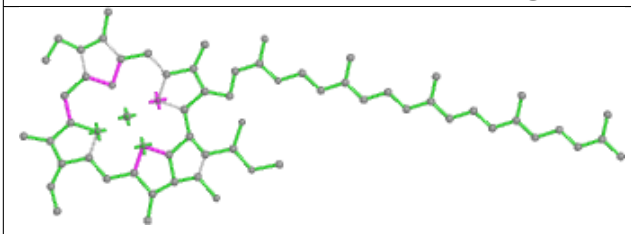


Torsions

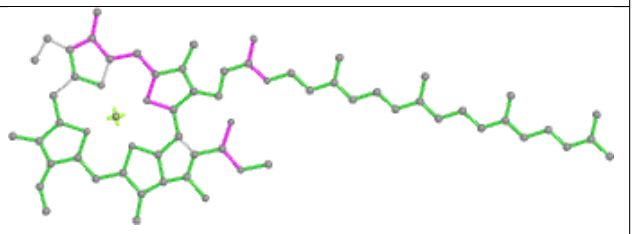


Rings

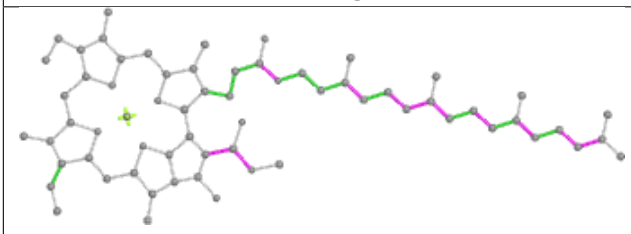
Ligand CLA C 505



Bond lengths



Bond angles



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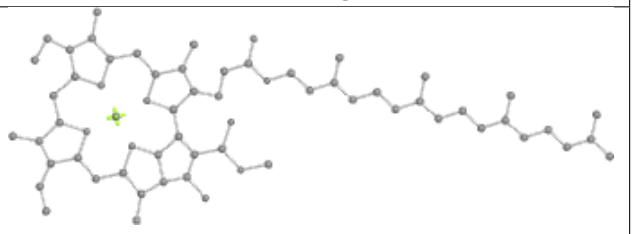
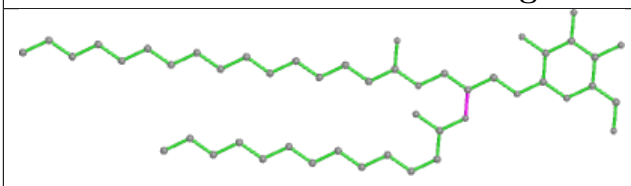
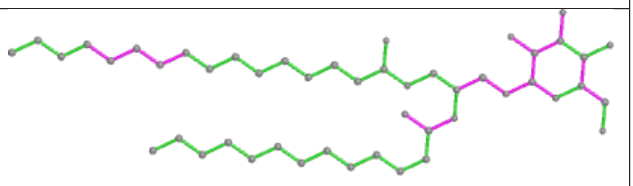


Rings

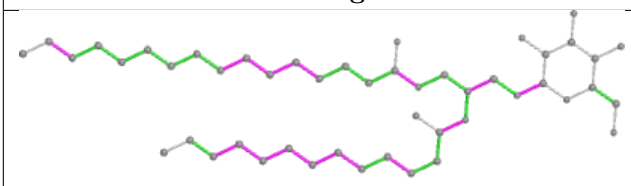
Ligand LMG C 518



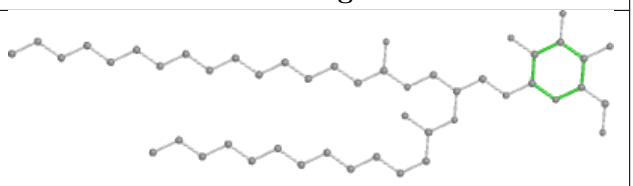
Bond lengths



Bond angles

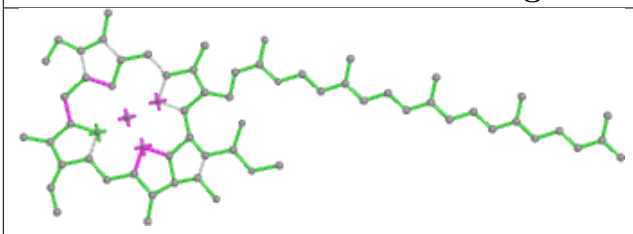


Torsions

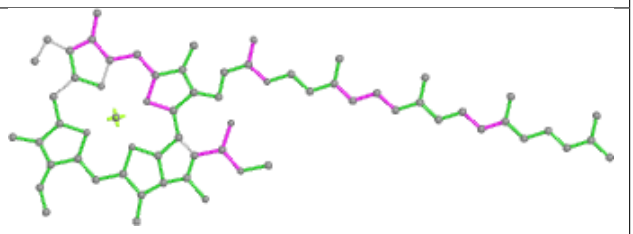


Rings

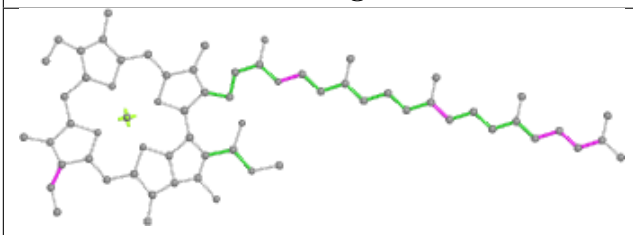
Ligand CLA A 606



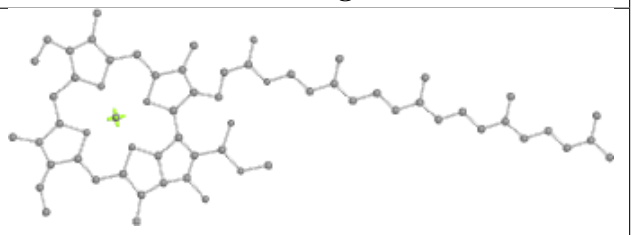
Bond lengths



Bond angles

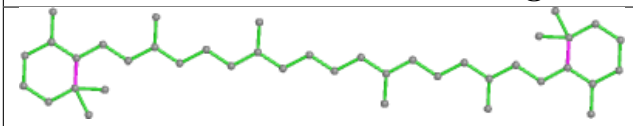


Torsions

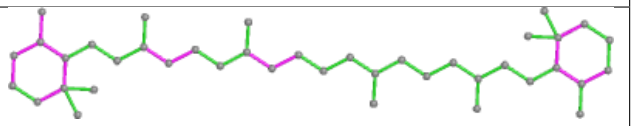


Rings

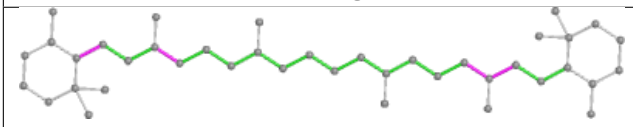
Ligand BCR b 617



Bond lengths



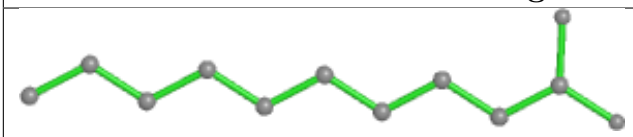
Bond angles



Torsions

Rings

Ligand STE B 625



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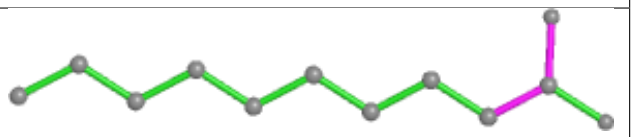
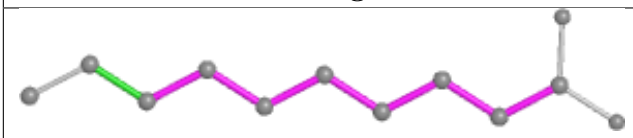
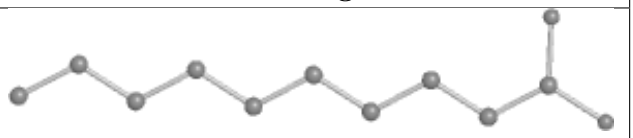


Bond angles

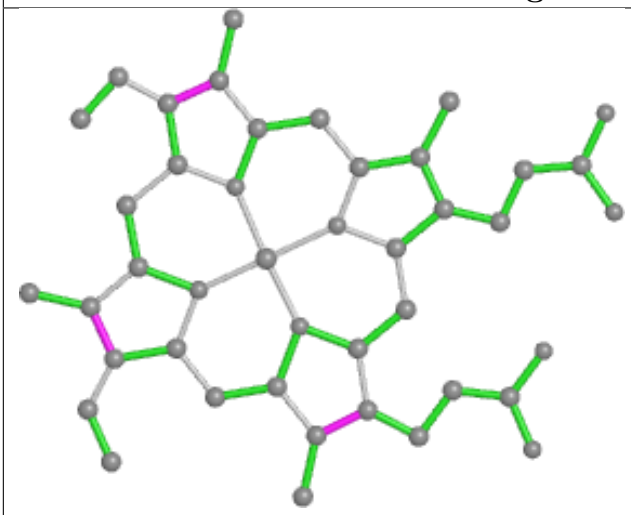


Torsions

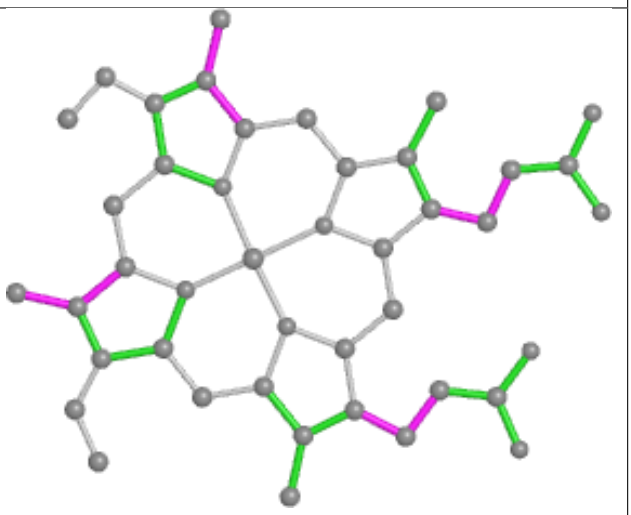


Rings

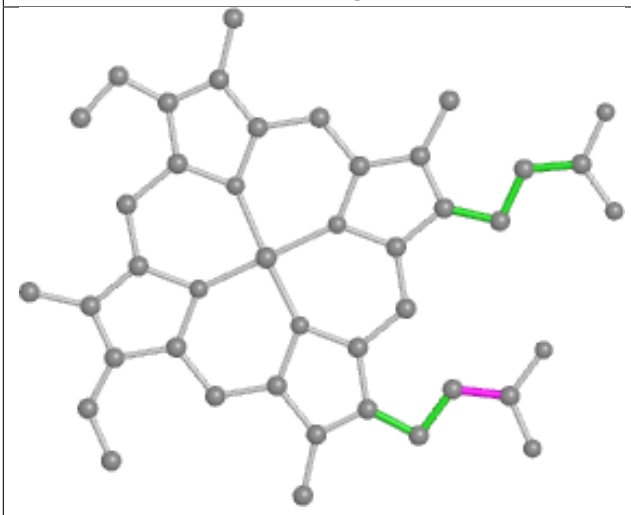
Ligand HEC v 201



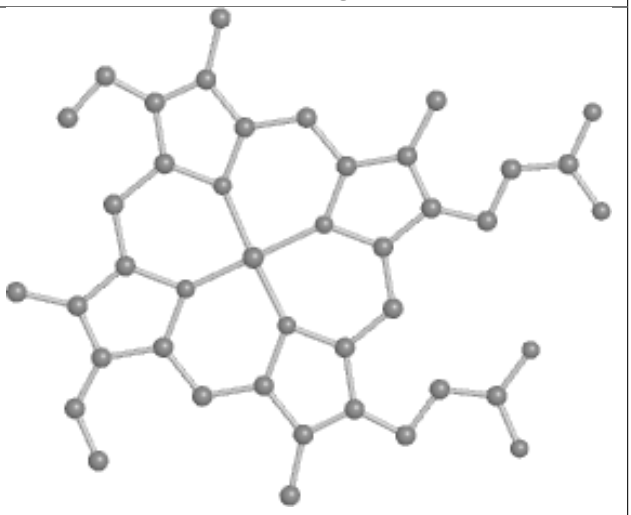
Bond lengths



Bond angles

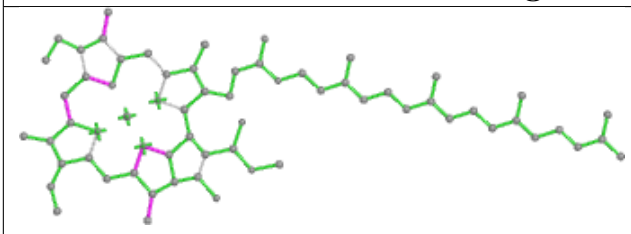


Torsions

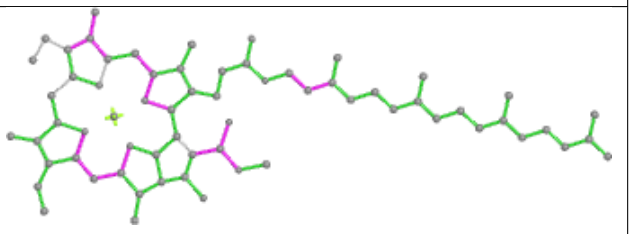


Rings

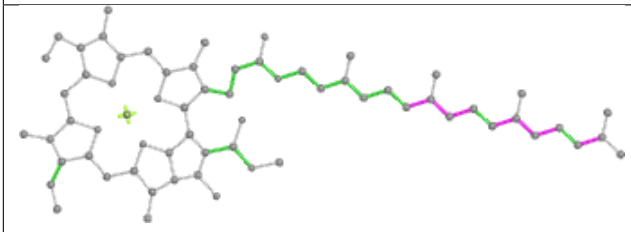
Ligand CLA B 611



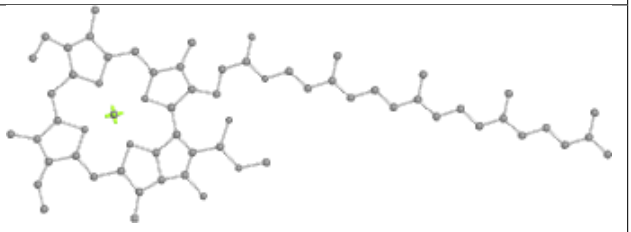
Bond lengths



Bond angles

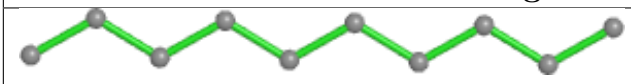


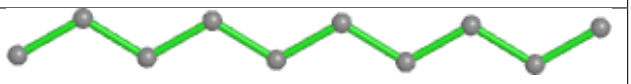
Torsions

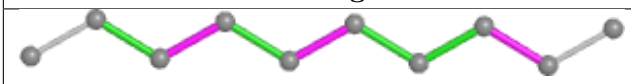


Rings

Ligand STE M 103


Bond lengths


Bond angles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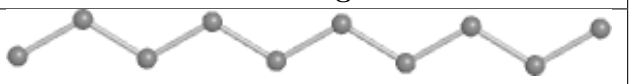
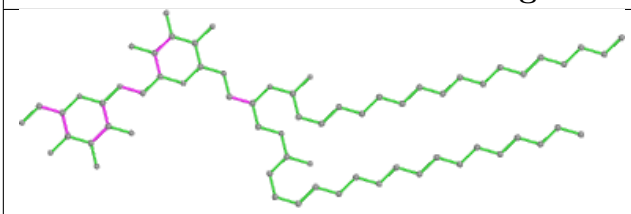

Rings

Ligand DGD A 617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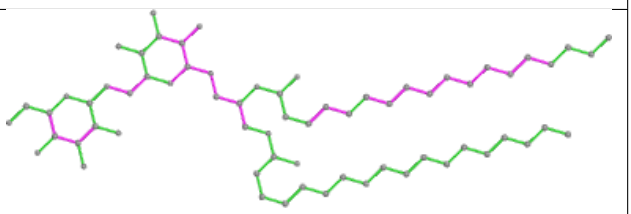
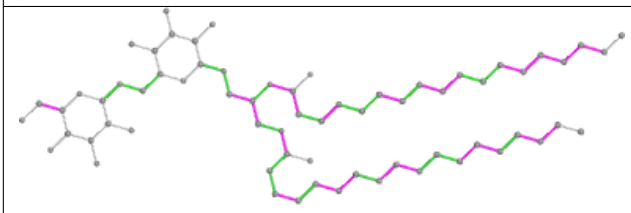
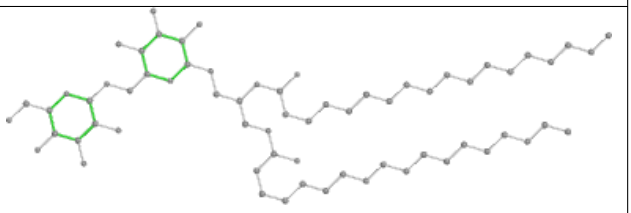

Bond angles


Torsions


Rings

Ligand STE I 101

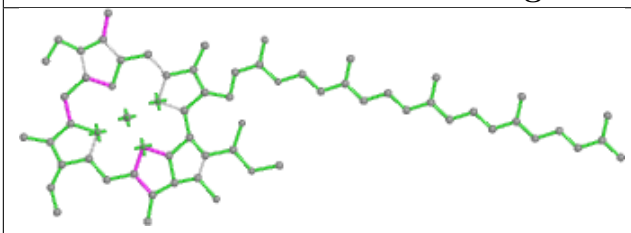

Bond lengths

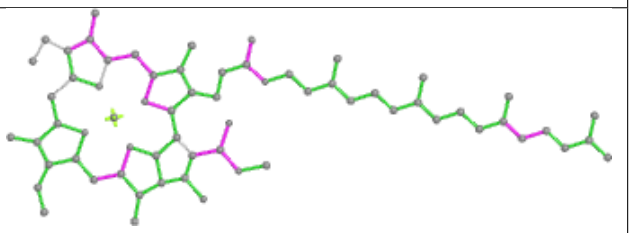

Bond angles

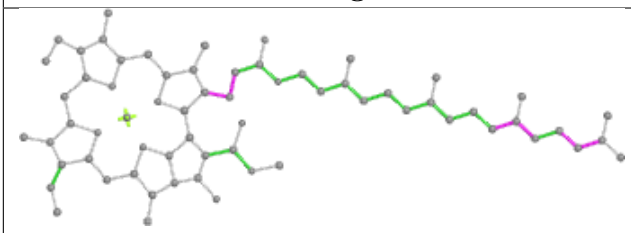

Torsions


Rings

Ligand CLA B 602


Bond lengths


Bond angles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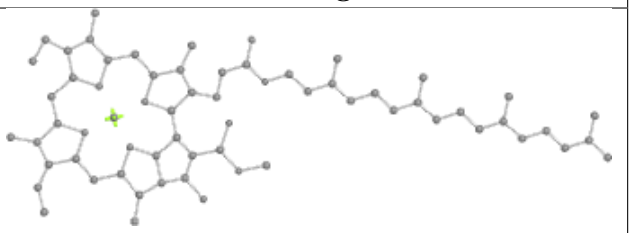
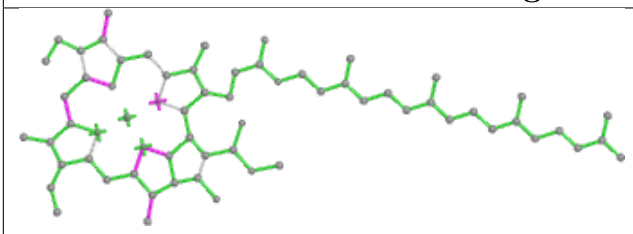
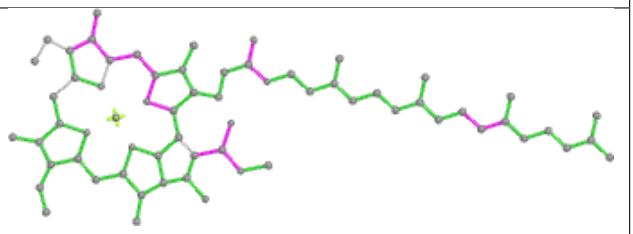

Rings

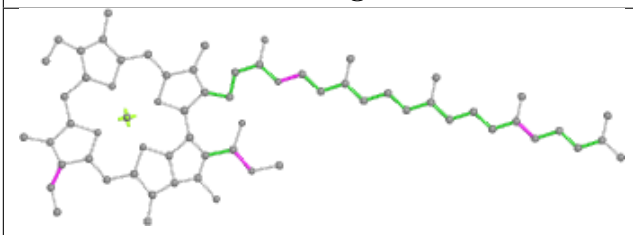
Ligand CLA D 404



Bond lengths



Bond angles



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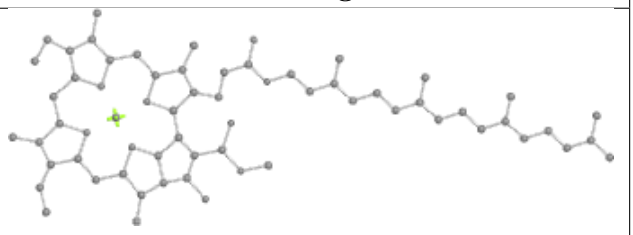
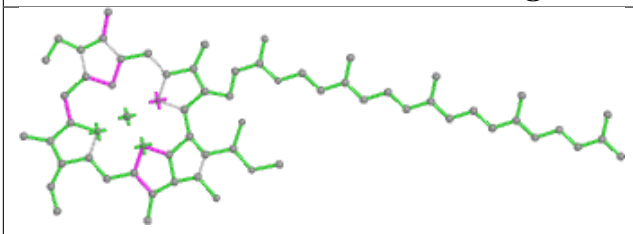
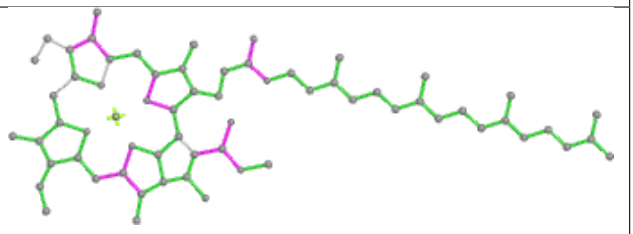


Rings

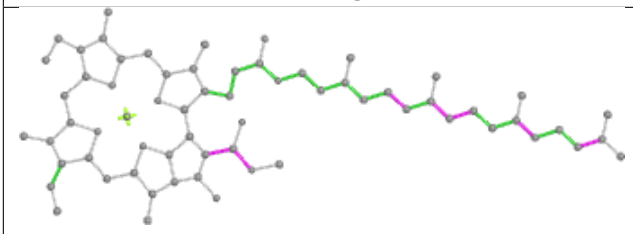
Ligand CLA C 508



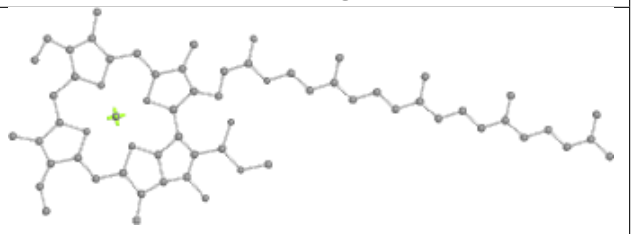
Bond lengths



Bond angles

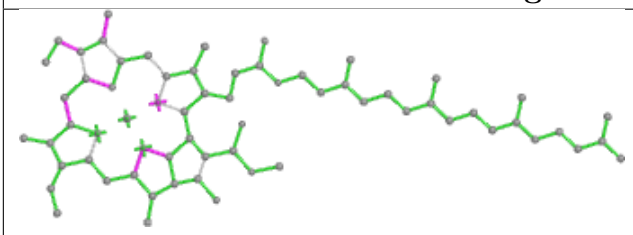


Torsions

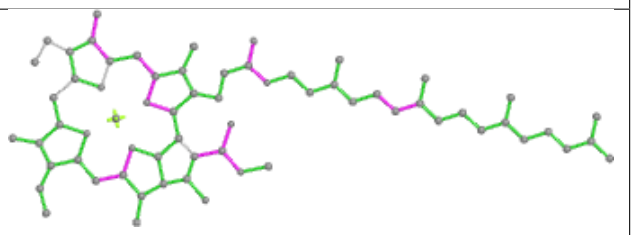


Rings

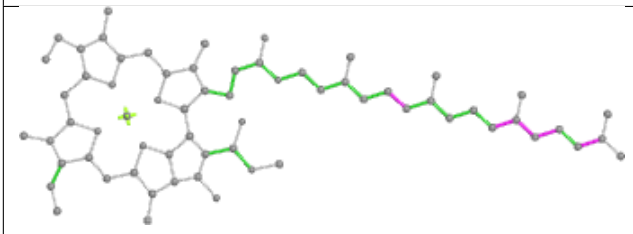
Ligand CLA B 615



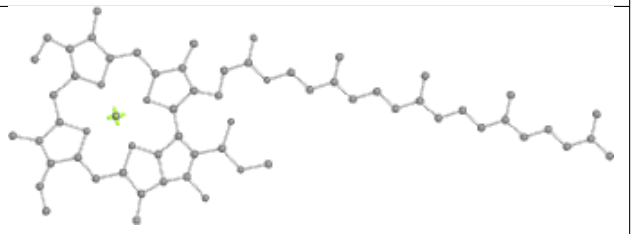
Bond lengths



Bond angles

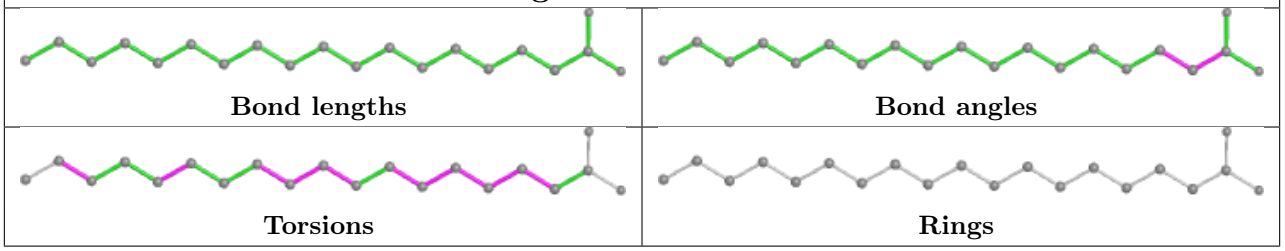


Torsions

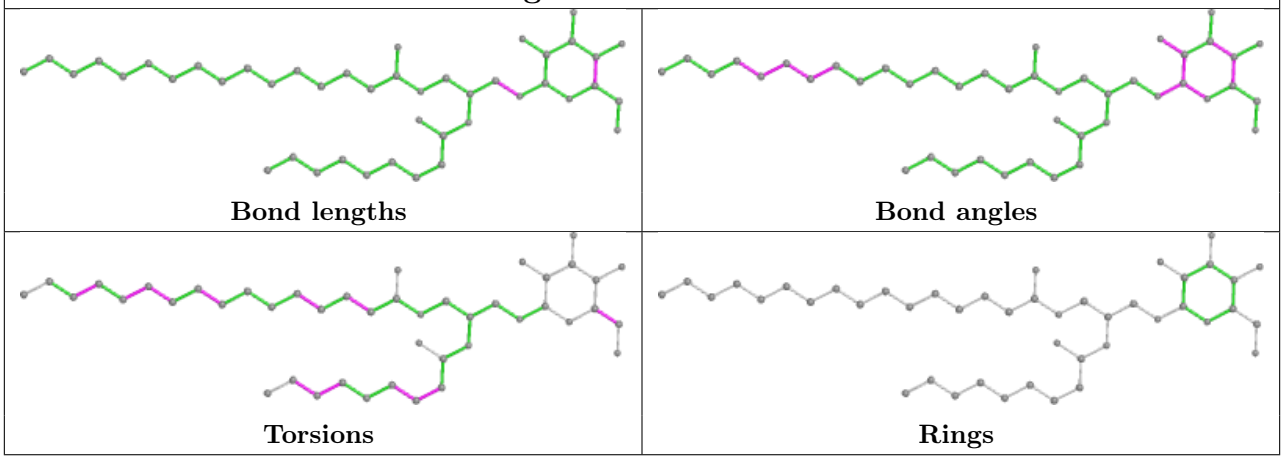


Rings

Ligand STE x 102



Ligand LMG d 411



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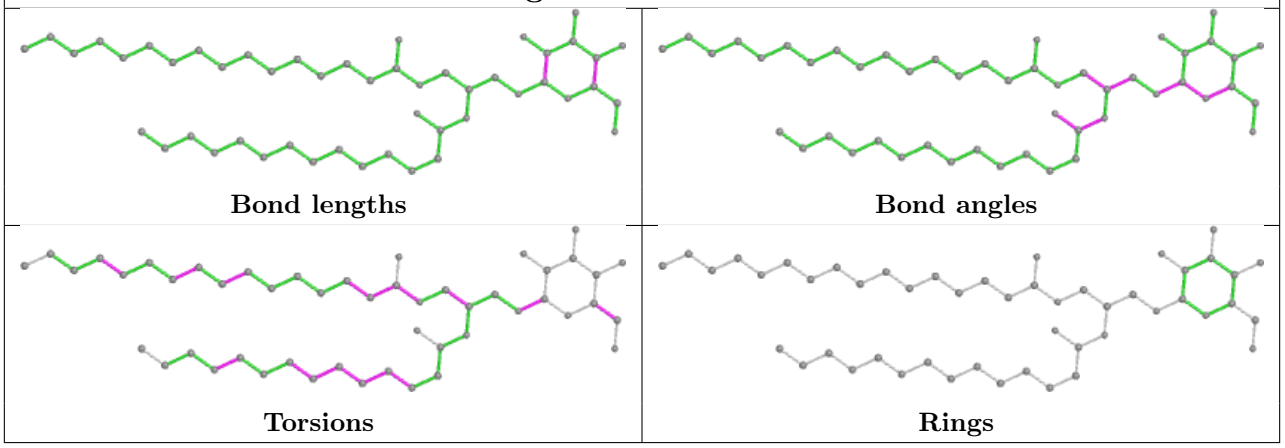

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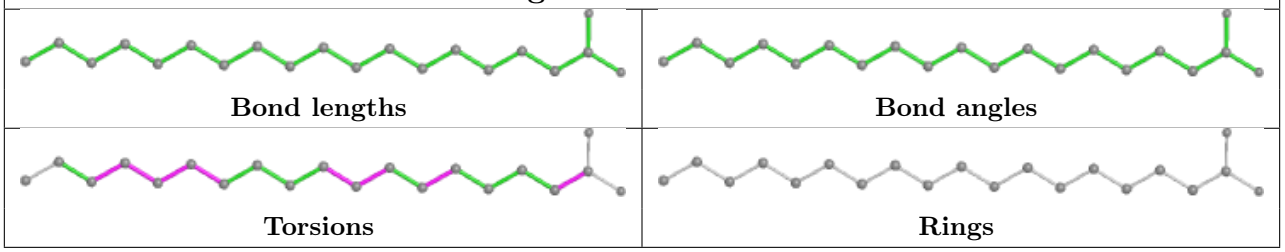
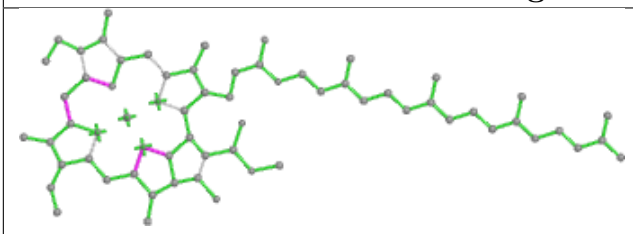
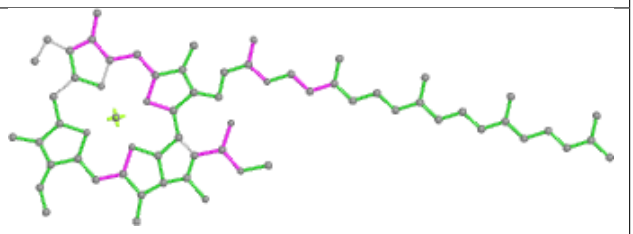


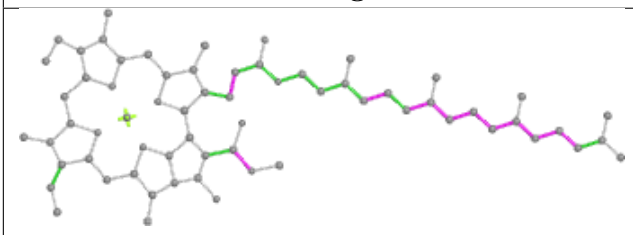
Ligand CLA b 602



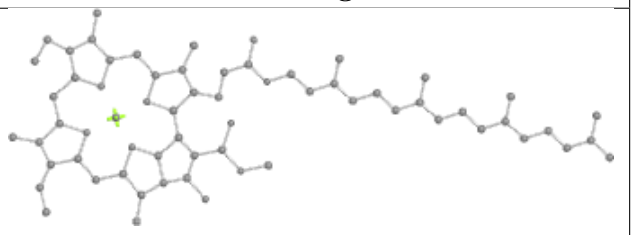
Bond lengths



Bond angles

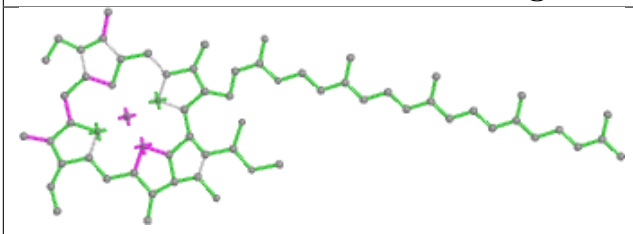


Torsions

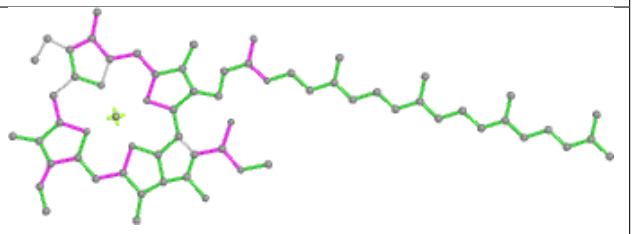


Rings

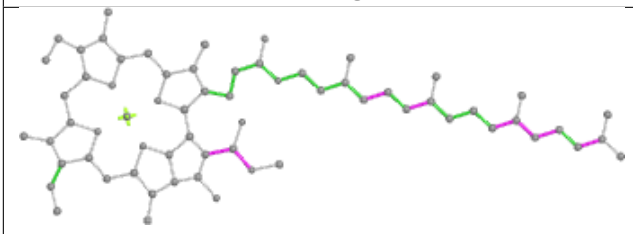
Ligand CLA a 608



Bond lengths



Bond angles



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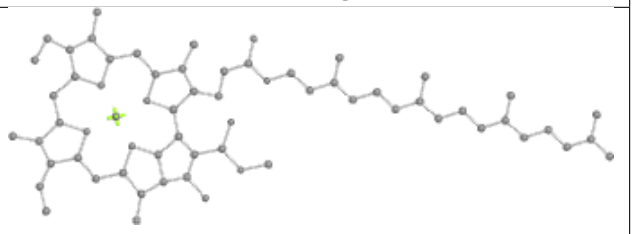
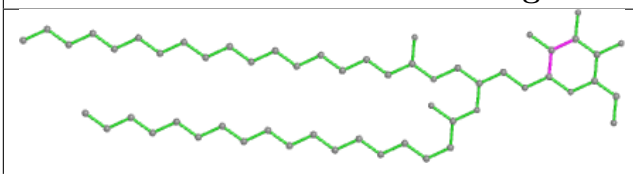
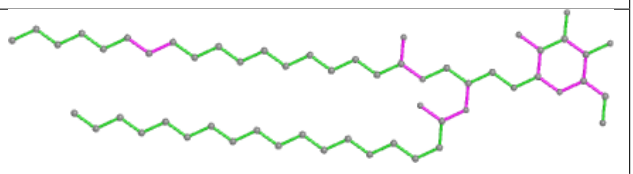


Rings

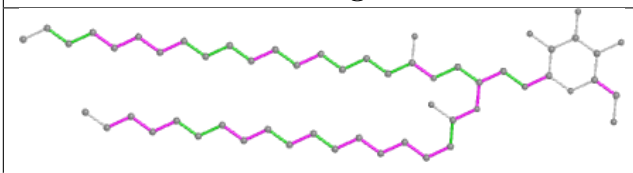
Ligand LMG b 621



Bond lengths



Bond angles



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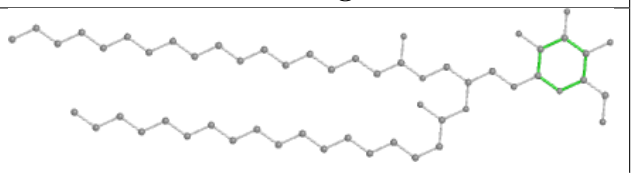
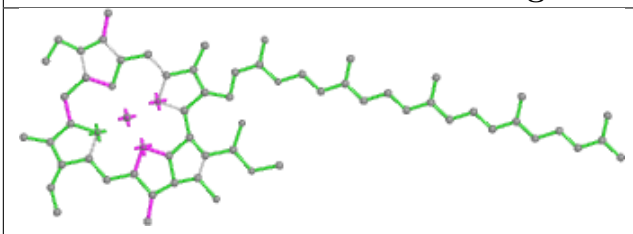
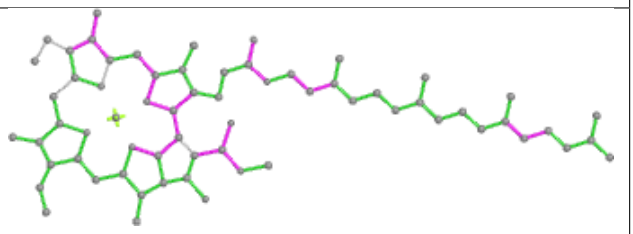


Rings

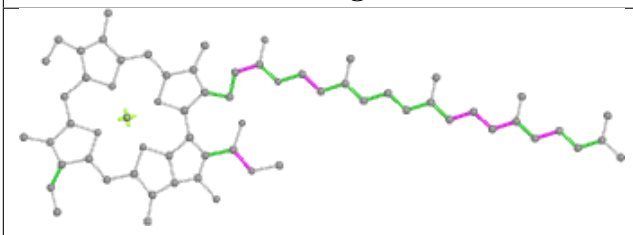
Ligand CLA b 613



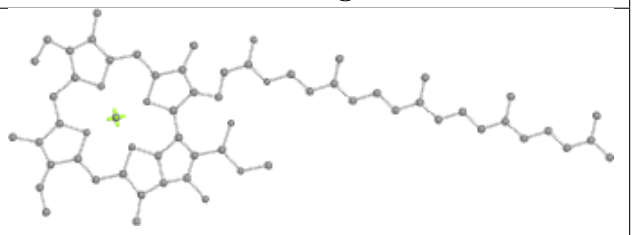
Bond lengths



Bond angles

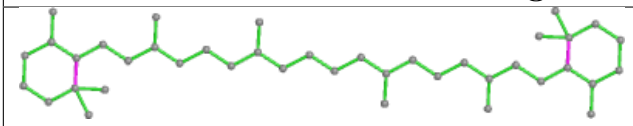


Torsions

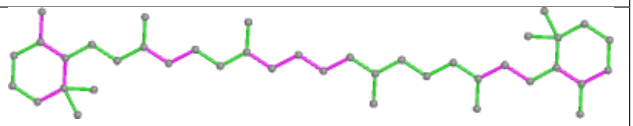


Rings

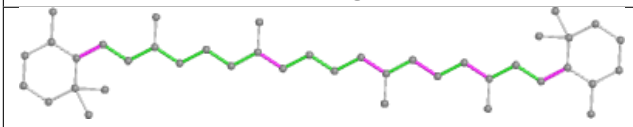
Ligand BCR c 514



Bond lengths



Bond angles

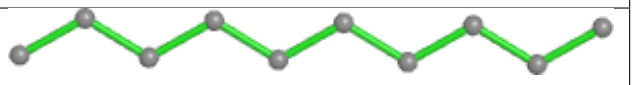


Torsions

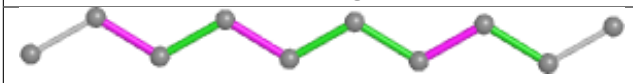
Rings

Ligand STE a 616

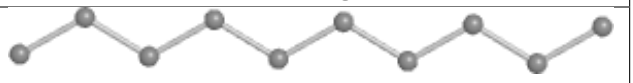
Bond lengths



Bond angles

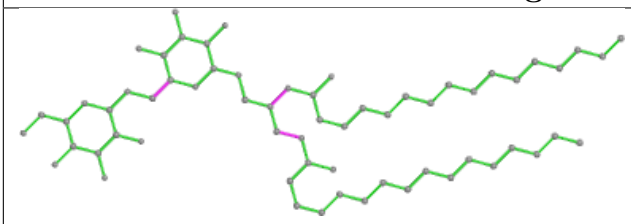


Torsions

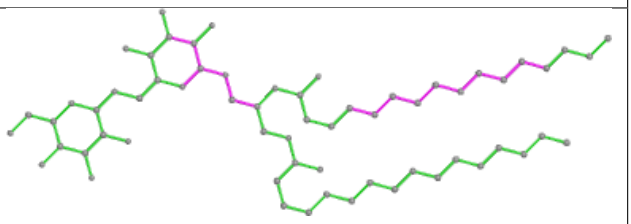


Rings

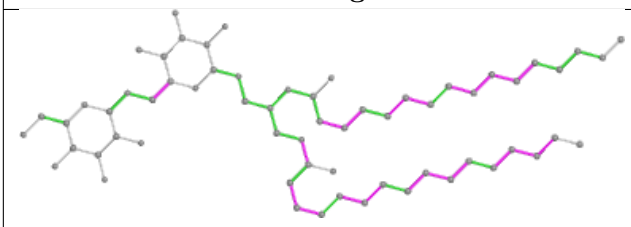
Ligand DGD c 519



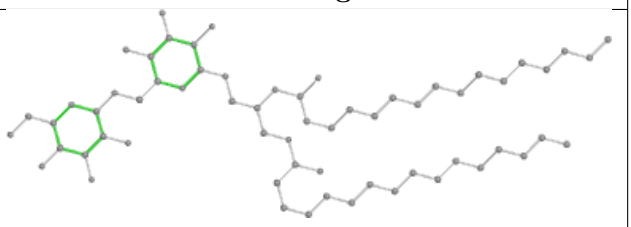
Bond lengths



Bond angles

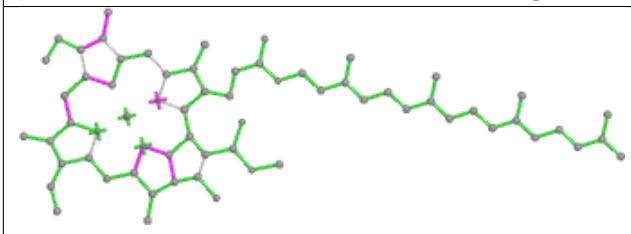


Torsions

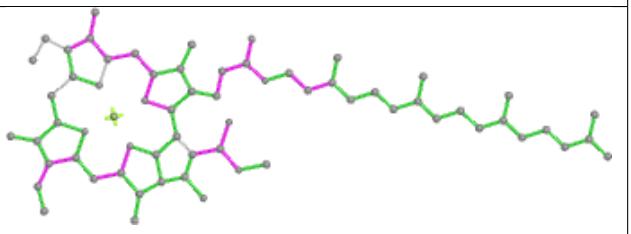


Rings

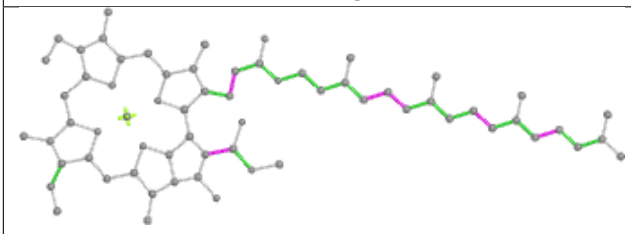
Ligand CLA b 610



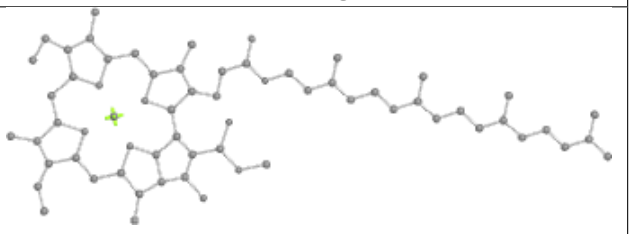
Bond lengths



Bond angles

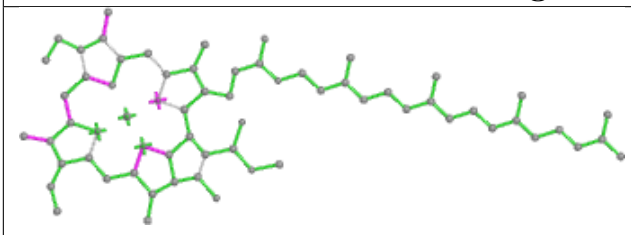


Torsions

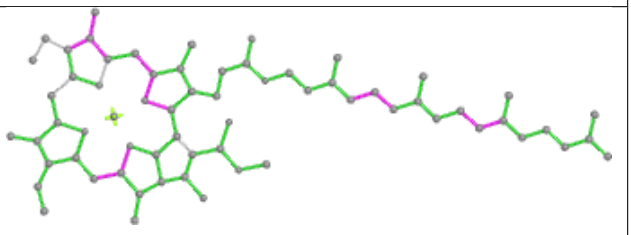


Rings

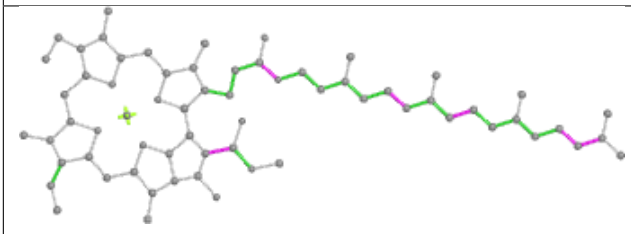
Ligand CLA c 503



Bond lengths



Bond angles



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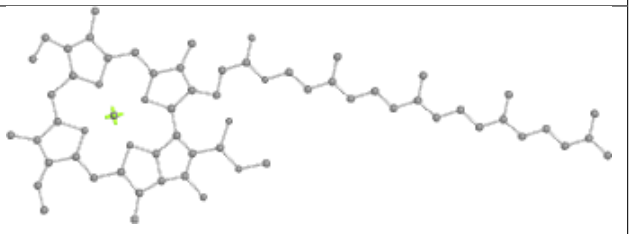
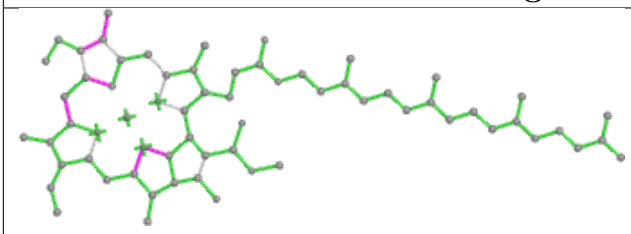


Rings

Ligand CLA B 610



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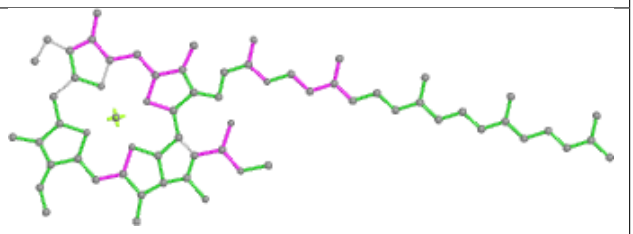
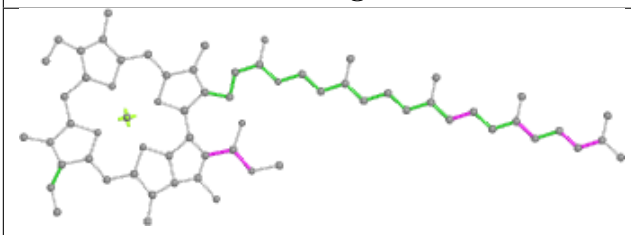
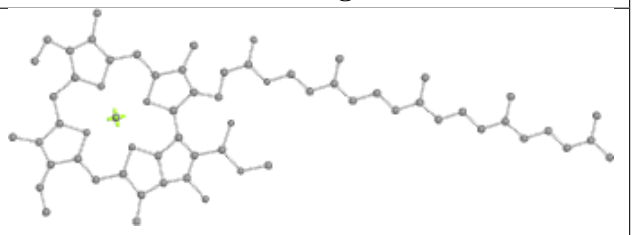


Bond angles

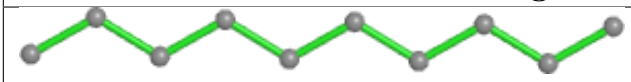


Torsions

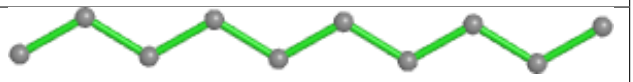


Rings

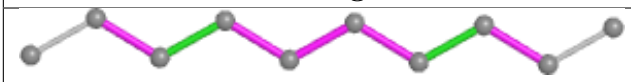
Ligand STE b 623



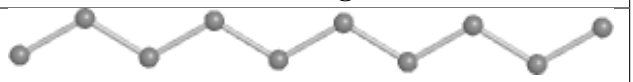
Bond lengths



Bond angles

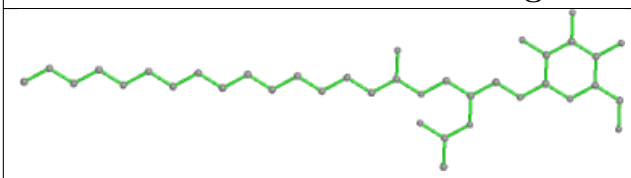


Torsions

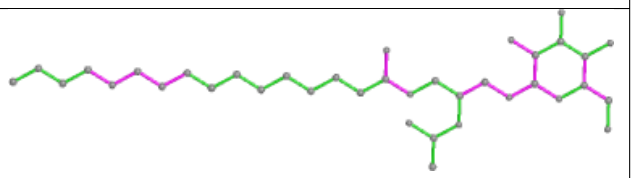


Rings

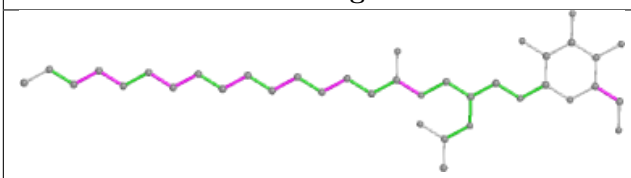
Ligand LMG c 520



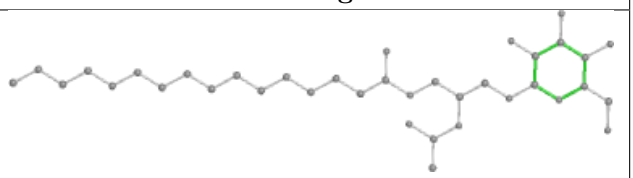
Bond lengths



Bond angles

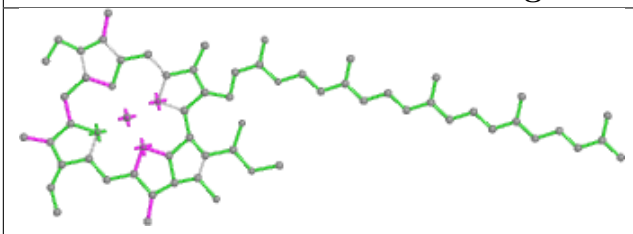


Torsions

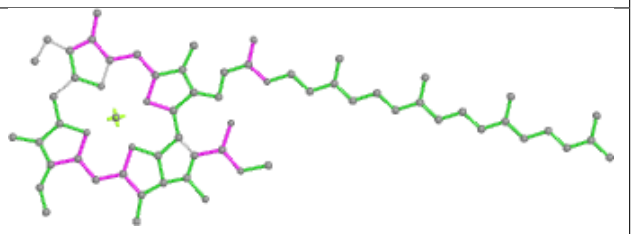


Rings

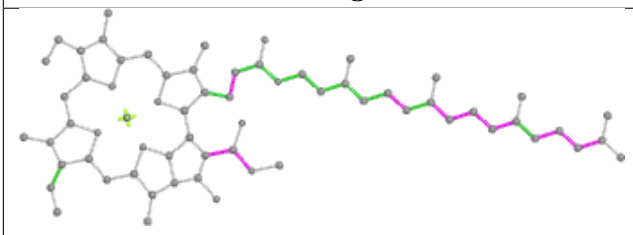
Ligand CLA B 603



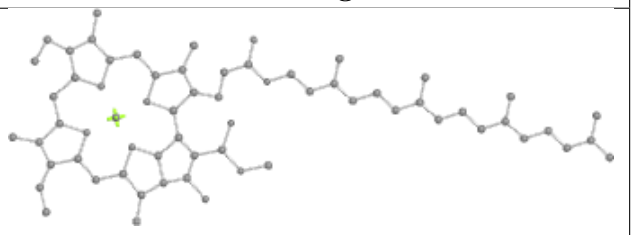
Bond lengths



Bond angles

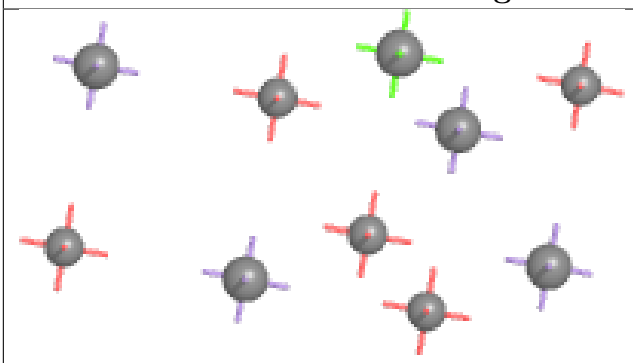


Torsions

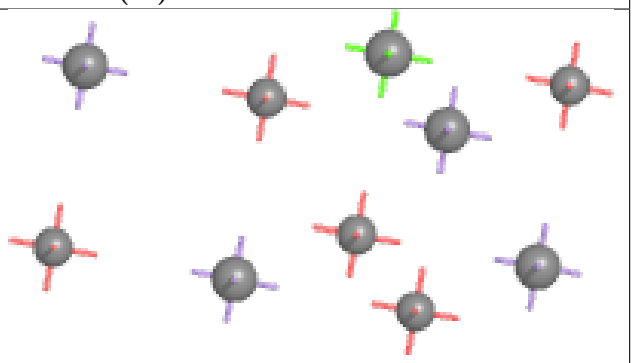


Rings

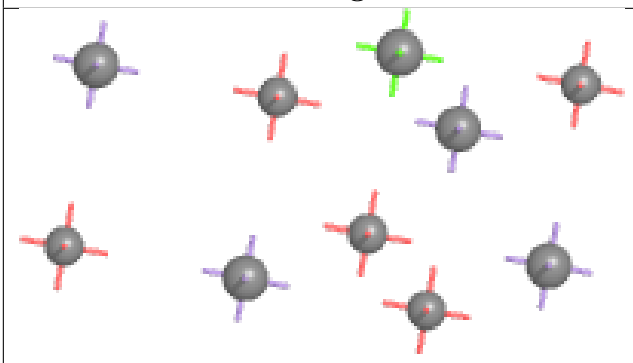
Ligand OEX a 602 (A)



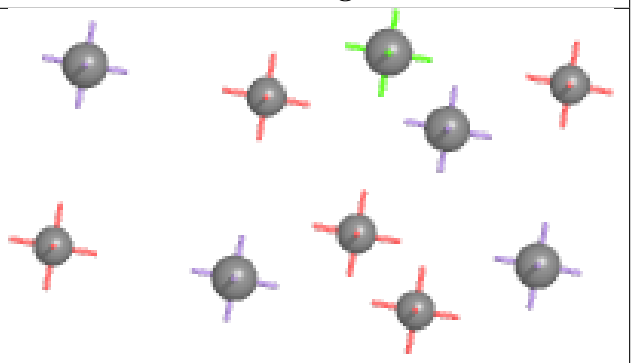
Bond lengths



Bond angles

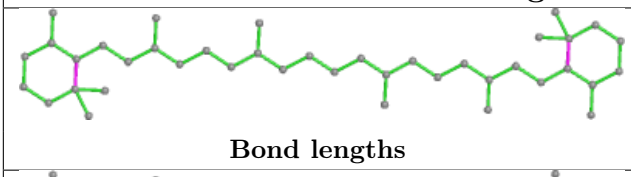


Torsions

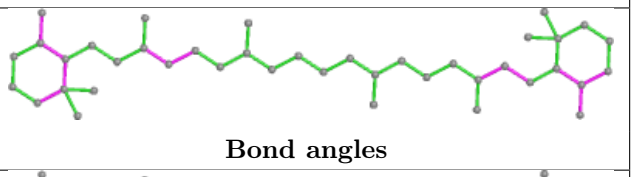


Rings

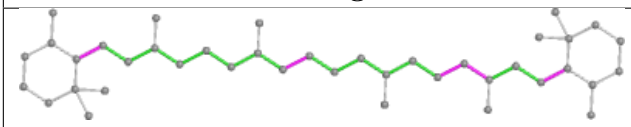
Ligand BCR c 516



Bond lengths



Bond angles



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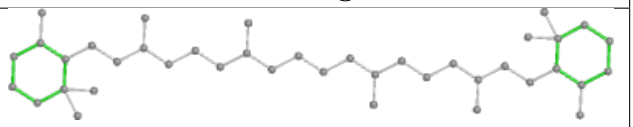
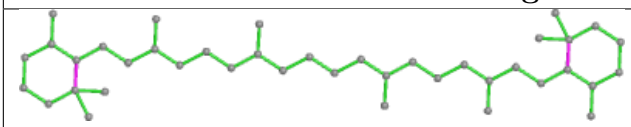


Rings

Ligand BCR D 406



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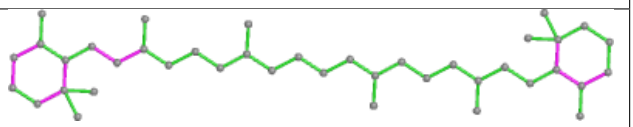
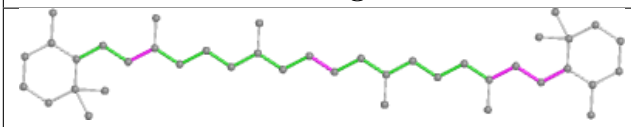


Bond angles



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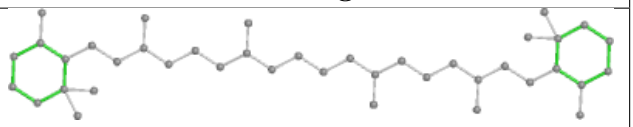
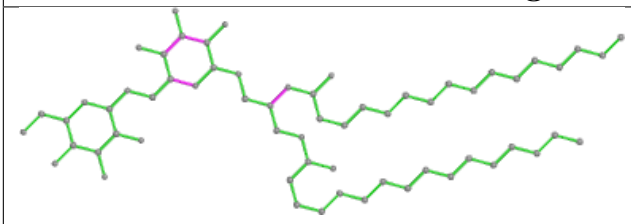
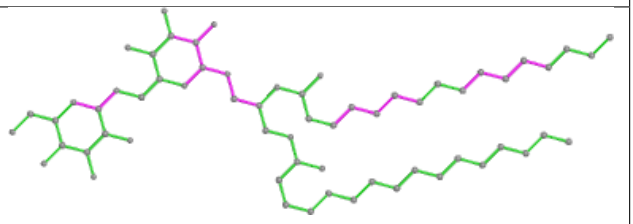


Rings

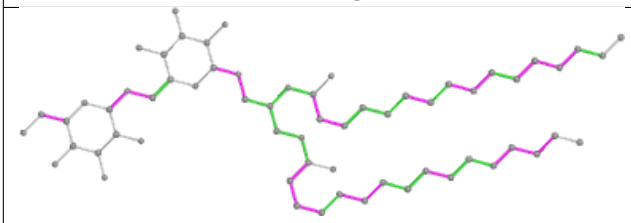
Ligand DGD c 518



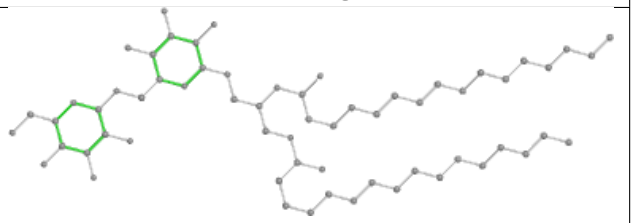
Bond lengths



Bond angles

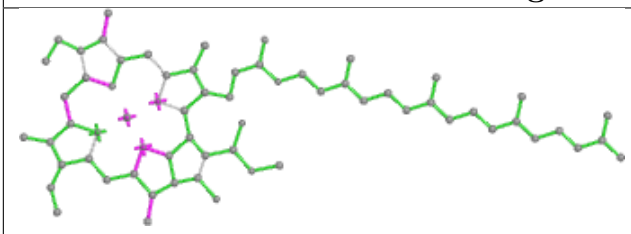


Torsions

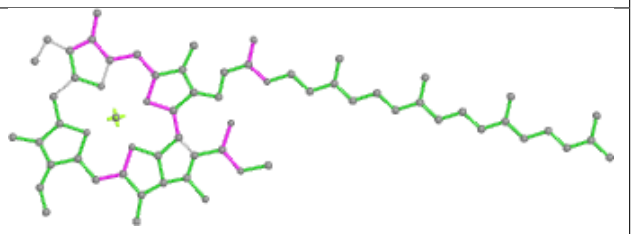


Rings

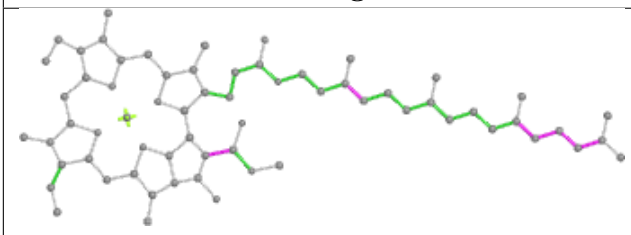
Ligand CLA b 609



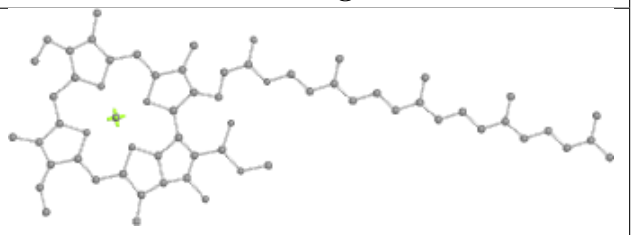
Bond lengths



Bond angles

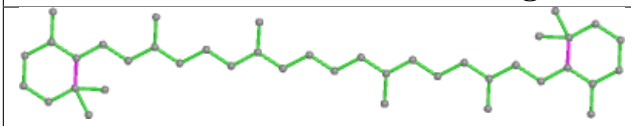


Torsions

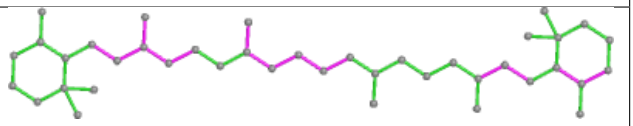


Rings

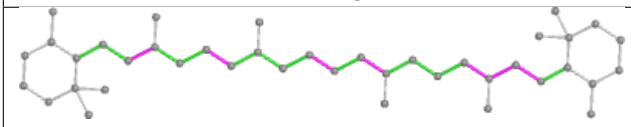
Ligand BCR K 101



Bond lengths



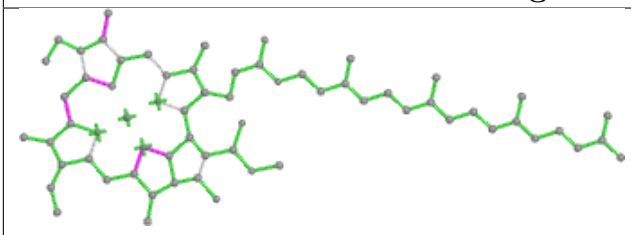
Bond angles



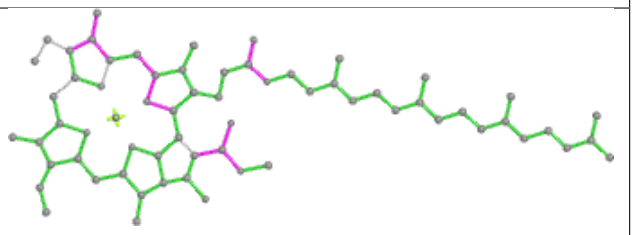
Torsions

Rings

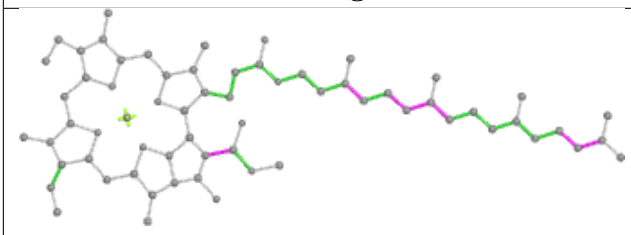
Ligand CLA c 505



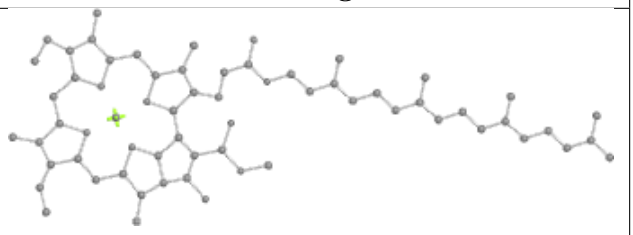
Bond lengths



Bond angles

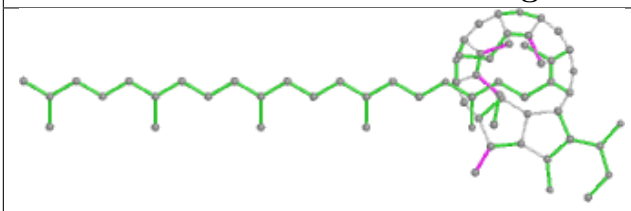


Torsions



Rings

Ligand PHO D 402



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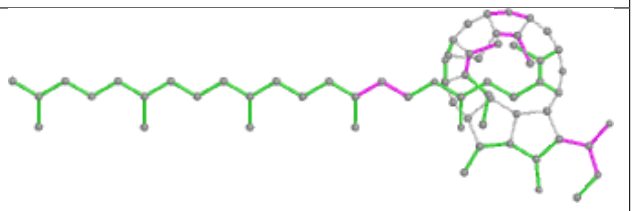
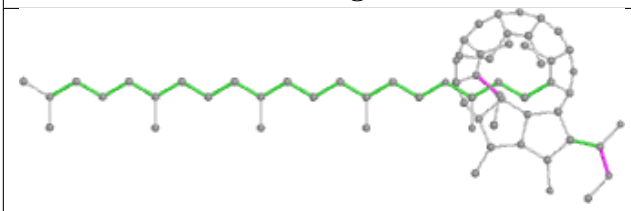
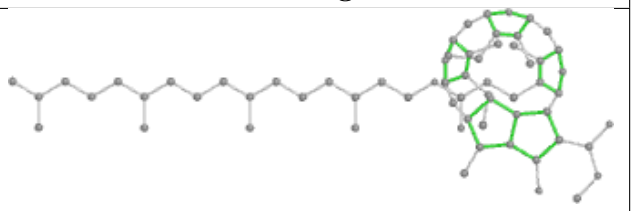


Bond angles

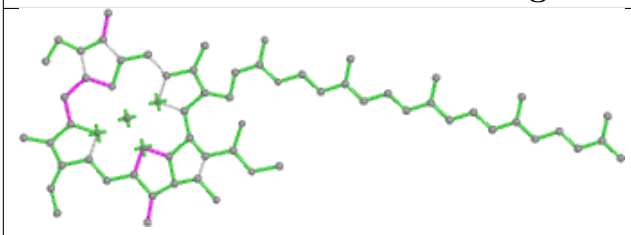


Torsions

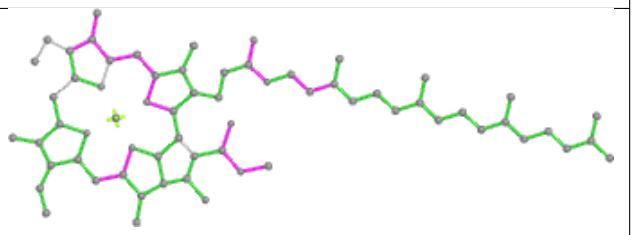


Rings

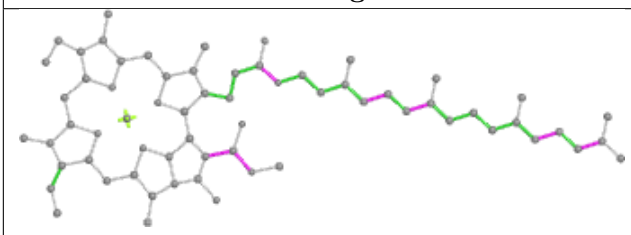
Ligand CLA c 502



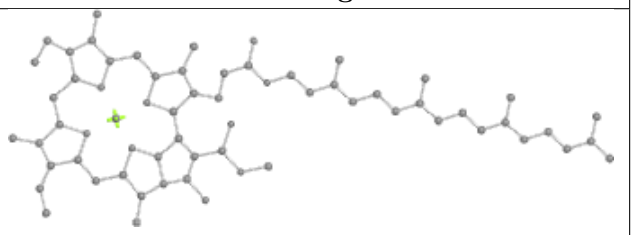
Bond lengths



Bond angles

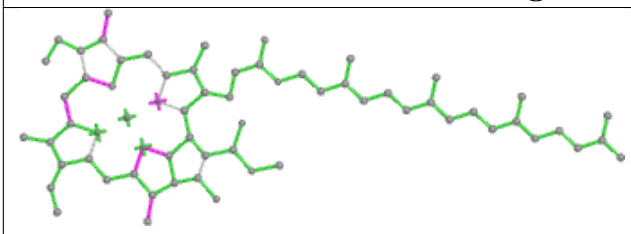


Torsions

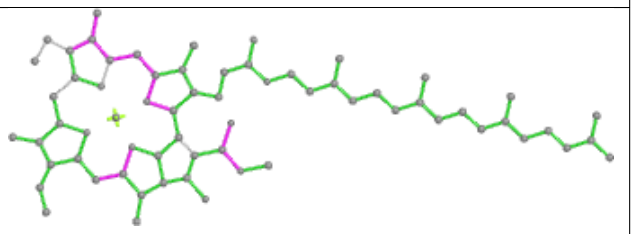


Rings

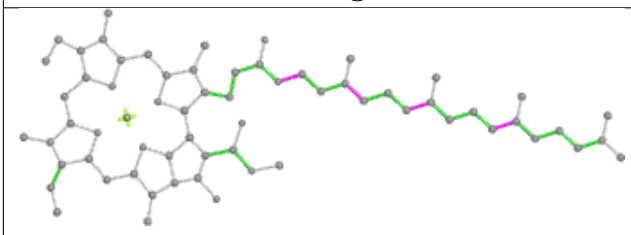
Ligand CLA d 403



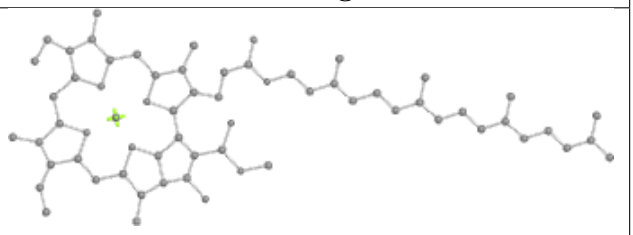
Bond lengths



Bond angles

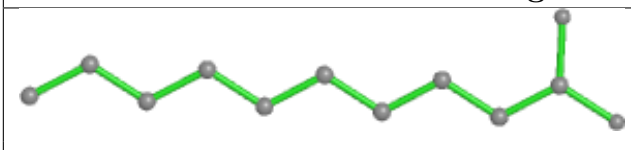


Torsions



Rings

Ligand STE C 519



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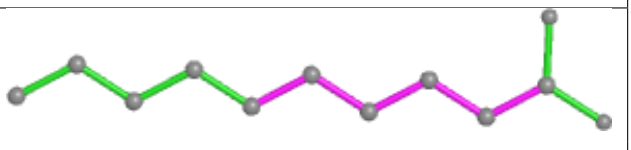
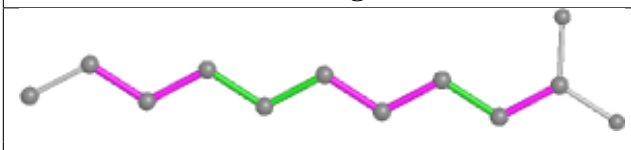


Bond angles



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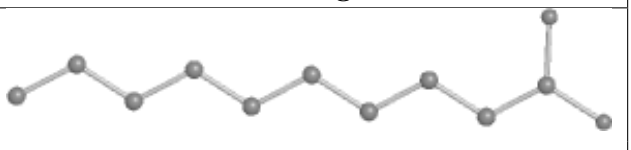
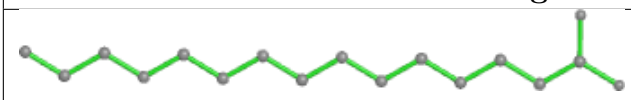
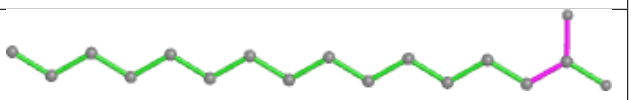


Rings

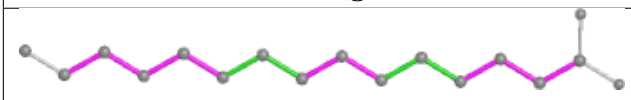
Ligand STE d 413



Bond lengths



Bond angles



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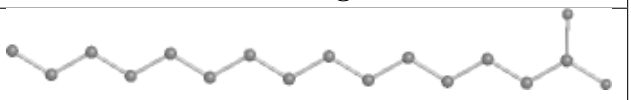
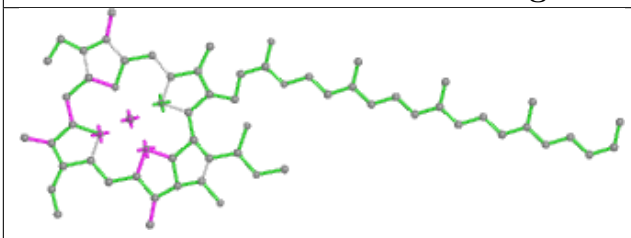
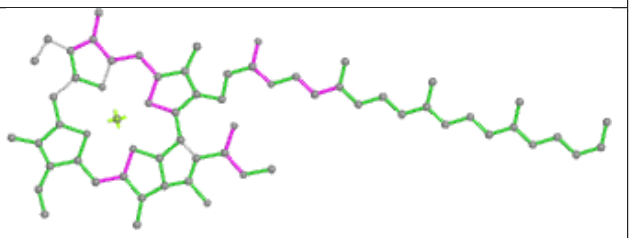


Rings

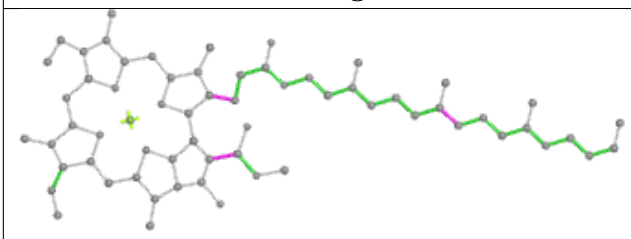
Ligand CLA c 508



Bond lengths



Bond angles



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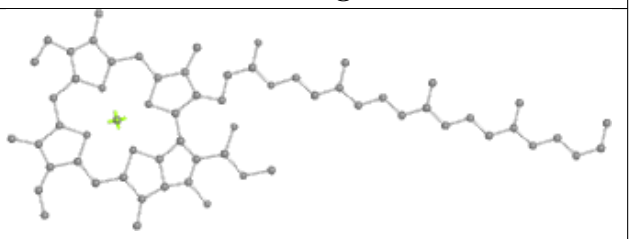
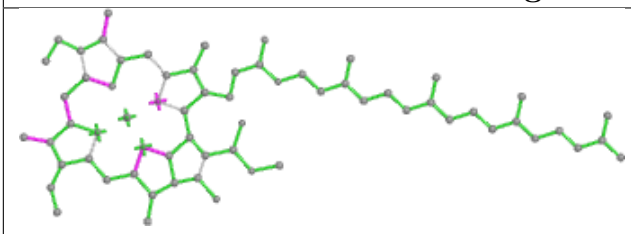


Rings

Ligand CLA C 513



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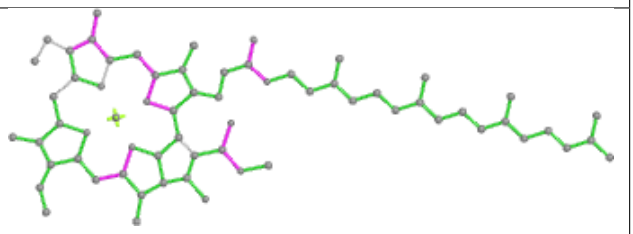
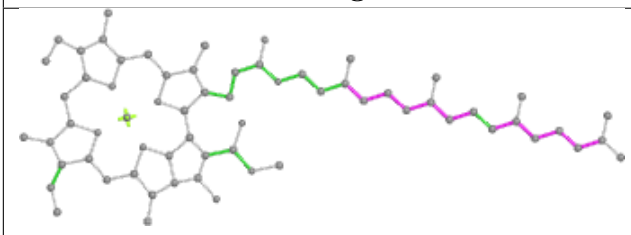
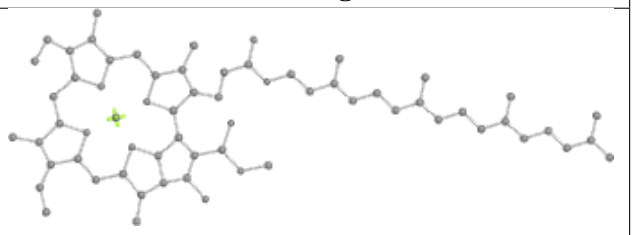


Bond angles

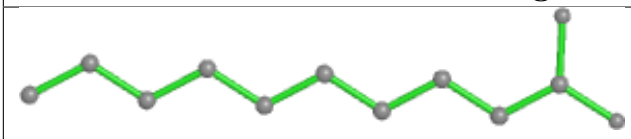


Torsions

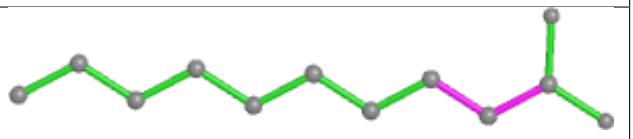


Rings

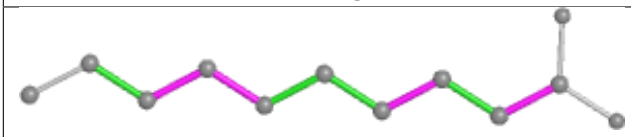
Ligand STE c 523



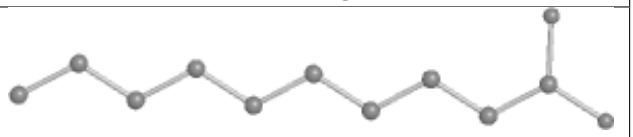
Bond lengths



Bond angles

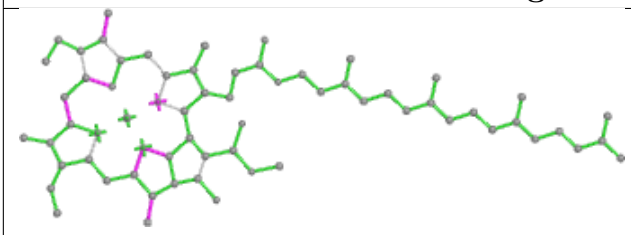


Torsions



Rings

Ligand CLA b 611



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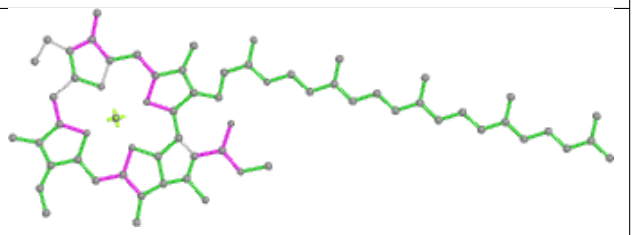
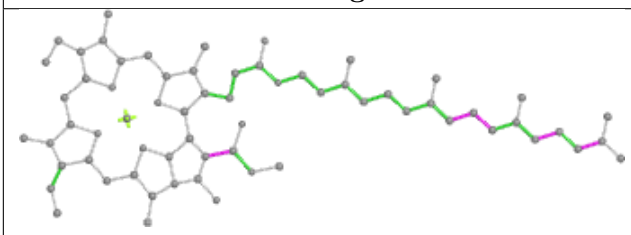


Bond angles



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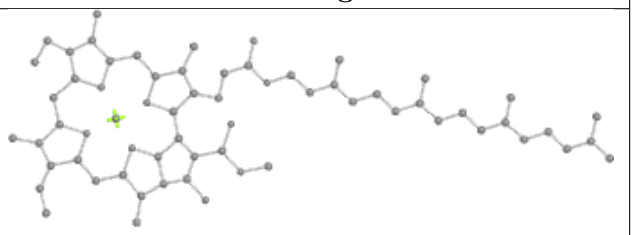
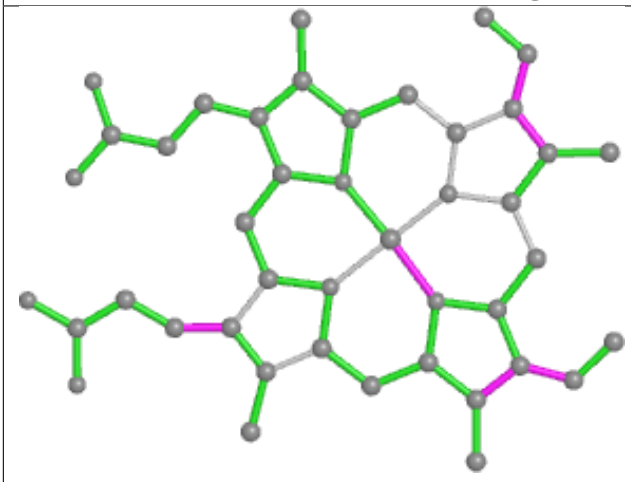
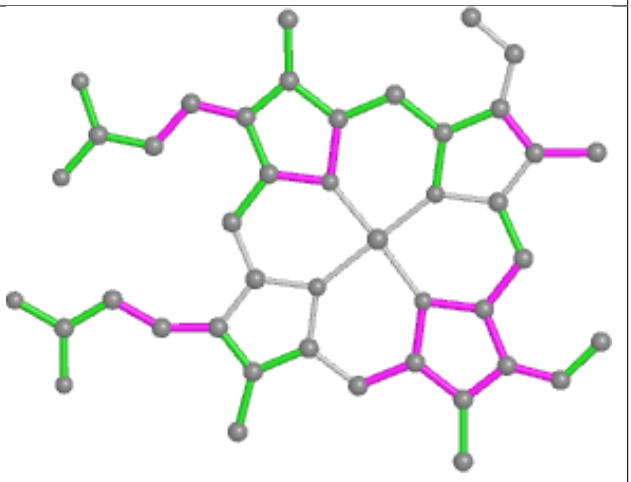


Rings

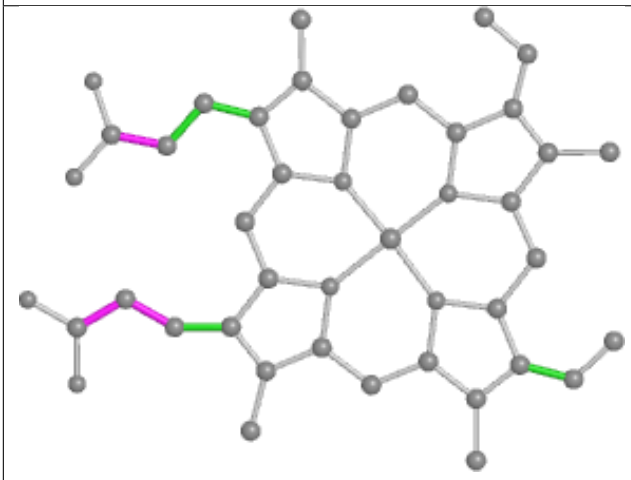
Ligand HEM f 101



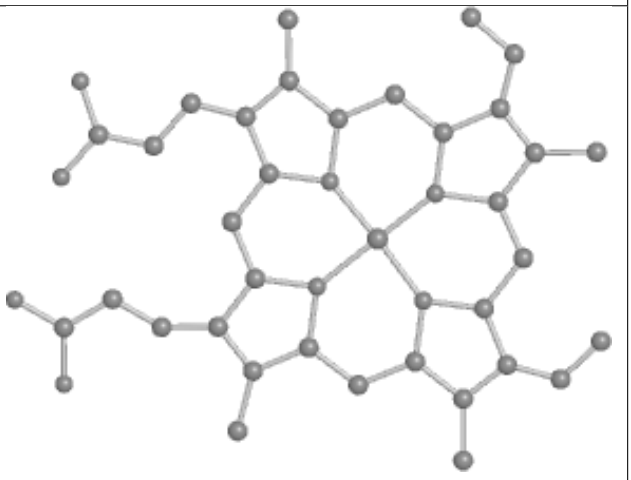
Bond lengths



Bond angles

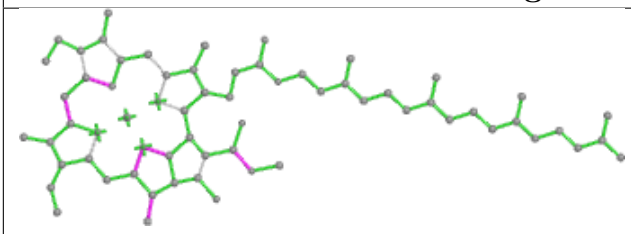


Torsions

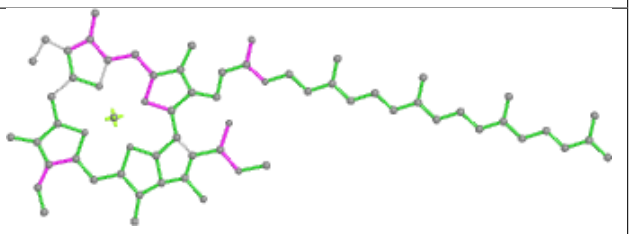


Rings

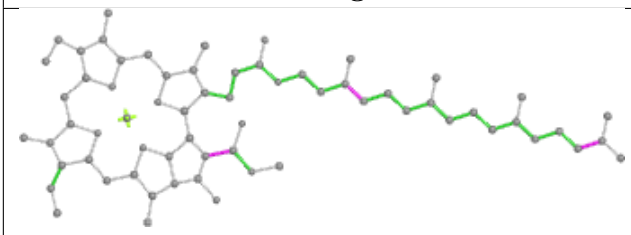
Ligand CLA B 609



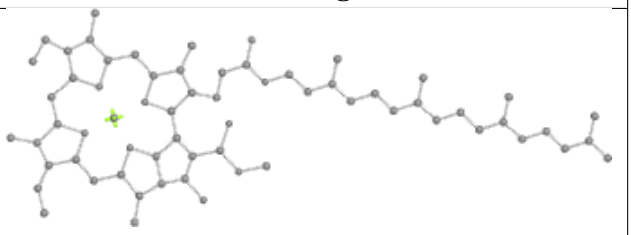
Bond lengths



Bond angles

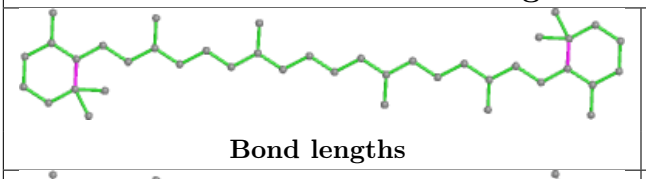


Torsions

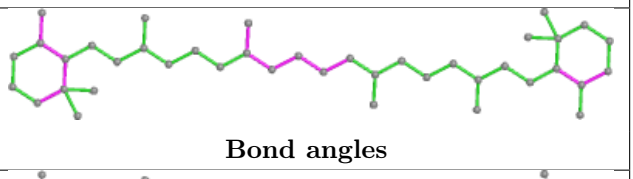


Rings

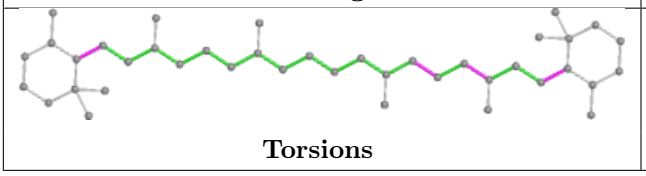
Ligand BCR C 514



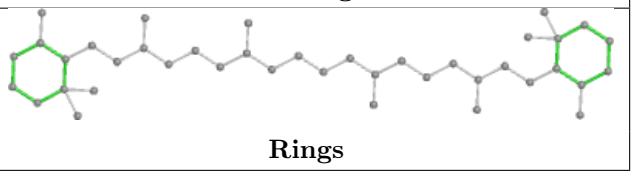
Bond lengths



Bond angles

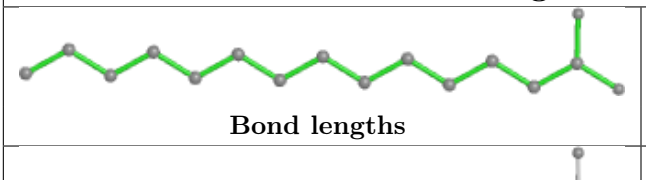


Torsions

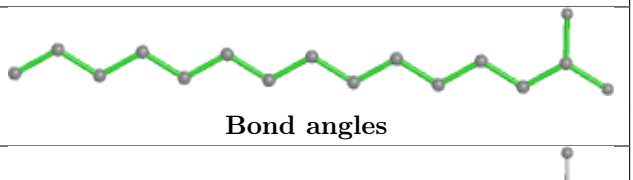


Rings

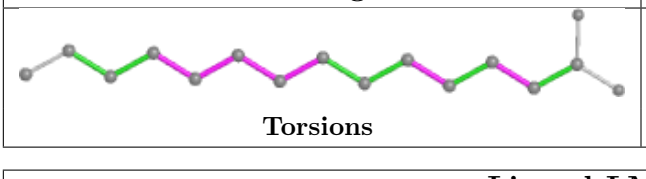
Ligand STE d 412



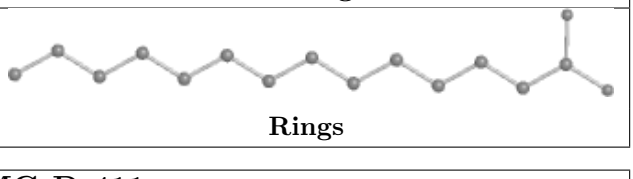
Bond lengths



Bond angles

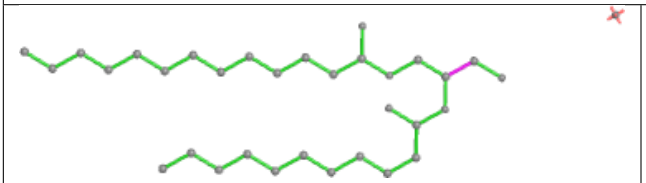


Torsions

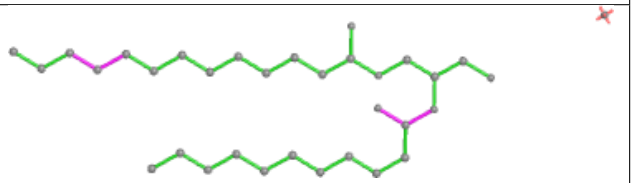


Rings

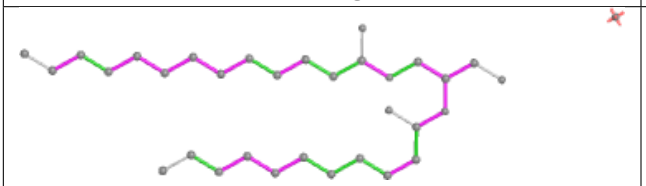
Ligand LMG D 411



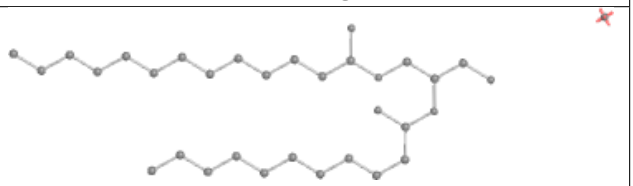
Bond lengths



Bond angles

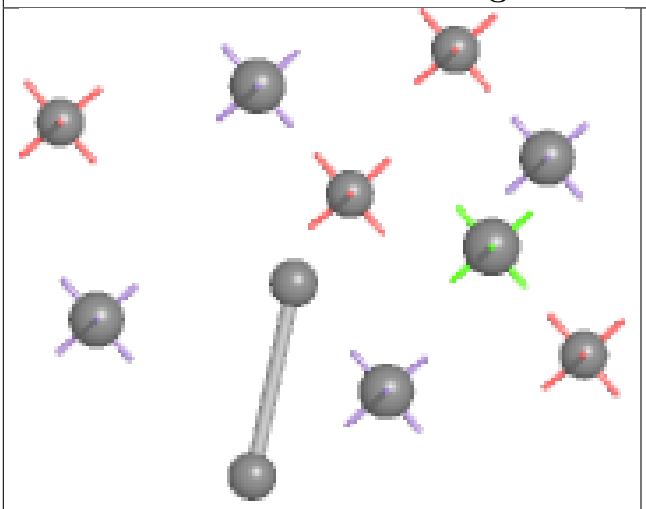


Torsions



Rings

Ligand OEY A 601 (B)



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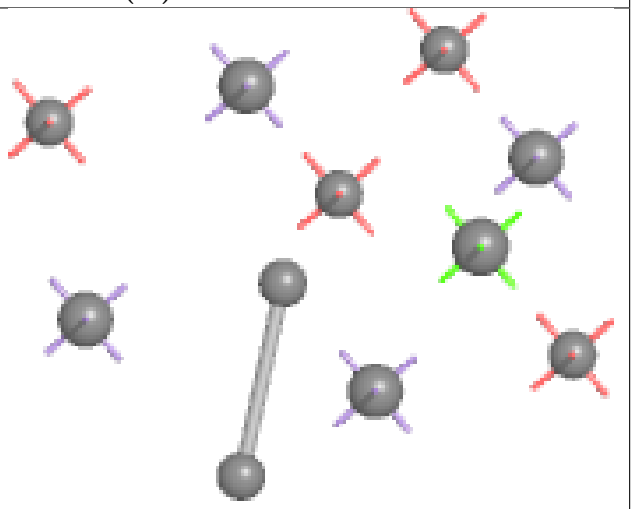
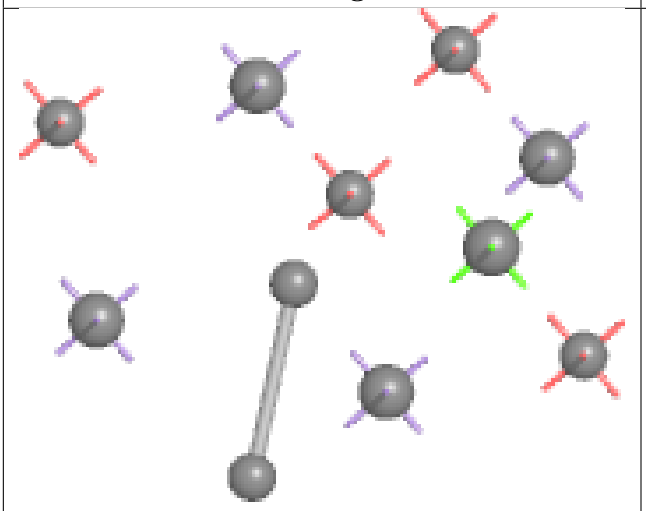
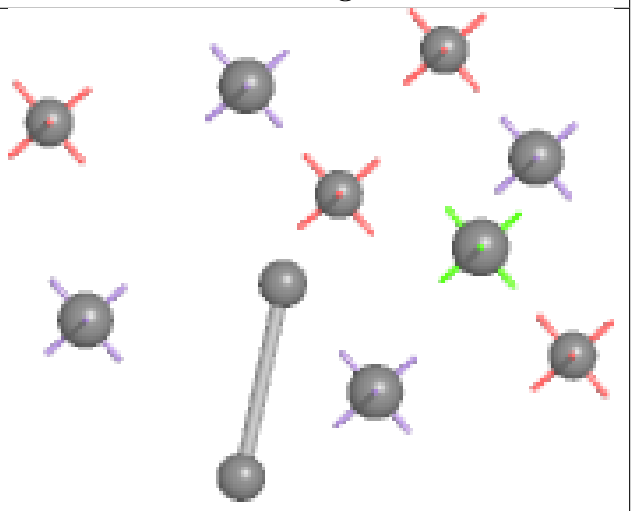


Bond angles

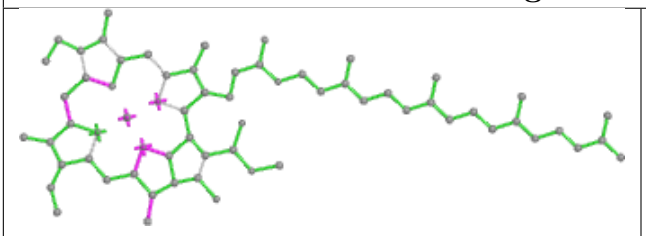


Torsions

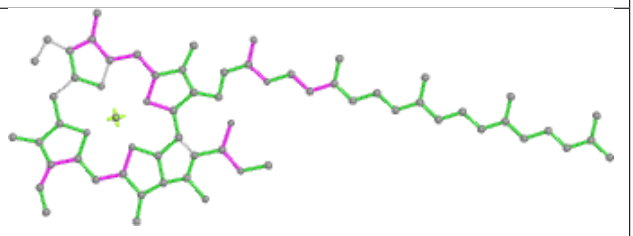


Rings

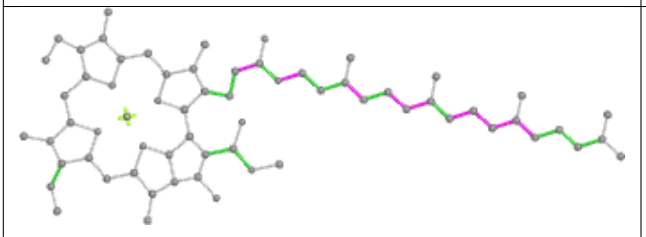
Ligand CLA B 613



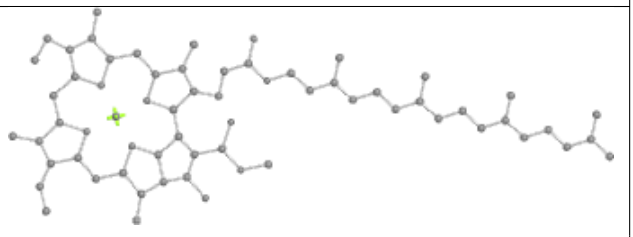
Bond lengths



Bond angles

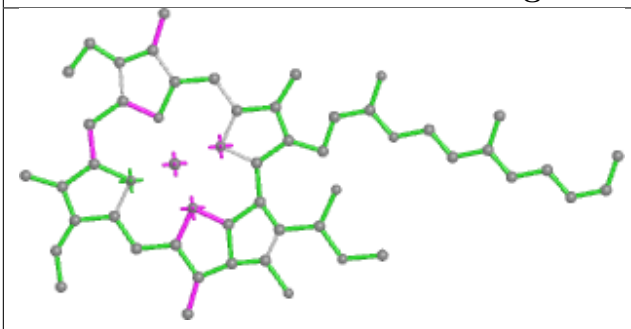


Torsions

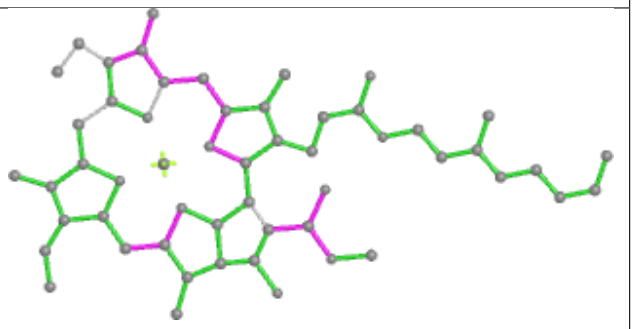


Rings

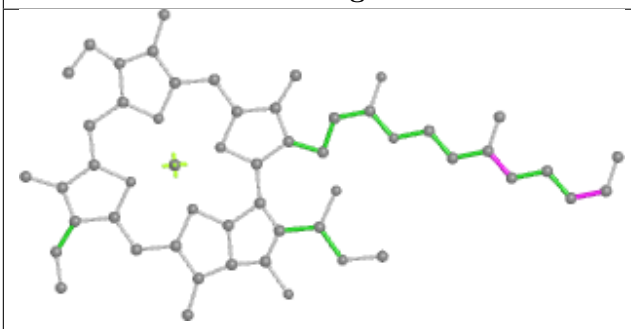
Ligand CLA A 609



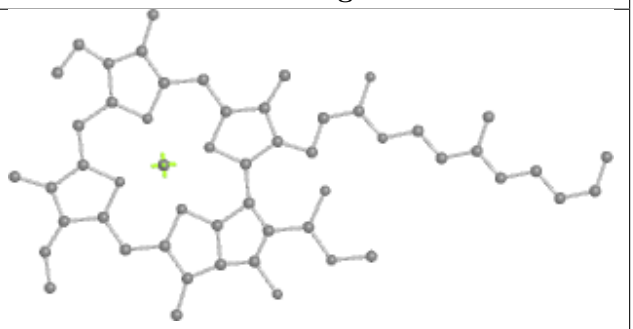
Bond lengths



Bond angles

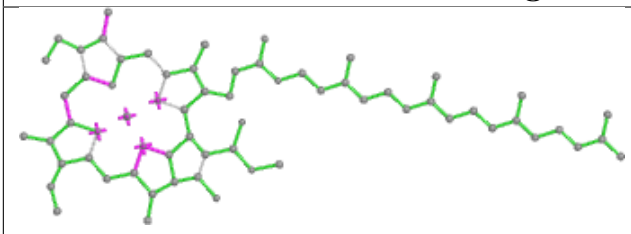


Torsions

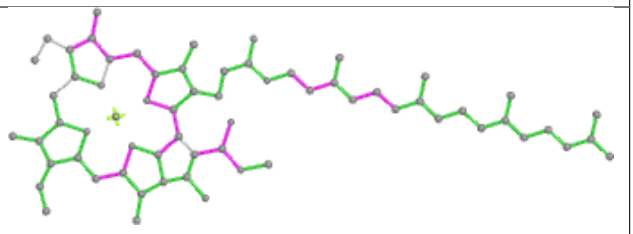


Rings

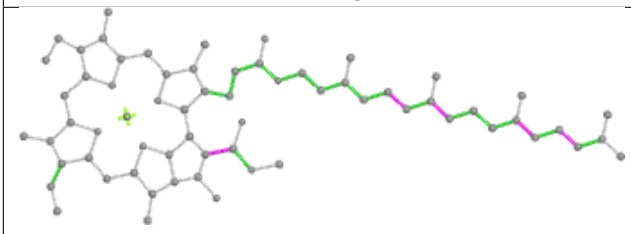
Ligand CLA C 503



Bond lengths



Bond angles



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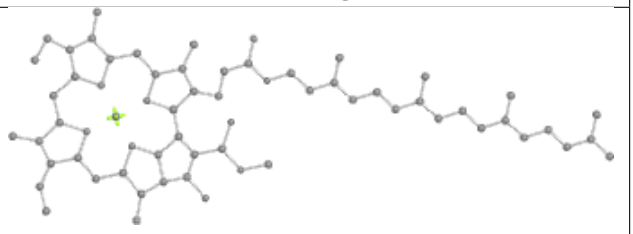
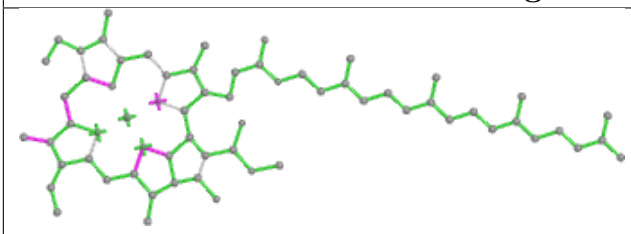
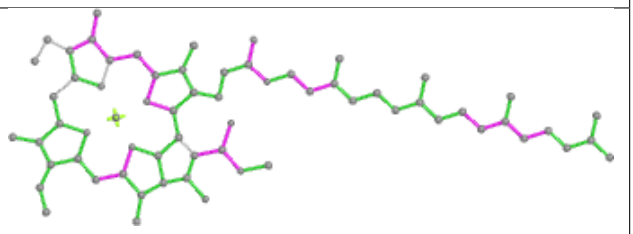


Rings

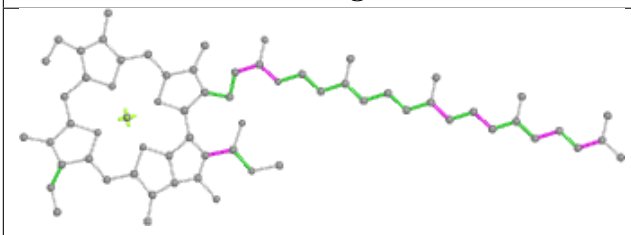
Ligand CLA B 612



Bond lengths



Bond angles



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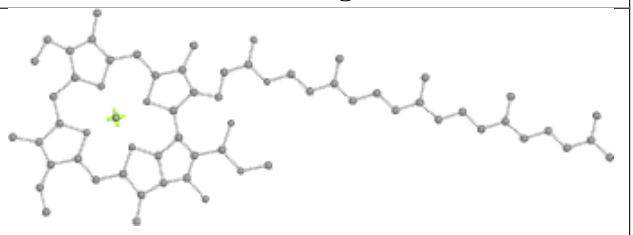
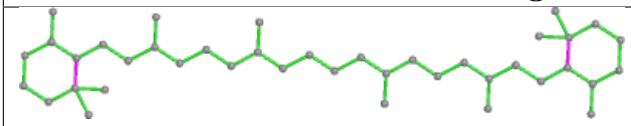
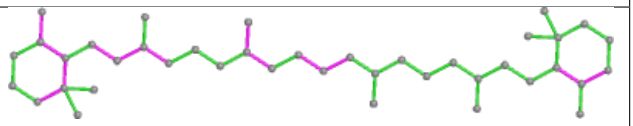


Rings

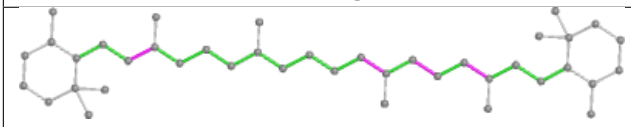
Ligand BCR c 515



Bond lengths



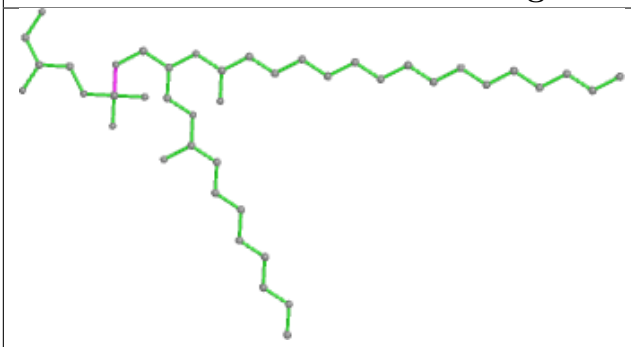
Bond angles



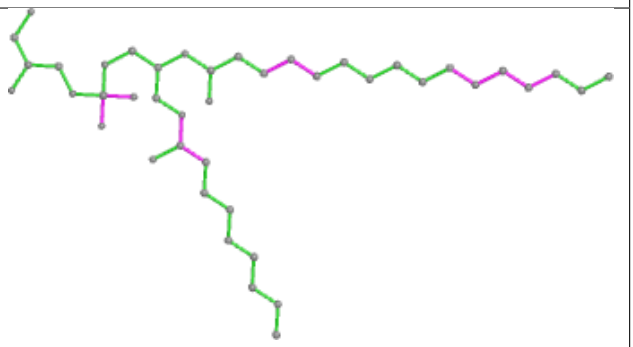
Torsions

Rings

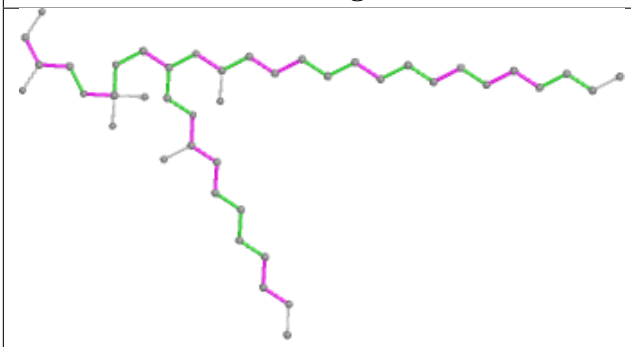
Ligand LHG e 101



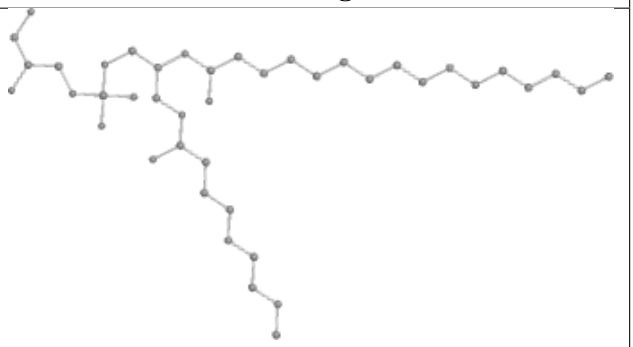
Bond lengths



Bond angles

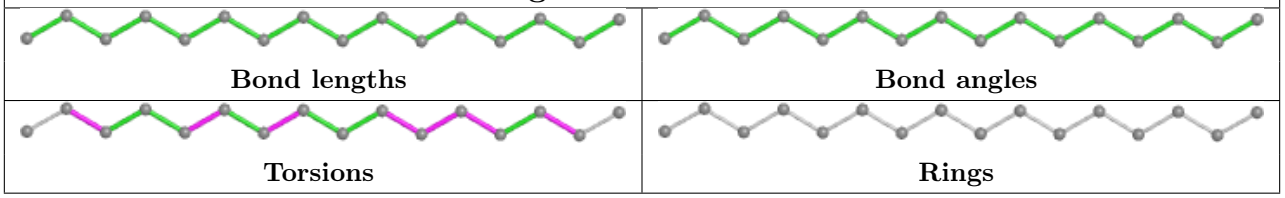


Torsions

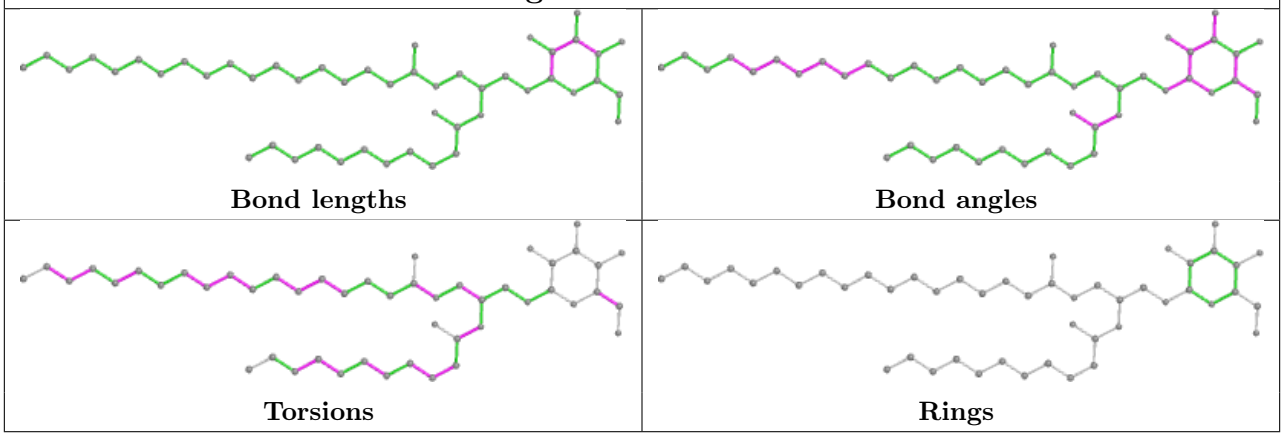


Rings

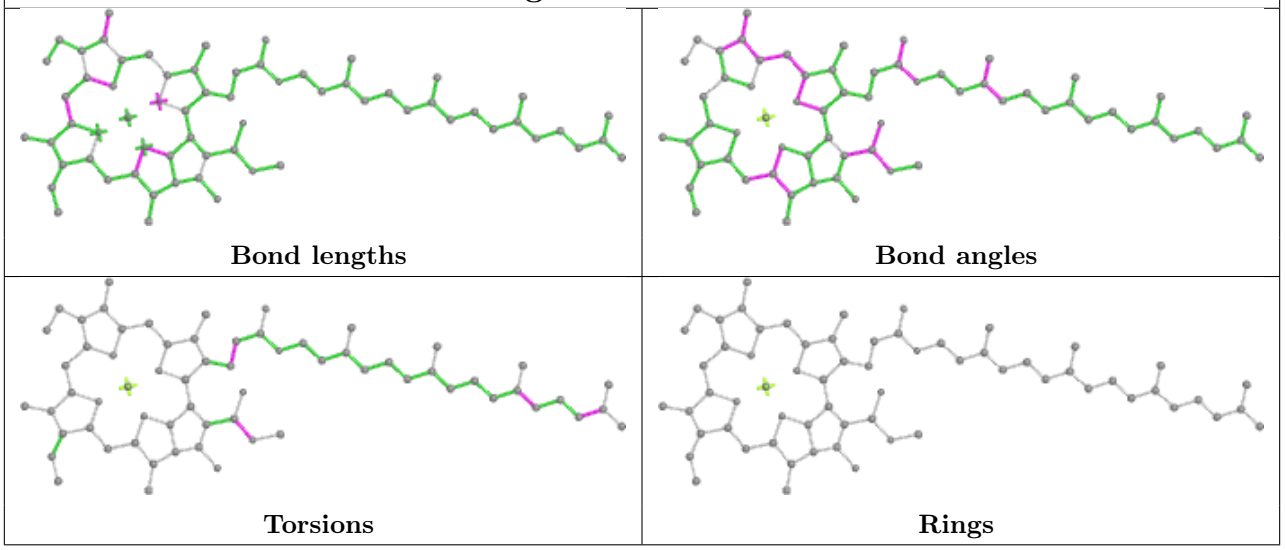
Ligand STE T 102



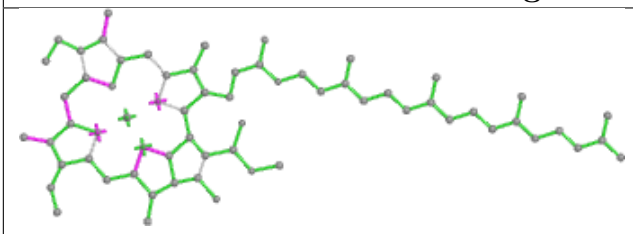
Ligand LMG c 522



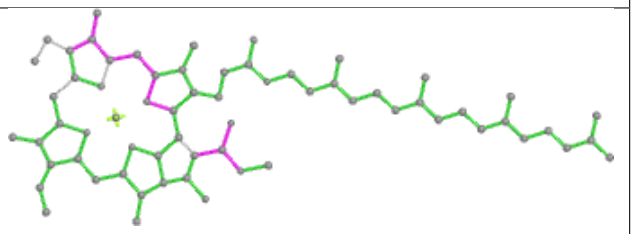
Ligand CLA C 501



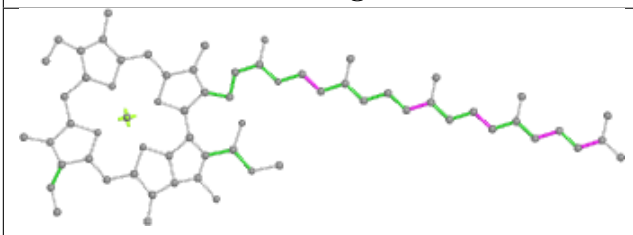
Ligand CLA D 405



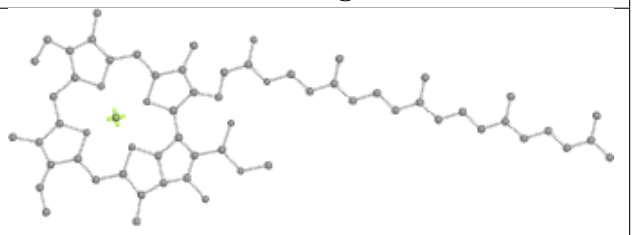
Bond lengths



Bond angles

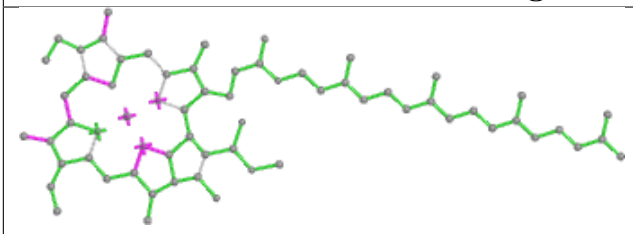


Torsions



Rings

Ligand CLA b 614



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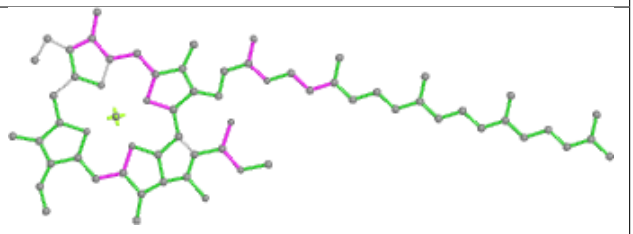
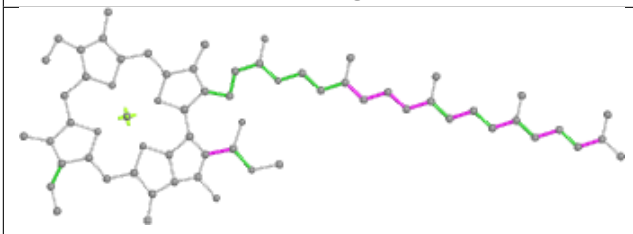
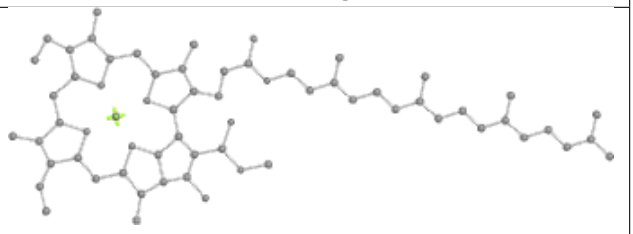


Bond angles

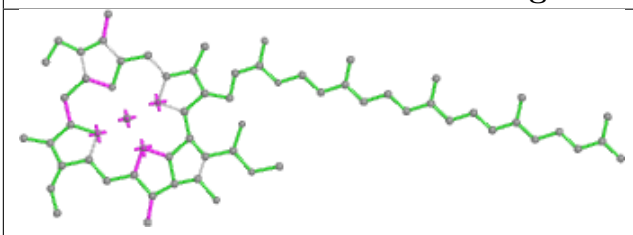


Torsions



Rings

Ligand CLA c 510



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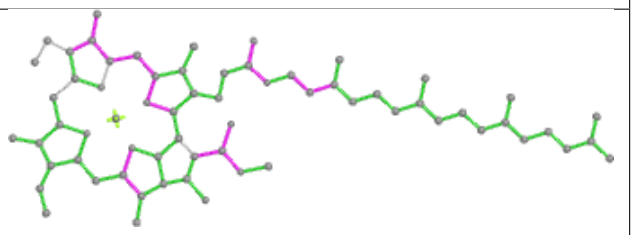
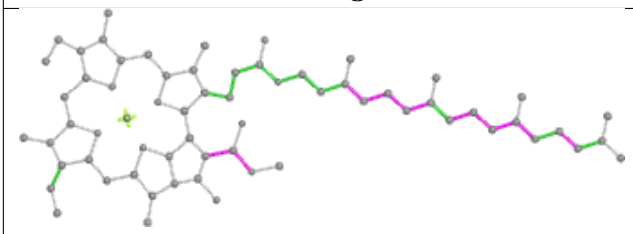


Bond angles



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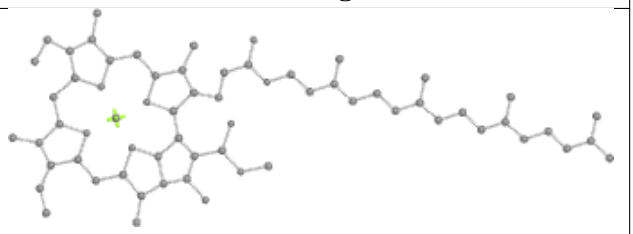
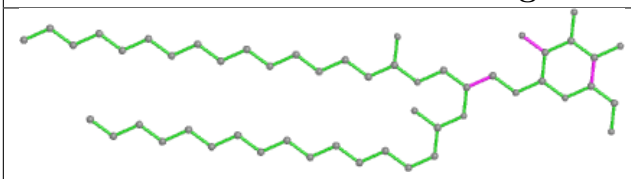
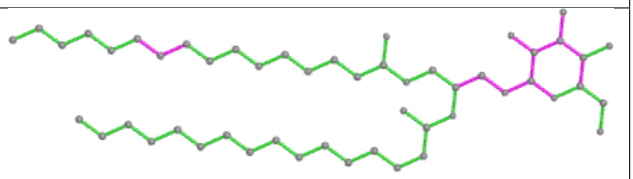


Rings

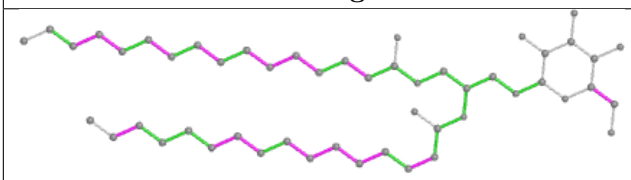
Ligand LMG D 408



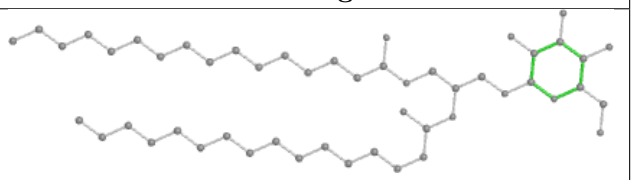
Bond lengths



Bond angles

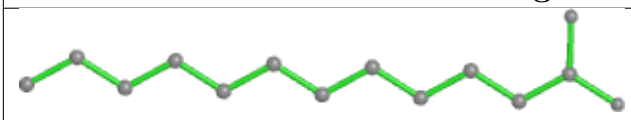


Torsions

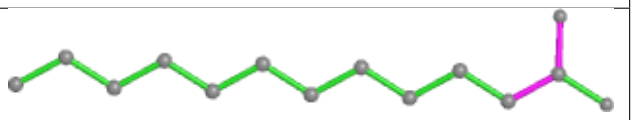


Rings

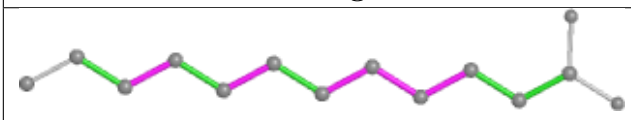
Ligand STE t 102



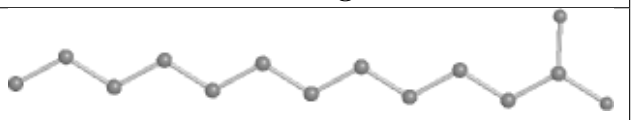
Bond lengths



Bond angles

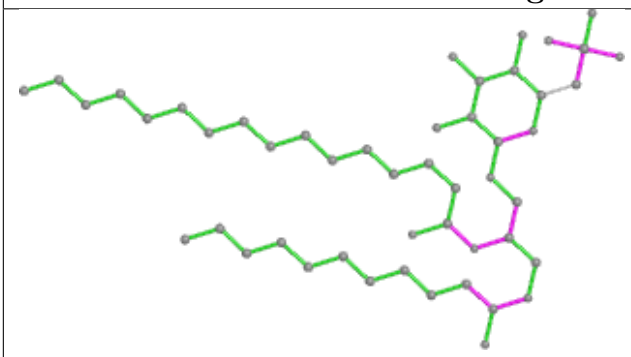


Torsions

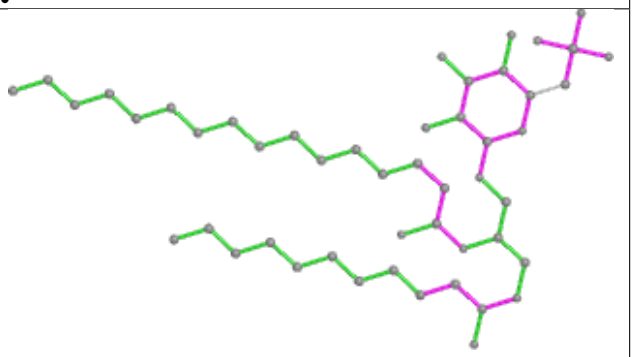


Rings

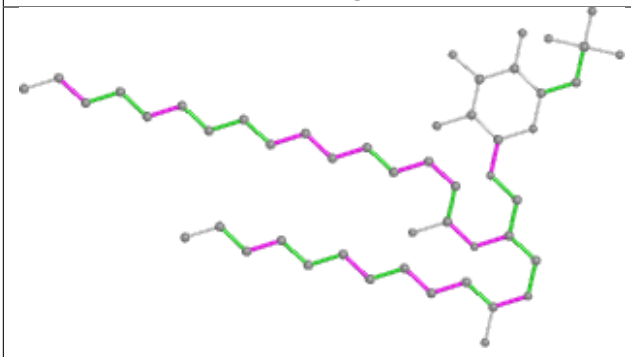
Ligand SQD L 101



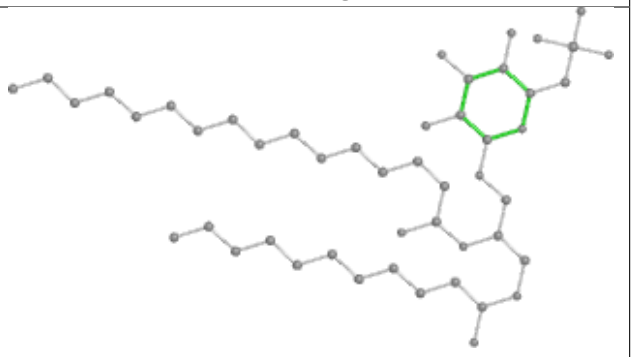
Bond lengths



Bond angles

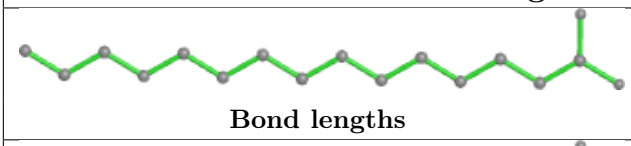


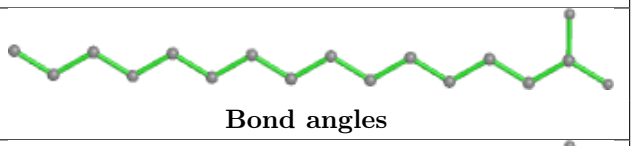
Torsions

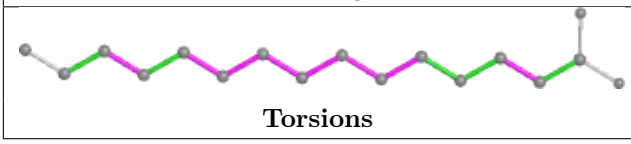


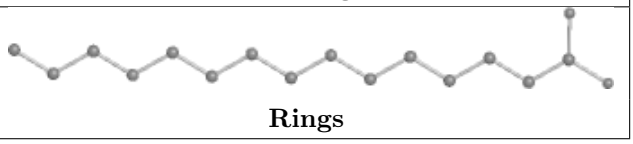
Rings

Ligand STE B 620

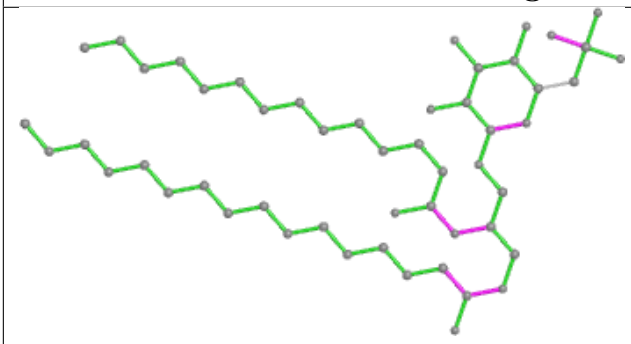

Bond lengths

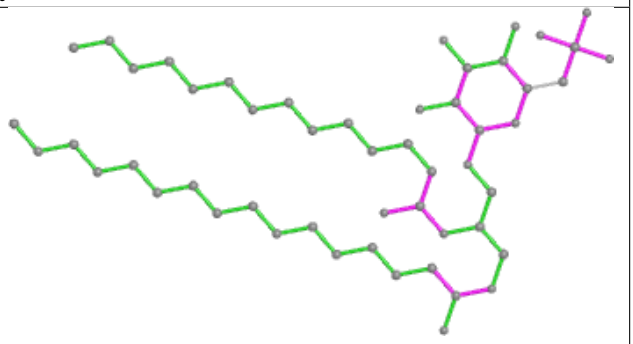

Bond angles

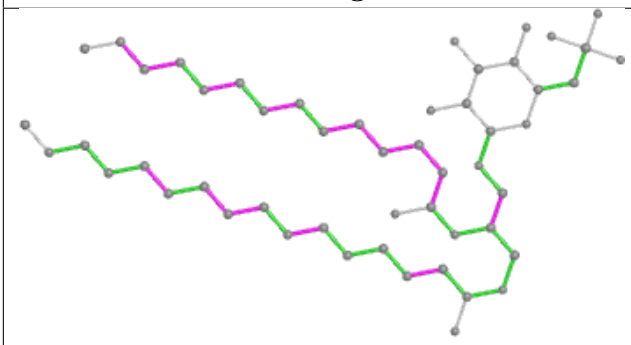

Torsions

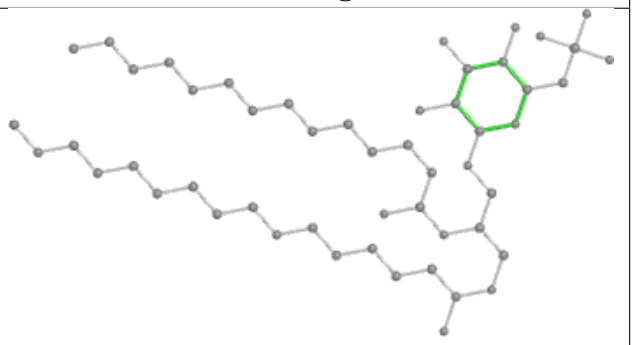

Rings

Ligand SQD A 613

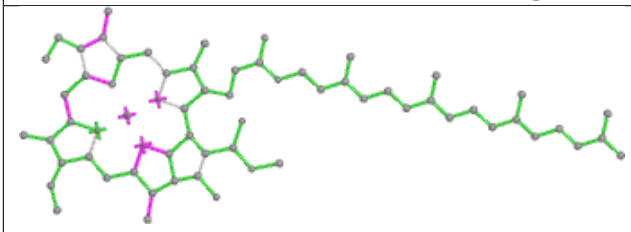

Bond lengths

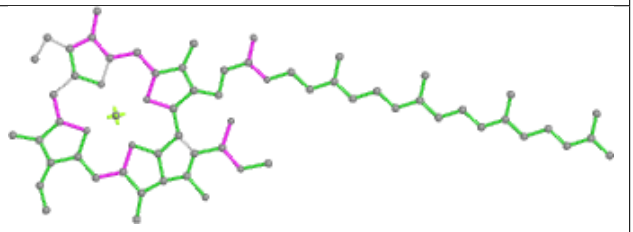

Bond angles

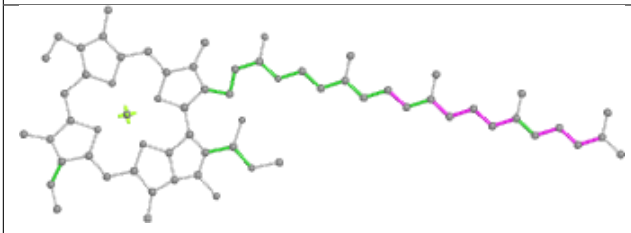

Torsions

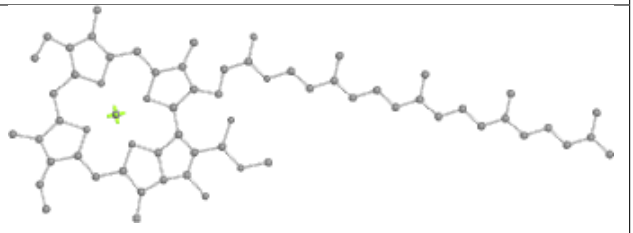

Rings

Ligand CLA b 615

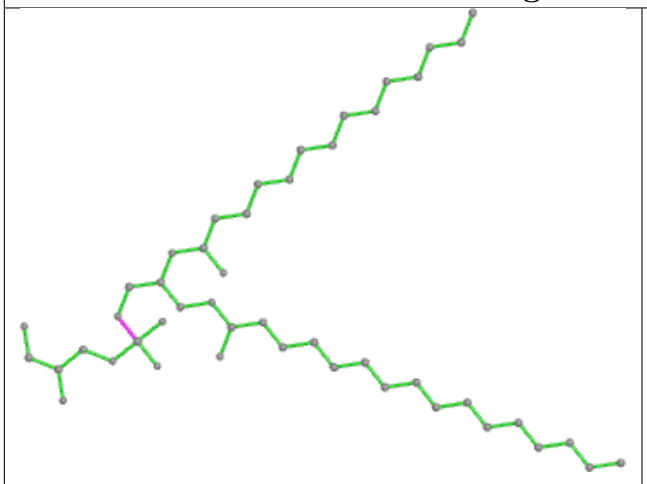

Bond lengths


Bond angles

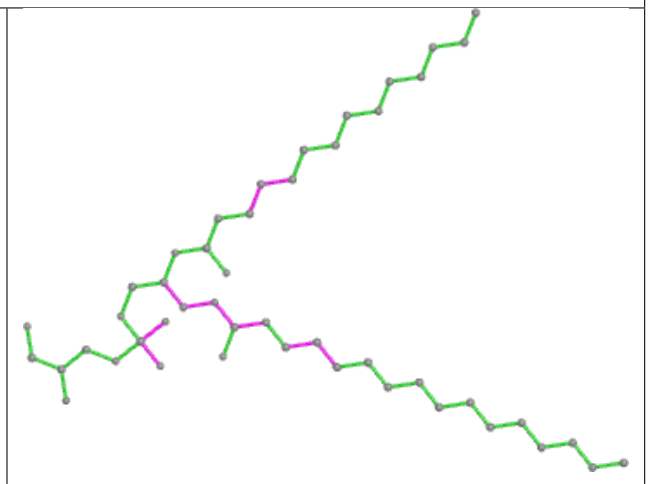

Torsions


Rings

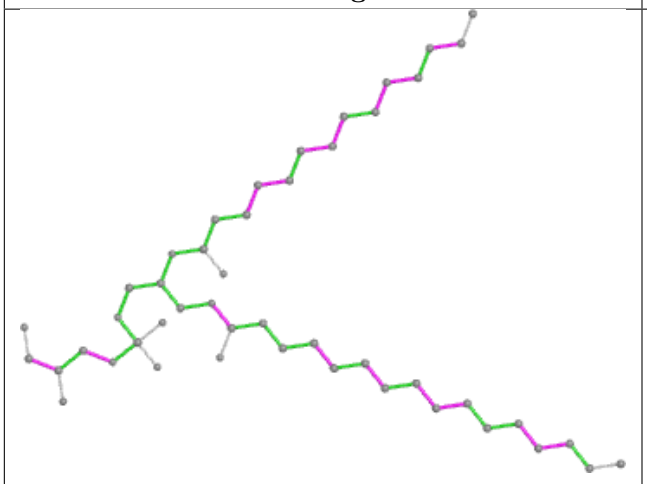
Ligand LHG D 410



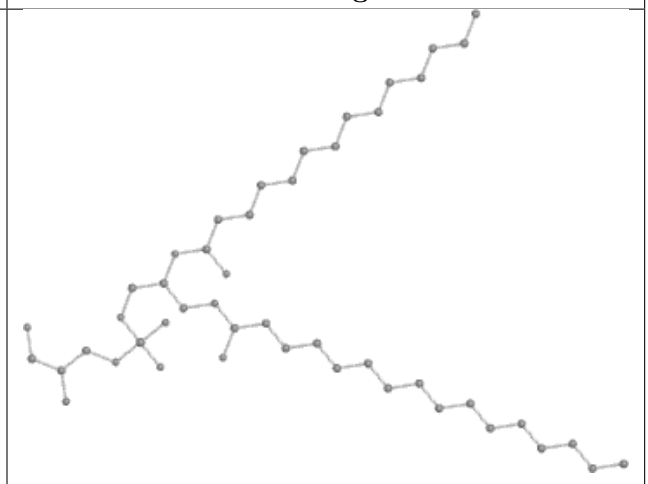
Bond lengths



Bond angles

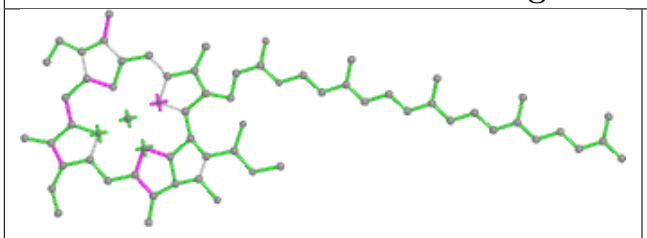


Torsions

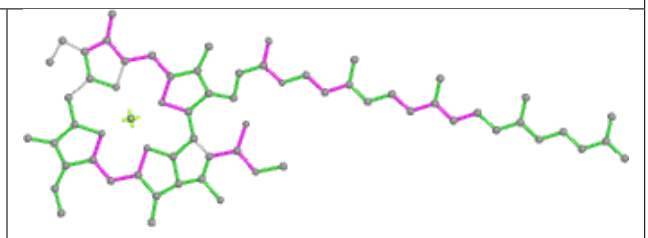


Rings

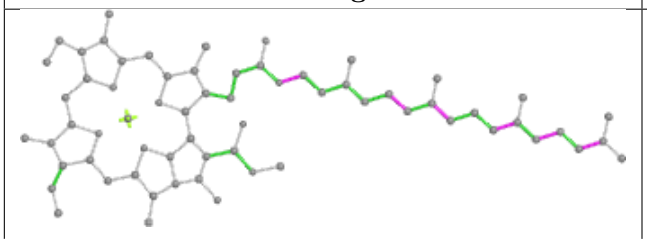
Ligand CLA b 608



Bond lengths



Bond angles



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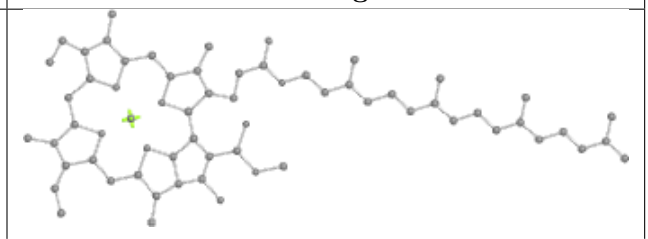
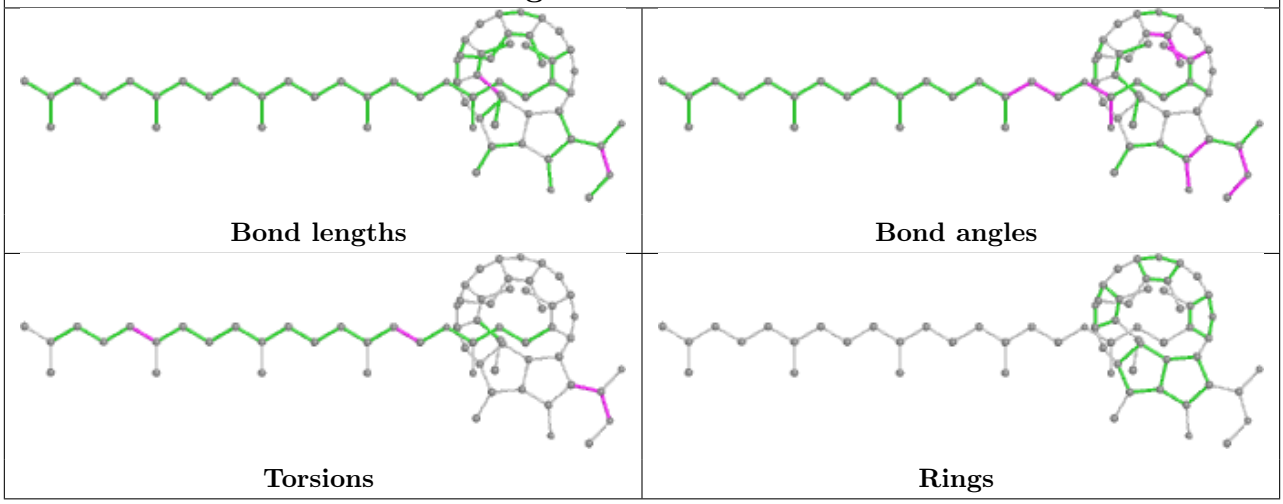
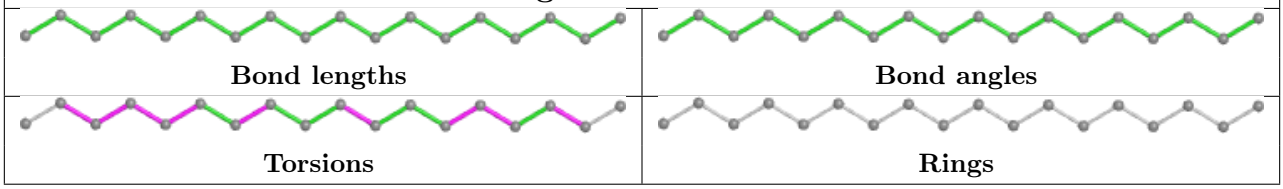


Rings

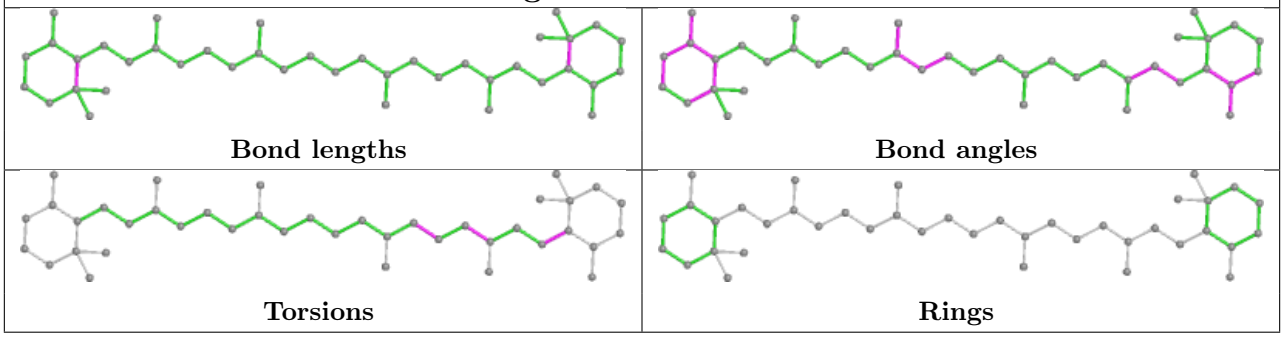
Ligand PHO d 401



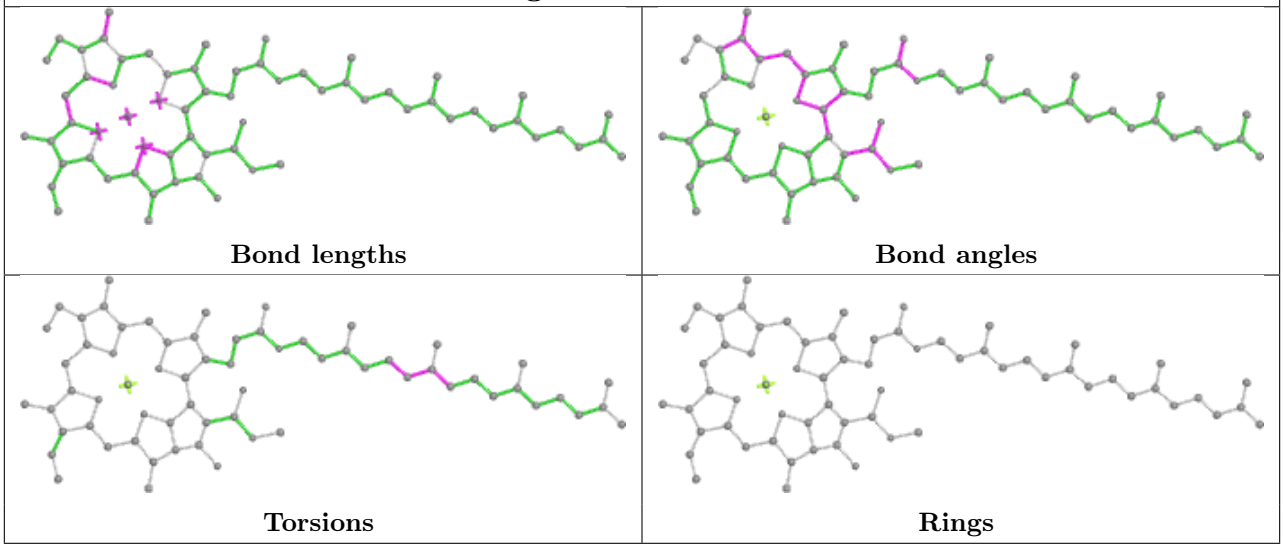
Ligand STE l 102



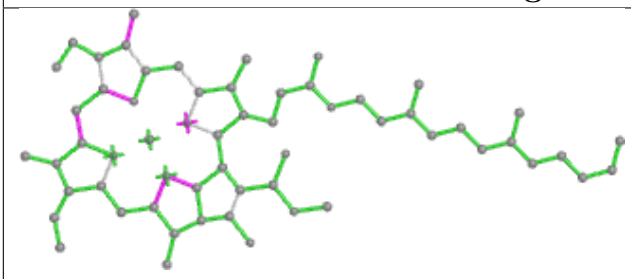
Ligand BCR B 618



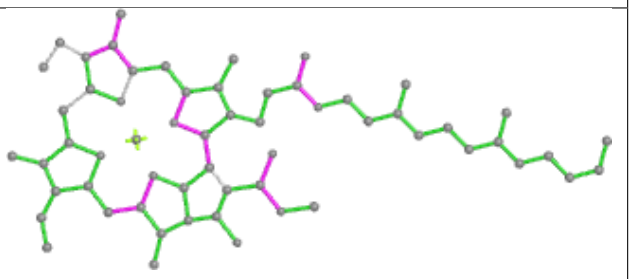
Ligand CLA C 507



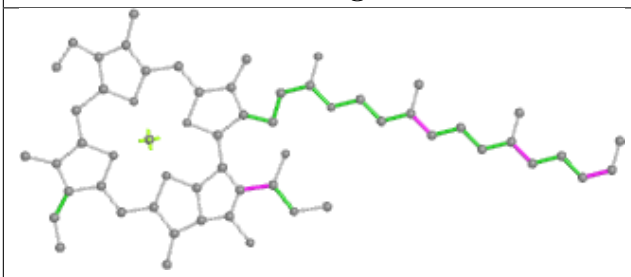
Ligand CLA C 504



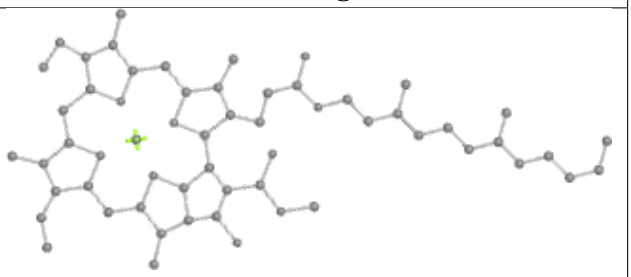
Bond lengths



Bond angles

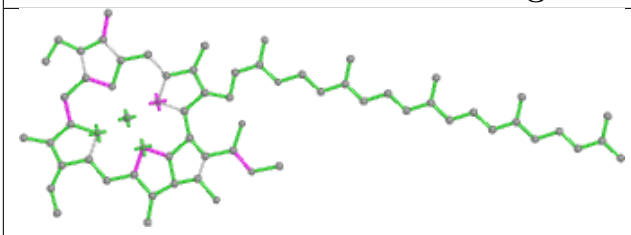


Torsions

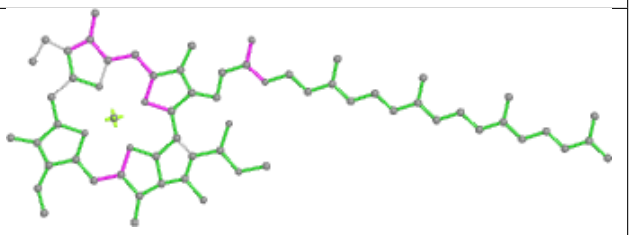


Rings

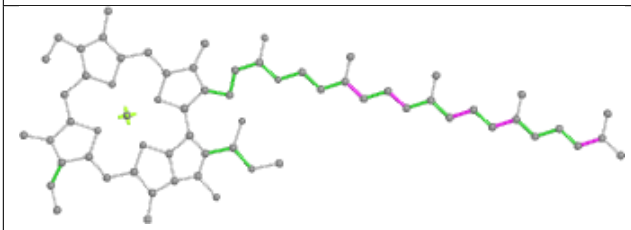
Ligand CLA d 404



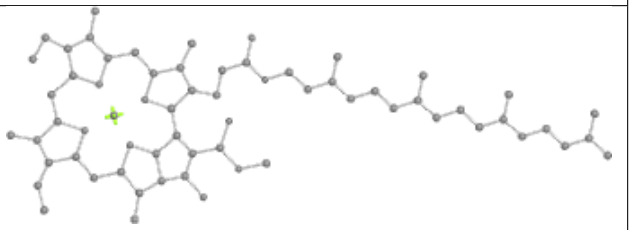
Bond lengths



Bond angles

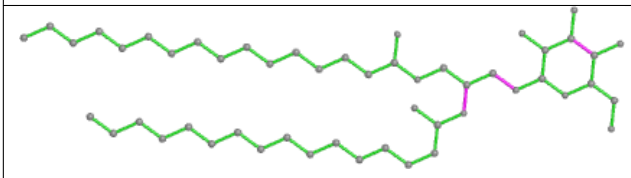


Torsions

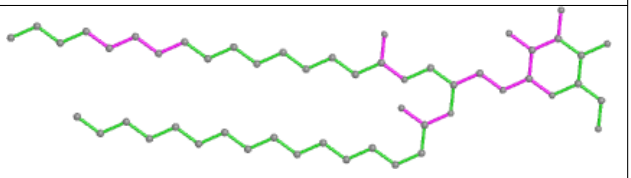


Rings

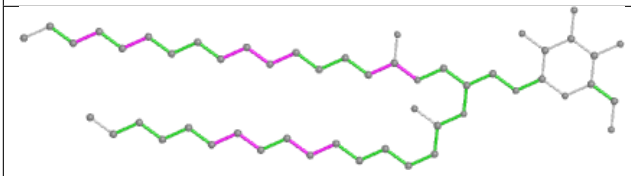
Ligand LMG m 101



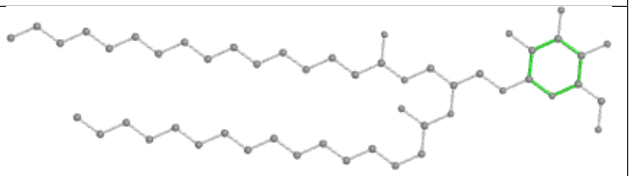
Bond lengths



Bond angles

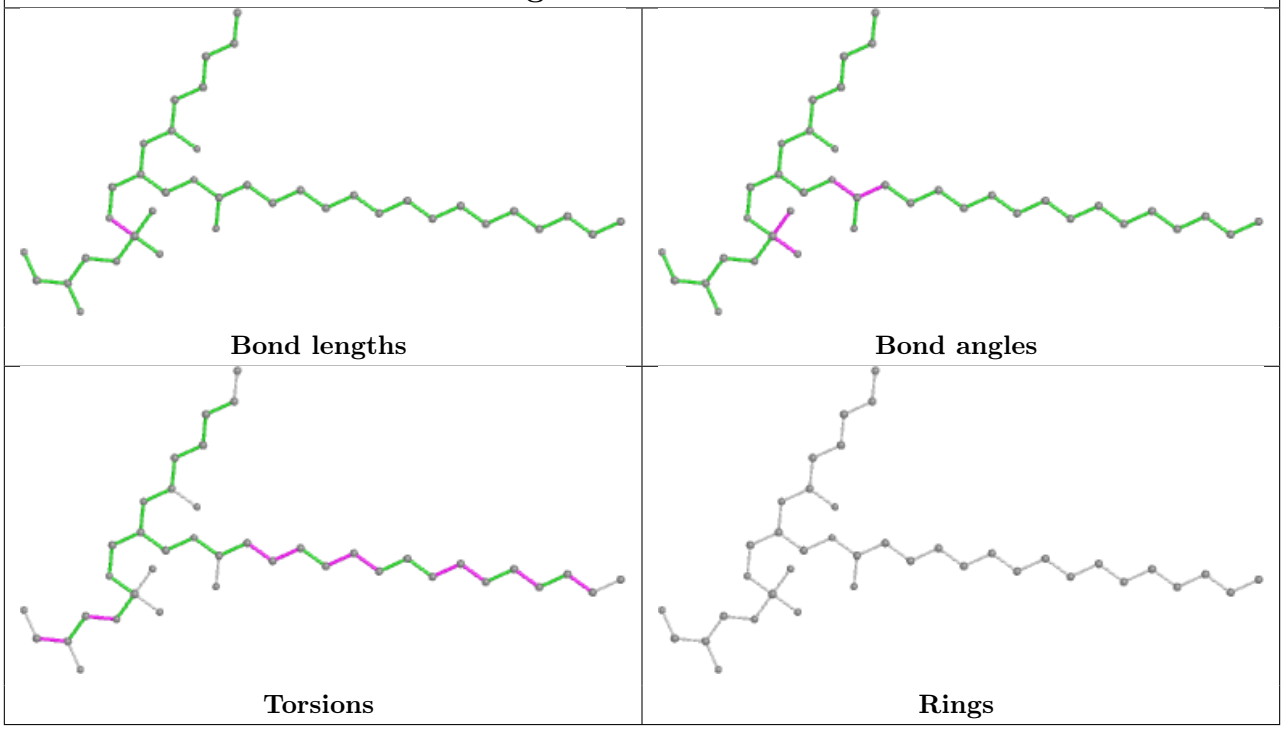


Torsions

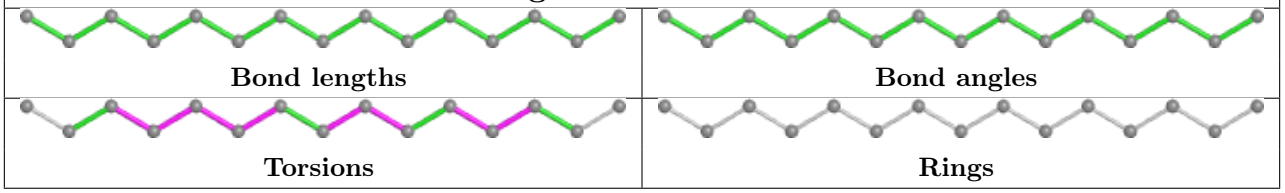


Rings

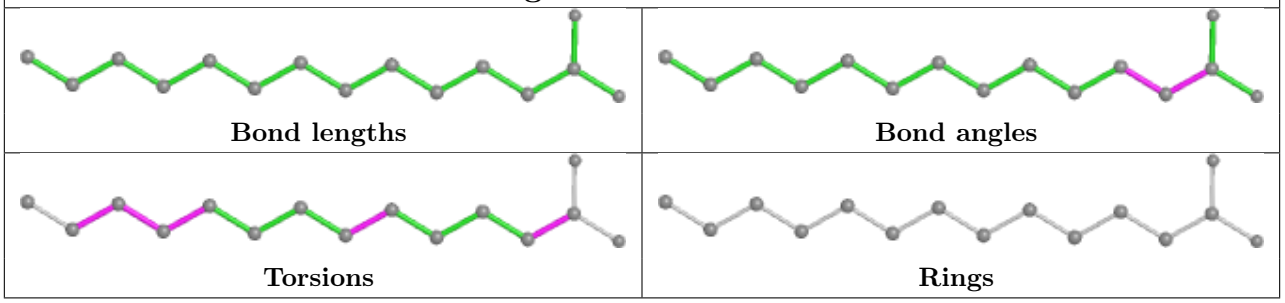
Ligand LHG d 409



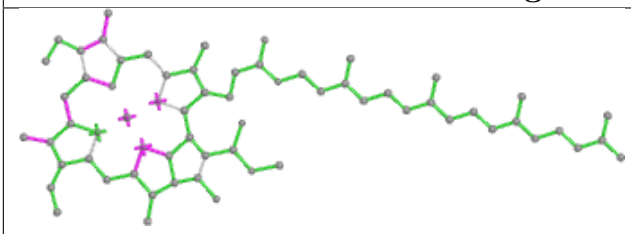
Ligand STE T 103



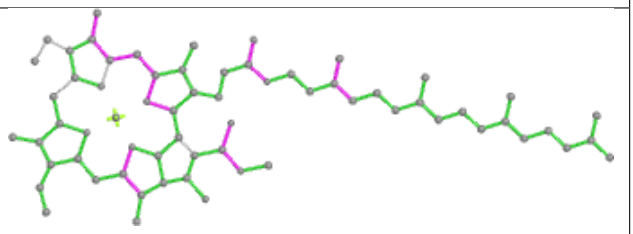
Ligand STE M 102



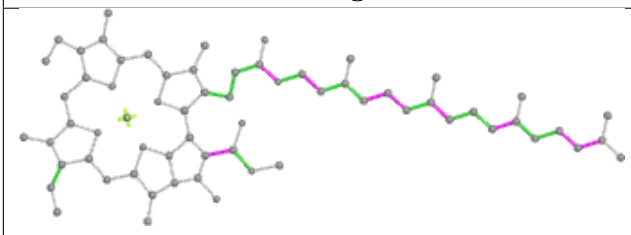
Ligand CLA B 601



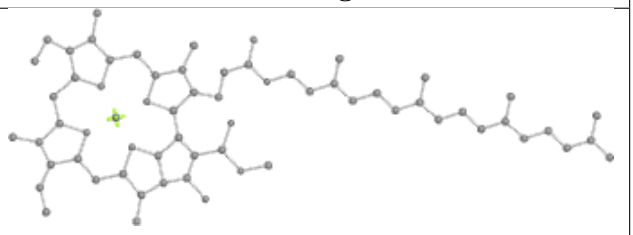
Bond lengths



Bond angles

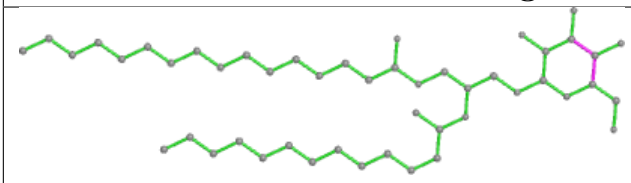


Torsions



Rings

Ligand LMG A 612



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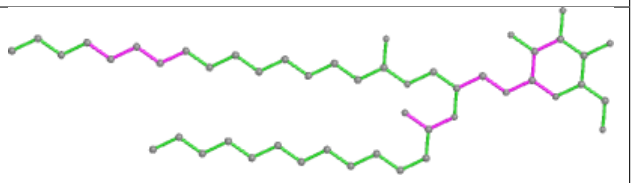
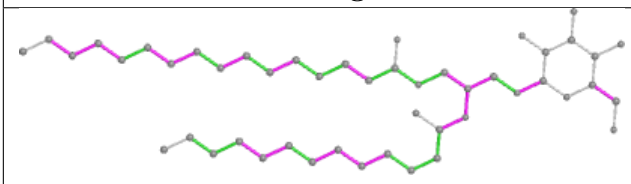
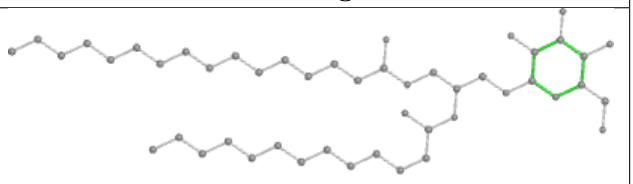


Bond angles

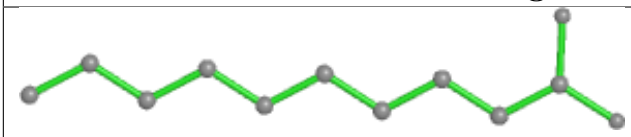


Torsions

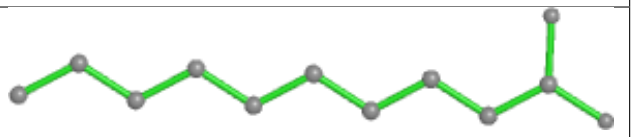


Rings

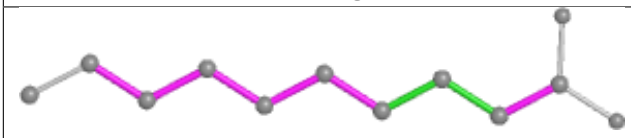
Ligand STE B 623



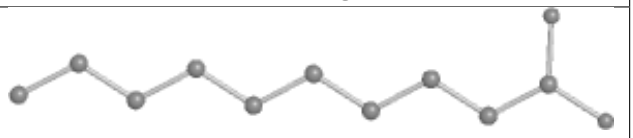
Bond lengths



Bond angles

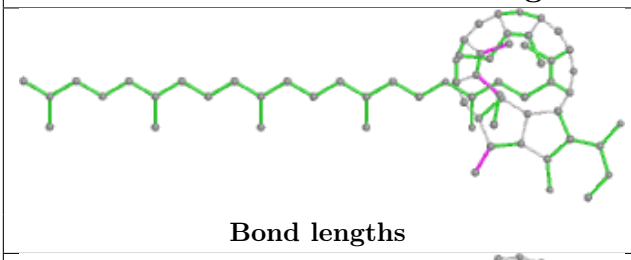


Torsions

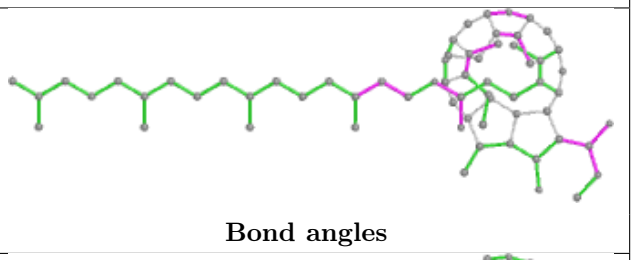


Rings

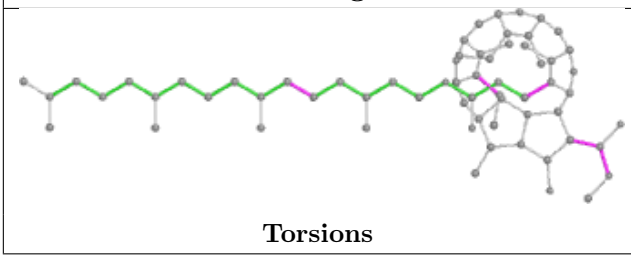
Ligand PHO d 402



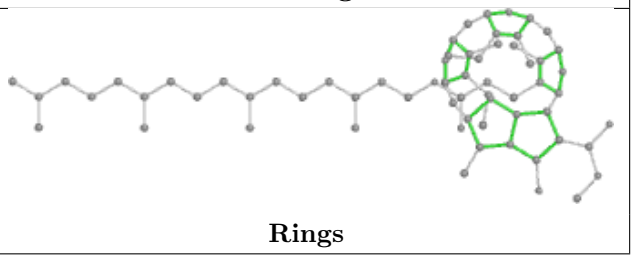
Bond lengths



Bond angles

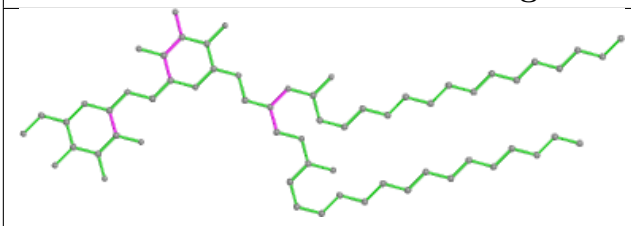


Torsions

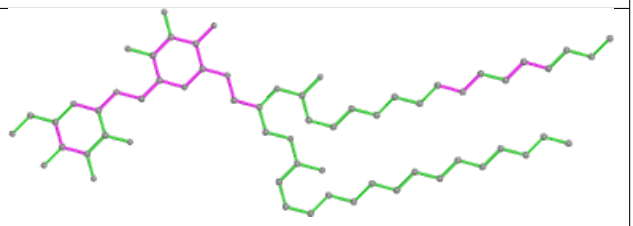


Rings

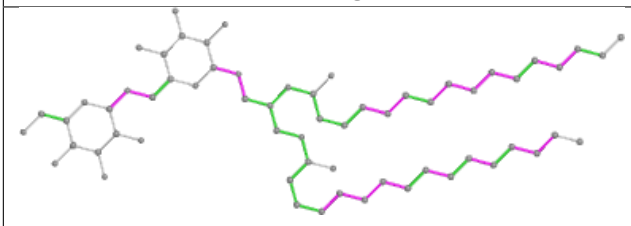
Ligand DGD C 516



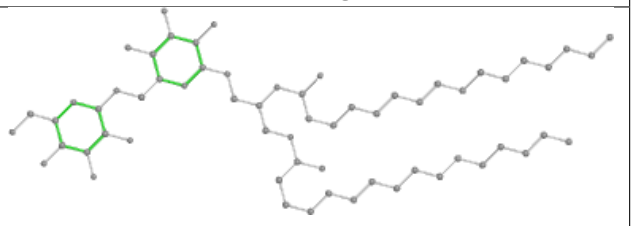
Bond lengths



Bond angles

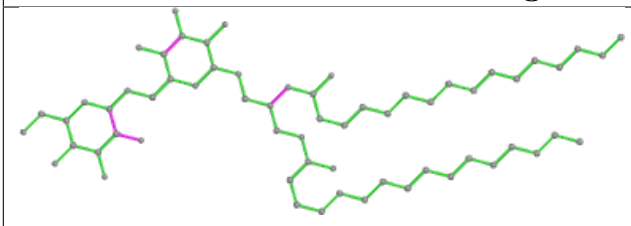


Torsions

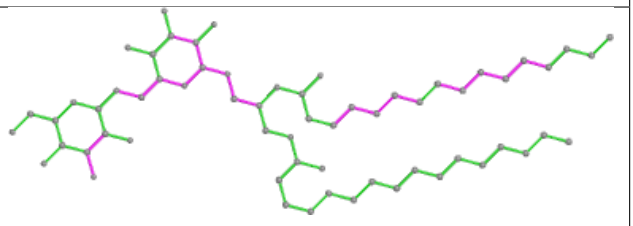


Rings

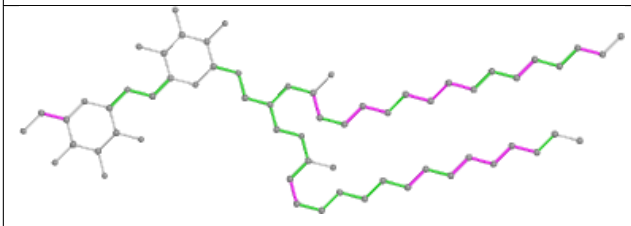
Ligand DGD h 101



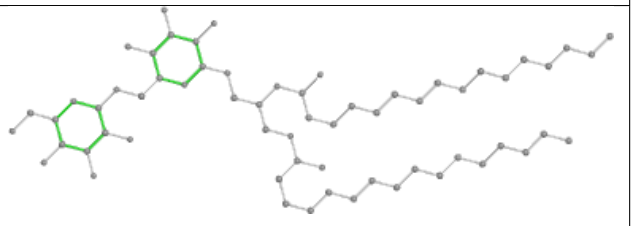
Bond lengths



Bond angles

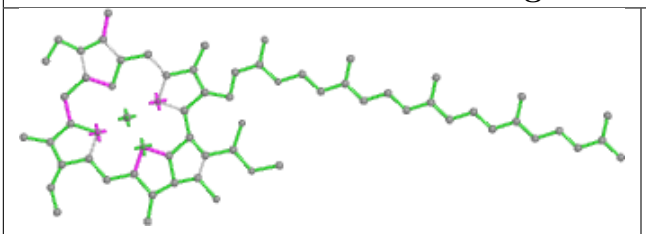


Torsions



Rings

Ligand CLA C 510



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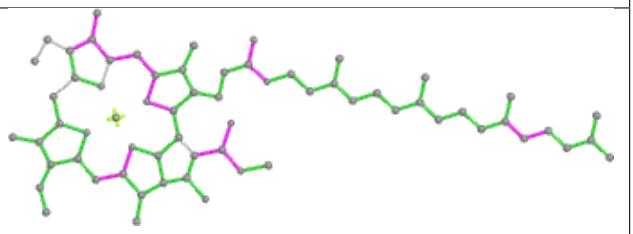

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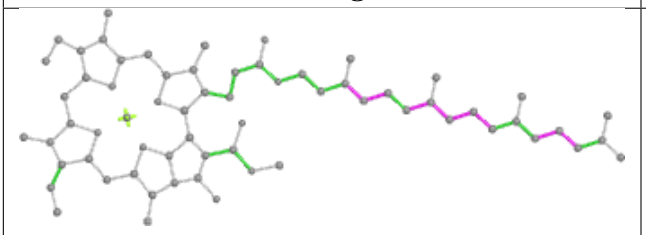

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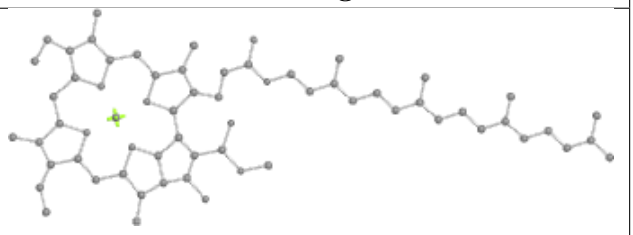
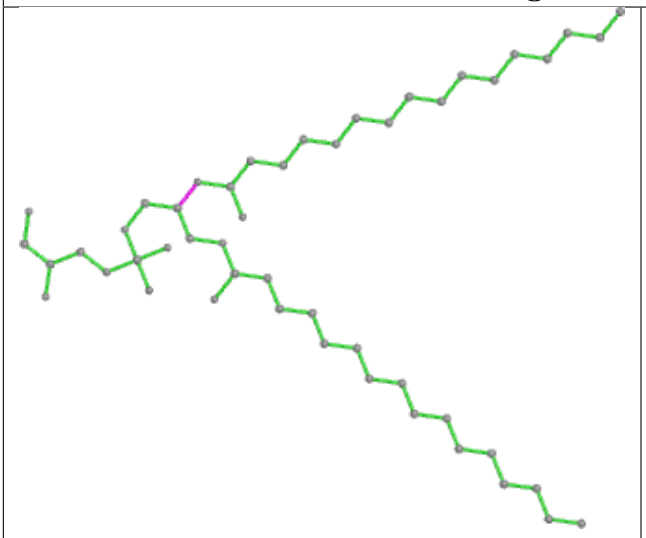


Rings

Ligand LHG d 408



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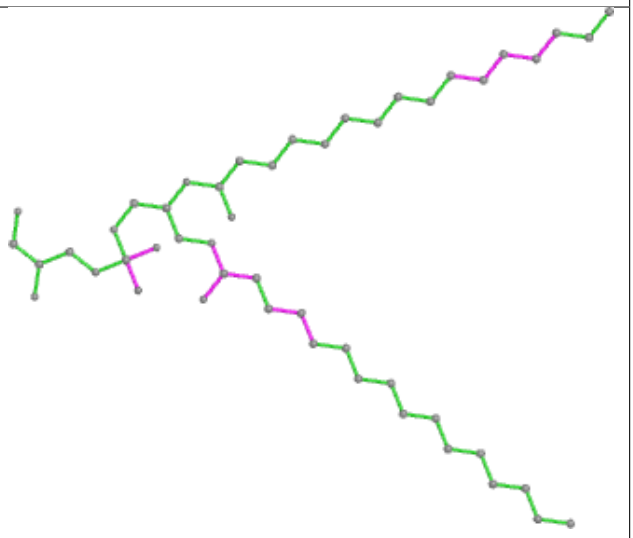
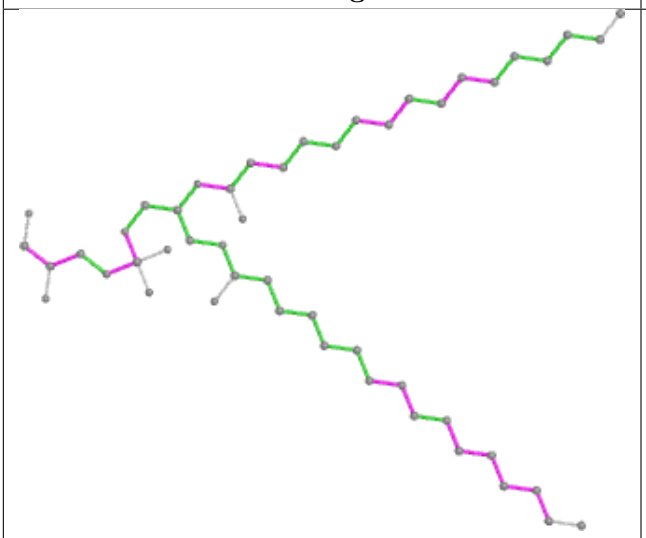


Bond angles



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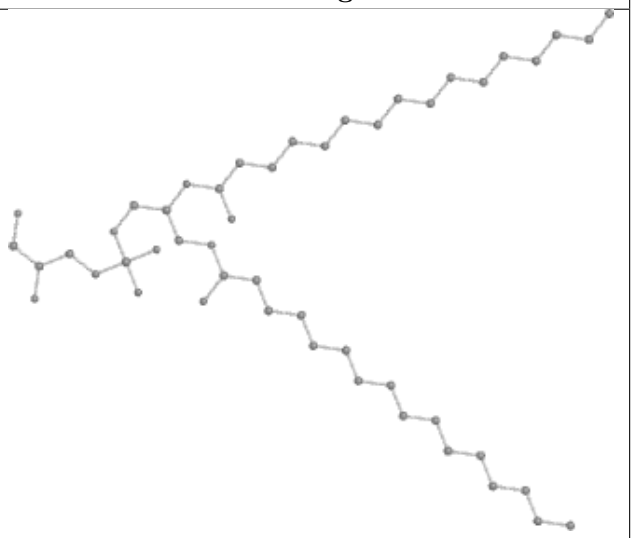
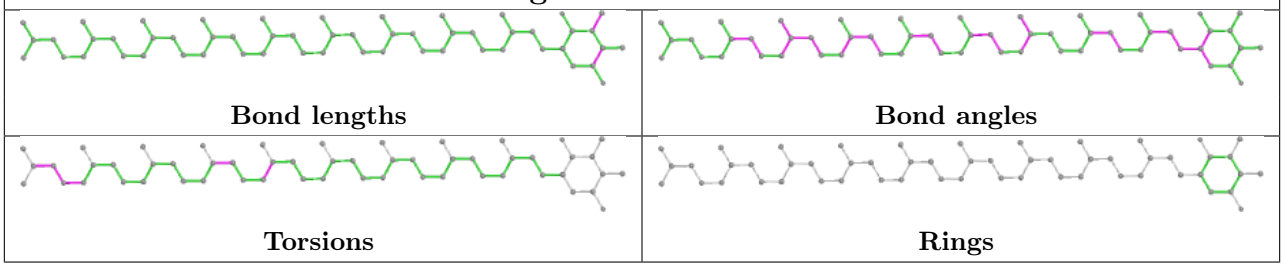


Rings

Ligand PL9 D 407



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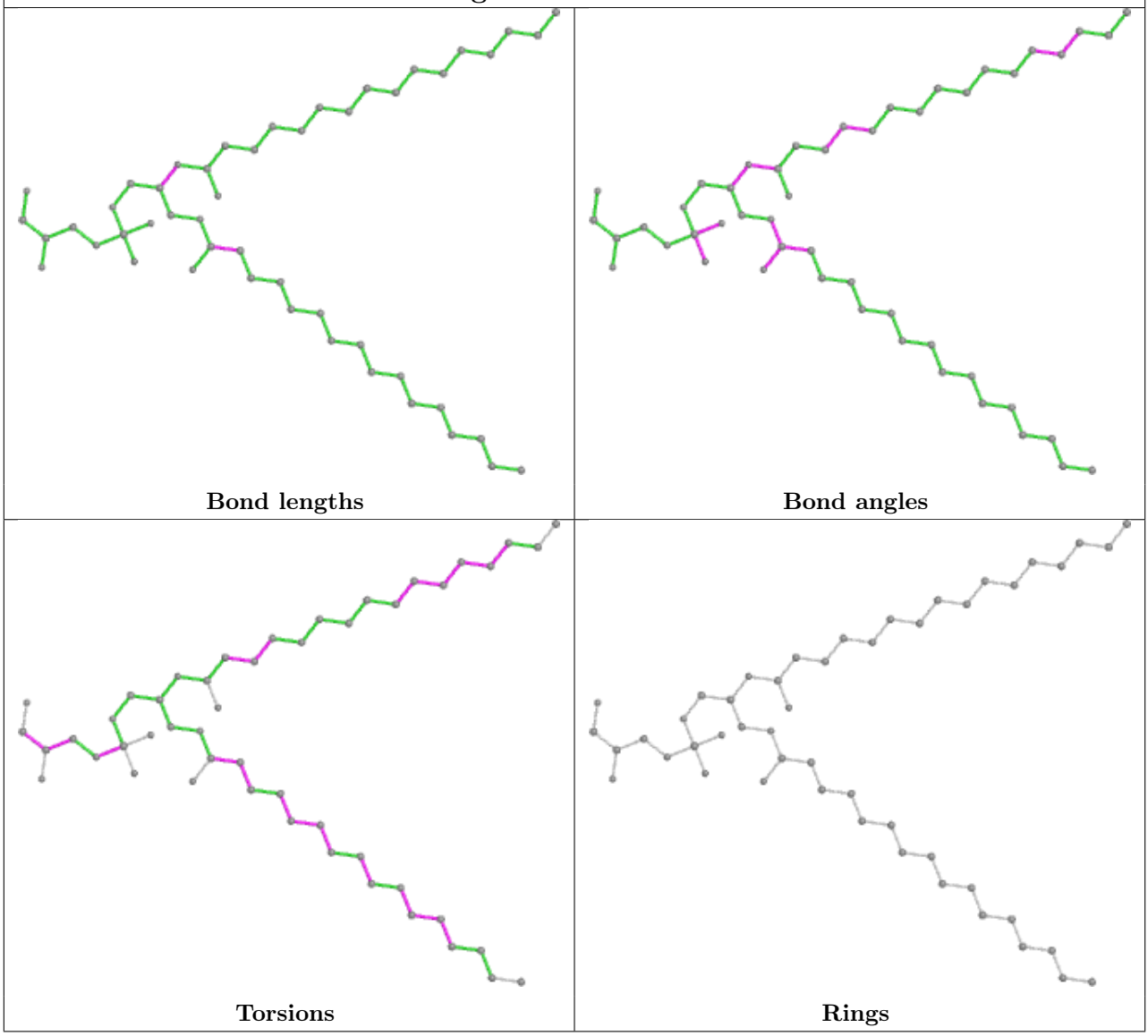
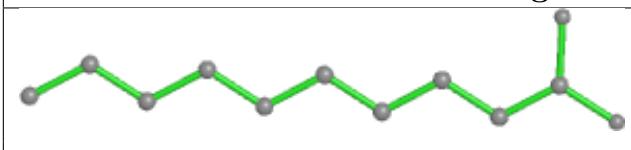
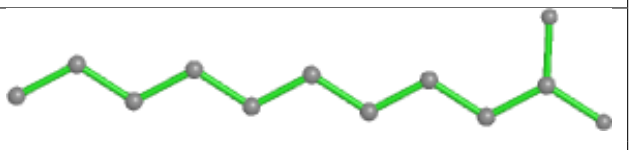
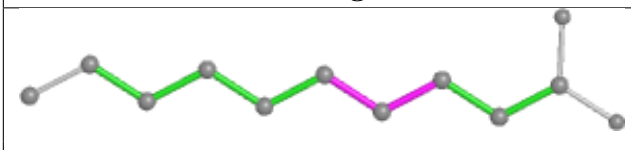


Ligand STE J 101


Bond lengths


Bond angles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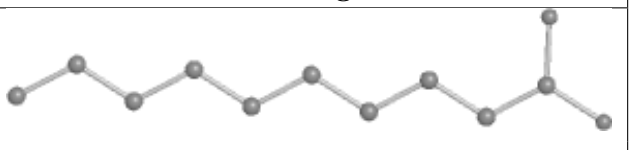
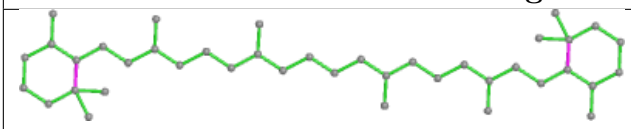

Rings

Ligand BCR b 619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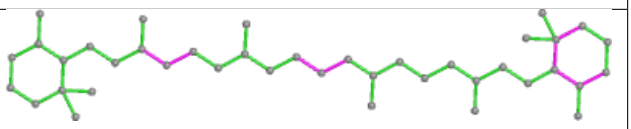
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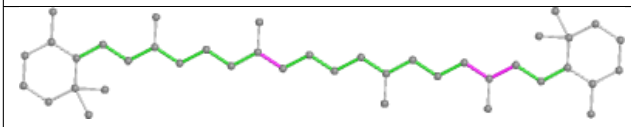
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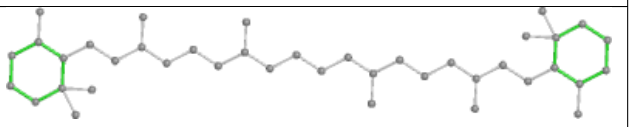
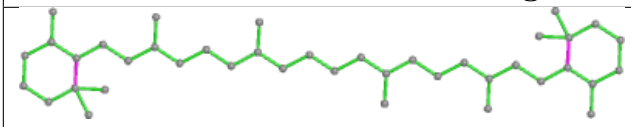

Rings

Ligand BCR Y 101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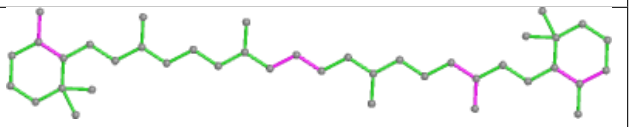
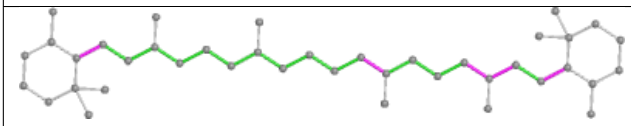

Bond angles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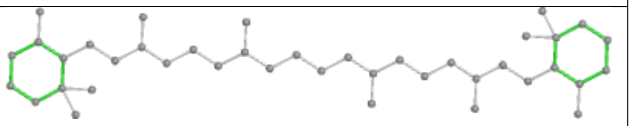
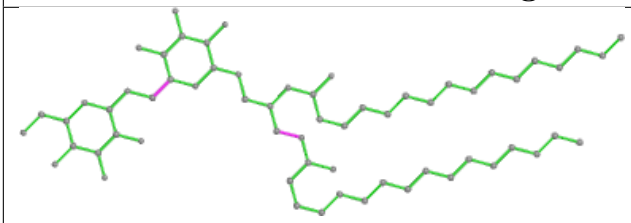

Rings

Ligand DGD C 517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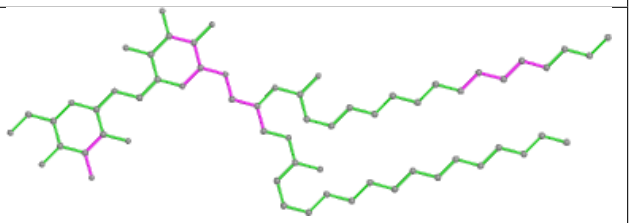
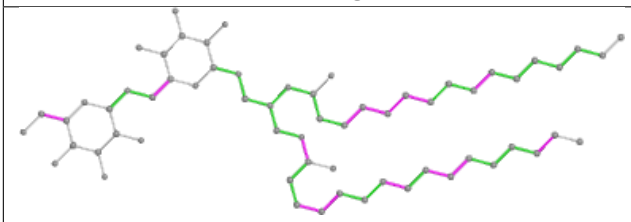

Bond angles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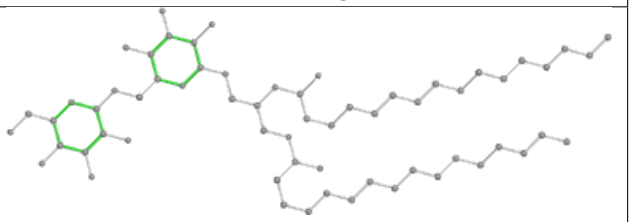
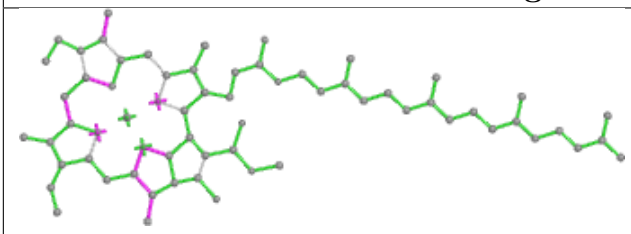

Rings

Ligand CLA B 608



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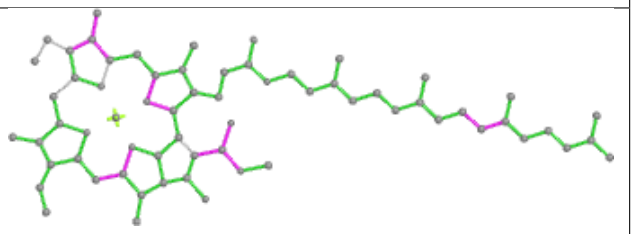
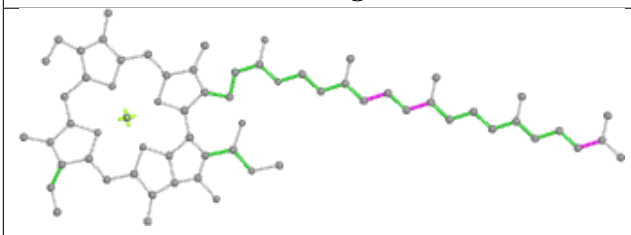


Bond angles



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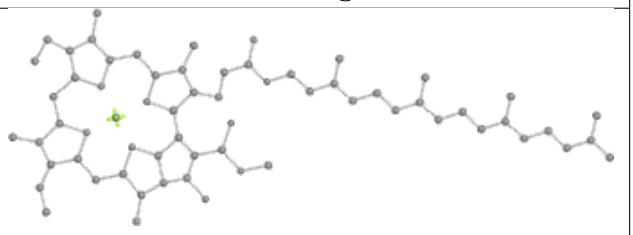
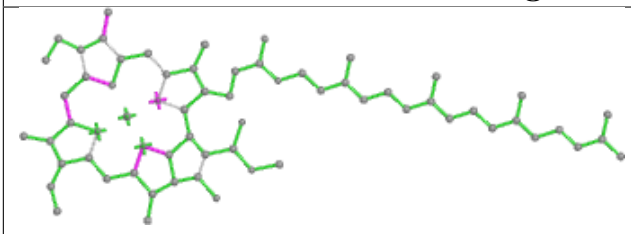


Rings

Ligand CLA C 511



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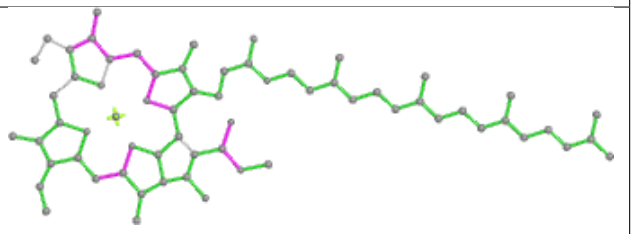
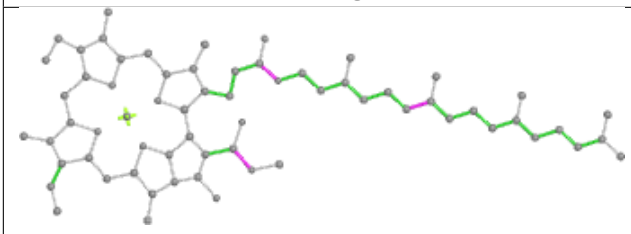


Bond angles



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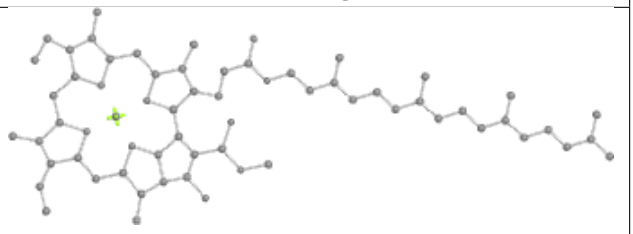
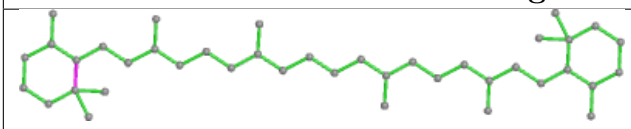


Rings

Ligand BCR t 101



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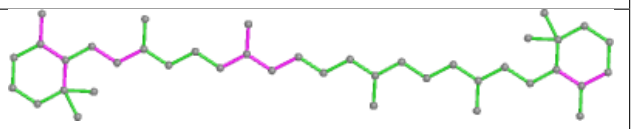

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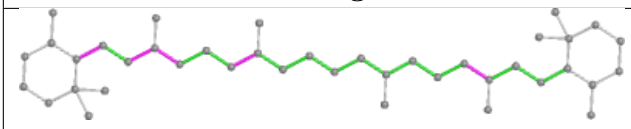
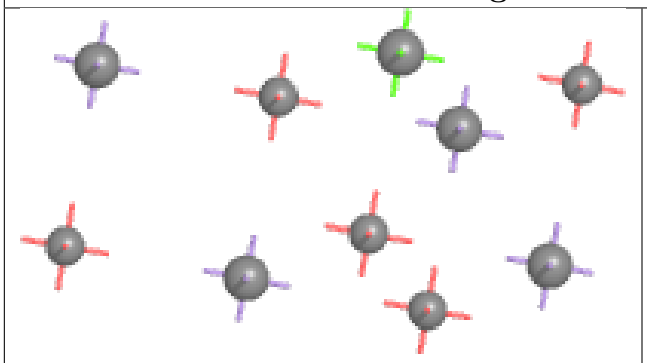


Torsions

Rings

Ligand OEX A 602 (A)



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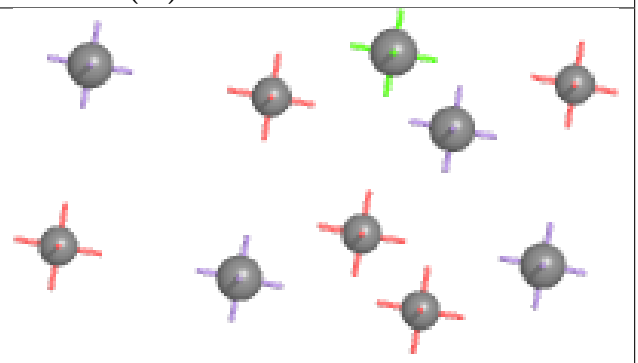

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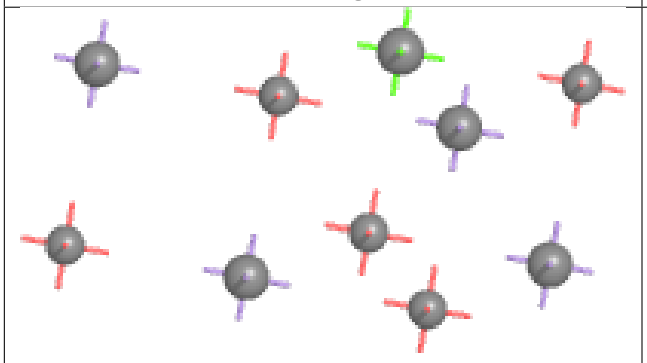

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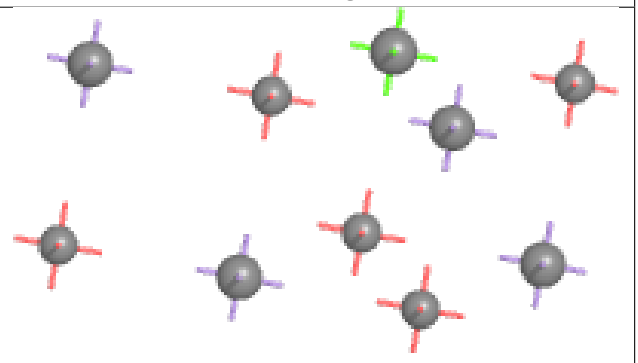
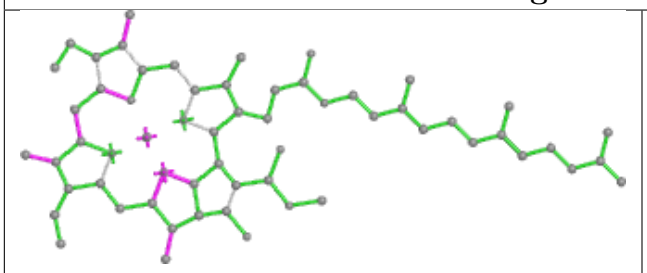


Rings

Ligand CLA c 504



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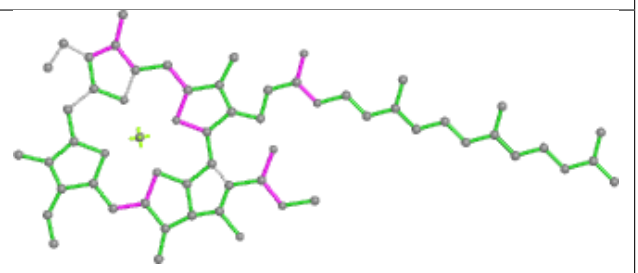
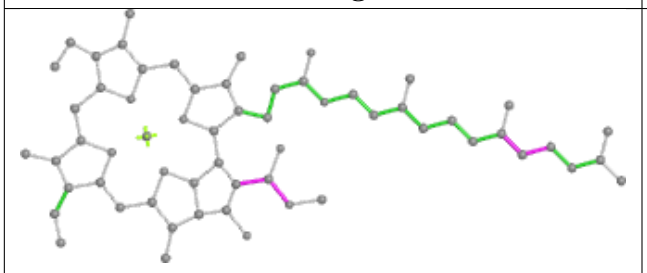


Bond angles



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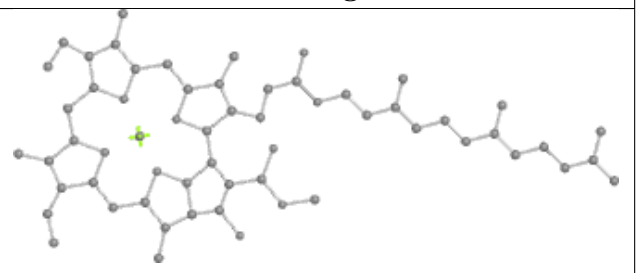
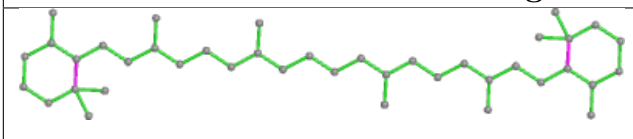


Rings

Ligand BCR b 618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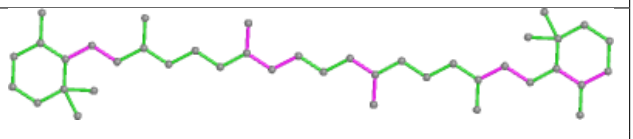
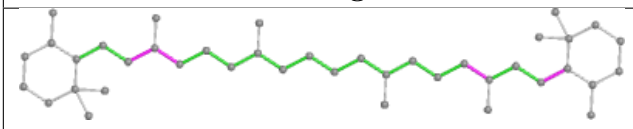

Bond angles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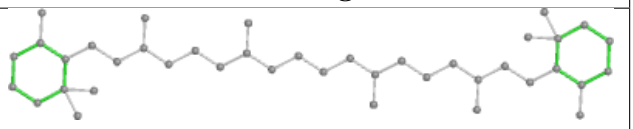
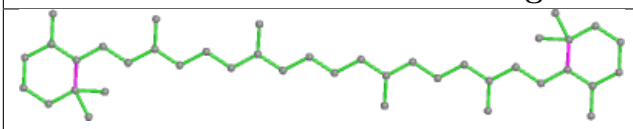
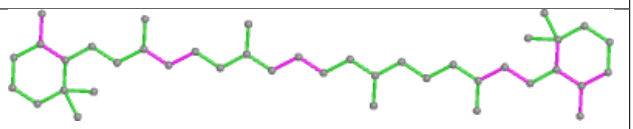
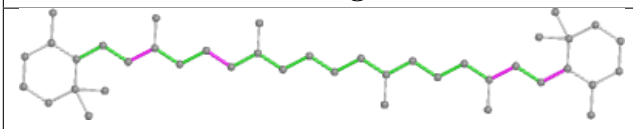
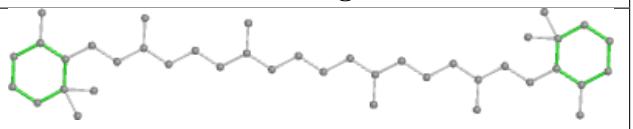

Rings

Ligand BCR d 405

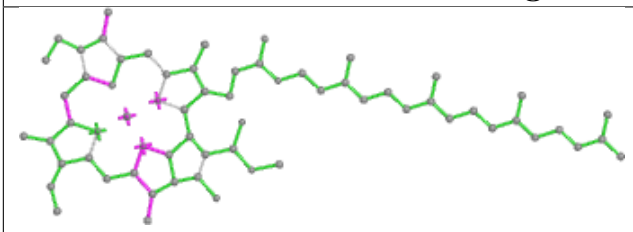

Bond lengths

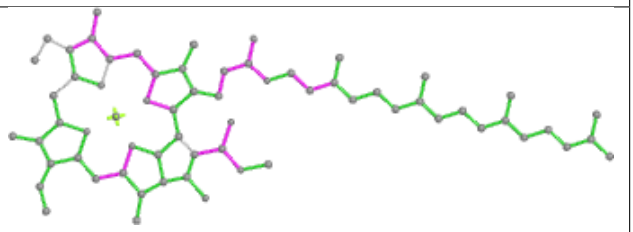

Bond angles

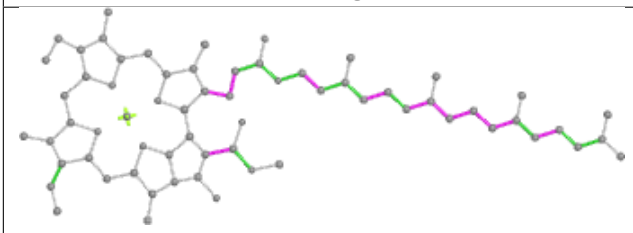

Torsions

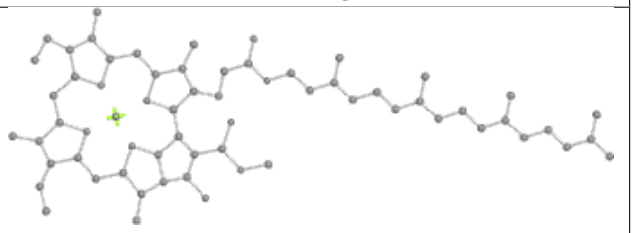

Rings

Ligand CLA C 512

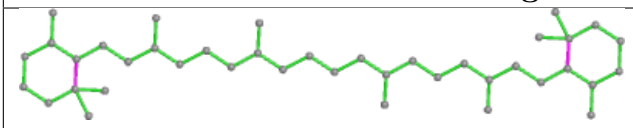

Bond lengths

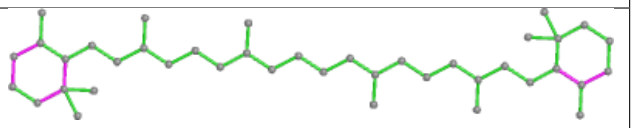

Bond angles

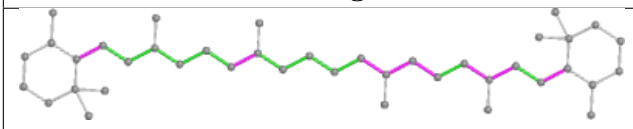

Torsions


Rings

Ligand BCR K 102


Bond lengths


Bond angles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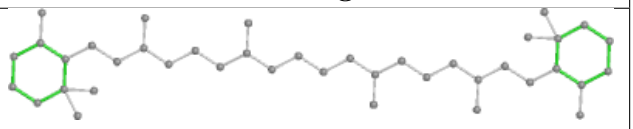
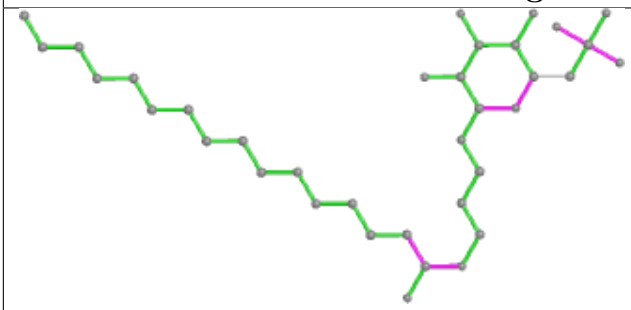

Rings

Ligand SQD F 101



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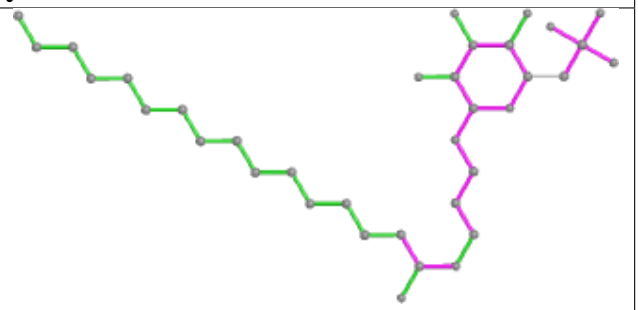
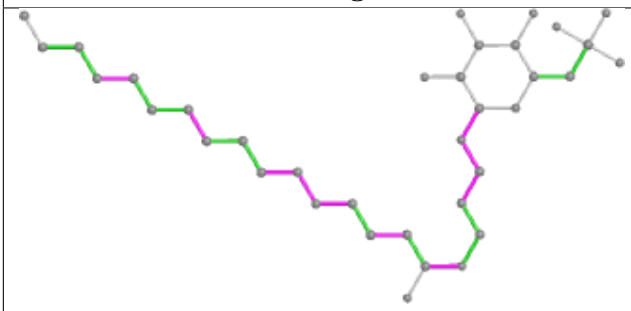


Bond angles



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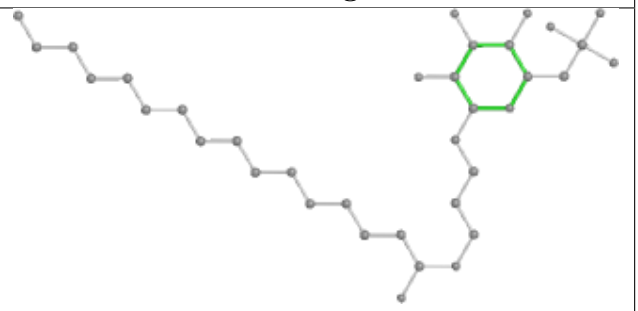
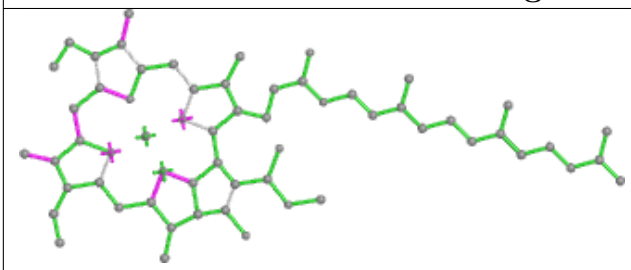


Rings

Ligand CLA B 616



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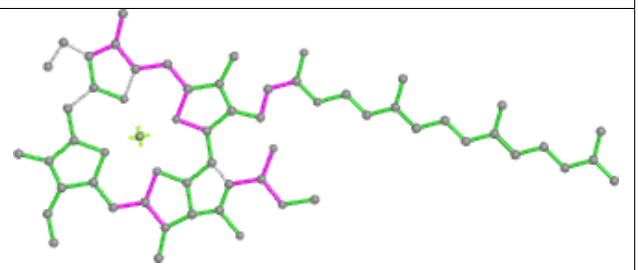
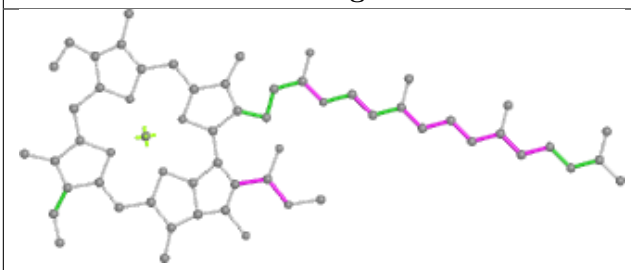


Bond angles



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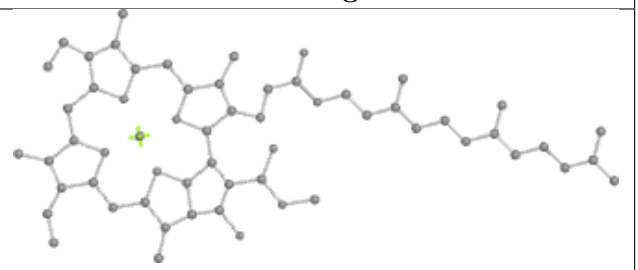
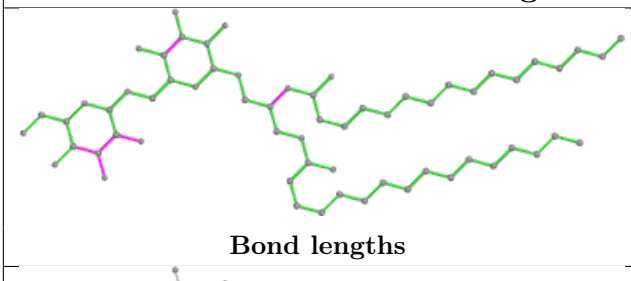
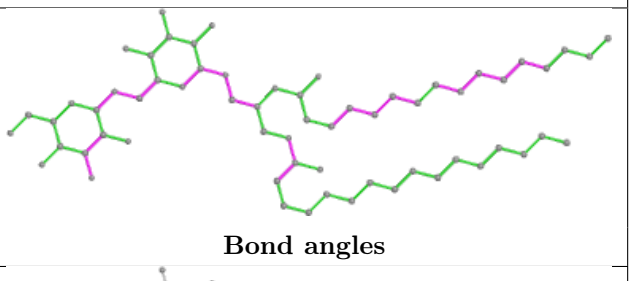


Rings

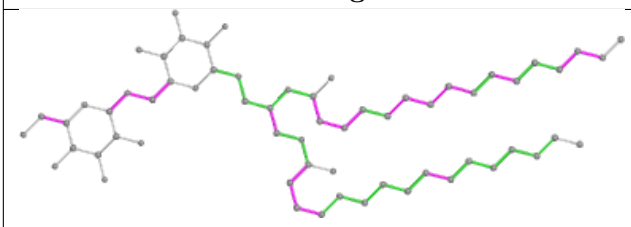
Ligand DGD C 515



Bond lengths



Bond angles



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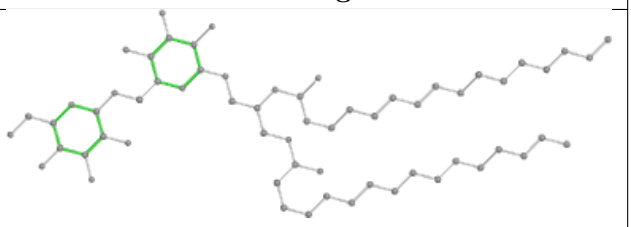
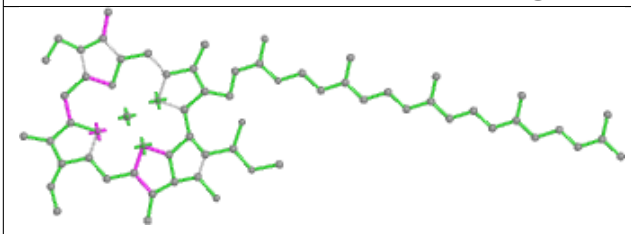


Rings

Ligand CLA c 501



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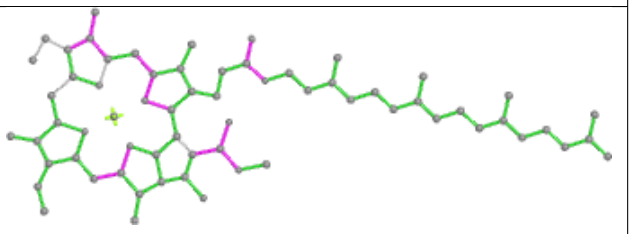
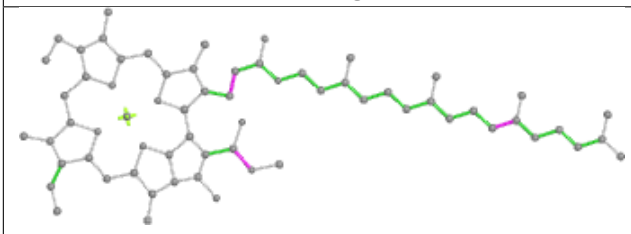


Bond angles



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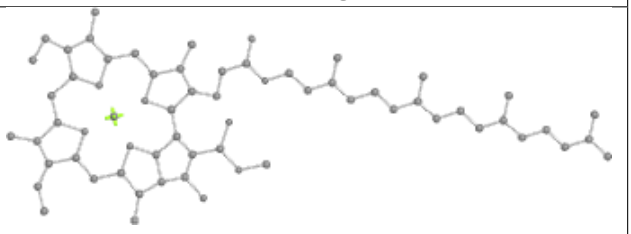
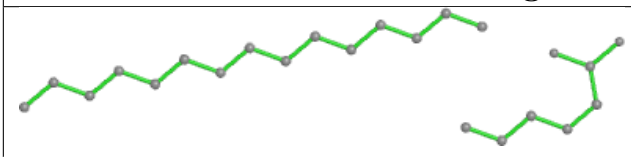


Rings

Ligand LMG d 410



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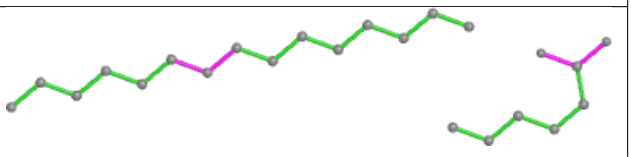
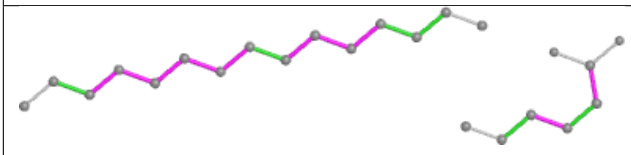


Bond angles



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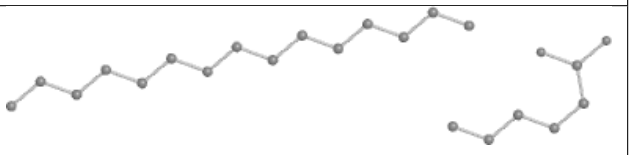
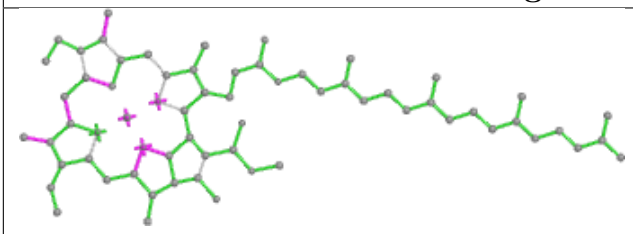


Rings

Ligand CLA C 506



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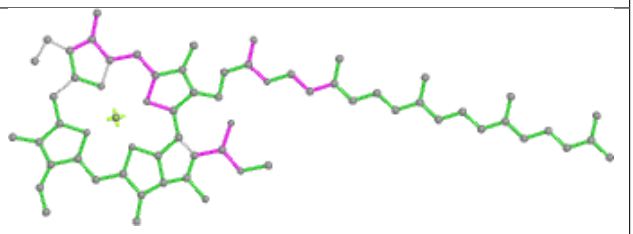
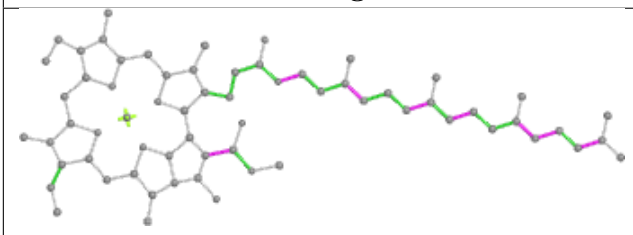


Bond angles



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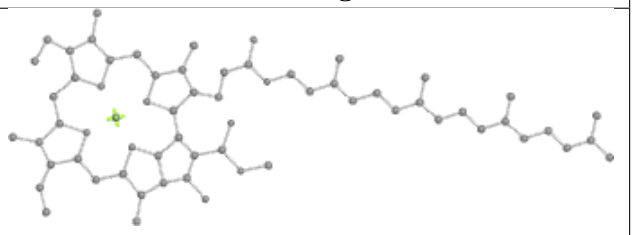
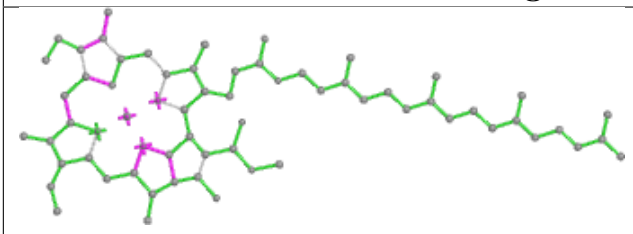


Rings

Ligand CLA C 502



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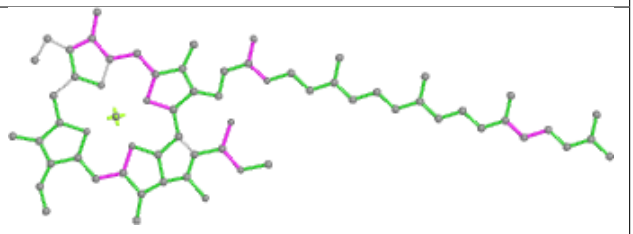
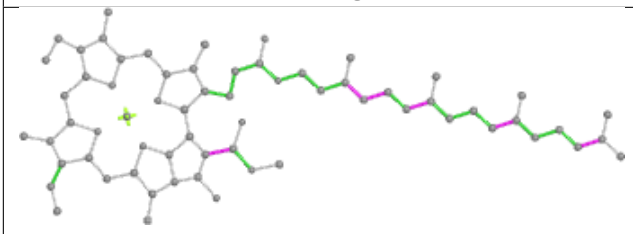


Bond angles



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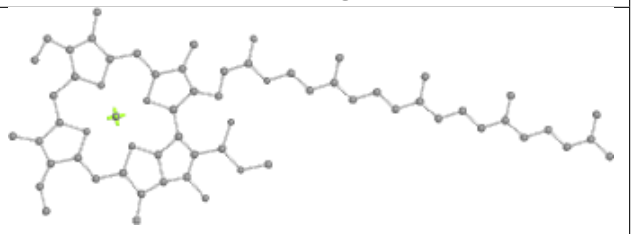
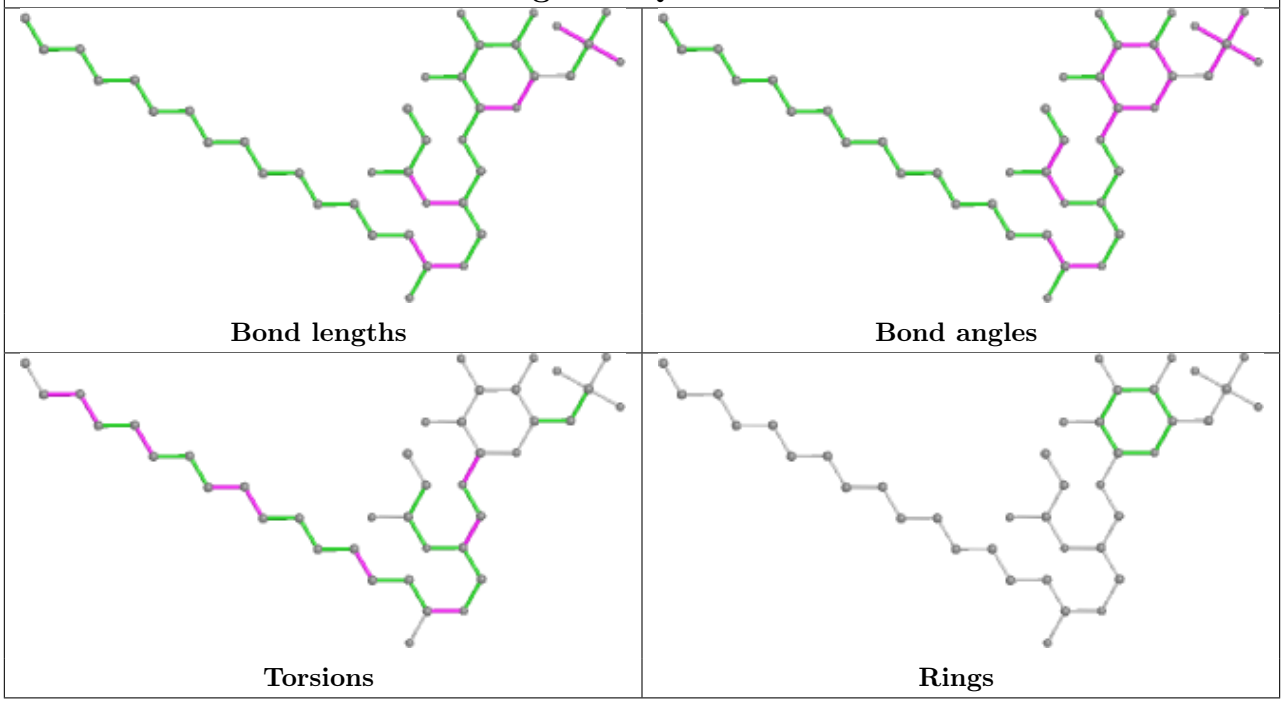
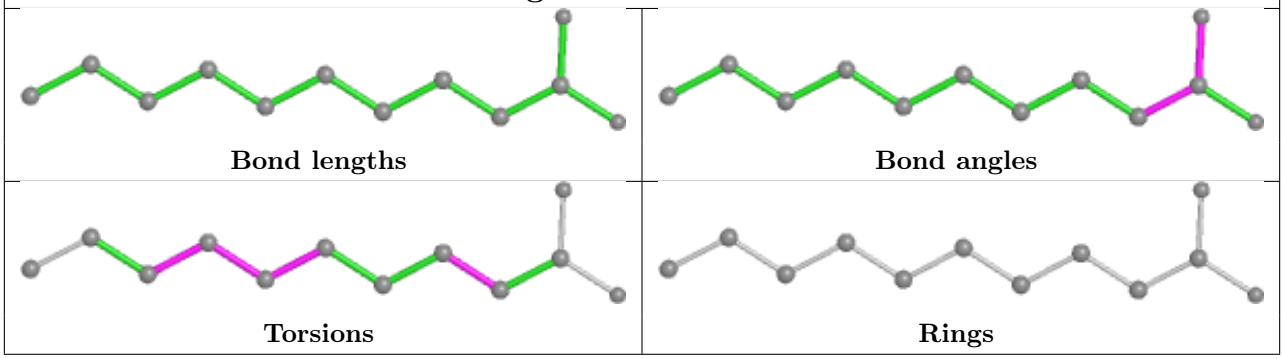


Rings

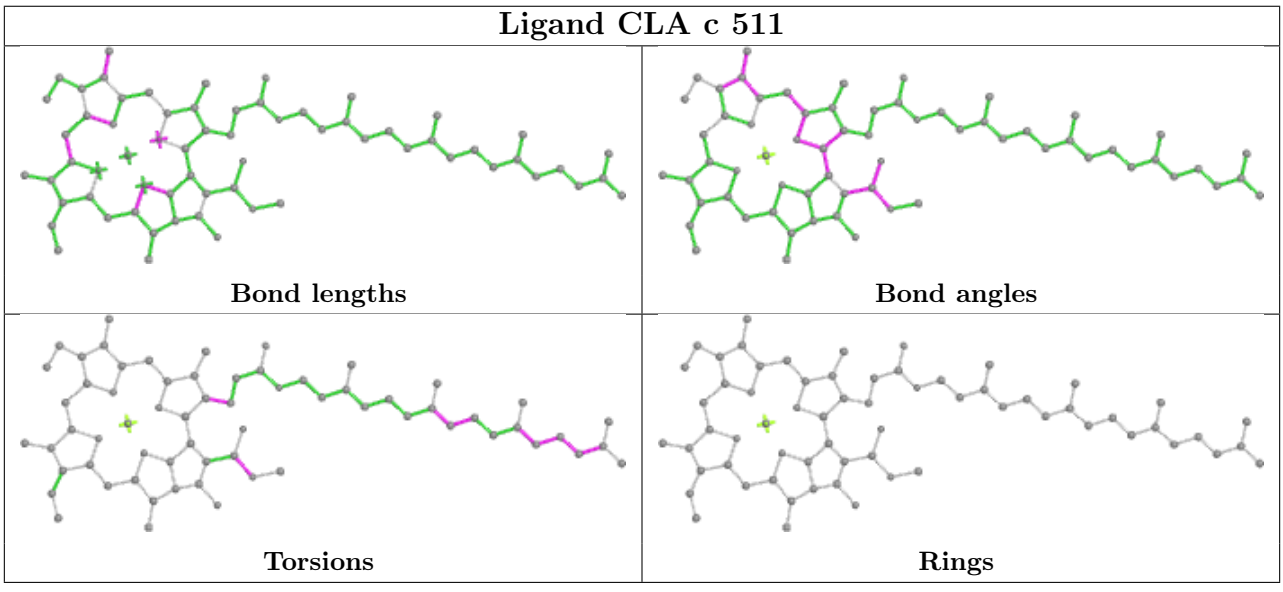
Ligand SQD f 102



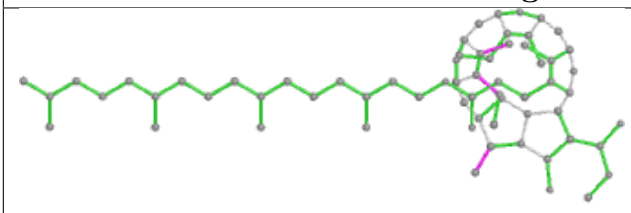
Ligand STE m 102



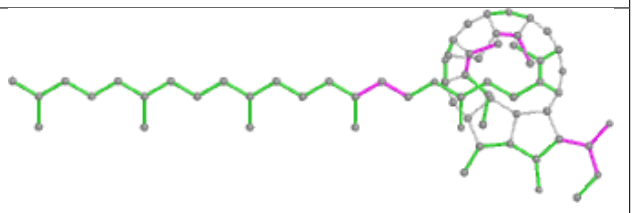
Ligand CLA c 511



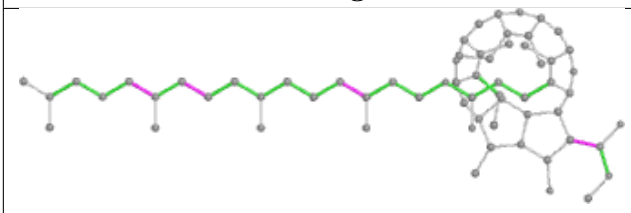
Ligand PHO A 608



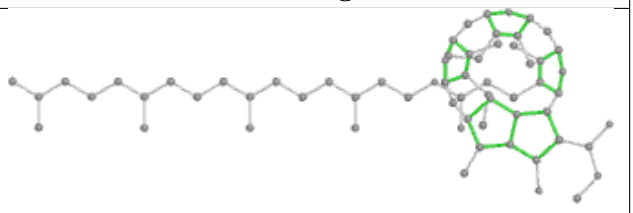
Bond lengths



Bond angles



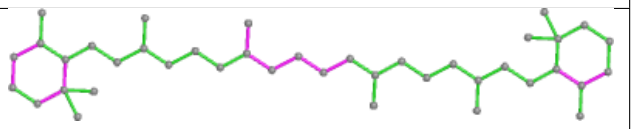
Torsions



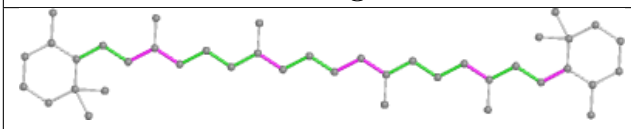
Rings

Ligand BCR x 101

Bond lengths



Bond angles



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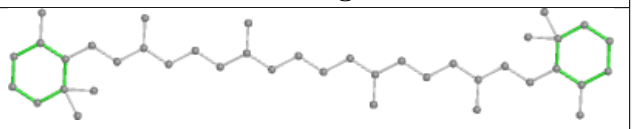
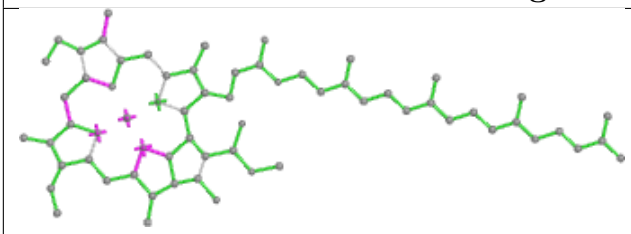


Rings

Ligand CLA c 509



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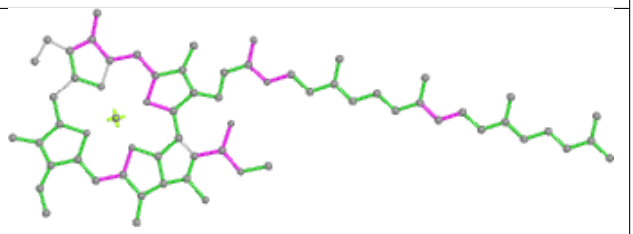
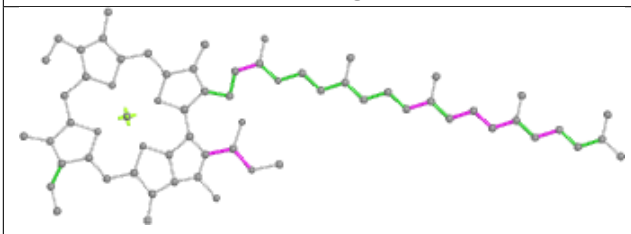


Bond angles



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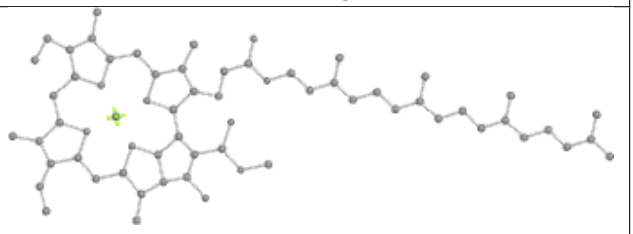
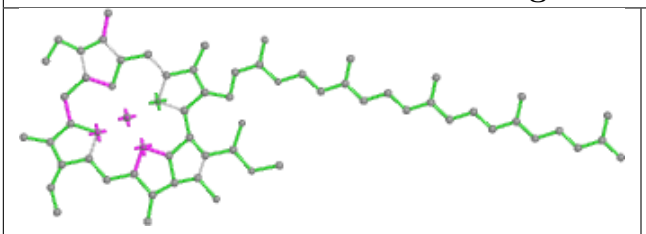
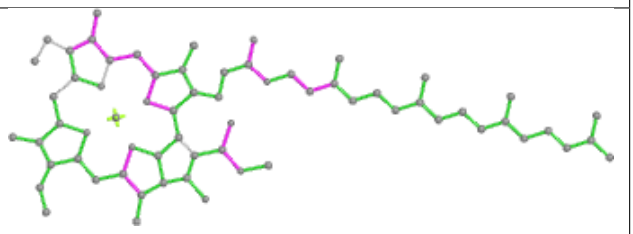


Rings

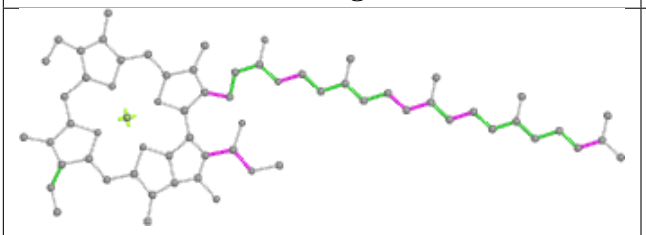
Ligand CLA c 513



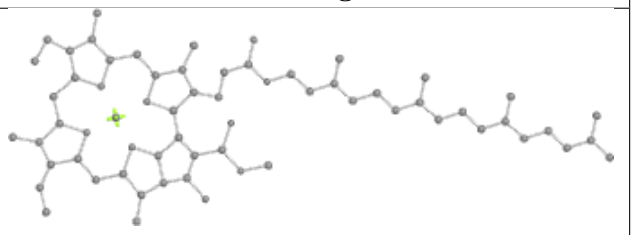
Bond lengths



Bond angles

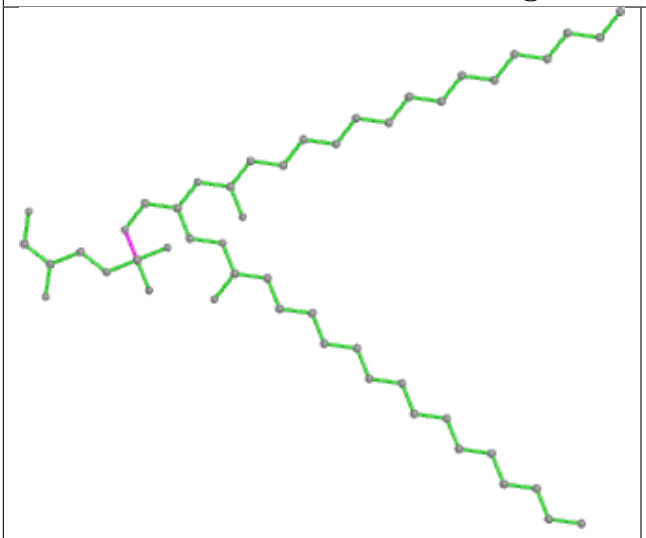


Torsions



Rings

Ligand LHG A 614



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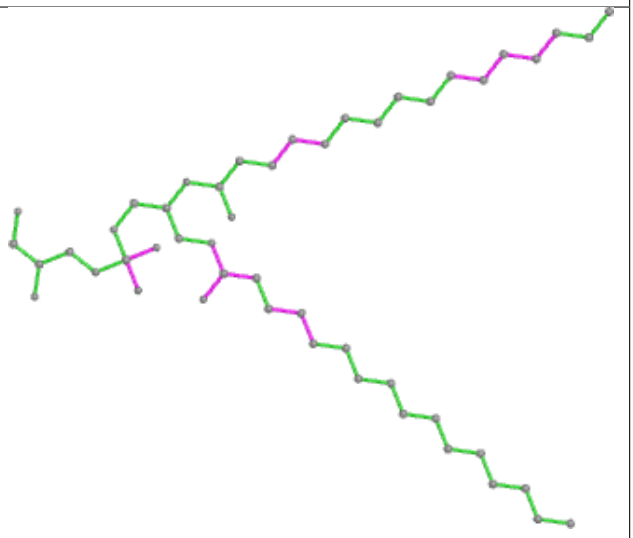
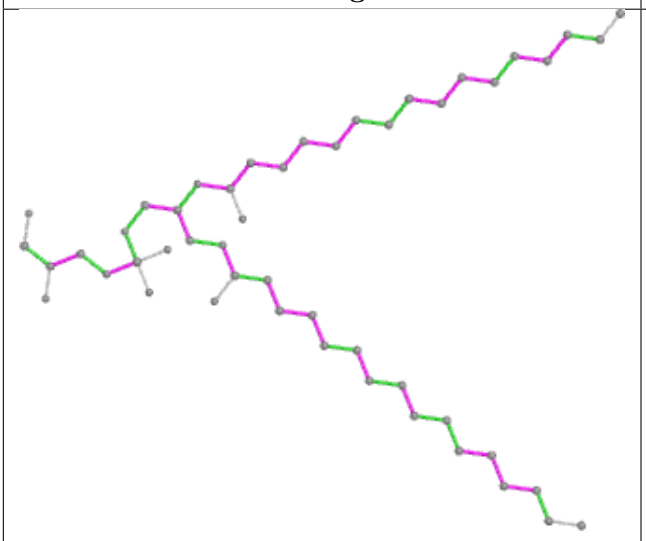
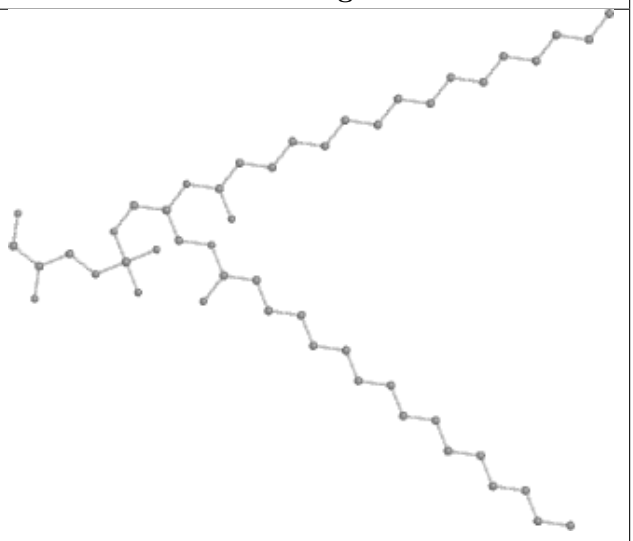


Bond angles

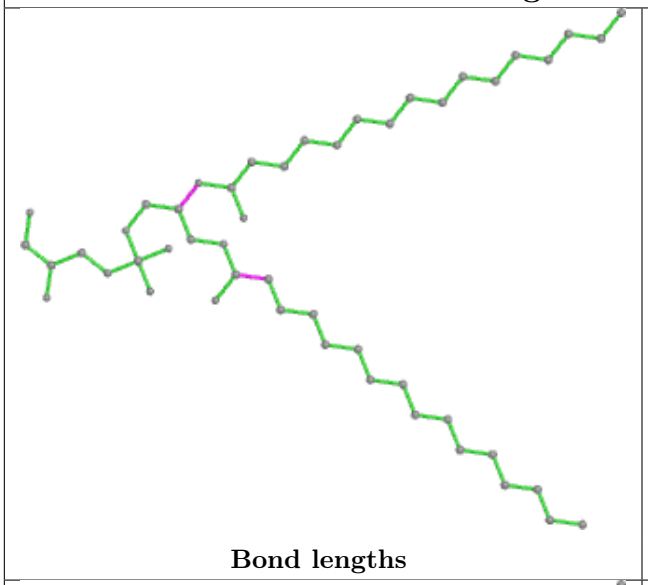


Torsions

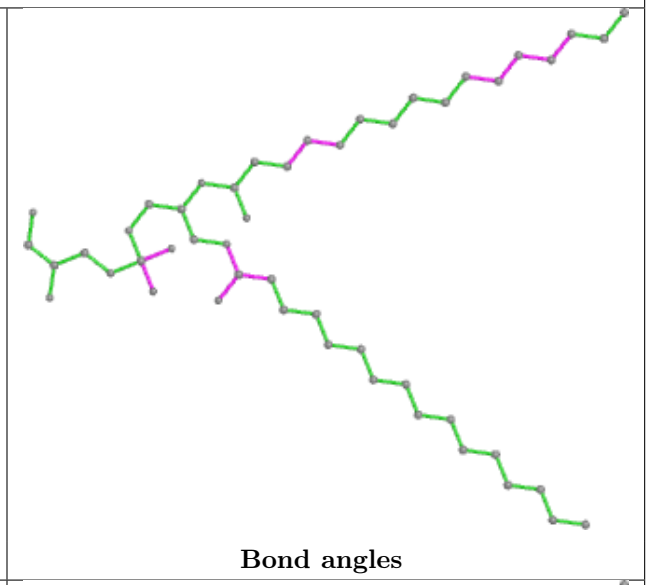


Rings

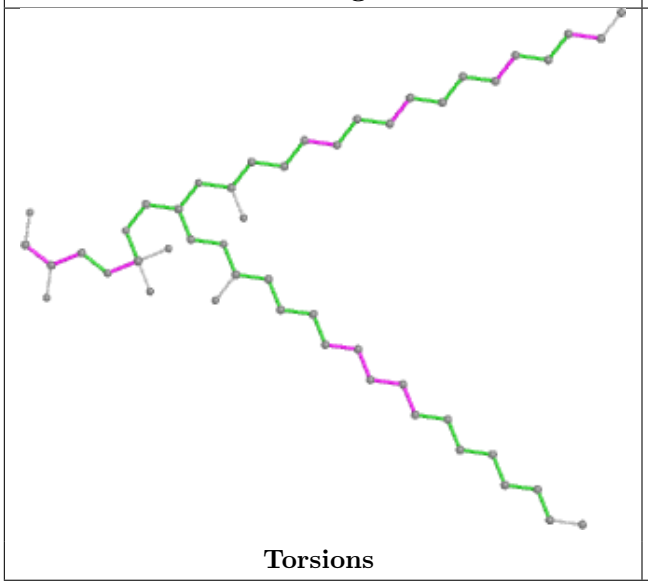
Ligand LHG D 412



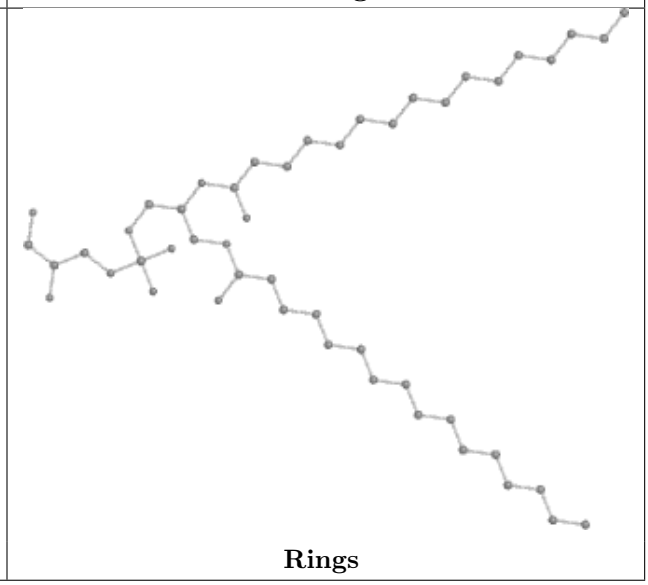
Bond lengths



Bond angles

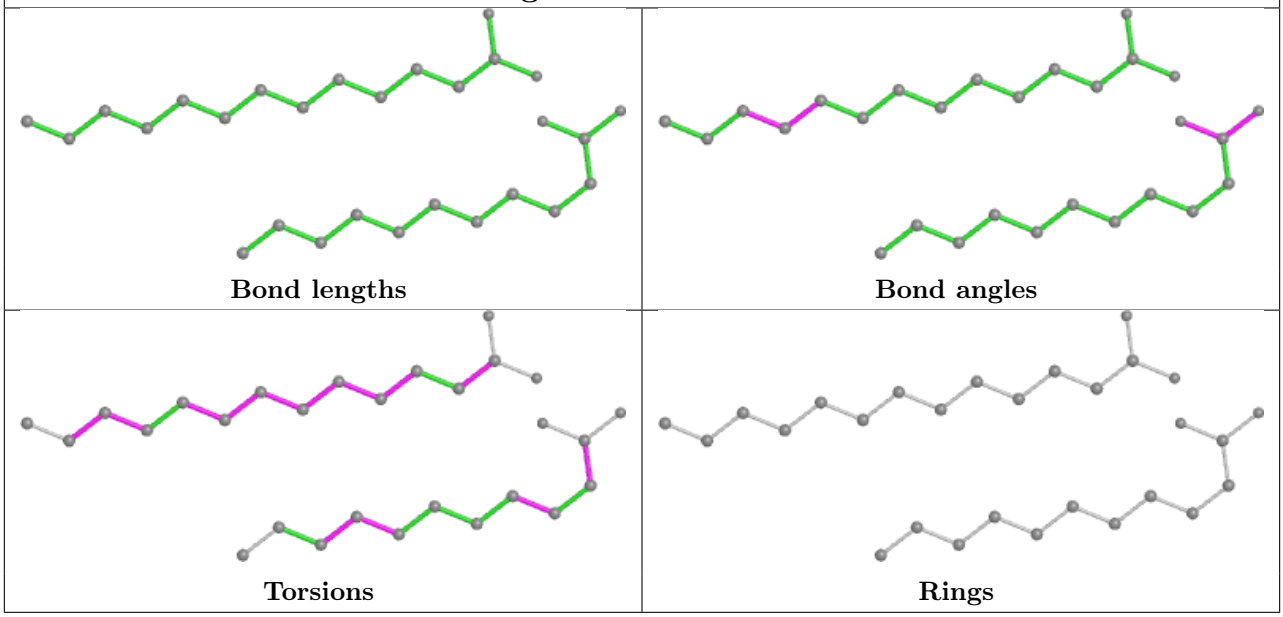


Torsions

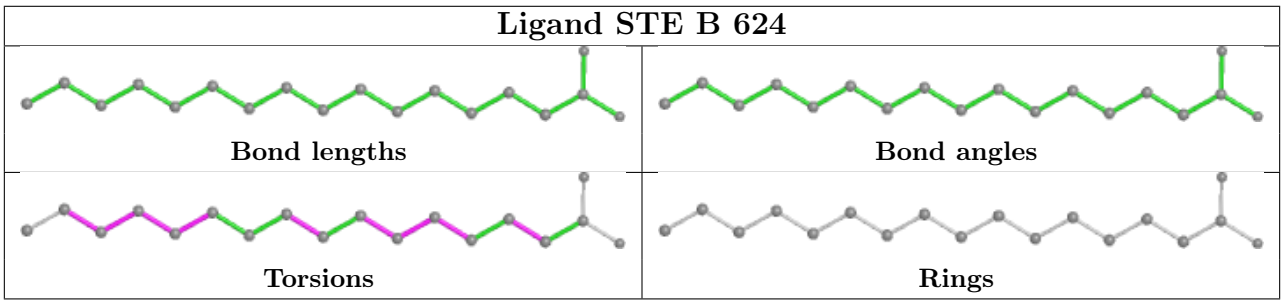


Rings

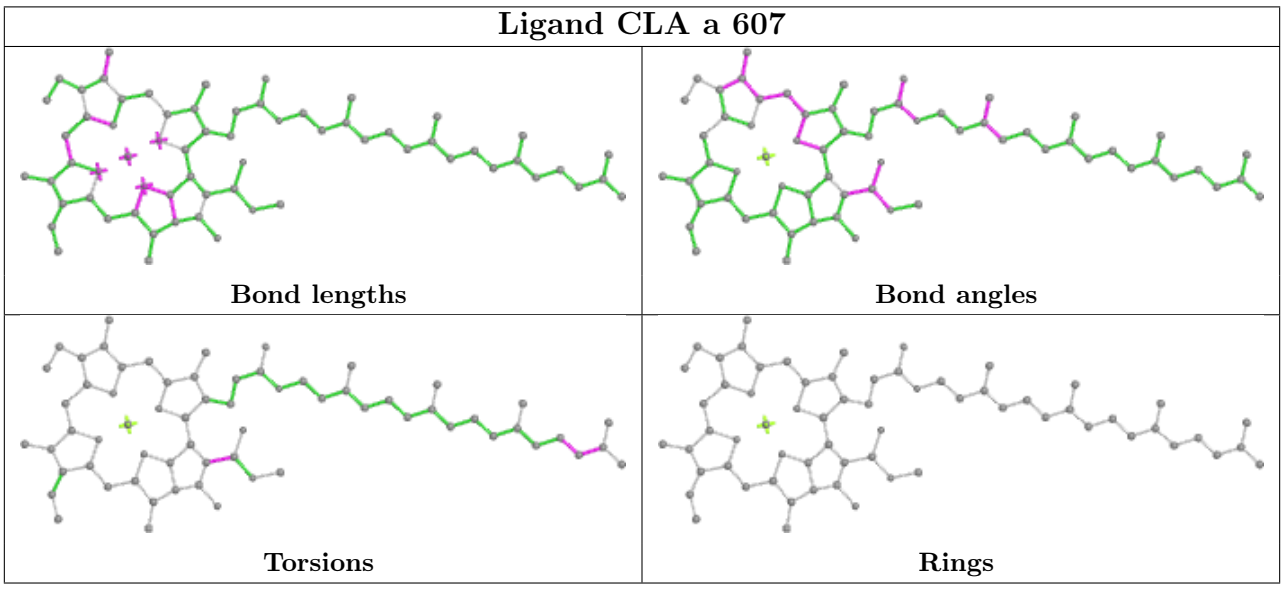
Ligand LMG B 621



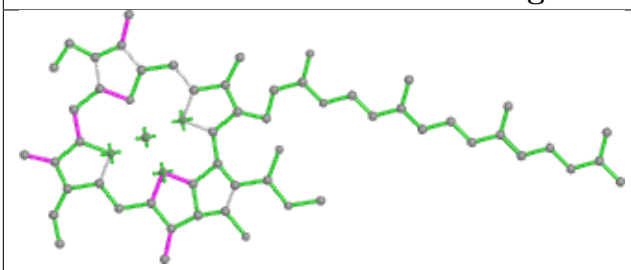
Ligand STE B 624

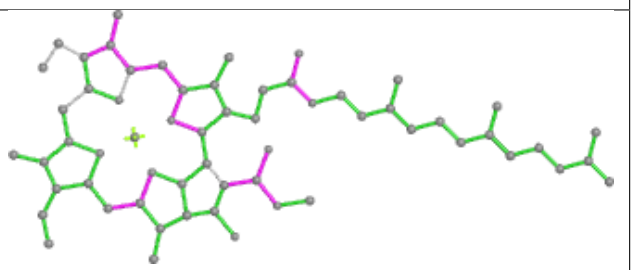


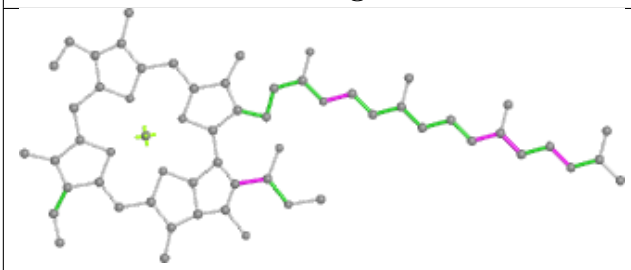
Ligand CLA a 607

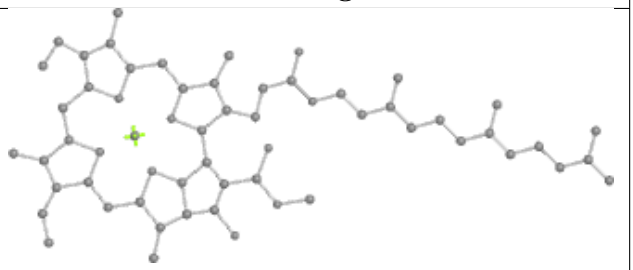


Ligand CLA b 616

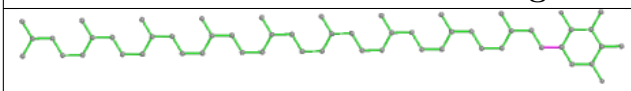

Bond lengths


Bond angles


Torsions


Rings

Ligand PL9 A 611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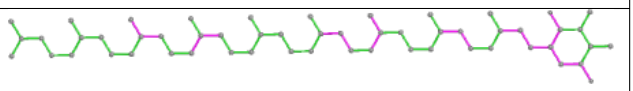
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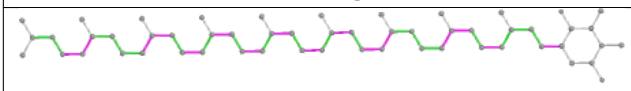
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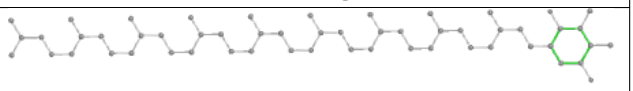
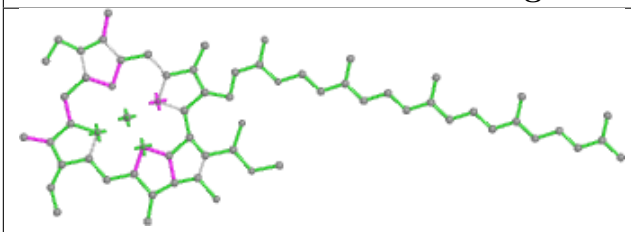

Rings

Ligand CLA B 607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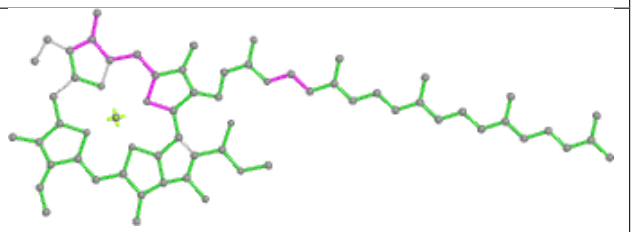
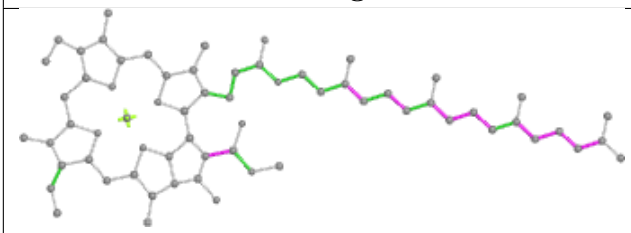

Bond angles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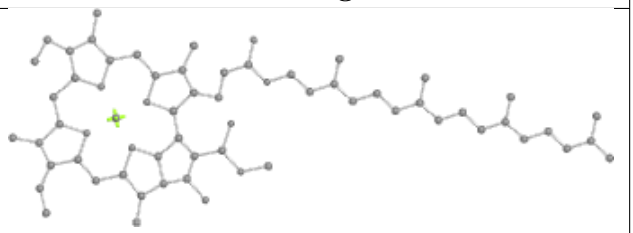
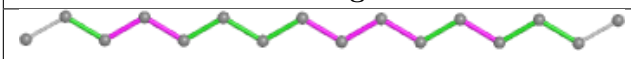

Rings

Ligand STE C 521


Bond lengths


Bond angles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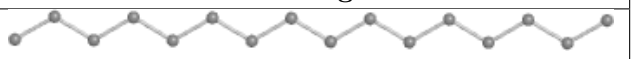
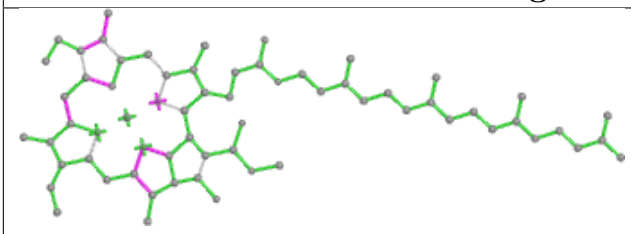
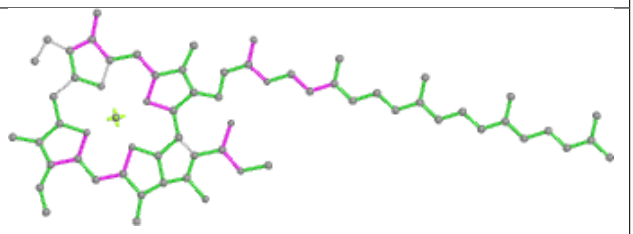

Rings

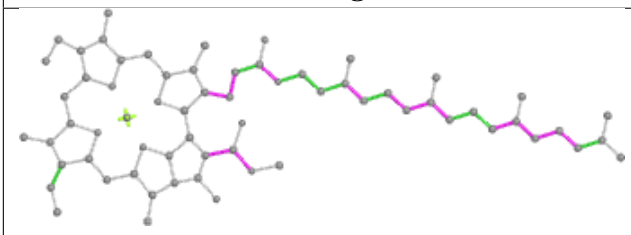
Ligand CLA c 512



Bond lengths



Bond angles



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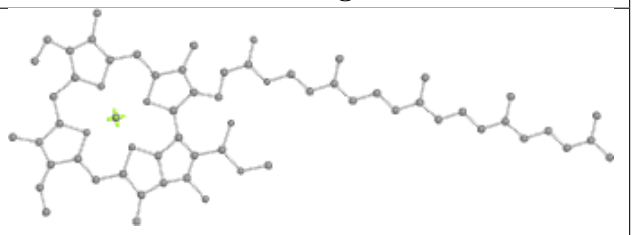
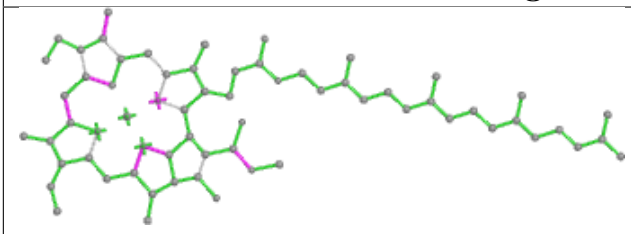


Rings

Ligand CLA C 509



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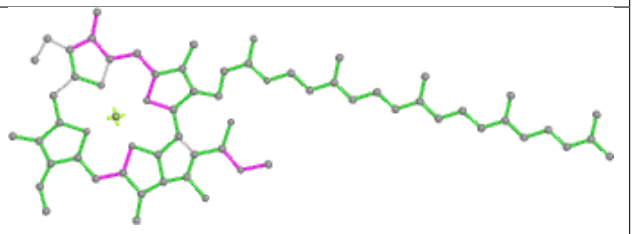
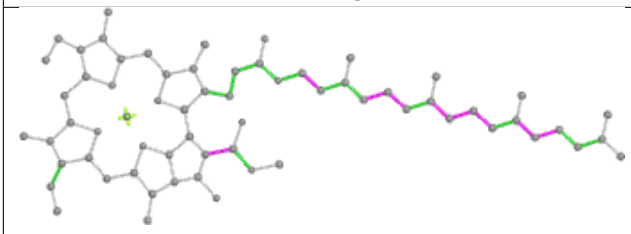


Bond angles



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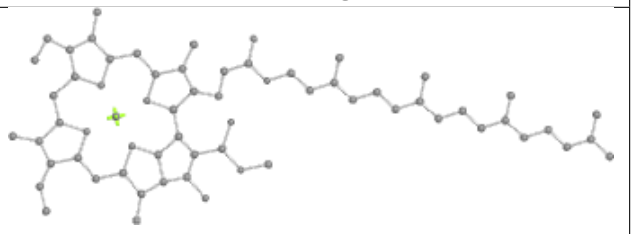
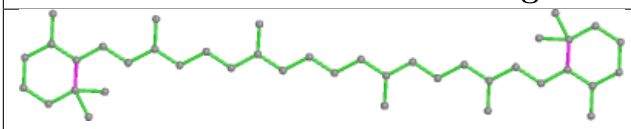


Rings

Ligand BCR H 101



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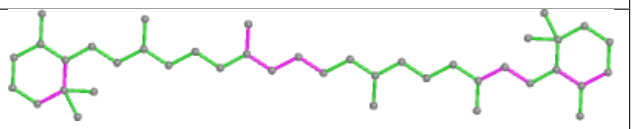
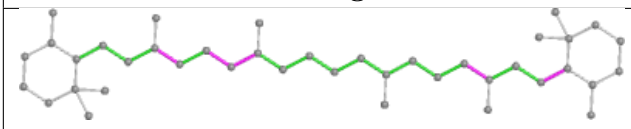


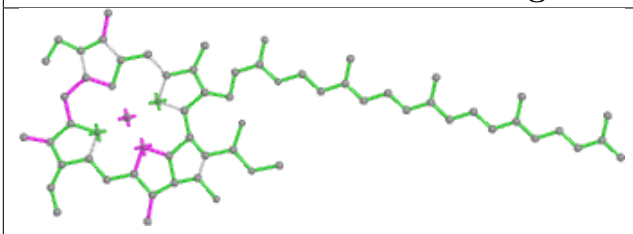
Bond angles



Torsions

Rings

Ligand CLA a 609



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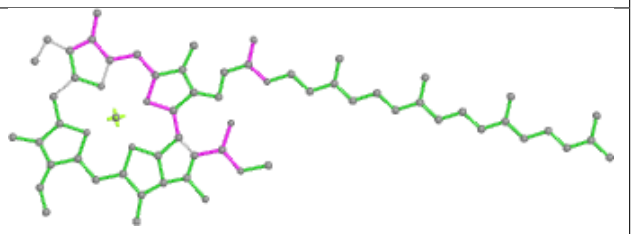
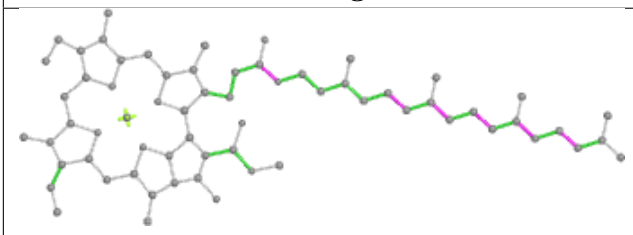
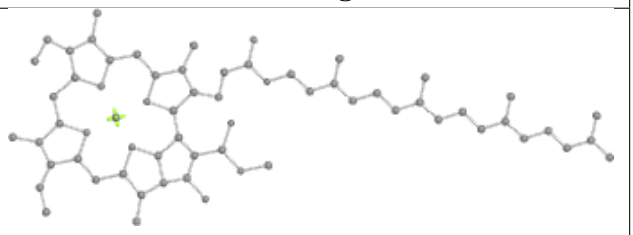


Bond angles

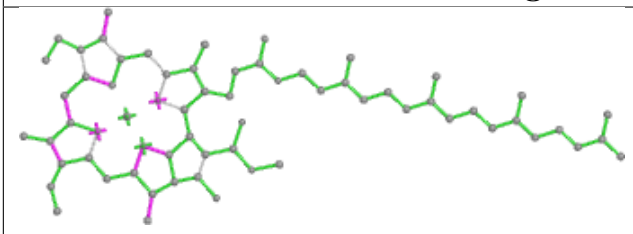


Torsions



Rings

Ligand CLA B 604



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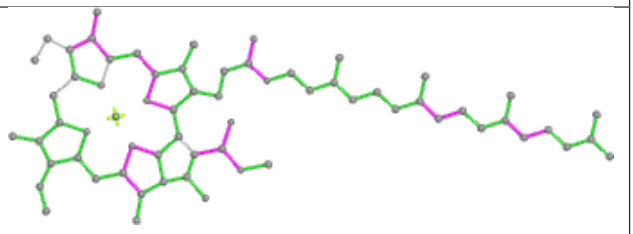
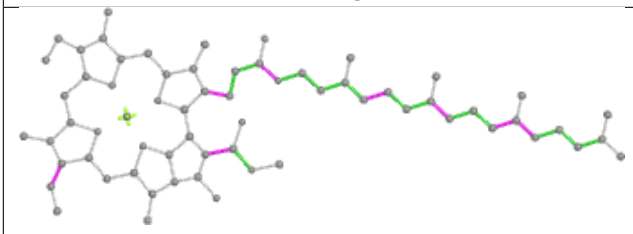
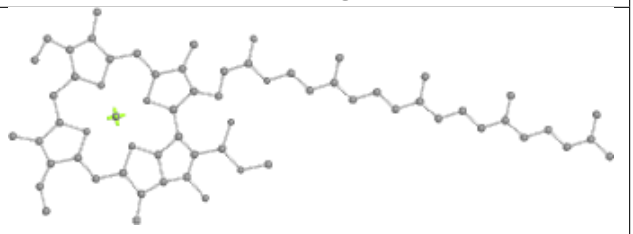


Bond angles

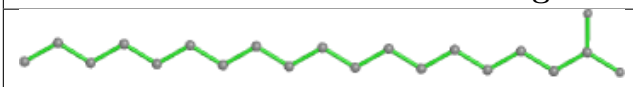


Torsions



Rings

Ligand STE c 521



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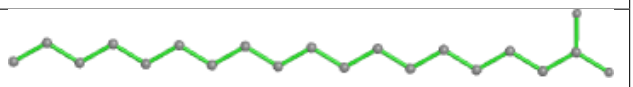
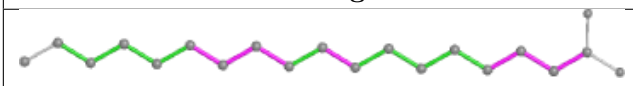


Bond angles



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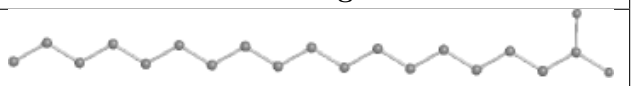
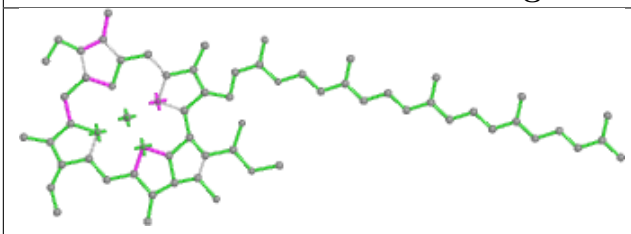


Rings

Ligand CLA A 607



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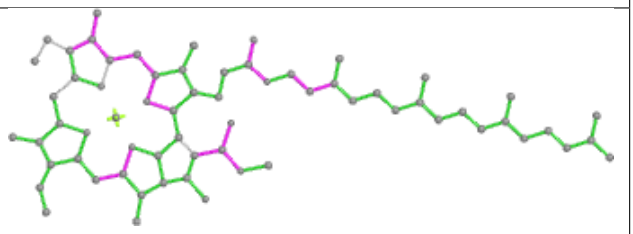
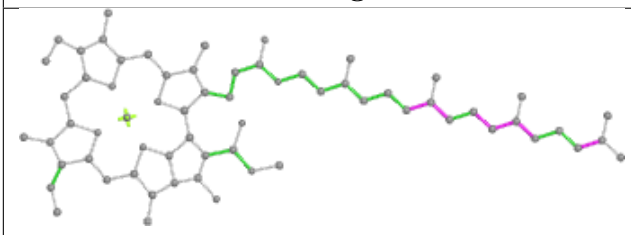
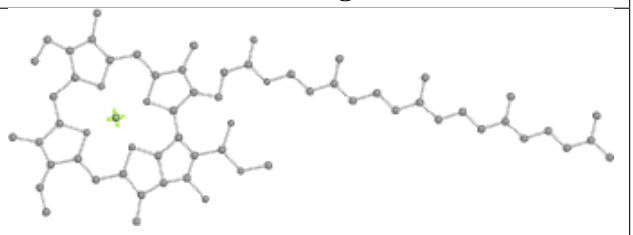


Bond angles

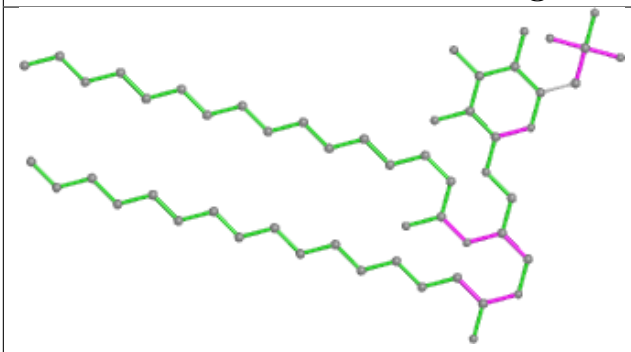


Torsions



Rings

Ligand SQD a 613



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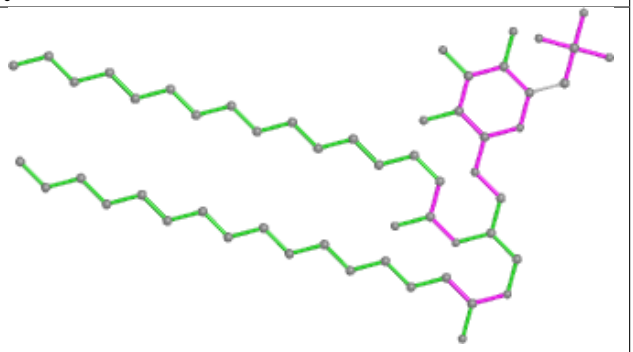
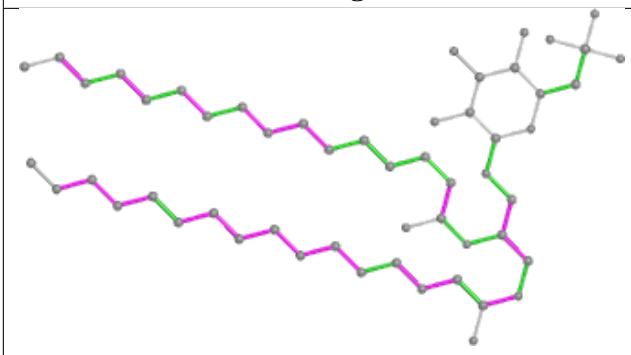
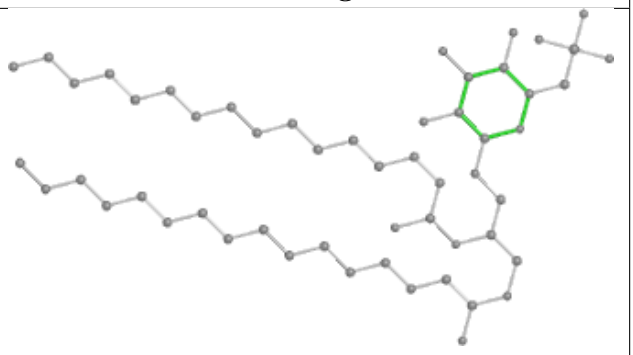


Bond angles

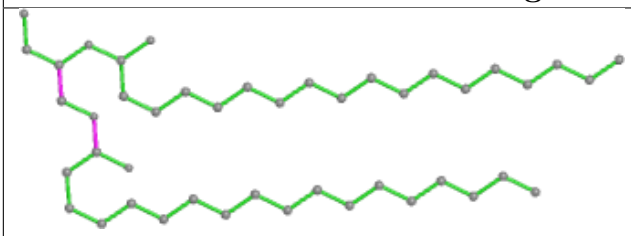


Torsions

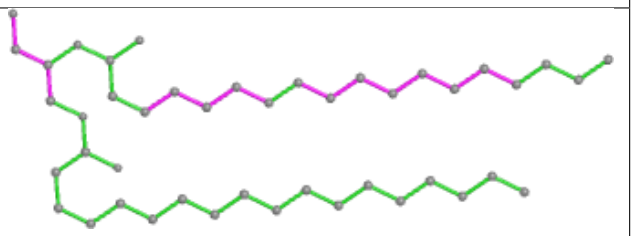


Rings

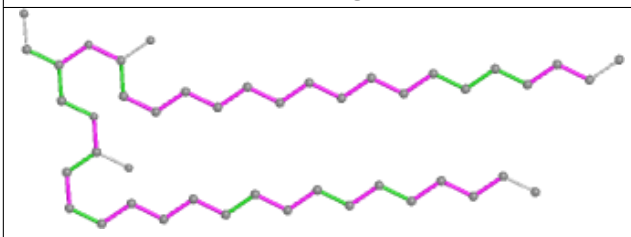
Ligand DGD a 615



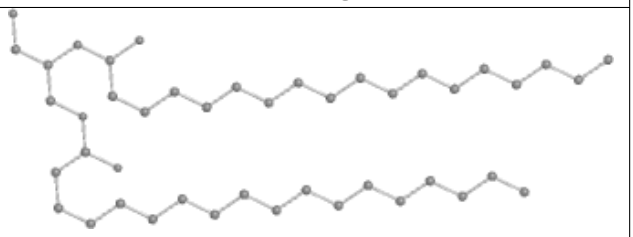
Bond lengths



Bond angles

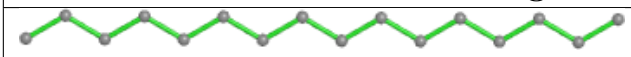


Torsions



Rings

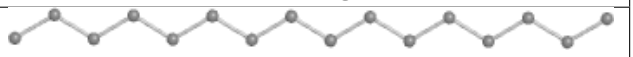
Ligand STE B 626



Bond lengths

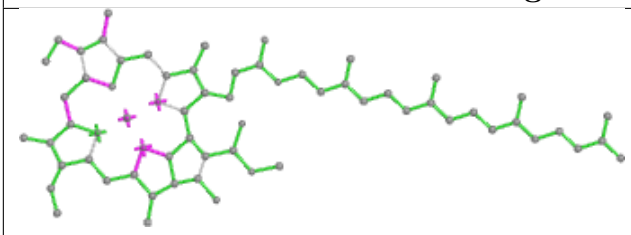
Bond angles

Torsions

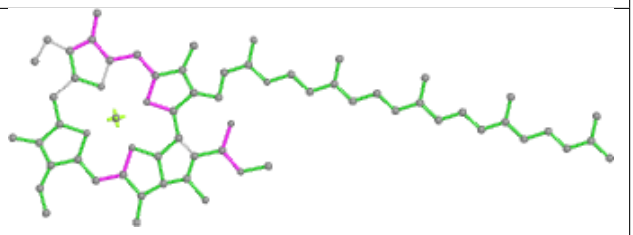


Rings

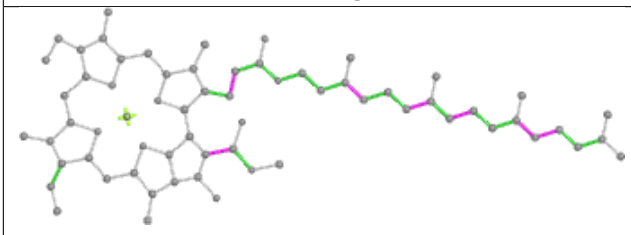
Ligand CLA B 614



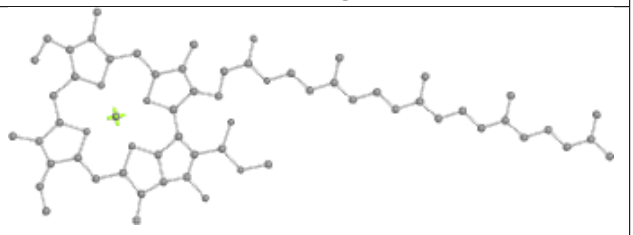
Bond lengths



Bond angles

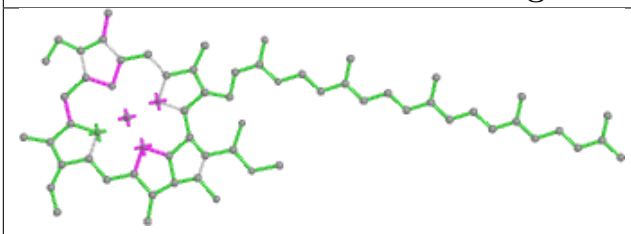


Torsions

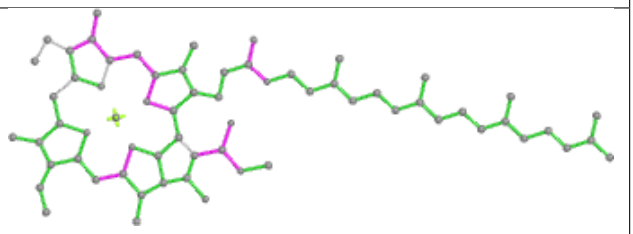


Rings

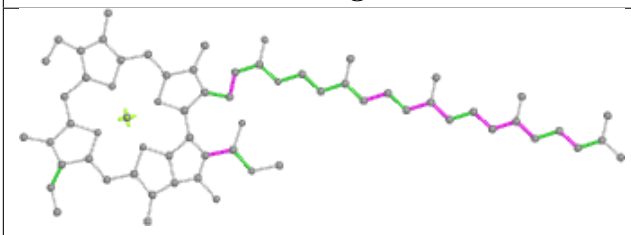
Ligand CLA b 606



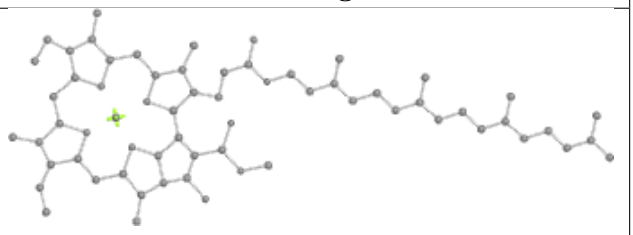
Bond lengths



Bond angles

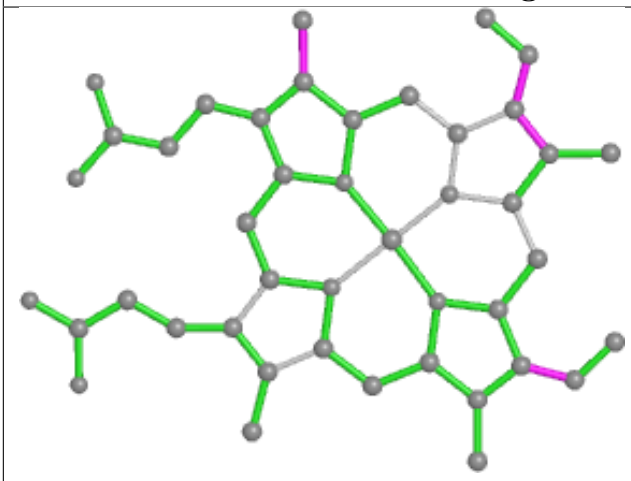


Torsions

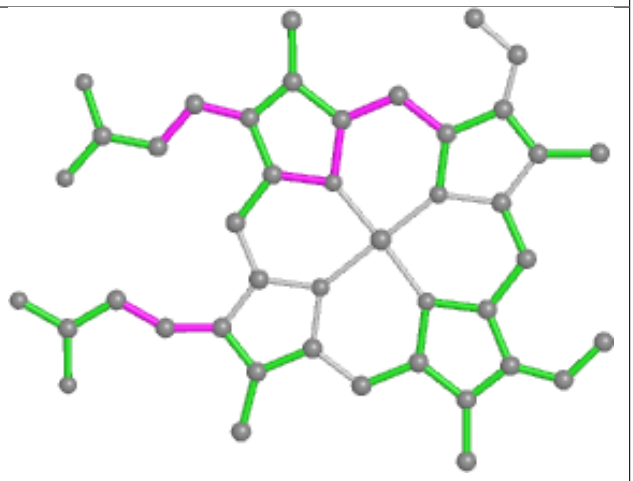


Rings

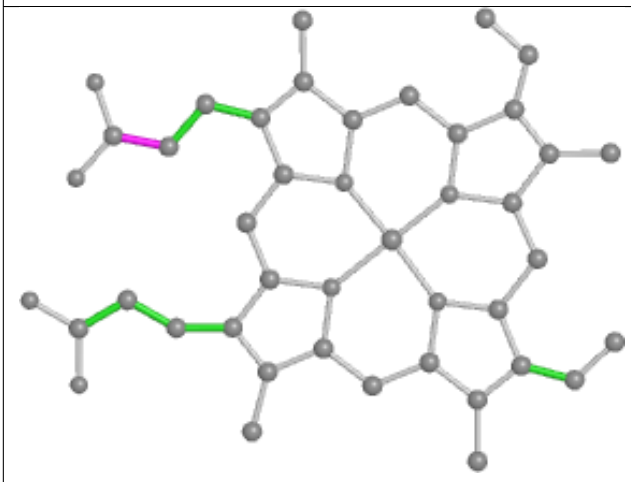
Ligand HEM E 101



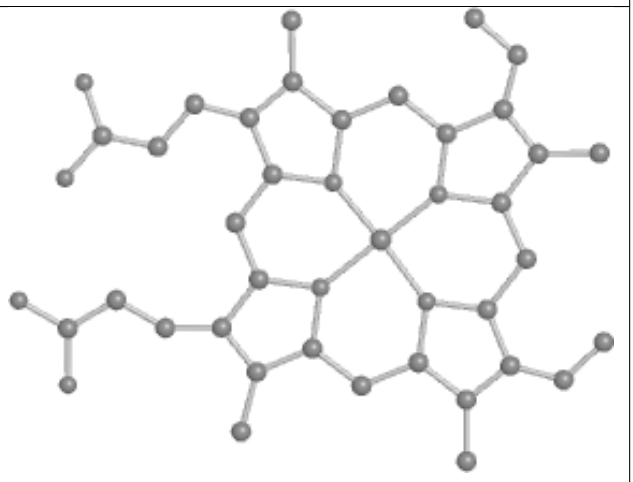
Bond lengths



Bond angles

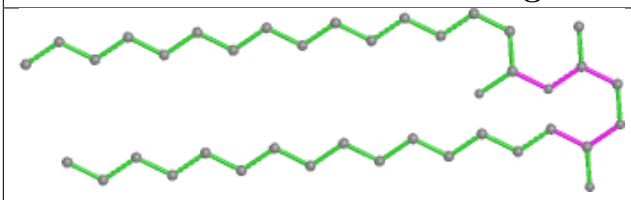


Torsions

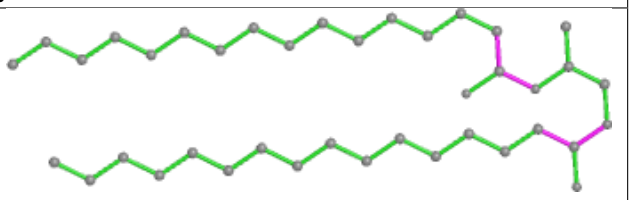


Rings

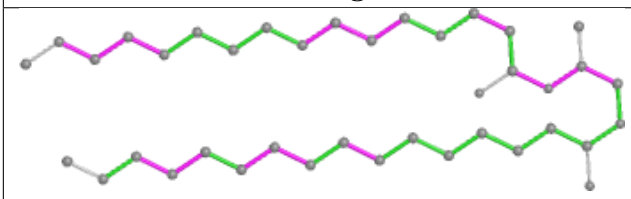
Ligand SQD A 616



Bond lengths



Bond angles



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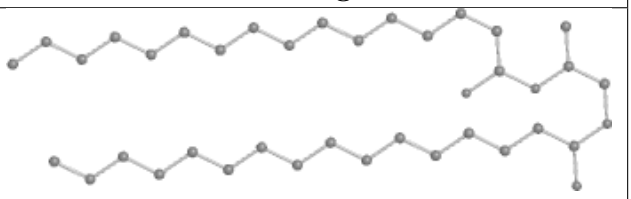
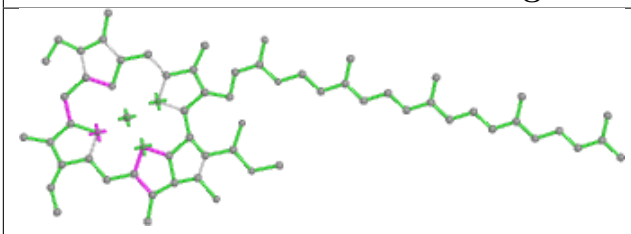
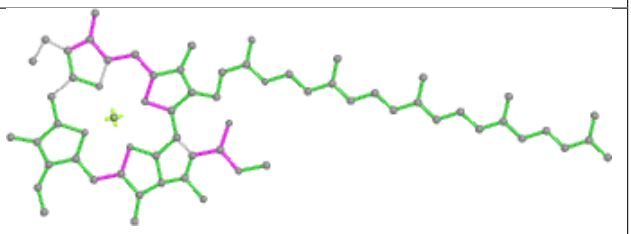


Rings

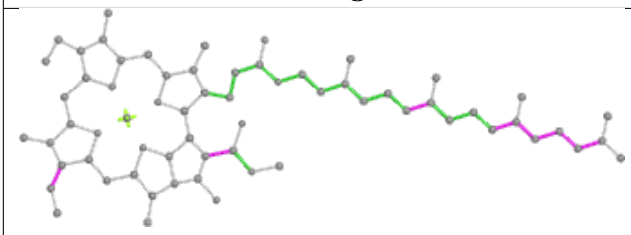
Ligand CLA D 403



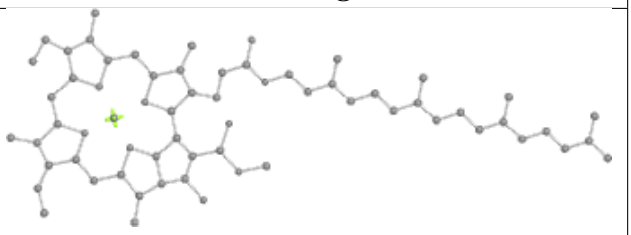
Bond lengths



Bond angles

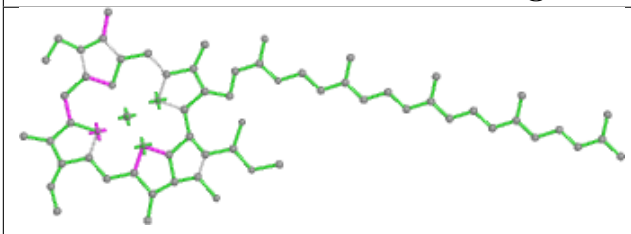


Torsions

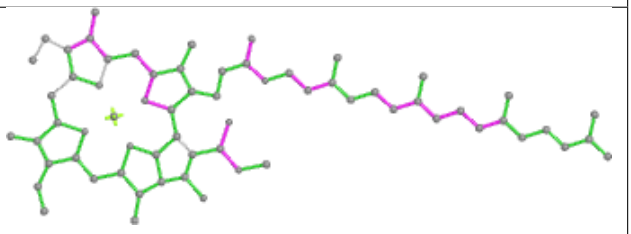


Rings

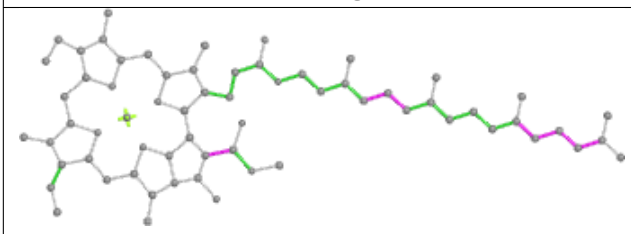
Ligand CLA b 604



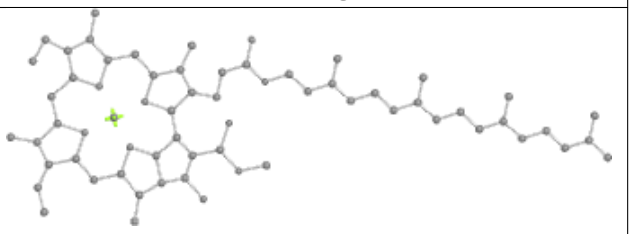
Bond lengths



Bond angles

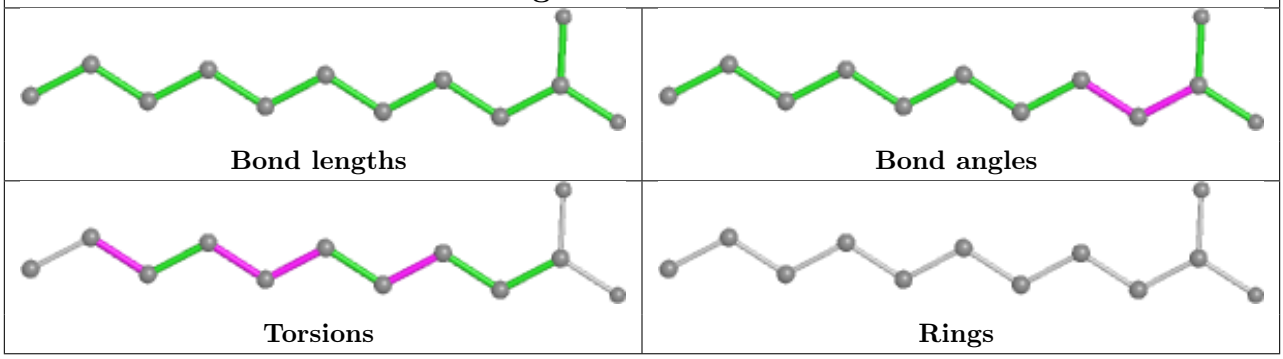


Torsions

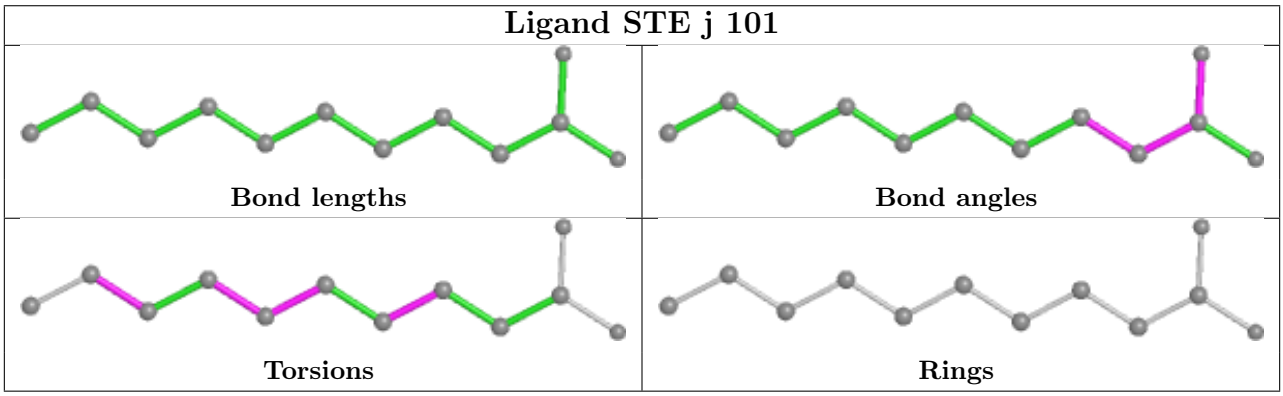


Rings

Ligand STE a 617



Ligand STE j 101



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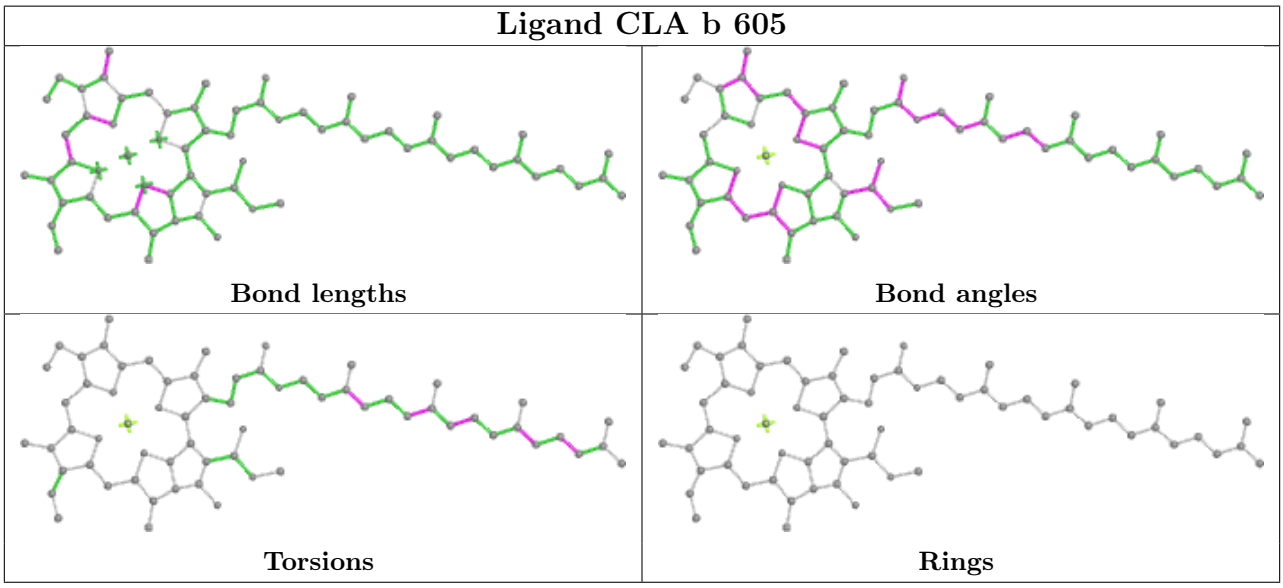
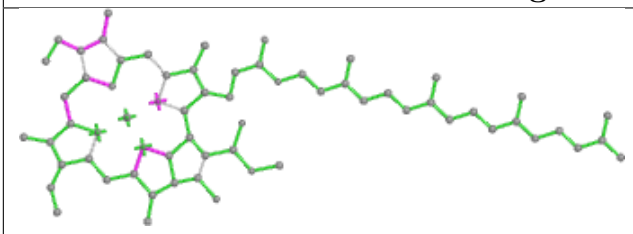
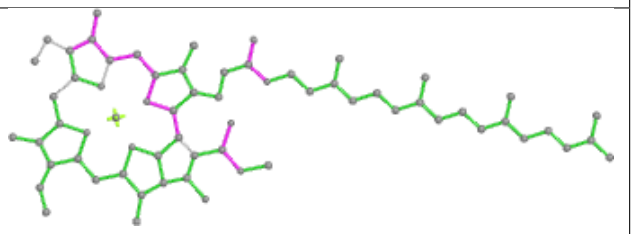


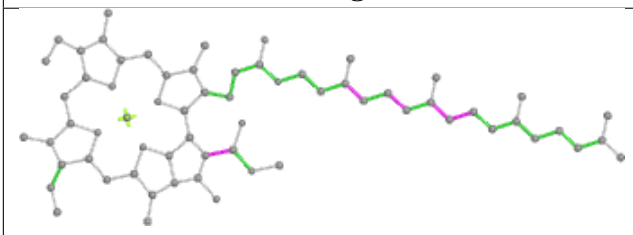
Ligand CLA c 507



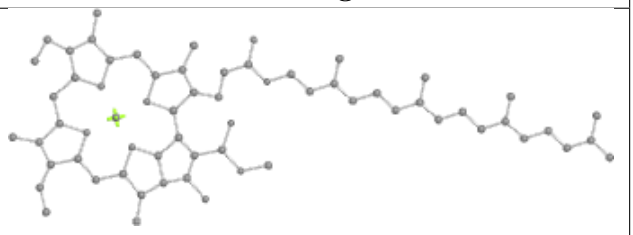
Bond lengths



Bond angles

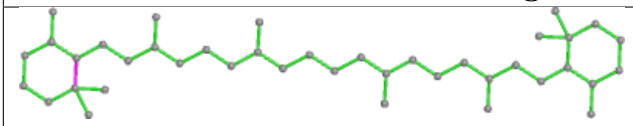


Torsions

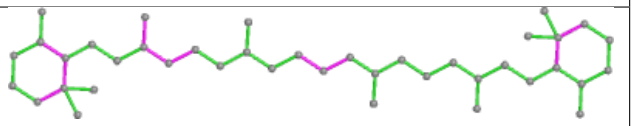


Rings

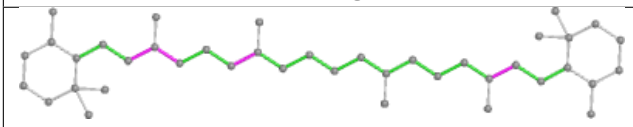
Ligand BCR B 619



Bond lengths



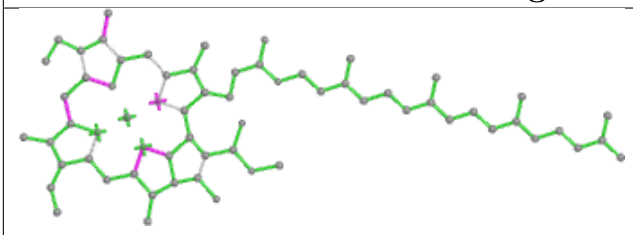
Bond angles



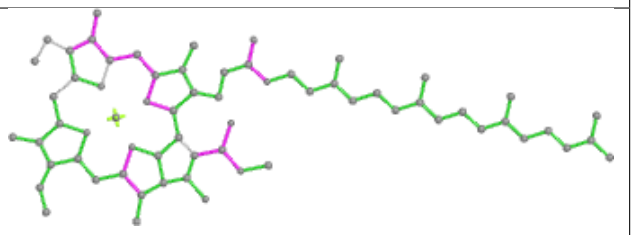
Torsions

Rings

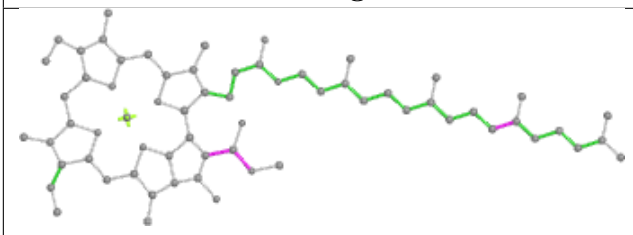
Ligand CLA a 612



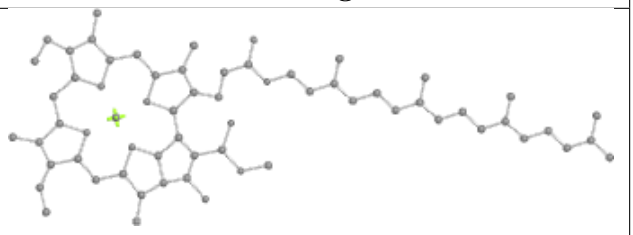
Bond lengths



Bond angles

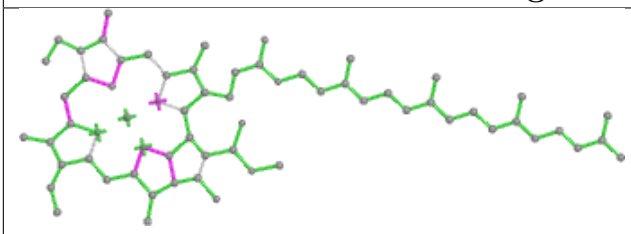


Torsions

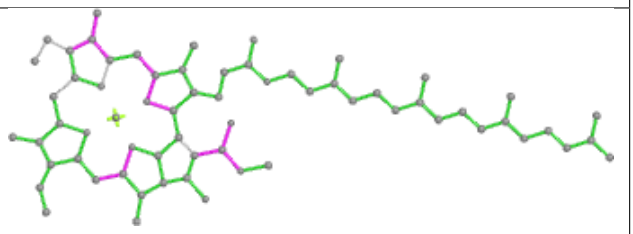


Rings

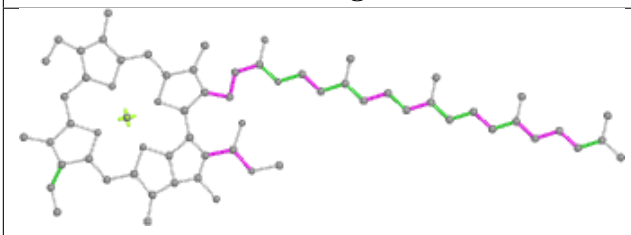
Ligand CLA b 601



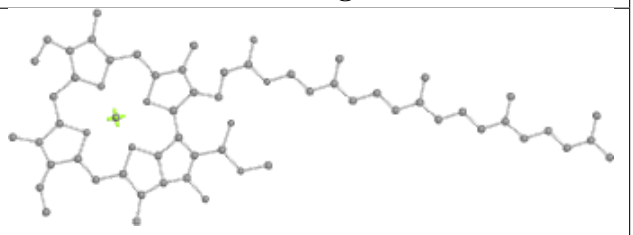
Bond lengths



Bond angles

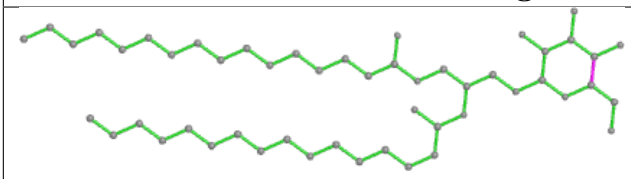


Torsions



Rings

Ligand LMG M 101



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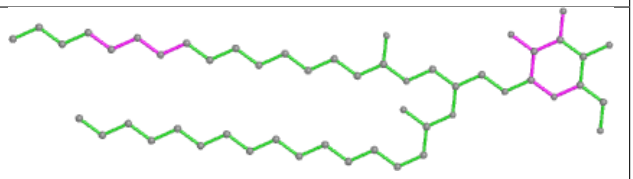
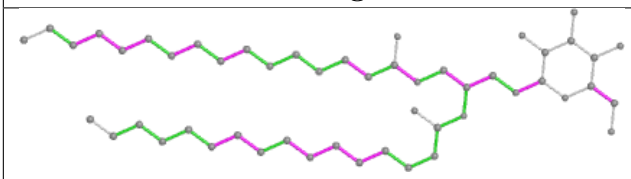
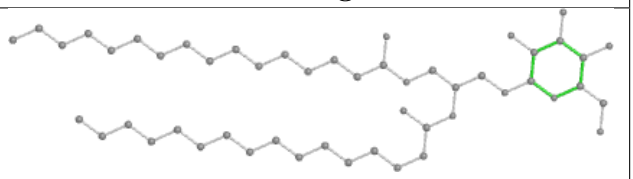


Bond angles

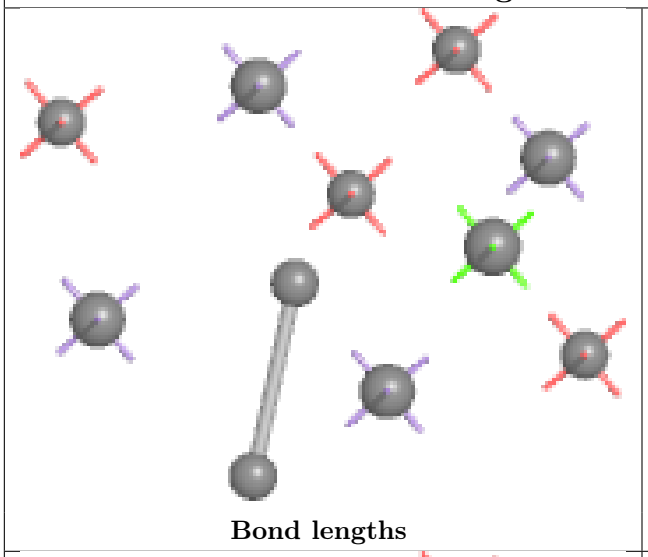


Torsions

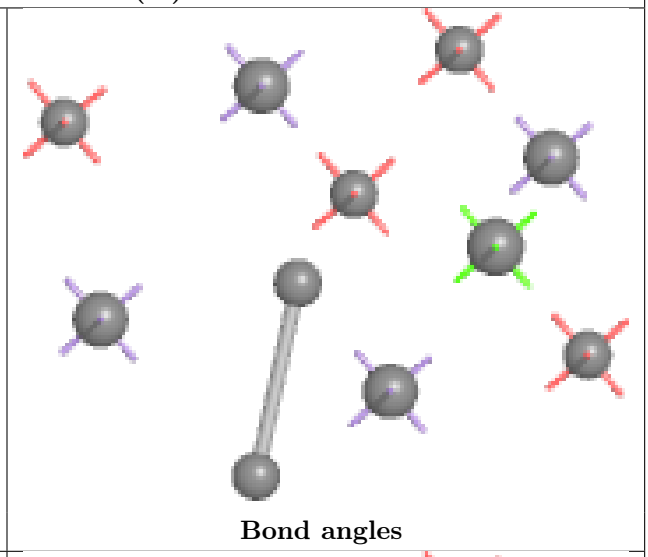


Rings

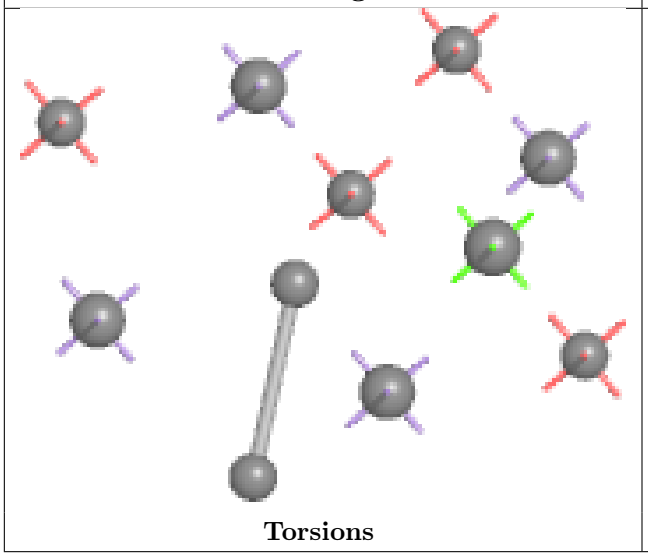
Ligand OEY a 601 (B)



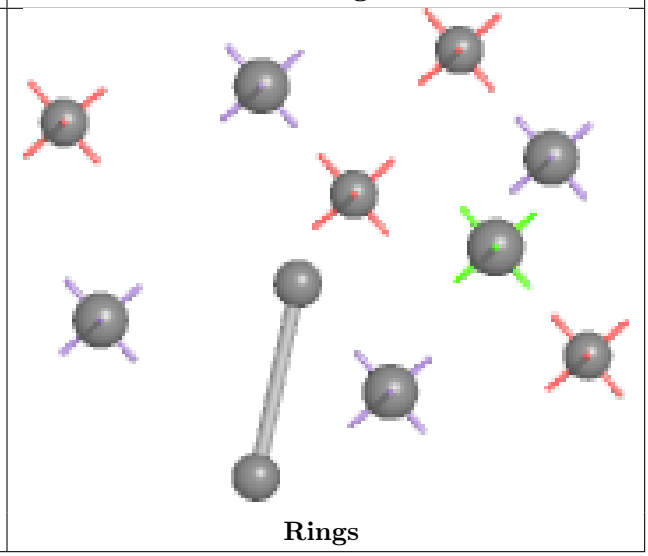
Bond lengths



Bond angles

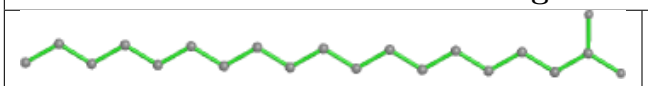


Torsions

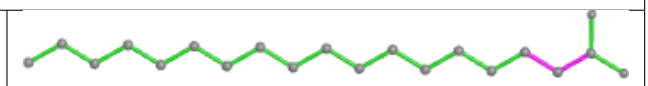


Rings

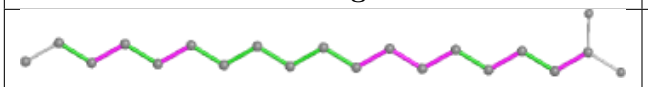
Ligand STE b 622



Bond lengths



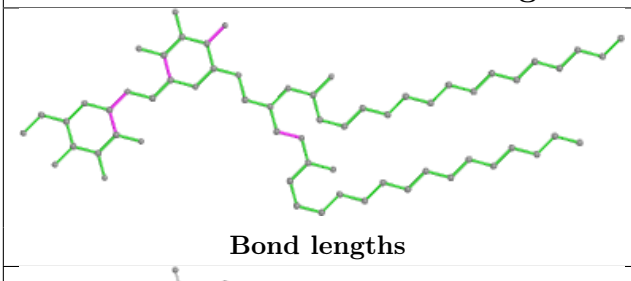
Bond angles

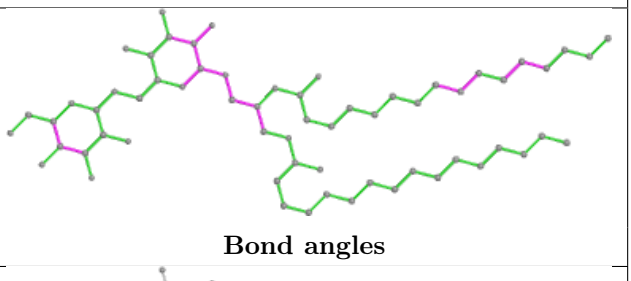


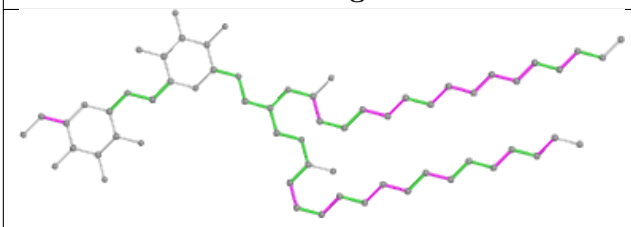
Torsions

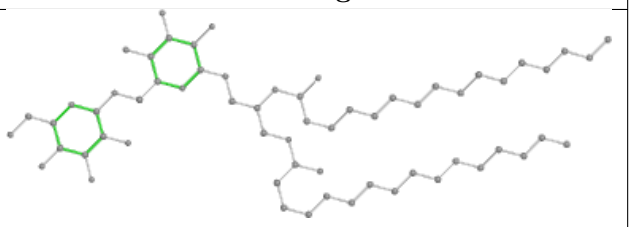
Rings

Ligand DGD H 102

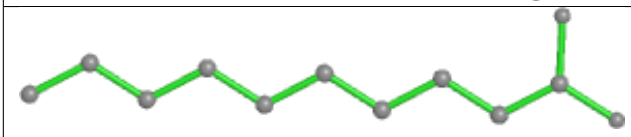

Bond lengths

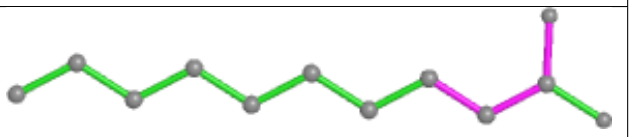

Bond angles

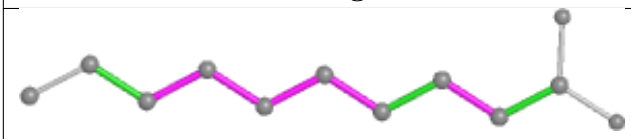

Torsions

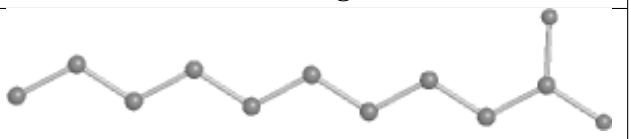

Rings

Ligand STE C 520

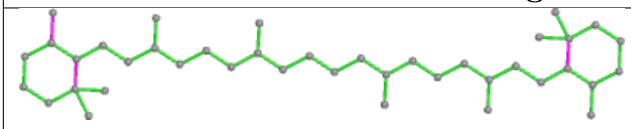

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR k 101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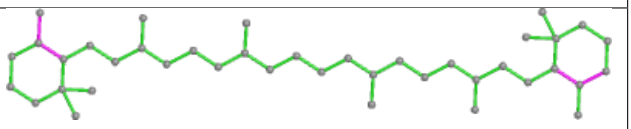
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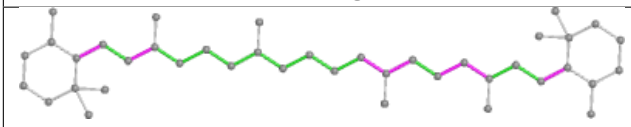
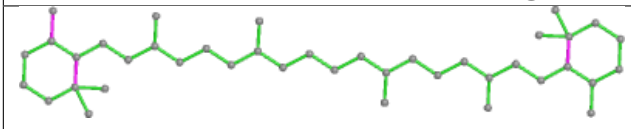
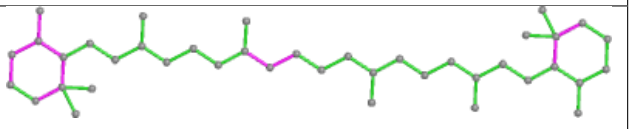
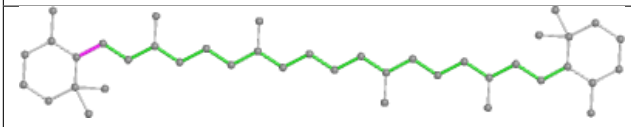

Torsions

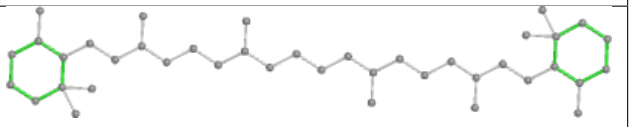

Rings

Ligand BCR B 617

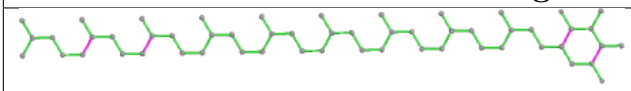

Bond lengths


Bond angles


Torsions


Rings

Ligand PL9 d 406



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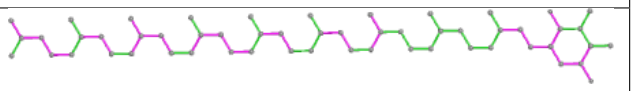
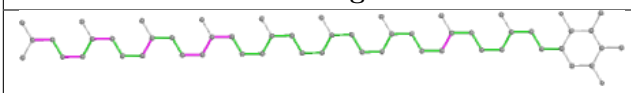
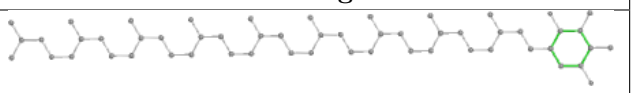


Bond angles

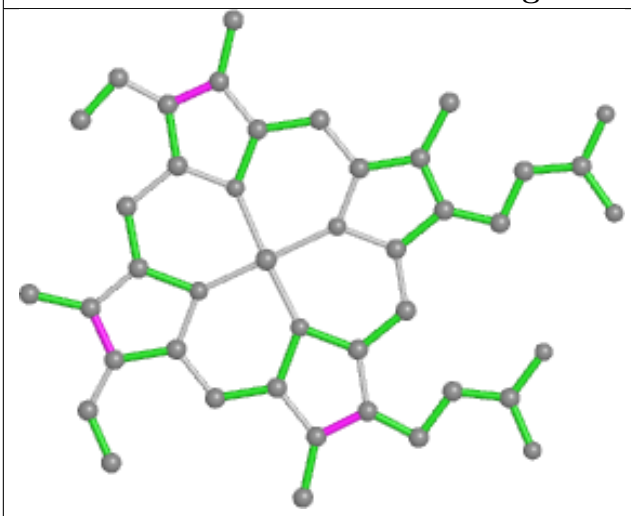


Torsions



Rings

Ligand HEC V 201



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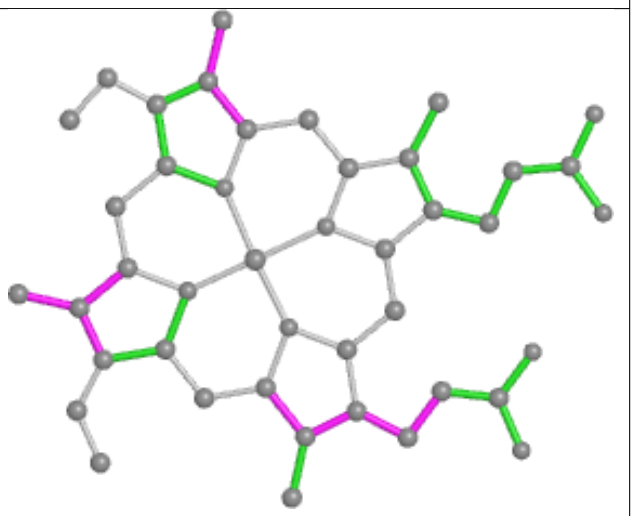
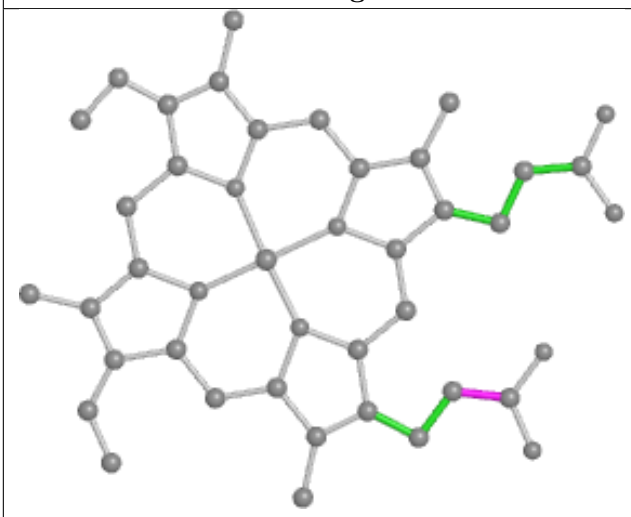


Bond angles



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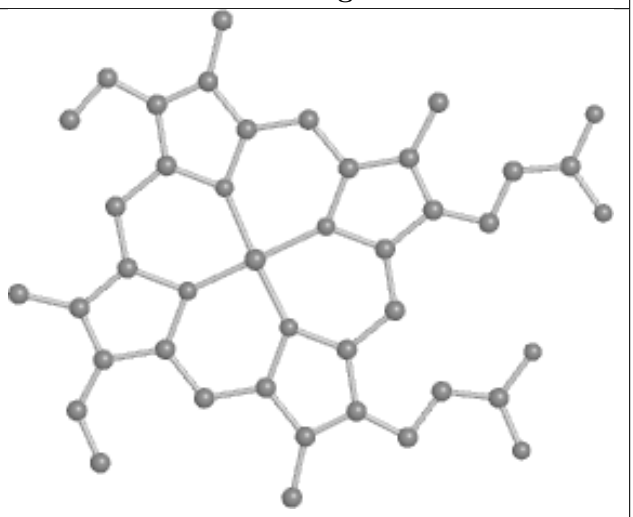
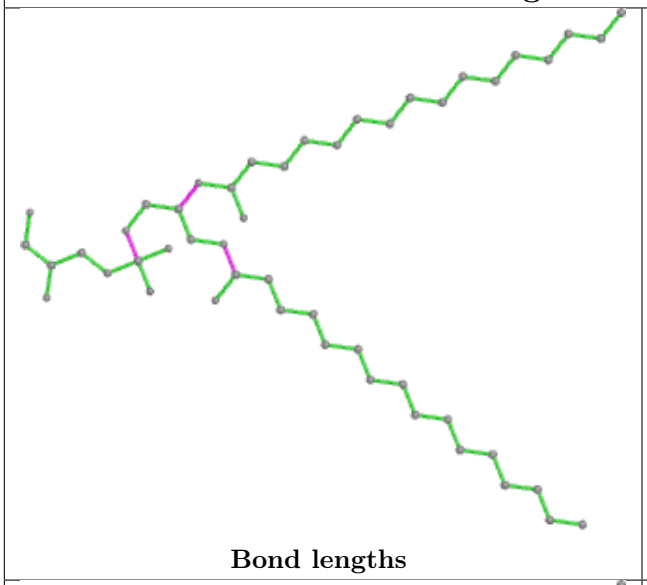


Rings

Ligand LHG A 615



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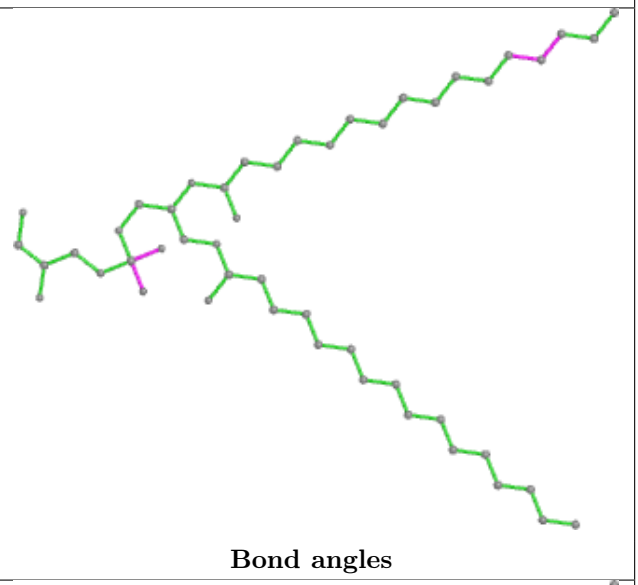

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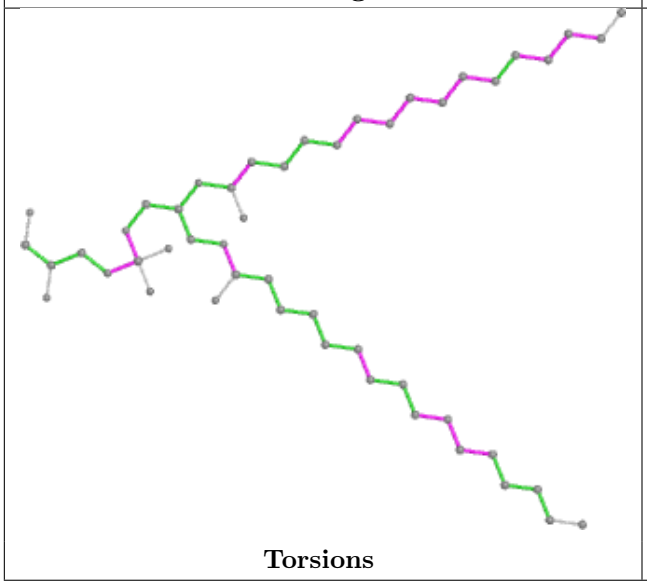

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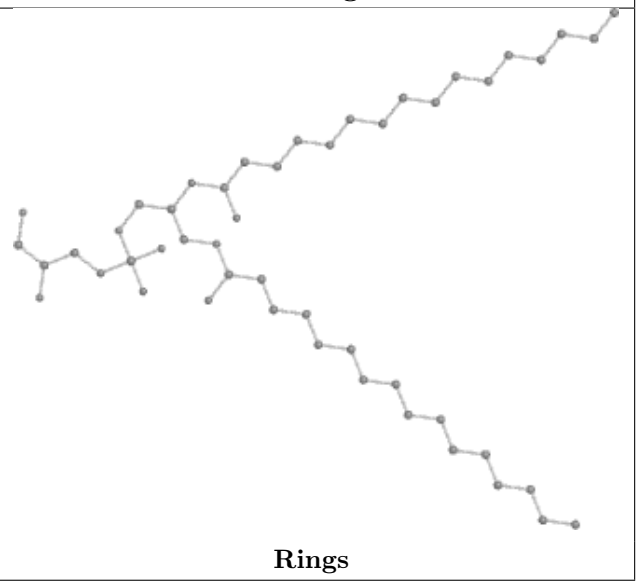
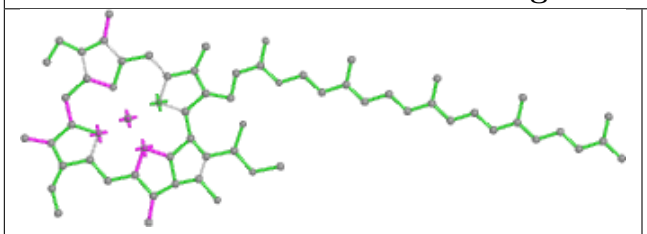


Rings

Ligand CLA c 506



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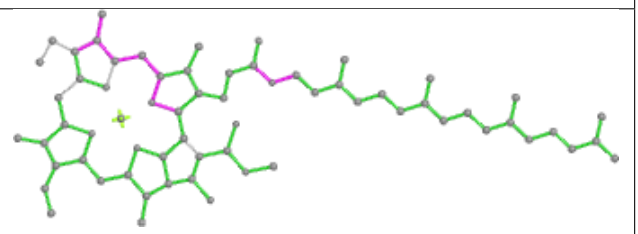
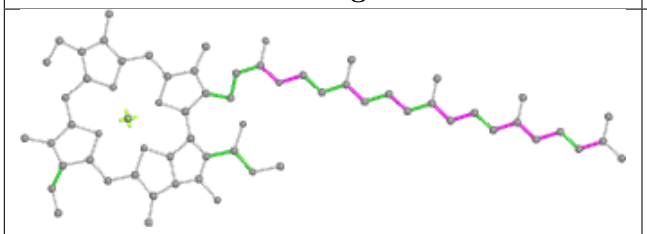


Bond angles



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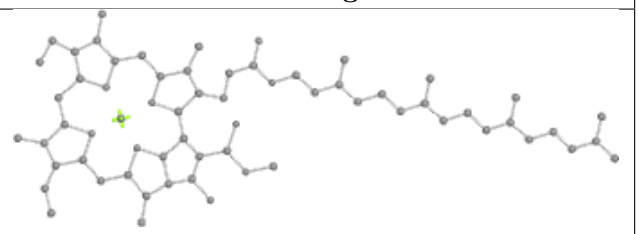
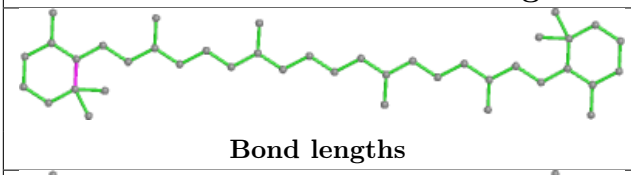


Rings

Ligand BCR A 610



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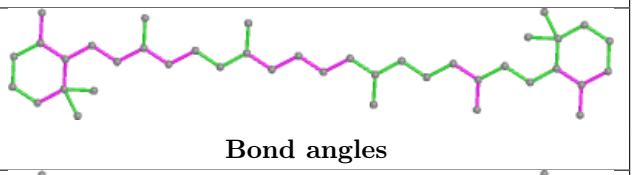
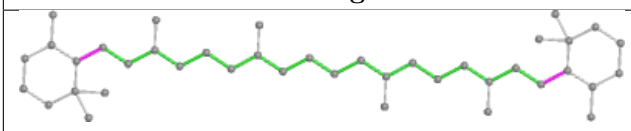


Bond angles



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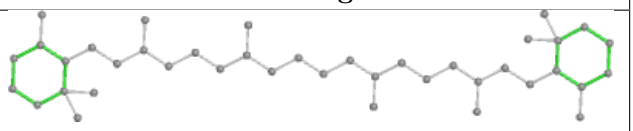
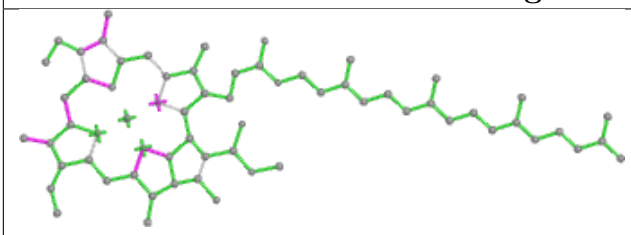


Rings

Ligand CLA B 605



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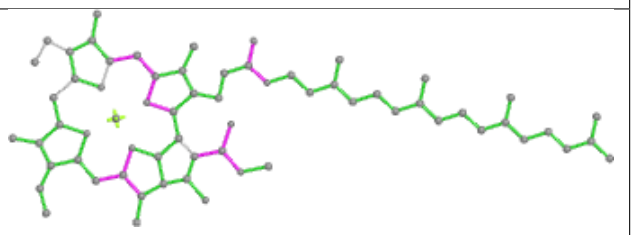
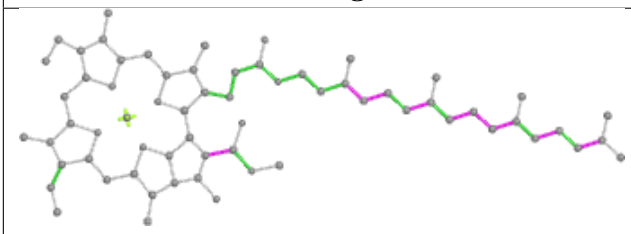


Bond angles



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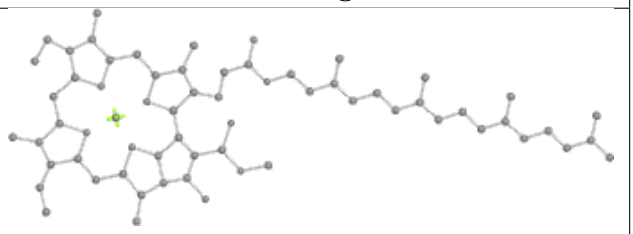
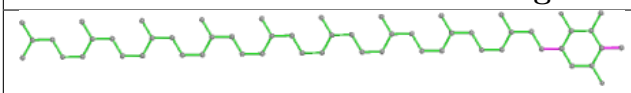


Rings

Ligand PL9 a 611



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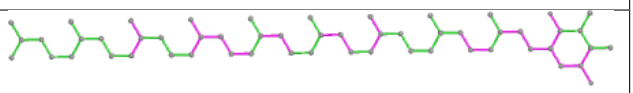
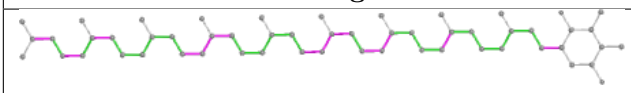


Bond angles



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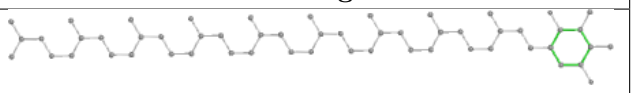
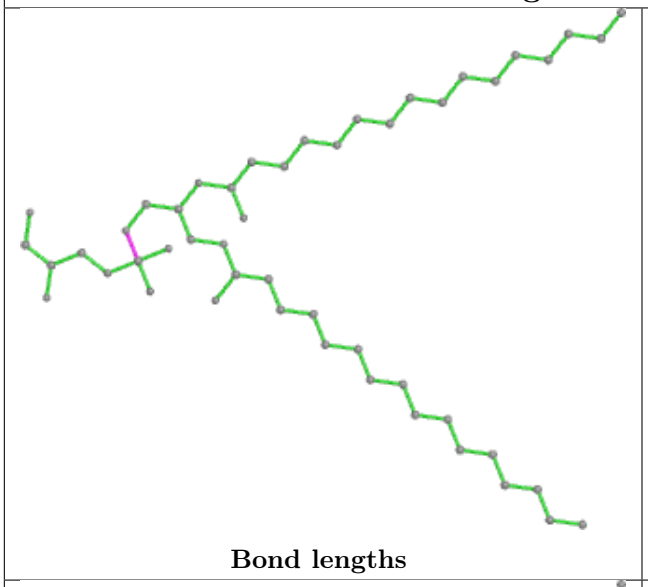


Rings

Ligand LHG D 409



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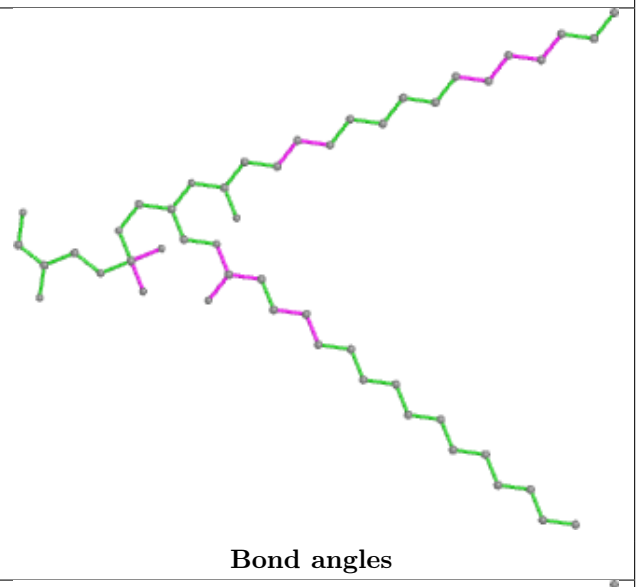
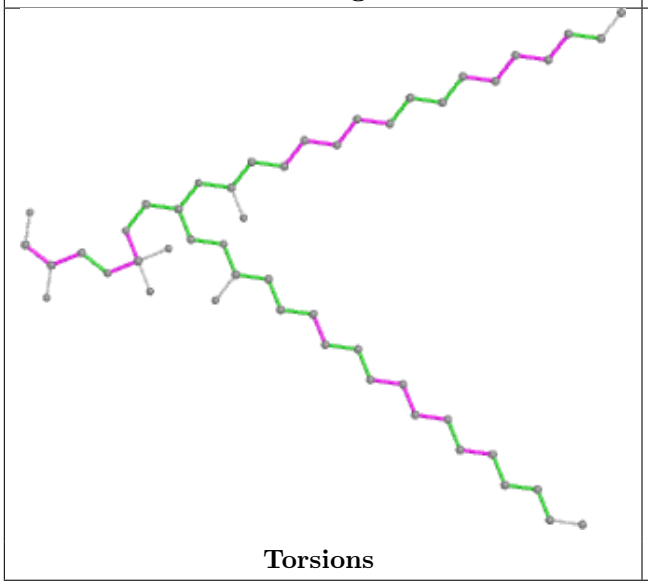


Bond angles



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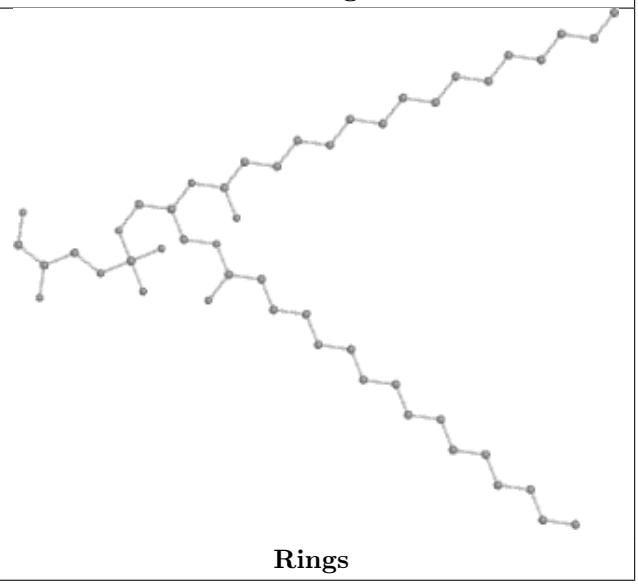
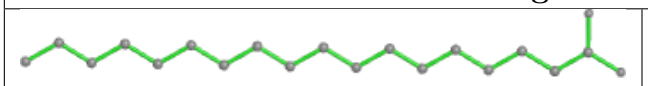


Rings

Ligand STE b 620



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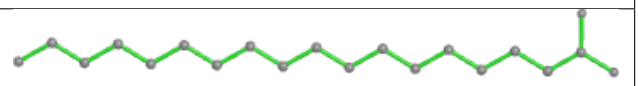
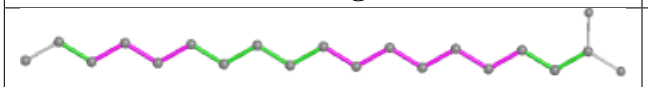


Bond angles



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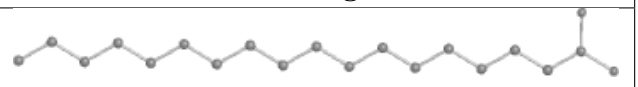
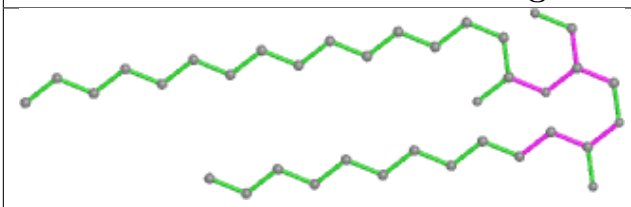


Rings

Ligand SQD a 614



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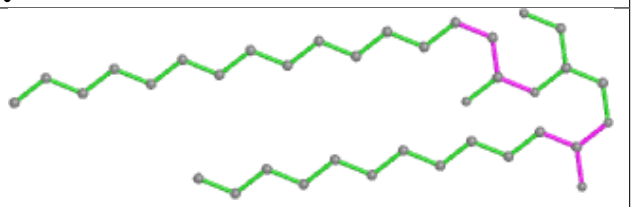
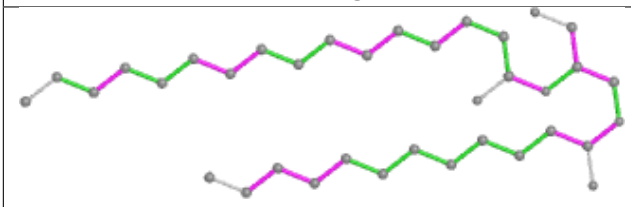
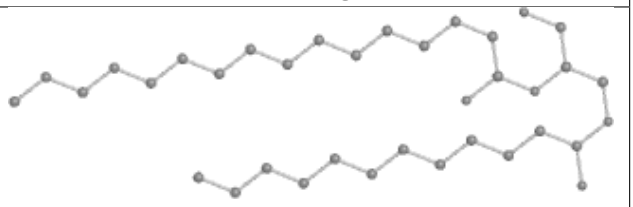


Bond angles

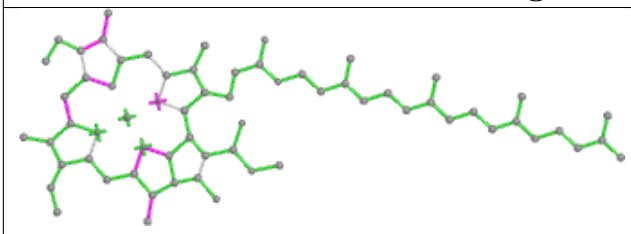


Torsions



Rings

Ligand CLA b 607



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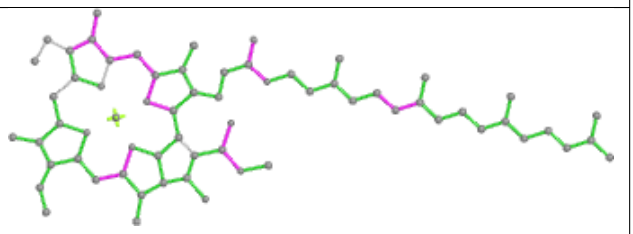
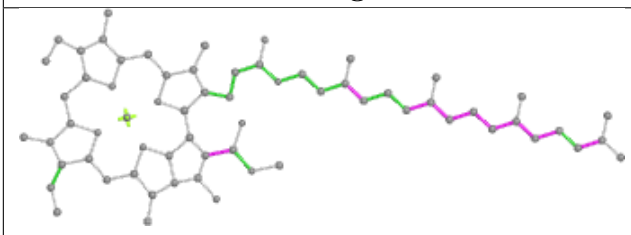


Bond angles



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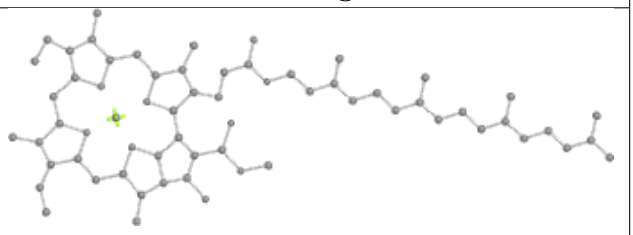
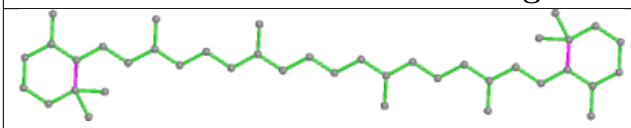
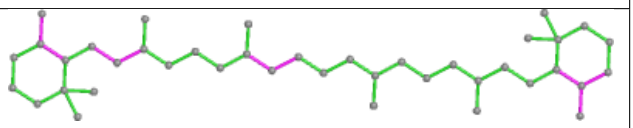


Rings

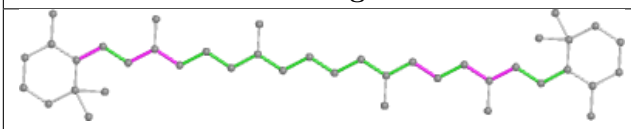
Ligand BCR T 101



Bond lengths



Bond angles



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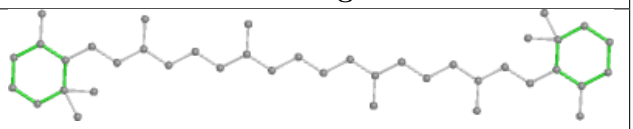
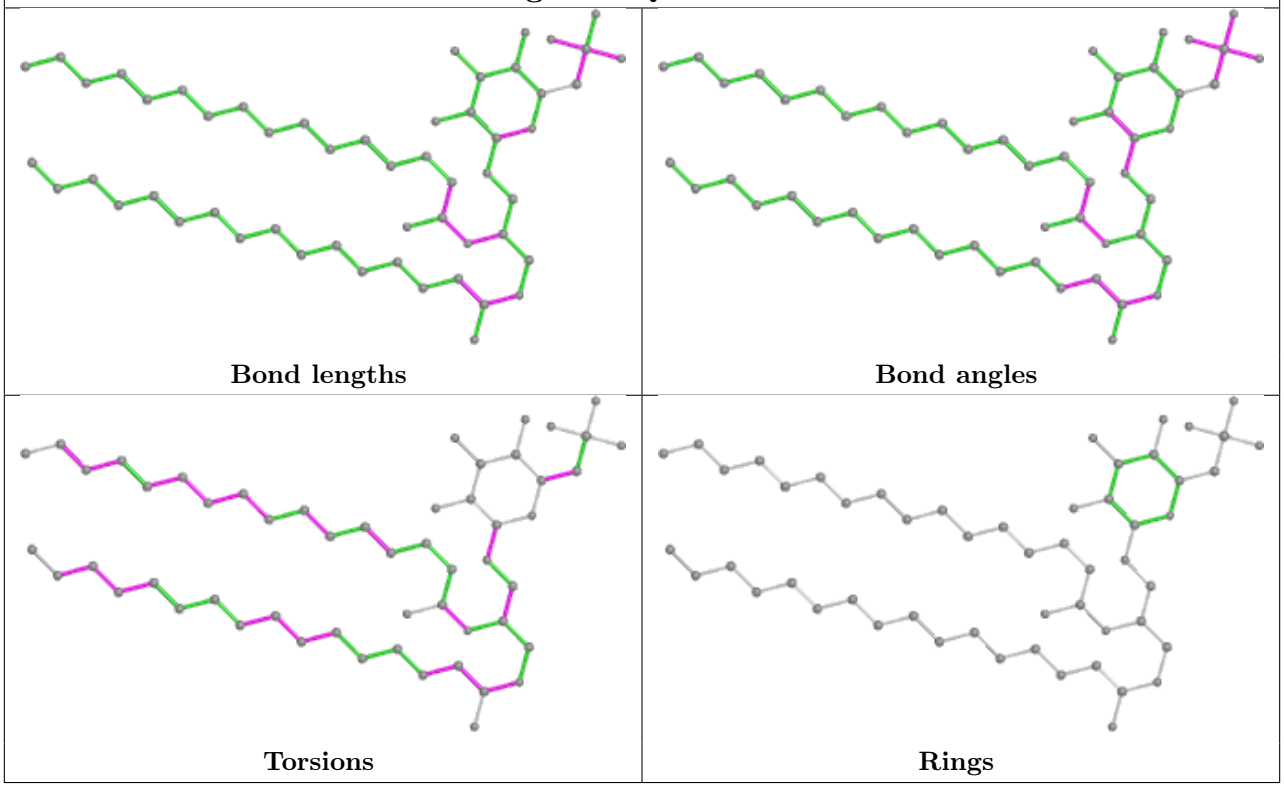
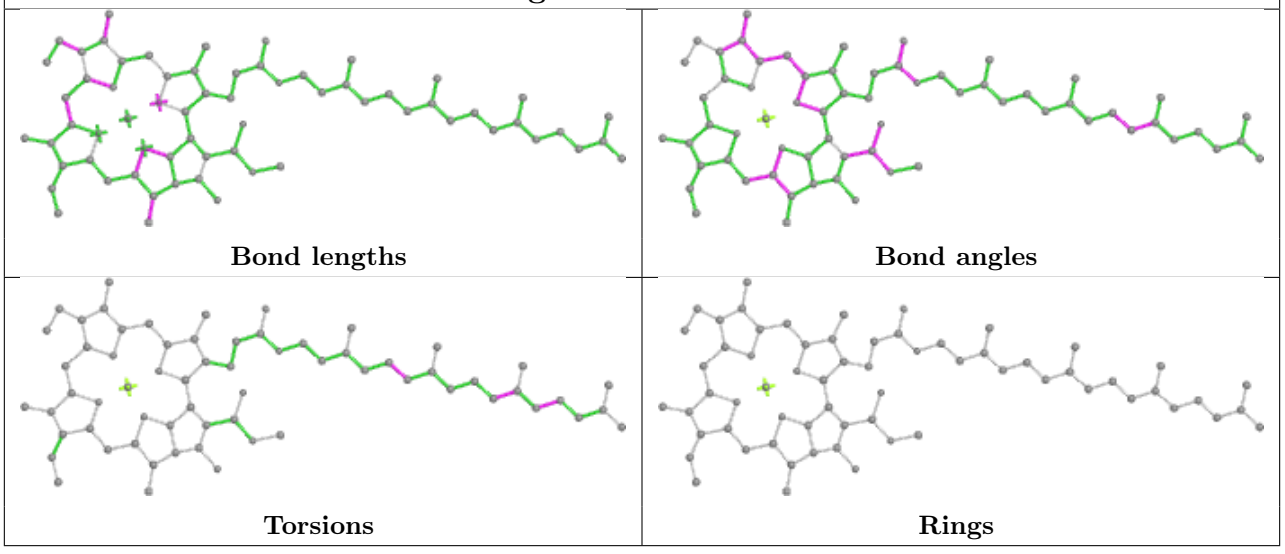


Rings

Ligand SQD B 622



Ligand CLA b 603



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%)	-0.37	4 (1%) 79 82	23, 31, 52, 80	0
1	a	334/344 (97%)	-0.37	1 (0%) 94 94	25, 33, 58, 76	0
2	B	505/510 (99%)	-0.37	7 (1%) 75 78	26, 35, 62, 88	0
2	b	505/510 (99%)	-0.21	13 (2%) 56 61	27, 38, 71, 111	0
3	C	442/461 (95%)	-0.31	6 (1%) 75 78	27, 38, 54, 79	0
3	c	451/461 (97%)	-0.18	11 (2%) 59 64	28, 42, 62, 97	0
4	D	341/352 (96%)	-0.33	2 (0%) 89 91	25, 33, 50, 78	0
4	d	341/352 (96%)	-0.31	0 100 100	27, 36, 60, 81	0
5	E	82/84 (97%)	0.10	5 (6%) 21 26	36, 54, 69, 85	0
5	e	82/84 (97%)	0.17	4 (4%) 29 35	41, 59, 79, 85	0
6	F	34/45 (75%)	-0.33	2 (5%) 22 27	41, 47, 63, 85	0
6	f	34/45 (75%)	-0.23	2 (5%) 22 27	44, 52, 78, 94	0
7	H	65/66 (98%)	-0.14	3 (4%) 32 38	36, 42, 58, 75	0
7	h	63/66 (95%)	0.16	4 (6%) 20 24	41, 50, 61, 64	0
8	I	35/38 (92%)	-0.33	1 (2%) 51 57	34, 40, 67, 83	0
8	i	35/38 (92%)	-0.19	2 (5%) 23 29	33, 42, 72, 80	0
9	J	36/40 (90%)	-0.08	3 (8%) 11 14	36, 51, 78, 88	0
9	j	36/40 (90%)	0.23	5 (13%) 2 3	42, 53, 86, 98	0
10	K	37/46 (80%)	0.18	1 (2%) 54 60	46, 54, 71, 83	0
10	k	37/46 (80%)	-0.05	0 100 100	49, 56, 70, 83	0
11	L	37/37 (100%)	-0.36	0 100 100	27, 32, 63, 68	0
11	l	36/37 (97%)	-0.30	3 (8%) 11 14	28, 33, 66, 88	0
12	M	32/36 (88%)	-0.11	0 100 100	30, 36, 58, 70	0
12	m	31/36 (86%)	-0.25	0 100 100	28, 35, 52, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.08	14 (5%) 23 29	29, 43, 79, 132	0
13	o	244/272 (89%)	-0.09	14 (5%) 23 29	29, 42, 82, 123	0
14	T	29/32 (90%)	-0.32	2 (6%) 16 21	29, 34, 60, 72	0
14	t	29/32 (90%)	-0.24	2 (6%) 16 21	29, 34, 73, 89	0
15	U	97/134 (72%)	-0.32	1 (1%) 82 85	33, 45, 69, 86	0
15	u	97/134 (72%)	-0.43	0 100 100	32, 42, 58, 87	0
16	V	137/163 (84%)	-0.50	0 100 100	32, 42, 55, 80	0
16	v	137/163 (84%)	-0.18	1 (0%) 87 89	35, 48, 67, 85	0
17	Y	27/46 (58%)	1.23	10 (37%) 0 0	55, 72, 92, 96	0
17	y	30/46 (65%)	0.40	4 (13%) 3 4	62, 75, 88, 94	0
18	X	38/41 (92%)	-0.10	2 (5%) 26 32	42, 52, 69, 78	0
18	x	39/41 (95%)	0.24	4 (10%) 6 8	51, 61, 87, 99	0
19	Z	62/62 (100%)	0.95	15 (24%) 0 0	55, 69, 108, 124	0
19	z	62/62 (100%)	0.68	10 (16%) 1 2	61, 71, 112, 117	0
20	R	34/41 (82%)	2.02	15 (44%) 0 0	64, 75, 84, 93	0
20	r	31/41 (75%)	3.97	28 (90%) 0 0	75, 94, 112, 117	0
All	All	5302/5700 (93%)	-0.17	201 (3%) 40 46	23, 40, 74, 132	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	j	6	GLY	7.7
19	Z	33	TRP	7.2
13	o	58	ASN	6.9
20	r	26	TYR	6.8
20	r	28	VAL	6.6
20	r	3	TRP	6.4
20	r	10	LEU	6.4
20	r	29	LYS	6.3
13	O	60	ARG	6.1
20	r	18	TRP	6.0
2	b	495	PHE	5.9
20	R	3	TRP	5.6
20	r	15	ALA	5.6
3	c	23	ALA	5.4
20	r	9	LEU	5.4

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Mol	Chain	Res	Type	RSRZ
13	O	3	GLN	5.4
20	r	14	LEU	5.4
14	t	30	THR	5.4
20	r	24	LEU	5.3
20	R	6	LEU	5.3
17	Y	20	ALA	5.0
13	O	56	PRO	5.0
13	o	3	GLN	4.9
20	r	25	PRO	4.9
14	T	30	THR	4.8
18	X	2	THR	4.8
8	i	36	ASP	4.7
1	A	13	LEU	4.6
13	O	59	LYS	4.6
20	r	6	LEU	4.5
5	e	79	PHE	4.5
19	z	33	TRP	4.5
19	Z	32	ASP	4.3
19	Z	62	VAL	4.3
18	x	2	THR	4.3
20	r	31	VAL	4.2
6	F	12	SER	4.2
13	o	60	ARG	4.1
19	Z	41	PHE	4.1
2	b	506	ARG	4.0
20	R	13	LEU	4.0
13	o	4	THR	4.0
3	c	24	THR	4.0
20	r	2	ASP	4.0
17	Y	25	ILE	3.9
2	b	127	ARG	3.9
17	Y	22	LEU	3.9
19	Z	34	ASP	3.9
13	O	5	LEU	3.8
13	O	4	THR	3.8
19	Z	61	VAL	3.8
19	Z	3	ILE	3.7
13	o	62	GLU	3.7
13	O	62	GLU	3.6
19	z	35	ARG	3.6
9	J	6	GLY	3.6
17	y	40	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	227	GLU	3.6
19	Z	35	ARG	3.5
6	f	12	SER	3.5
20	R	32	GLN	3.5
20	r	13	LEU	3.5
3	c	143	TYR	3.5
13	o	61	GLN	3.4
18	X	3	ILE	3.4
20	R	18	TRP	3.4
20	r	27	ALA	3.4
20	R	24	LEU	3.3
19	z	36	SER	3.3
2	b	505	ARG	3.3
17	Y	43	ARG	3.3
20	r	19	ALA	3.2
20	R	31	VAL	3.2
9	j	7	ARG	3.2
9	j	8	ILE	3.2
20	r	8	VAL	3.2
20	R	21	ARG	3.2
19	Z	31	GLN	3.1
20	R	26	TYR	3.1
19	Z	7	LEU	3.1
2	b	289	GLN	3.1
20	r	7	VAL	3.1
20	R	29	LYS	3.0
13	O	61	GLN	3.0
13	o	63	ALA	3.0
20	r	32	GLN	3.0
20	R	2	ASP	3.0
19	Z	1	MET	2.9
20	r	4	ARG	2.9
5	E	83	LEU	2.9
19	z	62	VAL	2.9
7	h	6	TRP	2.9
13	o	59	LYS	2.9
8	I	36	ASP	2.9
20	r	12	VAL	2.8
18	x	38	GLN	2.8
5	e	61	ARG	2.8
2	B	293	ALA	2.8
19	z	30	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
5	e	82	GLN	2.8
20	r	23	ILE	2.8
20	R	20	VAL	2.8
9	j	5	GLY	2.8
13	o	207	ARG	2.8
20	R	25	PRO	2.8
20	r	11	PRO	2.8
9	J	5	GLY	2.8
11	l	3	PRO	2.7
5	E	17	VAL	2.7
19	Z	60	PHE	2.7
7	H	66	GLY	2.7
2	B	495	PHE	2.7
2	b	487	SER	2.7
20	r	5	VAL	2.7
5	E	3	GLY	2.7
3	C	146	PHE	2.6
13	O	246	ALA	2.6
4	D	12	ARG	2.6
9	J	7	ARG	2.6
2	b	128	THR	2.6
17	Y	37	PHE	2.6
2	B	505	ARG	2.6
5	E	79	PHE	2.6
2	B	490	GLN	2.6
15	U	8	GLU	2.6
2	B	506	ARG	2.5
11	l	2	GLU	2.5
8	i	34	ARG	2.5
19	z	41	PHE	2.5
13	O	63	ALA	2.5
7	H	65	LEU	2.5
20	r	16	ALA	2.5
19	Z	4	LEU	2.4
14	t	29	ILE	2.4
13	o	57	LYS	2.4
3	c	146	PHE	2.4
19	z	60	PHE	2.4
7	H	41	PHE	2.4
3	c	262	ARG	2.4
17	Y	42	ARG	2.4
17	y	19	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	486	LEU	2.3
19	Z	42	LEU	2.3
19	z	7	LEU	2.3
20	R	9	LEU	2.3
7	h	10	ILE	2.3
19	z	3	ILE	2.3
17	Y	21	GLN	2.3
17	y	41	VAL	2.3
1	a	11	ALA	2.3
2	b	85	GLY	2.3
3	c	147	PHE	2.3
13	o	56	PRO	2.3
20	r	22	ASN	2.3
5	e	74	GLN	2.3
13	o	246	ALA	2.3
20	r	21	ARG	2.3
13	o	54	GLU	2.3
16	v	17	LYS	2.3
3	c	25	ASN	2.3
2	b	485	GLU	2.3
10	K	17	ILE	2.3
6	f	16	PHE	2.2
13	O	132	ASN	2.2
5	E	84	LYS	2.2
18	x	40	SER	2.2
17	Y	40	ALA	2.2
2	b	374	ASN	2.2
2	B	487	SER	2.2
13	O	35	SER	2.2
3	C	143	TYR	2.2
1	A	12	ASN	2.2
17	Y	41	VAL	2.2
17	Y	45	ASN	2.2
2	b	161	LEU	2.1
3	C	61	VAL	2.1
3	C	57	ALA	2.1
18	x	3	ILE	2.1
3	c	142	GLU	2.1
3	C	60	ILE	2.1
14	T	29	ILE	2.1
11	l	7	ARG	2.1
13	o	5	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
7	h	21	VAL	2.1
7	h	56	ASP	2.1
3	C	126	GLY	2.1
19	z	4	LEU	2.1
3	c	191	PRO	2.1
2	B	127	ARG	2.1
9	j	11	TRP	2.1
2	b	126	PRO	2.0
13	O	54	GLU	2.0
19	Z	37	LYS	2.0
1	A	15	GLU	2.0
20	R	28	VAL	2.0
17	y	37	PHE	2.0
3	c	152	LYS	2.0
6	F	13	TYR	2.0
13	O	55	GLU	2.0
1	A	11	ALA	2.0
3	c	55	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.92	0.10	33,40,56,70	0
14	FME	T	1	10/11	0.94	0.11	29,41,54,64	0
8	FME	I	1	10/11	0.94	0.16	38,46,49,50	0
12	FME	m	1	10/11	0.95	0.14	30,46,64,66	0
12	FME	M	1	10/11	0.95	0.13	39,47,62,64	0
8	FME	i	1	10/11	0.96	0.18	36,49,53,53	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	STE	H	103	18/20	0.66	0.27	47,63,69,73	0
33	STE	c	521	20/20	0.69	0.20	42,54,83,83	0
33	STE	b	622	20/20	0.71	0.20	47,58,69,70	0
32	DGD	a	615	44/66	0.73	0.18	36,51,70,72	0
33	STE	a	616	10/20	0.74	0.20	37,55,60,62	0
33	STE	B	626	16/20	0.74	0.28	42,59,71,72	0
29	LMG	D	411	33/55	0.74	0.20	41,52,69,74	0
33	STE	B	620	17/20	0.76	0.18	38,47,64,66	0
33	STE	E	102	12/20	0.76	0.32	60,67,83,84	0
30	SQD	a	614	36/54	0.78	0.18	35,55,66,72	0
31	LHG	A	614	49/49	0.78	0.24	54,76,98,103	0
28	PL9	A	611	55/55	0.79	0.29	42,61,74,85	0
33	STE	c	523	12/20	0.79	0.20	54,62,72,77	0
29	LMG	b	621	55/55	0.80	0.26	53,65,77,85	0
33	STE	C	521	16/20	0.80	0.15	37,49,64,65	0
33	STE	d	412	16/20	0.80	0.18	48,54,75,77	0
29	LMG	d	410	23/55	0.81	0.21	41,59,69,72	0
33	STE	a	617	12/20	0.81	0.21	52,58,64,66	0
33	STE	D	413	20/20	0.82	0.17	37,46,70,81	0
33	STE	b	620	20/20	0.82	0.20	38,52,71,73	0
33	STE	B	624	18/20	0.82	0.14	40,49,78,85	0
29	LMG	c	522	48/55	0.82	0.23	45,69,89,93	0
33	STE	T	102	16/20	0.82	0.17	36,47,61,66	0
28	PL9	a	611	55/55	0.82	0.24	43,64,79,85	0
27	BCR	x	101	40/40	0.83	0.14	42,54,65,71	0
29	LMG	A	612	48/55	0.83	0.17	45,57,68,75	0
31	LHG	e	101	42/49	0.83	0.23	57,77,97,102	0
32	DGD	A	617	66/66	0.83	0.18	45,57,67,74	0
33	STE	j	101	12/20	0.83	0.12	49,55,61,67	0
27	BCR	H	101	40/40	0.84	0.14	35,43,50,55	0
30	SQD	A	616	39/54	0.84	0.18	39,49,72,77	0
33	STE	I	101	15/20	0.84	0.14	39,48,61,65	0
33	STE	l	102	18/20	0.84	0.19	36,44,63,66	0
33	STE	m	102	12/20	0.84	0.20	50,56,67,69	0
33	STE	x	102	20/20	0.84	0.20	45,53,60,64	0
25	CLA	b	601	65/65	0.85	0.17	49,64,78,89	0
29	LMG	c	524	49/55	0.85	0.16	40,56,68,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	SQD	B	622	54/54	0.85	0.17	40,57,82,93	0
33	STE	d	413	17/20	0.85	0.17	46,51,62,65	0
33	STE	C	519	12/20	0.86	0.12	34,42,52,53	0
33	STE	T	103	15/20	0.86	0.16	44,53,64,66	0
29	LMG	M	101	51/55	0.86	0.13	31,46,62,65	0
33	STE	b	623	10/20	0.86	0.20	43,50,62,63	0
30	SQD	L	101	49/54	0.87	0.14	37,55,73,77	0
25	CLA	C	512	65/65	0.87	0.16	35,51,68,77	0
33	STE	B	623	12/20	0.88	0.13	41,51,60,68	0
33	STE	J	101	12/20	0.88	0.14	46,54,61,64	0
33	STE	M	103	10/20	0.88	0.18	41,44,50,50	0
30	SQD	f	102	41/54	0.88	0.18	63,78,89,92	0
25	CLA	c	512	65/65	0.88	0.15	45,53,76,81	0
29	LMG	B	621	28/55	0.88	0.15	38,48,58,70	0
25	CLA	C	513	65/65	0.89	0.17	44,56,83,89	0
33	STE	M	102	15/20	0.89	0.14	37,46,62,67	0
25	CLA	c	513	65/65	0.89	0.17	47,61,81,86	0
27	BCR	D	406	40/40	0.89	0.12	34,41,66,70	0
25	CLA	B	601	65/65	0.89	0.14	37,53,75,87	0
29	LMG	m	101	51/55	0.89	0.12	34,49,64,70	0
27	BCR	c	516	40/40	0.89	0.17	45,53,58,66	0
27	BCR	d	405	40/40	0.89	0.13	39,49,78,87	0
27	BCR	k	101	40/40	0.89	0.11	47,57,64,68	0
33	STE	C	520	12/20	0.90	0.13	43,49,57,58	0
27	BCR	Y	101	40/40	0.90	0.12	46,52,61,64	0
29	LMG	C	518	48/55	0.90	0.14	45,63,73,78	0
33	STE	B	625	12/20	0.90	0.38	44,59,64,67	0
29	LMG	D	408	51/55	0.90	0.16	33,47,64,71	0
27	BCR	K	101	40/40	0.90	0.13	49,56,60,61	0
29	LMG	c	520	37/55	0.91	0.17	45,64,74,77	0
33	STE	t	102	14/20	0.91	0.11	36,49,54,61	0
27	BCR	c	514	40/40	0.91	0.14	44,55,64,66	0
25	CLA	c	503	65/65	0.92	0.15	33,44,49,53	0
27	BCR	K	102	40/40	0.92	0.16	39,49,63,65	0
25	CLA	c	508	64/65	0.92	0.13	32,43,73,90	0
30	SQD	F	101	36/54	0.92	0.16	49,66,74,77	0
25	CLA	D	405	65/65	0.92	0.13	28,36,81,92	0
25	CLA	C	503	65/65	0.92	0.13	33,42,47,53	0
25	CLA	d	404	65/65	0.92	0.13	32,41,75,81	0
27	BCR	B	619	40/40	0.92	0.09	32,40,46,49	0
27	BCR	C	514	40/40	0.92	0.11	32,39,47,47	0
25	CLA	b	616	60/65	0.92	0.12	32,40,70,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	DGD	H	102	62/66	0.92	0.12	34,42,49,53	0
28	PL9	D	407	55/55	0.92	0.11	23,32,38,45	0
32	DGD	c	518	62/66	0.92	0.12	37,48,74,80	0
32	DGD	h	101	62/66	0.92	0.12	38,45,53,53	0
25	CLA	c	502	65/65	0.92	0.12	32,41,53,60	0
25	CLA	C	511	65/65	0.93	0.11	36,48,57,65	0
25	CLA	B	616	60/65	0.93	0.14	26,36,74,85	0
25	CLA	C	502	65/65	0.93	0.12	32,39,48,53	0
30	SQD	a	613	54/54	0.93	0.13	40,57,71,73	0
25	CLA	c	509	65/65	0.93	0.16	38,45,55,58	0
27	BCR	b	619	40/40	0.93	0.09	33,42,57,60	0
25	CLA	c	510	65/65	0.93	0.14	37,47,53,61	0
25	CLA	B	606	65/65	0.93	0.12	26,36,57,62	0
25	CLA	a	609	65/65	0.93	0.12	23,30,63,67	0
32	DGD	C	516	62/66	0.93	0.12	38,47,83,95	0
25	CLA	C	506	65/65	0.93	0.11	29,42,72,76	0
27	BCR	B	618	40/40	0.93	0.11	29,36,47,50	0
25	CLA	b	614	65/65	0.93	0.13	25,37,60,65	0
25	CLA	b	615	65/65	0.93	0.13	29,40,50,51	0
25	CLA	C	507	65/65	0.93	0.12	28,36,48,51	0
30	SQD	A	613	52/54	0.94	0.13	32,53,75,79	0
27	BCR	c	515	40/40	0.94	0.11	34,41,48,55	0
25	CLA	B	614	65/65	0.94	0.15	27,35,61,74	0
25	CLA	c	511	65/65	0.94	0.11	40,52,61,64	0
25	CLA	b	604	65/65	0.94	0.12	25,33,63,76	0
27	BCR	t	101	40/40	0.94	0.10	28,36,46,47	0
25	CLA	b	605	65/65	0.94	0.11	22,35,43,46	0
25	CLA	b	609	65/65	0.94	0.13	33,41,55,63	0
27	BCR	A	610	40/40	0.94	0.09	27,34,40,43	0
27	BCR	B	617	40/40	0.94	0.12	32,38,49,50	0
25	CLA	B	615	65/65	0.94	0.10	29,36,53,63	0
32	DGD	C	515	62/66	0.94	0.13	27,37,65,71	0
25	CLA	C	508	65/65	0.94	0.11	30,39,82,89	0
32	DGD	C	517	62/66	0.94	0.11	34,43,66,71	0
25	CLA	A	607	65/65	0.94	0.12	26,32,83,88	0
25	CLA	C	501	65/65	0.94	0.11	25,33,44,48	0
25	CLA	B	604	65/65	0.94	0.11	23,31,58,61	0
32	DGD	c	519	62/66	0.94	0.13	32,45,68,76	0
25	CLA	c	505	65/65	0.94	0.14	29,39,54,58	0
25	CLA	c	506	65/65	0.94	0.10	36,44,74,78	0
27	BCR	T	101	40/40	0.94	0.09	31,37,49,53	0
25	CLA	c	507	65/65	0.94	0.12	30,40,50,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	BCR	b	618	40/40	0.94	0.10	28,38,48,53	0
25	CLA	A	609	54/65	0.94	0.10	21,28,58,62	0
25	CLA	C	505	65/65	0.94	0.13	27,36,59,61	0
32	DGD	c	517	62/66	0.95	0.10	29,38,60,66	0
28	PL9	d	406	55/55	0.95	0.11	27,33,37,41	0
25	CLA	d	403	65/65	0.95	0.10	25,33,46,55	0
25	CLA	C	504	59/65	0.95	0.11	32,39,66,71	0
26	PHO	d	401	64/64	0.95	0.12	24,31,36,38	0
25	CLA	B	610	65/65	0.95	0.13	23,30,38,41	0
25	CLA	b	606	65/65	0.95	0.09	28,38,58,64	0
25	CLA	b	608	65/65	0.95	0.12	33,41,51,53	0
25	CLA	B	611	65/65	0.95	0.13	22,29,41,46	0
25	CLA	b	610	65/65	0.95	0.16	29,37,42,46	0
25	CLA	b	611	65/65	0.95	0.12	26,33,46,53	0
25	CLA	b	613	65/65	0.95	0.13	23,31,61,67	0
25	CLA	B	612	65/65	0.95	0.14	24,31,39,44	0
29	LMG	d	411	44/55	0.95	0.11	39,45,71,76	0
25	CLA	B	613	65/65	0.95	0.12	22,30,55,60	0
25	CLA	C	509	65/65	0.95	0.15	31,39,52,58	0
25	CLA	c	501	65/65	0.95	0.12	30,38,45,50	0
27	BCR	a	610	40/40	0.95	0.07	24,31,40,44	0
27	BCR	b	617	40/40	0.95	0.10	30,38,43,43	0
25	CLA	C	510	65/65	0.95	0.12	32,42,51,54	0
25	CLA	B	603	65/65	0.95	0.14	24,31,49,53	0
25	CLA	c	504	60/65	0.95	0.09	35,42,72,73	0
25	CLA	A	606	65/65	0.95	0.09	22,27,37,43	0
25	CLA	B	605	65/65	0.95	0.13	23,31,40,42	0
31	LHG	D	412	49/49	0.95	0.12	30,40,54,58	0
31	LHG	d	407	49/49	0.95	0.12	32,46,58,65	0
31	LHG	d	408	49/49	0.95	0.11	30,40,47,57	0
25	CLA	B	602	65/65	0.95	0.13	29,37,48,53	0
31	LHG	l	101	49/49	0.95	0.11	31,42,48,53	0
25	CLA	a	608	65/65	0.95	0.12	31,38,79,85	0
25	CLA	B	607	65/65	0.95	0.10	20,29,52,58	0
25	CLA	a	612	65/65	0.95	0.10	22,30,36,42	0
25	CLA	B	609	65/65	0.95	0.12	28,37,43,48	0
25	CLA	b	602	65/65	0.95	0.13	30,39,51,55	0
25	CLA	b	603	65/65	0.95	0.12	25,33,55,62	0
25	CLA	a	607	65/65	0.96	0.09	23,30,38,50	0
25	CLA	D	403	65/65	0.96	0.08	21,27,38,44	0
31	LHG	A	615	49/49	0.96	0.12	30,37,47,57	0
31	LHG	D	409	49/49	0.96	0.10	27,36,44,52	0

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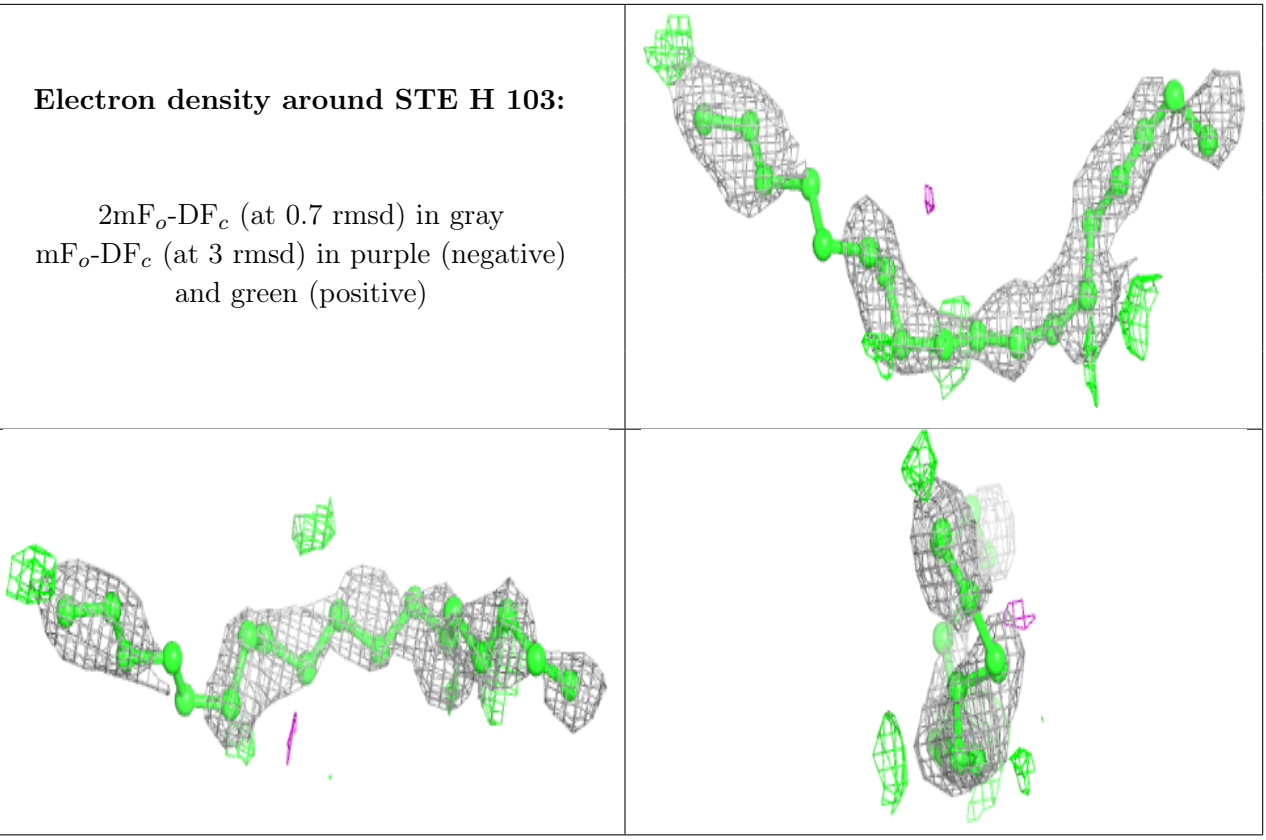
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LHG	D	410	47/49	0.96	0.10	28,39,66,77	0
25	CLA	b	612	65/65	0.96	0.15	27,33,43,51	0
25	CLA	b	607	65/65	0.96	0.11	22,32,50,58	0
26	PHO	A	608	64/64	0.96	0.09	20,28,33,39	0
31	LHG	d	409	39/49	0.96	0.10	32,43,54,58	0
26	PHO	D	402	64/64	0.96	0.13	25,32,38,42	0
25	CLA	D	404	65/65	0.96	0.10	21,29,45,48	0
26	PHO	d	402	64/64	0.96	0.09	29,38,43,49	0
25	CLA	B	608	65/65	0.96	0.10	24,31,45,50	0
34	BCT	a	606	4/4	0.96	0.13	34,40,44,49	0
35	HEM	E	101	43/43	0.96	0.11	44,50,62,68	0
35	HEM	f	101	43/43	0.96	0.12	47,59,75,85	0
34	BCT	D	401	4/4	0.97	0.16	34,39,39,40	0
36	HEC	V	201	43/43	0.97	0.11	27,34,41,45	0
36	HEC	v	201	43/43	0.97	0.12	31,38,43,50	0
22	OEX	a	602[A]	10/10	0.98	0.09	29,32,36,37	10
23	FE2	a	603	1/1	0.98	0.04	38,38,38,38	0
21	OEY	A	601[B]	11/11	0.98	0.12	26,29,33,34	11
21	OEY	a	601[B]	11/11	0.98	0.09	27,30,33,38	11
22	OEX	A	602[A]	10/10	0.98	0.12	31,32,36,38	10
24	CL	a	604	1/1	0.99	0.04	32,32,32,32	0
24	CL	a	605	1/1	0.99	0.05	33,33,33,33	0
24	CL	A	604	1/1	0.99	0.03	33,33,33,33	0
24	CL	A	605	1/1	0.99	0.05	34,34,34,34	0
23	FE2	A	603	1/1	1.00	0.07	32,32,32,32	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.

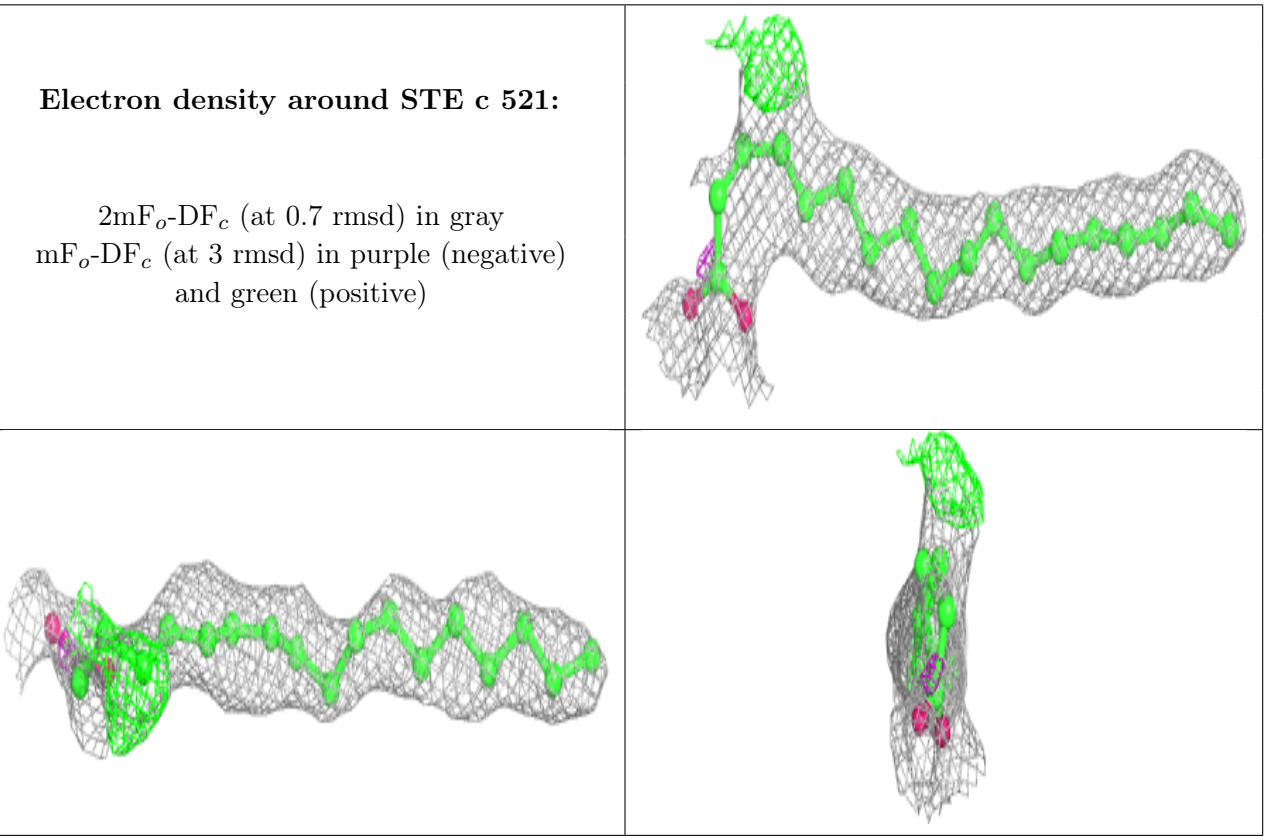
Electron density around STE H 103:

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



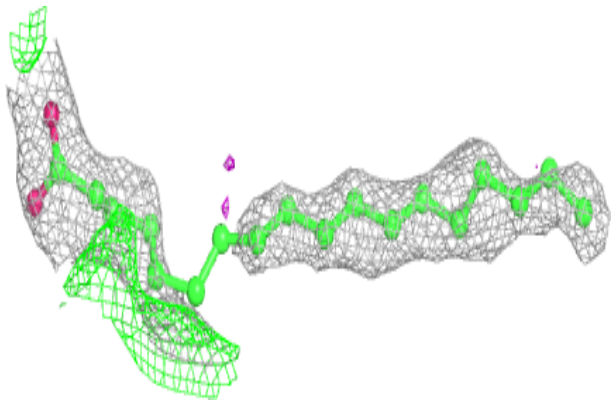
Electron density around STE c 521:

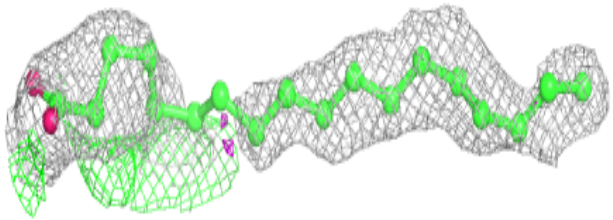
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

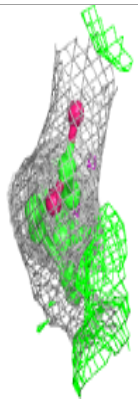


Electron density around STE b 622:

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

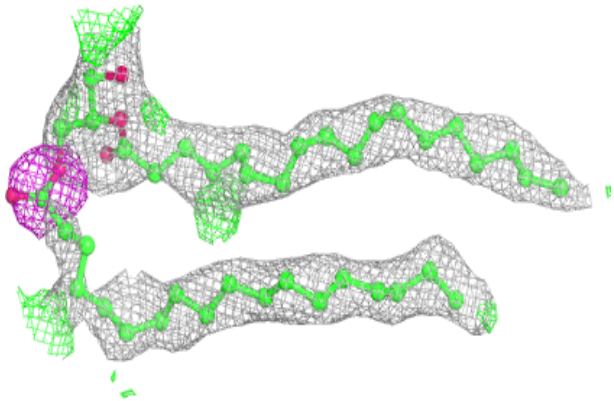


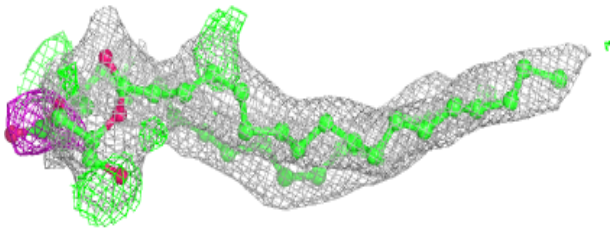


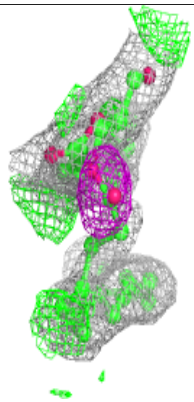


Electron density around DGD a 615:

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

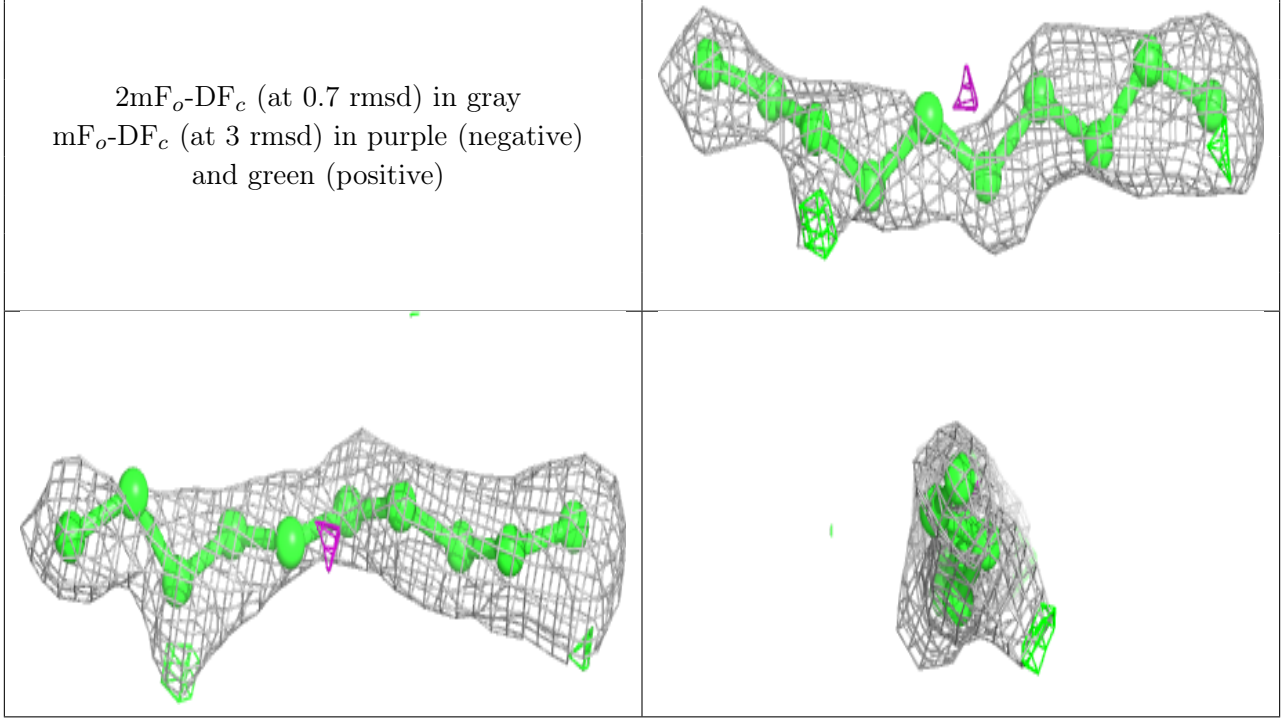






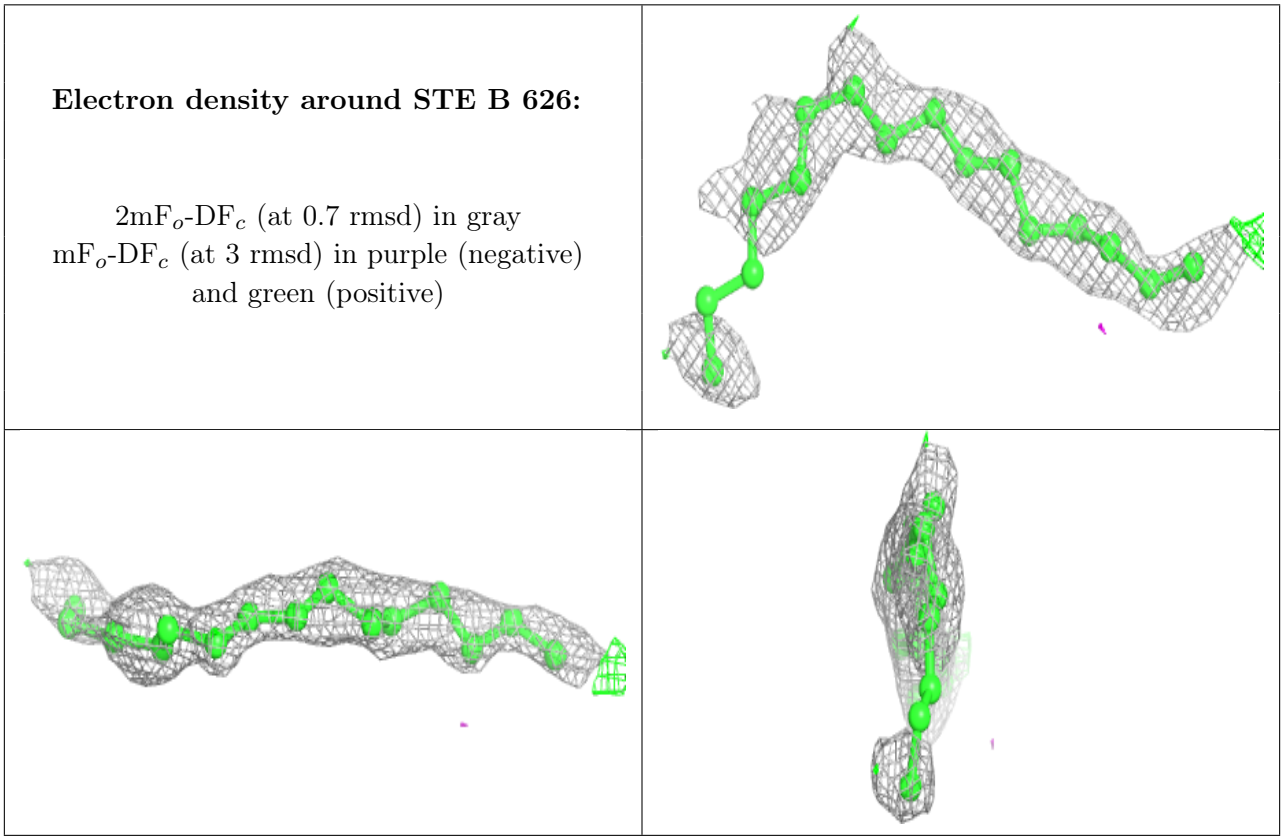
Electron density around STE a 616:

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



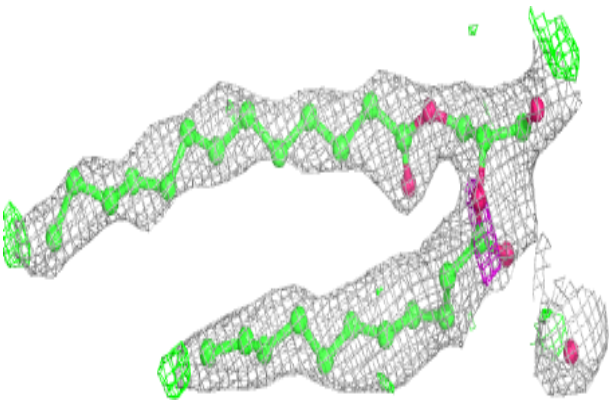
Electron density around STE B 626:

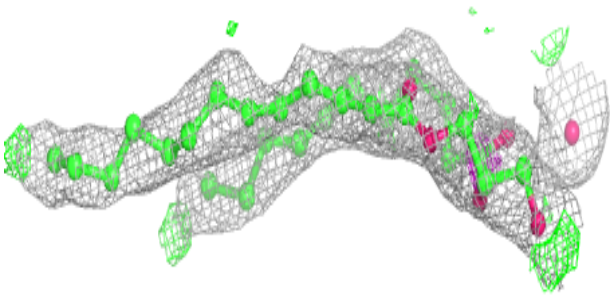
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

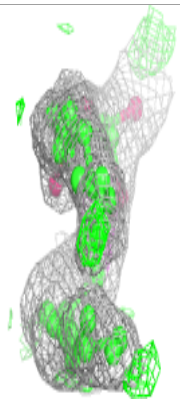


Electron density around LMG D 411:

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

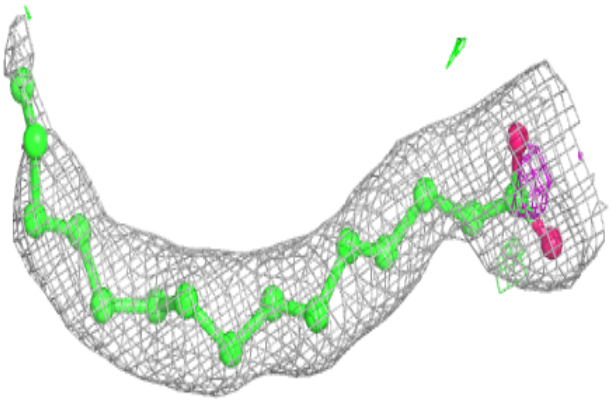


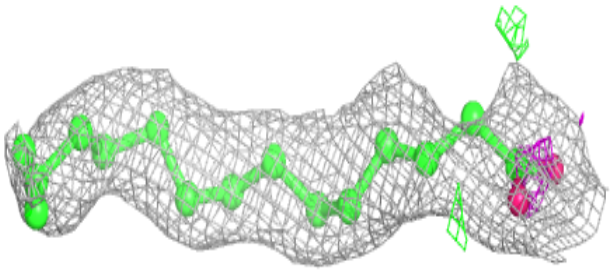


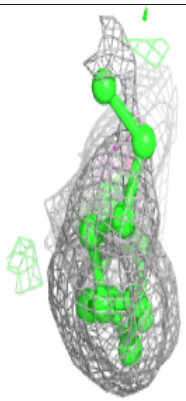


Electron density around STE B 620:

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

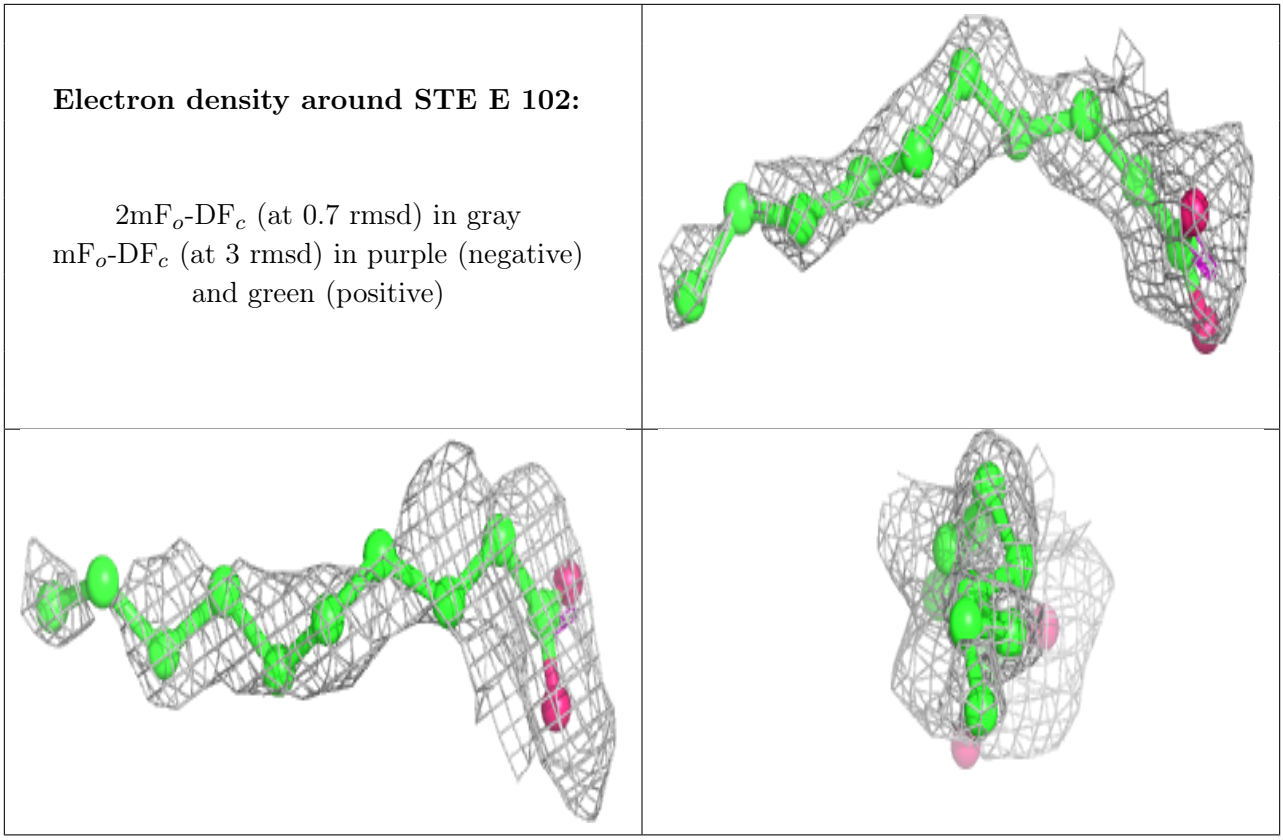






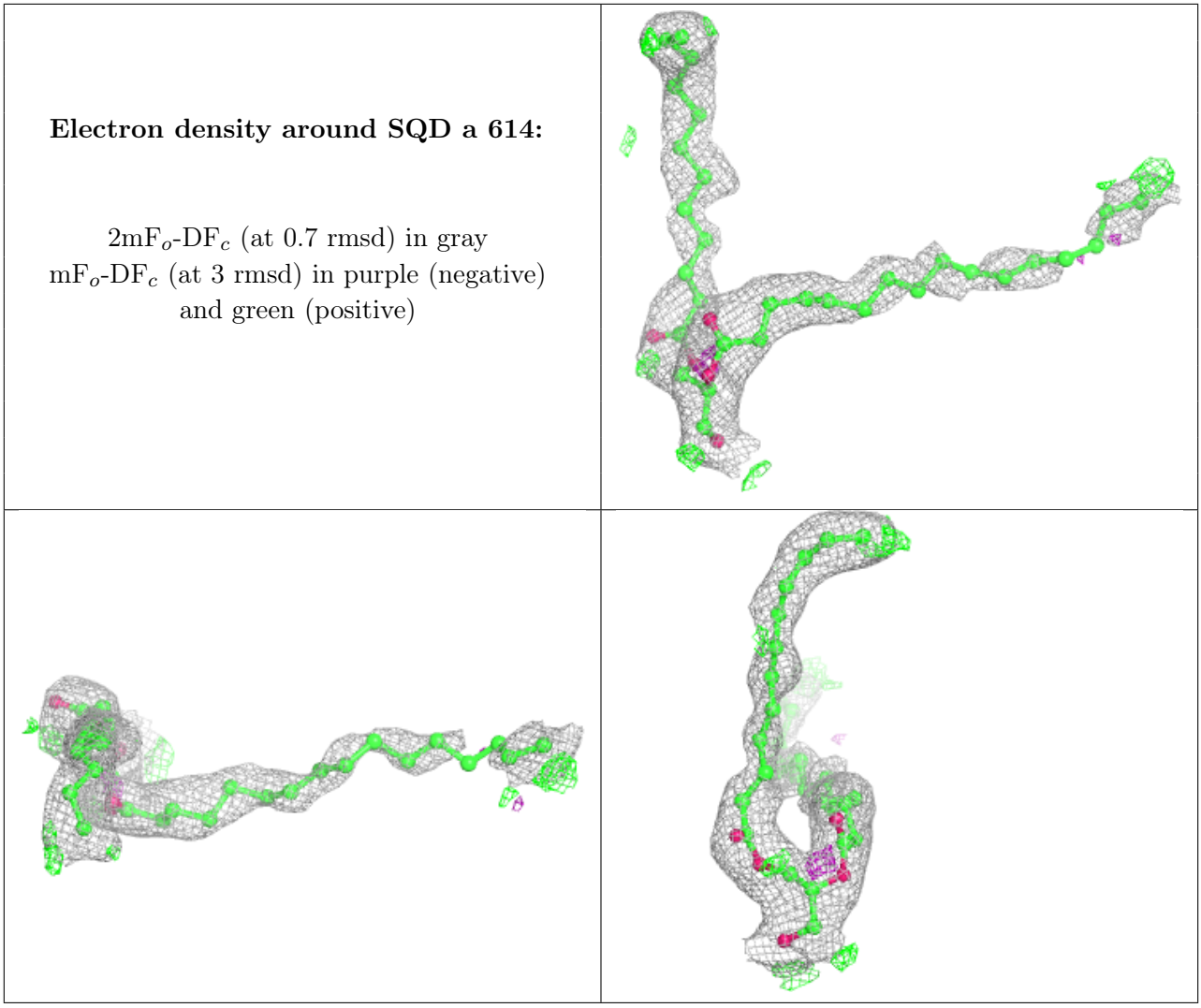
Electron density around STE E 102:

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



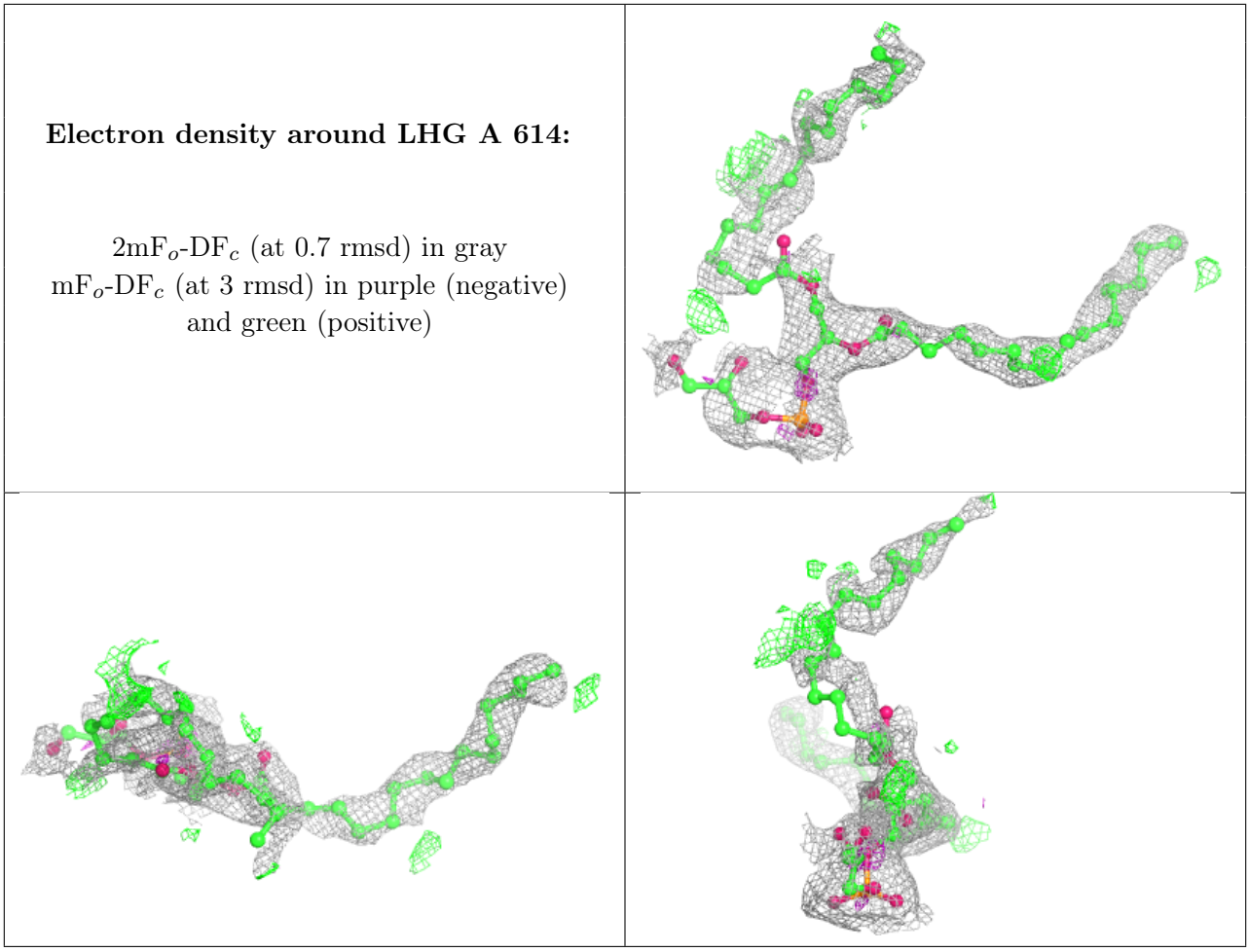
Electron density around SQD a 614:

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



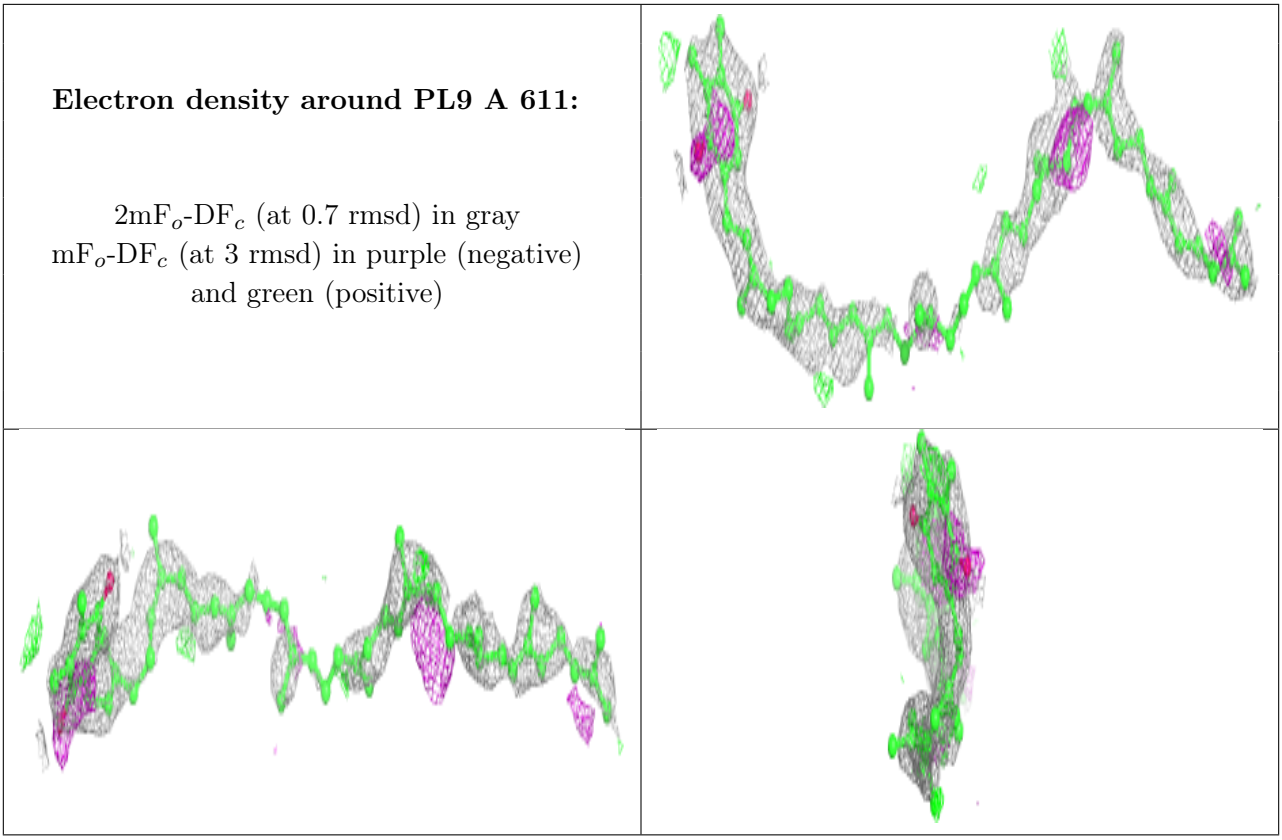
Electron density around LHG A 614:

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



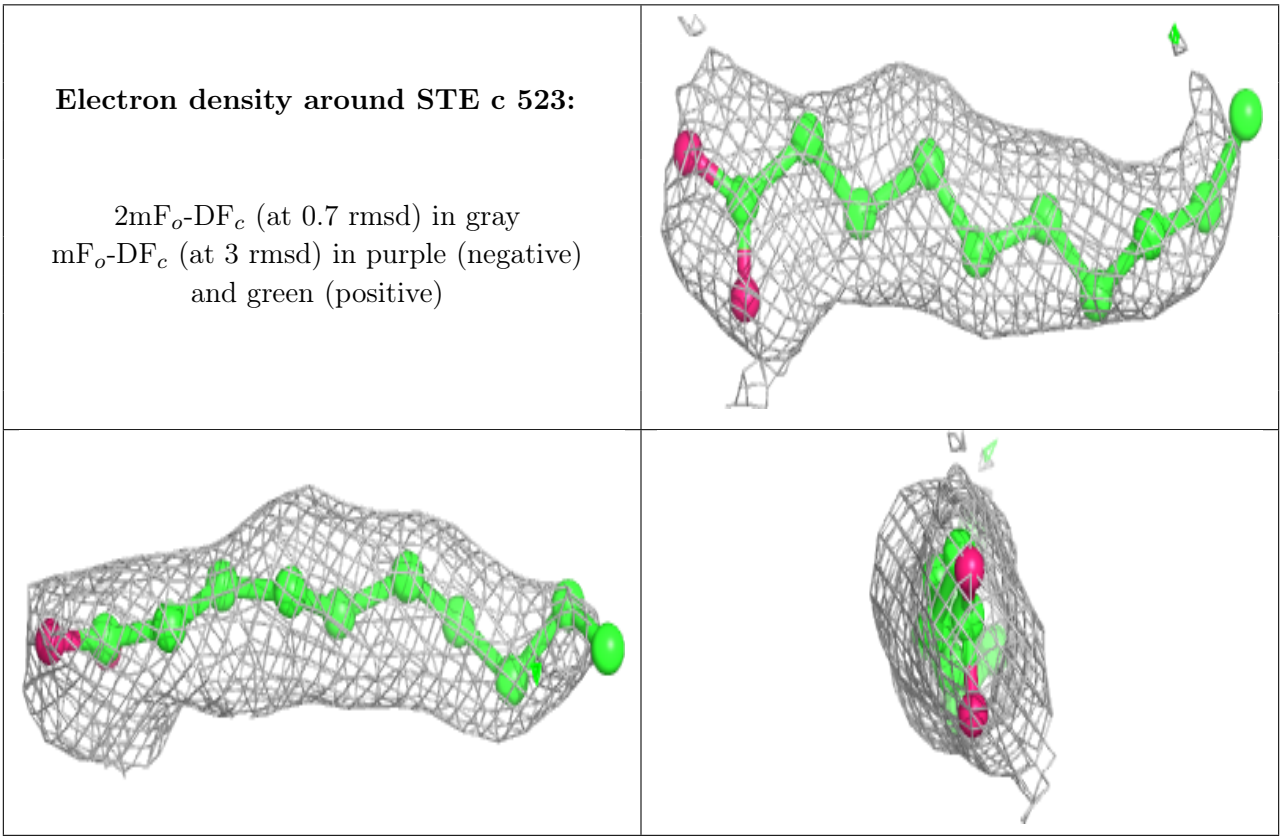
Electron density around PL9 A 611:

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



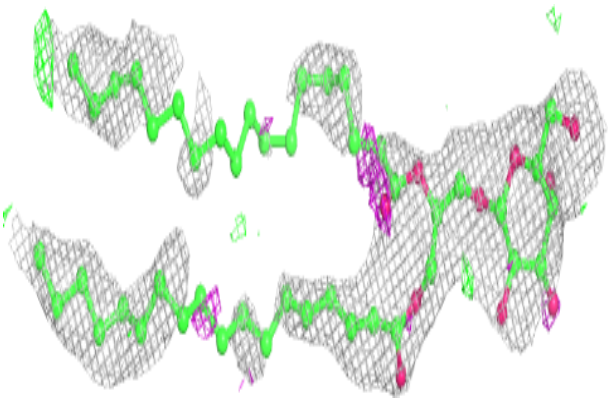
Electron density around STE c 523:

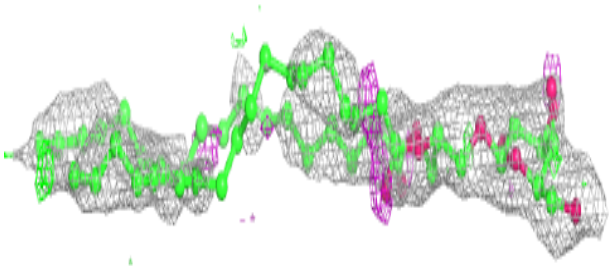
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

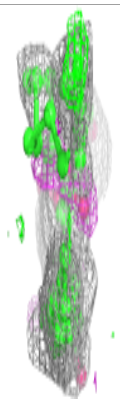


Electron density around LMG b 621:

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

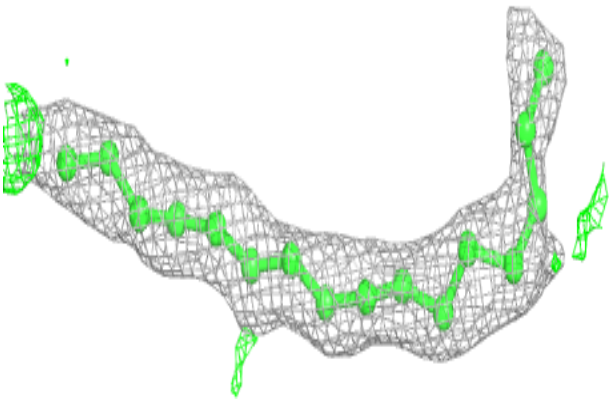


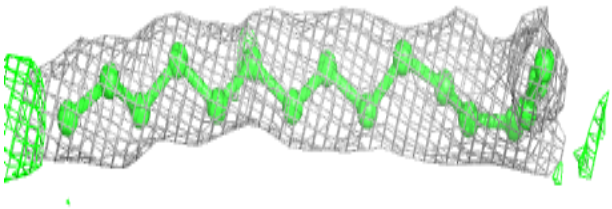


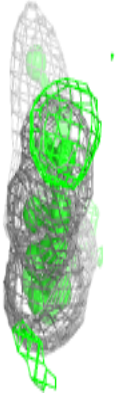


Electron density around STE C 521:

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

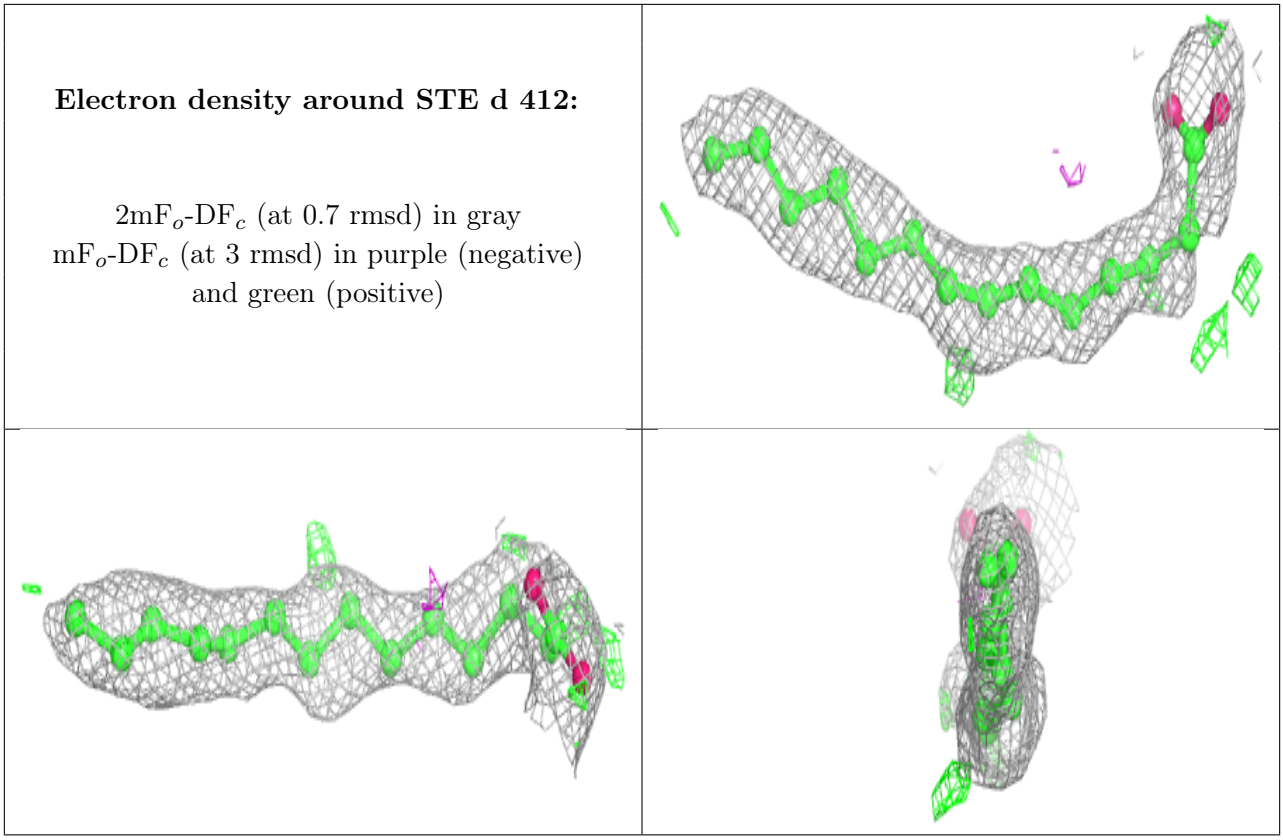






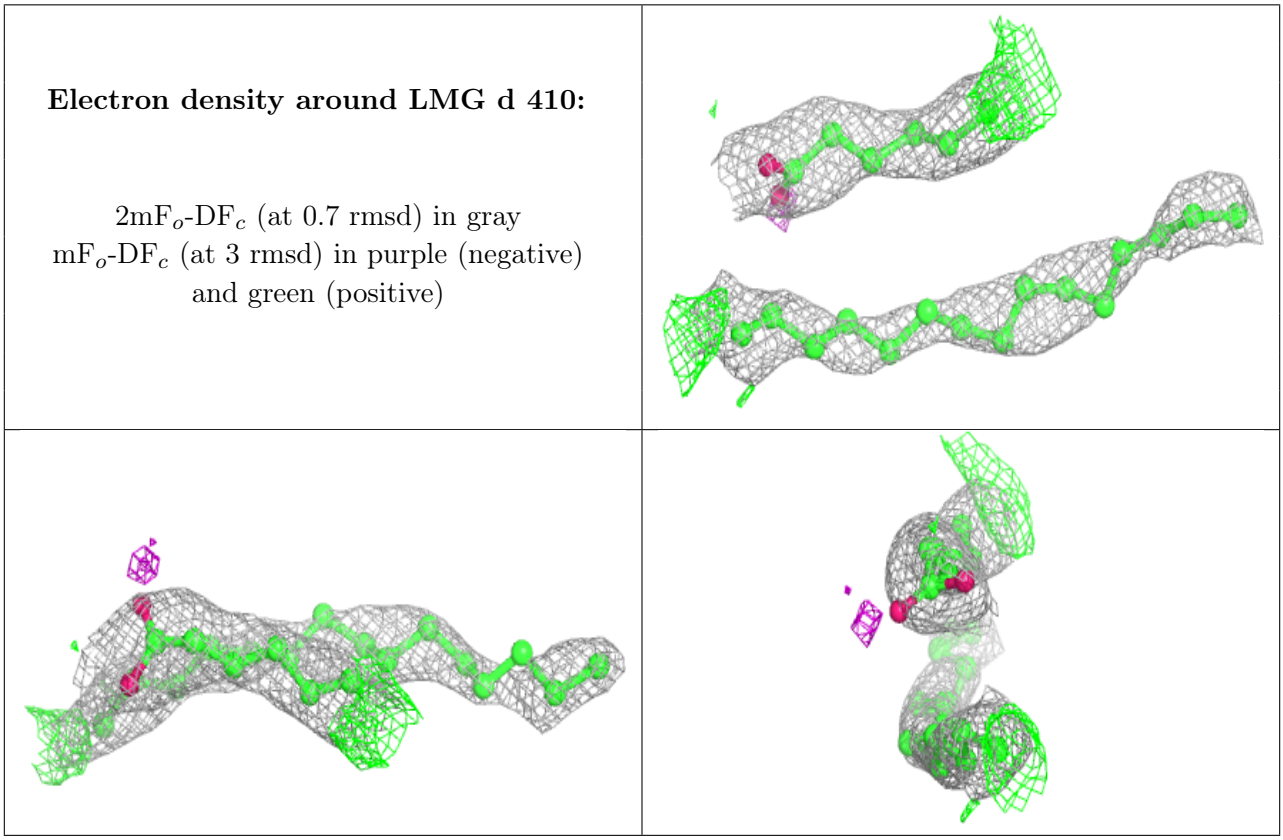
Electron density around STE d 412:

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



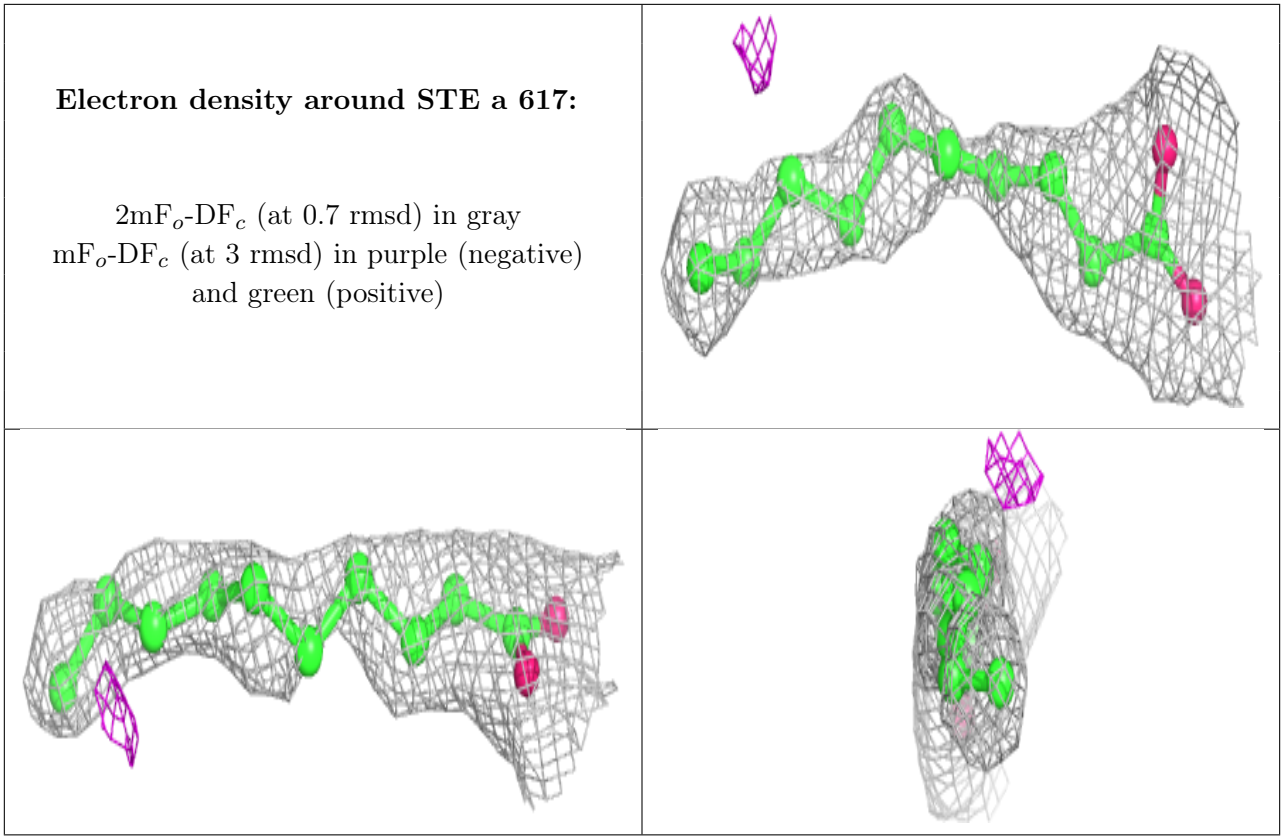
Electron density around LMG d 410:

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



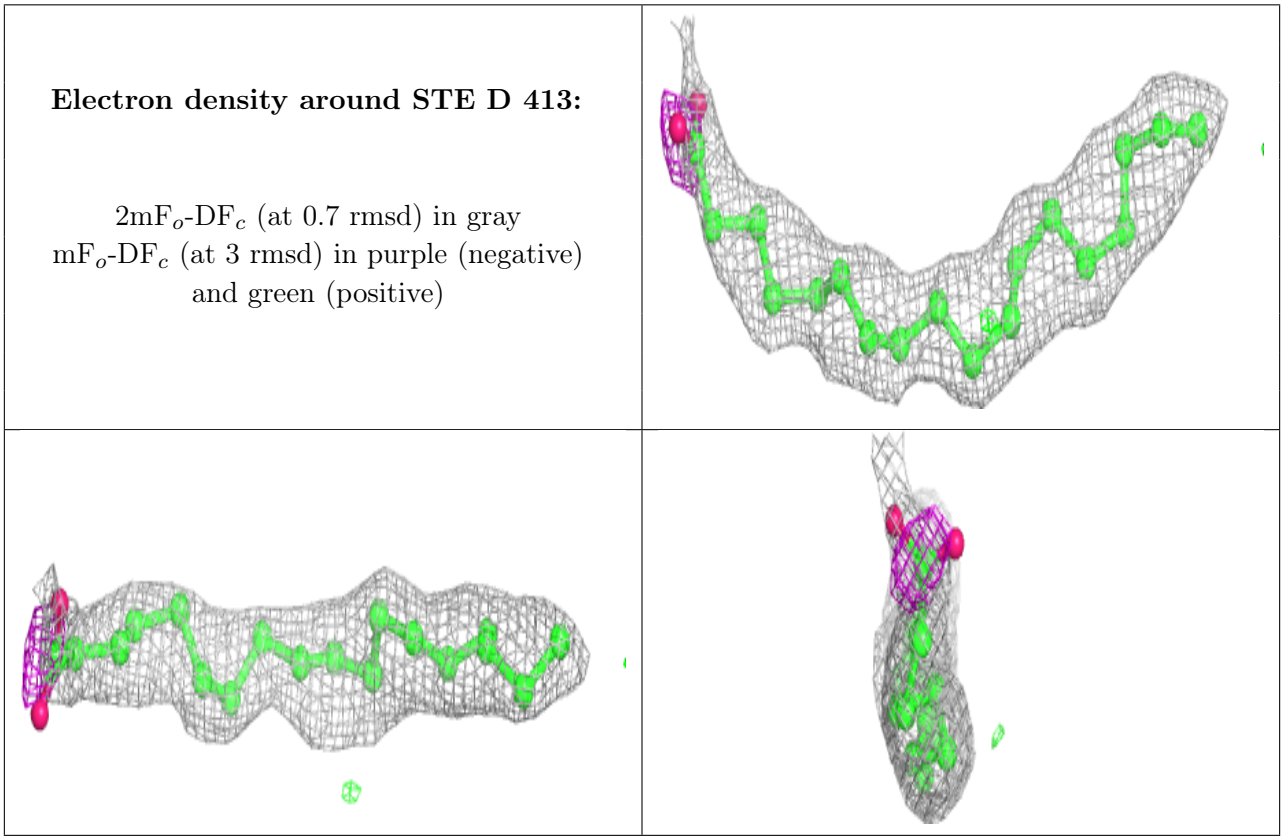
Electron density around STE a 617:

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



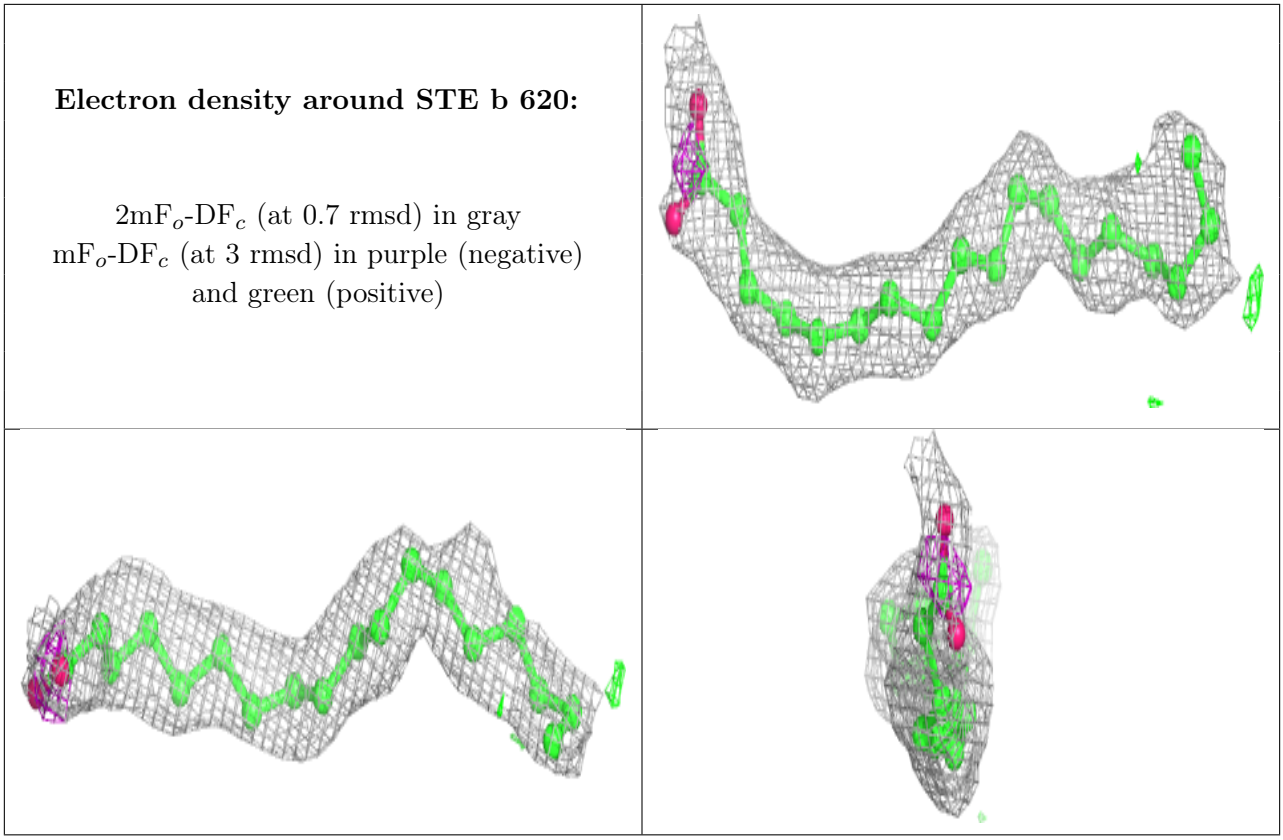
Electron density around STE D 413:

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



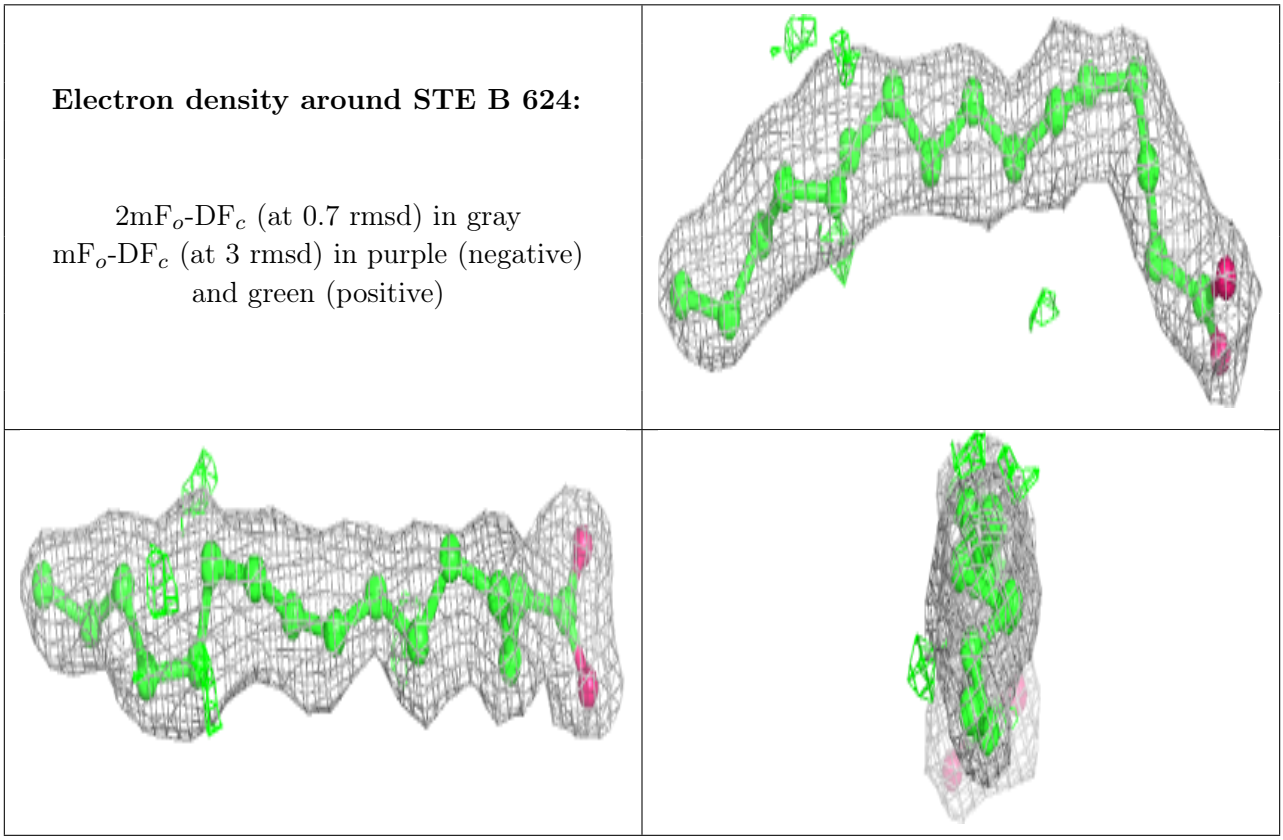
Electron density around STE b 620:

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



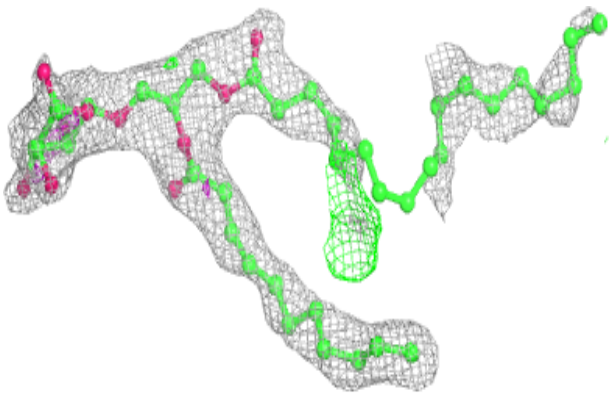
Electron density around STE B 624:

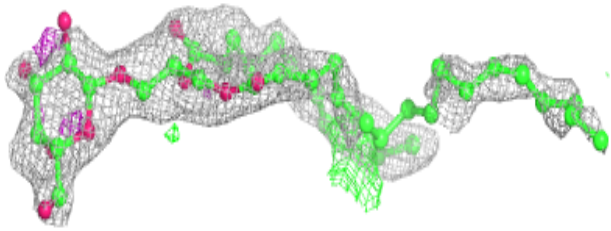
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

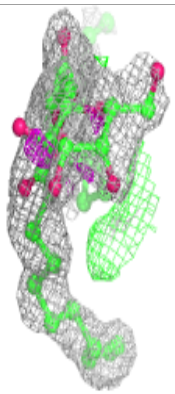


Electron density around LMG c 522:

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

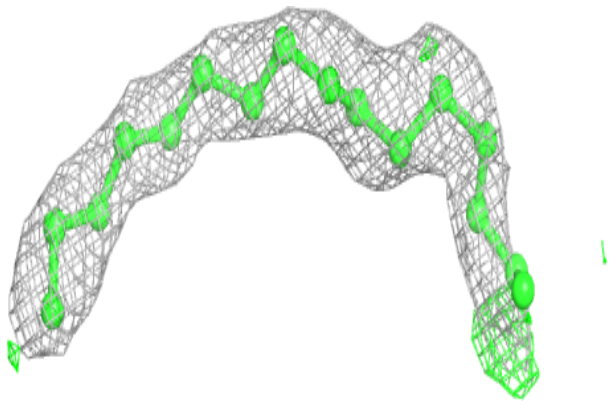


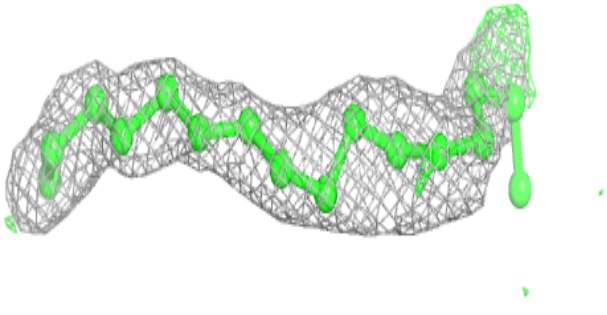


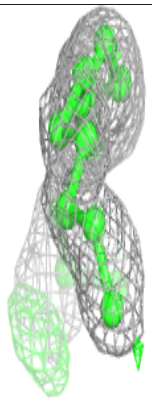


Electron density around STE T 102:

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

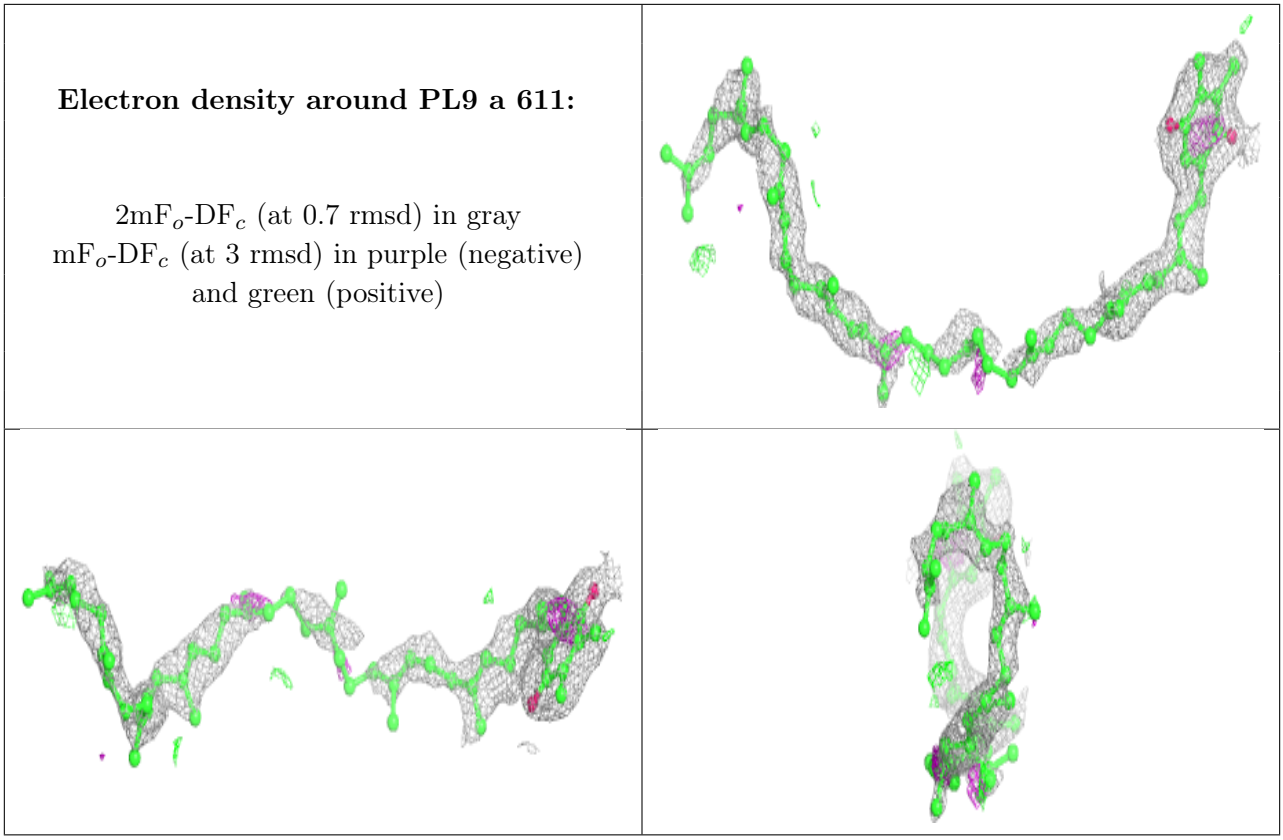






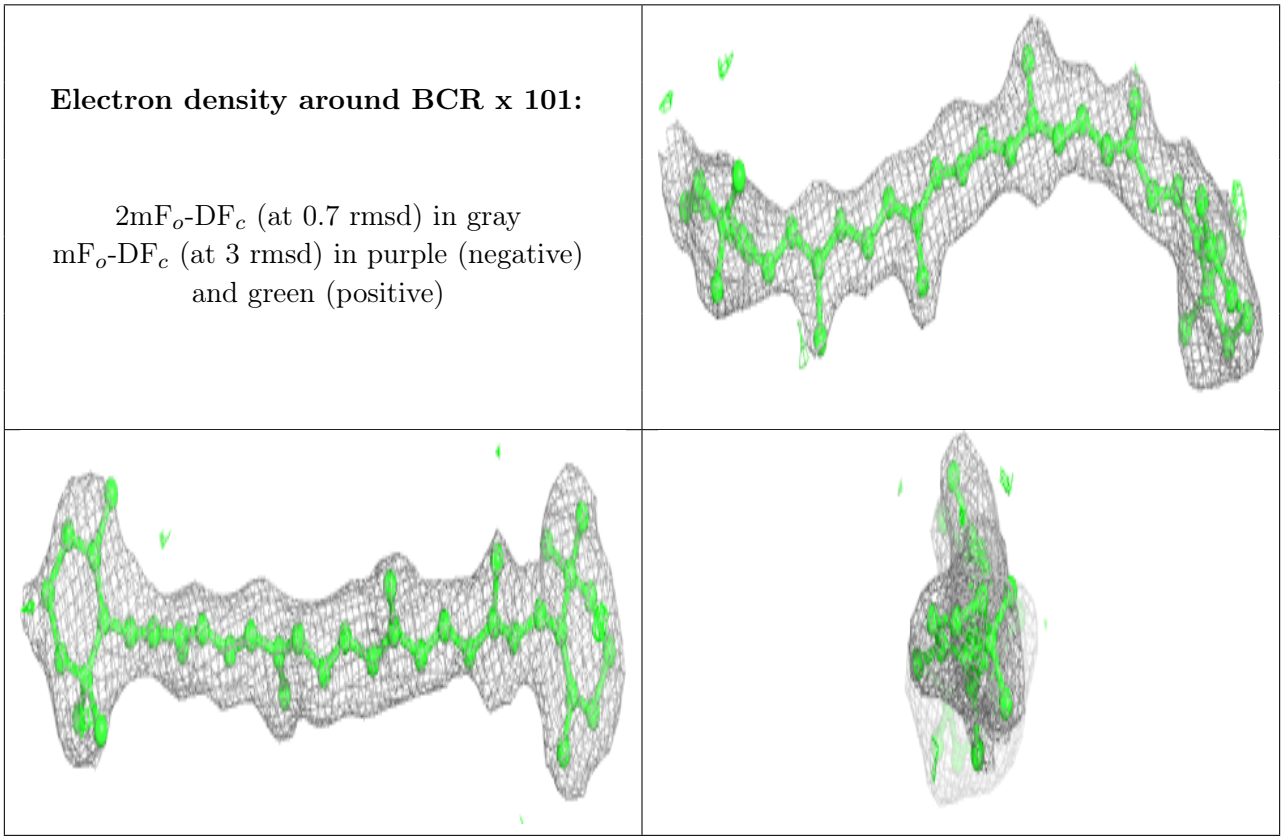
Electron density around PL9 a 611:

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



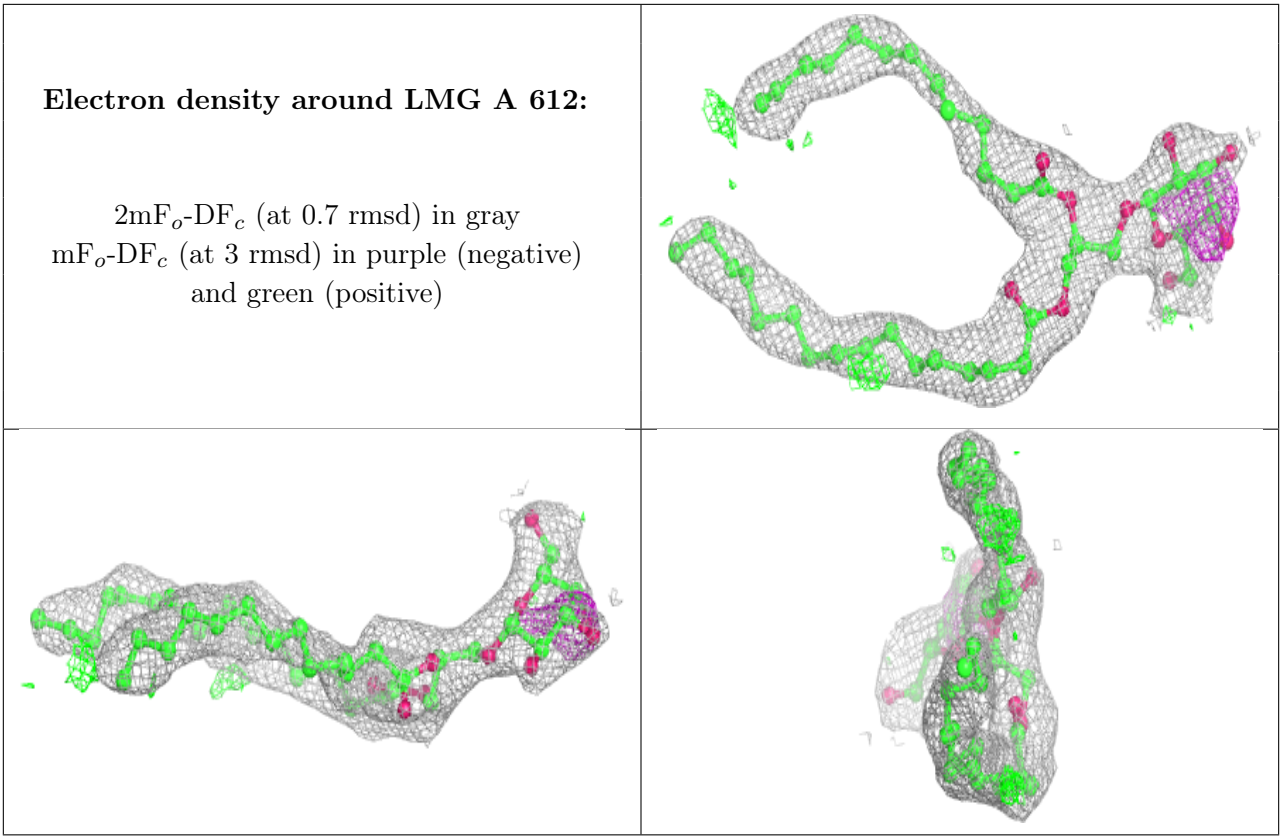
Electron density around BCR x 101:

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



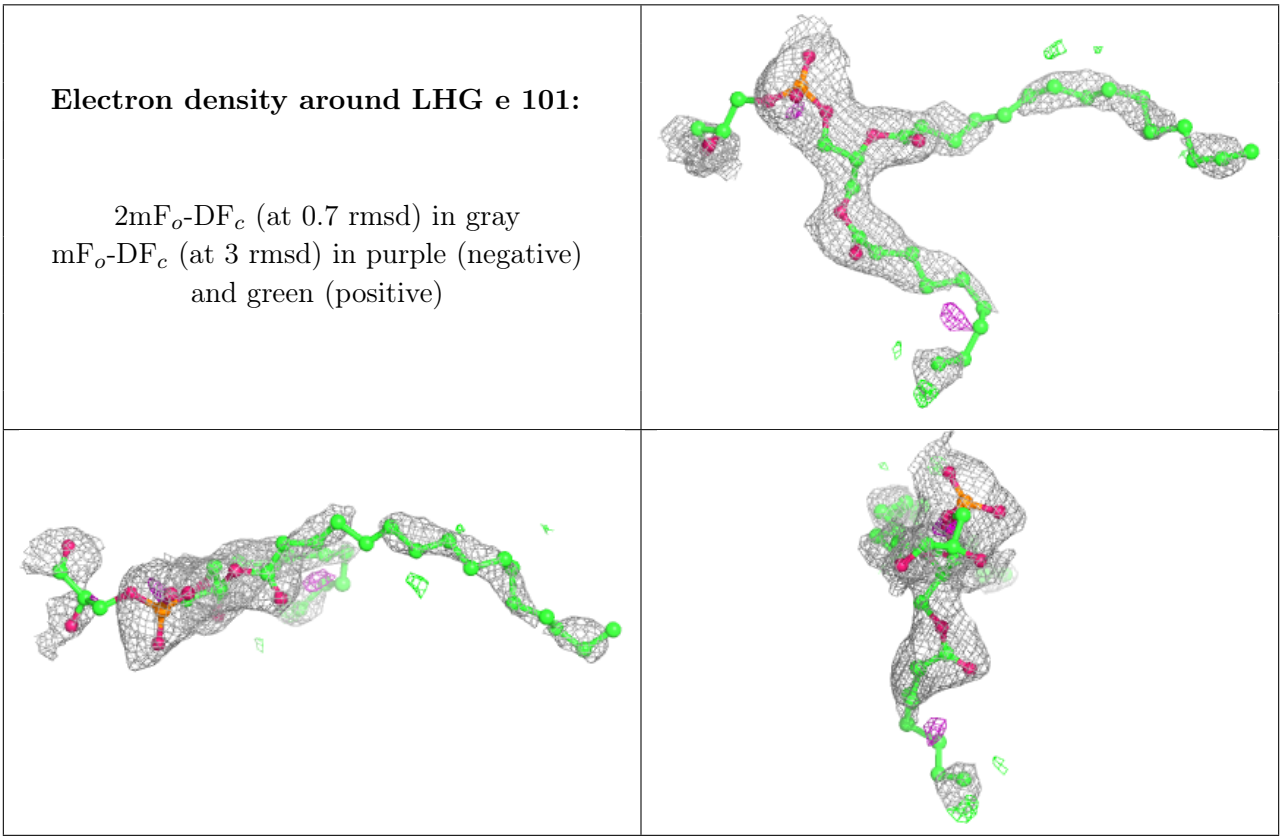
Electron density around LMG A 612:

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



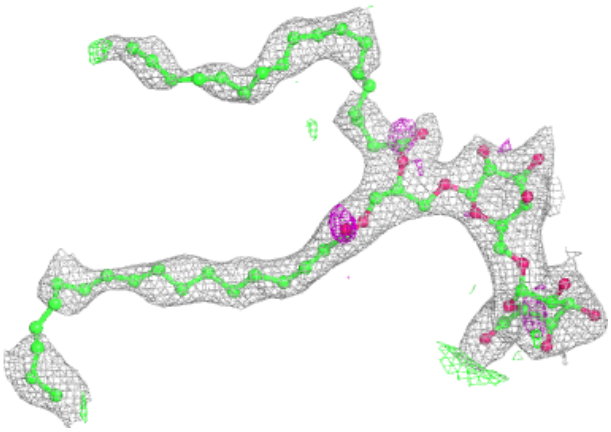
Electron density around LHG e 101:

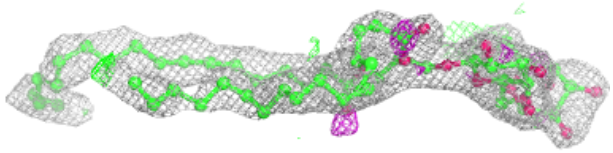
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD A 617:

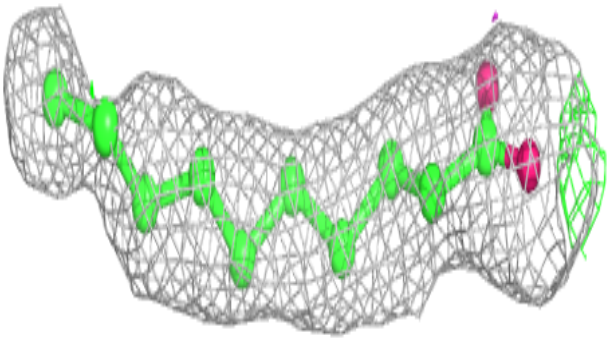
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

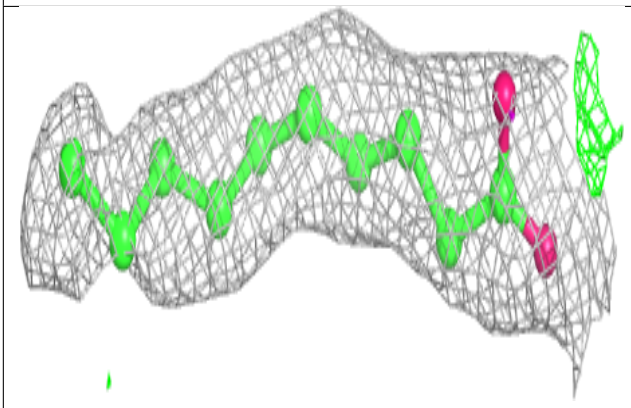


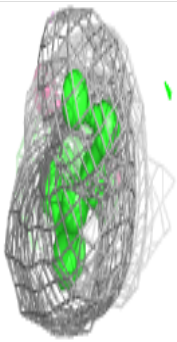


Electron density around STE j 101:

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

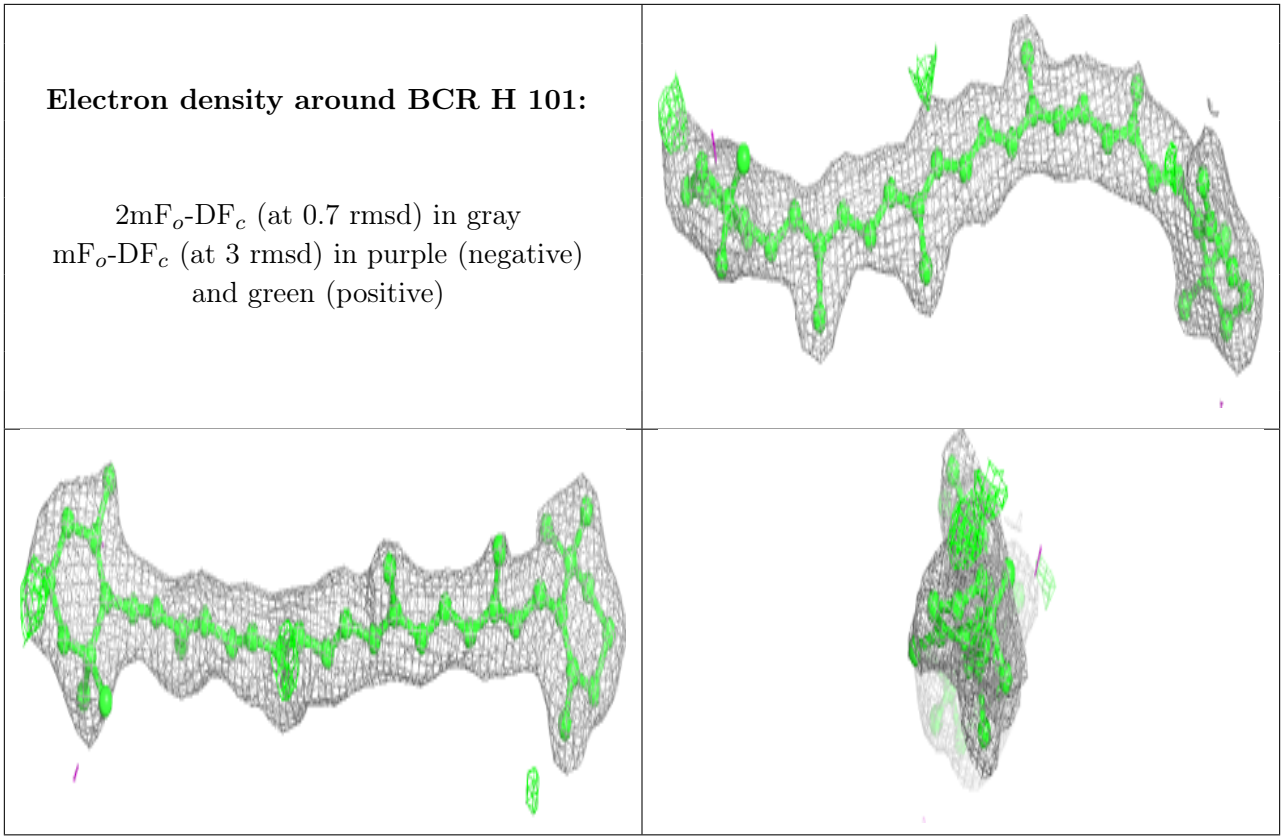






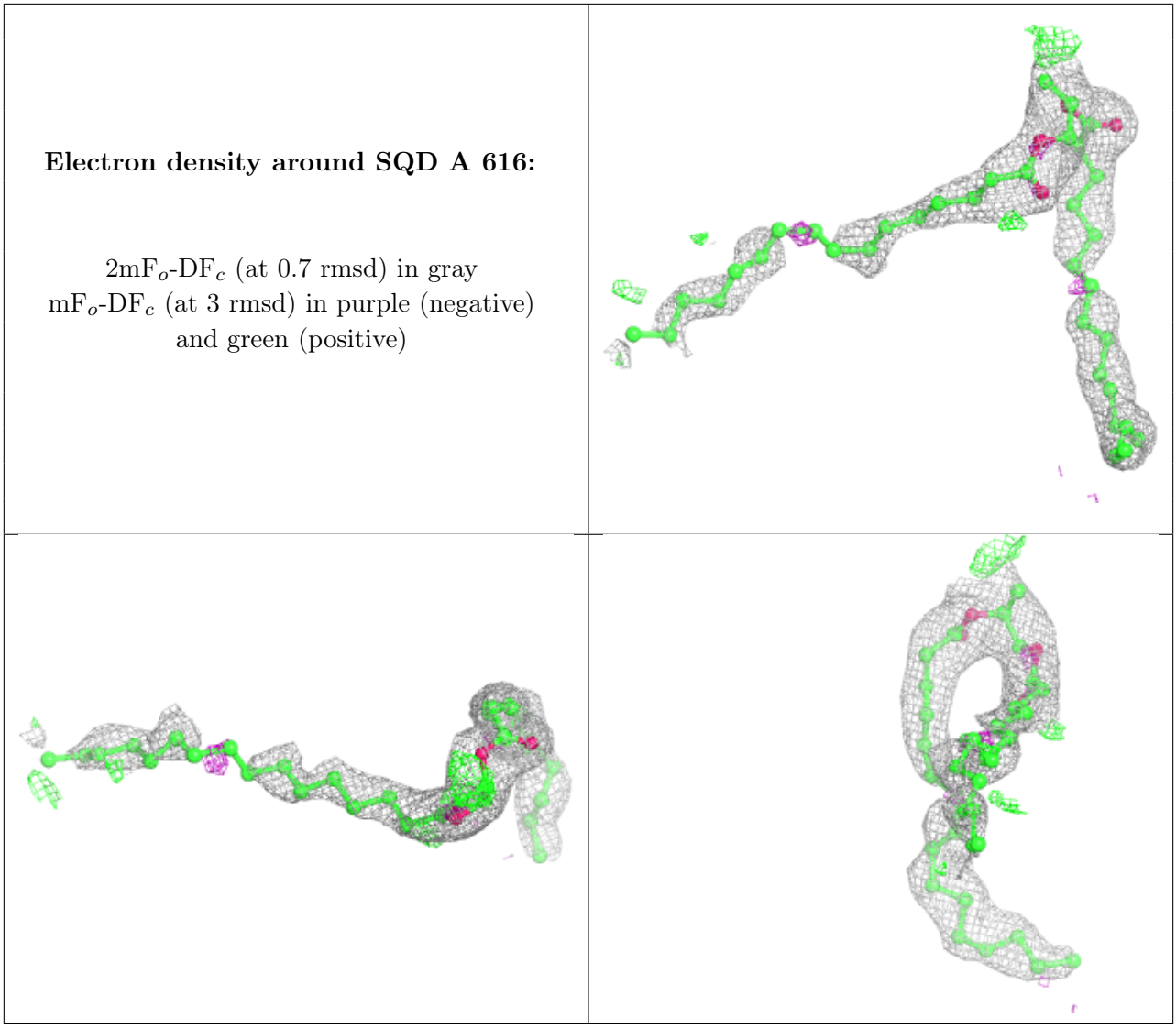
Electron density around BCR H 101:

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



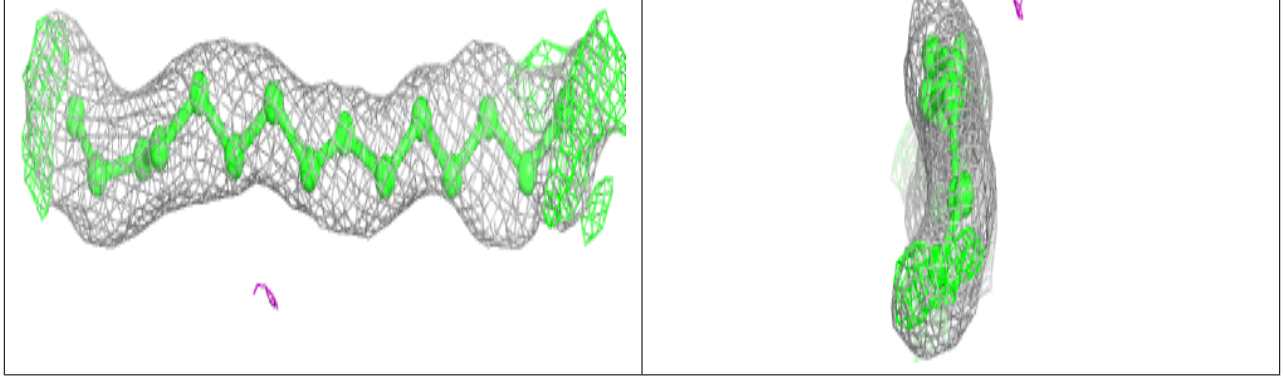
Electron density around SQD A 616:

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



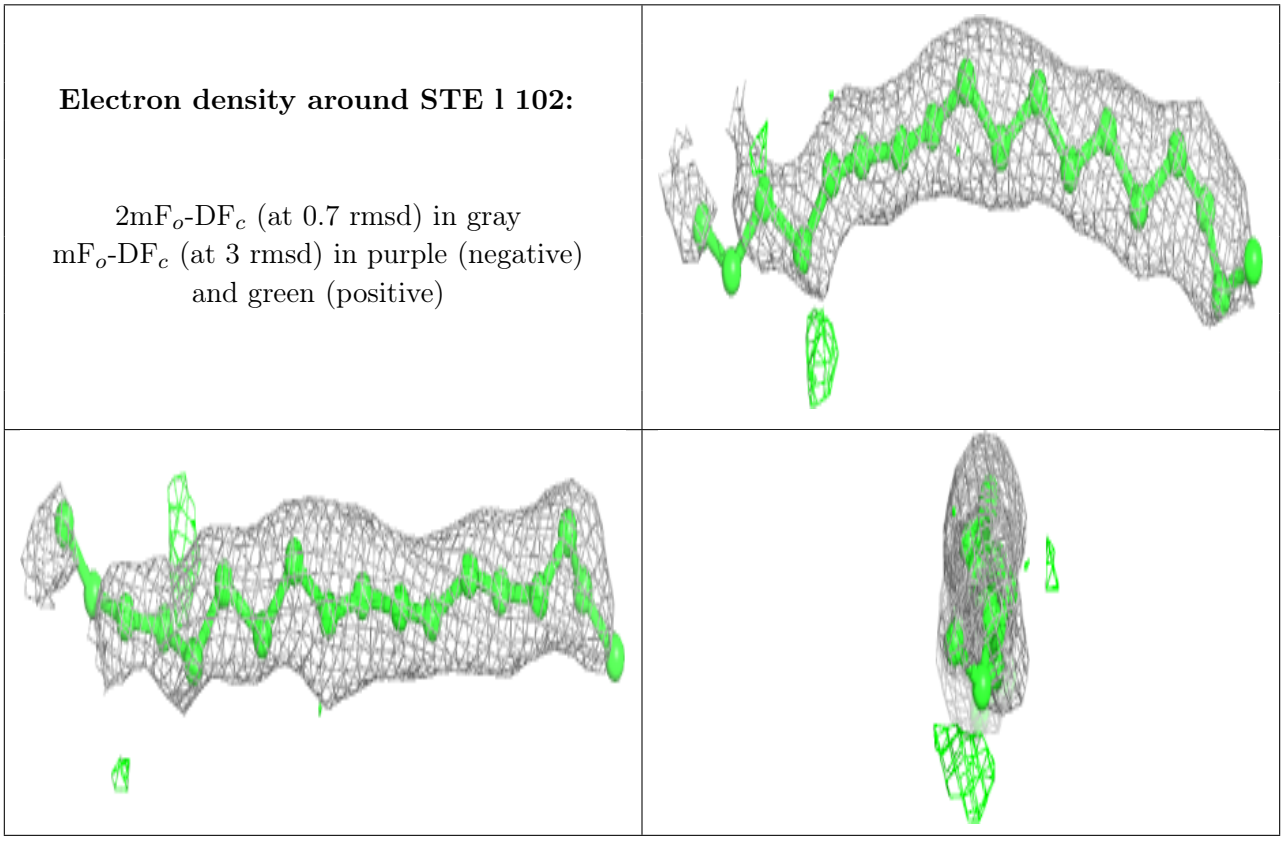
Electron density around STE I 101:

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



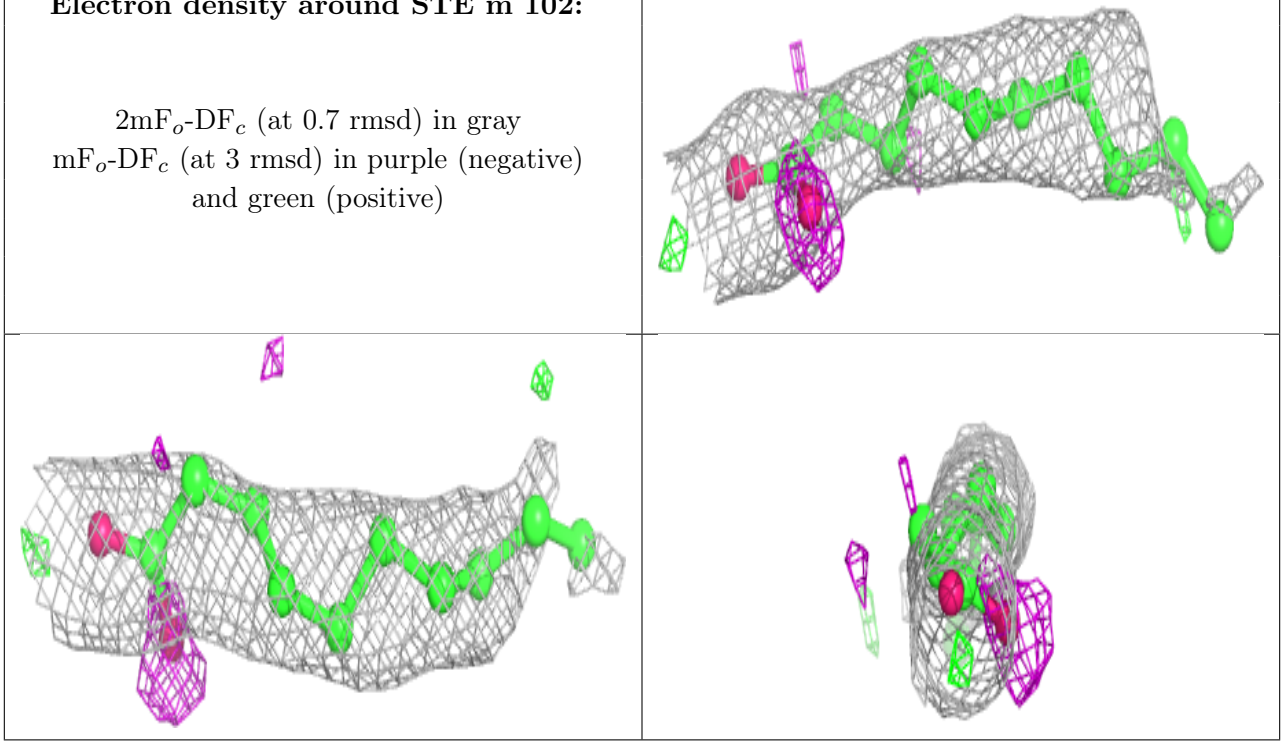
Electron density around STE l 102:

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



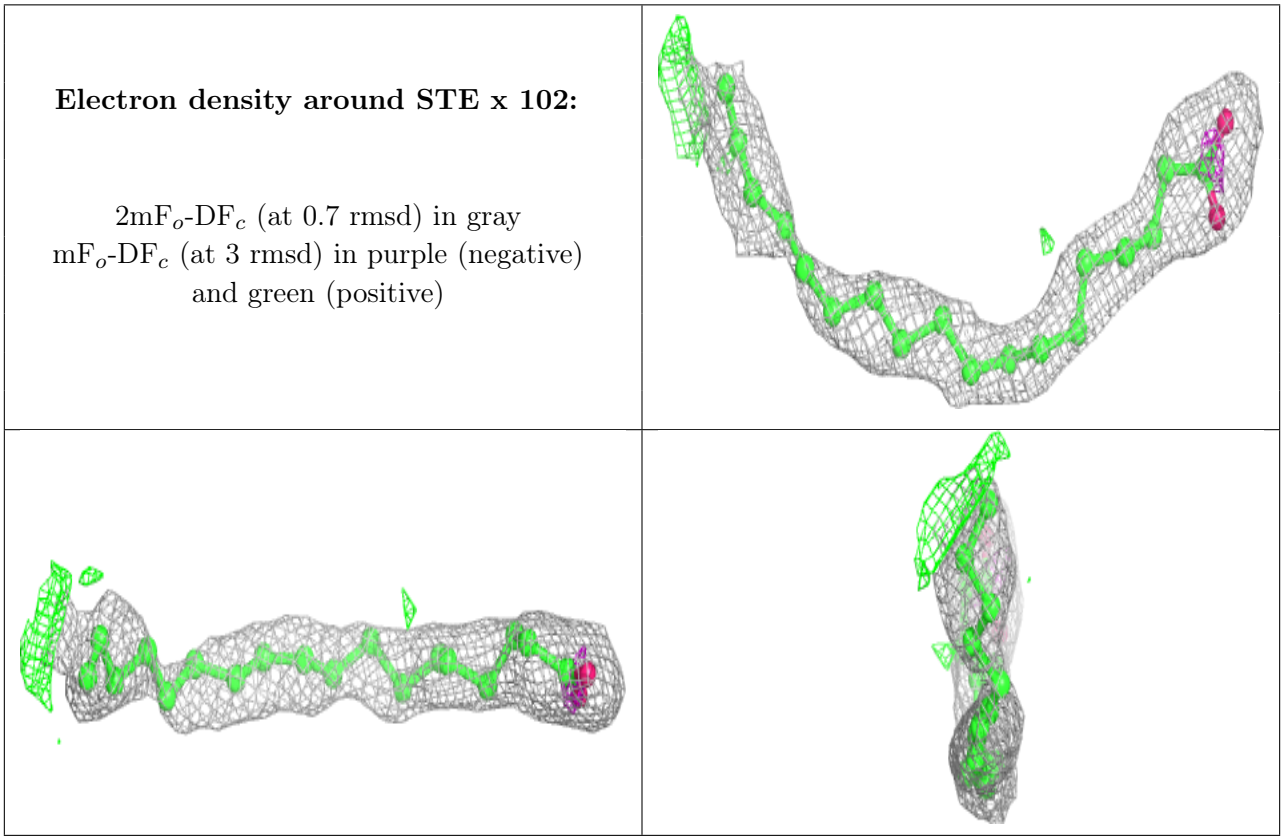
Electron density around STE m 102:

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



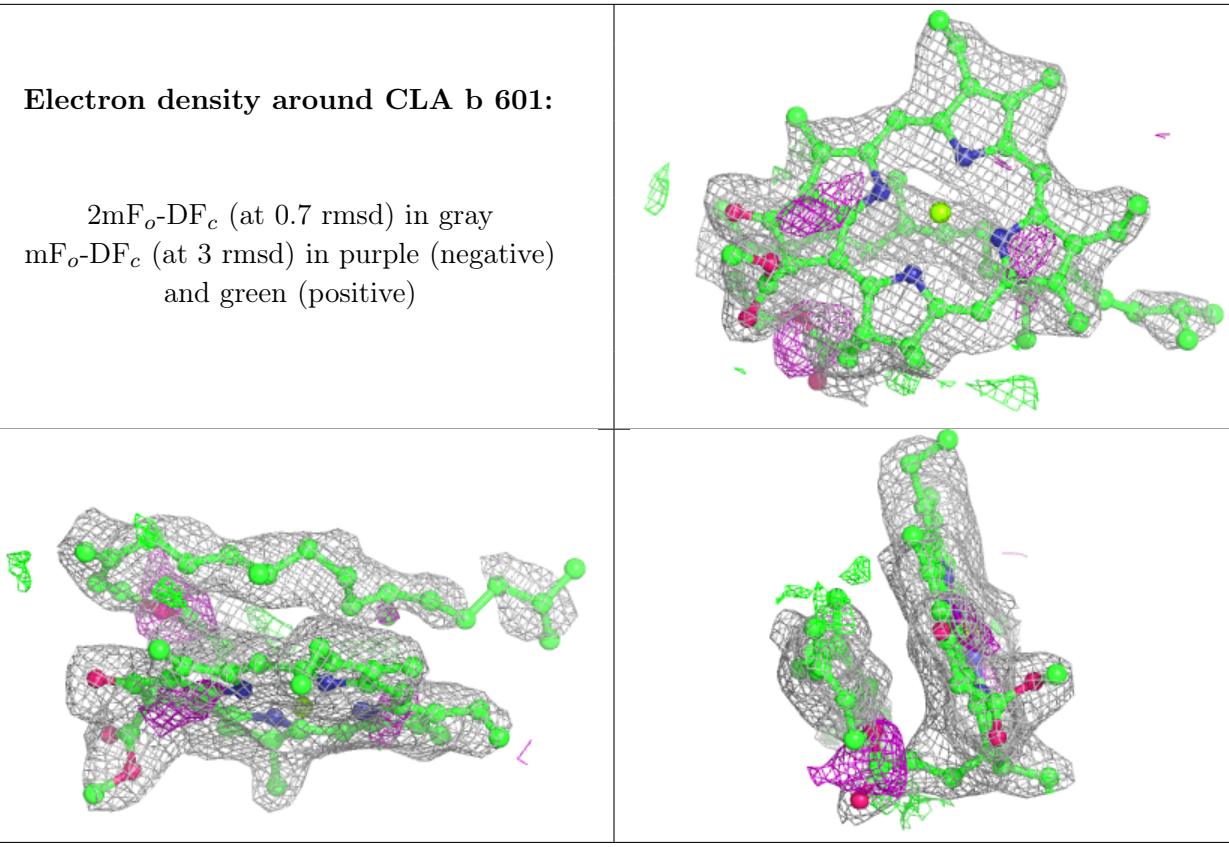
Electron density around STE x 102:

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



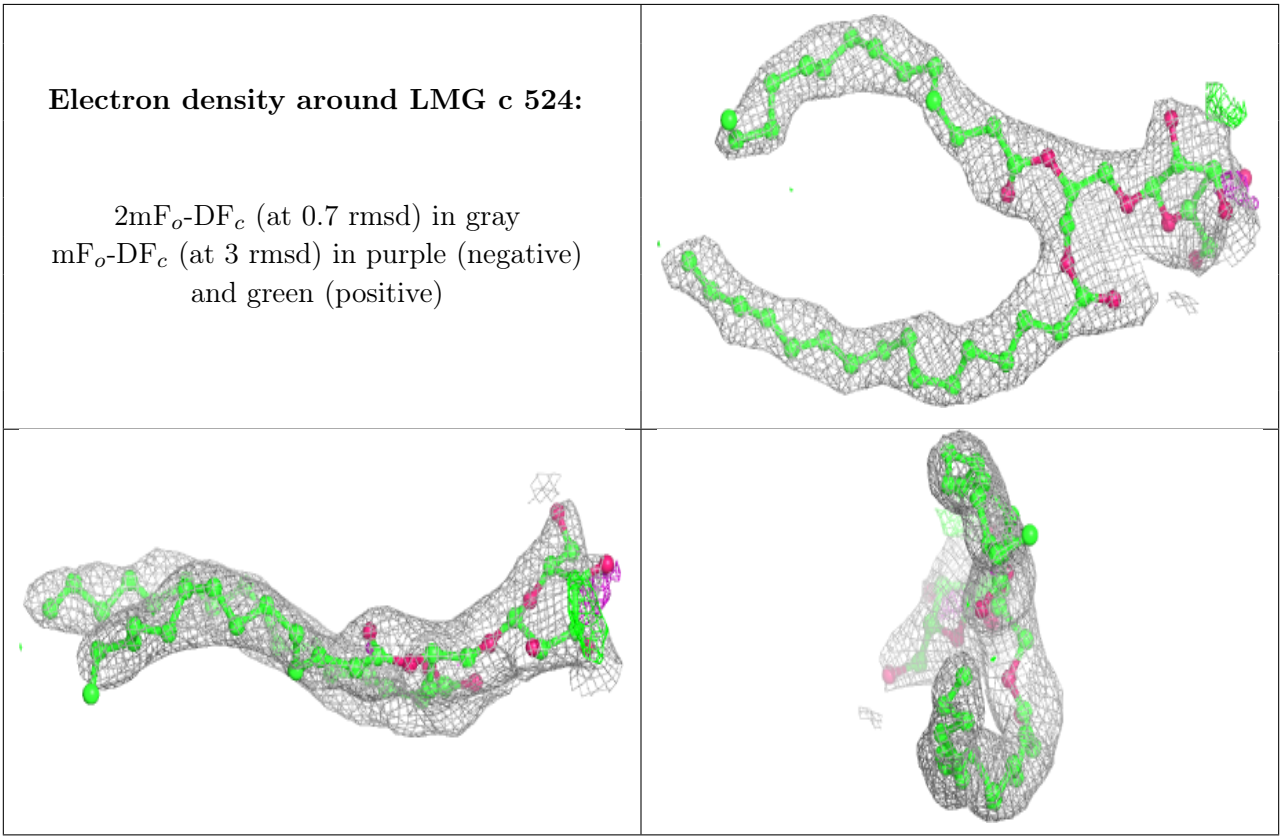
Electron density around CLA b 601:

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



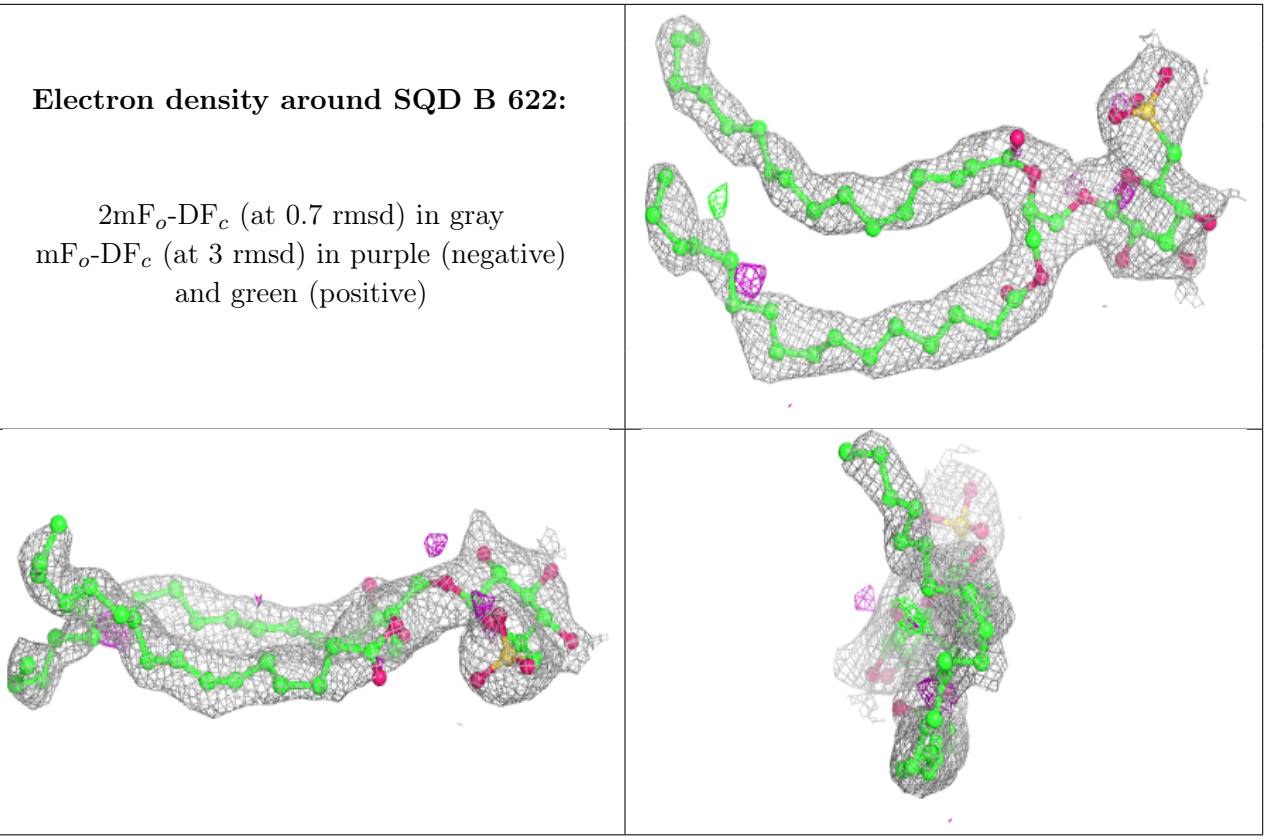
Electron density around LMG c 524:

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



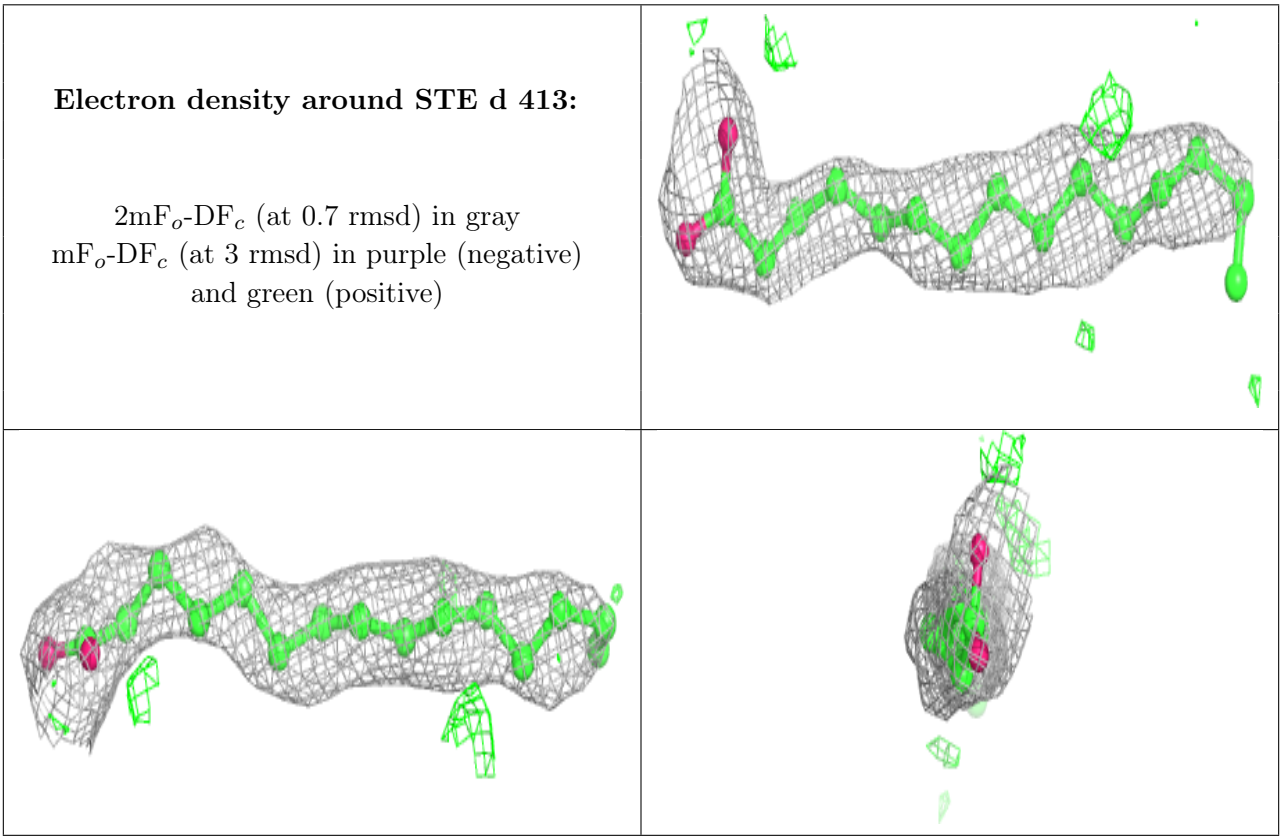
Electron density around SQD B 622:

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



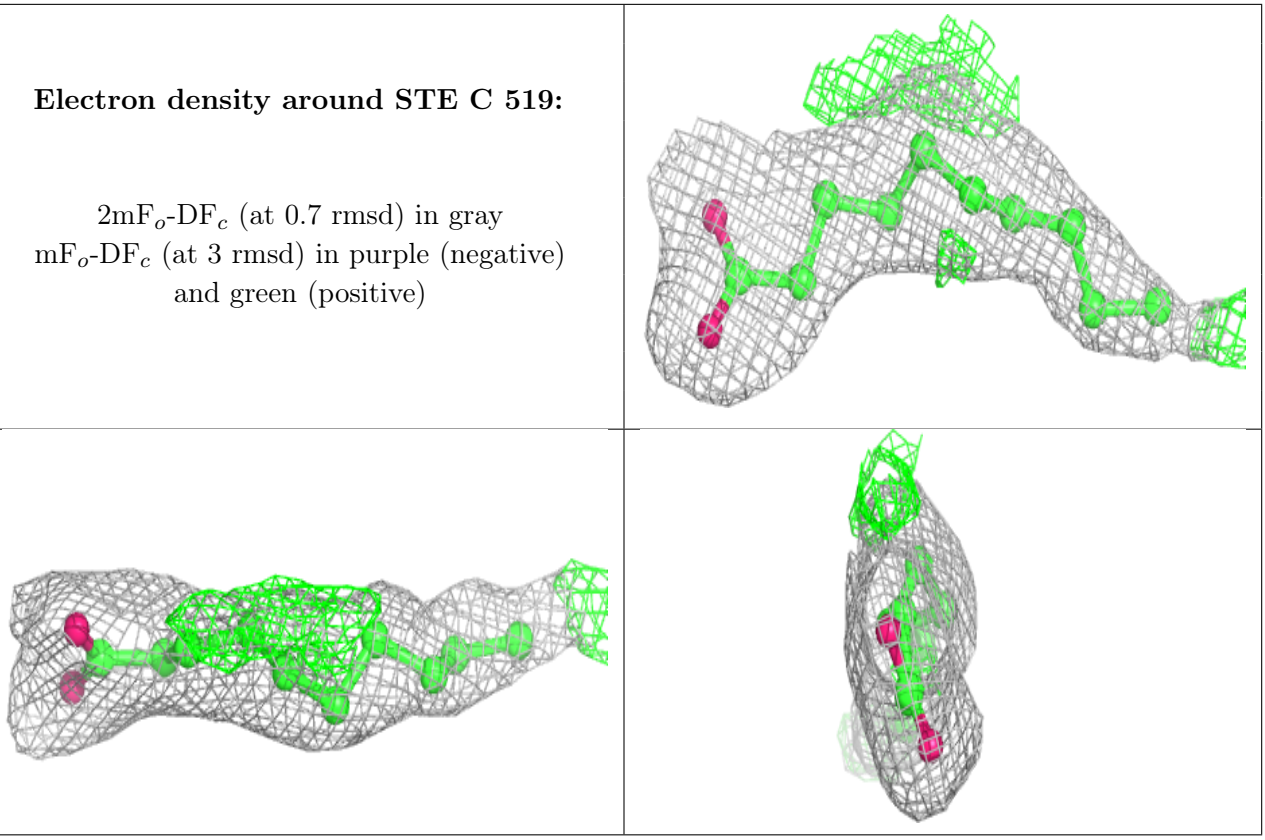
Electron density around STE d 413:

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



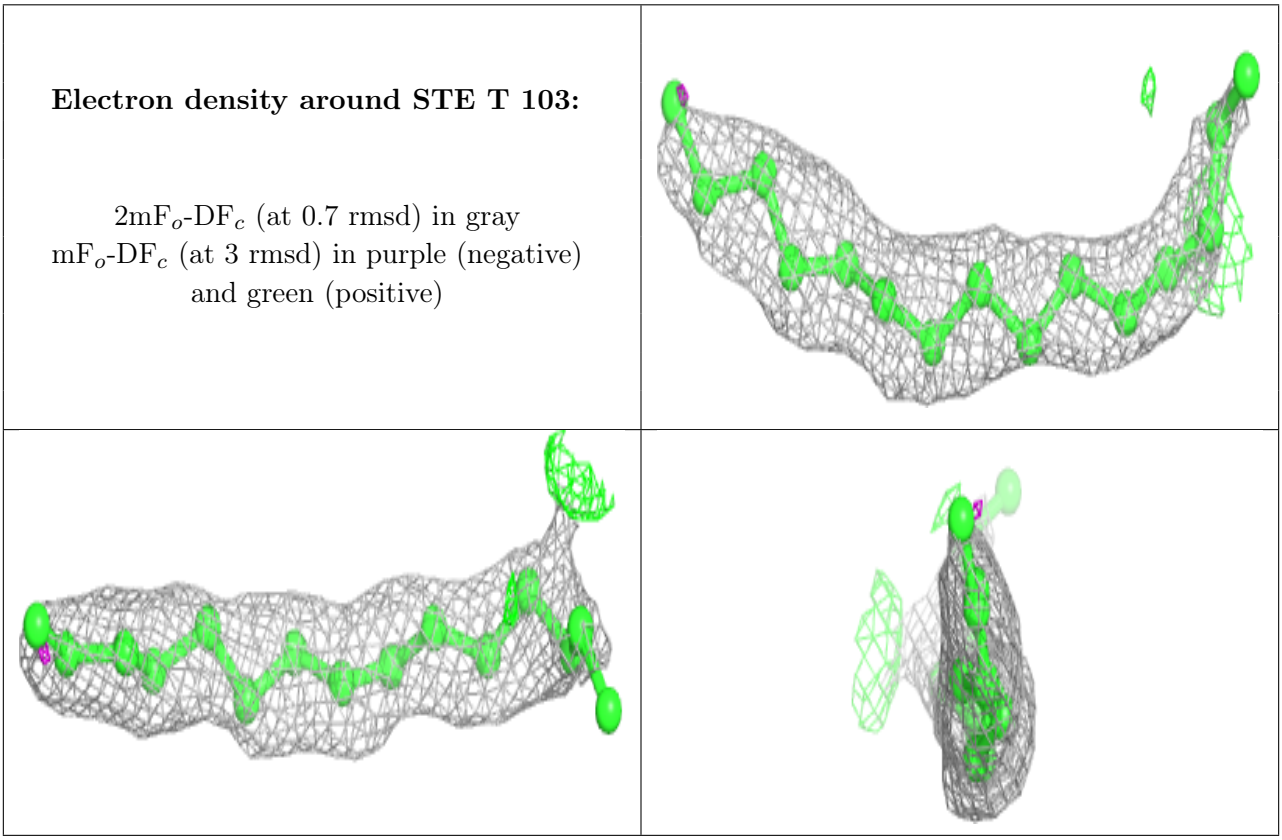
Electron density around STE C 519:

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



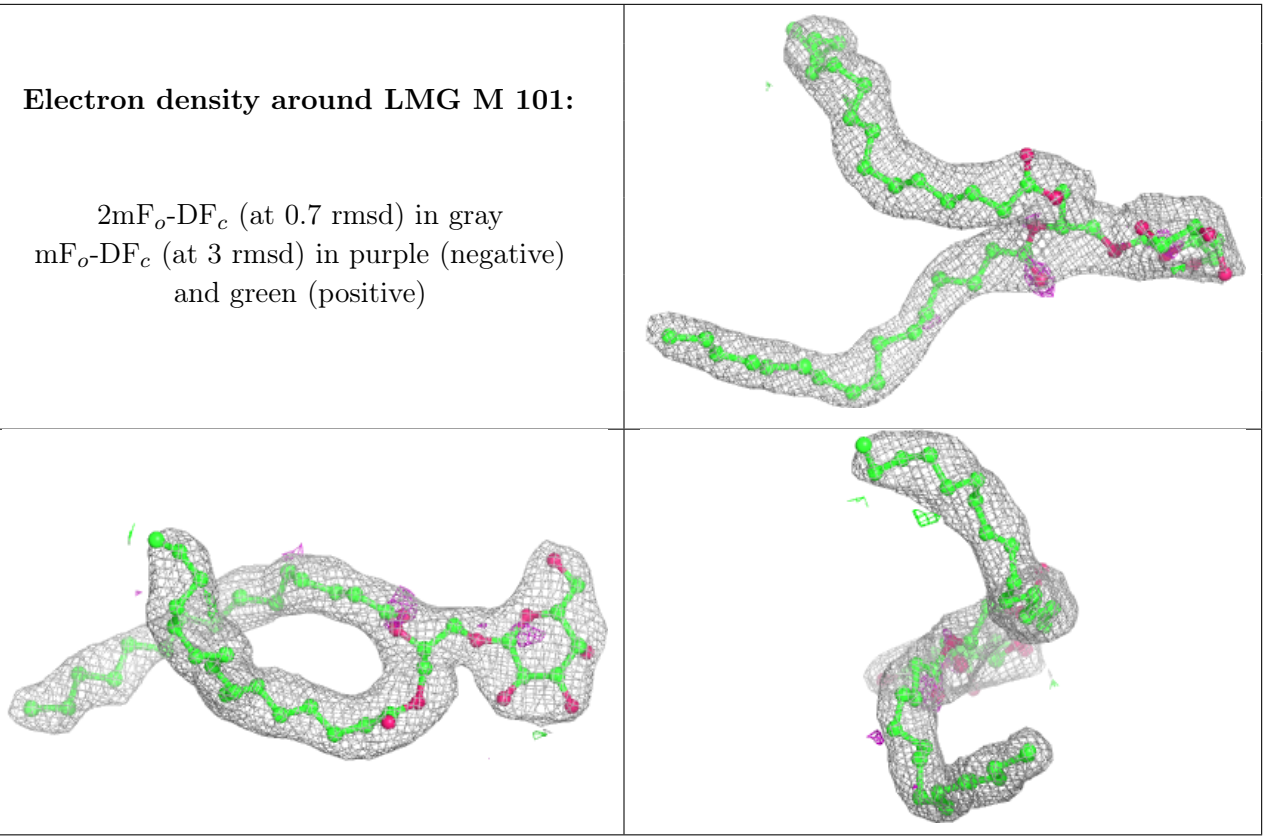
Electron density around STE T 103:

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



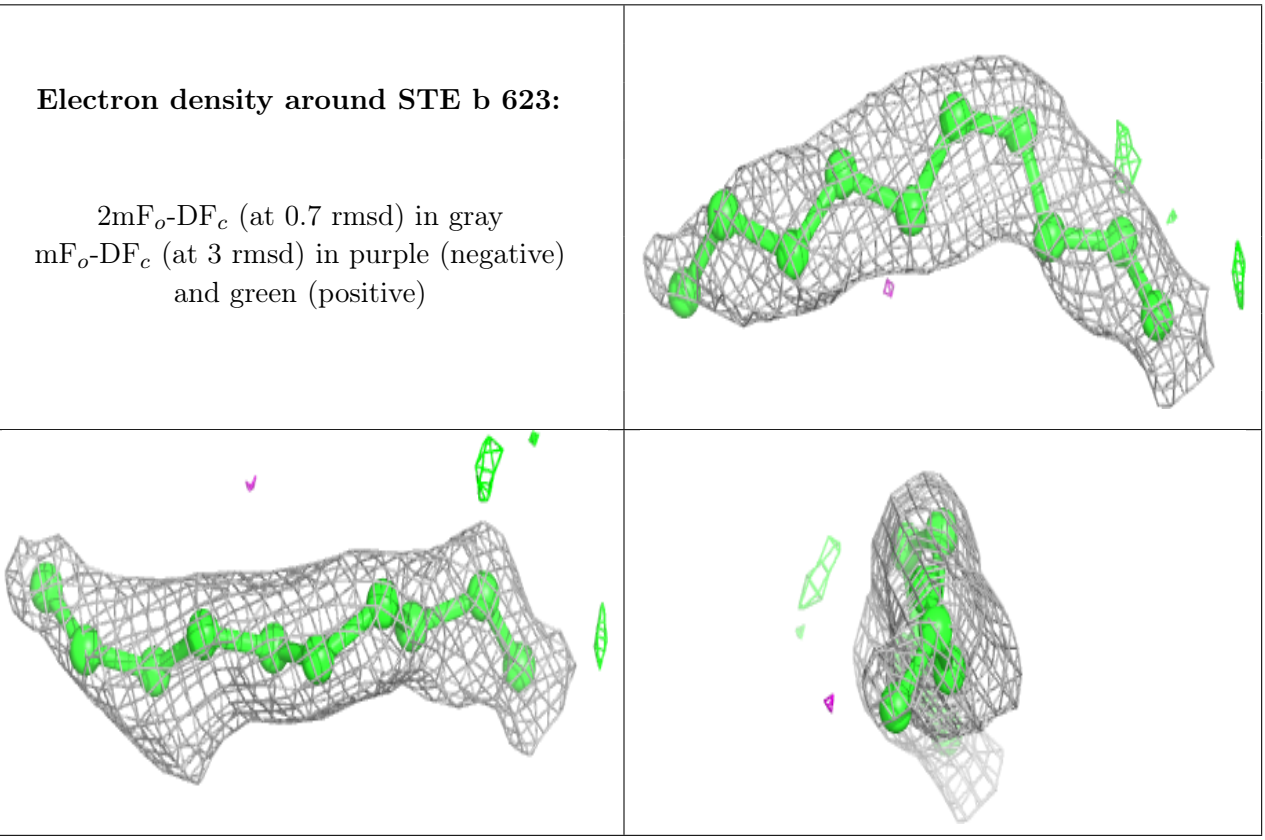
Electron density around LMG M 101:

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



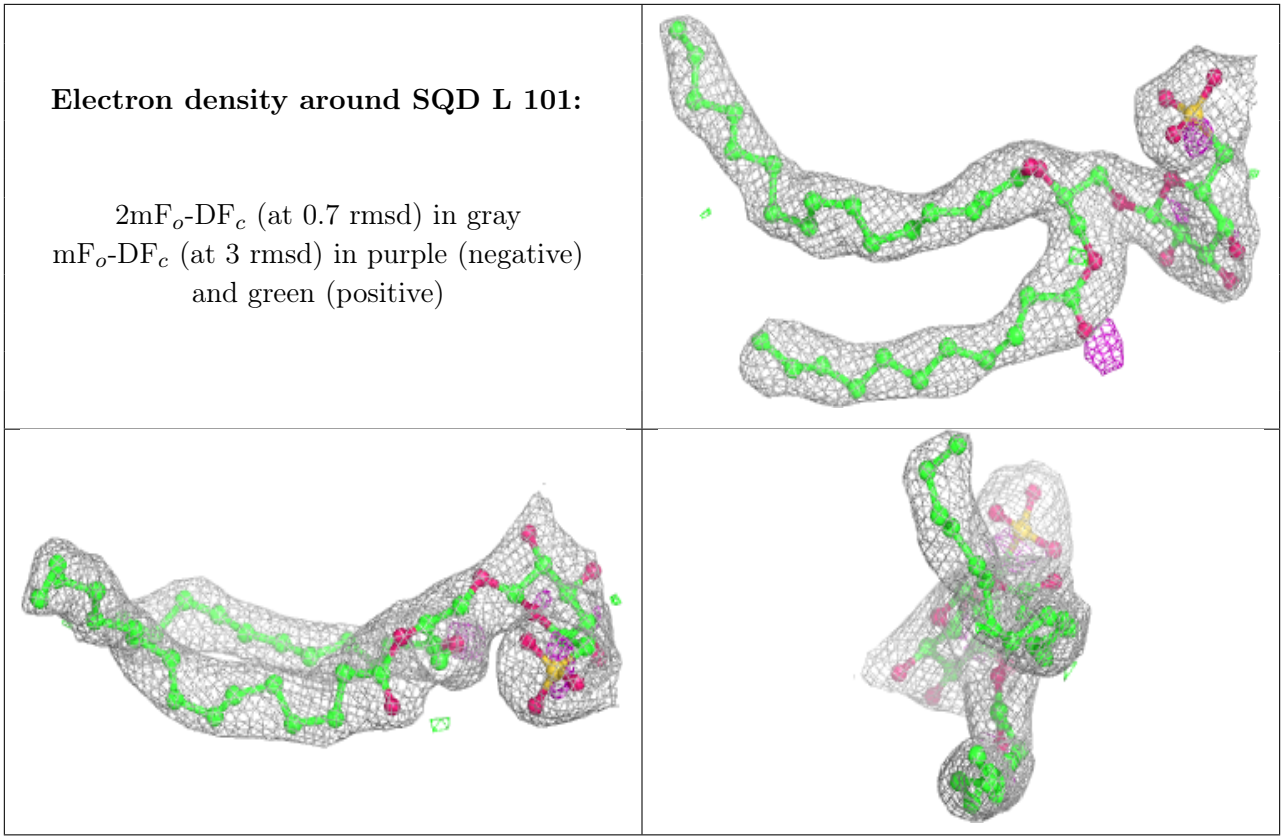
Electron density around STE b 623:

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



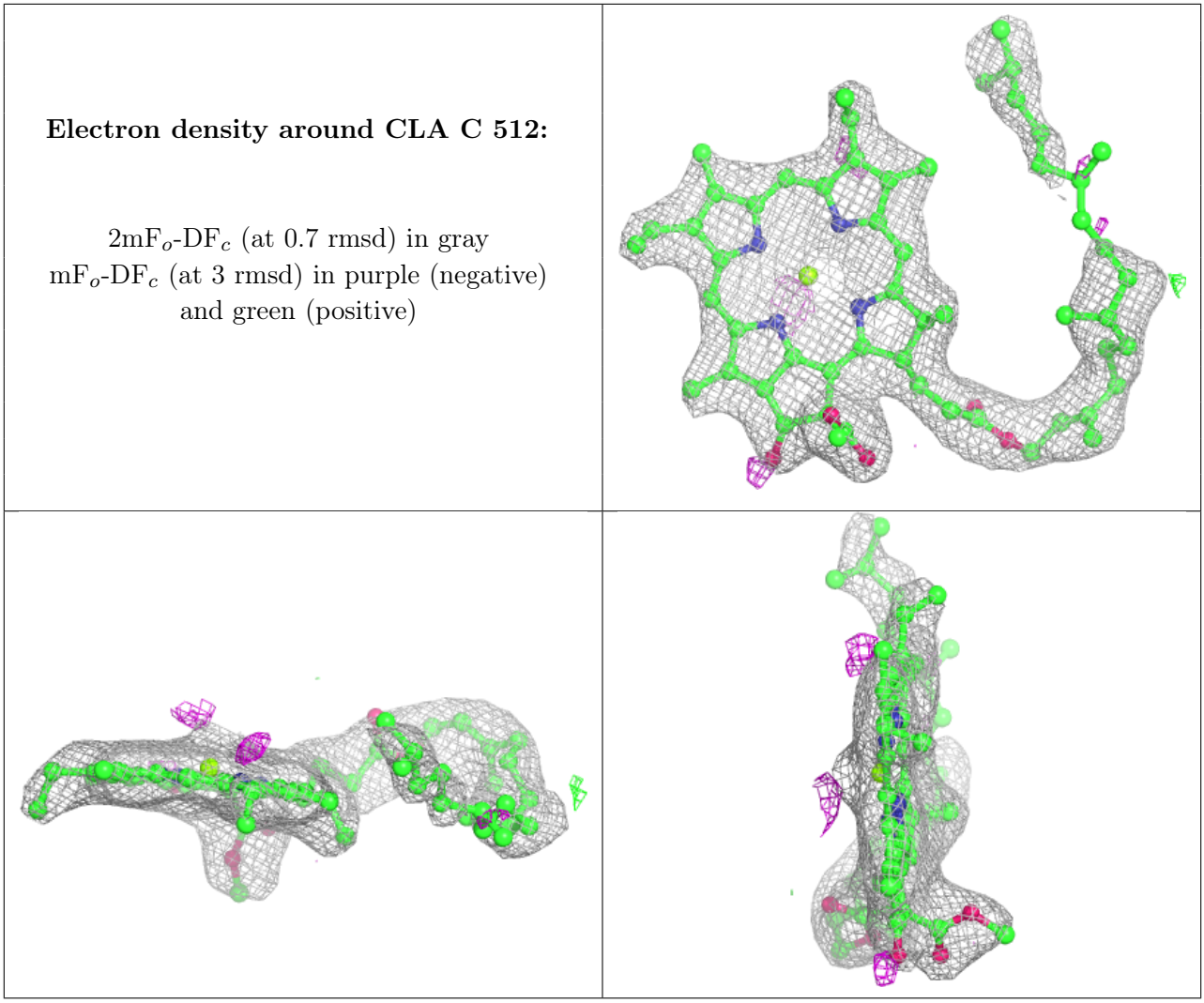
Electron density around SQD L 101:

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



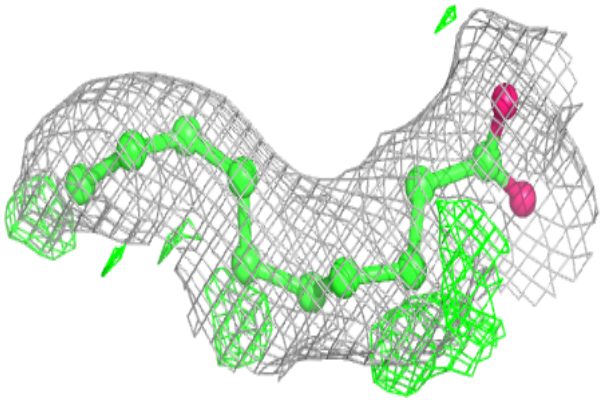
Electron density around CLA C 512:

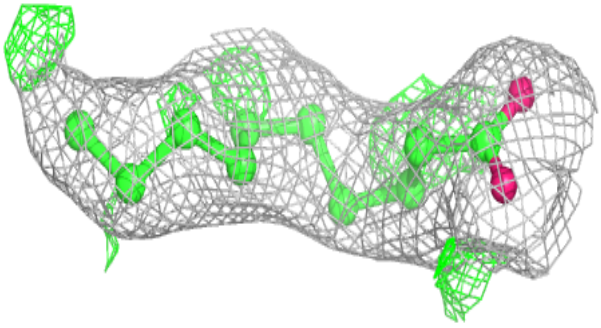
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

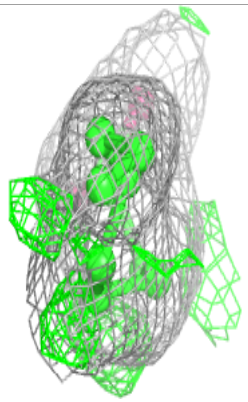


Electron density around STE B 623:

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

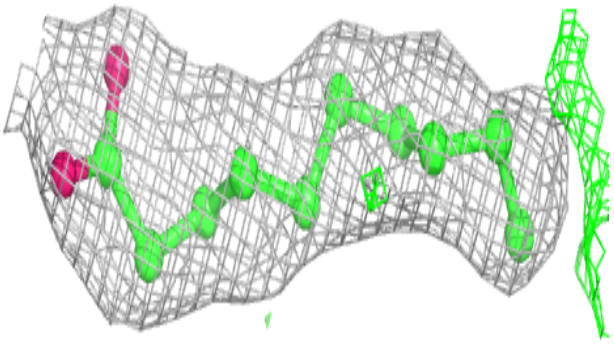


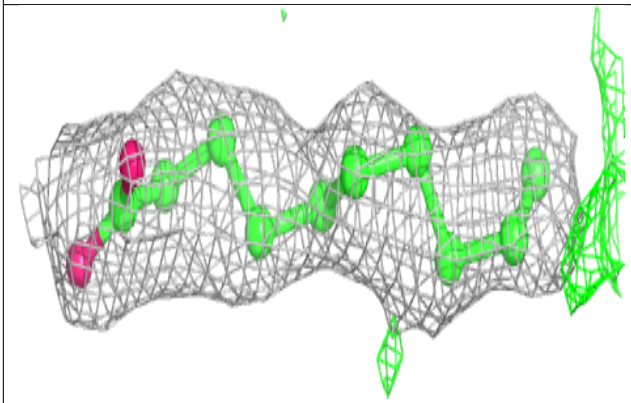


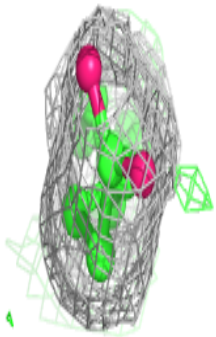


Electron density around STE J 101:

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

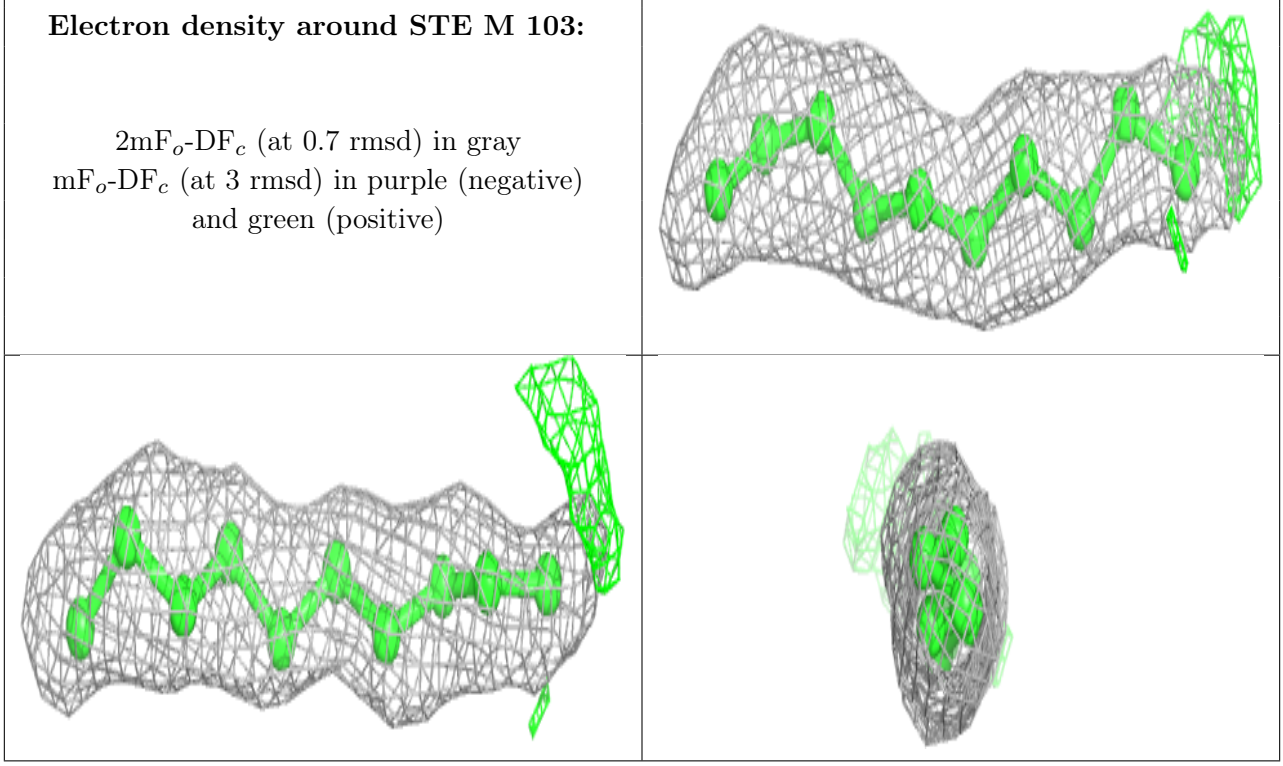






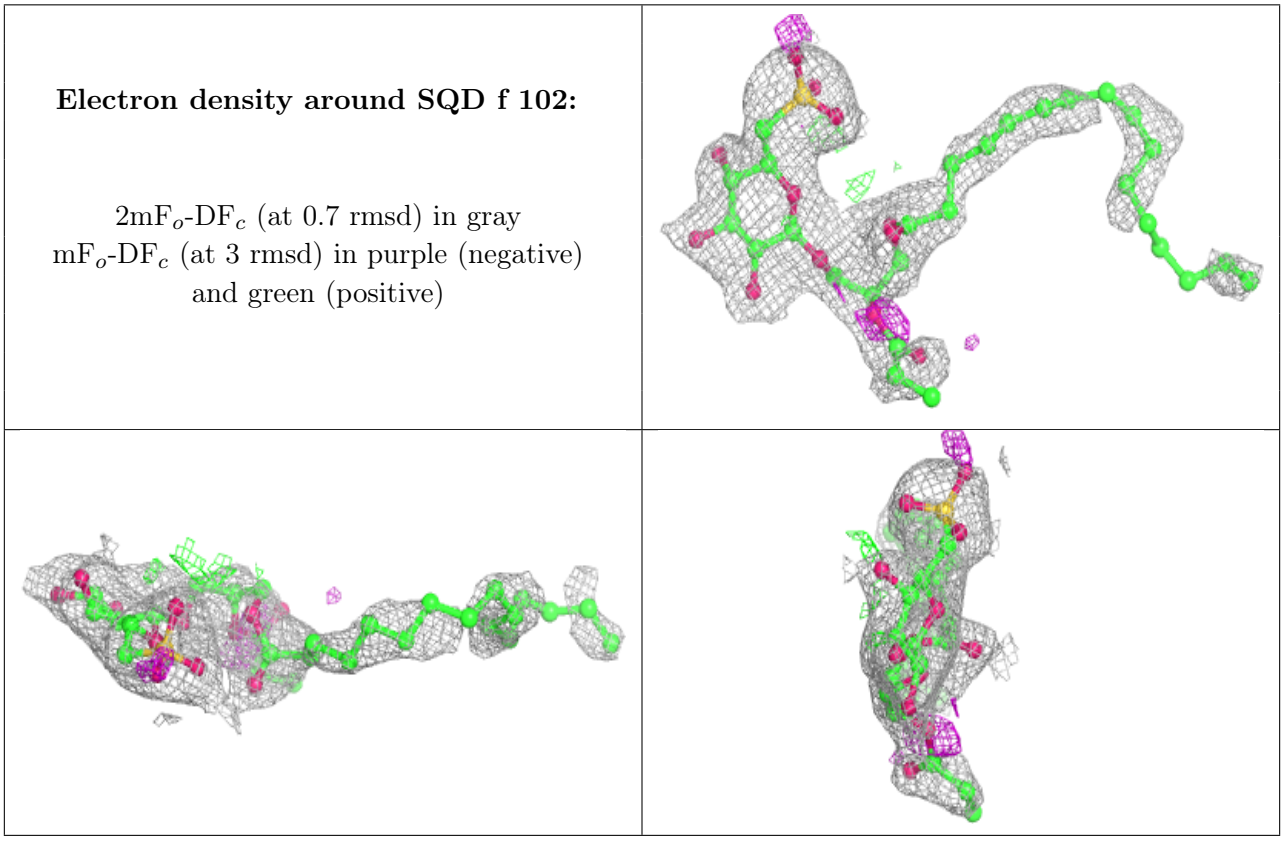
Electron density around STE M 103:

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



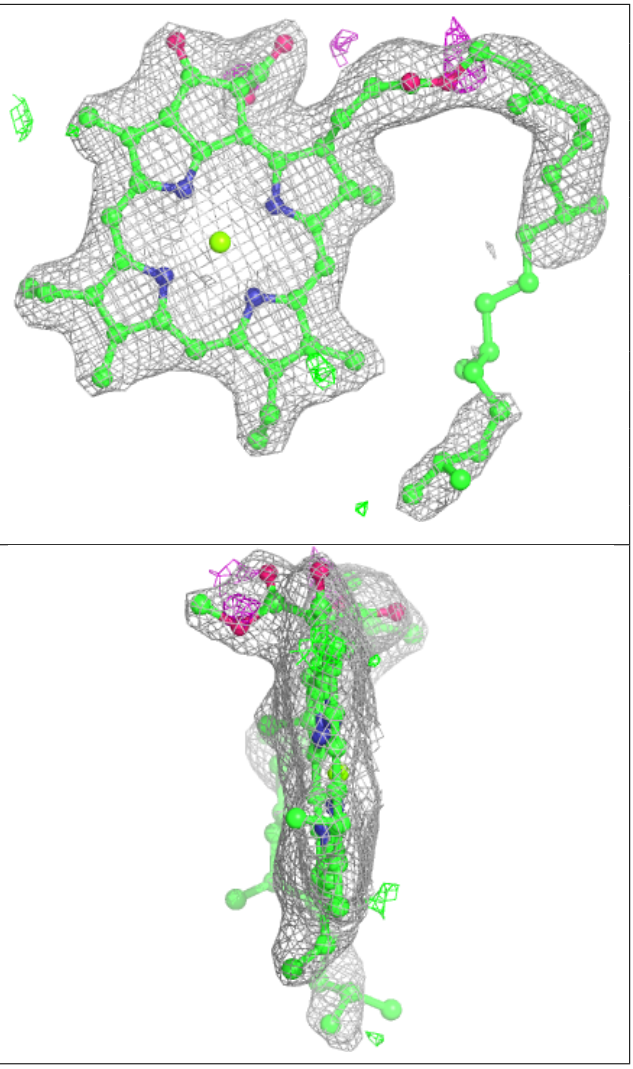
Electron density around SQD f 102:

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



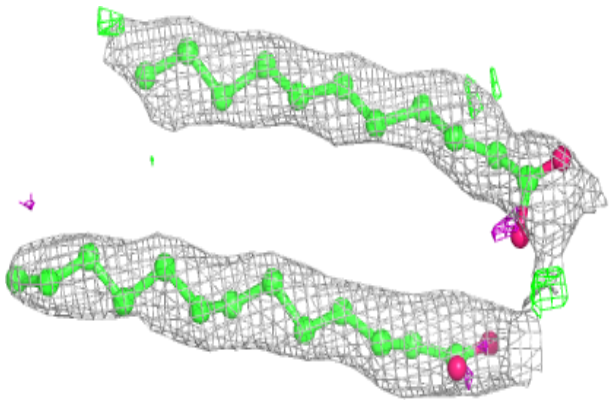
Electron density around CLA c 512:

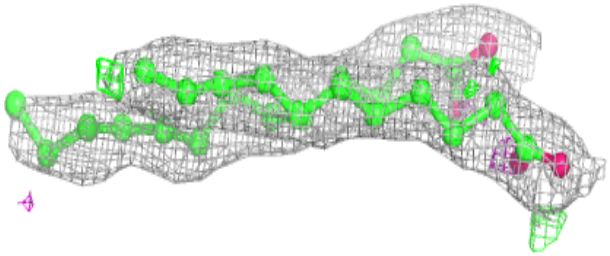
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

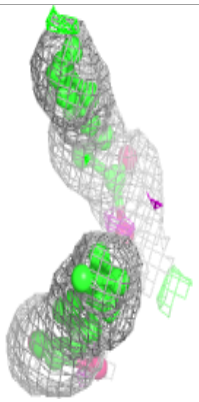


Electron density around LMG B 621:

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

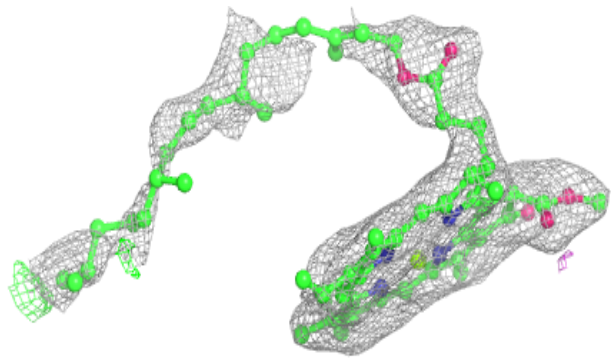


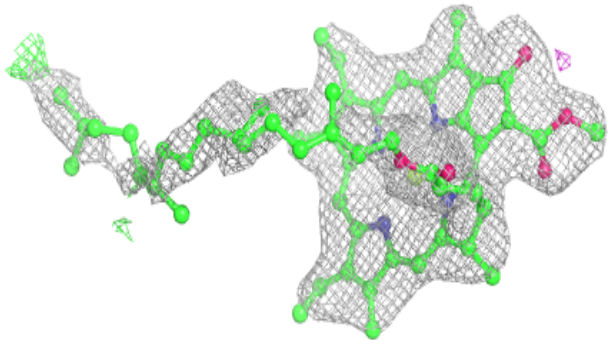


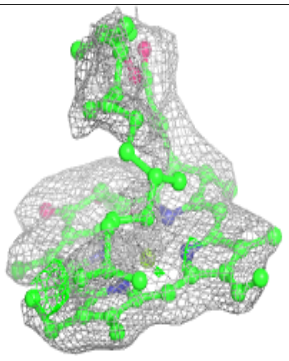


Electron density around CLA C 513:

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

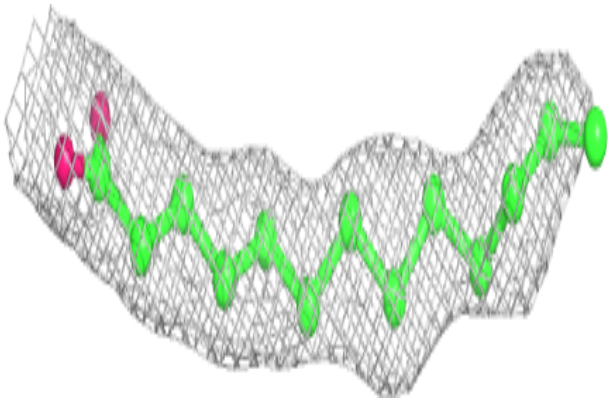


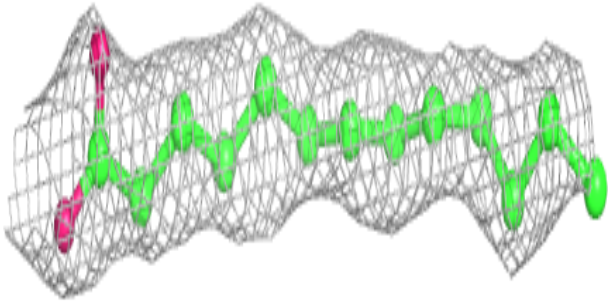


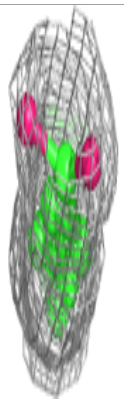


Electron density around STE M 102:

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

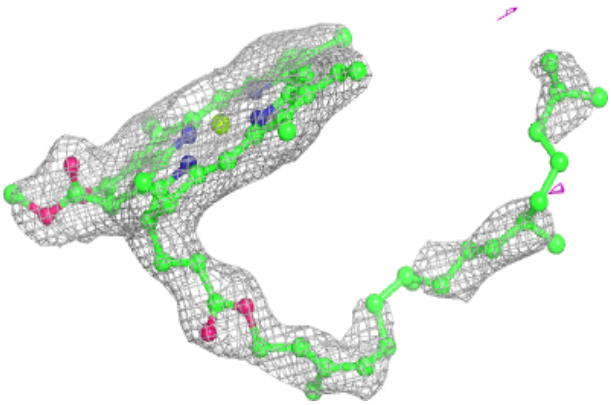


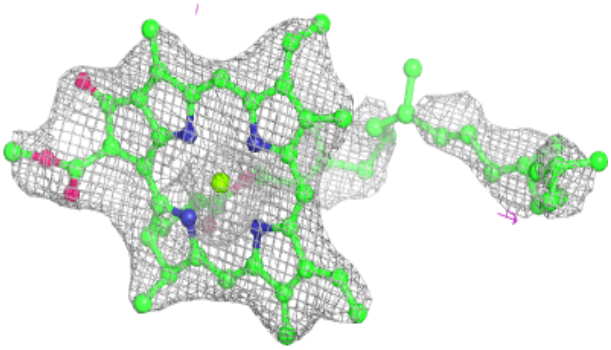


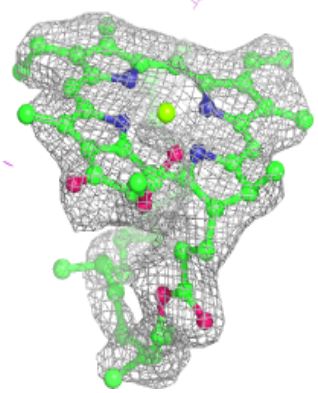


Electron density around CLA c 513:

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

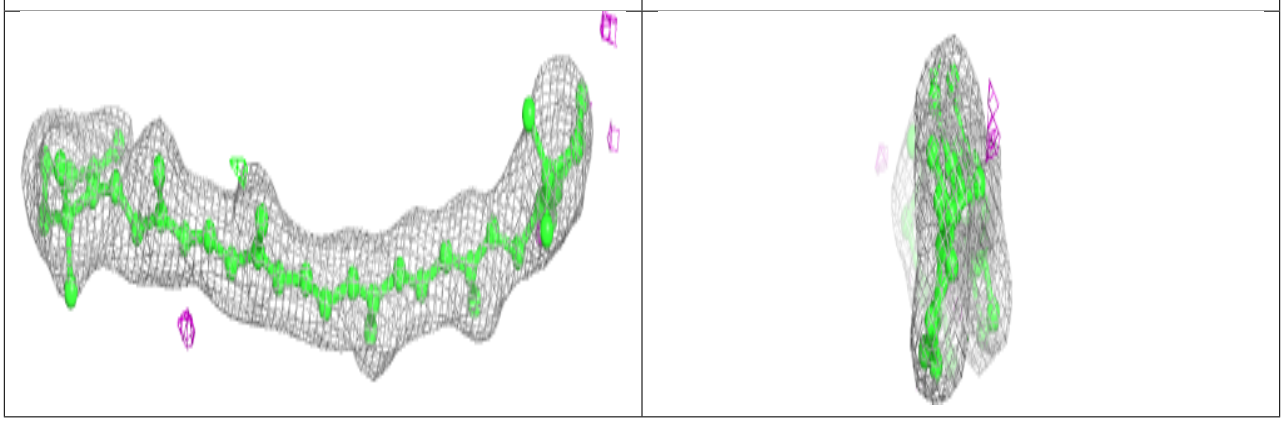






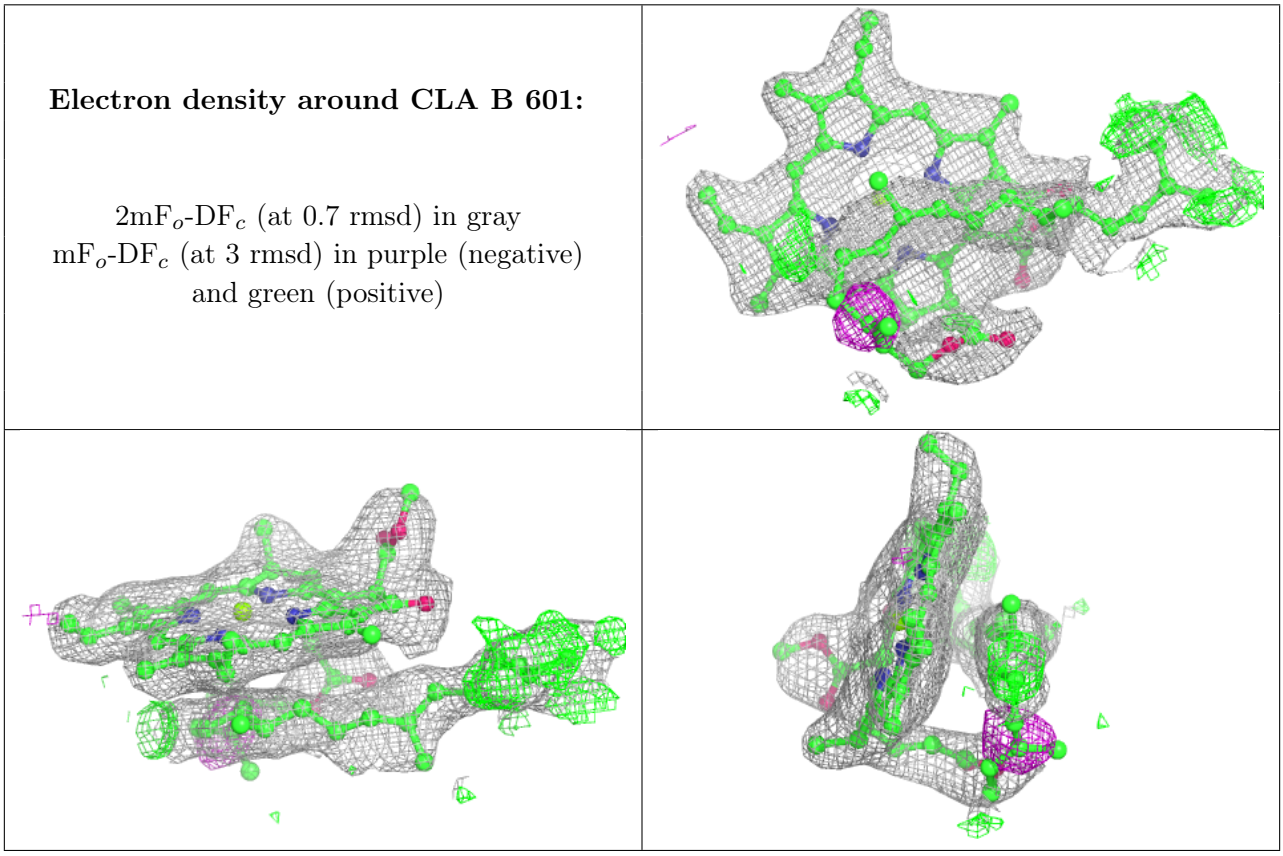
Electron density around BCR D 406:

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



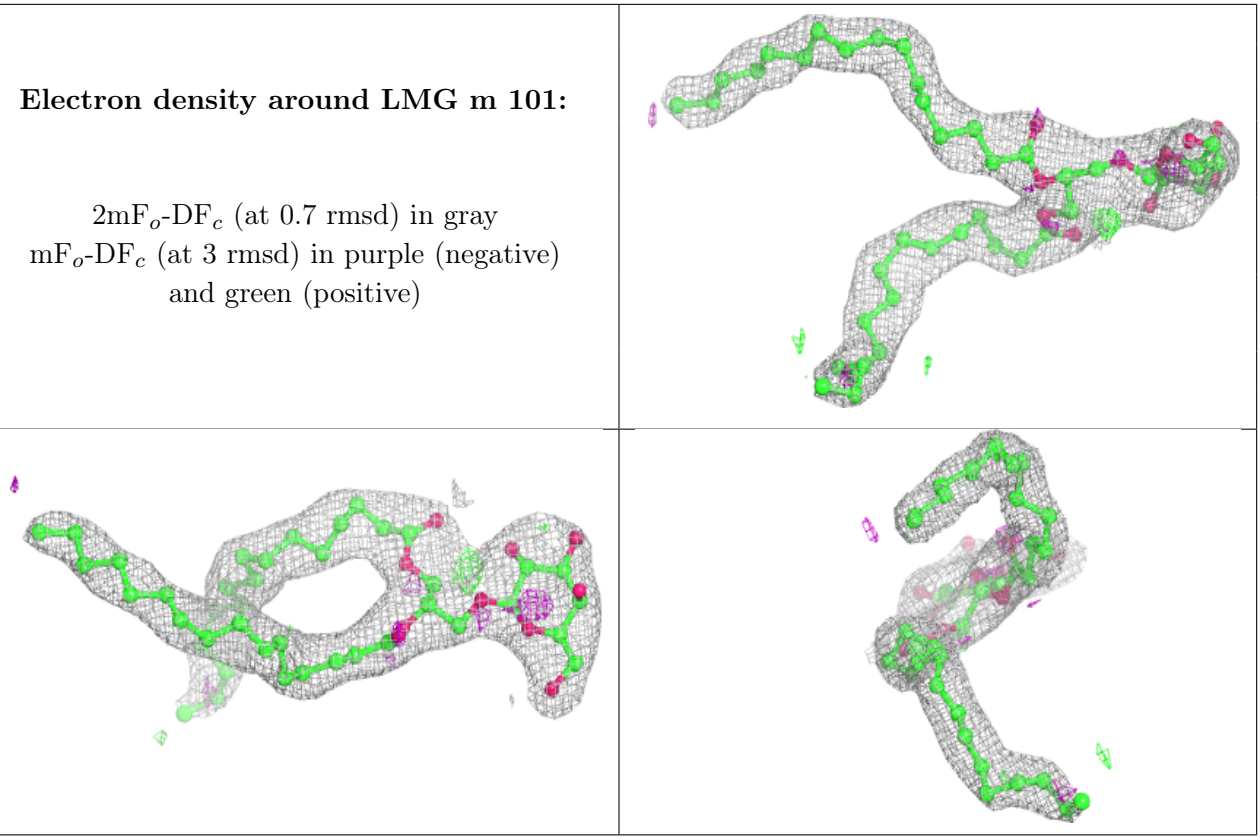
Electron density around CLA B 601:

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



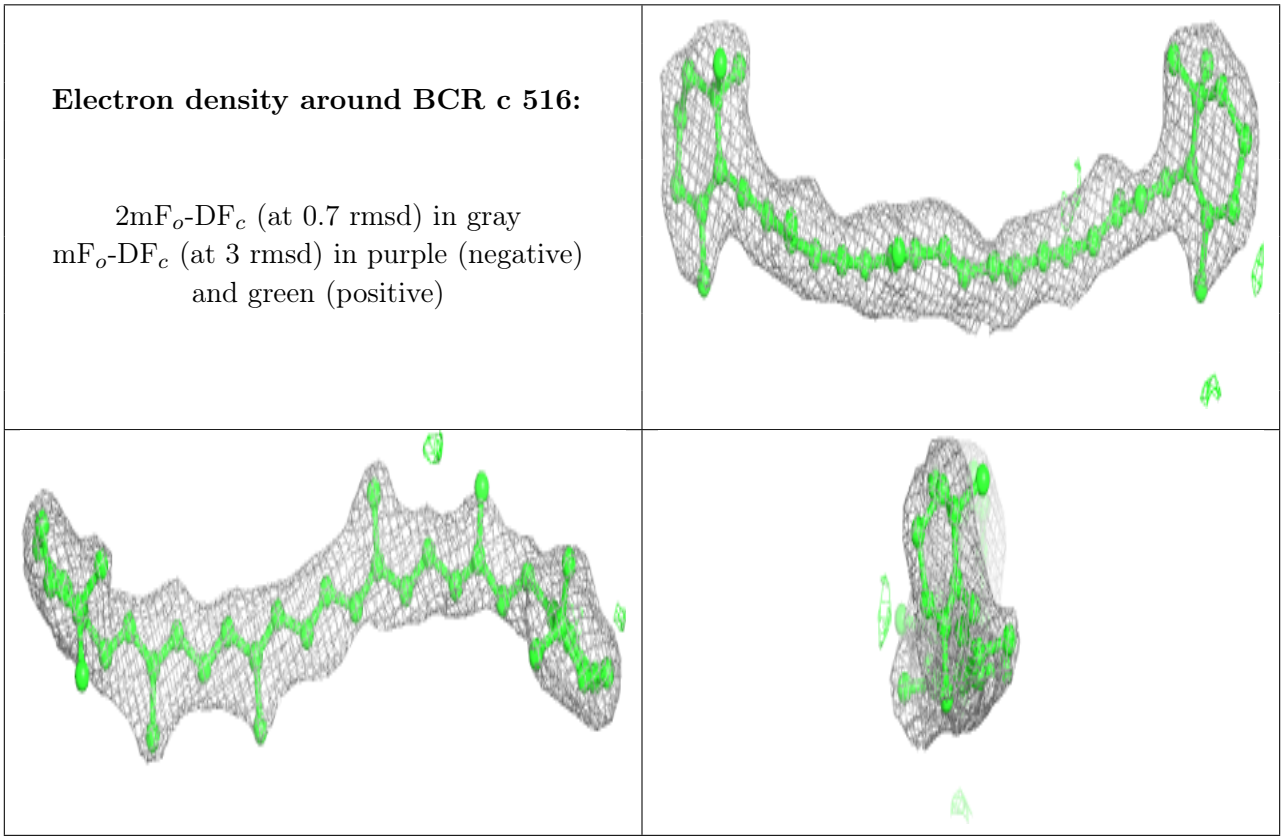
Electron density around LMG m 101:

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



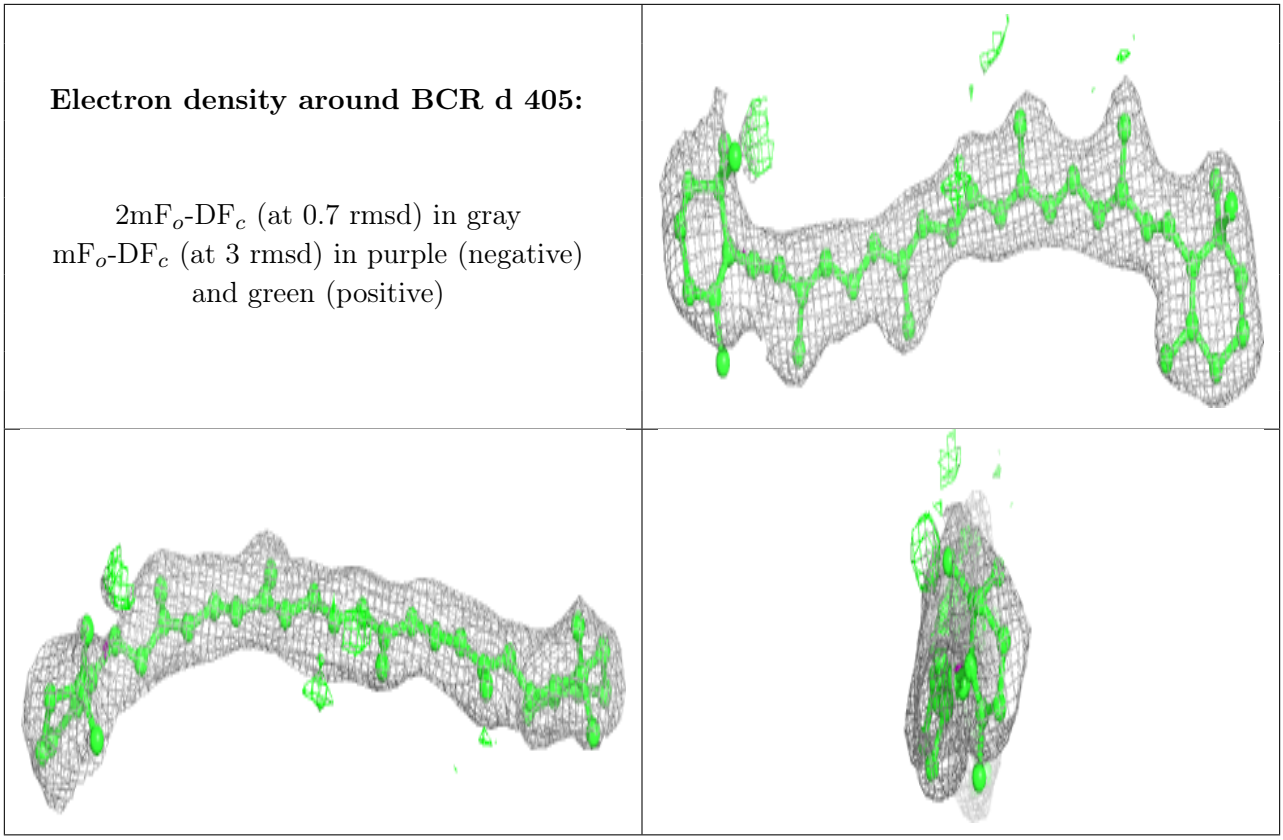
Electron density around BCR c 516:

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



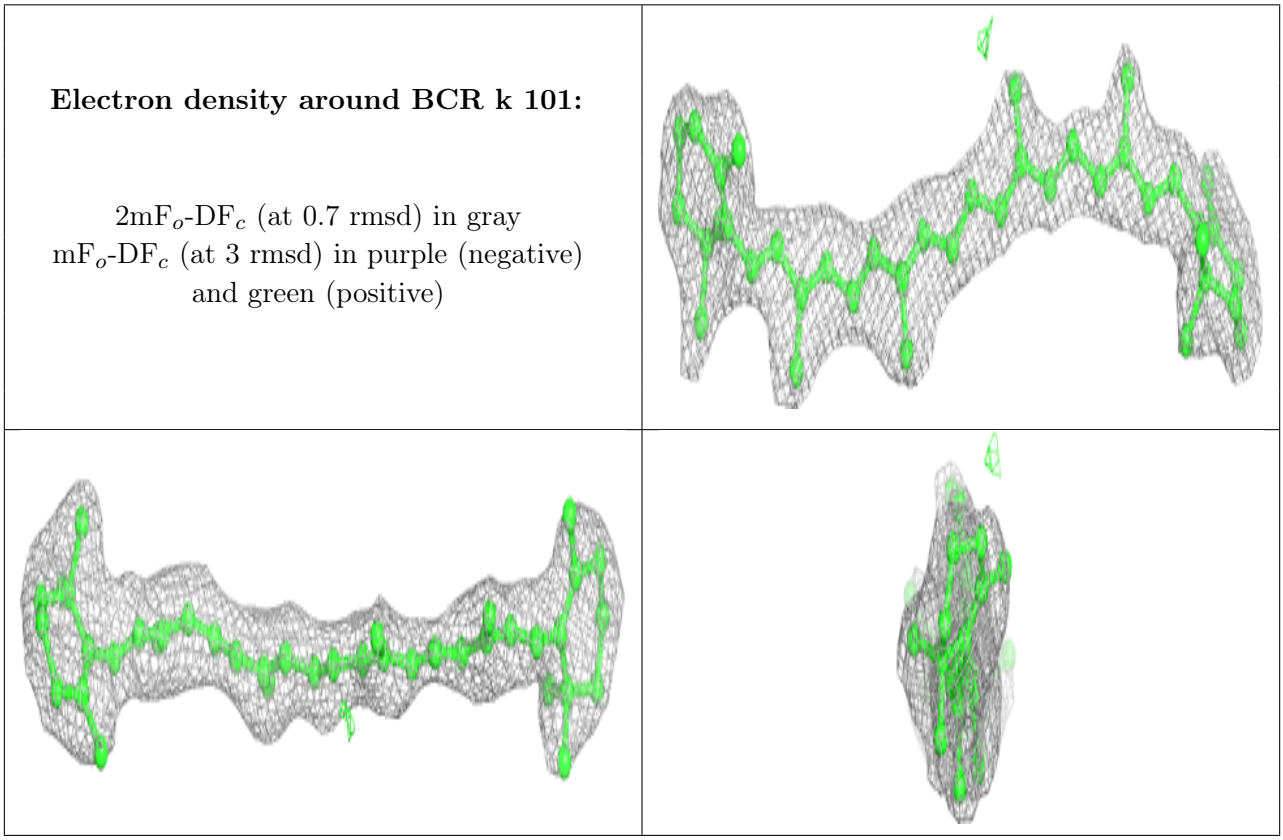
Electron density around BCR d 405:

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



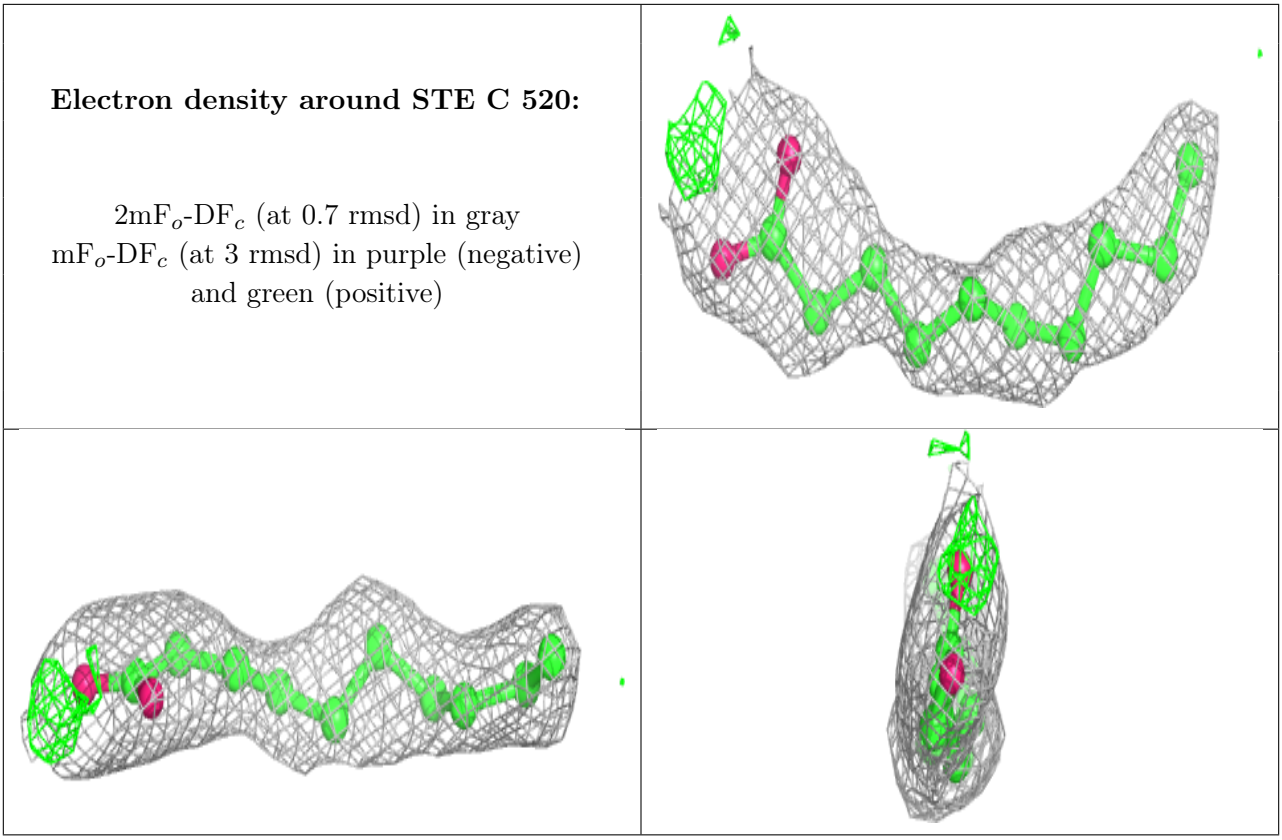
Electron density around BCR k 101:

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



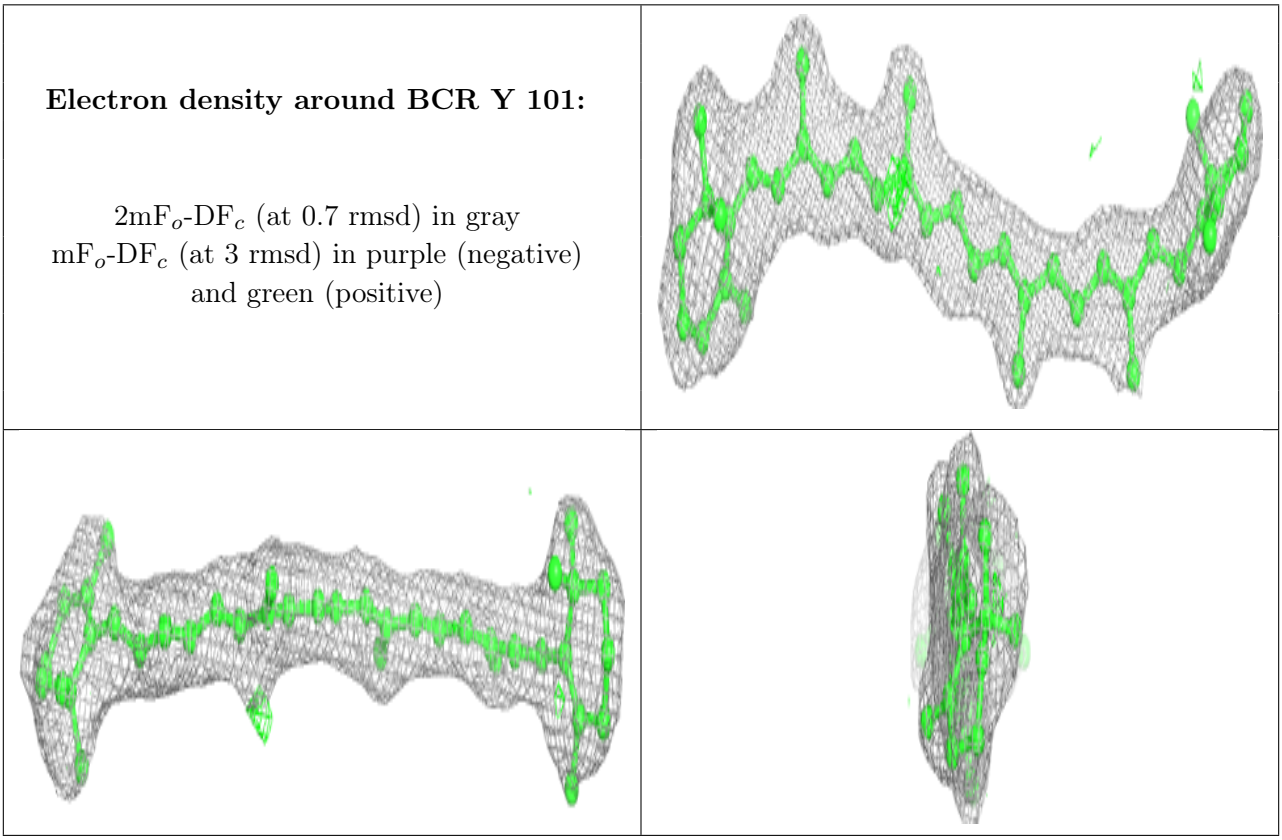
Electron density around STE C 520:

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



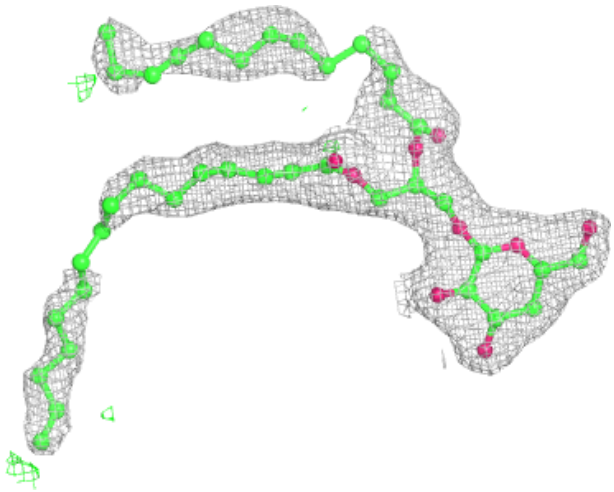
Electron density around BCR Y 101:

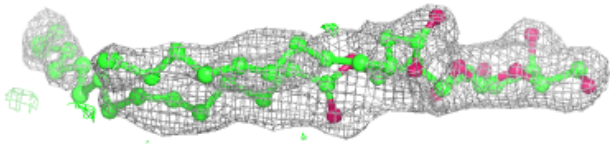
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

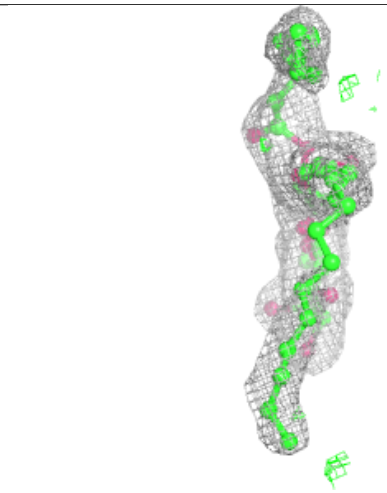


Electron density around LMG C 518:

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

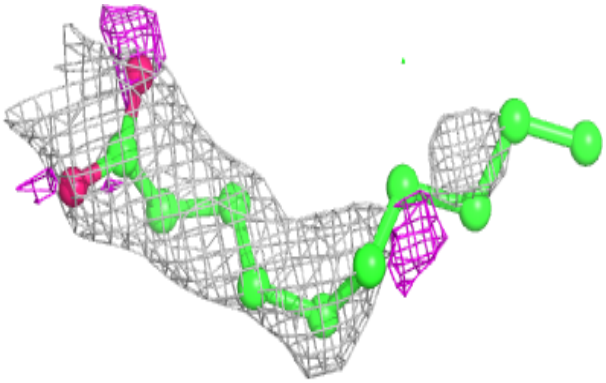


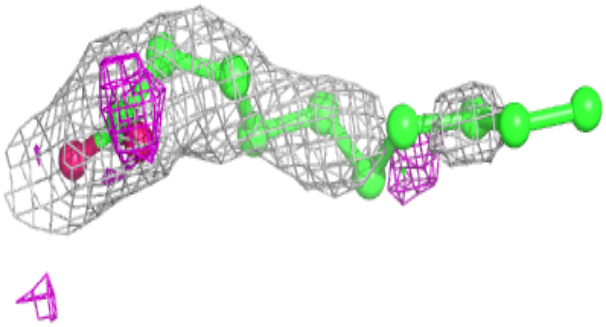


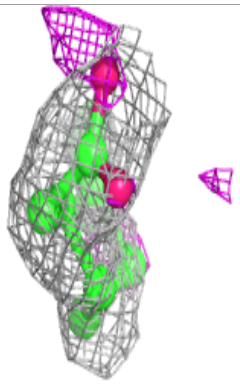


Electron density around STE B 625:

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

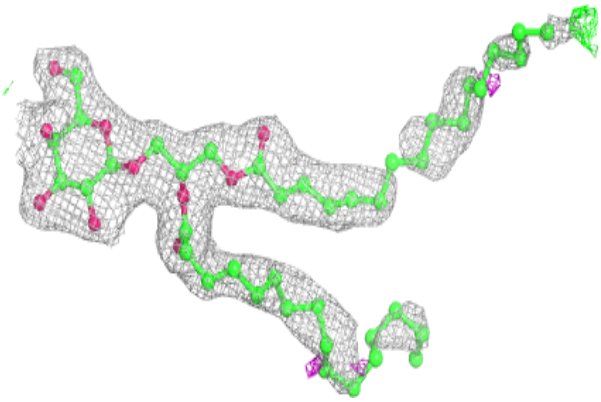


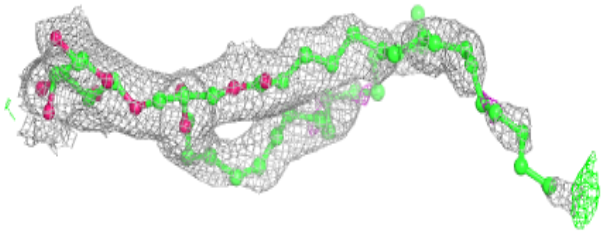


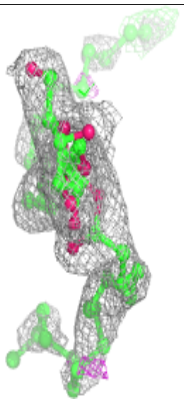


Electron density around LMG D 408:

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

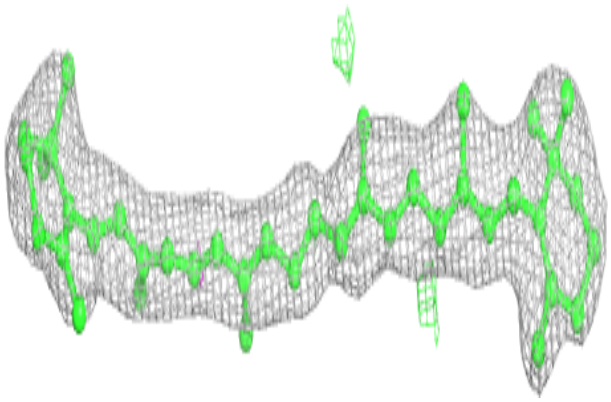


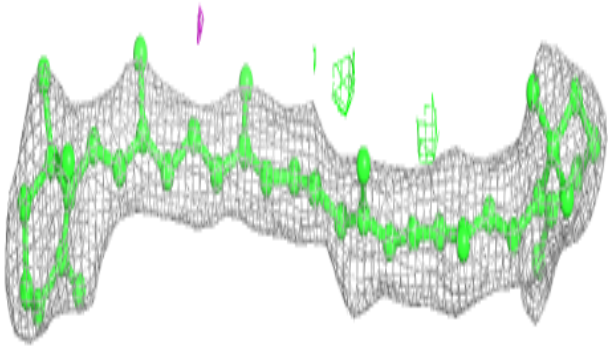


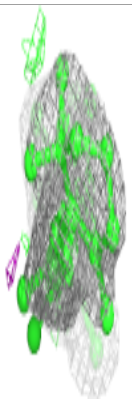


Electron density around BCR K 101:

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

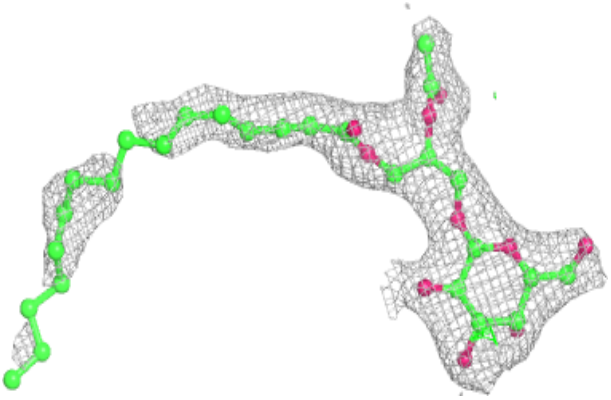


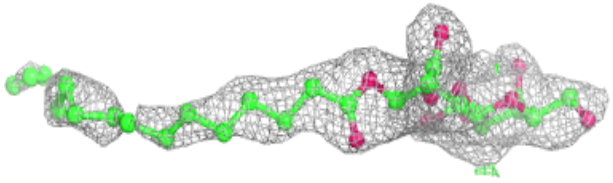




Electron density around LMG c 520:

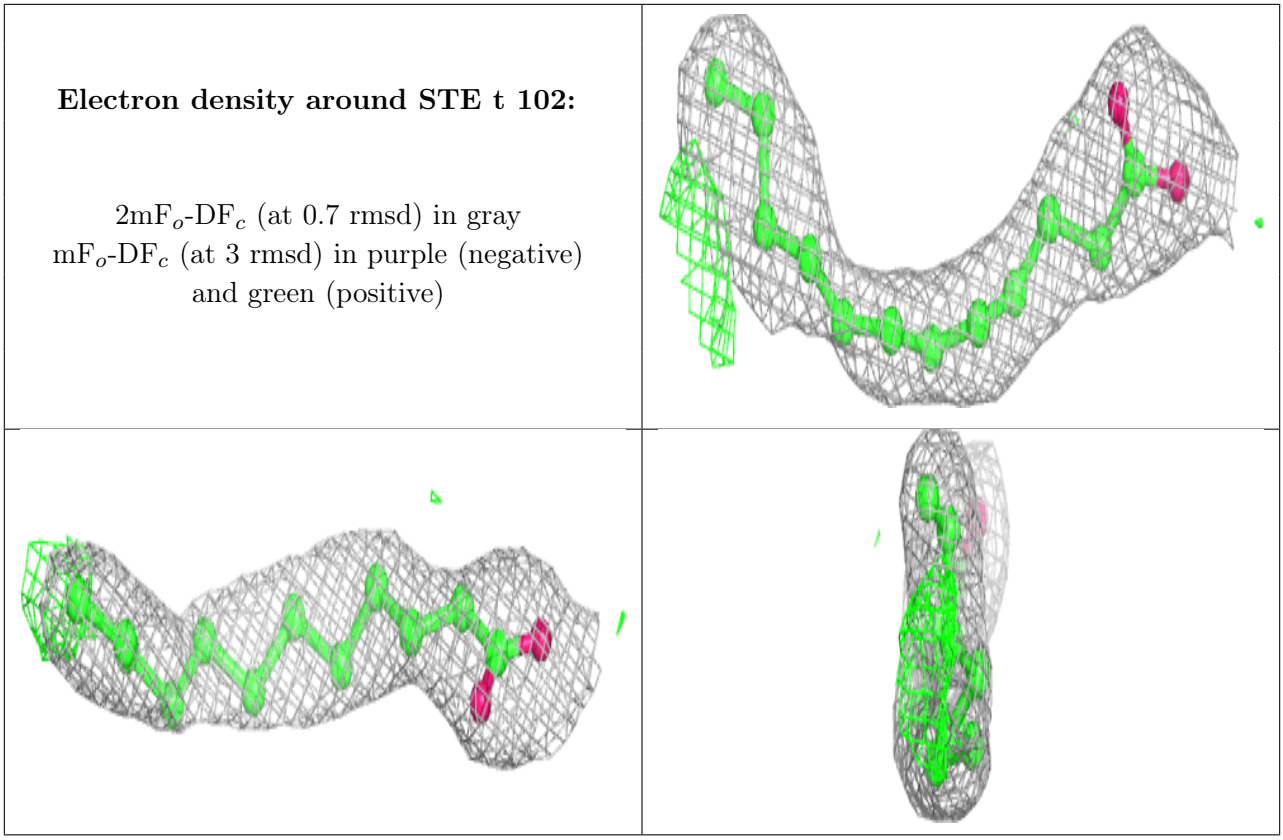
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





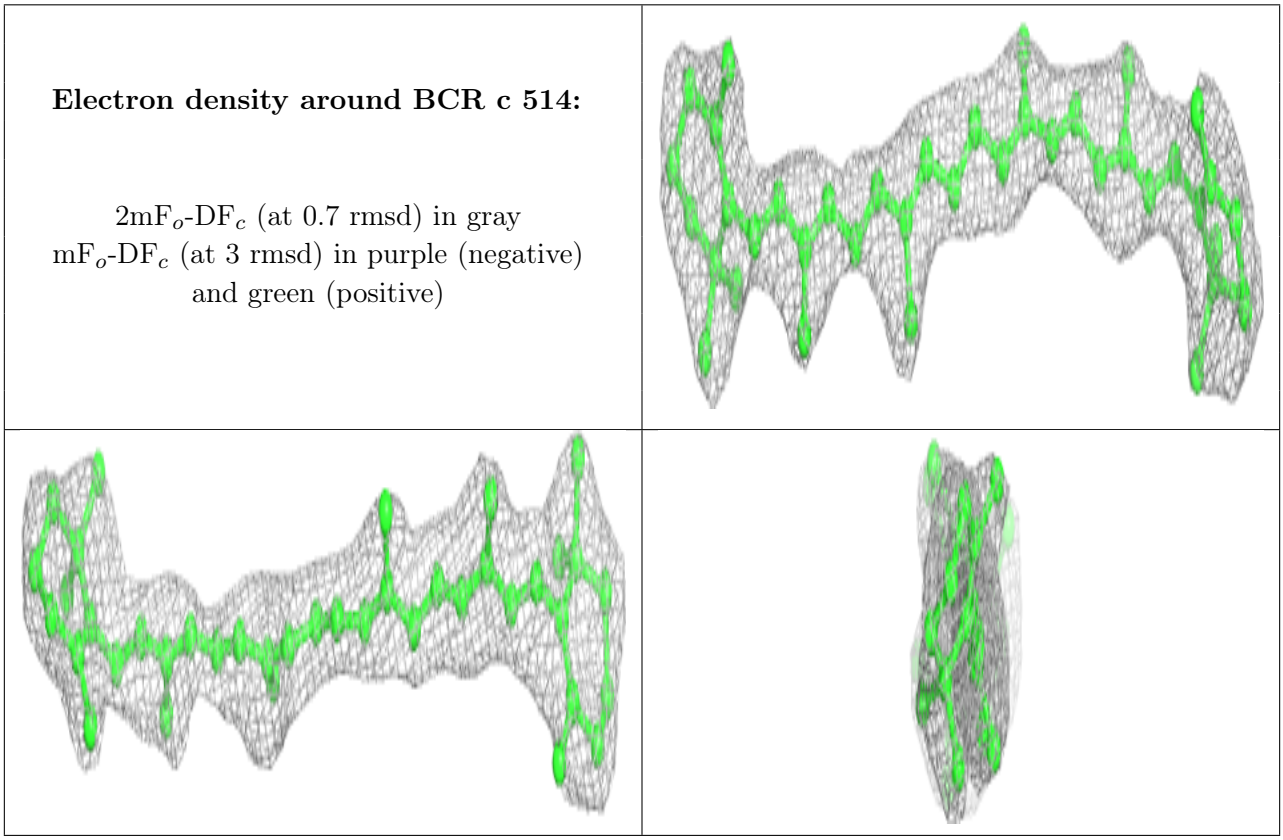
Electron density around STE t 102:

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



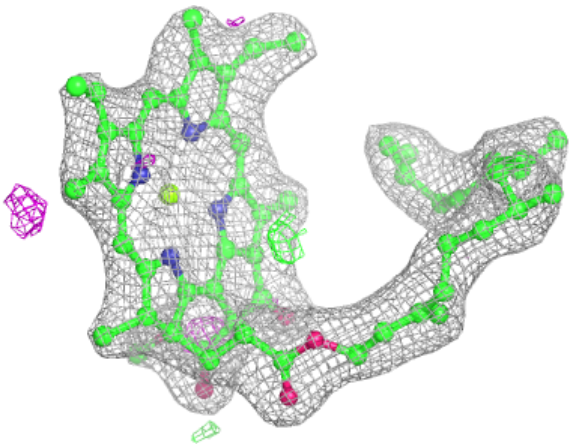
Electron density around BCR c 514:

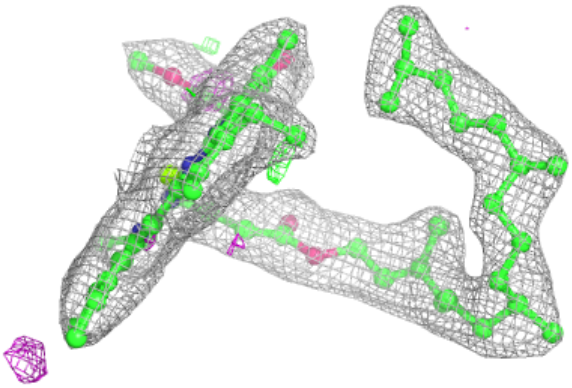
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

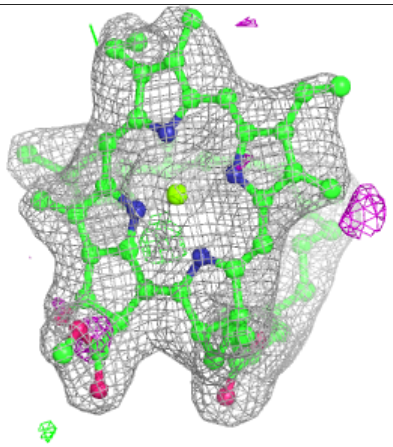


Electron density around CLA c 503:

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

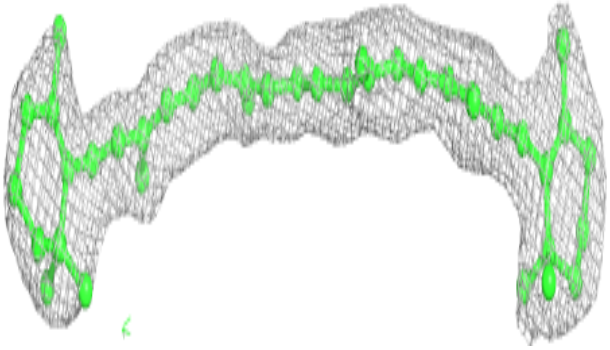


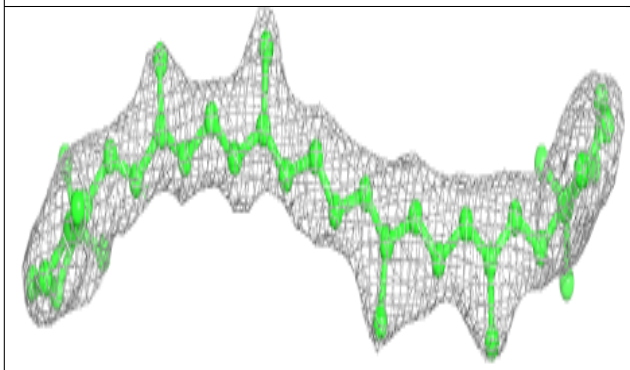


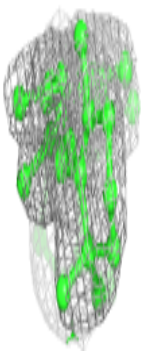


Electron density around BCR K 102:

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

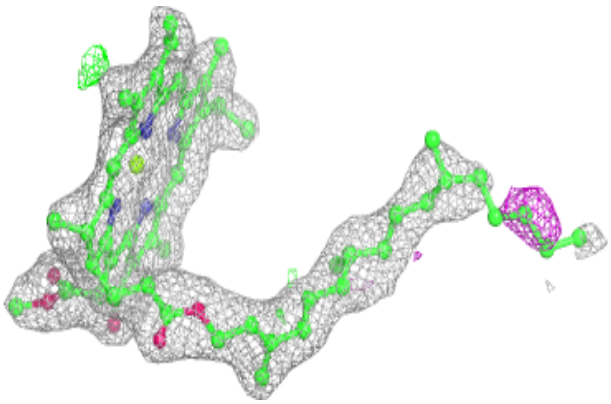


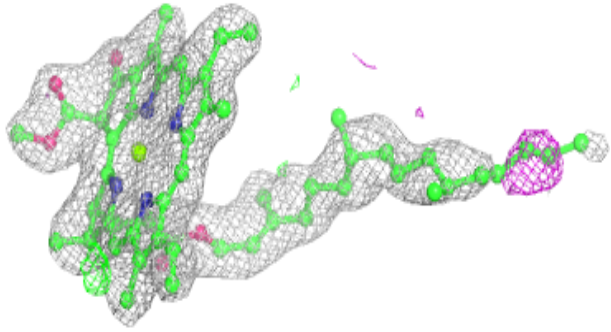


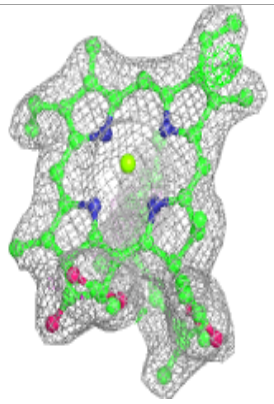


Electron density around CLA c 508:

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

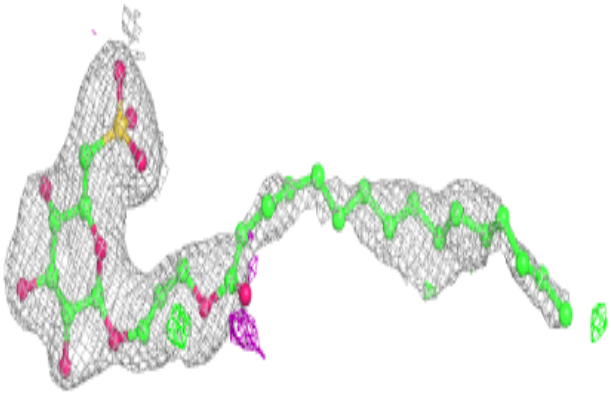


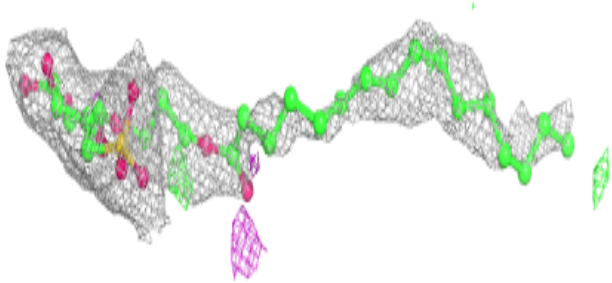


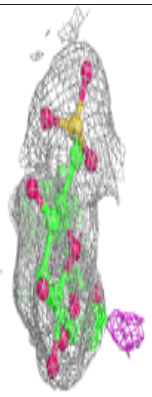


Electron density around SQD F 101:

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

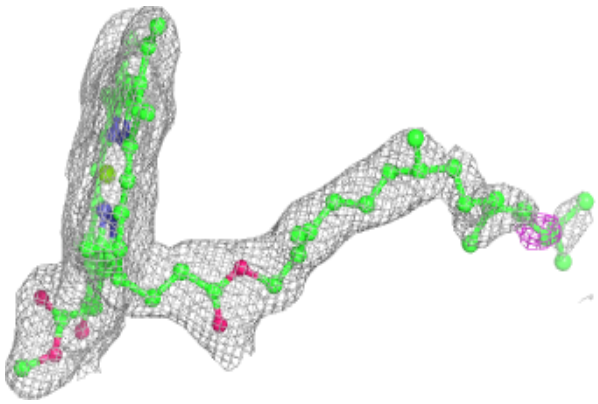


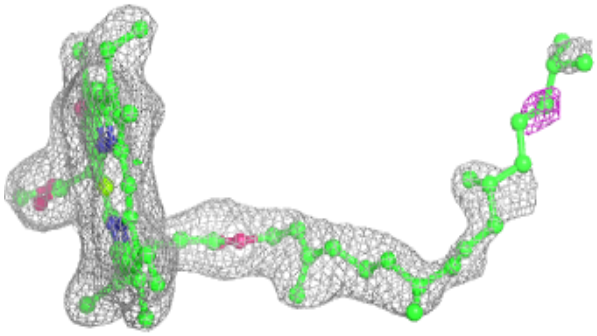


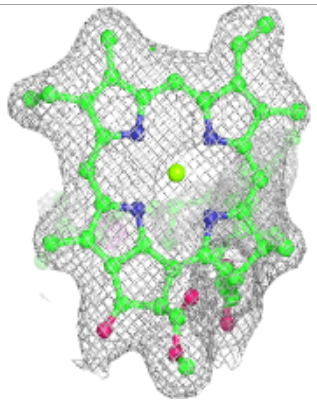


Electron density around CLA D 405:

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

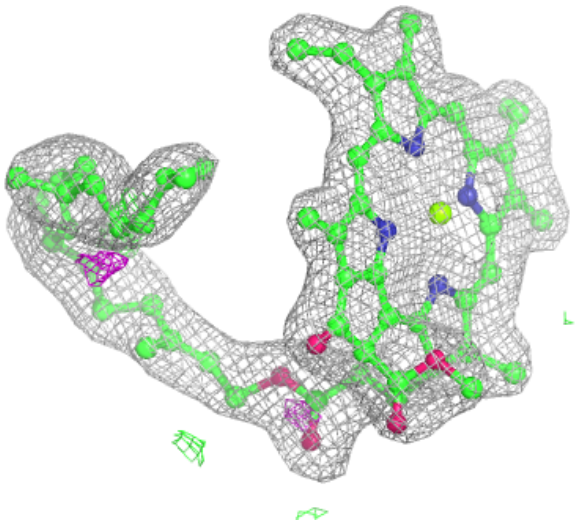


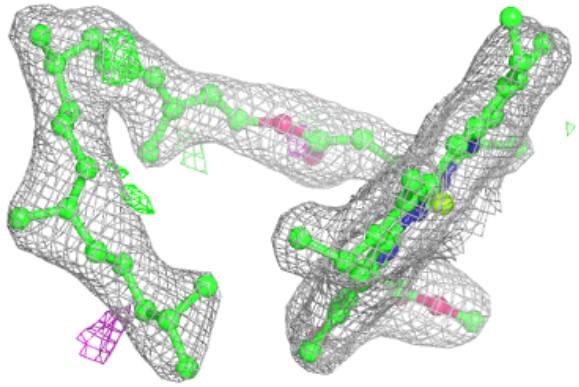


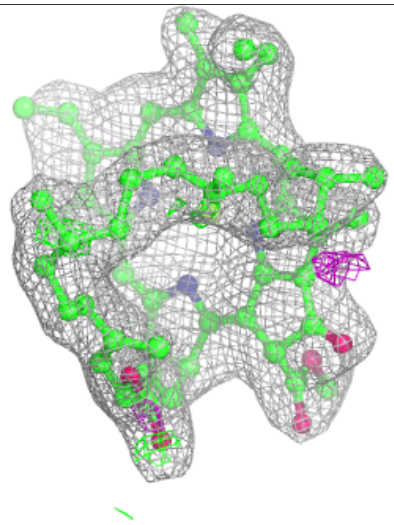


Electron density around CLA C 503:

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

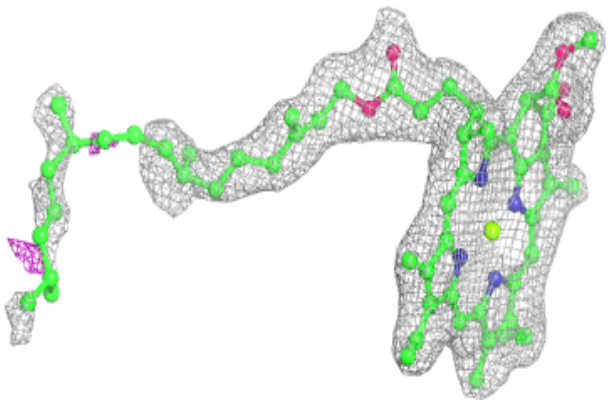


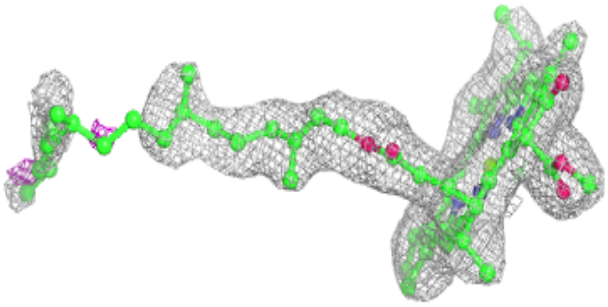


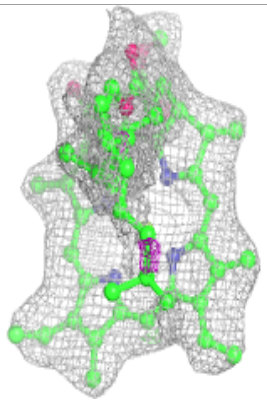


Electron density around CLA d 404:

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

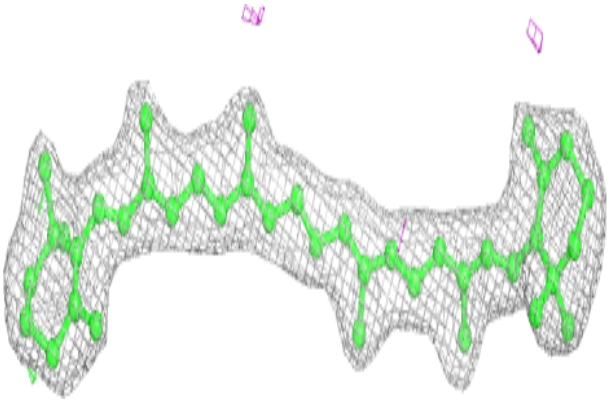


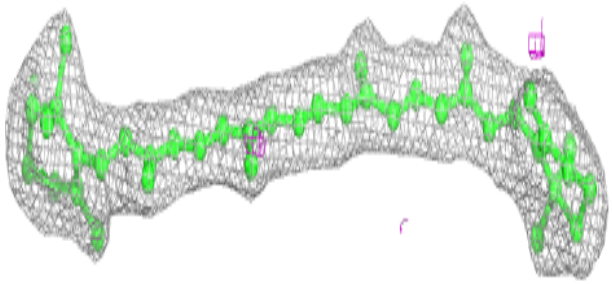


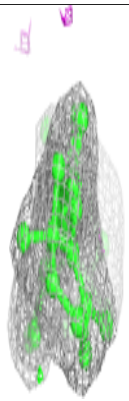


Electron density around BCR B 619:

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

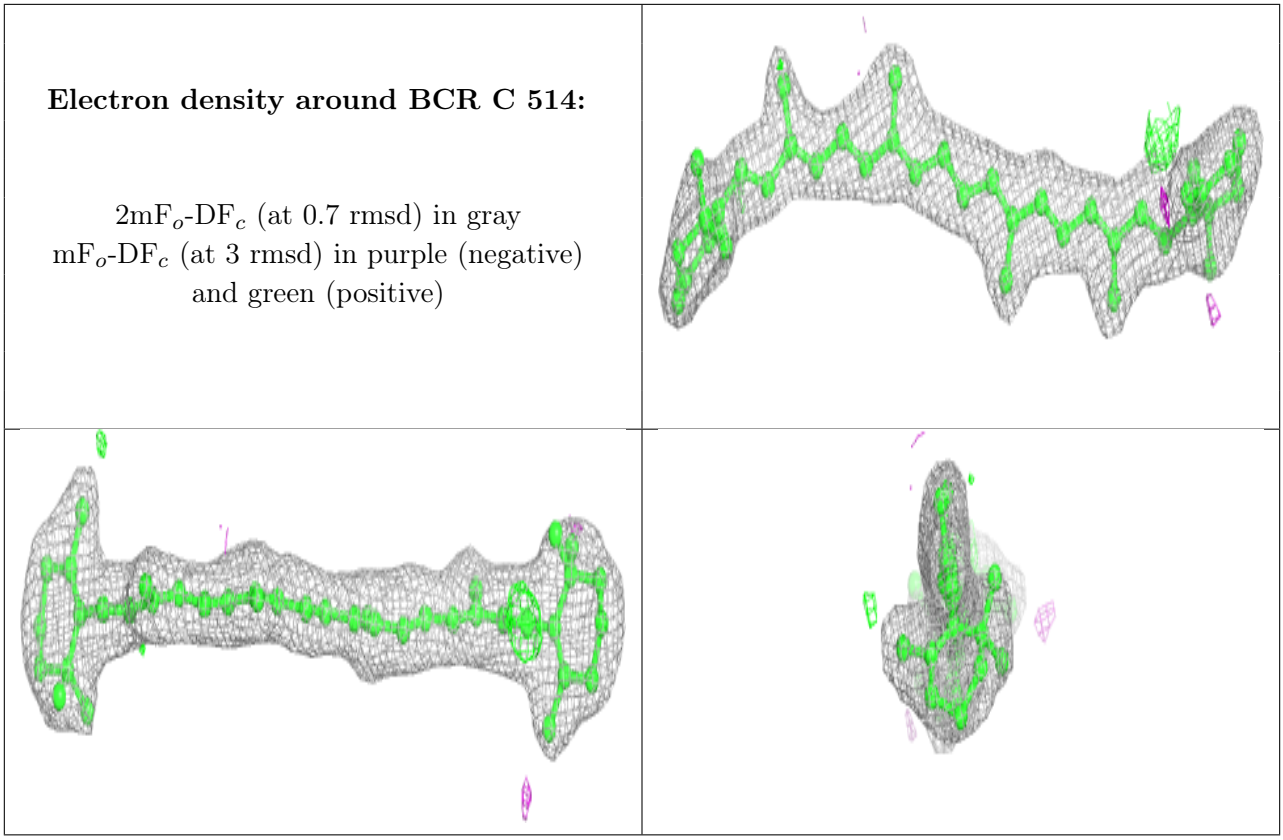






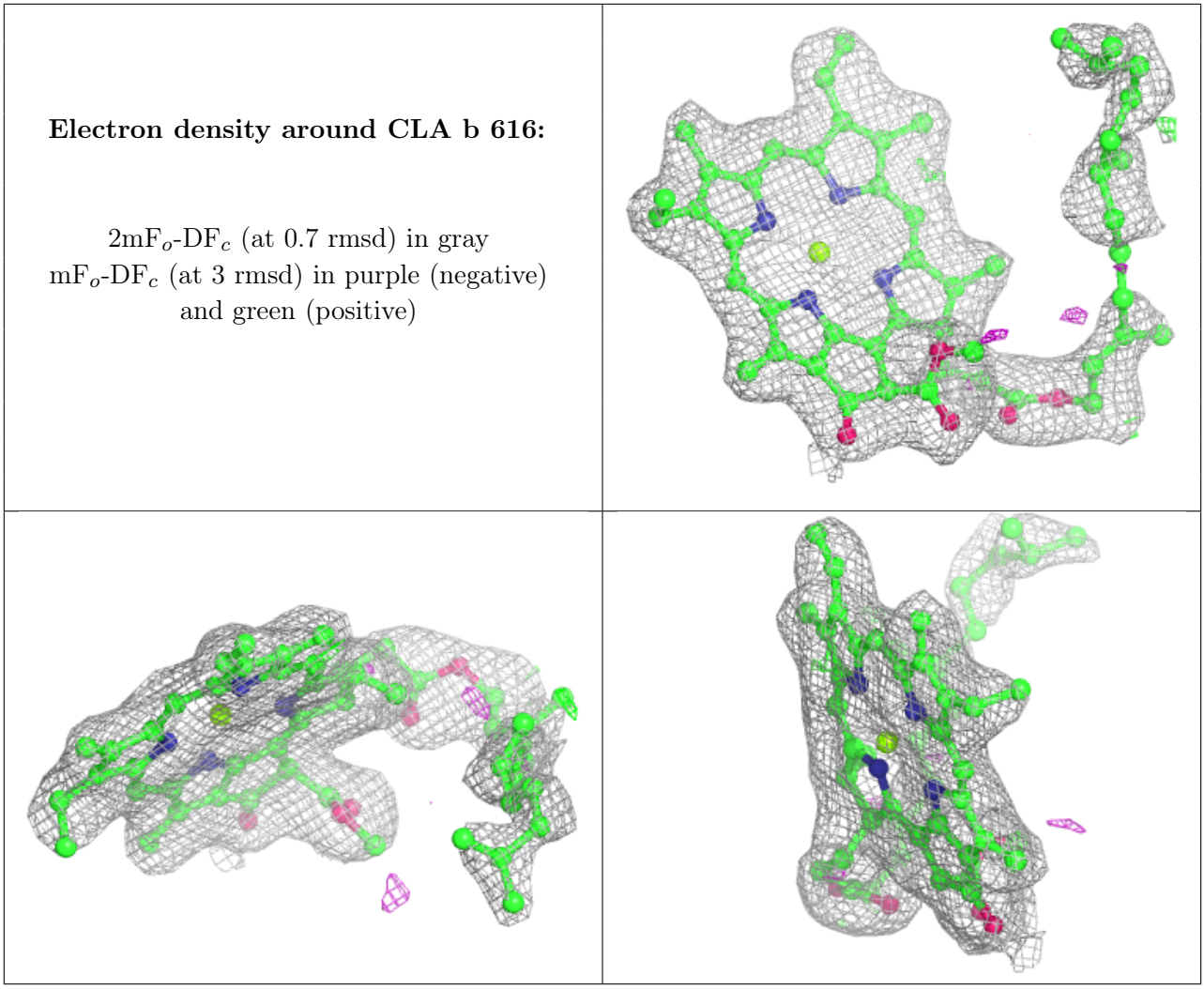
Electron density around BCR C 514:

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



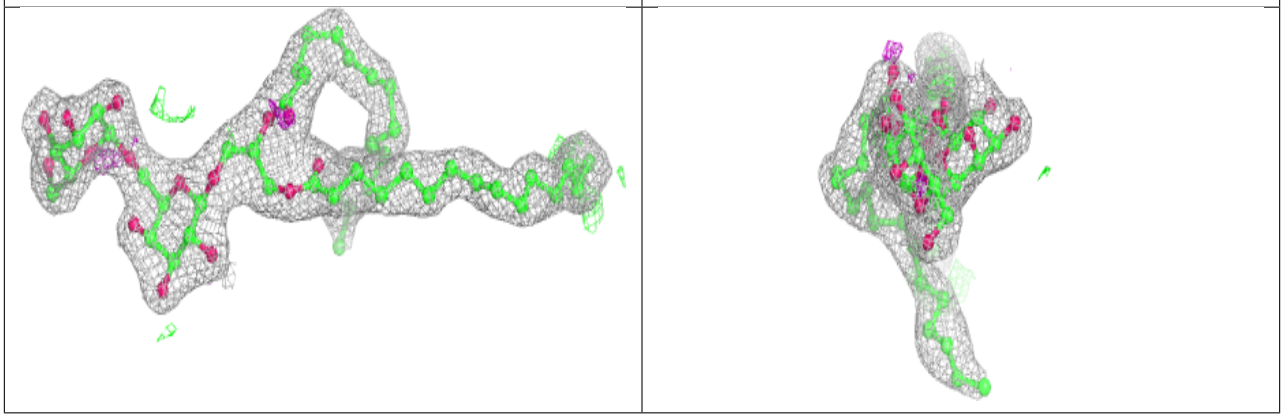
Electron density around CLA b 616:

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



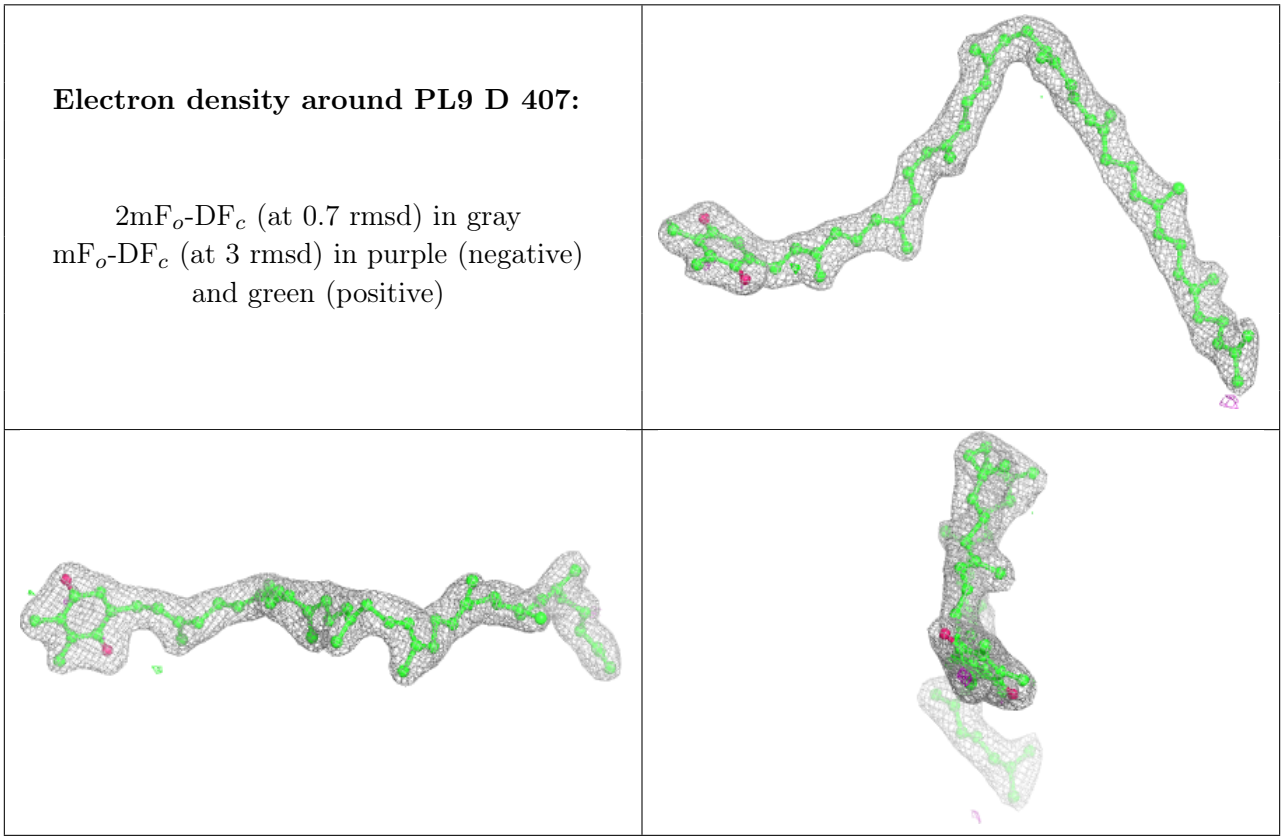
Electron density around DGD H 102:

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



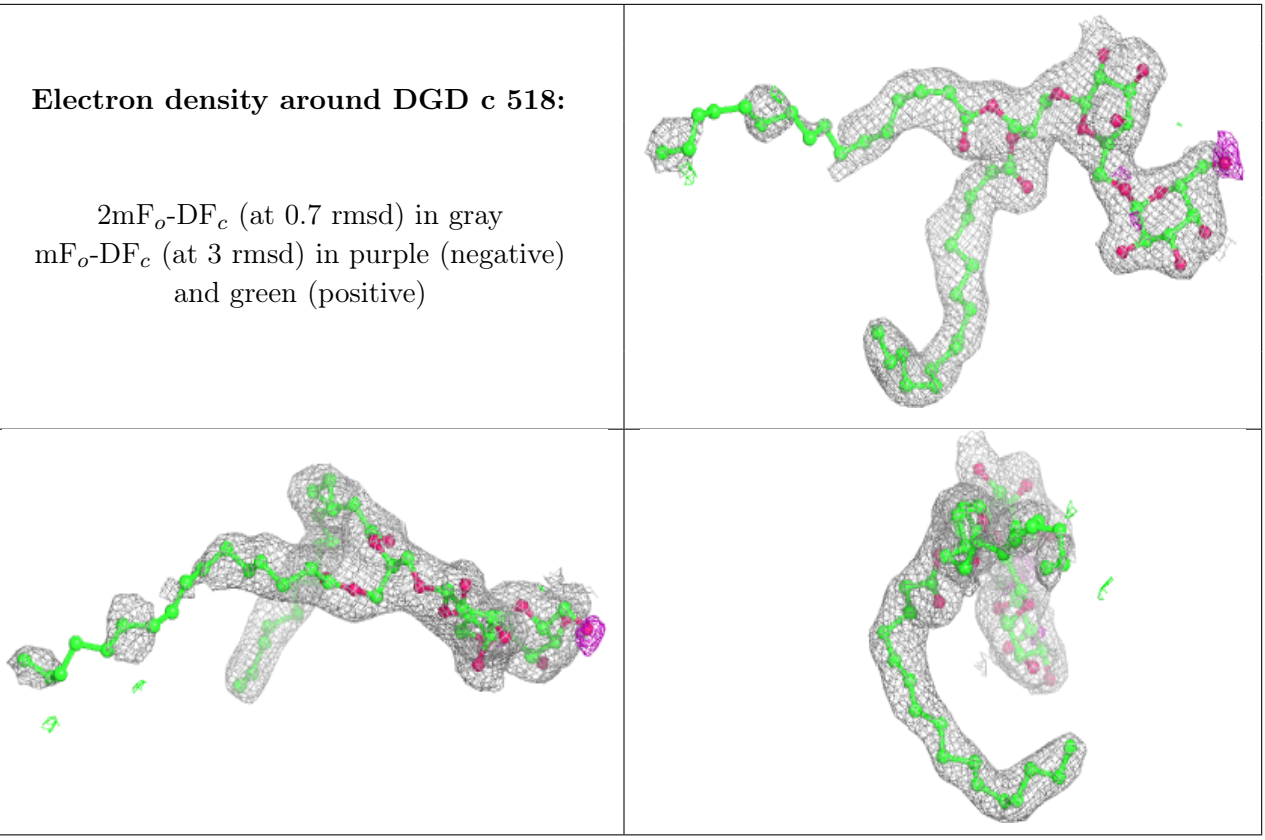
Electron density around PL9 D 407:

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



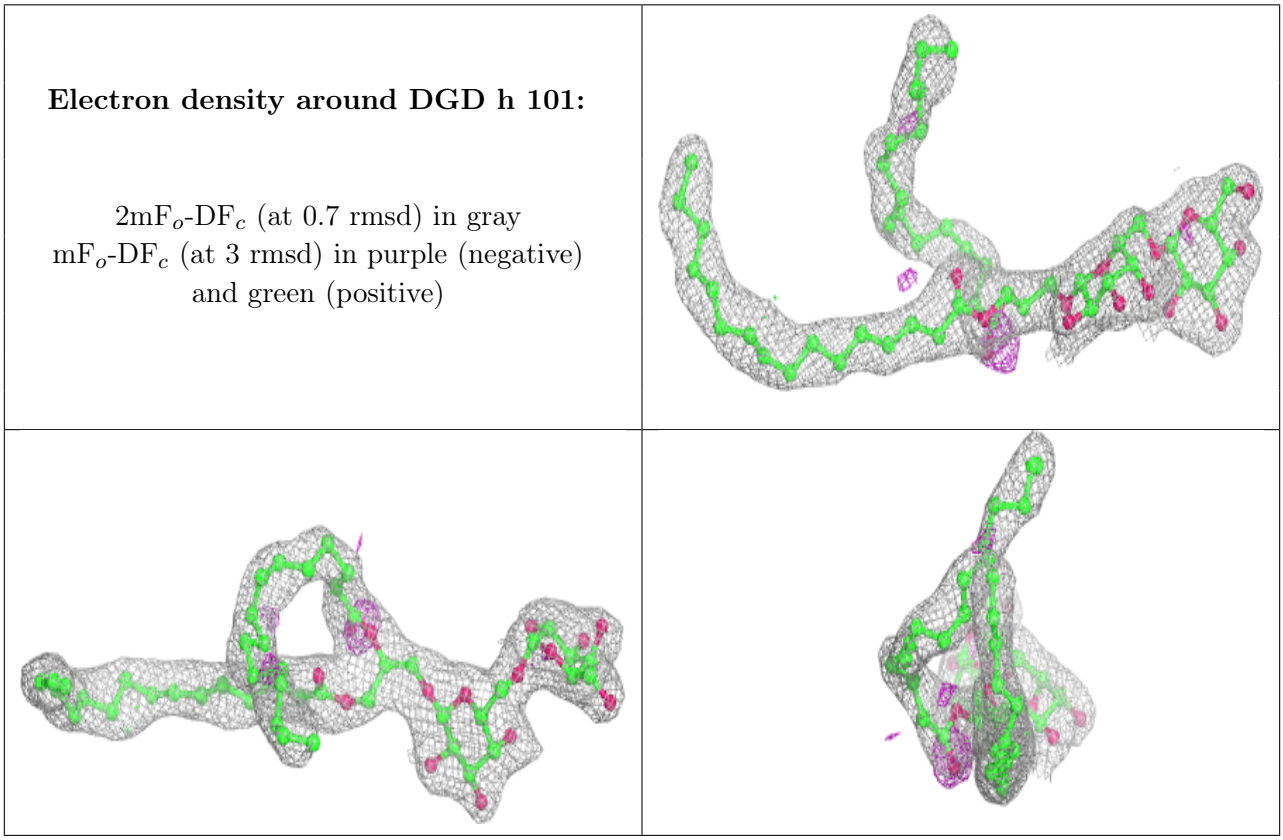
Electron density around DGD c 518:

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



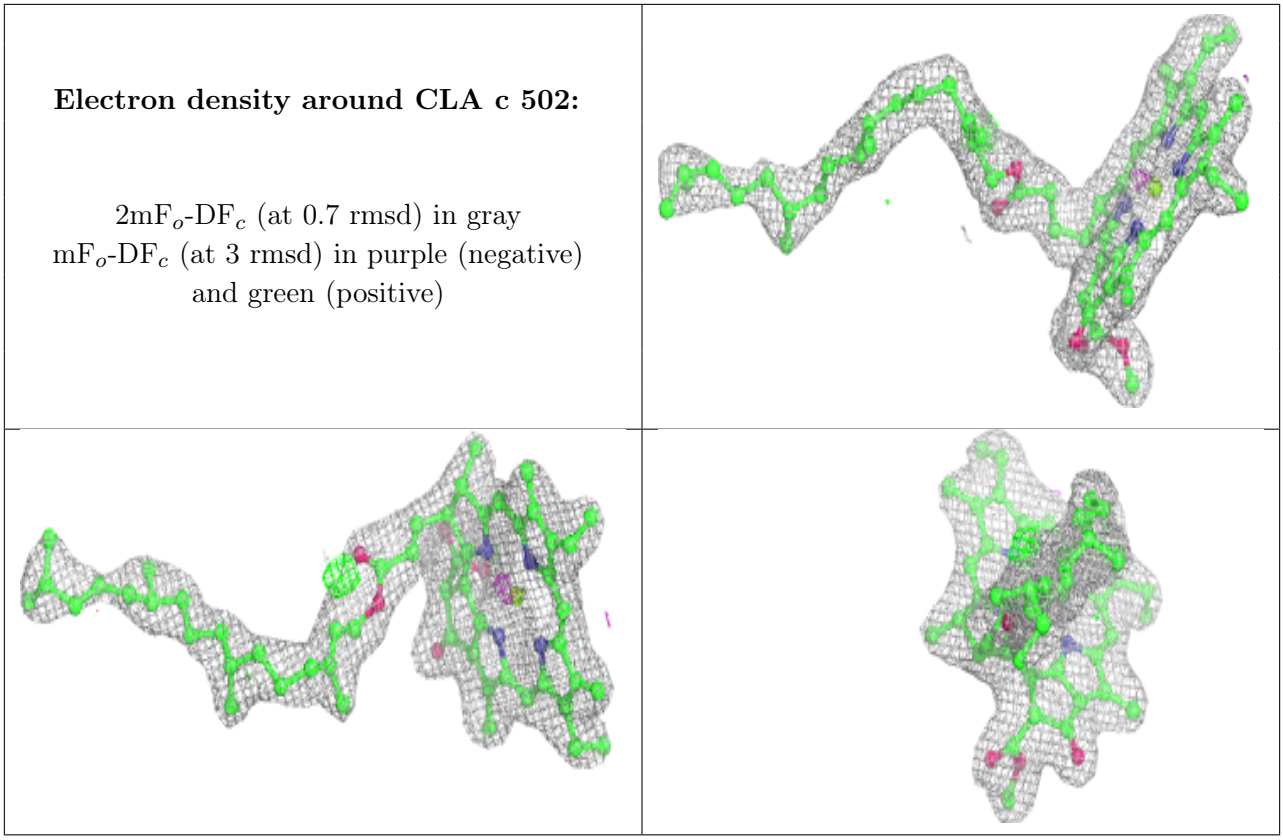
Electron density around DGD h 101:

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



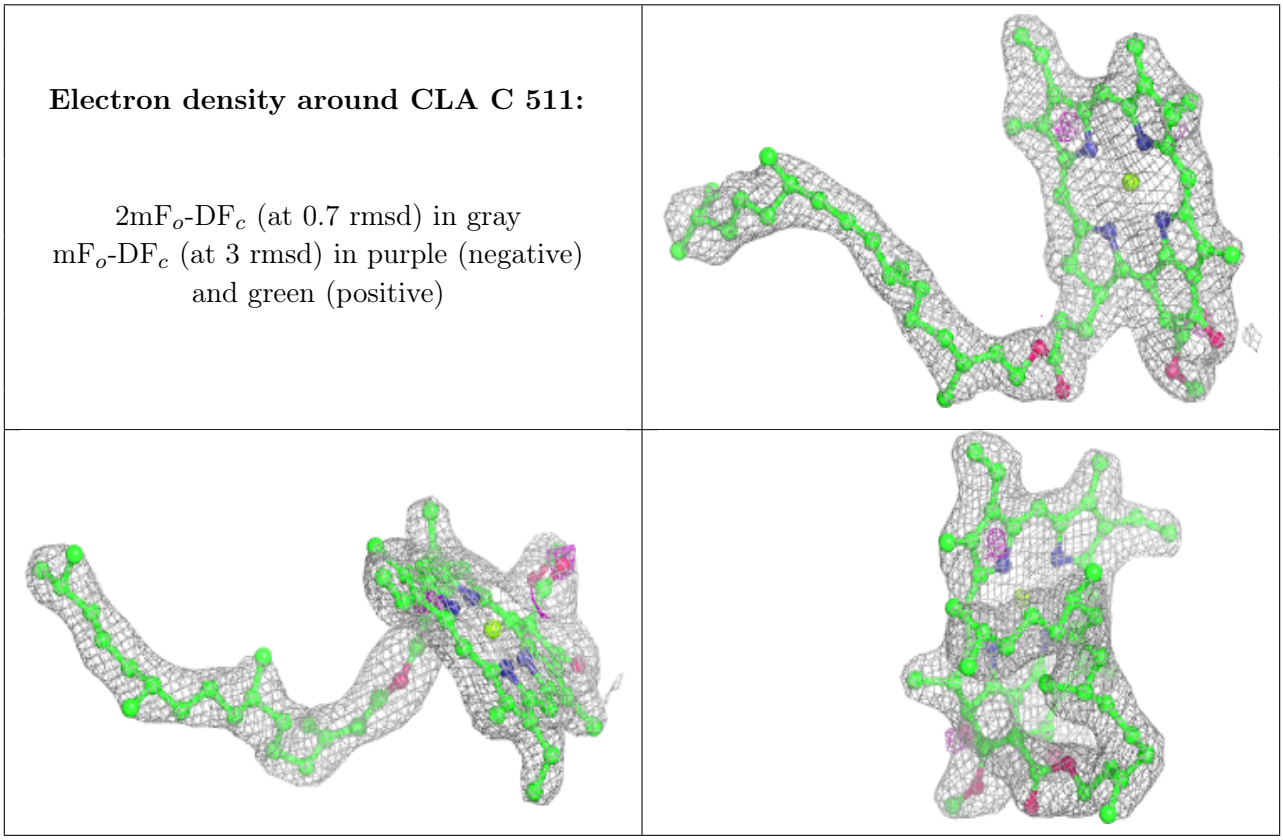
Electron density around CLA c 502:

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



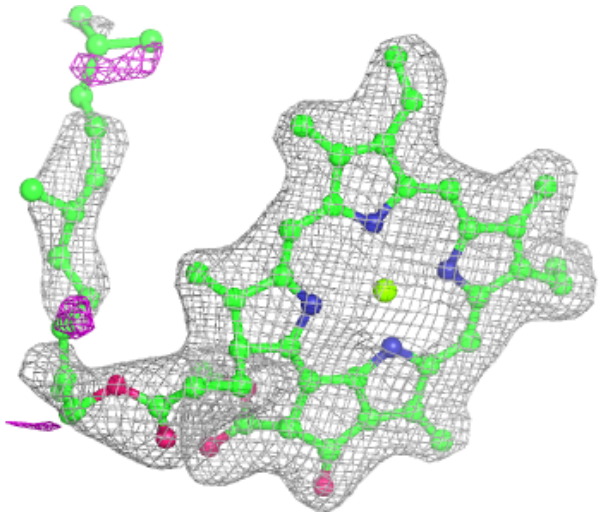
Electron density around CLA C 511:

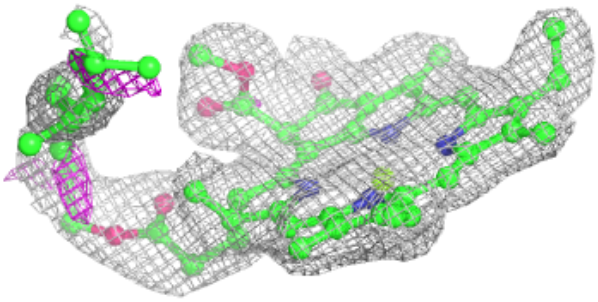
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

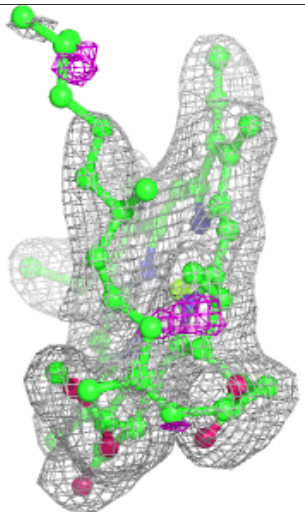


Electron density around CLA B 616:

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

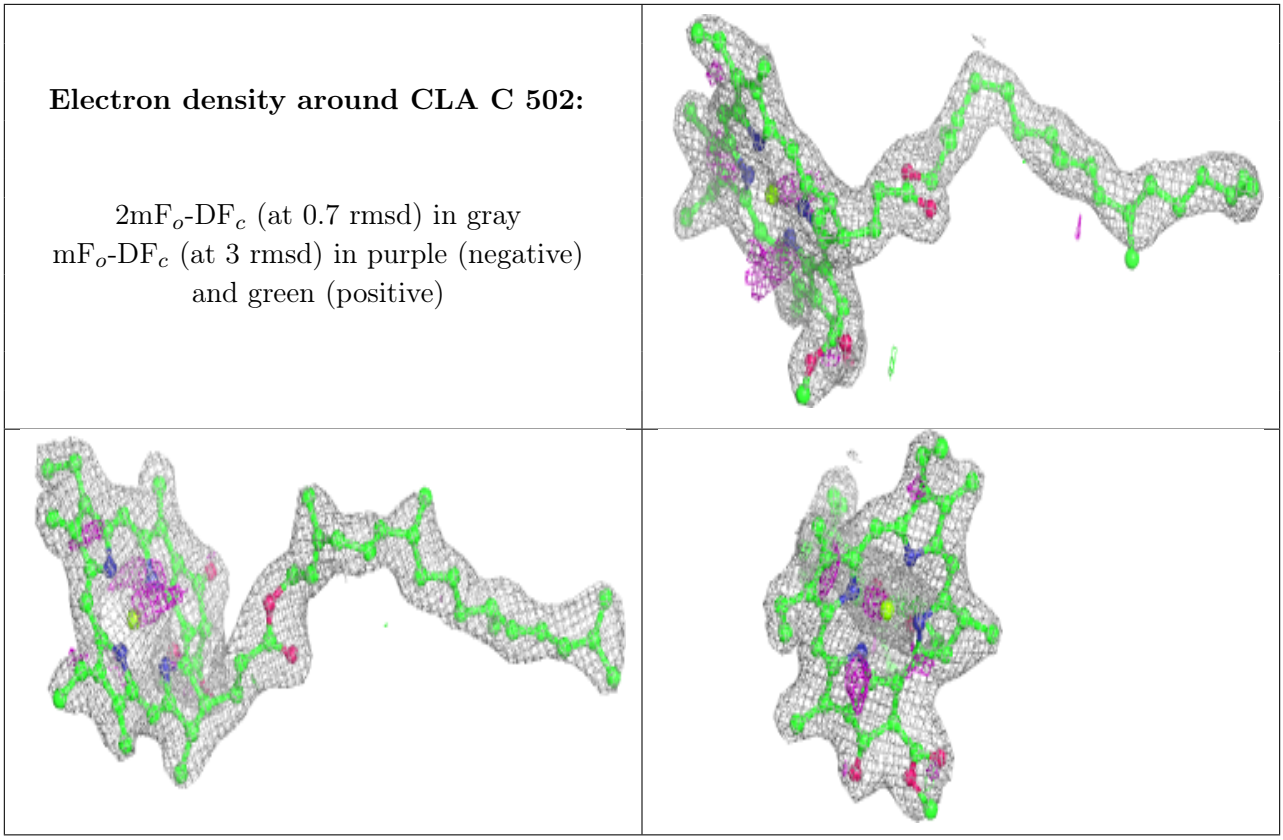






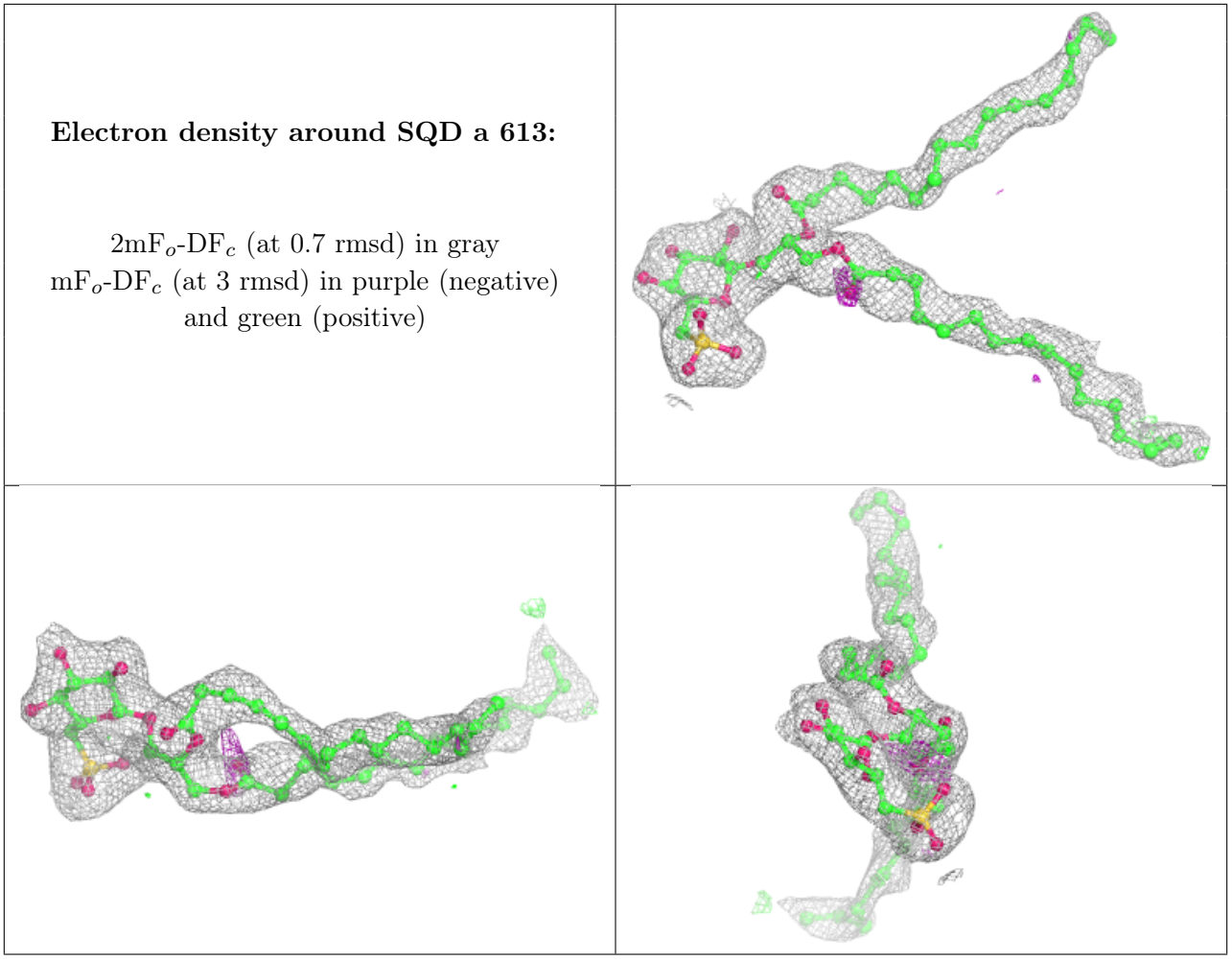
Electron density around CLA C 502:

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



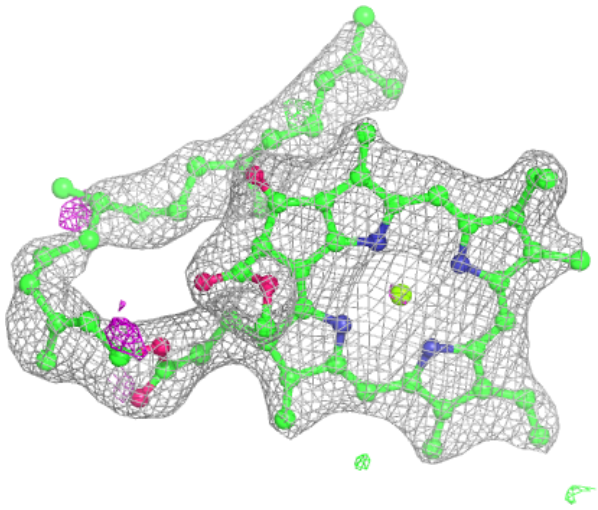
Electron density around SQD a 613:

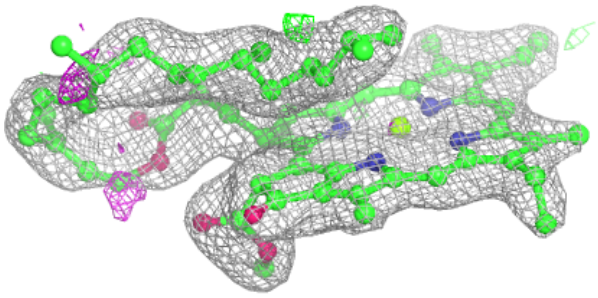
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

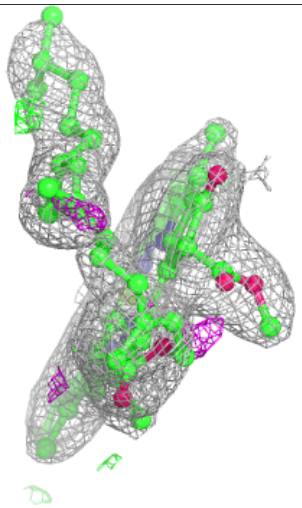


Electron density around CLA c 509:

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

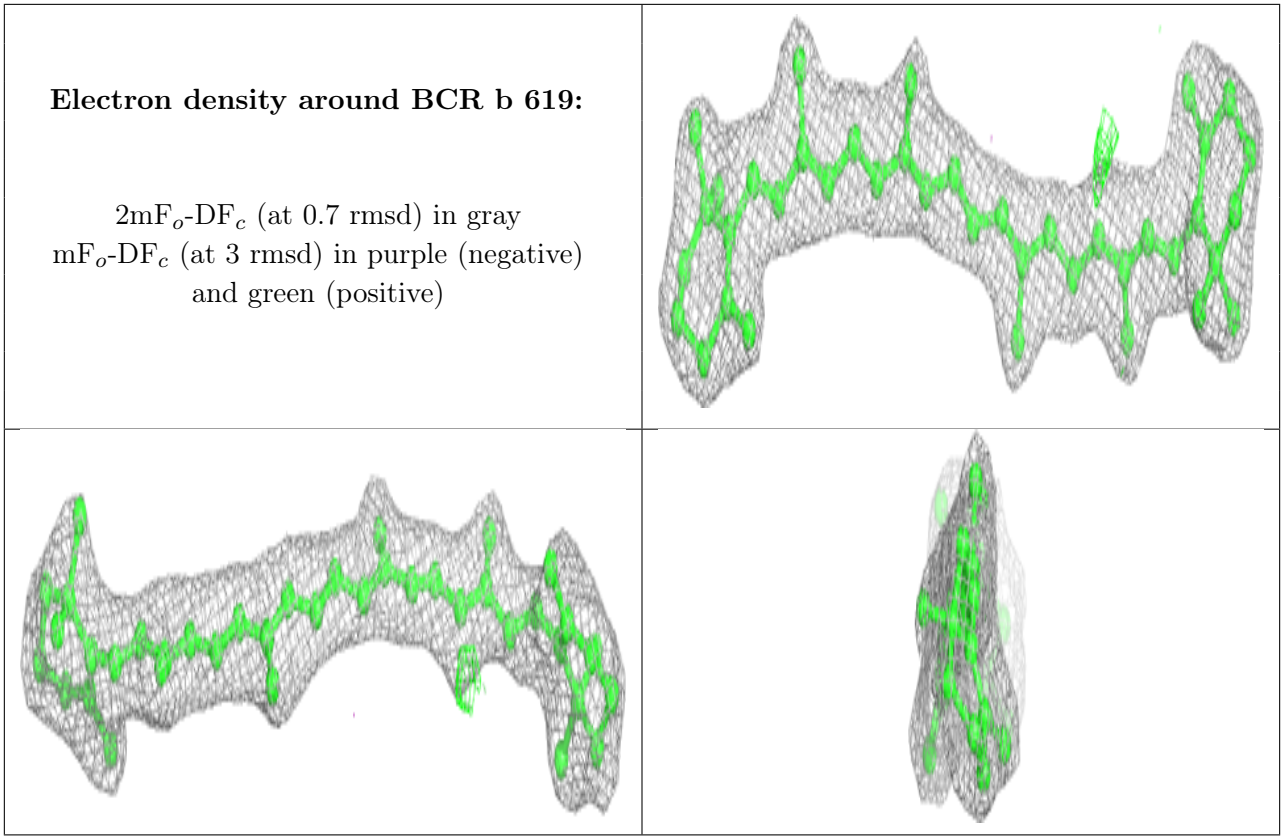






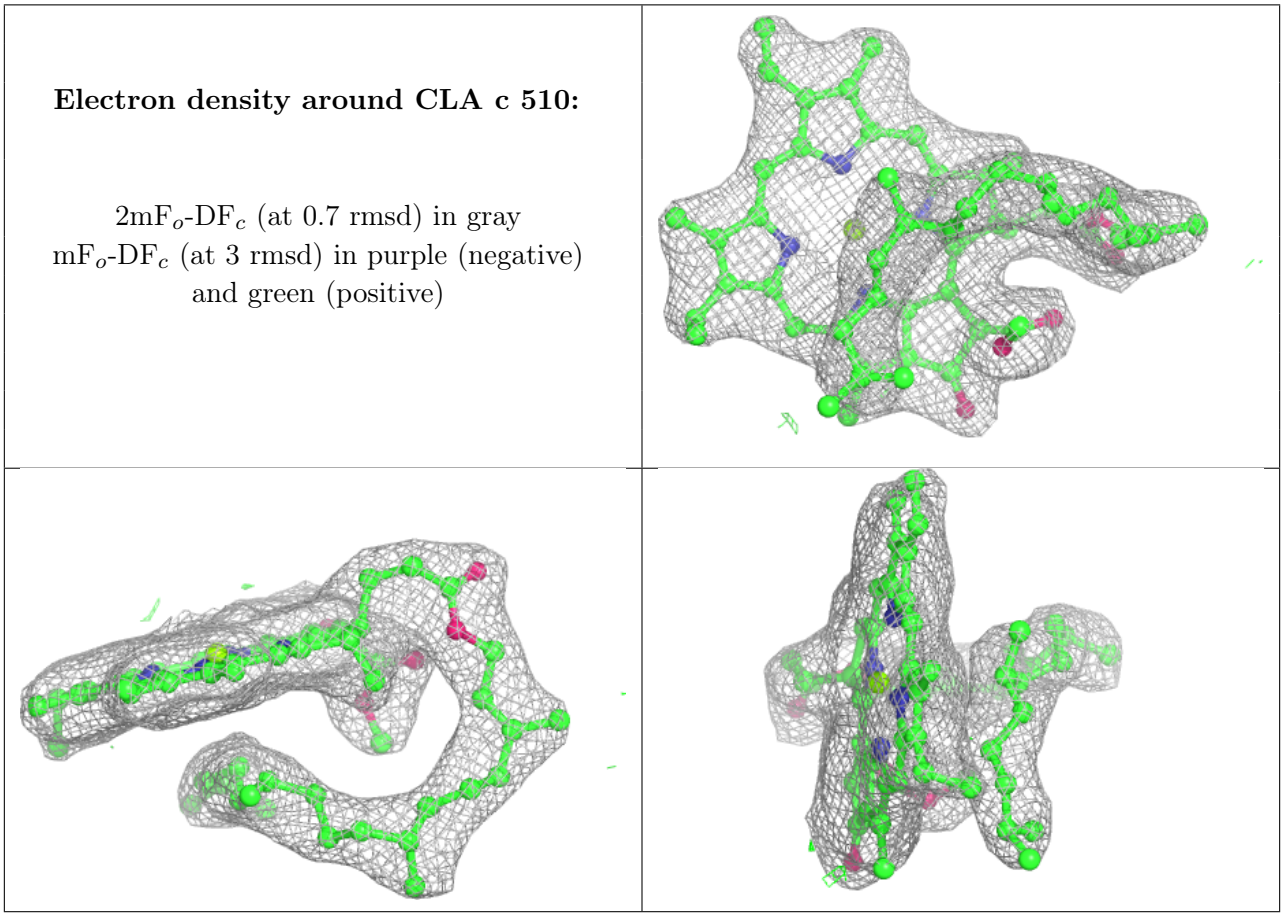
Electron density around BCR b 619:

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



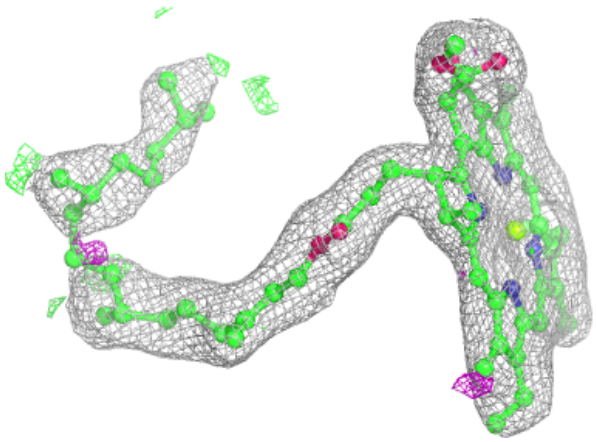
Electron density around CLA c 510:

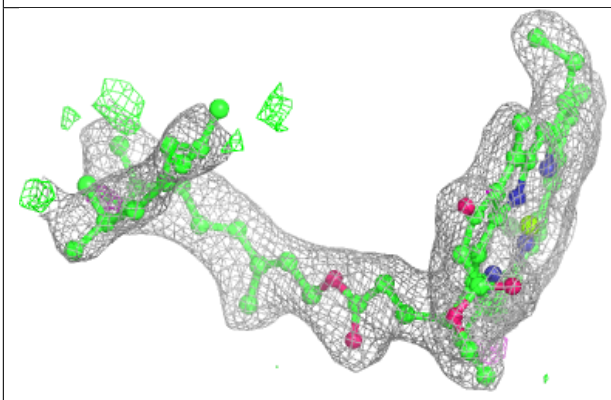
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

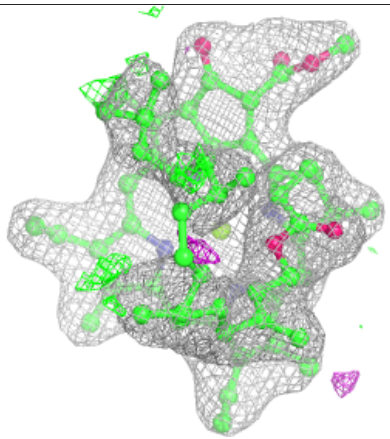


Electron density around CLA B 606:

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

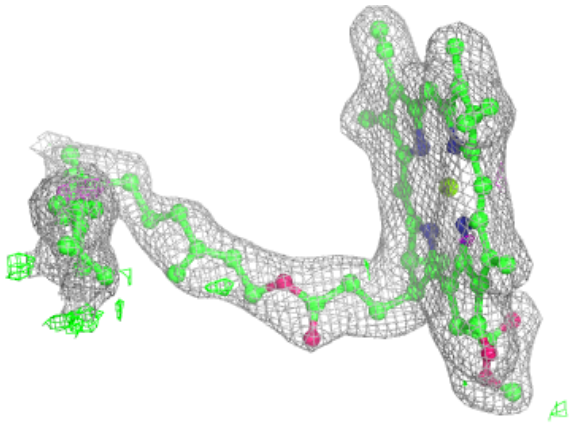


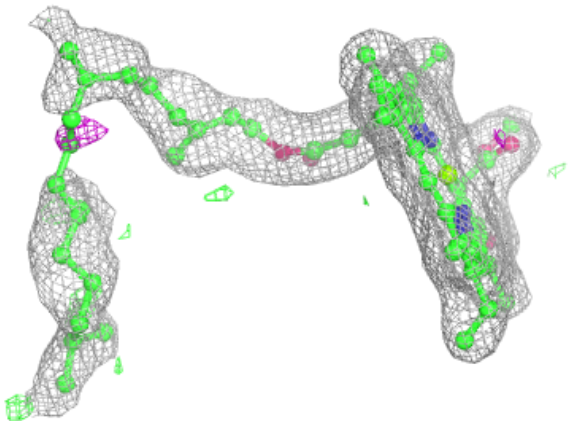


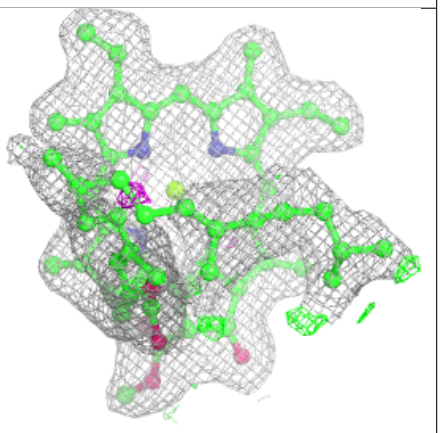


Electron density around CLA a 609:

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

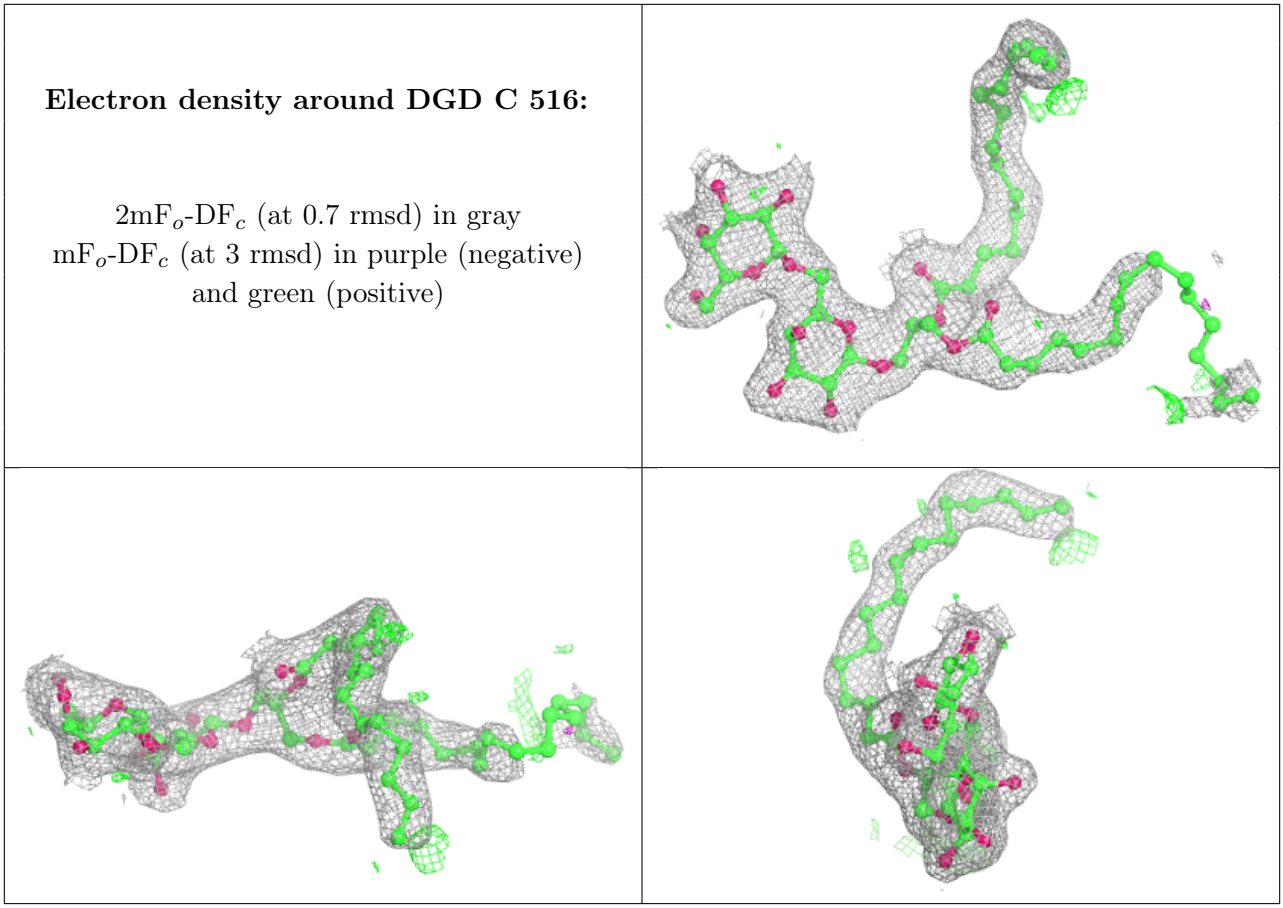






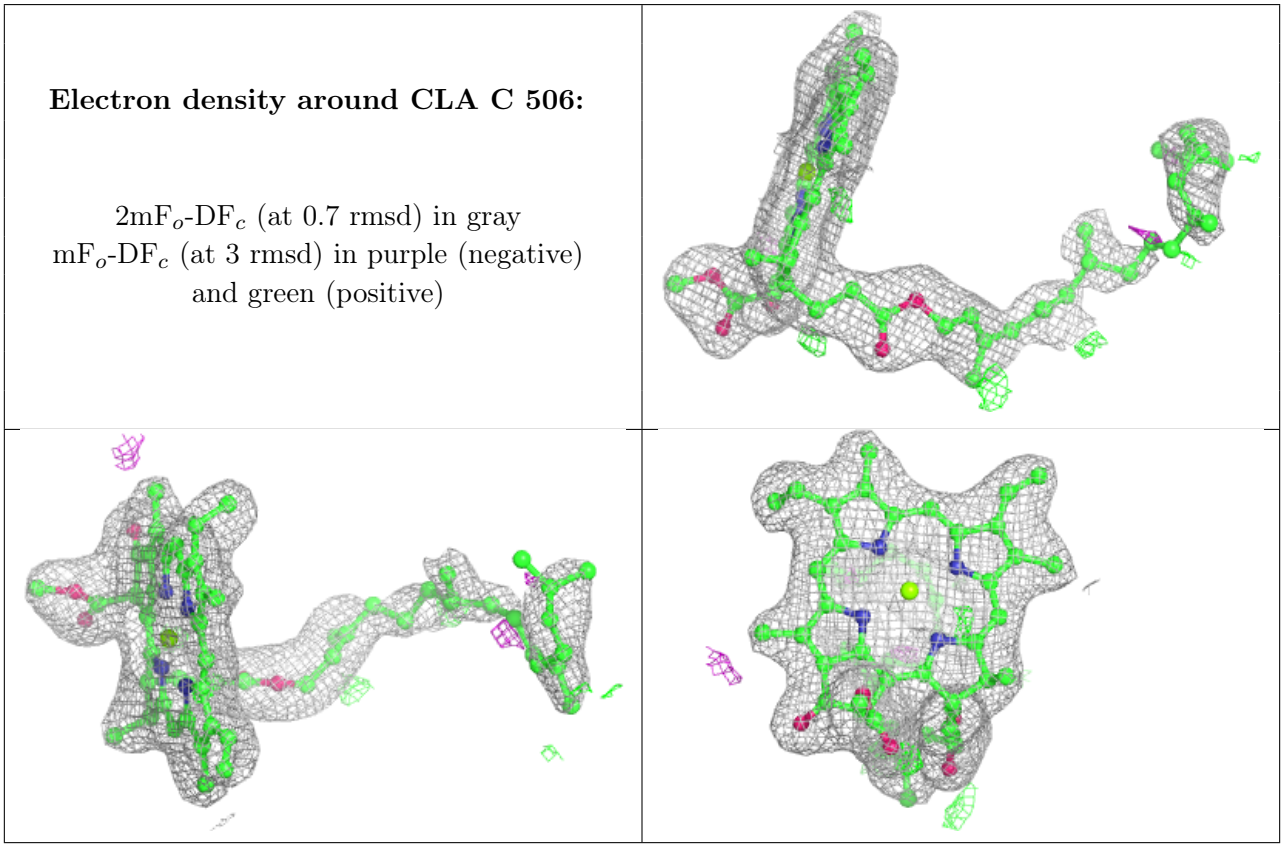
Electron density around DGD C 516:

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



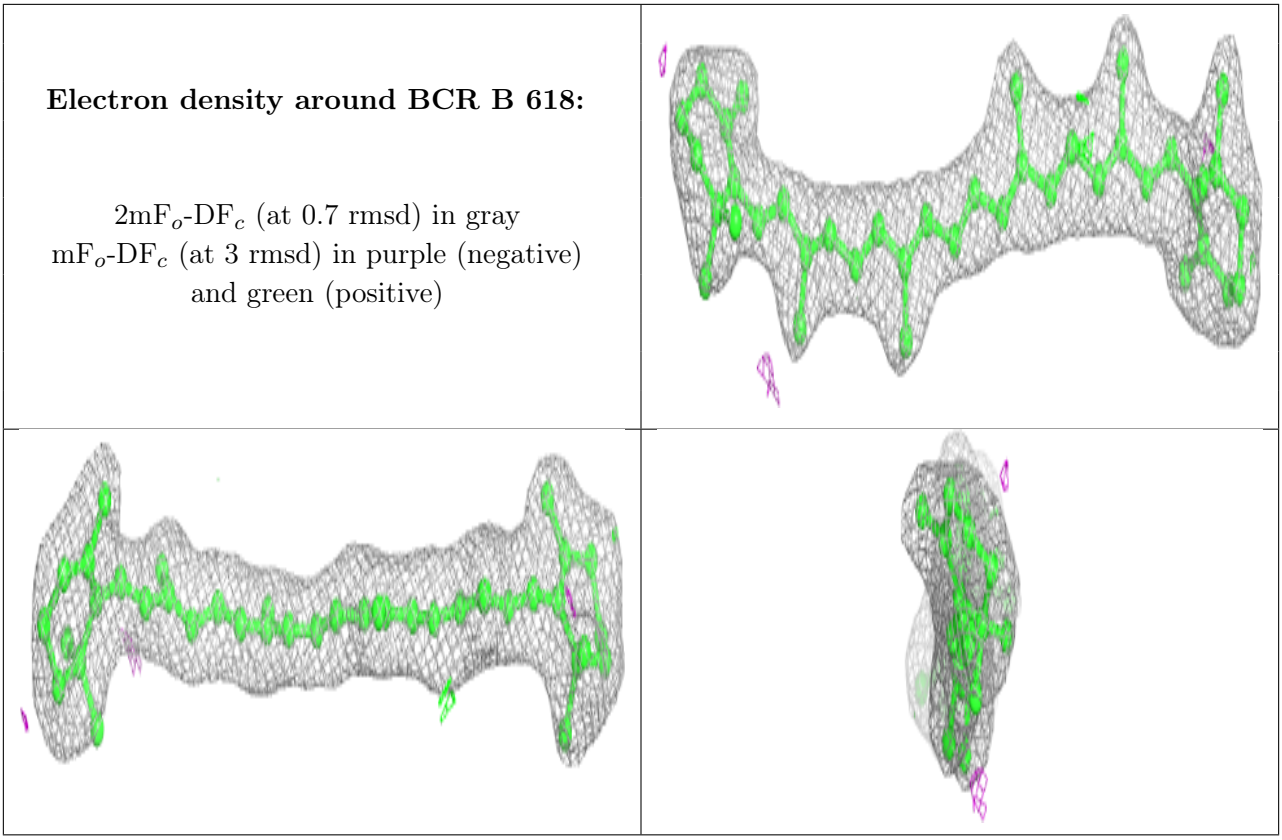
Electron density around CLA C 506:

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



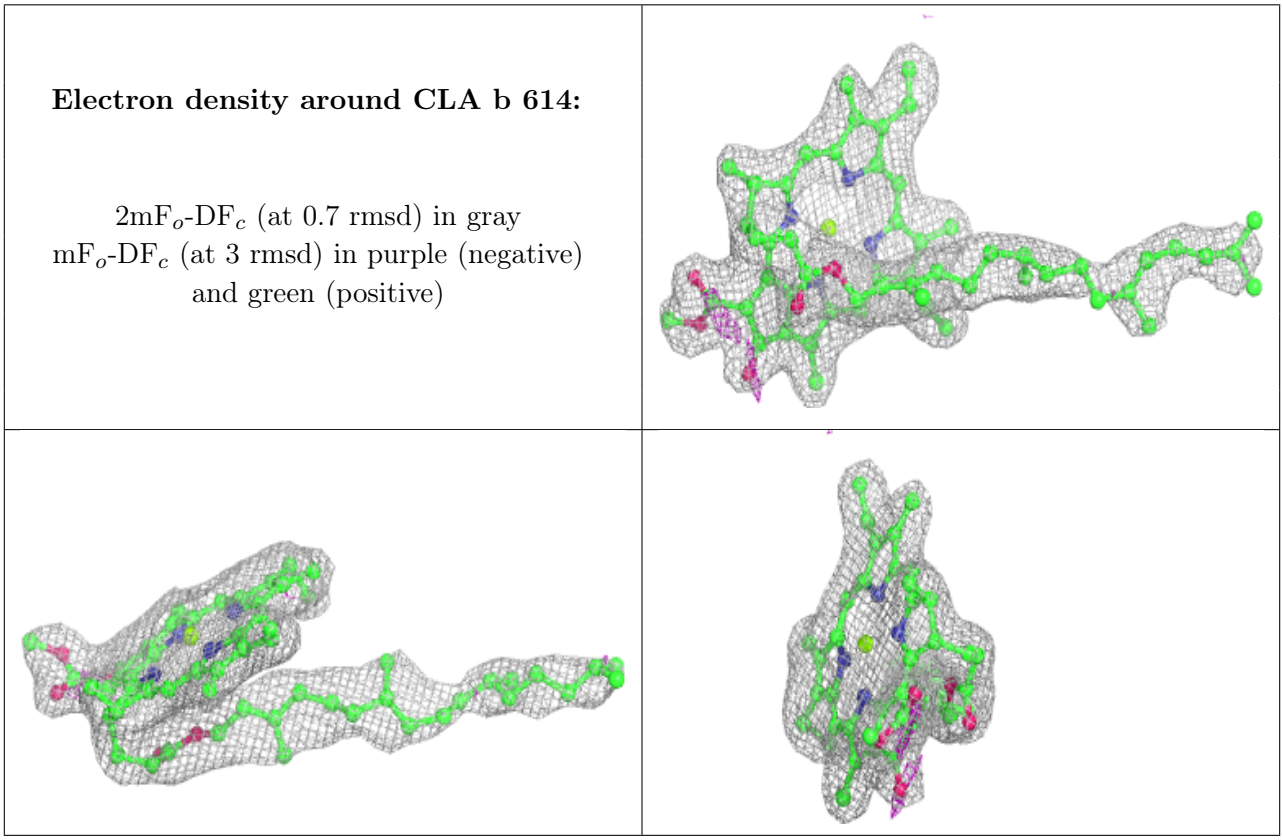
Electron density around BCR B 618:

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



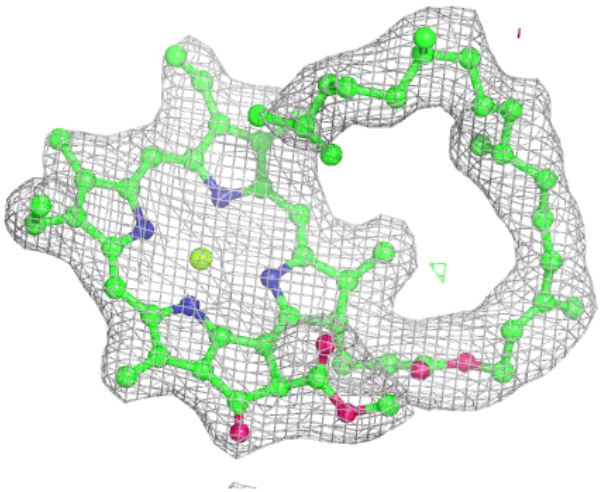
Electron density around CLA b 614:

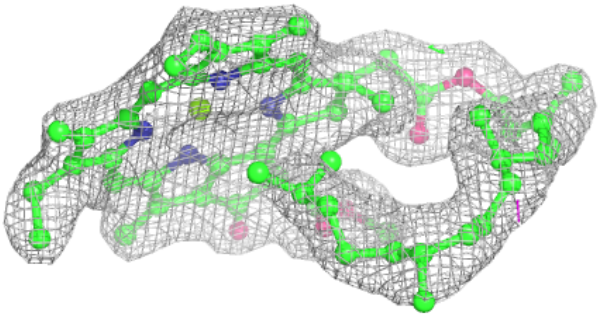
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

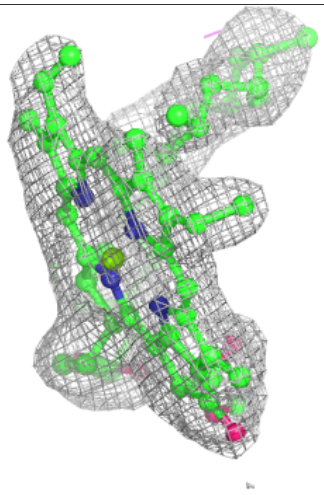


Electron density around CLA b 615:

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

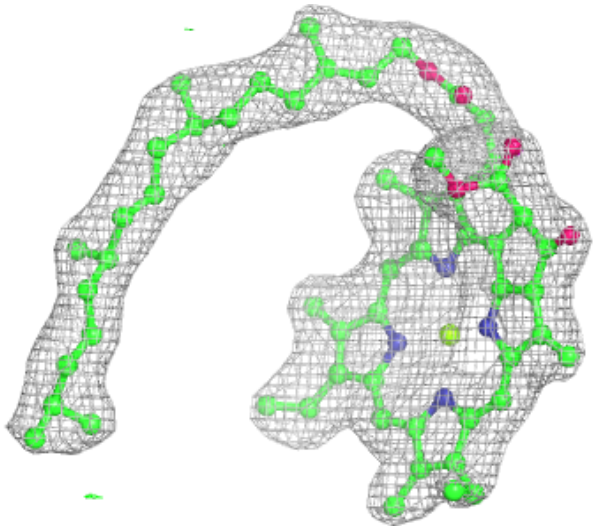


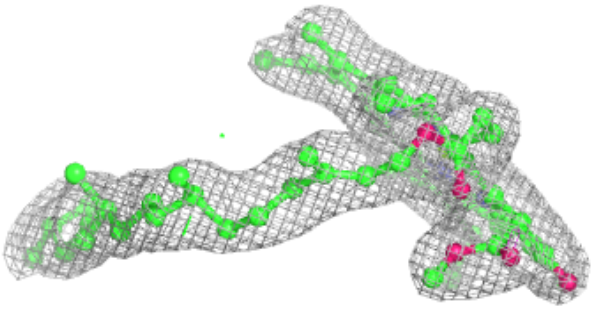


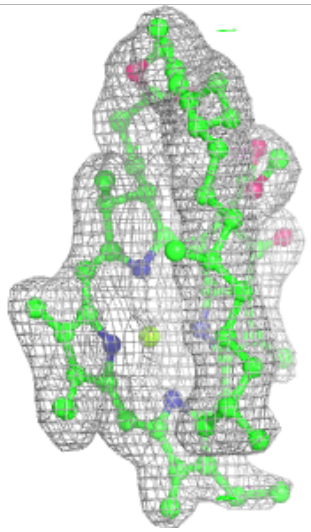


Electron density around CLA C 507:

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

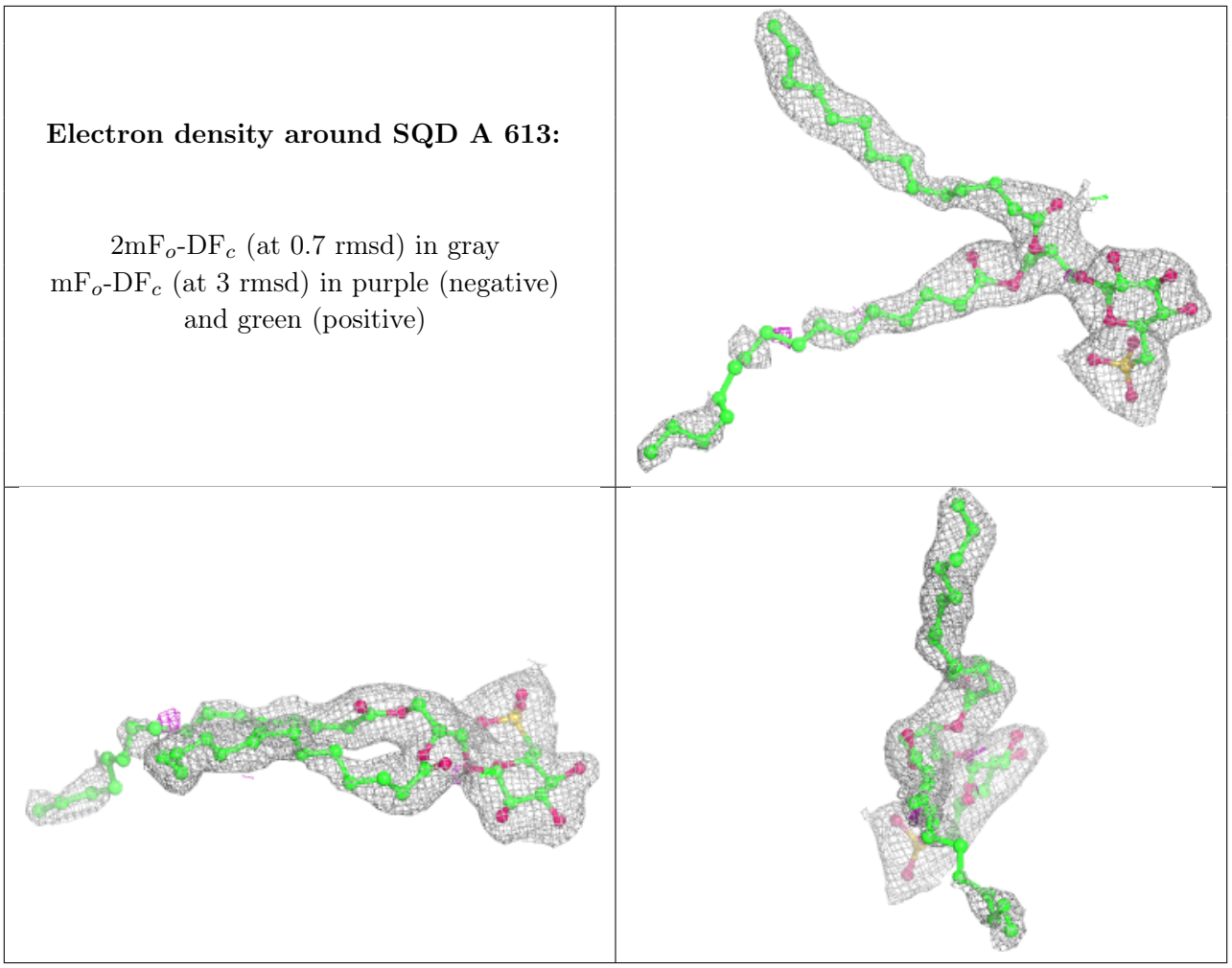






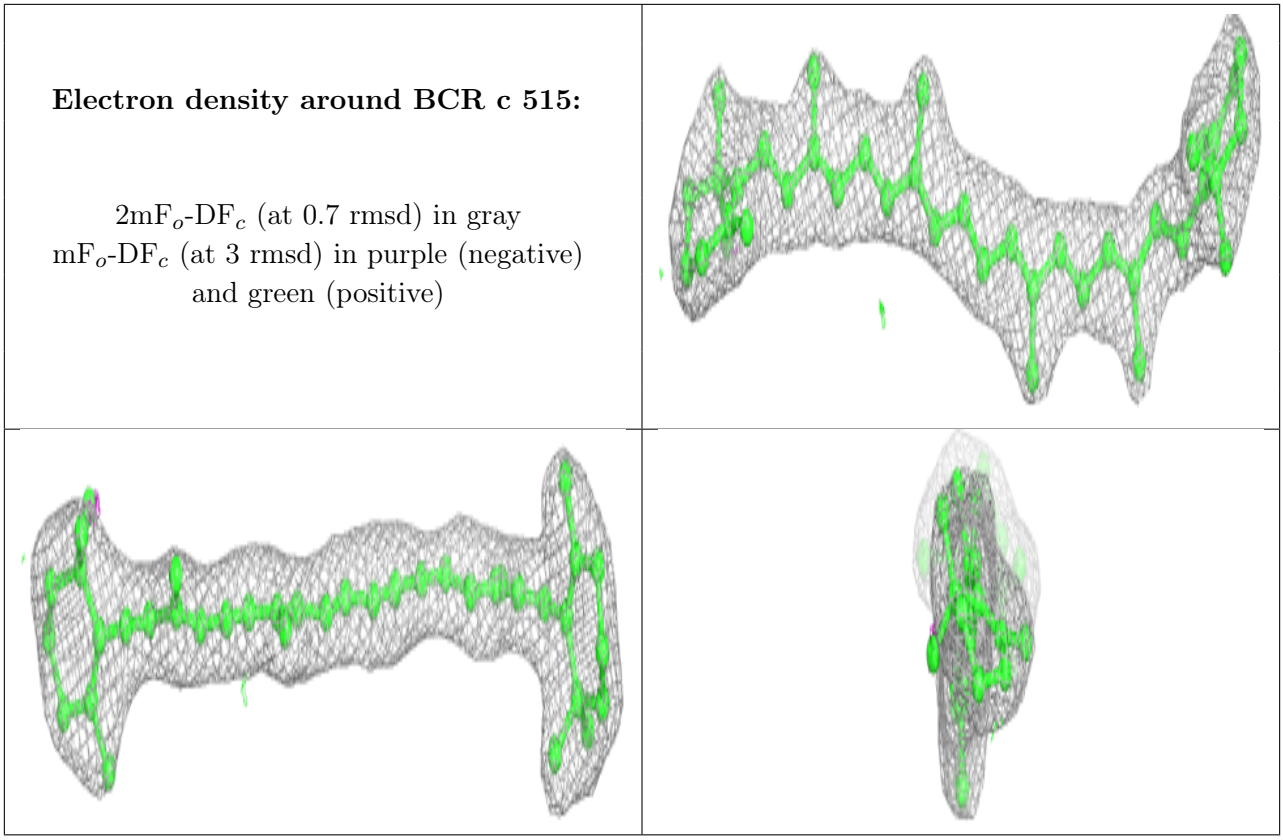
Electron density around SQD A 613:

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



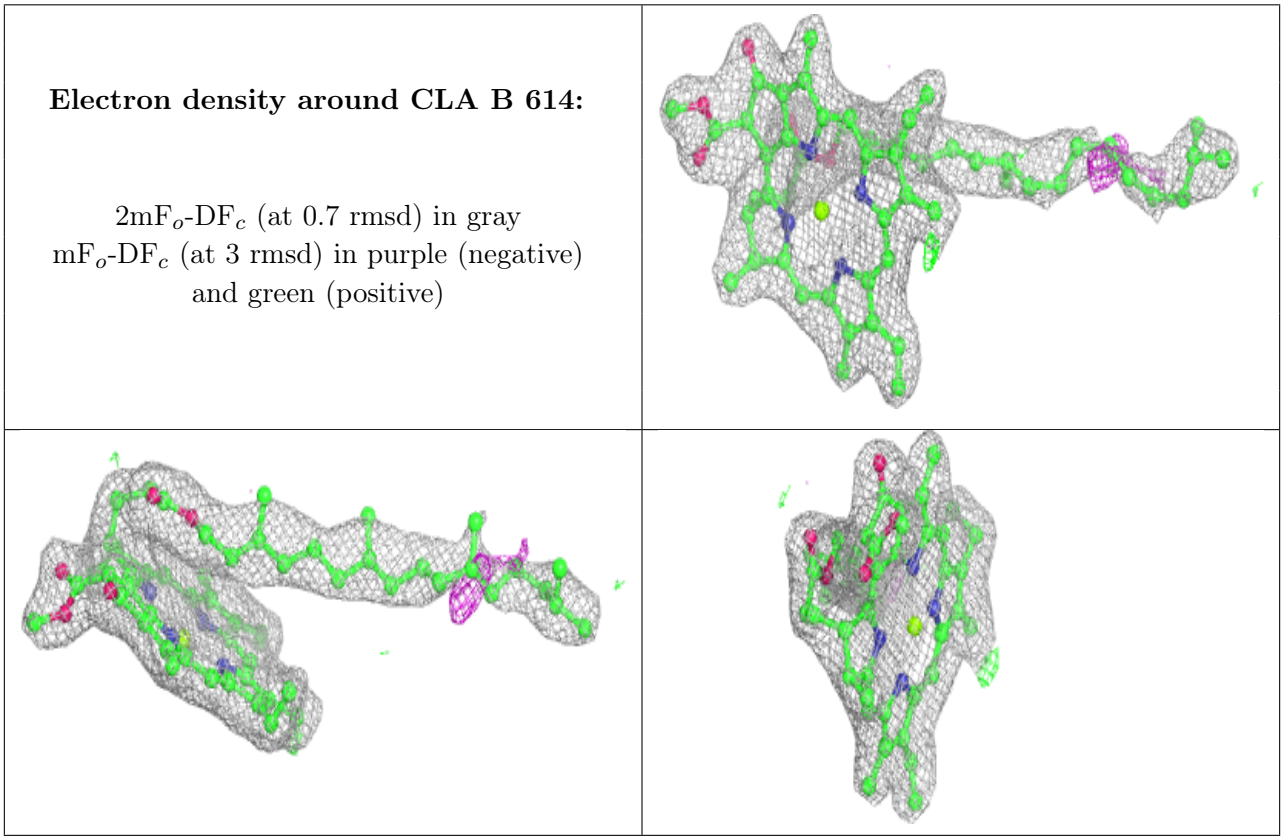
Electron density around BCR c 515:

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



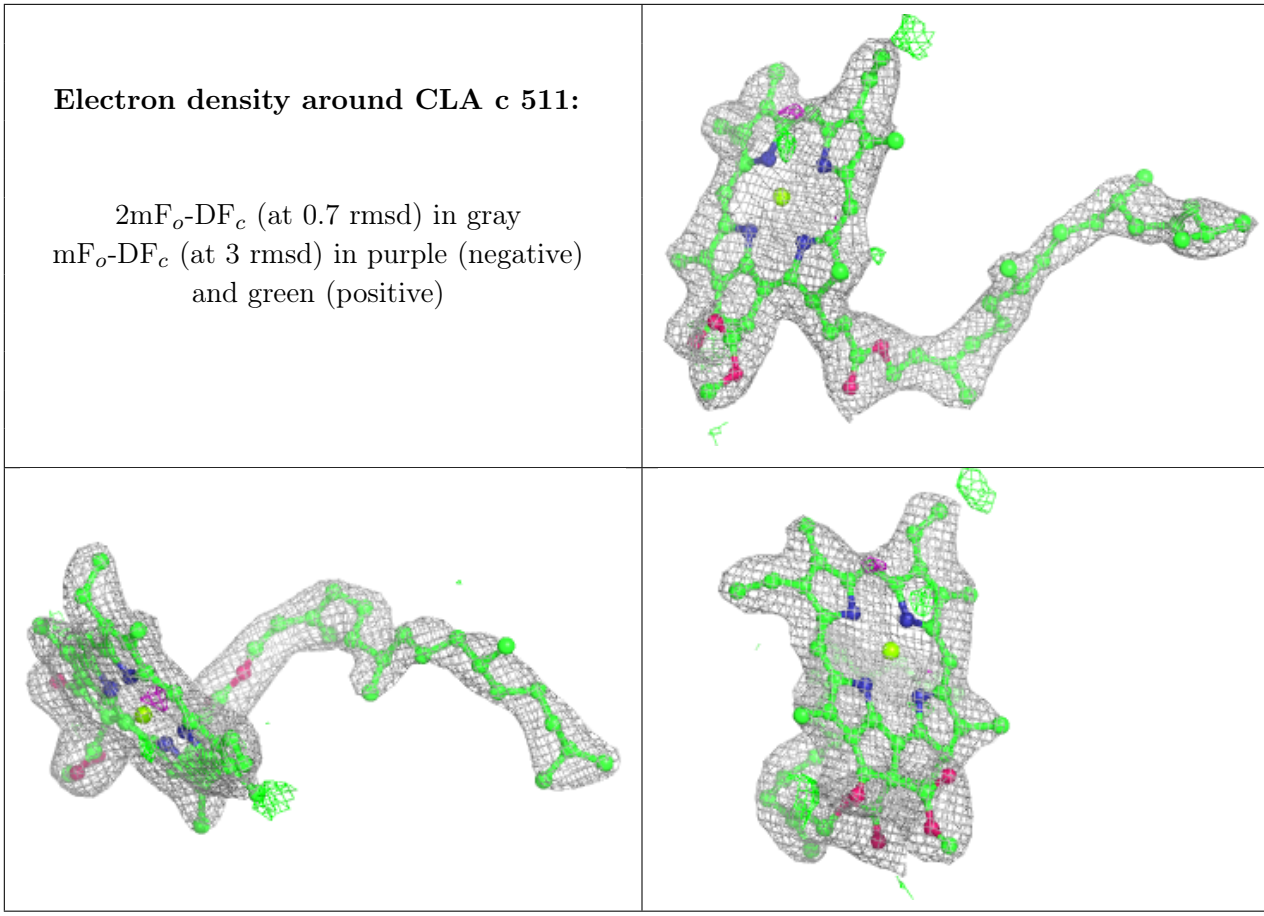
Electron density around CLA B 614:

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



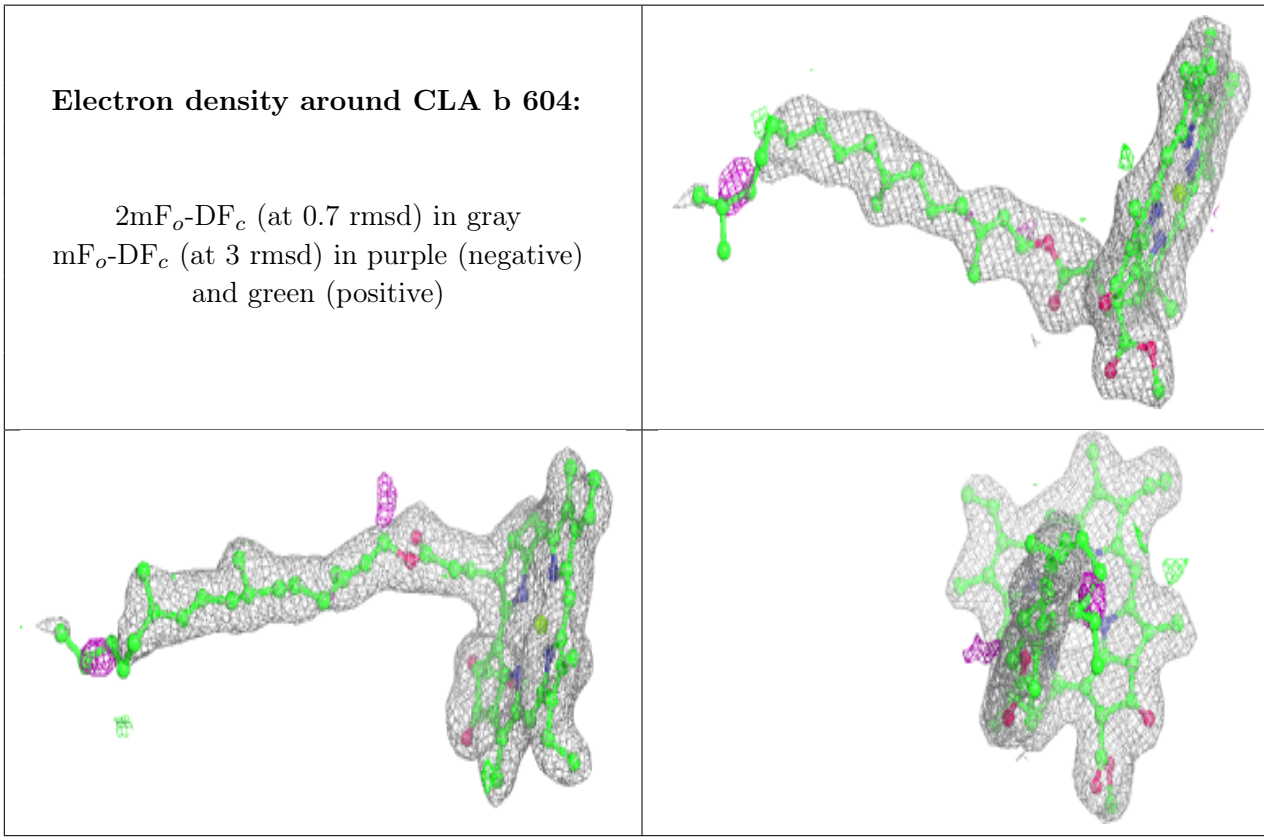
Electron density around CLA c 511:

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



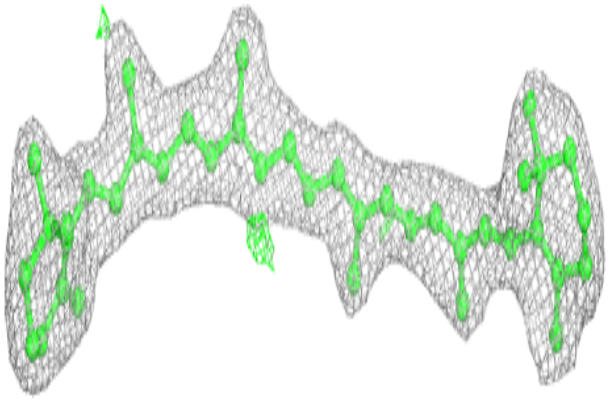
Electron density around CLA b 604:

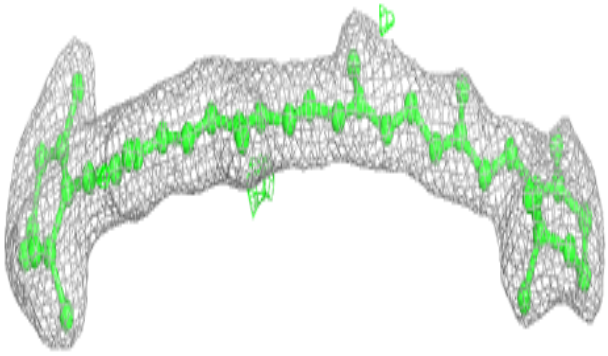
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

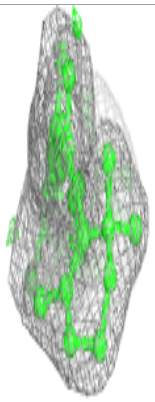


Electron density around BCR t 101:

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

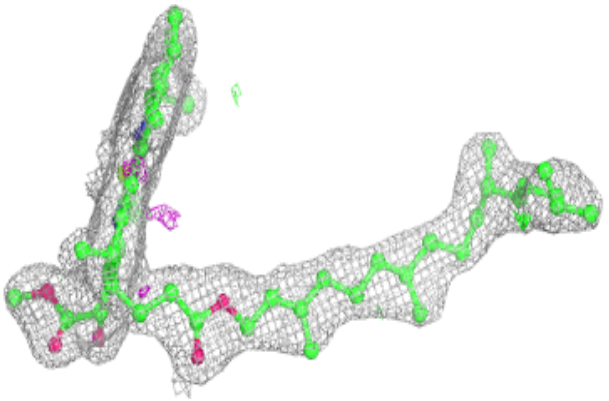


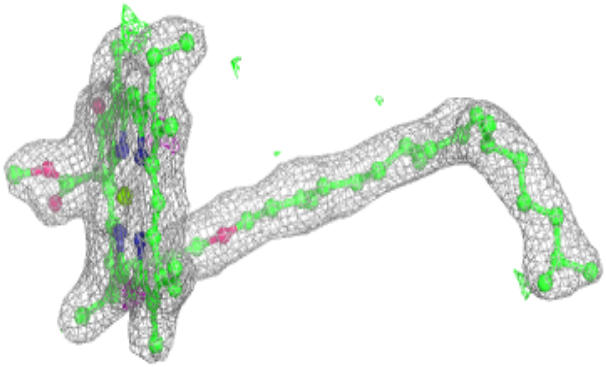


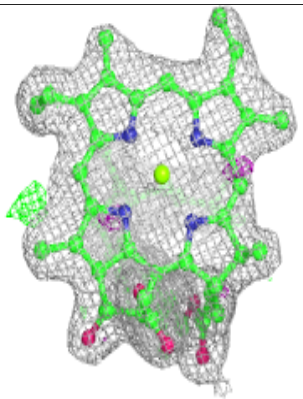


Electron density around CLA b 605:

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

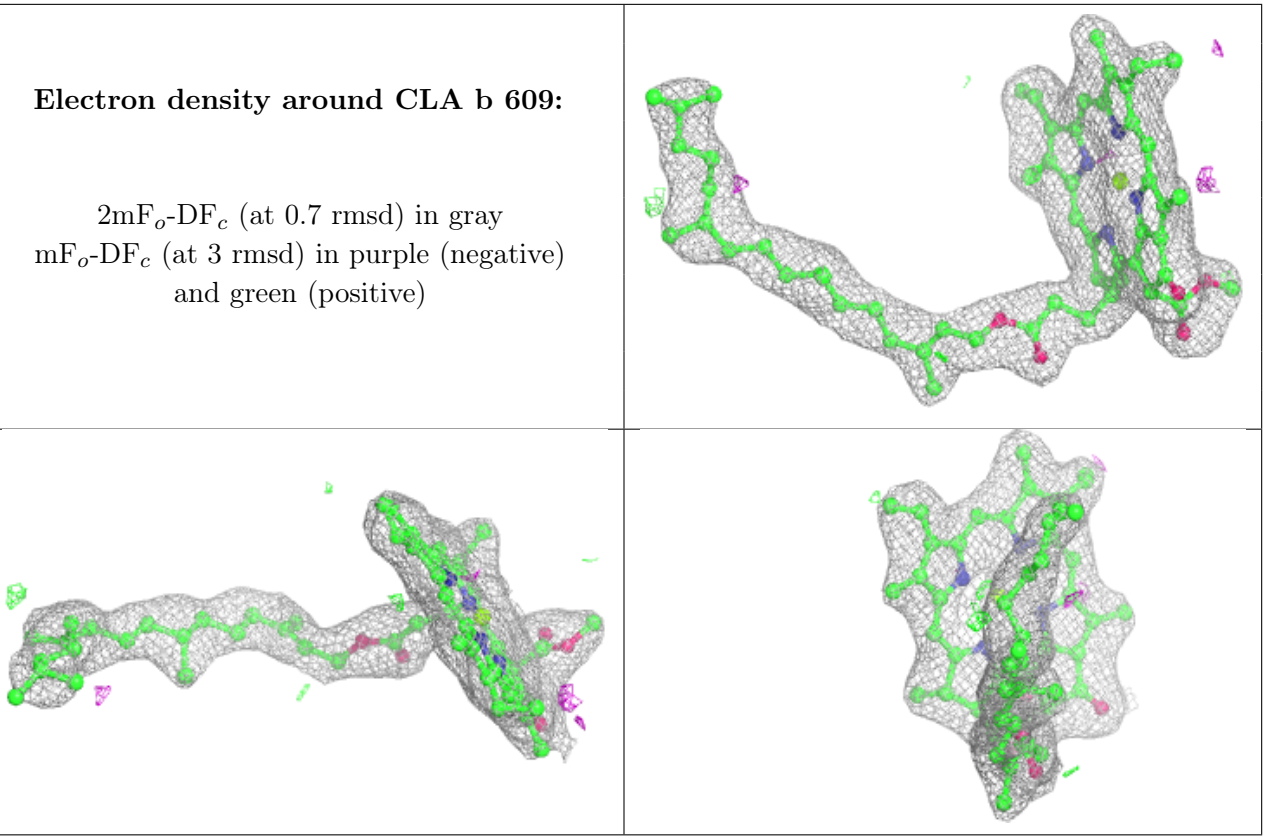






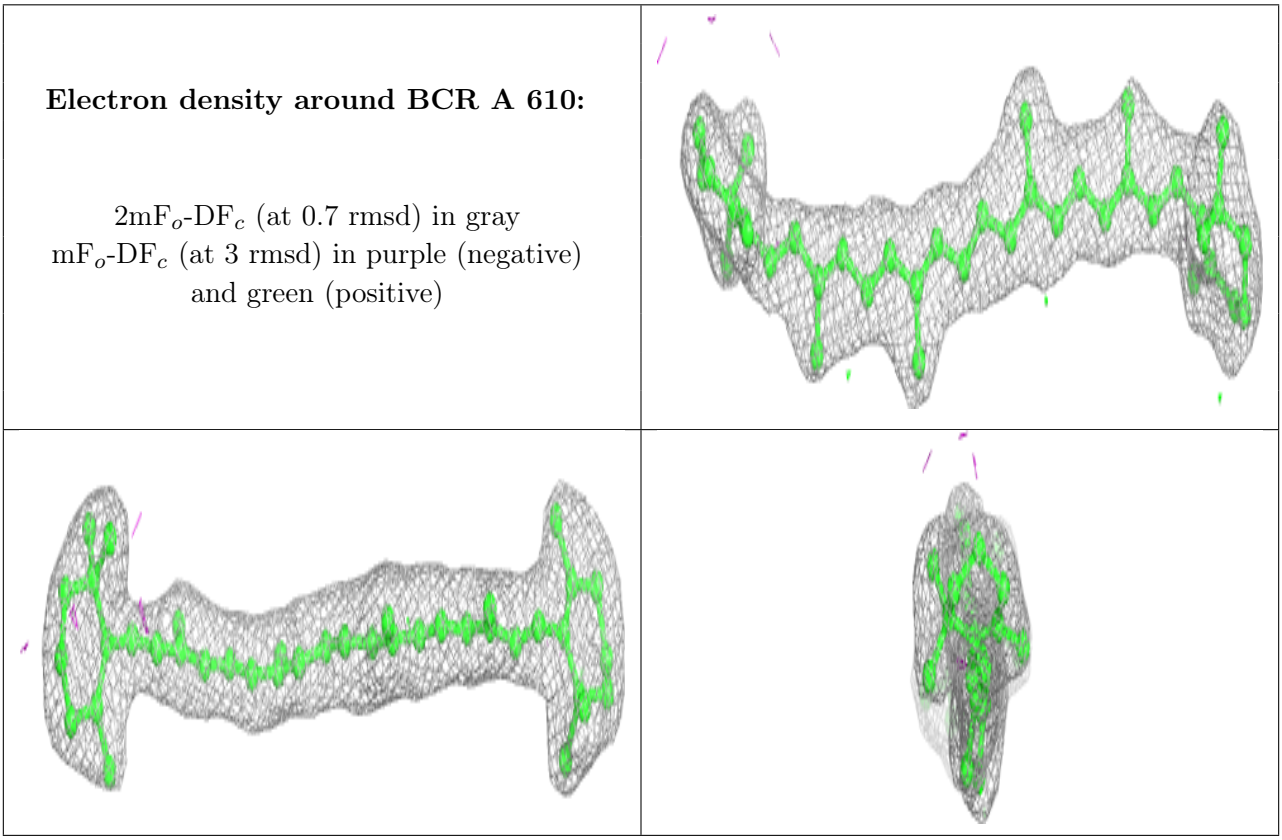
Electron density around CLA b 609:

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



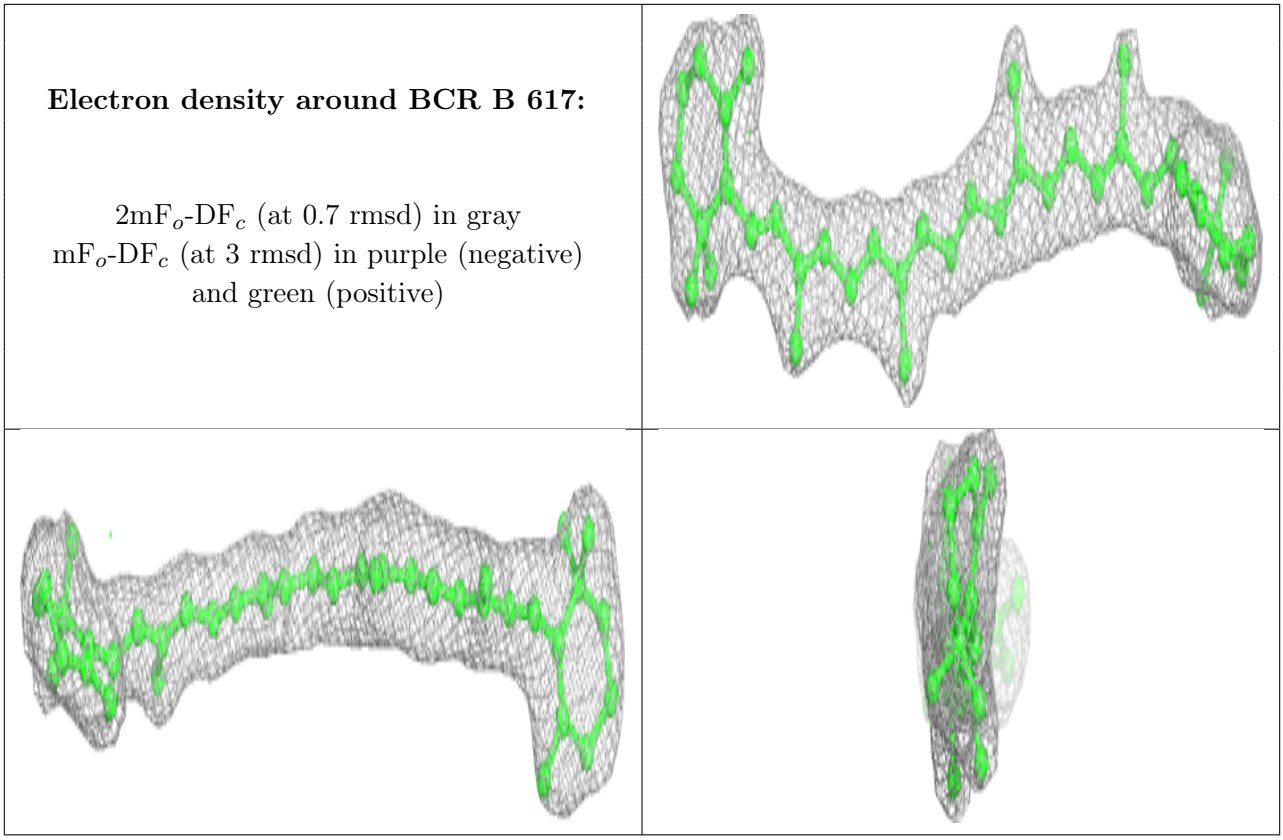
Electron density around BCR A 610:

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



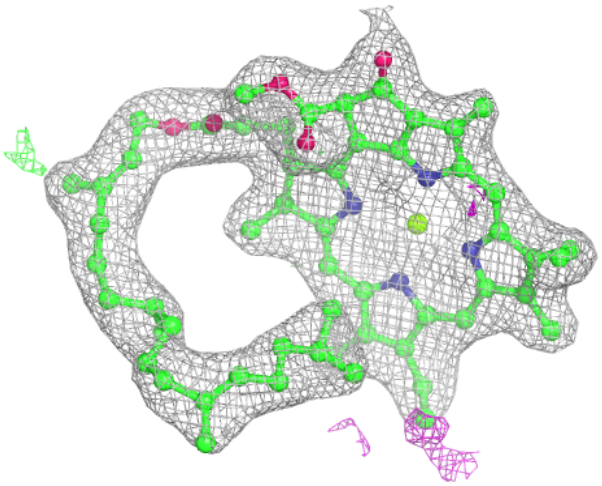
Electron density around BCR B 617:

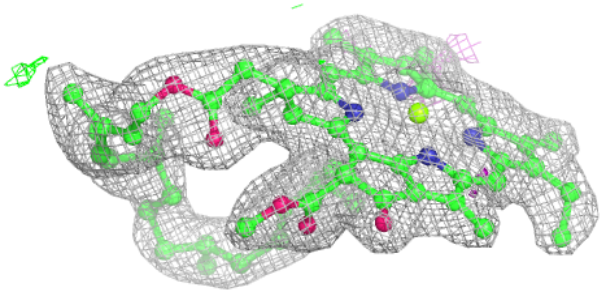
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

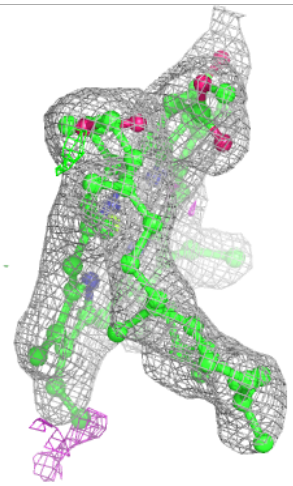


Electron density around CLA B 615:

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

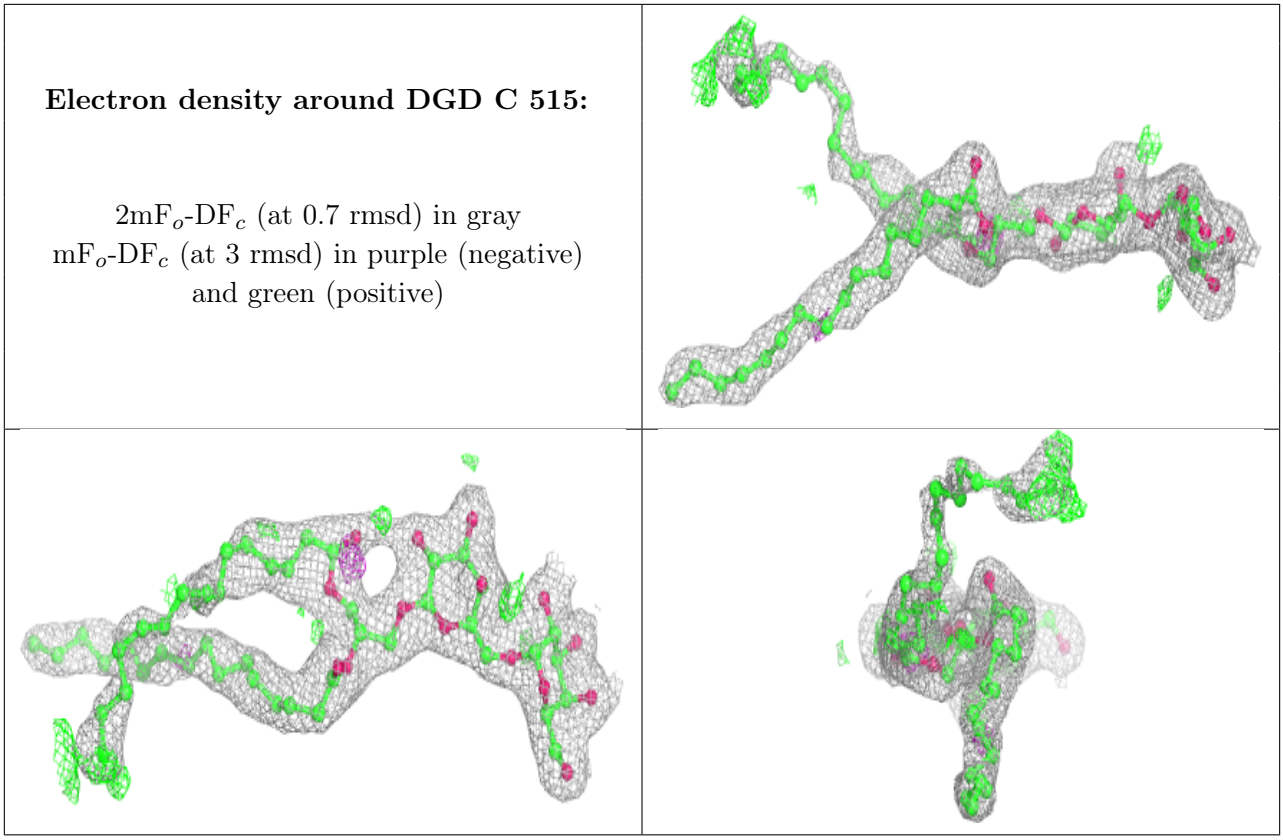






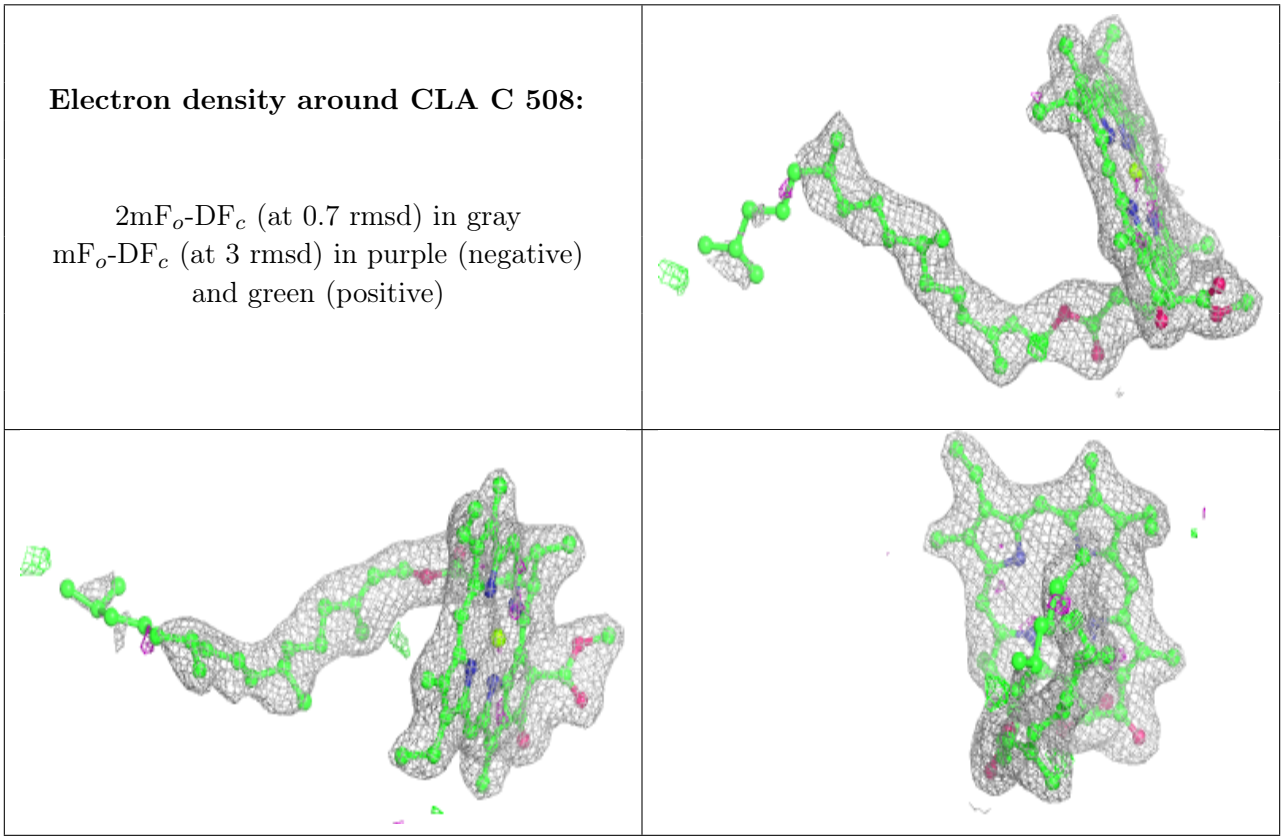
Electron density around DGD C 515:

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



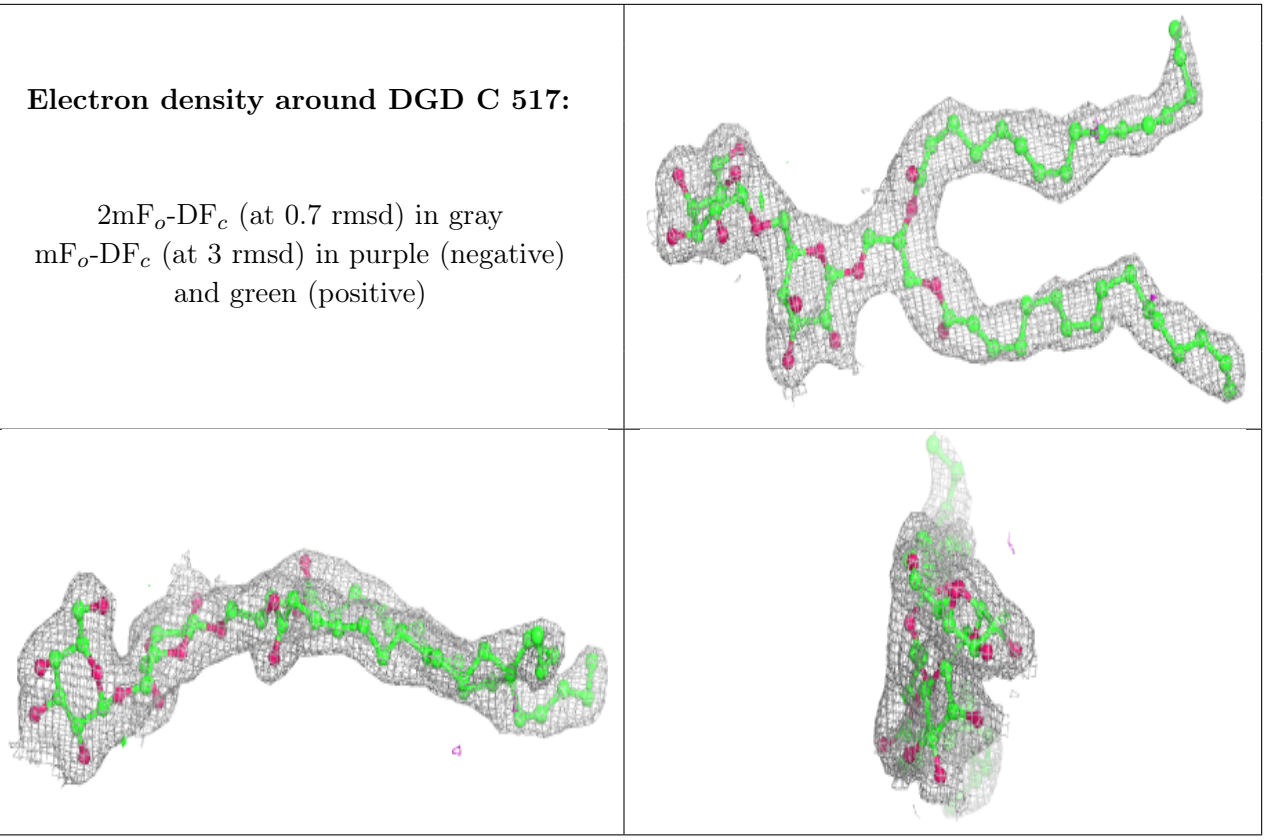
Electron density around CLA C 508:

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



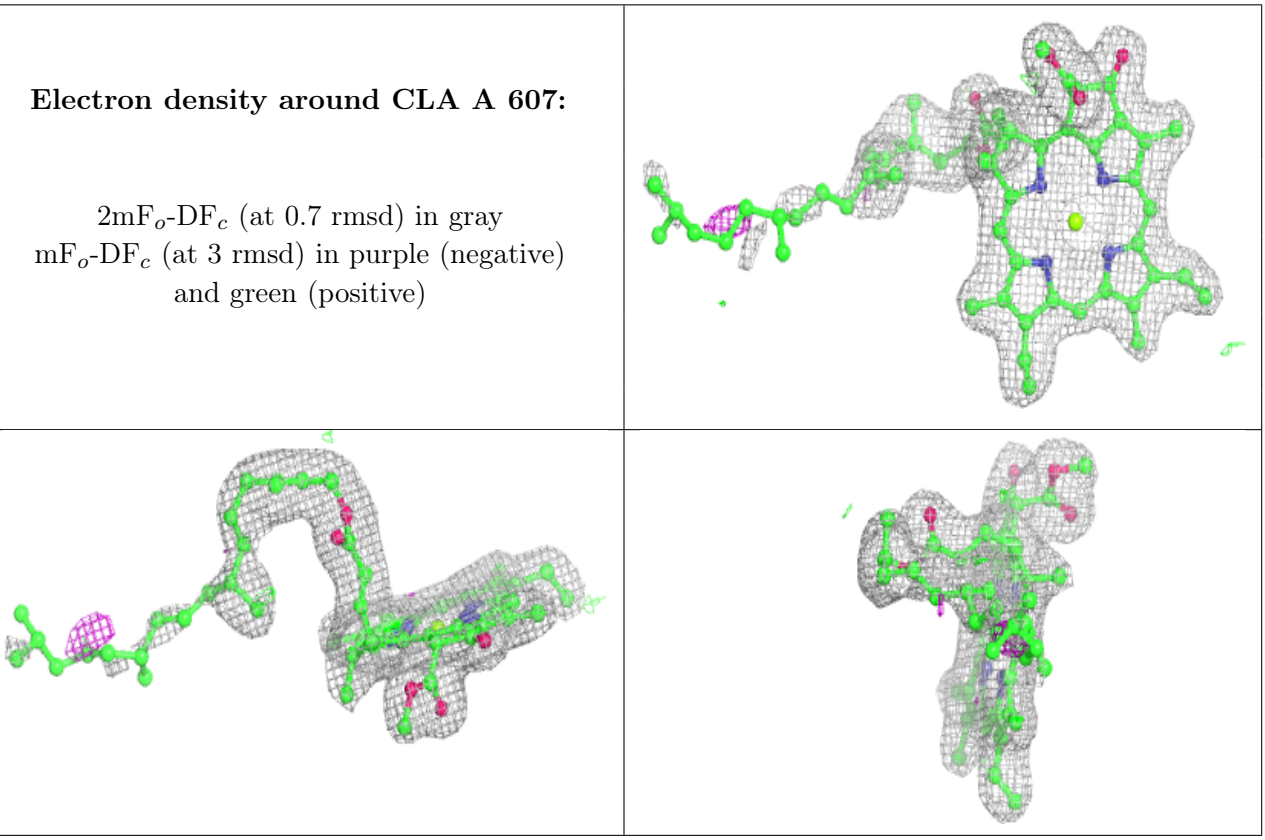
Electron density around DGD C 517:

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



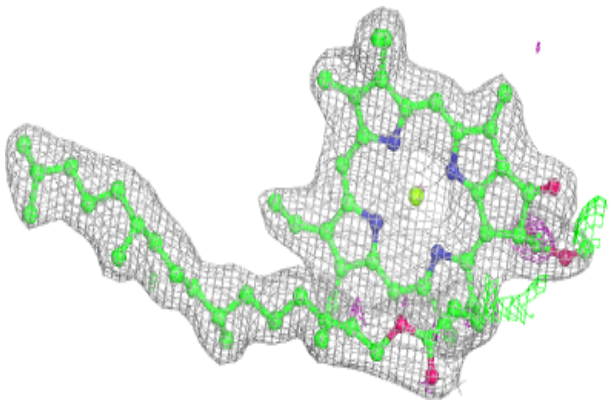
Electron density around CLA A 607:

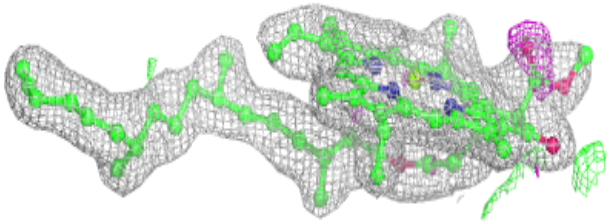
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

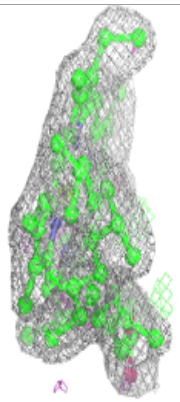


Electron density around CLA C 501:

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

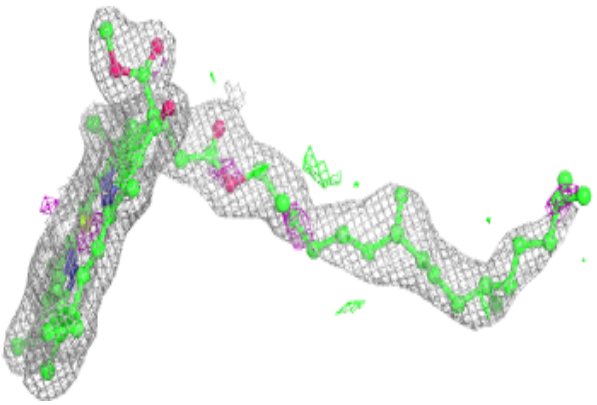


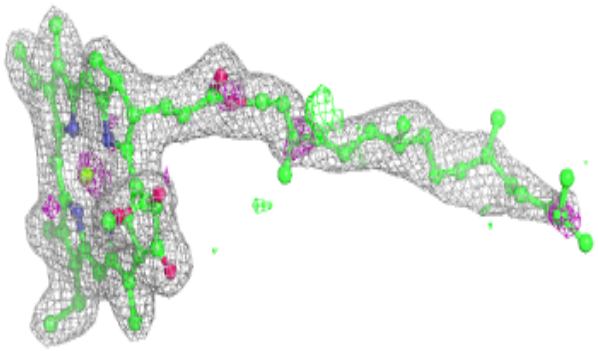


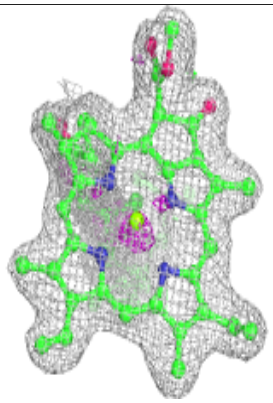


Electron density around CLA B 604:

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

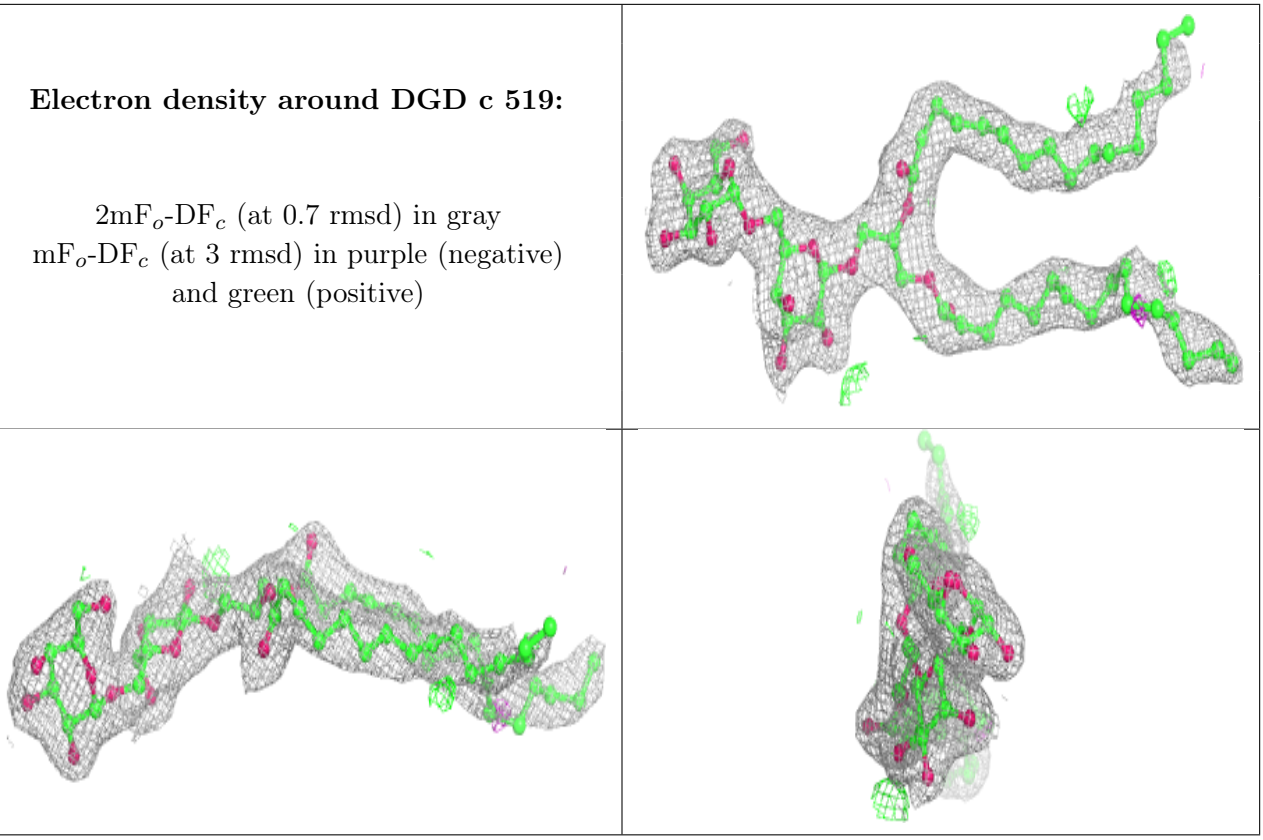






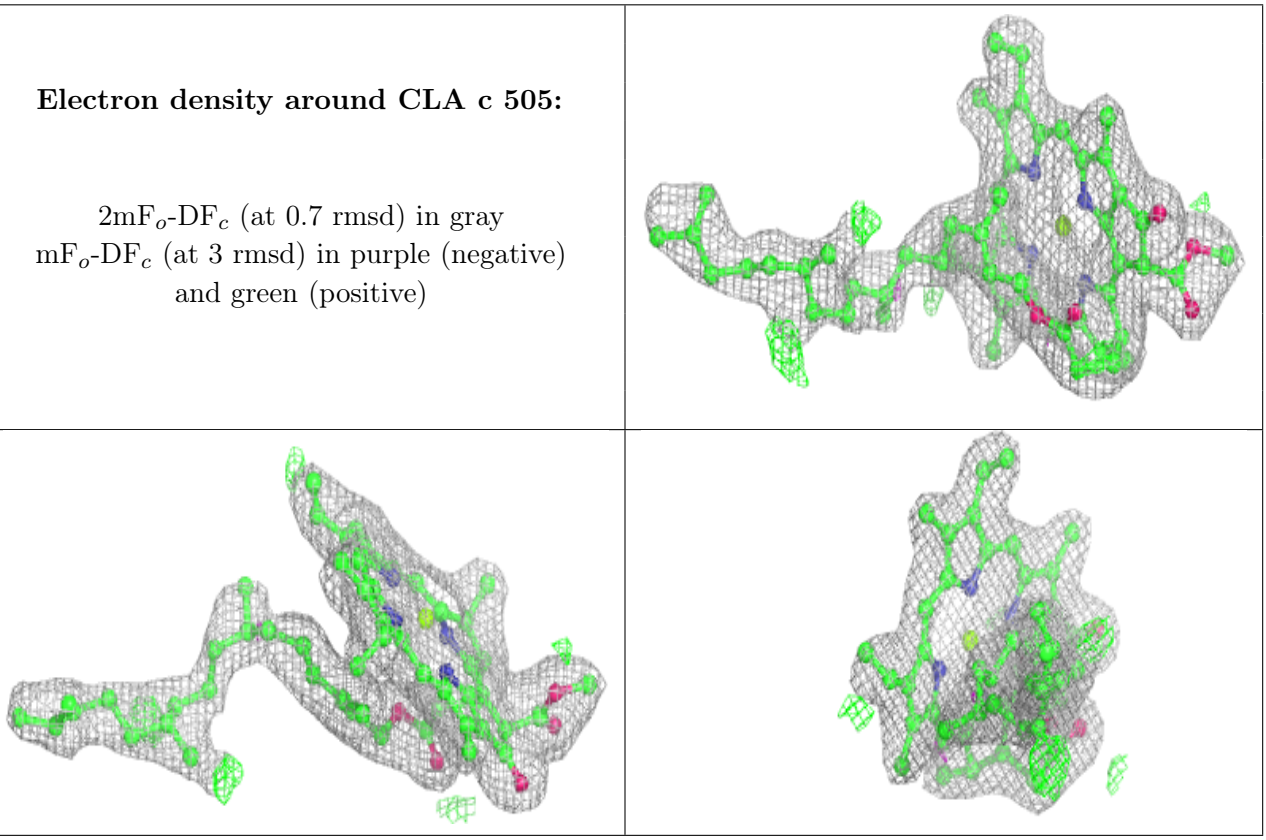
Electron density around DGD c 519:

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



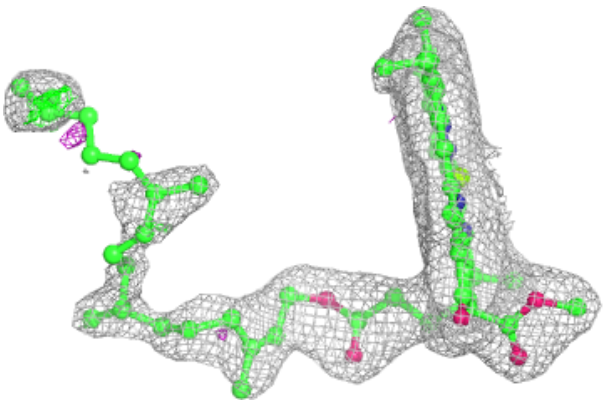
Electron density around CLA c 505:

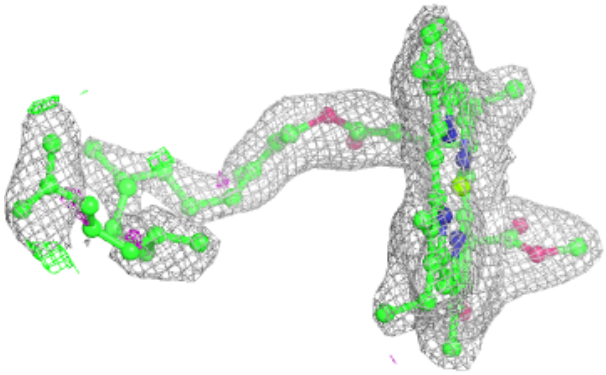
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

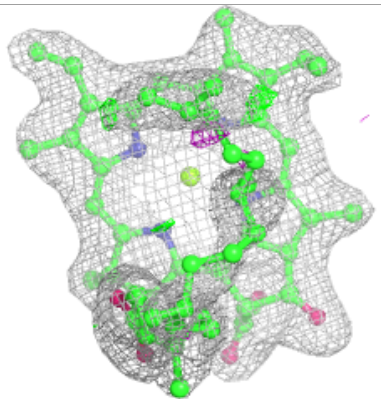


Electron density around CLA c 506:

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

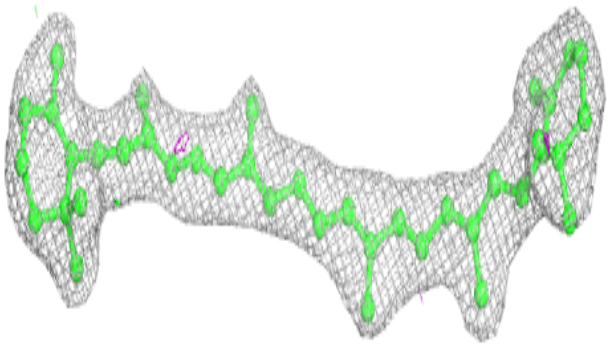


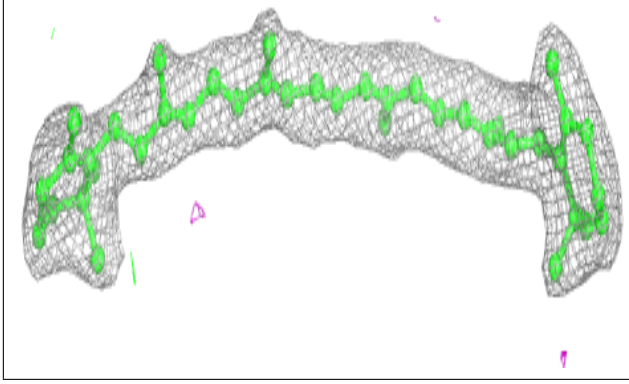


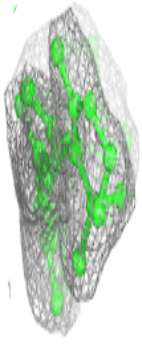


Electron density around BCR T 101:

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

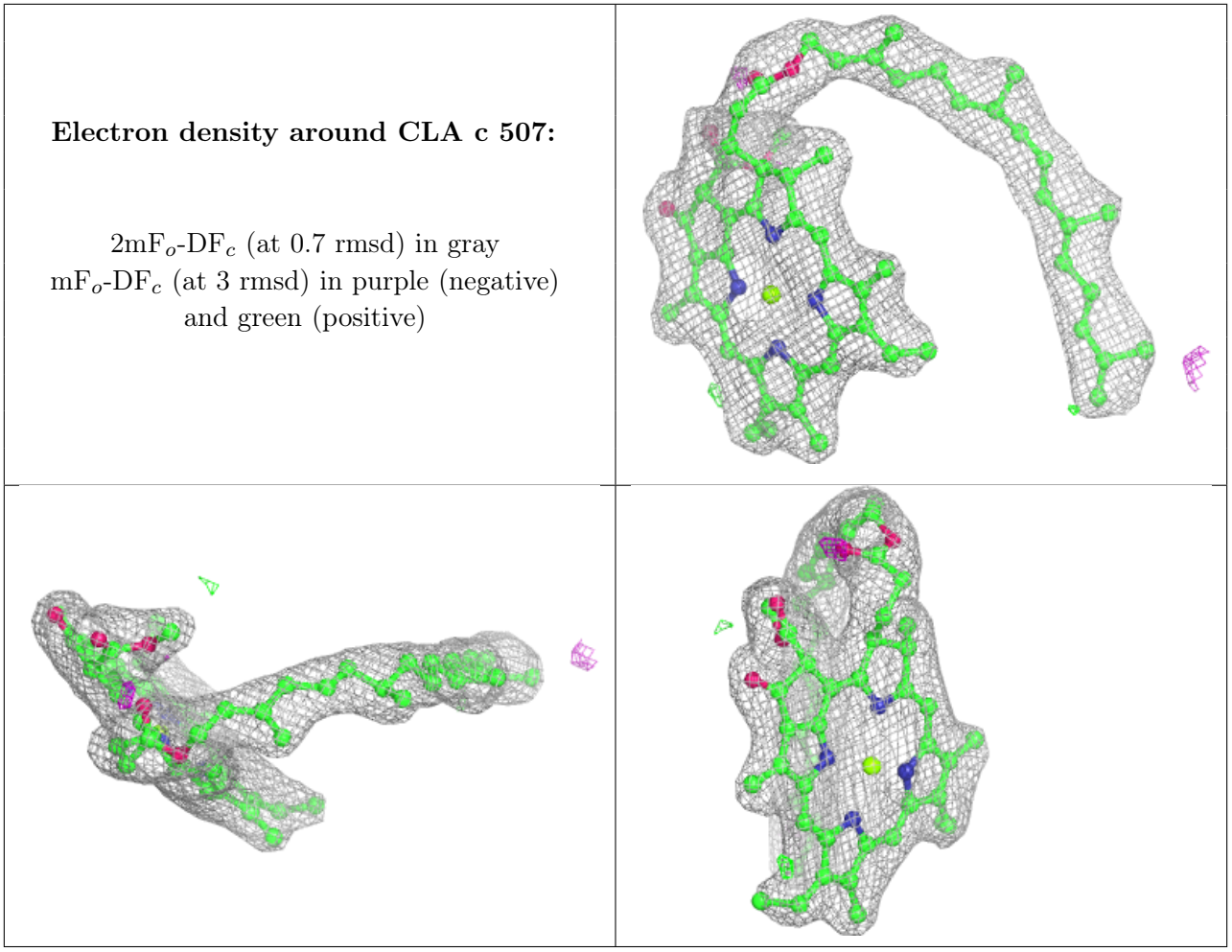






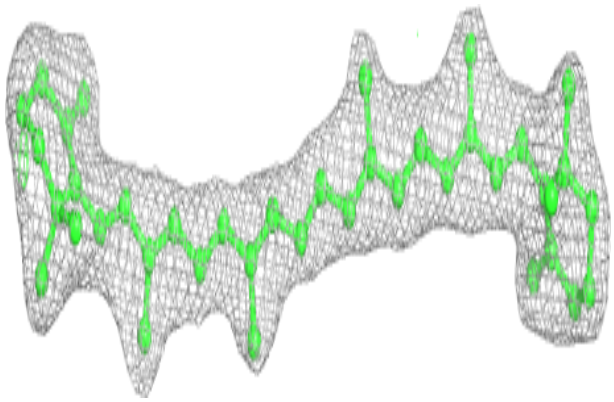
Electron density around CLA c 507:

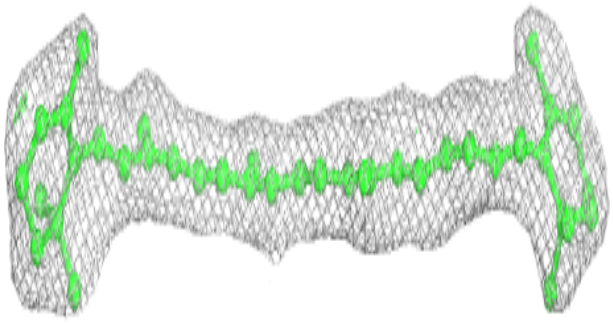
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

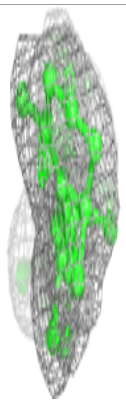


Electron density around BCR b 618:

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

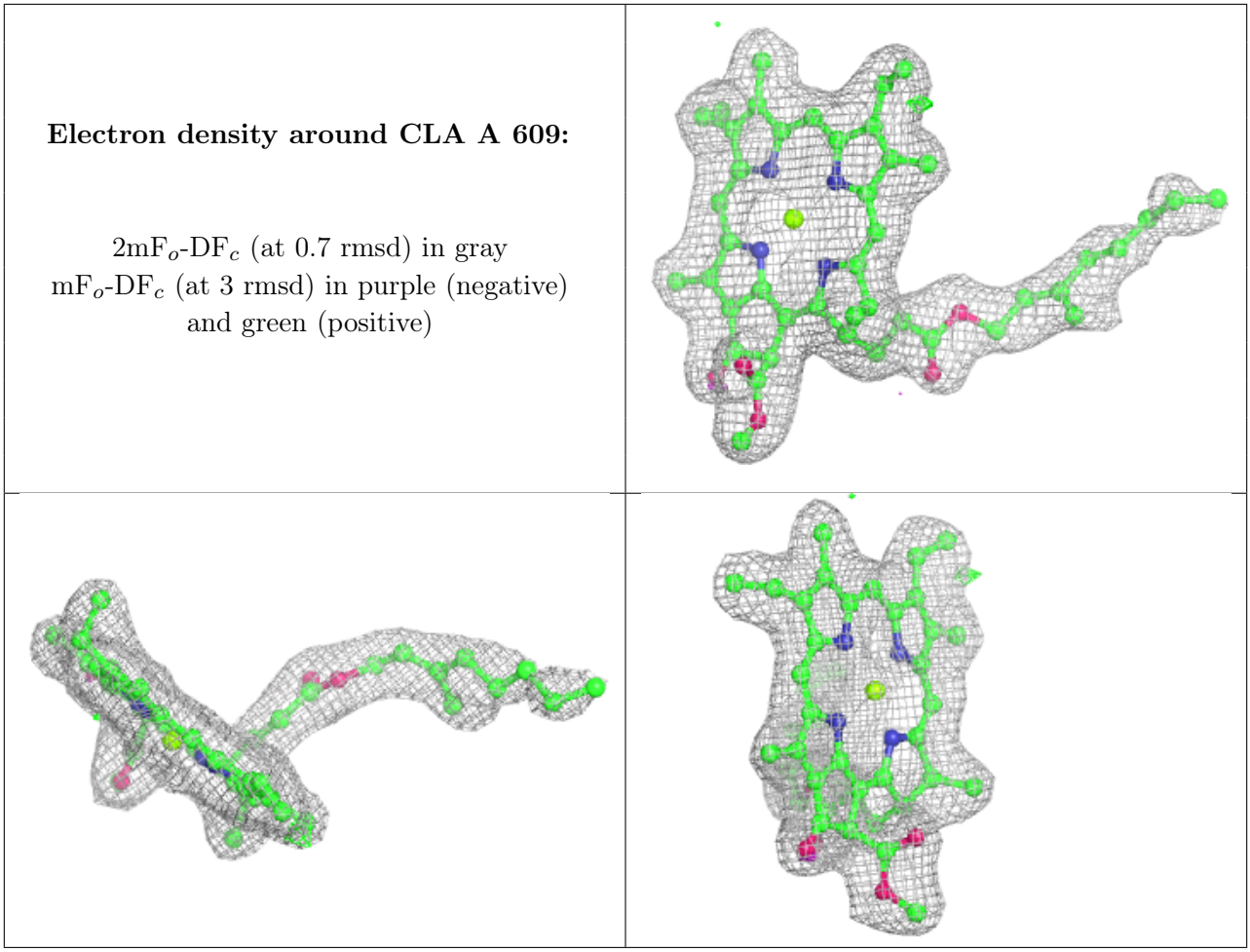






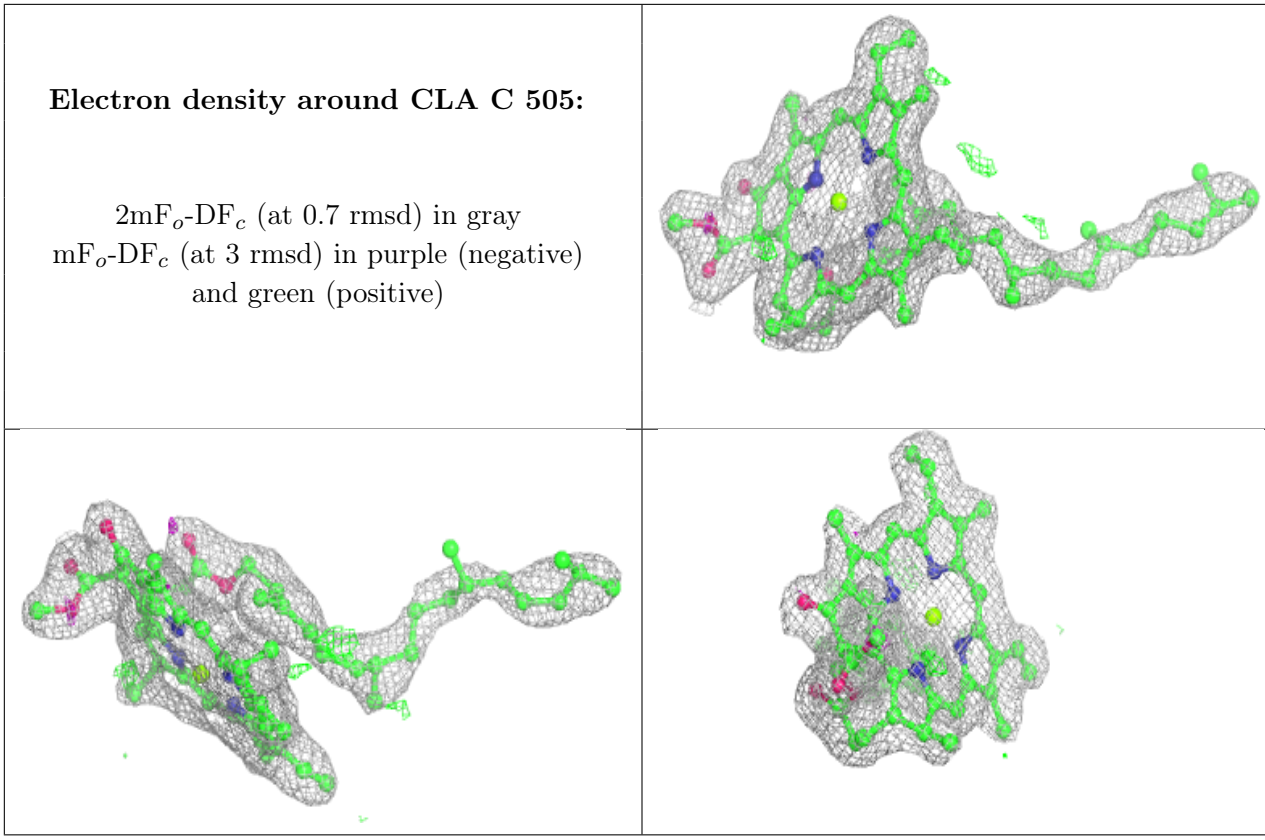
Electron density around CLA A 609:

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



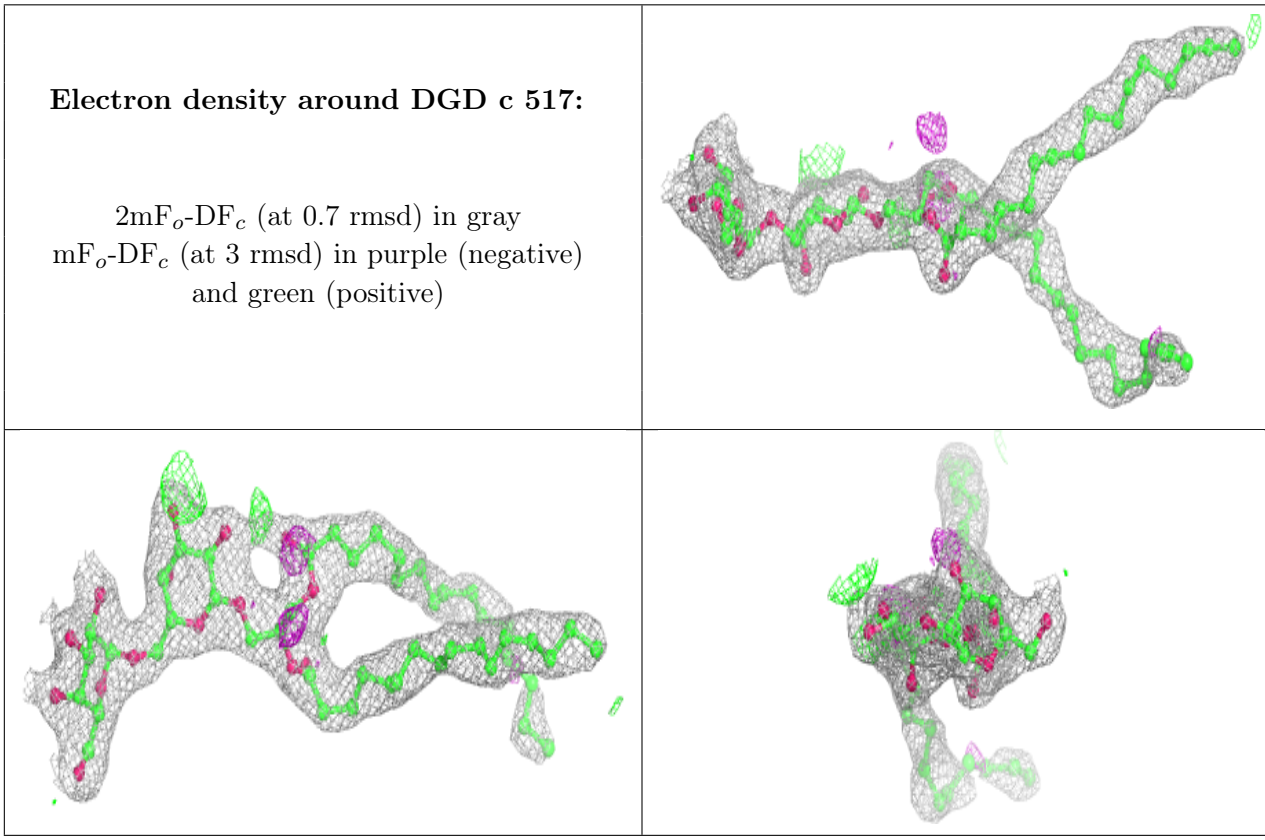
Electron density around CLA C 505:

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



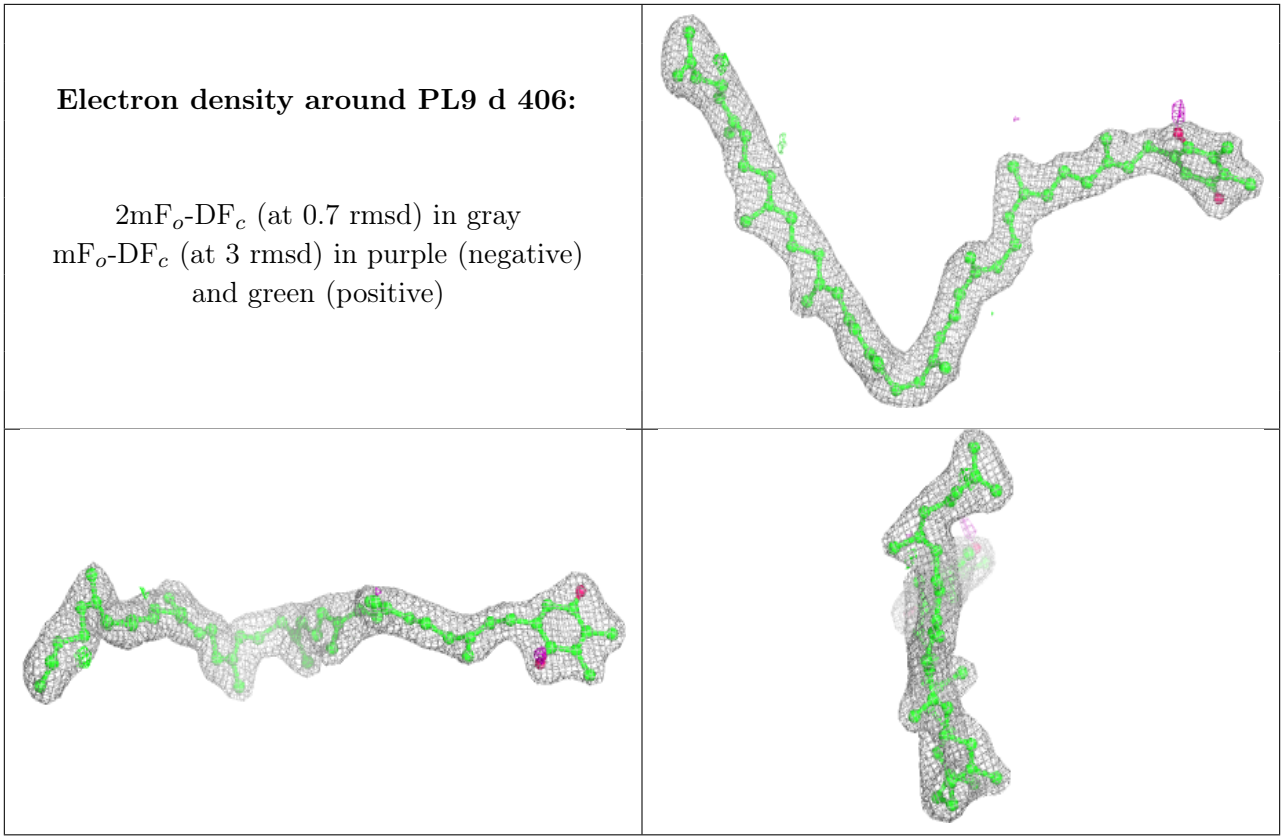
Electron density around DGD c 517:

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



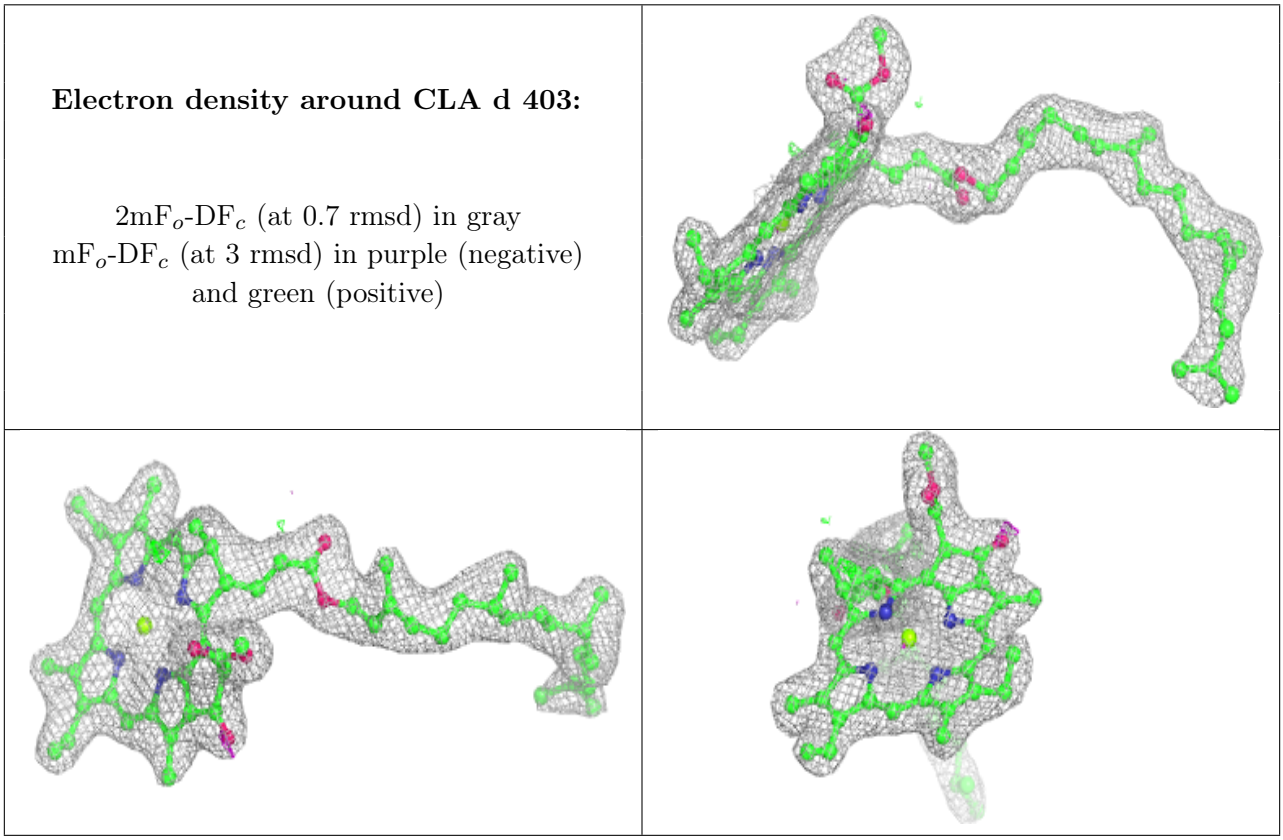
Electron density around PL9 d 406:

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



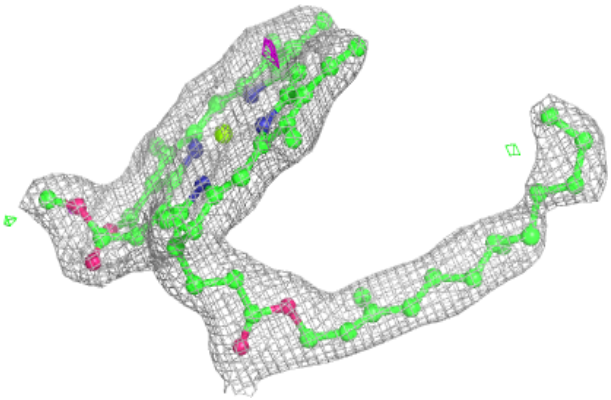
Electron density around CLA d 403:

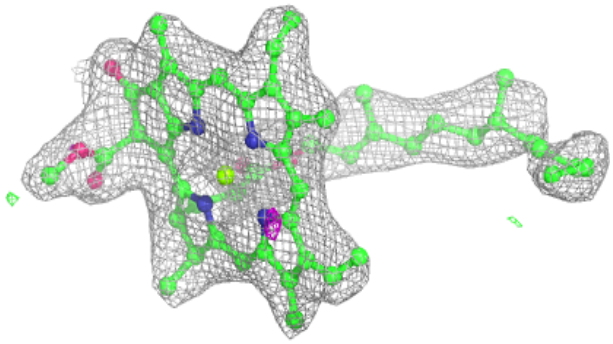
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

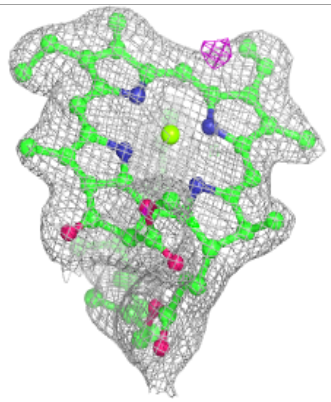


Electron density around CLA C 504:

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

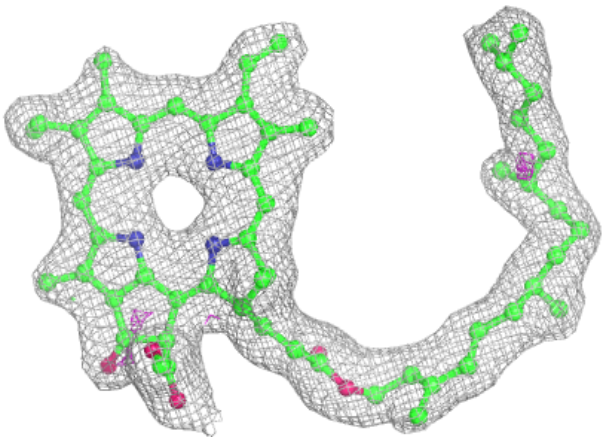


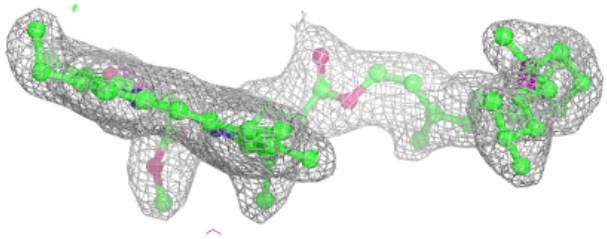


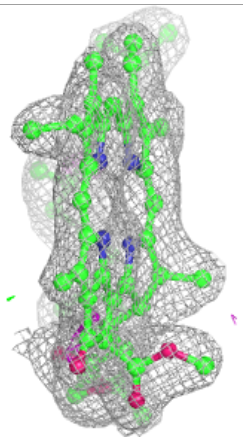


Electron density around PHO d 401:

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

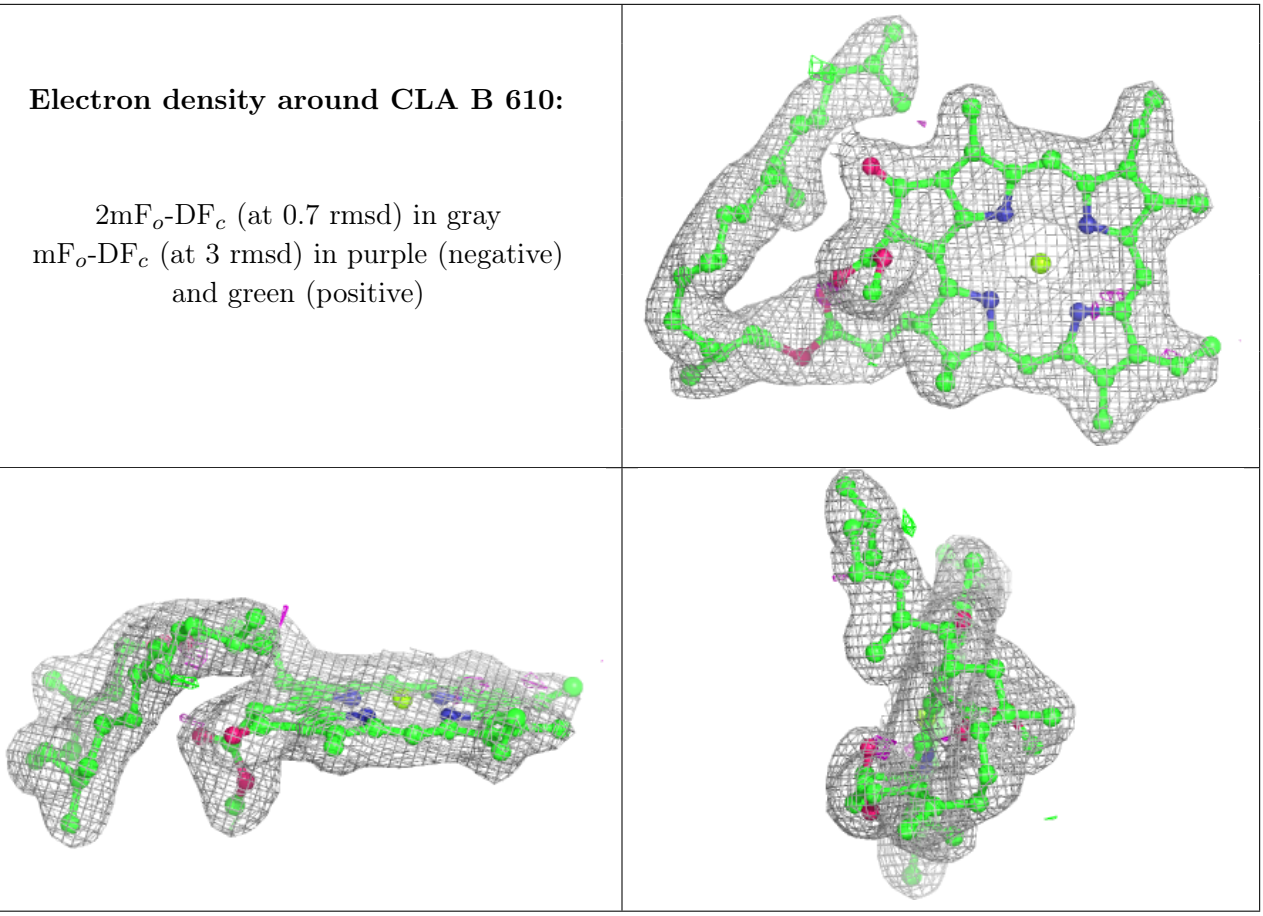






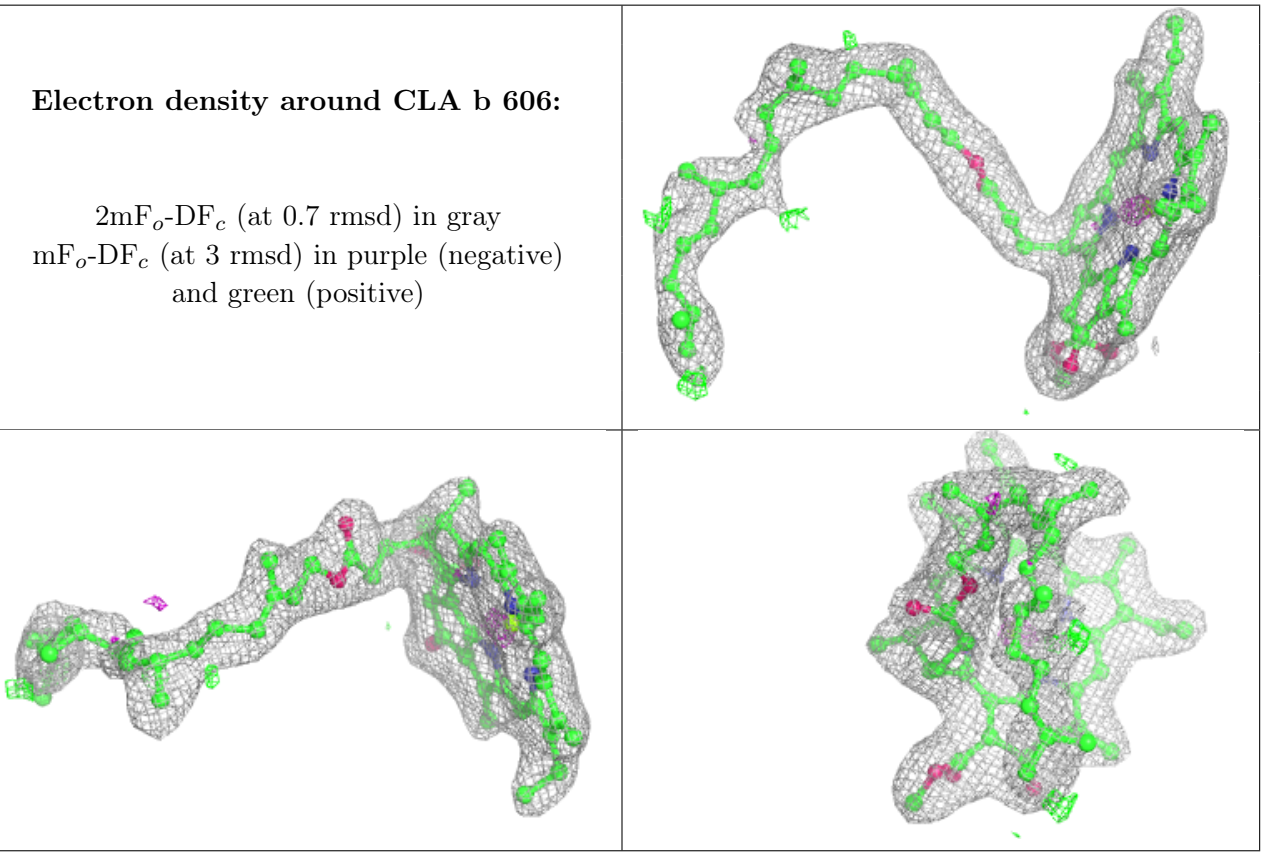
Electron density around CLA B 610:

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



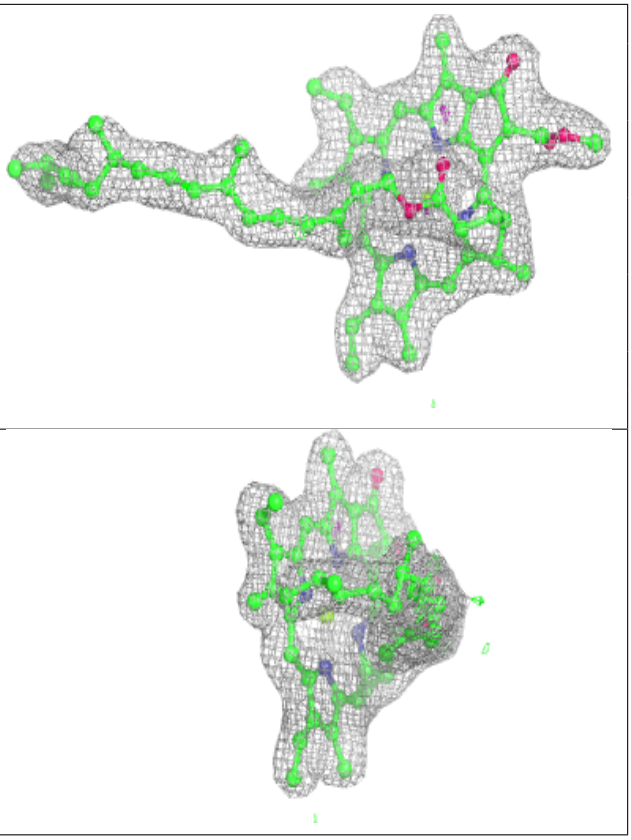
Electron density around CLA b 606:

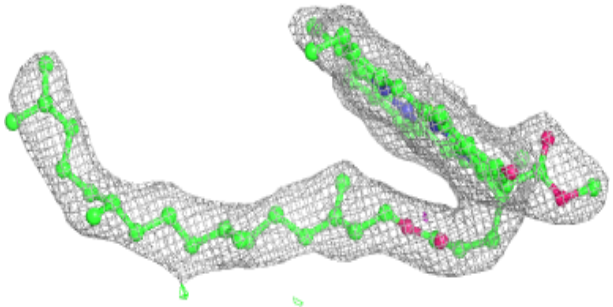
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 608:

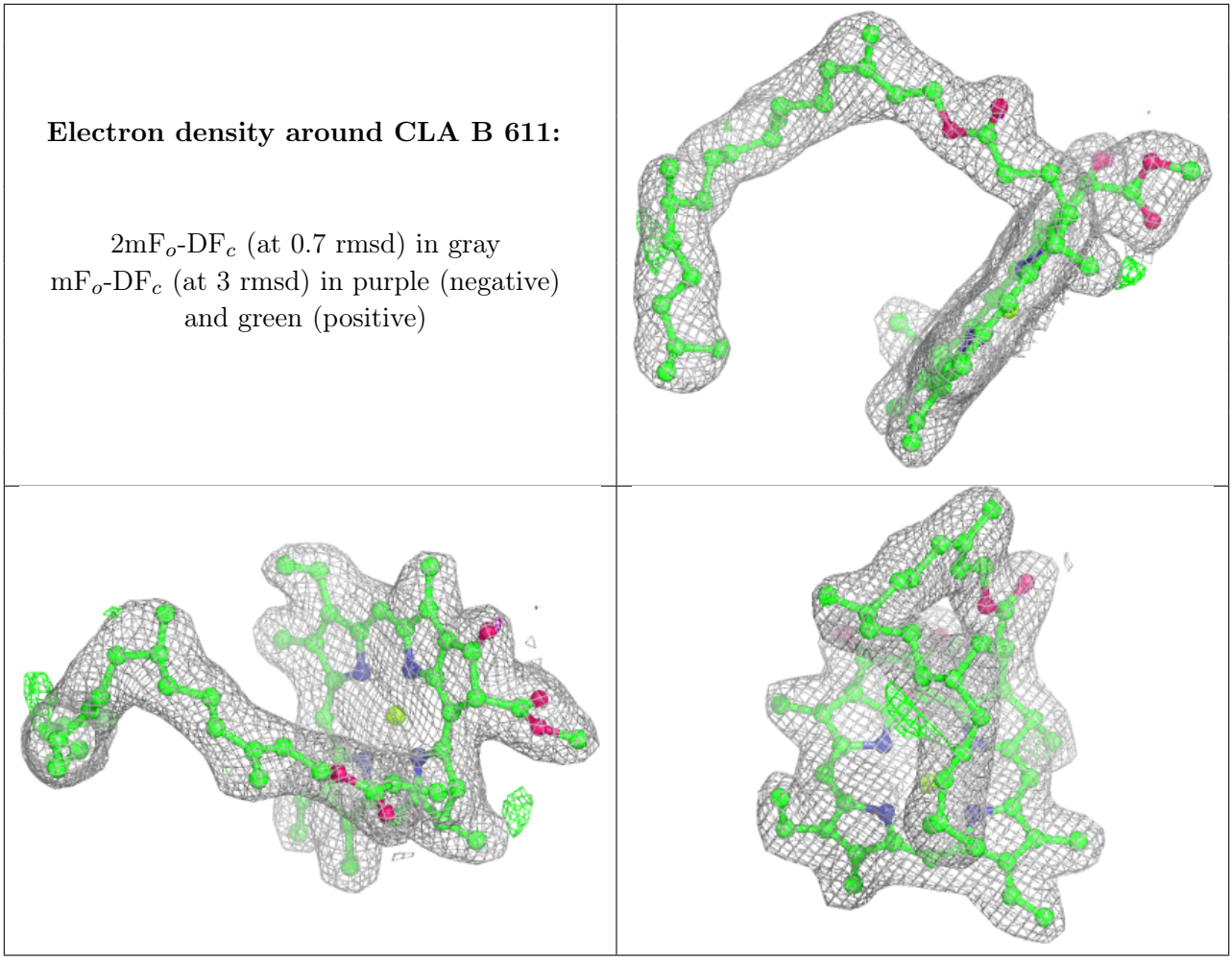
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





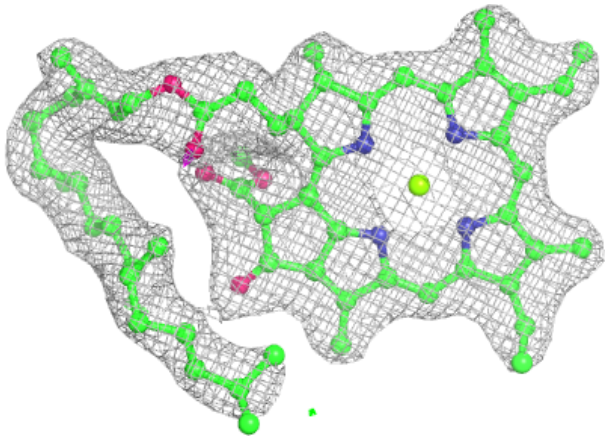
Electron density around CLA B 611:

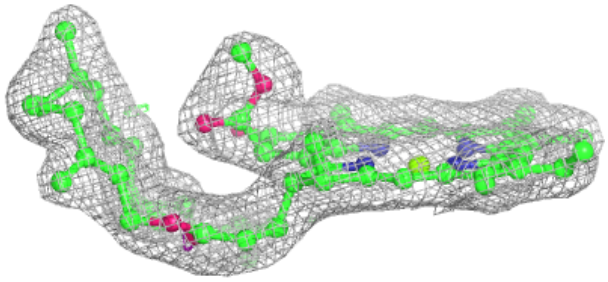
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

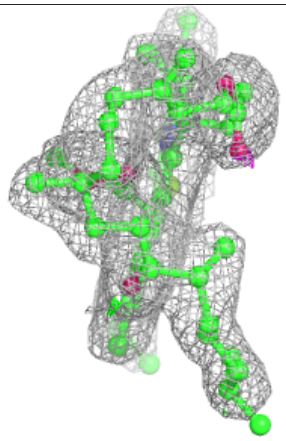


Electron density around CLA b 610:

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

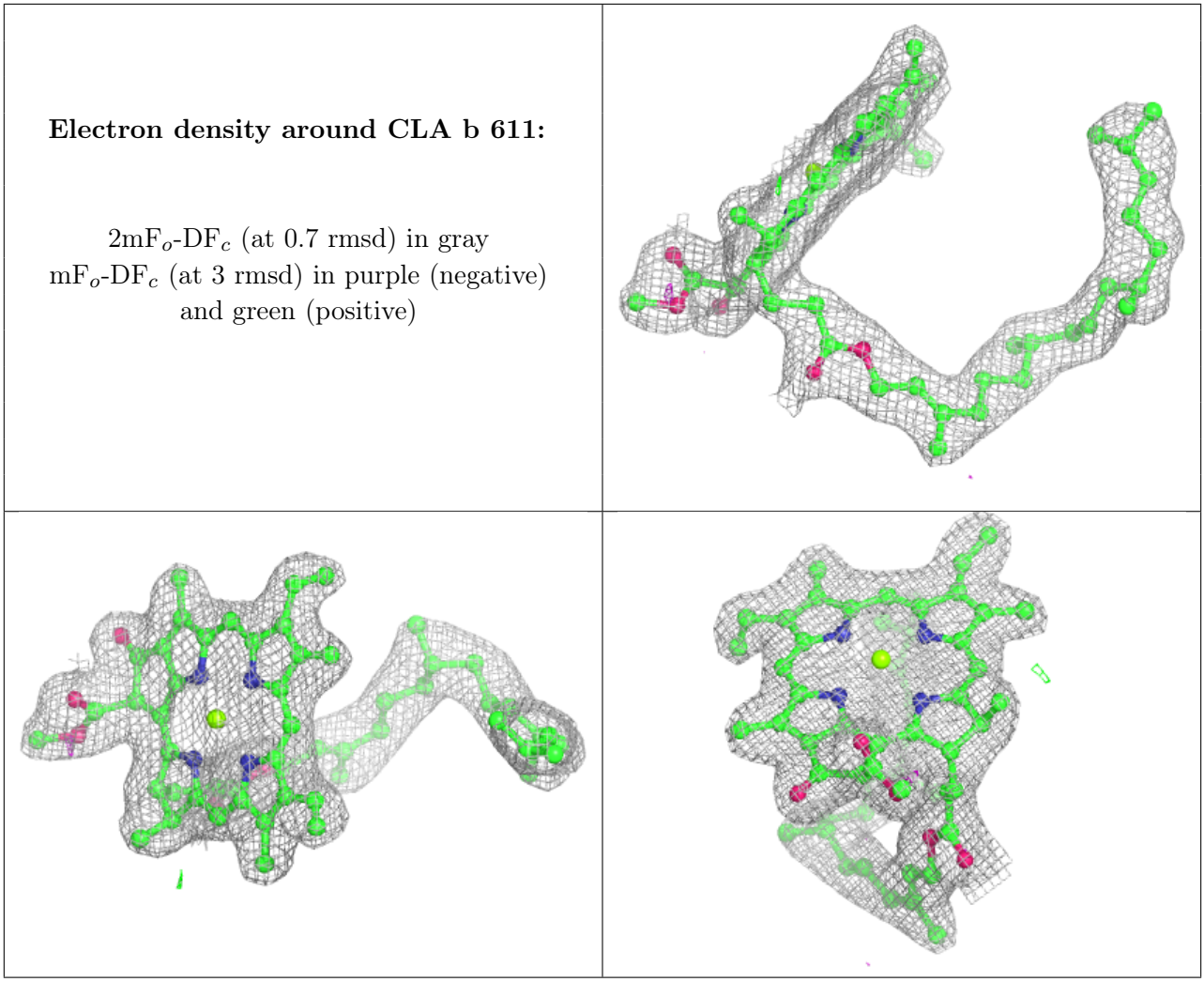






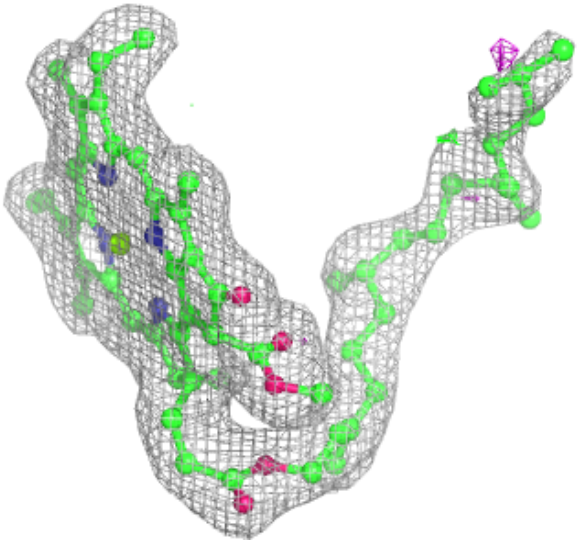
Electron density around CLA b 611:

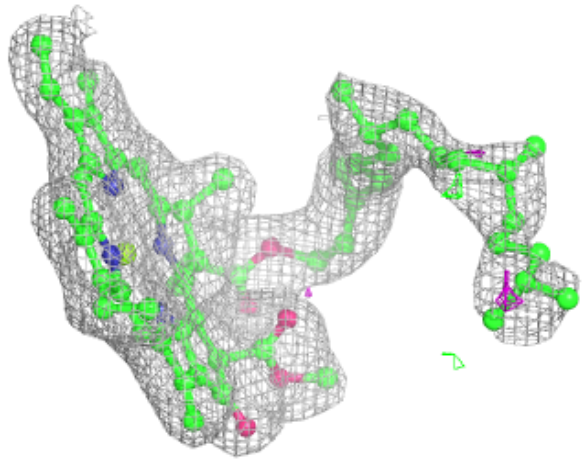
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

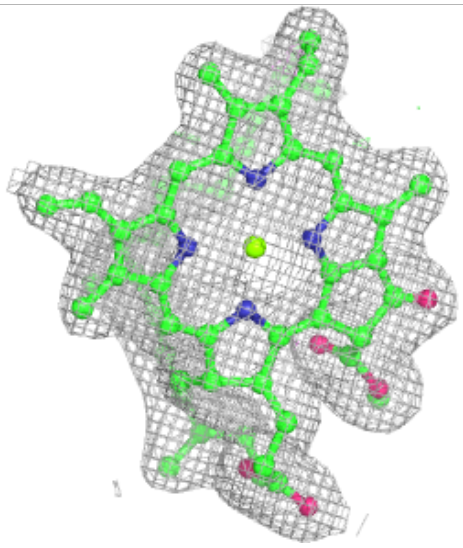


Electron density around CLA b 613:

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

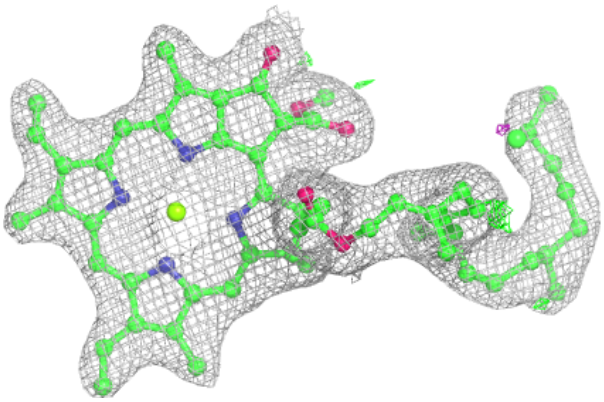


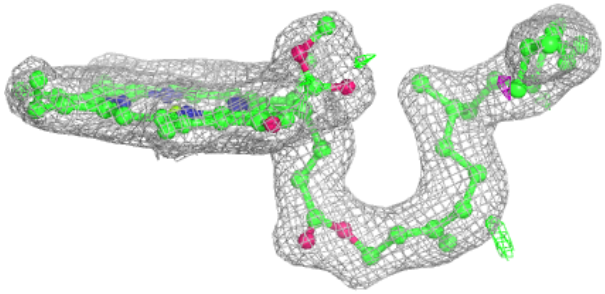


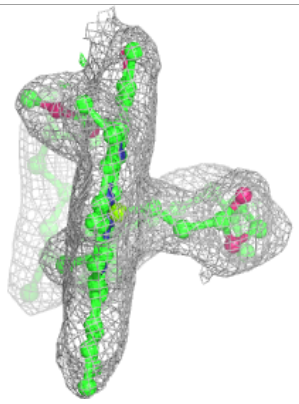


Electron density around CLA B 612:

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

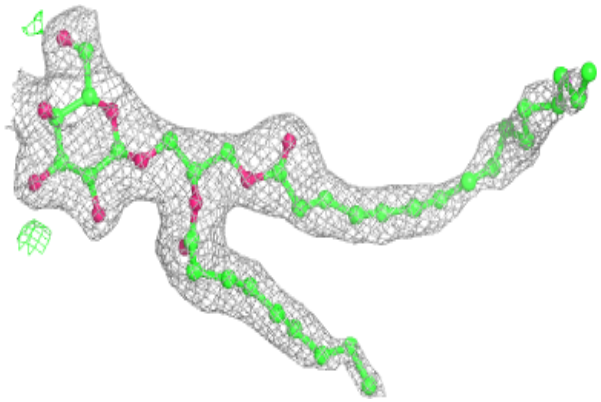


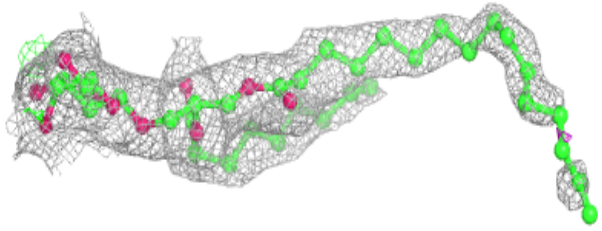


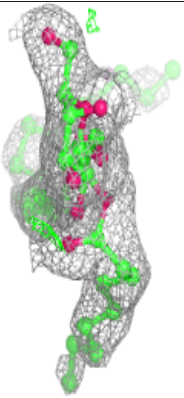


Electron density around LMG d 411:

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

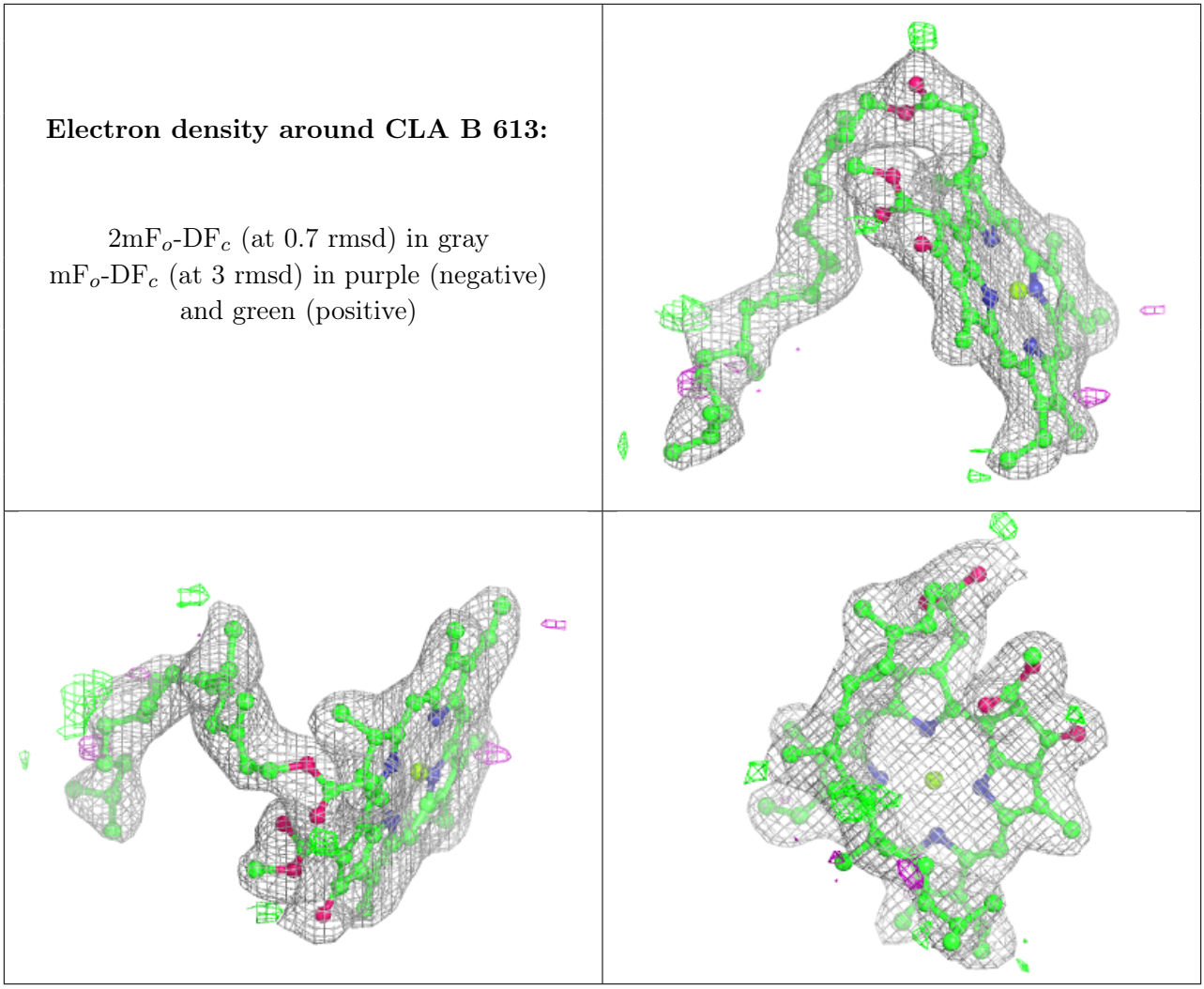






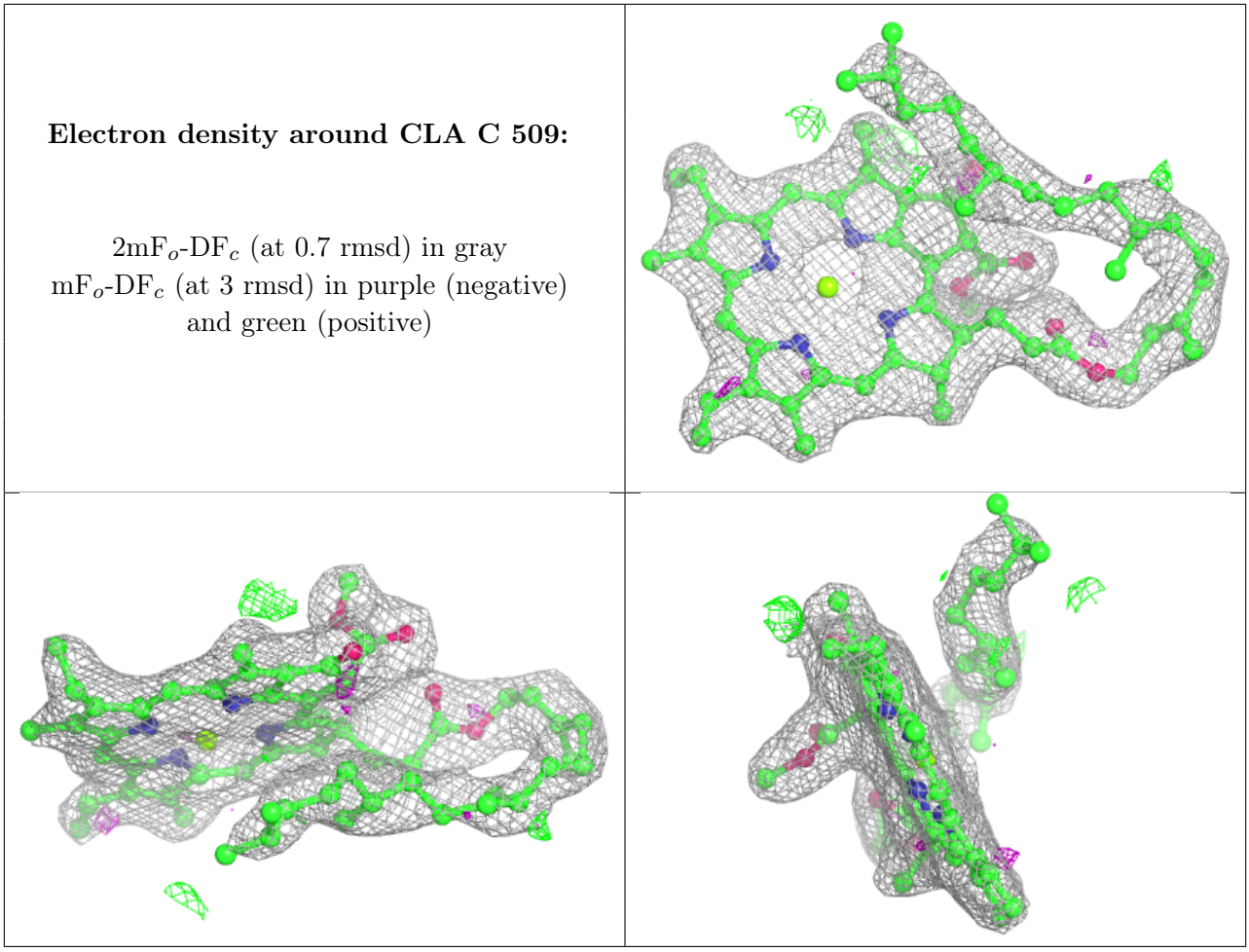
Electron density around CLA B 613:

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



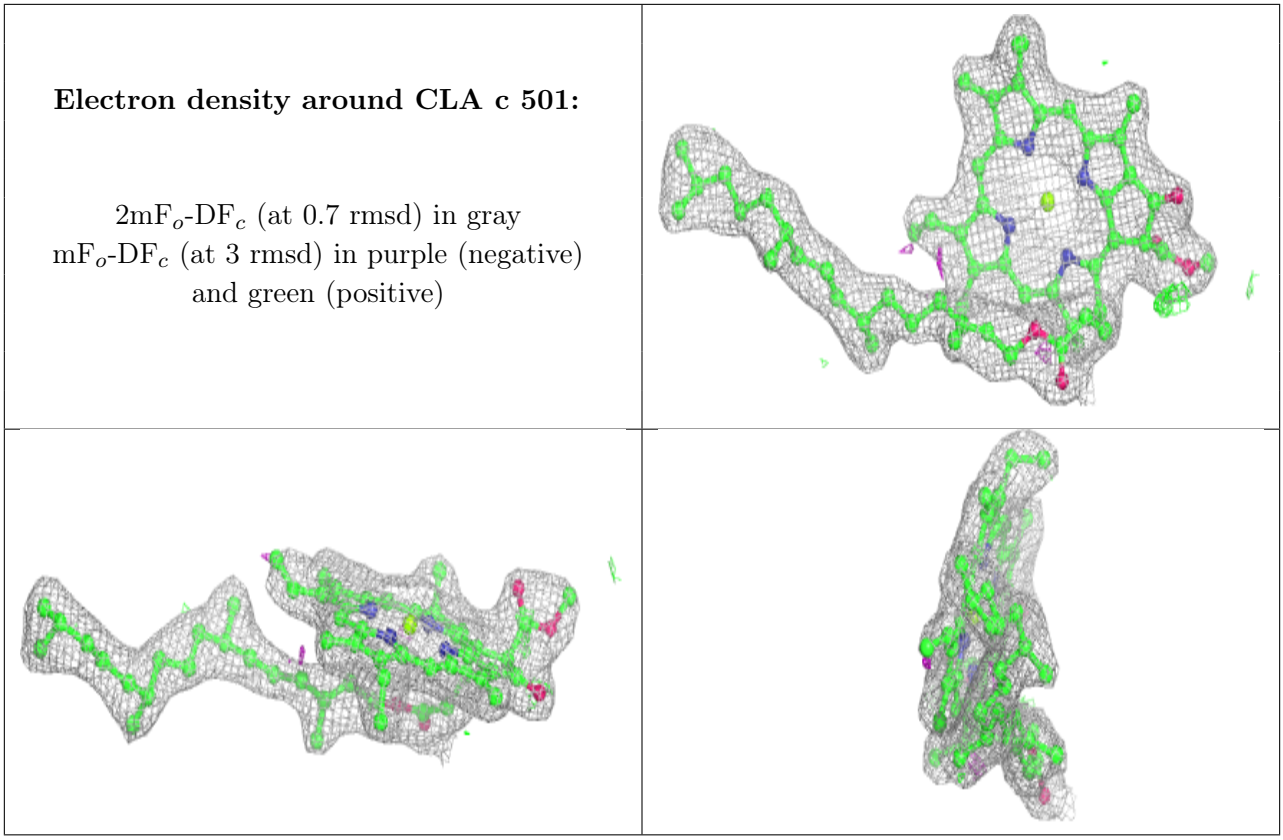
Electron density around CLA C 509:

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



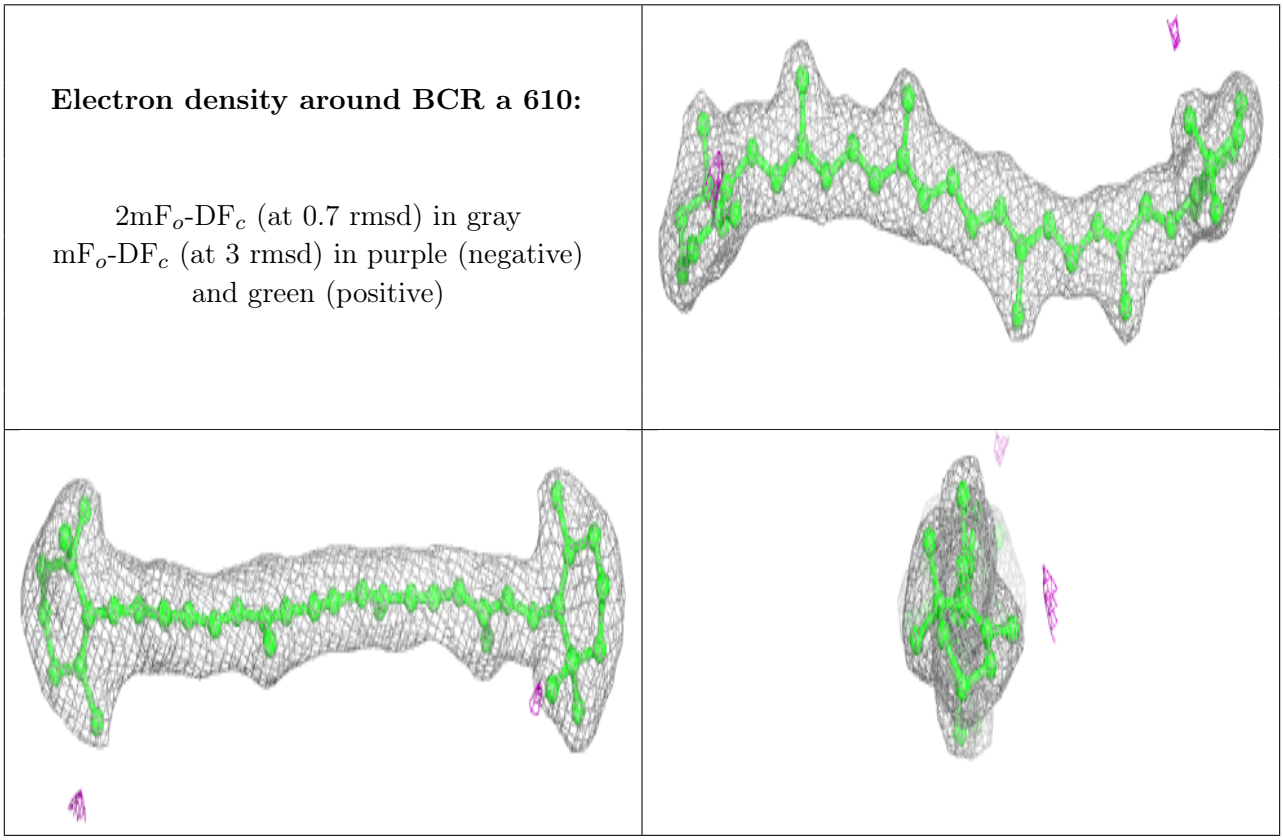
Electron density around CLA c 501:

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



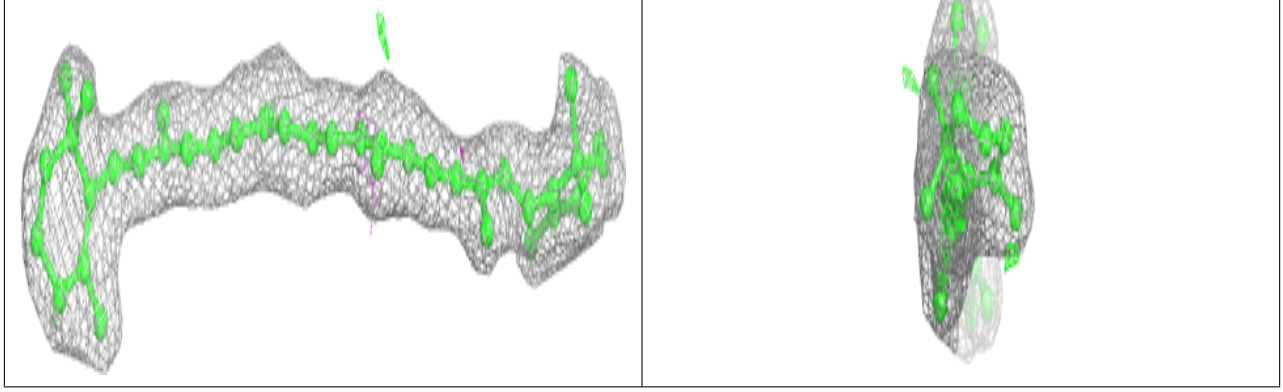
Electron density around BCR a 610:

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



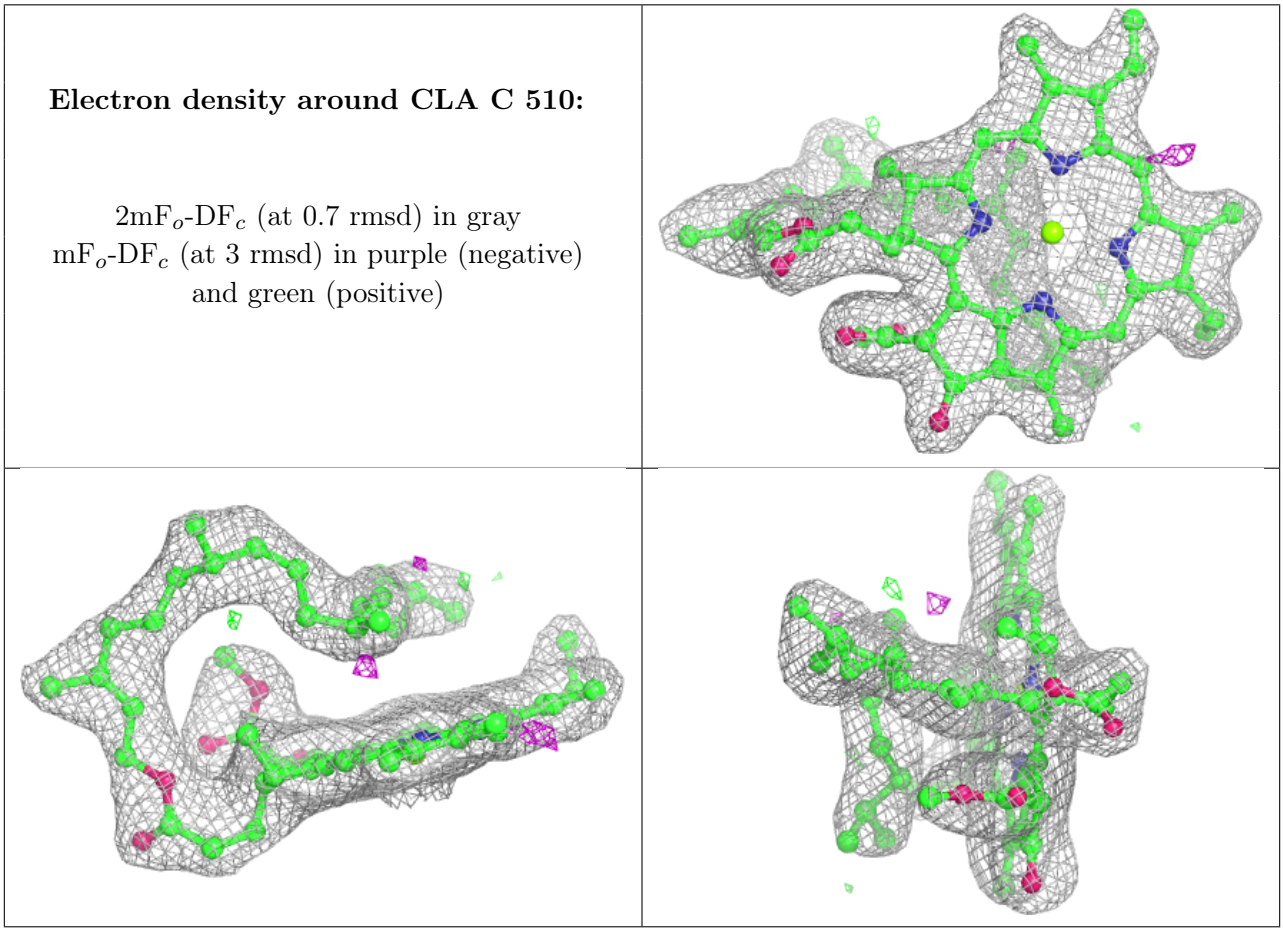
Electron density around BCR b 617:

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



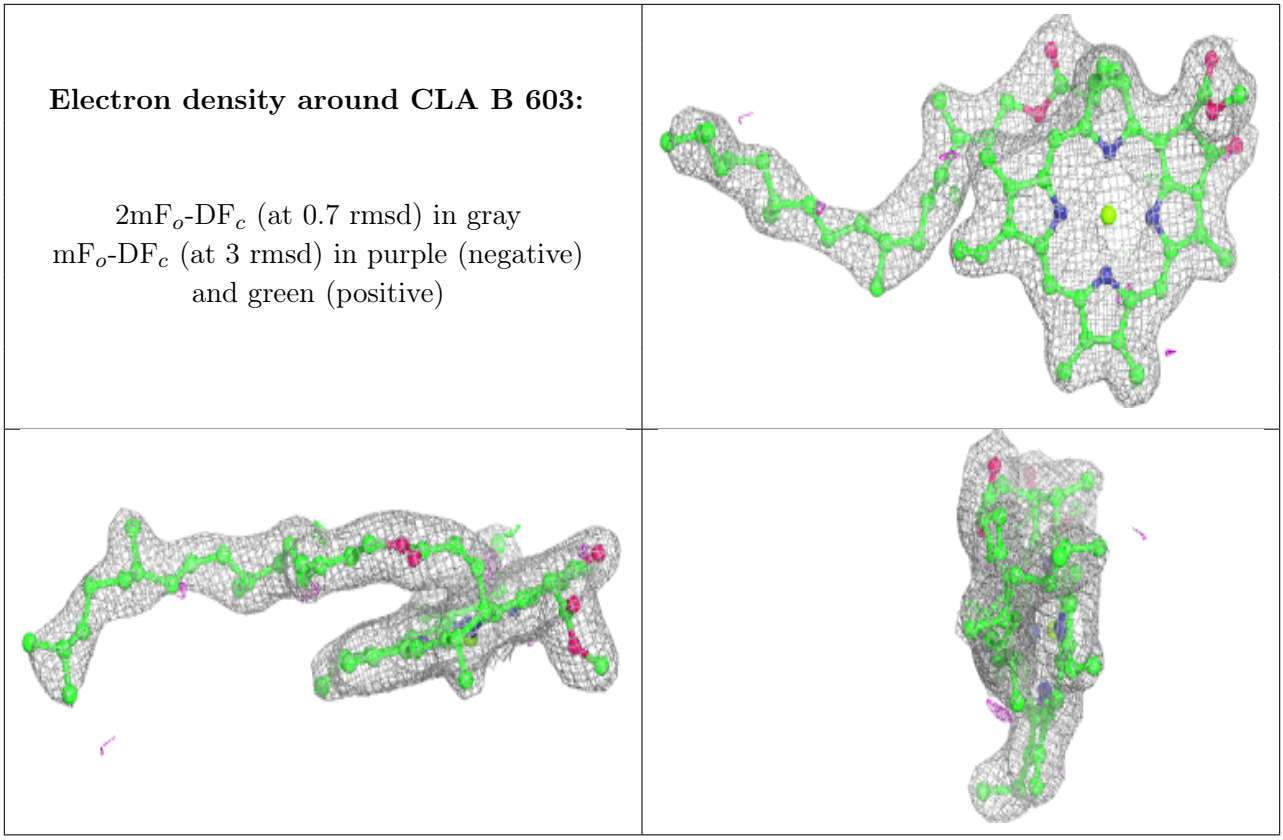
Electron density around CLA C 510:

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



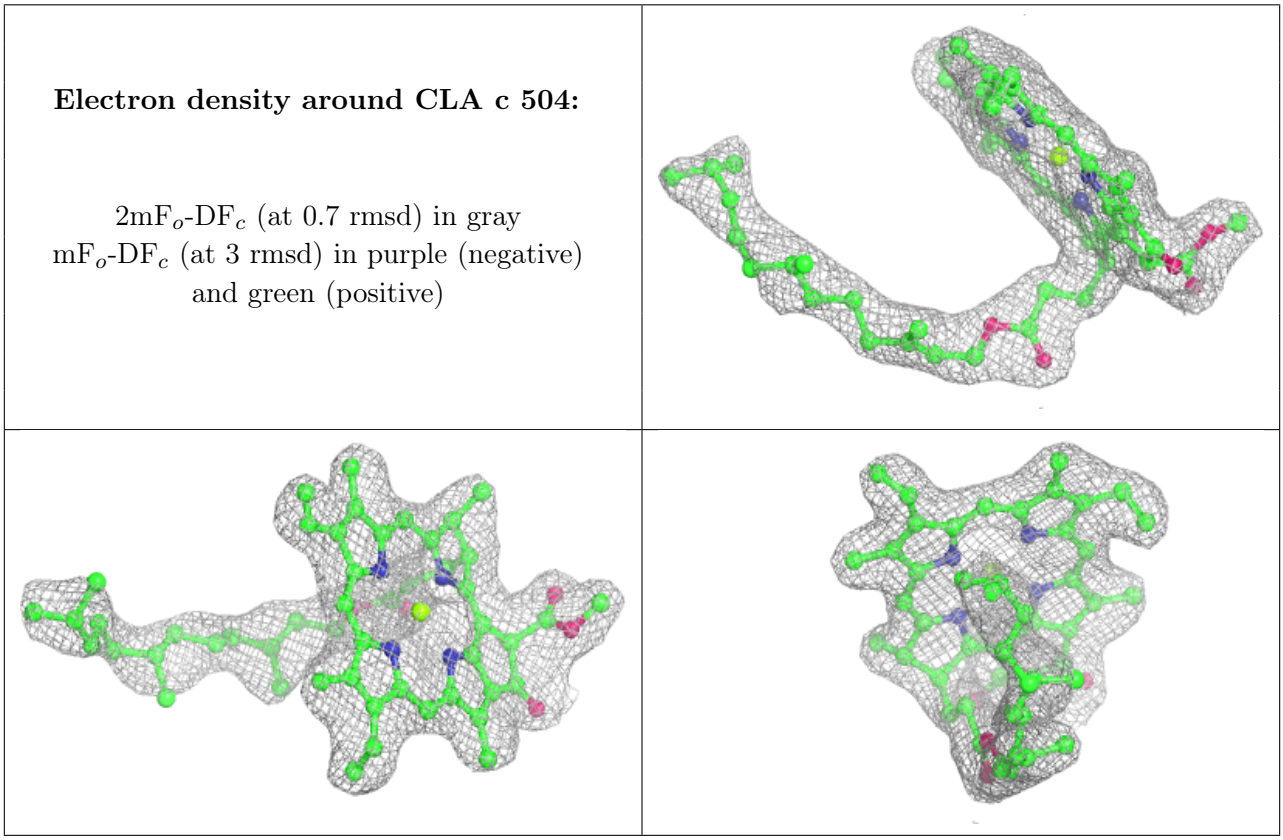
Electron density around CLA B 603:

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



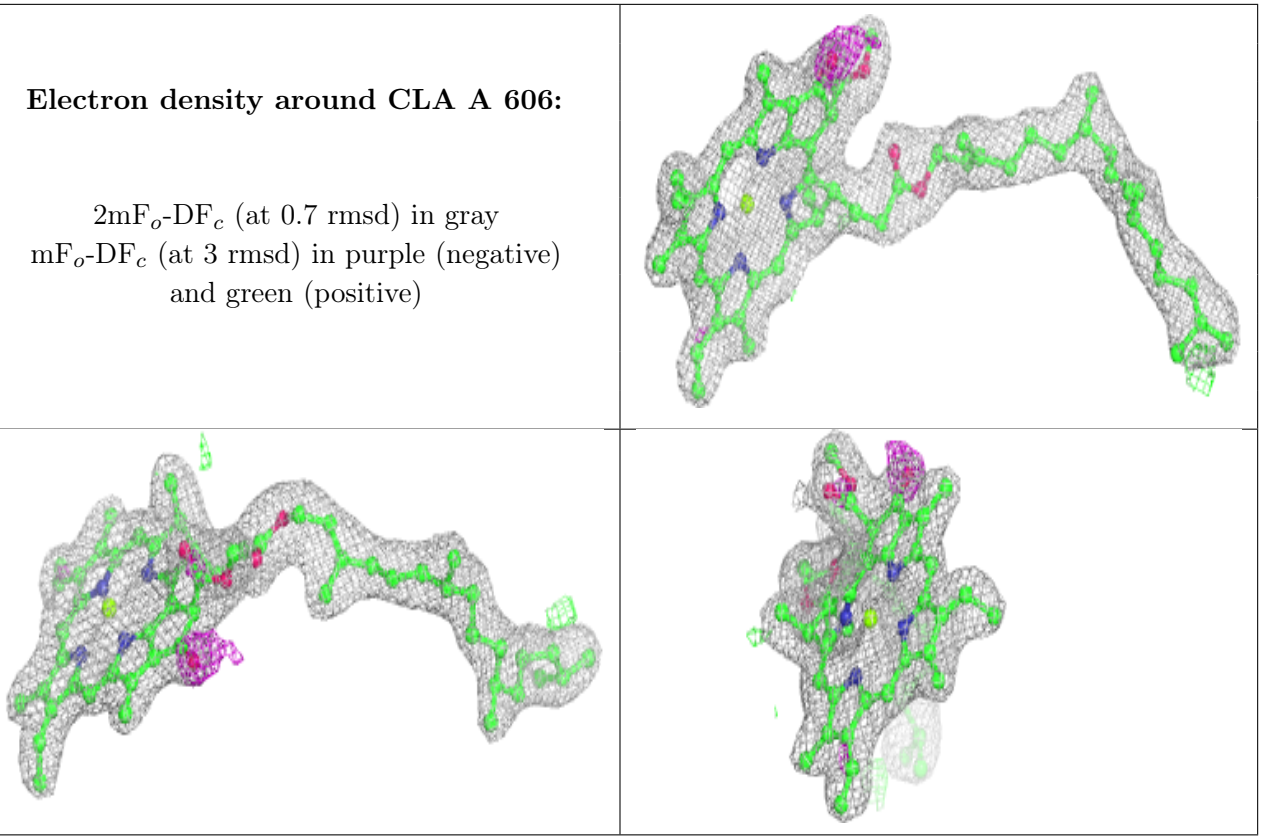
Electron density around CLA c 504:

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



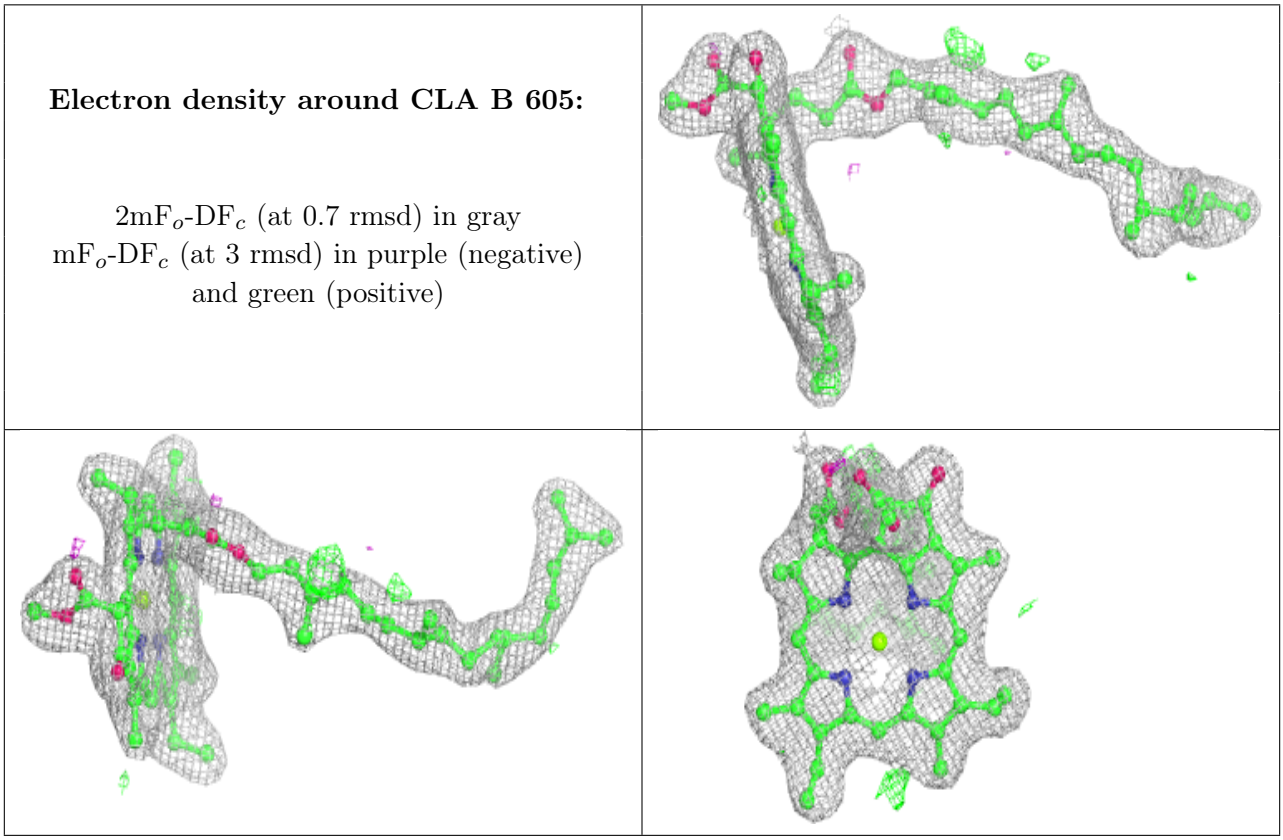
Electron density around CLA A 606:

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



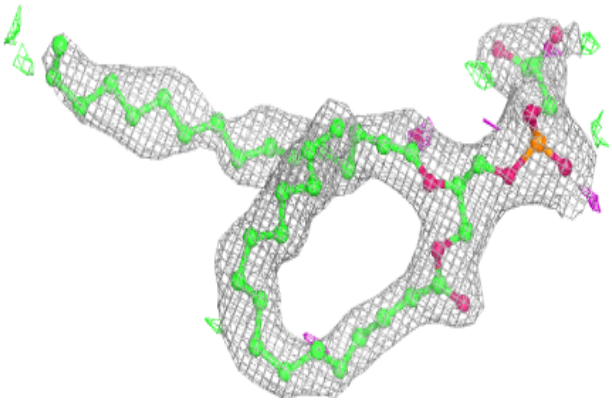
Electron density around CLA B 605:

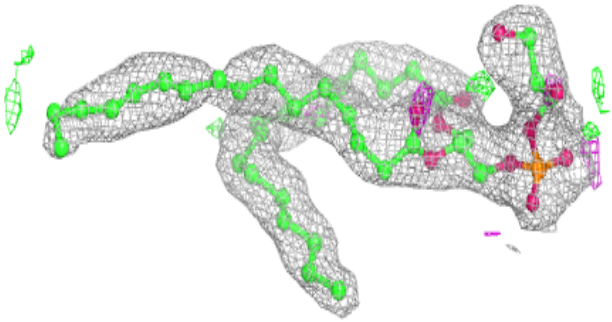
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

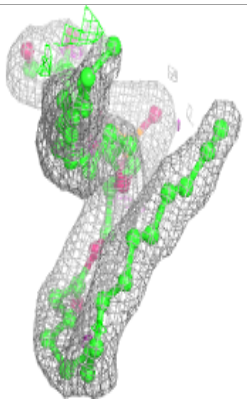


Electron density around LHG D 412:

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

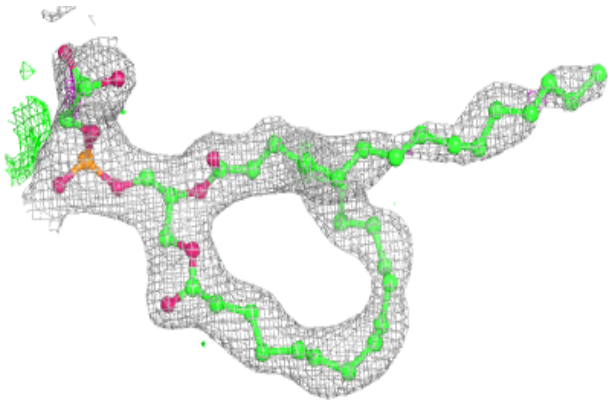


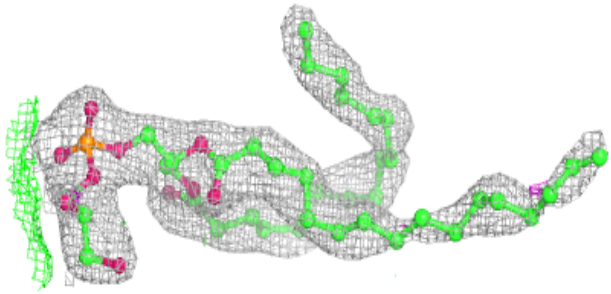


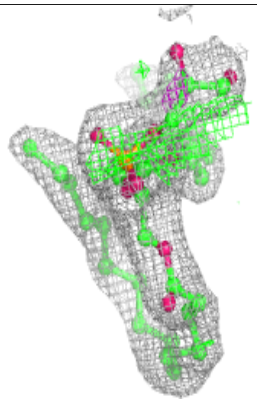


Electron density around LHG d 407:

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

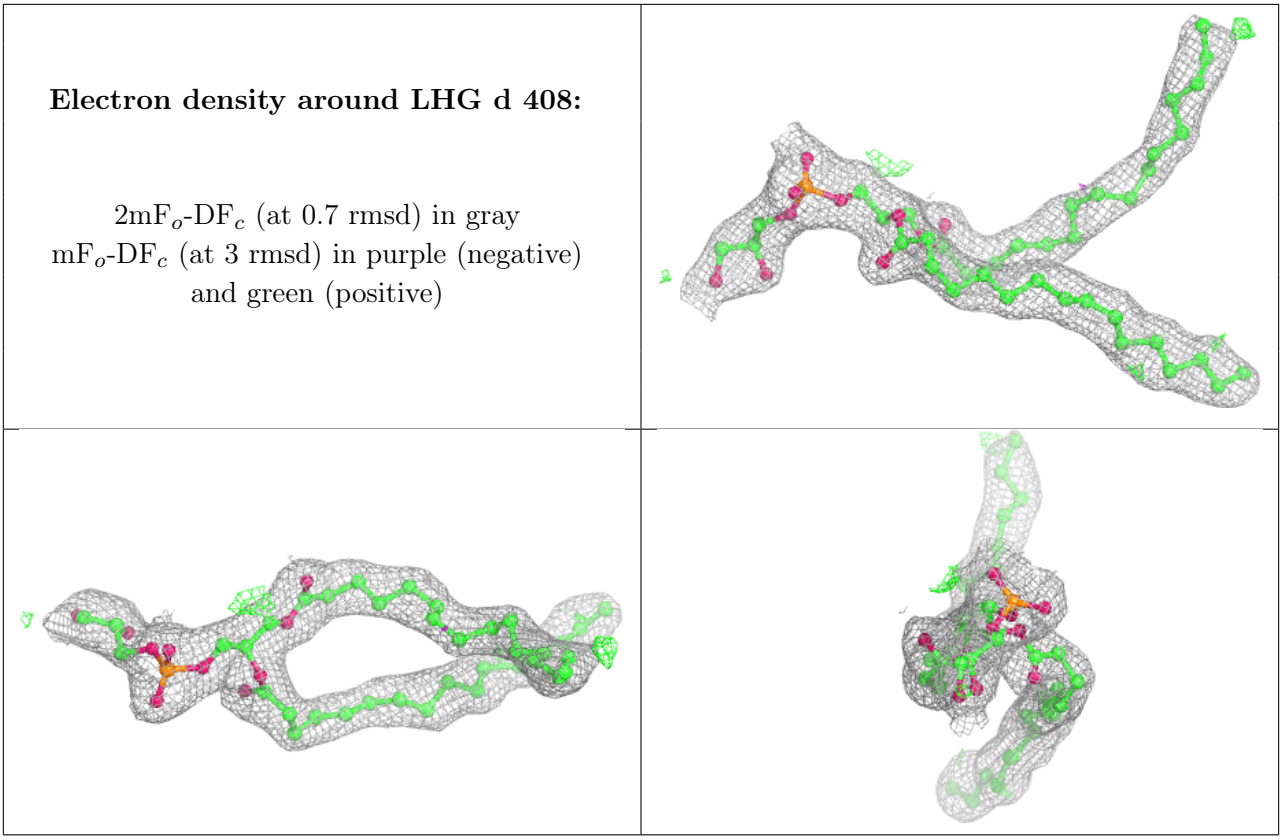






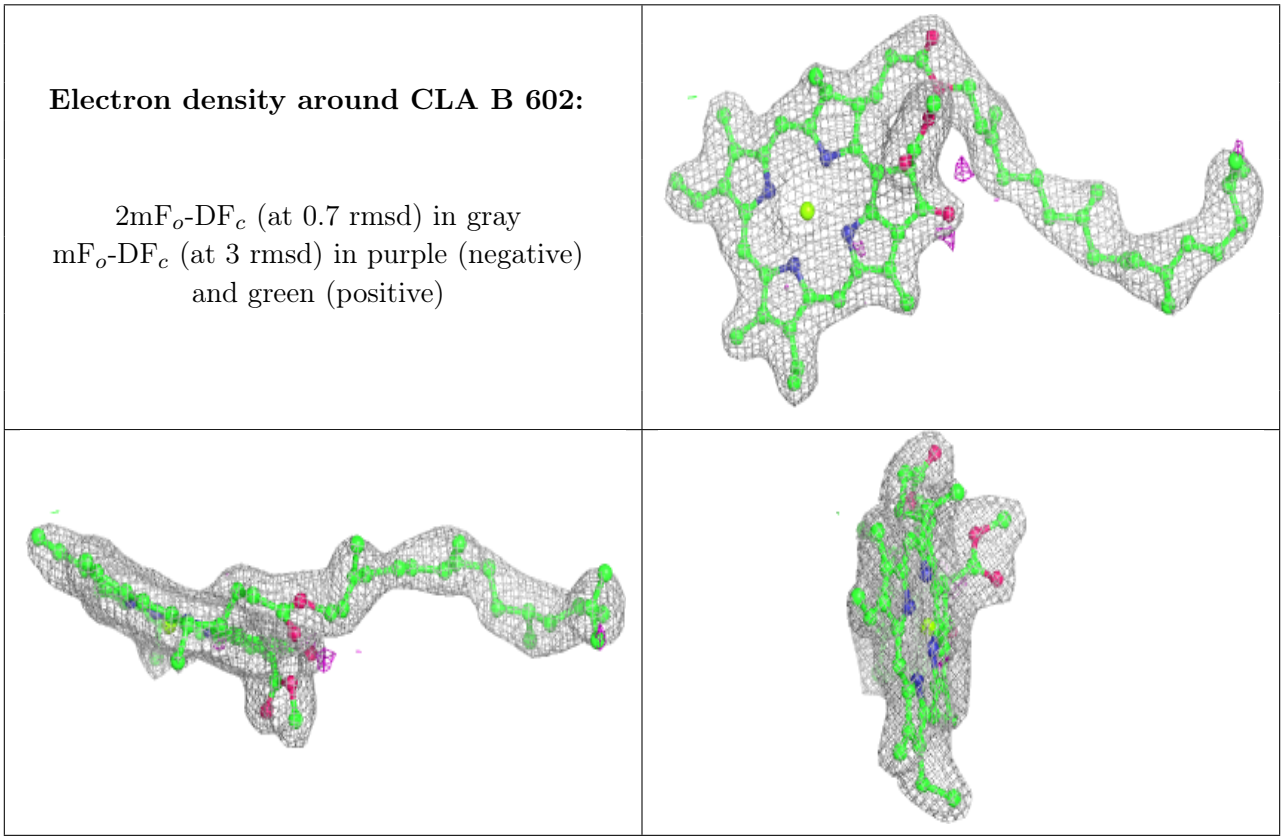
Electron density around LHG d 408:

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



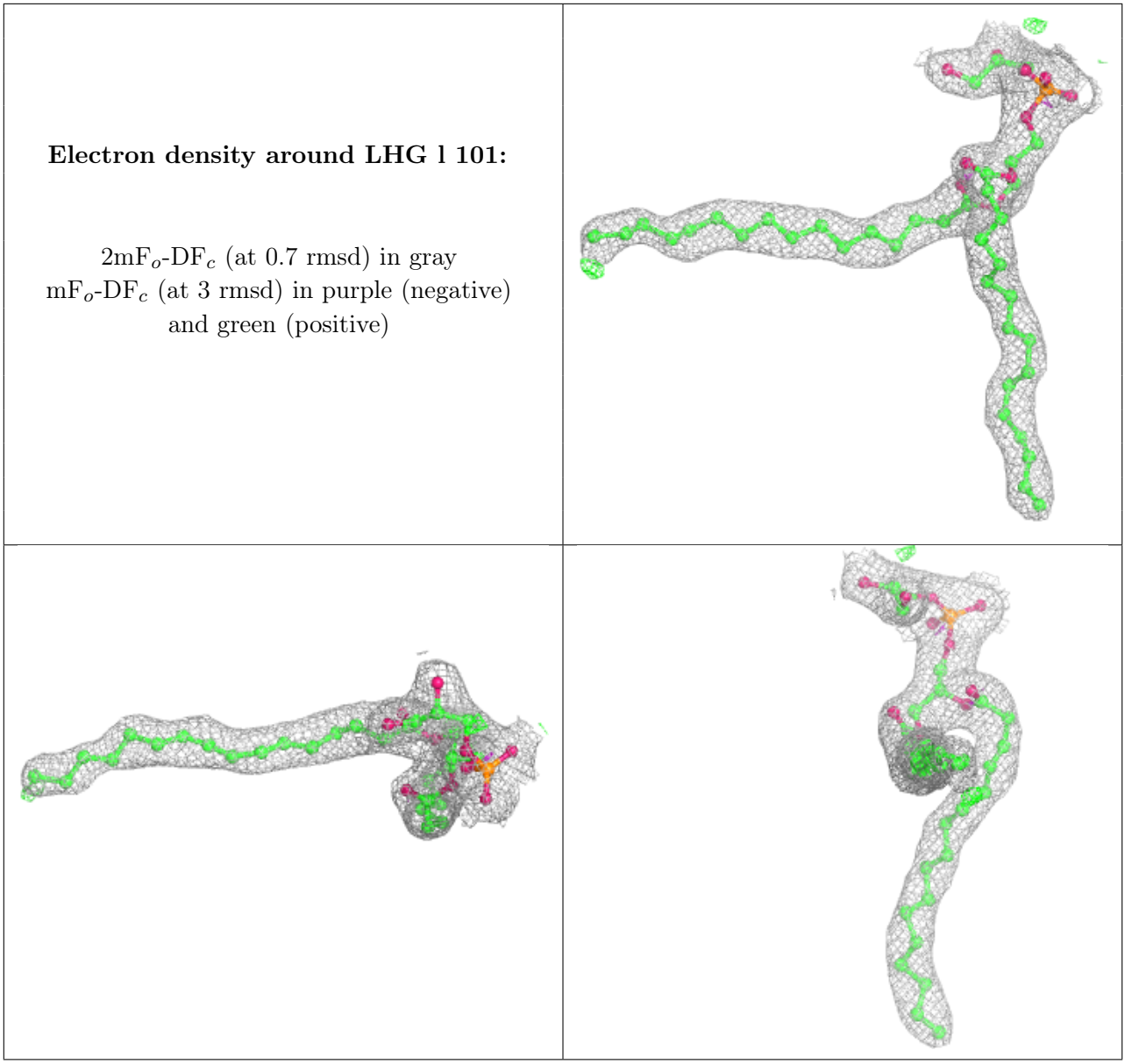
Electron density around CLA B 602:

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



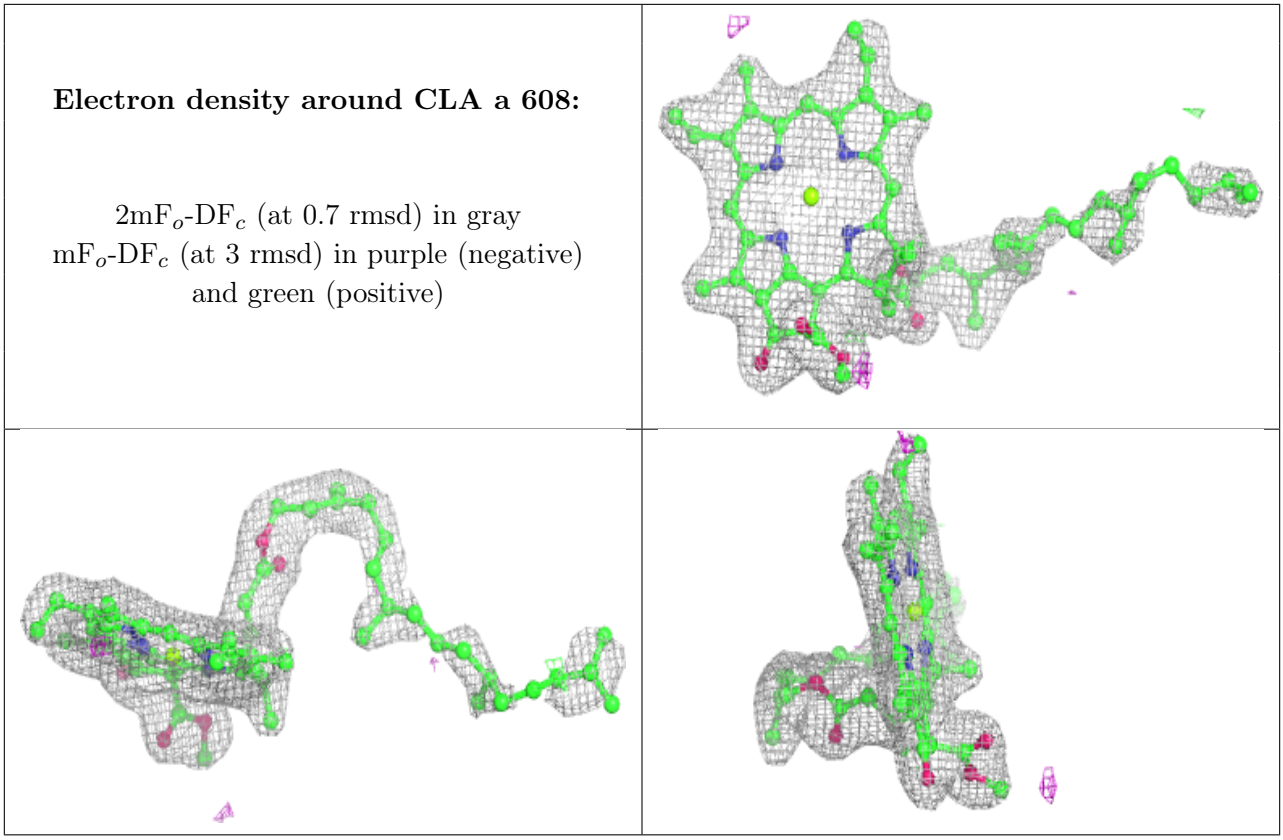
Electron density around LHG l 101:

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



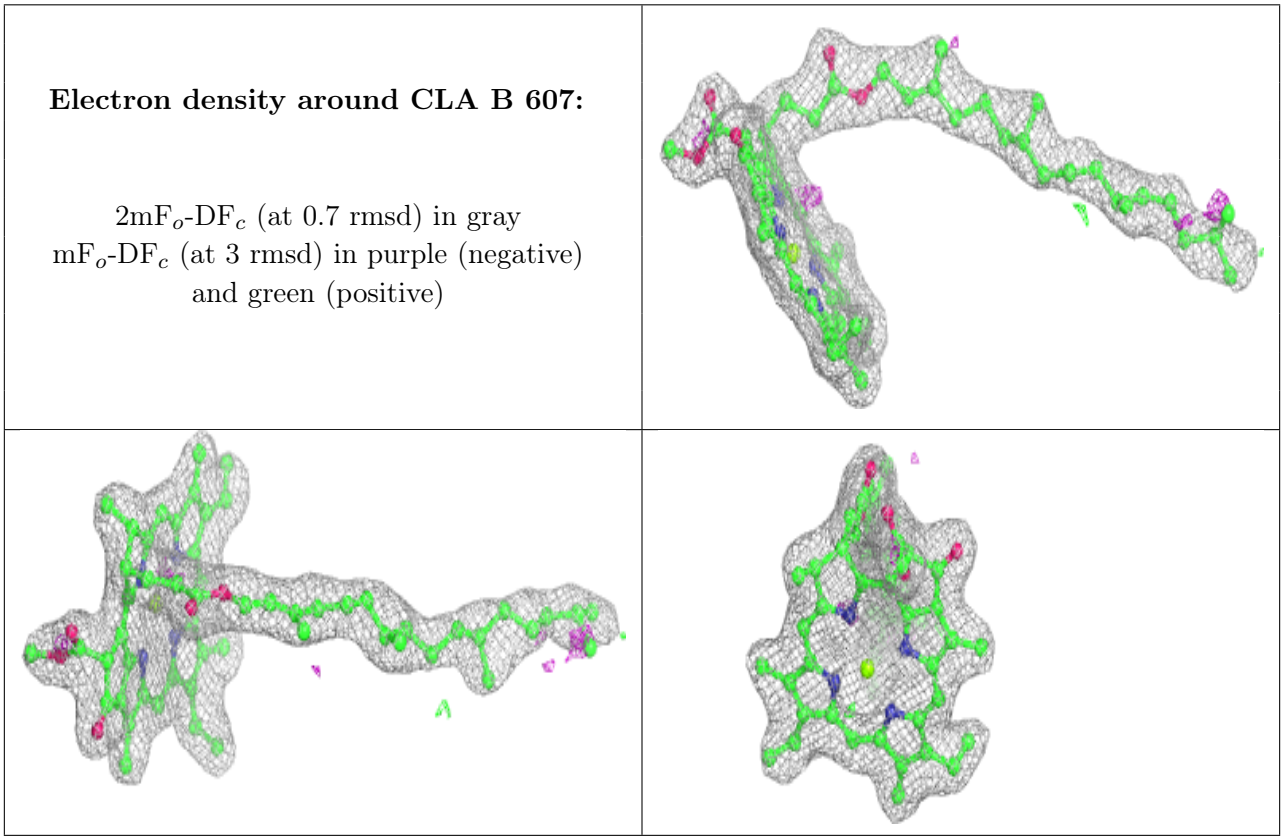
Electron density around CLA a 608:

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



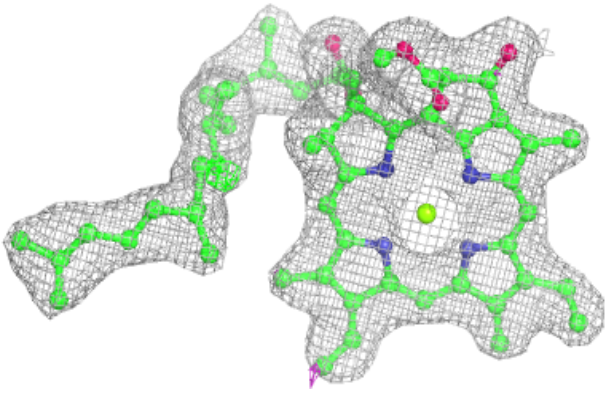
Electron density around CLA B 607:

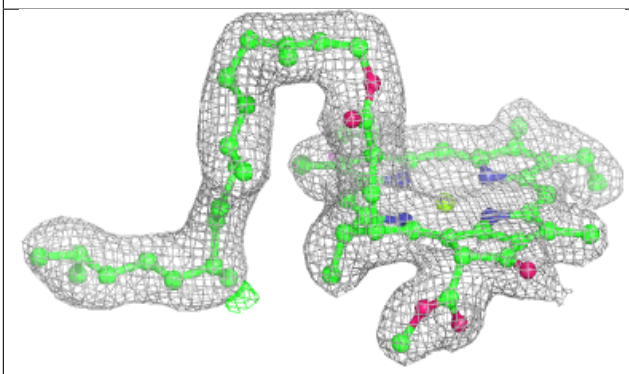
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

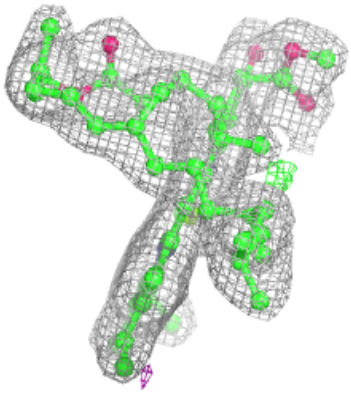


Electron density around CLA a 612:

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

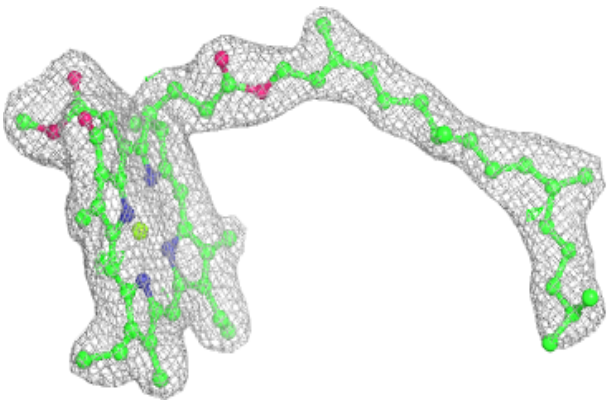


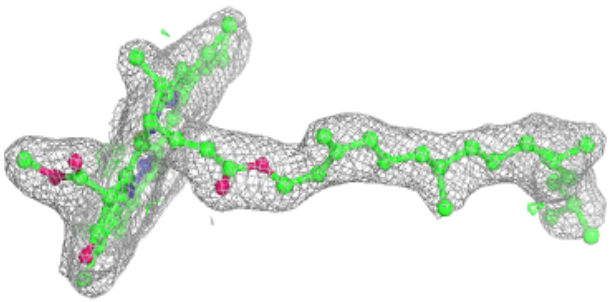


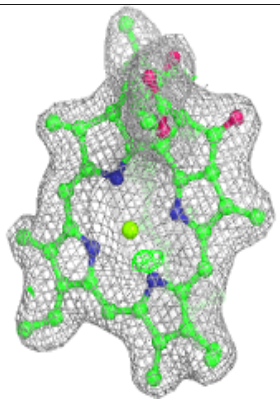


Electron density around CLA B 609:

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

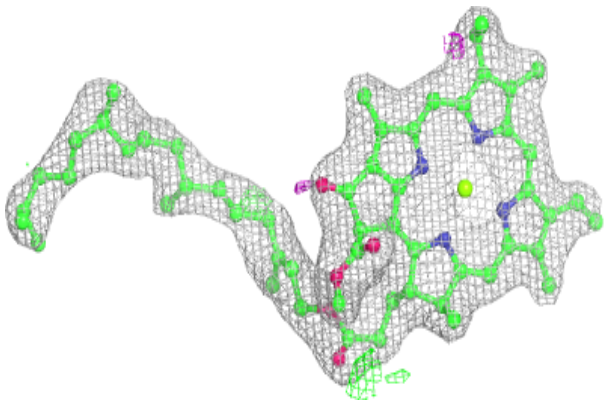


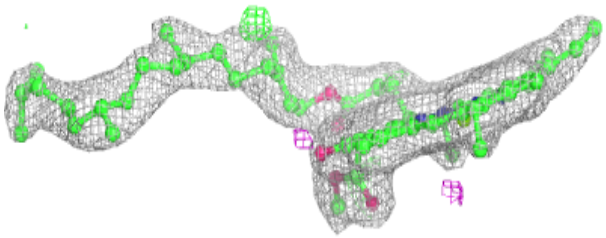


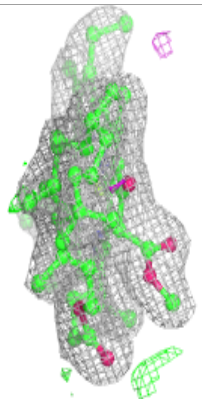


Electron density around CLA b 602:

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

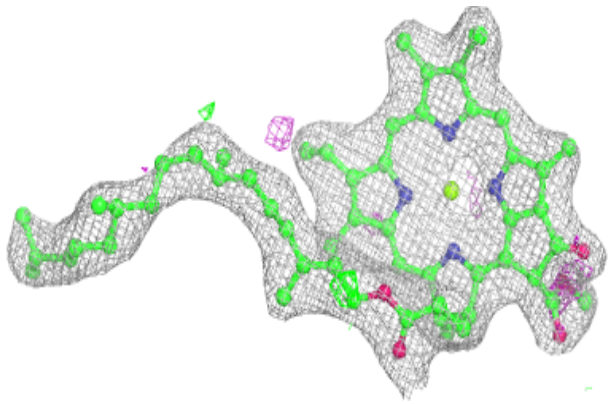


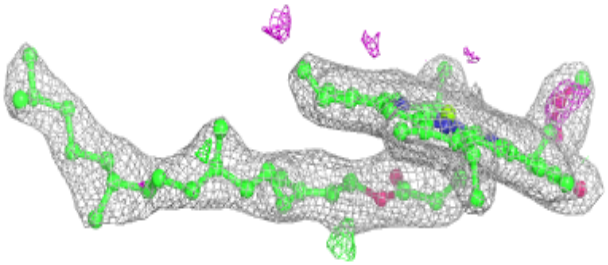


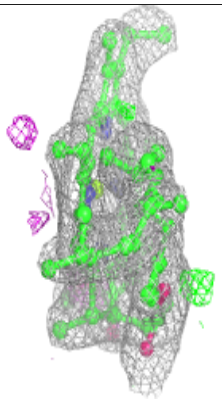


Electron density around CLA b 603:

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

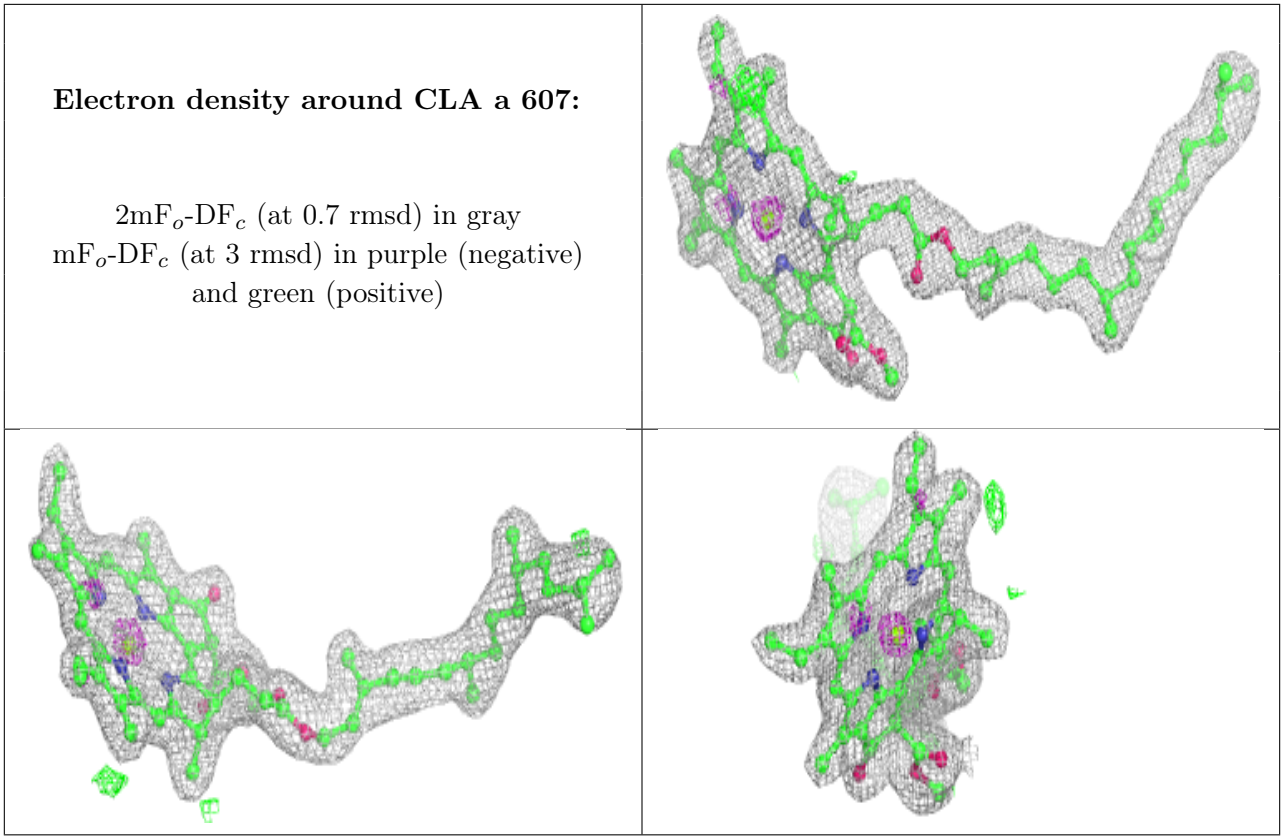






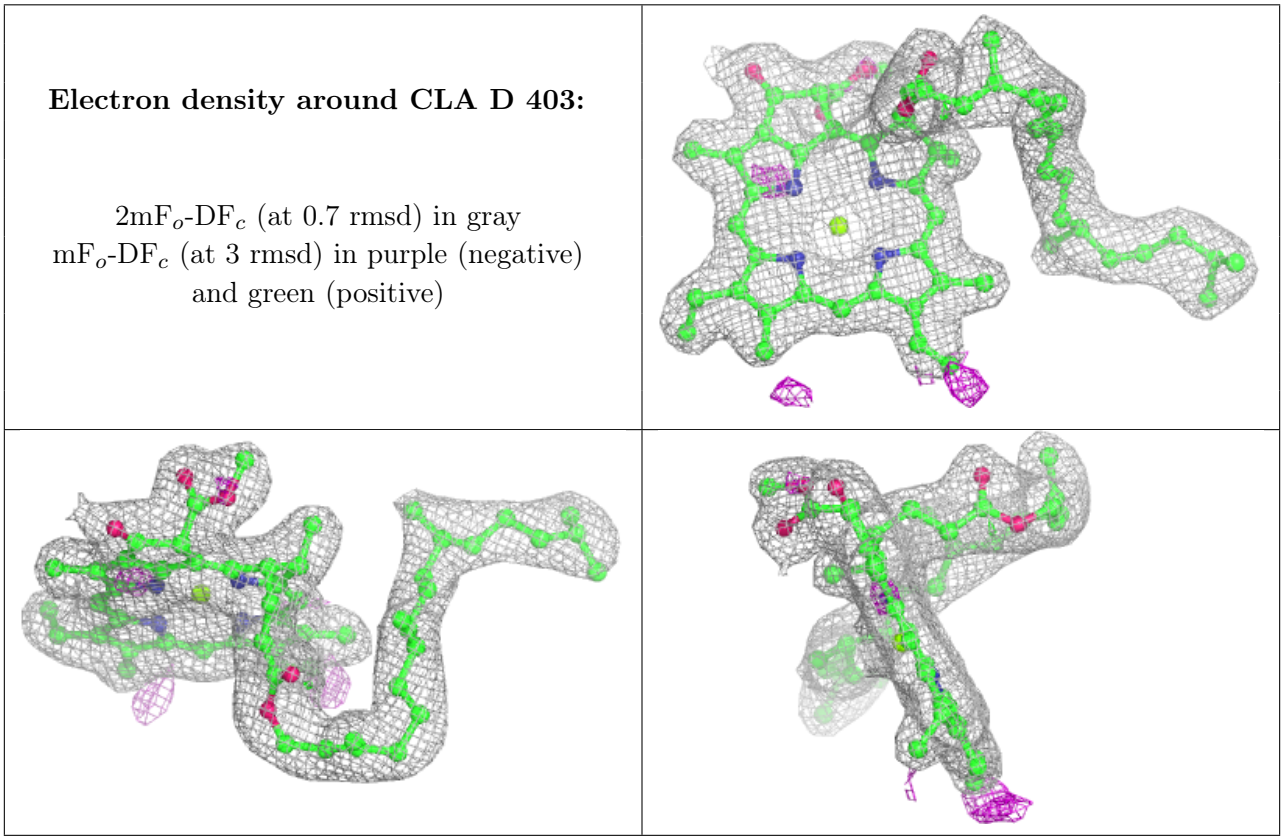
Electron density around CLA a 607:

$2mF_o$-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 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)

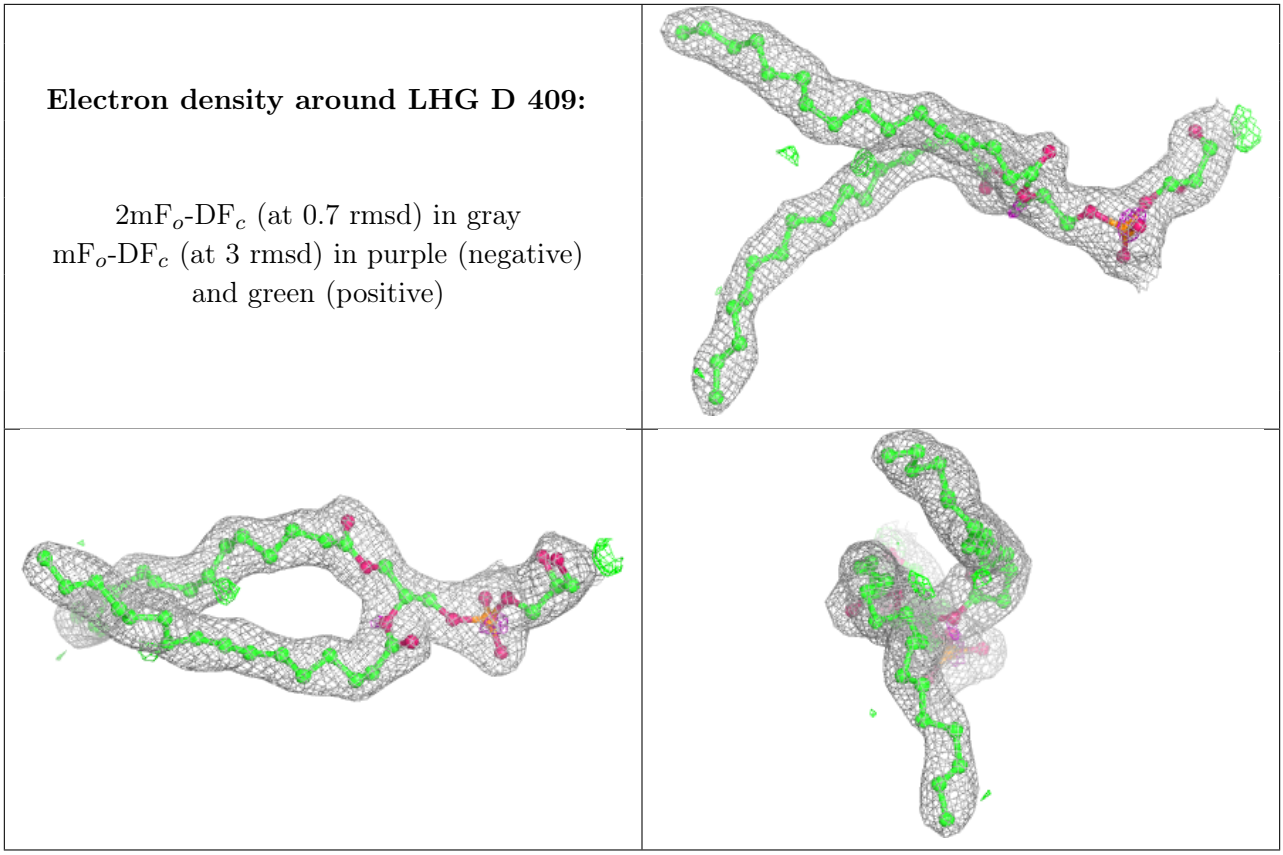


Electron density around LHG A 615:

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

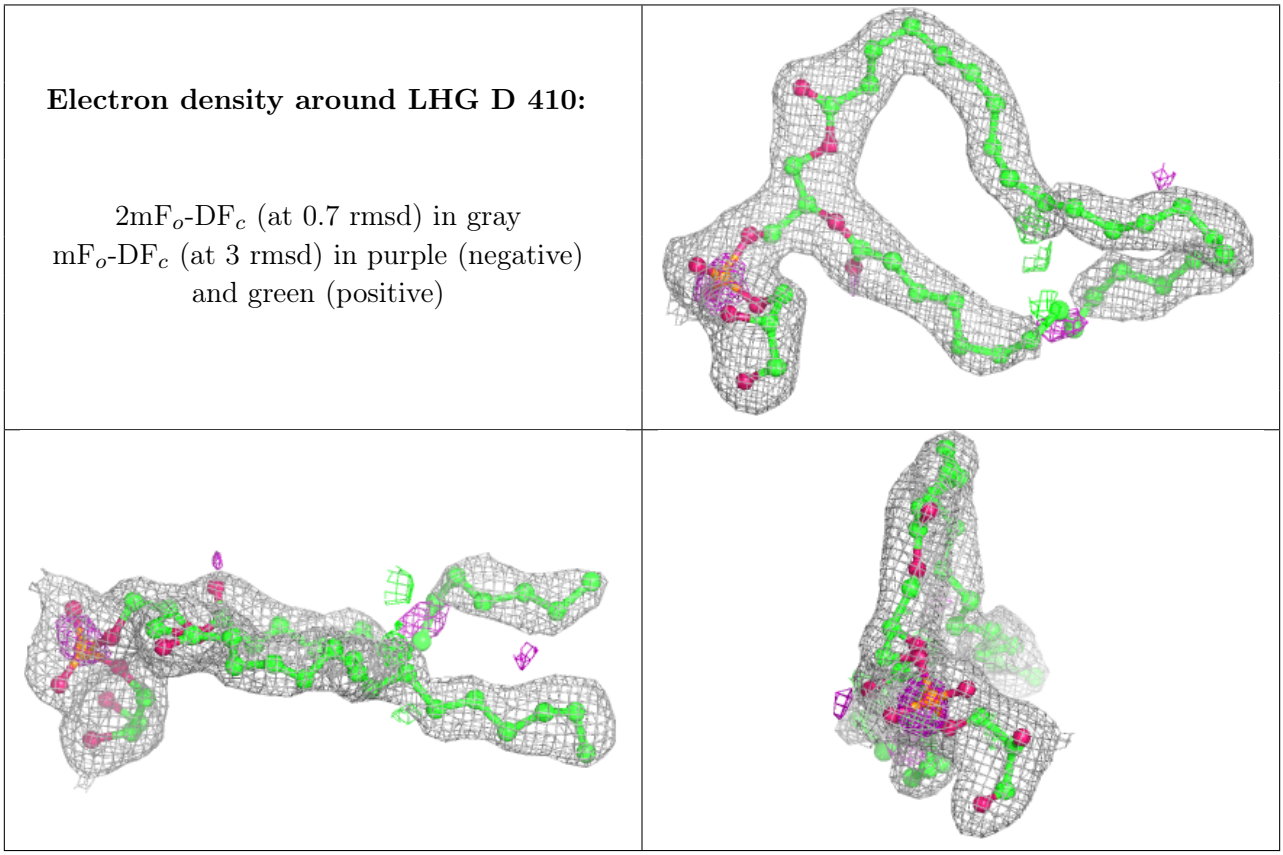
Electron density around LHG D 409:

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



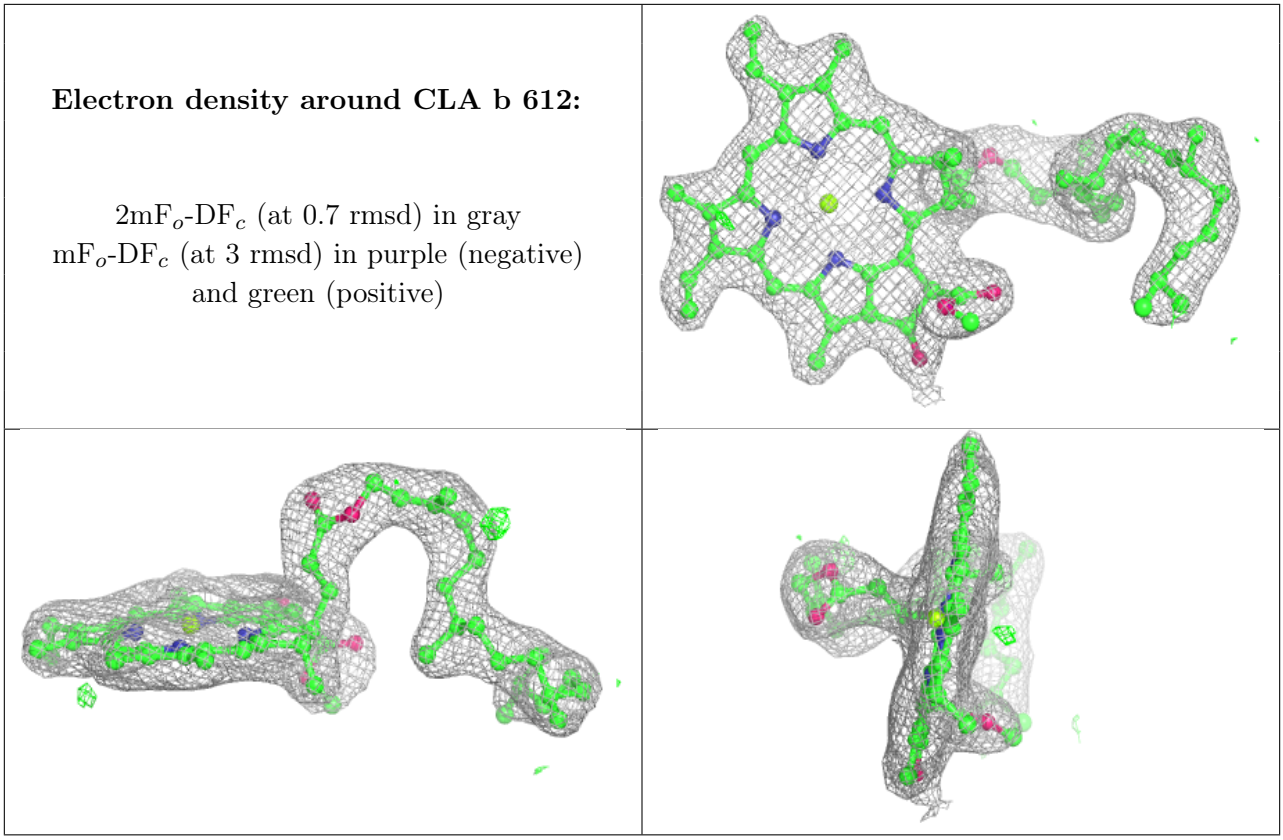
Electron density around LHG D 410:

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



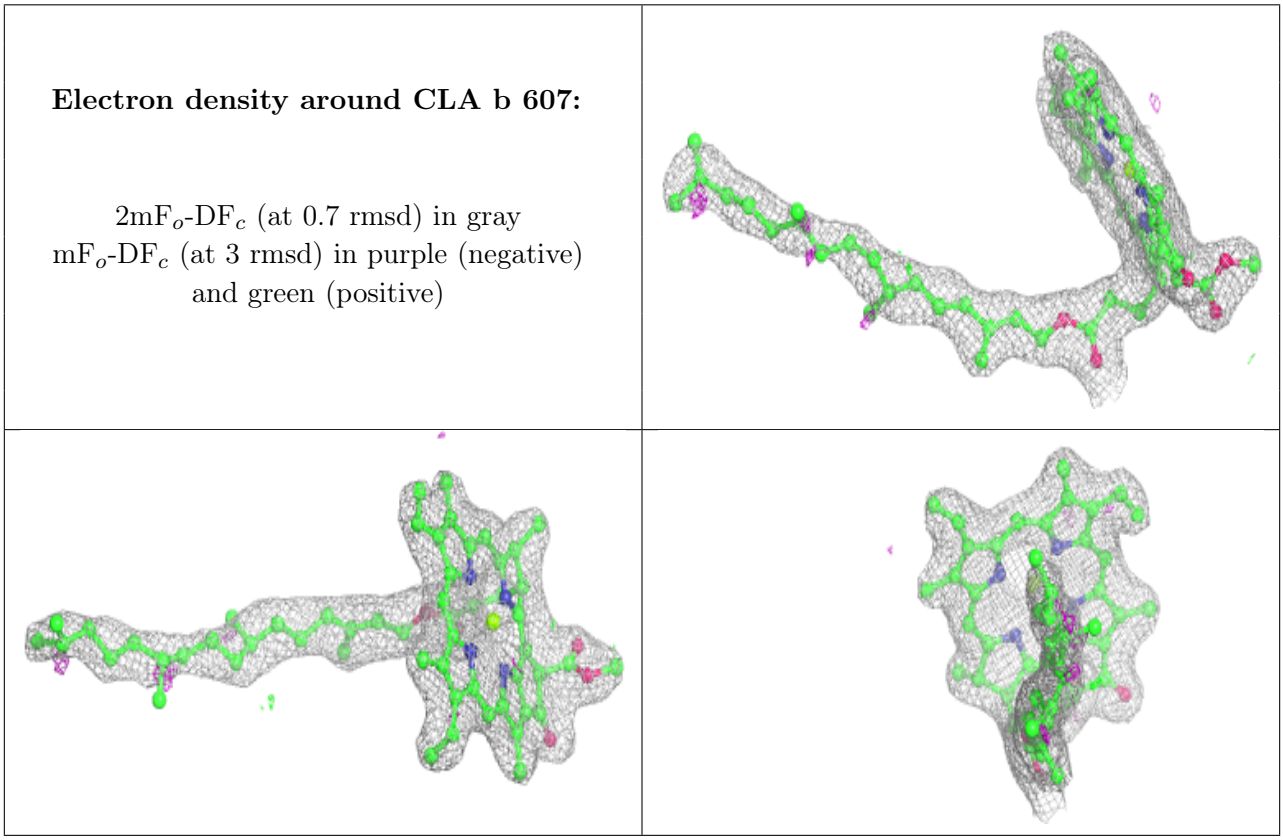
Electron density around CLA b 612:

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



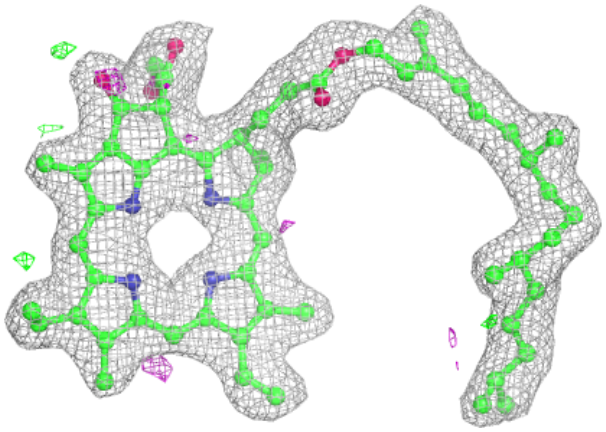
Electron density around CLA b 607:

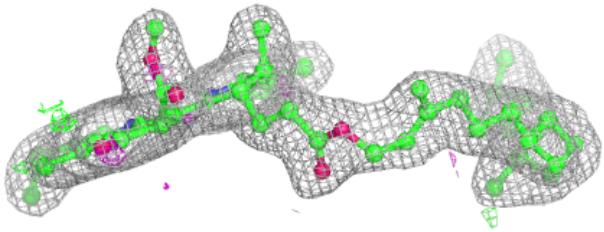
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

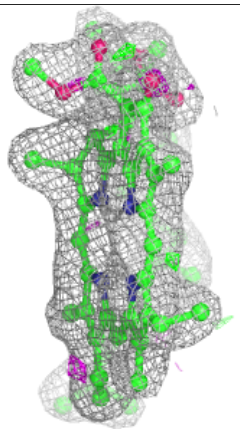


Electron density around PHO A 608:

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

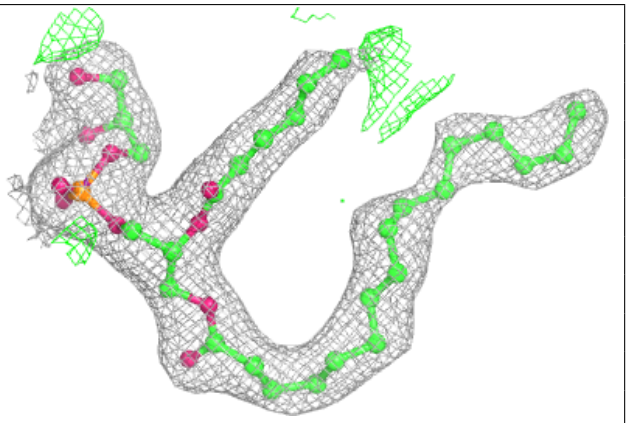


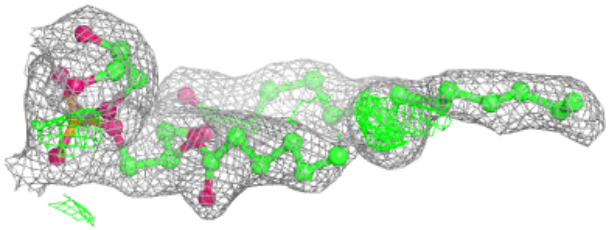


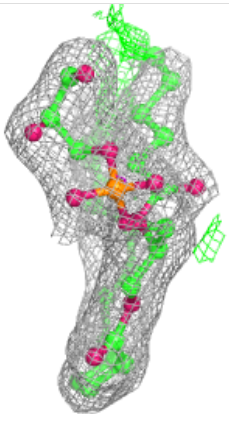


Electron density around LHG d 409:

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

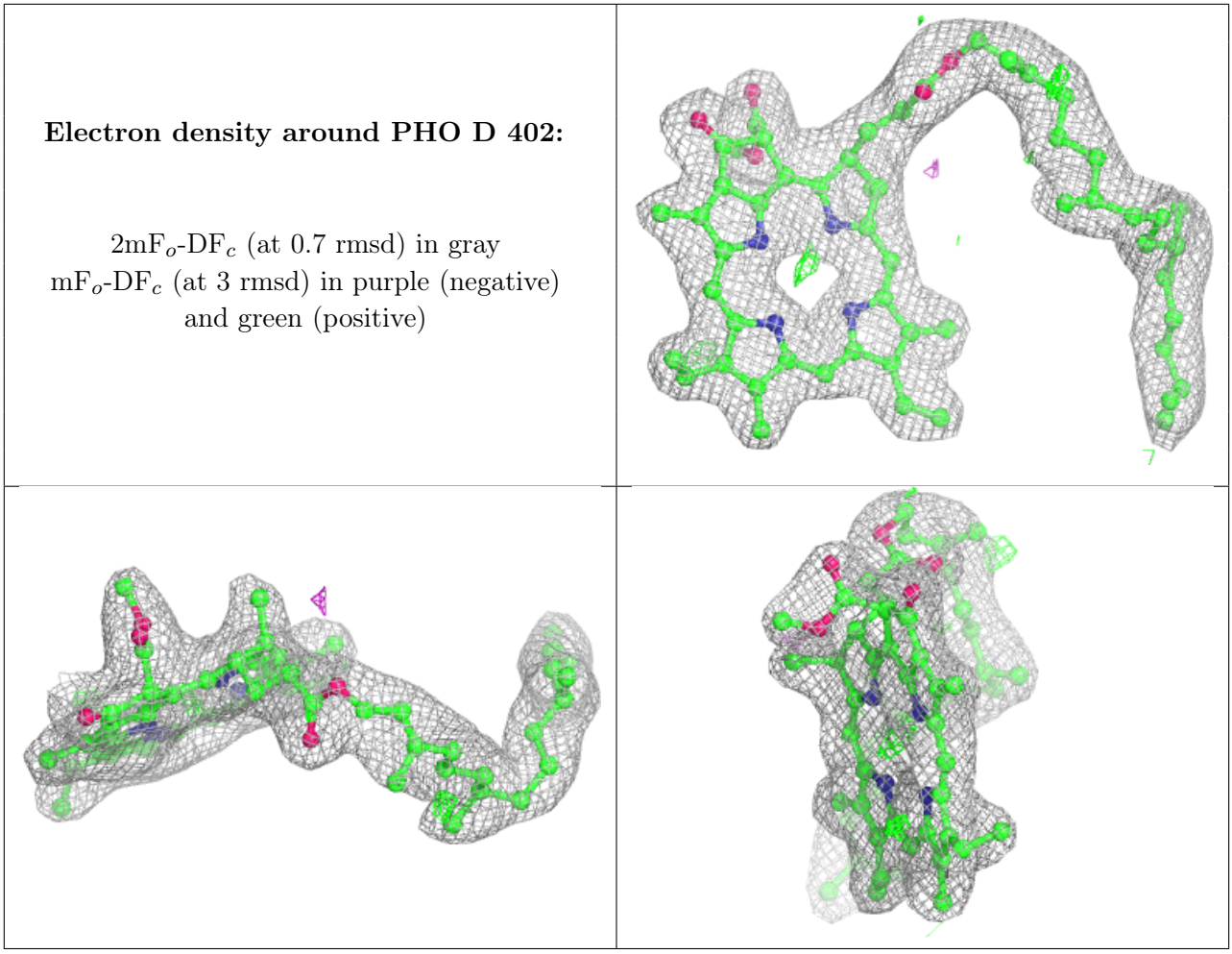






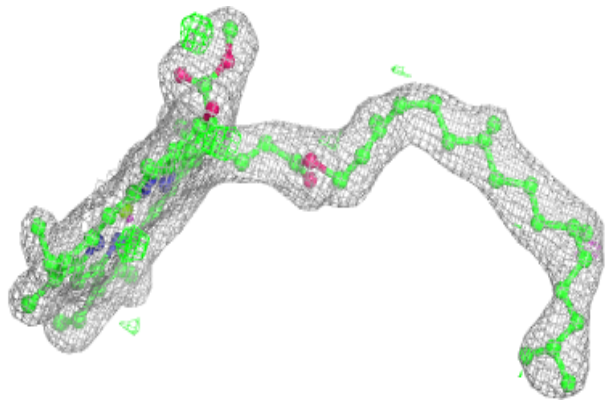
Electron density around PHO D 402:

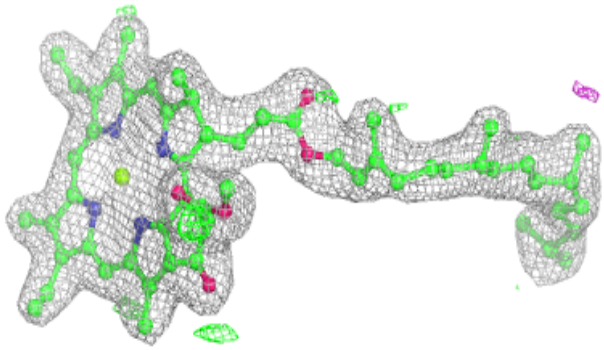
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

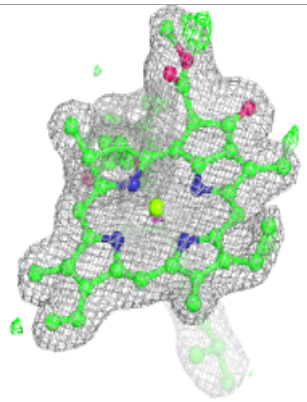


Electron density around CLA D 404:

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

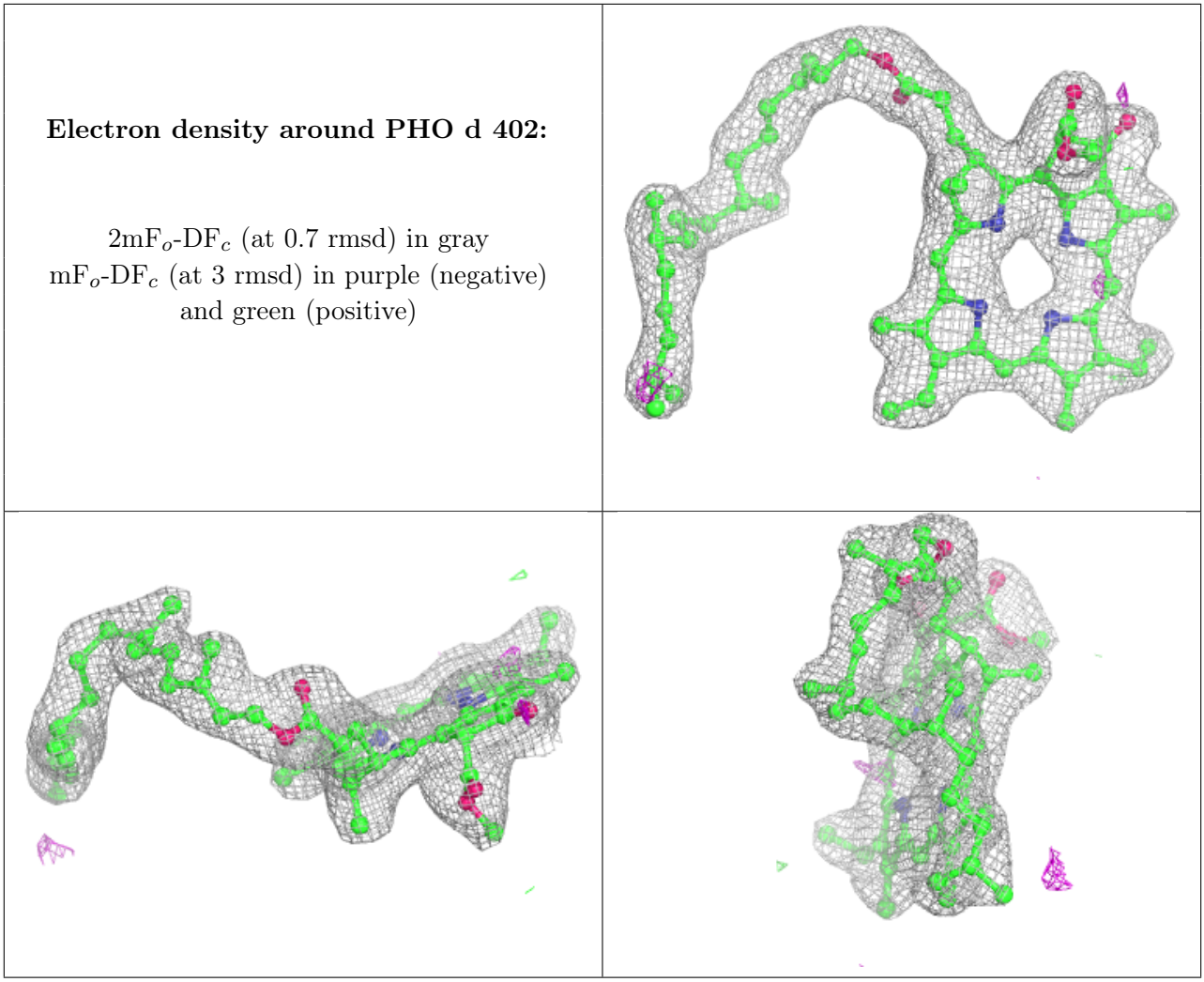






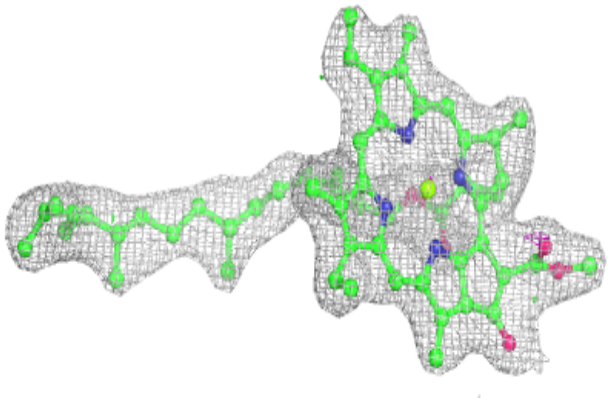
Electron density around PHO d 402:

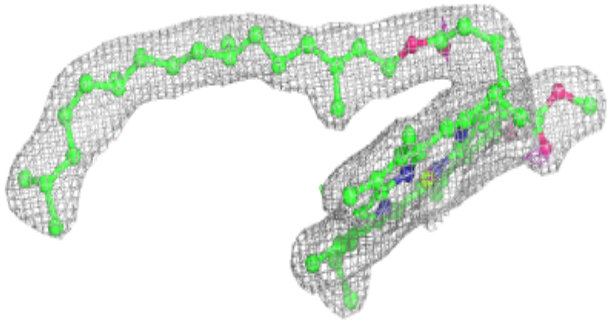
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

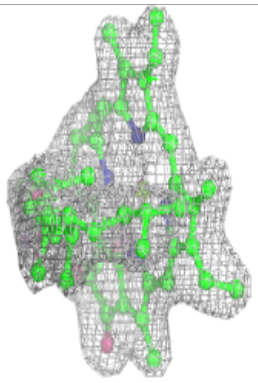


Electron density around CLA B 608:

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

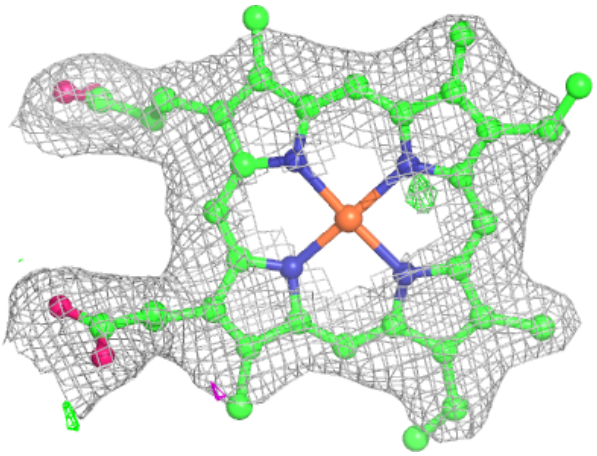


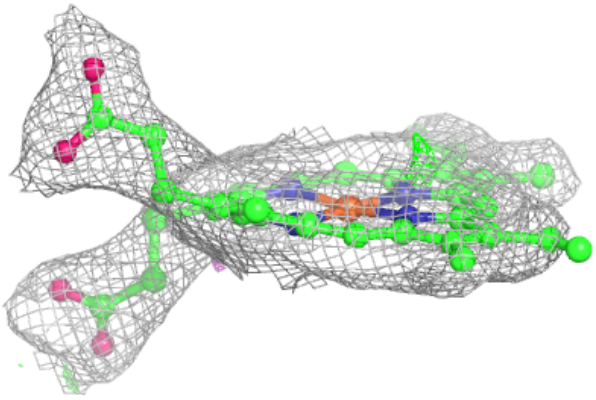


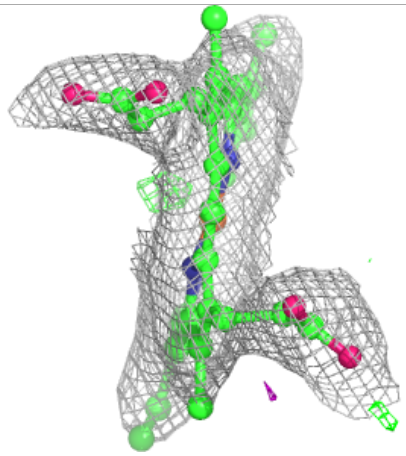


Electron density around HEM E 101:

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

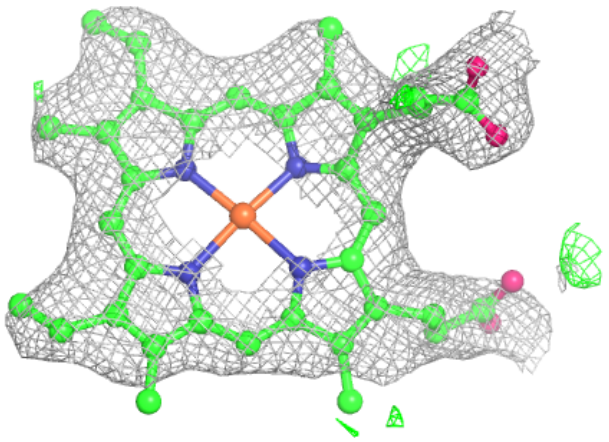


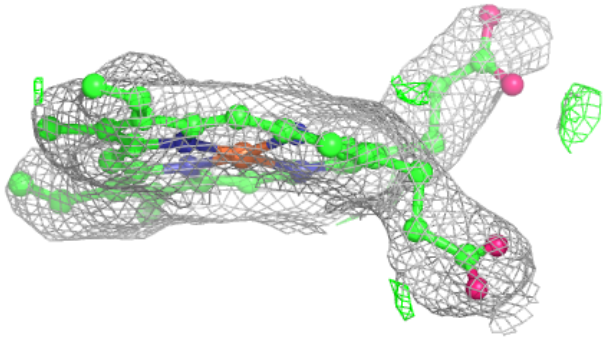


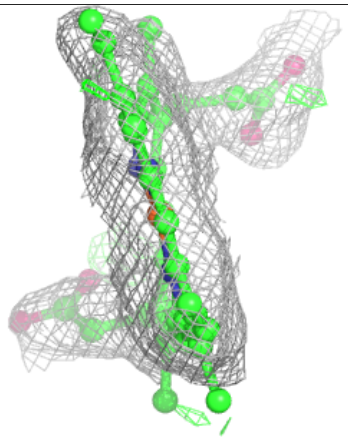


Electron density around HEM f 101:

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

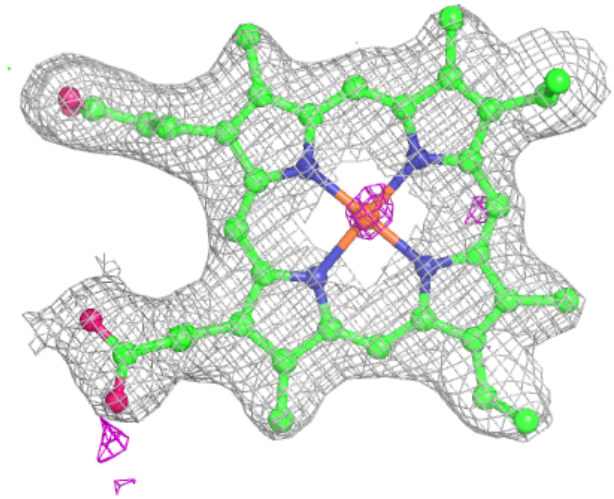


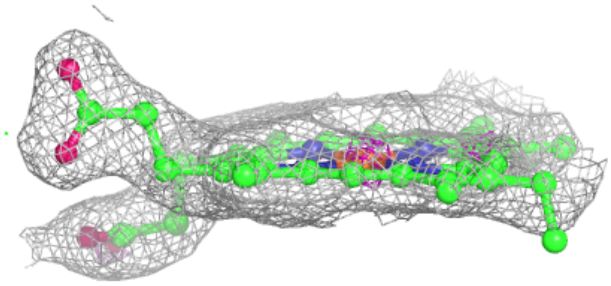


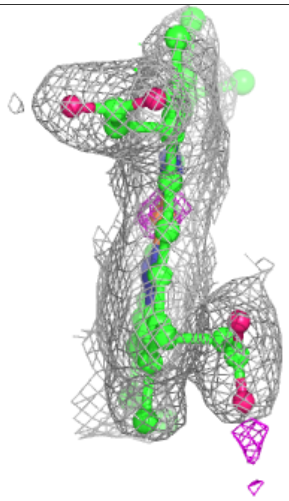


Electron density around HEC V 201:

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

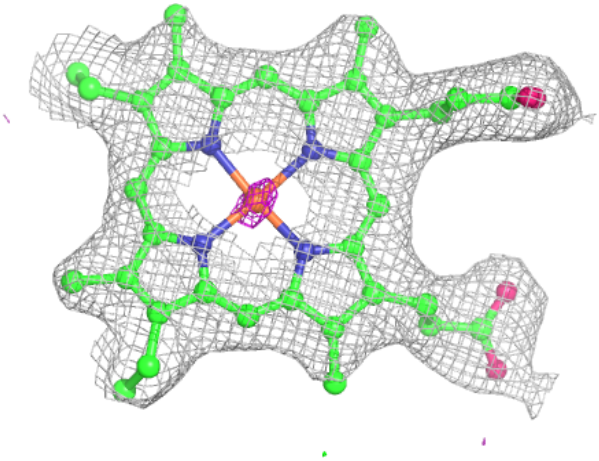


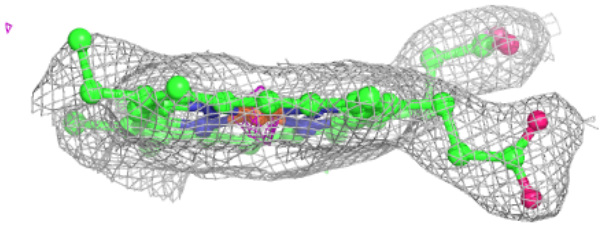




Electron density around HEC v 201:

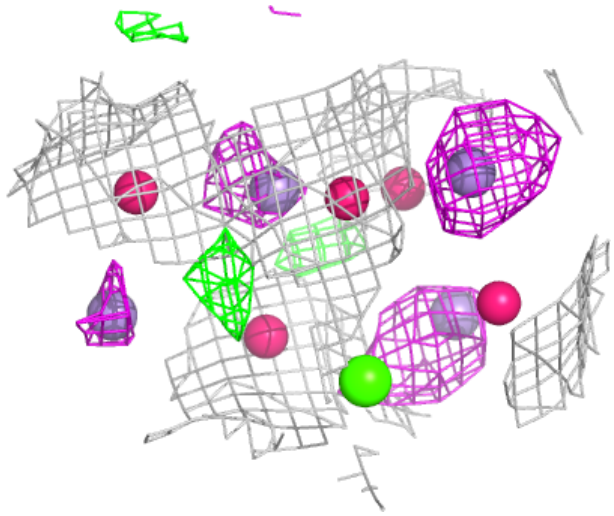
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

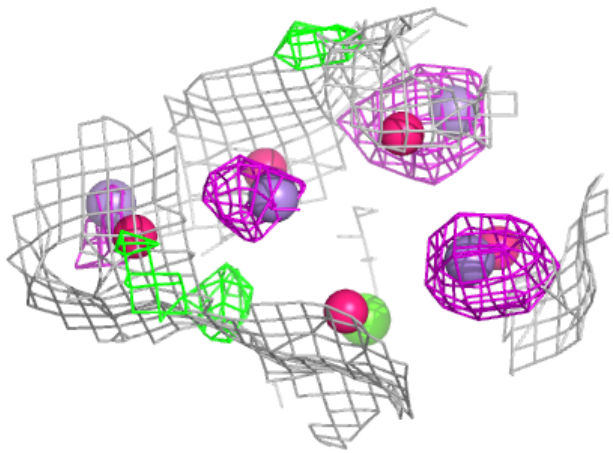


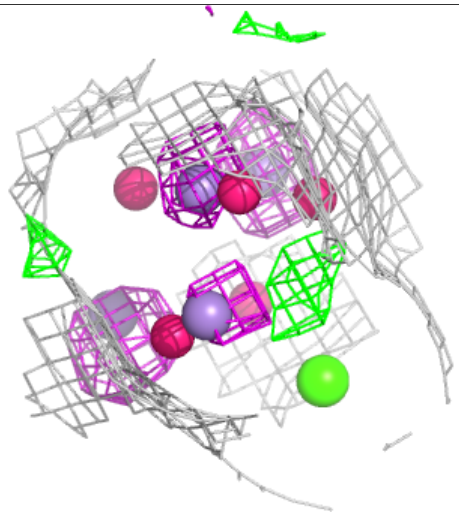


Electron density around OEX a 602 (A):

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

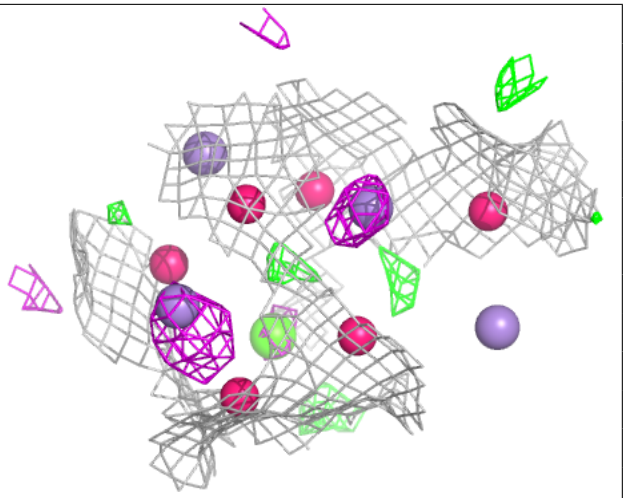


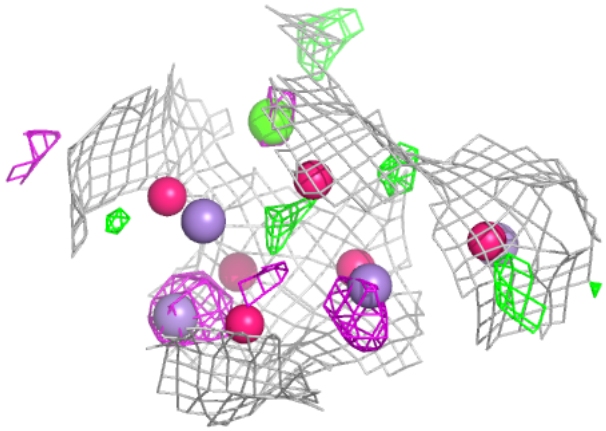


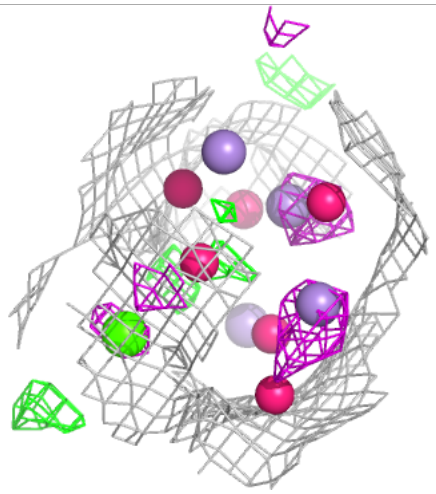


Electron density around OEY A 601 (B):

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

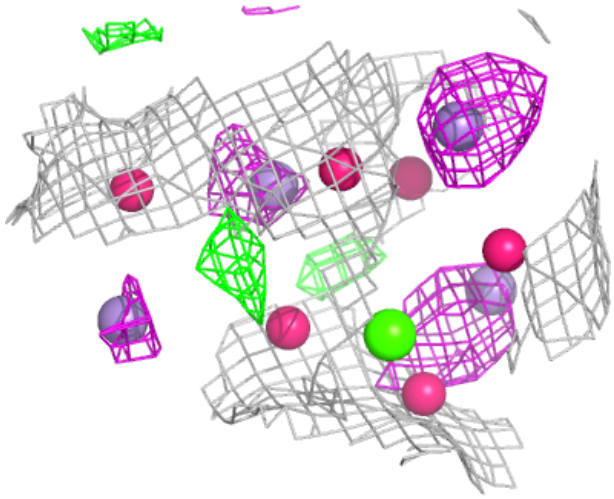


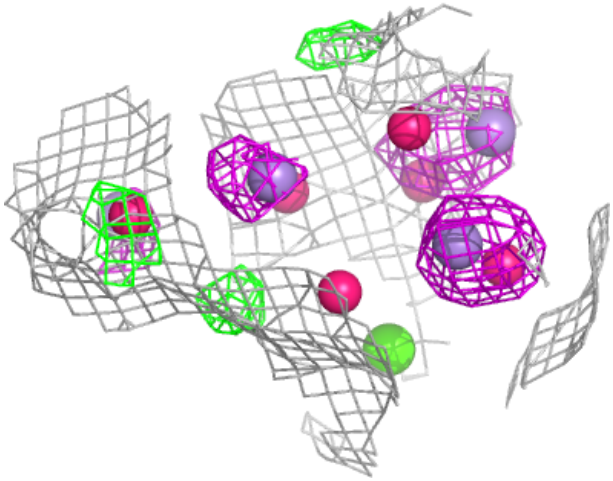


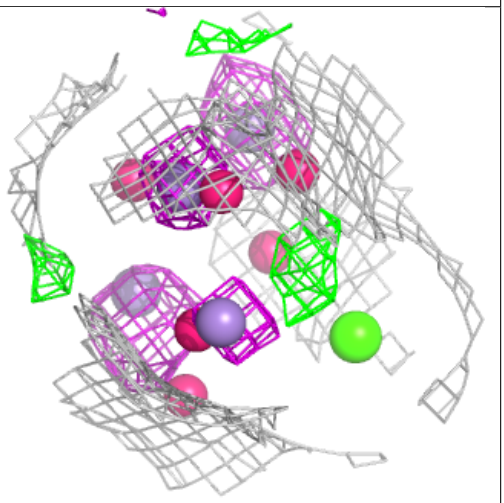


Electron density around OEY a 601 (B):

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

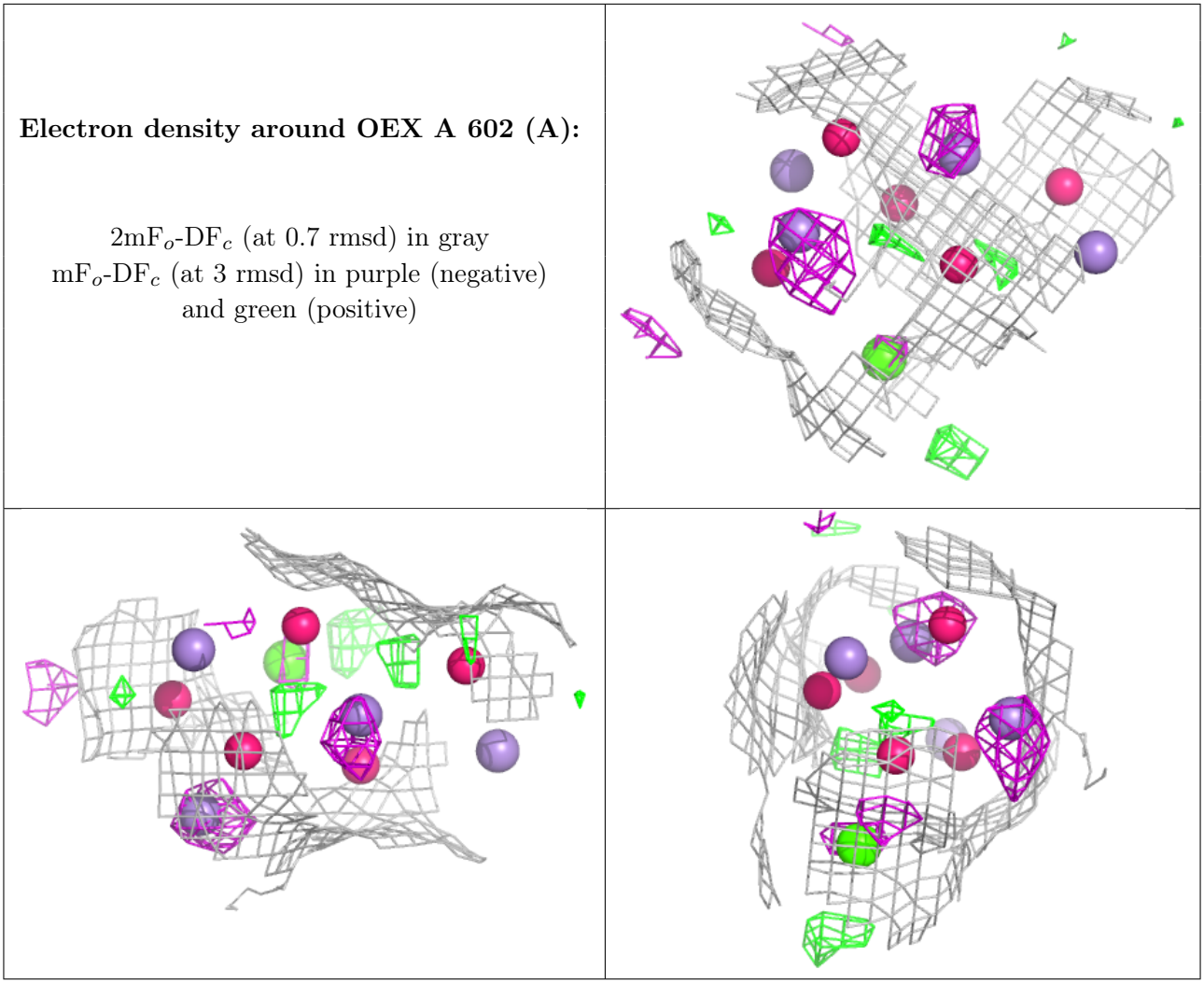






Electron density around OEX A 602 (A):

$2mF_o$-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 (i)

There are no such residues in this entry.