Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2024 – 06:36 AM EST

PDB ID	:	6DHE
Title	:	RT XFEL structure of the dark-stable state of Photosystem II (0F, S1-rich) at 2.05 Angstrom resolution
Authors	:	Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on	:	2018-05-20
Resolution	:	2.05 Å(reported)

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

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

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

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

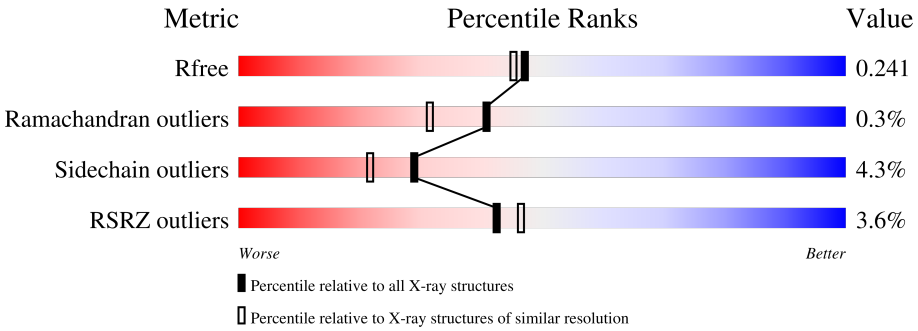
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36

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 2.05 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	1692 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	334	99%
1	a	334	97%

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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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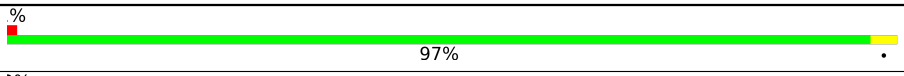
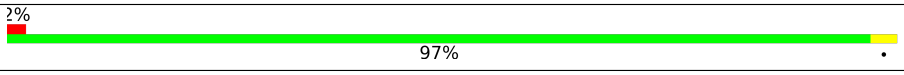
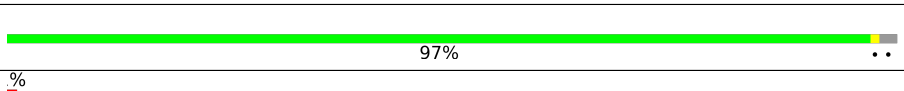
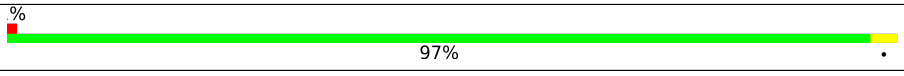
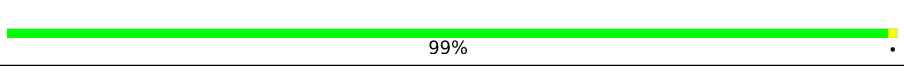
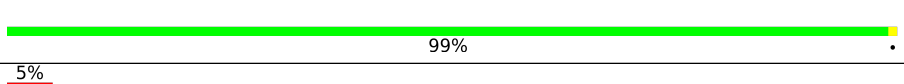
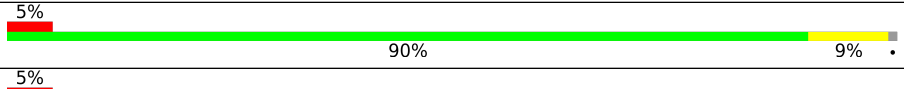
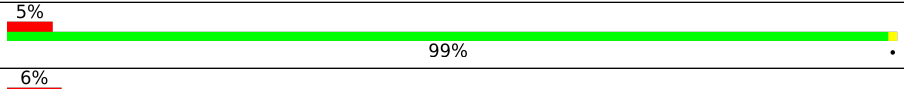
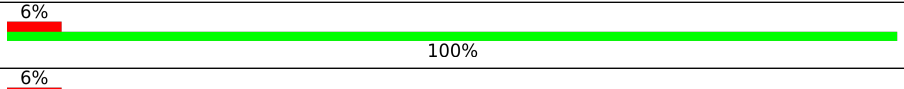
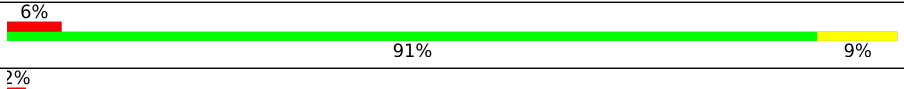
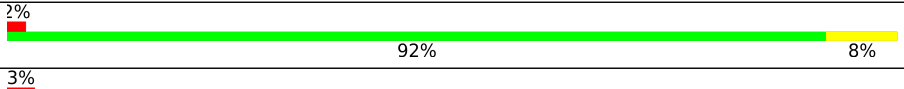
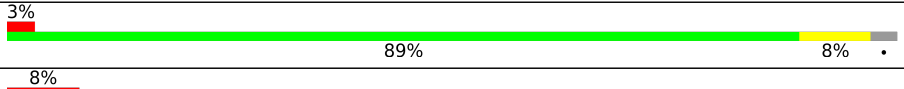
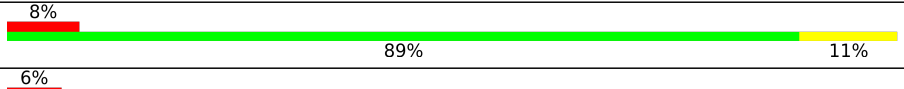
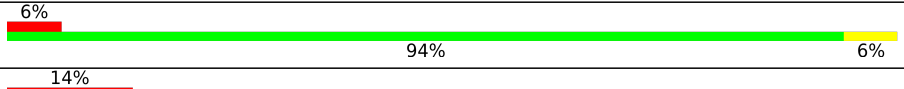
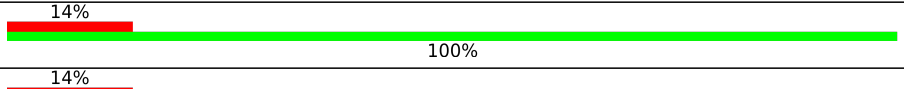
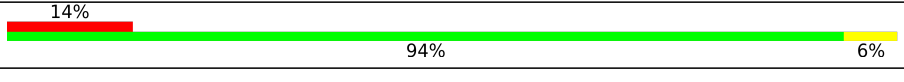
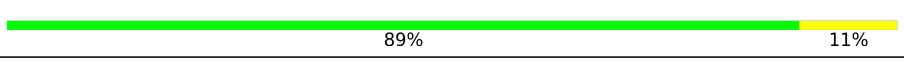
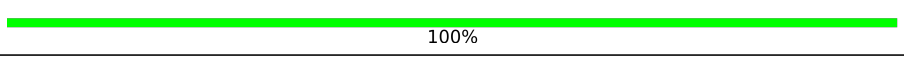
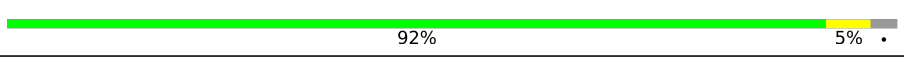
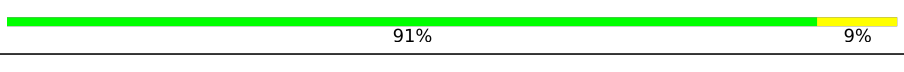
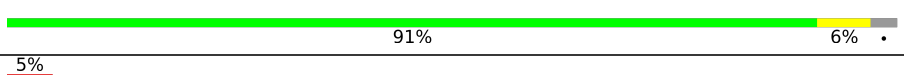
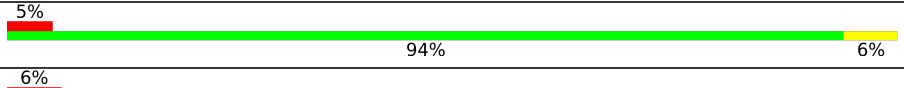
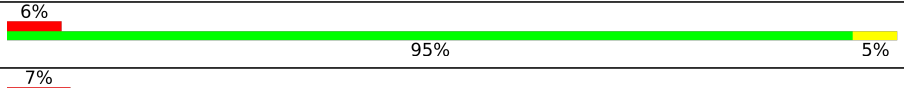
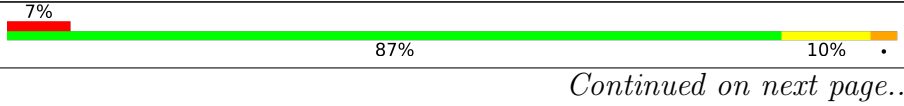
Mol	Chain	Length	Quality of chain
2	B	505	
2	b	505	
3	C	451	
3	c	451	
4	D	341	
4	d	341	
5	E	82	
5	e	82	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	36	
8	i	36	
9	J	36	
9	j	36	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	33	
12	m	33	
13	O	244	
13	o	244	
14	T	30	

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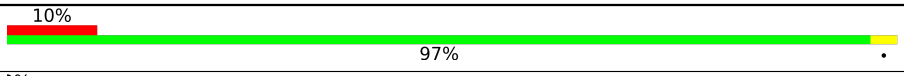
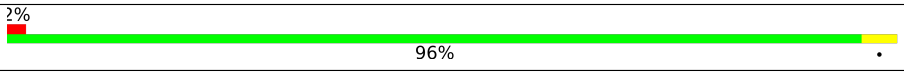
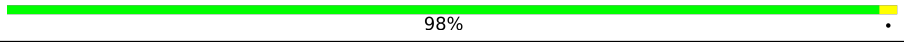
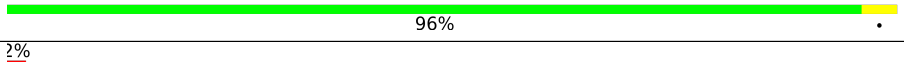
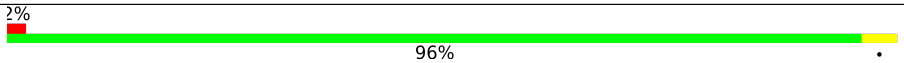
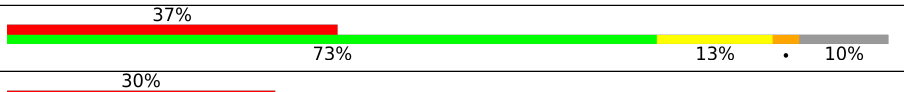
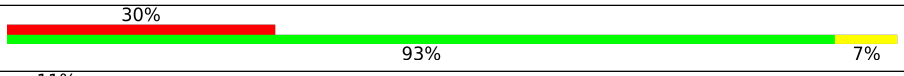
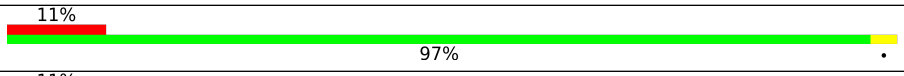
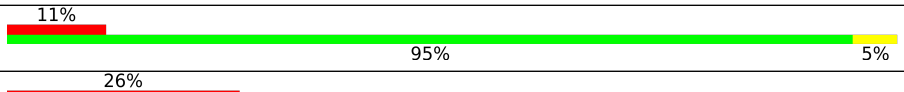
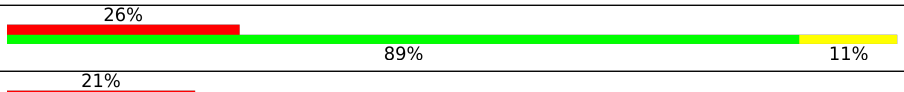
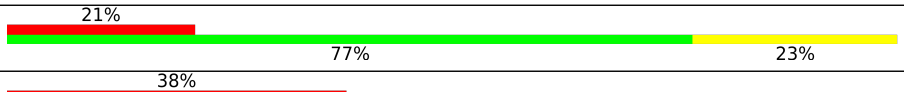
Mol	Chain	Length	Quality of chain
14	t	30	
15	U	97	
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
23	CLA	A	404	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	404	X	-	-	-
25	8CT	A	408	X	-	-	-
25	8CT	B	617	X	-	-	-
25	8CT	B	619	X	-	-	-
25	8CT	C	514	X	-	-	-
25	8CT	C	515	X	-	-	-
25	8CT	C	520	X	-	-	-
25	8CT	D	405	X	-	-	-
25	8CT	b	620	X	-	-	-
25	8CT	c	514	X	-	-	-
25	8CT	d	405	X	-	-	-
25	8CT	k	101	X	-	-	-
25	8CT	t	101	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 103686 atoms, of which 51480 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	0	0
			6752	2244	3335	570	590	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6911	2290	3411	587	610	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	S	0	0	0
			1030	338	523	82	85	2			
7	h	63	Total	C	H	N	O	S	0	0	0
			1016	333	518	80	83	2			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	S	0	0	0
			525	174	268	40	42	1			
9	j	36	Total	C	H	N	O	S	0	0	0
			516	172	261	40	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1	0
			3730	1174	1850	317	385	4			
13	o	244	Total	C	H	N	O	S	0	0	0
			3718	1170	1844	317	383	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	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	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	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	H	N	O	0	0	0
			593	188	312	45	48			
18	x	38	Total	C	H	N	O	0	0	0
			593	188	312	45	48			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	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	H	N	O	0	0	0
			569	184	298	47	40			
20	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

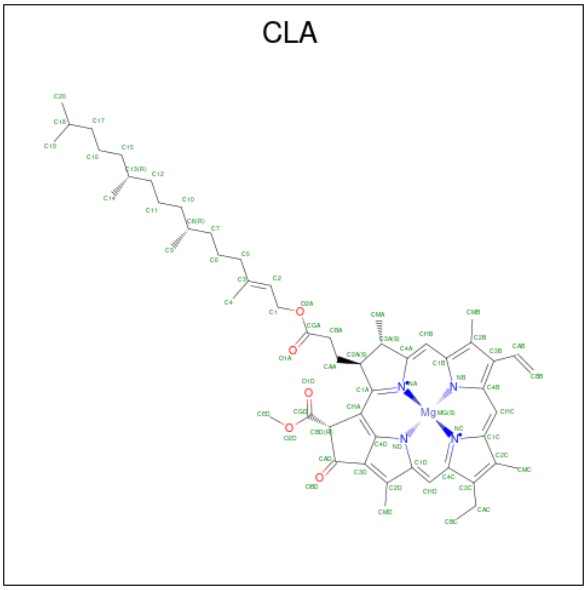
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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

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

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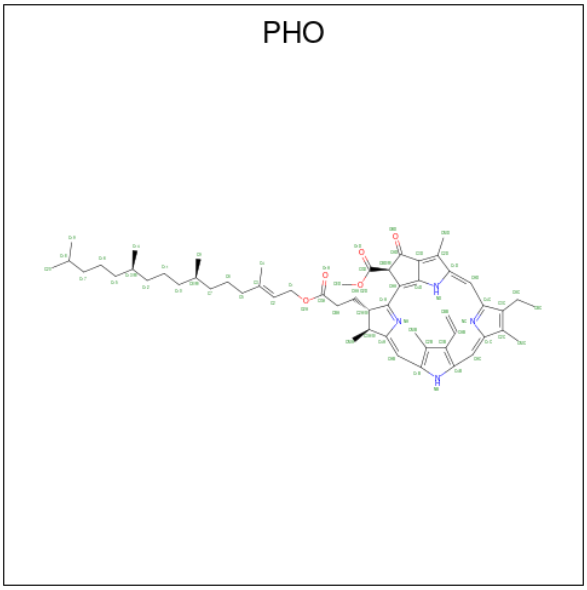
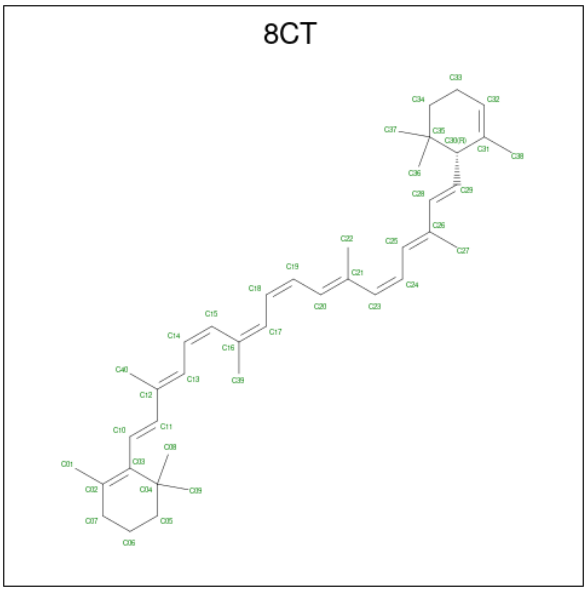
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

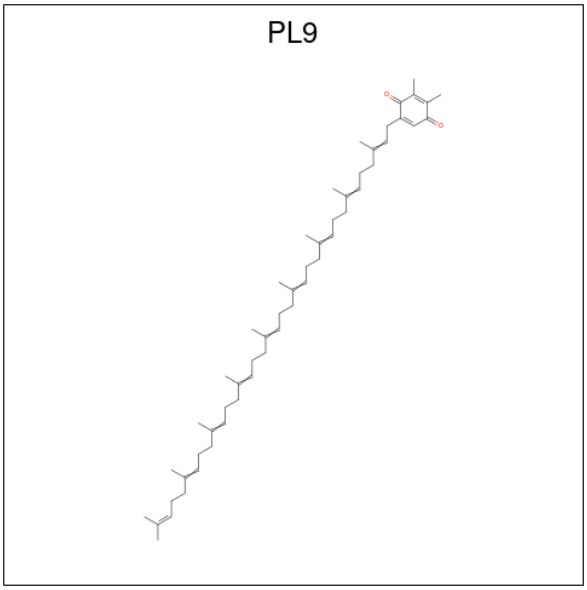
- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	D	1	Total C H 96 40 56	0	0
25	b	1	Total C H 96 40 56	0	0
25	c	1	Total C H 96 40 56	0	0
25	d	1	Total C H 96 40 56	0	0
25	k	1	Total C H 96 40 56	0	0
25	t	1	Total C H 96 40 56	0	0

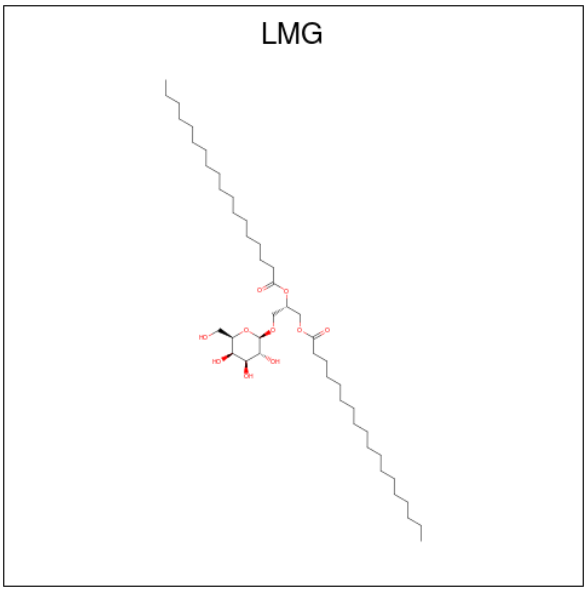
- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:

$C_{53}H_{80}O_2$).



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

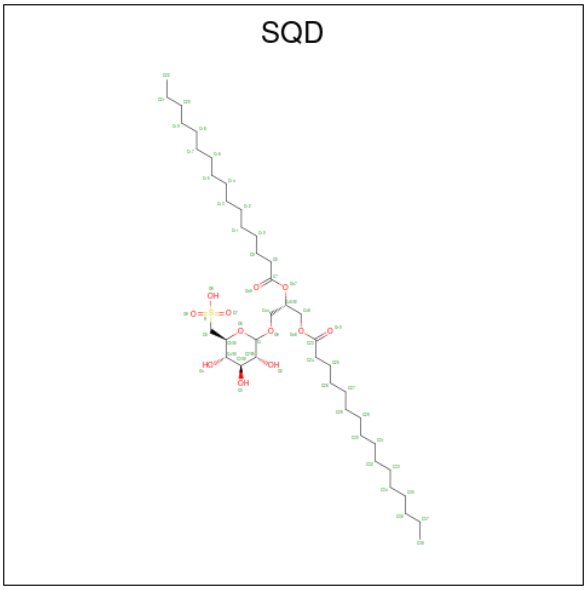
- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			123	41	72	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	b	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		

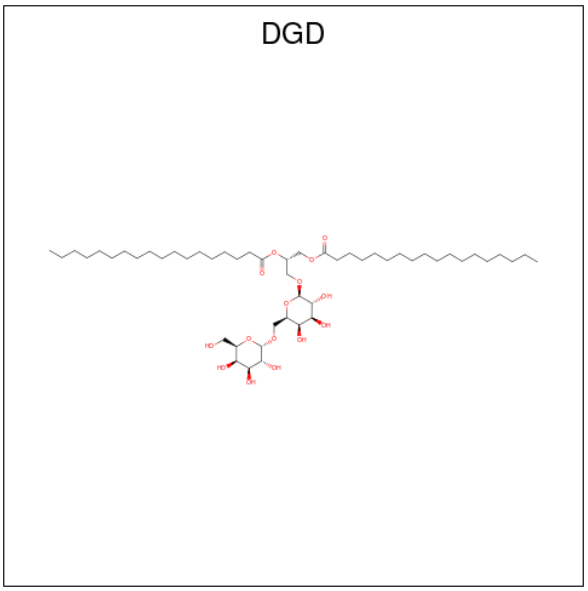
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



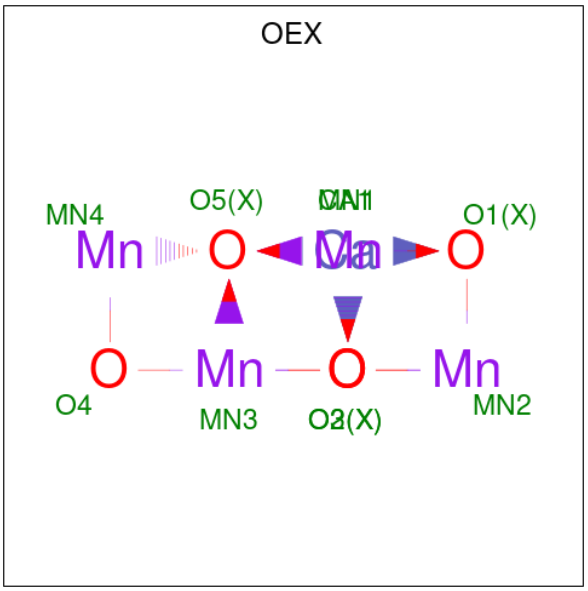
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C H O S 122 39 70 12 1	0	0
28	A	1	Total C H O 104 35 65 4	0	0
28	B	1	Total C H O S 132 41 78 12 1	0	0
28	D	1	Total C H O S 81 25 45 10 1	0	0
28	a	1	Total C H O S 132 41 78 12 1	0	0
28	a	1	Total C H O 92 31 56 5	0	0
28	b	1	Total C H O S 114 36 65 12 1	0	0
28	f	1	Total C H O S 90 28 49 12 1	0	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



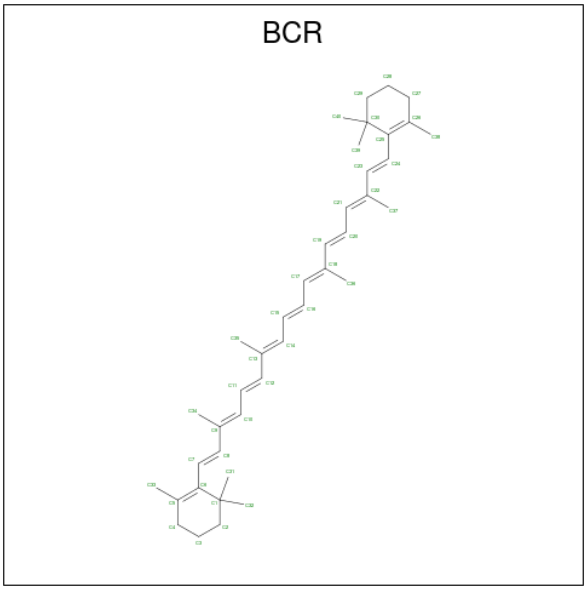
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		
29	o	1	Total	C	H	O	0	0
			119	39	75	5		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	H	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	T	1	Total C H 96 40 56	0	0
31	Y	1	Total C H 96 40 56	0	0
31	a	1	Total C H 96 40 56	0	0
31	b	1	Total C H 96 40 56	0	0
31	b	1	Total C H 96 40 56	0	0
31	c	1	Total C H 96 40 56	0	0
31	c	1	Total C H 96 40 56	0	0
31	h	1	Total C H 96 40 56	0	0

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	5	Total C H O 192 67 117 8	0	0
32	C	3	Total C H O 103 36 63 4	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	2	Total C H O 63 23 38 2	0	0
32	T	2	Total C H 91 31 60	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	4	Total C H O 176 60 110 6	0	0

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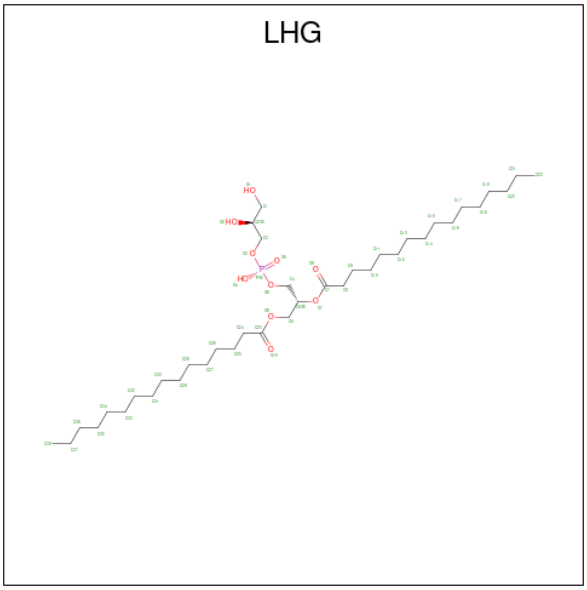
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	c	2	Total C H O 83 28 51 4	0	0
32	d	2	Total C H O 98 33 61 4	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	m	1	Total C H O 28 10 16 2	0	0
32	t	2	Total C H O 60 22 36 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C H O P 123 38 74 10 1	0	0
33	D	1	Total C H O P 123 38 74 10 1	0	0
33	D	1	Total C H O P 114 36 67 10 1	0	0
33	E	1	Total C H O P 123 38 74 10 1	0	0
33	L	1	Total C H O P 123 38 74 10 1	0	0

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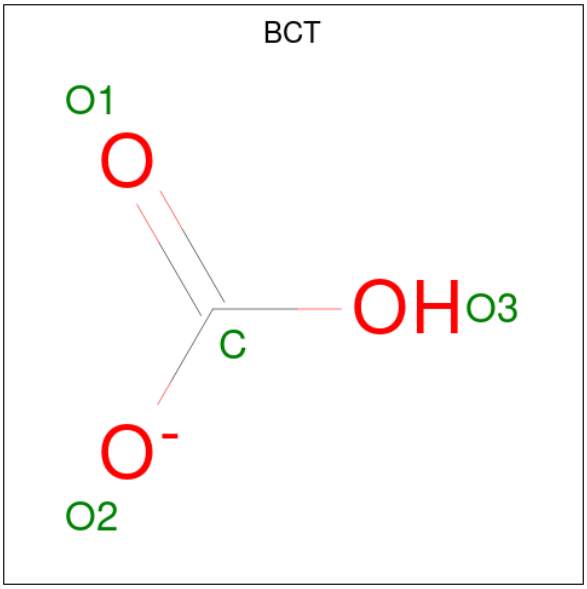
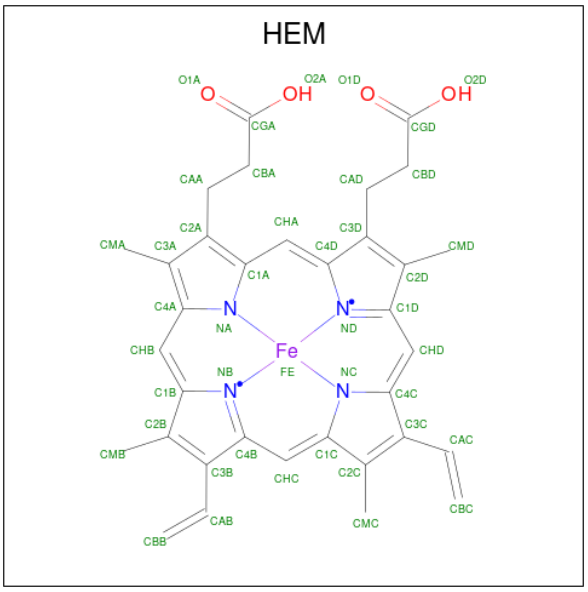
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



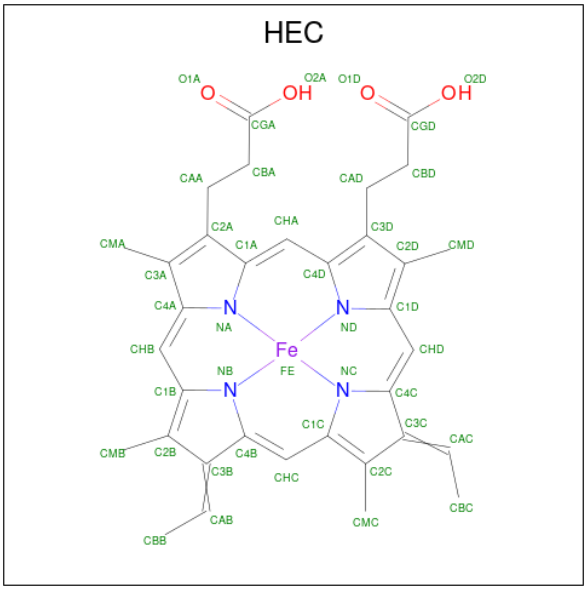
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	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	H	N	O	0	0
			73	34	1	30	4	4		
36	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	140	Total O 140 140	0	0
37	B	214	Total O 214 214	0	0
37	C	199	Total O 199 199	0	0
37	D	137	Total O 137 137	0	0
37	E	28	Total O 28 28	0	0
37	F	12	Total O 12 12	0	0
37	H	26	Total O 26 26	0	0
37	I	15	Total O 15 15	0	0
37	J	12	Total O 12 12	0	0
37	K	2	Total O 2 2	0	0
37	L	7	Total O 7 7	0	0
37	M	5	Total O 5 5	0	0
37	O	129	Total O 129 129	0	0
37	T	13	Total O 13 13	0	0
37	U	49	Total O 49 49	0	0
37	V	72	Total O 72 72	0	0
37	Y	5	Total O 5 5	0	0
37	X	9	Total O 9 9	0	0
37	Z	5	Total O 5 5	0	0
37	R	3	Total O 3 3	0	0
37	a	124	Total O 124 124	0	0

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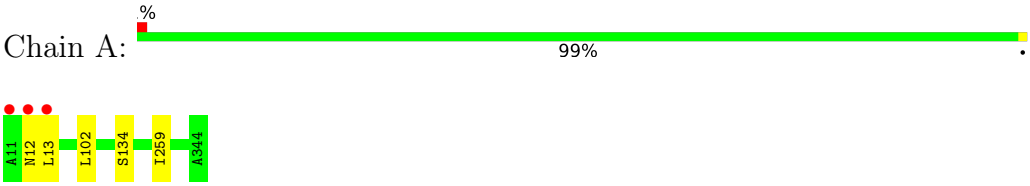
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	b	191	Total O 191 191	0	0
37	c	161	Total O 161 161	0	0
37	d	123	Total O 123 123	0	0
37	e	24	Total O 24 24	0	0
37	f	6	Total O 6 6	0	0
37	h	17	Total O 17 17	0	0
37	i	9	Total O 9 9	0	0
37	j	7	Total O 7 7	0	0
37	k	5	Total O 5 5	0	0
37	l	10	Total O 10 10	0	0
37	m	8	Total O 8 8	0	0
37	o	111	Total O 111 111	0	0
37	t	10	Total O 10 10	0	0
37	u	50	Total O 50 50	0	0
37	v	61	Total O 61 61	0	0
37	y	4	Total O 4 4	0	0
37	x	11	Total O 11 11	0	0
37	z	1	Total O 1 1	0	0
37	r	6	Total O 6 6	0	0

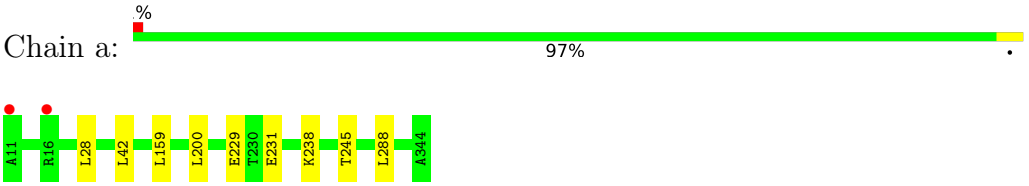
3 Residue-property plots (i)

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

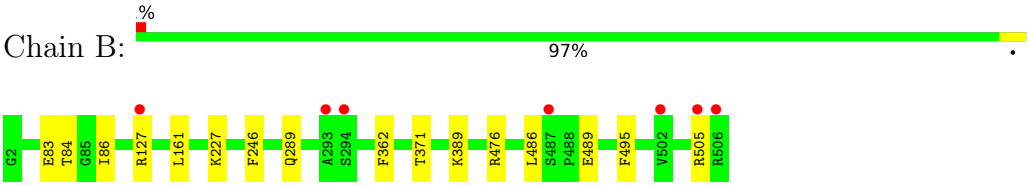
• Molecule 1: Photosystem II protein D1 1



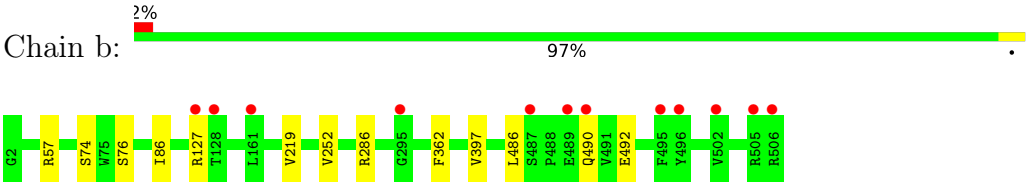
• Molecule 1: Photosystem II protein D1 1



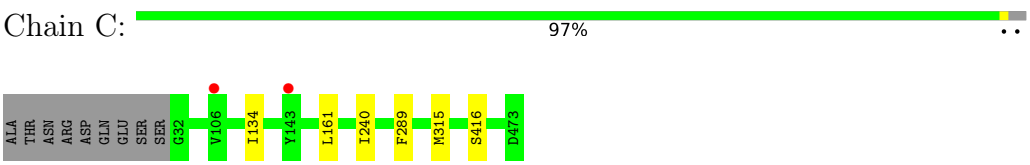
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

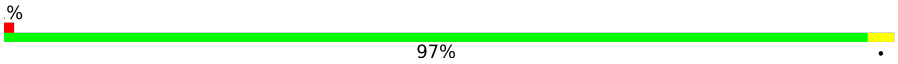


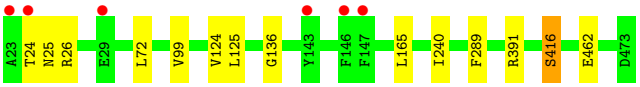
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

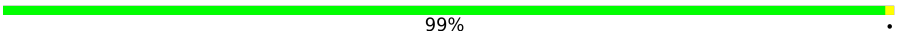
Chain c:





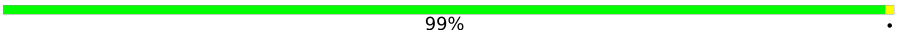
• Molecule 4: Photosystem II D2 protein

Chain D:



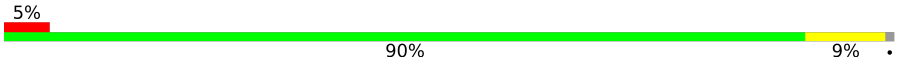
• Molecule 4: Photosystem II D2 protein

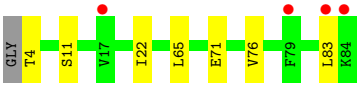
Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

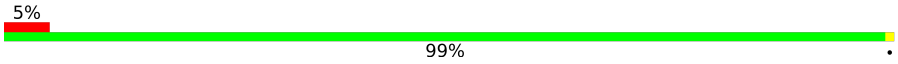
Chain E:

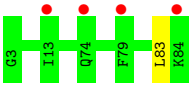




• Molecule 5: Cytochrome b559 subunit alpha

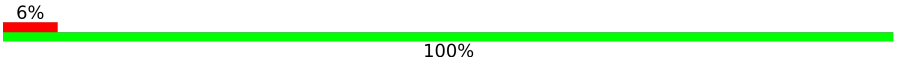
Chain e:





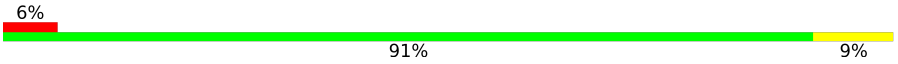
• Molecule 6: Cytochrome b559 subunit beta

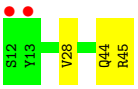
Chain F:



• Molecule 6: Cytochrome b559 subunit beta

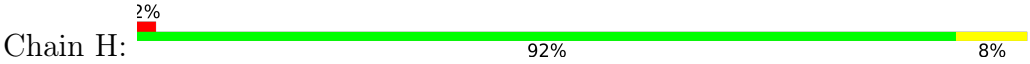
Chain f:





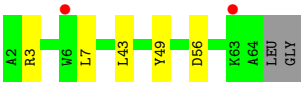
• Molecule 7: Photosystem II reaction center protein H

Chain H:



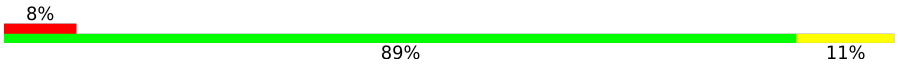
• Molecule 7: Photosystem II reaction center protein H

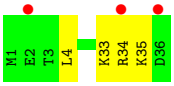
Chain h:



• Molecule 8: Photosystem II reaction center protein I

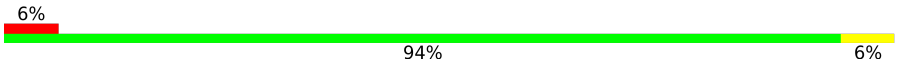
Chain I:

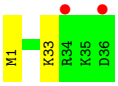




• Molecule 8: Photosystem II reaction center protein I

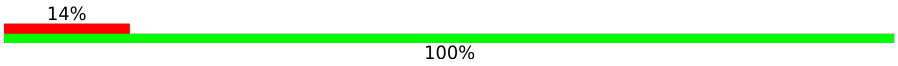
Chain i:

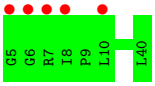




• Molecule 9: Photosystem II reaction center protein J

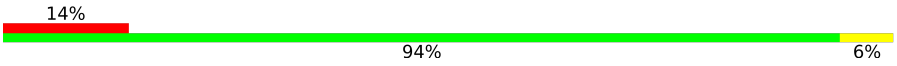
Chain J:

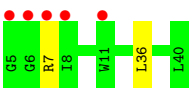




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

• Molecule 10: Photosystem II reaction center protein K

Chain k:

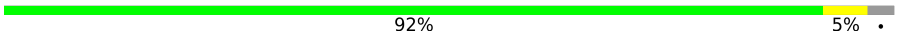
• Molecule 11: Photosystem II reaction center protein L

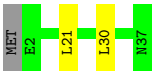
Chain L:

There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem II reaction center protein L

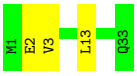
Chain l:





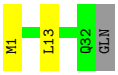
• Molecule 12: Photosystem II reaction center protein M

Chain M:



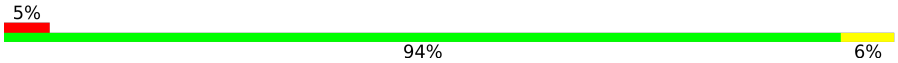
• Molecule 12: Photosystem II reaction center protein M

Chain m:



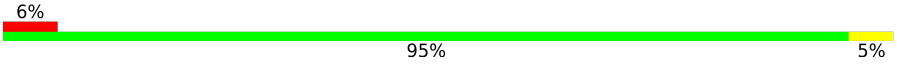
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

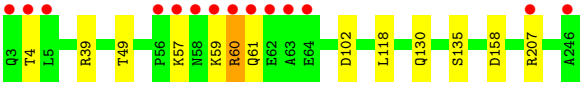
Chain O:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

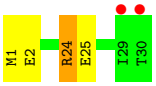
Chain o:





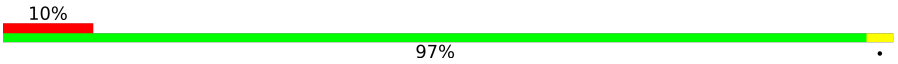
• Molecule 14: Photosystem II reaction center protein T

Chain T:



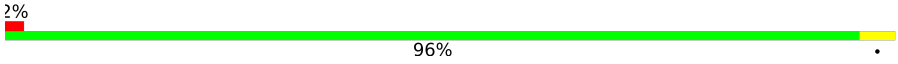
• Molecule 14: Photosystem II reaction center protein T

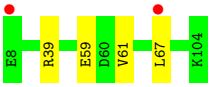
Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

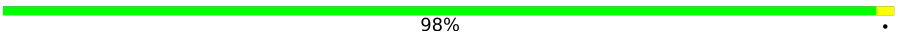
Chain U:





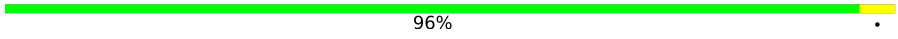
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



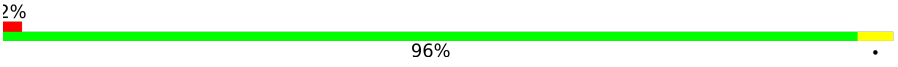
• Molecule 16: Cytochrome c-550

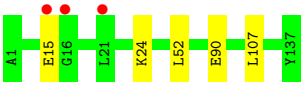
Chain V:



• Molecule 16: Cytochrome c-550

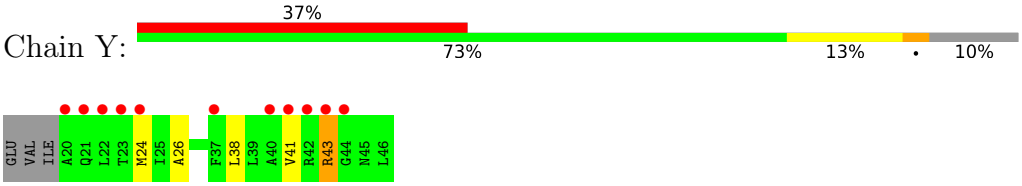
Chain v:





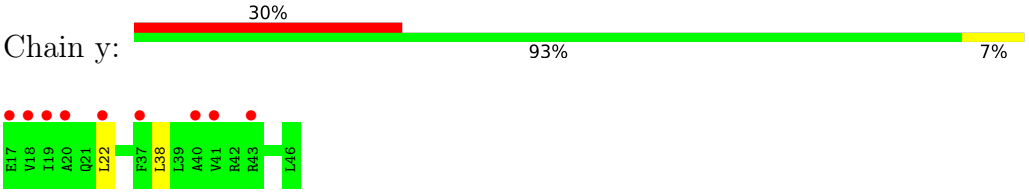
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



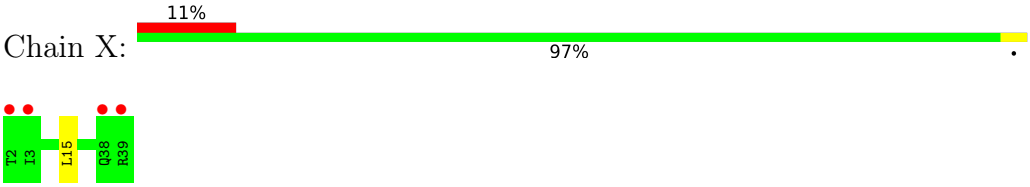
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



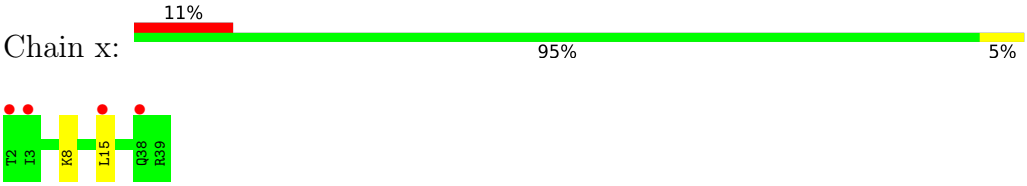
• Molecule 18: Photosystem II reaction center X protein

Chain X:



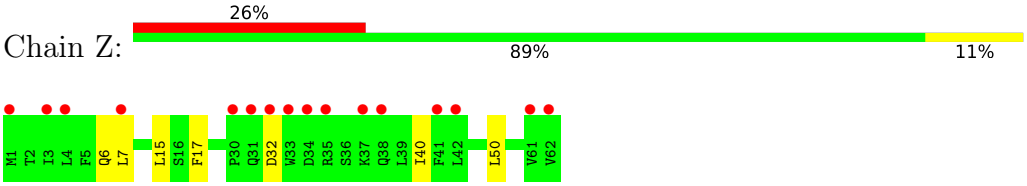
• Molecule 18: Photosystem II reaction center X protein

Chain x:



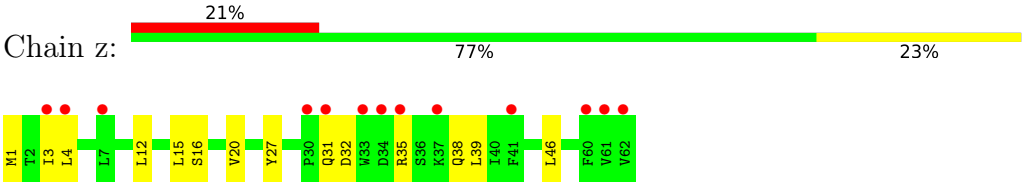
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



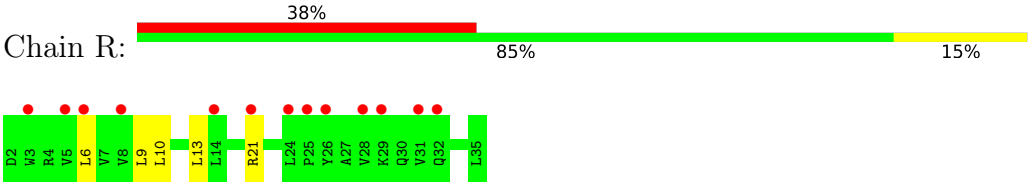
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



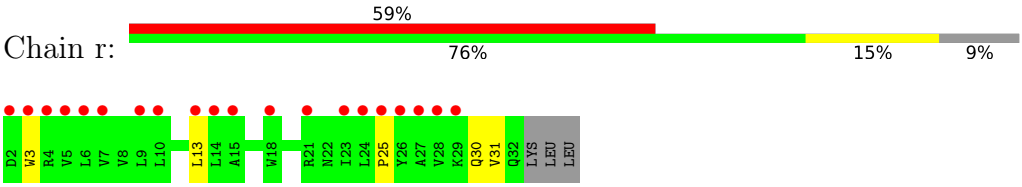
• Molecule 20: Photosystem II protein Y

Chain R:



• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.91Å 221.41Å 308.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.55 – 2.05 30.55 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.55-2.05) 87.7 (30.55-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.185 , 0.241 0.185 , 0.241	Depositor DCC
R_{free} test set	4419 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	103686	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: CLA, OEX, CL, UNL, 8CT, FME, PHO, SQD, BCR, PL9, HEC, LMG, BCT, FE2, HEM, DGD, LHG

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	0.64	0/2707	0.70	0/3692
1	a	0.61	0/2704	0.67	0/3688
2	B	0.62	0/4160	0.68	0/5668
2	b	0.60	0/4118	0.66	1/5611 (0.0%)
3	C	0.63	0/3530	0.67	0/4807
3	c	0.54	0/3619	0.65	0/4926
4	D	0.63	0/2812	0.67	0/3832
4	d	0.60	0/2821	0.68	0/3844
5	E	0.51	0/684	0.65	0/935
5	e	0.49	0/683	0.57	0/932
6	F	0.51	0/284	0.59	0/387
6	f	0.51	0/284	0.57	0/387
7	H	0.60	0/520	0.67	0/709
7	h	0.54	0/511	0.68	0/697
8	I	0.61	0/293	0.63	0/396
8	i	0.67	0/293	0.72	0/396
9	J	0.52	0/263	0.70	0/356
9	j	0.49	0/261	0.63	0/353
10	K	0.44	0/314	0.67	0/427
10	k	0.44	0/303	0.65	0/416
11	L	0.62	0/311	0.65	0/422
11	l	0.64	0/303	0.70	0/412
12	M	0.57	0/249	0.70	0/341
12	m	0.61	0/244	0.63	0/334
13	O	0.56	0/1914	0.70	0/2596
13	o	0.57	0/1905	0.74	2/2583 (0.1%)
14	T	0.63	0/257	0.79	2/349 (0.6%)
14	t	0.66	0/255	0.58	0/346
15	U	0.54	0/785	0.65	0/1064
15	u	0.57	0/785	0.69	0/1064
16	V	0.56	0/1085	0.65	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.50	0/1085	0.64	0/1473
17	Y	0.39	0/197	0.59	0/264
17	y	0.36	0/219	0.56	0/294
18	X	0.51	0/284	0.63	0/384
18	x	0.37	0/284	0.54	0/384
19	Z	0.46	0/490	0.58	0/669
19	z	0.41	0/488	0.55	0/666
20	R	0.39	0/277	0.65	0/380
20	r	0.34	0/233	0.49	0/323
All	All	0.58	0/42814	0.67	5/58280 (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
15	u	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	24	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	b	57	ARG	NE-CZ-NH1	-6.30	117.15	120.30
13	o	158	ASP	CB-CG-OD1	5.42	123.18	118.30
13	o	102	ASP	CB-CG-OD1	5.20	122.98	118.30
14	T	24	ARG	NE-CZ-NH2	-5.15	117.72	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	u	52	ASN	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	332/334 (99%)	324 (98%)	7 (2%)	1 (0%)	41 31
1	a	332/334 (99%)	325 (98%)	7 (2%)	0	100 100
2	B	508/505 (101%)	499 (98%)	9 (2%)	0	100 100
2	b	503/505 (100%)	493 (98%)	10 (2%)	0	100 100
3	C	440/451 (98%)	426 (97%)	13 (3%)	1 (0%)	47 39
3	c	451/451 (100%)	436 (97%)	13 (3%)	2 (0%)	34 24
4	D	339/341 (99%)	329 (97%)	10 (3%)	0	100 100
4	d	340/341 (100%)	330 (97%)	10 (3%)	0	100 100
5	E	80/82 (98%)	77 (96%)	3 (4%)	0	100 100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100 100
6	F	32/34 (94%)	32 (100%)	0	0	100 100
6	f	32/34 (94%)	32 (100%)	0	0	100 100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100 100
7	h	61/65 (94%)	57 (93%)	4 (7%)	0	100 100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100 100
8	i	34/36 (94%)	33 (97%)	1 (3%)	0	100 100
9	J	34/36 (94%)	32 (94%)	2 (6%)	0	100 100
9	j	34/36 (94%)	31 (91%)	3 (9%)	0	100 100
10	K	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4 0
10	k	35/37 (95%)	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	31/33 (94%)	30 (97%)	1 (3%)	0	100 100
12	m	30/33 (91%)	30 (100%)	0	0	100 100
13	O	243/244 (100%)	230 (95%)	11 (4%)	2 (1%)	19 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	19 10
14	T	28/30 (93%)	28 (100%)	0	0	100 100
14	t	28/30 (93%)	26 (93%)	2 (7%)	0	100 100
15	U	95/97 (98%)	92 (97%)	3 (3%)	0	100 100
15	u	95/97 (98%)	90 (95%)	5 (5%)	0	100 100
16	V	135/137 (98%)	130 (96%)	5 (4%)	0	100 100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100 100
17	Y	25/30 (83%)	16 (64%)	6 (24%)	3 (12%)	0 0
17	y	28/30 (93%)	25 (89%)	3 (11%)	0	100 100
18	X	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
19	Z	60/62 (97%)	55 (92%)	4 (7%)	1 (2%)	9 2
19	z	60/62 (97%)	53 (88%)	6 (10%)	1 (2%)	9 2
20	R	32/34 (94%)	30 (94%)	2 (6%)	0	100 100
20	r	29/34 (85%)	24 (83%)	2 (7%)	3 (10%)	0 0
All	All	5236/5326 (98%)	5051 (96%)	168 (3%)	17 (0%)	41 31

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	62	GLU
17	Y	41	VAL
17	Y	43	ARG
3	c	416	SER
13	o	60	ARG
13	o	61	GLN
20	r	30	GLN
20	r	31	VAL
19	z	15	LEU
17	Y	26	ALA
19	Z	6	GLN
13	O	73	ARG
3	c	136	GLY
1	A	259	ILE
20	r	25	PRO

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	270/270 (100%)	266 (98%)	4 (2%)	65 62
1	a	269/270 (100%)	260 (97%)	9 (3%)	38 31
2	B	407/403 (101%)	391 (96%)	16 (4%)	32 25
2	b	402/403 (100%)	390 (97%)	12 (3%)	41 34
3	C	344/352 (98%)	339 (98%)	5 (2%)	65 62
3	c	354/352 (101%)	340 (96%)	14 (4%)	31 24
4	D	276/276 (100%)	273 (99%)	3 (1%)	73 73
4	d	277/276 (100%)	272 (98%)	5 (2%)	59 55
5	E	72/72 (100%)	64 (89%)	8 (11%)	6 1
5	e	71/72 (99%)	70 (99%)	1 (1%)	67 65
6	F	28/28 (100%)	28 (100%)	0	100 100
6	f	28/28 (100%)	25 (89%)	3 (11%)	6 2
7	H	53/54 (98%)	48 (91%)	5 (9%)	8 3
7	h	53/54 (98%)	48 (91%)	5 (9%)	8 3
8	I	32/32 (100%)	28 (88%)	4 (12%)	4 1
8	i	32/32 (100%)	31 (97%)	1 (3%)	40 33
9	J	24/24 (100%)	24 (100%)	0	100 100
9	j	23/24 (96%)	21 (91%)	2 (9%)	10 4
10	K	31/30 (103%)	27 (87%)	4 (13%)	4 1
10	k	30/30 (100%)	26 (87%)	4 (13%)	4 1
11	L	35/35 (100%)	35 (100%)	0	100 100
11	l	34/35 (97%)	32 (94%)	2 (6%)	19 11
12	M	28/29 (97%)	25 (89%)	3 (11%)	6 2
12	m	28/29 (97%)	27 (96%)	1 (4%)	35 28
13	O	208/207 (100%)	195 (94%)	13 (6%)	18 9
13	o	207/207 (100%)	197 (95%)	10 (5%)	25 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	T	26/26 (100%)	23 (88%)	3 (12%)	5 1
14	t	25/26 (96%)	25 (100%)	0	100 100
15	U	84/84 (100%)	80 (95%)	4 (5%)	25 18
15	u	84/84 (100%)	83 (99%)	1 (1%)	71 70
16	V	117/117 (100%)	112 (96%)	5 (4%)	29 22
16	v	117/117 (100%)	112 (96%)	5 (4%)	29 22
17	Y	19/23 (83%)	16 (84%)	3 (16%)	2 0
17	y	22/23 (96%)	20 (91%)	2 (9%)	9 3
18	X	31/31 (100%)	30 (97%)	1 (3%)	39 32
18	x	31/31 (100%)	29 (94%)	2 (6%)	17 9
19	Z	52/52 (100%)	46 (88%)	6 (12%)	5 1
19	z	51/52 (98%)	38 (74%)	13 (26%)	0 0
20	R	28/29 (97%)	23 (82%)	5 (18%)	2 0
20	r	19/29 (66%)	17 (90%)	2 (10%)	7 2
All	All	4322/4348 (99%)	4136 (96%)	186 (4%)	29 22

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	102	LEU
1	A	134	SER
2	B	83	GLU
2	B	84	THR
2	B	86	ILE
2	B	127	ARG
2	B	161	LEU
2	B	227	LYS
2	B	246	PHE
2	B	289	GLN
2	B	362	PHE
2	B	371	THR
2	B	389	LYS
2	B	476	ARG
2	B	486	LEU
2	B	489	GLU

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Mol	Chain	Res	Type
2	B	495	PHE
2	B	505	ARG
3	C	134	ILE
3	C	161	LEU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	76	VAL
4	D	180	ARG
5	E	4	THR
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU
5	E	71	GLU
5	E	76	VAL
5	E	83	LEU
7	H	20	LYS
7	H	41	PHE
7	H	49	TYR
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	34	ARG
8	I	35	LYS
10	K	10	LYS
10	K	19	ASP
10	K	25	LEU
10	K	43	VAL
12	M	2	GLU
12	M	3	VAL
12	M	13	LEU
13	O	3	GLN
13	O	23	ASP
13	O	35	SER
13	O	39	ARG
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU

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Mol	Chain	Res	Type
13	O	135	SER
13	O	207	ARG
13	O	214	THR
13	O	234	LYS
13	O	240	TYR
14	T	2	GLU
14	T	24	ARG
14	T	25	GLU
15	U	39	ARG
15	U	59	GLU
15	U	61	VAL
15	U	67	LEU
16	V	2	GLU
16	V	3	LEU
16	V	14	SER
16	V	23	GLU
16	V	31	ARG
17	Y	24	MET
17	Y	38	LEU
17	Y	43	ARG
18	X	15	LEU
19	Z	7	LEU
19	Z	15	LEU
19	Z	17	PHE
19	Z	32	ASP
19	Z	40	ILE
19	Z	50	LEU
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
20	R	21	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	229	GLU
1	a	231	GLU
1	a	238	LYS
1	a	245	THR
1	a	288	LEU
2	b	74	SER

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Mol	Chain	Res	Type
2	b	76	SER
2	b	86	ILE
2	b	127	ARG
2	b	219	VAL
2	b	252	VAL
2	b	286	ARG
2	b	362	PHE
2	b	397	VAL
2	b	486	LEU
2	b	490	GLN
2	b	492	GLU
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
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	289	PHE
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	416	SER
3	c	462	GLU
4	d	90	LEU
4	d	180	ARG
4	d	291	LEU
4	d	321	LEU
4	d	329	MET
5	e	83	LEU
6	f	28	VAL
6	f	44	GLN
6	f	45	ARG
7	h	3	ARG
7	h	7	LEU
7	h	43	LEU
7	h	49	TYR
7	h	56	ASP
8	i	33	LYS
9	j	7	ARG
9	j	36	LEU

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Mol	Chain	Res	Type
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	46	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	4	THR
13	o	39	ARG
13	o	49	THR
13	o	57	LYS
13	o	59	LYS
13	o	60	ARG
13	o	118	LEU
13	o	130	GLN
13	o	135	SER
13	o	207	ARG
15	u	23	GLU
16	v	15	GLU
16	v	24	LYS
16	v	52	LEU
16	v	90	GLU
16	v	107	LEU
17	y	22	LEU
17	y	38	LEU
18	x	8	LYS
18	x	15	LEU
19	z	1	MET
19	z	3	ILE
19	z	4	LEU
19	z	12	LEU
19	z	16	SER
19	z	20	VAL
19	z	27	TYR
19	z	31	GLN
19	z	32	ASP
19	z	35	ARG
19	z	38	GLN
19	z	39	LEU
19	z	46	LEU
20	r	3	TRP
20	r	13	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	289	GLN
13	O	88	ASN
13	O	231	HIS
17	Y	21	GLN
2	b	497	GLN
3	c	25	ASN
13	o	58	ASN
19	z	38	GLN
19	z	58	ASN

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	$\#\|Z\| > 2$
14	FME	T	1	14	8,9,10	0.97	0	7,9,11	1.61	2 (28%)
8	FME	I	1	8	8,9,10	0.96	0	7,9,11	0.95	0
8	FME	i	1	8	8,9,10	1.07	0	7,9,11	1.36	1 (14%)
12	FME	M	1	12	8,9,10	0.99	0	7,9,11	0.84	0
12	FME	m	1	12	8,9,10	0.99	1 (12%)	7,9,11	0.97	1 (14%)
14	FME	t	1	14	8,9,10	0.93	0	7,9,11	1.15	1 (14%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	m	1	FME	CA-N	-2.18	1.43	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	CA-N-CN	-2.57	118.87	122.82
14	T	1	FME	C-CA-N	2.23	113.76	109.73
14	t	1	FME	C-CA-N	2.17	113.65	109.73
14	T	1	FME	O1-CN-N	-2.13	119.66	125.27
12	m	1	FME	C-CA-N	-2.08	105.99	109.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

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 186 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 149 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	$\#\|Z\|>2$
23	CLA	c	511	3	65,73,73	1.81	8 (12%)	76,113,113	1.42	5 (6%)
25	8CT	b	620	-	40,41,41	1.70	4 (10%)	50,56,56	2.27	11 (22%)
23	CLA	C	506	-	65,73,73	1.83	8 (12%)	76,113,113	1.28	6 (7%)
27	LMG	D	411	-	31,31,55	1.38	5 (16%)	33,33,63	1.13	3 (9%)
33	LHG	D	410	-	46,46,48	1.05	3 (6%)	49,52,54	1.25	3 (6%)
23	CLA	a	406	37	65,73,73	1.62	11 (16%)	76,113,113	1.60	14 (18%)
33	LHG	D	409	-	48,48,48	1.01	4 (8%)	51,54,54	1.19	5 (9%)
24	PHO	d	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.44	5 (10%)
23	CLA	b	606	-	65,73,73	1.37	6 (9%)	76,113,113	1.64	11 (14%)
23	CLA	b	612	-	65,73,73	1.51	9 (13%)	76,113,113	1.60	14 (18%)
25	8CT	C	520	-	40,41,41	1.62	4 (10%)	50,56,56	2.44	10 (20%)
31	BCR	c	521	-	41,41,41	0.98	1 (2%)	56,56,56	1.30	7 (12%)
34	BCT	a	404	21	2,3,3	1.45	0	2,3,3	3.11	2 (100%)
23	CLA	b	604	-	65,73,73	1.61	10 (15%)	76,113,113	1.64	12 (15%)
33	LHG	L	101	-	48,48,48	0.86	1 (2%)	51,54,54	1.19	3 (5%)
34	BCT	D	401	21	2,3,3	1.08	0	2,3,3	3.53	2 (100%)
27	LMG	B	622	-	26,26,55	0.82	1 (3%)	26,26,63	0.99	1 (3%)
31	BCR	c	515	-	41,41,41	1.22	3 (7%)	56,56,56	1.32	9 (16%)
23	CLA	B	607	37	65,73,73	1.49	7 (10%)	76,113,113	1.47	9 (11%)
23	CLA	B	615	-	65,73,73	1.60	11 (16%)	76,113,113	1.37	10 (13%)
24	PHO	a	407	-	51,69,69	1.13	6 (11%)	47,99,99	1.32	6 (12%)
25	8CT	C	514	-	40,41,41	1.67	4 (10%)	50,56,56	2.59	11 (22%)
23	CLA	C	502	-	65,73,73	1.55	7 (10%)	76,113,113	1.39	9 (11%)
23	CLA	C	504	37	59,67,73	1.57	8 (13%)	68,105,113	1.48	10 (14%)
28	SQD	a	412	-	35,35,54	1.12	2 (5%)	37,37,65	1.39	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	503	-	65,73,73	1.65	7 (10%)	76,113,113	1.57	13 (17%)
31	BCR	a	409	-	41,41,41	1.14	3 (7%)	56,56,56	1.29	4 (7%)
27	LMG	c	519	-	37,37,55	1.17	5 (13%)	45,45,63	1.28	4 (8%)
29	DGD	C	516	-	63,63,67	1.16	5 (7%)	77,77,81	1.38	11 (14%)
23	CLA	b	611	37	65,73,73	1.62	11 (16%)	76,113,113	1.37	13 (17%)
27	LMG	b	621	-	51,51,55	0.86	1 (1%)	59,59,63	1.53	7 (11%)
27	LMG	D	407	-	51,51,55	1.04	1 (1%)	59,59,63	1.25	5 (8%)
23	CLA	b	613	-	65,73,73	1.34	5 (7%)	76,113,113	1.55	13 (17%)
31	BCR	H	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.28	6 (10%)
23	CLA	B	601	37	65,73,73	1.98	9 (13%)	76,113,113	1.62	12 (15%)
23	CLA	A	405	37	65,73,73	1.55	10 (15%)	76,113,113	1.70	13 (17%)
33	LHG	d	409	-	38,38,48	0.95	2 (5%)	41,44,54	1.11	2 (4%)
25	8CT	A	408	-	40,41,41	1.72	4 (10%)	50,56,56	2.42	13 (26%)
33	LHG	E	101	-	48,48,48	0.90	3 (6%)	51,54,54	1.15	2 (3%)
28	SQD	A	413	-	38,38,54	1.05	3 (7%)	40,40,65	1.33	2 (5%)
23	CLA	c	505	-	65,73,73	1.67	10 (15%)	76,113,113	1.27	10 (13%)
29	DGD	c	517	-	63,63,67	1.14	7 (11%)	77,77,81	1.38	9 (11%)
23	CLA	B	613	-	65,73,73	1.61	10 (15%)	76,113,113	1.51	10 (13%)
23	CLA	c	503	-	65,73,73	1.62	9 (13%)	76,113,113	1.55	12 (15%)
23	CLA	b	616	-	65,73,73	1.73	11 (16%)	76,113,113	1.59	14 (18%)
23	CLA	d	403	-	65,73,73	1.52	9 (13%)	76,113,113	1.44	9 (11%)
29	DGD	o	301	-	43,43,67	1.10	4 (9%)	45,45,81	1.26	3 (6%)
27	LMG	c	522	-	48,48,55	1.14	6 (12%)	56,56,63	1.26	6 (10%)
23	CLA	C	501	-	65,73,73	1.97	10 (15%)	76,113,113	1.45	5 (6%)
36	HEC	v	201	16	32,50,50	2.25	5 (15%)	24,82,82	1.61	4 (16%)
28	SQD	a	411	-	53,54,54	0.99	4 (7%)	62,65,65	1.96	14 (22%)
29	DGD	A	414	-	67,67,67	1.33	8 (11%)	81,81,81	1.39	11 (13%)
28	SQD	B	624	-	53,54,54	0.92	3 (5%)	62,65,65	1.76	12 (19%)
25	8CT	B	617	-	40,41,41	1.75	5 (12%)	50,56,56	2.56	11 (22%)
31	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.19	6 (10%)
28	SQD	D	408	-	35,36,54	1.02	3 (8%)	42,45,65	1.73	10 (23%)
27	LMG	b	623	-	55,55,55	0.92	3 (5%)	63,63,63	1.35	7 (11%)
23	CLA	B	609	-	65,73,73	1.56	12 (18%)	76,113,113	1.42	9 (11%)
23	CLA	c	509	-	65,73,73	1.56	7 (10%)	76,113,113	1.47	9 (11%)
29	DGD	c	516	-	63,63,67	1.05	6 (9%)	77,77,81	1.36	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	508	-	65,73,73	1.62	9 (13%)	76,113,113	1.48	11 (14%)
25	8CT	B	619	-	40,41,41	1.77	5 (12%)	50,56,56	2.51	11 (22%)
33	LHG	d	408	-	48,48,48	0.72	0	51,54,54	1.22	4 (7%)
24	PHO	A	406	-	51,69,69	1.07	5 (9%)	47,99,99	1.34	6 (12%)
25	8CT	D	405	-	40,41,41	1.72	4 (10%)	50,56,56	2.65	8 (16%)
23	CLA	C	513	-	65,73,73	1.55	8 (12%)	76,113,113	1.56	11 (14%)
28	SQD	f	101	-	40,41,54	1.14	5 (12%)	49,52,65	1.59	10 (20%)
23	CLA	B	610	37	65,73,73	1.81	9 (13%)	76,113,113	1.60	13 (17%)
31	BCR	b	618	-	41,41,41	1.20	3 (7%)	56,56,56	1.35	6 (10%)
33	LHG	d	407	-	48,48,48	0.76	1 (2%)	51,54,54	1.25	5 (9%)
27	LMG	B	620	-	51,51,55	0.99	3 (5%)	59,59,63	1.51	12 (20%)
35	HEM	e	102	6,5	41,50,50	1.44	5 (12%)	45,82,82	1.66	8 (17%)
23	CLA	B	611	-	65,73,73	1.58	11 (16%)	76,113,113	1.45	13 (17%)
23	CLA	b	609	-	65,73,73	1.41	10 (15%)	76,113,113	1.41	12 (15%)
29	DGD	c	518	-	63,63,67	1.13	5 (7%)	77,77,81	1.43	15 (19%)
26	PL9	a	410	-	55,55,55	1.12	2 (3%)	68,69,69	1.62	13 (19%)
27	LMG	b	624	-	21,21,55	0.76	0	20,20,63	0.98	0
23	CLA	b	607	-	65,73,73	1.83	10 (15%)	76,113,113	1.65	17 (22%)
23	CLA	b	615	-	65,73,73	1.52	10 (15%)	76,113,113	1.52	11 (14%)
30	OEX	a	414	3,37,1	0,15,15	-	-	-		
23	CLA	C	505	-	65,73,73	1.52	7 (10%)	76,113,113	1.41	11 (14%)
33	LHG	e	101	-	41,41,48	0.80	1 (2%)	44,47,54	1.27	5 (11%)
23	CLA	a	405	-	65,73,73	1.55	9 (13%)	76,113,113	1.53	12 (15%)
23	CLA	B	608	-	65,73,73	1.56	11 (16%)	76,113,113	1.48	11 (14%)
23	CLA	c	508	-	64,72,73	1.52	9 (14%)	74,111,113	1.29	7 (9%)
27	LMG	d	410	-	44,44,55	0.99	3 (6%)	52,52,63	1.34	7 (13%)
23	CLA	C	511	3	65,73,73	1.75	11 (16%)	76,113,113	1.38	5 (6%)
23	CLA	C	512	-	65,73,73	1.52	8 (12%)	76,113,113	1.34	10 (13%)
23	CLA	b	610	-	65,73,73	1.53	9 (13%)	76,113,113	1.32	7 (9%)
23	CLA	D	403	-	65,73,73	1.29	7 (10%)	76,113,113	1.26	9 (11%)
26	PL9	D	406	-	55,55,55	1.51	10 (18%)	68,69,69	1.54	14 (20%)
23	CLA	c	506	-	65,73,73	1.86	9 (13%)	76,113,113	1.34	12 (15%)
23	CLA	c	512	-	65,73,73	1.57	9 (13%)	76,113,113	1.42	10 (13%)
30	OEX	A	415	3,37,1	0,15,15	-	-	-		
33	LHG	l	101	-	48,48,48	0.67	0	51,54,54	1.25	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	501	-	65,73,73	1.38	7 (10%)	76,113,113	1.68	11 (14%)
23	CLA	d	404	-	65,73,73	1.76	10 (15%)	76,113,113	1.24	10 (13%)
23	CLA	B	604	-	65,73,73	1.74	11 (16%)	76,113,113	1.64	8 (10%)
23	CLA	c	502	-	65,73,73	1.63	9 (13%)	76,113,113	1.67	9 (11%)
28	SQD	A	412	-	51,52,54	1.05	5 (9%)	60,63,65	2.27	14 (23%)
23	CLA	B	605	-	65,73,73	1.22	7 (10%)	76,113,113	1.53	10 (13%)
29	DGD	h	102	-	63,63,67	1.17	9 (14%)	77,77,81	1.55	16 (20%)
35	HEM	F	101	6,5	41,50,50	1.56	3 (7%)	45,82,82	1.25	4 (8%)
23	CLA	b	614	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	13 (17%)
25	8CT	C	515	-	40,41,41	1.75	6 (15%)	50,56,56	2.36	14 (28%)
23	CLA	A	411	37	65,73,73	1.56	10 (15%)	76,113,113	1.24	7 (9%)
25	8CT	d	405	-	40,41,41	1.71	5 (12%)	50,56,56	2.45	9 (18%)
23	CLA	B	606	-	65,73,73	1.98	10 (15%)	76,113,113	1.39	9 (11%)
23	CLA	B	612	-	65,73,73	1.48	6 (9%)	76,113,113	1.65	10 (13%)
23	CLA	B	602	-	65,73,73	1.47	8 (12%)	76,113,113	1.43	9 (11%)
23	CLA	B	603	-	65,73,73	1.38	8 (12%)	76,113,113	1.47	12 (15%)
23	CLA	b	617	-	60,68,73	1.56	9 (15%)	70,107,113	1.59	10 (14%)
23	CLA	c	507	37	65,73,73	1.54	11 (16%)	76,113,113	1.57	12 (15%)
29	DGD	C	517	-	63,63,67	1.23	8 (12%)	77,77,81	1.49	9 (11%)
23	CLA	C	507	37	65,73,73	1.65	10 (15%)	76,113,113	1.34	11 (14%)
33	LHG	B	623	-	48,48,48	0.83	1 (2%)	51,54,54	1.36	6 (11%)
23	CLA	C	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.45	9 (11%)
25	8CT	k	101	-	40,41,41	1.65	5 (12%)	50,56,56	2.33	7 (14%)
23	CLA	a	408	-	65,73,73	1.70	11 (16%)	76,113,113	1.41	12 (15%)
23	CLA	b	603	-	65,73,73	1.49	8 (12%)	76,113,113	1.69	10 (13%)
23	CLA	d	402	37	65,73,73	1.56	8 (12%)	76,113,113	1.46	7 (9%)
23	CLA	D	404	-	65,73,73	1.54	9 (13%)	76,113,113	1.17	5 (6%)
29	DGD	C	518	-	63,63,67	0.99	3 (4%)	77,77,81	1.46	12 (15%)
23	CLA	b	608	37	65,73,73	1.39	10 (15%)	76,113,113	1.19	7 (9%)
23	CLA	c	510	-	65,73,73	1.42	8 (12%)	76,113,113	1.69	7 (9%)
26	PL9	d	406	-	55,55,55	1.35	6 (10%)	68,69,69	1.85	22 (32%)
31	BCR	Y	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	9 (16%)
23	CLA	B	614	-	65,73,73	1.50	7 (10%)	76,113,113	1.36	9 (11%)
26	PL9	A	409	-	55,55,55	1.10	3 (5%)	68,69,69	1.75	12 (17%)
23	CLA	A	407	-	54,62,73	1.85	10 (18%)	62,99,113	1.64	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	8CT	c	514	-	40,41,41	1.69	3 (7%)	50,56,56	2.41	13 (26%)
24	PHO	D	402	-	51,69,69	1.13	3 (5%)	47,99,99	1.20	6 (12%)
23	CLA	B	616	-	60,68,73	1.80	11 (18%)	70,107,113	1.70	11 (15%)
23	CLA	c	513	-	65,73,73	1.51	6 (9%)	76,113,113	1.22	6 (7%)
27	LMG	c	524	-	49,49,55	1.02	4 (8%)	57,57,63	1.21	4 (7%)
31	BCR	h	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.33	7 (12%)
23	CLA	C	509	-	65,73,73	1.47	7 (10%)	76,113,113	1.49	11 (14%)
23	CLA	b	602	37	65,73,73	1.78	13 (20%)	76,113,113	1.44	10 (13%)
25	8CT	t	101	-	40,41,41	1.63	4 (10%)	50,56,56	2.67	17 (34%)
23	CLA	b	605	-	65,73,73	1.68	9 (13%)	76,113,113	1.61	13 (17%)
28	SQD	b	601	-	48,49,54	0.97	3 (6%)	57,60,65	2.02	13 (22%)
29	DGD	H	102	-	63,63,67	1.34	9 (14%)	77,77,81	1.48	13 (16%)
27	LMG	C	519	-	48,48,55	0.94	3 (6%)	56,56,63	1.27	7 (12%)
23	CLA	A	404	-	65,73,73	1.42	10 (15%)	76,113,113	1.40	7 (9%)
27	LMG	A	410	-	48,48,55	0.92	4 (8%)	56,56,63	1.34	8 (14%)
31	BCR	T	101	-	41,41,41	1.16	4 (9%)	56,56,56	1.39	8 (14%)
31	BCR	b	619	-	41,41,41	1.28	3 (7%)	56,56,56	1.24	5 (8%)
23	CLA	c	504	37	60,68,73	1.55	7 (11%)	70,107,113	1.58	10 (14%)
36	HEC	V	201	16	32,50,50	2.13	5 (15%)	24,82,82	1.54	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	511	3	1/1/20/20	7/37/115/115	-
25	8CT	b	620	-	1/1/25/25	9/29/63/63	0/2/2/2
23	CLA	C	506	-	1/1/20/20	14/37/115/115	-
27	LMG	D	411	-	-	18/33/33/70	-
33	LHG	D	410	-	-	20/51/51/53	-
23	CLA	a	406	37	-	11/37/115/115	-
33	LHG	D	409	-	-	18/53/53/53	-
24	PHO	d	401	-	-	1/37/103/103	0/5/6/6
23	CLA	b	606	-	1/1/20/20	9/37/115/115	-
23	CLA	b	612	-	1/1/20/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	C	520	-	1/1/25/25	8/29/63/63	0/2/2/2
31	BCR	c	521	-	-	9/29/63/63	0/2/2/2
23	CLA	b	604	-	1/1/20/20	9/37/115/115	-
33	LHG	L	101	-	-	22/53/53/53	-
27	LMG	B	622	-	-	10/22/22/70	-
31	BCR	c	515	-	-	7/29/63/63	0/2/2/2
23	CLA	B	607	37	1/1/20/20	12/37/115/115	-
23	CLA	B	615	-	1/1/20/20	11/37/115/115	-
24	PHO	a	407	-	-	5/37/103/103	0/5/6/6
25	8CT	C	514	-	1/1/25/25	8/29/63/63	0/2/2/2
23	CLA	C	502	-	1/1/20/20	10/37/115/115	-
23	CLA	C	504	37	1/1/18/20	9/30/108/115	-
28	SQD	a	412	-	-	19/37/37/69	-
23	CLA	C	503	-	1/1/20/20	5/37/115/115	-
31	BCR	a	409	-	-	1/29/63/63	0/2/2/2
27	LMG	c	519	-	-	13/31/51/70	0/1/1/1
29	DGD	C	516	-	-	18/51/91/95	0/2/2/2
23	CLA	b	611	37	1/1/20/20	5/37/115/115	-
27	LMG	b	621	-	-	18/46/66/70	0/1/1/1
27	LMG	D	407	-	-	14/46/66/70	0/1/1/1
23	CLA	b	613	-	1/1/20/20	9/37/115/115	-
31	BCR	H	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	601	37	1/1/20/20	14/37/115/115	-
23	CLA	A	405	37	-	6/37/115/115	-
33	LHG	d	409	-	-	12/43/43/53	-
25	8CT	A	408	-	1/1/25/25	6/29/63/63	0/2/2/2
33	LHG	E	101	-	-	27/53/53/53	-
28	SQD	A	413	-	-	11/39/39/69	-
23	CLA	c	505	-	1/1/20/20	11/37/115/115	-
29	DGD	c	517	-	-	18/51/91/95	0/2/2/2
23	CLA	B	613	-	1/1/20/20	5/37/115/115	-
23	CLA	c	503	-	-	5/37/115/115	-
23	CLA	b	616	-	1/1/20/20	9/37/115/115	-
23	CLA	d	403	-	-	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	o	301	-	-	23/45/45/95	-
27	LMG	c	522	-	-	22/43/63/70	0/1/1/1
23	CLA	C	501	-	1/1/20/20	2/37/115/115	-
36	HEC	v	201	16	-	2/10/54/54	-
28	SQD	a	411	-	-	19/49/69/69	0/1/1/1
29	DGD	A	414	-	-	26/55/95/95	0/2/2/2
28	SQD	B	624	-	-	22/49/69/69	0/1/1/1
25	8CT	B	617	-	1/1/25/25	10/29/63/63	0/2/2/2
31	BCR	B	618	-	-	4/29/63/63	0/2/2/2
28	SQD	D	408	-	-	17/28/48/69	0/1/1/1
27	LMG	b	623	-	-	19/50/70/70	0/1/1/1
23	CLA	B	609	-	-	5/37/115/115	-
23	CLA	c	509	-	1/1/20/20	12/37/115/115	-
29	DGD	c	516	-	-	26/51/91/95	0/2/2/2
23	CLA	C	508	-	-	7/37/115/115	-
25	8CT	B	619	-	1/1/25/25	7/29/63/63	0/2/2/2
33	LHG	d	408	-	-	24/53/53/53	-
24	PHO	A	406	-	-	7/37/103/103	0/5/6/6
25	8CT	D	405	-	1/1/25/25	6/29/63/63	0/2/2/2
23	CLA	C	513	-	1/1/20/20	11/37/115/115	-
28	SQD	f	101	-	-	17/36/56/69	0/1/1/1
23	CLA	B	610	37	1/1/20/20	4/37/115/115	-
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2
33	LHG	d	407	-	-	22/53/53/53	-
27	LMG	B	620	-	-	19/46/66/70	0/1/1/1
35	HEM	e	102	6,5	-	3/12/54/54	-
23	CLA	B	611	-	-	6/37/115/115	-
23	CLA	b	609	-	-	6/37/115/115	-
29	DGD	c	518	-	-	17/51/91/95	0/2/2/2
26	PL9	a	410	-	-	19/53/73/73	0/1/1/1
27	LMG	b	624	-	-	10/17/17/70	-
23	CLA	b	607	-	1/1/20/20	9/37/115/115	-
23	CLA	b	615	-	1/1/20/20	14/37/115/115	-
23	CLA	C	505	-	1/1/20/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	e	101	-	-	28/46/46/53	-
23	CLA	a	405	-	1/1/20/20	7/37/115/115	-
23	CLA	B	608	-	-	6/37/115/115	-
23	CLA	c	508	-	-	9/36/114/115	-
27	LMG	d	410	-	-	11/39/59/70	0/1/1/1
23	CLA	C	511	3	1/1/20/20	8/37/115/115	-
23	CLA	C	512	-	1/1/20/20	9/37/115/115	-
23	CLA	b	610	-	1/1/20/20	9/37/115/115	-
23	CLA	D	403	-	1/1/20/20	8/37/115/115	-
26	PL9	D	406	-	-	13/53/73/73	0/1/1/1
23	CLA	c	506	-	1/1/20/20	18/37/115/115	-
23	CLA	c	512	-	1/1/20/20	19/37/115/115	-
33	LHG	l	101	-	-	16/53/53/53	-
23	CLA	c	501	-	1/1/20/20	6/37/115/115	-
23	CLA	d	404	-	1/1/20/20	8/37/115/115	-
23	CLA	B	604	-	1/1/20/20	11/37/115/115	-
23	CLA	c	502	-	-	3/37/115/115	-
28	SQD	A	412	-	-	22/47/67/69	0/1/1/1
23	CLA	B	605	-	1/1/20/20	13/37/115/115	-
29	DGD	h	102	-	-	20/51/91/95	0/2/2/2
35	HEM	F	101	6,5	-	2/12/54/54	-
23	CLA	b	614	-	1/1/20/20	5/37/115/115	-
25	8CT	C	515	-	1/1/25/25	8/29/63/63	0/2/2/2
23	CLA	A	411	37	-	2/37/115/115	-
25	8CT	d	405	-	1/1/25/25	11/29/63/63	0/2/2/2
23	CLA	B	606	-	1/1/20/20	11/37/115/115	-
23	CLA	B	612	-	1/1/20/20	12/37/115/115	-
23	CLA	B	602	-	1/1/20/20	5/37/115/115	-
23	CLA	B	603	-	1/1/20/20	7/37/115/115	-
23	CLA	b	617	-	1/1/19/20	9/31/109/115	-
23	CLA	c	507	37	1/1/20/20	9/37/115/115	-
29	DGD	C	517	-	-	21/51/91/95	0/2/2/2
23	CLA	C	507	37	1/1/20/20	6/37/115/115	-
33	LHG	B	623	-	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	510	-	1/1/20/20	13/37/115/115	-
25	8CT	k	101	-	1/1/25/25	13/29/63/63	0/2/2/2
23	CLA	a	408	-	1/1/20/20	8/37/115/115	-
23	CLA	b	603	-	1/1/20/20	10/37/115/115	-
23	CLA	d	402	37	1/1/20/20	8/37/115/115	-
23	CLA	D	404	-	1/1/20/20	11/37/115/115	-
29	DGD	C	518	-	-	15/51/91/95	0/2/2/2
23	CLA	b	608	37	1/1/20/20	14/37/115/115	-
23	CLA	c	510	-	1/1/20/20	15/37/115/115	-
26	PL9	d	406	-	-	18/53/73/73	0/1/1/1
31	BCR	Y	101	-	-	9/29/63/63	0/2/2/2
23	CLA	B	614	-	1/1/20/20	9/37/115/115	-
26	PL9	A	409	-	-	21/53/73/73	0/1/1/1
23	CLA	A	407	-	1/1/17/20	4/24/102/115	-
25	8CT	c	514	-	1/1/25/25	15/29/63/63	0/2/2/2
24	PHO	D	402	-	-	2/37/103/103	0/5/6/6
23	CLA	B	616	-	1/1/19/20	9/31/109/115	-
23	CLA	c	513	-	1/1/20/20	11/37/115/115	-
27	LMG	c	524	-	-	22/44/64/70	0/1/1/1
31	BCR	h	101	-	-	7/29/63/63	0/2/2/2
23	CLA	C	509	-	1/1/20/20	14/37/115/115	-
23	CLA	b	602	37	1/1/20/20	18/37/115/115	-
25	8CT	t	101	-	1/1/25/25	8/29/63/63	0/2/2/2
23	CLA	b	605	-	1/1/20/20	10/37/115/115	-
28	SQD	b	601	-	-	20/44/64/69	0/1/1/1
29	DGD	H	102	-	-	19/51/91/95	0/2/2/2
27	LMG	C	519	-	-	13/43/63/70	0/1/1/1
23	CLA	A	404	-	1/1/20/20	4/37/115/115	-
27	LMG	A	410	-	-	22/43/63/70	0/1/1/1
31	BCR	T	101	-	-	1/29/63/63	0/2/2/2
31	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	c	504	37	1/1/19/20	6/31/109/115	-
36	HEC	V	201	16	-	2/10/54/54	-

All (905) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	MG-NA	9.72	2.29	2.06
23	c	506	CLA	MG-ND	-9.38	1.87	2.05
23	B	601	CLA	C4B-NB	9.09	1.43	1.35
23	B	610	CLA	C4B-NB	8.81	1.43	1.35
23	b	605	CLA	C4B-NB	8.66	1.42	1.35
25	A	408	8CT	C32-C31	8.42	1.49	1.32
25	c	514	8CT	C32-C31	8.09	1.48	1.32
23	b	607	CLA	MG-NA	8.06	2.25	2.06
23	C	501	CLA	MG-NA	7.94	2.25	2.06
25	b	620	8CT	C32-C31	7.91	1.48	1.32
25	d	405	8CT	C32-C31	7.90	1.48	1.32
23	a	408	CLA	C4B-NB	7.89	1.42	1.35
23	C	506	CLA	MG-ND	-7.87	1.90	2.05
25	C	514	8CT	C32-C31	7.84	1.48	1.32
25	B	617	8CT	C32-C31	7.79	1.48	1.32
23	B	604	CLA	MG-NA	7.77	2.24	2.06
23	a	405	CLA	C4B-NB	7.76	1.42	1.35
23	B	616	CLA	MG-NA	7.76	2.24	2.06
25	k	101	8CT	C32-C31	7.75	1.48	1.32
23	c	504	CLA	C4B-NB	7.71	1.42	1.35
25	C	520	8CT	C32-C31	7.70	1.47	1.32
25	t	101	8CT	C32-C31	7.65	1.47	1.32
23	c	511	CLA	C4B-NB	7.65	1.42	1.35
23	c	513	CLA	C4B-NB	7.64	1.42	1.35
23	C	505	CLA	C4B-NB	7.63	1.42	1.35
36	v	201	HEC	C2B-C3B	-7.60	1.32	1.40
25	C	515	8CT	C32-C31	7.58	1.47	1.32
23	A	407	CLA	C4B-NB	7.52	1.41	1.35
25	D	405	8CT	C32-C31	7.48	1.47	1.32
23	b	604	CLA	C4B-NB	7.42	1.41	1.35
23	C	503	CLA	C4B-NB	7.39	1.41	1.35
23	d	404	CLA	MG-ND	-7.38	1.91	2.05
23	B	612	CLA	C4B-NB	7.37	1.41	1.35
23	c	512	CLA	C4B-NB	7.29	1.41	1.35
25	B	619	8CT	C32-C31	7.28	1.47	1.32
23	b	614	CLA	C4B-NB	7.28	1.41	1.35
23	B	616	CLA	C4B-NB	7.25	1.41	1.35
23	d	403	CLA	C4B-NB	7.24	1.41	1.35
23	C	506	CLA	C4B-NB	7.23	1.41	1.35
23	C	511	CLA	C4B-NB	7.21	1.41	1.35
23	A	405	CLA	C4B-NB	7.18	1.41	1.35
23	a	406	CLA	C4B-NB	7.12	1.41	1.35
23	c	511	CLA	MG-NA	7.10	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	C4B-NB	7.09	1.41	1.35
23	C	513	CLA	C4B-NB	7.07	1.41	1.35
23	C	501	CLA	C4B-NB	7.03	1.41	1.35
23	b	616	CLA	MG-NA	7.02	2.23	2.06
23	B	615	CLA	C4B-NB	7.02	1.41	1.35
23	b	611	CLA	C4B-NB	7.01	1.41	1.35
23	b	602	CLA	MG-NA	6.99	2.22	2.06
23	B	606	CLA	C4B-NB	6.98	1.41	1.35
23	B	613	CLA	C4B-NB	6.98	1.41	1.35
23	c	508	CLA	C4B-NB	6.98	1.41	1.35
23	B	601	CLA	MG-NA	6.97	2.22	2.06
23	b	607	CLA	C4B-NB	6.96	1.41	1.35
23	b	610	CLA	C4B-NB	6.95	1.41	1.35
23	C	502	CLA	C4B-NB	6.94	1.41	1.35
23	b	603	CLA	C4B-NB	6.94	1.41	1.35
23	C	504	CLA	C4B-NB	6.88	1.41	1.35
23	b	602	CLA	C4B-NB	6.86	1.41	1.35
23	C	510	CLA	C4B-NB	6.85	1.41	1.35
23	b	616	CLA	C4B-NB	6.85	1.41	1.35
23	c	505	CLA	C4B-NB	6.83	1.41	1.35
23	c	501	CLA	C4B-NB	6.83	1.41	1.35
23	B	614	CLA	C4B-NB	6.80	1.41	1.35
23	c	507	CLA	C4B-NB	6.77	1.41	1.35
23	C	508	CLA	C4B-NB	6.76	1.41	1.35
23	d	404	CLA	C4B-NB	6.76	1.41	1.35
23	C	509	CLA	C4B-NB	6.75	1.41	1.35
23	C	507	CLA	C4B-NB	6.68	1.41	1.35
23	A	411	CLA	C4B-NB	6.65	1.41	1.35
23	c	502	CLA	MG-ND	6.63	2.18	2.05
23	B	602	CLA	C4B-NB	6.59	1.41	1.35
23	C	501	CLA	MG-ND	-6.57	1.92	2.05
23	c	509	CLA	C4B-NB	6.56	1.41	1.35
23	b	617	CLA	C4B-NB	6.55	1.41	1.35
23	c	502	CLA	C4B-NB	6.51	1.41	1.35
23	c	503	CLA	C4B-NB	6.46	1.41	1.35
23	C	512	CLA	C4B-NB	6.46	1.41	1.35
23	b	615	CLA	C4B-NB	6.45	1.41	1.35
23	c	510	CLA	C4B-NB	6.44	1.41	1.35
36	V	201	HEC	C2B-C3B	-6.40	1.34	1.40
23	c	506	CLA	C4B-NB	6.31	1.40	1.35
23	C	511	CLA	MG-NA	6.31	2.21	2.06
23	B	609	CLA	C4B-NB	6.30	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	MG-NA	6.09	2.20	2.06
36	v	201	HEC	C3C-C2C	-6.08	1.34	1.40
36	V	201	HEC	C3C-C2C	-5.94	1.34	1.40
23	b	606	CLA	C4B-NB	5.88	1.40	1.35
23	B	601	CLA	MG-ND	-5.86	1.94	2.05
23	C	503	CLA	MG-NA	5.86	2.20	2.06
23	b	612	CLA	C4B-NB	5.81	1.40	1.35
23	A	407	CLA	MG-ND	-5.79	1.94	2.05
23	B	610	CLA	MG-NC	-5.76	1.92	2.06
23	B	613	CLA	MG-ND	-5.74	1.94	2.05
23	B	604	CLA	C4B-NB	5.74	1.40	1.35
23	C	507	CLA	MG-NA	5.73	2.19	2.06
23	B	611	CLA	C4B-NB	5.66	1.40	1.35
23	d	402	CLA	C4B-NB	5.53	1.40	1.35
23	B	607	CLA	C4B-NB	5.51	1.40	1.35
23	B	612	CLA	C4D-ND	-5.36	1.30	1.37
35	F	101	HEM	C3C-C2C	-5.29	1.33	1.40
23	b	613	CLA	C4B-NB	5.17	1.39	1.35
26	d	406	PL9	C7-C8	-5.10	1.43	1.50
23	c	505	CLA	C4D-ND	-5.10	1.30	1.37
23	B	608	CLA	C4B-NB	5.02	1.39	1.35
23	A	404	CLA	C4B-NB	4.95	1.39	1.35
23	B	603	CLA	C4B-NB	4.92	1.39	1.35
29	A	414	DGD	C4D-C5D	4.84	1.63	1.53
23	c	503	CLA	C1D-ND	4.81	1.43	1.37
23	b	612	CLA	MG-NC	-4.80	1.94	2.06
29	H	102	DGD	O5D-C1E	4.78	1.48	1.40
23	d	402	CLA	C4D-ND	-4.76	1.31	1.37
23	B	610	CLA	C3B-C2B	-4.76	1.33	1.40
23	C	508	CLA	MG-NA	4.68	2.17	2.06
23	c	512	CLA	MG-NC	4.68	2.17	2.06
26	D	406	PL9	C6-C1	-4.67	1.40	1.48
26	D	406	PL9	C11-C9	-4.65	1.41	1.51
23	a	408	CLA	C1D-ND	4.65	1.43	1.37
23	b	613	CLA	C4D-ND	-4.60	1.31	1.37
23	b	615	CLA	C4D-ND	-4.60	1.31	1.37
23	C	502	CLA	C4D-ND	-4.59	1.31	1.37
23	c	509	CLA	C1D-ND	4.58	1.43	1.37
23	C	504	CLA	MG-NA	4.52	2.17	2.06
23	d	402	CLA	MG-NA	4.49	2.16	2.06
23	B	608	CLA	MG-NA	4.46	2.16	2.06
23	c	509	CLA	C4D-ND	-4.40	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	MG-ND	-4.39	1.97	2.05
23	b	609	CLA	C4B-NB	4.35	1.39	1.35
35	e	102	HEM	C3C-C2C	-4.35	1.34	1.40
23	B	614	CLA	C4D-ND	-4.34	1.31	1.37
23	C	512	CLA	C4D-ND	-4.33	1.31	1.37
23	c	503	CLA	MG-NC	4.33	2.16	2.06
23	c	508	CLA	C4D-ND	-4.32	1.31	1.37
23	b	611	CLA	C4D-ND	-4.23	1.31	1.37
23	a	406	CLA	MG-NC	4.20	2.16	2.06
23	B	609	CLA	C1D-ND	4.18	1.42	1.37
31	h	101	BCR	C30-C25	-4.17	1.48	1.53
23	c	507	CLA	C4D-ND	-4.16	1.32	1.37
23	A	405	CLA	C1D-ND	4.16	1.42	1.37
27	D	407	LMG	C4-C5	4.14	1.61	1.53
23	B	605	CLA	C4D-ND	-4.12	1.32	1.37
25	B	617	8CT	C04-C03	-4.12	1.48	1.53
23	B	603	CLA	C4D-ND	-4.11	1.32	1.37
25	C	515	8CT	C04-C03	-4.11	1.48	1.53
23	B	611	CLA	MG-NC	-4.11	1.96	2.06
23	C	501	CLA	C1D-ND	4.09	1.42	1.37
23	c	511	CLA	C1D-ND	4.09	1.42	1.37
26	a	410	PL9	C7-C3	4.04	1.55	1.51
33	D	410	LHG	P-O6	4.03	1.75	1.59
23	A	404	CLA	MG-ND	-4.03	1.97	2.05
23	B	604	CLA	C1D-ND	4.02	1.42	1.37
23	B	606	CLA	MG-NC	-4.02	1.96	2.06
31	c	515	BCR	C30-C25	-4.01	1.48	1.53
23	b	607	CLA	C1D-ND	3.98	1.42	1.37
23	d	404	CLA	MG-NA	3.97	2.15	2.06
23	b	611	CLA	C1D-ND	3.96	1.42	1.37
23	b	605	CLA	C1D-ND	3.96	1.42	1.37
23	b	608	CLA	C4B-NB	3.95	1.38	1.35
31	b	618	BCR	C1-C6	-3.94	1.48	1.53
23	b	603	CLA	C4D-ND	-3.93	1.32	1.37
28	a	411	SQD	O48-C23	3.93	1.44	1.33
23	b	609	CLA	CHC-C1C	3.93	1.45	1.35
23	c	505	CLA	MG-NA	-3.92	1.97	2.06
26	d	406	PL9	C6-C1	-3.91	1.41	1.48
23	B	607	CLA	C4D-ND	-3.91	1.32	1.37
23	C	512	CLA	MG-ND	-3.91	1.98	2.05
23	C	502	CLA	MG-NC	3.91	2.15	2.06
36	V	201	HEC	CBB-CAB	-3.91	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C4B-NB	3.89	1.38	1.35
23	B	606	CLA	MG-ND	-3.88	1.98	2.05
23	B	602	CLA	C1D-ND	3.87	1.42	1.37
25	B	619	8CT	C30-C29	-3.87	1.44	1.50
23	C	507	CLA	MG-ND	-3.87	1.98	2.05
23	c	505	CLA	CHC-C1C	3.86	1.44	1.35
23	b	604	CLA	MG-ND	-3.86	1.98	2.05
23	c	511	CLA	CHC-C1C	3.85	1.44	1.35
31	b	619	BCR	C1-C6	-3.84	1.48	1.53
23	B	607	CLA	C1D-ND	3.84	1.42	1.37
23	A	411	CLA	C3B-C2B	-3.81	1.35	1.40
23	A	411	CLA	C4D-ND	-3.81	1.32	1.37
29	o	301	DGD	O1G-C1A	3.81	1.44	1.33
23	C	508	CLA	MG-ND	3.81	2.13	2.05
23	c	512	CLA	C1D-ND	3.80	1.42	1.37
23	c	502	CLA	C4D-ND	-3.80	1.32	1.37
23	B	608	CLA	MG-ND	-3.78	1.98	2.05
25	B	619	8CT	C04-C03	-3.77	1.48	1.53
27	D	411	LMG	C7-C8	3.77	1.60	1.51
25	D	405	8CT	C04-C03	-3.76	1.48	1.53
23	C	513	CLA	C1D-ND	3.76	1.42	1.37
31	Y	101	BCR	C1-C6	-3.76	1.48	1.53
23	C	510	CLA	C4D-ND	-3.75	1.32	1.37
29	c	517	DGD	O3D-C3D	-3.75	1.34	1.43
23	B	603	CLA	C1D-ND	3.75	1.42	1.37
23	a	405	CLA	MG-NA	3.75	2.15	2.06
23	A	407	CLA	C1D-ND	3.74	1.42	1.37
23	B	608	CLA	C4D-ND	-3.73	1.32	1.37
36	V	201	HEC	CBC-CAC	-3.73	1.35	1.49
23	b	612	CLA	C4D-ND	-3.72	1.32	1.37
23	c	503	CLA	C4D-ND	-3.71	1.32	1.37
23	C	508	CLA	C4D-ND	-3.71	1.32	1.37
23	b	608	CLA	C3B-C2B	-3.70	1.35	1.40
23	c	506	CLA	C1D-ND	3.70	1.42	1.37
31	Y	101	BCR	C30-C25	-3.69	1.48	1.53
29	C	518	DGD	O2G-C2G	-3.68	1.37	1.46
23	A	404	CLA	MG-NA	3.68	2.15	2.06
23	C	513	CLA	C4D-ND	-3.67	1.32	1.37
23	b	608	CLA	MG-NC	3.67	2.15	2.06
29	C	517	DGD	C4D-C3D	3.66	1.61	1.52
23	C	505	CLA	MG-ND	-3.65	1.98	2.05
23	B	616	CLA	C1D-ND	3.64	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	C4E-C3E	3.63	1.61	1.52
28	a	412	SQD	O47-C7	3.63	1.44	1.34
23	c	505	CLA	MG-ND	3.62	2.13	2.05
23	C	509	CLA	MG-ND	3.62	2.13	2.05
23	c	508	CLA	C1D-ND	3.62	1.42	1.37
23	A	405	CLA	C4D-ND	-3.61	1.32	1.37
23	D	404	CLA	C1D-ND	3.60	1.42	1.37
23	C	506	CLA	CHC-C1C	3.60	1.44	1.35
23	B	601	CLA	C1D-ND	3.59	1.42	1.37
28	a	412	SQD	O48-C23	3.59	1.43	1.33
23	b	607	CLA	MG-ND	-3.58	1.98	2.05
23	b	617	CLA	MG-ND	-3.58	1.98	2.05
23	C	506	CLA	C1D-ND	3.57	1.42	1.37
23	C	510	CLA	C1D-ND	3.56	1.42	1.37
23	B	614	CLA	CHC-C1C	3.55	1.44	1.35
31	a	409	BCR	C1-C6	-3.55	1.48	1.53
23	C	511	CLA	C1D-ND	3.55	1.42	1.37
23	B	613	CLA	C4D-ND	-3.54	1.32	1.37
31	H	101	BCR	C30-C25	-3.54	1.48	1.53
31	b	618	BCR	C30-C25	-3.54	1.48	1.53
23	c	504	CLA	C4D-ND	-3.53	1.32	1.37
23	B	602	CLA	MG-ND	-3.53	1.98	2.05
23	c	506	CLA	C4D-ND	-3.52	1.32	1.37
25	D	405	8CT	C30-C29	-3.52	1.45	1.50
23	b	603	CLA	CMD-C2D	-3.51	1.43	1.50
26	a	410	PL9	C53-C6	-3.51	1.43	1.50
25	c	514	8CT	C04-C03	-3.50	1.49	1.53
23	b	604	CLA	C4D-ND	-3.49	1.32	1.37
23	C	512	CLA	CHC-C1C	3.49	1.43	1.35
27	c	522	LMG	O1-C1	3.49	1.46	1.40
31	c	515	BCR	C1-C6	-3.48	1.49	1.53
23	C	503	CLA	C4D-ND	-3.48	1.32	1.37
24	D	402	PHO	CAC-C3C	-3.47	1.46	1.52
27	d	410	LMG	O7-C8	-3.46	1.37	1.46
36	v	201	HEC	CBB-CAB	-3.46	1.36	1.49
23	a	405	CLA	C1D-ND	3.45	1.42	1.37
28	A	413	SQD	O48-C23	3.45	1.43	1.33
23	b	616	CLA	CHC-C1C	3.43	1.43	1.35
23	c	513	CLA	C1D-ND	3.43	1.42	1.37
26	d	406	PL9	C3-C4	-3.43	1.43	1.49
23	B	615	CLA	C1D-ND	3.43	1.42	1.37
23	C	503	CLA	CHC-C1C	3.42	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C4D-ND	-3.42	1.33	1.37
23	b	605	CLA	CHC-C1C	3.42	1.43	1.35
23	b	616	CLA	C1D-ND	3.42	1.42	1.37
23	b	602	CLA	C1D-ND	3.41	1.42	1.37
23	c	509	CLA	MG-ND	3.41	2.12	2.05
23	C	501	CLA	CHC-C1C	3.41	1.43	1.35
23	B	614	CLA	MG-ND	-3.41	1.99	2.05
23	b	617	CLA	CMB-C2B	-3.41	1.44	1.51
23	a	406	CLA	CHC-C1C	3.41	1.43	1.35
23	B	605	CLA	C4B-NB	3.40	1.38	1.35
29	A	414	DGD	C1E-C2E	3.40	1.62	1.52
25	d	405	8CT	C04-C03	-3.39	1.49	1.53
23	C	509	CLA	C1D-ND	3.39	1.42	1.37
23	b	603	CLA	CHC-C1C	3.39	1.43	1.35
29	A	414	DGD	C4D-C3D	3.39	1.61	1.52
28	f	101	SQD	O47-C7	3.39	1.43	1.34
28	b	601	SQD	O48-C23	3.38	1.43	1.33
23	A	411	CLA	C1D-ND	3.38	1.41	1.37
23	b	608	CLA	MG-ND	-3.38	1.99	2.05
31	B	618	BCR	C30-C25	-3.37	1.49	1.53
35	F	101	HEM	C3C-CAC	3.37	1.54	1.47
23	b	611	CLA	MG-ND	-3.37	1.99	2.05
29	c	518	DGD	C4D-C5D	3.36	1.60	1.53
23	C	506	CLA	MG-NC	3.36	2.14	2.06
23	B	615	CLA	CMB-C2B	-3.35	1.44	1.51
23	d	403	CLA	CMB-C2B	-3.35	1.44	1.51
23	c	510	CLA	C4D-ND	-3.34	1.33	1.37
23	A	411	CLA	CHC-C1C	3.34	1.43	1.35
36	v	201	HEC	CBC-CAC	-3.34	1.37	1.49
23	b	610	CLA	MG-NA	3.34	2.14	2.06
23	C	505	CLA	C1D-ND	3.33	1.41	1.37
28	D	408	SQD	O48-C23	3.33	1.43	1.33
25	A	408	8CT	C04-C03	-3.33	1.49	1.53
23	B	609	CLA	C3B-CAB	-3.31	1.41	1.47
23	a	406	CLA	C1D-ND	3.29	1.41	1.37
23	B	607	CLA	C3B-C2B	-3.27	1.35	1.40
23	c	503	CLA	CMB-C2B	-3.27	1.44	1.51
23	c	508	CLA	CHC-C1C	3.27	1.43	1.35
23	C	506	CLA	C4D-ND	-3.26	1.33	1.37
23	B	602	CLA	CHC-C1C	3.25	1.43	1.35
23	B	610	CLA	CHC-C1C	3.25	1.43	1.35
29	c	518	DGD	C6D-C5D	3.25	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	C4D-ND	-3.25	1.33	1.37
23	C	511	CLA	MG-NC	3.24	2.14	2.06
24	A	406	PHO	C3B-C2B	-3.23	1.35	1.40
23	c	510	CLA	C1D-ND	3.23	1.41	1.37
26	D	406	PL9	C21-C22	3.23	1.64	1.53
23	C	511	CLA	CHC-C1C	3.23	1.43	1.35
23	C	510	CLA	CHC-C1C	3.22	1.43	1.35
23	C	501	CLA	C3B-C2B	-3.22	1.35	1.40
29	c	518	DGD	C2A-C1A	-3.21	1.41	1.50
23	a	408	CLA	C3B-C2B	-3.20	1.35	1.40
25	C	514	8CT	C30-C29	-3.20	1.45	1.50
31	T	101	BCR	C30-C25	-3.20	1.49	1.53
23	a	405	CLA	CHC-C1C	3.19	1.43	1.35
23	b	610	CLA	C4D-ND	-3.19	1.33	1.37
23	d	403	CLA	C1D-ND	3.19	1.41	1.37
23	C	502	CLA	C1D-ND	3.18	1.41	1.37
28	A	412	SQD	O48-C23	3.18	1.42	1.33
23	b	617	CLA	C1D-ND	3.18	1.41	1.37
25	b	620	8CT	C30-C29	-3.17	1.45	1.50
23	d	402	CLA	MG-ND	3.17	2.12	2.05
28	B	624	SQD	O47-C7	3.17	1.43	1.34
23	C	513	CLA	MG-ND	3.16	2.12	2.05
23	b	615	CLA	MG-NA	-3.16	1.98	2.06
23	B	615	CLA	C3B-C2B	-3.16	1.36	1.40
23	C	507	CLA	MG-NC	-3.15	1.98	2.06
23	D	404	CLA	MG-NC	3.15	2.13	2.06
23	A	407	CLA	C4D-ND	-3.14	1.33	1.37
23	B	608	CLA	CMD-C2D	-3.14	1.44	1.50
33	d	409	LHG	P-O6	3.14	1.72	1.59
27	c	524	LMG	O8-C9	-3.14	1.38	1.45
23	b	606	CLA	CMD-C2D	-3.14	1.44	1.50
23	b	617	CLA	C4D-ND	-3.14	1.33	1.37
31	B	618	BCR	C1-C6	-3.13	1.49	1.53
23	B	606	CLA	C3B-C2B	-3.13	1.36	1.40
23	B	605	CLA	CHC-C1C	3.13	1.43	1.35
29	H	102	DGD	C4D-C5D	3.12	1.59	1.53
29	H	102	DGD	C1E-C2E	3.12	1.61	1.52
28	B	624	SQD	O48-C23	3.12	1.42	1.33
23	b	610	CLA	MG-ND	-3.11	1.99	2.05
28	A	413	SQD	O47-C7	3.11	1.43	1.34
26	A	409	PL9	C53-C6	-3.10	1.44	1.50
23	B	606	CLA	C4D-ND	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CMB-C2B	-3.10	1.45	1.51
23	C	510	CLA	MG-NC	3.10	2.13	2.06
25	b	620	8CT	C04-C03	-3.09	1.49	1.53
23	c	513	CLA	CHC-C1C	3.09	1.42	1.35
23	C	502	CLA	CHC-C1C	3.08	1.42	1.35
23	a	408	CLA	C4B-CHC	-3.08	1.32	1.41
23	A	407	CLA	CMB-C2B	-3.07	1.45	1.51
23	b	602	CLA	MG-ND	-3.07	1.99	2.05
23	c	513	CLA	C4D-ND	-3.06	1.33	1.37
27	D	411	LMG	C9-C8	3.06	1.60	1.50
23	D	403	CLA	C4D-ND	-3.06	1.33	1.37
23	b	606	CLA	CHC-C1C	3.05	1.42	1.35
23	C	507	CLA	C3B-C2B	-3.05	1.36	1.40
23	C	507	CLA	C4D-ND	-3.05	1.33	1.37
23	b	605	CLA	C4D-ND	-3.03	1.33	1.37
23	C	509	CLA	C4D-ND	-3.03	1.33	1.37
23	D	404	CLA	CMD-C2D	-3.02	1.44	1.50
23	b	611	CLA	C3B-C2B	-3.02	1.36	1.40
23	c	507	CLA	C3B-C2B	-3.02	1.36	1.40
23	d	403	CLA	CHC-C1C	3.02	1.42	1.35
23	a	408	CLA	CMC-C2C	-3.01	1.44	1.50
23	c	507	CLA	MG-NC	-2.99	1.99	2.06
23	A	407	CLA	CMD-C2D	-2.99	1.44	1.50
23	c	513	CLA	MG-NA	2.98	2.13	2.06
23	c	509	CLA	CHC-C1C	2.98	1.42	1.35
23	b	615	CLA	CHC-C1C	2.98	1.42	1.35
23	B	609	CLA	C3B-C2B	-2.97	1.36	1.40
23	b	614	CLA	C1D-ND	2.97	1.41	1.37
23	d	402	CLA	CHC-C1C	2.97	1.42	1.35
23	C	508	CLA	CHC-C1C	2.97	1.42	1.35
23	d	404	CLA	CHC-C1C	2.97	1.42	1.35
31	T	101	BCR	C1-C6	-2.96	1.49	1.53
23	c	507	CLA	CHC-C1C	2.96	1.42	1.35
23	d	404	CLA	C4D-ND	-2.96	1.33	1.37
23	b	607	CLA	C4D-ND	-2.95	1.33	1.37
25	C	515	8CT	C30-C29	-2.95	1.46	1.50
23	D	403	CLA	CHC-C1C	2.94	1.42	1.35
23	D	403	CLA	C1D-ND	2.94	1.41	1.37
23	B	611	CLA	CHC-C1C	2.94	1.42	1.35
23	C	504	CLA	CMB-C2B	-2.94	1.45	1.51
29	c	516	DGD	C3G-C2G	2.94	1.59	1.50
23	c	504	CLA	MG-ND	-2.94	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	410	LHG	O3-C3	-2.94	1.33	1.44
25	k	101	8CT	C04-C03	-2.93	1.49	1.53
23	c	504	CLA	CHC-C1C	2.93	1.42	1.35
23	B	602	CLA	C4D-ND	-2.93	1.33	1.37
31	h	101	BCR	C1-C6	-2.93	1.49	1.53
23	b	609	CLA	C1D-ND	2.93	1.41	1.37
23	B	615	CLA	C3B-CAB	-2.93	1.42	1.47
29	C	517	DGD	C1E-C2E	2.93	1.60	1.52
23	c	512	CLA	CHC-C1C	2.92	1.42	1.35
29	A	414	DGD	O2G-C1B	2.91	1.42	1.34
23	B	607	CLA	CHC-C1C	2.91	1.42	1.35
28	f	101	SQD	O48-C23	2.90	1.41	1.33
23	B	611	CLA	C4D-ND	-2.90	1.33	1.37
23	b	609	CLA	MG-NA	2.90	2.13	2.06
23	c	507	CLA	C1D-ND	2.90	1.41	1.37
23	c	506	CLA	CHC-C1C	2.90	1.42	1.35
23	d	404	CLA	C3B-C2B	-2.90	1.36	1.40
23	B	606	CLA	CHC-C1C	2.90	1.42	1.35
23	C	506	CLA	C3B-C2B	-2.89	1.36	1.40
23	c	505	CLA	C3B-C2B	-2.89	1.36	1.40
29	C	518	DGD	O1G-C1G	-2.89	1.38	1.45
23	A	405	CLA	MG-NA	2.89	2.13	2.06
23	B	608	CLA	CHC-C1C	2.89	1.42	1.35
23	b	603	CLA	MG-ND	2.89	2.11	2.05
23	C	508	CLA	C1D-ND	2.89	1.41	1.37
23	B	607	CLA	MG-NC	2.88	2.13	2.06
23	b	605	CLA	C1B-NB	2.88	1.37	1.35
23	A	404	CLA	CMD-C2D	-2.88	1.44	1.50
27	c	522	LMG	C7-C8	2.88	1.59	1.50
23	C	505	CLA	CHC-C1C	2.87	1.42	1.35
33	D	409	LHG	O8-C6	-2.87	1.38	1.45
29	H	102	DGD	C4E-C5E	2.87	1.59	1.53
23	c	510	CLA	CMB-C2B	-2.87	1.45	1.51
27	c	524	LMG	C3-C2	2.87	1.59	1.52
35	F	101	HEM	CAB-C3B	2.87	1.55	1.47
23	b	615	CLA	MG-ND	2.86	2.11	2.05
29	h	102	DGD	O1G-C1G	-2.85	1.38	1.45
29	C	517	DGD	O2G-C2G	-2.85	1.39	1.46
23	a	406	CLA	C3B-C2B	-2.85	1.36	1.40
23	b	602	CLA	CHC-C1C	2.85	1.42	1.35
25	C	514	8CT	C04-C03	-2.84	1.49	1.53
23	b	602	CLA	MG-NC	-2.84	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C4D-ND	-2.84	1.33	1.37
35	e	102	HEM	CAB-C3B	2.83	1.55	1.47
29	A	414	DGD	C3E-C2E	2.83	1.59	1.52
24	d	401	PHO	CAC-C3C	-2.83	1.47	1.52
25	t	101	8CT	C04-C03	-2.83	1.49	1.53
23	b	617	CLA	C3B-CAB	-2.83	1.42	1.47
23	b	613	CLA	CMC-C2C	-2.82	1.44	1.50
23	B	613	CLA	C1D-ND	2.82	1.41	1.37
23	C	501	CLA	C4D-ND	-2.82	1.33	1.37
23	b	616	CLA	C1B-NB	2.82	1.37	1.35
28	A	413	SQD	O47-C45	-2.81	1.42	1.47
23	b	608	CLA	CHC-C1C	2.81	1.42	1.35
23	b	610	CLA	C1D-ND	2.81	1.41	1.37
23	B	615	CLA	MG-NA	2.81	2.12	2.06
31	b	619	BCR	C30-C25	-2.80	1.49	1.53
23	C	511	CLA	CMB-C2B	-2.80	1.45	1.51
23	b	613	CLA	CHC-C1C	2.80	1.42	1.35
23	C	504	CLA	CHC-C1C	2.79	1.42	1.35
23	b	604	CLA	CHC-C1C	2.79	1.42	1.35
23	b	604	CLA	CMD-C2D	-2.79	1.44	1.50
28	b	601	SQD	O47-C7	2.79	1.42	1.34
29	C	516	DGD	O2G-C2G	-2.79	1.39	1.46
23	B	606	CLA	C1D-ND	2.79	1.41	1.37
23	C	511	CLA	C1B-NB	2.79	1.37	1.35
29	A	414	DGD	C3G-C2G	2.79	1.59	1.50
23	b	605	CLA	CMB-C2B	-2.78	1.45	1.51
25	t	101	8CT	C30-C29	-2.78	1.46	1.50
23	B	609	CLA	MG-NA	2.78	2.12	2.06
29	C	517	DGD	O6D-C5D	-2.78	1.37	1.44
31	a	409	BCR	C30-C25	-2.78	1.49	1.53
29	c	517	DGD	O3G-C1D	-2.78	1.35	1.40
23	C	505	CLA	C3B-C2B	-2.77	1.36	1.40
23	B	612	CLA	CHC-C1C	2.77	1.42	1.35
29	H	102	DGD	O2D-C2D	-2.77	1.36	1.43
23	d	403	CLA	MG-NC	2.76	2.12	2.06
26	d	406	PL9	C11-C9	-2.76	1.45	1.51
23	c	501	CLA	CHC-C1C	2.76	1.42	1.35
23	c	513	CLA	CMB-C2B	-2.76	1.45	1.51
23	b	607	CLA	CHC-C1C	2.76	1.42	1.35
28	A	412	SQD	O2-C2	-2.76	1.36	1.43
23	B	609	CLA	MG-ND	-2.74	2.00	2.05
35	e	102	HEM	C3C-CAC	2.74	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C4D-ND	-2.74	1.33	1.37
23	B	604	CLA	C4D-ND	-2.74	1.33	1.37
23	b	612	CLA	CMB-C2B	-2.74	1.45	1.51
23	C	507	CLA	CHC-C1C	2.74	1.42	1.35
23	c	507	CLA	C3B-CAB	-2.73	1.42	1.47
23	b	609	CLA	C3B-CAB	-2.73	1.42	1.47
29	h	102	DGD	C4D-C3D	2.73	1.59	1.52
23	b	617	CLA	C3B-C2B	-2.72	1.36	1.40
23	b	603	CLA	CMB-C2B	-2.72	1.46	1.51
23	b	613	CLA	CMB-C2B	-2.72	1.46	1.51
23	d	403	CLA	MG-NA	2.72	2.12	2.06
27	B	620	LMG	C1-C2	2.72	1.60	1.52
23	c	510	CLA	CHC-C1C	2.71	1.41	1.35
25	k	101	8CT	C30-C29	-2.71	1.46	1.50
23	c	512	CLA	C4D-ND	-2.71	1.34	1.37
27	B	620	LMG	C9-C8	2.70	1.59	1.50
23	B	607	CLA	CMB-C2B	-2.70	1.46	1.51
24	a	407	PHO	O2D-CGD	2.70	1.39	1.33
27	C	519	LMG	O7-C8	-2.70	1.39	1.46
27	c	524	LMG	C4-C5	2.70	1.58	1.53
23	B	601	CLA	CMB-C2B	-2.70	1.46	1.51
23	b	610	CLA	CHC-C1C	2.69	1.41	1.35
23	c	504	CLA	C1D-ND	2.69	1.41	1.37
23	c	503	CLA	CHC-C1C	2.68	1.41	1.35
23	C	505	CLA	C4D-ND	-2.68	1.34	1.37
23	C	504	CLA	C4D-ND	-2.68	1.34	1.37
23	b	604	CLA	C1D-ND	2.67	1.41	1.37
26	D	406	PL9	C11-C12	-2.67	1.44	1.53
33	E	101	LHG	O8-C23	2.67	1.41	1.33
23	B	601	CLA	CHC-C1C	2.67	1.41	1.35
24	a	407	PHO	C3B-C2B	-2.67	1.36	1.40
23	c	507	CLA	CMB-C2B	-2.66	1.46	1.51
23	d	404	CLA	C1D-ND	2.66	1.41	1.37
23	B	609	CLA	C4D-ND	-2.66	1.34	1.37
23	b	609	CLA	C3B-C2B	-2.66	1.36	1.40
23	D	404	CLA	MG-ND	-2.65	2.00	2.05
23	B	604	CLA	MG-ND	-2.65	2.00	2.05
23	A	411	CLA	MG-NC	2.65	2.12	2.06
28	A	412	SQD	O47-C7	2.65	1.41	1.34
23	B	615	CLA	CHC-C1C	2.64	1.41	1.35
23	b	608	CLA	CMD-C2D	-2.64	1.45	1.50
33	L	101	LHG	O7-C5	-2.64	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	515	BCR	C33-C5	-2.63	1.46	1.50
23	a	408	CLA	C4D-ND	-2.63	1.34	1.37
23	b	612	CLA	C4B-CHC	-2.63	1.33	1.41
25	D	405	8CT	C35-C30	-2.62	1.49	1.56
23	b	611	CLA	C3B-CAB	-2.62	1.42	1.47
23	B	613	CLA	CMB-C2B	-2.62	1.46	1.51
25	A	408	8CT	C01-C02	-2.62	1.46	1.50
25	B	617	8CT	C01-C02	-2.62	1.46	1.50
23	a	406	CLA	MG-ND	2.62	2.11	2.05
27	D	411	LMG	O8-C28	2.61	1.41	1.33
29	H	102	DGD	C3E-C2E	2.61	1.59	1.52
23	b	607	CLA	C3B-C2B	-2.61	1.36	1.40
27	b	623	LMG	C3-C2	2.61	1.59	1.52
23	c	502	CLA	CHC-C1C	2.61	1.41	1.35
23	d	404	CLA	CMD-C2D	-2.61	1.45	1.50
23	b	614	CLA	C4D-ND	-2.61	1.34	1.37
23	b	611	CLA	CHC-C1C	2.61	1.41	1.35
23	b	609	CLA	CMB-C2B	-2.60	1.46	1.51
23	C	505	CLA	CMB-C2B	-2.60	1.46	1.51
27	A	410	LMG	C4-C3	2.60	1.58	1.52
23	b	603	CLA	C1D-ND	2.60	1.41	1.37
23	D	404	CLA	CMB-C2B	-2.60	1.46	1.51
24	D	402	PHO	CMD-C2D	-2.60	1.45	1.51
33	B	623	LHG	O7-C5	-2.60	1.40	1.46
23	C	511	CLA	CMC-C2C	-2.60	1.45	1.50
25	B	619	8CT	C35-C30	-2.60	1.49	1.56
23	A	411	CLA	CMB-C2B	-2.60	1.46	1.51
23	b	611	CLA	CMB-C2B	-2.59	1.46	1.51
23	B	601	CLA	C3B-C2B	-2.59	1.36	1.40
23	b	614	CLA	CMB-C2B	-2.58	1.46	1.51
23	A	405	CLA	C1B-NB	2.58	1.37	1.35
23	b	606	CLA	C1D-ND	2.58	1.41	1.37
27	C	519	LMG	C4-C3	2.58	1.58	1.52
25	b	620	8CT	C35-C30	-2.57	1.49	1.56
23	B	604	CLA	CHC-C1C	2.57	1.41	1.35
23	B	613	CLA	C3B-CAB	-2.56	1.42	1.47
23	C	509	CLA	MG-NC	2.56	2.12	2.06
23	b	616	CLA	CMC-C2C	-2.56	1.45	1.50
33	D	409	LHG	C24-C23	2.55	1.58	1.50
23	C	513	CLA	CHC-C1C	2.55	1.41	1.35
23	d	402	CLA	C1D-ND	2.55	1.40	1.37
24	a	407	PHO	CMB-C2B	-2.55	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	524	LMG	C7-C8	2.54	1.58	1.50
29	A	414	DGD	C6D-C5D	2.54	1.59	1.51
31	c	521	BCR	C1-C6	-2.53	1.50	1.53
28	D	408	SQD	O2-C2	-2.53	1.37	1.43
23	a	406	CLA	MG-NA	2.53	2.12	2.06
25	B	617	8CT	C30-C29	-2.52	1.46	1.50
24	A	406	PHO	CMD-C2D	-2.52	1.45	1.51
23	d	403	CLA	C4D-ND	-2.52	1.34	1.37
29	c	516	DGD	C4D-C3D	2.52	1.58	1.52
23	b	612	CLA	C3B-C2B	-2.52	1.36	1.40
23	b	610	CLA	CMB-C2B	-2.52	1.46	1.51
29	C	516	DGD	C4D-C3D	2.52	1.58	1.52
23	c	502	CLA	CMC-C2C	-2.52	1.45	1.50
23	A	405	CLA	CMB-C2B	-2.51	1.46	1.51
23	b	617	CLA	CMD-C2D	-2.51	1.45	1.50
25	C	520	8CT	C35-C30	-2.51	1.49	1.56
23	C	501	CLA	CMD-C2D	-2.51	1.45	1.50
23	B	610	CLA	CMB-C2B	-2.51	1.46	1.51
23	c	509	CLA	MG-NC	2.51	2.12	2.06
25	C	514	8CT	C35-C30	-2.51	1.49	1.56
27	c	519	LMG	C1-C2	2.50	1.59	1.52
25	d	405	8CT	C35-C30	-2.50	1.49	1.56
29	A	414	DGD	C6E-C5E	2.50	1.60	1.51
23	b	612	CLA	C1D-ND	2.50	1.40	1.37
23	B	610	CLA	C1D-ND	2.50	1.40	1.37
23	B	616	CLA	CMD-C2D	-2.50	1.45	1.50
23	b	604	CLA	CMB-C2B	-2.49	1.46	1.51
28	f	101	SQD	O2-C2	-2.49	1.37	1.43
25	k	101	8CT	C35-C30	-2.49	1.49	1.56
23	b	608	CLA	C3B-CAB	-2.48	1.42	1.47
23	C	508	CLA	CMB-C2B	-2.48	1.46	1.51
23	B	615	CLA	C4B-CHC	-2.48	1.34	1.41
23	C	507	CLA	CMB-C2B	-2.47	1.46	1.51
26	D	406	PL9	C7-C3	-2.47	1.48	1.51
29	c	518	DGD	O5D-C1E	2.47	1.44	1.40
23	c	508	CLA	CMD-C2D	-2.47	1.45	1.50
23	B	609	CLA	CHC-C1C	2.47	1.41	1.35
33	D	409	LHG	O7-C5	-2.47	1.40	1.46
31	a	409	BCR	C33-C5	-2.47	1.46	1.50
23	c	502	CLA	CMD-C2D	-2.47	1.45	1.50
23	b	606	CLA	C4B-CHC	-2.47	1.34	1.41
23	c	508	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	C1D-C2D	2.47	1.59	1.52
23	B	605	CLA	C1D-ND	2.46	1.40	1.37
23	c	501	CLA	CAC-C3C	-2.46	1.44	1.51
25	C	515	8CT	C35-C30	-2.46	1.49	1.56
28	D	408	SQD	O3-C3	-2.46	1.37	1.43
23	C	509	CLA	CMB-C2B	-2.46	1.46	1.51
23	b	608	CLA	C1D-ND	2.46	1.40	1.37
28	a	411	SQD	O47-C7	2.45	1.41	1.34
24	d	401	PHO	CMD-C2D	-2.45	1.45	1.51
26	D	406	PL9	C52-C5	-2.45	1.45	1.50
23	D	403	CLA	C3B-C2B	-2.45	1.37	1.40
23	b	604	CLA	CMC-C2C	-2.45	1.45	1.50
28	a	411	SQD	O3-C3	-2.44	1.37	1.43
29	h	102	DGD	C1E-C2E	2.44	1.59	1.52
23	b	616	CLA	O2D-CGD	2.44	1.39	1.33
23	C	513	CLA	C4B-CHC	-2.44	1.34	1.41
29	c	517	DGD	C4D-C3D	2.44	1.58	1.52
23	c	501	CLA	C4D-ND	-2.44	1.34	1.37
28	f	101	SQD	O3-C3	-2.44	1.37	1.43
23	b	608	CLA	CMB-C2B	-2.43	1.46	1.51
25	C	520	8CT	C04-C03	-2.43	1.50	1.53
23	B	614	CLA	C3B-C2B	-2.43	1.37	1.40
23	b	607	CLA	CAC-C3C	-2.43	1.44	1.51
23	B	605	CLA	C3B-C2B	-2.43	1.37	1.40
23	b	616	CLA	CMB-C2B	-2.43	1.46	1.51
24	d	401	PHO	CMC-C2C	-2.43	1.45	1.51
29	o	301	DGD	O2G-C1B	2.43	1.41	1.34
23	A	407	CLA	CHC-C1C	2.42	1.41	1.35
27	c	519	LMG	C4-C5	2.42	1.58	1.53
27	B	620	LMG	O6-C1	2.42	1.48	1.41
23	b	602	CLA	O2A-CGA	2.42	1.40	1.33
25	C	520	8CT	C30-C29	-2.42	1.46	1.50
23	a	408	CLA	C1C-NC	-2.42	1.34	1.37
33	D	409	LHG	O6-C4	-2.41	1.35	1.44
23	c	506	CLA	C3B-CAB	-2.41	1.43	1.47
23	b	609	CLA	CMD-C2D	-2.41	1.45	1.50
23	C	503	CLA	C1D-C2D	2.41	1.50	1.45
23	b	615	CLA	MG-NC	2.40	2.12	2.06
29	C	517	DGD	C4D-C5D	2.40	1.58	1.53
23	b	605	CLA	C3B-CAB	-2.40	1.43	1.47
23	B	611	CLA	CMD-C2D	-2.40	1.45	1.50
23	B	611	CLA	C3B-C2B	-2.40	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C4B-CHC	-2.40	1.34	1.41
23	d	402	CLA	CMD-C2D	-2.40	1.45	1.50
23	c	508	CLA	CMC-C2C	-2.40	1.45	1.50
23	b	602	CLA	C1B-NB	2.40	1.37	1.35
27	c	519	LMG	O2-C2	-2.40	1.37	1.43
29	o	301	DGD	C1G-C2G	2.39	1.58	1.50
29	h	102	DGD	C4E-C5E	2.39	1.58	1.53
23	A	404	CLA	C5-C3	-2.39	1.46	1.51
28	a	411	SQD	O2-C2	-2.39	1.37	1.43
23	a	408	CLA	C3D-C4D	2.39	1.49	1.44
23	B	609	CLA	C4B-CHC	-2.39	1.34	1.41
23	B	613	CLA	CHC-C1C	2.39	1.41	1.35
23	c	511	CLA	MG-ND	-2.38	2.01	2.05
23	C	512	CLA	CMB-C2B	-2.38	1.46	1.51
23	A	411	CLA	CMC-C2C	-2.38	1.45	1.50
35	e	102	HEM	C3B-C2B	-2.38	1.32	1.37
23	b	607	CLA	CMB-C2B	-2.38	1.46	1.51
23	B	616	CLA	C3B-C2B	-2.38	1.37	1.40
23	b	614	CLA	MG-NC	2.37	2.11	2.06
23	c	505	CLA	CMB-C2B	-2.37	1.46	1.51
29	C	516	DGD	C2B-C1B	-2.37	1.43	1.50
23	c	504	CLA	CMD-C2D	-2.36	1.45	1.50
28	A	412	SQD	O3-C3	-2.36	1.37	1.43
23	b	610	CLA	CMA-C3A	-2.36	1.48	1.53
26	d	406	PL9	C46-C44	-2.36	1.46	1.51
27	D	411	LMG	C30-C29	2.35	1.60	1.52
23	B	609	CLA	CMD-C2D	-2.35	1.45	1.50
23	B	616	CLA	CMC-C2C	-2.35	1.45	1.50
29	h	102	DGD	O3G-C1D	2.34	1.44	1.40
25	C	515	8CT	C01-C02	-2.34	1.47	1.50
27	d	410	LMG	C4-C3	2.34	1.58	1.52
23	B	614	CLA	C1D-ND	2.34	1.40	1.37
23	B	603	CLA	C3B-CAB	-2.34	1.43	1.47
24	A	406	PHO	C1C-NC	-2.34	1.31	1.38
23	A	407	CLA	C4B-CHC	-2.33	1.34	1.41
23	c	503	CLA	C3B-CAB	-2.33	1.43	1.47
23	c	501	CLA	CMD-C2D	-2.33	1.45	1.50
23	B	615	CLA	C4D-ND	-2.33	1.34	1.37
25	d	405	8CT	C30-C29	-2.33	1.46	1.50
29	c	516	DGD	C6D-C5D	2.33	1.58	1.51
31	H	101	BCR	C33-C5	-2.32	1.47	1.50
23	a	405	CLA	CMB-C2B	-2.32	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	517	DGD	C1G-C2G	2.32	1.57	1.50
23	b	608	CLA	C4D-ND	-2.31	1.34	1.37
23	c	502	CLA	C1D-ND	2.31	1.40	1.37
23	B	604	CLA	C3C-C2C	2.31	1.41	1.36
23	A	404	CLA	O2D-CGD	2.30	1.38	1.33
26	D	406	PL9	C10-C9	-2.30	1.44	1.50
27	d	410	LMG	O6-C5	-2.30	1.38	1.44
23	c	505	CLA	CMC-C2C	-2.30	1.45	1.50
23	B	616	CLA	CMB-C2B	-2.30	1.46	1.51
25	C	515	8CT	C22-C21	-2.30	1.46	1.50
23	C	501	CLA	CMB-C2B	-2.30	1.46	1.51
23	d	404	CLA	C3B-CAB	-2.29	1.43	1.47
23	B	611	CLA	C4B-CHC	-2.29	1.34	1.41
27	b	621	LMG	O7-C8	-2.29	1.40	1.46
24	a	407	PHO	CAC-C3C	-2.29	1.48	1.52
23	b	615	CLA	CMB-C2B	-2.29	1.46	1.51
23	b	611	CLA	CMD-C2D	-2.29	1.46	1.50
23	b	615	CLA	C1D-ND	2.28	1.40	1.37
23	b	616	CLA	C4D-ND	-2.28	1.34	1.37
23	B	608	CLA	C1D-ND	2.28	1.40	1.37
23	a	406	CLA	CMB-C2B	-2.28	1.46	1.51
23	B	613	CLA	CMC-C2C	-2.28	1.46	1.50
23	B	608	CLA	C3B-C2B	-2.28	1.37	1.40
23	b	614	CLA	C4B-CHC	-2.28	1.34	1.41
23	B	604	CLA	C3B-CAB	-2.28	1.43	1.47
23	C	512	CLA	CMD-C2D	-2.28	1.46	1.50
23	D	403	CLA	MG-ND	-2.28	2.01	2.05
27	c	519	LMG	C7-C8	2.28	1.57	1.50
23	B	610	CLA	CMD-C2D	-2.27	1.46	1.50
27	D	411	LMG	O8-C9	2.27	1.50	1.45
27	b	623	LMG	C1-C2	2.27	1.59	1.52
26	D	406	PL9	C25-C24	-2.27	1.44	1.50
23	a	405	CLA	C4D-ND	-2.27	1.34	1.37
23	b	602	CLA	C3B-CAB	-2.27	1.43	1.47
29	o	301	DGD	C2B-C1B	2.27	1.57	1.50
23	c	501	CLA	C1D-ND	2.27	1.40	1.37
23	b	611	CLA	C1C-NC	-2.27	1.34	1.37
23	B	609	CLA	CMC-C2C	-2.27	1.46	1.50
23	B	612	CLA	C1D-ND	2.26	1.40	1.37
29	c	517	DGD	C4E-C3E	2.26	1.58	1.52
23	B	612	CLA	CMC-C2C	-2.26	1.46	1.50
23	C	512	CLA	C3B-CAB	-2.26	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1D-ND	2.26	1.40	1.37
23	B	614	CLA	CMB-C2B	-2.25	1.47	1.51
27	c	522	LMG	C1-C2	2.25	1.59	1.52
23	B	602	CLA	CMB-C2B	-2.25	1.47	1.51
23	A	411	CLA	CMD-C2D	-2.25	1.46	1.50
23	a	405	CLA	MG-NC	2.25	2.11	2.06
23	A	404	CLA	C4D-ND	-2.25	1.34	1.37
23	c	512	CLA	CMD-C2D	-2.25	1.46	1.50
33	E	101	LHG	O7-C5	-2.25	1.41	1.46
27	A	410	LMG	C1-C2	2.24	1.59	1.52
29	h	102	DGD	O2D-C2D	-2.24	1.37	1.43
27	c	522	LMG	C3-C2	2.24	1.58	1.52
23	c	507	CLA	CMC-C2C	-2.24	1.46	1.50
23	c	512	CLA	CMB-C2B	-2.24	1.47	1.51
23	c	512	CLA	C3B-CAB	-2.24	1.43	1.47
23	A	404	CLA	O2D-CED	-2.24	1.40	1.45
23	C	508	CLA	C1D-C2D	2.24	1.49	1.45
26	D	406	PL9	C53-C6	-2.24	1.46	1.50
23	B	616	CLA	CHC-C1C	2.23	1.40	1.35
24	A	406	PHO	O2D-CGD	2.23	1.38	1.33
31	T	101	BCR	C27-C26	-2.23	1.46	1.51
23	C	509	CLA	CHC-C1C	2.23	1.40	1.35
23	B	603	CLA	C3B-C2B	-2.23	1.37	1.40
29	c	517	DGD	C6E-C5E	2.23	1.59	1.51
23	A	407	CLA	CAC-C3C	-2.22	1.45	1.51
23	b	612	CLA	CHC-C1C	2.22	1.40	1.35
23	B	603	CLA	CMB-C2B	-2.22	1.47	1.51
23	B	603	CLA	CMD-C2D	-2.22	1.46	1.50
23	B	605	CLA	C1C-NC	-2.21	1.34	1.37
23	a	408	CLA	CHC-C1C	2.21	1.40	1.35
23	B	609	CLA	O2D-CGD	2.21	1.38	1.33
23	c	506	CLA	C3B-C2B	-2.21	1.37	1.40
23	b	616	CLA	MG-ND	-2.21	2.01	2.05
29	C	517	DGD	O5D-C6D	-2.21	1.39	1.43
29	c	516	DGD	O3G-C3G	-2.21	1.39	1.43
33	e	101	LHG	P-O6	2.21	1.68	1.59
29	c	516	DGD	O1G-C1G	-2.20	1.40	1.45
29	H	102	DGD	O6E-C1E	2.20	1.47	1.41
23	c	510	CLA	MG-NA	2.20	2.11	2.06
23	c	502	CLA	C4B-CHC	-2.20	1.34	1.41
23	c	504	CLA	CMB-C2B	-2.20	1.47	1.51
23	b	602	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C3B-CAB	-2.19	1.43	1.47
23	d	403	CLA	C3B-C2B	-2.19	1.37	1.40
23	b	604	CLA	C1B-NB	2.19	1.37	1.35
23	A	411	CLA	MG-ND	-2.19	2.01	2.05
23	B	606	CLA	CMB-C2B	-2.19	1.47	1.51
27	A	410	LMG	O1-C7	-2.19	1.39	1.43
28	B	624	SQD	O2-C2	-2.19	1.37	1.43
24	D	402	PHO	C3B-C2B	-2.19	1.37	1.40
23	B	612	CLA	MG-NA	2.18	2.11	2.06
29	h	102	DGD	O3G-C3G	-2.18	1.39	1.43
31	b	619	BCR	C4-C5	-2.18	1.46	1.51
23	b	611	CLA	C3D-C4D	2.18	1.49	1.44
24	A	406	PHO	CMC-C2C	-2.18	1.46	1.51
23	B	616	CLA	C4B-CHC	-2.18	1.34	1.41
23	B	611	CLA	CMB-C2B	-2.18	1.47	1.51
23	C	504	CLA	MG-NC	-2.17	2.01	2.06
25	c	514	8CT	C35-C30	-2.17	1.50	1.56
24	a	407	PHO	C3B-CAB	-2.17	1.43	1.47
23	c	505	CLA	C3B-CAB	-2.17	1.43	1.47
29	C	518	DGD	C4D-C5D	2.17	1.57	1.53
23	d	403	CLA	CMC-C2C	-2.16	1.46	1.50
26	A	409	PL9	C25-C24	-2.16	1.45	1.50
23	C	510	CLA	CMB-C2B	-2.16	1.47	1.51
27	B	622	LMG	O8-C28	2.16	1.38	1.30
23	A	405	CLA	CHC-C1C	2.16	1.40	1.35
23	c	506	CLA	CMC-C2C	-2.15	1.46	1.50
23	b	604	CLA	MG-NA	2.15	2.11	2.06
23	C	511	CLA	CMD-C2D	-2.15	1.46	1.50
23	C	511	CLA	C3B-C2B	-2.15	1.37	1.40
25	B	617	8CT	C35-C30	-2.15	1.50	1.56
27	c	522	LMG	C4-C3	2.15	1.57	1.52
23	d	404	CLA	CMC-C2C	-2.15	1.46	1.50
23	C	504	CLA	C1D-ND	2.14	1.40	1.37
23	c	511	CLA	C3C-C2C	2.14	1.41	1.36
23	b	612	CLA	CMD-C2D	-2.14	1.46	1.50
29	C	517	DGD	C6D-C5D	2.14	1.58	1.51
23	B	610	CLA	C3D-C4D	2.14	1.49	1.44
23	D	404	CLA	C4D-ND	-2.14	1.34	1.37
26	A	409	PL9	C7-C3	-2.13	1.49	1.51
23	B	616	CLA	C4D-ND	-2.13	1.34	1.37
33	E	101	LHG	C24-C23	2.13	1.56	1.50
29	H	102	DGD	C6E-C5E	2.13	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C5-C3	-2.13	1.46	1.51
24	a	407	PHO	C1C-NC	-2.13	1.32	1.38
23	b	615	CLA	C1B-NB	-2.13	1.33	1.35
23	D	404	CLA	CHC-C1C	2.12	1.40	1.35
23	d	402	CLA	CMB-C2B	-2.12	1.47	1.51
27	A	410	LMG	C4-C5	2.12	1.57	1.53
23	A	405	CLA	CAC-C3C	-2.12	1.45	1.51
23	b	616	CLA	CMD-C2D	-2.12	1.46	1.50
23	C	507	CLA	CMD-C2D	-2.12	1.46	1.50
23	C	506	CLA	CAA-C2A	-2.12	1.50	1.54
23	b	602	CLA	C1D-C2D	2.12	1.49	1.45
23	B	608	CLA	C3B-CAB	-2.11	1.43	1.47
23	c	505	CLA	C3C-C2C	2.11	1.41	1.36
25	k	101	8CT	C01-C02	-2.11	1.47	1.50
23	B	608	CLA	O2D-CED	-2.11	1.40	1.45
23	B	616	CLA	C3B-CAB	-2.10	1.43	1.47
23	B	608	CLA	CMA-C3A	-2.10	1.48	1.53
23	a	405	CLA	CMC-C2C	-2.10	1.46	1.50
23	C	504	CLA	CMD-C2D	-2.10	1.46	1.50
25	A	408	8CT	C35-C30	-2.10	1.50	1.56
23	B	602	CLA	C4B-CHC	-2.10	1.35	1.41
36	v	201	HEC	CMD-C2D	2.10	1.56	1.51
23	a	408	CLA	CMB-C2B	-2.10	1.47	1.51
35	e	102	HEM	C4A-CHB	-2.10	1.35	1.41
23	b	605	CLA	MG-NA	2.10	2.11	2.06
23	C	503	CLA	CMB-C2B	-2.10	1.47	1.51
25	d	405	8CT	C01-C02	-2.09	1.47	1.50
23	C	501	CLA	C3D-C4D	2.09	1.48	1.44
23	D	404	CLA	C3B-C2B	-2.09	1.37	1.40
23	b	614	CLA	CMD-C2D	-2.09	1.46	1.50
23	B	611	CLA	C3B-CAB	-2.09	1.43	1.47
23	b	605	CLA	CMD-C2D	-2.09	1.46	1.50
29	c	518	DGD	O4E-C4E	-2.09	1.38	1.43
23	c	501	CLA	CMB-C2B	-2.08	1.47	1.51
26	D	406	PL9	C35-C34	-2.08	1.45	1.50
23	C	502	CLA	CMC-C2C	-2.08	1.46	1.50
23	c	509	CLA	CMB-C2B	-2.08	1.47	1.51
23	c	507	CLA	C4B-CHC	-2.08	1.35	1.41
36	V	201	HEC	C2A-C1A	2.08	1.47	1.42
23	b	602	CLA	C4D-ND	-2.08	1.34	1.37
26	d	406	PL9	C53-C6	-2.08	1.46	1.50
23	c	507	CLA	MG-NA	2.08	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	T	101	BCR	C38-C26	-2.08	1.47	1.50
23	b	615	CLA	CMC-C2C	-2.07	1.46	1.50
29	c	517	DGD	O4E-C4E	-2.07	1.38	1.43
23	B	606	CLA	CMC-C2C	-2.07	1.46	1.50
23	A	405	CLA	CMC-C2C	-2.07	1.46	1.50
23	c	510	CLA	CMD-C2D	-2.07	1.46	1.50
27	c	519	LMG	O1-C1	2.07	1.43	1.40
23	A	404	CLA	C1D-ND	2.07	1.40	1.37
23	B	601	CLA	C1D-C2D	2.07	1.49	1.45
27	C	519	LMG	C7-C8	2.06	1.57	1.50
27	c	522	LMG	C4-C5	2.06	1.57	1.53
23	a	406	CLA	C1D-C2D	2.06	1.49	1.45
23	a	405	CLA	C1D-C2D	2.05	1.49	1.45
23	b	609	CLA	C4B-CHC	-2.05	1.35	1.41
23	a	406	CLA	CMD-C2D	-2.05	1.46	1.50
23	B	610	CLA	C4D-ND	-2.05	1.34	1.37
29	h	102	DGD	C6D-C5D	2.05	1.58	1.51
23	b	610	CLA	O2D-CGD	2.05	1.38	1.33
25	t	101	8CT	C35-C30	-2.05	1.50	1.56
23	C	508	CLA	C3B-CAB	-2.05	1.43	1.47
23	C	503	CLA	MG-ND	-2.05	2.01	2.05
23	B	602	CLA	MG-NC	2.04	2.11	2.06
23	B	604	CLA	C3B-C2B	-2.04	1.37	1.40
23	b	617	CLA	CAC-C3C	-2.04	1.45	1.51
23	B	603	CLA	CMC-C2C	-2.04	1.46	1.50
33	D	410	LHG	C3-C2	2.04	1.58	1.51
23	B	601	CLA	C4B-CHC	-2.04	1.35	1.41
29	H	102	DGD	C6D-C5D	2.04	1.58	1.51
23	C	511	CLA	C3B-CAB	-2.04	1.43	1.47
23	c	508	CLA	C3B-CAB	-2.04	1.43	1.47
23	b	602	CLA	CMB-C2B	-2.03	1.47	1.51
23	c	503	CLA	C1D-C2D	2.03	1.49	1.45
29	c	516	DGD	O4E-C4E	2.03	1.47	1.43
23	C	512	CLA	C1A-CHA	-2.03	1.34	1.43
33	d	407	LHG	O7-C5	-2.03	1.41	1.46
27	b	623	LMG	O1-C7	-2.03	1.40	1.43
29	h	102	DGD	O2G-C1B	2.03	1.40	1.34
23	b	603	CLA	CAC-C3C	-2.03	1.45	1.51
23	D	403	CLA	CMB-C2B	-2.03	1.47	1.51
28	b	601	SQD	O2-C2	-2.03	1.38	1.43
25	B	619	8CT	C39-C16	-2.03	1.46	1.50
23	B	613	CLA	C3B-C2B	-2.02	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	MG-NA	2.02	2.11	2.06
29	c	517	DGD	C3E-C2E	2.02	1.57	1.52
23	c	512	CLA	CMC-C2C	-2.02	1.46	1.50
23	C	502	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	508	CLA	MG-NA	2.02	2.11	2.06
23	B	604	CLA	CAA-C2A	-2.02	1.50	1.54
23	B	615	CLA	C1D-C2D	2.02	1.49	1.45
23	A	405	CLA	C3B-C2B	-2.02	1.37	1.40
23	c	511	CLA	CMB-C2B	-2.01	1.47	1.51
23	c	503	CLA	C3D-C4D	2.01	1.48	1.44
28	A	412	SQD	O47-C45	-2.01	1.41	1.46
23	B	604	CLA	CMA-C3A	-2.01	1.48	1.53
23	B	613	CLA	CMD-C2D	-2.01	1.46	1.50
23	c	506	CLA	MG-NA	2.01	2.11	2.06
33	d	409	LHG	O8-C23	2.01	1.39	1.33
31	b	618	BCR	C33-C5	-2.01	1.47	1.50
23	A	407	CLA	CMC-C2C	-2.00	1.46	1.50
23	c	510	CLA	C4B-CHC	-2.00	1.35	1.41
28	f	101	SQD	O4-C4	-2.00	1.38	1.43
23	B	611	CLA	CMA-C3A	-2.00	1.48	1.53
23	B	605	CLA	C4B-CHC	-2.00	1.35	1.41
23	A	404	CLA	CHC-C1C	2.00	1.40	1.35

All (1320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	405	8CT	C33-C32-C31	-14.89	110.57	124.85
25	C	514	8CT	C33-C32-C31	-13.80	111.62	124.85
25	B	617	8CT	C33-C32-C31	-13.56	111.85	124.85
25	t	101	8CT	C33-C32-C31	-13.35	112.05	124.85
25	d	405	8CT	C33-C32-C31	-12.71	112.67	124.85
25	C	520	8CT	C33-C32-C31	-12.59	112.78	124.85
25	B	619	8CT	C33-C32-C31	-12.29	113.07	124.85
25	k	101	8CT	C33-C32-C31	-12.07	113.28	124.85
25	A	408	8CT	C33-C32-C31	-11.80	113.54	124.85
25	c	514	8CT	C33-C32-C31	-11.41	113.91	124.85
25	b	620	8CT	C33-C32-C31	-11.30	114.01	124.85
25	C	515	8CT	C33-C32-C31	-10.59	114.70	124.85
28	A	412	SQD	O6-C1-C2	10.15	124.16	108.30
23	B	604	CLA	C4A-NA-C1A	9.89	111.15	106.71
23	c	502	CLA	C4A-NA-C1A	9.44	110.95	106.71
23	B	601	CLA	C4A-NA-C1A	8.80	110.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	C4A-NA-C1A	8.64	110.59	106.71
28	b	601	SQD	O6-C1-C2	8.43	121.46	108.30
28	a	411	SQD	O6-C1-C2	8.31	121.28	108.30
26	A	409	PL9	C7-C3-C4	8.18	123.53	116.88
23	A	405	CLA	C4A-NA-C1A	8.14	110.37	106.71
23	C	501	CLA	C4A-NA-C1A	8.10	110.35	106.71
23	b	607	CLA	C4A-NA-C1A	7.91	110.26	106.71
23	c	511	CLA	C4A-NA-C1A	7.90	110.26	106.71
23	c	503	CLA	C4A-NA-C1A	7.76	110.20	106.71
23	B	616	CLA	C4A-NA-C1A	7.56	110.10	106.71
23	B	606	CLA	C4A-NA-C1A	7.41	110.04	106.71
23	C	511	CLA	C4A-NA-C1A	7.32	110.00	106.71
23	C	510	CLA	C4A-NA-C1A	7.27	109.97	106.71
23	B	613	CLA	C4A-NA-C1A	7.02	109.86	106.71
23	d	402	CLA	C4A-NA-C1A	6.98	109.85	106.71
28	A	412	SQD	O7-S-C6	6.93	115.18	106.94
23	C	513	CLA	C4A-NA-C1A	6.91	109.81	106.71
23	B	608	CLA	C4A-NA-C1A	6.88	109.80	106.71
23	a	406	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	d	403	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	c	510	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	b	612	CLA	CHD-C1D-ND	-6.61	118.38	124.45
26	a	410	PL9	C7-C3-C4	6.58	122.22	116.88
23	B	612	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	b	605	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	C	506	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	a	405	CLA	C4A-NA-C1A	6.46	109.61	106.71
23	c	507	CLA	C4A-NA-C1A	6.09	109.45	106.71
25	C	514	8CT	C35-C30-C31	6.00	122.17	111.42
23	C	503	CLA	C4A-NA-C1A	5.97	109.39	106.71
23	c	509	CLA	C4A-NA-C1A	5.94	109.38	106.71
23	c	504	CLA	C4A-NA-C1A	5.91	109.36	106.71
23	A	404	CLA	C4A-NA-C1A	5.91	109.36	106.71
23	B	609	CLA	C4A-NA-C1A	5.88	109.35	106.71
23	b	606	CLA	C4A-NA-C1A	5.83	109.33	106.71
23	C	509	CLA	C4A-NA-C1A	5.78	109.30	106.71
35	e	102	HEM	CBA-CAA-C2A	-5.75	102.81	112.62
25	D	405	8CT	C35-C30-C31	5.73	121.69	111.42
25	A	408	8CT	C35-C30-C31	5.71	121.65	111.42
26	d	406	PL9	C7-C3-C4	5.69	121.50	116.88
28	a	412	SQD	O47-C7-C8	5.52	123.41	111.50
25	b	620	8CT	C35-C30-C31	5.51	121.29	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	407	CLA	CMB-C2B-C1B	-5.50	120.00	128.46
23	c	513	CLA	C4A-NA-C1A	5.45	109.15	106.71
28	B	624	SQD	O7-S-C6	5.43	113.39	106.94
23	b	617	CLA	C4A-NA-C1A	5.43	109.15	106.71
25	C	515	8CT	C35-C30-C31	5.41	121.10	111.42
25	C	520	8CT	C35-C30-C31	5.39	121.07	111.42
25	B	619	8CT	C35-C30-C31	5.33	120.96	111.42
23	B	614	CLA	O2D-CGD-O1D	-5.29	113.49	123.84
23	b	615	CLA	CMB-C2B-C1B	-5.25	120.40	128.46
28	A	413	SQD	C45-O47-C7	5.21	124.58	117.88
23	c	510	CLA	O2D-CGD-CBD	5.18	120.47	111.27
23	B	612	CLA	CMB-C2B-C1B	-5.16	120.53	128.46
23	b	603	CLA	O2D-CGD-O1D	-5.16	113.75	123.84
25	c	514	8CT	C35-C30-C29	5.16	119.22	112.70
23	b	604	CLA	O2D-CGD-O1D	-5.15	113.76	123.84
23	c	512	CLA	C4A-NA-C1A	5.13	109.01	106.71
23	c	501	CLA	O2D-CGD-O1D	-5.09	113.88	123.84
23	b	617	CLA	O2D-CGD-O1D	-5.09	113.89	123.84
25	t	101	8CT	C35-C30-C31	5.03	120.43	111.42
23	b	613	CLA	CMB-C2B-C1B	-5.03	120.73	128.46
28	B	624	SQD	O6-C1-C2	5.00	116.11	108.30
26	D	406	PL9	C7-C3-C4	4.98	120.93	116.88
25	B	619	8CT	C35-C30-C29	4.97	118.99	112.70
23	c	510	CLA	O2D-CGD-O1D	-4.97	114.11	123.84
25	c	514	8CT	C30-C31-C32	4.97	127.58	121.47
28	f	101	SQD	O9-S-C6	4.90	112.76	106.94
23	b	603	CLA	O2D-CGD-CBD	4.87	119.92	111.27
25	d	405	8CT	C35-C30-C29	4.87	118.85	112.70
23	B	610	CLA	O2D-CGD-O1D	-4.84	114.37	123.84
28	D	408	SQD	O8-S-C6	4.81	113.41	105.74
23	B	607	CLA	C4A-NA-C1A	4.81	108.87	106.71
23	b	603	CLA	C4A-NA-C1A	4.78	108.86	106.71
23	c	501	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
23	C	504	CLA	CMB-C2B-C1B	-4.72	121.20	128.46
28	a	411	SQD	O8-S-C6	4.72	113.26	105.74
23	C	507	CLA	C4A-NA-C1A	4.72	108.83	106.71
23	B	610	CLA	CHD-C1D-ND	-4.72	120.12	124.45
25	k	101	8CT	C35-C30-C31	4.69	119.82	111.42
23	b	615	CLA	CMB-C2B-C3B	4.68	133.44	124.68
28	A	412	SQD	C1-C2-C3	-4.68	100.25	110.00
29	C	517	DGD	O3G-C3G-C2G	-4.68	99.61	110.90
23	B	607	CLA	CMB-C2B-C1B	-4.61	121.38	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	CHD-C1D-ND	-4.61	120.22	124.45
23	b	606	CLA	O2D-CGD-O1D	-4.60	114.84	123.84
25	d	405	8CT	C35-C30-C31	4.60	119.65	111.42
23	B	616	CLA	O2D-CGD-O1D	-4.59	114.86	123.84
24	d	401	PHO	O1D-CGD-CBD	4.57	132.35	124.74
23	c	501	CLA	O2D-CGD-CBD	4.56	119.36	111.27
23	b	604	CLA	C4A-NA-C1A	4.55	108.75	106.71
23	B	602	CLA	O2D-CGD-O1D	-4.54	114.95	123.84
29	H	102	DGD	O3G-C3G-C2G	-4.53	99.97	110.90
26	A	409	PL9	C7-C3-C2	-4.52	117.36	123.30
23	c	501	CLA	C4A-NA-C1A	4.47	108.72	106.71
23	C	503	CLA	CHD-C1D-ND	-4.47	120.35	124.45
23	a	408	CLA	C4A-NA-C1A	4.46	108.71	106.71
34	D	401	BCT	O2-C-O1	4.45	131.08	119.55
29	C	518	DGD	O3G-C3G-C2G	-4.43	100.21	110.90
23	C	513	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
26	a	410	PL9	C35-C34-C36	4.42	122.70	115.27
23	B	612	CLA	CMB-C2B-C3B	4.41	132.94	124.68
25	B	617	8CT	C35-C30-C31	4.40	119.30	111.42
23	c	507	CLA	CHD-C1D-ND	-4.40	120.42	124.45
23	b	613	CLA	CMB-C2B-C3B	4.38	132.87	124.68
23	A	404	CLA	CMB-C2B-C3B	4.38	132.87	124.68
23	B	610	CLA	C1B-CHB-C4A	-4.34	121.53	130.12
25	k	101	8CT	C30-C31-C32	4.34	126.80	121.47
29	A	414	DGD	C3G-C2G-C1G	-4.33	101.55	111.79
26	d	406	PL9	C40-C39-C41	4.32	122.54	115.27
25	A	408	8CT	C30-C31-C32	4.31	126.78	121.47
23	C	509	CLA	CMB-C2B-C1B	-4.29	121.87	128.46
23	C	508	CLA	O2D-CGD-O1D	-4.29	115.45	123.84
25	C	515	8CT	C35-C30-C29	4.28	118.11	112.70
23	b	607	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
23	A	407	CLA	CMB-C2B-C3B	4.27	132.68	124.68
23	b	602	CLA	O2D-CGD-O1D	-4.27	115.48	123.84
23	A	405	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
23	c	510	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
28	D	408	SQD	O9-S-C6	4.26	112.00	106.94
25	t	101	8CT	C30-C31-C32	4.24	126.69	121.47
25	C	520	8CT	C30-C31-C32	4.23	126.67	121.47
23	b	614	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
23	b	603	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
33	e	101	LHG	O4-P-O5	4.21	133.03	112.24
23	C	505	CLA	CMB-C2B-C1B	-4.19	122.03	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	515	8CT	C30-C31-C32	4.18	126.61	121.47
23	c	508	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
33	B	623	LHG	O4-P-O5	4.15	132.78	112.24
23	C	508	CLA	CHD-C1D-ND	-4.14	120.64	124.45
23	c	504	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
28	A	412	SQD	O9-S-O7	-4.12	99.68	113.95
23	c	509	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
23	B	615	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
23	b	614	CLA	C2C-C1C-NC	4.10	113.81	109.97
23	b	604	CLA	O2D-CGD-CBD	4.09	118.54	111.27
23	C	508	CLA	C4A-NA-C1A	4.09	108.55	106.71
23	B	608	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
33	d	409	LHG	O4-P-O5	4.09	132.44	112.24
25	C	514	8CT	C30-C31-C32	4.08	126.49	121.47
28	D	408	SQD	O6-C1-C2	4.08	114.68	108.30
23	b	613	CLA	C4A-NA-C1A	4.08	108.54	106.71
23	d	402	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
23	D	404	CLA	C1B-CHB-C4A	-4.07	122.06	130.12
23	b	610	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
23	A	411	CLA	C4A-NA-C1A	4.06	108.53	106.71
25	D	405	8CT	C35-C30-C29	4.06	117.83	112.70
23	B	610	CLA	CHB-C4A-NA	4.04	130.10	124.51
25	d	405	8CT	C30-C31-C32	4.04	126.43	121.47
23	C	509	CLA	CMB-C2B-C3B	4.03	132.22	124.68
25	t	101	8CT	C35-C30-C29	4.03	117.79	112.70
29	c	516	DGD	O3G-C3G-C2G	-4.03	101.18	110.90
25	c	514	8CT	C35-C30-C31	4.02	118.63	111.42
23	B	602	CLA	C4A-NA-C1A	4.02	108.52	106.71
28	f	101	SQD	O6-C1-C2	4.02	114.58	108.30
25	k	101	8CT	C35-C30-C29	4.02	117.78	112.70
23	c	512	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
23	c	509	CLA	CMB-C2B-C3B	4.01	132.18	124.68
23	b	603	CLA	CHB-C4A-NA	4.01	130.06	124.51
33	l	101	LHG	O4-P-O5	4.00	132.04	112.24
33	E	101	LHG	O4-P-O5	4.00	132.03	112.24
23	B	605	CLA	C16-C15-C13	-4.00	103.00	115.92
23	c	502	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
33	d	408	LHG	O4-P-O5	3.98	131.93	112.24
33	L	101	LHG	O4-P-O5	3.98	131.91	112.24
25	B	619	8CT	C37-C35-C34	-3.97	100.85	109.03
28	b	601	SQD	O9-S-C6	3.97	111.66	106.94
25	b	620	8CT	C35-C30-C29	3.97	117.72	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	624	SQD	O47-C7-C8	3.96	120.03	111.50
23	b	615	CLA	C4A-NA-C1A	3.96	108.49	106.71
33	D	410	LHG	O4-P-O5	3.95	131.78	112.24
23	c	501	CLA	CMB-C2B-C3B	3.95	132.07	124.68
23	C	505	CLA	CAC-C3C-C4C	3.92	129.89	124.81
23	C	512	CLA	C4A-NA-C1A	3.91	108.46	106.71
23	C	508	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	c	507	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
33	d	407	LHG	O4-P-O5	3.90	131.50	112.24
33	D	409	LHG	O4-P-O5	3.89	131.48	112.24
28	b	601	SQD	O7-S-C6	3.89	111.56	106.94
23	B	602	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
23	a	405	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
23	b	604	CLA	C4-C3-C5	3.89	121.81	115.27
28	b	601	SQD	O5-C5-C4	3.88	116.74	109.69
28	a	411	SQD	O47-C7-C8	3.88	119.85	111.50
28	b	601	SQD	C1-C2-C3	-3.86	101.95	110.00
23	B	610	CLA	C1D-ND-C4D	-3.86	103.60	106.33
28	A	412	SQD	O47-C7-C8	3.85	119.80	111.50
23	A	405	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
23	C	502	CLA	O2D-CGD-O1D	-3.85	116.32	123.84
27	b	621	LMG	O7-C10-O9	-3.84	114.41	123.70
23	A	407	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
23	c	501	CLA	CHD-C1D-ND	-3.84	120.93	124.45
23	b	617	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
23	b	610	CLA	C4A-NA-C1A	3.83	108.43	106.71
23	b	617	CLA	O1D-CGD-CBD	3.81	132.28	124.48
25	A	408	8CT	C35-C30-C29	3.81	117.52	112.70
23	b	616	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
34	a	404	BCT	O2-C-O1	3.80	129.41	119.55
28	a	411	SQD	O9-S-C6	3.80	111.45	106.94
23	A	404	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
23	a	406	CLA	O2D-CGD-CBD	3.78	117.98	111.27
23	B	609	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
23	B	602	CLA	CHB-C4A-NA	3.77	129.73	124.51
29	h	102	DGD	O2D-C2D-C1D	-3.76	100.91	110.05
29	h	102	DGD	O3G-C3G-C2G	-3.76	101.83	110.90
35	e	102	HEM	CBD-CAD-C3D	-3.75	102.22	112.63
23	d	403	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
25	B	617	8CT	C35-C30-C29	3.74	117.42	112.70
25	B	617	8CT	C30-C31-C32	3.74	126.06	121.47
23	b	617	CLA	C1B-CHB-C4A	-3.73	122.73	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CMB-C2B-C1B	-3.71	122.75	128.46
23	C	503	CLA	C7-C6-C5	-3.71	103.28	113.36
25	t	101	8CT	C38-C31-C32	-3.71	109.14	122.33
23	b	602	CLA	O2D-CGD-CBD	3.70	117.85	111.27
23	C	502	CLA	C4A-NA-C1A	3.70	108.37	106.71
23	B	612	CLA	C11-C12-C13	-3.69	103.99	115.92
23	B	605	CLA	CHD-C1D-ND	-3.69	121.06	124.45
23	b	609	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
23	B	614	CLA	O1D-CGD-CBD	3.68	132.02	124.48
24	A	406	PHO	CMA-C3A-C4A	-3.68	106.31	114.38
23	a	406	CLA	CMA-C3A-C4A	-3.68	101.88	111.77
23	B	605	CLA	C4A-NA-C1A	3.68	108.36	106.71
23	B	605	CLA	C4-C3-C5	3.67	121.45	115.27
28	B	624	SQD	C1-O5-C5	-3.67	106.48	113.69
23	c	508	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
23	B	602	CLA	O2D-CGD-CBD	3.67	117.78	111.27
31	b	618	BCR	C2-C1-C6	3.66	116.12	110.48
23	B	611	CLA	C4A-NA-C1A	3.64	108.34	106.71
23	B	614	CLA	C4A-NA-C1A	3.64	108.34	106.71
23	b	611	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
26	a	410	PL9	C7-C3-C2	-3.64	118.51	123.30
23	b	602	CLA	CHD-C1D-ND	-3.63	121.12	124.45
23	B	603	CLA	CMB-C2B-C3B	3.63	131.47	124.68
28	b	601	SQD	C3-C4-C5	3.63	116.72	110.24
23	C	502	CLA	CHD-C1D-ND	-3.63	121.12	124.45
25	C	520	8CT	C35-C30-C29	3.62	117.28	112.70
33	B	623	LHG	O8-C23-C24	3.62	123.27	111.91
23	d	402	CLA	CMB-C2B-C3B	3.61	131.43	124.68
23	B	605	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	b	602	CLA	C4A-NA-C1A	3.59	108.32	106.71
29	C	517	DGD	O5D-C1E-C2E	3.59	113.91	108.30
24	d	401	PHO	CMC-C2C-C3C	3.58	131.69	124.94
29	C	516	DGD	O3G-C3G-C2G	-3.57	102.28	110.90
23	b	612	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
23	B	607	CLA	CMB-C2B-C3B	3.56	131.35	124.68
23	C	512	CLA	CHB-C4A-NA	3.56	129.44	124.51
36	v	201	HEC	CMC-C2C-C1C	-3.56	122.99	128.46
31	c	515	BCR	C35-C13-C14	-3.56	117.94	122.92
24	a	407	PHO	C1-C2-C3	-3.55	119.89	126.04
23	c	503	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
23	c	511	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
25	B	619	8CT	C30-C31-C32	3.53	125.81	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	603	CLA	C4A-NA-C1A	3.53	108.29	106.71
23	B	612	CLA	O2A-CGA-O1A	-3.52	114.71	123.59
28	A	412	SQD	C1-O5-C5	-3.52	106.78	113.69
23	C	512	CLA	CMB-C2B-C3B	3.52	131.26	124.68
23	b	604	CLA	C1B-CHB-C4A	-3.52	123.15	130.12
23	B	613	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
23	c	506	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
23	c	507	CLA	CHB-C4A-NA	3.50	129.35	124.51
26	d	406	PL9	C7-C3-C2	-3.49	118.71	123.30
27	B	620	LMG	O1-C1-C2	-3.49	102.85	108.30
23	b	606	CLA	C1-C2-C3	-3.48	120.02	126.04
23	c	502	CLA	C4D-CHA-C1A	3.48	125.49	121.25
23	b	613	CLA	CHD-C1D-ND	-3.48	121.25	124.45
31	T	101	BCR	C38-C26-C27	-3.48	106.93	113.62
31	T	101	BCR	C27-C26-C25	3.47	127.77	122.73
23	B	609	CLA	CMB-C2B-C3B	3.47	131.17	124.68
25	B	617	8CT	C38-C31-C32	-3.47	110.00	122.33
23	C	510	CLA	O2D-CGD-CBD	3.47	117.43	111.27
25	b	620	8CT	C30-C31-C32	3.47	125.73	121.47
23	b	617	CLA	CMB-C2B-C3B	3.47	131.16	124.68
23	B	612	CLA	CHB-C4A-NA	3.46	129.30	124.51
25	C	515	8CT	C01-C02-C03	-3.46	120.65	124.53
23	B	610	CLA	O2A-CGA-O1A	-3.46	114.87	123.59
28	b	601	SQD	O48-C23-C24	3.45	122.74	111.91
23	b	604	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
23	c	506	CLA	CMB-C2B-C3B	3.45	131.13	124.68
28	a	411	SQD	O48-C23-C24	3.45	122.73	111.91
25	B	619	8CT	C05-C04-C03	3.44	115.78	110.48
23	A	411	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
23	b	606	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
25	c	514	8CT	C38-C31-C32	-3.44	110.09	122.33
23	A	405	CLA	CED-O2D-CGD	-3.44	108.17	115.94
23	b	609	CLA	CMB-C2B-C3B	3.44	131.10	124.68
23	a	406	CLA	C2D-C1D-ND	-3.43	107.57	110.10
23	b	603	CLA	CMB-C2B-C3B	3.43	131.10	124.68
23	B	613	CLA	CHB-C4A-NA	3.43	129.25	124.51
23	C	513	CLA	CMB-C2B-C3B	3.43	131.09	124.68
23	c	504	CLA	O2D-CGD-CBD	3.43	117.36	111.27
23	b	612	CLA	CHD-C1D-C2D	3.43	132.66	125.48
23	c	508	CLA	CMB-C2B-C3B	3.42	131.08	124.68
25	D	405	8CT	C30-C31-C32	3.42	125.67	121.47
23	d	403	CLA	O2D-CGD-O1D	-3.42	117.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	521	BCR	C27-C26-C25	3.41	127.69	122.73
23	C	513	CLA	CHD-C1D-ND	-3.40	121.33	124.45
23	b	603	CLA	C2D-C1D-ND	-3.40	107.60	110.10
23	b	606	CLA	O1D-CGD-CBD	3.40	131.44	124.48
23	A	411	CLA	CMB-C2B-C3B	3.40	131.03	124.68
26	d	406	PL9	C41-C39-C38	-3.39	114.25	121.12
23	c	512	CLA	CHB-C4A-NA	3.39	129.20	124.51
23	C	504	CLA	C4A-NA-C1A	3.39	108.23	106.71
23	c	510	CLA	CHB-C4A-NA	3.38	129.19	124.51
29	H	102	DGD	C1E-O6E-C5E	3.38	120.33	113.69
23	b	607	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
33	d	407	LHG	O8-C23-C24	3.36	122.44	111.91
23	B	615	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
36	V	201	HEC	CMC-C2C-C1C	-3.35	123.32	128.46
23	c	504	CLA	CMB-C2B-C3B	3.35	130.94	124.68
23	c	509	CLA	O2A-CGA-O1A	-3.34	115.15	123.59
23	B	615	CLA	C4A-NA-C1A	3.34	108.21	106.71
25	k	101	8CT	C38-C31-C32	-3.33	110.47	122.33
23	c	502	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
28	B	624	SQD	O5-C5-C4	3.33	115.74	109.69
25	C	520	8CT	C38-C31-C32	-3.33	110.50	122.33
23	D	403	CLA	CMB-C2B-C3B	3.32	130.89	124.68
25	B	617	8CT	C05-C04-C03	3.32	115.59	110.48
23	b	611	CLA	C1B-CHB-C4A	-3.31	123.55	130.12
23	B	607	CLA	CHD-C1D-ND	-3.31	121.41	124.45
23	D	403	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
23	C	504	CLA	C1-O2A-CGA	3.30	125.11	116.44
23	C	511	CLA	CAC-C3C-C4C	3.30	129.09	124.81
29	c	518	DGD	O3G-C3G-C2G	-3.30	102.94	110.90
23	b	605	CLA	C1-C2-C3	-3.30	120.34	126.04
26	d	406	PL9	C50-C49-C48	-3.29	113.13	122.65
24	d	401	PHO	CMB-C2B-C3B	3.29	130.84	124.68
23	C	513	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
28	A	412	SQD	O2-C2-C1	3.28	118.01	110.05
28	B	624	SQD	O8-S-C6	3.27	110.96	105.74
29	C	516	DGD	C3D-C4D-C5D	-3.27	104.41	110.24
23	B	601	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
25	t	101	8CT	C37-C35-C34	-3.26	102.31	109.03
23	c	504	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
33	d	409	LHG	C25-C24-C23	3.25	125.45	113.62
23	a	408	CLA	C1D-ND-C4D	-3.25	104.03	106.33
27	b	621	LMG	O6-C1-O1	-3.24	102.29	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	PL9	C37-C38-C39	-3.24	119.85	127.66
25	C	514	8CT	C35-C30-C29	3.24	116.80	112.70
29	C	516	DGD	O6D-C1D-O3G	-3.23	102.31	109.97
25	C	515	8CT	C38-C31-C32	-3.23	110.85	122.33
23	B	616	CLA	C1-O2A-CGA	3.22	124.89	116.44
23	b	609	CLA	CHD-C1D-ND	-3.22	121.50	124.45
23	D	403	CLA	CED-O2D-CGD	3.21	123.20	115.94
23	B	607	CLA	C1-C2-C3	-3.21	120.49	126.04
23	b	610	CLA	CMB-C2B-C3B	3.21	130.68	124.68
23	a	406	CLA	CHB-C4A-NA	3.21	128.94	124.51
23	a	406	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
23	b	605	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
23	B	616	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
23	c	502	CLA	CMB-C2B-C3B	3.20	130.66	124.68
27	c	524	LMG	C1-O6-C5	-3.19	107.42	113.69
23	B	601	CLA	O1D-CGD-CBD	3.19	131.01	124.48
23	C	504	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
29	H	102	DGD	C1D-O6D-C5D	-3.18	107.44	113.69
23	C	505	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
23	B	616	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
24	D	402	PHO	O1D-CGD-CBD	3.18	130.03	124.74
23	c	505	CLA	O2D-CGD-CBD	3.17	116.91	111.27
23	b	602	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
23	c	510	CLA	CMB-C2B-C3B	3.17	130.61	124.68
28	a	412	SQD	O48-C23-C24	3.17	121.85	111.91
29	A	414	DGD	C1D-C2D-C3D	-3.17	103.40	110.00
29	C	518	DGD	O3G-C1D-C2D	-3.17	103.36	108.30
23	B	615	CLA	CMB-C2B-C3B	3.16	130.60	124.68
33	E	101	LHG	O8-C23-C24	3.16	121.83	111.91
27	b	623	LMG	O1-C1-C2	-3.16	103.37	108.30
29	c	517	DGD	O3G-C3G-C2G	-3.15	103.29	110.90
23	A	404	CLA	CHB-C4A-NA	3.15	128.87	124.51
23	c	512	CLA	C1-C2-C3	-3.15	120.60	126.04
26	A	409	PL9	O2-C1-C2	-3.15	114.57	121.78
35	e	102	HEM	CHB-C1B-NB	3.14	128.26	124.38
36	V	201	HEC	CBD-CAD-C3D	-3.14	107.26	112.62
23	A	405	CLA	CHB-C4A-NA	3.14	128.85	124.51
23	C	509	CLA	CHB-C4A-NA	3.14	128.85	124.51
25	t	101	8CT	C39-C16-C17	-3.13	118.53	122.92
35	F	101	HEM	CHC-C4B-NB	3.13	127.84	124.43
25	A	408	8CT	C38-C31-C32	-3.13	111.19	122.33
23	A	407	CLA	CHD-C1D-ND	-3.13	121.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	618	BCR	C33-C5-C6	-3.13	121.02	124.53
23	a	406	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	A	405	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
28	a	411	SQD	O5-C1-C2	-3.12	103.74	110.35
23	C	505	CLA	CMB-C2B-C3B	3.12	130.51	124.68
23	C	507	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
28	B	624	SQD	O9-S-O7	-3.12	103.16	113.95
31	H	101	BCR	C29-C30-C25	3.12	115.28	110.48
29	H	102	DGD	O2D-C2D-C1D	-3.12	102.48	110.05
29	c	518	DGD	C3E-C4E-C5E	-3.12	104.68	110.24
23	B	603	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
23	B	604	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
23	c	507	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
24	D	402	PHO	CMB-C2B-C3B	3.11	130.50	124.68
26	d	406	PL9	C45-C44-C46	-3.11	110.04	115.27
23	b	605	CLA	CHB-C4A-NA	3.11	128.81	124.51
25	B	617	8CT	C37-C35-C34	-3.11	102.64	109.03
23	b	616	CLA	CHC-C1C-NC	3.10	128.91	124.20
23	b	614	CLA	CMB-C2B-C3B	3.10	130.48	124.68
23	B	610	CLA	O2D-CGD-CBD	3.10	116.77	111.27
23	D	403	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
23	b	611	CLA	CMB-C2B-C3B	3.09	130.46	124.68
31	a	409	BCR	C33-C5-C6	-3.09	121.06	124.53
23	B	602	CLA	CMB-C2B-C3B	3.09	130.45	124.68
23	C	509	CLA	C1-C2-C3	-3.08	120.71	126.04
23	C	503	CLA	C5-C3-C2	-3.08	114.89	121.12
31	b	619	BCR	C15-C14-C13	-3.08	122.92	127.31
23	B	603	CLA	C1D-ND-C4D	3.08	108.52	106.33
29	C	517	DGD	O5D-C6D-C5D	-3.07	103.36	109.05
25	b	620	8CT	C37-C35-C34	-3.07	102.71	109.03
23	C	504	CLA	CHD-C1D-ND	-3.07	121.64	124.45
23	C	505	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
28	f	101	SQD	O9-S-O7	-3.06	103.35	113.95
29	C	518	DGD	O3E-C3E-C2E	-3.06	103.28	110.35
23	b	612	CLA	CHB-C4A-NA	3.06	128.74	124.51
27	A	410	LMG	C1-O6-C5	-3.06	107.69	113.69
29	C	516	DGD	O1G-C1A-C2A	-3.05	102.33	111.91
23	d	403	CLA	CMB-C2B-C3B	3.05	130.38	124.68
31	a	409	BCR	C27-C26-C25	3.05	127.16	122.73
23	B	611	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	b	618	BCR	C15-C16-C17	-3.04	117.25	123.47
29	C	517	DGD	O6D-C1D-O3G	-3.03	102.80	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	O1D-CGD-CBD	3.03	130.68	124.48
23	D	403	CLA	C4A-NA-C1A	3.03	108.07	106.71
23	b	608	CLA	CMB-C2B-C3B	3.02	130.34	124.68
25	C	514	8CT	C38-C31-C32	-3.02	111.57	122.33
23	b	612	CLA	CMD-C2D-C1D	3.02	130.04	124.71
23	C	511	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
29	C	517	DGD	O6E-C1E-O5D	-3.02	102.83	109.97
25	k	101	8CT	C01-C02-C03	-3.02	121.14	124.53
23	b	604	CLA	O2A-C1-C2	-3.01	100.72	108.64
23	b	604	CLA	CMB-C2B-C3B	3.01	130.31	124.68
36	v	201	HEC	CMD-C2D-C1D	-3.01	123.84	128.46
26	d	406	PL9	C22-C23-C24	-3.01	120.42	127.66
23	b	602	CLA	CHB-C4A-NA	3.00	128.66	124.51
25	d	405	8CT	C38-C31-C32	-3.00	111.66	122.33
23	b	608	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
23	c	503	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
23	a	405	CLA	CMB-C2B-C3B	2.99	130.27	124.68
29	c	517	DGD	O3D-C3D-C4D	-2.99	103.45	110.35
23	c	511	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
27	D	407	LMG	O8-C28-O10	-2.98	116.06	123.59
24	A	406	PHO	CMB-C2B-C3B	2.97	130.24	124.68
23	b	614	CLA	O1D-CGD-CBD	2.97	130.57	124.48
23	B	604	CLA	CHB-C4A-NA	2.97	128.62	124.51
28	A	412	SQD	O5-C1-C2	-2.97	104.06	110.35
28	B	624	SQD	C1-C2-C3	-2.97	103.81	110.00
23	b	608	CLA	C6-C7-C8	-2.97	106.32	115.92
28	b	601	SQD	O9-S-O7	-2.97	103.68	113.95
23	C	505	CLA	C2D-C1D-ND	-2.97	107.92	110.10
23	B	613	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
27	d	410	LMG	O6-C1-O1	-2.96	102.97	109.97
23	C	504	CLA	CMB-C2B-C3B	2.95	130.20	124.68
23	C	506	CLA	CHB-C4A-NA	2.95	128.59	124.51
23	B	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	B	615	CLA	CHB-C4A-NA	2.95	128.59	124.51
28	a	411	SQD	O9-S-O7	-2.94	103.76	113.95
23	b	602	CLA	CMB-C2B-C3B	2.94	130.19	124.68
28	b	601	SQD	O2-C2-C1	2.94	117.19	110.05
23	B	614	CLA	CHB-C4A-NA	2.93	128.56	124.51
26	A	409	PL9	C22-C23-C24	-2.93	120.61	127.66
23	C	508	CLA	CMB-C2B-C3B	2.93	130.16	124.68
28	b	601	SQD	O8-S-C6	2.93	110.41	105.74
23	c	509	CLA	CHB-C4A-NA	2.92	128.56	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	O2A-CGA-O1A	-2.92	116.21	123.59
26	a	410	PL9	C32-C33-C34	-2.92	120.62	127.66
23	c	508	CLA	O2D-CGD-CBD	2.92	116.46	111.27
28	B	624	SQD	C3-C4-C5	2.92	115.45	110.24
23	c	508	CLA	CHD-C1D-ND	-2.92	121.77	124.45
23	b	612	CLA	O2D-CGD-CBD	2.91	116.45	111.27
23	c	508	CLA	CHB-C4A-NA	2.91	128.54	124.51
24	a	407	PHO	OBD-CAD-CBD	-2.91	121.55	125.82
23	C	503	CLA	O2A-C1-C2	-2.91	100.99	108.64
23	b	613	CLA	C11-C12-C13	-2.91	106.53	115.92
23	B	611	CLA	C2D-C1D-ND	-2.91	107.96	110.10
23	B	608	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
29	c	517	DGD	O6D-C1D-O3G	-2.90	103.10	109.97
31	a	409	BCR	C38-C26-C27	-2.90	108.04	113.62
23	B	611	CLA	C14-C13-C15	-2.90	100.81	111.29
23	C	506	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
23	c	511	CLA	CMB-C2B-C3B	2.89	130.08	124.68
28	A	412	SQD	O47-C7-O49	-2.89	116.72	123.70
23	c	506	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
25	t	101	8CT	C10-C11-C12	-2.88	121.88	126.23
23	b	606	CLA	C16-C15-C13	-2.88	106.61	115.92
25	B	619	8CT	C38-C31-C32	-2.88	112.10	122.33
36	v	201	HEC	CMC-C2C-C3C	2.87	129.20	125.82
33	e	101	LHG	O8-C23-C24	2.87	120.92	111.91
23	C	507	CLA	CHD-C1D-ND	-2.87	121.82	124.45
31	H	101	BCR	C16-C15-C14	-2.87	117.59	123.47
25	c	514	8CT	C01-C02-C03	-2.87	121.31	124.53
23	B	616	CLA	C2D-C1D-ND	-2.87	107.99	110.10
31	h	101	BCR	C27-C26-C25	2.87	126.89	122.73
28	a	411	SQD	C1-C2-C3	-2.86	104.04	110.00
23	B	616	CLA	CAA-CBA-CGA	-2.86	104.90	113.25
28	D	408	SQD	O9-S-O7	-2.86	104.06	113.95
33	d	408	LHG	O8-C23-C24	2.86	120.87	111.91
23	C	510	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
26	D	406	PL9	C42-C43-C44	-2.85	120.80	127.66
23	b	611	CLA	CAA-CBA-CGA	-2.85	104.93	113.25
23	B	615	CLA	CHD-C1D-ND	-2.85	121.84	124.45
23	C	501	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	b	609	CLA	O2D-CGD-CBD	2.84	116.32	111.27
23	c	512	CLA	CMB-C2B-C3B	2.84	130.00	124.68
25	D	405	8CT	C19-C18-C17	-2.84	117.65	123.47
23	c	506	CLA	C4A-NA-C1A	2.84	107.98	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404	CLA	CMB-C2B-C3B	2.84	129.98	124.68
29	h	102	DGD	C1D-O6D-C5D	-2.83	108.12	113.69
27	D	407	LMG	O3-C3-C2	-2.83	103.80	110.35
27	d	410	LMG	O1-C1-C2	-2.83	103.88	108.30
23	c	509	CLA	CHD-C1D-ND	-2.82	121.86	124.45
23	c	503	CLA	C4-C3-C5	2.82	120.02	115.27
25	A	408	8CT	C18-C19-C20	-2.82	117.70	123.47
23	A	404	CLA	C7-C6-C5	-2.82	105.70	113.36
24	d	401	PHO	C1-C2-C3	-2.82	121.17	126.04
23	d	404	CLA	C1-C2-C3	-2.82	121.17	126.04
23	D	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	b	616	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	c	505	CLA	CHD-C1D-ND	-2.81	121.87	124.45
23	C	501	CLA	O2D-CGD-CBD	2.81	116.26	111.27
25	C	515	8CT	C22-C21-C20	-2.81	118.99	122.92
29	h	102	DGD	C3D-C4D-C5D	-2.81	105.23	110.24
23	b	611	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
25	C	520	8CT	C18-C19-C20	-2.80	117.73	123.47
23	C	510	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
23	a	406	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
23	B	611	CLA	CHD-C1D-ND	-2.80	121.88	124.45
27	A	410	LMG	O8-C28-O10	-2.80	116.53	123.59
35	F	101	HEM	CBD-CAD-C3D	-2.80	104.86	112.63
23	C	505	CLA	O1D-CGD-CBD	2.80	130.20	124.48
23	c	502	CLA	C1-C2-C3	-2.79	121.22	126.04
29	C	517	DGD	C1D-C2D-C3D	-2.79	104.19	110.00
23	B	611	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
23	b	612	CLA	C1-C2-C3	-2.79	121.22	126.04
25	D	405	8CT	C38-C31-C32	-2.78	112.43	122.33
28	D	408	SQD	O48-C23-C24	2.78	120.64	111.91
23	c	504	CLA	C7-C6-C5	-2.78	105.82	113.36
29	c	516	DGD	CDB-CCB-CBB	-2.77	100.34	114.42
28	A	413	SQD	O47-C7-C8	2.76	117.46	111.50
23	b	607	CLA	C4-C3-C5	2.76	119.92	115.27
23	b	614	CLA	C4A-NA-C1A	2.76	107.95	106.71
26	d	406	PL9	C35-C34-C36	2.76	119.92	115.27
29	A	414	DGD	O5D-C6D-C5D	-2.76	103.94	109.05
23	a	405	CLA	CHD-C1D-ND	-2.76	121.92	124.45
27	d	410	LMG	O2-C2-C1	-2.76	103.35	110.05
23	B	616	CLA	O1D-CGD-CBD	2.75	130.12	124.48
23	d	404	CLA	CMB-C2B-C1B	-2.75	124.23	128.46
23	B	606	CLA	CHD-C1D-ND	-2.75	121.92	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	O1D-CGD-CBD	2.75	130.12	124.48
23	a	405	CLA	C7-C6-C5	-2.75	105.89	113.36
26	a	410	PL9	C22-C23-C24	-2.75	121.05	127.66
25	C	514	8CT	C05-C04-C03	2.75	114.71	110.48
27	C	519	LMG	C3-C4-C5	-2.74	105.34	110.24
23	B	611	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
31	Y	101	BCR	C23-C22-C21	-2.74	114.74	118.94
28	a	411	SQD	C1-O5-C5	-2.73	108.32	113.69
29	o	301	DGD	O3G-C3G-C2G	-2.73	104.53	111.78
29	c	518	DGD	C3D-C4D-C5D	-2.73	105.36	110.24
28	a	412	SQD	O49-C7-C8	-2.73	113.08	123.73
23	c	502	CLA	CHD-C1D-ND	-2.73	121.95	124.45
23	b	614	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
23	c	505	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
31	H	101	BCR	C27-C26-C25	2.73	126.69	122.73
23	b	612	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
31	c	515	BCR	C27-C26-C25	2.72	126.68	122.73
29	h	102	DGD	C3G-C2G-C1G	-2.72	105.35	111.79
23	B	616	CLA	CMB-C2B-C3B	2.72	129.76	124.68
31	Y	101	BCR	C27-C26-C25	2.72	126.67	122.73
27	B	620	LMG	C40-C39-C38	-2.72	100.64	114.42
23	c	504	CLA	O2A-CGA-O1A	-2.72	116.74	123.59
33	d	408	LHG	C20-C19-C18	-2.71	100.65	114.42
23	B	604	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
23	C	503	CLA	C6-C7-C8	-2.71	107.16	115.92
23	B	614	CLA	CHD-C1D-ND	-2.71	121.97	124.45
23	b	605	CLA	CMB-C2B-C3B	2.71	129.74	124.68
25	t	101	8CT	C18-C19-C20	-2.70	117.94	123.47
28	f	101	SQD	O8-S-C6	2.70	110.04	105.74
27	c	519	LMG	O2-C2-C1	-2.70	103.49	110.05
33	D	409	LHG	C20-C19-C18	-2.70	100.72	114.42
23	B	601	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	b	607	CLA	C2A-C1A-CHA	2.70	128.58	123.86
23	c	507	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
23	b	617	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	d	406	PL9	C37-C38-C39	-2.70	121.17	127.66
23	B	605	CLA	O1D-CGD-CBD	2.69	129.99	124.48
23	C	507	CLA	CMB-C2B-C3B	2.69	129.71	124.68
31	c	515	BCR	C33-C5-C6	-2.68	121.51	124.53
23	d	404	CLA	CHD-C1D-ND	-2.68	121.99	124.45
29	C	516	DGD	C6B-C5B-C4B	-2.68	100.80	114.42
23	b	602	CLA	CBA-CAA-C2A	2.68	121.78	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	C4-C3-C5	2.68	119.78	115.27
23	d	404	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
27	c	522	LMG	O6-C1-O1	-2.68	103.63	109.97
27	b	621	LMG	O1-C7-C8	-2.68	104.44	110.90
23	b	611	CLA	C4A-NA-C1A	2.68	107.91	106.71
29	c	518	DGD	O6D-C1D-O3G	-2.68	103.64	109.97
23	b	605	CLA	CHC-C1C-NC	2.67	128.26	124.20
23	c	503	CLA	CHD-C1D-ND	-2.67	122.00	124.45
23	b	613	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	C	502	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
23	c	506	CLA	CGD-CBD-CAD	-2.67	102.10	110.73
23	b	613	CLA	O1D-CGD-CBD	2.67	129.94	124.48
23	a	408	CLA	OBD-CAD-C3D	2.67	134.93	128.52
23	B	611	CLA	C1-C2-C3	-2.66	121.43	126.04
23	B	609	CLA	CHA-C1A-NA	-2.66	120.30	126.40
33	l	101	LHG	C29-C28-C27	-2.66	100.90	114.42
28	D	408	SQD	O5-C5-C4	2.66	114.53	109.69
35	e	102	HEM	C3B-C2B-C1B	2.66	108.46	106.49
33	D	410	LHG	O8-C6-C5	-2.66	100.70	108.43
23	b	610	CLA	CHD-C1D-ND	-2.65	122.02	124.45
31	B	618	BCR	C29-C30-C25	2.65	114.56	110.48
23	C	508	CLA	O2D-CGD-CBD	2.65	115.98	111.27
31	c	515	BCR	C2-C1-C6	2.65	114.56	110.48
23	A	411	CLA	CHB-C4A-NA	2.65	128.17	124.51
29	H	102	DGD	O5D-C1E-C2E	2.64	112.43	108.30
23	b	606	CLA	CMB-C2B-C3B	2.64	129.62	124.68
25	C	515	8CT	C39-C16-C17	-2.64	119.23	122.92
26	D	406	PL9	C12-C13-C14	-2.64	121.31	127.66
27	b	621	LMG	O1-C1-C2	-2.64	104.19	108.30
29	C	517	DGD	O5E-C6E-C5E	-2.63	102.25	111.29
28	b	601	SQD	C45-O47-C7	2.63	124.27	117.79
27	D	407	LMG	O1-C7-C8	-2.63	104.55	110.90
23	b	612	CLA	C4A-NA-C1A	2.63	107.89	106.71
33	D	410	LHG	O8-C23-C24	2.63	120.16	111.91
23	A	407	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
23	c	503	CLA	CMB-C2B-C3B	2.63	129.59	124.68
28	D	408	SQD	C1-C2-C3	-2.63	104.53	110.00
31	b	618	BCR	C29-C30-C25	2.63	114.52	110.48
27	b	623	LMG	O6-C1-O1	-2.63	103.76	109.97
27	b	623	LMG	O1-C7-C8	-2.62	104.57	110.90
33	d	407	LHG	C11-C10-C9	-2.62	101.11	114.42
23	c	505	CLA	CMB-C2B-C1B	-2.62	124.44	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	PL9	C20-C19-C21	2.62	119.67	115.27
23	B	603	CLA	C2C-C1C-NC	2.61	112.42	109.97
29	C	518	DGD	CDB-CCB-CBB	-2.61	101.16	114.42
23	B	601	CLA	CED-O2D-CGD	2.61	121.84	115.94
25	B	619	8CT	C01-C02-C03	-2.61	121.60	124.53
23	B	606	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	a	406	CLA	CMB-C2B-C3B	2.60	129.55	124.68
29	C	518	DGD	C3G-O3G-C1D	-2.60	108.66	113.74
31	b	618	BCR	C27-C26-C25	2.60	126.50	122.73
23	c	512	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
23	b	617	CLA	C2C-C1C-NC	2.60	112.41	109.97
29	H	102	DGD	O6E-C5E-C4E	2.59	114.41	109.69
25	b	620	8CT	C38-C31-C32	-2.59	113.10	122.33
33	d	407	LHG	O8-C23-O10	-2.59	117.05	123.59
31	h	101	BCR	C30-C25-C26	-2.59	118.97	122.61
23	A	405	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	B	603	CLA	C2D-C1D-ND	-2.58	108.20	110.10
23	c	512	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
23	d	402	CLA	CHD-C1D-ND	-2.58	122.08	124.45
31	Y	101	BCR	C15-C16-C17	-2.58	118.19	123.47
31	Y	101	BCR	C39-C30-C25	-2.58	106.11	110.30
33	L	101	LHG	C20-C19-C18	-2.58	101.33	114.42
29	A	414	DGD	C6D-O5D-C1E	2.58	118.77	113.74
23	B	611	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
29	c	517	DGD	C8B-C7B-C6B	-2.57	101.36	114.42
29	C	517	DGD	CDB-CCB-CBB	-2.57	101.39	114.42
23	C	507	CLA	CHB-C4A-NA	2.57	128.06	124.51
36	V	201	HEC	CMB-C2B-C1B	-2.56	124.53	128.46
25	c	514	8CT	C14-C13-C12	-2.56	123.66	127.31
23	C	512	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
28	f	101	SQD	O7-S-C6	2.56	109.98	106.94
31	H	101	BCR	C38-C26-C25	-2.56	121.66	124.53
25	C	520	8CT	C05-C04-C03	2.55	114.41	110.48
26	A	409	PL9	C21-C19-C18	-2.55	115.95	121.12
23	b	614	CLA	CED-O2D-CGD	2.55	121.71	115.94
23	b	602	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
25	t	101	8CT	C39-C16-C15	2.55	122.09	118.08
23	b	609	CLA	CHA-C1A-NA	-2.55	120.56	126.40
25	C	515	8CT	C40-C12-C13	-2.55	119.36	122.92
25	B	617	8CT	C14-C13-C12	-2.55	123.68	127.31
23	c	501	CLA	O2A-CGA-O1A	-2.55	117.17	123.59
26	d	406	PL9	C20-C19-C21	2.54	119.55	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	O1D-CGD-CBD	2.54	129.69	124.48
23	B	601	CLA	C2A-C1A-CHA	2.54	128.31	123.86
23	A	404	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
23	A	411	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
33	d	408	LHG	C18-C17-C16	-2.54	101.55	114.42
23	c	504	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	C	503	CLA	C6-C5-C3	2.53	120.10	113.45
26	d	406	PL9	C46-C47-C48	-2.53	103.56	111.88
27	A	410	LMG	O7-C10-O9	-2.53	117.58	123.70
23	c	513	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	c	505	CLA	C4A-NA-C1A	2.53	107.84	106.71
29	h	102	DGD	C3E-C4E-C5E	-2.53	105.73	110.24
23	a	408	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	B	602	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
31	B	618	BCR	C8-C7-C6	-2.52	120.12	127.20
26	A	409	PL9	C40-C39-C41	2.52	119.51	115.27
23	C	512	CLA	CAA-CBA-CGA	-2.52	105.89	113.25
23	b	609	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
31	Y	101	BCR	C40-C30-C25	2.52	114.38	110.30
29	h	102	DGD	C1E-O6E-C5E	2.52	118.63	113.69
23	B	610	CLA	CHD-C4C-NC	2.51	128.16	124.20
31	Y	101	BCR	C33-C5-C6	-2.51	121.70	124.53
23	c	509	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
25	A	408	8CT	C37-C35-C36	-2.51	104.19	107.89
23	B	614	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
33	e	101	LHG	O8-C23-O10	-2.51	117.25	123.59
26	d	406	PL9	C42-C43-C44	-2.51	121.62	127.66
35	F	101	HEM	CAD-CBD-CGD	2.51	119.00	113.60
28	f	101	SQD	C45-O47-C7	2.51	123.97	117.79
26	D	406	PL9	C7-C3-C2	-2.51	120.00	123.30
29	H	102	DGD	CDB-CCB-CBB	-2.51	101.69	114.42
36	V	201	HEC	CMC-C2C-C3C	2.51	128.77	125.82
26	A	409	PL9	O2-C1-C6	2.51	124.93	120.59
23	B	608	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	B	615	CLA	C6-C7-C8	-2.50	107.83	115.92
23	C	510	CLA	CMB-C2B-C3B	2.50	129.36	124.68
23	C	502	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	C	508	CLA	CHD-C1D-C2D	2.50	130.72	125.48
23	b	607	CLA	CMB-C2B-C3B	2.49	129.34	124.68
23	d	403	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
23	b	612	CLA	C2C-C1C-NC	2.49	112.31	109.97
23	B	604	CLA	CMB-C2B-C3B	2.49	129.33	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	410	LMG	C36-C35-C34	-2.49	101.80	114.42
24	d	401	PHO	O2D-CGD-O1D	-2.49	118.98	123.84
27	D	407	LMG	O6-C1-O1	-2.49	104.09	109.97
23	d	402	CLA	CHB-C4A-NA	2.48	127.95	124.51
23	b	609	CLA	CHD-C4C-NC	2.48	128.12	124.20
23	B	601	CLA	C2D-C1D-ND	-2.48	108.28	110.10
23	A	411	CLA	O2D-CGD-CBD	2.48	115.68	111.27
25	C	514	8CT	C01-C02-C03	-2.48	121.74	124.53
24	A	406	PHO	OBD-CAD-CBD	-2.48	122.19	125.82
25	b	620	8CT	C14-C13-C12	-2.48	123.78	127.31
23	C	513	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	a	405	CLA	CAC-C3C-C4C	2.47	128.02	124.81
27	D	411	LMG	O8-C28-O10	-2.47	117.36	123.59
26	d	406	PL9	C8-C7-C3	2.47	118.96	111.98
23	b	615	CLA	C1-C2-C3	-2.47	121.77	126.04
31	c	521	BCR	C38-C26-C27	-2.47	108.88	113.62
23	b	609	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
29	C	518	DGD	C6D-O5D-C1E	2.47	118.56	113.74
23	b	616	CLA	CHA-C4D-ND	2.47	137.66	132.50
23	d	402	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	a	405	CLA	C2A-C1A-CHA	2.46	128.16	123.86
23	a	405	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
23	B	602	CLA	C1-C2-C3	-2.46	121.79	126.04
29	C	518	DGD	O6D-C1D-O3G	-2.46	104.15	109.97
23	C	502	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
23	C	512	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
24	a	407	PHO	O2A-CGA-O1A	-2.45	117.40	123.59
25	d	405	8CT	C27-C26-C25	-2.45	119.49	122.92
23	B	608	CLA	O1D-CGD-CBD	2.45	129.50	124.48
23	b	614	CLA	CHB-C4A-NA	2.45	127.90	124.51
33	L	101	LHG	C12-C11-C10	-2.45	102.00	114.42
23	c	502	CLA	C3A-C2A-C1A	2.45	105.00	101.34
29	H	102	DGD	C8B-C7B-C6B	-2.45	102.01	114.42
23	B	605	CLA	CMB-C2B-C3B	2.45	129.25	124.68
23	C	506	CLA	CMB-C2B-C3B	2.44	129.25	124.68
23	b	615	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	b	621	LMG	C40-C39-C38	-2.44	102.03	114.42
31	T	101	BCR	C15-C14-C13	-2.44	123.83	127.31
29	h	102	DGD	C1D-C2D-C3D	-2.44	104.91	110.00
26	D	406	PL9	C22-C23-C24	-2.44	121.79	127.66
23	A	407	CLA	O2D-CGD-CBD	2.44	115.60	111.27
25	A	408	8CT	C05-C04-C03	2.44	114.23	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	412	SQD	O9-S-C6	2.44	109.83	106.94
23	d	404	CLA	CHB-C4A-NA	2.43	127.88	124.51
23	d	404	CLA	CHA-C1A-NA	-2.43	120.83	126.40
25	A	408	8CT	C01-C02-C03	-2.43	121.80	124.53
29	c	516	DGD	O3E-C3E-C2E	-2.43	104.73	110.35
26	d	406	PL9	C31-C32-C33	-2.43	103.90	111.88
29	o	301	DGD	C2G-O2G-C1B	2.43	123.77	117.79
23	B	609	CLA	C7-C6-C5	-2.43	106.77	113.36
26	a	410	PL9	C37-C38-C39	-2.43	121.82	127.66
23	b	608	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
23	b	615	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
23	C	507	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
29	C	516	DGD	O5D-C6D-C5D	-2.42	104.57	109.05
23	b	613	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	b	604	CLA	CHD-C1D-ND	-2.42	122.23	124.45
23	c	507	CLA	CMA-C3A-C4A	-2.42	105.28	111.77
23	B	606	CLA	O2D-CGD-CBD	2.42	115.56	111.27
23	c	513	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
31	c	521	BCR	C15-C16-C17	-2.41	118.53	123.47
23	b	607	CLA	CHA-C1A-NA	-2.41	120.87	126.40
23	B	603	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
26	d	406	PL9	C7-C8-C9	-2.41	122.78	126.79
23	b	614	CLA	CHA-C1A-NA	-2.41	120.88	126.40
29	c	518	DGD	O3E-C3E-C2E	-2.41	104.78	110.35
23	c	513	CLA	CHD-C1D-ND	-2.41	122.24	124.45
23	b	613	CLA	C1-C2-C3	-2.41	121.88	126.04
28	f	101	SQD	O47-C7-C8	2.40	117.49	110.80
29	c	518	DGD	C5B-C4B-C3B	-2.40	102.24	114.42
29	H	102	DGD	C3E-C4E-C5E	-2.40	105.96	110.24
23	c	507	CLA	CMB-C2B-C3B	2.40	129.16	124.68
23	b	602	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
28	D	408	SQD	C3-C4-C5	2.40	114.52	110.24
23	b	603	CLA	C11-C12-C13	-2.40	108.17	115.92
24	D	402	PHO	O2D-CGD-O1D	-2.40	119.15	123.84
27	B	620	LMG	C38-C37-C36	-2.40	102.26	114.42
25	C	520	8CT	C18-C17-C16	-2.40	123.89	127.31
23	C	507	CLA	CHA-C1A-NA	-2.40	120.91	126.40
26	d	406	PL9	C11-C9-C8	-2.39	116.28	121.12
25	C	515	8CT	C18-C19-C20	-2.39	118.58	123.47
27	C	519	LMG	O1-C7-C8	-2.39	105.13	110.90
27	d	410	LMG	O1-C7-C8	-2.39	105.13	110.90
28	f	101	SQD	O5-C1-O6	2.39	115.64	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	H	101	BCR	C35-C13-C14	-2.39	119.58	122.92
23	c	501	CLA	CHB-C4A-NA	2.39	127.81	124.51
23	b	614	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
23	d	402	CLA	C1-O2A-CGA	2.38	122.70	116.44
29	c	516	DGD	O5D-C6D-C5D	-2.38	104.64	109.05
29	c	517	DGD	CDB-CCB-CBB	-2.38	102.32	114.42
23	C	508	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
25	c	514	8CT	C10-C11-C12	-2.38	122.64	126.23
23	B	613	CLA	CAC-C3C-C4C	2.38	127.90	124.81
31	b	619	BCR	C30-C25-C26	-2.38	119.26	122.61
23	b	616	CLA	C1D-CHD-C4C	-2.38	120.93	126.06
27	c	522	LMG	O8-C28-O10	-2.38	117.59	123.59
23	d	403	CLA	C4-C3-C5	2.37	119.27	115.27
25	C	520	8CT	C37-C35-C34	-2.37	104.14	109.03
31	T	101	BCR	C35-C13-C14	-2.37	119.60	122.92
23	B	606	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
31	B	618	BCR	C7-C8-C9	-2.37	122.65	126.23
29	h	102	DGD	O3E-C3E-C2E	-2.37	104.86	110.35
23	c	506	CLA	CHA-C1A-NA	-2.37	120.97	126.40
31	b	619	BCR	C8-C7-C6	-2.37	120.54	127.20
25	C	515	8CT	C37-C35-C34	-2.37	104.15	109.03
24	A	406	PHO	O2D-CGD-O1D	-2.37	119.20	123.84
27	b	623	LMG	C1-O6-C5	-2.37	109.03	113.69
25	b	620	8CT	C11-C10-C03	-2.37	120.55	127.20
23	C	508	CLA	C7-C6-C5	-2.37	106.93	113.36
27	c	519	LMG	O6-C1-O1	-2.37	104.37	109.97
27	d	410	LMG	C3-C4-C5	-2.37	106.02	110.24
27	B	620	LMG	C6-C5-C4	-2.36	107.47	113.00
31	B	618	BCR	C33-C5-C6	-2.36	121.88	124.53
27	c	519	LMG	C40-C39-C38	-2.36	102.43	114.42
27	A	410	LMG	C38-C37-C36	-2.36	102.44	114.42
23	C	510	CLA	CHD-C1D-ND	-2.36	122.28	124.45
31	c	515	BCR	C8-C9-C10	2.36	122.56	118.94
25	A	408	8CT	C39-C16-C17	-2.36	119.62	122.92
23	C	509	CLA	C2D-C1D-ND	-2.36	108.37	110.10
27	c	522	LMG	O7-C10-O9	-2.36	118.01	123.70
23	B	601	CLA	C1-C2-C3	-2.35	121.97	126.04
28	b	601	SQD	O48-C23-O10	-2.35	117.65	123.59
23	B	613	CLA	CHC-C1C-NC	2.35	127.77	124.20
31	T	101	BCR	C7-C8-C9	-2.35	122.69	126.23
31	h	101	BCR	C7-C8-C9	-2.35	122.69	126.23
23	a	405	CLA	O1D-CGD-CBD	2.35	129.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	h	102	DGD	CDB-CCB-CBB	-2.35	102.51	114.42
23	C	507	CLA	C2A-C1A-CHA	2.35	127.96	123.86
23	b	605	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	c	507	CLA	CHD-C4C-NC	2.35	127.90	124.20
23	D	404	CLA	CED-O2D-CGD	2.35	121.24	115.94
23	C	508	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
23	B	607	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
27	c	524	LMG	C9-C8-C7	-2.34	106.25	111.79
31	h	101	BCR	C35-C13-C14	-2.34	119.64	122.92
23	C	503	CLA	CHD-C1D-C2D	2.34	130.39	125.48
29	c	516	DGD	C3G-C2G-C1G	-2.34	106.25	111.79
23	c	501	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	b	605	CLA	CHD-C1D-ND	-2.34	122.31	124.45
23	C	505	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	B	607	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	B	608	CLA	CHA-C1A-NA	-2.34	121.05	126.40
27	B	622	LMG	O7-C10-O9	-2.34	117.48	123.30
27	c	519	LMG	C9-C8-C7	-2.33	106.27	111.79
29	C	518	DGD	O2D-C2D-C1D	-2.33	104.38	110.05
29	c	517	DGD	O5D-C6D-C5D	-2.33	104.73	109.05
31	Y	101	BCR	C38-C26-C25	-2.33	121.91	124.53
23	b	605	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
33	l	101	LHG	C11-C10-C9	-2.33	102.60	114.42
27	C	519	LMG	O7-C10-O9	-2.33	118.07	123.70
28	D	408	SQD	C46-C45-C44	-2.33	105.96	113.70
25	k	101	8CT	C10-C11-C12	-2.32	122.72	126.23
23	C	509	CLA	C2A-C3A-C4A	2.32	105.62	101.87
23	A	405	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
23	c	512	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
23	a	405	CLA	CAA-C2A-C1A	-2.32	104.37	111.97
27	b	621	LMG	C31-C30-C29	-2.32	104.85	113.19
23	b	613	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
23	b	607	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
25	B	619	8CT	C06-C07-C02	-2.32	109.94	114.08
23	b	615	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
28	B	624	SQD	O48-C23-O10	-2.32	117.75	123.59
23	D	403	CLA	C1-C2-C3	-2.31	122.04	126.04
23	B	613	CLA	CMB-C2B-C3B	2.31	129.01	124.68
23	B	607	CLA	CHA-C1A-NA	-2.31	121.10	126.40
25	C	515	8CT	C05-C04-C03	2.31	114.04	110.48
25	t	101	8CT	C37-C35-C36	-2.31	104.49	107.89
23	A	407	CLA	CHD-C4C-NC	2.31	127.84	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C2C-C1C-NC	2.31	112.14	109.97
23	A	405	CLA	O1D-CGD-CBD	2.31	129.21	124.48
23	c	506	CLA	CED-O2D-CGD	2.31	121.15	115.94
35	e	102	HEM	C2C-C3C-C4C	2.31	108.51	106.90
23	c	506	CLA	O2A-C1-C2	-2.30	102.58	108.64
23	b	615	CLA	OBD-CAD-C3D	2.30	134.06	128.52
31	c	521	BCR	C37-C22-C21	-2.30	119.70	122.92
29	A	414	DGD	O3G-C1D-C2D	-2.30	104.72	108.30
23	a	408	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
23	c	506	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
23	c	505	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
23	C	503	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
35	F	101	HEM	O2D-CGD-CBD	2.30	121.40	114.03
23	C	509	CLA	C4-C3-C5	2.29	119.13	115.27
23	C	513	CLA	C6-C7-C8	-2.29	108.51	115.92
29	c	516	DGD	C4A-C3A-C2A	-2.29	104.96	113.19
29	c	517	DGD	O2D-C2D-C1D	-2.29	104.48	110.05
23	b	607	CLA	O2D-CGD-CBD	2.29	115.33	111.27
27	A	410	LMG	O6-C1-O1	-2.29	104.56	109.97
23	b	606	CLA	CHD-C4C-NC	2.29	127.81	124.20
23	b	607	CLA	C3C-C4C-NC	-2.29	108.01	110.57
31	Y	101	BCR	C23-C24-C25	-2.28	120.79	127.20
23	b	607	CLA	CED-O2D-CGD	-2.28	110.77	115.94
24	a	407	PHO	CMB-C2B-C3B	2.28	128.95	124.68
23	c	506	CLA	C6-C5-C3	-2.28	107.47	113.45
29	C	518	DGD	C3G-C2G-C1G	-2.28	106.39	111.79
23	d	404	CLA	C4-C3-C5	2.28	119.11	115.27
23	D	404	CLA	C2D-C1D-ND	-2.28	108.42	110.10
26	a	410	PL9	C11-C12-C13	-2.28	104.39	111.88
24	A	406	PHO	C4-C3-C2	-2.28	117.83	123.68
27	d	410	LMG	C1-C2-C3	-2.28	105.25	110.00
28	f	101	SQD	O48-C23-O10	-2.28	117.84	123.59
23	A	404	CLA	C5-C3-C2	-2.28	116.51	121.12
23	a	405	CLA	C11-C10-C8	-2.28	108.56	115.92
26	A	409	PL9	C20-C19-C21	2.28	119.10	115.27
25	C	520	8CT	C27-C26-C25	-2.27	119.74	122.92
23	B	601	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
28	A	412	SQD	O8-S-C6	2.27	109.36	105.74
23	c	507	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	B	602	CLA	CHA-C1A-NA	-2.27	121.20	126.40
23	c	505	CLA	C3B-C4B-NB	-2.27	106.27	109.21
25	b	620	8CT	C19-C18-C17	-2.27	118.82	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	514	8CT	C36-C35-C30	2.27	112.98	109.55
27	b	623	LMG	O3-C3-C2	-2.27	105.11	110.35
28	a	411	SQD	C3-C4-C5	2.27	114.28	110.24
23	a	408	CLA	CHA-C1A-NA	-2.27	121.21	126.40
23	b	616	CLA	C1-O2A-CGA	2.27	122.39	116.44
23	B	603	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
25	D	405	8CT	C10-C11-C12	-2.26	122.81	126.23
23	C	502	CLA	O2D-CGD-CBD	2.26	115.29	111.27
23	c	508	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
29	C	518	DGD	C4A-C3A-C2A	-2.26	105.06	113.19
28	a	412	SQD	O48-C23-O10	-2.26	117.88	123.59
23	a	406	CLA	C3C-C4C-NC	-2.26	108.03	110.57
28	f	101	SQD	O5-C5-C4	2.26	113.80	109.69
23	B	610	CLA	C3D-C4D-ND	2.26	113.89	110.24
25	C	515	8CT	C14-C13-C12	-2.26	124.09	127.31
23	c	504	CLA	C4-C3-C5	2.26	119.07	115.27
28	A	412	SQD	O48-C23-C24	2.26	118.99	111.91
27	c	522	LMG	O3-C3-C2	-2.26	105.13	110.35
26	a	410	PL9	O2-C1-C2	-2.26	116.61	121.78
23	A	405	CLA	O2D-CGD-CBD	2.26	115.28	111.27
23	C	502	CLA	CHA-C1A-NA	-2.25	121.23	126.40
26	D	406	PL9	C27-C28-C29	-2.25	122.23	127.66
23	D	403	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
31	T	101	BCR	C1-C6-C5	-2.25	119.44	122.61
34	D	401	BCT	O3-C-O1	-2.25	113.71	119.55
23	B	609	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	D	403	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	b	615	CLA	CHD-C1D-C2D	2.24	130.19	125.48
23	B	615	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
25	C	514	8CT	C18-C19-C20	-2.24	118.88	123.47
23	b	611	CLA	CED-O2D-CGD	-2.24	110.87	115.94
27	C	519	LMG	O1-C1-C2	-2.24	104.81	108.30
23	B	615	CLA	C6-C5-C3	-2.24	107.58	113.45
23	C	504	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
31	Y	101	BCR	C8-C7-C6	-2.24	120.92	127.20
29	c	516	DGD	O2E-C2E-C1E	-2.24	104.61	110.05
23	B	613	CLA	C2A-C3A-C4A	2.24	105.48	101.87
23	A	405	CLA	C2A-C1A-CHA	2.23	127.77	123.86
31	c	515	BCR	C15-C16-C17	-2.23	118.90	123.47
26	D	406	PL9	C7-C8-C9	-2.23	123.08	126.79
23	b	613	CLA	CHB-C4A-NA	2.23	127.60	124.51
23	B	611	CLA	O2D-CGD-CBD	2.23	115.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414	DGD	CDB-CCB-CBB	-2.23	103.12	114.42
26	D	406	PL9	C40-C39-C38	-2.23	117.96	123.68
23	b	608	CLA	O1D-CGD-CBD	2.23	129.04	124.48
25	B	619	8CT	C09-C04-C03	-2.23	106.69	110.30
23	B	607	CLA	C2C-C1C-NC	2.23	112.06	109.97
33	d	407	LHG	O8-C6-C5	-2.23	101.95	108.43
23	B	601	CLA	CHA-C4D-ND	2.23	137.16	132.50
23	c	505	CLA	CHB-C4A-NA	2.23	127.59	124.51
29	h	102	DGD	O5E-C6E-C5E	-2.22	103.66	111.29
23	B	613	CLA	C1-C2-C3	-2.22	122.20	126.04
27	b	621	LMG	O2-C2-C1	-2.22	104.64	110.05
26	D	406	PL9	C11-C9-C8	-2.22	116.62	121.12
23	a	408	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
23	B	609	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
23	C	503	CLA	O1D-CGD-CBD	2.22	129.03	124.48
29	c	518	DGD	C3G-C2G-C1G	-2.22	106.54	111.79
23	C	504	CLA	CHD-C4C-NC	2.22	127.70	124.20
23	a	408	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
24	a	407	PHO	O2D-CGD-CBD	2.22	113.80	111.00
25	d	405	8CT	C04-C03-C02	-2.22	119.49	122.61
34	a	404	BCT	O3-C-O1	-2.21	113.81	119.55
23	a	408	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
23	d	404	CLA	CED-O2D-CGD	2.21	120.94	115.94
23	b	615	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
31	h	101	BCR	C38-C26-C25	-2.21	122.05	124.53
31	b	618	BCR	C15-C14-C13	-2.21	124.16	127.31
23	C	503	CLA	C4D-CHA-C1A	2.21	123.94	121.25
29	c	516	DGD	O6E-C5E-C6E	-2.21	100.94	106.44
23	b	607	CLA	O1D-CGD-CBD	2.21	129.01	124.48
23	b	612	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
23	B	605	CLA	OBD-CAD-C3D	2.21	133.83	128.52
23	d	403	CLA	O1D-CGD-CBD	2.21	129.00	124.48
24	D	402	PHO	C1-C2-C3	-2.20	122.23	126.04
25	D	405	8CT	C06-C07-C02	-2.20	110.14	114.08
23	c	503	CLA	CAC-C3C-C4C	2.20	127.67	124.81
23	c	513	CLA	CMB-C2B-C3B	2.20	128.80	124.68
29	A	414	DGD	CCB-CBB-CAB	-2.20	103.24	114.42
23	D	404	CLA	C1-C2-C3	-2.20	122.23	126.04
28	a	411	SQD	O7-S-C6	2.20	109.56	106.94
23	A	407	CLA	CHB-C4A-NA	2.20	127.55	124.51
23	b	605	CLA	O1D-CGD-CBD	2.20	128.98	124.48
23	C	507	CLA	C1-O2A-CGA	2.20	122.21	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	t	101	8CT	C07-C02-C03	2.20	125.92	122.73
26	d	406	PL9	C31-C29-C28	2.20	125.56	121.12
33	B	623	LHG	O8-C23-O10	-2.20	118.05	123.59
26	a	410	PL9	C7-C8-C9	-2.19	123.14	126.79
29	c	516	DGD	O6D-C1D-O3G	-2.19	104.78	109.97
23	B	611	CLA	CHD-C1D-C2D	2.19	130.08	125.48
27	B	620	LMG	C17-C16-C15	-2.19	103.30	114.42
31	T	101	BCR	C2-C1-C6	2.19	113.85	110.48
25	b	620	8CT	C01-C02-C03	-2.19	122.07	124.53
29	c	518	DGD	C9B-C8B-C7B	-2.19	103.31	114.42
26	A	409	PL9	C31-C32-C33	-2.19	104.69	111.88
29	c	518	DGD	O1G-C1A-C2A	-2.19	105.04	111.91
23	C	505	CLA	CHA-C1A-NA	-2.19	121.39	126.40
23	b	609	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	B	611	CLA	CMB-C2B-C3B	2.19	128.77	124.68
23	b	616	CLA	O2D-CGD-CBD	2.19	115.15	111.27
23	B	613	CLA	C4-C3-C5	2.19	118.95	115.27
23	b	611	CLA	O1D-CGD-CBD	2.19	128.96	124.48
23	c	504	CLA	CED-O2D-CGD	2.18	120.88	115.94
23	C	510	CLA	CHB-C4A-NA	2.18	127.53	124.51
29	c	517	DGD	O3G-C1D-C2D	-2.18	104.89	108.30
23	B	603	CLA	O2A-C1-C2	-2.18	102.90	108.64
25	A	408	8CT	C11-C10-C03	-2.18	121.07	127.20
25	d	405	8CT	C01-C02-C03	-2.18	122.08	124.53
26	a	410	PL9	C27-C28-C29	-2.18	122.41	127.66
23	C	509	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	B	614	CLA	CHA-C1A-NA	-2.18	121.41	126.40
23	B	612	CLA	C16-C15-C13	-2.18	108.87	115.92
23	C	505	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
31	B	618	BCR	C15-C16-C17	-2.18	119.01	123.47
23	b	604	CLA	O1A-CGA-CBA	2.18	132.22	123.73
28	B	624	SQD	C45-O47-C7	2.18	123.15	117.79
23	c	506	CLA	CHB-C4A-NA	2.17	127.52	124.51
23	C	513	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
23	b	603	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
23	b	612	CLA	C5-C3-C2	2.17	125.51	121.12
27	B	620	LMG	O3-C3-C2	-2.17	105.33	110.35
31	T	101	BCR	C15-C16-C17	-2.17	119.03	123.47
27	C	519	LMG	O6-C1-O1	-2.17	104.84	109.97
31	c	515	BCR	C15-C14-C13	-2.17	124.22	127.31
26	D	406	PL9	C50-C49-C48	-2.17	116.39	122.65
29	C	516	DGD	CDB-CCB-CBB	-2.16	103.44	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	408	CLA	CHD-C1D-ND	-2.16	122.47	124.45
29	H	102	DGD	O3E-C3E-C2E	-2.16	105.35	110.35
29	c	518	DGD	CDB-CCB-CBB	-2.16	103.44	114.42
28	B	624	SQD	O47-C45-C46	2.16	116.23	108.40
25	c	514	8CT	C37-C35-C34	-2.16	104.58	109.03
25	C	514	8CT	C37-C35-C34	-2.16	104.58	109.03
23	b	605	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	d	404	CLA	O2A-C1-C2	-2.16	102.96	108.64
23	b	611	CLA	CHA-C1A-NA	-2.16	121.45	126.40
23	b	607	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
23	b	616	CLA	C4D-CHA-C1A	2.16	123.87	121.25
25	B	617	8CT	C40-C12-C13	-2.16	119.90	122.92
23	c	506	CLA	CHD-C1D-ND	-2.15	122.47	124.45
31	b	619	BCR	C15-C16-C17	-2.15	119.06	123.47
26	a	410	PL9	C36-C34-C33	-2.15	116.76	121.12
23	b	616	CLA	C7-C6-C5	-2.15	107.51	113.36
33	B	623	LHG	C18-C17-C16	-2.15	103.51	114.42
23	B	610	CLA	C11-C10-C8	-2.15	108.97	115.92
26	A	409	PL9	C36-C37-C38	-2.15	104.82	111.88
23	B	614	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
23	c	509	CLA	O1D-CGD-CBD	2.15	128.88	124.48
25	c	514	8CT	C05-C04-C03	2.15	113.79	110.48
25	t	101	8CT	C22-C21-C23	2.15	121.46	118.08
29	c	518	DGD	C1D-C2D-C3D	-2.14	105.53	110.00
23	b	607	CLA	C5-C3-C2	-2.14	116.78	121.12
23	C	503	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
23	B	611	CLA	CHB-C4A-NA	2.14	127.48	124.51
23	b	617	CLA	C1C-C2C-C3C	-2.14	104.70	106.96
29	C	516	DGD	CCB-CBB-CAB	-2.14	103.55	114.42
23	b	608	CLA	C2D-C1D-ND	-2.14	108.53	110.10
29	h	102	DGD	CBB-CAB-C9B	-2.14	103.55	114.42
23	b	616	CLA	CHC-C1C-C2C	-2.14	120.80	126.72
25	t	101	8CT	C36-C35-C34	2.14	113.44	109.03
23	B	612	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
27	d	410	LMG	O3-C3-C2	-2.14	105.41	110.35
23	b	613	CLA	C9-C8-C10	-2.14	103.55	111.29
28	A	412	SQD	O48-C23-O10	-2.14	118.20	123.59
26	d	406	PL9	C40-C39-C38	-2.14	118.20	123.68
25	b	620	8CT	C05-C04-C03	2.14	113.77	110.48
28	a	411	SQD	O10-C23-C24	-2.13	115.41	123.73
24	A	406	PHO	C5-C3-C2	2.13	125.43	121.12
23	C	507	CLA	C1B-CHB-C4A	-2.13	125.89	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C1-O2A-CGA	-2.13	110.85	116.44
33	D	409	LHG	O8-C23-C24	2.13	118.60	111.91
23	b	616	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
23	b	610	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
23	C	509	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
27	B	620	LMG	O7-C10-O9	-2.13	118.56	123.70
23	b	607	CLA	C2D-C1D-ND	-2.13	108.54	110.10
35	e	102	HEM	C4B-CHC-C1C	2.13	125.36	122.56
25	c	514	8CT	C18-C19-C20	-2.13	119.12	123.47
27	c	522	LMG	C6-C5-C4	-2.13	108.03	113.00
23	b	606	CLA	O1A-CGA-CBA	2.13	132.02	123.73
33	B	623	LHG	C20-C19-C18	-2.12	103.64	114.42
36	v	201	HEC	CBD-CAD-C3D	-2.12	109.00	112.62
23	c	510	CLA	C16-C15-C13	-2.12	109.06	115.92
23	C	513	CLA	O2A-C1-C2	-2.12	103.06	108.64
35	e	102	HEM	CAB-C3B-C2B	-2.12	121.61	128.60
23	B	614	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
27	B	620	LMG	C22-C21-C20	-2.12	103.66	114.42
23	b	607	CLA	C2C-C1C-NC	2.12	111.96	109.97
23	b	611	CLA	C6-C5-C3	2.12	119.02	113.45
31	h	101	BCR	C33-C5-C6	-2.12	122.15	124.53
29	c	517	DGD	CBB-CAB-C9B	-2.12	103.66	114.42
23	c	501	CLA	CED-O2D-CGD	-2.12	111.14	115.94
23	C	510	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
33	l	101	LHG	C20-C19-C18	-2.12	103.67	114.42
27	A	410	LMG	O6-C1-C2	-2.12	105.87	110.35
29	A	414	DGD	C1E-O6E-C5E	2.12	117.84	113.69
23	b	605	CLA	C3B-C4B-NB	-2.12	106.47	109.21
23	d	403	CLA	C1-C2-C3	-2.12	122.38	126.04
33	D	409	LHG	C27-C26-C25	-2.12	103.69	114.42
23	C	509	CLA	C2C-C1C-NC	2.11	111.95	109.97
27	B	620	LMG	O1-C7-C8	-2.11	105.80	110.90
23	A	407	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
24	a	407	PHO	C4A-C3A-C2A	-2.11	100.83	102.84
23	C	512	CLA	C7-C6-C5	-2.11	107.62	113.36
25	A	408	8CT	C14-C13-C12	-2.11	124.30	127.31
27	c	522	LMG	C35-C34-C33	-2.11	103.70	114.42
23	B	610	CLA	O1D-CGD-CBD	2.11	128.80	124.48
23	c	512	CLA	O2A-C1-C2	-2.11	103.09	108.64
31	h	101	BCR	C15-C16-C17	-2.11	119.16	123.47
23	b	612	CLA	CHD-C4C-NC	2.11	127.53	124.20
23	B	609	CLA	C2A-C1A-CHA	2.11	127.54	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	406	PL9	C27-C28-C29	-2.11	122.59	127.66
23	B	608	CLA	CHB-C4A-NA	2.10	127.42	124.51
31	c	515	BCR	C1-C6-C5	-2.10	119.65	122.61
29	C	516	DGD	O3E-C3E-C2E	-2.10	105.49	110.35
29	C	518	DGD	O3D-C3D-C4D	-2.10	105.49	110.35
28	a	412	SQD	C45-O47-C7	2.10	122.97	117.79
23	B	603	CLA	CHB-C4A-NA	2.10	127.42	124.51
27	B	620	LMG	C35-C34-C33	-2.10	103.77	114.42
33	B	623	LHG	C11-C10-C9	-2.10	103.77	114.42
23	c	503	CLA	C7-C6-C5	-2.10	107.66	113.36
23	B	608	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
23	B	604	CLA	O2A-C1-C2	2.10	114.15	108.64
23	c	503	CLA	C5-C3-C2	-2.10	116.87	121.12
29	c	518	DGD	C4D-C3D-C2D	-2.10	107.16	110.82
29	h	102	DGD	O6E-C5E-C4E	2.09	113.50	109.69
23	b	616	CLA	CHA-C1A-NA	-2.09	121.61	126.40
23	b	606	CLA	CMD-C2D-C1D	-2.09	121.03	124.71
23	B	616	CLA	O2D-CGD-CBD	2.09	114.99	111.27
27	B	620	LMG	C8-O7-C10	2.09	122.94	117.79
25	B	617	8CT	C27-C26-C28	2.09	121.37	118.08
23	A	411	CLA	CAA-C2A-C1A	-2.09	105.12	111.97
23	b	611	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
23	c	505	CLA	CMB-C2B-C3B	2.09	128.59	124.68
27	b	623	LMG	O2-C2-C1	-2.09	104.97	110.05
23	B	601	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
26	a	410	PL9	C40-C39-C38	-2.09	118.32	123.68
23	C	501	CLA	CHA-C1A-NA	-2.09	121.61	126.40
23	A	407	CLA	CHA-C1A-NA	-2.09	121.62	126.40
25	t	101	8CT	C04-C03-C02	-2.09	119.67	122.61
26	A	409	PL9	C27-C28-C29	-2.09	122.64	127.66
29	h	102	DGD	O6E-C1E-O5D	-2.09	105.03	109.97
24	D	402	PHO	C16-C15-C13	-2.09	109.17	115.92
31	c	521	BCR	C16-C15-C14	-2.09	119.20	123.47
23	b	610	CLA	CHD-C4C-NC	2.09	127.49	124.20
23	C	506	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
23	b	614	CLA	C11-C10-C8	-2.08	109.18	115.92
31	H	101	BCR	C24-C23-C22	-2.08	123.08	126.23
29	H	102	DGD	O6D-C1D-O3G	-2.08	105.04	109.97
23	a	406	CLA	O1A-CGA-CBA	2.08	131.86	123.73
23	A	407	CLA	C4A-NA-C1A	2.08	107.64	106.71
23	D	403	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	b	617	CLA	CHD-C1D-ND	-2.08	122.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	h	102	DGD	O5D-C1E-C2E	2.08	111.55	108.30
28	D	408	SQD	C1-O5-C5	-2.08	109.61	113.69
31	B	618	BCR	C38-C26-C25	-2.08	122.19	124.53
23	B	608	CLA	C6-C7-C8	-2.08	109.20	115.92
23	c	505	CLA	CHC-C1C-NC	2.08	127.36	124.20
29	H	102	DGD	CAB-C9B-C8B	-2.08	103.88	114.42
23	B	605	CLA	O2A-CGA-O1A	-2.08	118.36	123.59
23	a	408	CLA	C3D-C4D-ND	2.07	113.59	110.24
23	C	513	CLA	CHD-C4C-NC	2.07	127.47	124.20
31	c	521	BCR	C40-C30-C25	2.07	113.66	110.30
23	C	501	CLA	CHA-C4D-ND	2.07	136.83	132.50
29	C	516	DGD	CAB-C9B-C8B	-2.07	103.92	114.42
31	c	515	BCR	C38-C26-C27	-2.07	109.64	113.62
23	A	407	CLA	C2C-C1C-NC	2.07	111.91	109.97
23	B	603	CLA	CHA-C1A-NA	-2.07	121.67	126.40
23	b	611	CLA	CHB-C4A-NA	2.07	127.37	124.51
23	b	607	CLA	CHC-C1C-C2C	-2.06	121.01	126.72
23	B	606	CLA	CGD-CBD-CAD	-2.06	104.05	110.73
27	c	524	LMG	O2-C2-C1	-2.06	105.04	110.05
23	b	606	CLA	C4-C3-C2	-2.06	118.39	123.68
23	C	502	CLA	CHD-C1D-C2D	2.06	129.80	125.48
28	a	411	SQD	O8-S-O9	-2.06	106.24	111.27
23	C	505	CLA	CAC-C3C-C2C	-2.06	124.01	127.53
23	B	616	CLA	O2A-C1-C2	2.06	114.05	108.64
23	B	604	CLA	CHA-C4D-ND	2.06	136.81	132.50
23	C	510	CLA	C7-C6-C5	-2.06	107.77	113.36
23	b	609	CLA	C3B-C4B-NB	-2.06	106.55	109.21
33	e	101	LHG	C11-C10-C9	-2.06	103.99	114.42
27	D	411	LMG	O7-C10-O9	-2.05	118.74	123.70
23	B	606	CLA	CHA-C1A-NA	-2.05	121.69	126.40
25	C	514	8CT	C40-C12-C11	-2.05	114.84	118.08
23	B	609	CLA	CAC-C3C-C4C	2.05	127.47	124.81
23	b	616	CLA	C3B-C4B-NB	-2.05	106.56	109.21
23	C	511	CLA	C4-C3-C5	2.05	118.72	115.27
29	c	518	DGD	C7B-C6B-C5B	-2.05	104.01	114.42
23	c	509	CLA	O2A-CGA-CBA	2.05	118.34	111.91
23	B	610	CLA	C2D-C1D-ND	2.05	111.61	110.10
23	B	604	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	d	405	8CT	C07-C02-C03	2.05	125.71	122.73
23	A	405	CLA	C3C-C4C-NC	-2.05	108.27	110.57
23	a	408	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
29	A	414	DGD	O1G-C1A-O1A	-2.05	118.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	411	LMG	C8-O7-C10	2.05	122.83	117.79
23	c	502	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
29	C	517	DGD	C7B-C6B-C5B	-2.04	104.04	114.42
23	a	406	CLA	C4D-CHA-C1A	2.04	123.74	121.25
23	d	403	CLA	CHB-C4A-NA	2.04	127.34	124.51
27	C	519	LMG	C33-C32-C31	-2.04	104.05	114.42
35	e	102	HEM	CMC-C2C-C3C	2.04	128.50	124.68
29	A	414	DGD	CAB-C9B-C8B	-2.04	104.05	114.42
33	e	101	LHG	C18-C17-C16	-2.04	104.05	114.42
26	a	410	PL9	O2-C1-C6	2.04	124.13	120.59
23	C	513	CLA	CHD-C1D-C2D	2.04	129.76	125.48
25	C	515	8CT	C18-C17-C16	-2.04	124.40	127.31
26	D	406	PL9	C30-C29-C31	-2.04	111.84	115.27
23	C	504	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
23	B	606	CLA	CHD-C4C-NC	2.04	127.42	124.20
23	C	506	CLA	O1D-CGD-CBD	2.04	128.65	124.48
23	B	610	CLA	O1A-CGA-CBA	2.04	131.67	123.73
23	c	511	CLA	CHA-C1A-NA	-2.04	121.74	126.40
23	b	603	CLA	C1D-ND-C4D	2.04	107.78	106.33
23	a	405	CLA	C1-C2-C3	-2.04	122.52	126.04
23	b	614	CLA	C16-C15-C13	-2.04	109.34	115.92
23	B	608	CLA	CMA-C3A-C2A	-2.03	105.62	113.83
24	D	402	PHO	O2A-C1-C2	-2.03	103.29	108.64
27	b	623	LMG	C3-C4-C5	-2.03	106.61	110.24
23	B	615	CLA	CMD-C2D-C1D	2.03	128.30	124.71
23	C	504	CLA	C4-C3-C5	2.03	118.69	115.27
26	A	409	PL9	C36-C34-C33	-2.03	117.00	121.12
26	d	406	PL9	C36-C34-C33	-2.03	117.00	121.12
27	D	407	LMG	O2-C2-C3	-2.03	105.65	110.35
23	c	513	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	B	601	CLA	CHA-C1A-NA	-2.03	121.75	126.40
28	b	601	SQD	O10-C23-C24	-2.03	115.81	123.73
25	c	514	8CT	C19-C18-C17	-2.03	119.32	123.47
23	A	405	CLA	CBC-CAC-C3C	-2.03	106.84	112.43
23	B	612	CLA	C1-C2-C3	-2.03	122.53	126.04
25	C	514	8CT	C14-C13-C12	-2.03	124.42	127.31
26	D	406	PL9	C40-C39-C41	2.03	118.68	115.27
23	b	609	CLA	C6-C7-C8	-2.03	109.37	115.92
26	d	406	PL9	O2-C1-C2	-2.03	117.14	121.78
29	H	102	DGD	O1G-C1A-O1A	-2.03	118.48	123.59
28	A	412	SQD	C3-C4-C5	2.03	113.85	110.24
23	b	611	CLA	C1-C2-C3	-2.03	122.54	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	619	8CT	C18-C19-C20	-2.03	119.33	123.47
23	b	609	CLA	CMA-C3A-C4A	-2.03	106.33	111.77
23	b	613	CLA	C2C-C1C-NC	2.02	111.87	109.97
23	a	406	CLA	CHA-C1A-NA	-2.02	121.76	126.40
27	c	524	LMG	O8-C28-O10	-2.02	118.48	123.59
29	c	518	DGD	CBB-CAB-C9B	-2.02	104.15	114.42
27	A	410	LMG	C1-C2-C3	-2.02	105.78	110.00
29	C	516	DGD	CBB-CAB-C9B	-2.02	104.16	114.42
29	c	516	DGD	CBB-CAB-C9B	-2.02	104.17	114.42
23	C	512	CLA	CHA-C4D-ND	2.02	136.72	132.50
25	A	408	8CT	C10-C11-C12	-2.02	123.19	126.23
23	b	612	CLA	C4-C3-C2	-2.02	118.50	123.68
23	b	604	CLA	C5-C3-C2	-2.02	117.04	121.12
28	a	411	SQD	O48-C46-C45	2.02	114.30	108.43
23	C	508	CLA	C2D-C1D-ND	-2.02	108.62	110.10
23	c	503	CLA	O1D-CGD-CBD	2.02	128.61	124.48
23	B	608	CLA	C6-C5-C3	-2.01	108.17	113.45
23	c	507	CLA	O1A-CGA-CBA	2.01	131.59	123.73
31	b	619	BCR	C36-C18-C17	-2.01	120.10	122.92
29	o	301	DGD	C5B-C4B-C3B	-2.01	104.20	114.42
29	h	102	DGD	CAB-C9B-C8B	-2.01	104.20	114.42
29	A	414	DGD	O2D-C2D-C1D	-2.01	105.16	110.05
23	B	612	CLA	CGD-CBD-CAD	2.01	117.25	110.73
23	b	608	CLA	O2A-C1-C2	-2.01	103.35	108.64
23	B	606	CLA	C4-C3-C5	2.01	118.66	115.27
23	C	511	CLA	CHA-C1A-NA	-2.01	121.79	126.40
23	c	503	CLA	CMD-C2D-C1D	2.01	128.26	124.71
23	a	406	CLA	CHD-C1D-C2D	2.01	129.69	125.48
29	c	518	DGD	CCA-CBA-CAA	-2.01	104.22	114.42
25	t	101	8CT	C18-C17-C16	-2.01	124.44	127.31
23	c	501	CLA	CHD-C1D-C2D	2.01	129.69	125.48
23	b	614	CLA	C7-C6-C5	-2.01	107.90	113.36
23	C	512	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
27	B	620	LMG	C37-C36-C35	-2.01	104.24	114.42
25	t	101	8CT	C37-C35-C30	2.01	112.58	109.55
26	d	406	PL9	C17-C18-C19	-2.01	122.83	127.66
29	C	518	DGD	C6B-C5B-C4B	-2.01	104.24	114.42
23	b	605	CLA	C2A-C3A-C4A	2.01	105.11	101.87
27	C	519	LMG	C38-C37-C36	-2.00	104.25	114.42
31	c	521	BCR	C24-C23-C22	-2.00	123.21	126.23
31	a	409	BCR	C8-C7-C6	-2.00	121.58	127.20
23	c	503	CLA	C2C-C1C-NC	2.00	111.85	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	409	LHG	C18-C17-C16	-2.00	104.27	114.42
25	B	617	8CT	C01-C02-C03	-2.00	122.28	124.53

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	610	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	403	CLA	ND
23	D	404	CLA	ND
23	a	405	CLA	ND
23	a	408	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	c	501	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	d	404	CLA	ND
25	A	408	8CT	C30
25	B	617	8CT	C30
25	B	619	8CT	C30
25	C	514	8CT	C30
25	C	515	8CT	C30
25	C	520	8CT	C30
25	D	405	8CT	C30
25	b	620	8CT	C30
25	c	514	8CT	C30
25	d	405	8CT	C30
25	k	101	8CT	C30
25	t	101	8CT	C30

All (1646) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	411	CLA	CHA-CBD-CGD-O1D
23	A	411	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C11-C12-C13-C14
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	C2-C3-C5-C6
23	C	504	CLA	C4-C3-C5-C6
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	O2A-C1-C2-C3
23	a	406	CLA	CHA-CBD-CGD-O1D
23	b	602	CLA	C1A-C2A-CAA-CBA
23	b	603	CLA	CHA-CBD-CGD-O1D
23	b	603	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C11-C12-C13-C14
23	c	510	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C6-C7-C8-C9
25	A	408	8CT	C39-C16-C17-C18
25	B	617	8CT	C04-C03-C10-C11
25	B	617	8CT	C14-C15-C16-C39
25	B	617	8CT	C28-C29-C30-C31
25	B	619	8CT	C10-C11-C12-C40
25	B	619	8CT	C11-C12-C13-C14
25	B	619	8CT	C39-C16-C17-C18
25	B	619	8CT	C28-C29-C30-C31
25	C	514	8CT	C10-C11-C12-C40

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Mol	Chain	Res	Type	Atoms
25	C	514	8CT	C19-C20-C21-C22
25	C	514	8CT	C19-C20-C21-C23
25	C	514	8CT	C28-C29-C30-C31
25	C	520	8CT	C24-C25-C26-C27
25	D	405	8CT	C27-C26-C28-C29
25	D	405	8CT	C28-C29-C30-C35
25	b	620	8CT	C10-C11-C12-C40
25	b	620	8CT	C12-C13-C14-C15
25	b	620	8CT	C14-C15-C16-C17
25	b	620	8CT	C28-C29-C30-C31
25	c	514	8CT	C04-C03-C10-C11
25	c	514	8CT	C10-C11-C12-C13
25	c	514	8CT	C10-C11-C12-C40
25	c	514	8CT	C39-C16-C17-C18
25	c	514	8CT	C28-C29-C30-C31
25	d	405	8CT	C10-C11-C12-C40
25	d	405	8CT	C17-C18-C19-C20
25	d	405	8CT	C19-C20-C21-C22
25	d	405	8CT	C25-C26-C28-C29
25	d	405	8CT	C28-C29-C30-C31
25	k	101	8CT	C02-C03-C10-C11
25	k	101	8CT	C10-C11-C12-C40
25	k	101	8CT	C11-C12-C13-C14
25	k	101	8CT	C20-C21-C23-C24
25	k	101	8CT	C24-C25-C26-C27
25	k	101	8CT	C28-C29-C30-C31
25	t	101	8CT	C10-C11-C12-C40
25	t	101	8CT	C28-C29-C30-C31
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C13-C14-C16-C17
26	A	409	PL9	C17-C18-C19-C21
26	A	409	PL9	C18-C19-C21-C22
26	A	409	PL9	C22-C23-C24-C25
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C25-C24-C26-C27
26	A	409	PL9	C32-C33-C34-C35
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C37-C38-C39-C41
26	a	410	PL9	C12-C13-C14-C15
26	a	410	PL9	C16-C17-C18-C19
26	a	410	PL9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C22-C23-C24-C25
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C24-C26-C27-C28
26	d	406	PL9	C32-C33-C34-C35
26	d	406	PL9	C32-C33-C34-C36
26	d	406	PL9	C38-C39-C41-C42
26	d	406	PL9	C42-C43-C44-C45
26	d	406	PL9	C42-C43-C44-C46
27	A	410	LMG	O9-C10-O7-C8
27	A	410	LMG	C11-C10-O7-C8
27	C	519	LMG	C11-C10-O7-C8
27	D	411	LMG	C11-C10-O7-C8
27	b	623	LMG	C11-C10-O7-C8
27	c	524	LMG	O6-C1-O1-C7
28	B	624	SQD	C2-C1-O6-C44
28	B	624	SQD	O5-C1-O6-C44
28	B	624	SQD	O6-C44-C45-O47
28	B	624	SQD	O49-C7-O47-C45
28	B	624	SQD	C8-C7-O47-C45
28	D	408	SQD	C45-C44-O6-C1
28	a	411	SQD	O6-C44-C45-O47
28	a	412	SQD	O6-C44-C45-O47
28	a	412	SQD	O49-C7-O47-C45
28	f	101	SQD	O5-C1-O6-C44
29	A	414	DGD	O1B-C1B-O2G-C2G
29	A	414	DGD	O2G-C2G-C3G-O3G
31	B	618	BCR	C7-C8-C9-C34
31	H	101	BCR	C23-C24-C25-C30
31	Y	101	BCR	C7-C8-C9-C34
31	Y	101	BCR	C11-C12-C13-C35
31	Y	101	BCR	C37-C22-C23-C24
31	b	619	BCR	C37-C22-C23-C24
31	c	515	BCR	C11-C12-C13-C35
31	c	521	BCR	C20-C21-C22-C37
33	B	623	LHG	O1-C1-C2-O2
33	B	623	LHG	O1-C1-C2-C3
33	B	623	LHG	C3-O3-P-O4
33	D	409	LHG	C3-O3-P-O4
33	D	409	LHG	C4-O6-P-O4
33	D	410	LHG	C3-O3-P-O5
33	E	101	LHG	O1-C1-C2-C3
33	E	101	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C4-O6-P-O5
33	L	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	d	407	LHG	O1-C1-C2-C3
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C4-O6-P-O4
33	e	101	LHG	C1-C2-C3-O3
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O5
33	e	101	LHG	O10-C23-O8-C6
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O5
23	b	602	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	b	617	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	CBD-CGD-O2D-CED
23	b	602	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
27	c	522	LMG	O10-C28-O8-C9
33	E	101	LHG	O10-C23-O8-C6
23	C	509	CLA	O1D-CGD-O2D-CED
28	b	601	SQD	C24-C23-O48-C46
33	E	101	LHG	C24-C23-O8-C6
33	e	101	LHG	C24-C23-O8-C6
26	d	406	PL9	C47-C48-C49-C51
23	C	510	CLA	CBD-CGD-O2D-CED
23	D	404	CLA	CBD-CGD-O2D-CED
27	B	620	LMG	O10-C28-O8-C9
27	c	524	LMG	O10-C28-O8-C9
28	a	412	SQD	O10-C23-O48-C46
28	b	601	SQD	O10-C23-O48-C46
29	o	301	DGD	O1A-C1A-O1G-C1G
27	D	411	LMG	O9-C10-O7-C8
27	b	623	LMG	O9-C10-O7-C8
29	o	301	DGD	O1B-C1B-O2G-C2G
27	c	519	LMG	C11-C10-O7-C8
23	b	602	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
28	a	412	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
29	A	414	DGD	C2B-C1B-O2G-C2G
26	d	406	PL9	C47-C48-C49-C50
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
27	c	522	LMG	C29-C28-O8-C9
27	c	524	LMG	C29-C28-O8-C9
28	D	408	SQD	C24-C23-O48-C46
28	a	412	SQD	C24-C23-O48-C46
28	f	101	SQD	C24-C23-O48-C46
29	o	301	DGD	C2A-C1A-O1G-C1G
26	A	409	PL9	C12-C13-C14-C15
26	D	406	PL9	C32-C33-C34-C35
23	B	606	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
26	D	406	PL9	C32-C33-C34-C36
26	d	406	PL9	C37-C38-C39-C41
27	A	410	LMG	O6-C5-C6-O5
23	B	601	CLA	CBD-CGD-O2D-CED
33	D	410	LHG	O2-C2-C3-O3
23	C	506	CLA	C3-C5-C6-C7
23	c	506	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C13-C15-C16-C17
23	B	607	CLA	CBD-CGD-O2D-CED
23	C	501	CLA	CBD-CGD-O2D-CED
29	h	102	DGD	O6E-C5E-C6E-O5E
23	c	512	CLA	O1D-CGD-O2D-CED
24	D	402	PHO	CBD-CGD-O2D-CED
27	B	620	LMG	C29-C28-O8-C9
27	c	522	LMG	O6-C5-C6-O5
29	C	516	DGD	O6E-C5E-C6E-O5E
27	A	410	LMG	O10-C28-O8-C9
28	D	408	SQD	O10-C23-O48-C46
29	c	518	DGD	O1A-C1A-O1G-C1G
26	D	406	PL9	C47-C48-C49-C51
26	a	410	PL9	C47-C48-C49-C50
23	B	605	CLA	C4-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
26	a	410	PL9	C35-C34-C36-C37
23	B	605	CLA	C2-C3-C5-C6
23	b	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C2-C3-C5-C6
26	a	410	PL9	C33-C34-C36-C37
23	B	606	CLA	C2A-CAA-CBA-CGA
27	A	410	LMG	O6-C1-O1-C7
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C24-C26-C27-C28
26	A	409	PL9	C44-C46-C47-C48
26	a	410	PL9	C14-C16-C17-C18
26	a	410	PL9	C34-C36-C37-C38
26	d	406	PL9	C44-C46-C47-C48
28	B	624	SQD	C24-C23-O48-C46
23	C	510	CLA	O1D-CGD-O2D-CED
26	A	409	PL9	C47-C48-C49-C50
26	d	406	PL9	C37-C38-C39-C40
33	d	407	LHG	C1-C2-C3-O3
27	c	522	LMG	O9-C10-O7-C8
23	b	606	CLA	C10-C11-C12-C13
25	c	514	8CT	C12-C13-C14-C15
23	c	506	CLA	C13-C15-C16-C17
23	c	510	CLA	C15-C16-C17-C18
26	a	410	PL9	C47-C48-C49-C51
23	B	605	CLA	C10-C11-C12-C13
23	C	511	CLA	C8-C10-C11-C12
23	b	612	CLA	C8-C10-C11-C12
33	d	407	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
23	b	607	CLA	C3-C5-C6-C7
27	c	524	LMG	C2-C1-O1-C7
28	f	101	SQD	C2-C1-O6-C44
23	B	605	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C10-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	b	617	CLA	C11-C10-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
23	c	511	CLA	C14-C13-C15-C16
23	d	402	CLA	C14-C13-C15-C16
23	d	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C10-C11-C12-C13
25	C	514	8CT	C14-C15-C16-C39
25	c	514	8CT	C14-C15-C16-C39
25	d	405	8CT	C27-C26-C28-C29
31	c	521	BCR	C11-C12-C13-C35
27	B	622	LMG	C28-C29-C30-C31
27	D	411	LMG	C28-C29-C30-C31
29	c	518	DGD	C1A-C2A-C3A-C4A
23	C	505	CLA	C5-C6-C7-C8
23	b	616	CLA	C5-C6-C7-C8
23	c	506	CLA	C5-C6-C7-C8
23	B	602	CLA	C13-C15-C16-C17
23	B	607	CLA	C5-C6-C7-C8
23	B	612	CLA	C10-C11-C12-C13
23	b	615	CLA	C5-C6-C7-C8
23	c	509	CLA	C15-C16-C17-C18
23	c	512	CLA	C8-C10-C11-C12
23	c	512	CLA	C13-C15-C16-C17
27	D	411	LMG	C10-C11-C12-C13
23	A	404	CLA	C15-C16-C17-C18
23	B	604	CLA	C10-C11-C12-C13
23	B	612	CLA	C13-C15-C16-C17
23	B	613	CLA	C8-C10-C11-C12
23	C	509	CLA	C13-C15-C16-C17
23	b	602	CLA	C8-C10-C11-C12
23	b	607	CLA	C10-C11-C12-C13
23	c	509	CLA	C10-C11-C12-C13
33	d	407	LHG	O1-C1-C2-O2
27	b	621	LMG	C10-C11-C12-C13
27	b	623	LMG	C10-C11-C12-C13
28	A	412	SQD	C23-C24-C25-C26
28	D	408	SQD	C23-C24-C25-C26
33	d	407	LHG	C7-C8-C9-C10
33	d	407	LHG	C23-C24-C25-C26
33	e	101	LHG	C23-C24-C25-C26
23	B	601	CLA	CBA-CGA-O2A-C1
33	D	409	LHG	C28-C29-C30-C31
33	E	101	LHG	O9-C7-O7-C5
23	b	617	CLA	C2-C1-O2A-CGA
23	B	608	CLA	C15-C16-C17-C18
23	b	606	CLA	C5-C6-C7-C8
27	d	410	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	c	517	DGD	C1B-C2B-C3B-C4B
33	E	101	LHG	C23-C24-C25-C26
27	c	519	LMG	O6-C5-C6-O5
23	D	403	CLA	C12-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C15
23	C	512	CLA	C3-C5-C6-C7
25	C	515	8CT	C16-C17-C18-C19
25	c	514	8CT	C18-C19-C20-C21
23	B	605	CLA	C15-C16-C17-C18
23	a	408	CLA	C5-C6-C7-C8
23	c	507	CLA	C5-C6-C7-C8
28	D	408	SQD	O6-C44-C45-C46
23	B	614	CLA	C13-C15-C16-C17
23	b	608	CLA	C10-C11-C12-C13
23	D	404	CLA	O1D-CGD-O2D-CED
26	A	409	PL9	C34-C36-C37-C38
26	a	410	PL9	C44-C46-C47-C48
33	d	409	LHG	C23-C24-C25-C26
25	C	514	8CT	C13-C14-C15-C16
25	C	520	8CT	C13-C14-C15-C16
25	C	520	8CT	C21-C23-C24-C25
25	d	405	8CT	C13-C14-C15-C16
25	d	405	8CT	C21-C23-C24-C25
31	c	515	BCR	C18-C19-C20-C21
31	c	521	BCR	C18-C19-C20-C21
31	h	101	BCR	C18-C19-C20-C21
23	B	607	CLA	C13-C15-C16-C17
23	C	505	CLA	C8-C10-C11-C12
23	C	507	CLA	C10-C11-C12-C13
23	C	508	CLA	C13-C15-C16-C17
23	b	607	CLA	C15-C16-C17-C18
23	b	610	CLA	C15-C16-C17-C18
29	c	518	DGD	C2A-C1A-O1G-C1G
27	A	410	LMG	C4-C5-C6-O5
23	B	603	CLA	C5-C6-C7-C8
23	B	606	CLA	C15-C16-C17-C18
23	C	510	CLA	C15-C16-C17-C18
23	b	602	CLA	C15-C16-C17-C18
23	c	508	CLA	C13-C15-C16-C17
23	c	509	CLA	C8-C10-C11-C12
29	o	301	DGD	C2B-C1B-O2G-C2G
23	B	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	a	406	CLA	C8-C10-C11-C12
23	a	408	CLA	C10-C11-C12-C13
23	b	612	CLA	C13-C15-C16-C17
23	c	503	CLA	C5-C6-C7-C8
23	c	503	CLA	C8-C10-C11-C12
33	D	409	LHG	C3-O3-P-O6
33	D	410	LHG	C3-O3-P-O6
33	E	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O3
33	d	407	LHG	C3-O3-P-O6
33	d	408	LHG	C4-O6-P-O3
33	e	101	LHG	C3-O3-P-O6
33	L	101	LHG	C23-C24-C25-C26
27	A	410	LMG	C29-C28-O8-C9
23	C	513	CLA	C13-C15-C16-C17
23	B	601	CLA	O1A-CGA-O2A-C1
27	C	519	LMG	O9-C10-O7-C8
28	f	101	SQD	O49-C7-O47-C45
23	B	615	CLA	C16-C17-C18-C20
23	C	505	CLA	C10-C11-C12-C13
23	b	615	CLA	C8-C10-C11-C12
29	c	517	DGD	C1A-C2A-C3A-C4A
29	o	301	DGD	C1B-C2B-C3B-C4B
27	c	524	LMG	C16-C17-C18-C19
28	A	413	SQD	C12-C13-C14-C15
23	B	601	CLA	O1D-CGD-O2D-CED
25	B	617	8CT	C40-C12-C13-C14
25	B	617	8CT	C39-C16-C17-C18
25	B	617	8CT	C24-C25-C26-C27
25	B	619	8CT	C40-C12-C13-C14
25	C	515	8CT	C40-C12-C13-C14
25	C	515	8CT	C19-C20-C21-C22
25	C	520	8CT	C40-C12-C13-C14
25	D	405	8CT	C19-C20-C21-C22
25	D	405	8CT	C24-C25-C26-C27
25	b	620	8CT	C40-C12-C13-C14
25	b	620	8CT	C39-C16-C17-C18
25	k	101	8CT	C40-C12-C13-C14
25	k	101	8CT	C19-C20-C21-C22
25	t	101	8CT	C40-C12-C13-C14
31	B	618	BCR	C20-C21-C22-C37
31	H	101	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
31	Y	101	BCR	C20-C21-C22-C37
31	c	515	BCR	C35-C13-C14-C15
27	D	407	LMG	C20-C21-C22-C23
27	b	623	LMG	C31-C32-C33-C34
27	b	624	LMG	C36-C37-C38-C39
28	f	101	SQD	C31-C32-C33-C34
29	A	414	DGD	CAA-CBA-CCA-CDA
29	A	414	DGD	CEA-CFA-CGA-CHA
29	A	414	DGD	C2B-C3B-C4B-C5B
29	A	414	DGD	C8B-C9B-CAB-CBB
29	H	102	DGD	C7A-C8A-C9A-CAA
33	B	623	LHG	C18-C19-C20-C21
33	d	408	LHG	C33-C34-C35-C36
33	e	101	LHG	C12-C13-C14-C15
33	e	101	LHG	C14-C15-C16-C17
33	l	101	LHG	C29-C30-C31-C32
23	C	509	CLA	C16-C17-C18-C19
28	A	412	SQD	C30-C31-C32-C33
27	D	411	LMG	C9-C8-O7-C10
23	a	408	CLA	C13-C15-C16-C17
27	D	407	LMG	C18-C19-C20-C21
27	D	407	LMG	C30-C31-C32-C33
27	c	522	LMG	C32-C33-C34-C35
23	B	606	CLA	O1D-CGD-O2D-CED
27	c	524	LMG	C29-C30-C31-C32
28	A	412	SQD	C31-C32-C33-C34
28	B	624	SQD	C17-C18-C19-C20
29	c	516	DGD	C4B-C5B-C6B-C7B
33	d	409	LHG	C26-C27-C28-C29
33	e	101	LHG	C17-C18-C19-C20
28	a	411	SQD	C10-C11-C12-C13
33	d	408	LHG	C11-C12-C13-C14
33	d	408	LHG	C31-C32-C33-C34
25	C	515	8CT	C19-C20-C21-C23
25	C	520	8CT	C11-C12-C13-C14
25	c	514	8CT	C15-C16-C17-C18
25	d	405	8CT	C19-C20-C21-C23
25	k	101	8CT	C24-C25-C26-C28
29	C	517	DGD	C2E-C1E-O5D-C6D
29	c	517	DGD	C2E-C1E-O5D-C6D
28	A	413	SQD	C28-C29-C30-C31
28	a	412	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C6A-C7A-C8A-C9A
29	o	301	DGD	C4A-C5A-C6A-C7A
29	o	301	DGD	C5A-C6A-C7A-C8A
33	d	407	LHG	C10-C11-C12-C13
33	d	409	LHG	C30-C31-C32-C33
23	c	511	CLA	C15-C16-C17-C18
23	A	405	CLA	C16-C17-C18-C19
23	C	512	CLA	C16-C17-C18-C19
26	D	406	PL9	C7-C8-C9-C10
29	A	414	DGD	C5B-C6B-C7B-C8B
29	C	518	DGD	CCA-CDA-CEA-CFA
33	B	623	LHG	C12-C13-C14-C15
23	B	604	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C12-C13-C14
23	b	613	CLA	C6-C7-C8-C9
23	b	616	CLA	C14-C13-C15-C16
23	B	615	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C14-C15-C16-C17
27	A	410	LMG	C30-C31-C32-C33
27	B	622	LMG	C14-C15-C16-C17
27	C	519	LMG	C32-C33-C34-C35
27	b	621	LMG	C17-C18-C19-C20
27	b	624	LMG	C11-C12-C13-C14
28	A	413	SQD	C14-C15-C16-C17
28	D	408	SQD	C33-C34-C35-C36
29	H	102	DGD	CCB-CDB-CEB-CFB
29	c	518	DGD	CCB-CDB-CEB-CFB
29	h	102	DGD	C5B-C6B-C7B-C8B
33	B	623	LHG	C29-C30-C31-C32
33	D	410	LHG	C9-C10-C11-C12
33	E	101	LHG	C27-C28-C29-C30
33	e	101	LHG	C18-C19-C20-C21
23	b	611	CLA	C13-C15-C16-C17
23	c	505	CLA	C15-C16-C17-C18
28	a	411	SQD	O10-C23-O48-C46
28	f	101	SQD	O10-C23-O48-C46
25	b	620	8CT	C14-C15-C16-C39
28	A	412	SQD	C24-C25-C26-C27
28	a	412	SQD	C11-C12-C13-C14
33	B	623	LHG	C14-C15-C16-C17
33	D	409	LHG	C11-C10-C9-C8
33	d	409	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C8-C7-O7-C5
27	B	622	LMG	C29-C30-C31-C32
28	f	101	SQD	C28-C29-C30-C31
29	C	517	DGD	C8A-C9A-CAA-CBA
29	C	518	DGD	C8A-C9A-CAA-CBA
33	D	409	LHG	C12-C13-C14-C15
33	e	101	LHG	C26-C27-C28-C29
33	E	101	LHG	C7-C8-C9-C10
27	D	407	LMG	C14-C15-C16-C17
27	D	407	LMG	C35-C36-C37-C38
27	b	623	LMG	C16-C17-C18-C19
27	c	519	LMG	C31-C32-C33-C34
27	c	522	LMG	C36-C37-C38-C39
27	c	522	LMG	C40-C41-C42-C43
27	c	524	LMG	C30-C31-C32-C33
28	A	412	SQD	C28-C29-C30-C31
29	A	414	DGD	C2A-C3A-C4A-C5A
29	A	414	DGD	CEB-CFB-CGB-CHB
29	C	516	DGD	CCB-CDB-CEB-CFB
29	c	518	DGD	C5B-C6B-C7B-C8B
29	h	102	DGD	C3A-C4A-C5A-C6A
33	B	623	LHG	C25-C26-C27-C28
33	D	410	LHG	C27-C28-C29-C30
33	L	101	LHG	C30-C31-C32-C33
33	d	407	LHG	C16-C17-C18-C19
33	l	101	LHG	C9-C10-C11-C12
23	C	502	CLA	C16-C17-C18-C19
23	D	404	CLA	C16-C17-C18-C19
23	c	506	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
29	h	102	DGD	C4E-C5E-C6E-O5E
29	C	517	DGD	O6E-C1E-O5D-C6D
29	c	517	DGD	O6E-C1E-O5D-C6D
27	c	522	LMG	C11-C12-C13-C14
29	H	102	DGD	C3B-C4B-C5B-C6B
33	D	410	LHG	C25-C26-C27-C28
33	E	101	LHG	C33-C34-C35-C36
33	d	407	LHG	C27-C28-C29-C30
23	b	610	CLA	CBD-CGD-O2D-CED
27	B	622	LMG	C16-C17-C18-C19
27	D	407	LMG	C34-C35-C36-C37
27	b	623	LMG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	c	519	LMG	O9-C10-O7-C8
27	c	519	LMG	C39-C40-C41-C42
27	c	524	LMG	C11-C12-C13-C14
29	c	517	DGD	C6A-C7A-C8A-C9A
33	l	101	LHG	C31-C32-C33-C34
27	D	407	LMG	C11-C12-C13-C14
27	d	410	LMG	C34-C35-C36-C37
29	C	518	DGD	CAA-CBA-CCA-CDA
29	o	301	DGD	C3A-C4A-C5A-C6A
33	D	410	LHG	C11-C12-C13-C14
23	B	607	CLA	O1D-CGD-O2D-CED
28	a	412	SQD	C12-C13-C14-C15
28	a	412	SQD	C18-C19-C20-C21
29	o	301	DGD	C8B-C9B-CAB-CBB
33	d	407	LHG	C32-C33-C34-C35
23	c	501	CLA	O1D-CGD-O2D-CED
23	b	602	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
28	a	411	SQD	C30-C31-C32-C33
29	A	414	DGD	C6B-C7B-C8B-C9B
29	C	517	DGD	C5A-C6A-C7A-C8A
29	c	516	DGD	C5B-C6B-C7B-C8B
33	d	408	LHG	C12-C13-C14-C15
29	C	516	DGD	C4E-C5E-C6E-O5E
23	C	509	CLA	C16-C17-C18-C20
23	b	603	CLA	C16-C17-C18-C20
23	c	506	CLA	C16-C17-C18-C19
27	c	522	LMG	C12-C13-C14-C15
27	c	524	LMG	C12-C13-C14-C15
27	c	524	LMG	C32-C33-C34-C35
28	B	624	SQD	C34-C35-C36-C37
28	a	411	SQD	C26-C27-C28-C29
33	D	409	LHG	C15-C16-C17-C18
27	c	524	LMG	C34-C35-C36-C37
29	o	301	DGD	CBA-CCA-CDA-CEA
25	b	620	8CT	C17-C18-C19-C20
25	t	101	8CT	C17-C18-C19-C20
28	A	412	SQD	C32-C33-C34-C35
29	A	414	DGD	CDB-CEB-CFB-CGB
29	o	301	DGD	C5B-C6B-C7B-C8B
23	B	611	CLA	C8-C10-C11-C12
29	h	102	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	O1-C1-C2-O2
27	A	410	LMG	C38-C39-C40-C41
27	B	620	LMG	C36-C37-C38-C39
27	B	620	LMG	C38-C39-C40-C41
27	D	411	LMG	C11-C12-C13-C14
28	A	412	SQD	C25-C26-C27-C28
29	C	517	DGD	CCB-CDB-CEB-CFB
29	c	516	DGD	C9A-CAA-CBA-CCA
29	h	102	DGD	CCB-CDB-CEB-CFB
29	o	301	DGD	C7B-C8B-C9B-CAB
33	D	409	LHG	C29-C30-C31-C32
23	A	405	CLA	C16-C17-C18-C20
27	b	624	LMG	C31-C32-C33-C34
27	b	624	LMG	C37-C38-C39-C40
28	a	412	SQD	C11-C10-C9-C8
29	c	518	DGD	CBB-CCB-CDB-CEB
33	d	408	LHG	C14-C15-C16-C17
27	b	621	LMG	C15-C16-C17-C18
33	E	101	LHG	C16-C17-C18-C19
23	c	506	CLA	C2-C1-O2A-CGA
27	B	620	LMG	C13-C14-C15-C16
27	b	623	LMG	C18-C19-C20-C21
27	b	624	LMG	C32-C33-C34-C35
28	f	101	SQD	C25-C26-C27-C28
33	D	409	LHG	C30-C31-C32-C33
23	b	604	CLA	C13-C15-C16-C17
29	c	516	DGD	C8B-C9B-CAB-CBB
33	D	409	LHG	C11-C12-C13-C14
25	B	617	8CT	C02-C03-C10-C11
25	c	514	8CT	C02-C03-C10-C11
25	k	101	8CT	C04-C03-C10-C11
31	H	101	BCR	C23-C24-C25-C26
31	Y	101	BCR	C1-C6-C7-C8
31	Y	101	BCR	C5-C6-C7-C8
31	b	619	BCR	C23-C24-C25-C26
31	b	619	BCR	C23-C24-C25-C30
31	h	101	BCR	C23-C24-C25-C26
31	h	101	BCR	C23-C24-C25-C30
29	C	516	DGD	C4B-C5B-C6B-C7B
29	C	518	DGD	CBA-CCA-CDA-CEA
29	c	518	DGD	C8A-C9A-CAA-CBA
27	C	519	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	a	411	SQD	C24-C23-O48-C46
23	B	607	CLA	C8-C10-C11-C12
23	C	506	CLA	C15-C16-C17-C18
28	b	601	SQD	C16-C17-C18-C19
33	E	101	LHG	C11-C10-C9-C8
27	d	410	LMG	O6-C5-C6-O5
27	B	620	LMG	C28-C29-C30-C31
28	A	412	SQD	C7-C8-C9-C10
29	A	414	DGD	C1A-C2A-C3A-C4A
29	o	301	DGD	C1A-C2A-C3A-C4A
28	B	624	SQD	C9-C10-C11-C12
33	B	623	LHG	C9-C10-C11-C12
28	A	412	SQD	C14-C15-C16-C17
28	D	408	SQD	C27-C28-C29-C30
23	B	604	CLA	C11-C12-C13-C15
23	C	506	CLA	C2-C3-C5-C6
23	C	506	CLA	C6-C7-C8-C10
23	C	506	CLA	C11-C12-C13-C15
23	C	511	CLA	C6-C7-C8-C10
23	D	404	CLA	C11-C10-C8-C7
23	a	408	CLA	C11-C10-C8-C7
23	b	603	CLA	C12-C13-C15-C16
23	b	605	CLA	C6-C7-C8-C10
23	b	613	CLA	C6-C7-C8-C10
23	b	613	CLA	C12-C13-C15-C16
23	b	616	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C7
23	c	509	CLA	C12-C13-C15-C16
23	d	402	CLA	C12-C13-C15-C16
26	D	406	PL9	C13-C14-C16-C17
26	D	406	PL9	C28-C29-C31-C32
26	a	410	PL9	C13-C14-C16-C17
26	d	406	PL9	C28-C29-C31-C32
27	B	620	LMG	C31-C32-C33-C34
27	c	522	LMG	C34-C35-C36-C37
33	L	101	LHG	C31-C32-C33-C34
23	b	609	CLA	C13-C15-C16-C17
25	k	101	8CT	C23-C24-C25-C26
23	C	502	CLA	C16-C17-C18-C20
23	C	512	CLA	C16-C17-C18-C20
33	e	101	LHG	C7-C8-C9-C10
23	c	506	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	CBA-CGA-O2A-C1
27	c	522	LMG	C4-C5-C6-O5
23	B	606	CLA	C8-C10-C11-C12
27	b	621	LMG	C31-C32-C33-C34
27	c	524	LMG	C31-C32-C33-C34
27	c	522	LMG	C10-C11-C12-C13
29	c	516	DGD	C1A-C2A-C3A-C4A
27	D	407	LMG	C19-C20-C21-C22
29	h	102	DGD	C6A-C7A-C8A-C9A
33	D	409	LHG	C34-C35-C36-C37
33	e	101	LHG	C13-C14-C15-C16
28	A	413	SQD	C16-C17-C18-C19
28	a	411	SQD	C13-C14-C15-C16
27	A	410	LMG	C16-C17-C18-C19
33	B	623	LHG	C7-C8-C9-C10
27	c	522	LMG	C11-C10-O7-C8
28	b	601	SQD	C8-C7-O47-C45
27	B	620	LMG	C16-C17-C18-C19
23	C	502	CLA	C15-C16-C17-C18
23	C	509	CLA	C5-C6-C7-C8
27	c	524	LMG	C35-C36-C37-C38
33	e	101	LHG	O9-C7-O7-C5
29	H	102	DGD	C1A-C2A-C3A-C4A
27	B	620	LMG	C17-C18-C19-C20
28	a	412	SQD	C13-C14-C15-C16
29	C	518	DGD	C8B-C9B-CAB-CBB
28	A	412	SQD	O6-C44-C45-O47
29	H	102	DGD	C4B-C5B-C6B-C7B
33	d	409	LHG	C29-C30-C31-C32
27	B	622	LMG	C30-C31-C32-C33
27	c	519	LMG	C35-C36-C37-C38
29	H	102	DGD	C9A-CAA-CBA-CCA
23	B	610	CLA	C8-C10-C11-C12
23	A	407	CLA	C4-C3-C5-C6
23	b	615	CLA	C4-C3-C5-C6
26	d	406	PL9	C15-C14-C16-C17
26	d	406	PL9	C13-C14-C16-C17
27	c	524	LMG	C33-C34-C35-C36
33	L	101	LHG	C27-C28-C29-C30
33	d	408	LHG	C29-C30-C31-C32
23	C	506	CLA	C6-C7-C8-C9
23	C	510	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C6-C7-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	b	603	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C14
23	b	613	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C9
23	c	509	CLA	C14-C13-C15-C16
29	C	517	DGD	C7A-C8A-C9A-CAA
29	C	517	DGD	C9A-CAA-CBA-CCA
27	B	620	LMG	C12-C13-C14-C15
29	A	414	DGD	C8A-C9A-CAA-CBA
29	A	414	DGD	C9B-CAB-CBB-CCB
33	d	408	LHG	C32-C33-C34-C35
27	D	407	LMG	O6-C5-C6-O5
23	b	604	CLA	CBD-CGD-O2D-CED
28	A	413	SQD	C10-C11-C12-C13
28	A	413	SQD	C26-C27-C28-C29
29	h	102	DGD	C2B-C3B-C4B-C5B
23	c	506	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
27	b	621	LMG	O10-C28-O8-C9
23	C	508	CLA	C1A-C2A-CAA-CBA
23	a	408	CLA	C1A-C2A-CAA-CBA
28	D	408	SQD	C45-C46-O48-C23
23	b	608	CLA	C16-C17-C18-C20
23	b	616	CLA	C16-C17-C18-C20
29	A	414	DGD	CBA-CCA-CDA-CEA
29	H	102	DGD	C9B-CAB-CBB-CCB
33	E	101	LHG	C30-C31-C32-C33
23	C	509	CLA	C10-C11-C12-C13
33	d	408	LHG	C3-O3-P-O6
27	c	524	LMG	C38-C39-C40-C41
33	d	408	LHG	C26-C27-C28-C29
23	d	404	CLA	CBD-CGD-O2D-CED
28	b	601	SQD	C13-C14-C15-C16
23	c	512	CLA	C5-C6-C7-C8
26	a	410	PL9	C17-C18-C19-C20
27	b	621	LMG	C29-C30-C31-C32
27	c	522	LMG	C16-C17-C18-C19
27	d	410	LMG	C39-C40-C41-C42
29	H	102	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C28-C29-C30-C31
27	d	410	LMG	C13-C14-C15-C16
27	b	623	LMG	O6-C5-C6-O5
23	B	605	CLA	C5-C6-C7-C8
23	b	610	CLA	C13-C15-C16-C17
23	b	616	CLA	C8-C10-C11-C12
23	D	404	CLA	C16-C17-C18-C20
29	c	516	DGD	O6D-C5D-C6D-O5D
29	C	518	DGD	C2A-C3A-C4A-C5A
33	d	407	LHG	C15-C16-C17-C18
23	b	613	CLA	C3-C5-C6-C7
23	c	511	CLA	CBD-CGD-O2D-CED
28	B	624	SQD	C13-C14-C15-C16
23	c	503	CLA	CBA-CGA-O2A-C1
24	D	402	PHO	O1D-CGD-O2D-CED
23	C	506	CLA	C4-C3-C5-C6
27	b	624	LMG	C34-C35-C36-C37
28	D	408	SQD	C25-C26-C27-C28
33	d	409	LHG	C27-C28-C29-C30
23	B	613	CLA	C5-C6-C7-C8
23	b	606	CLA	C15-C16-C17-C18
23	d	404	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C12-C13-C14-C15
27	d	410	LMG	C14-C15-C16-C17
23	C	504	CLA	C11-C12-C13-C14
28	a	411	SQD	C34-C35-C36-C37
29	C	517	DGD	C8B-C9B-CAB-CBB
29	c	518	DGD	C3A-C4A-C5A-C6A
23	c	510	CLA	C16-C17-C18-C19
27	c	522	LMG	O1-C7-C8-C9
28	b	601	SQD	C44-C45-C46-O48
28	b	601	SQD	C19-C20-C21-C22
29	A	414	DGD	C1G-C2G-C3G-O3G
33	d	407	LHG	C18-C19-C20-C21
27	D	411	LMG	C15-C16-C17-C18
28	A	413	SQD	C9-C10-C11-C12
28	b	601	SQD	C12-C13-C14-C15
28	b	601	SQD	C30-C31-C32-C33
29	c	517	DGD	C3A-C4A-C5A-C6A
33	l	101	LHG	C7-C8-C9-C10
29	C	517	DGD	C2G-C3G-O3G-C1D
29	C	517	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
29	c	517	DGD	C2G-C3G-O3G-C1D
29	c	517	DGD	C5D-C6D-O5D-C1E
28	b	601	SQD	C26-C27-C28-C29
27	b	623	LMG	C24-C25-C26-C27
29	C	518	DGD	C5A-C6A-C7A-C8A
33	D	410	LHG	C16-C17-C18-C19
23	c	508	CLA	C15-C16-C17-C18
23	c	508	CLA	C16-C17-C18-C19
27	b	624	LMG	C39-C40-C41-C42
23	B	616	CLA	C3-C5-C6-C7
26	d	406	PL9	C39-C41-C42-C43
33	D	409	LHG	C32-C33-C34-C35
33	d	409	LHG	O1-C1-C2-O2
27	D	407	LMG	C38-C39-C40-C41
29	C	517	DGD	C6B-C7B-C8B-C9B
33	d	407	LHG	C29-C30-C31-C32
28	B	624	SQD	C11-C12-C13-C14
28	b	601	SQD	C10-C11-C12-C13
23	b	602	CLA	C10-C11-C12-C13
25	A	408	8CT	C24-C25-C26-C27
25	C	514	8CT	C40-C12-C13-C14
25	C	515	8CT	C24-C25-C26-C27
25	c	514	8CT	C24-C25-C26-C27
25	d	405	8CT	C24-C25-C26-C27
25	t	101	8CT	C19-C20-C21-C22
29	c	516	DGD	O6E-C5E-C6E-O5E
23	C	505	CLA	C4-C3-C5-C6
29	C	517	DGD	CDA-CEA-CFA-CGA
29	H	102	DGD	C8B-C9B-CAB-CBB
33	d	407	LHG	C19-C20-C21-C22
23	b	616	CLA	C16-C17-C18-C19
23	c	505	CLA	C2C-C3C-CAC-CBC
27	B	620	LMG	C29-C30-C31-C32
27	b	623	LMG	C34-C35-C36-C37
33	D	410	LHG	C17-C18-C19-C20
23	c	507	CLA	C2-C1-O2A-CGA
33	E	101	LHG	C35-C36-C37-C38
29	C	517	DGD	O6E-C5E-C6E-O5E
27	D	407	LMG	C13-C14-C15-C16
29	C	516	DGD	C5B-C6B-C7B-C8B
23	C	501	CLA	O1D-CGD-O2D-CED
25	D	405	8CT	C26-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C32-C33-C34-C35
29	h	102	DGD	CAB-CBB-CCB-CDB
27	c	519	LMG	C29-C28-O8-C9
33	E	101	LHG	O6-C4-C5-O7
23	b	608	CLA	C16-C17-C18-C19
29	c	518	DGD	C6B-C7B-C8B-C9B
27	c	519	LMG	C34-C35-C36-C37
23	B	614	CLA	C8-C10-C11-C12
23	c	513	CLA	C5-C6-C7-C8
25	B	617	8CT	C24-C25-C26-C28
25	C	515	8CT	C15-C16-C17-C18
25	C	520	8CT	C15-C16-C17-C18
23	b	610	CLA	O1D-CGD-O2D-CED
27	b	623	LMG	C11-C12-C13-C14
29	c	516	DGD	C2A-C3A-C4A-C5A
29	c	517	DGD	CAA-CBA-CCA-CDA
33	L	101	LHG	C18-C19-C20-C21
33	l	101	LHG	C17-C18-C19-C20
29	C	516	DGD	O6D-C5D-C6D-O5D
23	c	503	CLA	O1A-CGA-O2A-C1
33	L	101	LHG	O10-C23-O8-C6
29	C	518	DGD	CBB-CCB-CDB-CEB
33	B	623	LHG	C24-C25-C26-C27
33	L	101	LHG	C12-C13-C14-C15
26	D	406	PL9	C27-C28-C29-C30
26	d	406	PL9	C12-C13-C14-C15
23	B	611	CLA	C11-C12-C13-C15
23	B	615	CLA	C6-C7-C8-C10
23	B	616	CLA	C6-C7-C8-C10
23	C	506	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C10-C8-C7
23	a	406	CLA	C12-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C15
23	b	605	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	617	CLA	C11-C10-C8-C7
23	c	505	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C10-C8-C7
23	c	508	CLA	C12-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	C6-C7-C8-C10
23	c	512	CLA	C11-C12-C13-C15
23	c	513	CLA	C12-C13-C15-C16
23	d	403	CLA	C6-C7-C8-C10
27	D	411	LMG	C33-C34-C35-C36
28	A	412	SQD	C11-C12-C13-C14
23	B	604	CLA	C11-C10-C8-C9
23	B	615	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	a	406	CLA	C11-C10-C8-C9
23	a	406	CLA	C14-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C14
23	c	504	CLA	C11-C10-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	508	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C14
23	d	403	CLA	C6-C7-C8-C9
33	D	410	LHG	C32-C33-C34-C35
29	C	518	DGD	C3A-C4A-C5A-C6A
25	B	617	8CT	C10-C11-C12-C40
25	D	405	8CT	C10-C11-C12-C40
23	c	513	CLA	C16-C17-C18-C20
33	L	101	LHG	C26-C27-C28-C29
27	D	411	LMG	C12-C13-C14-C15
27	b	623	LMG	C15-C16-C17-C18
29	C	517	DGD	O1B-C1B-O2G-C2G
27	B	620	LMG	C40-C41-C42-C43
23	a	408	CLA	CBA-CGA-O2A-C1
27	c	524	LMG	C39-C40-C41-C42
29	C	516	DGD	C4A-C5A-C6A-C7A
29	c	517	DGD	CDA-CEA-CFA-CGA
27	A	410	LMG	C39-C40-C41-C42
29	c	518	DGD	CCA-CDA-CEA-CFA
29	o	301	DGD	O2G-C1B-C2B-C3B
29	c	516	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
29	A	414	DGD	CCA-CDA-CEA-CFA
27	b	621	LMG	C28-C29-C30-C31
23	d	403	CLA	C2C-C3C-CAC-CBC
33	e	101	LHG	C25-C26-C27-C28
27	b	621	LMG	C29-C28-O8-C9
27	D	407	LMG	C40-C41-C42-C43
23	c	510	CLA	C4-C3-C5-C6
26	a	410	PL9	C15-C14-C16-C17
26	d	406	PL9	C45-C44-C46-C47
23	C	505	CLA	C2-C3-C5-C6
28	A	413	SQD	C32-C33-C34-C35
27	b	621	LMG	C11-C12-C13-C14
28	A	412	SQD	C12-C13-C14-C15
28	a	411	SQD	C29-C30-C31-C32
28	f	101	SQD	C24-C25-C26-C27
23	B	601	CLA	C16-C17-C18-C20
23	b	608	CLA	CBA-CGA-O2A-C1
29	C	518	DGD	O1A-C1A-O1G-C1G
23	B	609	CLA	C3A-C2A-CAA-CBA
29	c	516	DGD	C4A-C5A-C6A-C7A
33	E	101	LHG	C19-C20-C21-C22
29	c	517	DGD	C8B-C9B-CAB-CBB
23	b	603	CLA	C16-C17-C18-C19
29	h	102	DGD	C5A-C6A-C7A-C8A
33	E	101	LHG	C9-C10-C11-C12
23	b	616	CLA	C15-C16-C17-C18
27	c	522	LMG	C7-C8-C9-O8
28	A	412	SQD	O6-C44-C45-C46
28	a	411	SQD	O6-C44-C45-C46
29	C	516	DGD	O1G-C1G-C2G-C3G
27	D	411	LMG	C14-C15-C16-C17
28	a	412	SQD	C31-C32-C33-C34
23	B	616	CLA	C5-C6-C7-C8
23	b	614	CLA	C8-C10-C11-C12
27	c	522	LMG	C31-C32-C33-C34
23	C	509	CLA	C3-C5-C6-C7
23	b	603	CLA	C3-C5-C6-C7
27	D	411	LMG	C31-C32-C33-C34
26	D	406	PL9	C30-C29-C31-C32
23	b	615	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
29	C	516	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
29	c	517	DGD	C7B-C8B-C9B-CAB
29	c	518	DGD	C7A-C8A-C9A-CAA
29	c	518	DGD	C4B-C5B-C6B-C7B
33	L	101	LHG	C15-C16-C17-C18
33	d	409	LHG	C25-C26-C27-C28
33	d	408	LHG	O1-C1-C2-O2
27	A	410	LMG	C37-C38-C39-C40
29	c	517	DGD	CAB-CBB-CCB-CDB
33	e	101	LHG	O6-C4-C5-O7
26	D	406	PL9	C22-C23-C24-C25
27	d	410	LMG	C10-C11-C12-C13
27	c	522	LMG	C38-C39-C40-C41
29	C	517	DGD	C3A-C4A-C5A-C6A
29	c	516	DGD	CDB-CEB-CFB-CGB
33	E	101	LHG	C25-C26-C27-C28
23	B	616	CLA	O1A-CGA-O2A-C1
28	B	624	SQD	O10-C23-O48-C46
33	d	407	LHG	C17-C18-C19-C20
33	d	407	LHG	C25-C26-C27-C28
29	c	516	DGD	C4D-C5D-C6D-O5D
29	C	516	DGD	CDA-CEA-CFA-CGA
33	L	101	LHG	C32-C33-C34-C35
27	A	410	LMG	O1-C7-C8-O7
27	B	620	LMG	O7-C8-C9-O8
27	c	522	LMG	O1-C7-C8-O7
28	a	411	SQD	O47-C45-C46-O48
28	f	101	SQD	O47-C45-C46-O48
27	B	622	LMG	C32-C33-C34-C35
28	A	412	SQD	C33-C34-C35-C36
23	c	513	CLA	C16-C17-C18-C19
27	D	411	LMG	C16-C17-C18-C19
28	D	408	SQD	O5-C1-O6-C44
23	b	608	CLA	C8-C10-C11-C12
23	b	617	CLA	C10-C11-C12-C13
23	c	511	CLA	C13-C15-C16-C17
33	D	410	LHG	C1-C2-C3-O3
27	C	519	LMG	C13-C14-C15-C16
28	a	411	SQD	C35-C36-C37-C38
27	C	519	LMG	C40-C41-C42-C43
23	C	508	CLA	C11-C10-C8-C9
23	C	509	CLA	C14-C13-C15-C16
23	C	510	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C11-C10-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	b	609	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
27	B	622	LMG	C31-C32-C33-C34
33	E	101	LHG	C2-C3-O3-P
27	c	519	LMG	C38-C39-C40-C41
33	l	101	LHG	C33-C34-C35-C36
23	B	615	CLA	C16-C17-C18-C19
23	B	616	CLA	C11-C12-C13-C14
31	b	618	BCR	C1-C6-C7-C8
31	b	618	BCR	C5-C6-C7-C8
23	C	503	CLA	C8-C10-C11-C12
23	A	407	CLA	C6-C7-C8-C9
27	A	410	LMG	C17-C18-C19-C20
33	d	408	LHG	C17-C18-C19-C20
33	D	410	LHG	C11-C10-C9-C8
25	B	617	8CT	C14-C15-C16-C17
25	B	619	8CT	C10-C11-C12-C13
25	c	514	8CT	C20-C21-C23-C24
31	Y	101	BCR	C7-C8-C9-C10
31	c	521	BCR	C11-C12-C13-C14
23	C	510	CLA	C10-C11-C12-C13
33	D	410	LHG	C30-C31-C32-C33
33	e	101	LHG	C28-C29-C30-C31
27	b	624	LMG	C28-C29-C30-C31
23	c	505	CLA	C5-C6-C7-C8
23	A	404	CLA	C4C-C3C-CAC-CBC
29	H	102	DGD	CDB-CEB-CFB-CGB
24	a	407	PHO	O1D-CGD-O2D-CED
33	E	101	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
28	a	412	SQD	C15-C16-C17-C18
23	B	604	CLA	C11-C10-C8-C7
23	B	604	CLA	C12-C13-C15-C16
23	B	605	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C12-C13-C15
23	C	504	CLA	C11-C10-C8-C7
23	C	505	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C10-C8-C7
23	C	508	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C12-C13-C15-C16
23	C	510	CLA	C12-C13-C15-C16
23	C	512	CLA	C12-C13-C15-C16
23	C	513	CLA	C12-C13-C15-C16
23	a	406	CLA	C11-C10-C8-C7
23	b	603	CLA	C6-C7-C8-C10
23	b	605	CLA	C12-C13-C15-C16
23	b	609	CLA	C11-C10-C8-C7
23	b	609	CLA	C11-C12-C13-C15
23	b	610	CLA	C12-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C10-C8-C7
23	c	509	CLA	C11-C12-C13-C15
28	D	408	SQD	C29-C30-C31-C32
33	d	408	LHG	C30-C31-C32-C33
25	c	514	8CT	C16-C17-C18-C19
23	c	512	CLA	C2A-CAA-CBA-CGA
23	B	601	CLA	C10-C11-C12-C13
25	C	514	8CT	C24-C25-C26-C27
31	T	101	BCR	C16-C17-C18-C36
31	a	409	BCR	C16-C17-C18-C36
31	c	515	BCR	C20-C21-C22-C37
31	h	101	BCR	C20-C21-C22-C37
33	d	408	LHG	C7-C8-C9-C10
23	b	602	CLA	C16-C17-C18-C20
29	o	301	DGD	CEB-CFB-CGB-CHB
28	A	412	SQD	C26-C27-C28-C29
29	C	518	DGD	C7B-C8B-C9B-CAB
33	D	409	LHG	C25-C26-C27-C28
23	b	604	CLA	C5-C6-C7-C8
29	c	517	DGD	C5B-C6B-C7B-C8B
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
28	b	601	SQD	C46-C45-O47-C7
28	B	624	SQD	C33-C34-C35-C36
29	h	102	DGD	C9A-CAA-CBA-CCA
33	D	409	LHG	C33-C34-C35-C36
27	C	519	LMG	C15-C16-C17-C18
25	b	620	8CT	C03-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	c	521	BCR	C6-C7-C8-C9
23	c	507	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
27	c	519	LMG	C36-C37-C38-C39
29	C	517	DGD	C3B-C4B-C5B-C6B
33	L	101	LHG	C11-C12-C13-C14
23	C	506	CLA	C13-C15-C16-C17
29	A	414	DGD	CFA-CGA-CHA-CIA
27	B	620	LMG	C7-C8-C9-O8
28	B	624	SQD	O6-C44-C45-C46
28	a	412	SQD	C44-C45-C46-O48
33	d	409	LHG	C2-C3-O3-P
23	C	511	CLA	CBD-CGD-O2D-CED
33	l	101	LHG	O6-C4-C5-O7
29	C	516	DGD	O1G-C1A-C2A-C3A
29	h	102	DGD	CAA-CBA-CCA-CDA
35	e	102	HEM	C4B-C3B-CAB-CBB
23	B	612	CLA	C16-C17-C18-C19
23	B	616	CLA	C11-C12-C13-C15
27	c	522	LMG	C29-C30-C31-C32
23	B	612	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O1D
33	l	101	LHG	C15-C16-C17-C18
23	b	608	CLA	O1A-CGA-O2A-C1
25	B	619	8CT	C19-C20-C21-C23
25	c	514	8CT	C19-C20-C21-C23
31	B	618	BCR	C11-C10-C9-C8
31	Y	101	BCR	C11-C10-C9-C8
31	c	515	BCR	C20-C21-C22-C23
28	b	601	SQD	O6-C44-C45-O47
23	B	616	CLA	CBA-CGA-O2A-C1
33	d	409	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
27	b	621	LMG	C19-C20-C21-C22
27	b	624	LMG	C33-C34-C35-C36
26	D	406	PL9	C15-C14-C16-C17
29	o	301	DGD	CFA-CGA-CHA-CIA
29	c	516	DGD	O1B-C1B-O2G-C2G
23	B	604	CLA	C14-C13-C15-C16
23	C	504	CLA	C11-C10-C8-C9
23	a	406	CLA	C6-C7-C8-C9
23	b	608	CLA	C6-C7-C8-C9
27	b	623	LMG	C38-C39-C40-C41
28	A	413	SQD	C30-C31-C32-C33
33	D	410	LHG	C24-C25-C26-C27
27	D	407	LMG	C39-C40-C41-C42
28	b	601	SQD	C18-C19-C20-C21
23	a	408	CLA	O1A-CGA-O2A-C1
25	C	520	8CT	C27-C26-C28-C29
33	l	101	LHG	C13-C14-C15-C16
25	k	101	8CT	C10-C11-C12-C13
33	d	407	LHG	C31-C32-C33-C34
33	d	408	LHG	C34-C35-C36-C37
23	C	502	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	c	509	CLA	C13-C15-C16-C17
23	B	612	CLA	C2-C1-O2A-CGA
29	o	301	DGD	CEA-CFA-CGA-CHA
25	C	515	8CT	C18-C19-C20-C21
28	D	408	SQD	C30-C31-C32-C33
23	A	407	CLA	C2-C3-C5-C6
27	D	411	LMG	O10-C28-O8-C9
27	c	519	LMG	O10-C28-O8-C9
33	d	407	LHG	C3-O3-P-O5
33	d	408	LHG	C3-O3-P-O4
33	d	408	LHG	C4-O6-P-O5
33	e	101	LHG	C3-O3-P-O4
23	b	602	CLA	C16-C17-C18-C19
29	C	516	DGD	C2B-C3B-C4B-C5B
29	C	517	DGD	O6D-C1D-O3G-C3G
27	B	622	LMG	C33-C34-C35-C36
33	L	101	LHG	C29-C30-C31-C32
28	a	411	SQD	C12-C13-C14-C15
23	B	601	CLA	C16-C17-C18-C19
29	o	301	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	513	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
28	f	101	SQD	C5-C6-S-O7
23	a	406	CLA	C15-C16-C17-C18
23	b	612	CLA	C15-C16-C17-C18
23	c	513	CLA	C8-C10-C11-C12
27	b	623	LMG	C19-C20-C21-C22
27	c	524	LMG	C14-C15-C16-C17
33	D	409	LHG	C13-C14-C15-C16
33	d	408	LHG	C25-C26-C27-C28
28	b	601	SQD	C25-C26-C27-C28
27	c	522	LMG	C28-C29-C30-C31
23	C	511	CLA	O1D-CGD-O2D-CED
33	B	623	LHG	C1-C2-C3-O3
29	C	518	DGD	C6B-C7B-C8B-C9B
29	c	518	DGD	C9A-CAA-CBA-CCA
23	B	606	CLA	C6-C7-C8-C10
23	B	607	CLA	C11-C10-C8-C7
23	B	608	CLA	C11-C12-C13-C15
23	C	505	CLA	C6-C7-C8-C10
23	C	509	CLA	C11-C10-C8-C7
23	D	404	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C7
23	b	602	CLA	C12-C13-C15-C16
23	b	608	CLA	C6-C7-C8-C10
23	b	615	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C12-C13-C15-C16
25	A	408	8CT	C28-C29-C30-C31
25	C	515	8CT	C28-C29-C30-C31
25	C	520	8CT	C28-C29-C30-C31
28	D	408	SQD	C26-C27-C28-C29
29	H	102	DGD	C3A-C4A-C5A-C6A
27	C	519	LMG	C37-C38-C39-C40
33	B	623	LHG	C32-C33-C34-C35
28	a	412	SQD	C19-C20-C21-C22
23	d	403	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	d	407	LHG	C26-C27-C28-C29
23	C	513	CLA	C10-C11-C12-C13
23	d	403	CLA	C16-C17-C18-C19
33	D	410	LHG	C7-C8-C9-C10
28	b	601	SQD	O6-C44-C45-C46
27	c	522	LMG	O7-C8-C9-O8
27	c	524	LMG	O7-C8-C9-O8
28	a	412	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
23	c	505	CLA	C4C-C3C-CAC-CBC
29	h	102	DGD	C7B-C8B-C9B-CAB
33	e	101	LHG	C10-C11-C12-C13
23	B	604	CLA	C2C-C3C-CAC-CBC
33	d	408	LHG	C10-C11-C12-C13
29	c	516	DGD	C7B-C8B-C9B-CAB
23	b	610	CLA	C3-C5-C6-C7
29	c	518	DGD	C8B-C9B-CAB-CBB
33	D	410	LHG	C2-C3-O3-P
28	B	624	SQD	C30-C31-C32-C33
33	e	101	LHG	C16-C17-C18-C19
23	B	603	CLA	C10-C11-C12-C13
33	D	409	LHG	C10-C11-C12-C13
29	c	516	DGD	CBA-CCA-CDA-CEA
23	B	610	CLA	C14-C13-C15-C16
23	C	505	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	C	512	CLA	C14-C13-C15-C16
23	b	605	CLA	C14-C13-C15-C16
23	b	607	CLA	C11-C10-C8-C9
23	b	608	CLA	C11-C10-C8-C9
23	b	609	CLA	C11-C10-C8-C9
23	c	510	CLA	C14-C13-C15-C16
23	c	513	CLA	C14-C13-C15-C16
27	D	411	LMG	C34-C35-C36-C37
26	d	406	PL9	C9-C11-C12-C13
29	h	102	DGD	C8B-C9B-CAB-CBB
28	a	412	SQD	C17-C18-C19-C20
33	B	623	LHG	C27-C28-C29-C30
28	A	412	SQD	C11-C10-C9-C8
29	A	414	DGD	C4B-C5B-C6B-C7B
33	L	101	LHG	C24-C25-C26-C27
33	L	101	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
28	A	413	SQD	C27-C28-C29-C30
29	c	517	DGD	C9A-CAA-CBA-CCA
23	b	604	CLA	O1D-CGD-O2D-CED
27	C	519	LMG	C30-C31-C32-C33
23	b	614	CLA	C13-C15-C16-C17
28	D	408	SQD	C31-C32-C33-C34
29	h	102	DGD	O2G-C1B-C2B-C3B
28	A	412	SQD	C13-C14-C15-C16
27	b	623	LMG	C9-C8-O7-C10
27	c	524	LMG	C9-C8-O7-C10
23	a	405	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C8-C10-C11-C12
23	B	615	CLA	C13-C15-C16-C17
25	A	408	8CT	C04-C03-C10-C11
26	A	409	PL9	C43-C44-C46-C47
27	d	410	LMG	C30-C31-C32-C33
29	H	102	DGD	O2G-C1B-C2B-C3B
23	B	603	CLA	C16-C17-C18-C20
23	B	608	CLA	C16-C17-C18-C20
28	f	101	SQD	C8-C7-O47-C45
29	c	516	DGD	O6E-C1E-O5D-C6D
33	E	101	LHG	C12-C13-C14-C15
28	b	601	SQD	O47-C45-C46-O48
29	c	516	DGD	O1G-C1G-C2G-O2G
33	D	409	LHG	C4-O6-P-O3
23	D	403	CLA	C2C-C3C-CAC-CBC
29	C	517	DGD	C5B-C6B-C7B-C8B
33	B	623	LHG	C31-C32-C33-C34
23	d	403	CLA	C16-C17-C18-C20
28	a	411	SQD	C44-C45-C46-O48
28	f	101	SQD	C44-C45-C46-O48
29	C	518	DGD	C9A-CAA-CBA-CCA
23	a	405	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	c	506	CLA	C6-C7-C8-C10
23	B	607	CLA	C11-C10-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	b	602	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	c	521	BCR	C9-C10-C11-C12
23	B	611	CLA	C16-C17-C18-C20
28	A	412	SQD	C35-C36-C37-C38
33	l	101	LHG	C30-C31-C32-C33
33	d	408	LHG	C19-C20-C21-C22
29	o	301	DGD	CDB-CEB-CFB-CGB
23	c	509	CLA	CAA-CBA-CGA-O2A
23	C	503	CLA	C5-C6-C7-C8
29	A	414	DGD	O6D-C5D-C6D-O5D
33	E	101	LHG	C14-C15-C16-C17
23	c	506	CLA	C4-C3-C5-C6
27	D	411	LMG	C29-C28-O8-C9
24	a	407	PHO	CBD-CGD-O2D-CED
28	a	411	SQD	C16-C17-C18-C19
29	h	102	DGD	C4B-C5B-C6B-C7B
33	d	408	LHG	C15-C16-C17-C18
23	c	501	CLA	C2A-CAA-CBA-CGA
29	C	516	DGD	O6E-C1E-O5D-C6D
29	c	516	DGD	CBB-CCB-CDB-CEB
23	B	607	CLA	C15-C16-C17-C18
27	A	410	LMG	C19-C20-C21-C22
28	f	101	SQD	C30-C31-C32-C33
26	A	409	PL9	C11-C12-C13-C14
29	h	102	DGD	C7A-C8A-C9A-CAA
29	h	102	DGD	CBB-CCB-CDB-CEB
24	A	406	PHO	C4-C3-C5-C6
23	B	609	CLA	C2-C3-C5-C6
23	d	402	CLA	C2C-C3C-CAC-CBC
29	o	301	DGD	CCB-CDB-CEB-CFB
35	F	101	HEM	CAD-CBD-CGD-O1D
36	V	201	HEC	CAD-CBD-CGD-O2D
23	c	511	CLA	O1D-CGD-O2D-CED
23	B	608	CLA	C16-C17-C18-C19
35	e	102	HEM	CAD-CBD-CGD-O1D
23	B	603	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	C2A-CAA-CBA-CGA
23	A	407	CLA	C5-C6-C7-C8
28	b	601	SQD	C24-C25-C26-C27
27	C	519	LMG	C34-C35-C36-C37
23	B	609	CLA	C4-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
27	B	620	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
29	C	518	DGD	C6A-C7A-C8A-C9A
23	B	608	CLA	C11-C12-C13-C14
23	C	502	CLA	C14-C13-C15-C16
23	C	503	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C12-C13-C14
23	C	512	CLA	C11-C10-C8-C9
23	b	614	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	511	CLA	C11-C10-C8-C9
24	A	406	PHO	C14-C13-C15-C16
24	a	407	PHO	C14-C13-C15-C16
23	A	404	CLA	C2C-C3C-CAC-CBC
28	f	101	SQD	C33-C34-C35-C36
28	B	624	SQD	C11-C10-C9-C8
27	D	411	LMG	C7-C8-C9-O8
29	c	516	DGD	O1G-C1G-C2G-C3G
31	Y	101	BCR	C35-C13-C14-C15
31	b	619	BCR	C11-C10-C9-C34
31	c	521	BCR	C11-C10-C9-C34
35	F	101	HEM	CAD-CBD-CGD-O2D
23	B	603	CLA	C16-C17-C18-C19
23	D	404	CLA	O2A-C1-C2-C3
23	b	602	CLA	O2A-C1-C2-C3
31	c	515	BCR	C37-C22-C23-C24
28	B	624	SQD	C29-C30-C31-C32
29	c	516	DGD	C1B-C2B-C3B-C4B
29	A	414	DGD	C7A-C8A-C9A-CAA
27	A	410	LMG	C9-C8-O7-C10
28	f	101	SQD	C44-C45-O47-C7
28	f	101	SQD	C46-C45-O47-C7
29	o	301	DGD	C3G-C2G-O2G-C1B
23	C	506	CLA	C10-C11-C12-C13
23	B	602	CLA	C1A-C2A-CAA-CBA
23	b	605	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	B	605	CLA	C12-C13-C15-C16
23	a	406	CLA	C6-C7-C8-C10
23	b	602	CLA	C11-C12-C13-C15
23	b	607	CLA	C11-C12-C13-C15
23	b	608	CLA	C11-C12-C13-C15
23	c	501	CLA	C11-C12-C13-C15
23	d	404	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	B	622	LMG	C34-C35-C36-C37
27	b	621	LMG	C36-C37-C38-C39
33	D	410	LHG	C31-C32-C33-C34
33	B	623	LHG	C16-C17-C18-C19
28	b	601	SQD	C14-C15-C16-C17
23	B	603	CLA	C13-C15-C16-C17
29	H	102	DGD	CBB-CCB-CDB-CEB
26	a	410	PL9	C3-C7-C8-C9
27	b	623	LMG	C42-C43-C44-C45
23	d	402	CLA	C15-C16-C17-C18
28	B	624	SQD	C31-C32-C33-C34
29	A	414	DGD	CDA-CEA-CFA-CGA
29	H	102	DGD	CAA-CBA-CCA-CDA
33	E	101	LHG	C26-C27-C28-C29
23	B	606	CLA	C16-C17-C18-C19
23	B	615	CLA	C4-C3-C5-C6
23	c	512	CLA	C4-C3-C5-C6
33	d	407	LHG	C28-C29-C30-C31
23	B	607	CLA	C10-C11-C12-C13
23	c	506	CLA	C10-C11-C12-C13
23	b	612	CLA	C2-C3-C5-C6
35	e	102	HEM	CAD-CBD-CGD-O2D
23	C	502	CLA	C10-C11-C12-C13
23	C	513	CLA	O1D-CGD-O2D-CED
29	c	517	DGD	C4A-C5A-C6A-C7A
31	c	521	BCR	C20-C21-C22-C23
27	d	410	LMG	C15-C16-C17-C18
33	e	101	LHG	O7-C5-C6-O8
28	A	412	SQD	C8-C7-O47-C45
27	C	519	LMG	O10-C28-O8-C9
33	e	101	LHG	C15-C16-C17-C18
23	a	405	CLA	C16-C17-C18-C20
23	b	611	CLA	C16-C17-C18-C19
27	b	623	LMG	C35-C36-C37-C38
29	C	516	DGD	C6A-C7A-C8A-C9A
29	H	102	DGD	CCA-CDA-CEA-CFA
33	E	101	LHG	C13-C14-C15-C16
33	L	101	LHG	C11-C10-C9-C8
36	v	201	HEC	CAD-CBD-CGD-O1D
27	c	519	LMG	C32-C33-C34-C35
23	A	404	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C2-C1-O2A-CGA
23	D	403	CLA	C2-C1-O2A-CGA
23	C	510	CLA	C2-C3-C5-C6
27	b	621	LMG	C39-C40-C41-C42
23	a	405	CLA	C14-C13-C15-C16
23	a	405	CLA	C2C-C3C-CAC-CBC
29	C	518	DGD	C2B-C3B-C4B-C5B
23	a	405	CLA	C4C-C3C-CAC-CBC
29	c	517	DGD	C3B-C4B-C5B-C6B
23	C	512	CLA	C8-C10-C11-C12
23	c	507	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C20
33	d	409	LHG	O10-C23-O8-C6
31	B	618	BCR	C23-C24-C25-C30
31	c	521	BCR	C1-C6-C7-C8
27	c	524	LMG	O1-C7-C8-C9
27	c	524	LMG	C7-C8-C9-O8
29	C	516	DGD	CBA-CCA-CDA-CEA
36	V	201	HEC	CAD-CBD-CGD-O1D
23	B	608	CLA	C13-C15-C16-C17
29	c	516	DGD	C6A-C7A-C8A-C9A
25	k	101	8CT	C16-C17-C18-C19
27	d	410	LMG	C35-C36-C37-C38
23	B	601	CLA	C4-C3-C5-C6
25	A	408	8CT	C20-C21-C23-C24
36	v	201	HEC	CAD-CBD-CGD-O2D
27	B	620	LMG	C8-C7-O1-C1
23	B	607	CLA	C16-C17-C18-C19
23	a	405	CLA	C16-C17-C18-C19
23	D	403	CLA	C10-C11-C12-C13
33	D	410	LHG	O6-C4-C5-O7
29	c	516	DGD	C3A-C4A-C5A-C6A
23	b	617	CLA	CBA-CGA-O2A-C1
23	B	604	CLA	O1D-CGD-O2D-CED
33	e	101	LHG	O6-C4-C5-C6
29	h	102	DGD	O1B-C1B-C2B-C3B
23	B	615	CLA	C2-C3-C5-C6
23	C	502	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C12-C13-C15
23	C	511	CLA	C11-C12-C13-C15
23	b	606	CLA	C12-C13-C15-C16
23	c	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	A	406	PHO	C2-C3-C5-C6
33	d	409	LHG	C9-C10-C11-C12
33	L	101	LHG	C14-C15-C16-C17
28	D	408	SQD	O48-C23-C24-C25
29	C	517	DGD	C2D-C1D-O3G-C3G
27	c	524	LMG	C18-C19-C20-C21
28	a	412	SQD	C9-C10-C11-C12
23	c	504	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	C15-C16-C17-C18
23	B	612	CLA	CBA-CGA-O2A-C1
29	A	414	DGD	C2A-C1A-O1G-C1G
23	d	403	CLA	C4-C3-C5-C6
26	d	406	PL9	C40-C39-C41-C42
23	B	601	CLA	C2-C3-C5-C6
23	c	512	CLA	C2-C3-C5-C6
23	b	613	CLA	CAA-CBA-CGA-O2A
27	b	621	LMG	O8-C28-C29-C30
28	a	411	SQD	O47-C7-C8-C9
23	B	605	CLA	C14-C13-C15-C16
23	B	612	CLA	C11-C10-C8-C9
23	B	613	CLA	C11-C12-C13-C14
23	D	404	CLA	C14-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C14
23	b	613	CLA	C11-C10-C8-C9
23	D	403	CLA	C3-C5-C6-C7
27	B	620	LMG	C20-C21-C22-C23
23	B	602	CLA	C3A-C2A-CAA-CBA
23	C	504	CLA	C10-C11-C12-C13
23	b	617	CLA	O1A-CGA-O2A-C1
29	c	516	DGD	O1G-C1A-C2A-C3A
33	D	409	LHG	C18-C19-C20-C21
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	B	609	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	CAD-CBD-CGD-O2D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	C16-C17-C18-C20
23	b	609	CLA	C2-C1-O2A-CGA
29	H	102	DGD	C7B-C8B-C9B-CAB
28	b	601	SQD	O47-C7-C8-C9
23	d	402	CLA	C4C-C3C-CAC-CBC
23	B	613	CLA	C4-C3-C5-C6
26	A	409	PL9	C40-C39-C41-C42
23	d	404	CLA	C5-C6-C7-C8
31	h	101	BCR	C11-C12-C13-C14
27	D	411	LMG	C29-C30-C31-C32
24	A	406	PHO	C2C-C3C-CAC-CBC
24	d	401	PHO	C2C-C3C-CAC-CBC
27	C	519	LMG	O1-C7-C8-C9
28	B	624	SQD	C25-C26-C27-C28
27	b	624	LMG	C29-C30-C31-C32
27	b	621	LMG	C14-C15-C16-C17
23	d	404	CLA	O2A-C1-C2-C3
24	A	406	PHO	O2A-C1-C2-C3
24	a	407	PHO	O2A-C1-C2-C3
33	e	101	LHG	C11-C10-C9-C8
23	C	509	CLA	C2A-CAA-CBA-CGA
23	B	612	CLA	CAA-CBA-CGA-O2A
28	D	408	SQD	C44-C45-C46-O48
27	c	519	LMG	C4-C5-C6-O5
23	C	511	CLA	C16-C17-C18-C19
29	c	518	DGD	O6D-C5D-C6D-O5D
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	CHA-CBD-CGD-O1D
23	d	402	CLA	CHA-CBD-CGD-O2D
31	H	101	BCR	C9-C10-C11-C12
23	C	513	CLA	C15-C16-C17-C18
27	b	621	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
28	A	412	SQD	O47-C7-C8-C9
23	B	611	CLA	C13-C15-C16-C17
27	B	622	LMG	O7-C10-C11-C12
28	B	624	SQD	C23-C24-C25-C26
27	b	623	LMG	O7-C10-C11-C12
28	A	413	SQD	C35-C36-C37-C38
29	H	102	DGD	C4E-C5E-C6E-O5E
24	A	406	PHO	CHA-CBD-CGD-O1D
27	d	410	LMG	C40-C41-C42-C43
27	D	411	LMG	C36-C37-C38-C39
33	l	101	LHG	C34-C35-C36-C37
23	B	605	CLA	C11-C12-C13-C15
23	B	612	CLA	C11-C10-C8-C7
23	D	403	CLA	C6-C7-C8-C10
23	c	512	CLA	C12-C13-C15-C16
23	d	403	CLA	C2-C3-C5-C6
26	A	409	PL9	C4-C3-C7-C8
26	a	410	PL9	C4-C3-C7-C8
23	b	614	CLA	CAA-CBA-CGA-O2A
23	B	601	CLA	C6-C7-C8-C9
23	B	605	CLA	C11-C12-C13-C14
23	C	510	CLA	C11-C12-C13-C14
23	b	602	CLA	C11-C12-C13-C14
23	c	501	CLA	C11-C12-C13-C14
23	c	513	CLA	C13-C15-C16-C17
23	c	510	CLA	CAA-CBA-CGA-O2A
28	a	411	SQD	C5-C6-S-O8
29	H	102	DGD	O1A-C1A-O1G-C1G
33	L	101	LHG	C19-C20-C21-C22
23	c	513	CLA	C2A-CAA-CBA-CGA
26	D	406	PL9	C21-C22-C23-C24
26	a	410	PL9	C21-C22-C23-C24
27	B	620	LMG	C33-C34-C35-C36
23	b	608	CLA	C13-C15-C16-C17
23	b	615	CLA	C16-C17-C18-C19
26	D	406	PL9	C12-C11-C9-C10
33	d	407	LHG	C33-C34-C35-C36
27	b	621	LMG	O10-C28-C29-C30
25	d	405	8CT	C10-C11-C12-C13
29	C	517	DGD	C9B-CAB-CBB-CCB
29	A	414	DGD	CBB-CCB-CDB-CEB
27	b	621	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	o	301	DGD	O1A-C1A-C2A-C3A
33	L	101	LHG	C17-C18-C19-C20
26	D	406	PL9	C46-C47-C48-C49
23	c	510	CLA	CAA-CBA-CGA-O1A
28	D	408	SQD	C35-C36-C37-C38
27	A	410	LMG	O1-C7-C8-C9
29	h	102	DGD	C1G-C2G-C3G-O3G
33	e	101	LHG	C4-C5-C6-O8
23	B	614	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	b	615	CLA	C2A-CAA-CBA-CGA
33	B	623	LHG	C3-O3-P-O6
23	b	613	CLA	CAA-CBA-CGA-O1A
28	a	411	SQD	O49-C7-C8-C9
29	c	516	DGD	O1B-C1B-C2B-C3B
23	b	615	CLA	C13-C15-C16-C17
29	c	517	DGD	CCB-CDB-CEB-CFB
23	C	510	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
27	C	519	LMG	O7-C10-C11-C12
29	H	102	DGD	C6B-C7B-C8B-C9B
29	A	414	DGD	C4A-C5A-C6A-C7A
29	C	516	DGD	C2E-C1E-O5D-C6D
23	C	505	CLA	C16-C17-C18-C19
23	B	612	CLA	CAA-CBA-CGA-O1A
27	b	623	LMG	O9-C10-C11-C12
29	c	518	DGD	O1B-C1B-C2B-C3B
25	c	514	8CT	C19-C20-C21-C22
33	D	410	LHG	O6-C4-C5-C6
25	A	408	8CT	C02-C03-C10-C11
25	t	101	8CT	C02-C03-C10-C11
25	t	101	8CT	C04-C03-C10-C11
29	c	518	DGD	C7B-C8B-C9B-CAB
33	l	101	LHG	C16-C17-C18-C19
23	a	406	CLA	C16-C17-C18-C19
25	t	101	8CT	C13-C14-C15-C16
23	c	508	CLA	C4-C3-C5-C6
31	h	101	BCR	C9-C10-C11-C12
23	A	405	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	608	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	d	402	CLA	CAD-CBD-CGD-O1D
27	A	410	LMG	C7-C8-O7-C10
28	A	412	SQD	C5-C6-S-O7
29	o	301	DGD	C1G-C2G-O2G-C1B
27	b	621	LMG	C32-C33-C34-C35
28	B	624	SQD	C35-C36-C37-C38
23	B	613	CLA	C13-C15-C16-C17
23	B	606	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
23	c	512	CLA	C14-C13-C15-C16
33	D	410	LHG	C15-C16-C17-C18
33	e	101	LHG	O10-C23-C24-C25
29	c	516	DGD	O2G-C1B-C2B-C3B
28	a	412	SQD	C28-C29-C30-C31
28	B	624	SQD	O47-C7-C8-C9
33	d	408	LHG	C23-C24-C25-C26
23	B	606	CLA	C16-C17-C18-C20
23	B	603	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C4-C3-C5-C6
23	b	612	CLA	C4-C3-C5-C6
23	B	601	CLA	C8-C10-C11-C12
23	c	507	CLA	C8-C10-C11-C12
23	B	601	CLA	C3A-C2A-CAA-CBA
23	B	611	CLA	C12-C13-C15-C16
23	C	503	CLA	C6-C7-C8-C10
23	C	505	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C10-C8-C7
23	b	613	CLA	C11-C10-C8-C7
28	A	412	SQD	C10-C11-C12-C13
29	C	516	DGD	O2G-C1B-C2B-C3B
31	c	515	BCR	C21-C22-C23-C24
31	h	101	BCR	C17-C18-C19-C20
23	c	501	CLA	CAA-CBA-CGA-O2A
28	a	411	SQD	O48-C23-C24-C25
29	c	516	DGD	O1A-C1A-O1G-C1G
27	B	620	LMG	O9-C10-O7-C8
23	b	614	CLA	CAA-CBA-CGA-O1A

Continued on next page...

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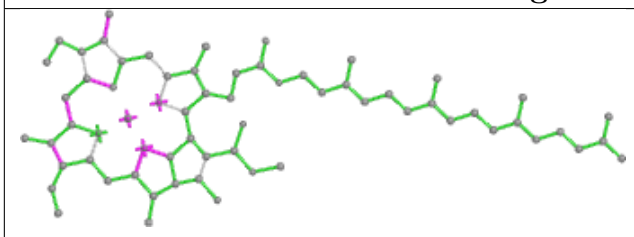
Mol	Chain	Res	Type	Atoms
23	C	513	CLA	CBD-CGD-O2D-CED
33	L	101	LHG	O7-C7-C8-C9
27	D	407	LMG	O7-C10-C11-C12
33	l	101	LHG	O7-C7-C8-C9

There are no ring outliers.

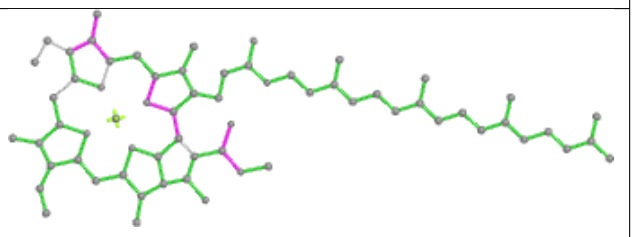
No monomer is involved in short contacts.

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

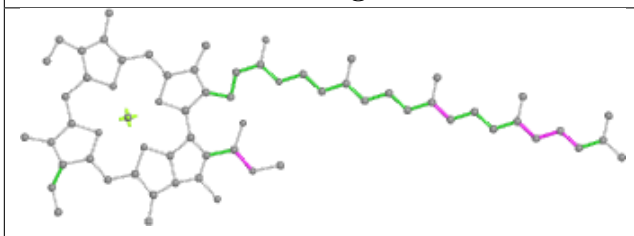
Ligand CLA c 511



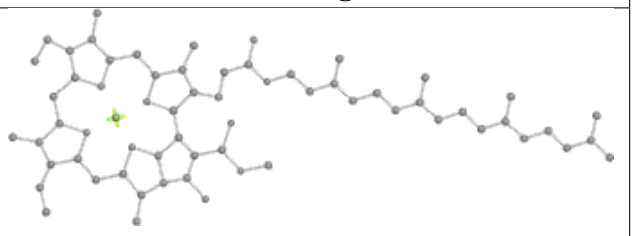
Bond lengths



Bond angles

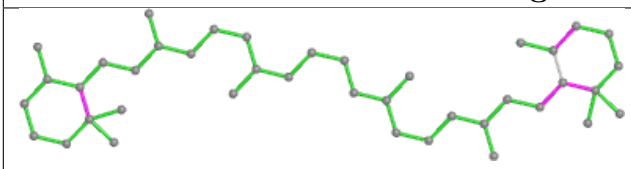


Torsions

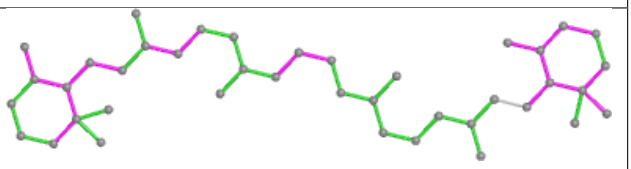


Rings

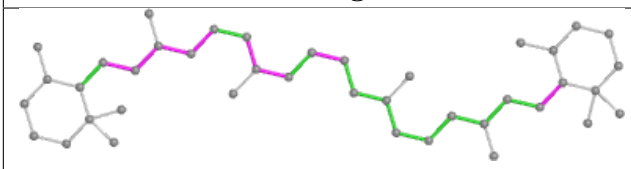
Ligand 8CT b 620



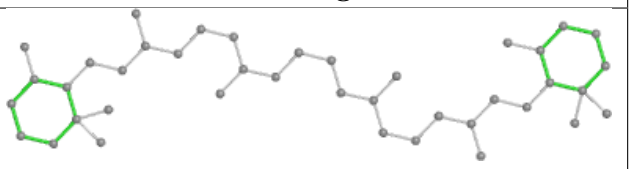
Bond lengths



Bond angles

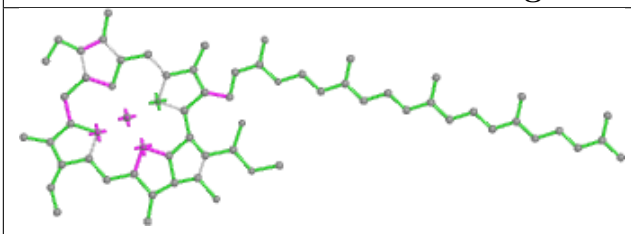


Torsions

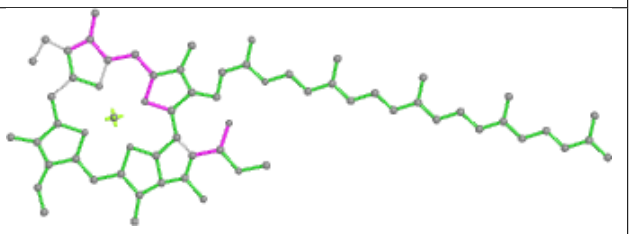


Rings

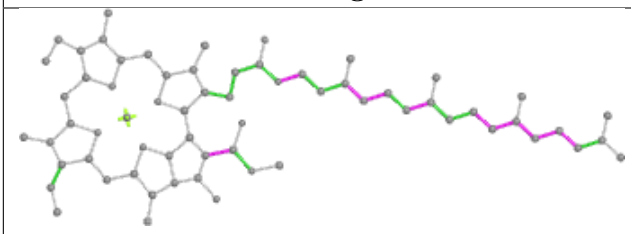
Ligand CLA C 506



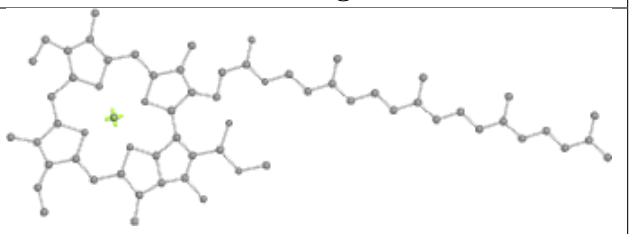
Bond lengths



Bond angles

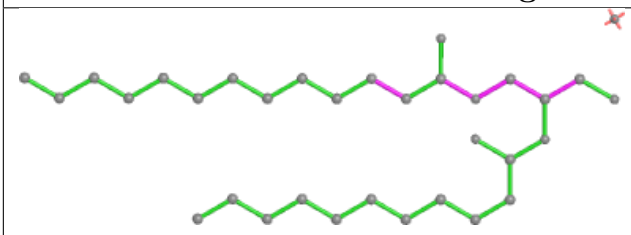


Torsions

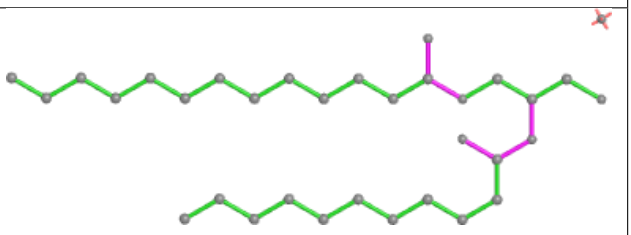


Rings

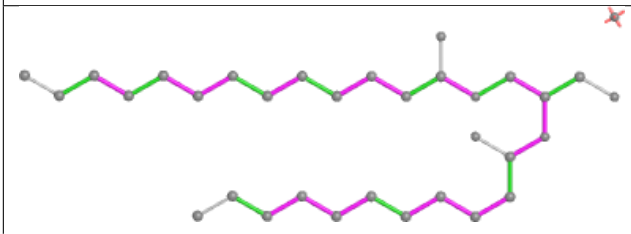
Ligand LMG D 411



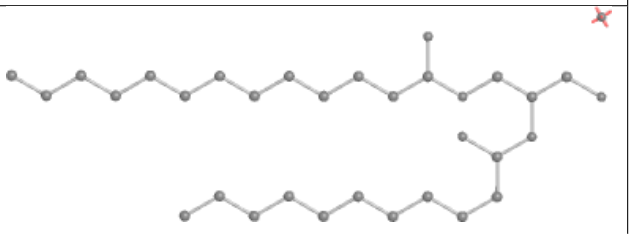
Bond lengths



Bond angles



Torsions



Rings

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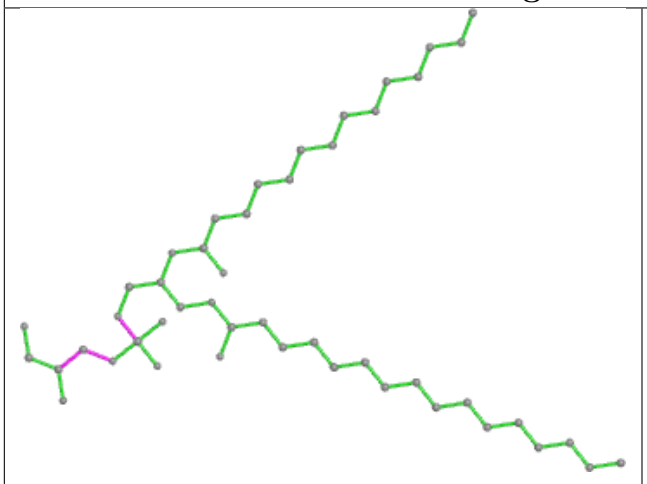

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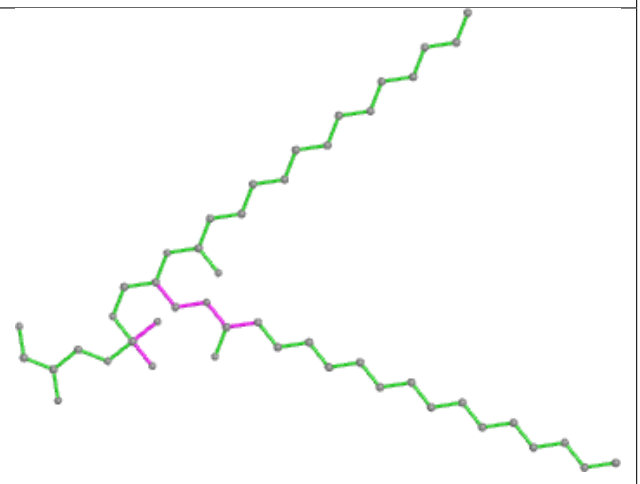
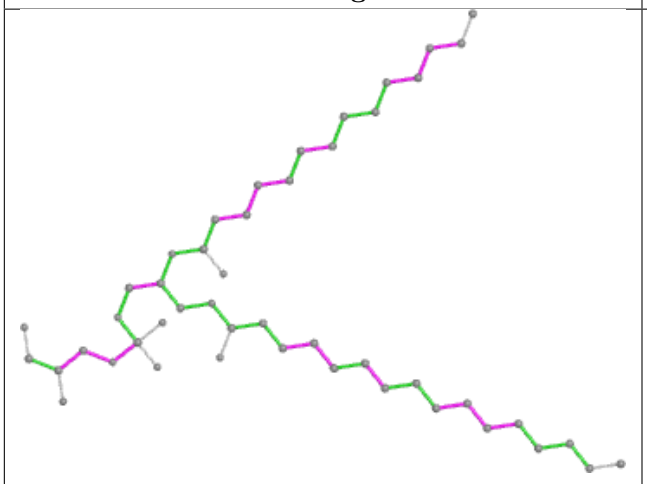


Bond angles



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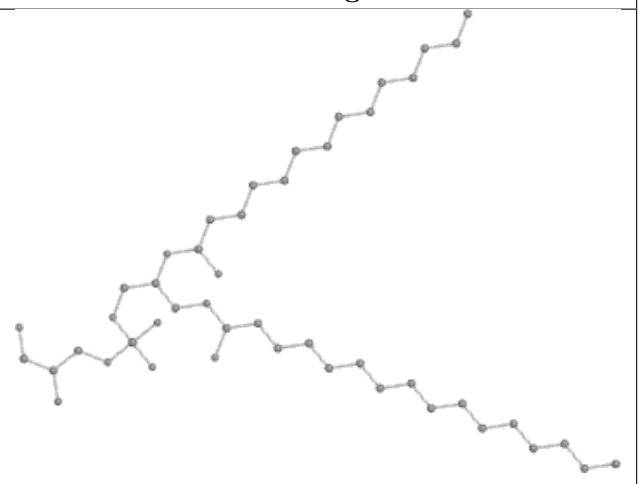
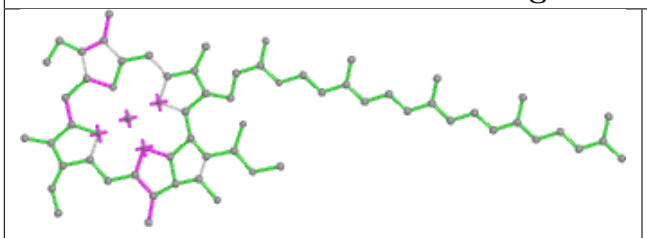


Rings

Ligand CLA a 406



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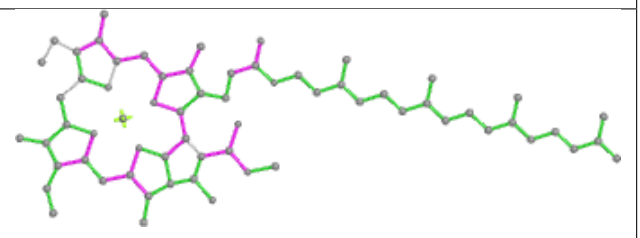
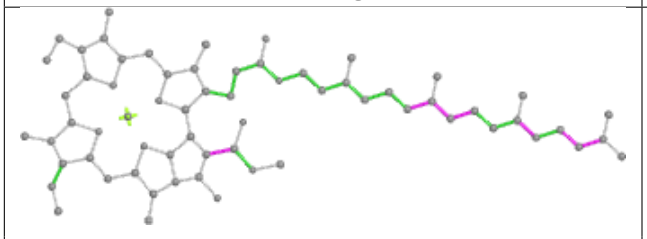


Bond angles



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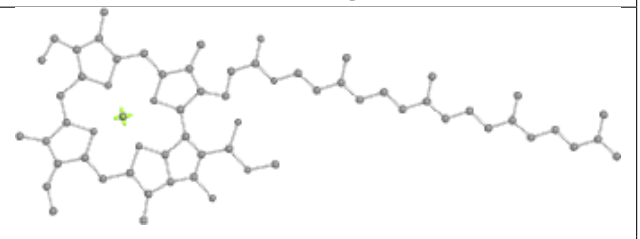

Rings

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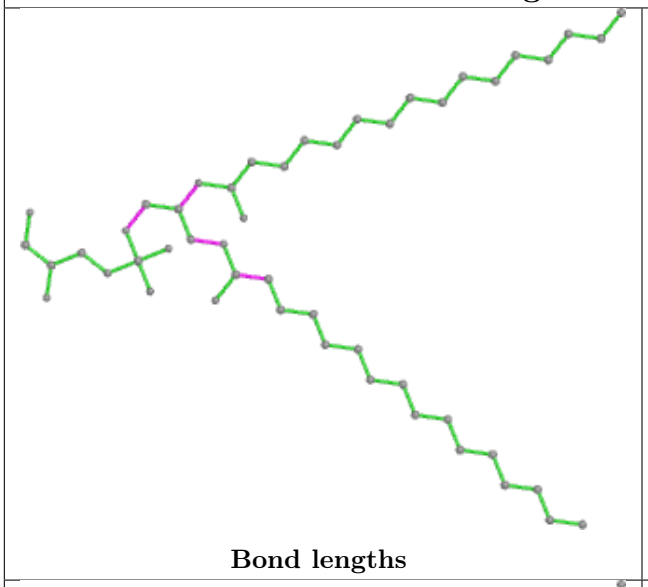

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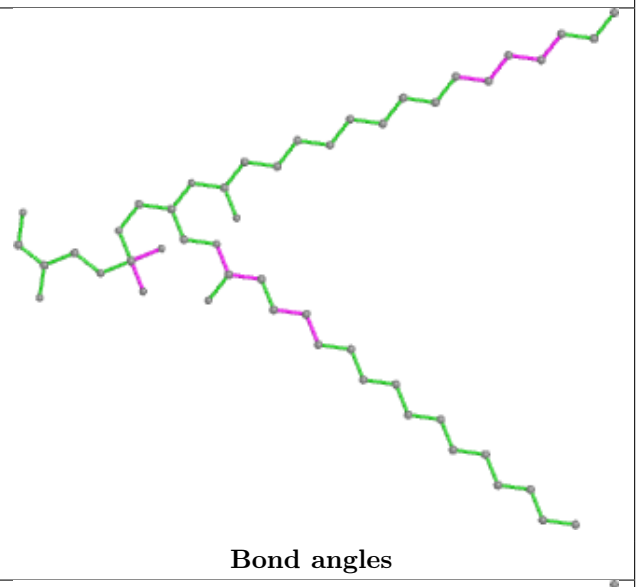
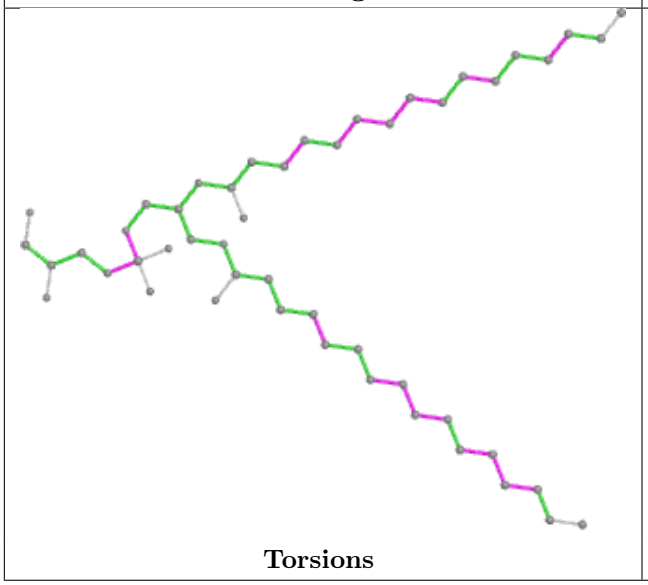


Bond angles



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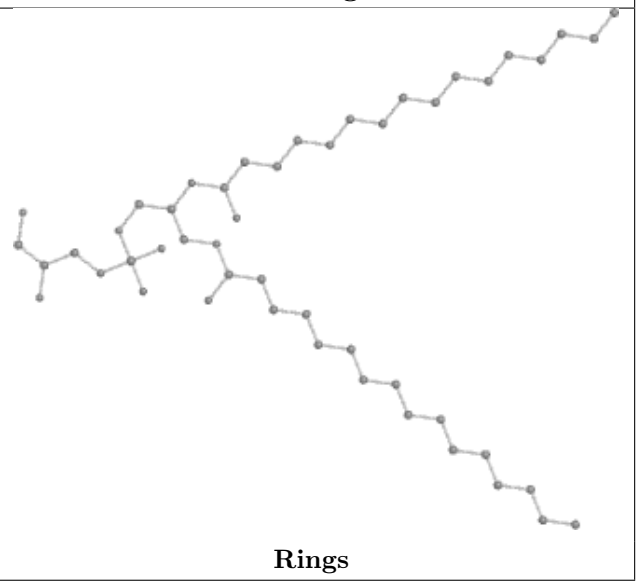
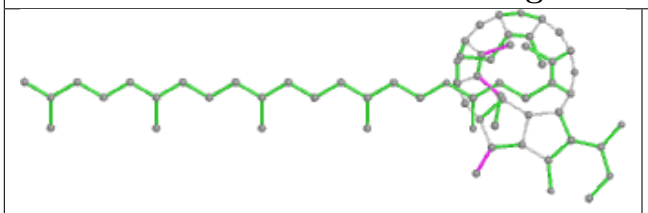


Rings

Ligand PHO d 401



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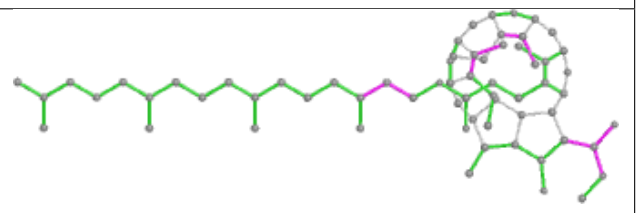
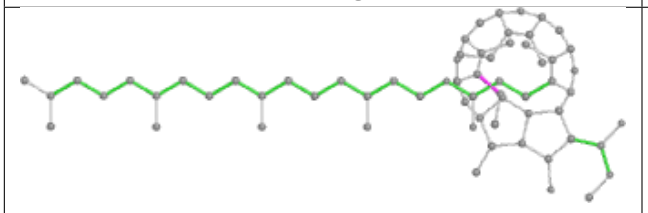
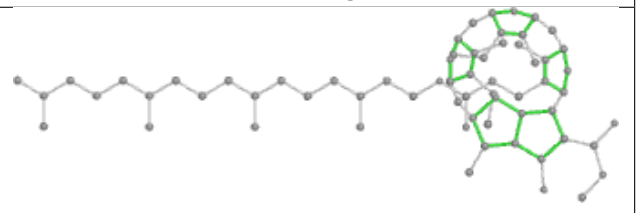


Bond angles

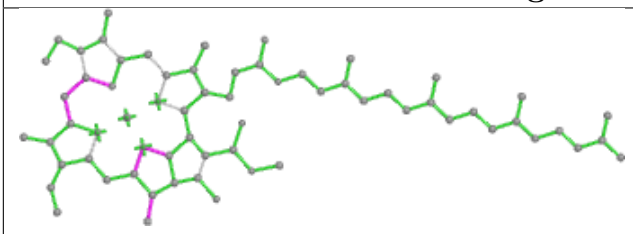


Torsions



Rings

Ligand CLA b 606



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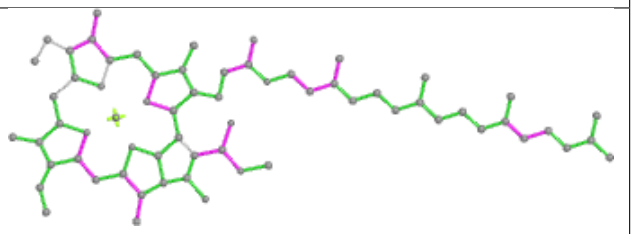
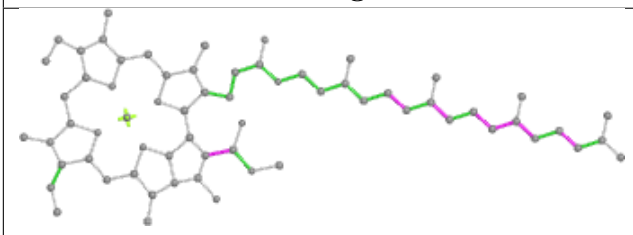


Bond angles



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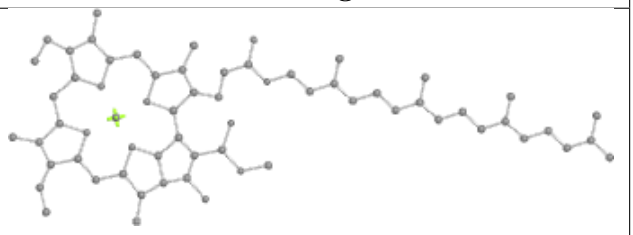
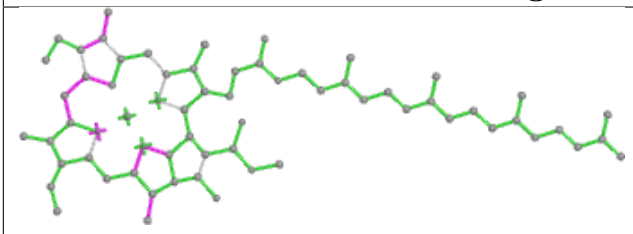


Rings

Ligand CLA b 612



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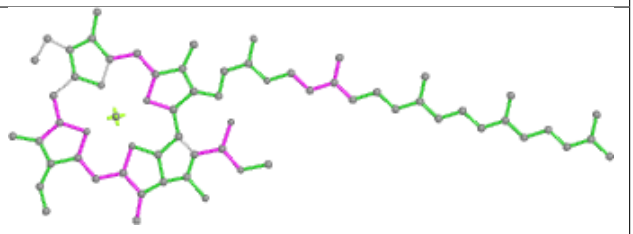
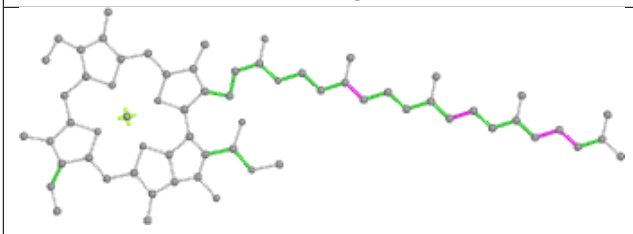
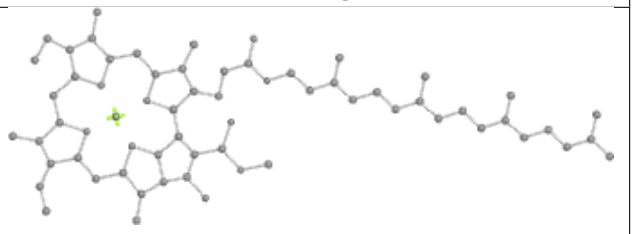


Bond angles

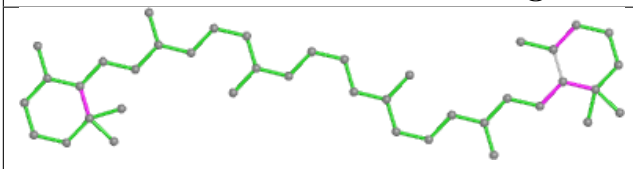


Torsions

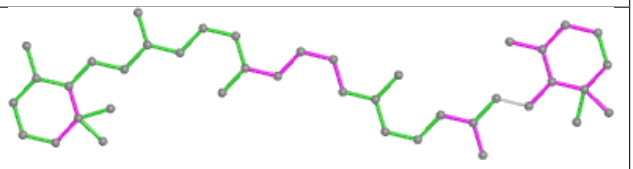


Rings

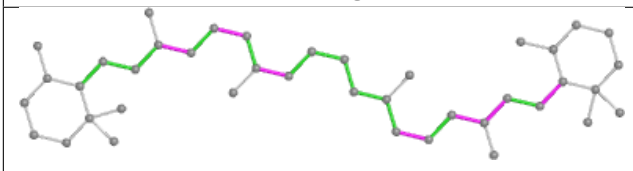
Ligand 8CT C 520



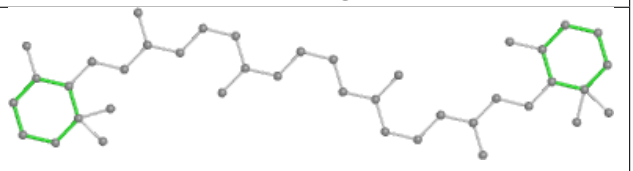
Bond lengths



Bond angles

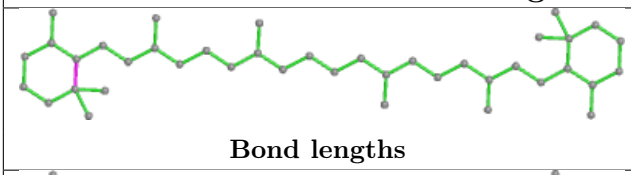


Torsions

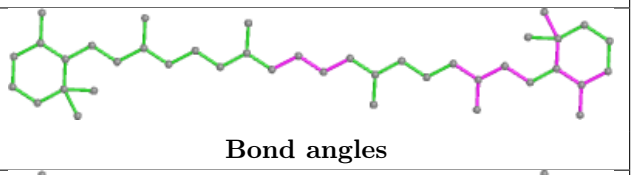


Rings

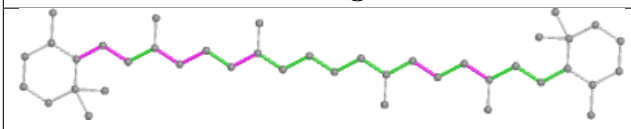
Ligand BCR c 521



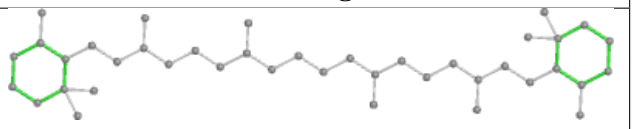
Bond lengths



Bond angles

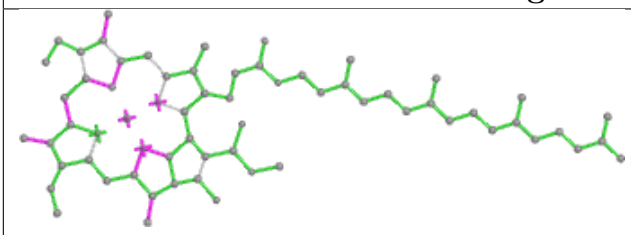


Torsions

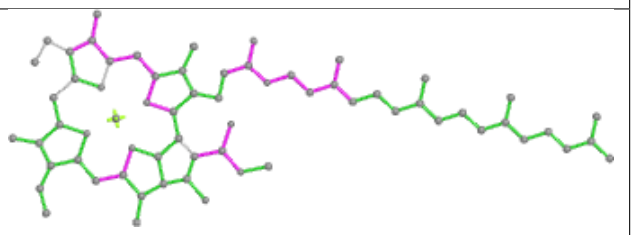


Rings

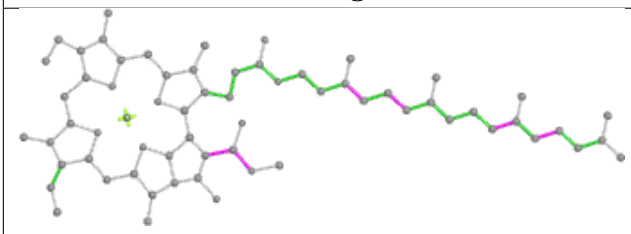
Ligand CLA b 604



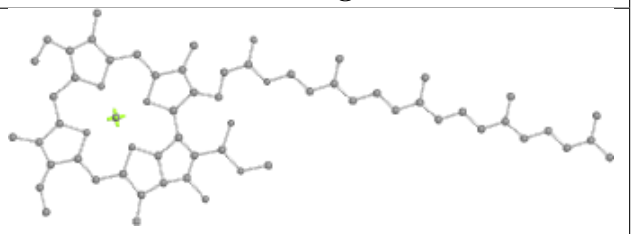
Bond lengths



Bond angles

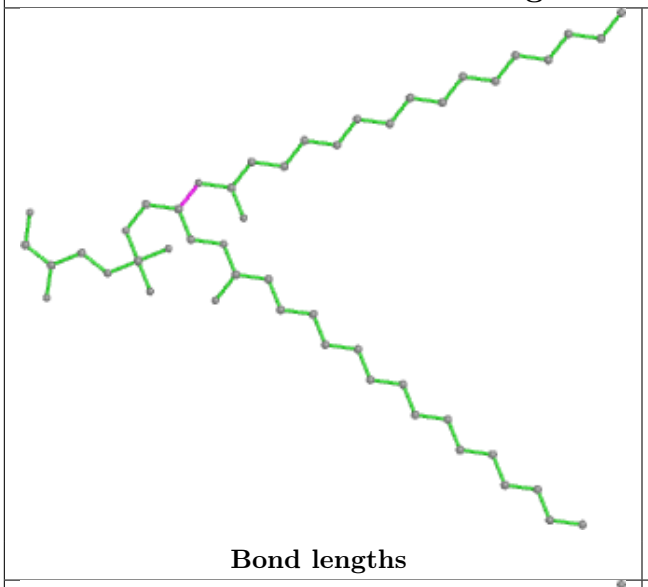


Torsions

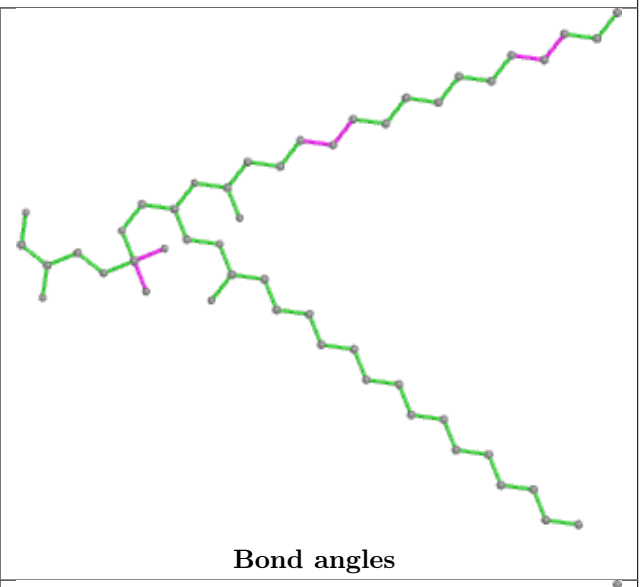


Rings

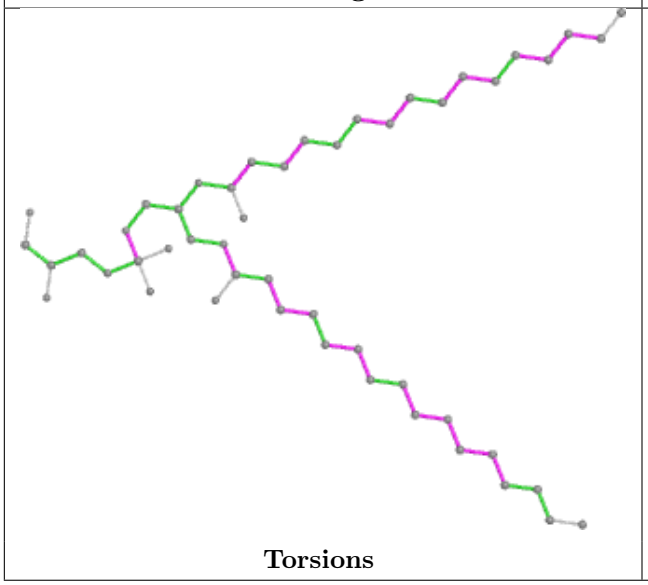
Ligand LHG L 101



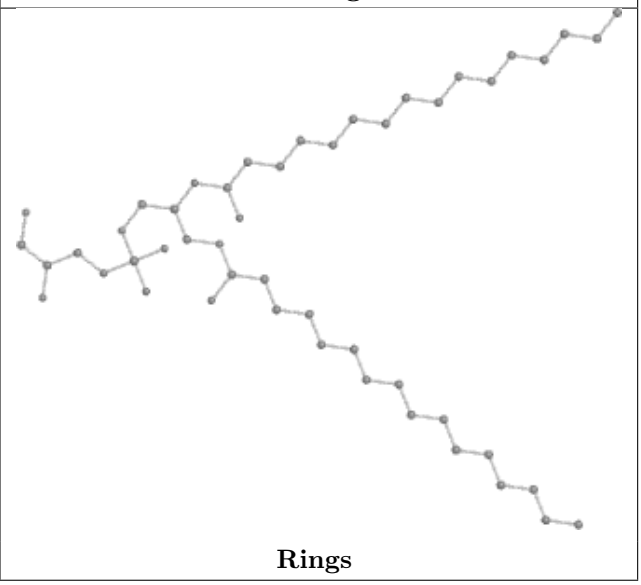
Bond lengths



Bond angles

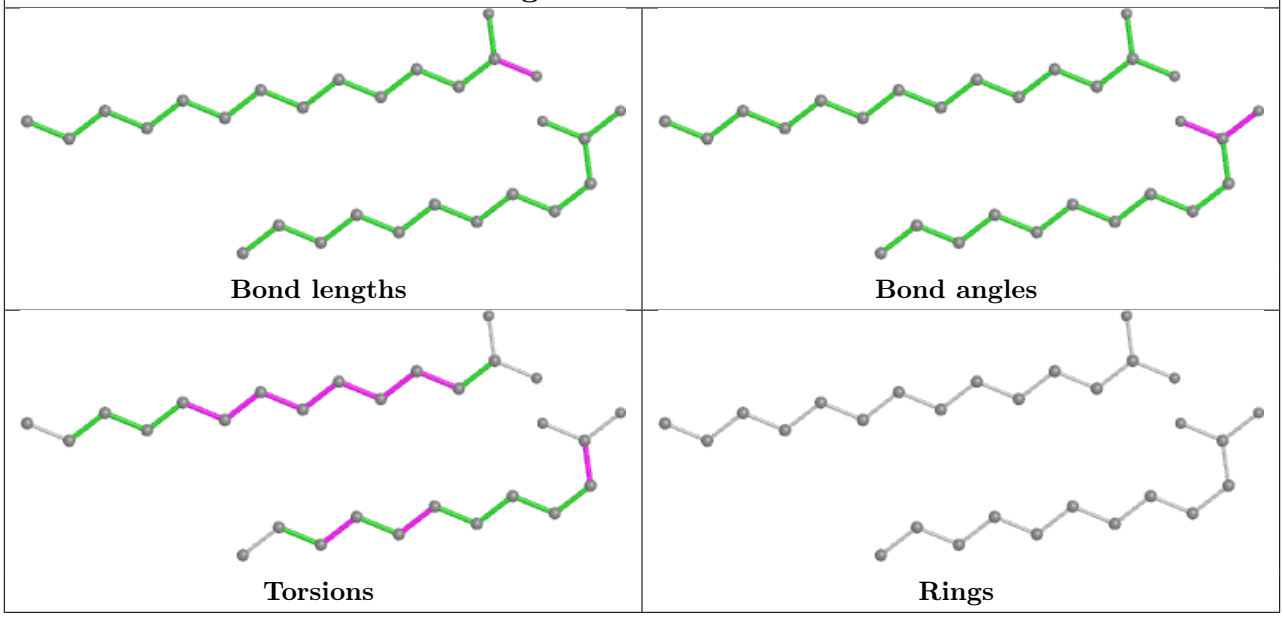


Torsions

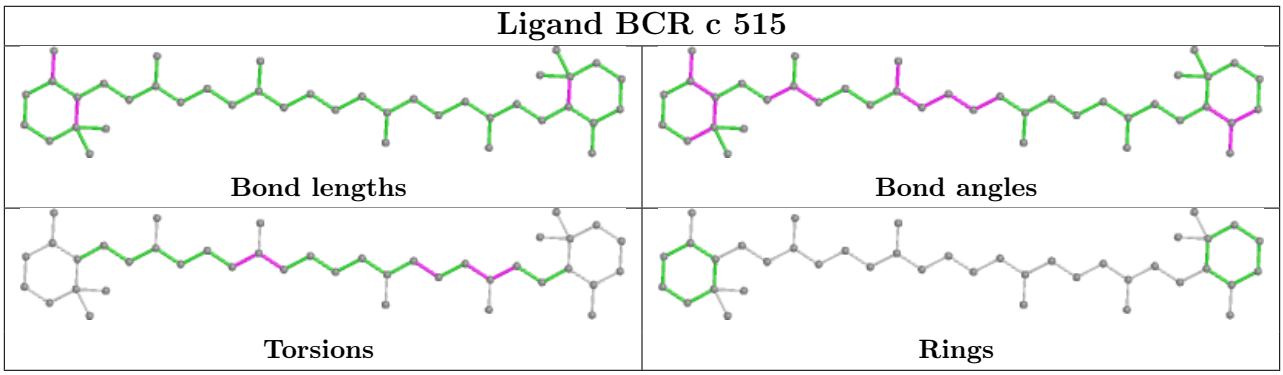


Rings

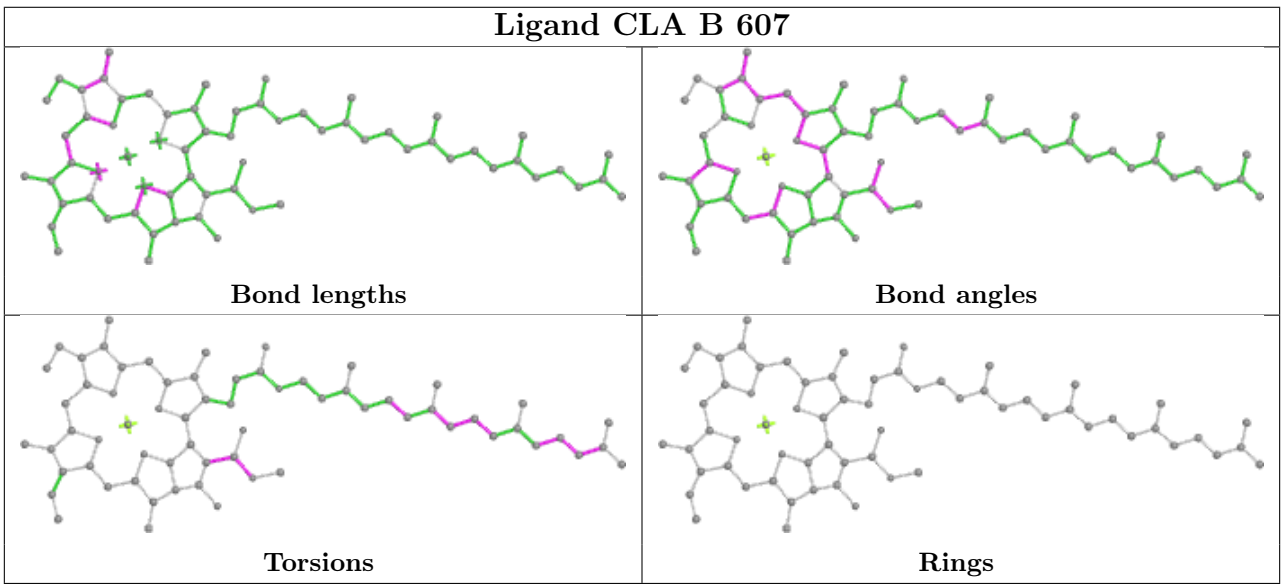
Ligand LMG B 622



Ligand BCR c 515



Ligand CLA B 607



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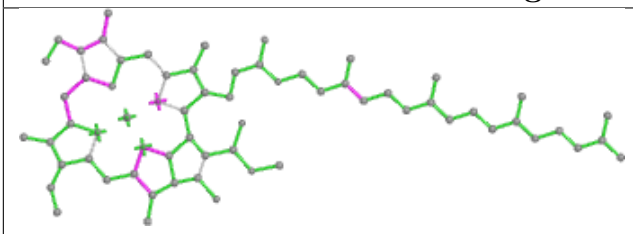
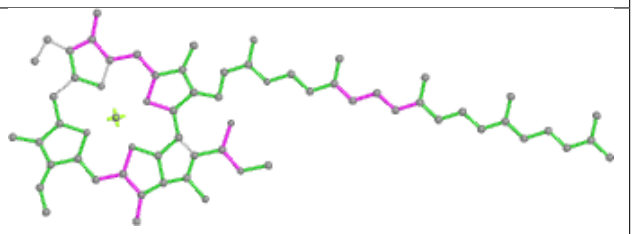
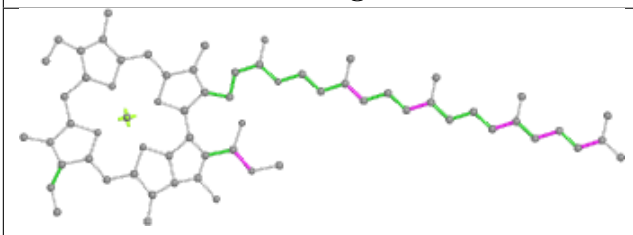


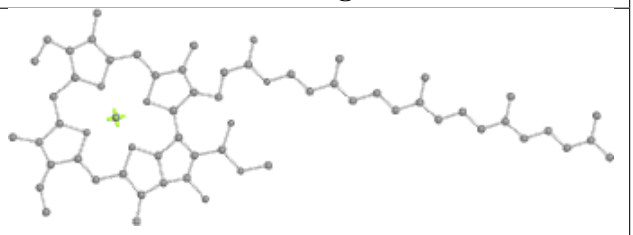
Bond lengths



Bond angles

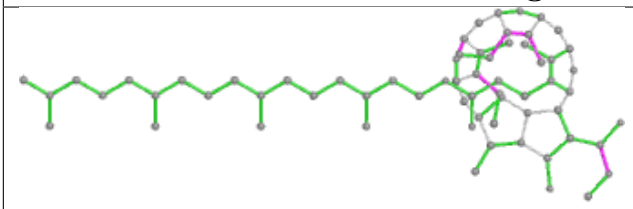


Torsions



Rings

Ligand PHO a 407



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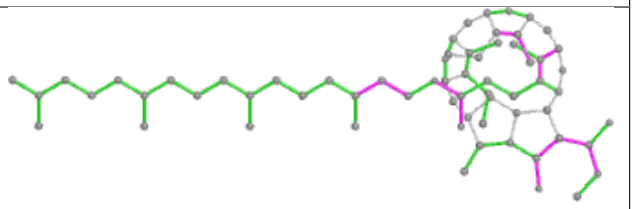
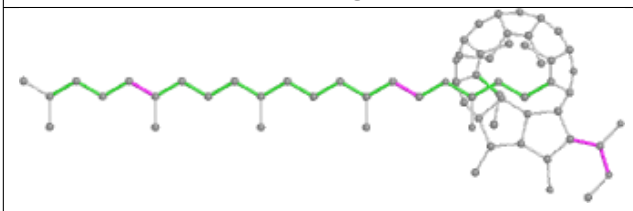


Bond angles



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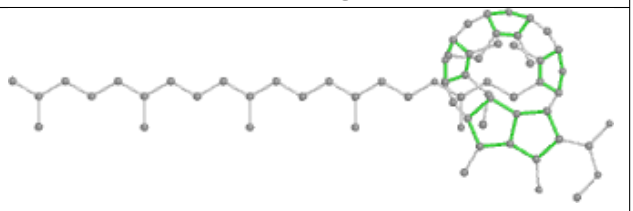
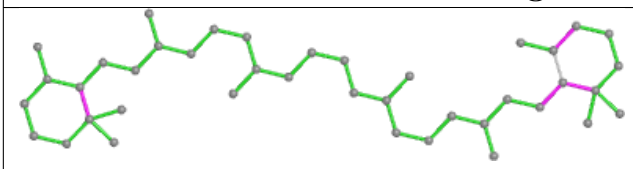


Rings

Ligand 8CT C 514



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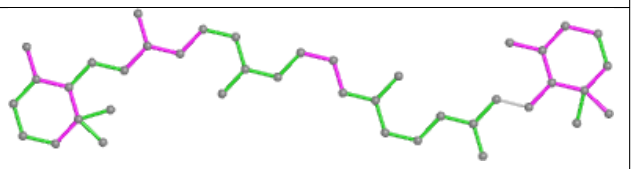
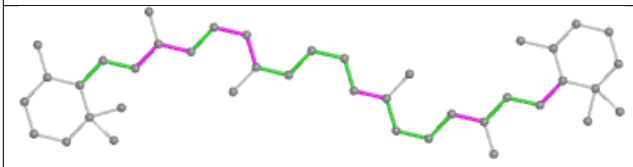


Bond angles



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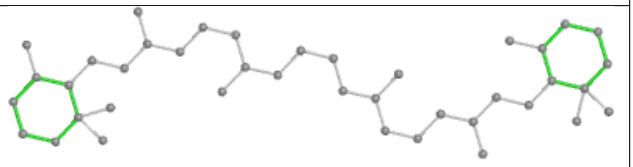
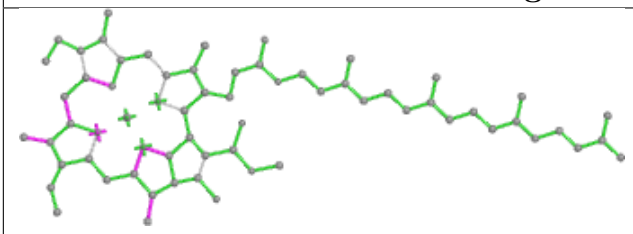
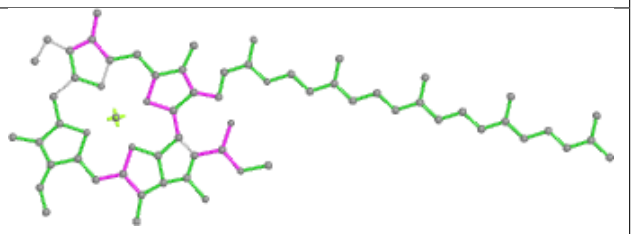


Rings

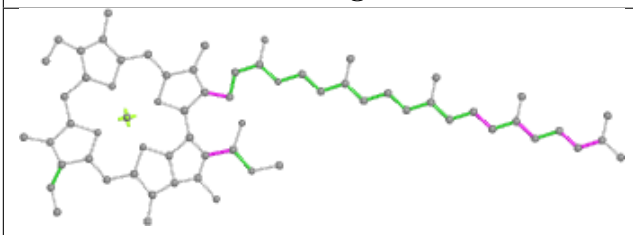
Ligand CLA C 502



Bond lengths



Bond angles



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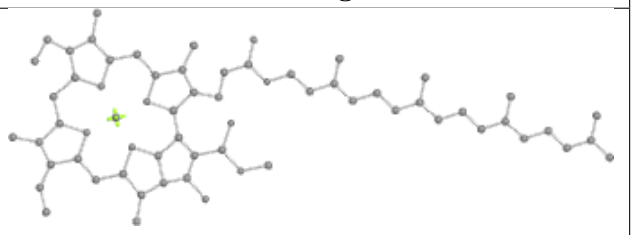

Rings

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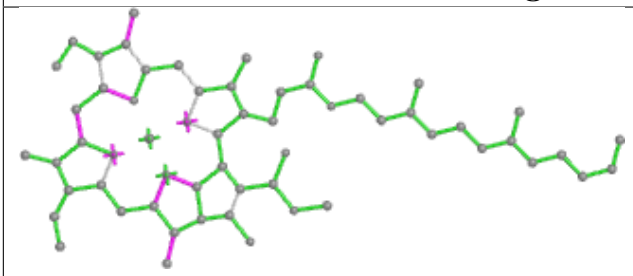

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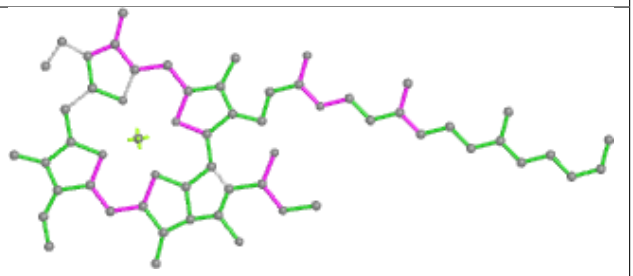
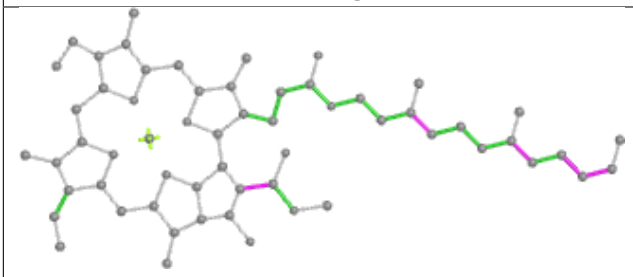
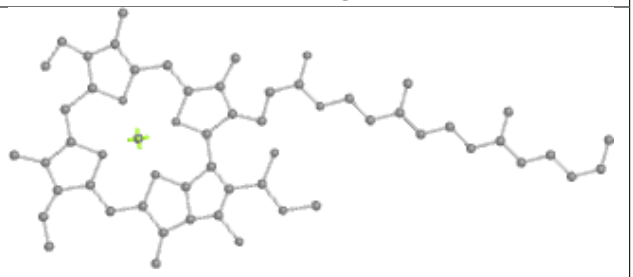


Bond angles

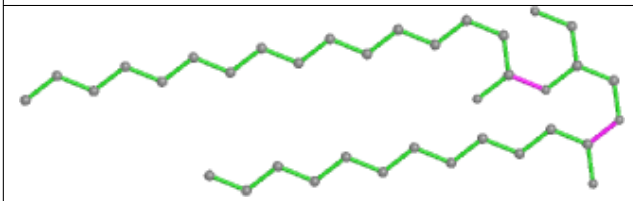


Torsions



Rings

Ligand SQD a 412



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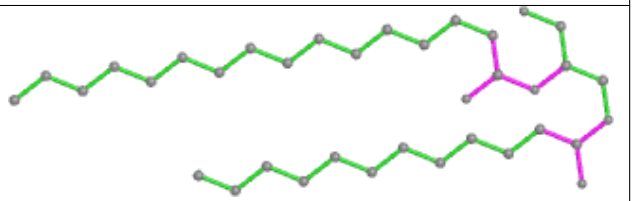
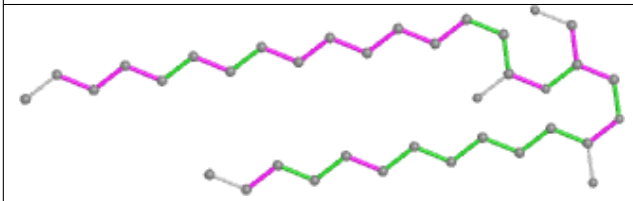


Bond angles



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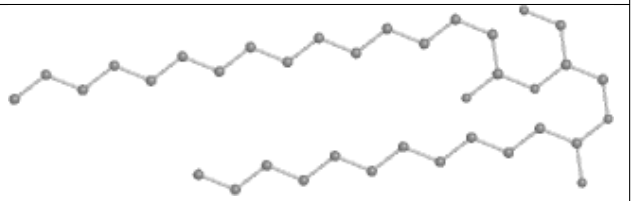

Rings

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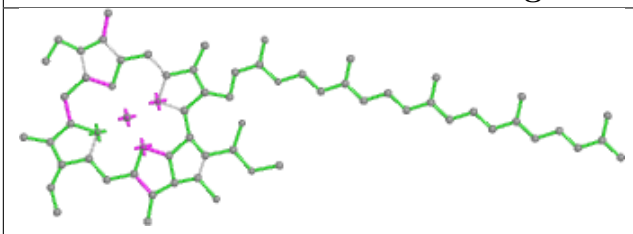

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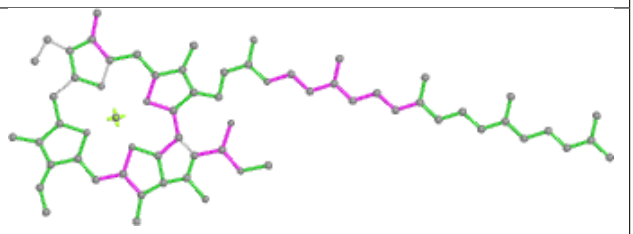
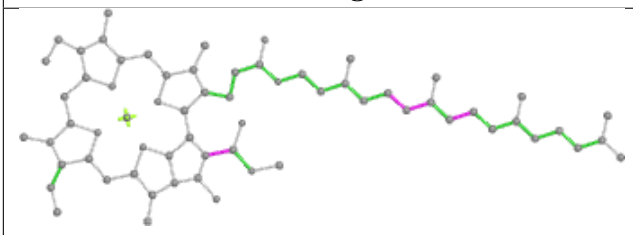


Bond angles



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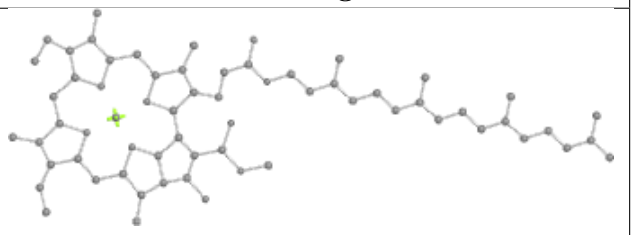
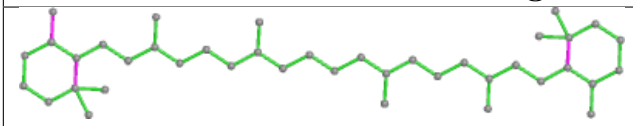


Rings

Ligand BCR a 409



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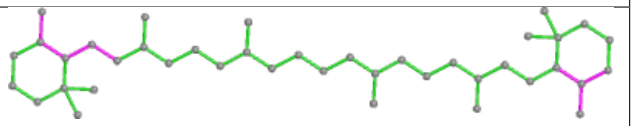
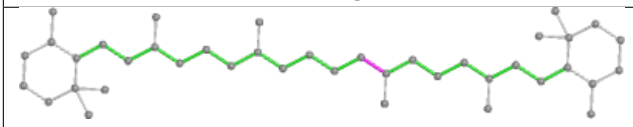


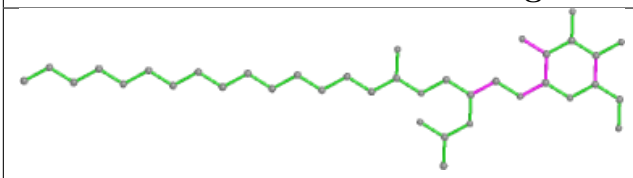
Bond angles



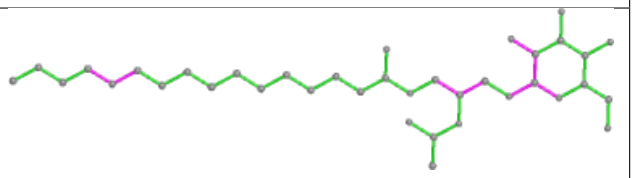
Torsions

Rings

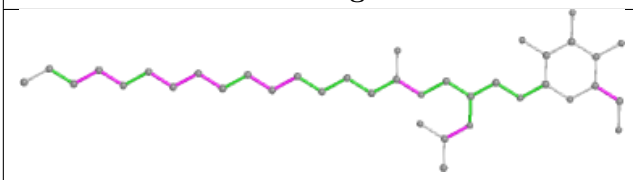
Ligand LMG c 519



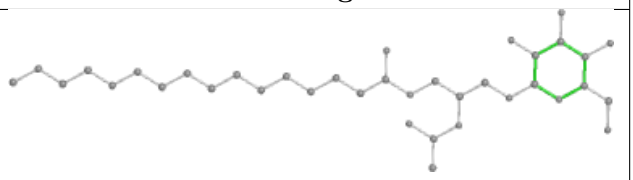
Bond lengths



Bond angles

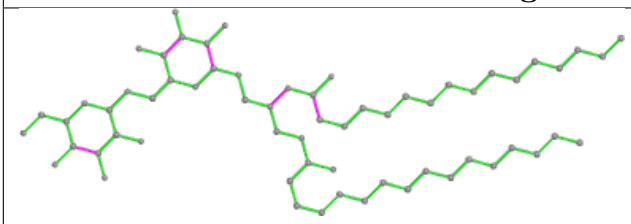


Torsions



Rings

Ligand DGD C 516



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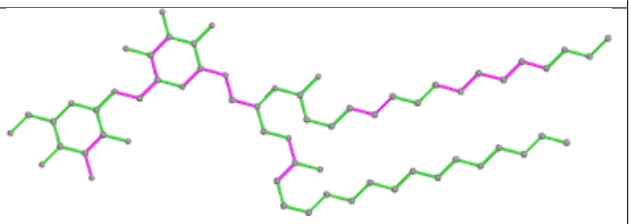
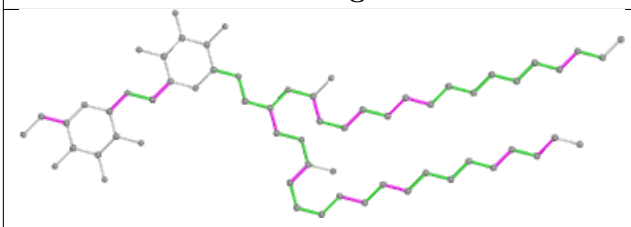
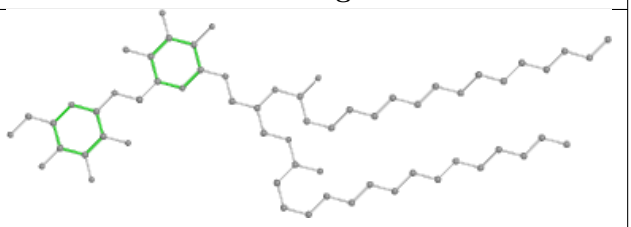


Bond angles

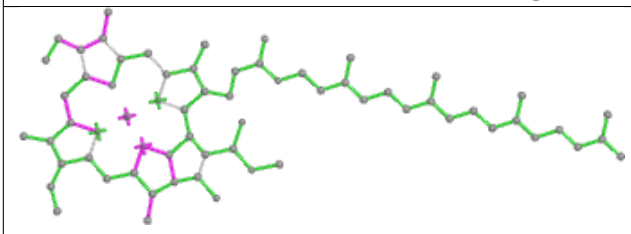


Torsions



Rings

Ligand CLA b 611



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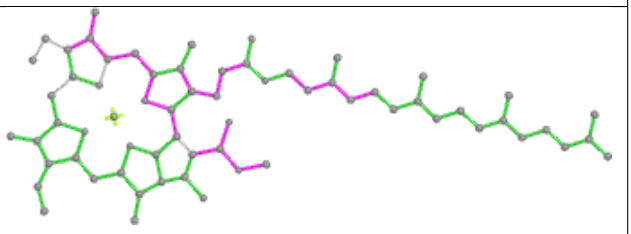
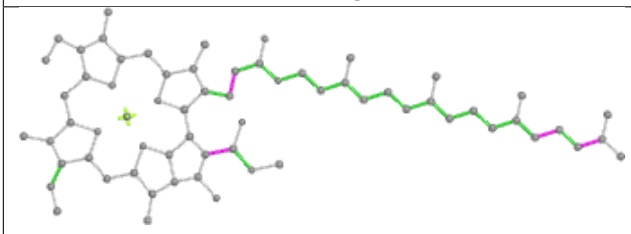
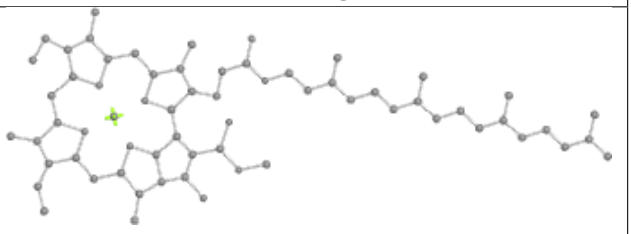


Bond angles

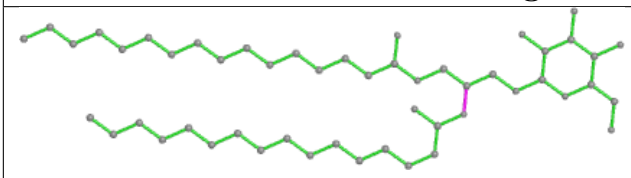


Torsions

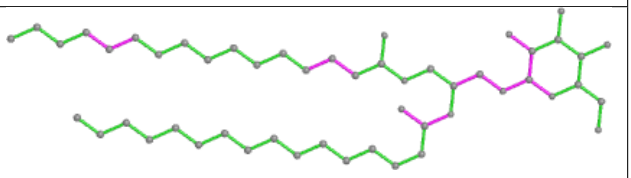


Rings

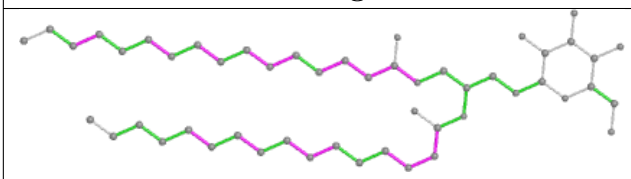
Ligand LMG b 621



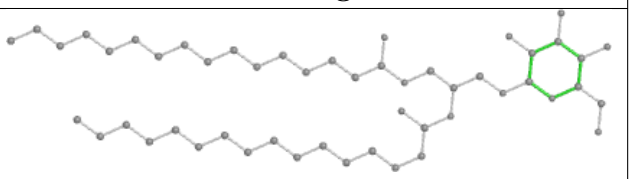
Bond lengths



Bond angles

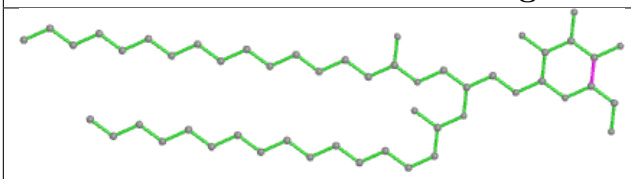


Torsions



Rings

Ligand LMG D 407



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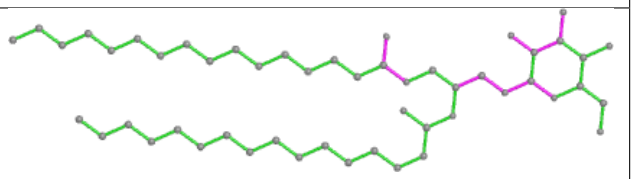

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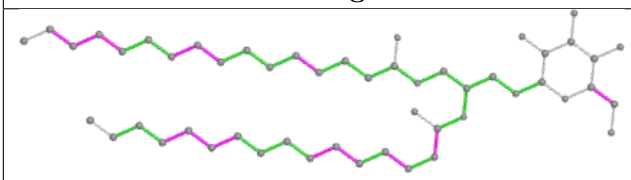
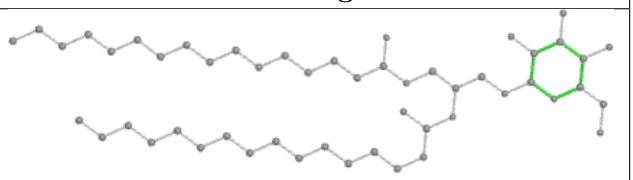
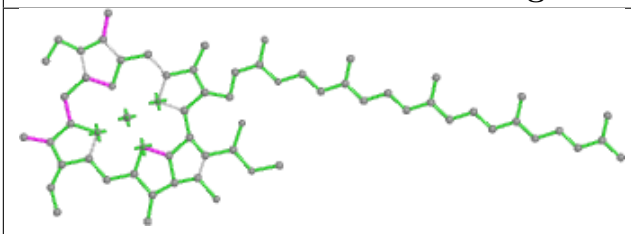


Torsions



Rings

Ligand CLA b 613



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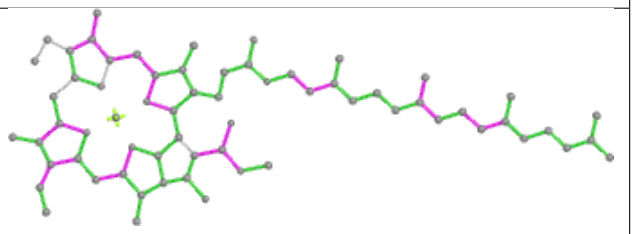
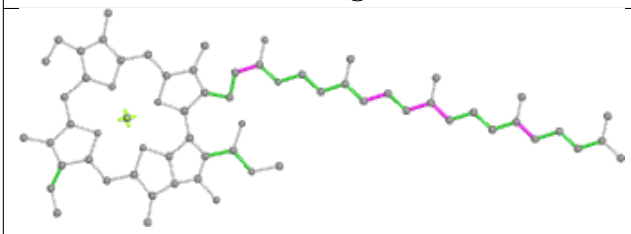


Bond angles



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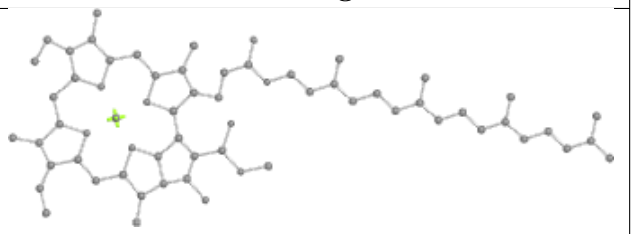
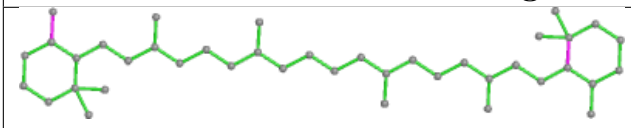


Rings

Ligand BCR H 101



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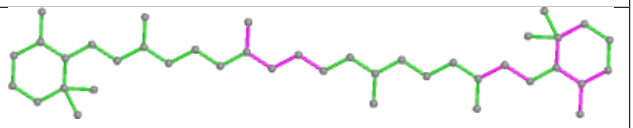
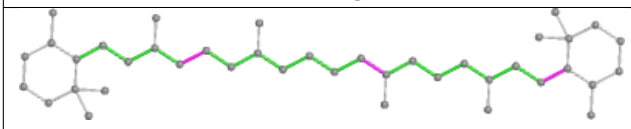


Bond angles



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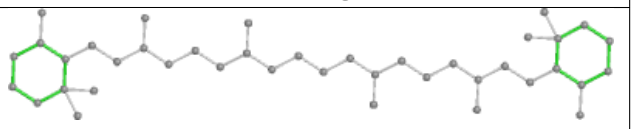
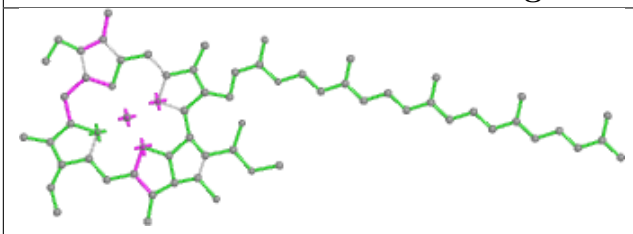
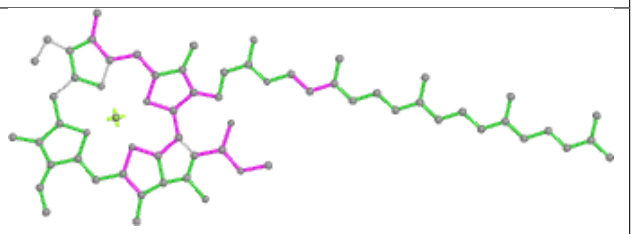


Rings

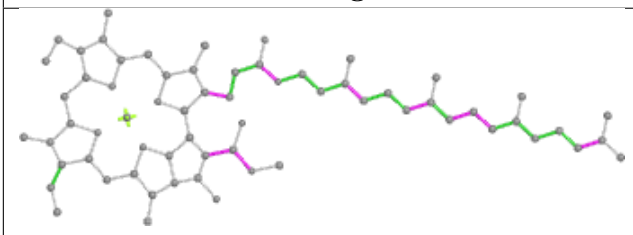
Ligand CLA B 601



Bond lengths



Bond angles



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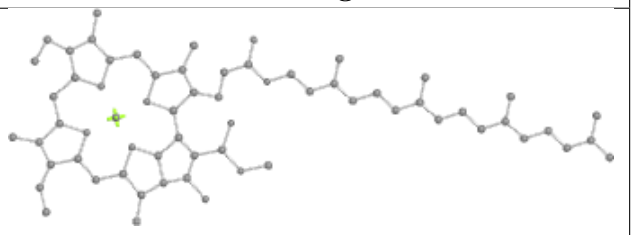
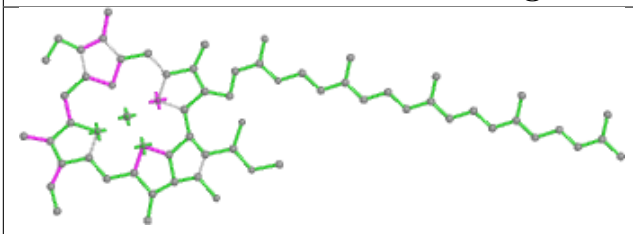


Rings

Ligand CLA A 405



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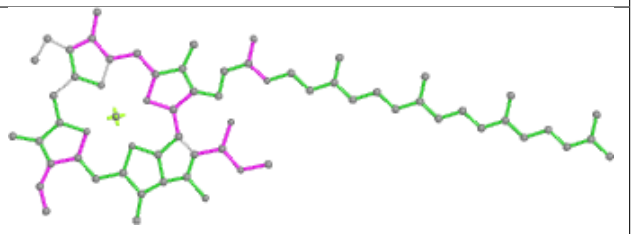
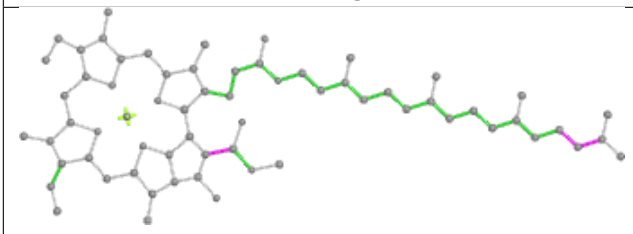


Bond angles



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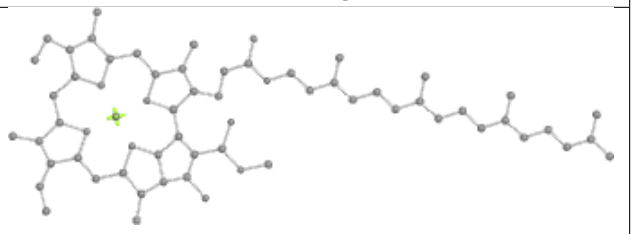
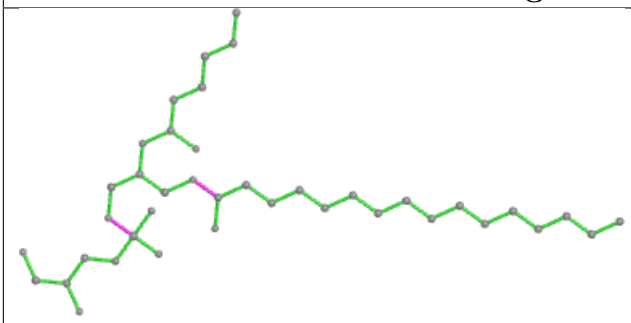


Rings

Ligand LHG d 409



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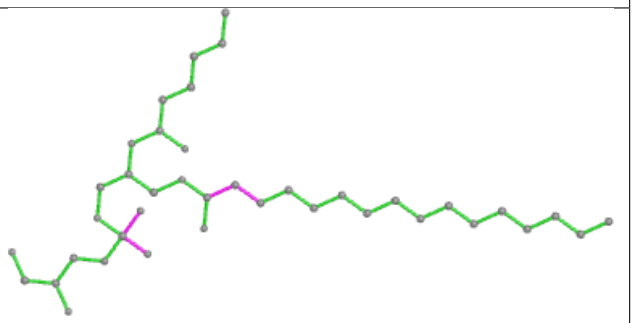

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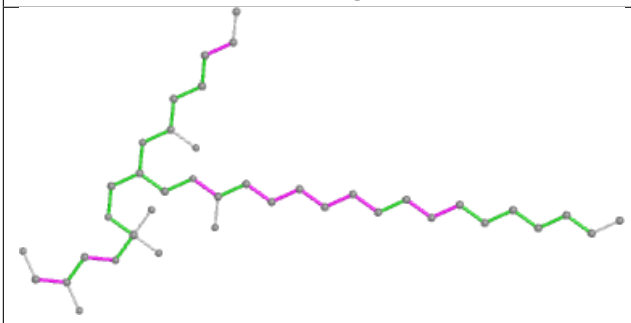

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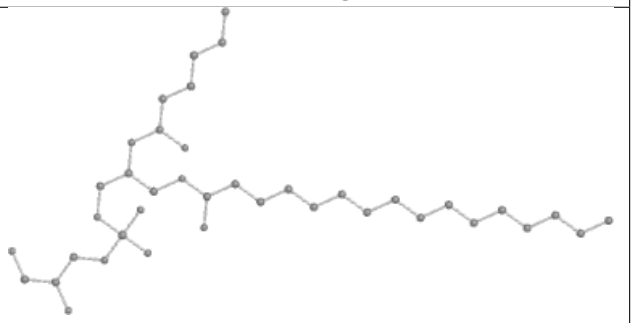
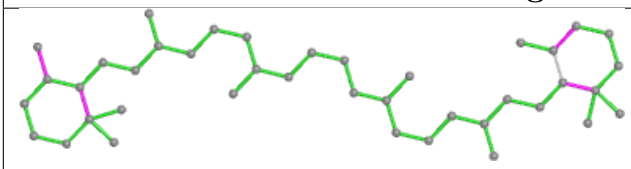


Rings

Ligand 8CT A 408



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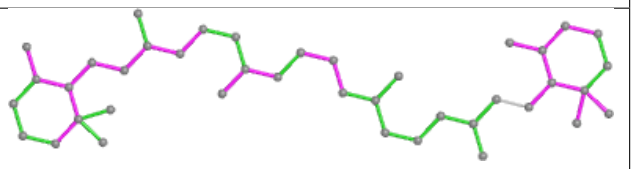
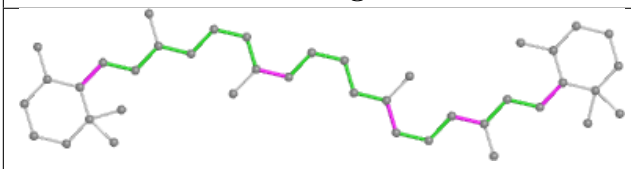


Bond angles



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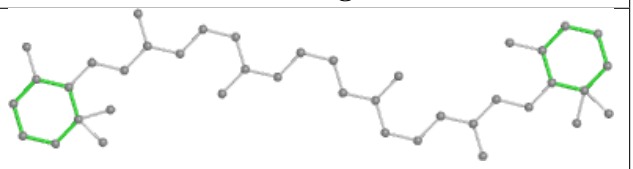
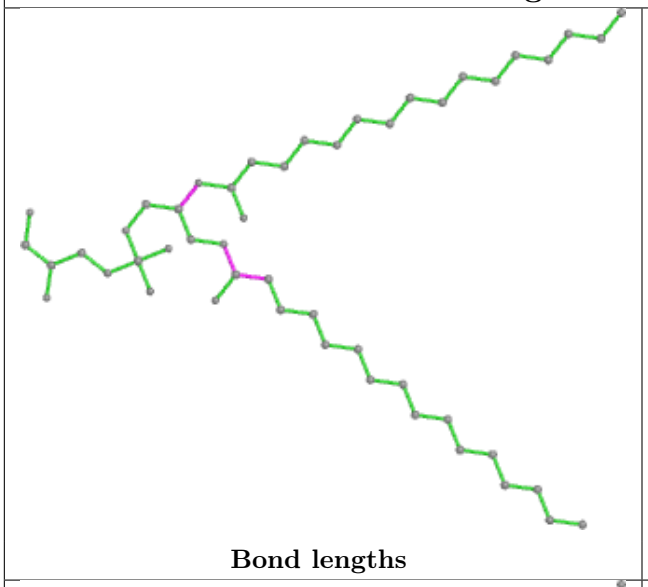


Rings

Ligand LHG E 101



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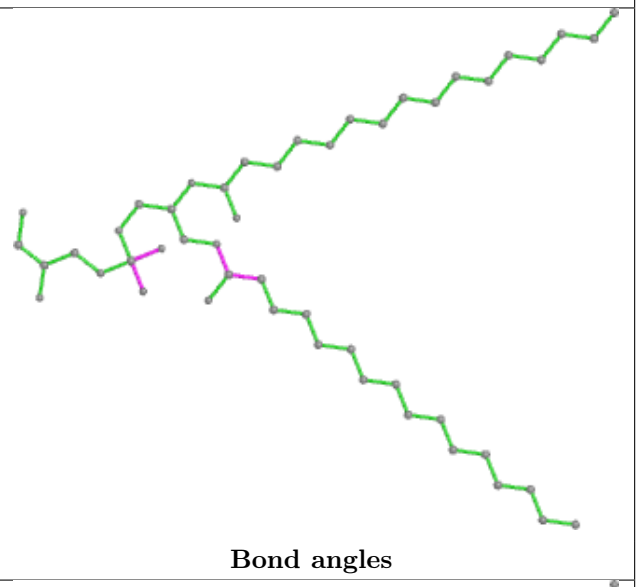
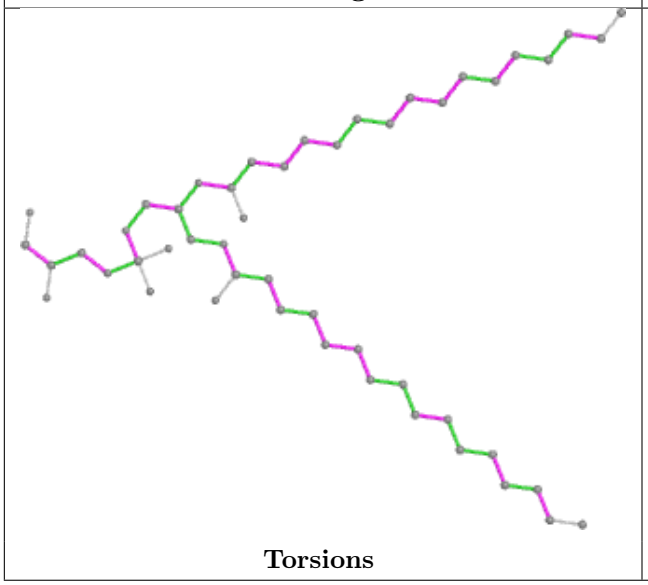


Bond angles



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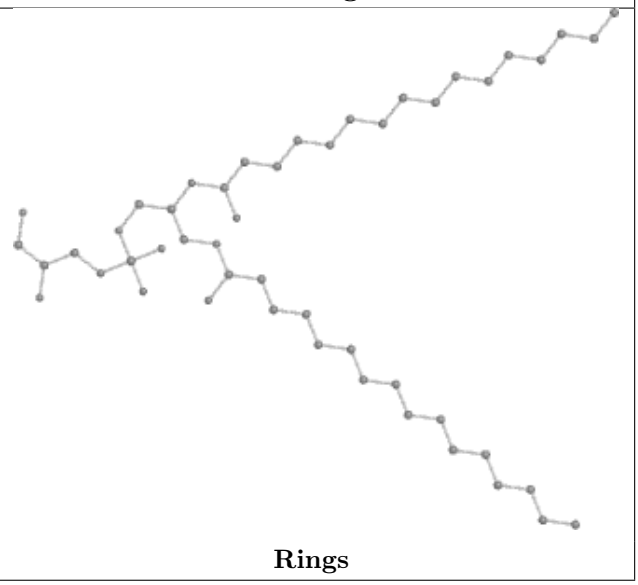
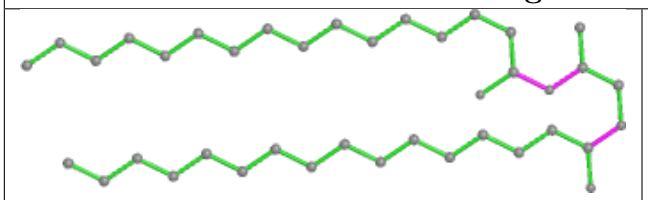


Rings

Ligand SQD A 413



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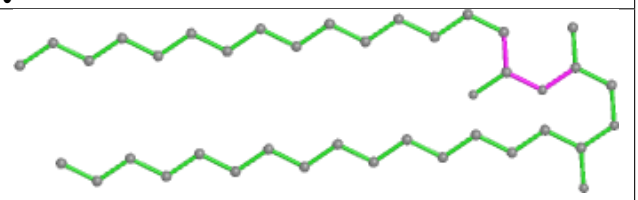
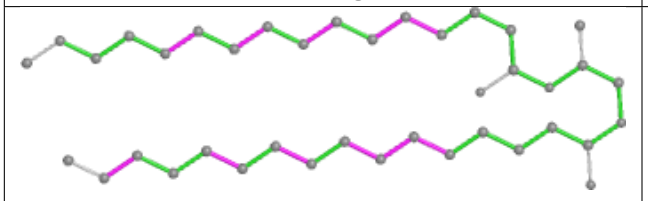


Bond angles



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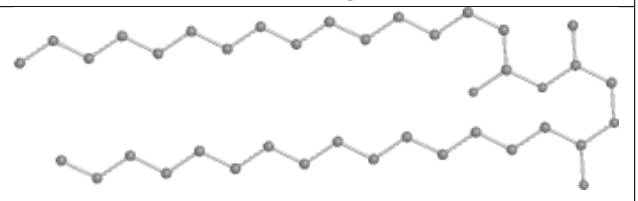
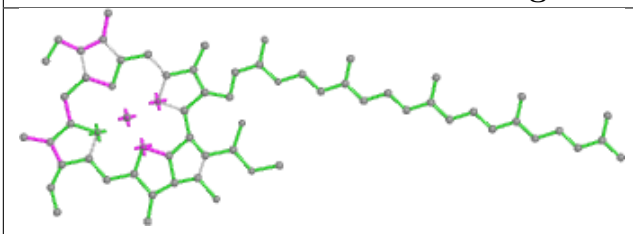


Rings

Ligand CLA c 505



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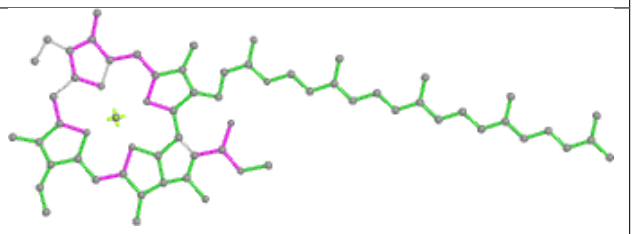
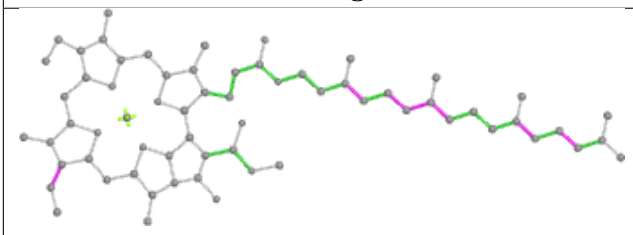


Bond angles



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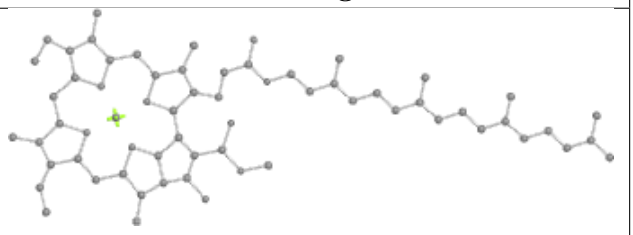

Rings

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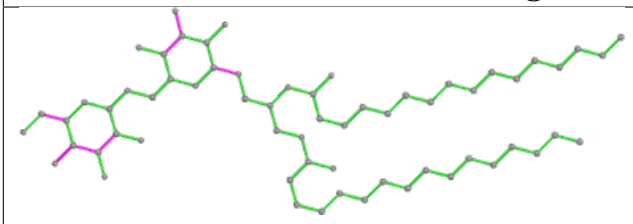
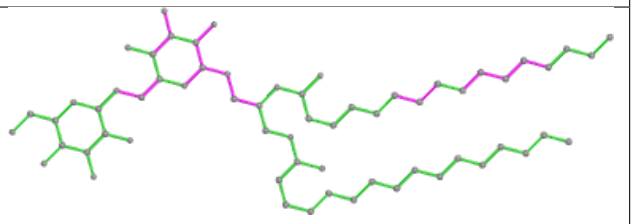
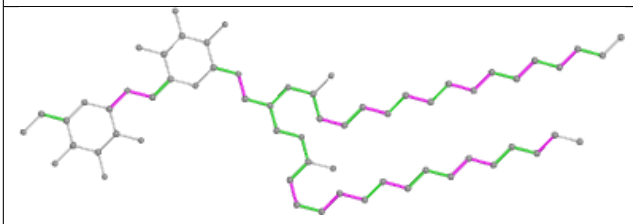


Bond lengths



Bond angles



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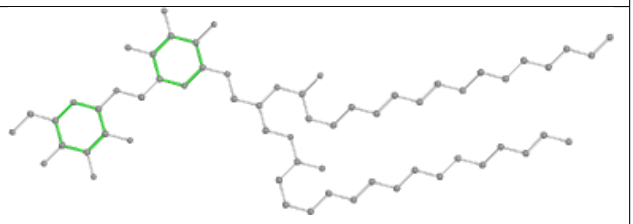
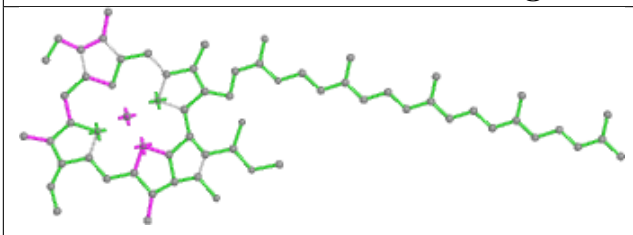


Rings

Ligand CLA B 613



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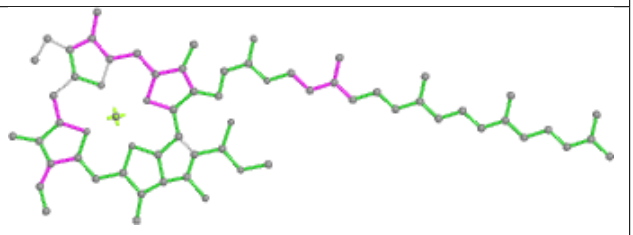
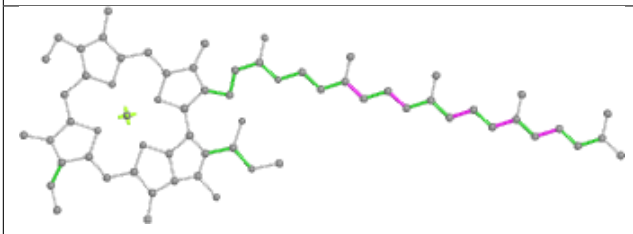


Bond angles



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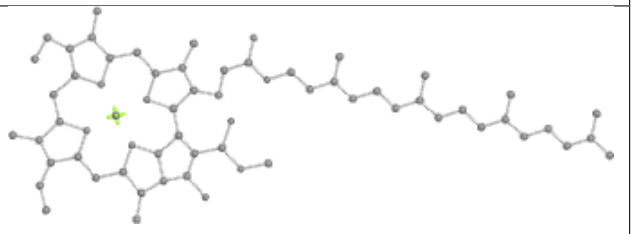
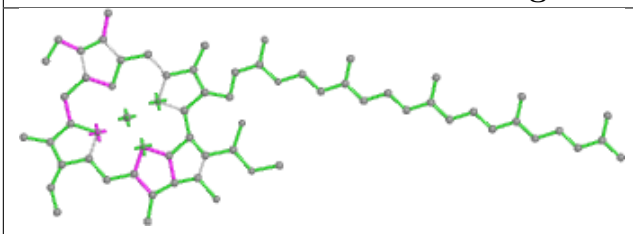
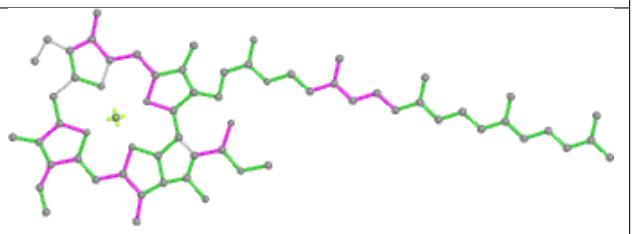


Rings

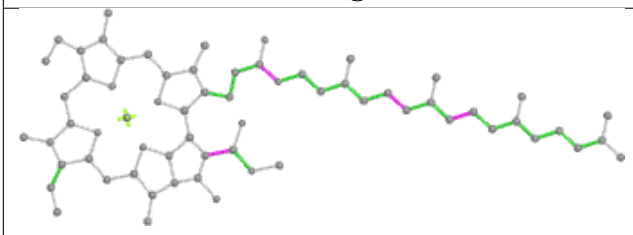
Ligand CLA c 503



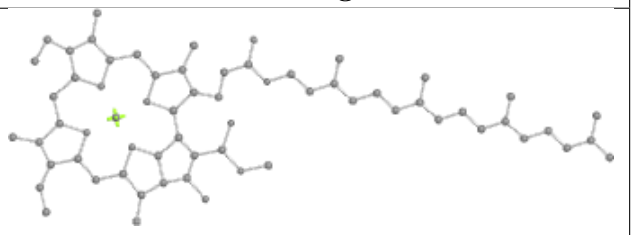
Bond lengths



Bond angles

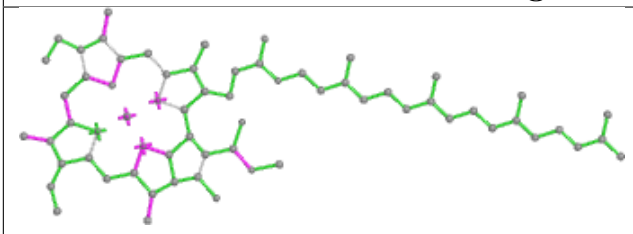


Torsions

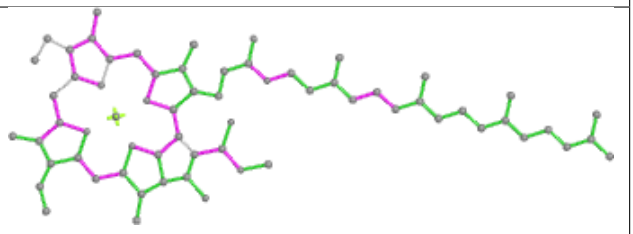


Rings

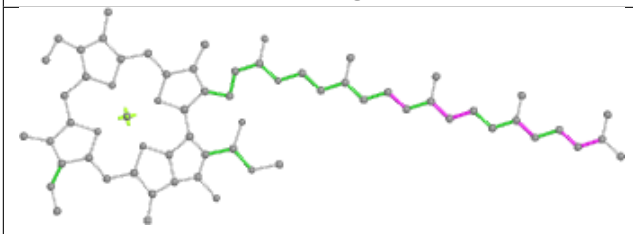
Ligand CLA b 616



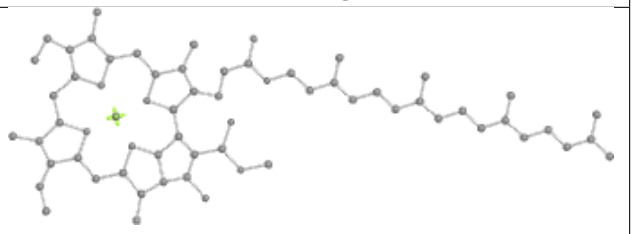
Bond lengths



Bond angles

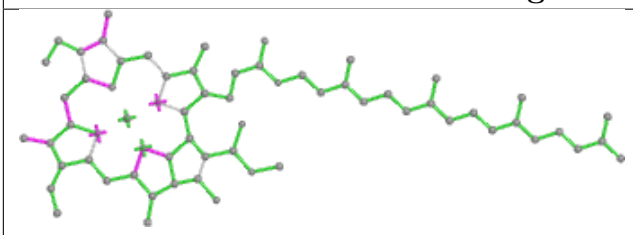


Torsions

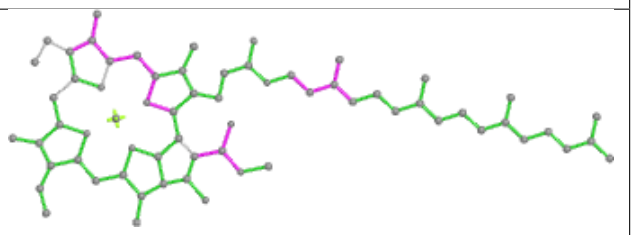


Rings

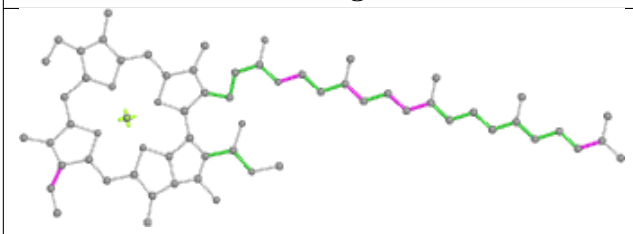
Ligand CLA d 403



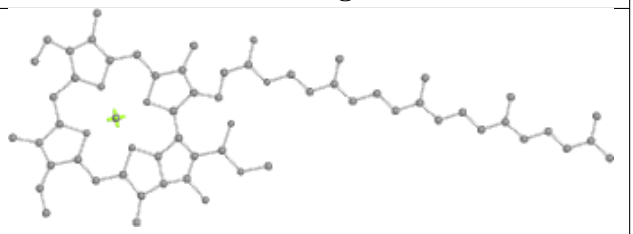
Bond lengths



Bond angles

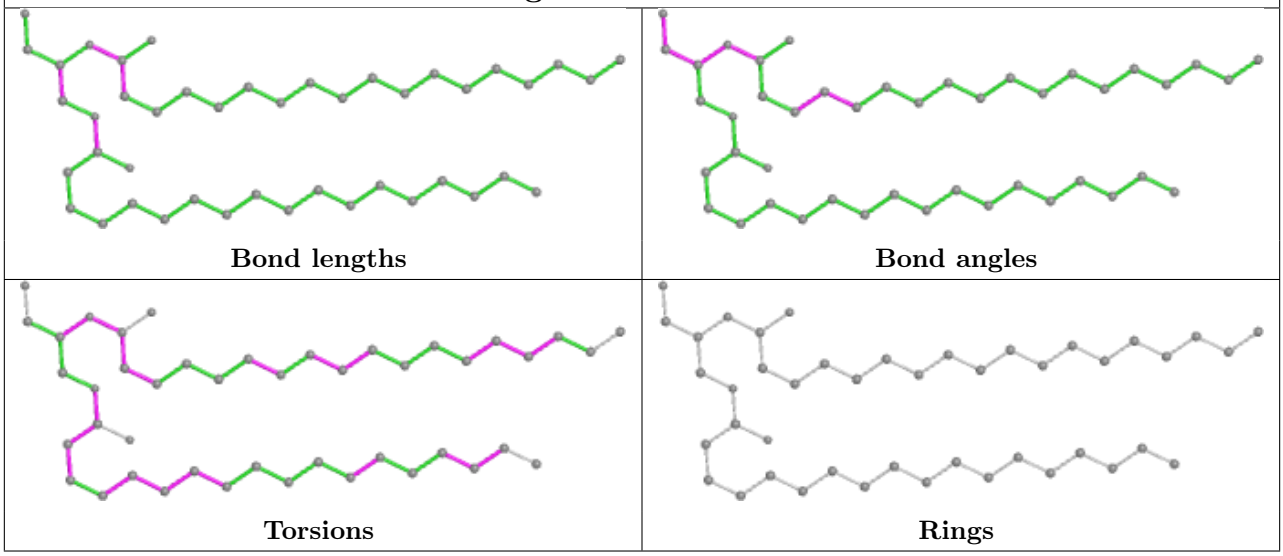


Torsions

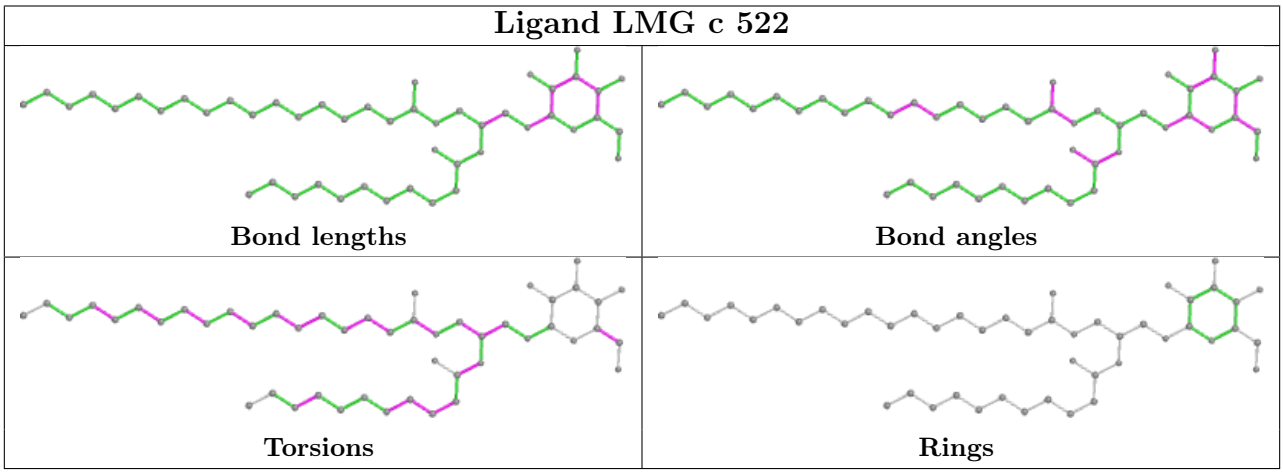


Rings

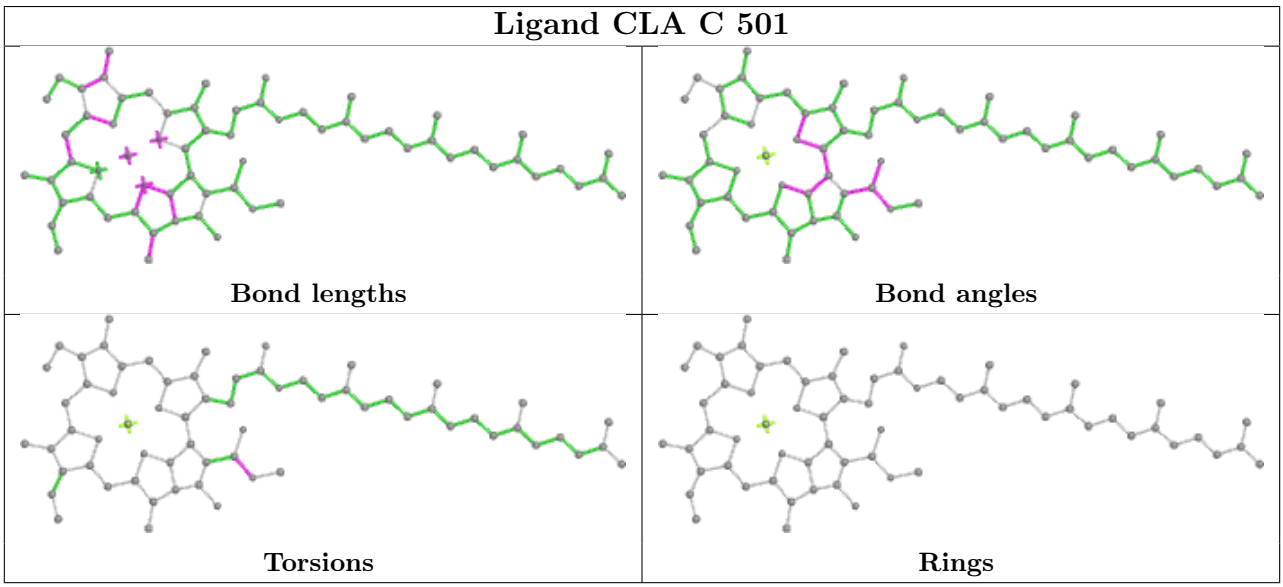
Ligand DGD o 301



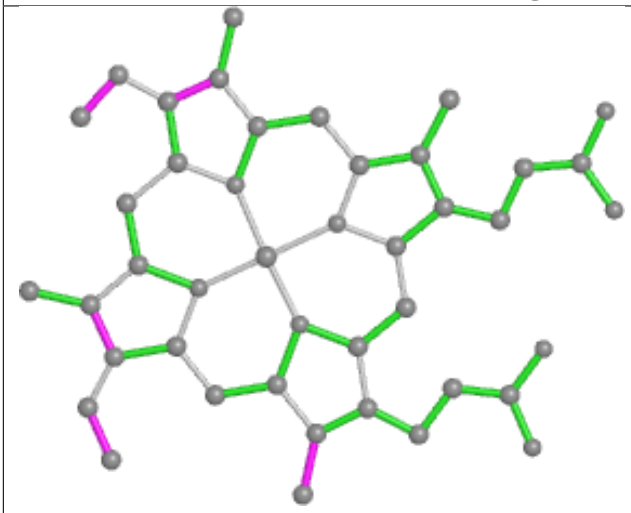
Ligand LMG c 522



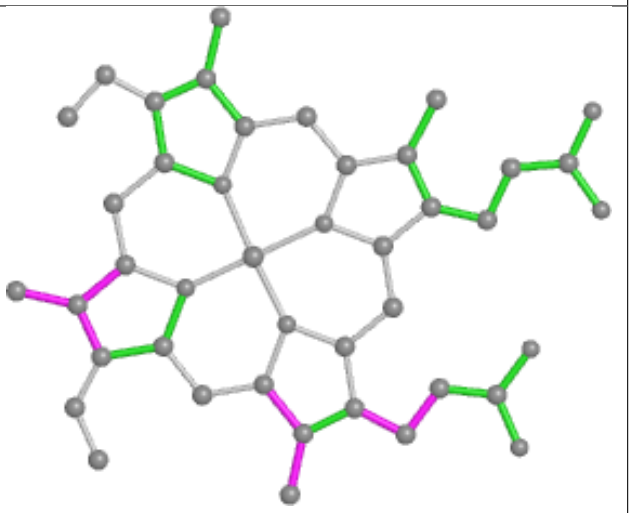
Ligand CLA C 501



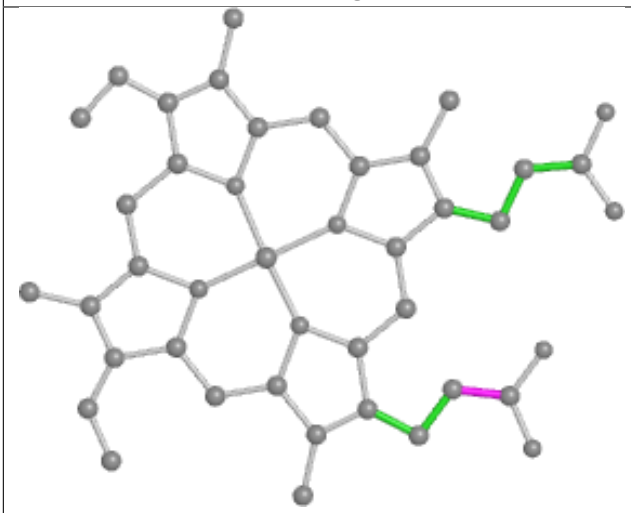
Ligand HEC v 201



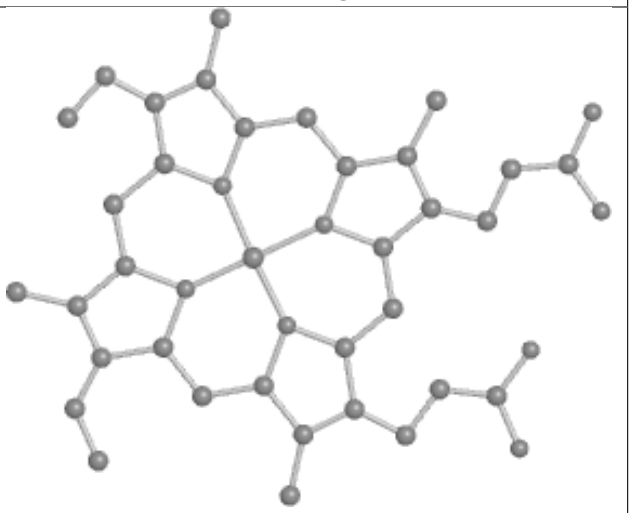
Bond lengths



Bond angles

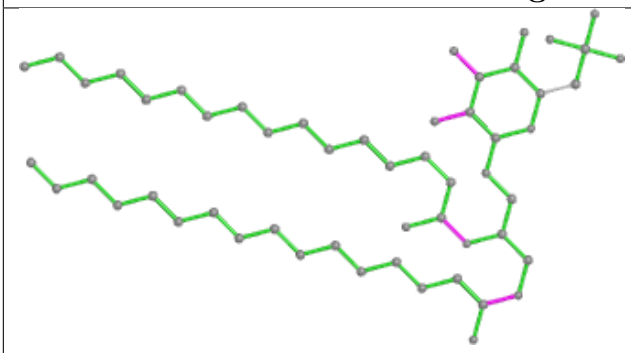


Torsions



Rings

Ligand SQD a 411



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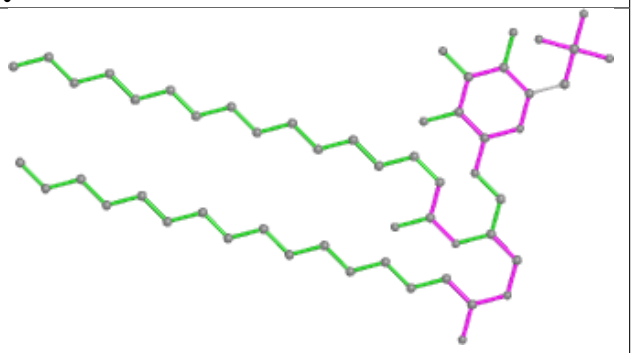
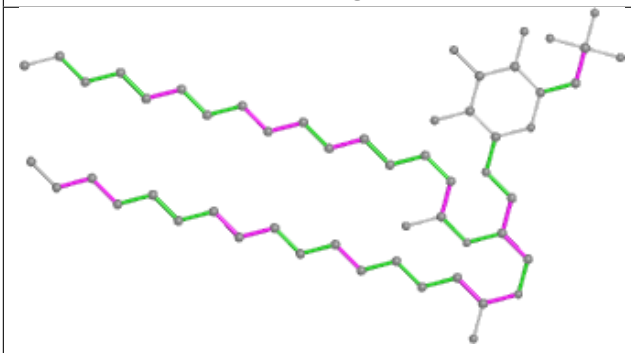
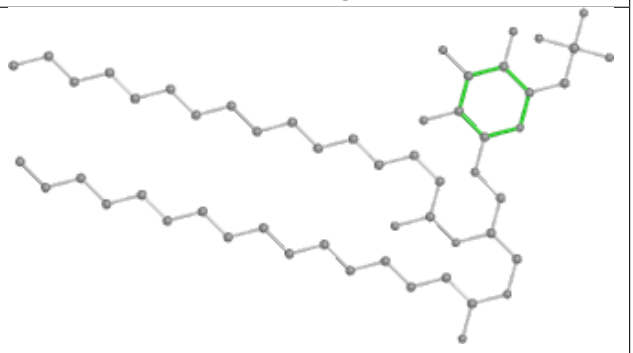


Bond angles

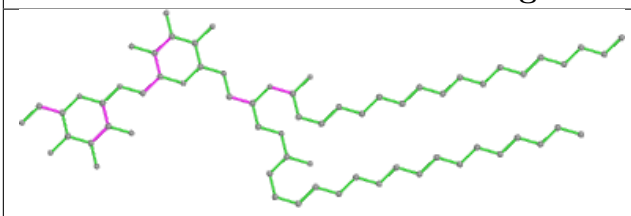


Torsions

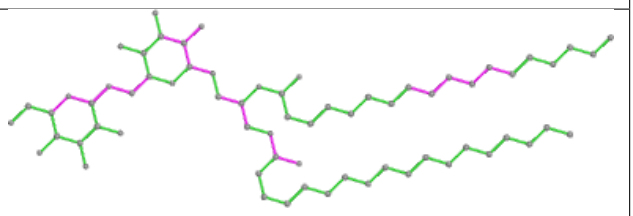


Rings

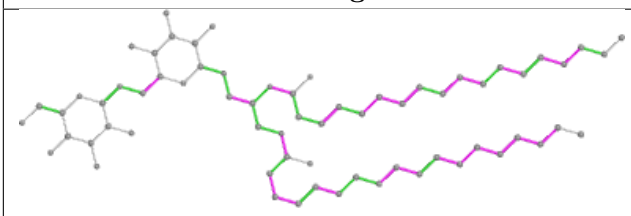
Ligand DGD A 414



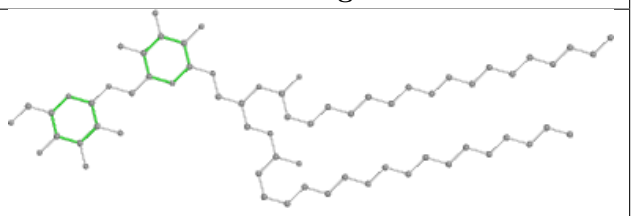
Bond lengths



Bond angles

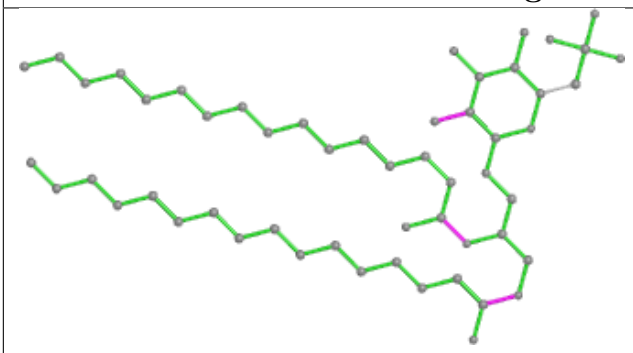


Torsions

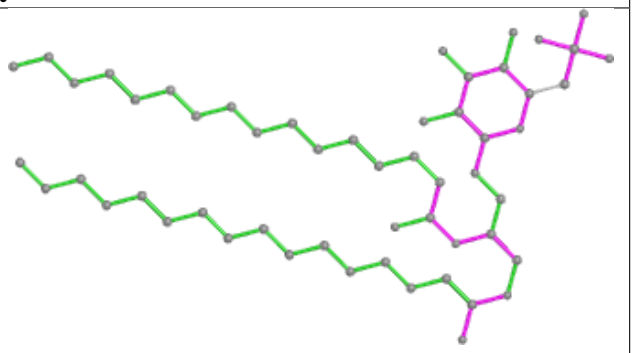


Rings

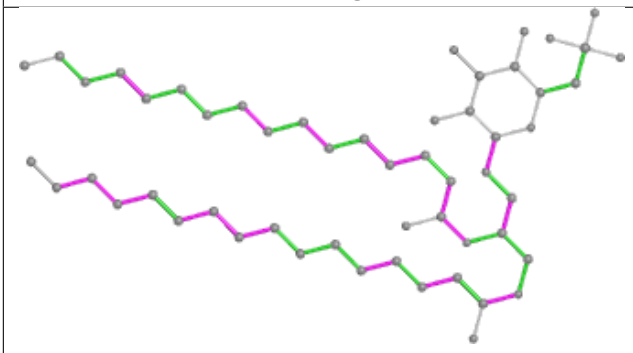
Ligand SQD B 624



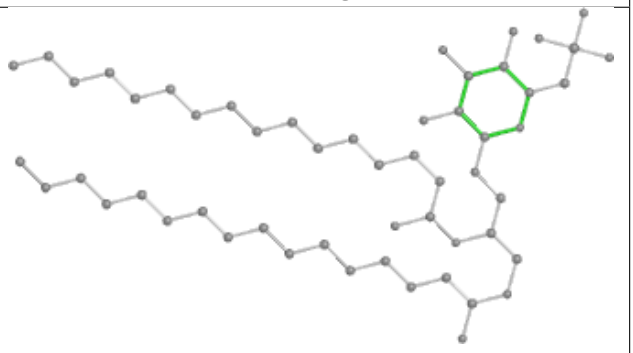
Bond lengths



Bond angles

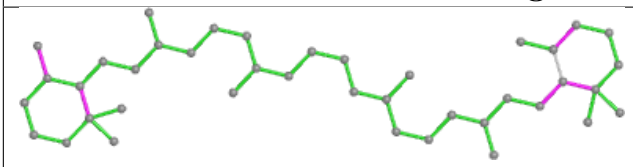


Torsions

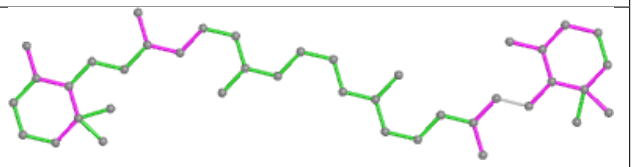


Rings

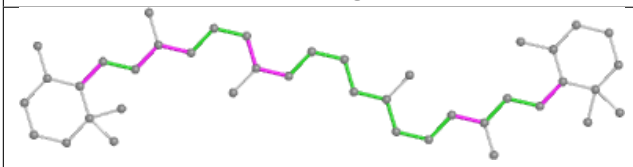
Ligand 8CT B 617



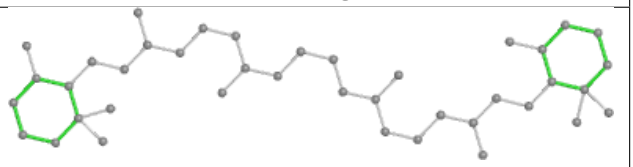
Bond lengths



Bond angles

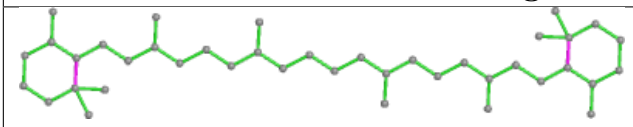


Torsions

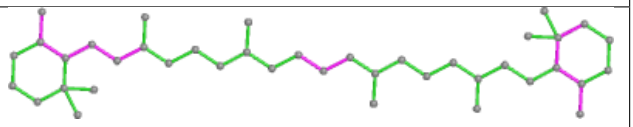


Rings

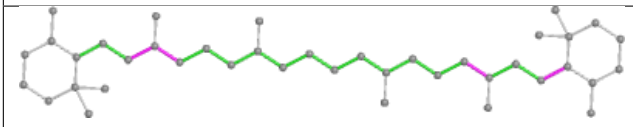
Ligand BCR B 618



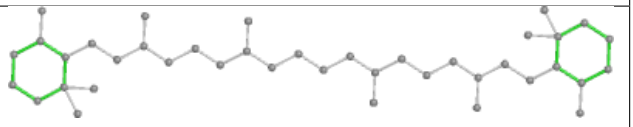
Bond lengths



Bond angles

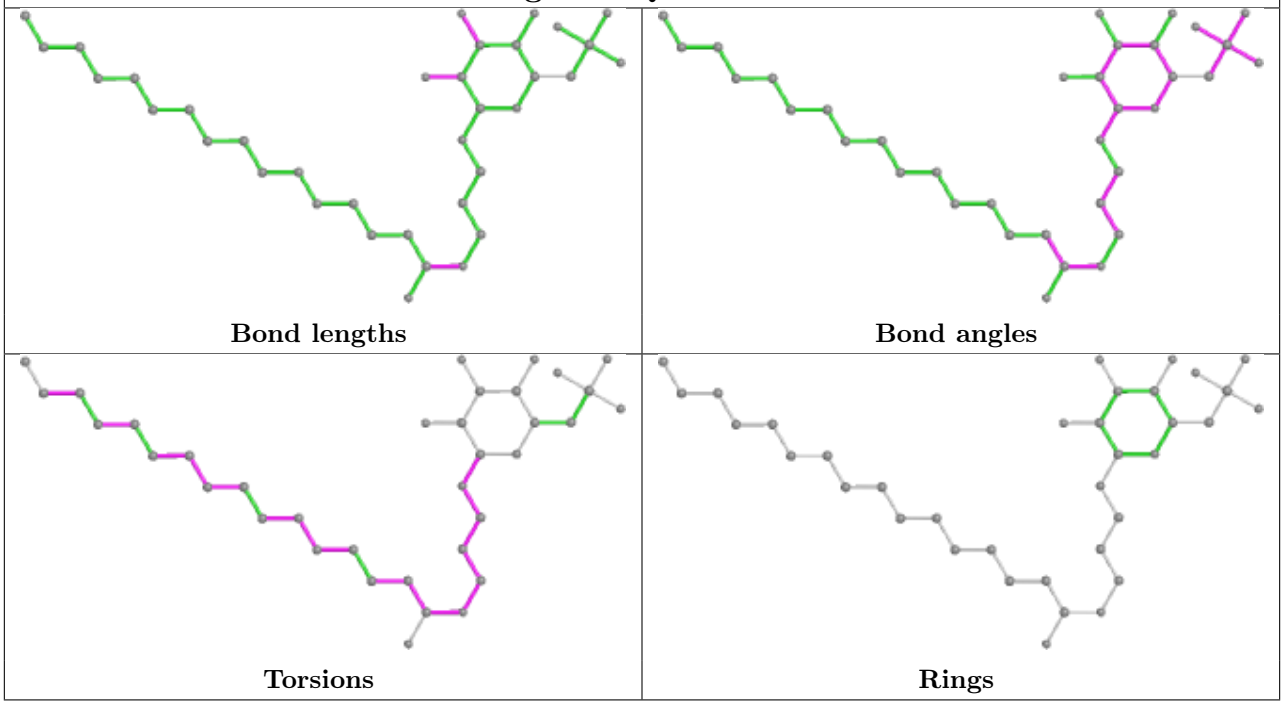


Torsions

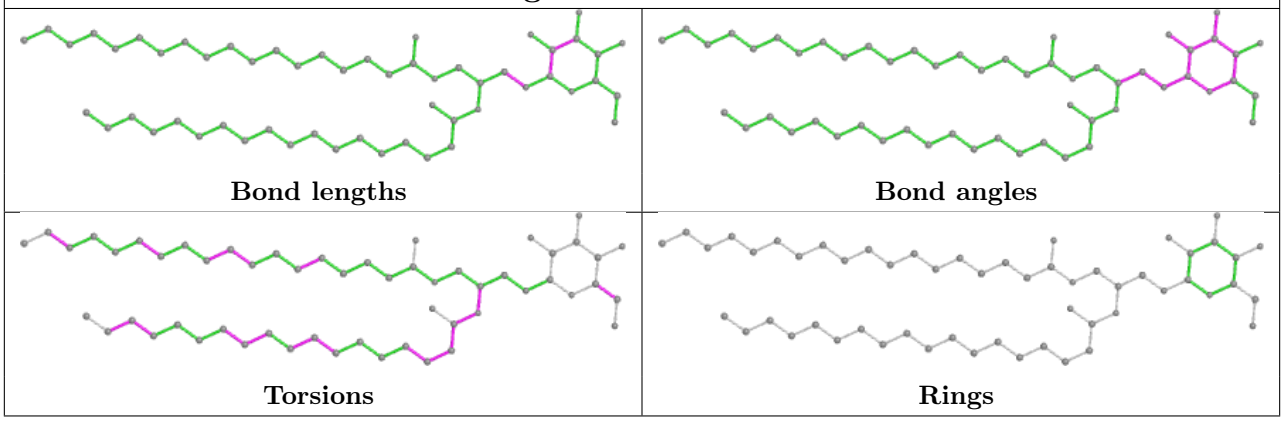


Rings

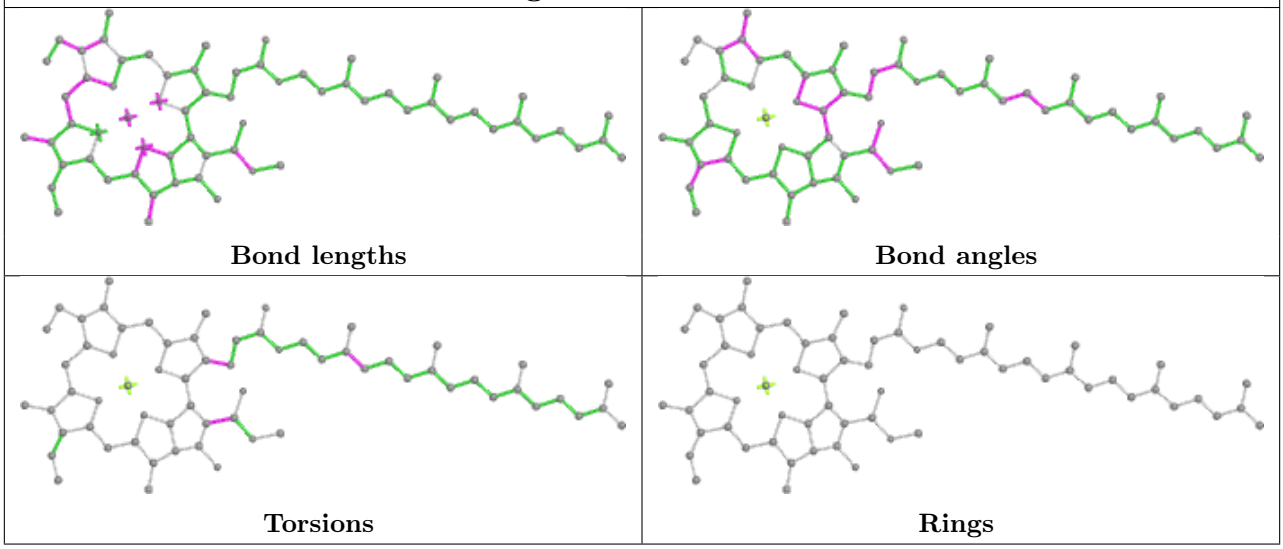
Ligand SQD D 408



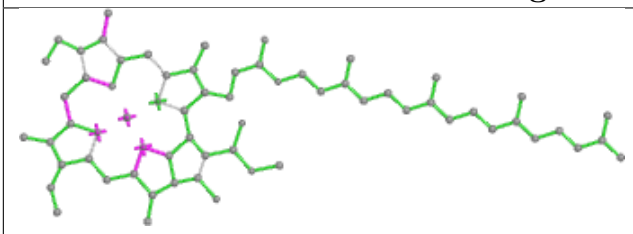
Ligand LMG b 623



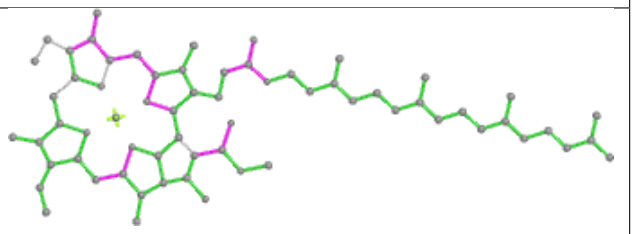
Ligand CLA B 609



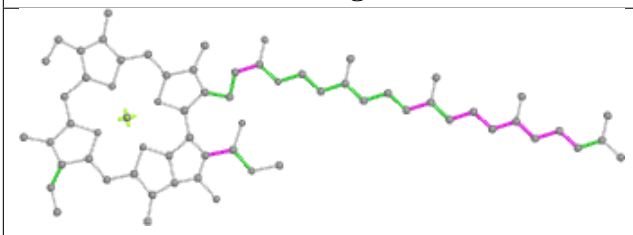
Ligand CLA c 509



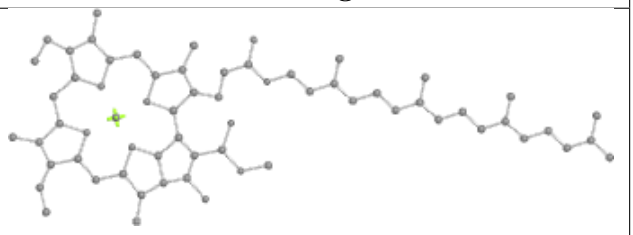
Bond lengths



Bond angles

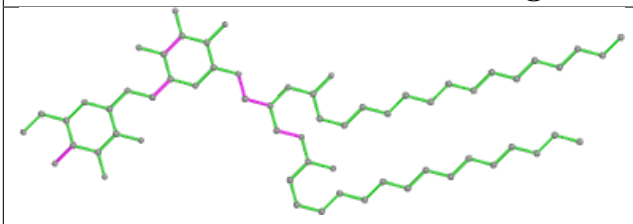


Torsions

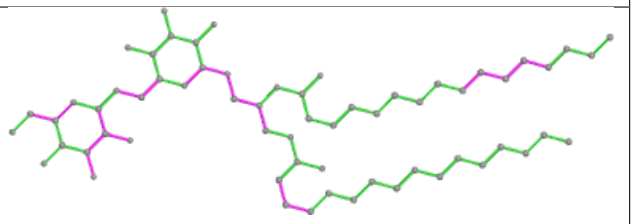


Rings

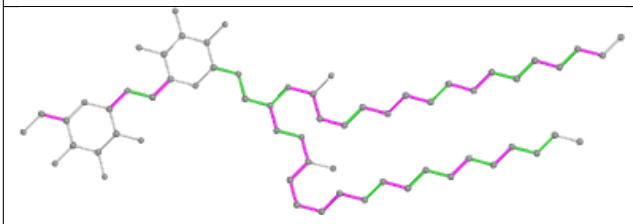
Ligand DGD c 516



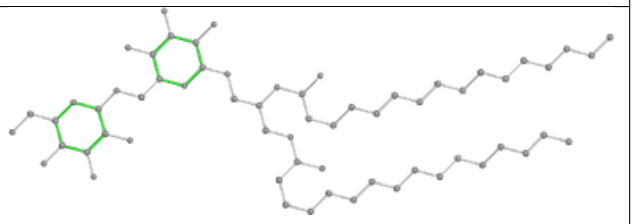
Bond lengths



Bond angles

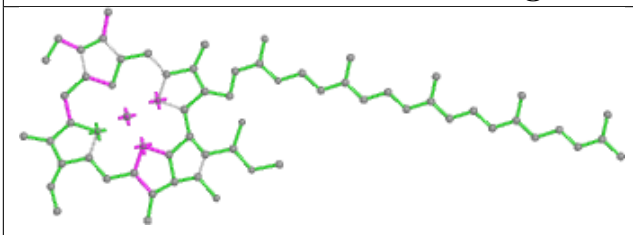


Torsions

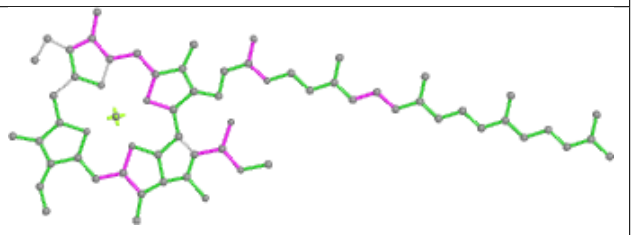


Rings

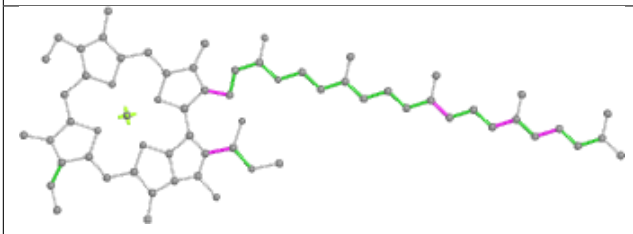
Ligand CLA C 508



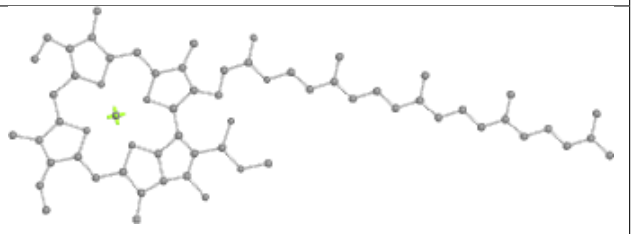
Bond lengths



Bond angles

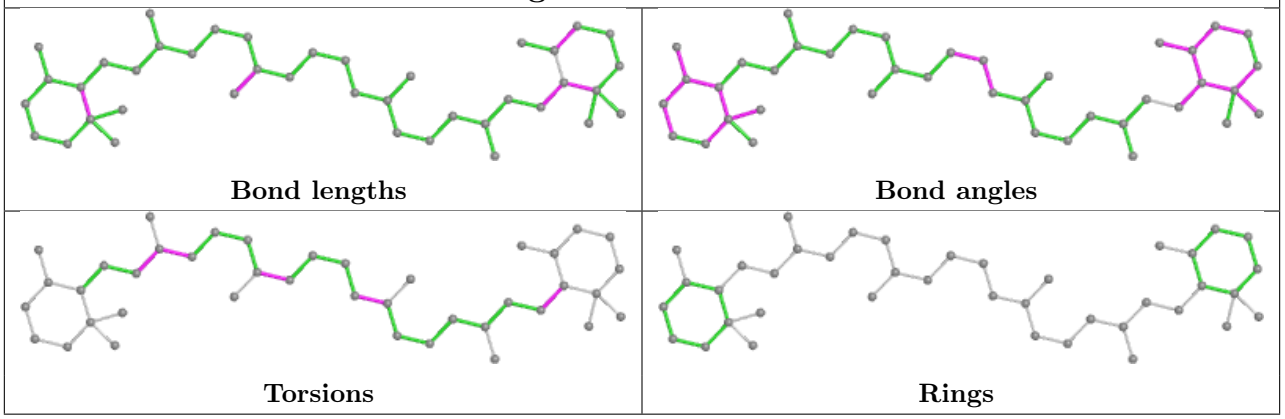


Torsions

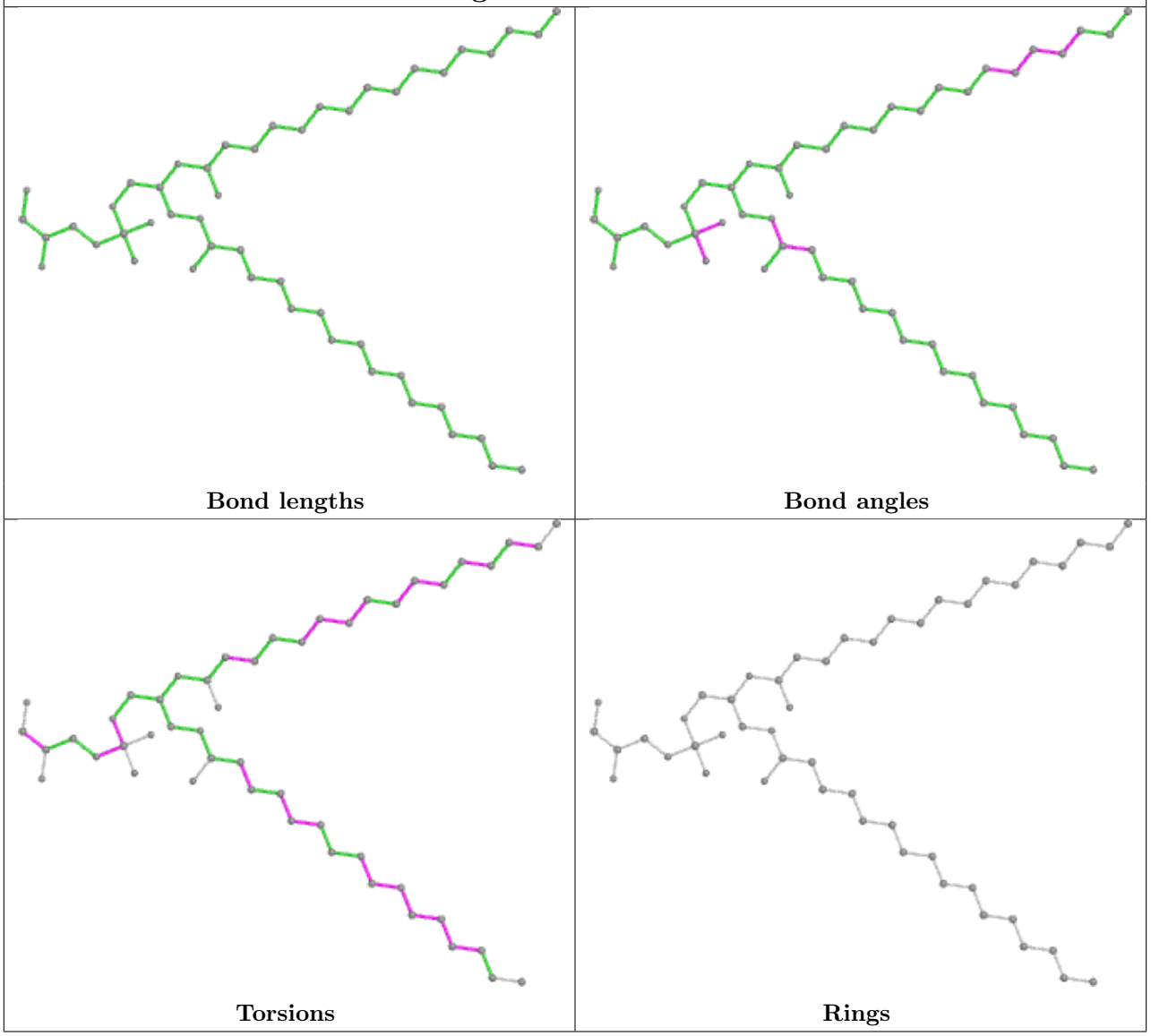


Rings

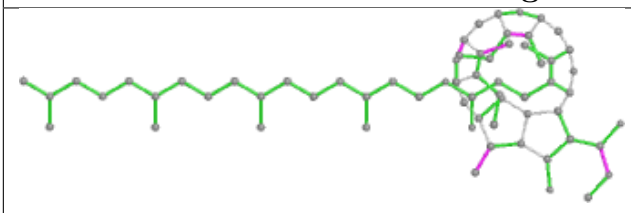
Ligand 8CT B 619



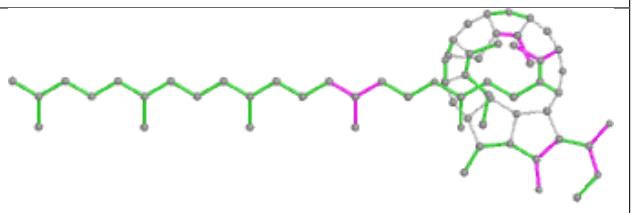
Ligand LHG d 408



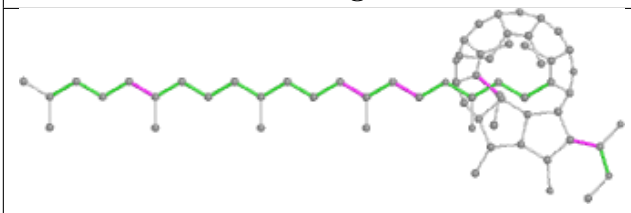
Ligand PHO A 406



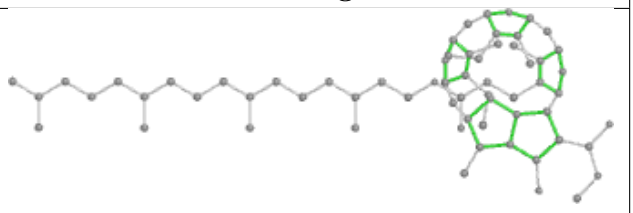
Bond lengths



Bond angles

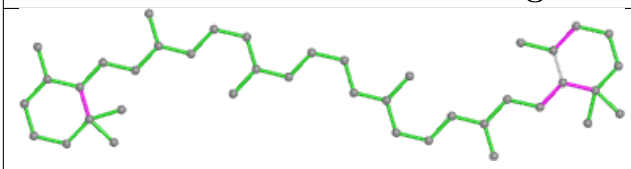


Torsions



Rings

Ligand 8CT D 405



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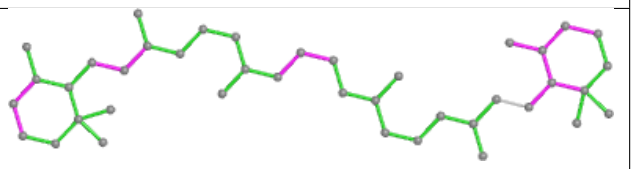
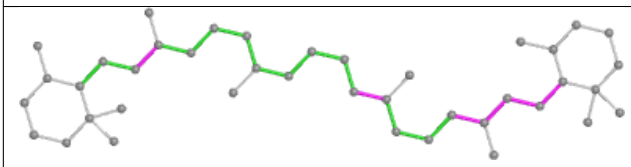


Bond angles



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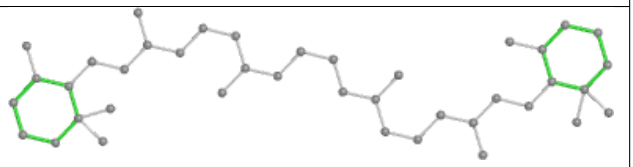
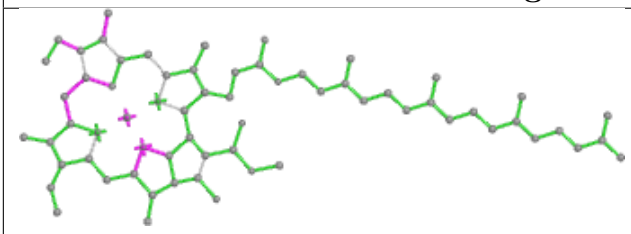


Rings

Ligand CLA C 513



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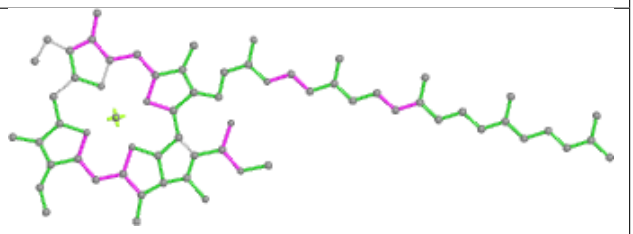
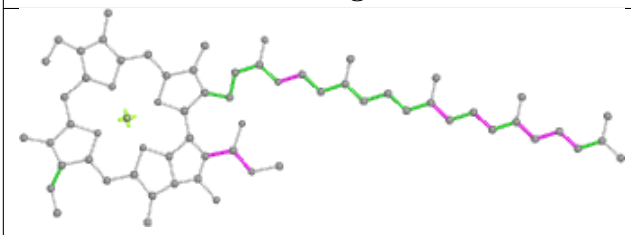
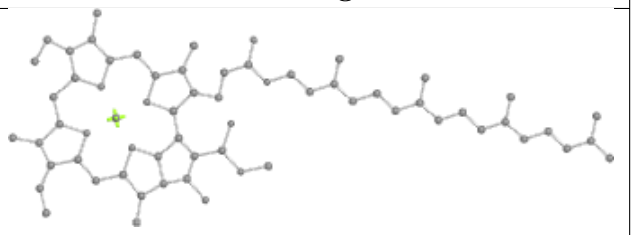


Bond angles

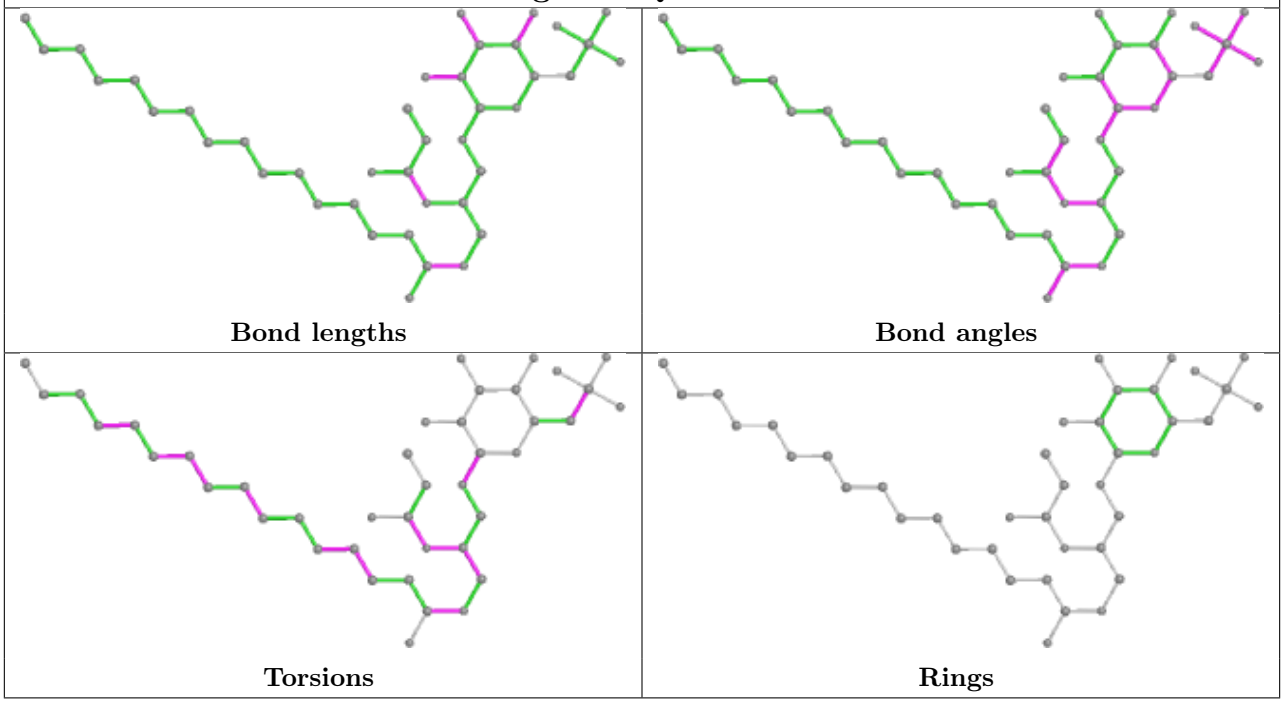


Torsions

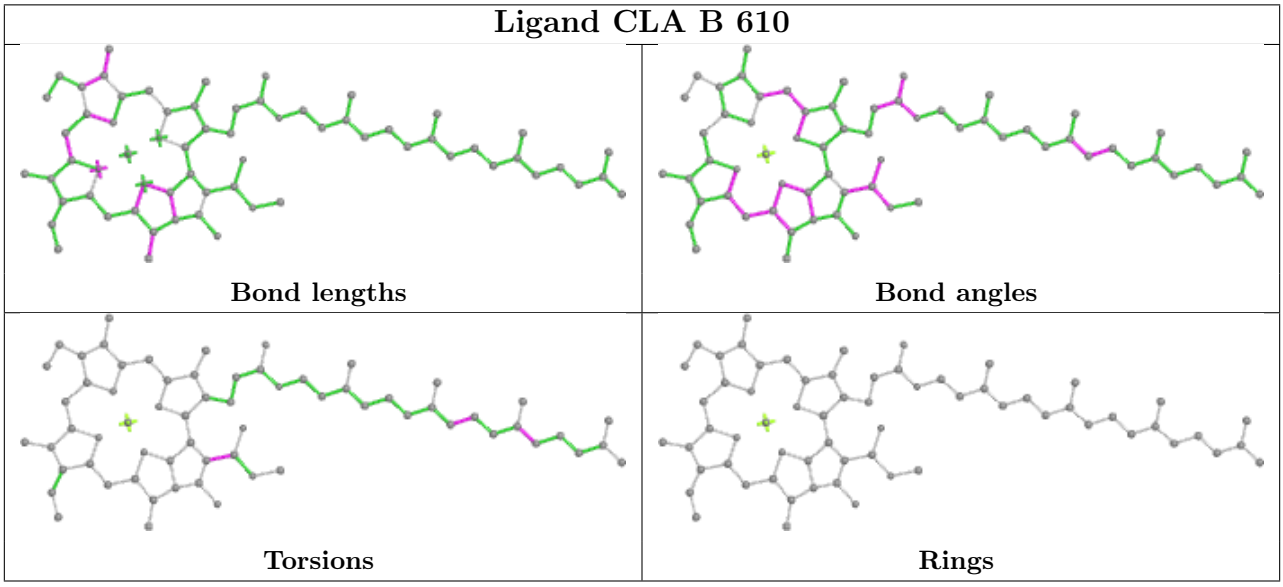


Rings

Ligand SQD f 101



Ligand CLA B 610



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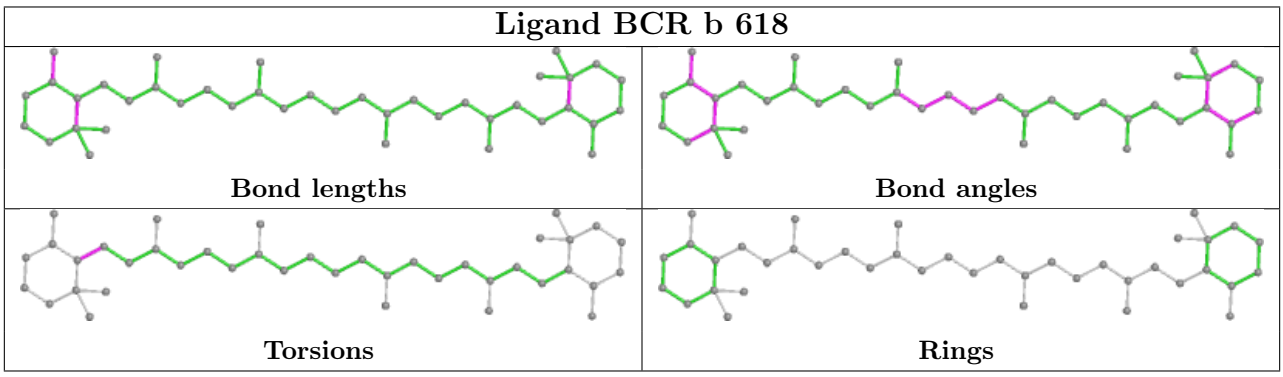
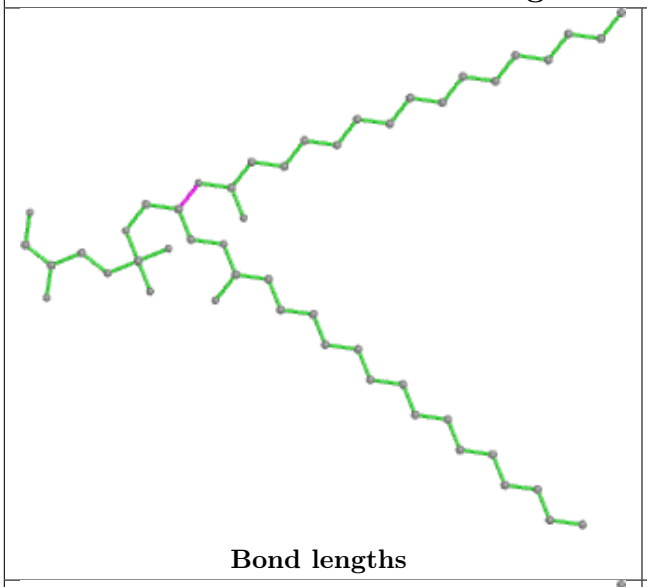
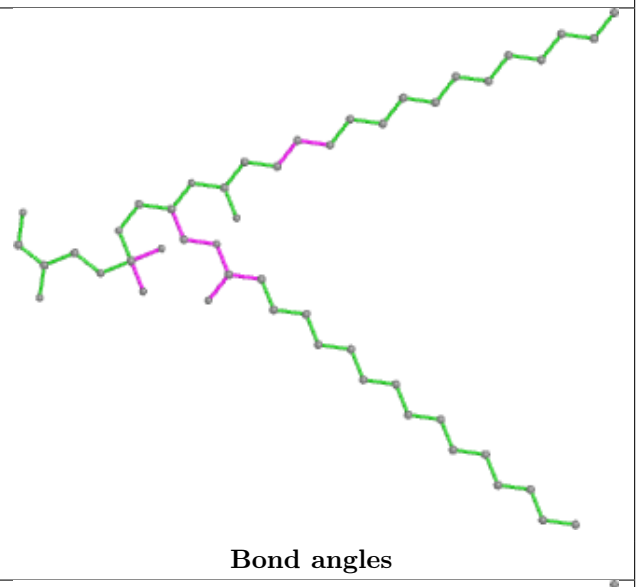


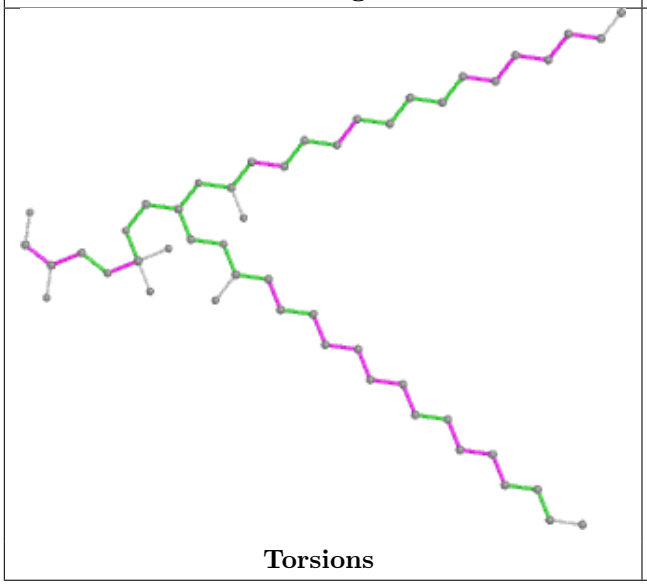
Ligand LHG d 407



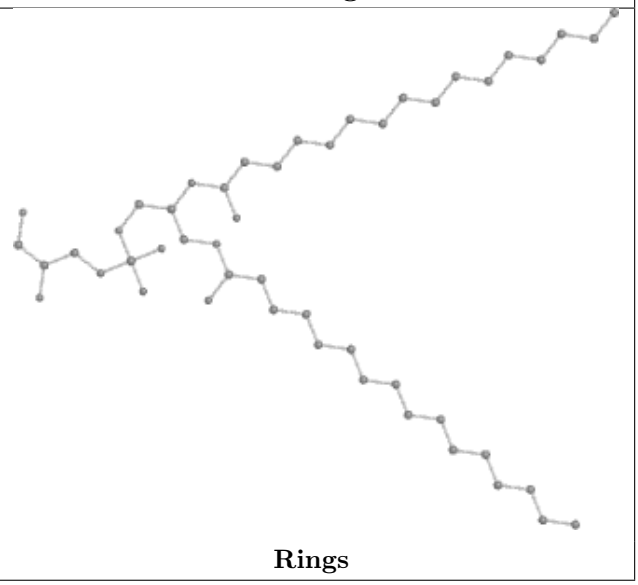
Bond lengths



Bond angles

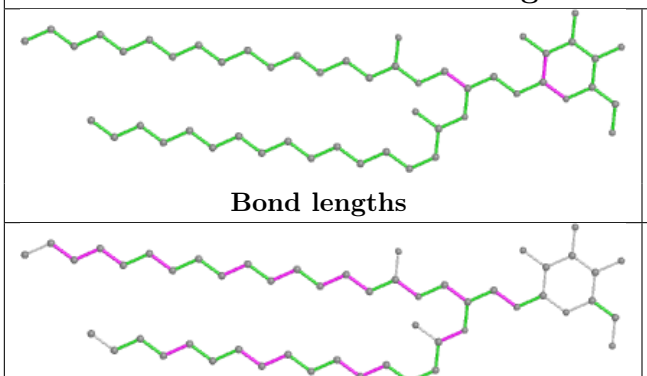


Torsions

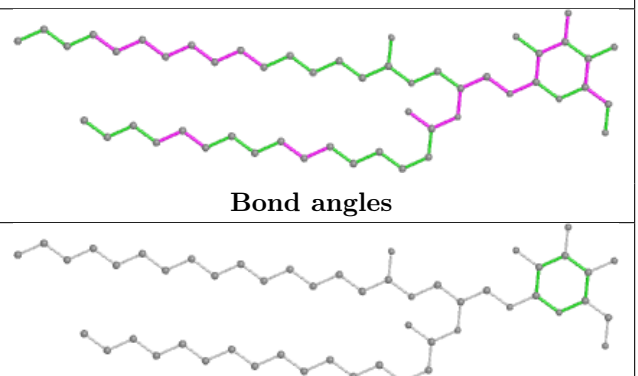


Rings

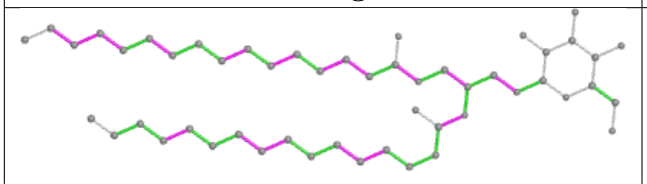
Ligand LMG B 620



Bond lengths



Bond angles



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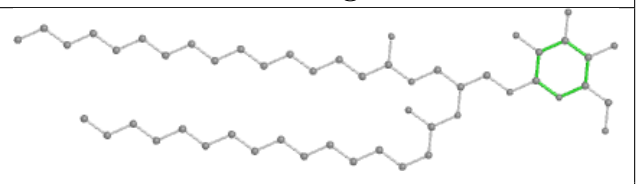
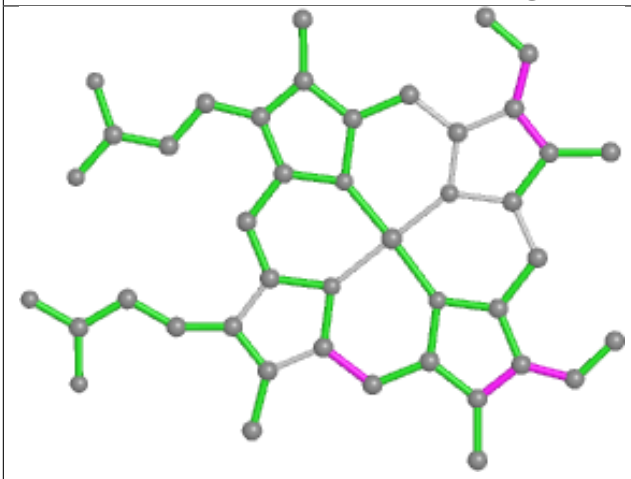


Rings

Ligand HEM e 102



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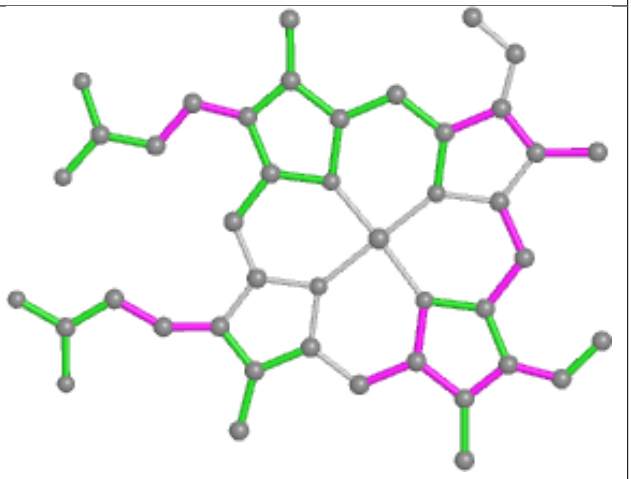
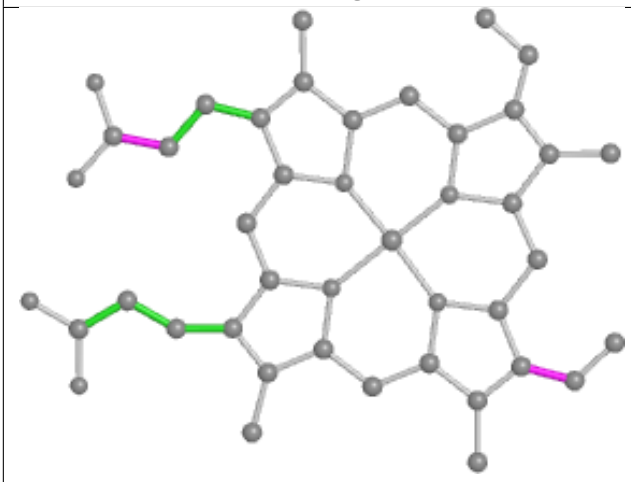


Bond angles



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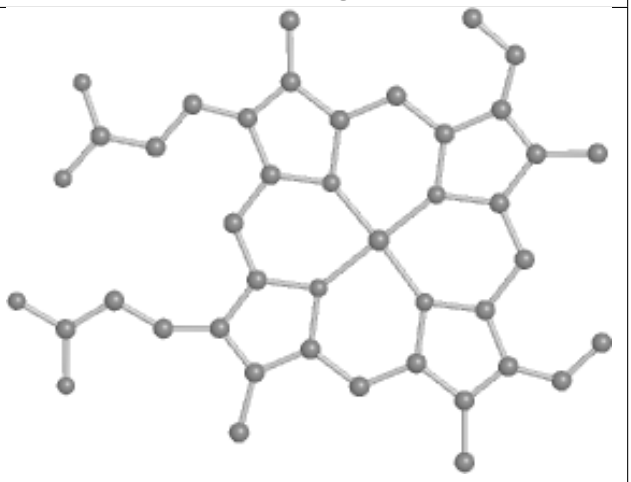
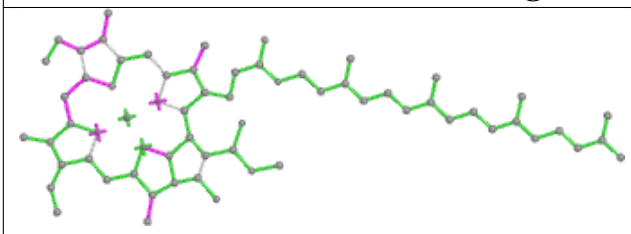


Rings

Ligand CLA B 611



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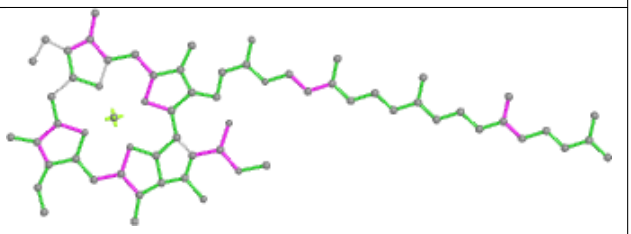
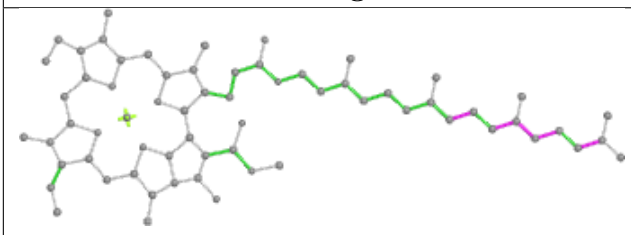
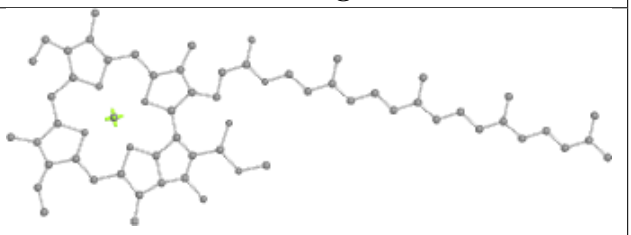


Bond angles

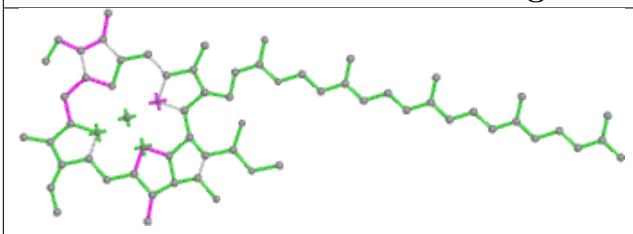


Torsions

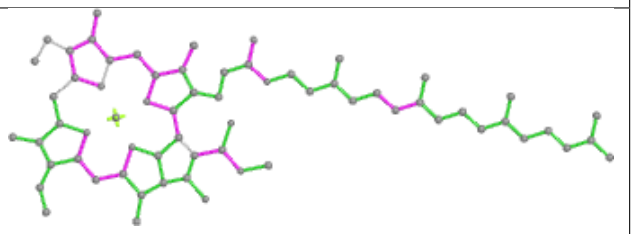


Rings

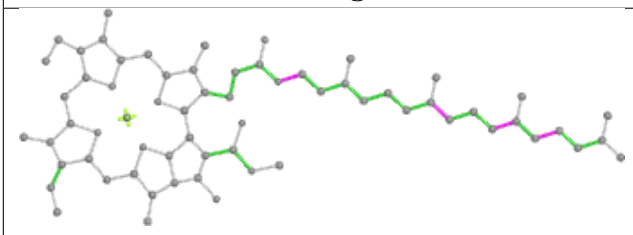
Ligand CLA b 609



Bond lengths



Bond angles



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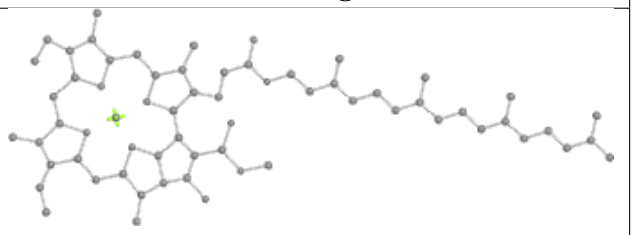
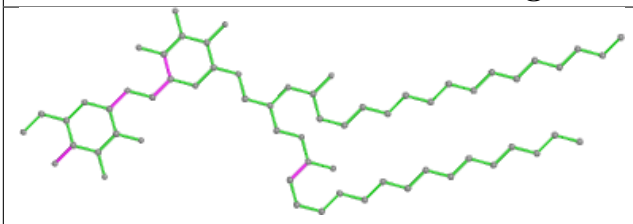


Rings

Ligand DGD c 518



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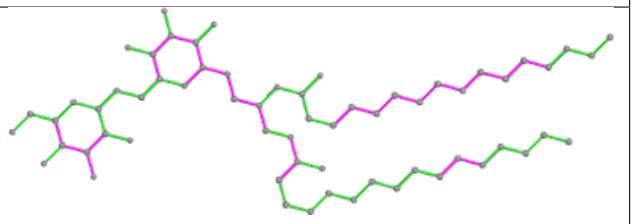
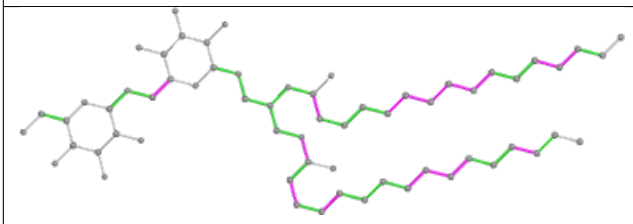
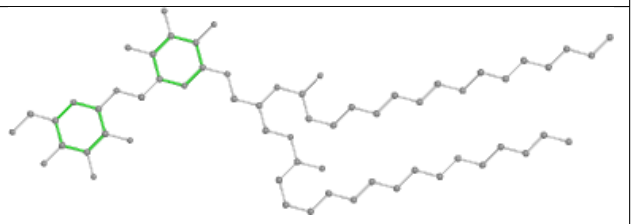


Bond angles

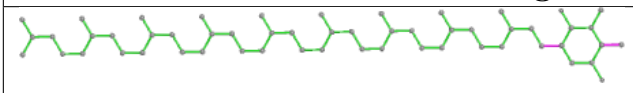


Torsions



Rings

Ligand PL9 a 410



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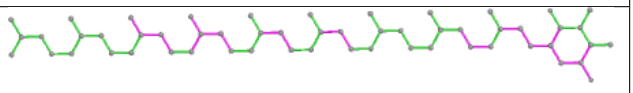
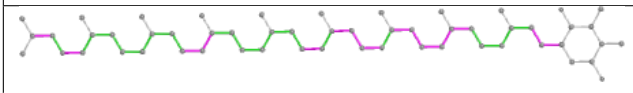
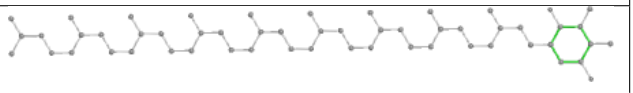


Bond angles

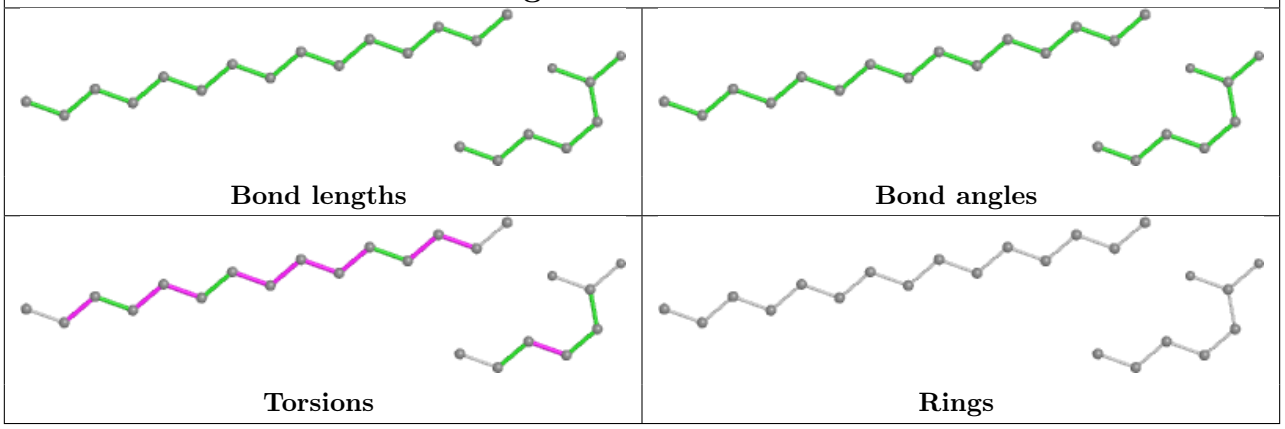


Torsions

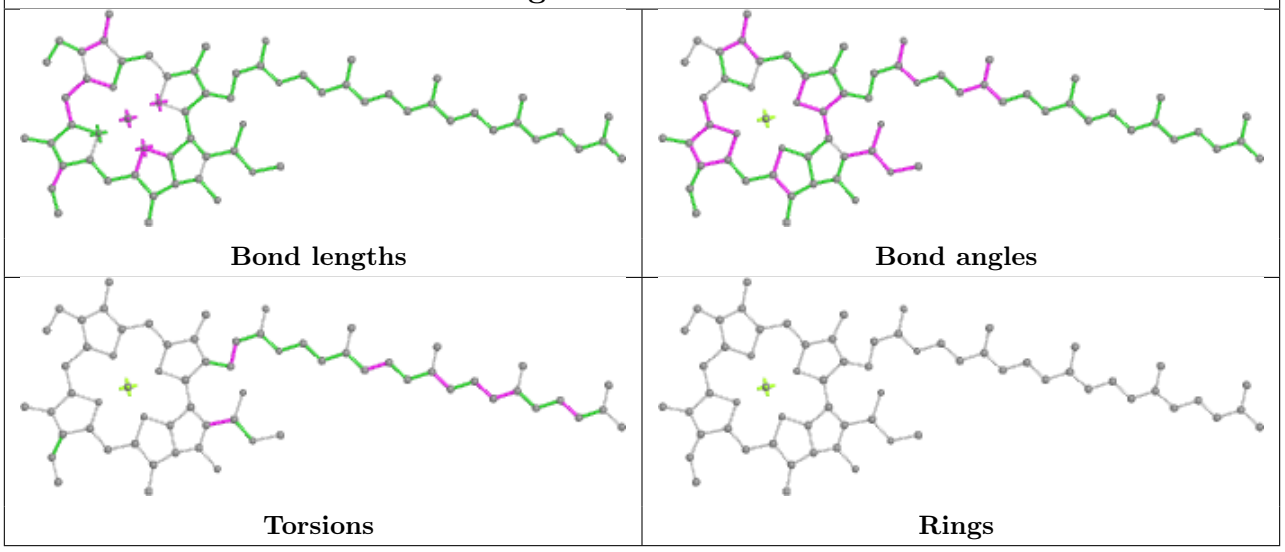


Rings

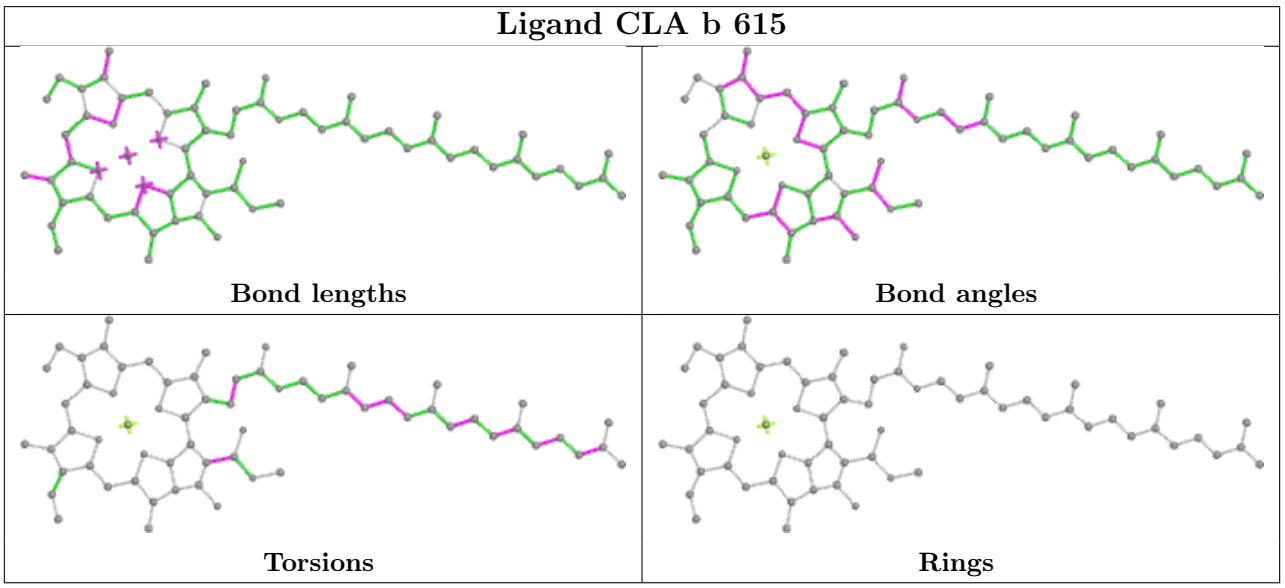
Ligand LMG b 624



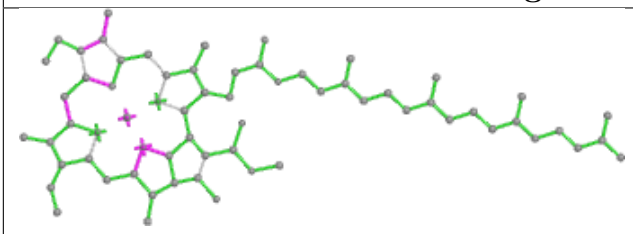
Ligand CLA b 607



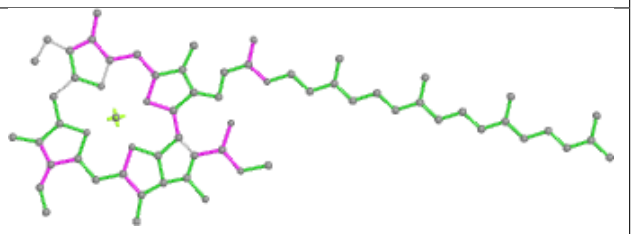
Ligand CLA b 615



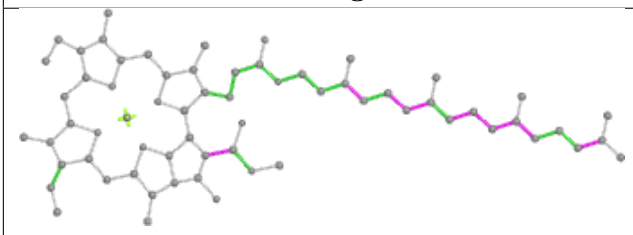
Ligand CLA C 505



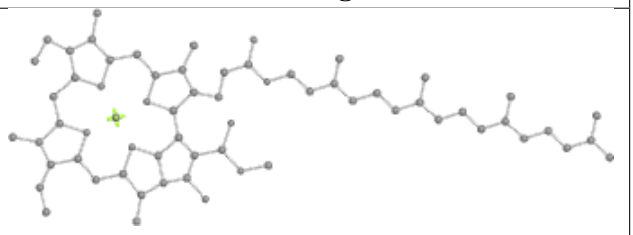
Bond lengths



Bond angles

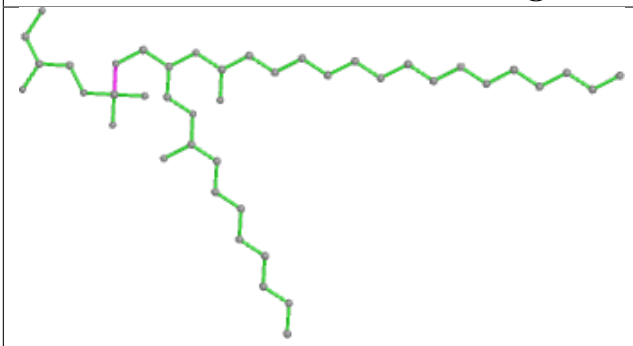


Torsions

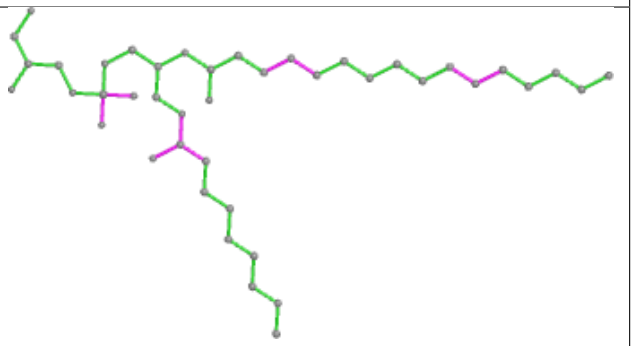


Rings

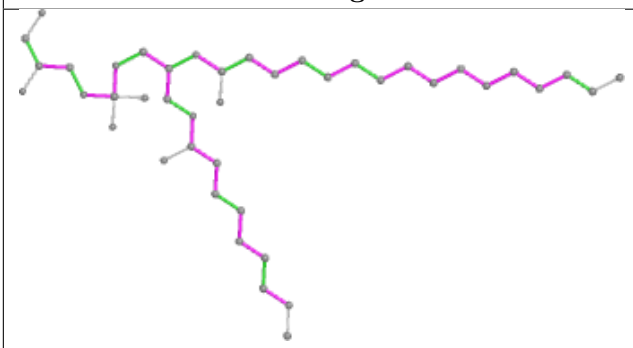
Ligand LHG e 101



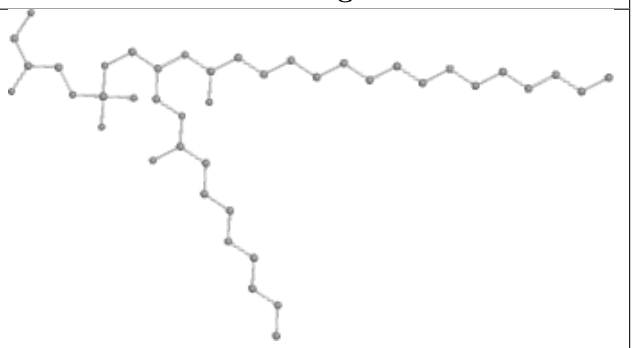
Bond lengths



Bond angles

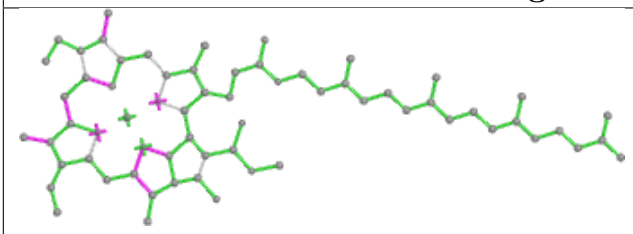


Torsions



Rings

Ligand CLA a 405



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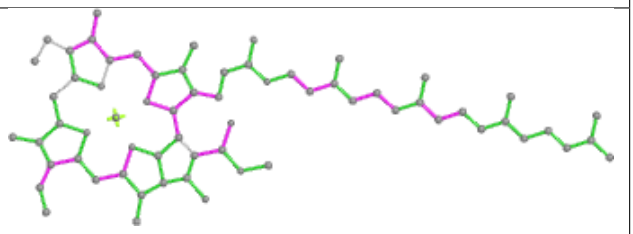
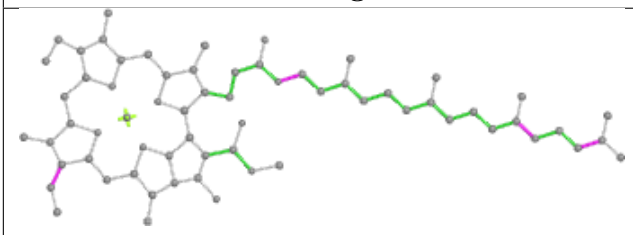


Bond angles



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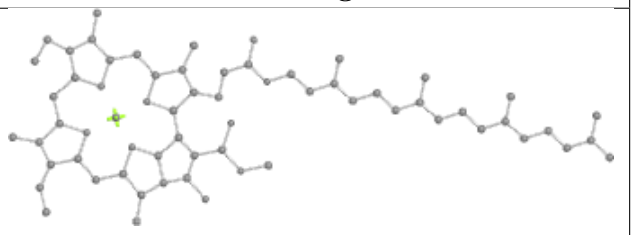
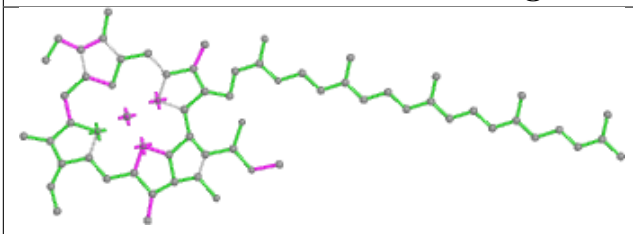


Rings

Ligand CLA B 608



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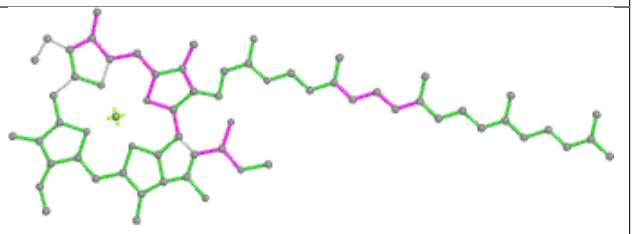
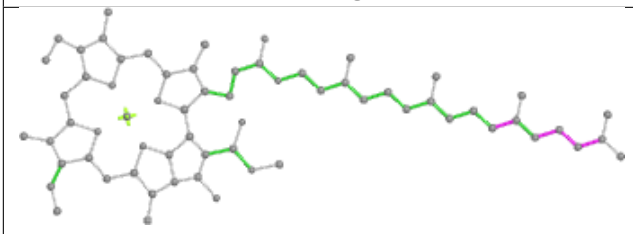
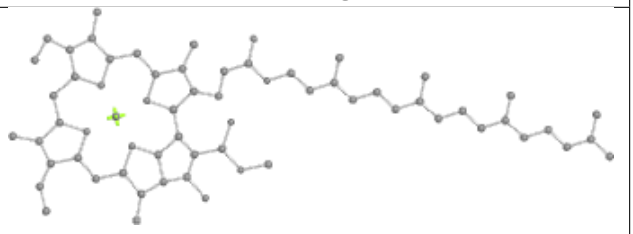


Bond angles

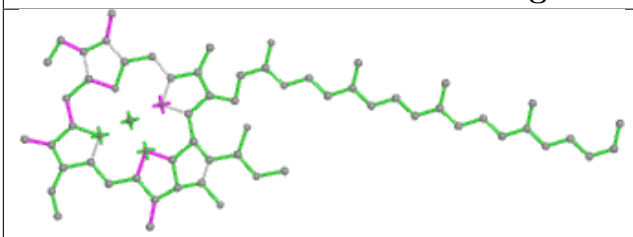


Torsions



Rings

Ligand CLA c 508



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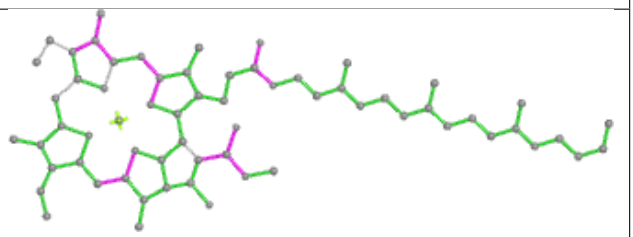
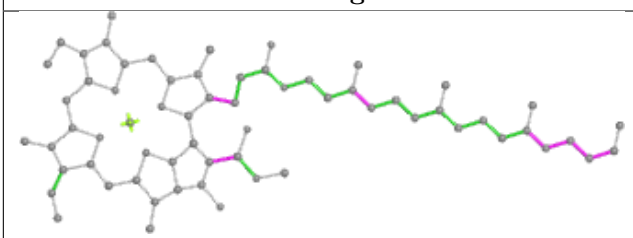


Bond angles



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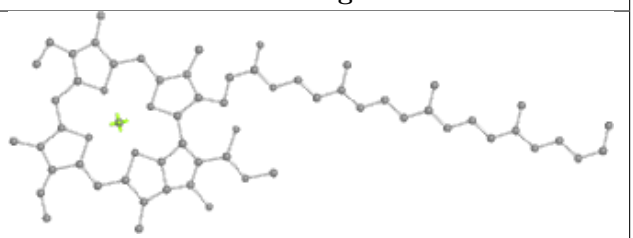
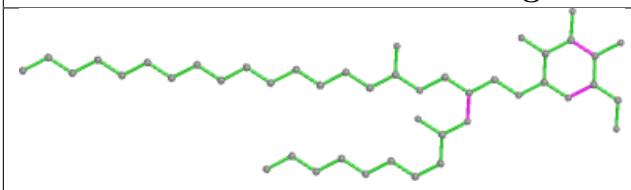


Rings

Ligand LMG d 410



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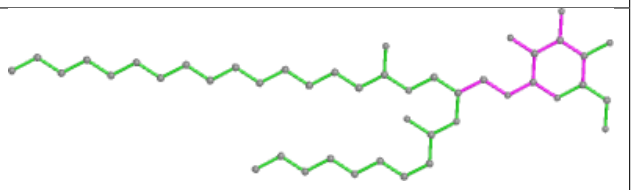
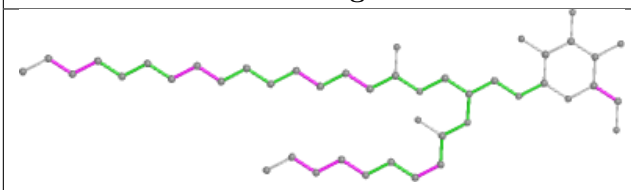


Bond angles



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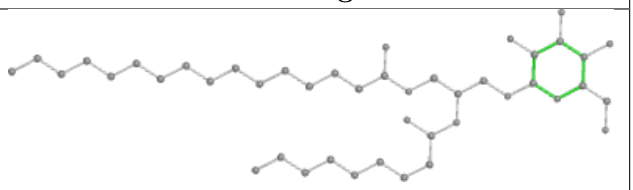
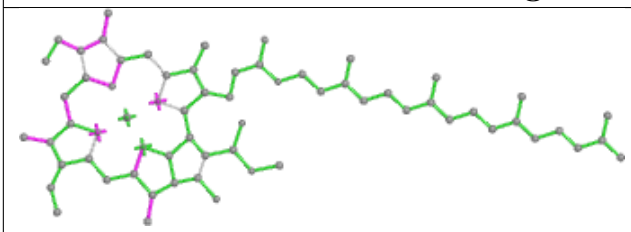


Rings

Ligand CLA C 511



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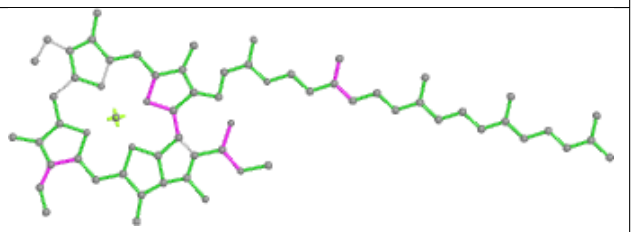
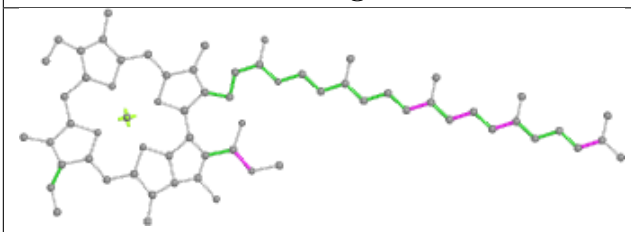


Bond angles



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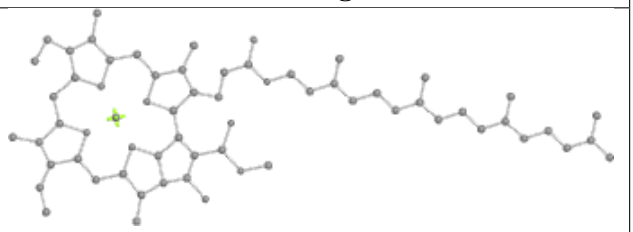
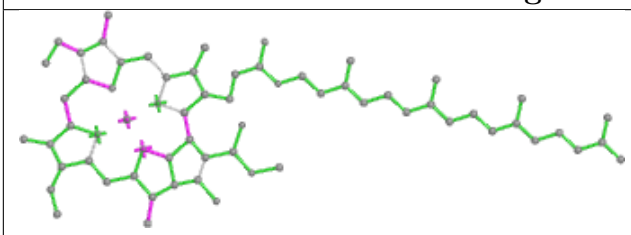


Rings

Ligand CLA C 512



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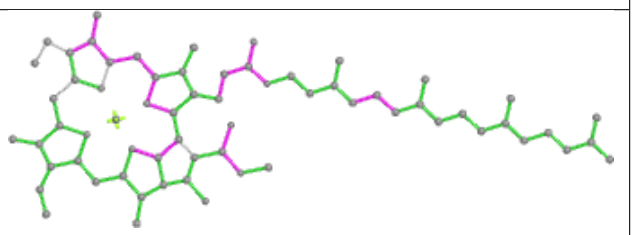
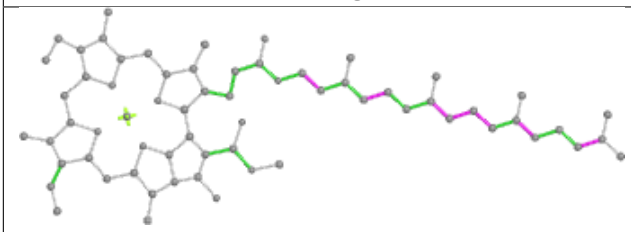


Bond angles



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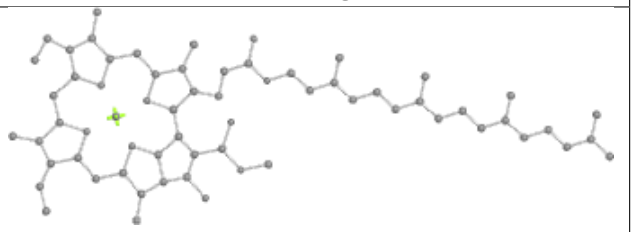
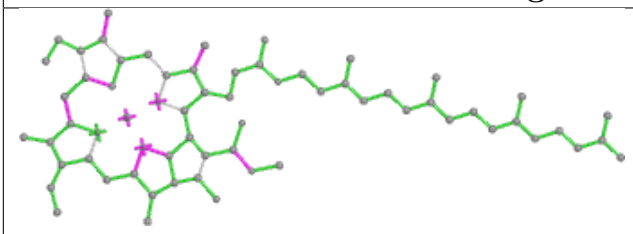


Rings

Ligand CLA b 610



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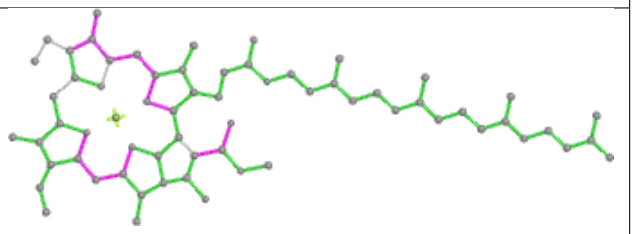
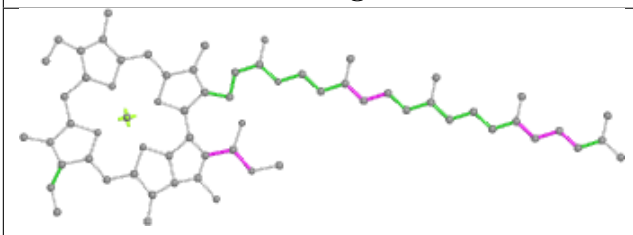


Bond angles



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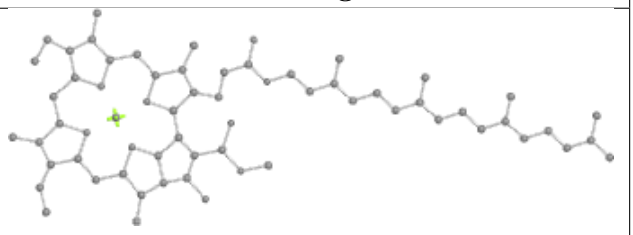
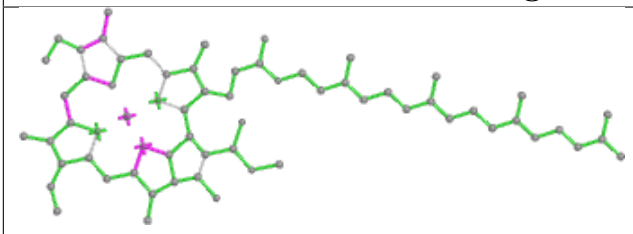


Rings

Ligand CLA D 403



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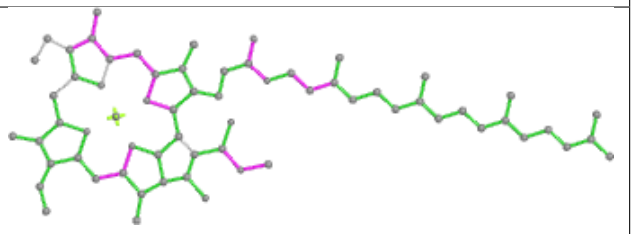
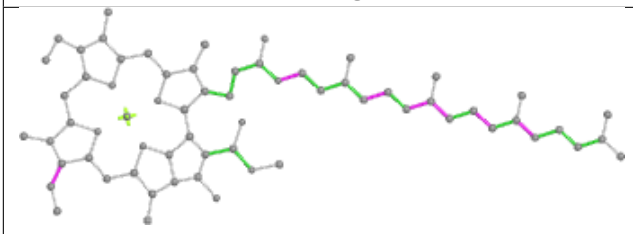


Bond angles



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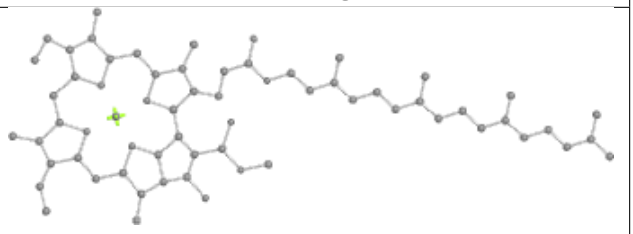
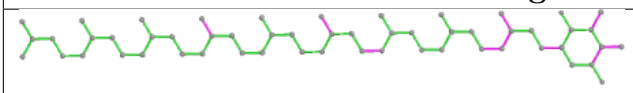


Rings

Ligand PL9 D 406



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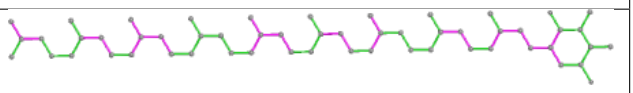
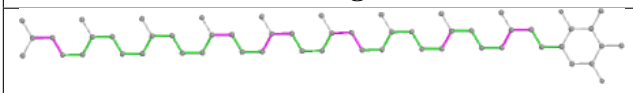


Bond angles



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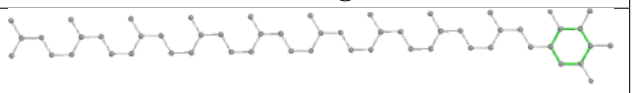
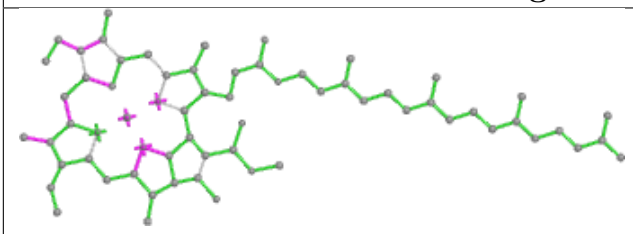


Rings

Ligand CLA c 506



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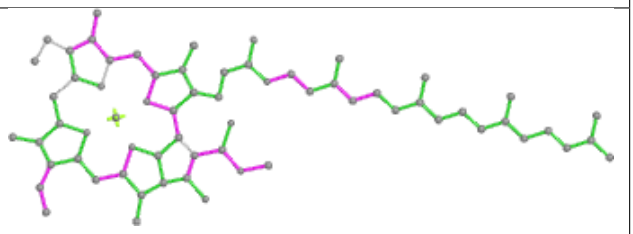
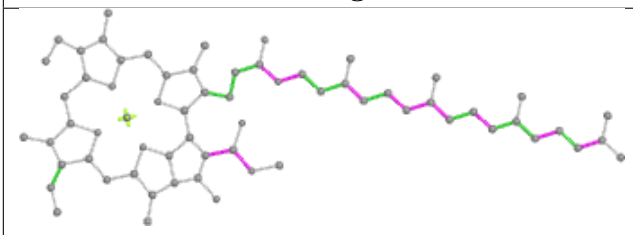


Bond angles



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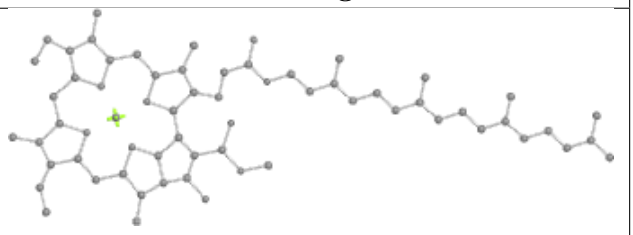
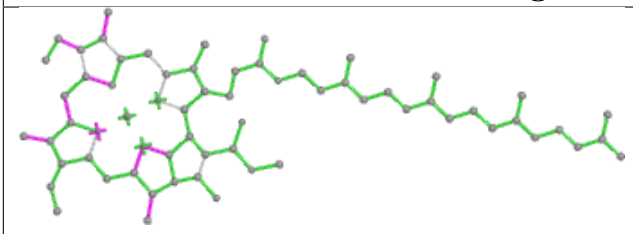


Rings

Ligand CLA c 512



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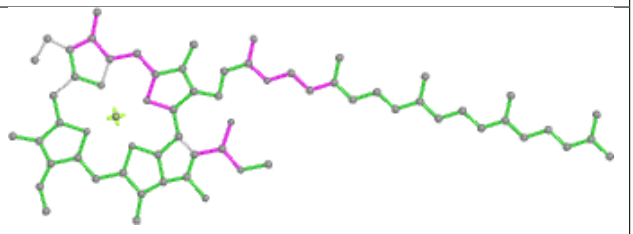
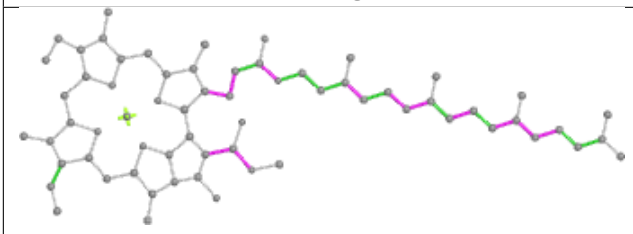
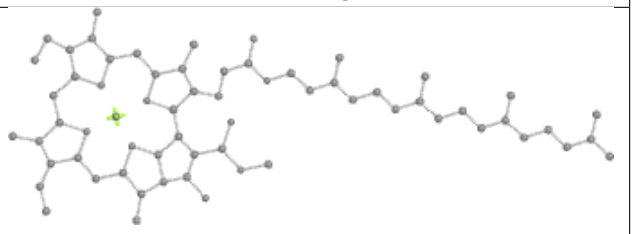


Bond angles

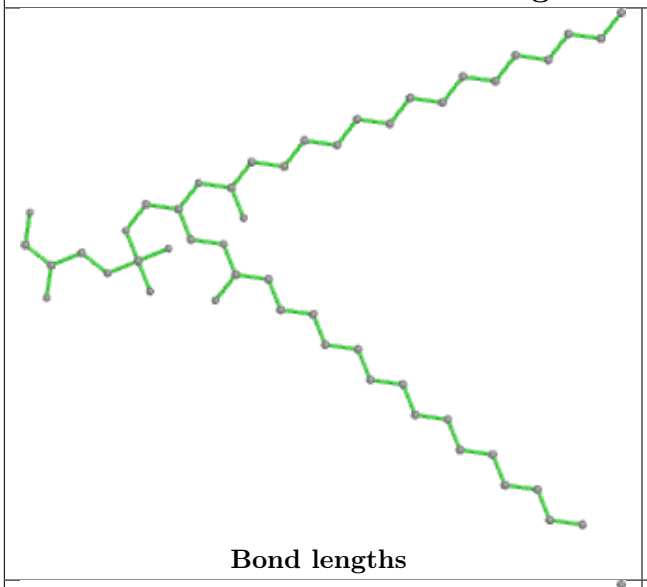


Torsions



Rings

Ligand LHG l 101



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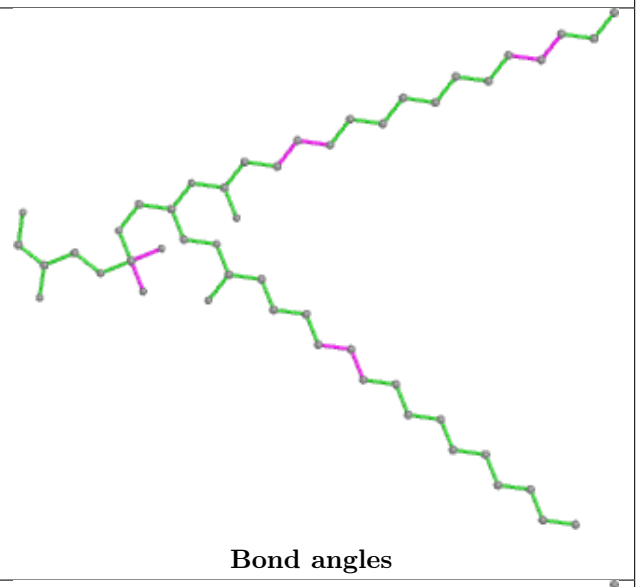
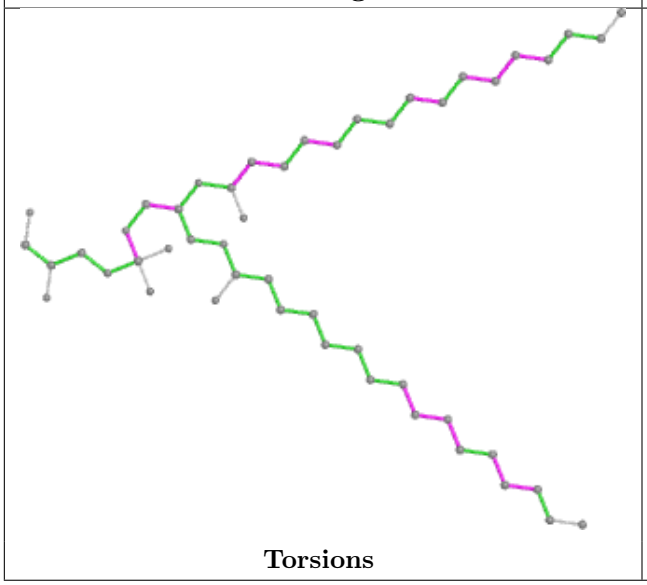
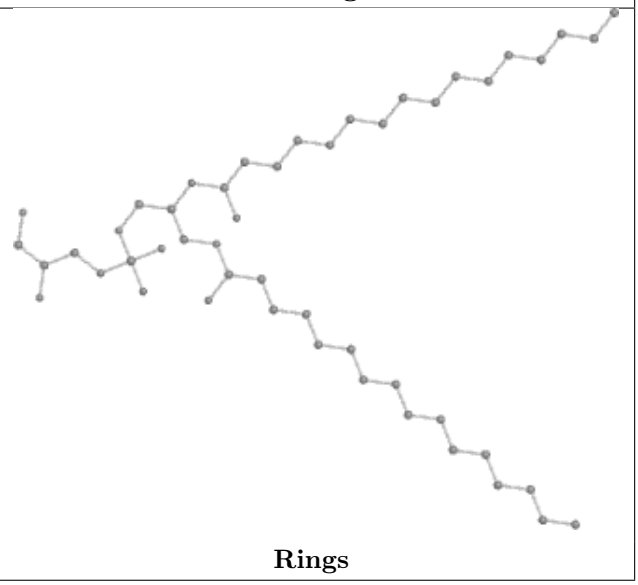


Bond angles

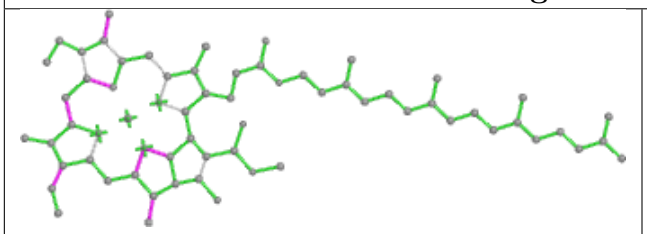


Torsions

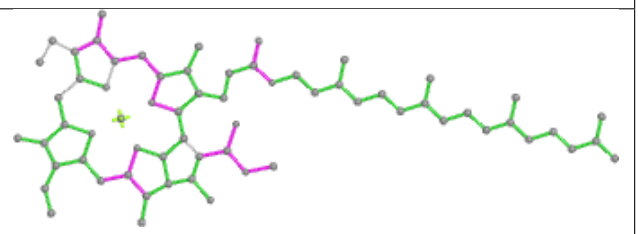


Rings

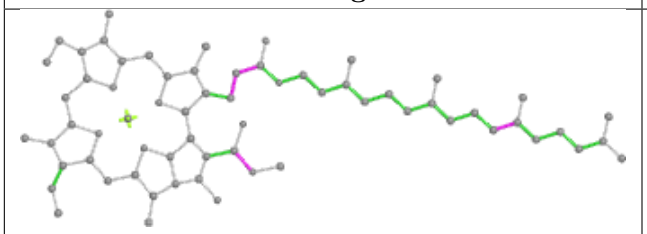
Ligand CLA c 501



Bond lengths



Bond angles



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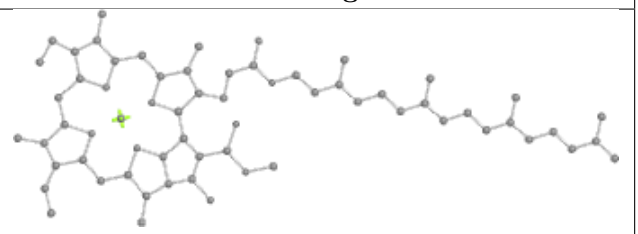
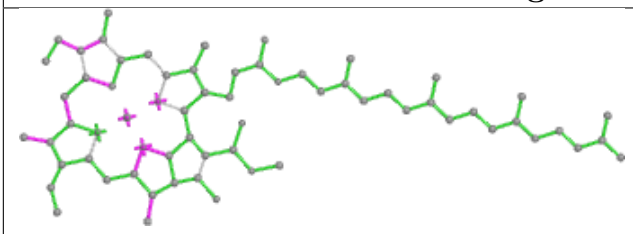


Rings

Ligand CLA d 404



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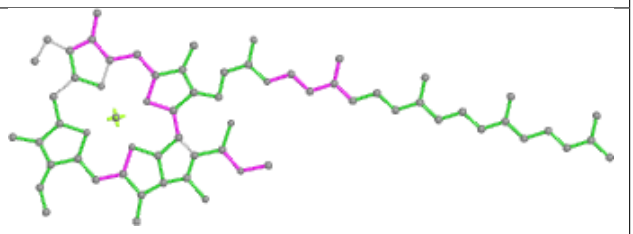
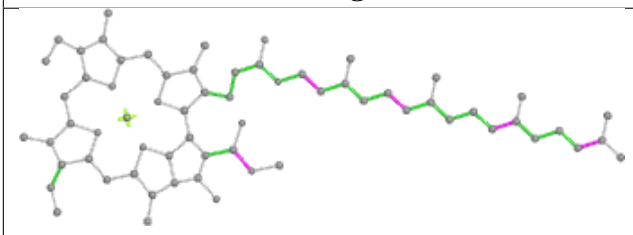
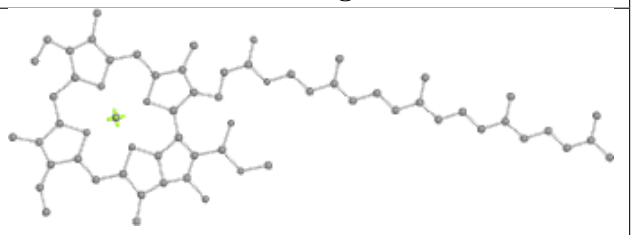


Bond angles

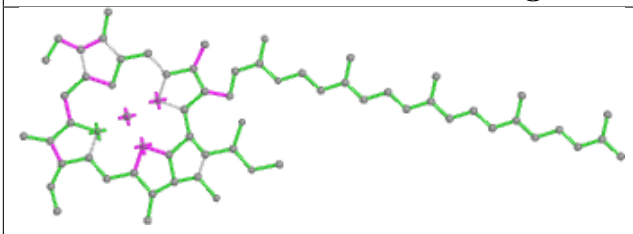


Torsions



Rings

Ligand CLA B 604



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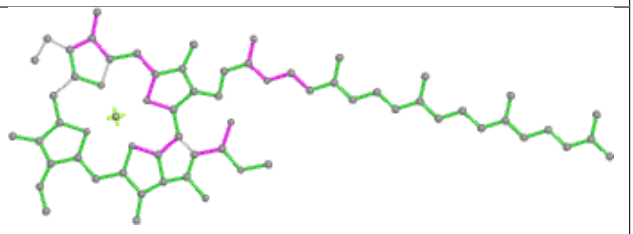
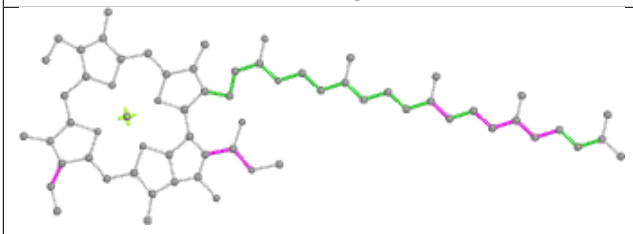


Bond angles



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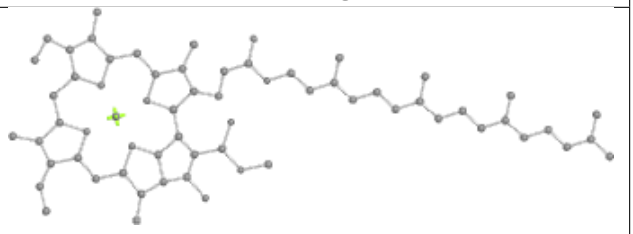
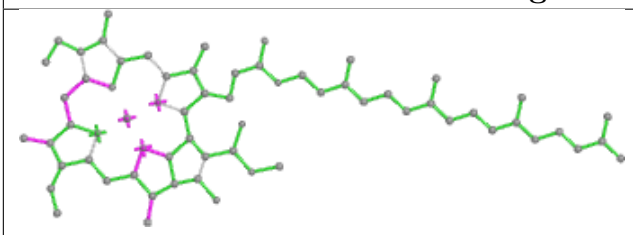


Rings

Ligand CLA c 502



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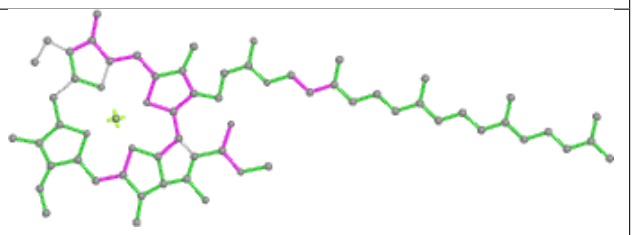
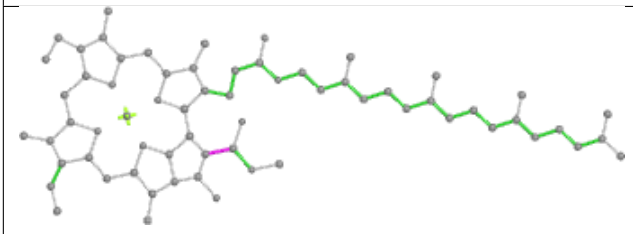


Bond angles



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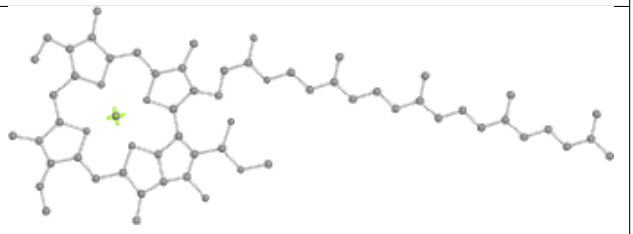
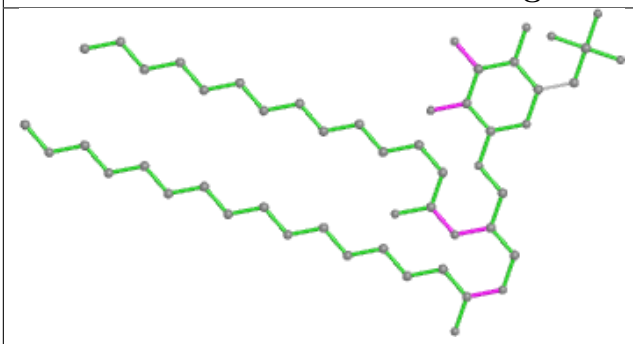


Rings

Ligand SQD A 412



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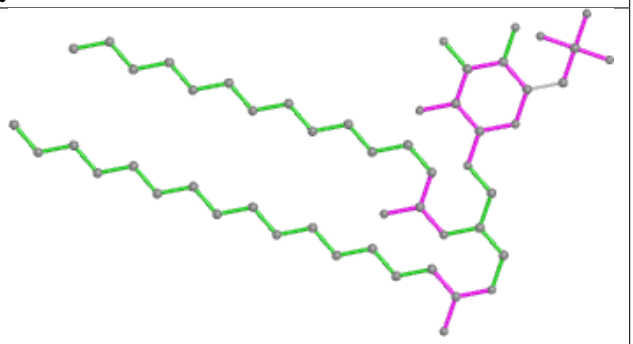
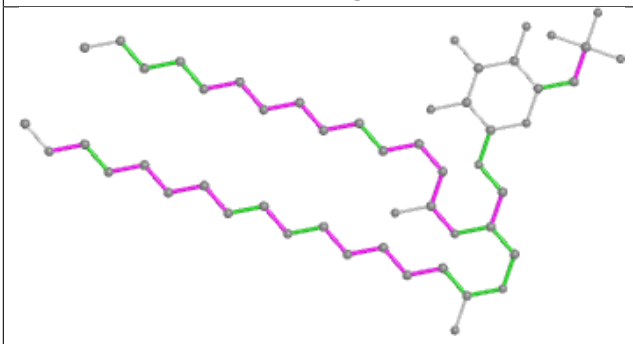


Bond angles



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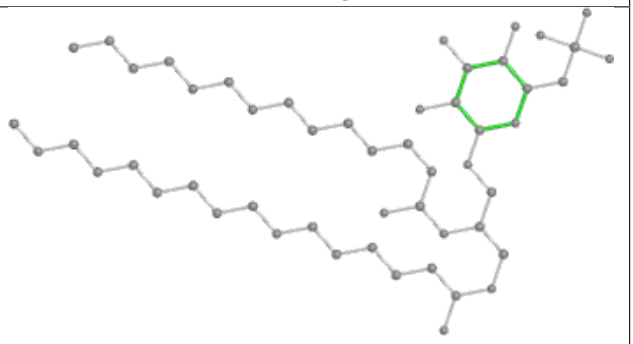
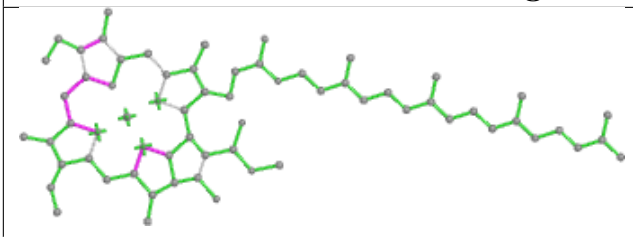


Rings

Ligand CLA B 605



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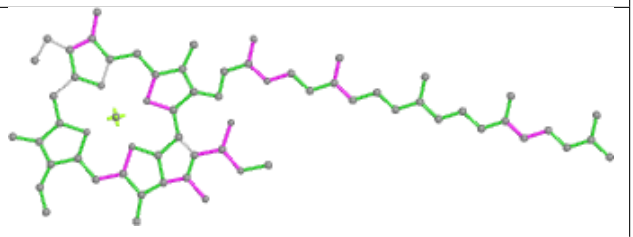
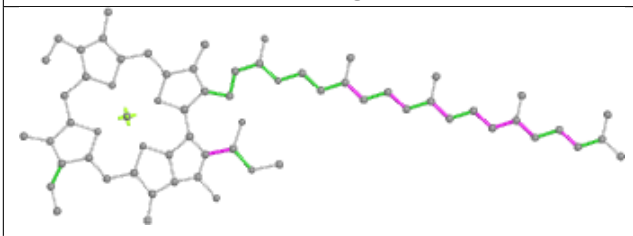


Bond angles



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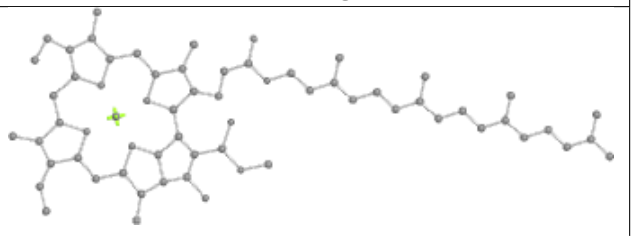
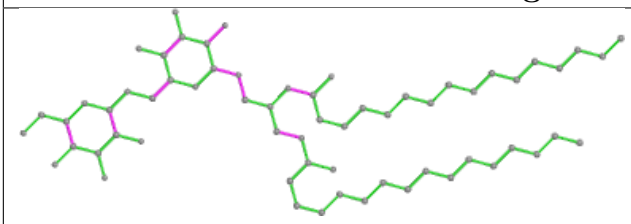


Rings

Ligand DGD h 102



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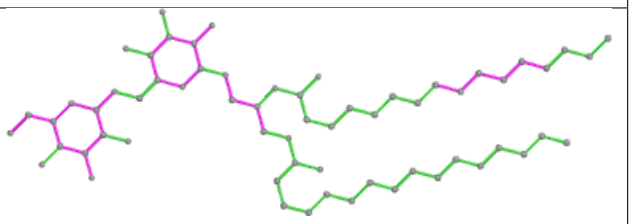

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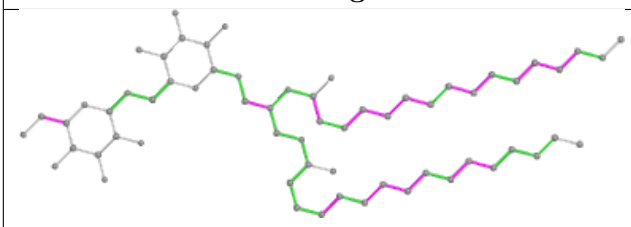

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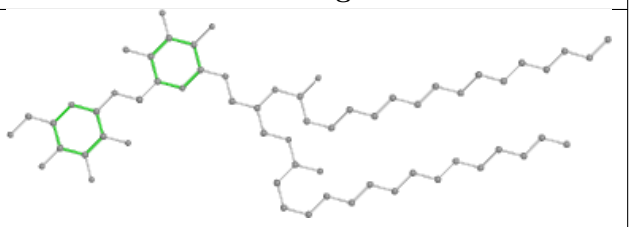
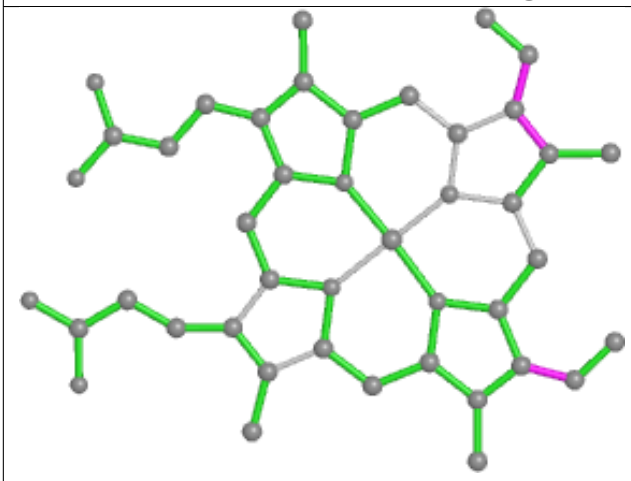


Rings

Ligand HEM F 101



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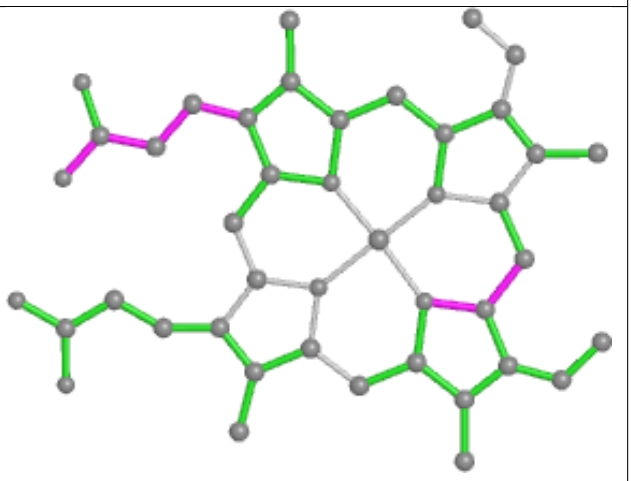
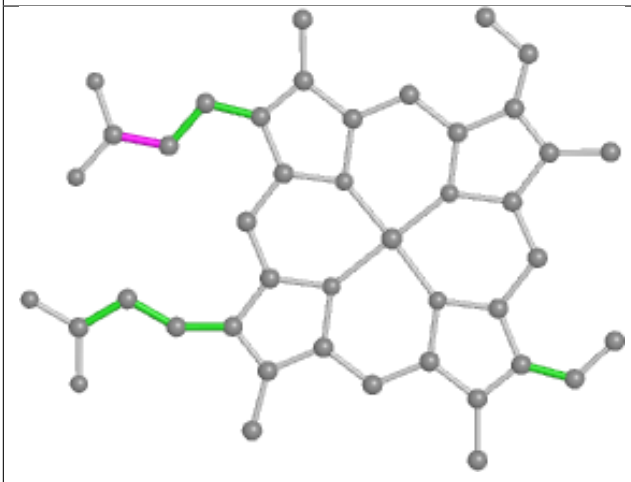
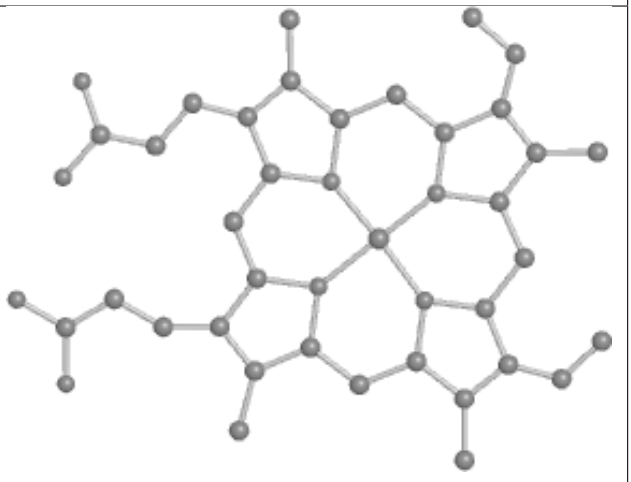


Bond angles

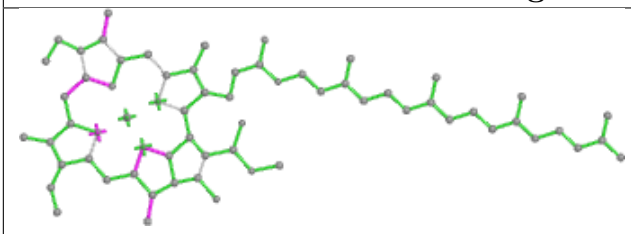


Torsions



Rings

Ligand CLA b 614



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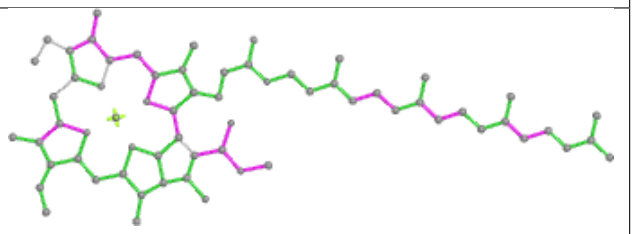
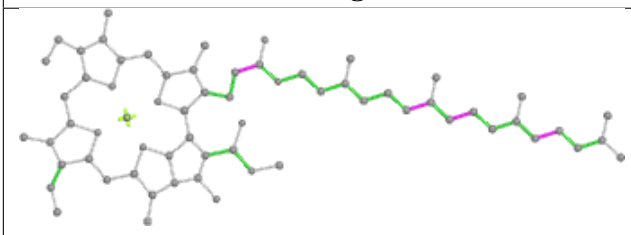


Bond angles



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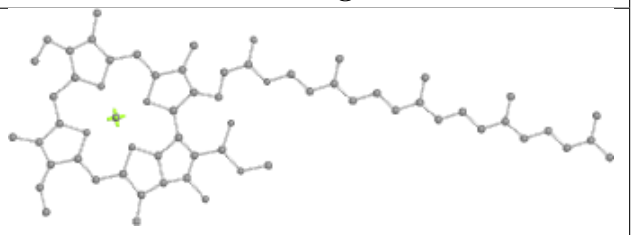
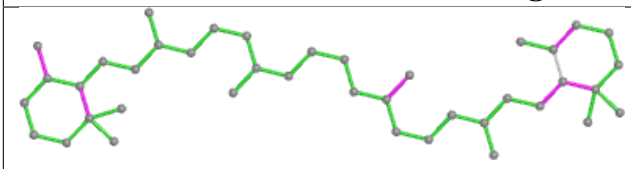


Rings

Ligand 8CT C 515



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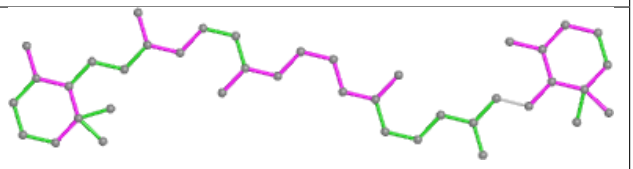
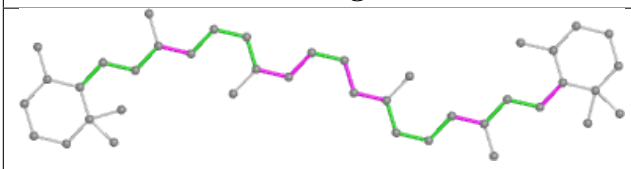


Bond angles



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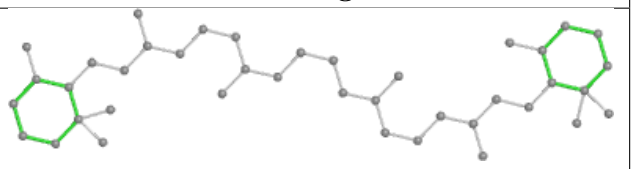
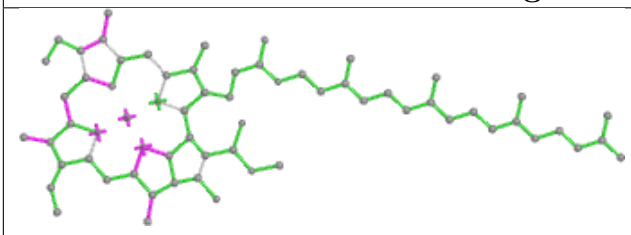


Rings

Ligand CLA A 411



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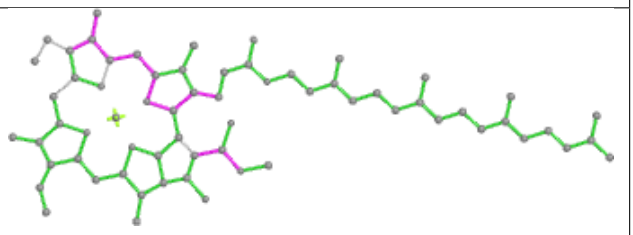
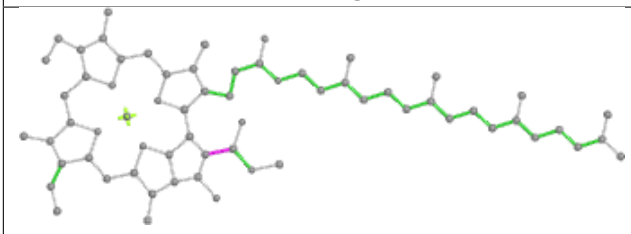
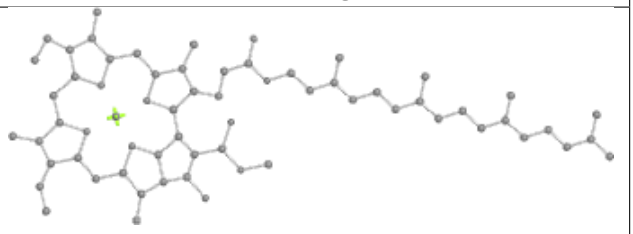


Bond angles

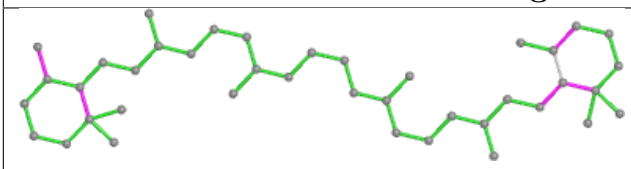


Torsions



Rings

Ligand 8CT d 405



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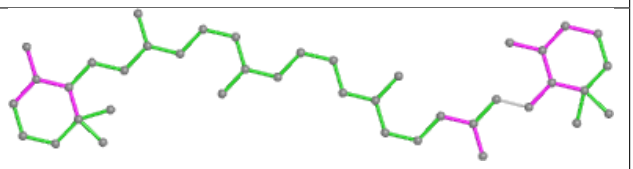
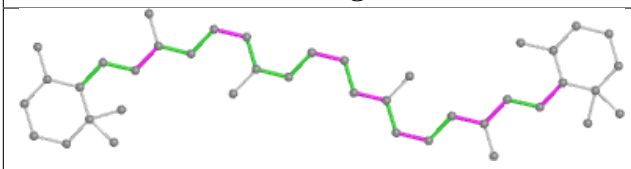


Bond angles



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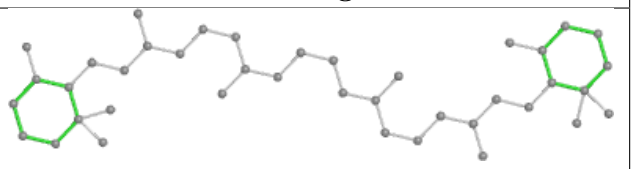
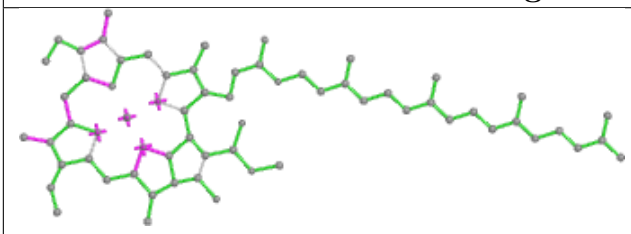
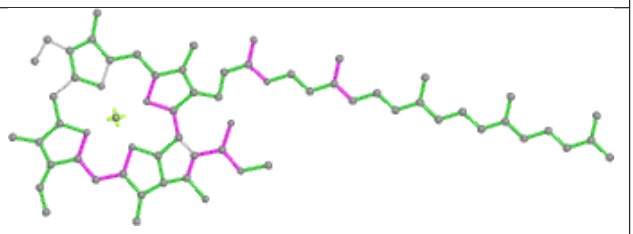


Rings

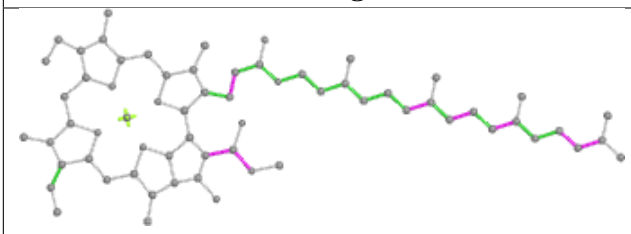
Ligand CLA B 606



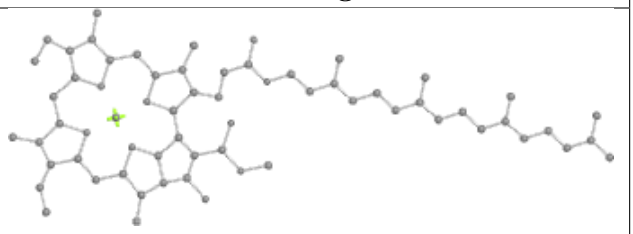
Bond lengths



Bond angles

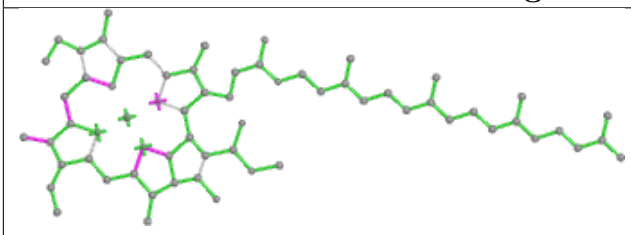


Torsions

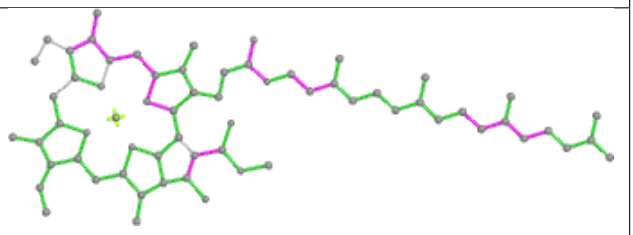


Rings

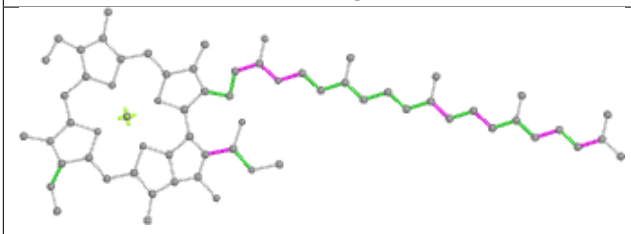
Ligand CLA B 612



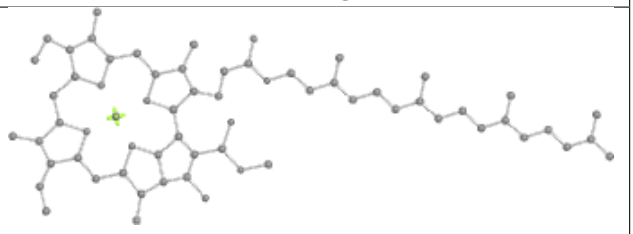
Bond lengths



Bond angles

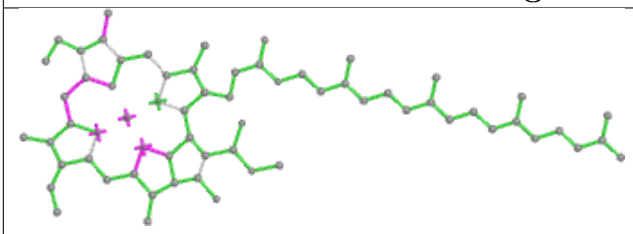


Torsions



Rings

Ligand CLA B 602



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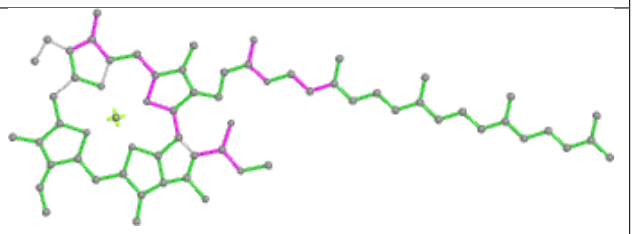
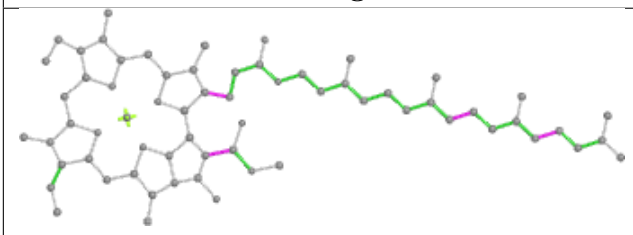


Bond angles



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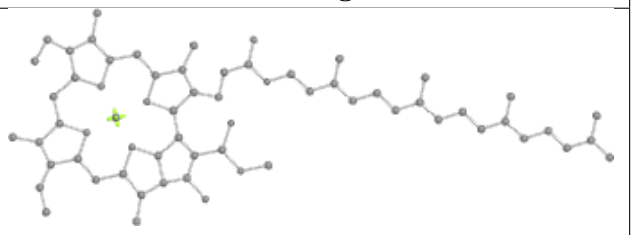
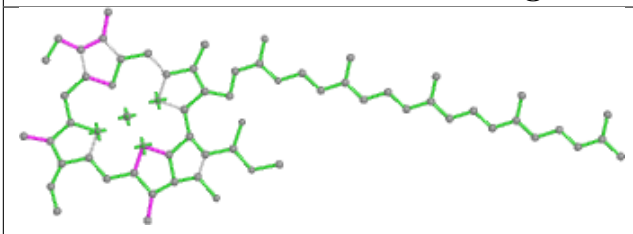


Rings

Ligand CLA B 603



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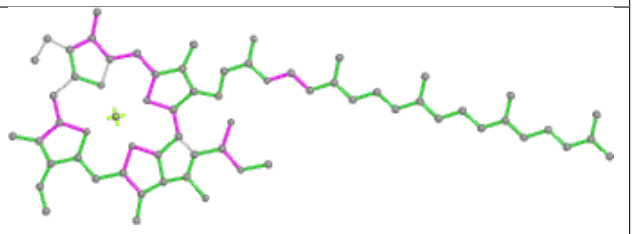
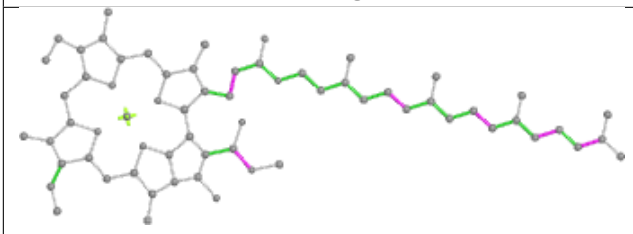


Bond angles



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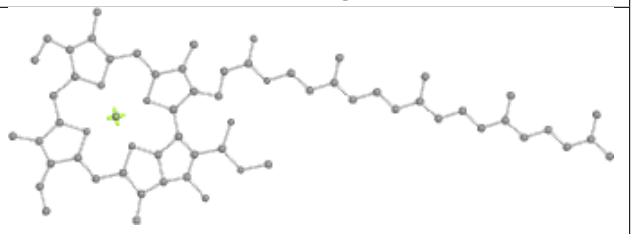
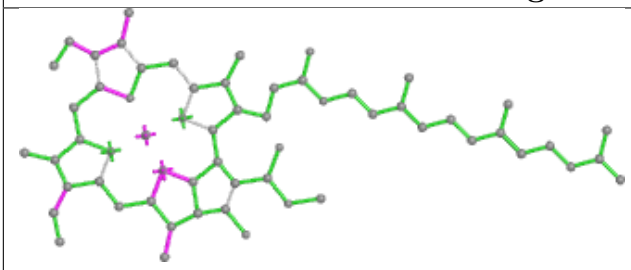


Rings

Ligand CLA b 617



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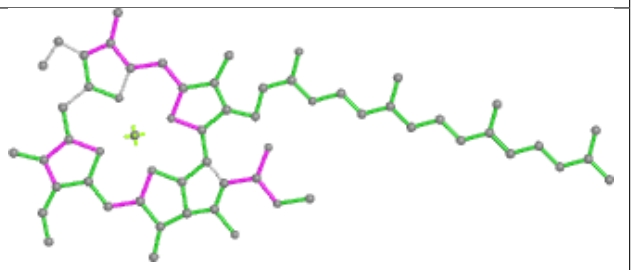
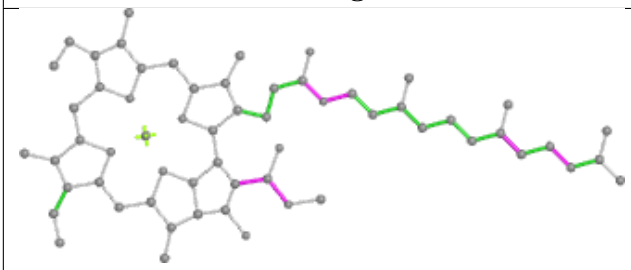


Bond angles



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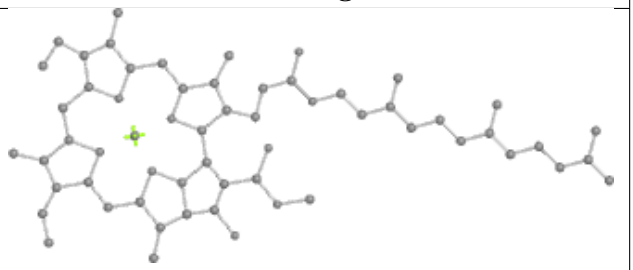
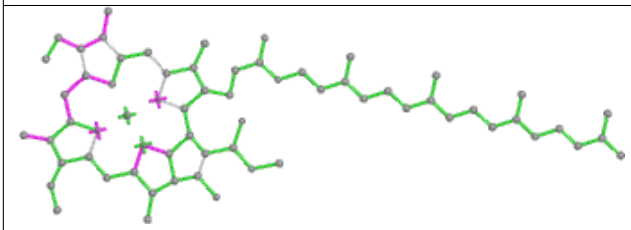


Rings

Ligand CLA c 507



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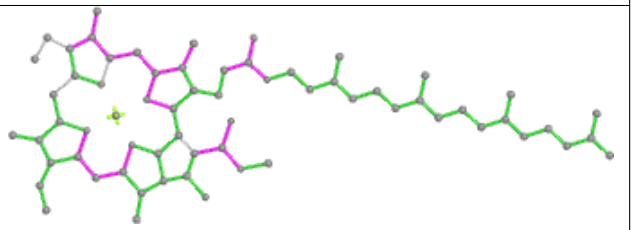
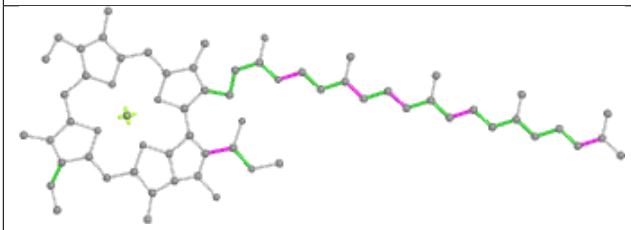


Bond angles



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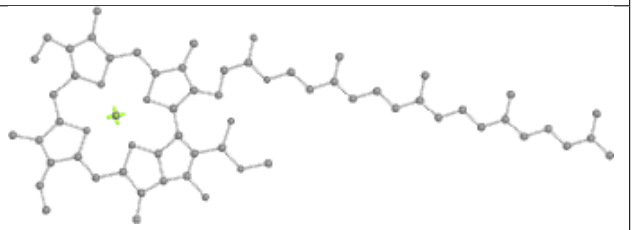
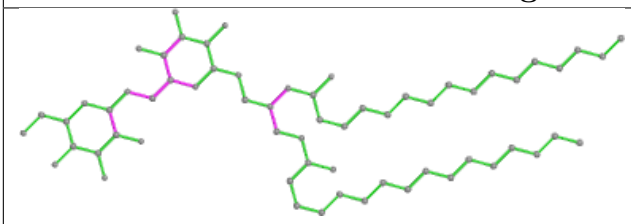


Rings

Ligand DGD C 517



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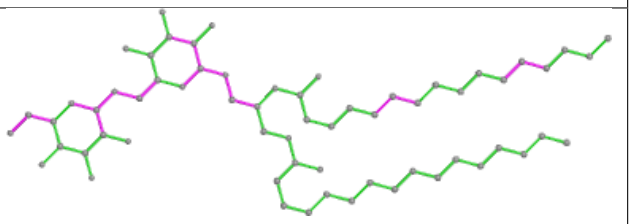
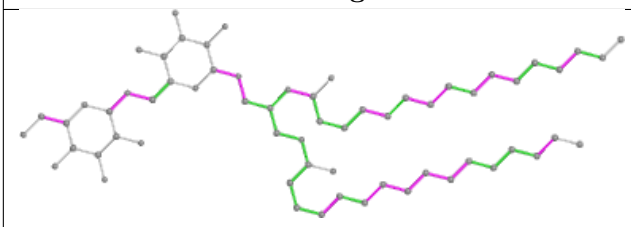


Bond angles



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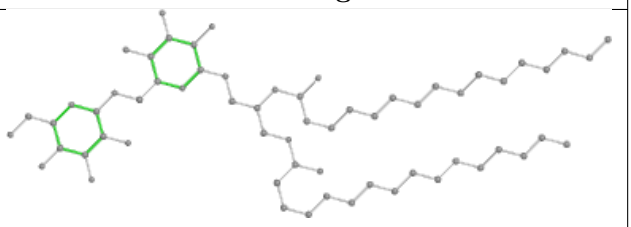

Rings

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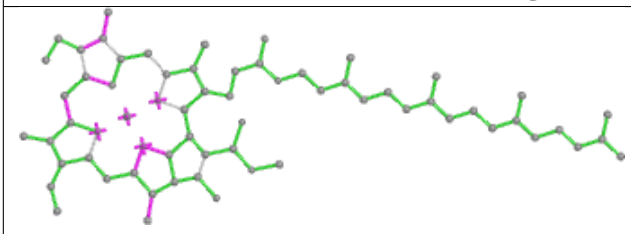

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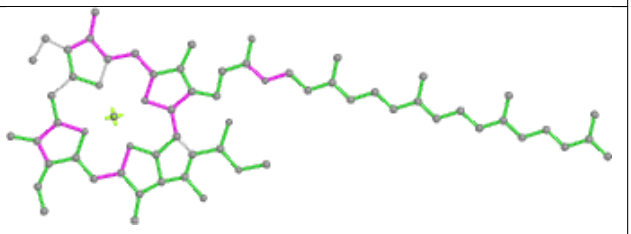
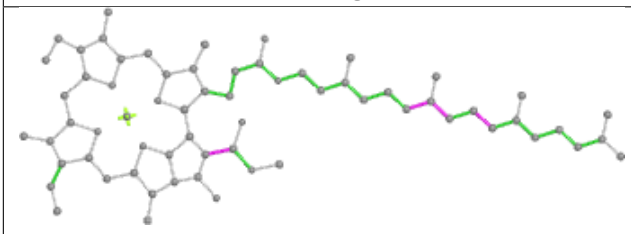


Bond angles



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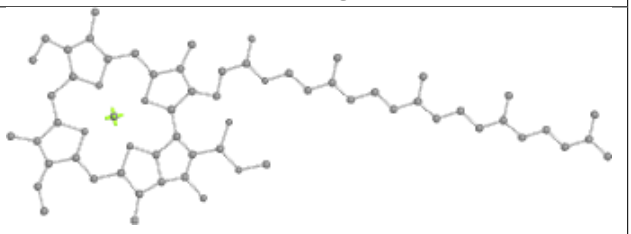
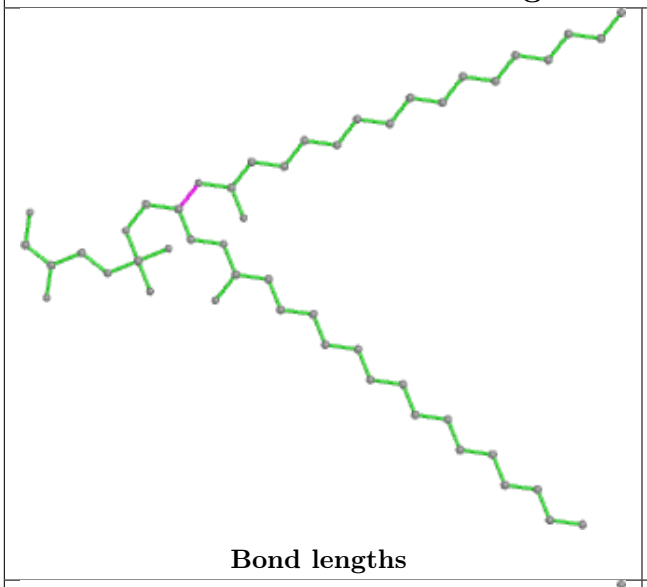


Rings

Ligand LHG B 623



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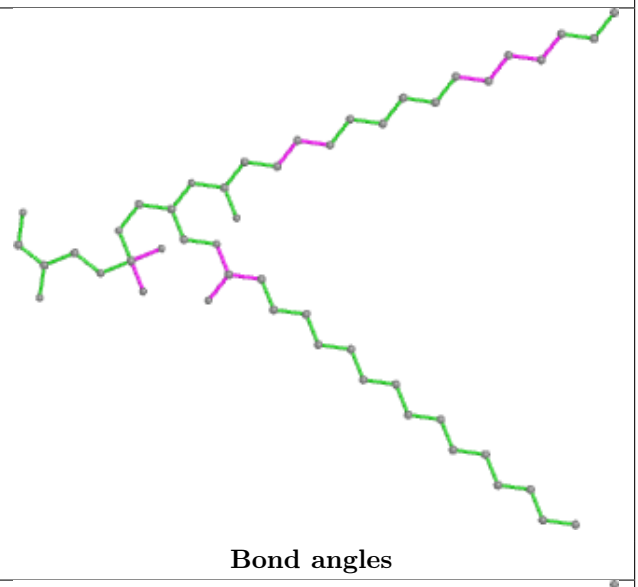

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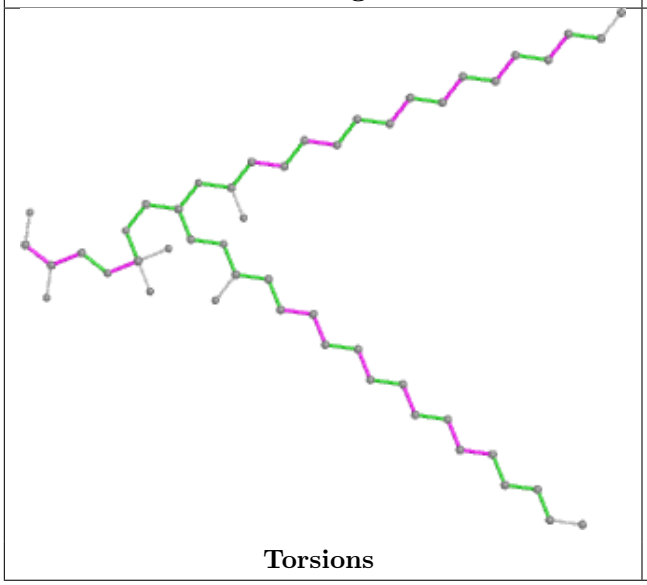

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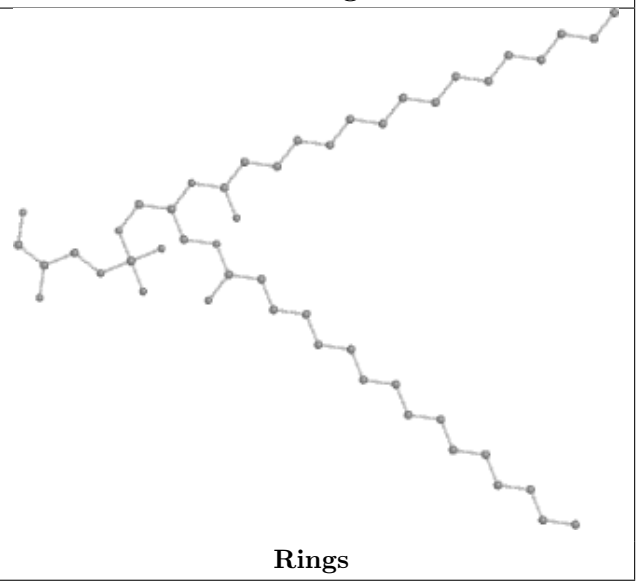
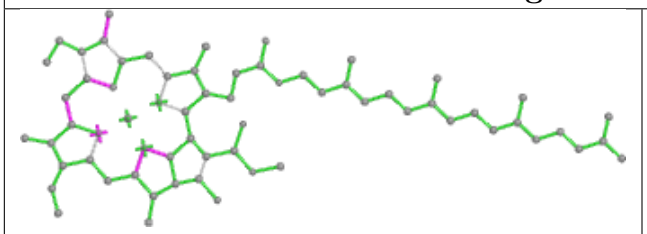


Rings

Ligand CLA C 510



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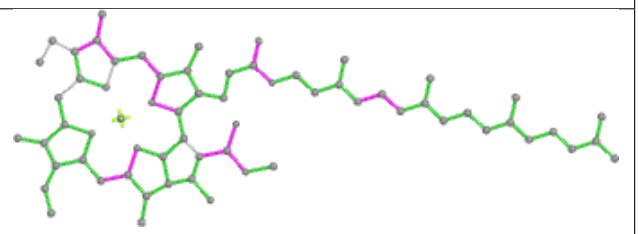
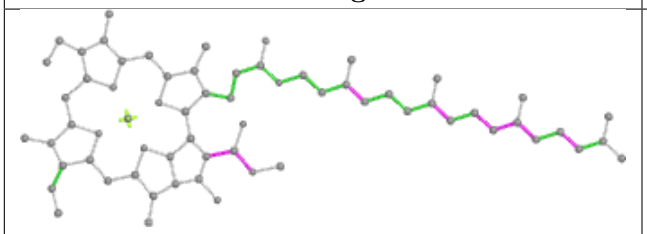


Bond angles



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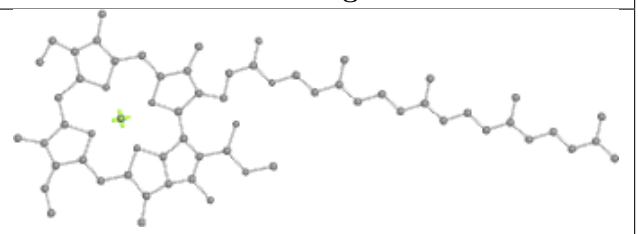
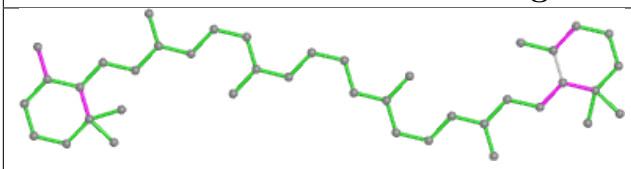


Rings

Ligand 8CT k 101



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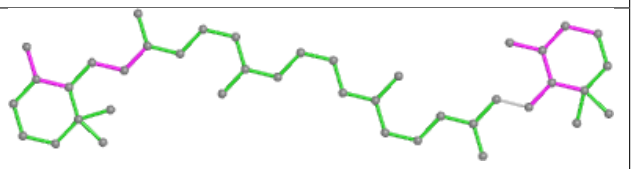
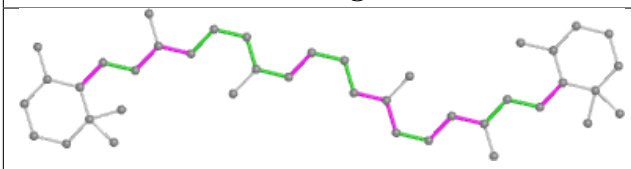


Bond angles



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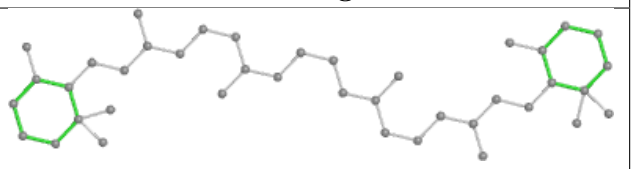
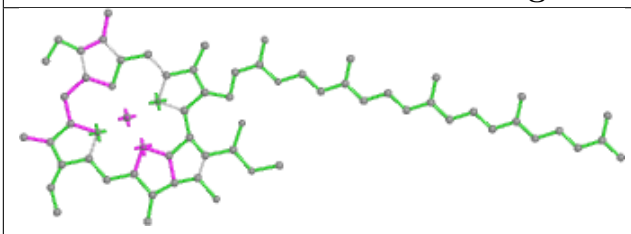


Rings

Ligand CLA a 408



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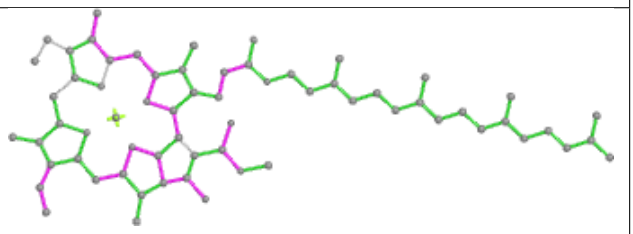
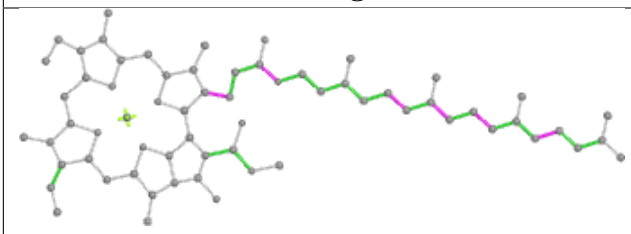


Bond angles



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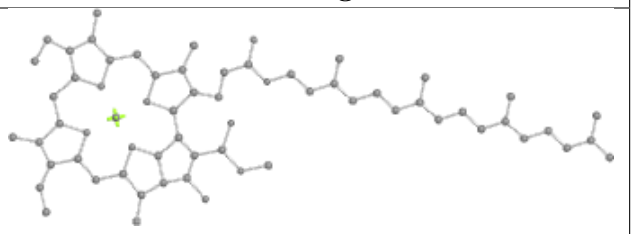
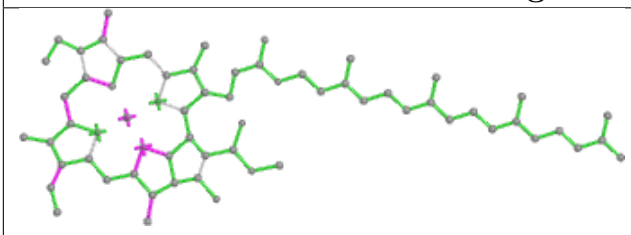
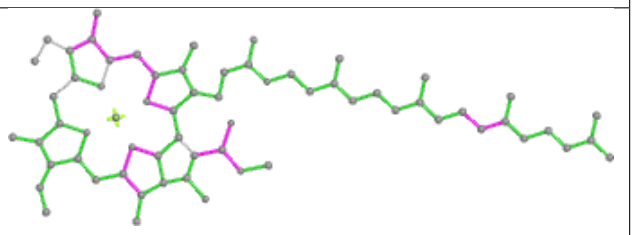


Rings

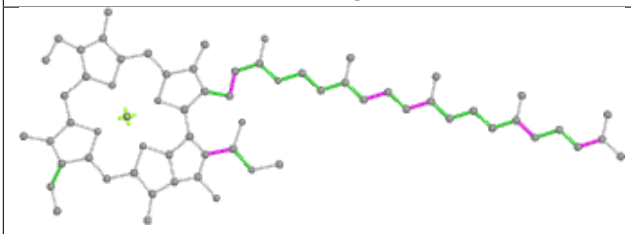
Ligand CLA b 603



Bond lengths



Bond angles



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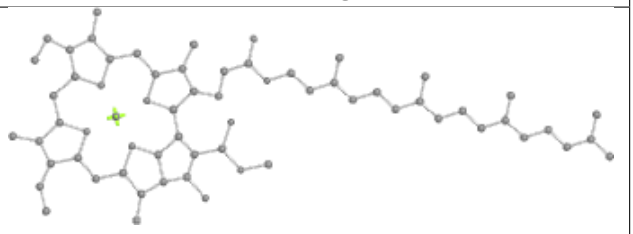
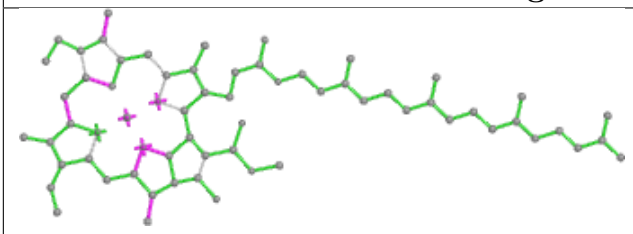


Rings

Ligand CLA d 402



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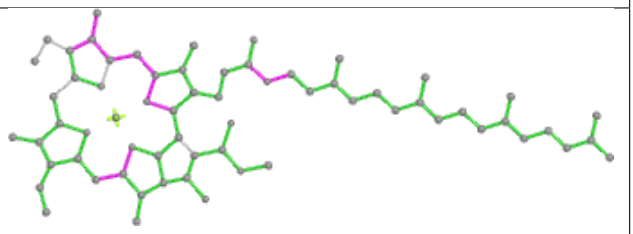
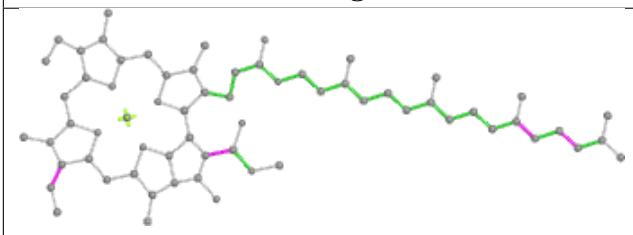


Bond angles



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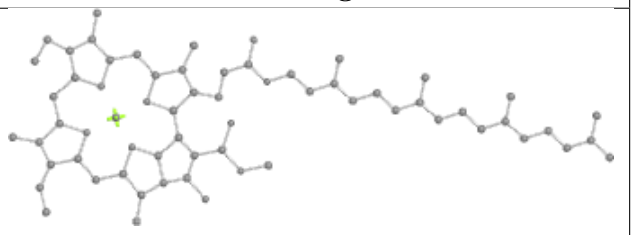
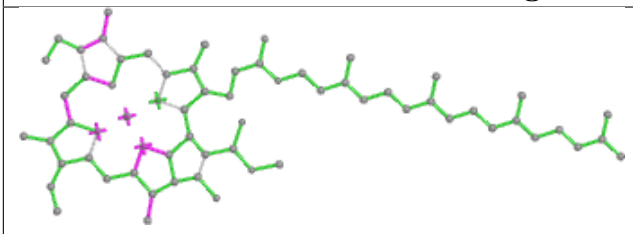
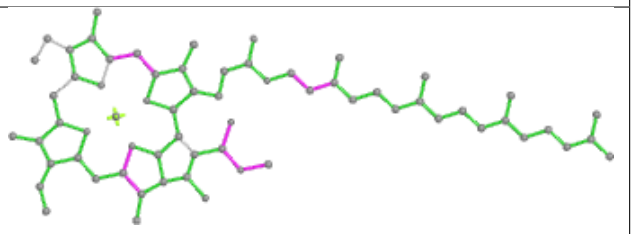


Rings

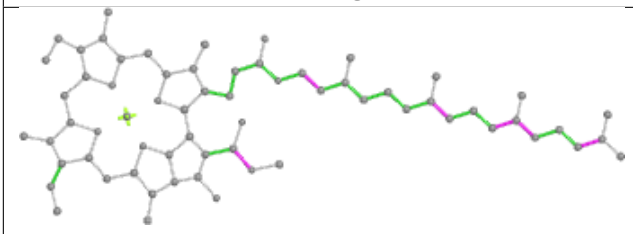
Ligand CLA D 404



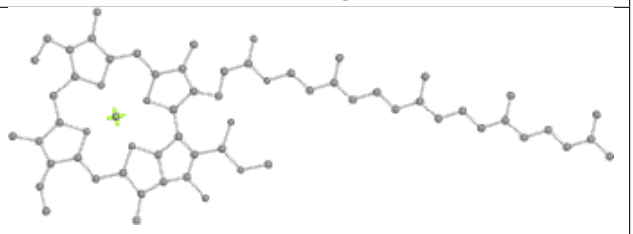
Bond lengths



Bond angles

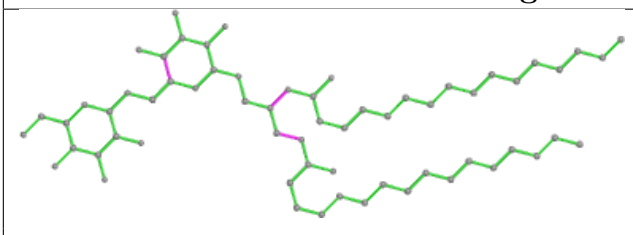


Torsions



Rings

Ligand DGD C 518



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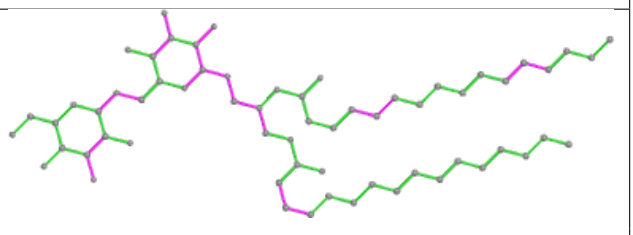
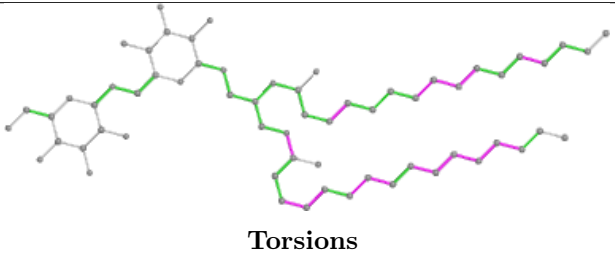


Bond angles



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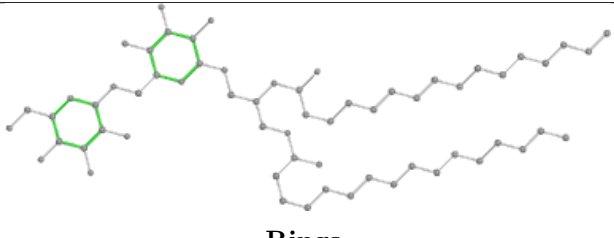
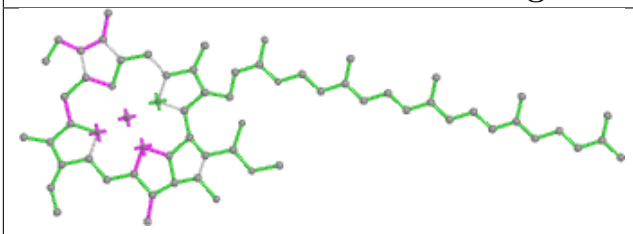
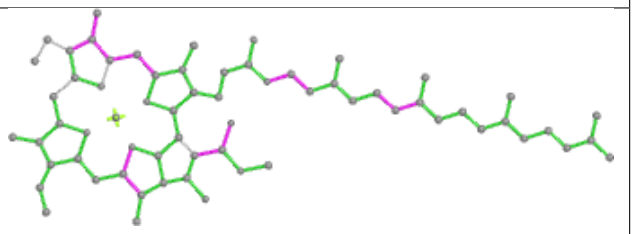


Rings

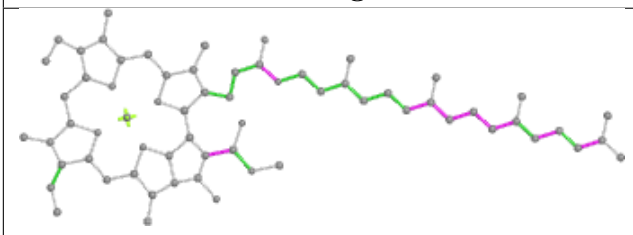
Ligand CLA b 608



Bond lengths



Bond angles



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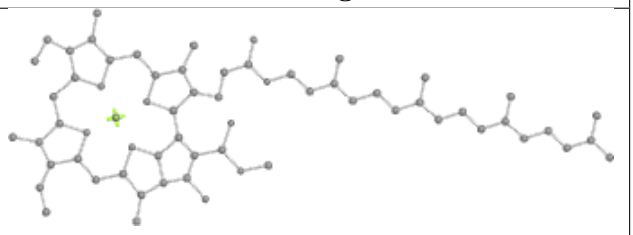
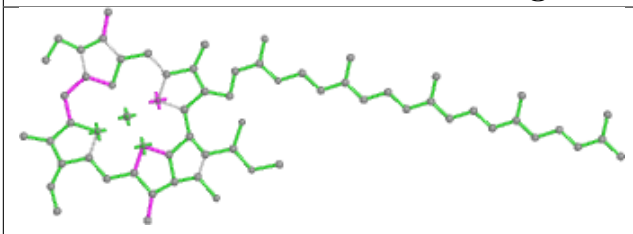


Rings

Ligand CLA c 510



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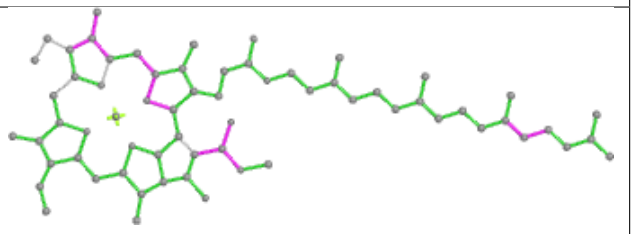
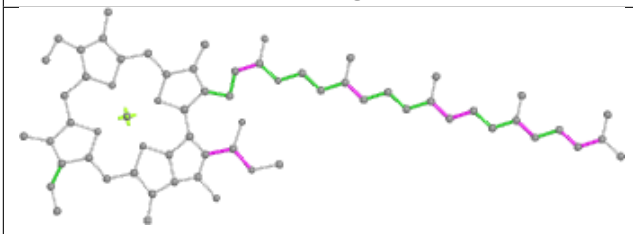
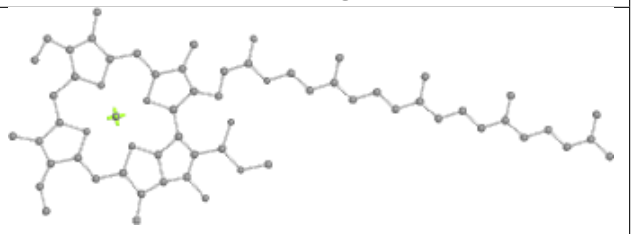


Bond angles

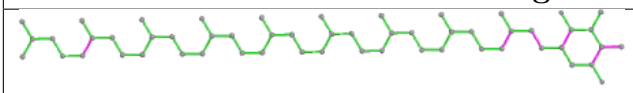


Torsions



Rings

Ligand PL9 d 406



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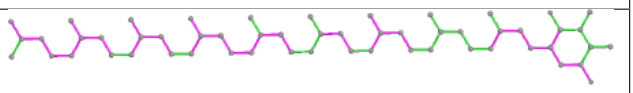
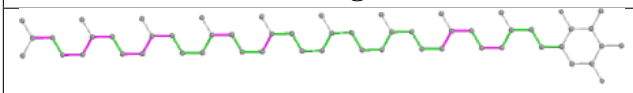


Bond angles



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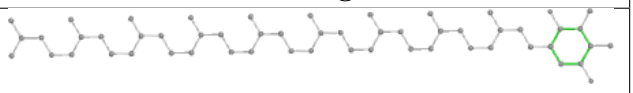
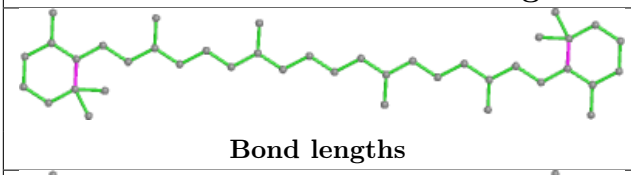
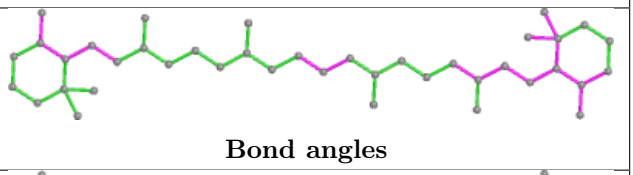


Rings

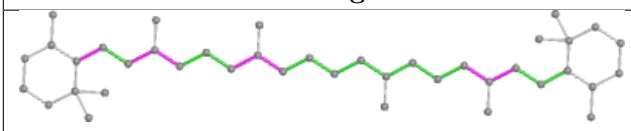
Ligand BCR Y 101



Bond lengths



Bond angles



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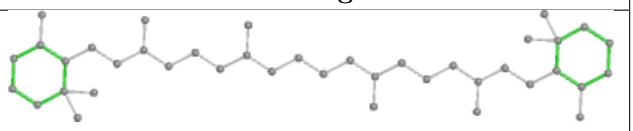
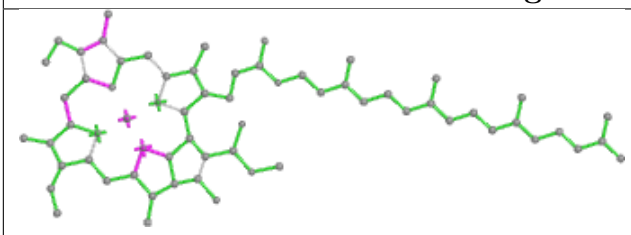


Rings

Ligand CLA B 614



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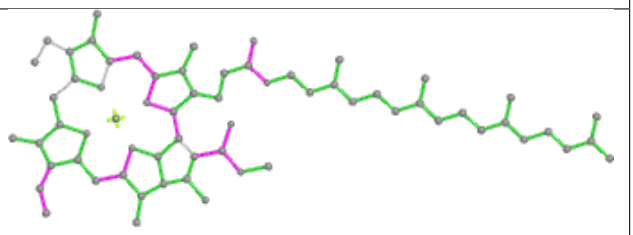
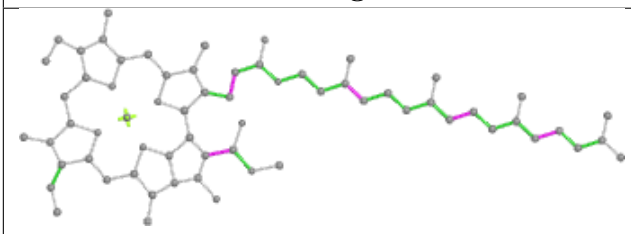
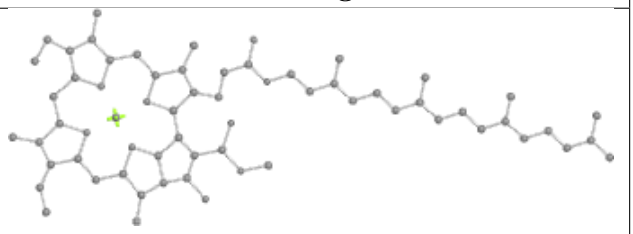


Bond angles

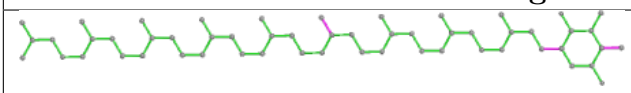


Torsions



Rings

Ligand PL9 A 409



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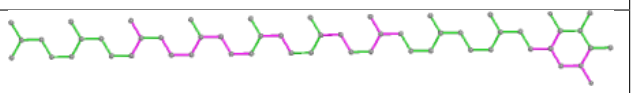
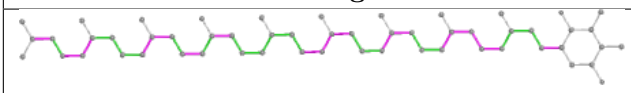
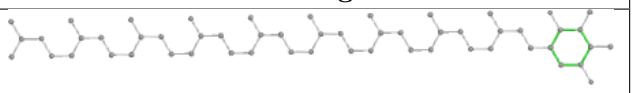


Bond angles

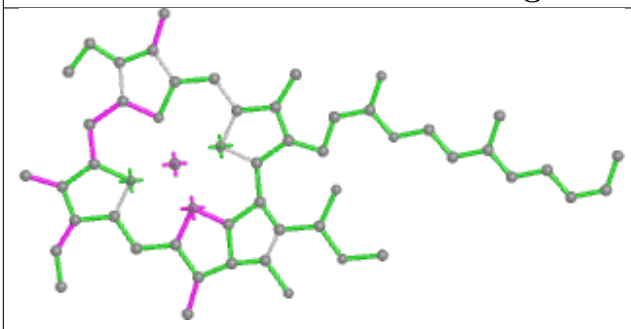


Torsions



Rings

Ligand CLA A 407



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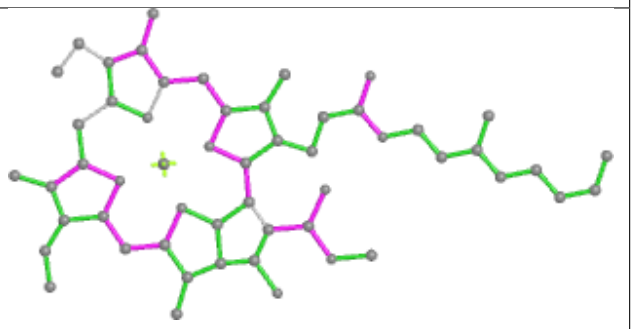
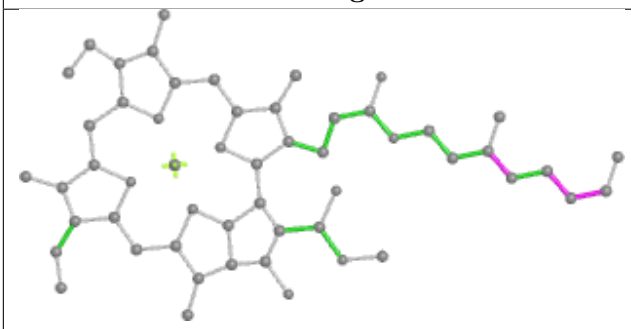


Bond angles



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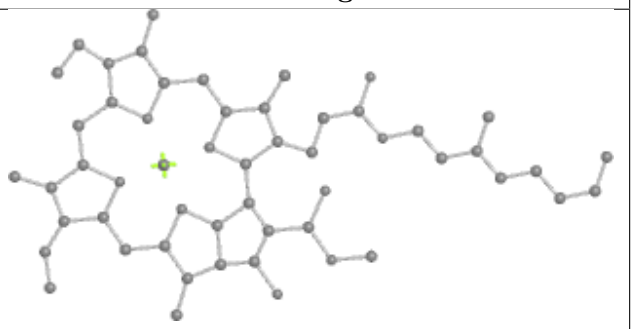
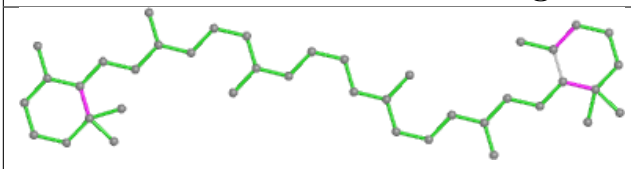


Rings

Ligand 8CT c 514



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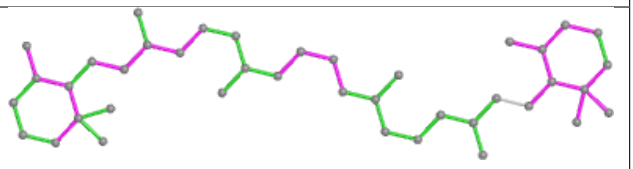
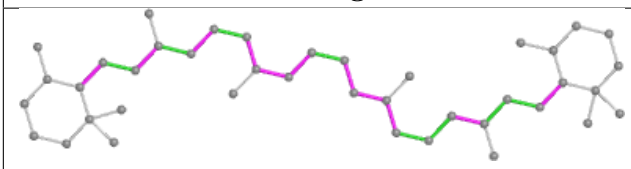


Bond angles



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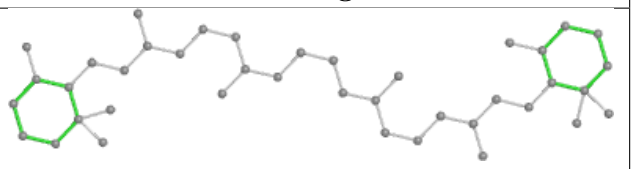
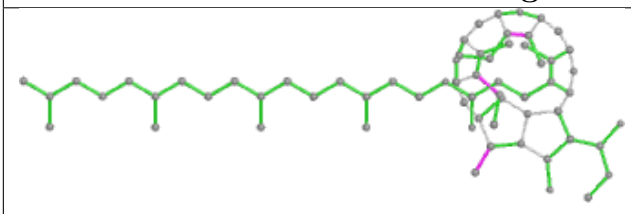


Rings

Ligand PHO D 402



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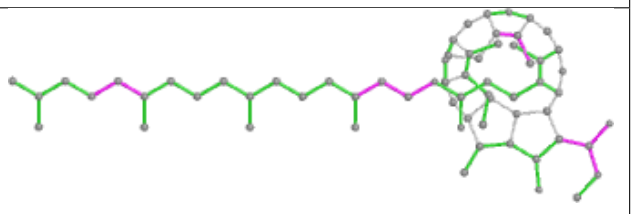
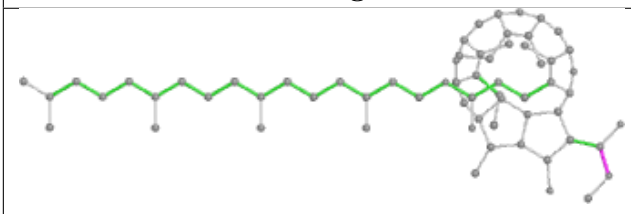


Bond angles



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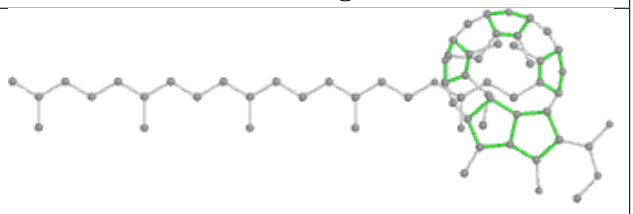
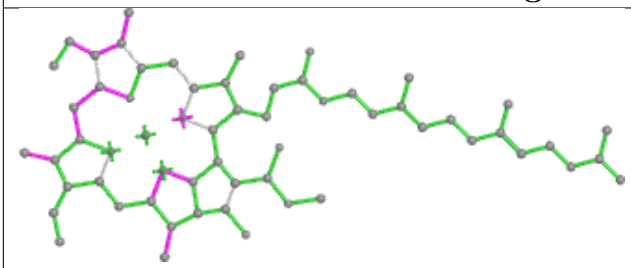


Rings

Ligand CLA B 616



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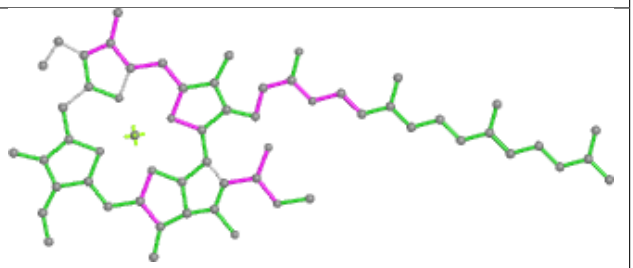
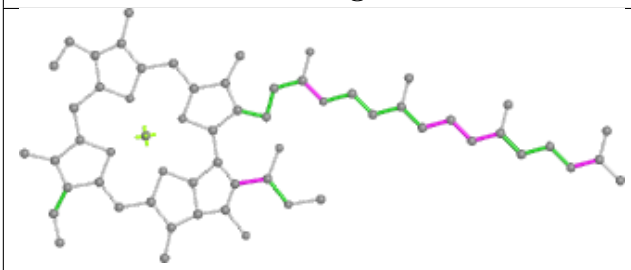


Bond angles



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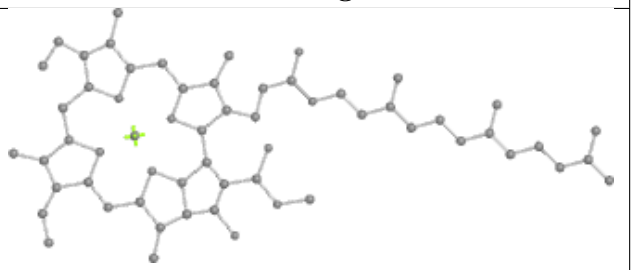
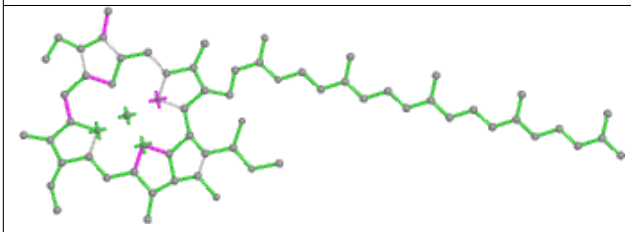
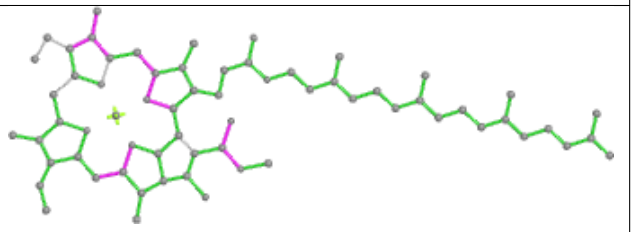


Rings

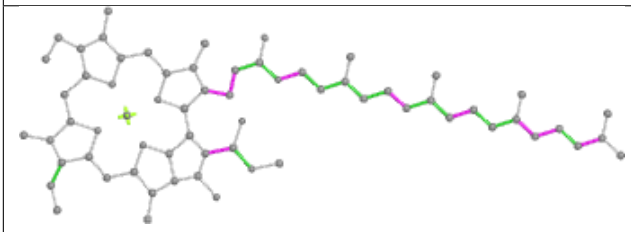
Ligand CLA c 513



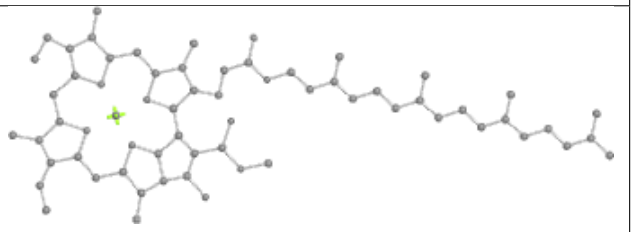
Bond lengths



Bond angles

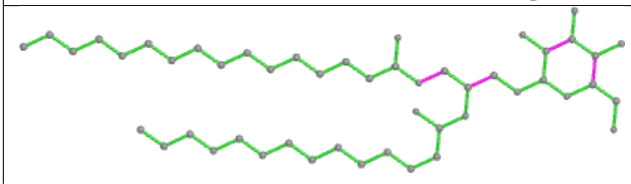


Torsions

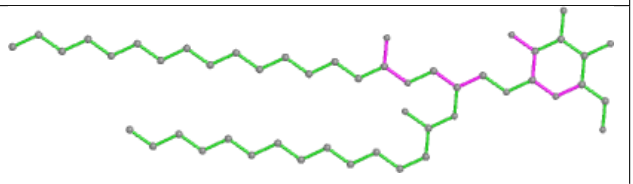


Rings

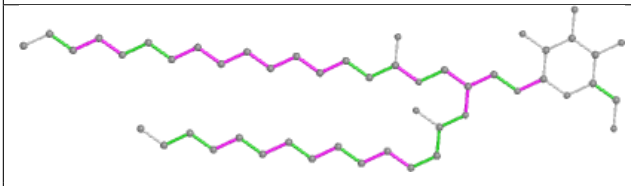
Ligand LMG c 524



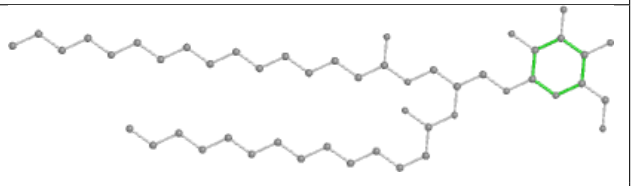
Bond lengths



Bond angles

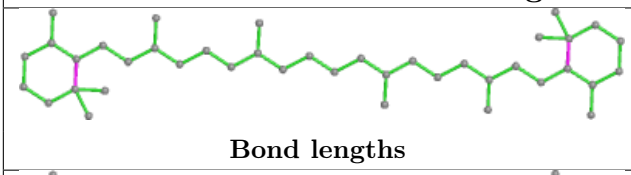


Torsions



Rings

Ligand BCR h 101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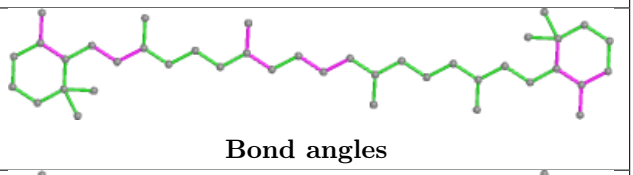
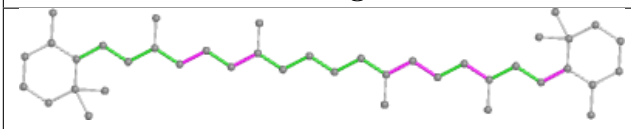
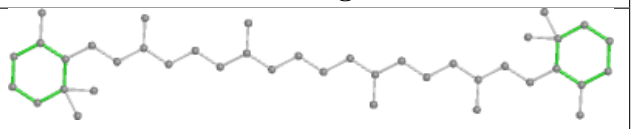
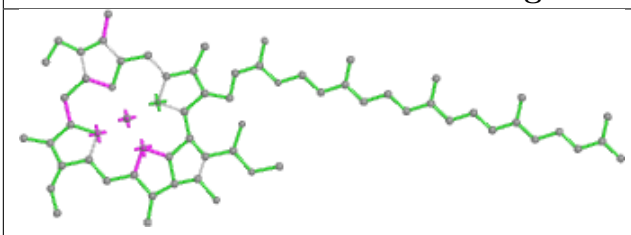

Bond angles


Torsions


Rings

Ligand CLA C 509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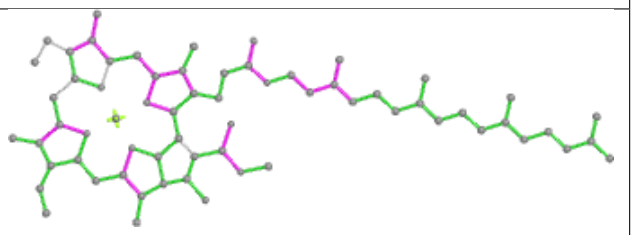
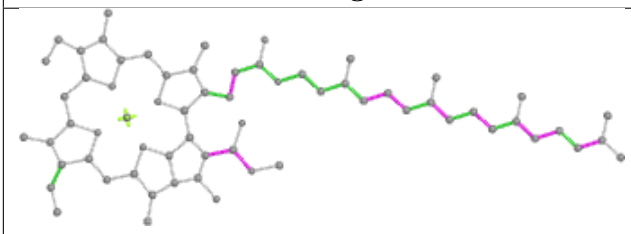
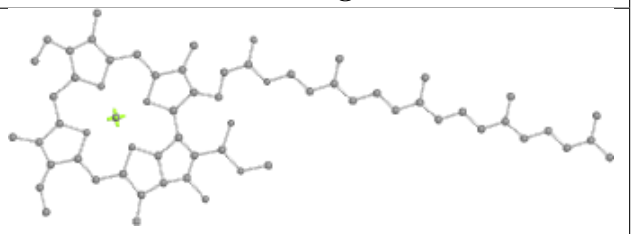
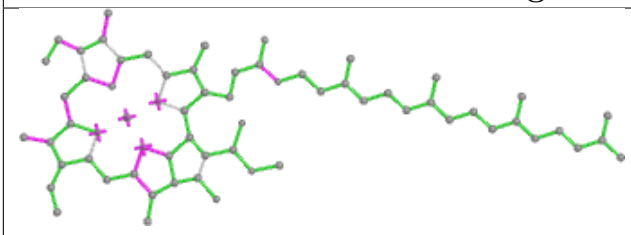

Bond angles


Torsions


Rings

Ligand CLA b 602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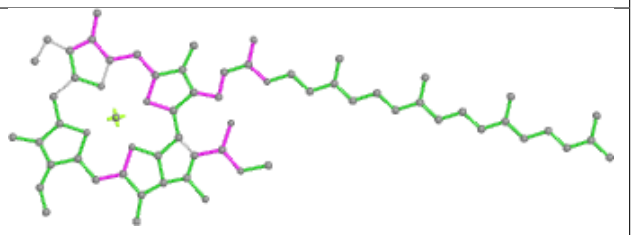
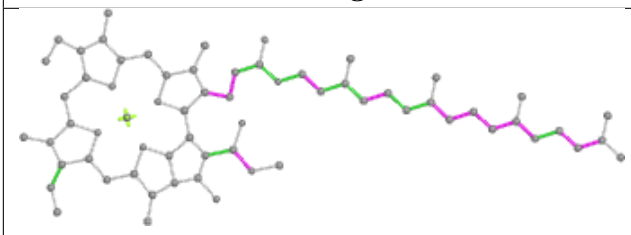
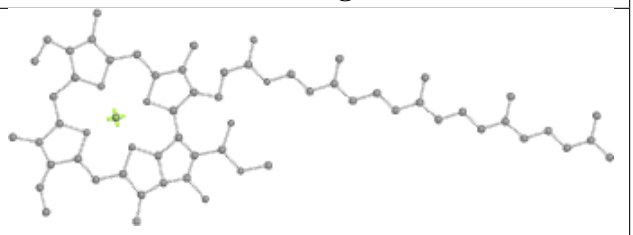
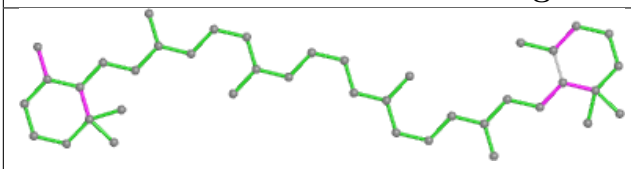

Bond angles


Torsions


Rings

Ligand 8CT t 101



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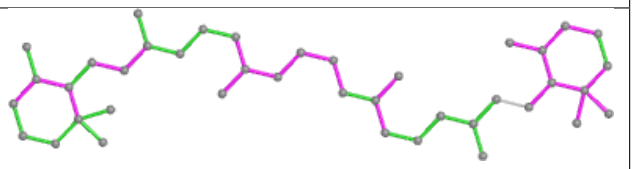
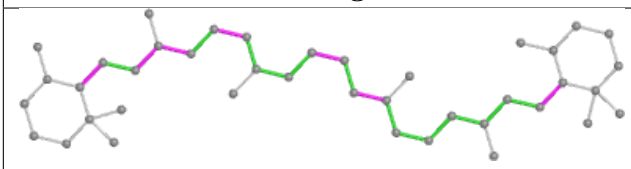


Bond angles



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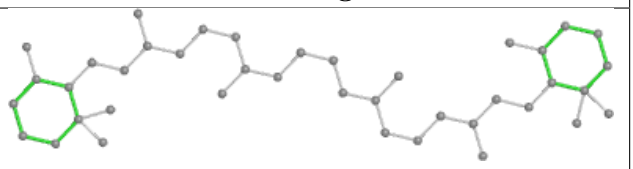
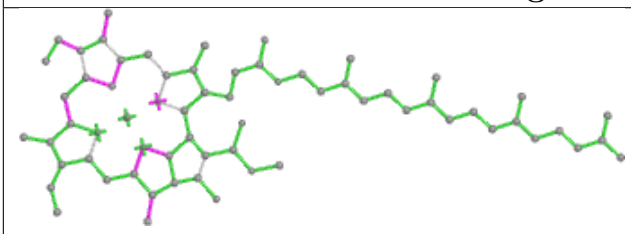


Rings

Ligand CLA b 605



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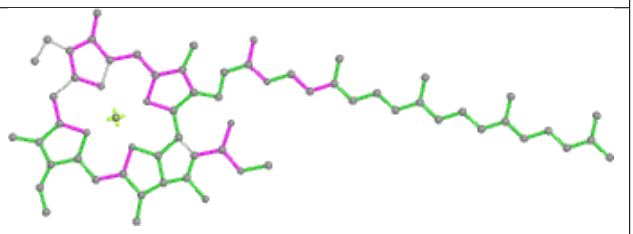
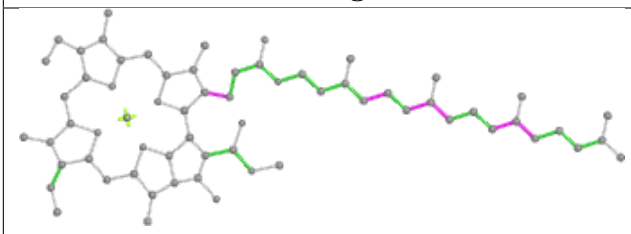


Bond angles



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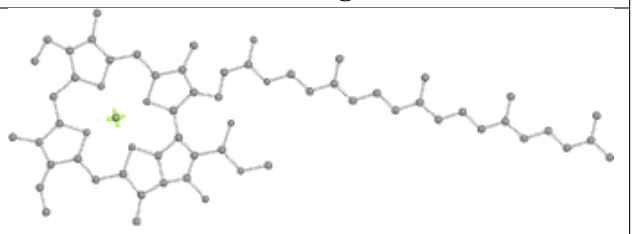
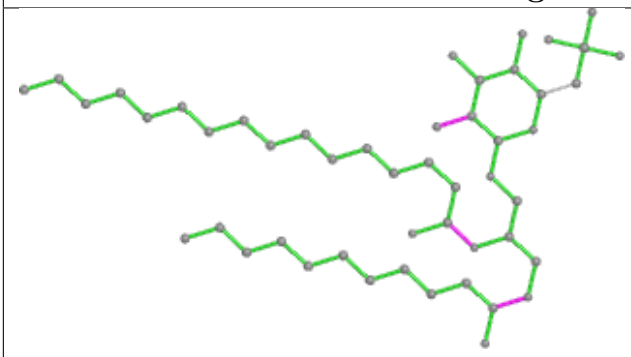


Rings

Ligand SQD b 601



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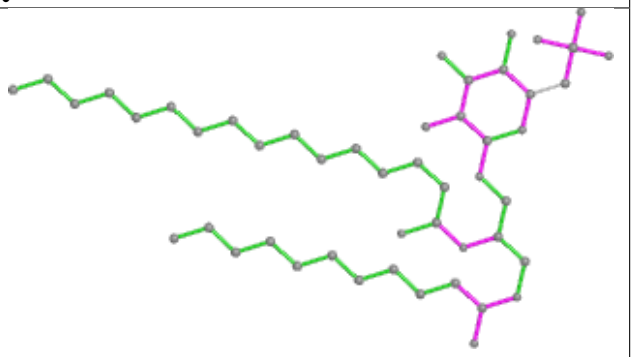
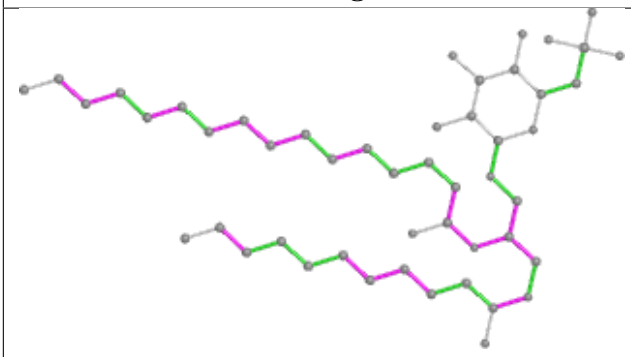


Bond angles



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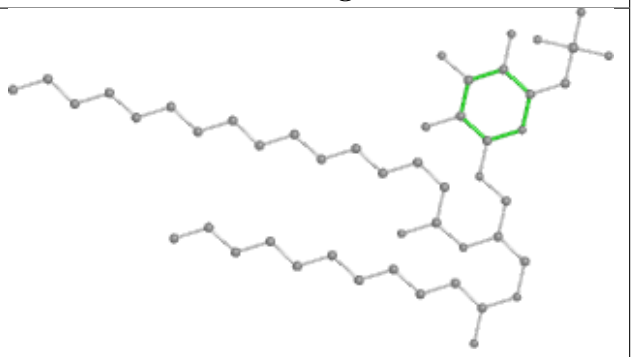
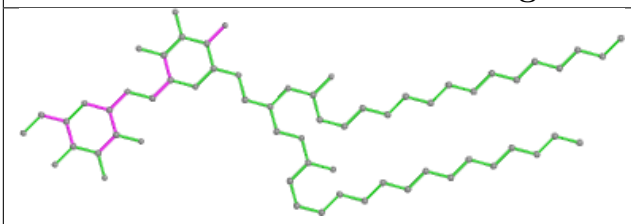


Rings

Ligand DGD H 102



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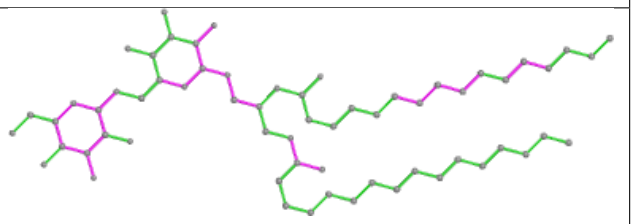
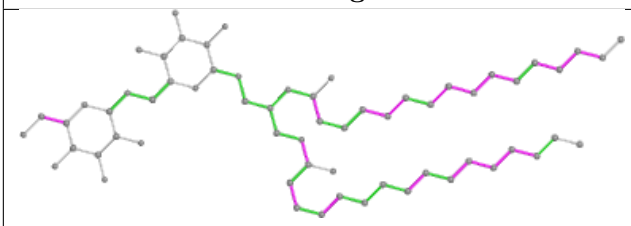
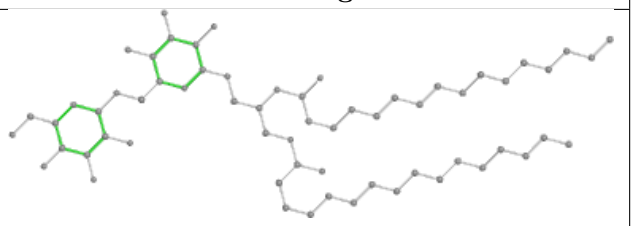


Bond angles

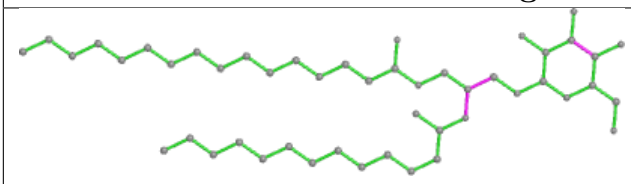


Torsions

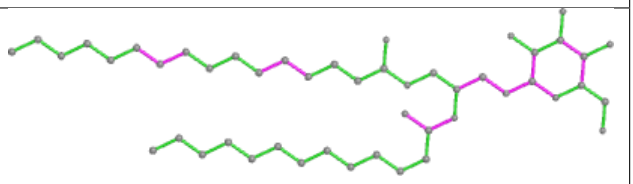


Rings

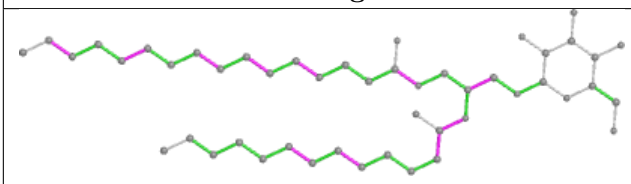
Ligand LMG C 519



Bond lengths



Bond angles



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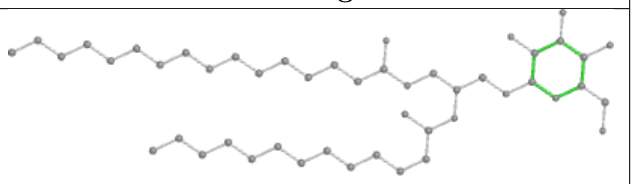
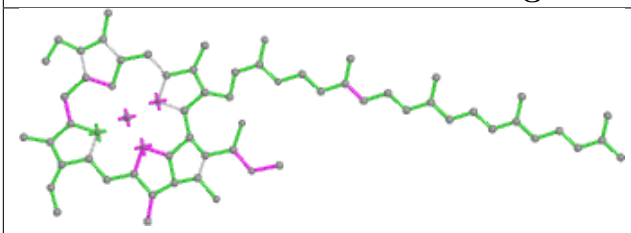


Rings

Ligand CLA A 404



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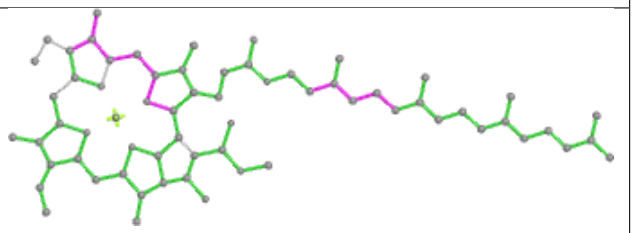
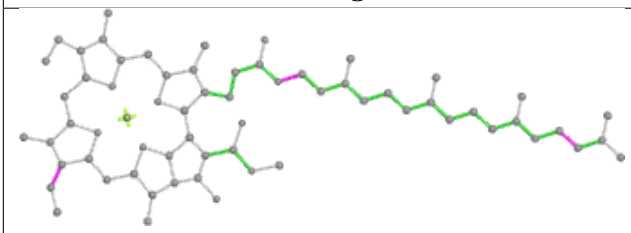


Bond angles



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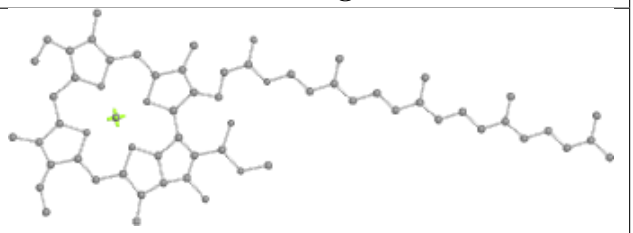
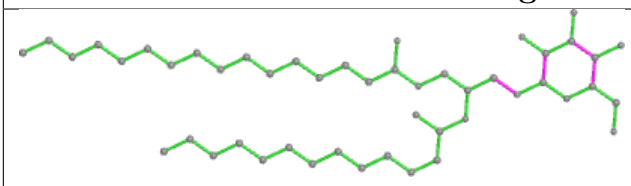


Rings

Ligand LMG A 410



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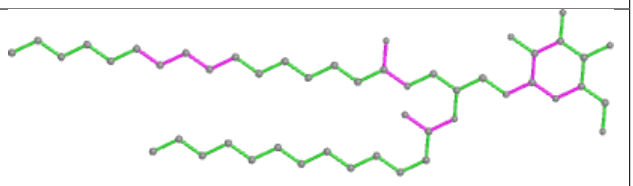
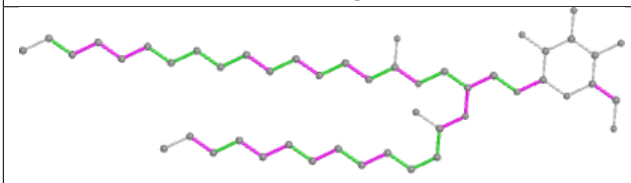


Bond angles



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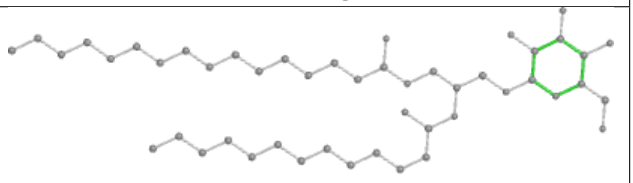
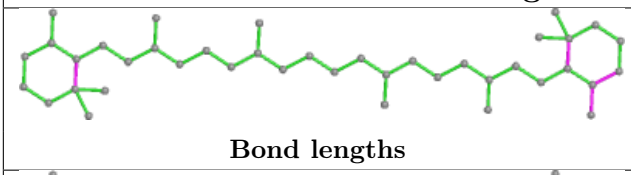


Rings

Ligand BCR T 101



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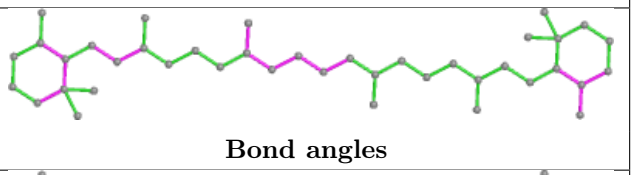
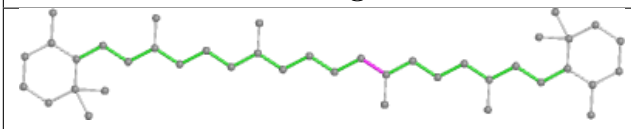
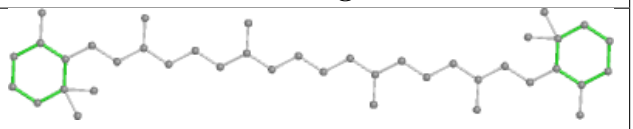


Bond angles

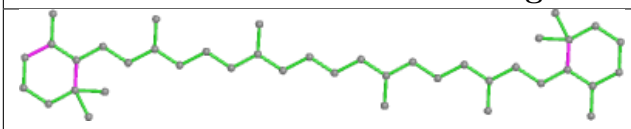


Torsions

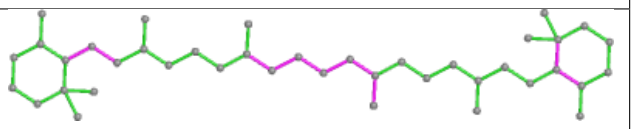


Rings

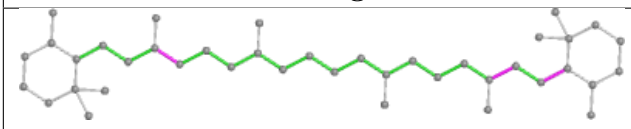
Ligand BCR b 619



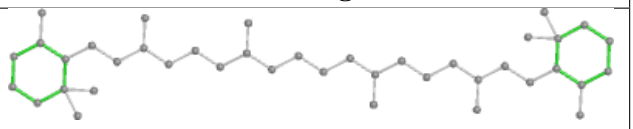
Bond lengths



Bond angles

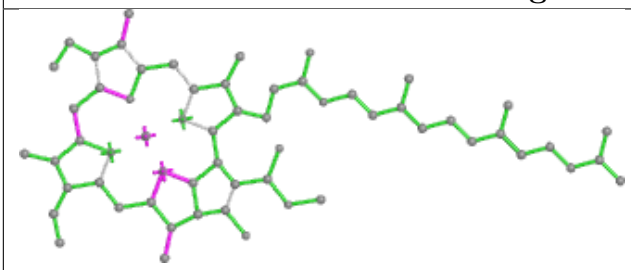


Torsions

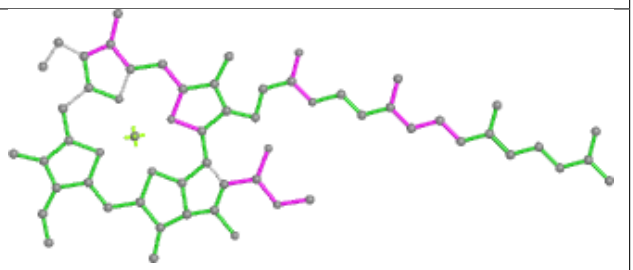


Rings

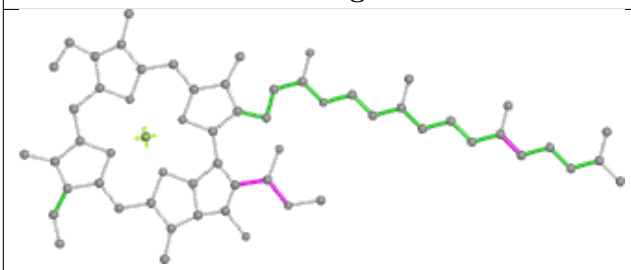
Ligand CLA c 504



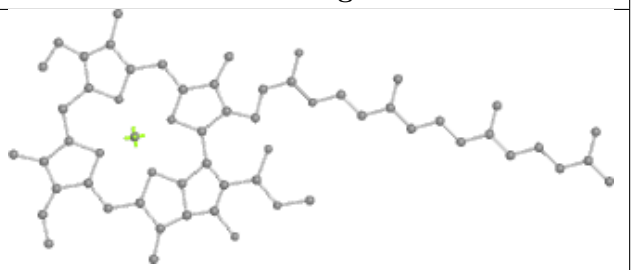
Bond lengths



Bond angles

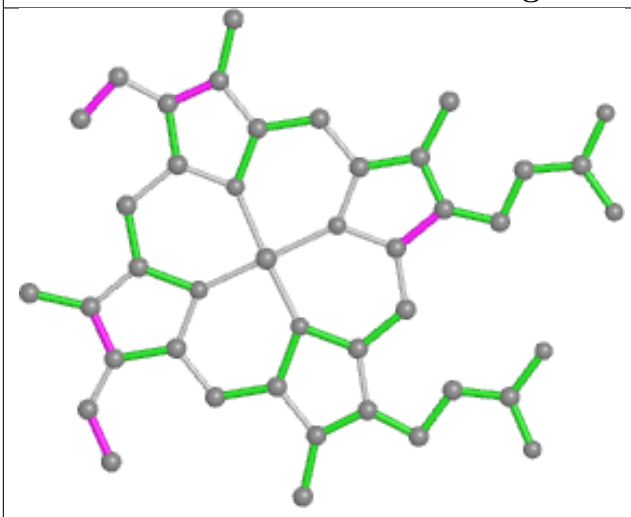


Torsions

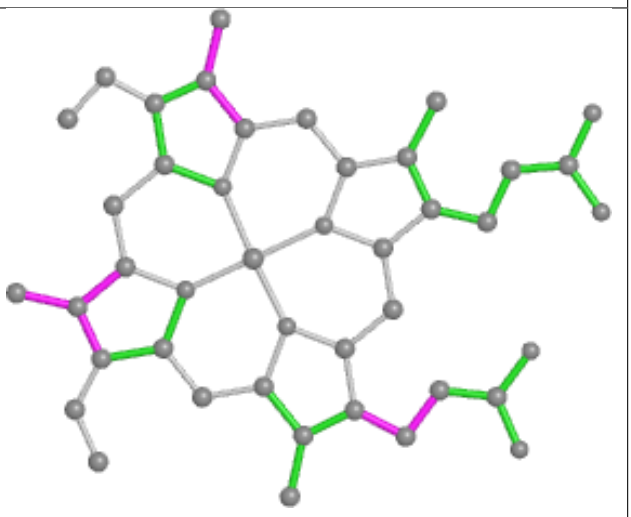


Rings

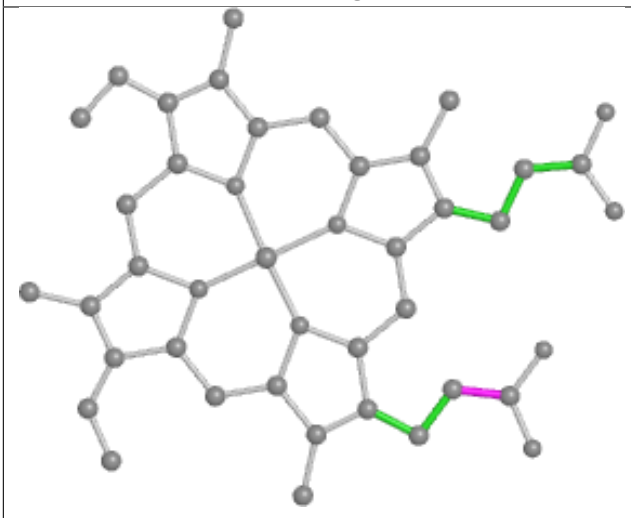
Ligand HEC V 201



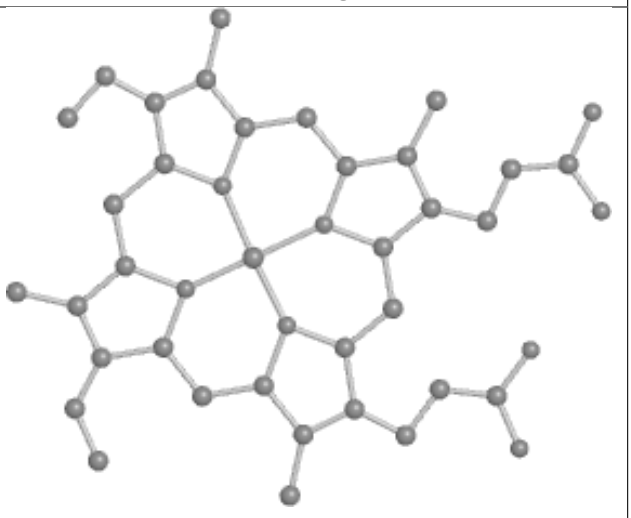
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/334 (100%)	-0.50	3 (0%) 84 86	19, 27, 46, 75	0
1	a	334/334 (100%)	-0.47	2 (0%) 89 91	21, 29, 55, 82	0
2	B	505/505 (100%)	-0.43	7 (1%) 75 78	19, 30, 60, 91	0
2	b	505/505 (100%)	-0.31	12 (2%) 59 63	22, 34, 67, 101	0
3	C	442/451 (98%)	-0.37	2 (0%) 91 92	22, 34, 51, 74	0
3	c	451/451 (100%)	-0.34	6 (1%) 77 79	23, 37, 58, 95	0
4	D	341/341 (100%)	-0.37	0 100 100	21, 28, 46, 80	0
4	d	341/341 (100%)	-0.39	1 (0%) 94 94	20, 32, 55, 75	0
5	E	81/82 (98%)	0.07	4 (4%) 29 31	31, 48, 65, 76	0
5	e	82/82 (100%)	0.27	4 (4%) 29 31	37, 57, 79, 87	0
6	F	34/34 (100%)	-0.33	2 (5%) 22 24	34, 40, 59, 79	0
6	f	34/34 (100%)	-0.12	2 (5%) 22 24	38, 48, 71, 82	0
7	H	65/65 (100%)	-0.08	1 (1%) 73 76	32, 37, 57, 69	0
7	h	63/65 (96%)	0.05	2 (3%) 47 52	38, 47, 60, 64	0
8	I	35/36 (97%)	-0.21	3 (8%) 10 11	28, 36, 67, 74	0
8	i	35/36 (97%)	-0.17	2 (5%) 23 25	30, 37, 68, 79	0
9	J	36/36 (100%)	0.24	5 (13%) 2 2	31, 47, 71, 86	0
9	j	36/36 (100%)	0.22	5 (13%) 2 2	35, 49, 83, 85	0
10	K	37/37 (100%)	-0.12	0 100 100	41, 49, 64, 72	0
10	k	37/37 (100%)	0.06	0 100 100	46, 56, 70, 77	0
11	L	37/37 (100%)	-0.33	0 100 100	23, 27, 60, 66	0
11	l	36/37 (97%)	-0.34	0 100 100	24, 29, 66, 77	0
12	M	32/33 (96%)	-0.31	0 100 100	25, 31, 60, 67	0
12	m	31/33 (93%)	-0.37	0 100 100	24, 32, 45, 60	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.08	12 (4%) 29 31	21, 39, 80, 130	0
13	o	244/244 (100%)	-0.18	14 (5%) 23 25	21, 38, 74, 128	0
14	T	29/30 (96%)	-0.60	2 (6%) 16 18	25, 29, 56, 72	0
14	t	29/30 (96%)	-0.31	3 (10%) 6 6	23, 29, 76, 92	0
15	U	97/97 (100%)	-0.30	2 (2%) 63 67	30, 40, 67, 93	0
15	u	97/97 (100%)	-0.48	0 100 100	30, 37, 56, 81	0
16	V	137/137 (100%)	-0.56	0 100 100	25, 37, 53, 78	0
16	v	137/137 (100%)	-0.26	3 (2%) 62 66	31, 44, 64, 83	0
17	Y	27/30 (90%)	1.84	11 (40%) 0 0	50, 69, 108, 115	0
17	y	30/30 (100%)	0.98	9 (30%) 0 0	58, 72, 94, 97	0
18	X	38/38 (100%)	0.12	4 (10%) 6 6	34, 47, 71, 80	0
18	x	38/38 (100%)	0.45	4 (10%) 6 6	47, 56, 80, 94	0
19	Z	62/62 (100%)	0.78	16 (25%) 0 0	48, 61, 108, 116	0
19	z	62/62 (100%)	1.11	13 (20%) 1 0	54, 69, 108, 119	0
20	R	34/34 (100%)	1.82	13 (38%) 0 0	56, 65, 82, 90	0
20	r	31/34 (91%)	2.43	20 (64%) 0 0	66, 81, 90, 95	0
All	All	5300/5326 (99%)	-0.23	189 (3%) 42 46	19, 35, 70, 130	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	33	TRP	9.7
17	Y	20	ALA	8.3
13	O	59	LYS	7.7
13	O	60	ARG	7.7
13	o	3	GLN	7.1
13	O	3	GLN	7.0
13	o	58	ASN	6.5
9	J	8	ILE	6.2
1	A	13	LEU	6.2
19	Z	62	VAL	6.2
20	R	3	TRP	5.9
19	z	35	ARG	5.8
18	X	2	THR	5.6
13	o	61	GLN	5.6
13	o	57	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
17	Y	21	GLN	5.4
17	Y	41	VAL	5.4
20	r	14	LEU	5.4
2	b	506	ARG	5.3
13	O	4	THR	5.3
17	Y	23	THR	5.3
20	R	6	LEU	5.2
13	O	56	PRO	5.0
17	y	19	ILE	4.8
6	F	12	SER	4.8
18	x	2	THR	4.7
20	r	3	TRP	4.7
17	Y	43	ARG	4.6
20	R	26	TYR	4.5
20	r	26	TYR	4.5
20	r	6	LEU	4.4
19	z	60	PHE	4.4
13	o	4	THR	4.3
9	J	6	GLY	4.3
9	j	5	GLY	4.2
9	J	7	ARG	4.2
13	O	62	GLU	4.2
14	t	29	ILE	4.2
13	o	5	LEU	4.1
2	B	506	ARG	4.1
2	b	127	ARG	4.1
20	r	5	VAL	4.0
6	f	13	TYR	4.0
19	Z	4	LEU	4.0
20	r	24	LEU	3.9
17	Y	37	PHE	3.9
2	b	495	PHE	3.9
13	O	61	GLN	3.8
19	Z	33	TRP	3.7
19	z	62	VAL	3.7
14	t	30	THR	3.7
20	r	13	LEU	3.7
19	z	41	PHE	3.7
15	U	8	GLU	3.6
17	y	18	VAL	3.6
19	Z	35	ARG	3.6
7	H	66	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
18	X	3	ILE	3.6
1	A	11	ALA	3.6
1	a	11	ALA	3.5
20	r	18	TRP	3.5
13	o	56	PRO	3.5
5	E	79	PHE	3.5
13	o	62	GLU	3.4
20	R	29	LYS	3.4
9	j	7	ARG	3.4
14	t	28	ARG	3.4
5	e	79	PHE	3.4
13	o	246	ALA	3.4
2	B	505	ARG	3.3
19	z	4	LEU	3.3
19	z	34	ASP	3.3
19	Z	42	LEU	3.3
20	r	28	VAL	3.3
3	c	23	ALA	3.3
20	r	10	LEU	3.3
17	y	20	ALA	3.2
17	Y	22	LEU	3.2
5	E	17	VAL	3.2
20	r	9	LEU	3.2
8	i	36	ASP	3.1
19	Z	7	LEU	3.1
2	b	490	GLN	3.1
3	c	24	THR	3.1
2	b	487	SER	3.1
17	Y	40	ALA	3.1
2	b	502	VAL	3.0
19	Z	3	ILE	3.0
19	Z	38	GLN	3.0
20	r	2	ASP	3.0
7	h	6	TRP	3.0
19	z	30	PRO	3.0
9	j	6	GLY	3.0
20	r	27	ALA	3.0
19	Z	34	ASP	3.0
16	v	15	GLU	3.0
3	c	147	PHE	2.9
17	Y	24	MET	2.9
13	O	63	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
9	J	5	GLY	2.9
20	r	23	ILE	2.9
2	b	505	ARG	2.9
3	C	143	TYR	2.9
19	Z	31	GLN	2.9
13	O	5	LEU	2.9
1	A	12	ASN	2.8
17	Y	42	ARG	2.8
19	z	37	LYS	2.8
19	Z	1	MET	2.8
4	d	227[A]	GLU	2.8
20	R	5	VAL	2.8
2	b	128	THR	2.7
7	h	63	LYS	2.7
20	R	24	LEU	2.7
20	R	32	GLN	2.7
3	C	106	VAL	2.7
9	j	8	ILE	2.6
20	R	21	ARG	2.6
3	c	143	TYR	2.6
17	y	41	VAL	2.6
19	Z	32	ASP	2.6
14	T	30	THR	2.6
2	B	502	VAL	2.6
6	f	12	SER	2.6
13	o	63	ALA	2.6
8	I	36	ASP	2.5
8	i	34	ARG	2.5
19	Z	61	VAL	2.5
2	b	161	LEU	2.5
17	y	40	ALA	2.5
13	O	57	LYS	2.5
9	J	10	LEU	2.5
13	O	246	ALA	2.5
13	o	207	ARG	2.5
2	b	496	TYR	2.5
2	B	487	SER	2.5
19	Z	41	PHE	2.5
20	r	29	LYS	2.5
2	B	127	ARG	2.5
17	y	43	ARG	2.5
19	z	31	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
17	y	17	GLU	2.4
15	U	67	LEU	2.4
18	X	39	ARG	2.4
20	r	25	PRO	2.4
20	r	4	ARG	2.4
6	F	13	TYR	2.4
13	o	60	ARG	2.4
5	e	13	ILE	2.4
13	o	59	LYS	2.3
2	B	293	ALA	2.3
20	R	25	PRO	2.3
17	y	37	PHE	2.3
13	O	36	GLN	2.2
20	R	31	VAL	2.2
2	B	294	SER	2.2
16	v	16	GLY	2.2
18	x	3	ILE	2.2
5	e	84	LYS	2.2
17	y	22	LEU	2.2
20	R	14	LEU	2.2
2	b	489	GLU	2.2
5	E	84	LYS	2.2
18	X	38	GLN	2.2
18	x	15	LEU	2.2
19	Z	37	LYS	2.2
20	r	7	VAL	2.2
19	z	3	ILE	2.1
5	E	83	LEU	2.1
3	c	29	GLU	2.1
19	z	7	LEU	2.1
2	b	295	GLY	2.1
3	c	146	PHE	2.1
8	I	34	ARG	2.1
19	z	61	VAL	2.1
9	j	11	TRP	2.1
14	T	29	ILE	2.1
1	a	16	ARG	2.1
19	Z	30	PRO	2.0
20	r	15	ALA	2.0
8	I	2	GLU	2.0
17	Y	44	GLY	2.0
5	e	74	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
18	x	38	GLN	2.0
13	o	64	GLU	2.0
16	v	21	LEU	2.0
20	R	8	VAL	2.0
20	R	28	VAL	2.0
20	r	21	ARG	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	0.94	0.09	28,37,65,65	0
14	FME	T	1	10/11	0.95	0.10	28,45,62,68	0
8	FME	I	1	10/11	0.96	0.14	36,54,63,65	0
8	FME	i	1	10/11	0.96	0.12	37,48,59,59	0
12	FME	m	1	10/11	0.96	0.14	32,46,70,77	0
12	FME	M	1	10/11	0.96	0.16	34,42,70,81	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	E	102	28/-	0.51	0.37	63,78,89,91	0
32	UNL	H	103	53/-	0.71	0.28	53,76,91,91	0
32	UNL	a	413	28/-	0.72	0.29	35,63,70,73	0
32	UNL	b	626	55/-	0.76	0.20	41,62,82,85	0
26	PL9	A	409	55/55	0.77	0.26	38,60,83,97	135
32	UNL	c	523	28/-	0.77	0.18	47,68,82,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LHG	E	101	49/49	0.77	0.25	44,85,112,121	0
32	UNL	b	625	40/-	0.78	0.18	52,69,87,92	0
26	PL9	a	410	55/55	0.79	0.22	40,68,89,93	0
32	UNL	c	520	55/-	0.80	0.18	41,56,75,82	0
32	UNL	B	628	47/-	0.80	0.30	44,67,86,86	0
27	LMG	D	411	33/55	0.80	0.16	35,56,88,94	0
29	DGD	A	414	66/66	0.81	0.19	41,64,84,113	0
27	LMG	b	624	23/55	0.81	0.23	34,70,96,100	0
27	LMG	c	522	48/55	0.82	0.21	42,73,112,117	0
27	LMG	b	623	55/55	0.82	0.26	44,75,99,109	0
32	UNL	j	101	28/-	0.82	0.14	46,59,70,74	0
32	UNL	t	103	26/-	0.82	0.20	47,65,79,84	0
32	UNL	B	627	28/-	0.82	0.33	47,68,85,91	0
32	UNL	d	411	43/-	0.83	0.18	48,60,70,78	0
29	DGD	o	301	44/66	0.83	0.15	31,56,79,85	0
23	CLA	c	512	65/65	0.84	0.16	43,60,98,114	0
32	UNL	C	523	47/-	0.84	0.12	41,54,66,67	0
32	UNL	J	101	28/-	0.84	0.19	49,62,75,83	0
28	SQD	a	412	36/54	0.85	0.15	29,62,85,87	0
28	SQD	f	101	41/54	0.86	0.22	58,84,117,131	0
23	CLA	b	602	65/65	0.86	0.14	39,63,87,98	0
28	SQD	b	601	49/54	0.86	0.14	40,62,98,102	0
31	BCR	Y	101	40/40	0.86	0.13	36,50,68,75	0
31	BCR	h	101	40/40	0.86	0.14	32,54,79,80	0
32	UNL	t	102	34/-	0.87	0.12	40,52,65,65	0
32	UNL	T	102	47/-	0.87	0.20	38,50,66,69	0
27	LMG	c	524	49/55	0.87	0.15	35,57,86,104	0
33	LHG	e	101	42/49	0.87	0.29	62,88,118,134	0
28	SQD	B	624	54/54	0.88	0.12	35,59,93,104	0
32	UNL	b	622	55/-	0.88	0.18	36,53,74,82	0
32	UNL	B	621	43/-	0.88	0.13	36,52,69,73	0
23	CLA	C	512	65/65	0.88	0.15	30,54,103,114	0
23	CLA	c	513	65/65	0.88	0.20	39,68,105,107	0
23	CLA	C	513	65/65	0.88	0.18	41,61,97,101	0
23	CLA	B	616	60/65	0.88	0.16	23,38,87,90	0
27	LMG	C	519	48/55	0.88	0.14	45,70,89,96	0
32	UNL	I	101	41/-	0.88	0.13	38,53,76,79	0
31	BCR	H	101	40/40	0.88	0.11	29,45,58,62	0
28	SQD	A	413	39/54	0.88	0.19	36,65,86,94	0
32	UNL	X	101	55/-	0.88	0.21	33,51,72,77	0
32	UNL	B	625	28/-	0.89	0.10	26,47,70,72	0
32	UNL	M	102	26/-	0.89	0.15	34,47,56,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	8CT	k	101	40/40	0.89	0.11	40,60,75,77	0
32	UNL	d	412	55/-	0.89	0.18	40,60,77,78	0
23	CLA	B	601	65/65	0.89	0.14	31,62,100,113	0
32	UNL	m	101	28/-	0.89	0.15	39,59,78,81	0
23	CLA	b	617	60/65	0.89	0.14	25,42,79,91	0
27	LMG	A	410	48/55	0.89	0.14	35,54,70,94	0
27	LMG	c	519	37/55	0.89	0.16	39,68,83,90	0
27	LMG	B	622	28/55	0.89	0.15	29,46,64,69	0
32	UNL	B	626	46/-	0.90	0.11	44,59,74,76	0
32	UNL	l	102	53/-	0.90	0.14	31,46,90,92	0
32	UNL	b	627	26/-	0.90	0.21	39,56,67,73	0
27	LMG	b	621	51/55	0.90	0.11	34,51,75,90	0
23	CLA	D	404	65/65	0.90	0.16	19,42,124,131	0
32	UNL	C	522	28/-	0.90	0.12	42,53,59,61	0
23	CLA	b	616	65/65	0.90	0.14	25,39,58,70	0
23	CLA	a	408	65/65	0.91	0.15	16,37,90,97	0
25	8CT	D	405	40/40	0.91	0.12	26,42,100,105	0
32	UNL	T	103	44/-	0.91	0.18	36,57,75,81	0
27	LMG	B	620	51/55	0.91	0.11	28,47,71,86	0
23	CLA	d	404	65/65	0.92	0.14	27,49,94,106	0
29	DGD	H	102	62/66	0.92	0.11	31,46,63,71	0
29	DGD	h	102	62/66	0.92	0.11	27,52,67,71	0
25	8CT	C	514	40/40	0.92	0.11	36,53,67,73	0
27	LMG	D	407	51/55	0.92	0.15	25,57,88,98	0
32	UNL	C	521	28/-	0.92	0.10	31,47,55,68	0
23	CLA	C	505	65/65	0.92	0.17	23,39,69,90	0
23	CLA	c	508	64/65	0.92	0.12	24,43,79,112	0
25	8CT	C	515	40/40	0.93	0.11	26,38,52,53	0
28	SQD	D	408	36/54	0.93	0.15	44,69,85,92	0
28	SQD	a	411	54/54	0.93	0.13	42,66,89,96	0
23	CLA	B	615	65/65	0.93	0.12	21,35,67,73	0
25	8CT	c	514	40/40	0.93	0.15	39,56,69,69	0
25	8CT	d	405	40/40	0.93	0.11	30,55,92,108	0
23	CLA	c	511	65/65	0.93	0.13	39,53,71,77	0
29	DGD	C	516	62/66	0.93	0.12	19,38,73,96	0
29	DGD	C	517	62/66	0.93	0.12	27,52,95,110	0
23	CLA	c	502	65/65	0.93	0.12	24,42,60,63	0
23	CLA	c	503	65/65	0.93	0.13	31,43,55,58	0
23	CLA	c	506	65/65	0.93	0.13	26,50,108,115	0
25	8CT	B	619	40/40	0.93	0.09	24,38,62,69	0
32	UNL	M	101	37/-	0.93	0.12	31,48,69,71	0
23	CLA	c	507	65/65	0.93	0.14	22,43,60,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	BCR	b	618	40/40	0.93	0.11	27,41,54,58	0
31	BCR	c	521	40/40	0.93	0.15	34,52,71,74	0
23	CLA	c	504	60/65	0.94	0.11	27,46,83,86	0
23	CLA	c	505	65/65	0.94	0.14	22,39,63,76	0
23	CLA	A	405	65/65	0.94	0.12	19,34,103,112	0
23	CLA	a	406	65/65	0.94	0.12	25,39,100,106	0
23	CLA	C	502	65/65	0.94	0.10	23,40,55,60	0
29	DGD	c	517	62/66	0.94	0.10	30,51,86,100	0
23	CLA	c	510	65/65	0.94	0.12	29,47,68,77	0
23	CLA	B	606	65/65	0.94	0.09	22,34,72,80	0
23	CLA	b	605	65/65	0.94	0.14	18,32,76,91	0
31	BCR	T	101	40/40	0.94	0.10	23,39,59,61	0
23	CLA	b	607	65/65	0.94	0.10	25,40,68,80	0
23	CLA	b	610	65/65	0.94	0.11	29,45,64,71	0
31	BCR	b	619	40/40	0.94	0.09	25,38,51,62	0
25	8CT	B	617	40/40	0.94	0.10	22,41,53,56	0
23	CLA	b	613	65/65	0.94	0.16	18,33,48,57	0
23	CLA	b	614	65/65	0.94	0.12	14,32,69,85	0
23	CLA	b	615	65/65	0.94	0.14	19,38,77,89	0
27	LMG	d	410	44/55	0.94	0.12	30,52,94,108	0
25	8CT	C	520	40/40	0.94	0.14	35,51,66,70	0
23	CLA	C	506	65/65	0.94	0.12	22,40,95,110	0
25	8CT	b	620	40/40	0.94	0.10	22,45,59,68	0
23	CLA	C	507	65/65	0.94	0.13	17,38,55,65	0
23	CLA	B	614	65/65	0.94	0.13	20,39,81,96	0
33	LHG	d	409	39/49	0.94	0.11	28,47,73,77	0
23	CLA	A	407	54/65	0.94	0.13	15,28,65,73	0
26	PL9	d	406	55/55	0.95	0.10	21,36,48,53	0
23	CLA	C	511	65/65	0.95	0.10	27,50,65,69	0
23	CLA	C	501	65/65	0.95	0.12	24,36,50,61	0
23	CLA	d	403	65/65	0.95	0.10	18,32,63,76	0
29	DGD	c	518	62/66	0.95	0.10	26,50,75,90	0
23	CLA	B	612	65/65	0.95	0.15	18,29,46,53	0
24	PHO	a	407	64/64	0.95	0.10	18,30,37,43	0
31	BCR	B	618	40/40	0.95	0.08	21,37,51,51	0
24	PHO	d	401	64/64	0.95	0.10	25,39,48,71	0
25	8CT	A	408	40/40	0.95	0.09	22,31,43,46	0
23	CLA	D	403	65/65	0.95	0.10	15,27,55,72	0
23	CLA	C	503	65/65	0.95	0.10	28,40,52,54	0
23	CLA	B	604	65/65	0.95	0.10	17,29,80,90	0
31	BCR	c	515	40/40	0.95	0.10	28,41,58,72	0
23	CLA	B	609	65/65	0.95	0.09	23,35,53,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	610	65/65	0.95	0.14	17,31,42,46	0
23	CLA	b	603	65/65	0.95	0.14	24,42,72,80	0
23	CLA	C	508	65/65	0.95	0.11	25,40,100,116	0
23	CLA	b	606	65/65	0.95	0.12	16,34,47,56	0
23	CLA	C	509	65/65	0.95	0.14	23,43,63,70	0
23	CLA	c	509	65/65	0.95	0.15	28,47,65,68	0
25	8CT	t	101	40/40	0.95	0.08	24,37,58,61	0
33	LHG	D	410	47/49	0.95	0.11	23,48,82,99	0
23	CLA	b	609	65/65	0.95	0.11	20,41,62,74	0
33	LHG	d	407	49/49	0.95	0.12	30,52,78,89	0
26	PL9	D	406	55/55	0.95	0.10	17,32,45,47	0
23	CLA	C	510	65/65	0.95	0.12	29,46,74,78	0
23	CLA	B	605	65/65	0.96	0.14	19,31,45,51	0
23	CLA	b	608	65/65	0.96	0.11	19,37,65,72	0
23	CLA	A	404	65/65	0.96	0.10	17,26,44,51	0
23	CLA	a	405	65/65	0.96	0.09	17,28,46,61	0
23	CLA	b	611	65/65	0.96	0.13	21,36,52,57	0
23	CLA	b	612	65/65	0.96	0.10	18,32,49,55	0
23	CLA	B	602	65/65	0.96	0.11	21,36,60,65	0
29	DGD	C	518	62/66	0.96	0.09	23,46,76,86	0
23	CLA	B	603	65/65	0.96	0.14	17,31,64,72	0
29	DGD	c	516	62/66	0.96	0.10	19,40,69,78	0
23	CLA	B	611	65/65	0.96	0.12	16,29,47,51	0
23	CLA	A	411	65/65	0.96	0.11	16,27,53,61	0
23	CLA	d	402	65/65	0.96	0.10	18,29,46,49	0
23	CLA	b	604	65/65	0.96	0.12	18,36,64,68	0
23	CLA	c	501	65/65	0.96	0.12	26,38,49,52	0
33	LHG	B	623	49/49	0.96	0.12	26,45,68,78	0
33	LHG	D	409	49/49	0.96	0.11	21,39,54,66	0
28	SQD	A	412	52/54	0.96	0.11	30,58,89,95	0
24	PHO	A	406	64/64	0.96	0.09	15,27,36,39	0
33	LHG	L	101	49/49	0.96	0.11	24,39,56,65	0
23	CLA	C	504	59/65	0.96	0.12	20,41,87,92	0
33	LHG	d	408	49/49	0.96	0.12	22,41,60,72	0
31	BCR	a	409	40/40	0.96	0.08	19,31,44,46	0
23	CLA	B	613	65/65	0.96	0.12	13,30,67,73	0
33	LHG	l	101	49/49	0.96	0.10	29,44,54,61	0
35	HEM	F	101	43/43	0.96	0.12	34,48,58,68	0
35	HEM	e	102	43/43	0.96	0.11	42,54,73,75	0
23	CLA	B	608	65/65	0.97	0.10	17,32,57,57	0
34	BCT	a	404	4/4	0.97	0.17	23,28,41,50	0
23	CLA	B	607	65/65	0.97	0.10	15,31,65,73	0

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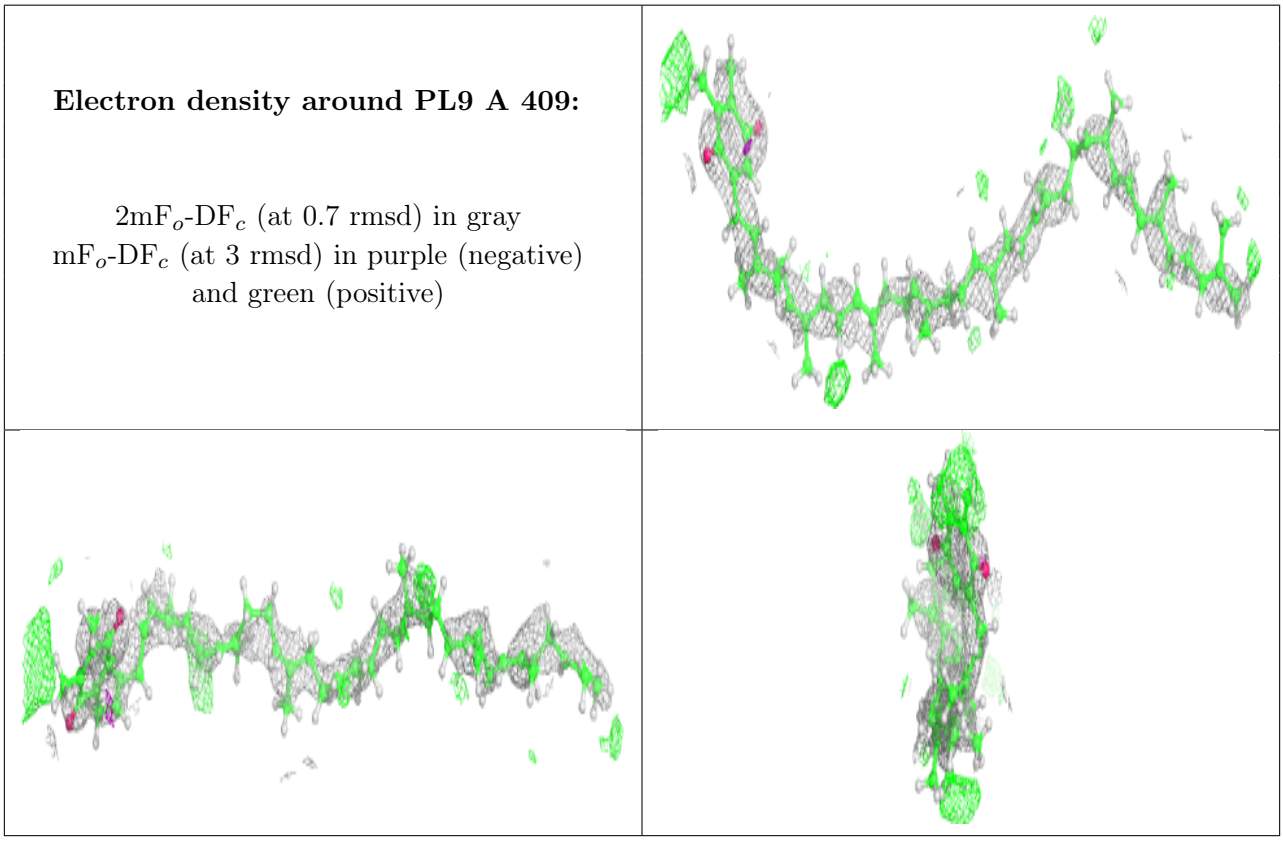
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PHO	D	402	64/64	0.97	0.08	17,31,43,49	0
36	HEC	v	201	43/43	0.97	0.12	27,35,46,55	0
30	OEX	A	415	10/10	0.98	0.11	22,25,27,28	0
36	HEC	V	201	43/43	0.98	0.11	20,32,42,44	0
34	BCT	D	401	4/4	0.98	0.22	28,28,35,42	0
21	FE2	a	401	1/1	0.99	0.06	31,31,31,31	0
22	CL	A	402	1/1	0.99	0.03	25,25,25,25	0
30	OEX	a	414	10/10	0.99	0.11	16,25,28,29	0
22	CL	a	402	1/1	0.99	0.08	28,28,28,28	0
22	CL	A	403	1/1	1.00	0.05	25,25,25,25	0
21	FE2	A	401	1/1	1.00	0.09	28,28,28,28	0
22	CL	a	403	1/1	1.00	0.02	27,27,27,27	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.

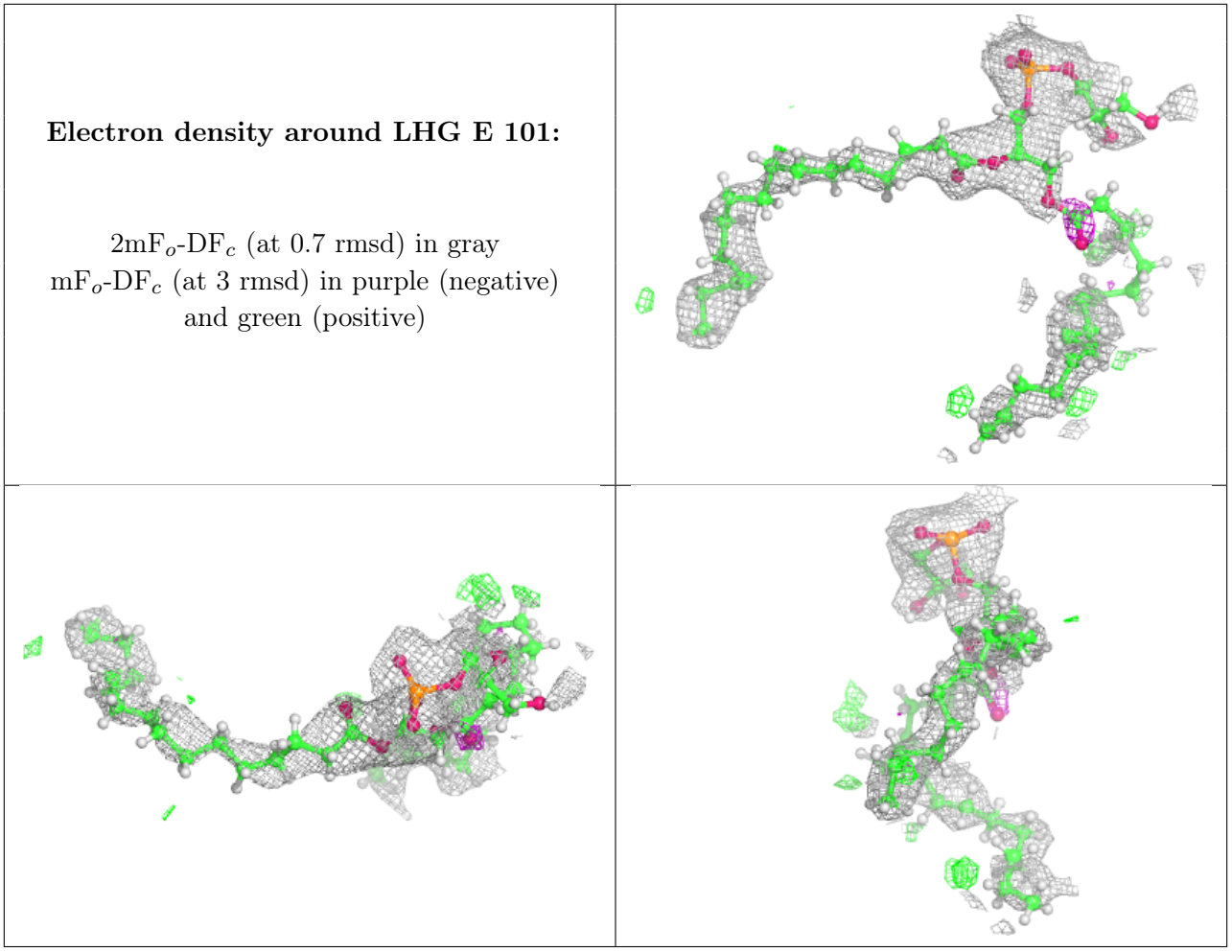
Electron density around PL9 A 409:

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



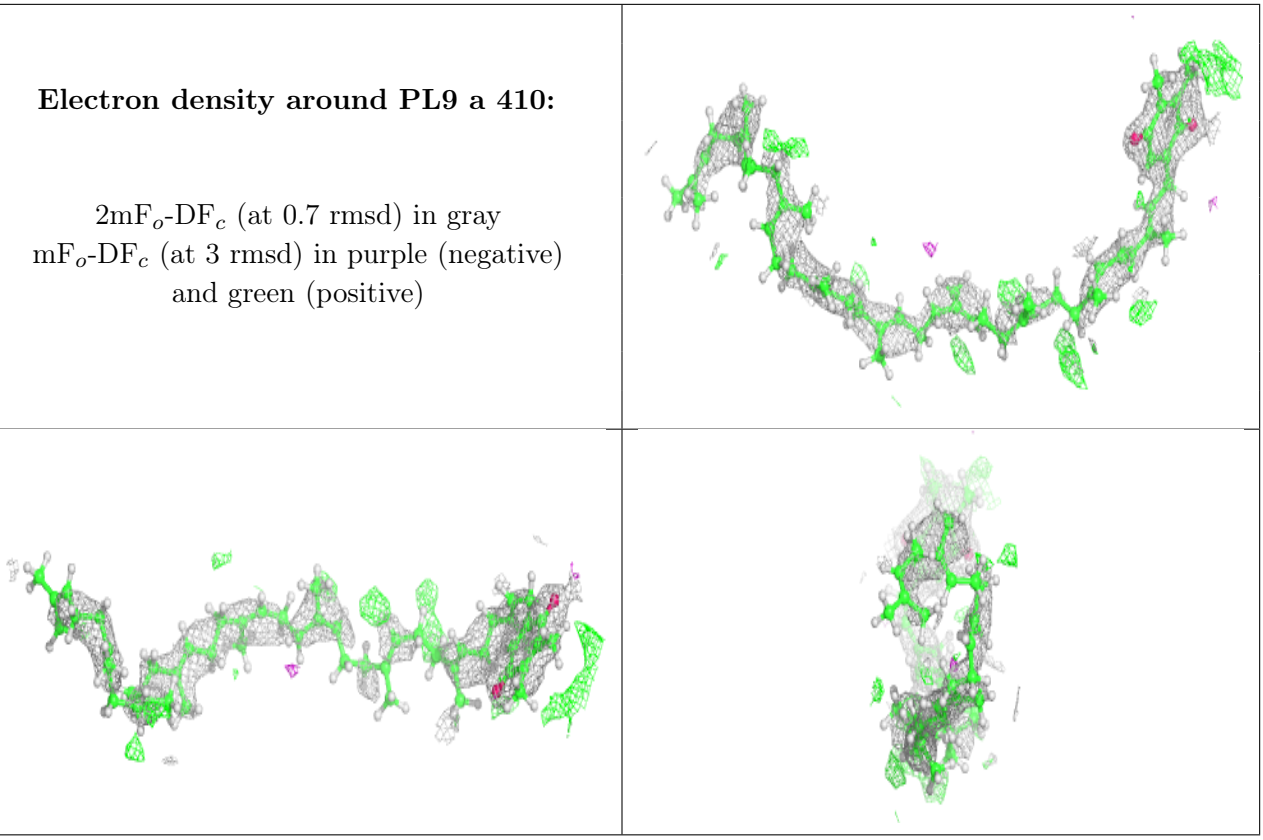
Electron density around LHG E 101:

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



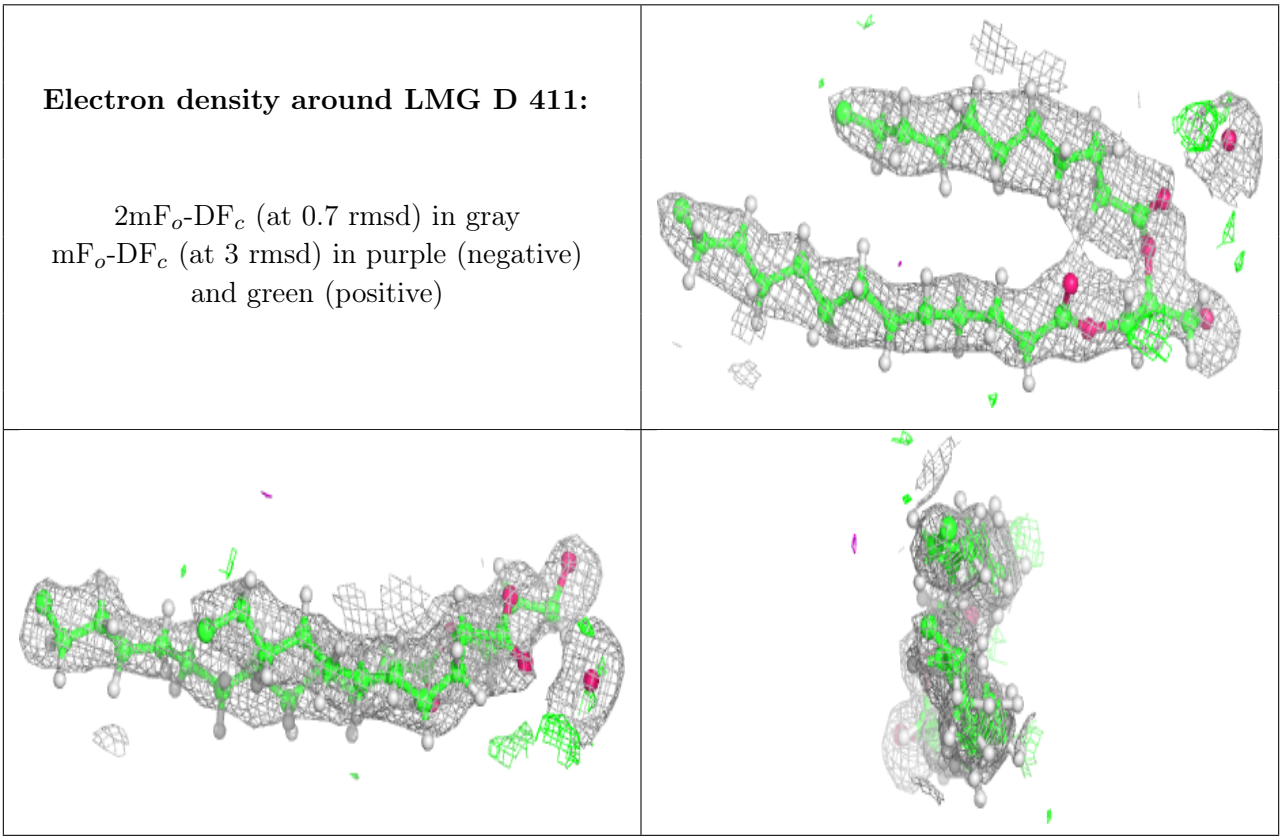
Electron density around PL9 a 410:

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



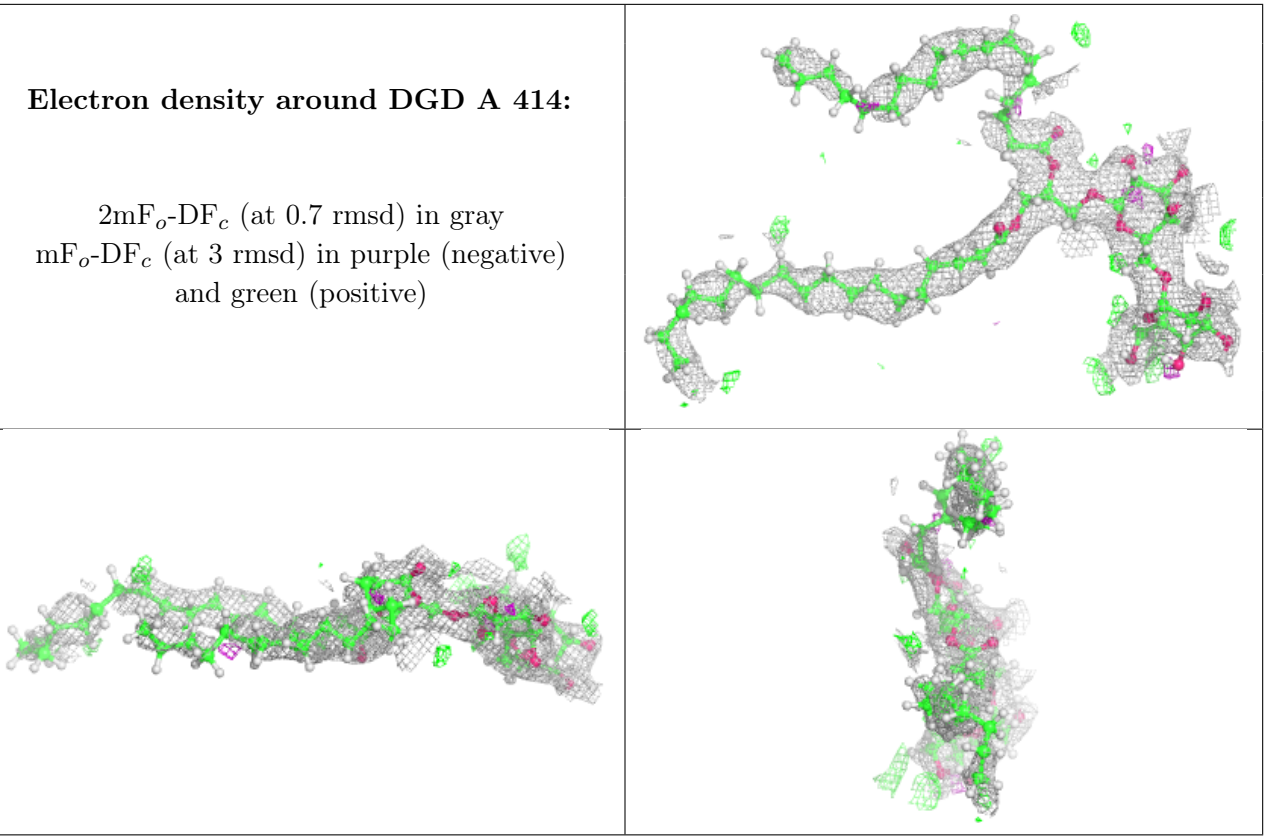
Electron density around LMG D 411:

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



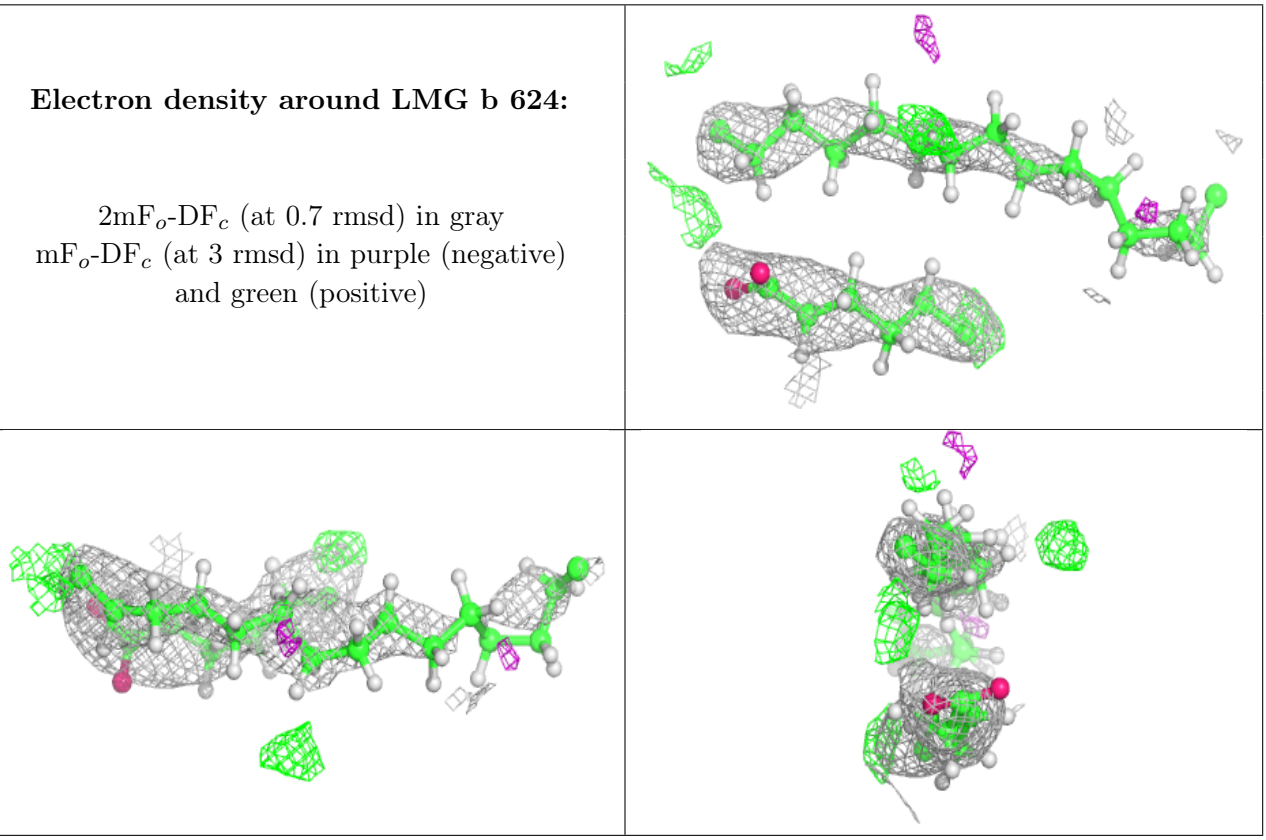
Electron density around DGD A 414:

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



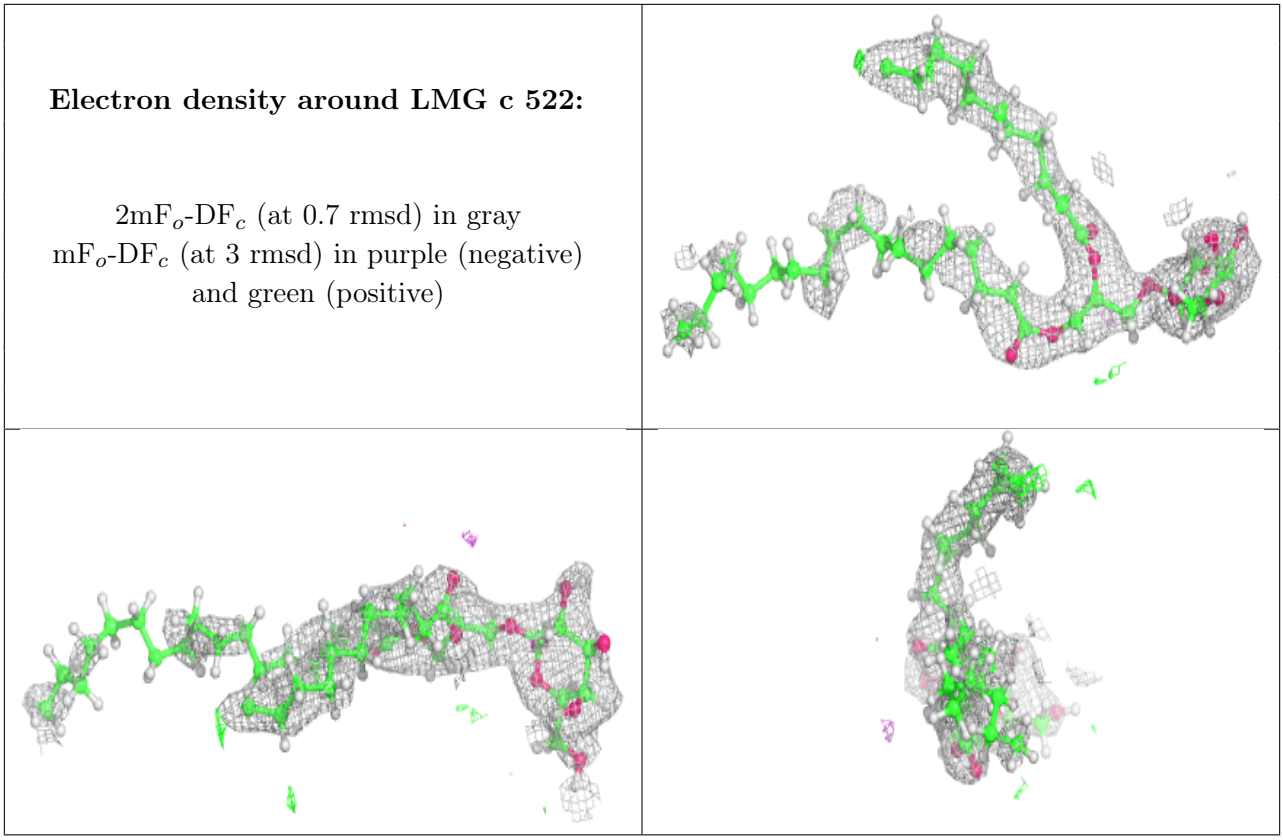
Electron density around LMG b 624:

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



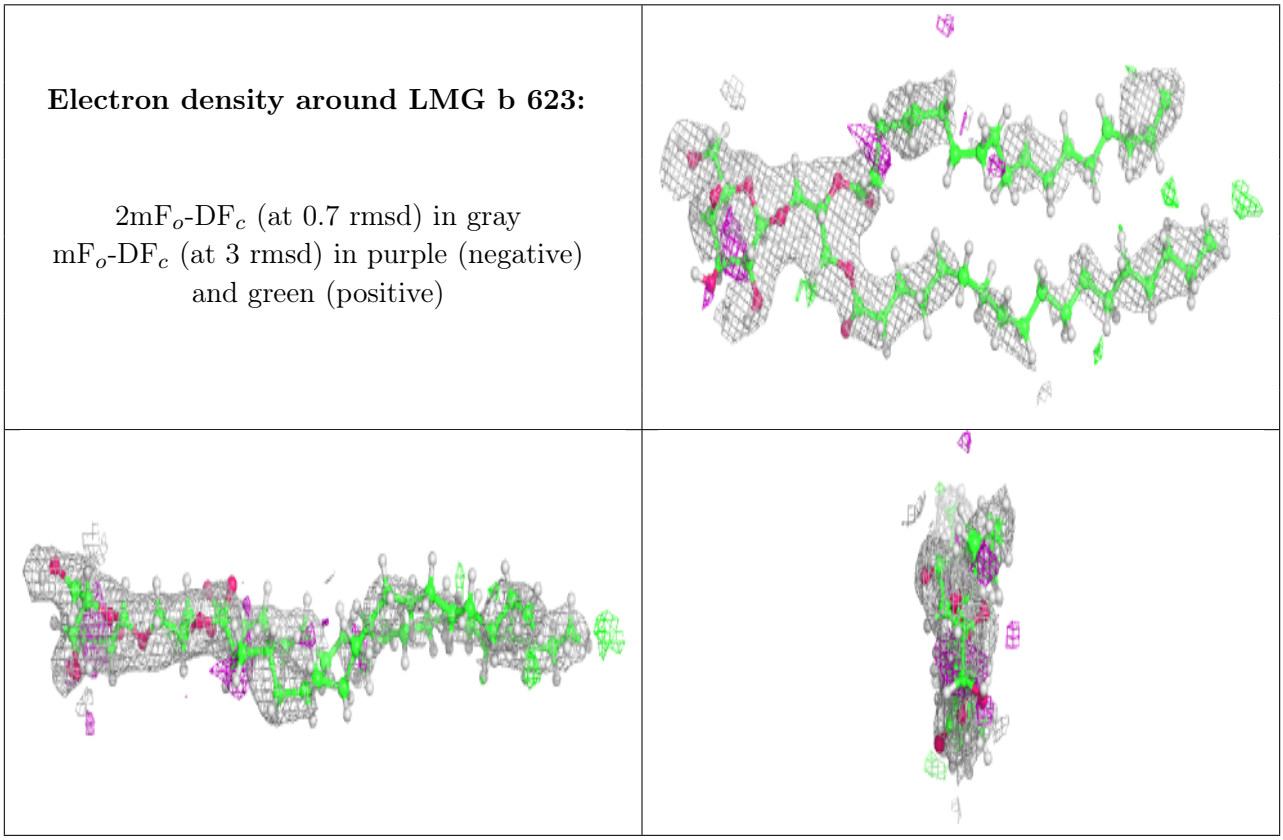
Electron density around LMG c 522:

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



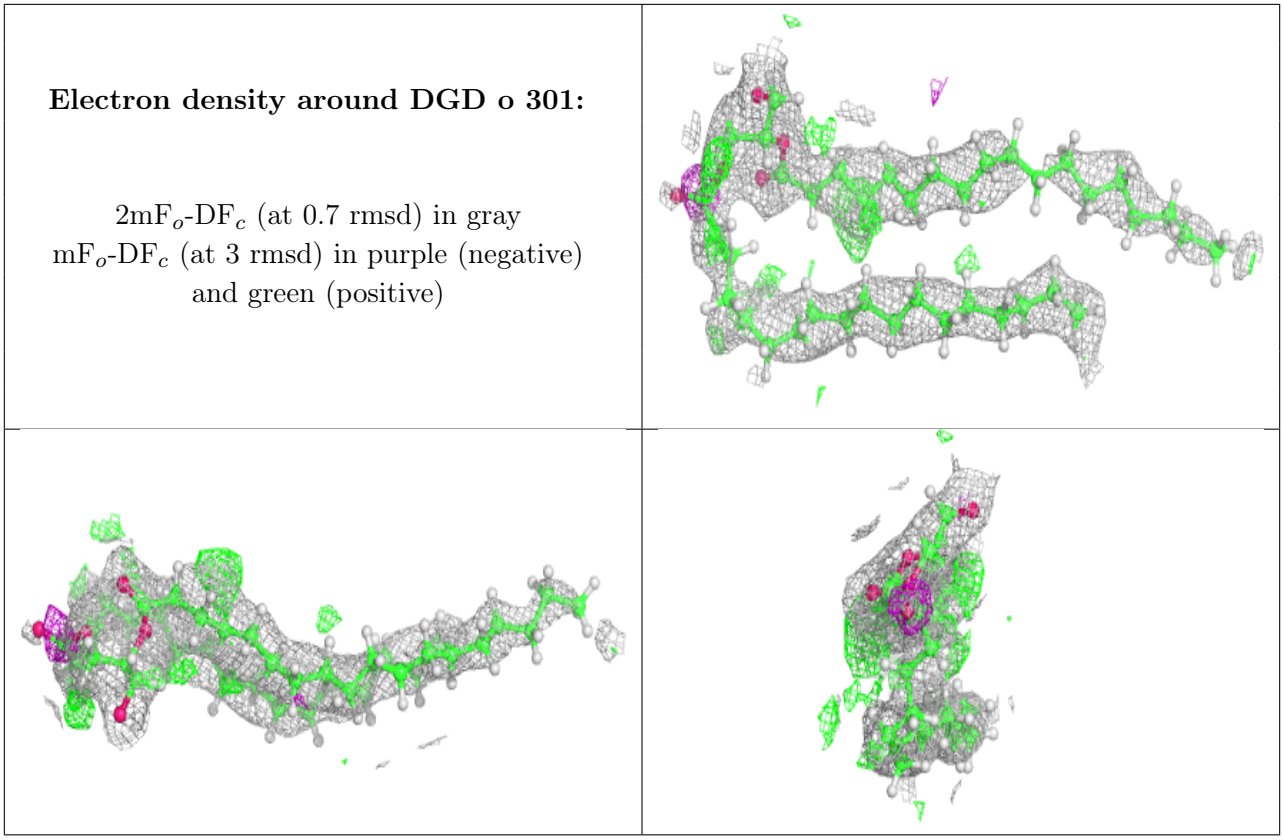
Electron density around LMG b 623:

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



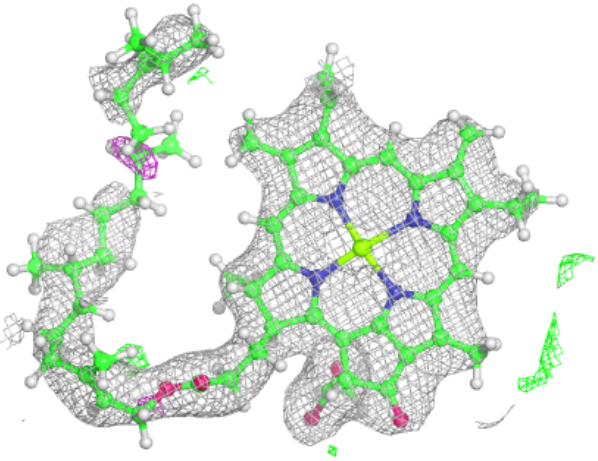
Electron density around DGD o 301:

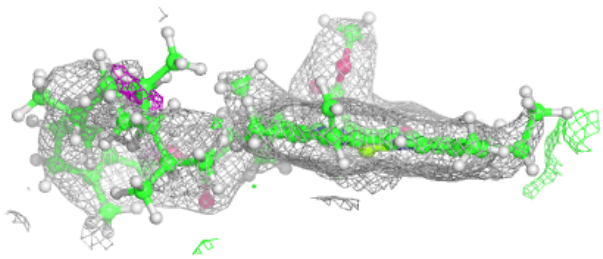
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

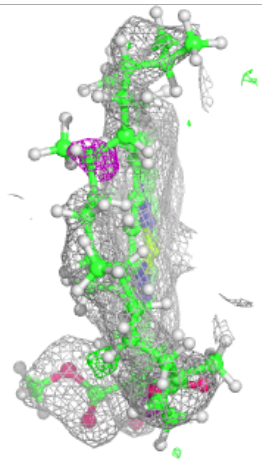


Electron density around CLA c 512:

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

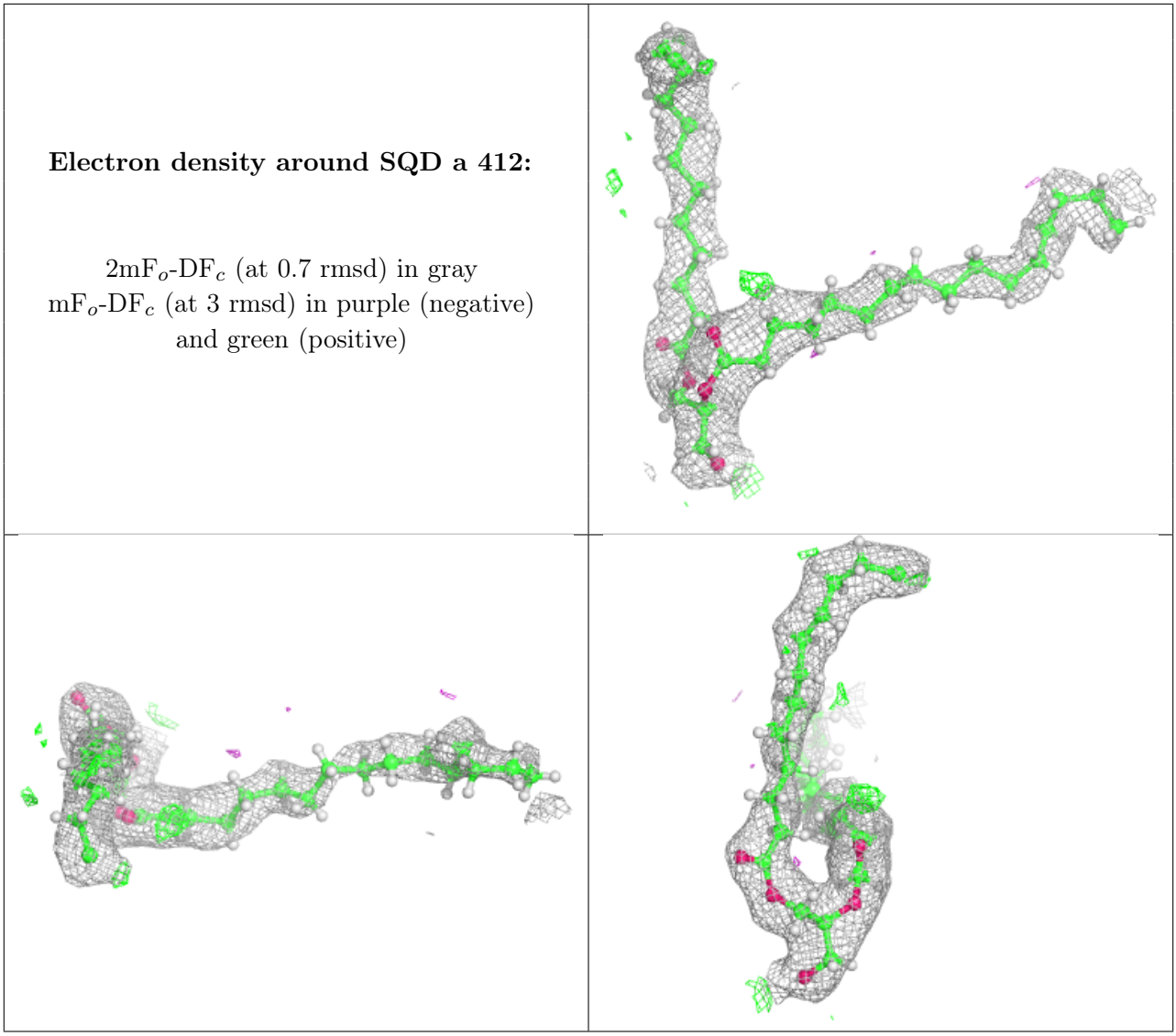






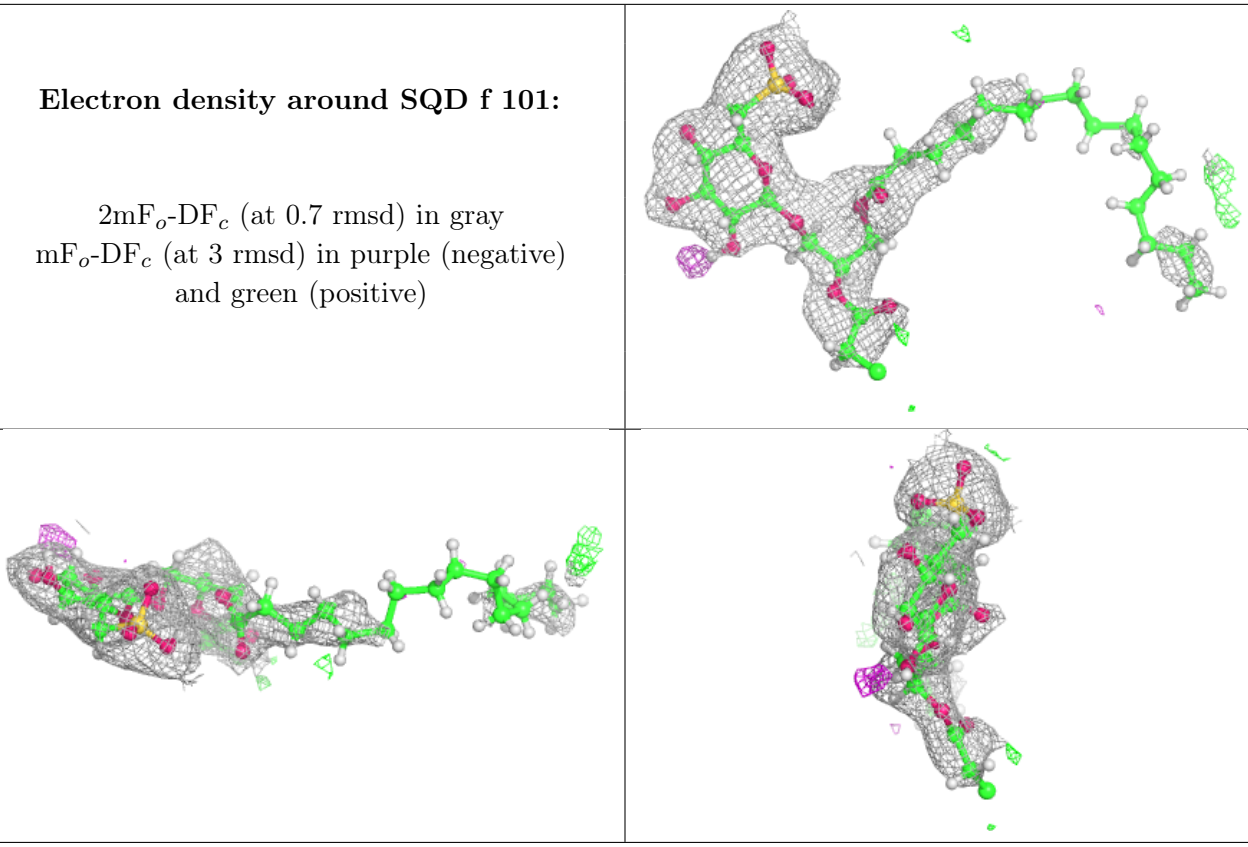
Electron density around SQD a 412:

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



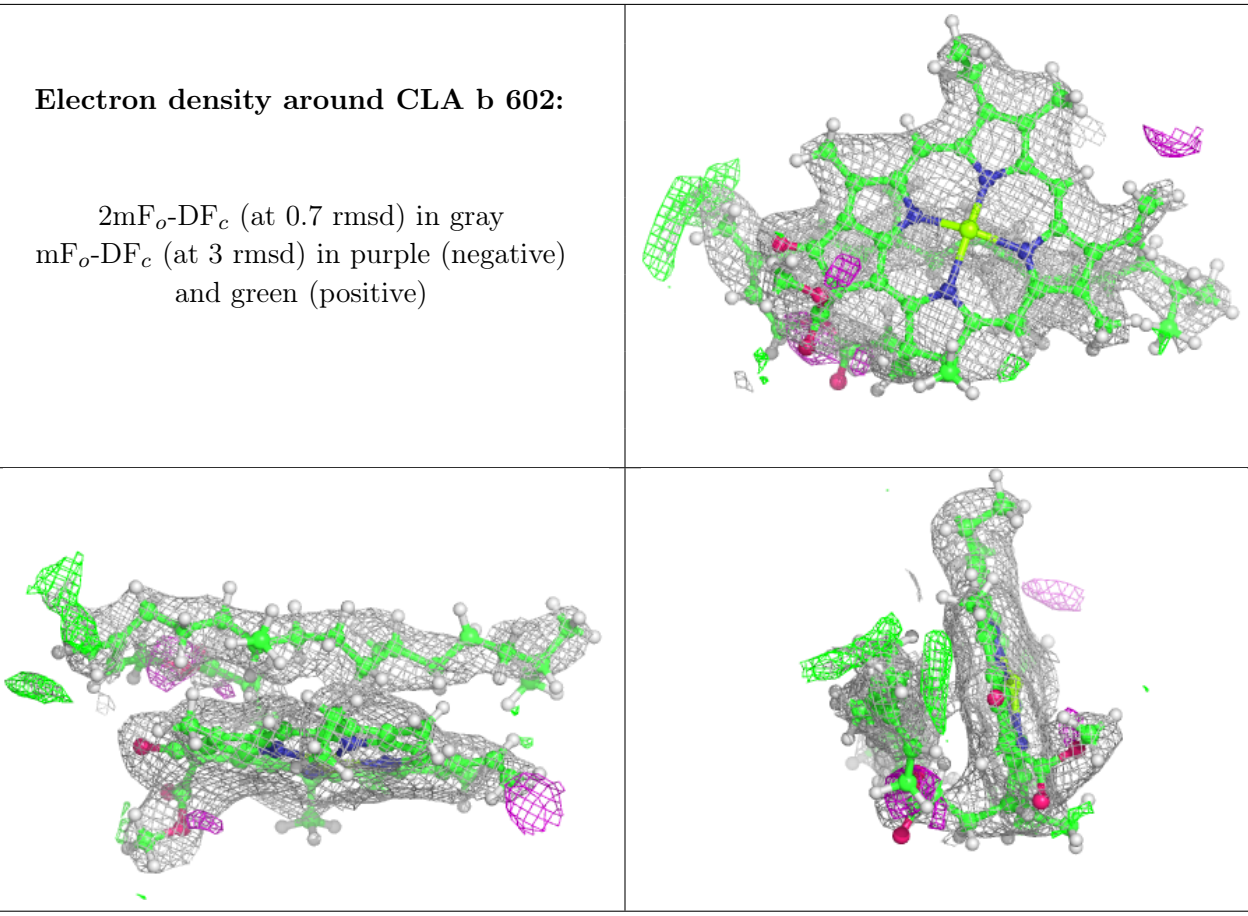
Electron density around SQD f 101:

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



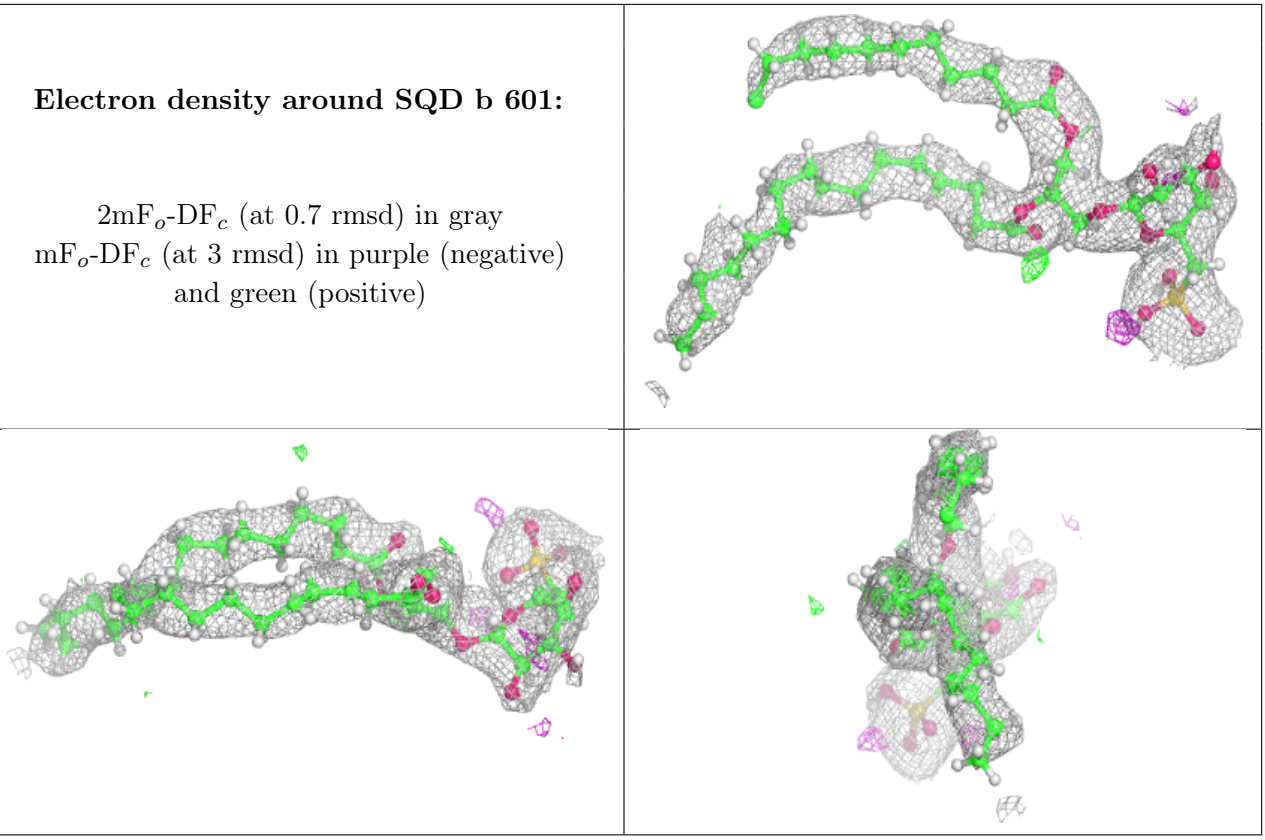
Electron density around CLA b 602:

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



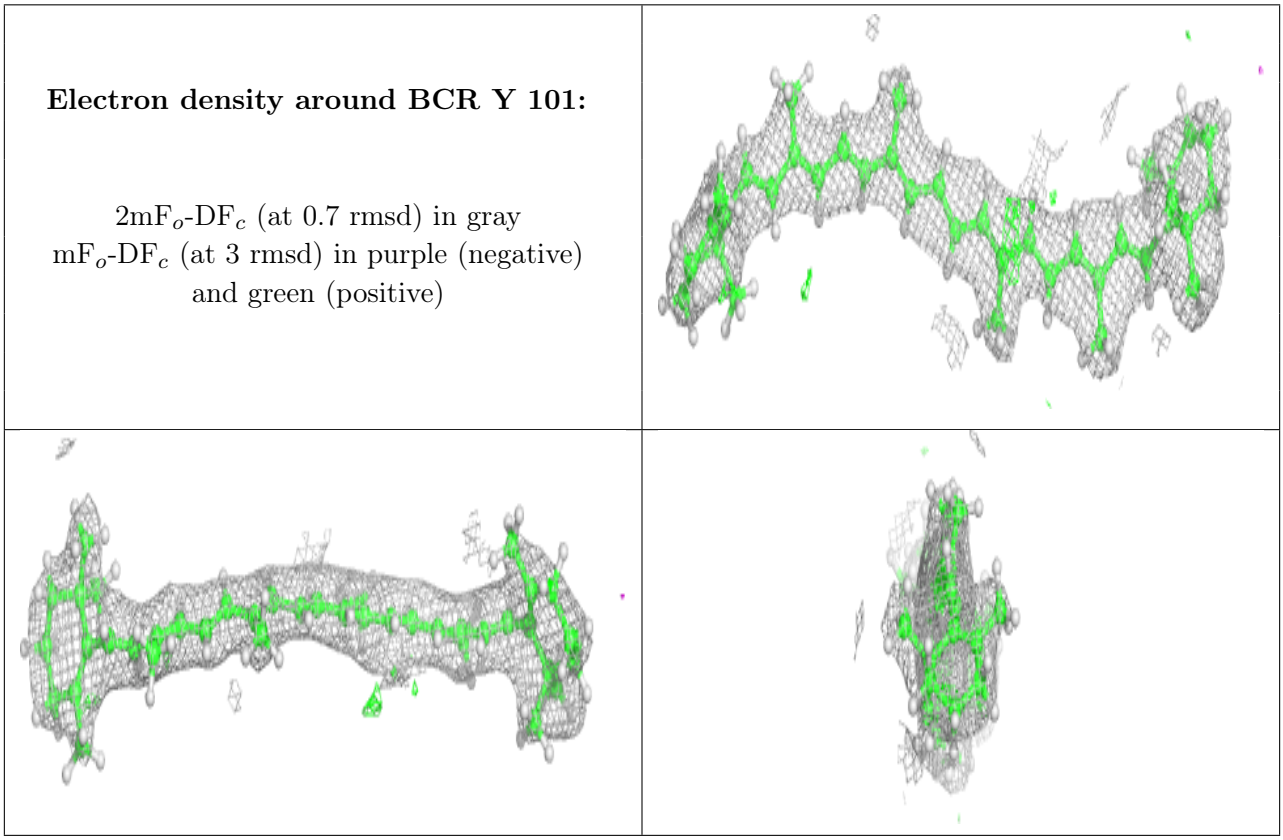
Electron density around SQD b 601:

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



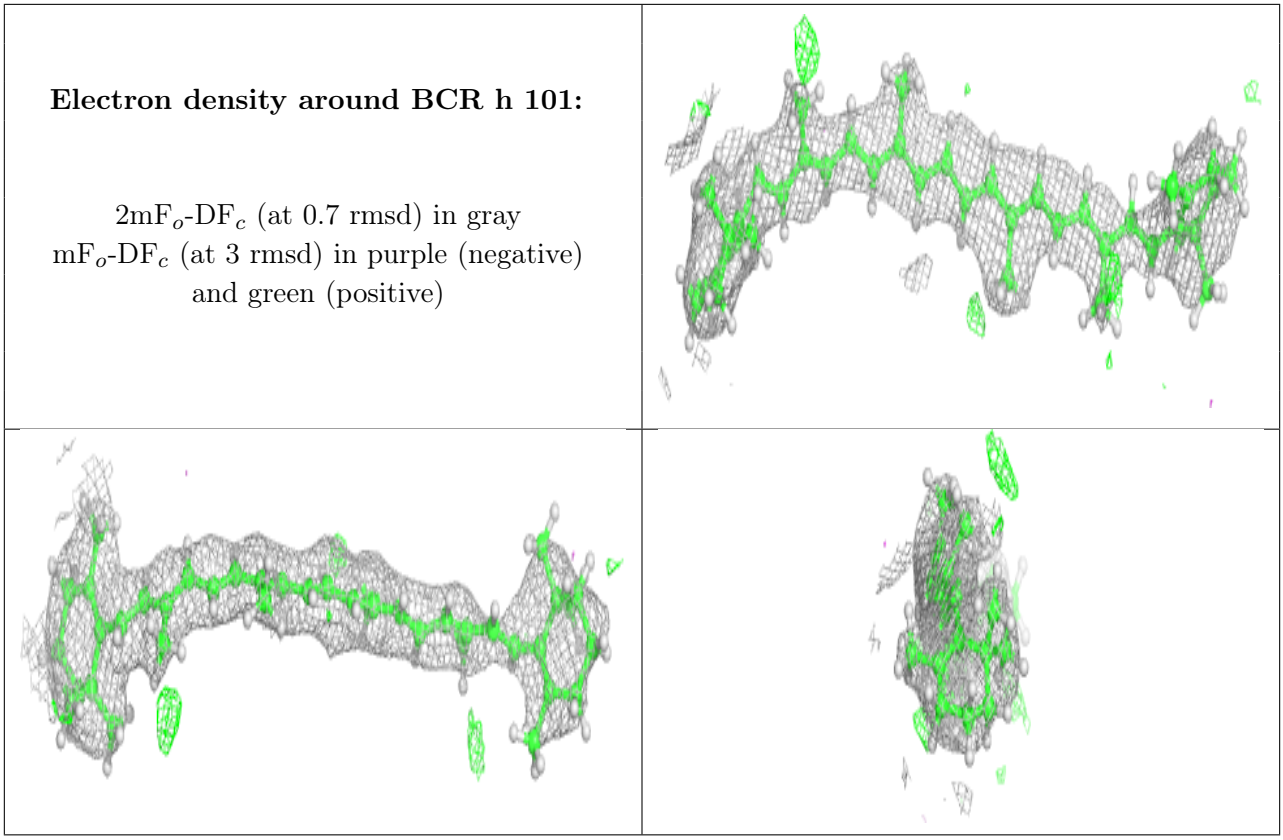
Electron density around BCR Y 101:

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



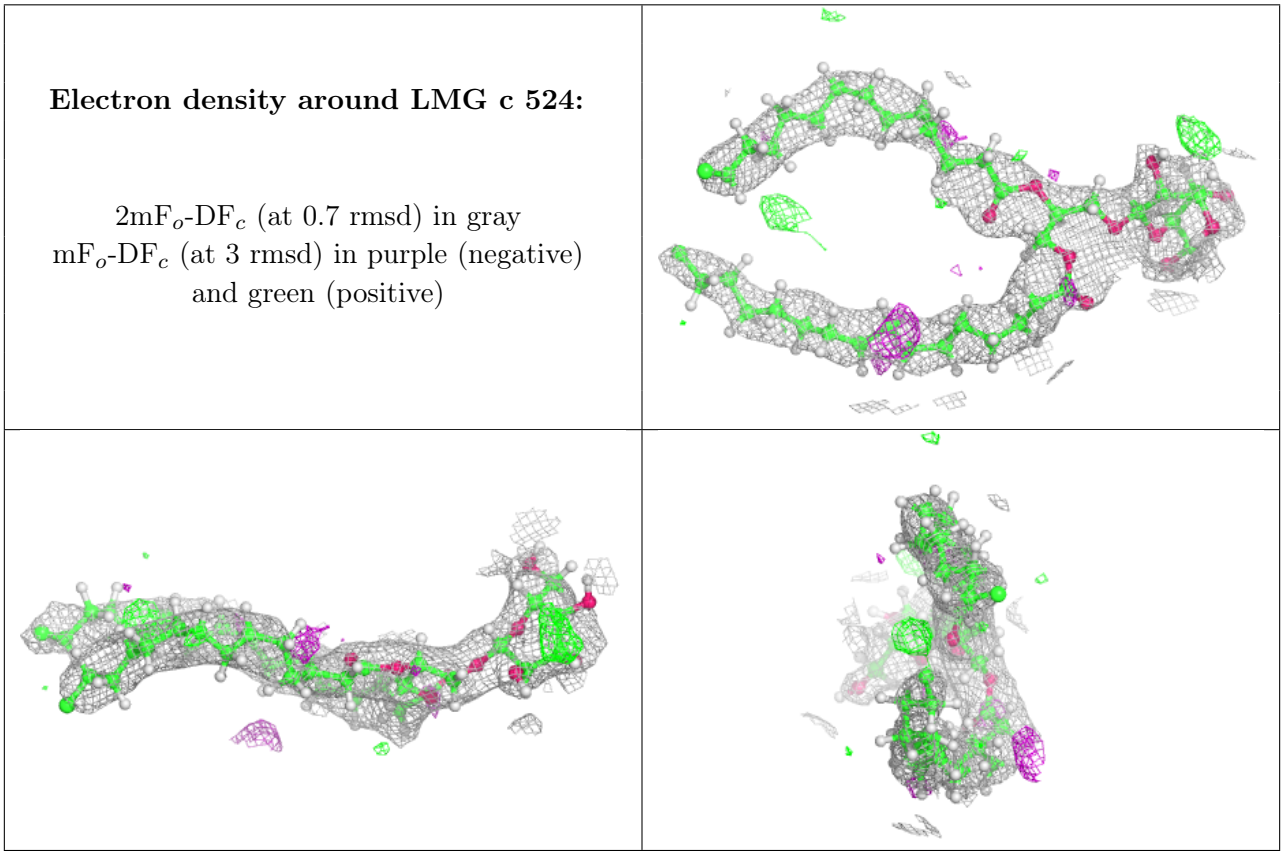
Electron density around BCR h 101:

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



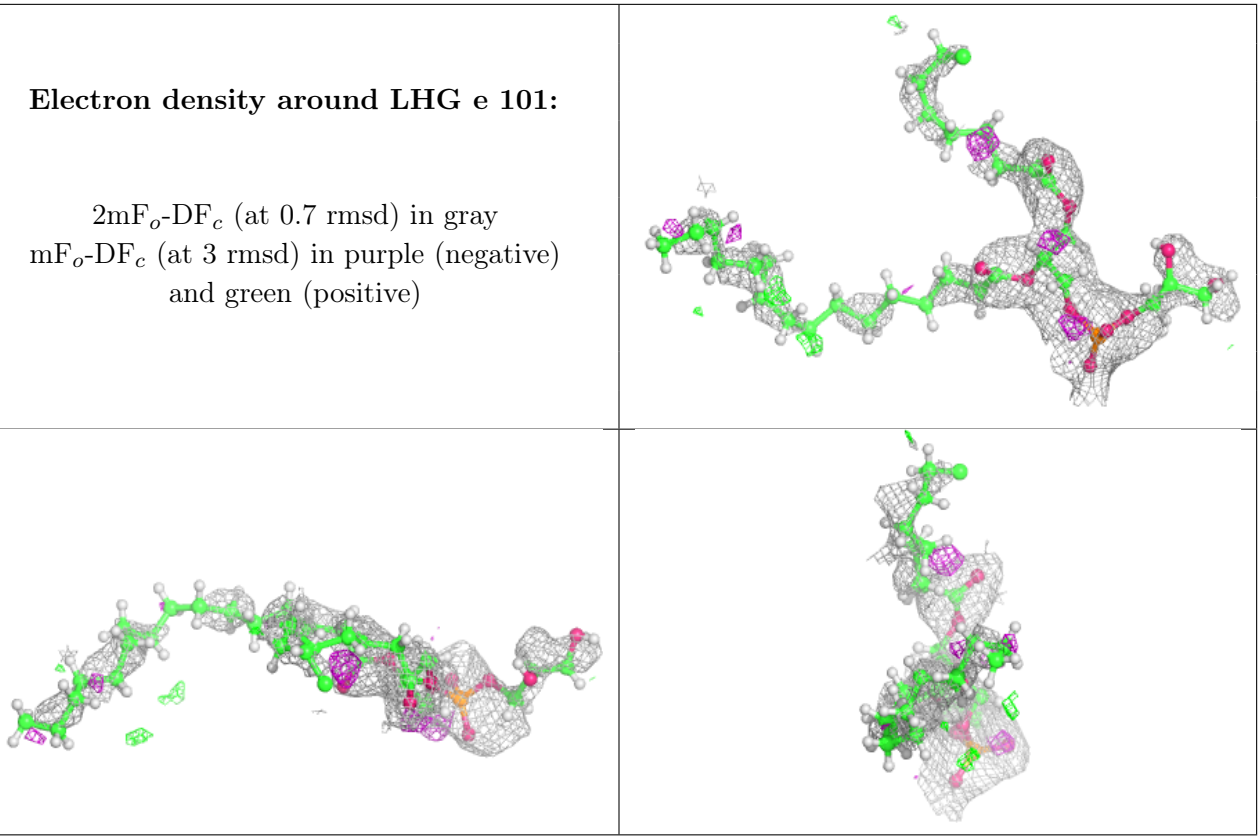
Electron density around LMG c 524:

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



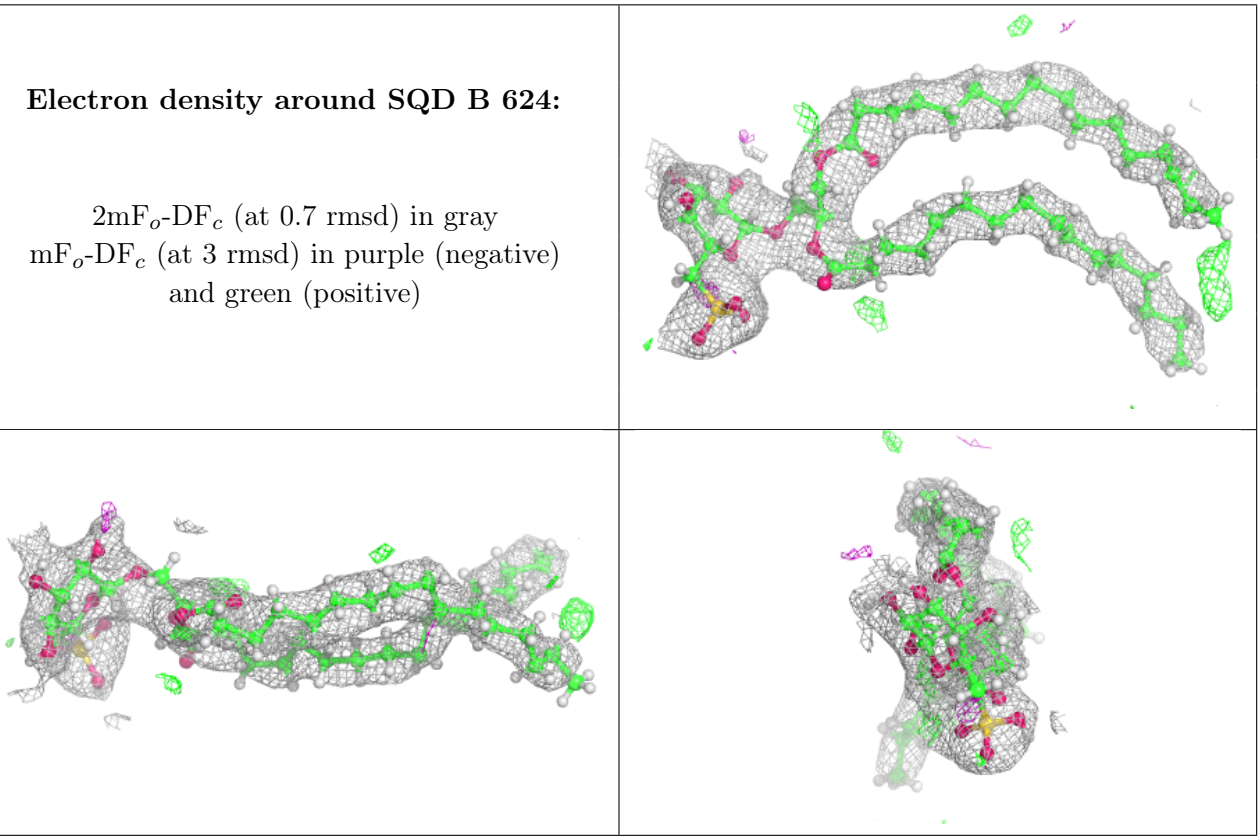
Electron density around LHG e 101:

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



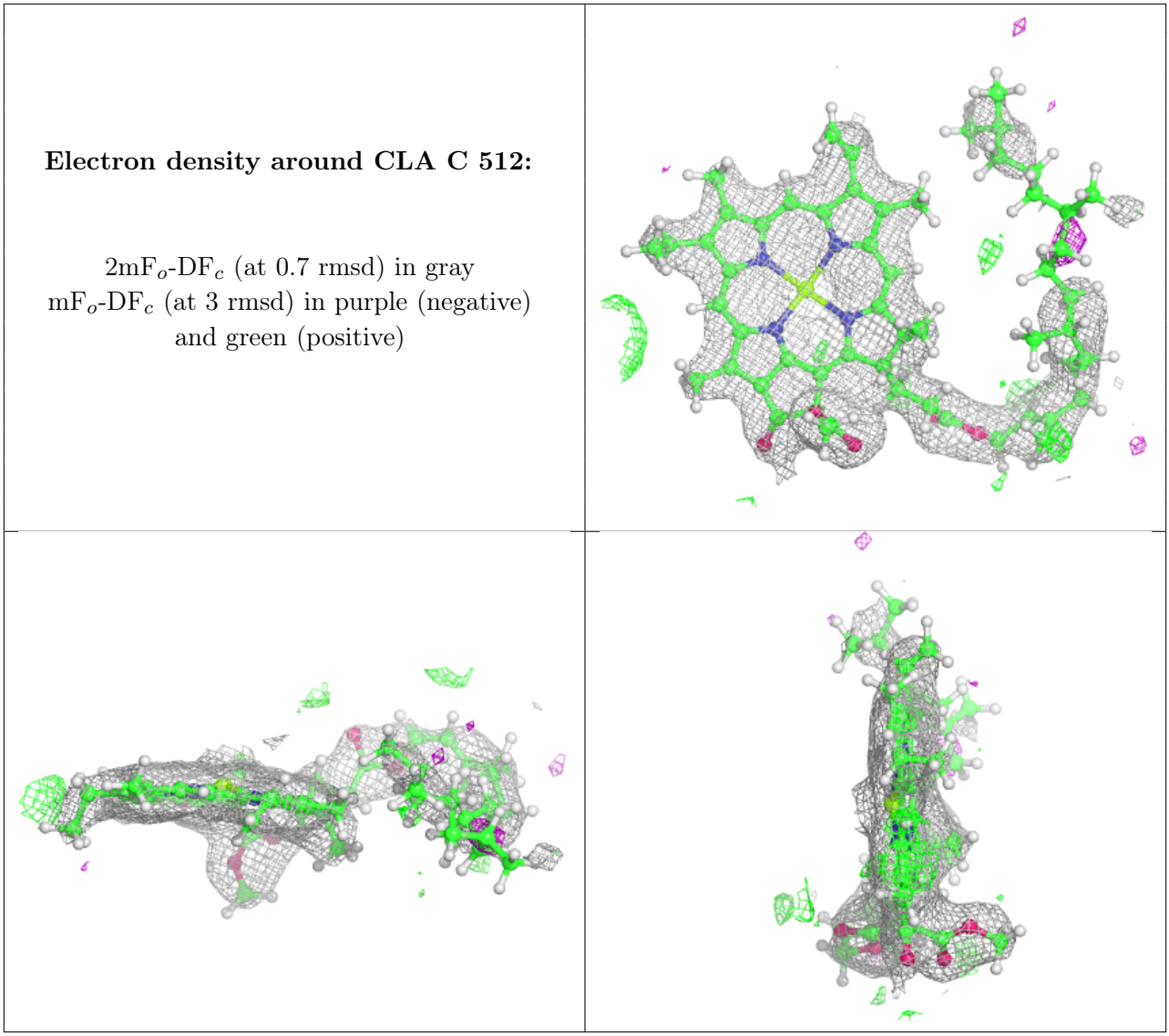
Electron density around SQD B 624:

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



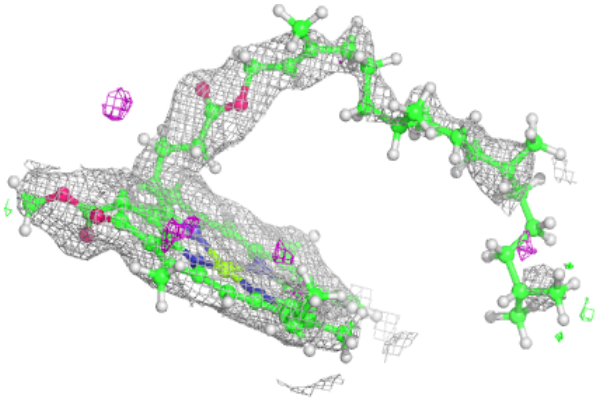
Electron density around CLA C 512:

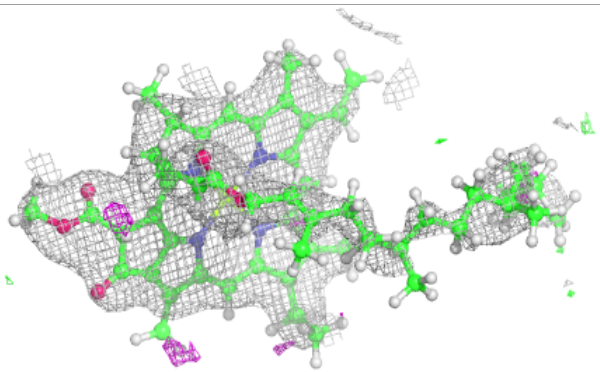
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

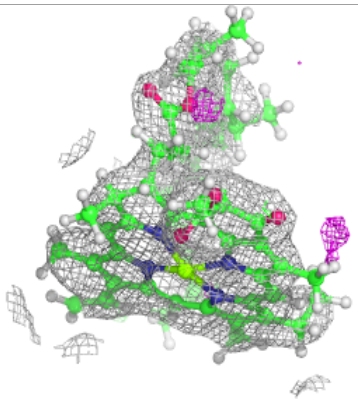


Electron density around CLA c 513:

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

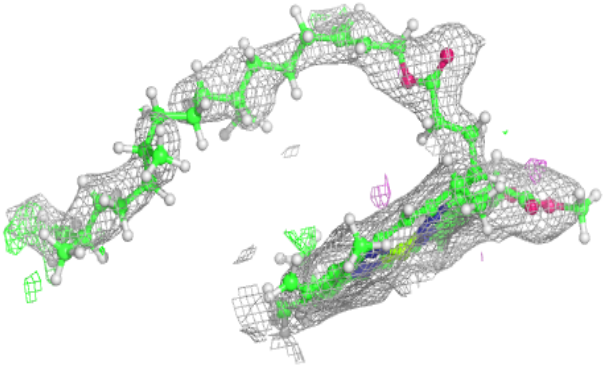


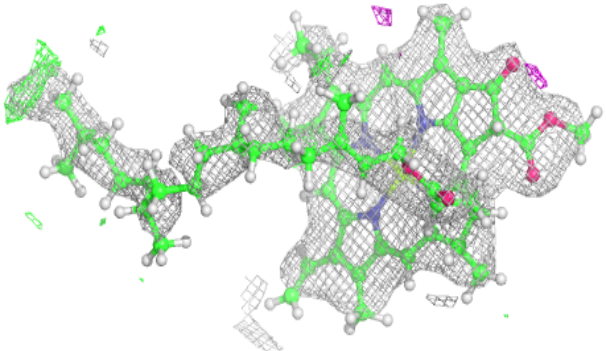


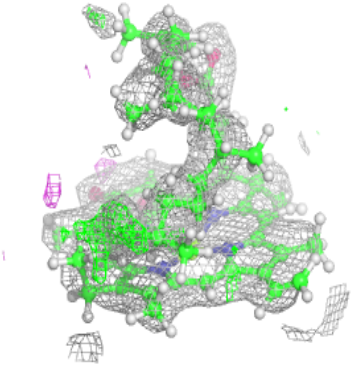


Electron density around CLA C 513:

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

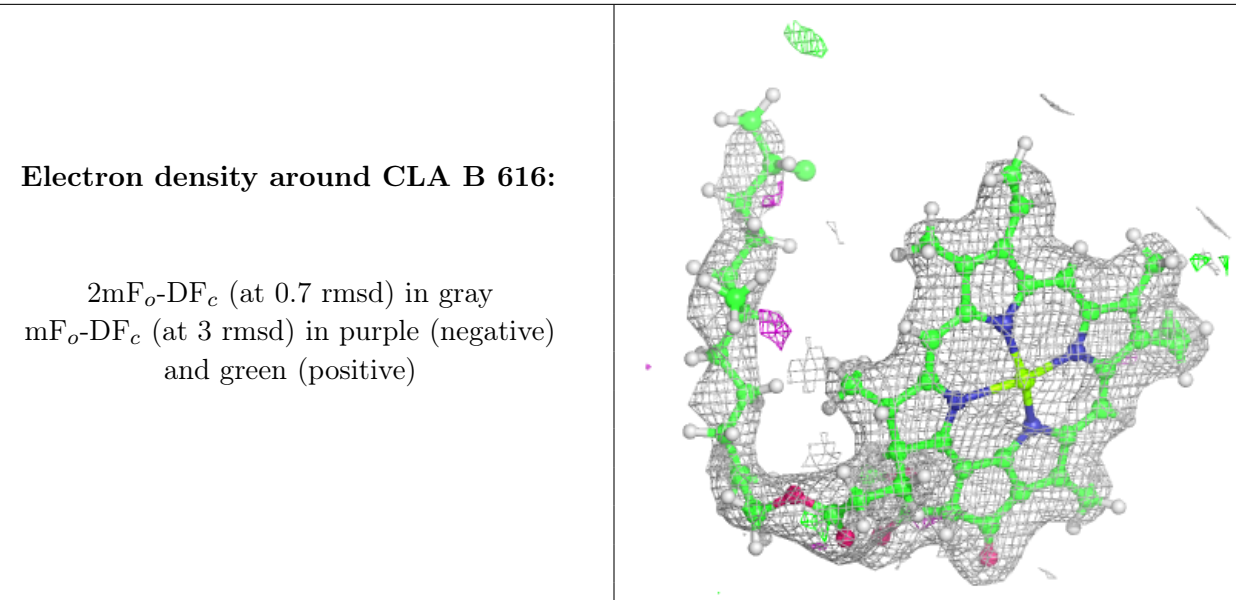


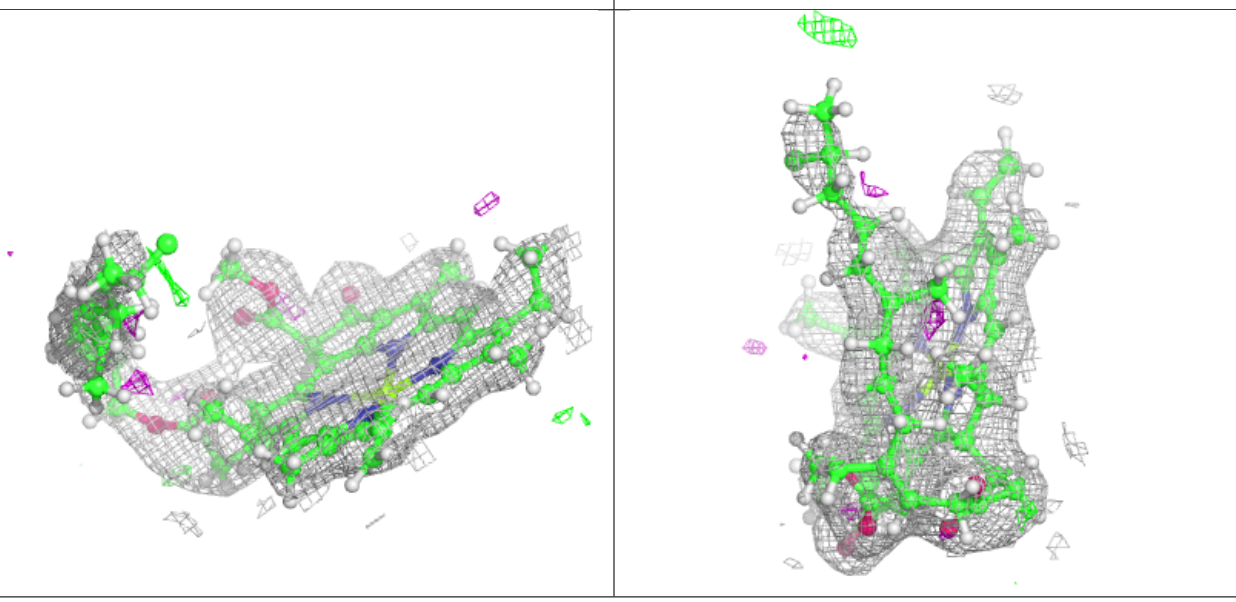




Electron density around CLA B 616:

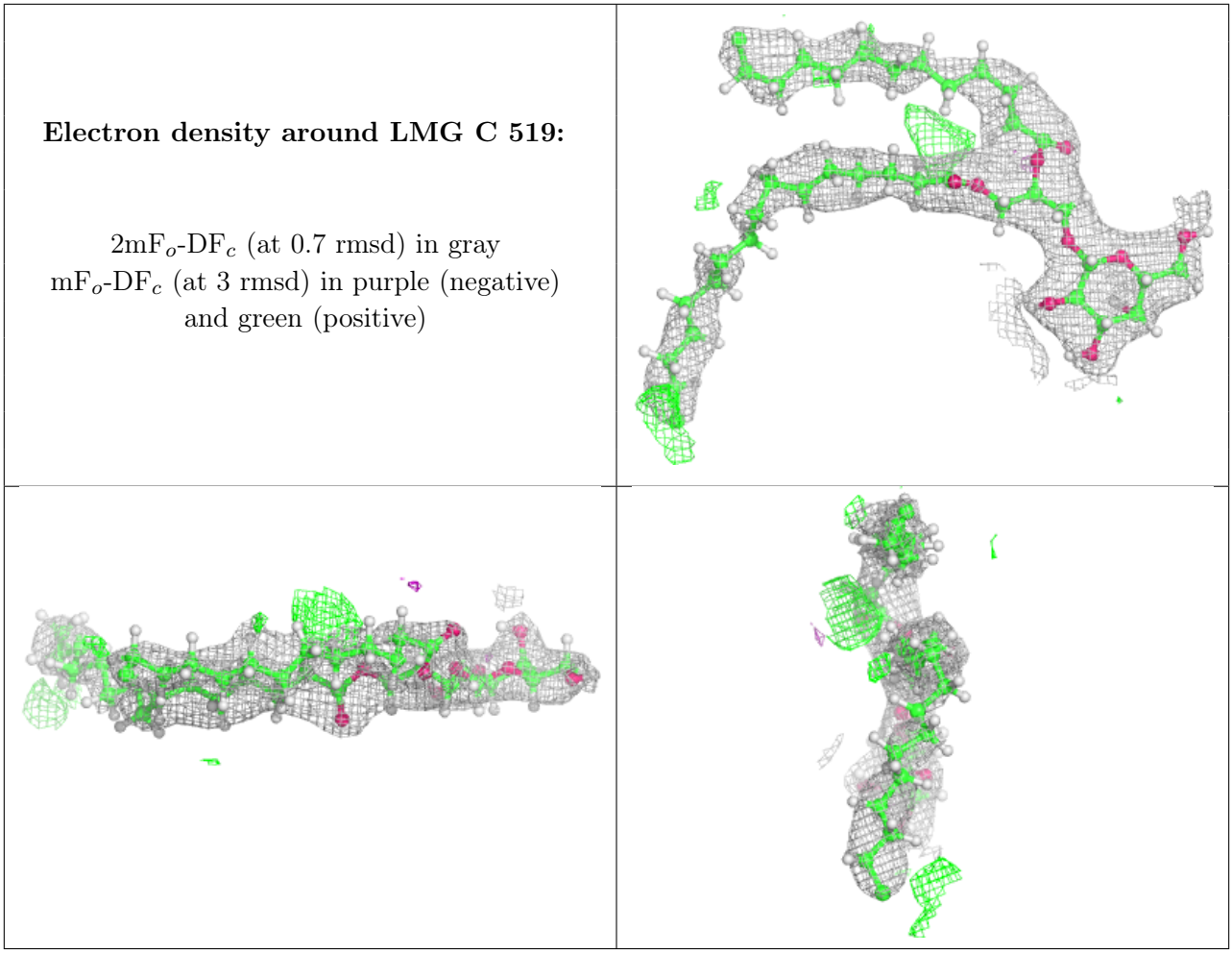
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





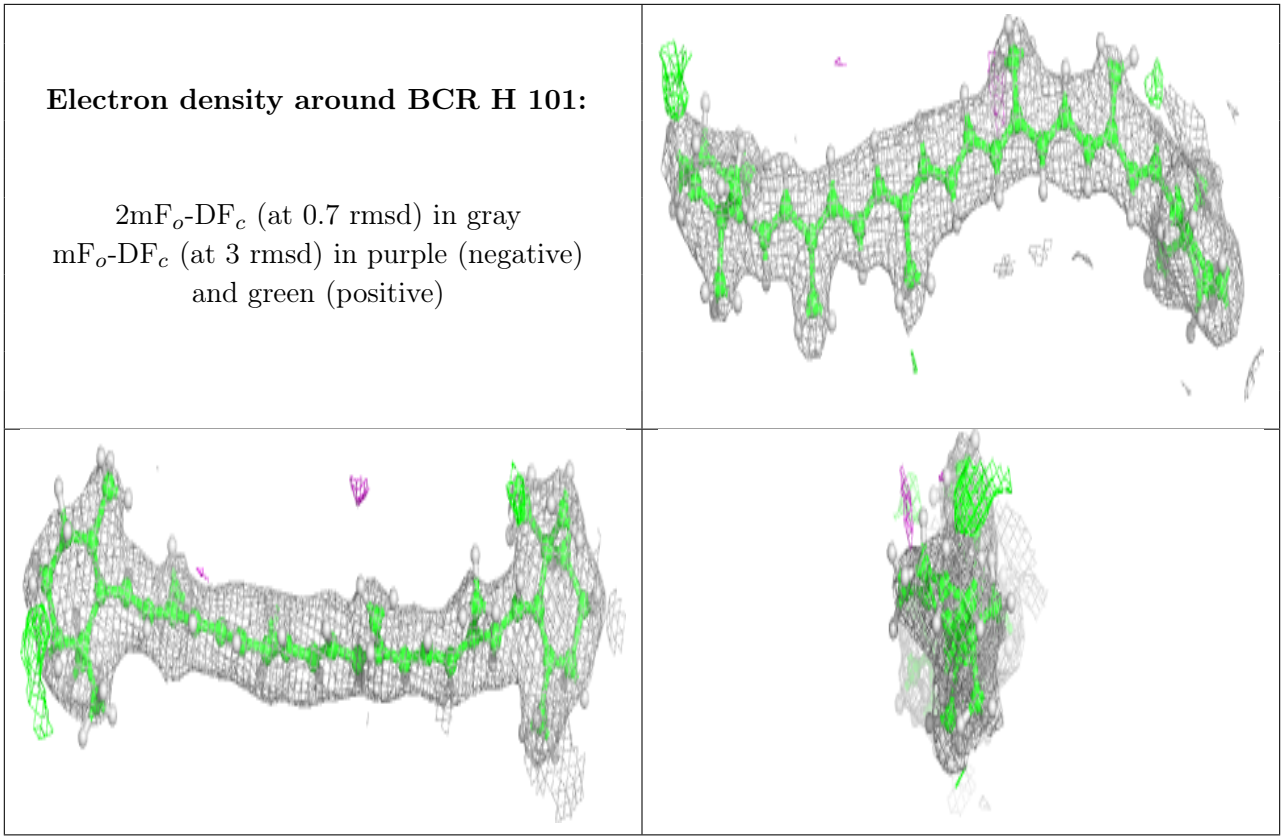
Electron density around LMG C 519:

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



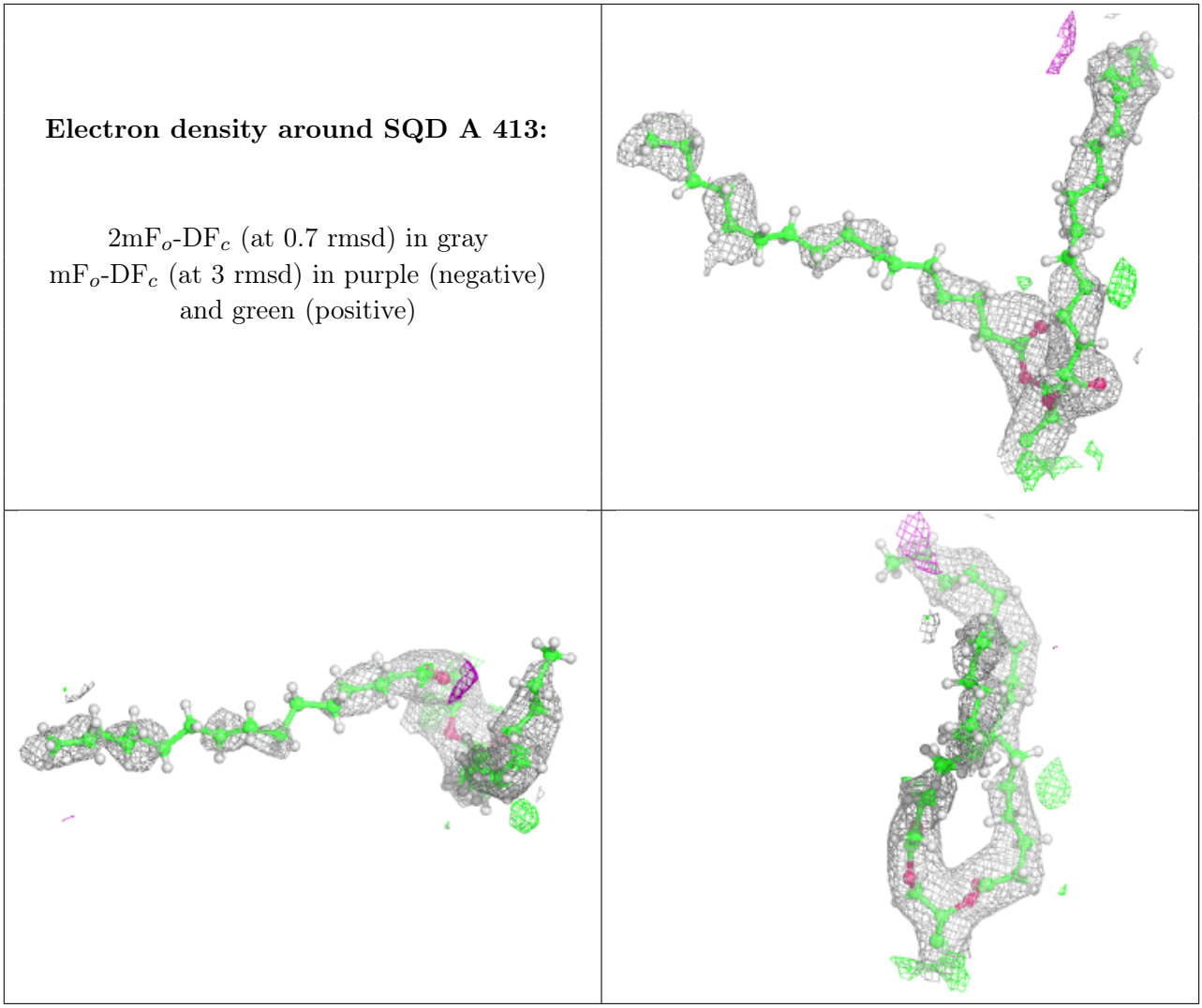
Electron density around BCR H 101:

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



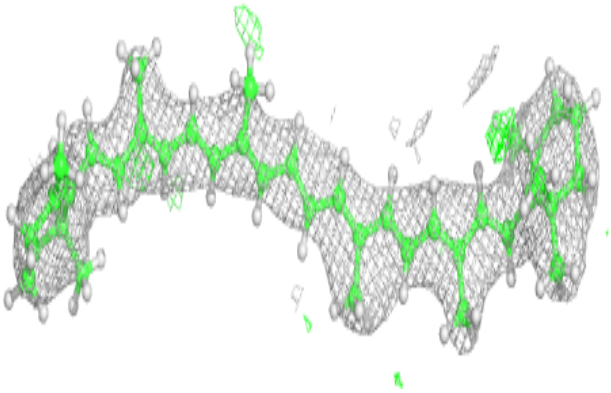
Electron density around SQD A 413:

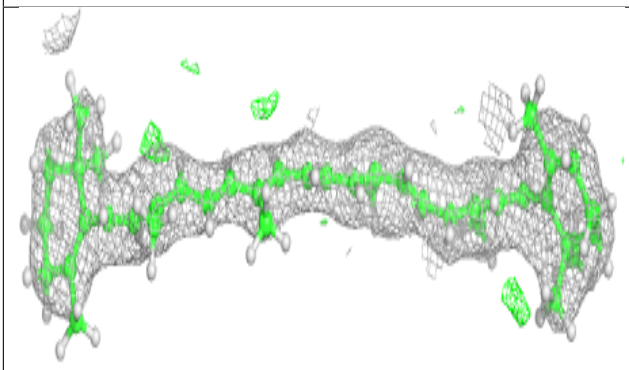
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

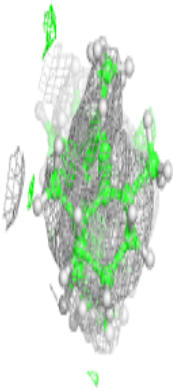


Electron density around 8CT k 101:

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

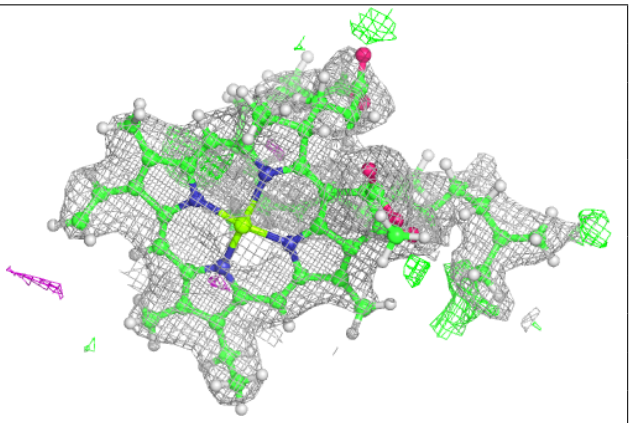


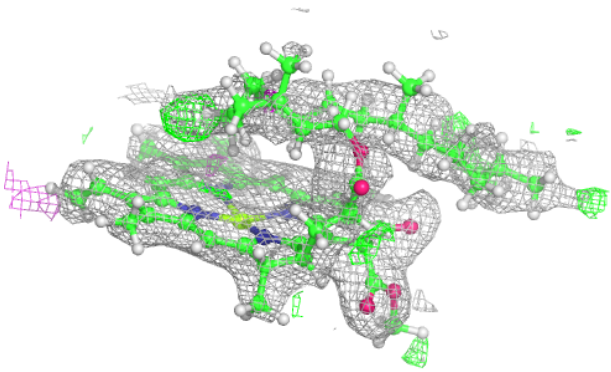


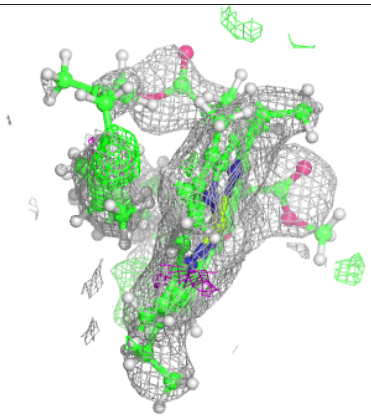


Electron density around CLA B 601:

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

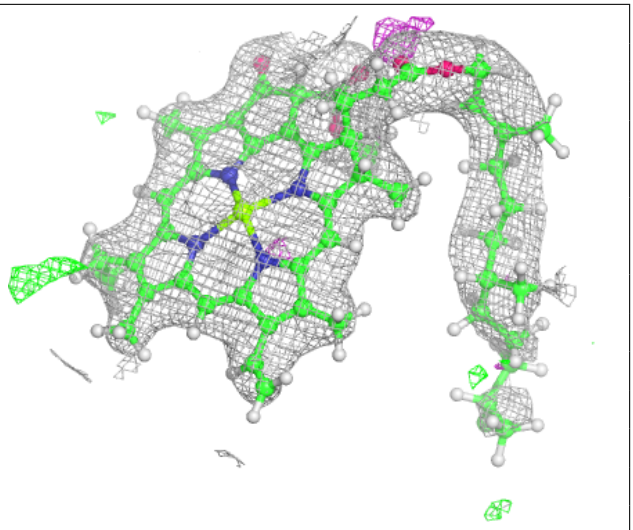


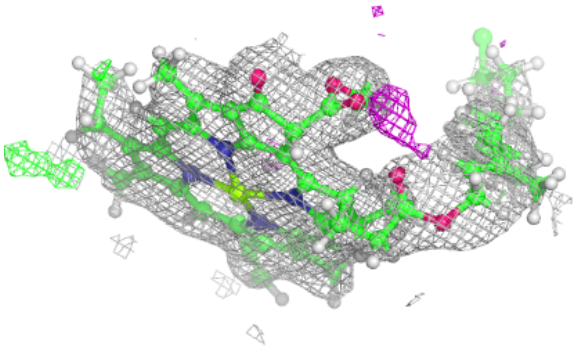


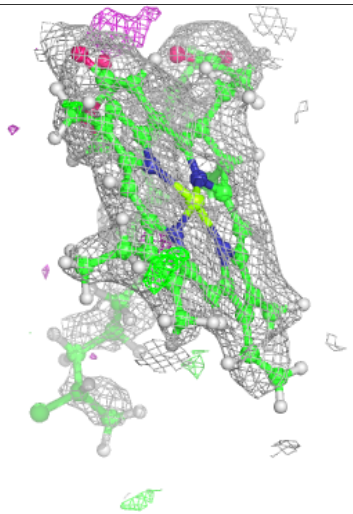


Electron density around CLA b 617:

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

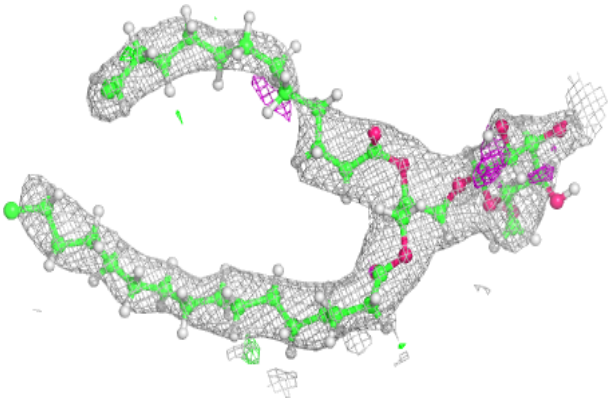


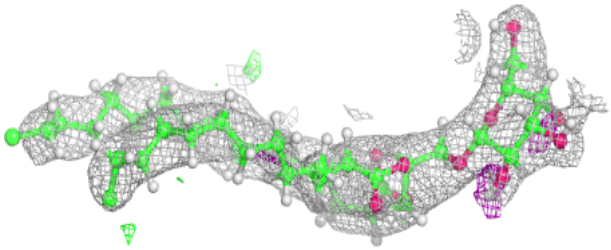


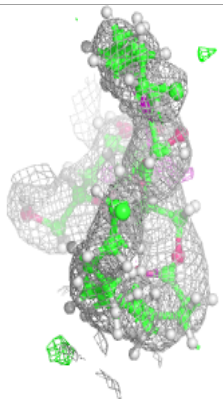


Electron density around LMG A 410:

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

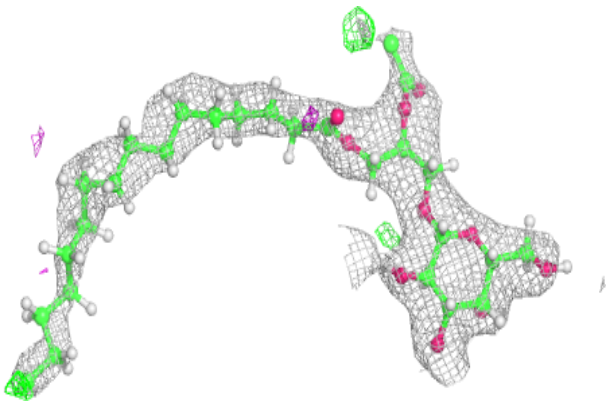


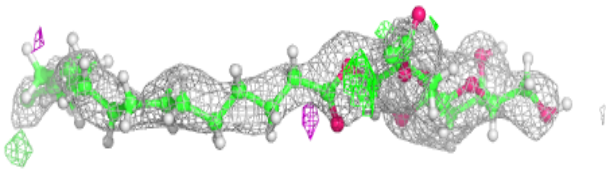


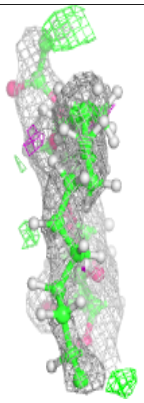


Electron density around LMG c 519:

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

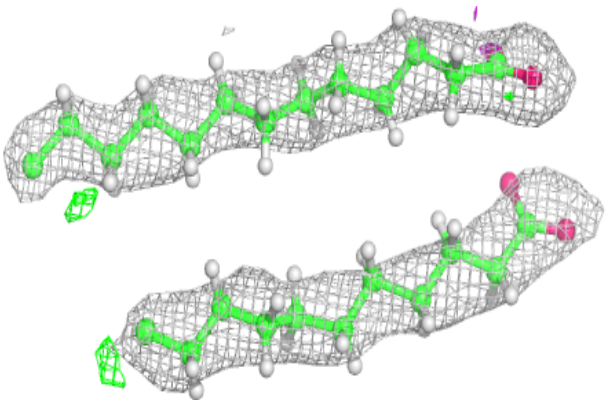


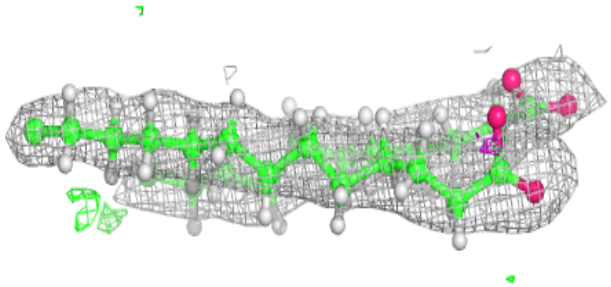


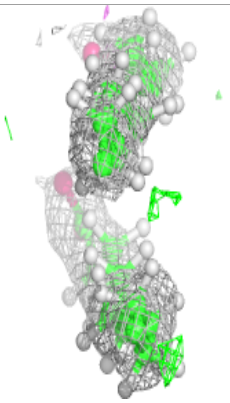


Electron density around LMG B 622:

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

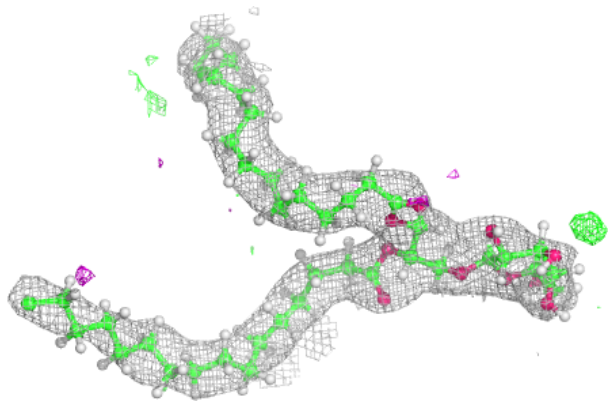


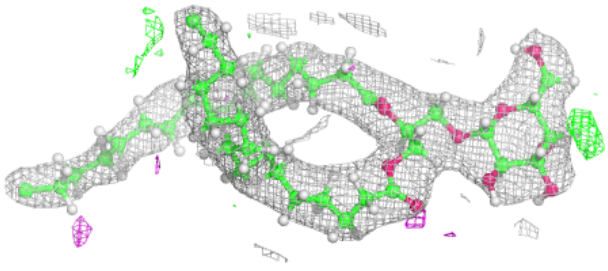


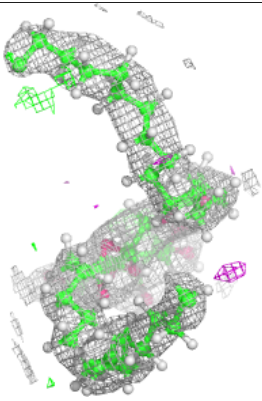


Electron density around LMG b 621:

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

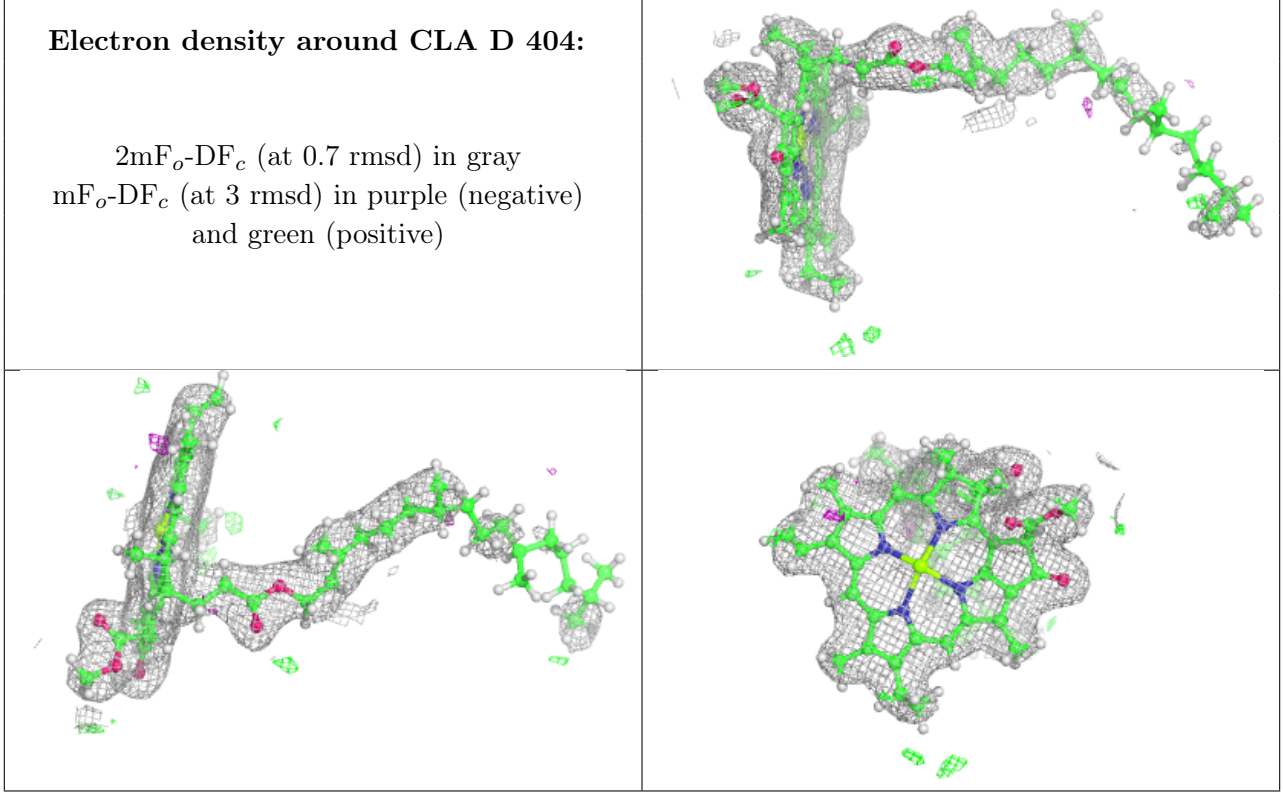






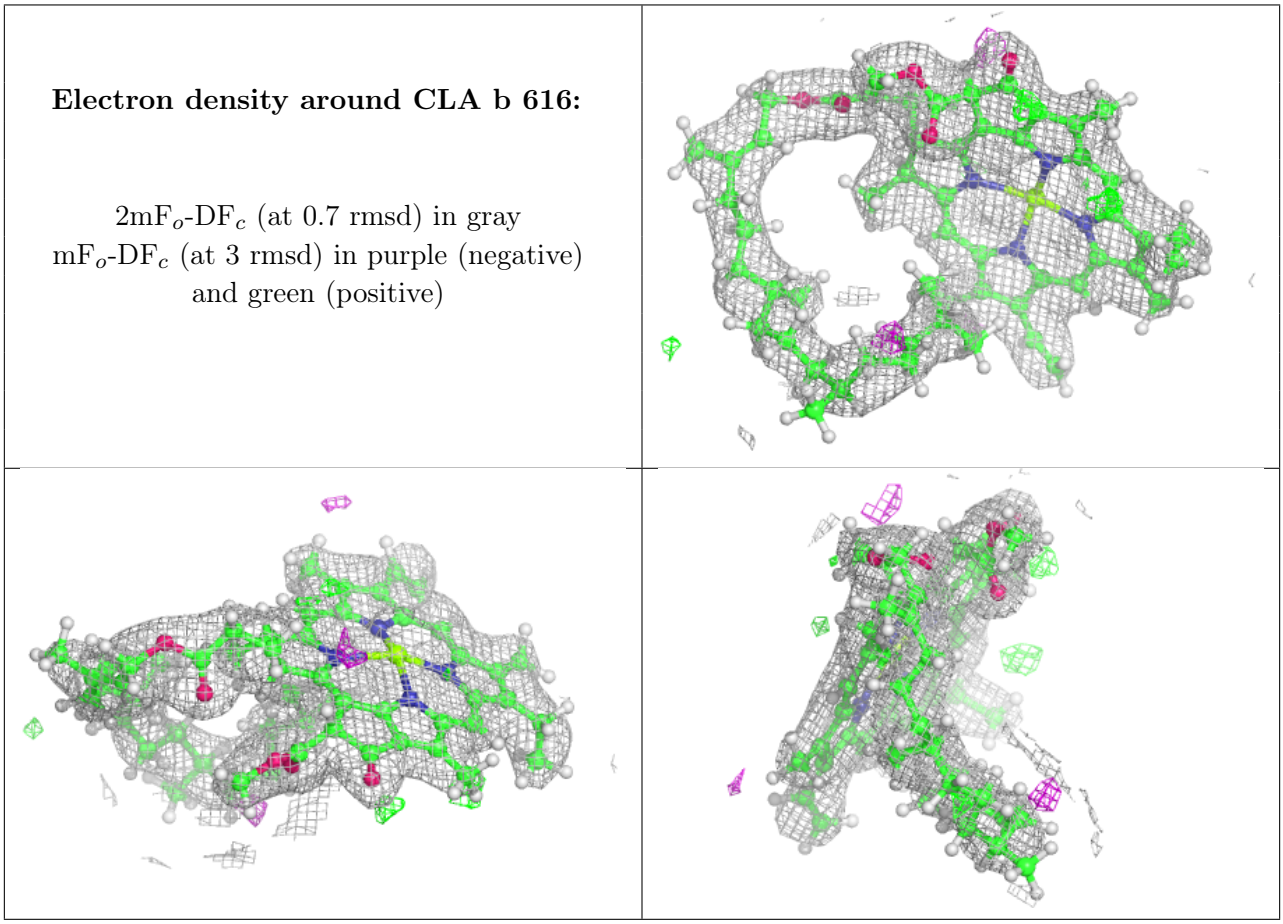
Electron density around CLA D 404:

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



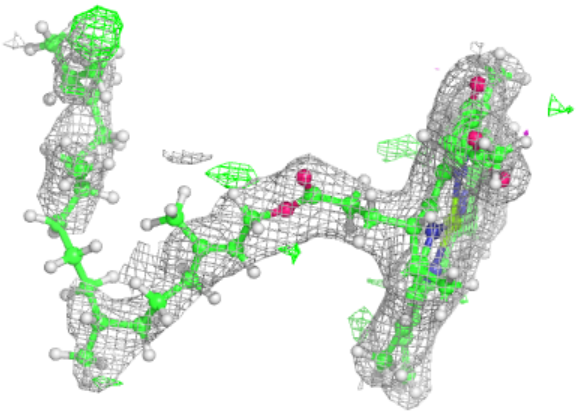
Electron density around CLA b 616:

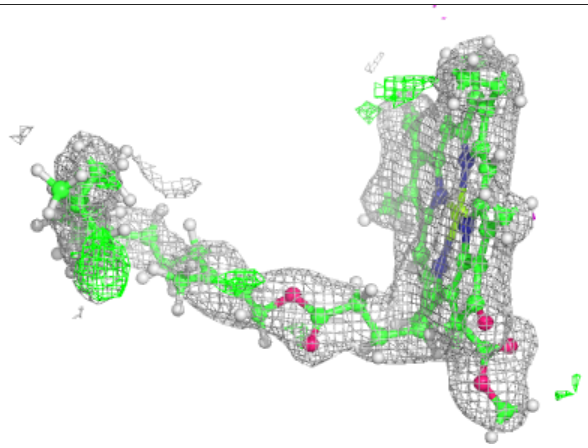
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

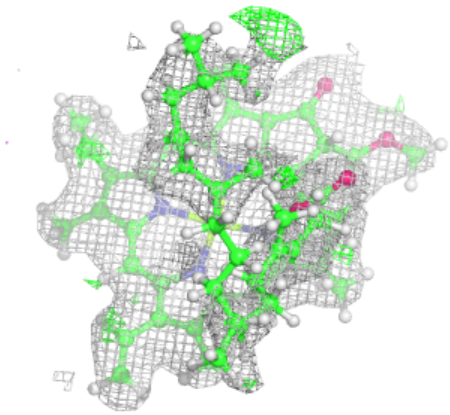


Electron density around CLA a 408:

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

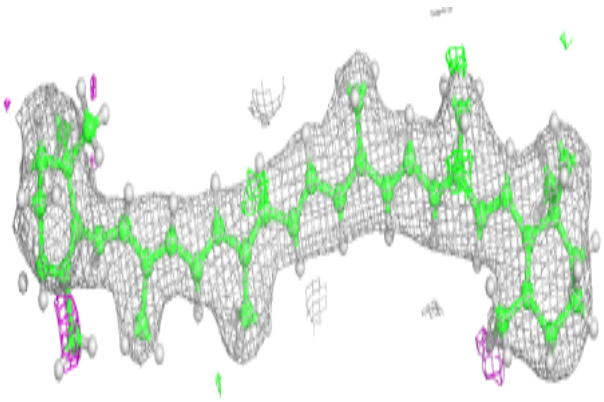


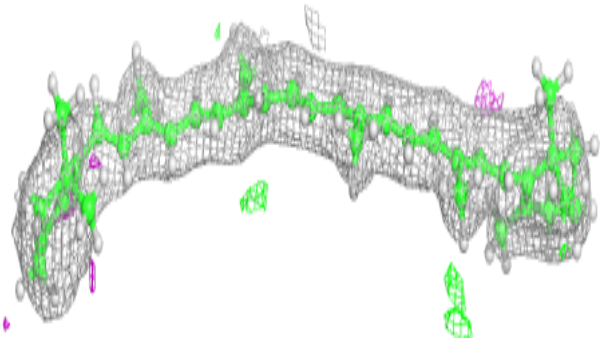


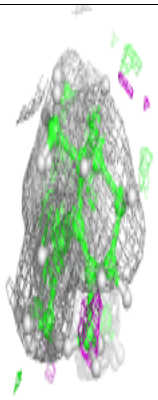


Electron density around 8CT D 405:

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

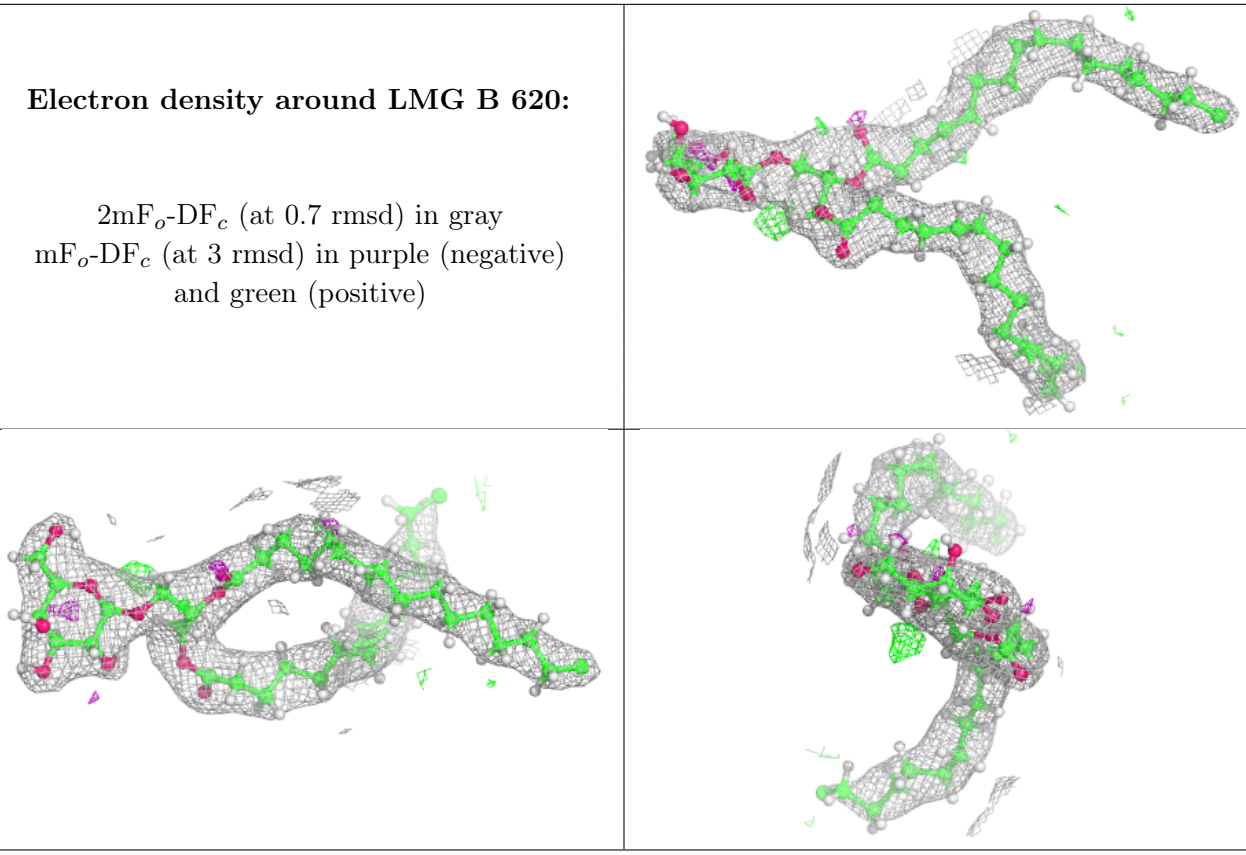






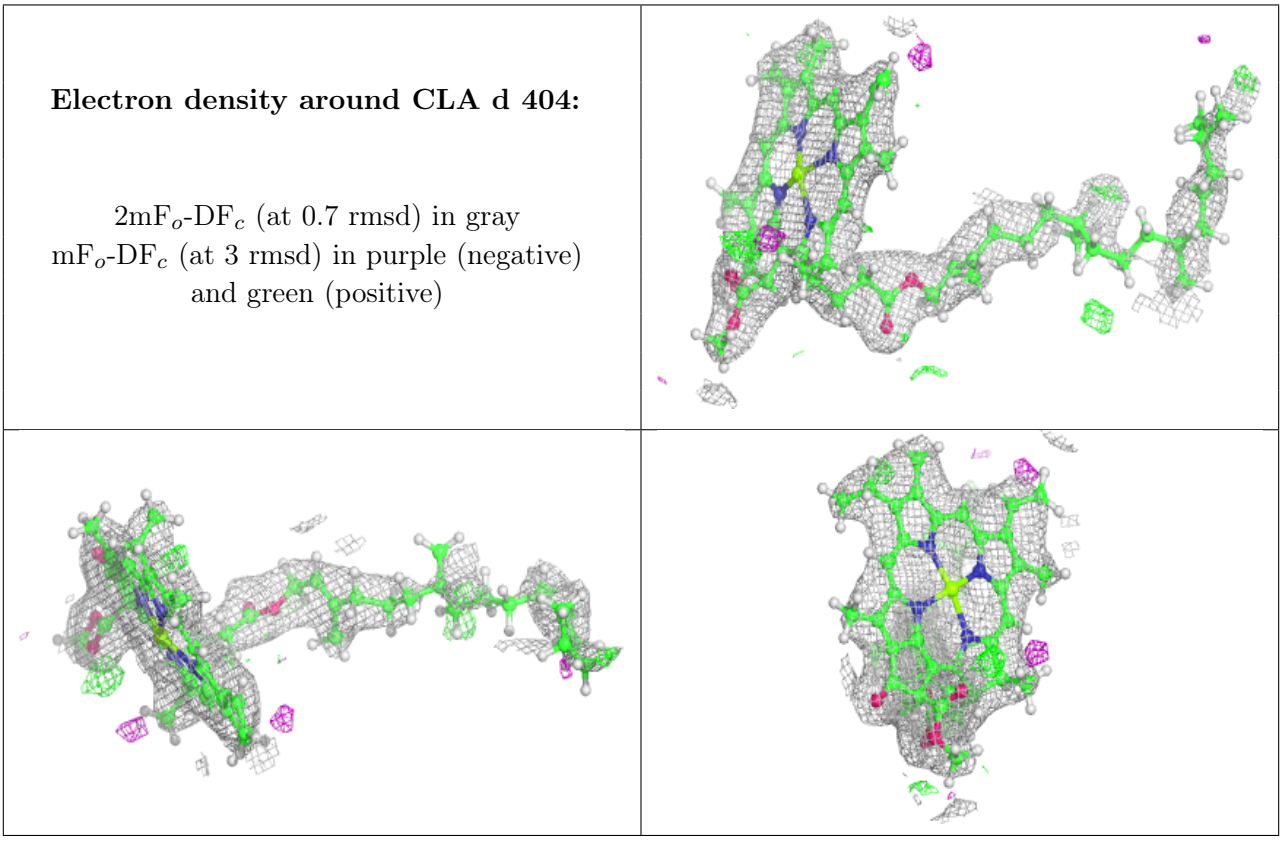
Electron density around LMG B 620:

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



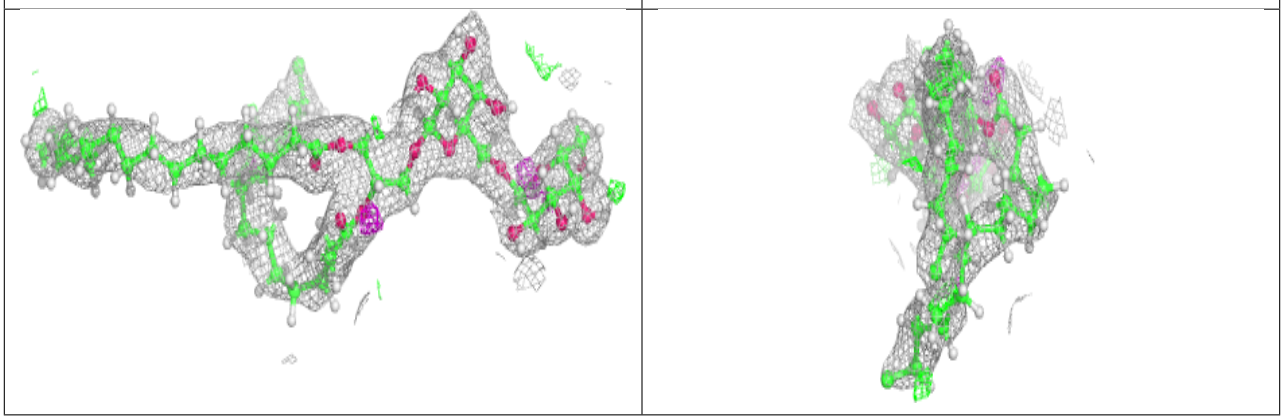
Electron density around CLA d 404:

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



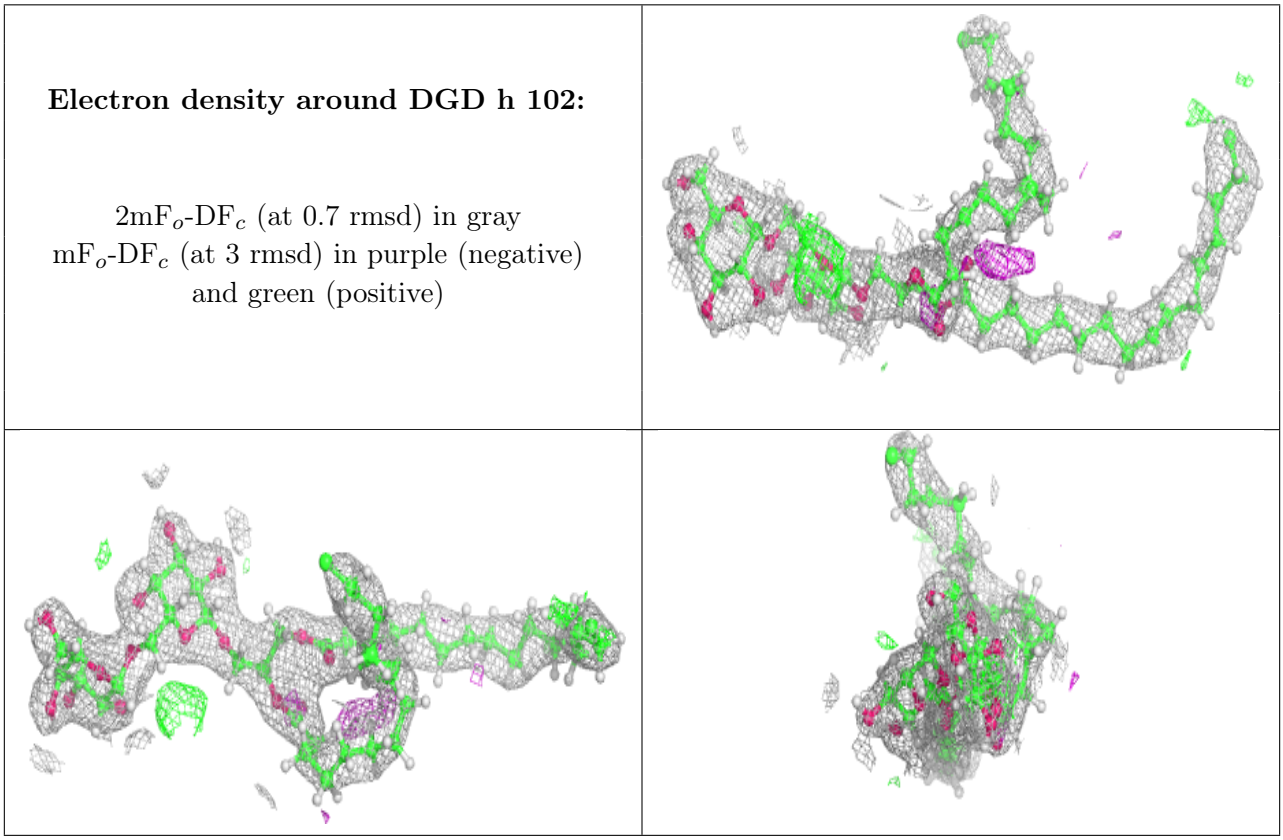
Electron density around DGD H 102:

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



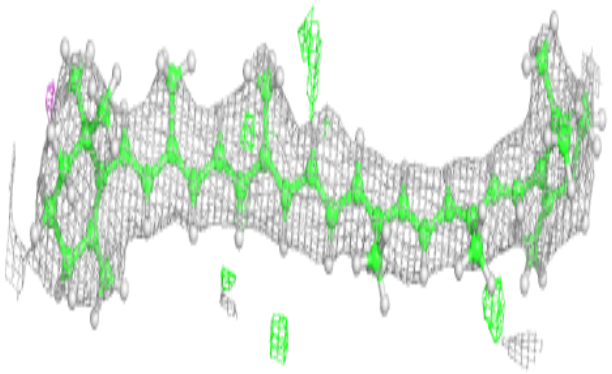
Electron density around DGD h 102:

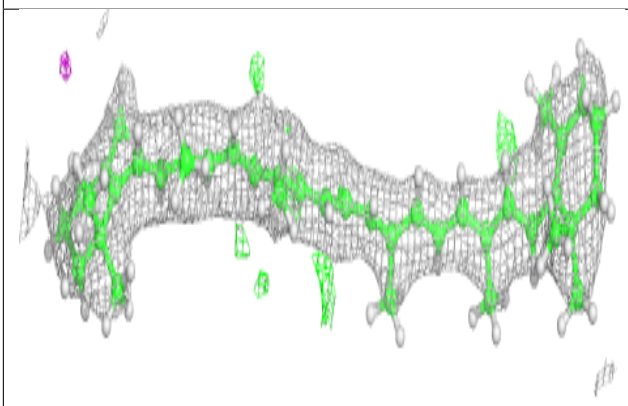
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

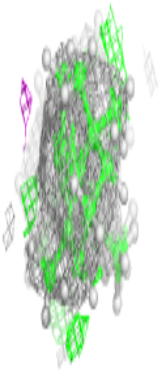


Electron density around 8CT C 514:

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

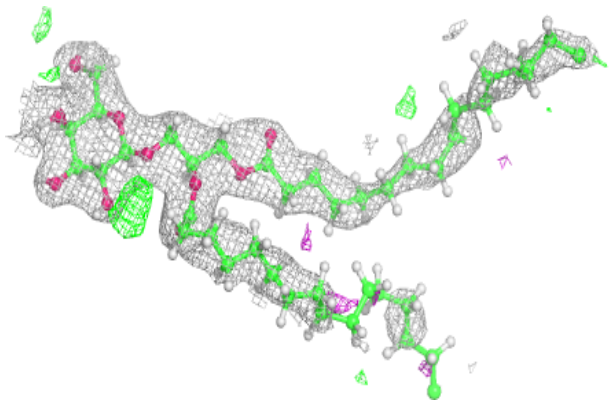


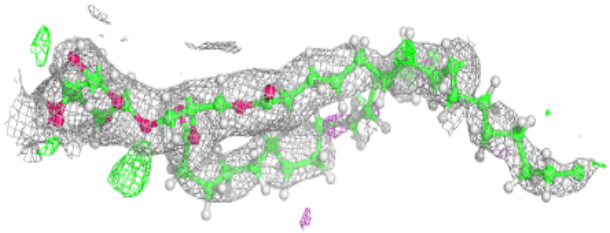




Electron density around LMG D 407:

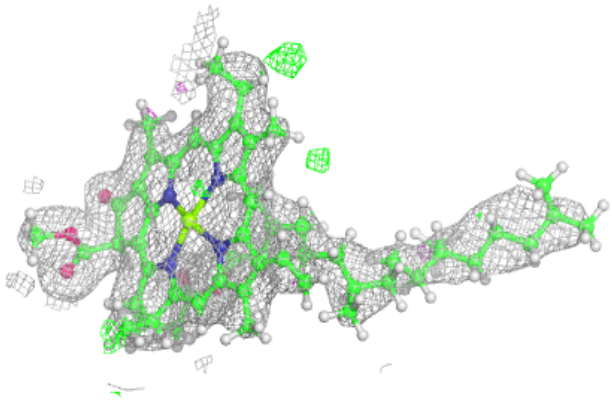
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

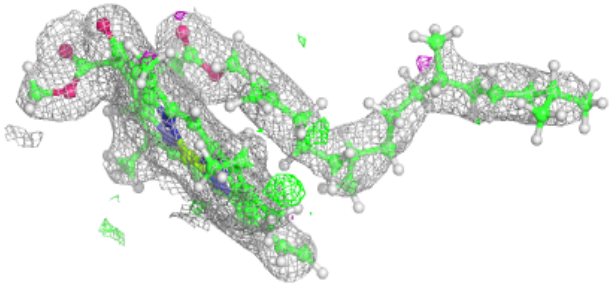


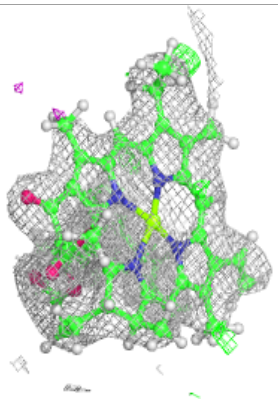


Electron density around CLA C 505:

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

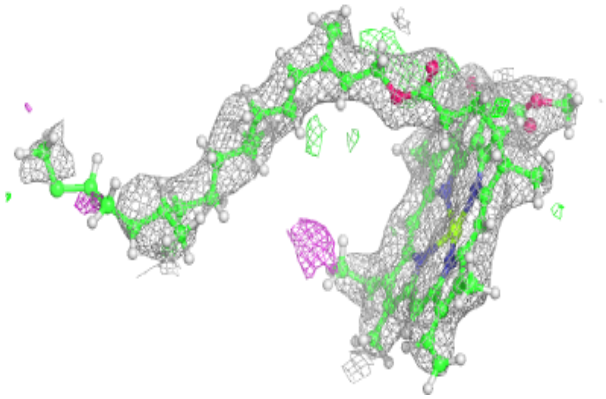


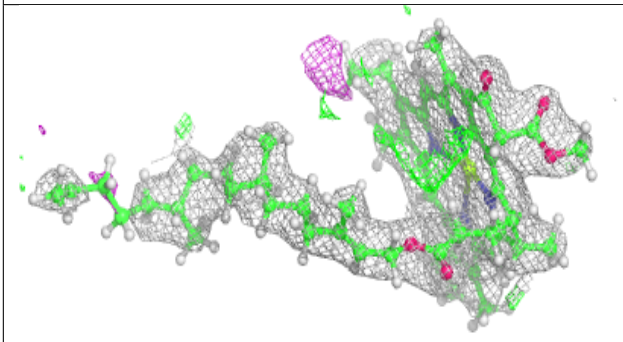


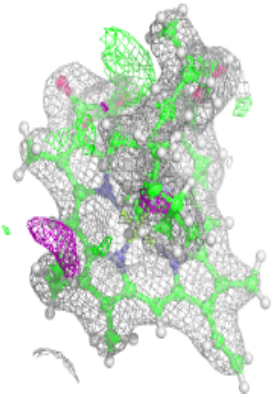


Electron density around CLA c 508:

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

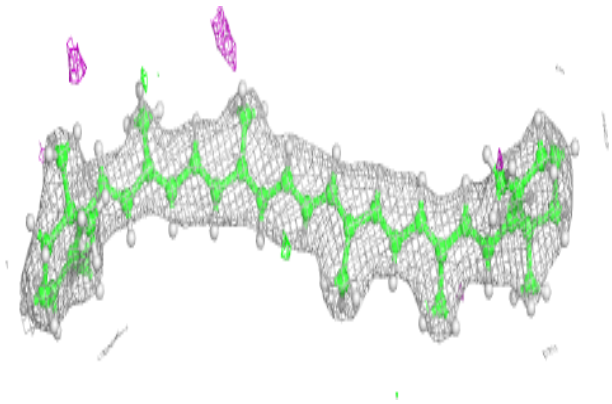


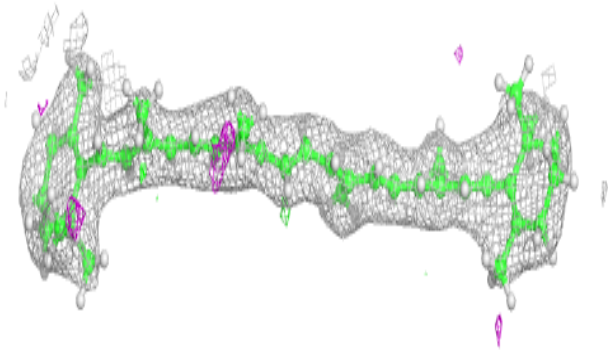


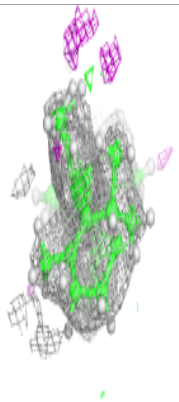


Electron density around 8CT C 515:

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

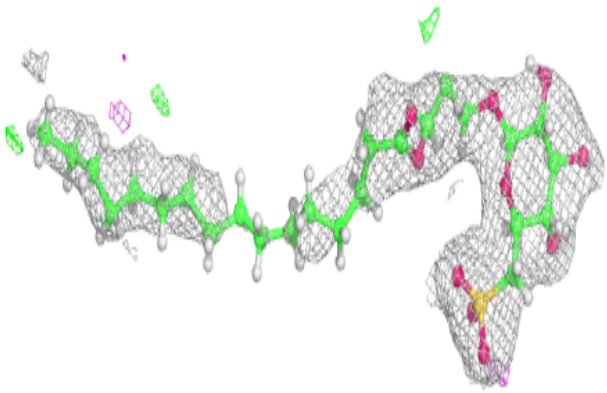


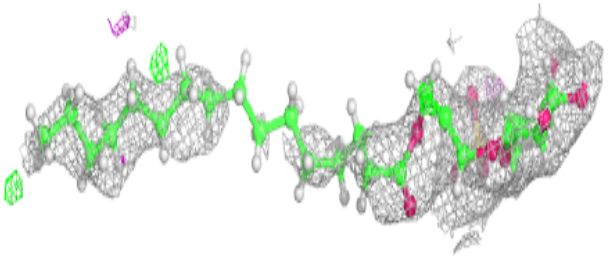


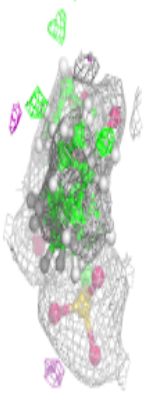


Electron density around SQD D 408:

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

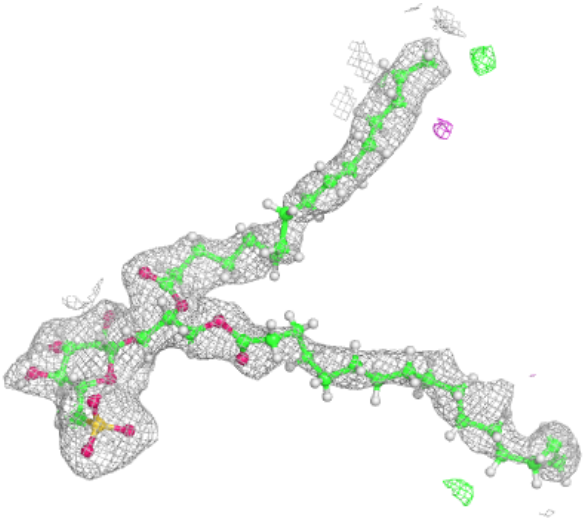


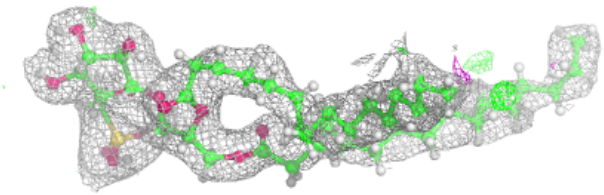




Electron density around SQD a 411:

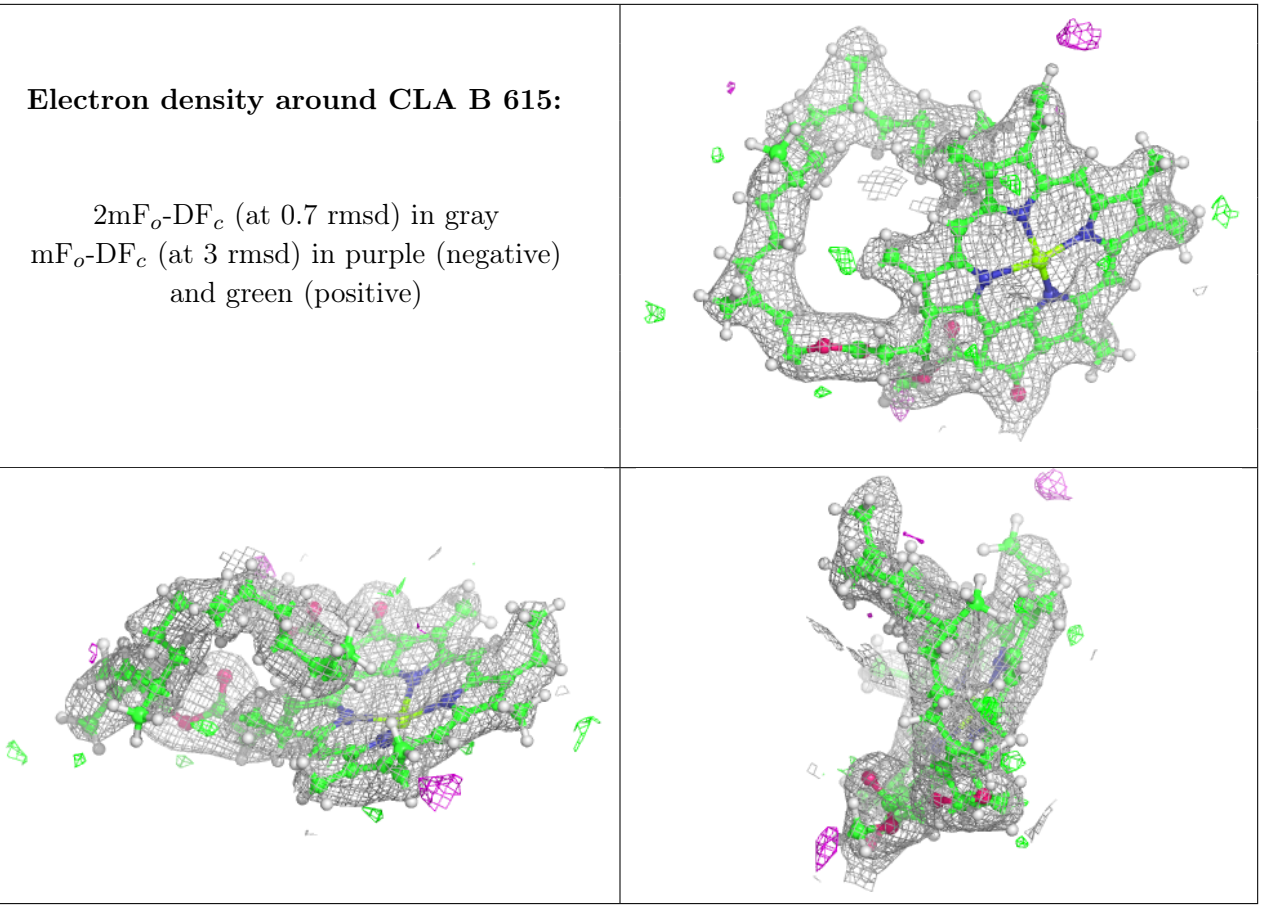
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





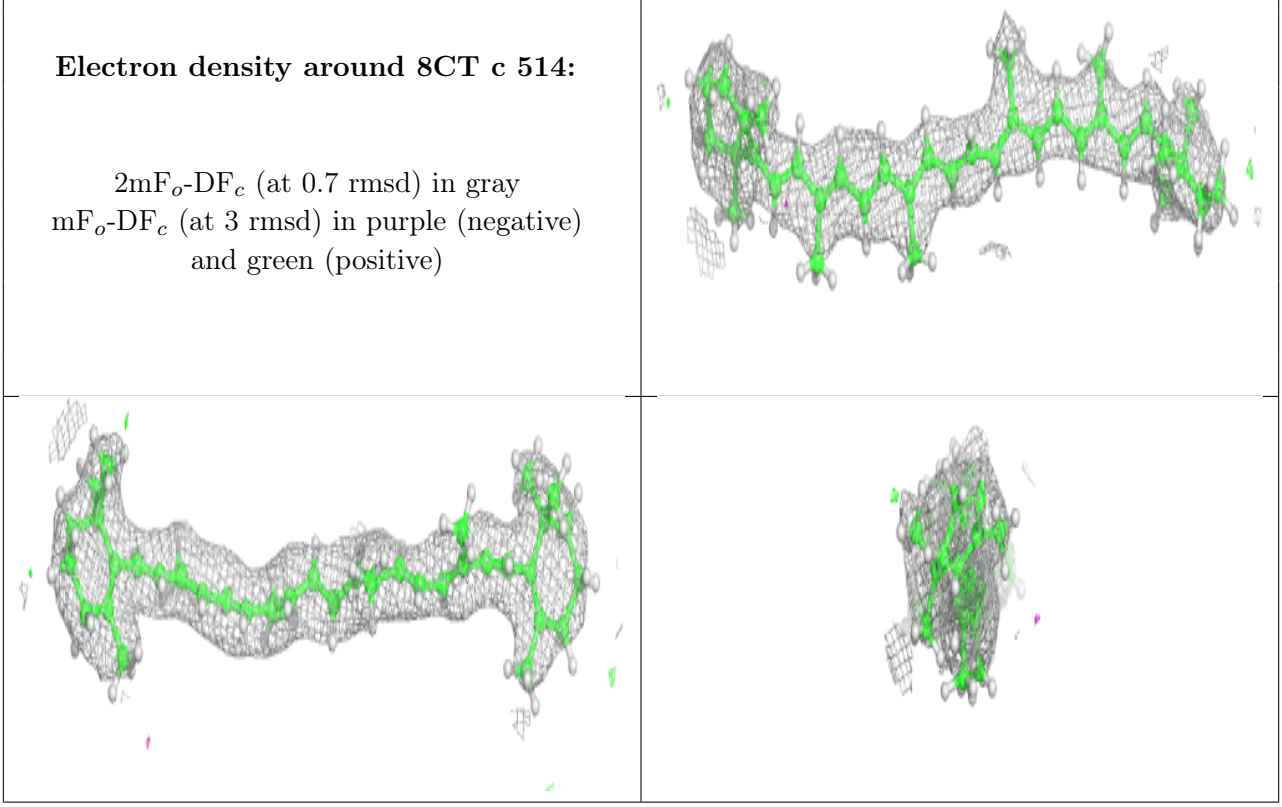
Electron density around CLA B 615:

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



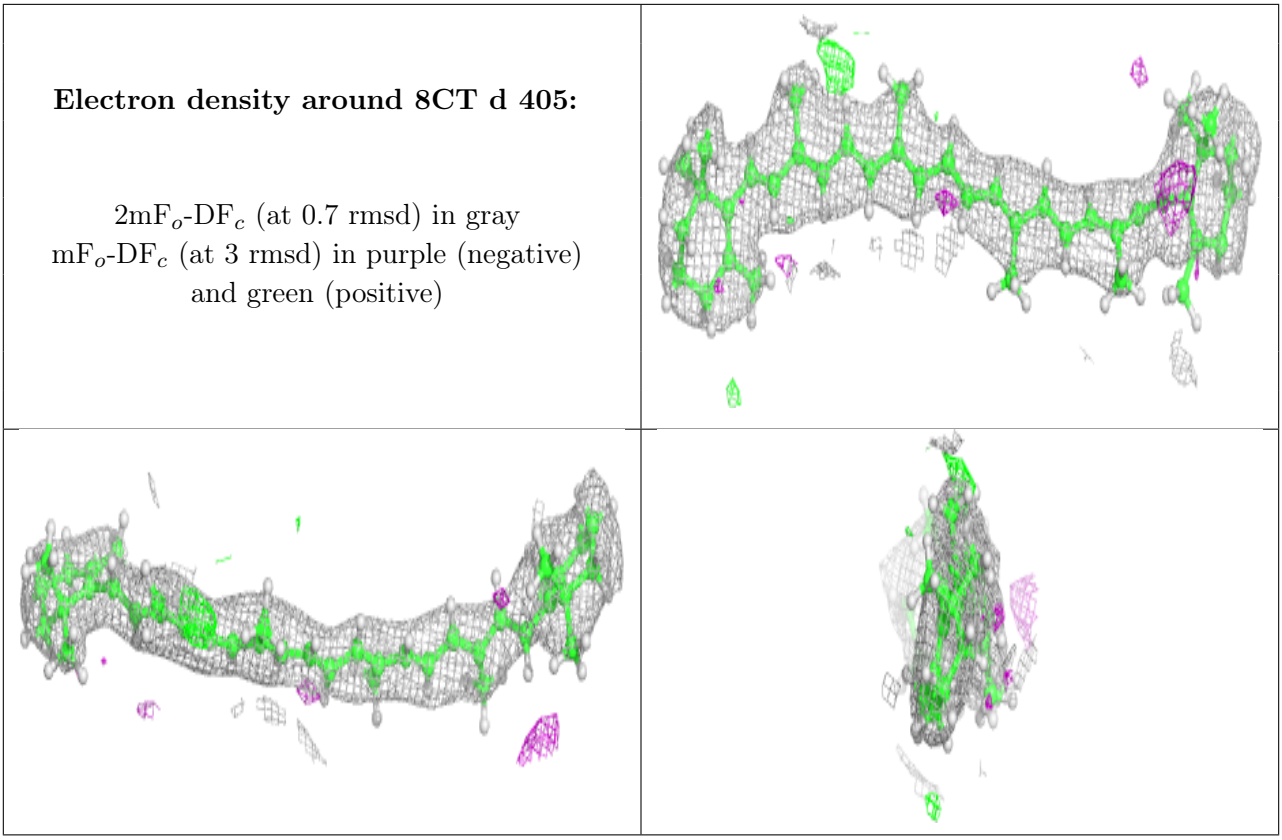
Electron density around 8CT c 514:

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



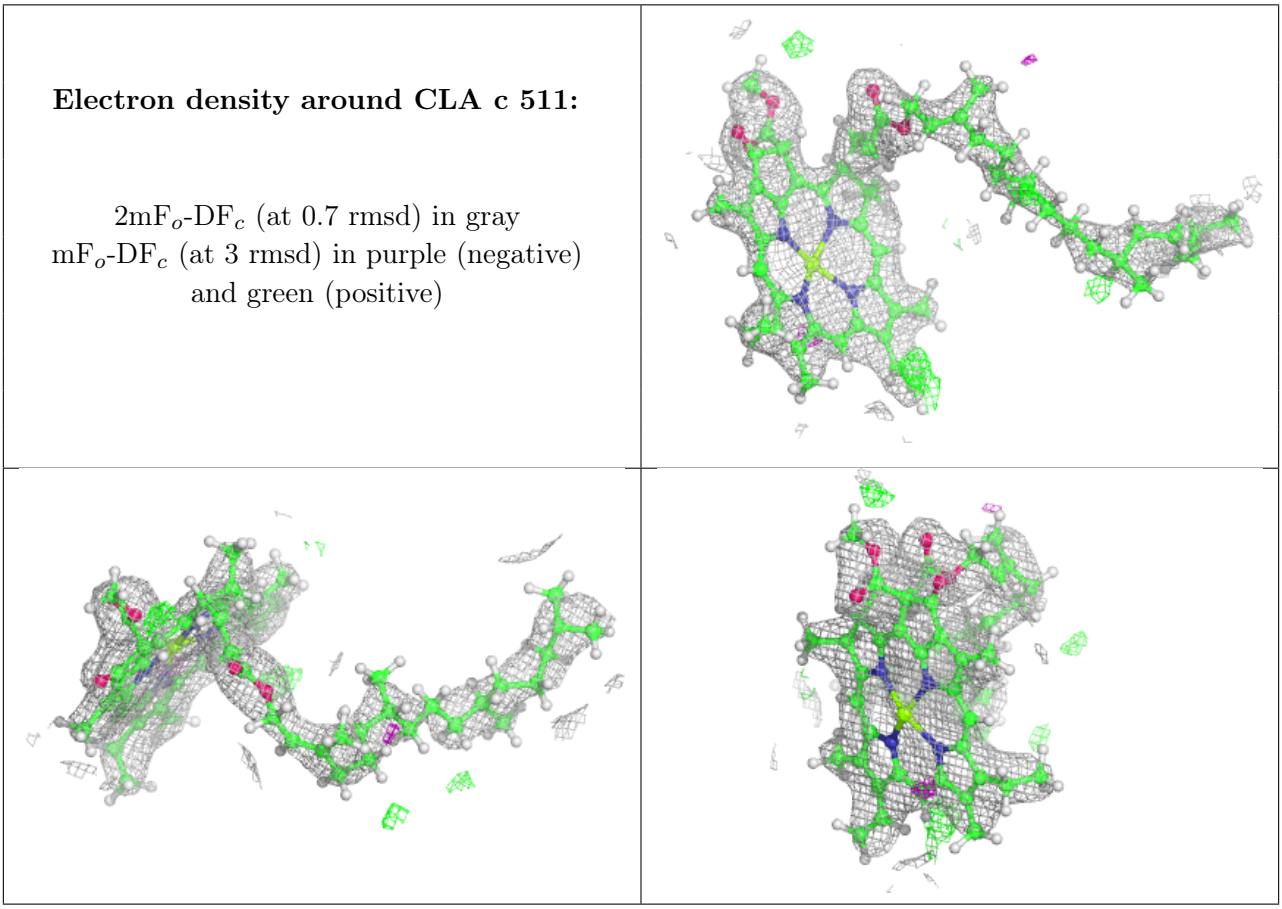
Electron density around 8CT d 405:

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



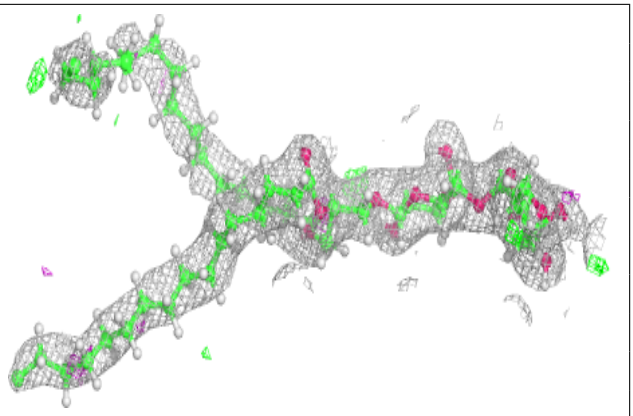
Electron density around CLA c 511:

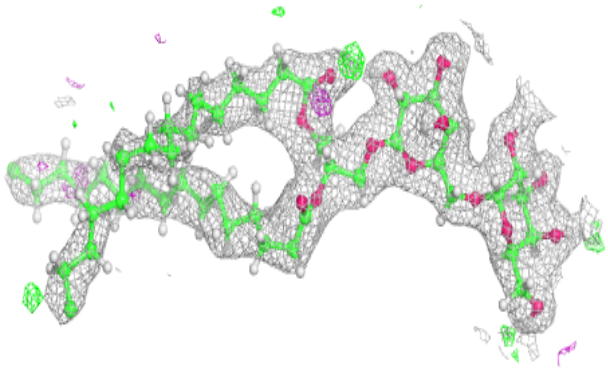
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

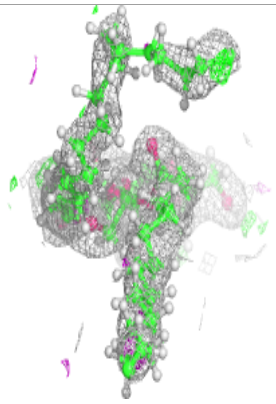


Electron density around DGD C 516:

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

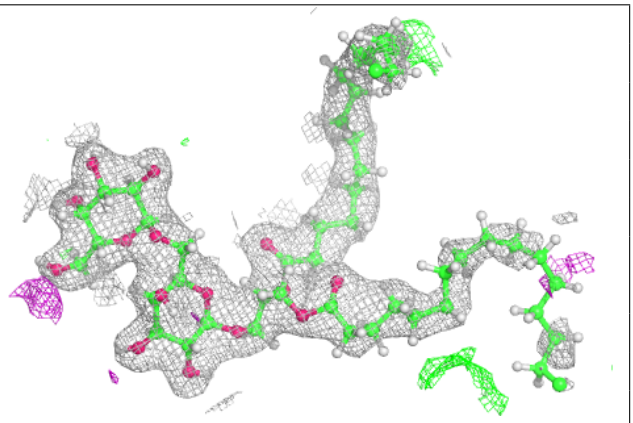


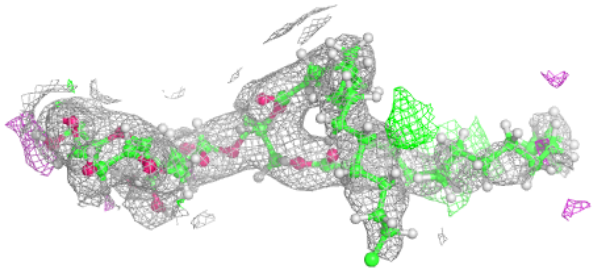


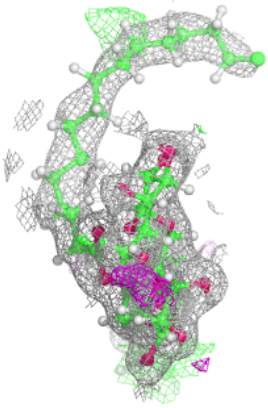


Electron density around DGD C 517:

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

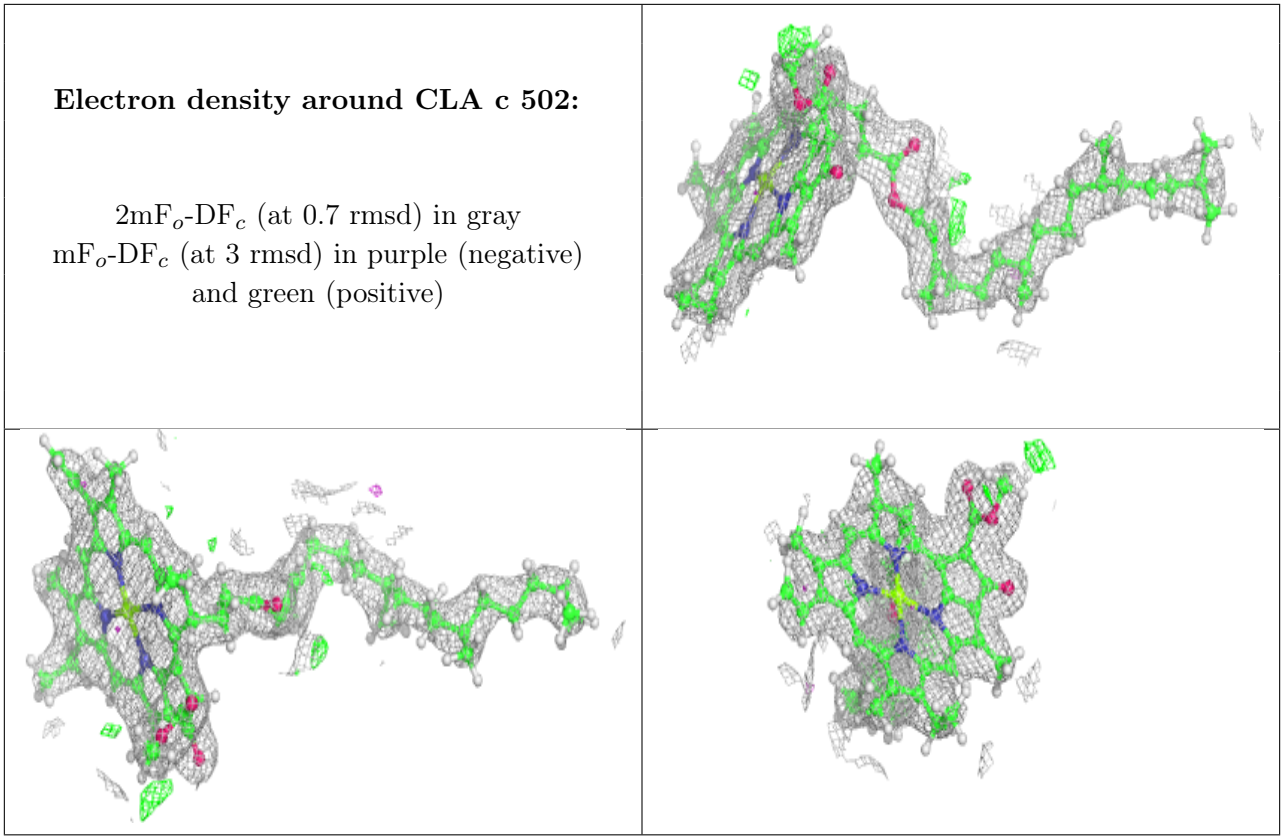






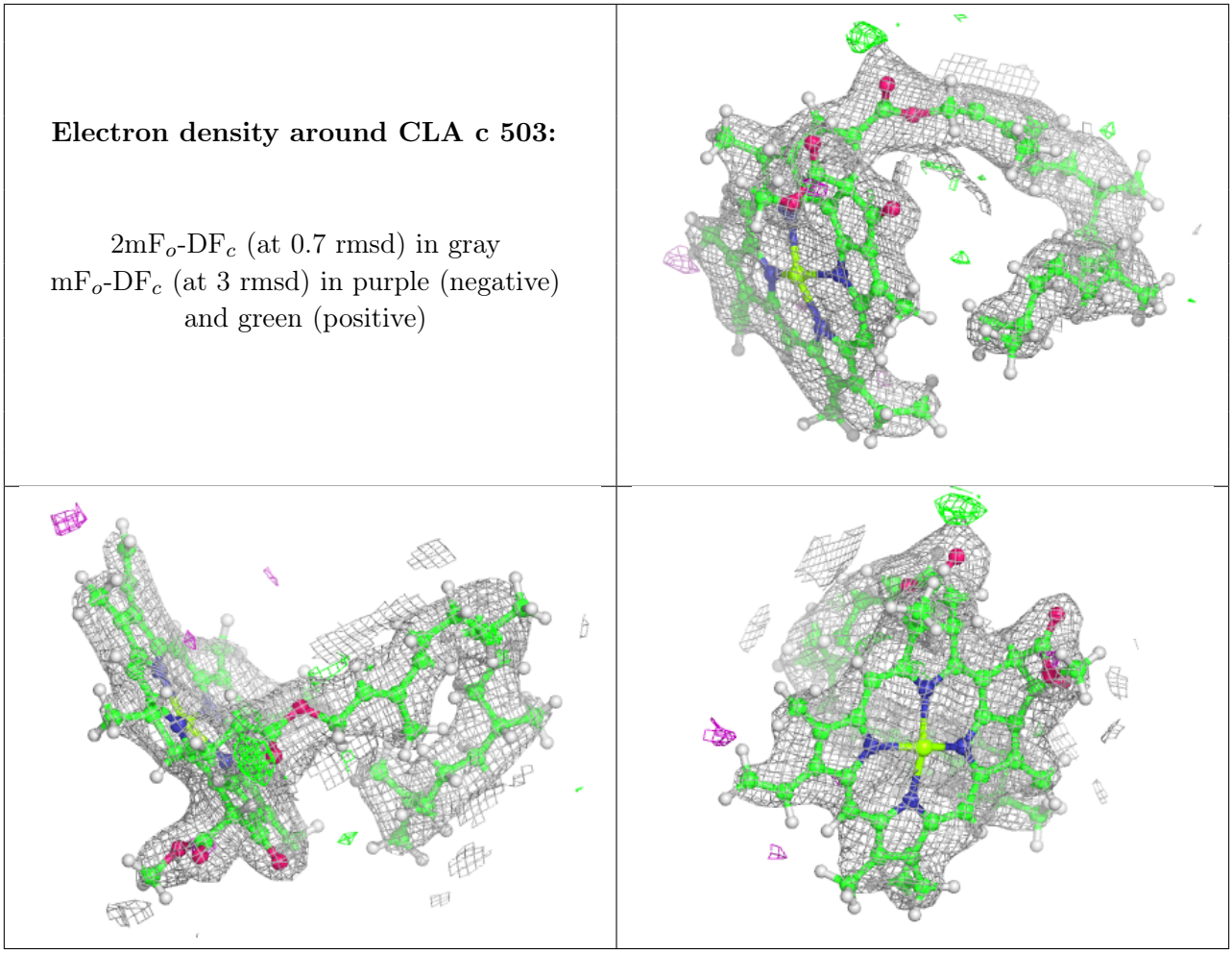
Electron density around CLA c 502:

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



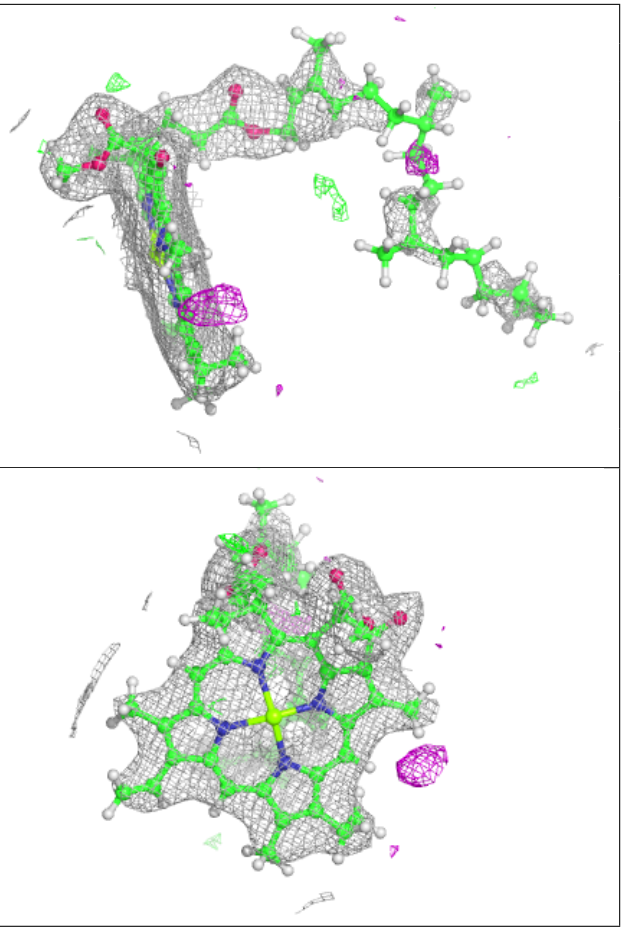
Electron density around CLA c 503:

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



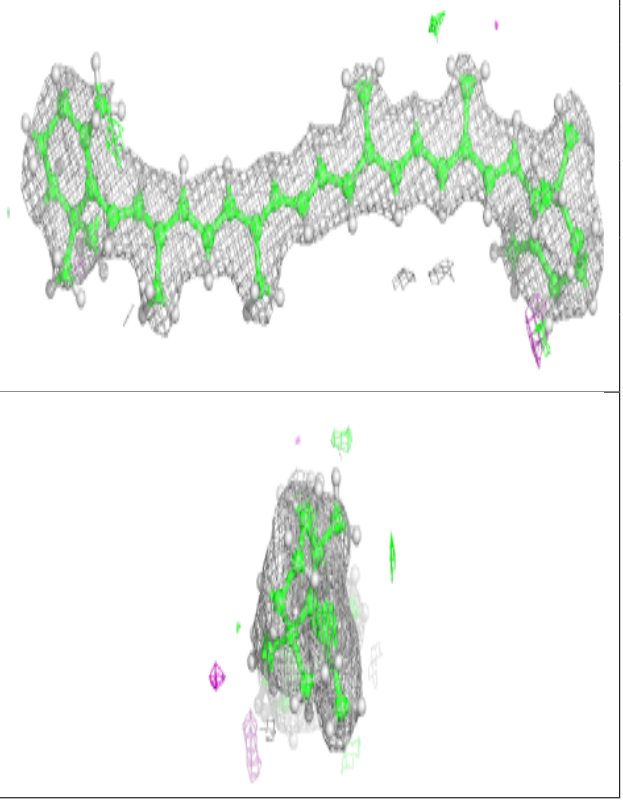
Electron density around CLA c 506:

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



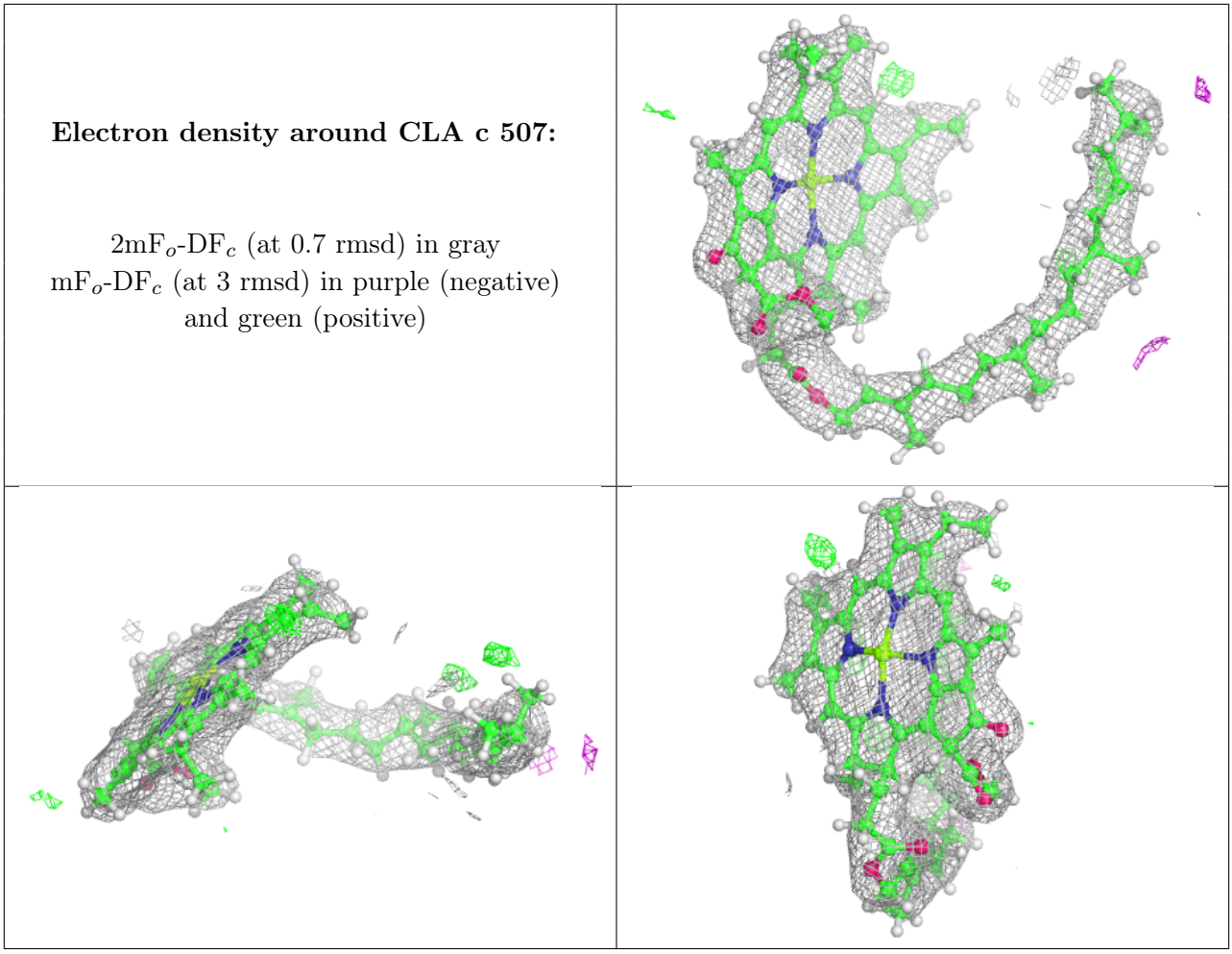
Electron density around 8CT B 619:

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



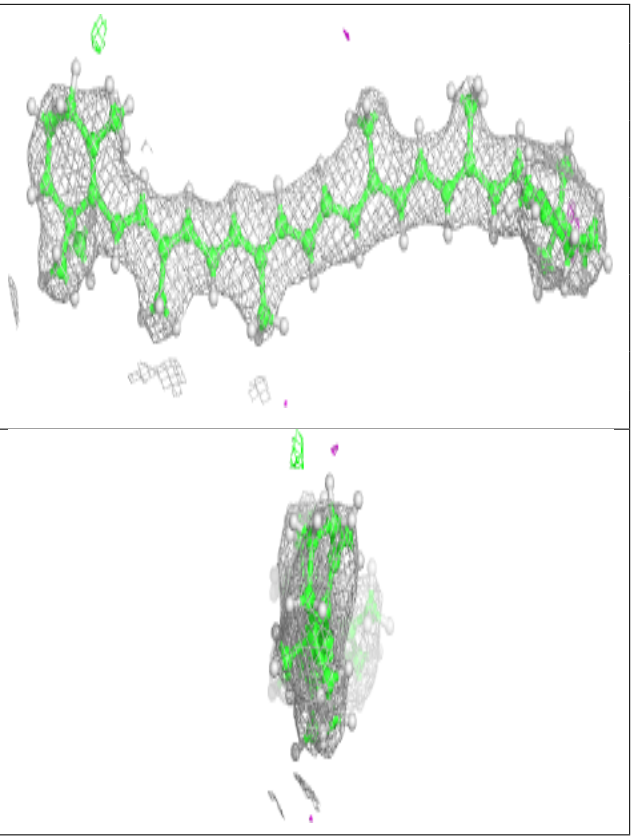
Electron density around CLA c 507:

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



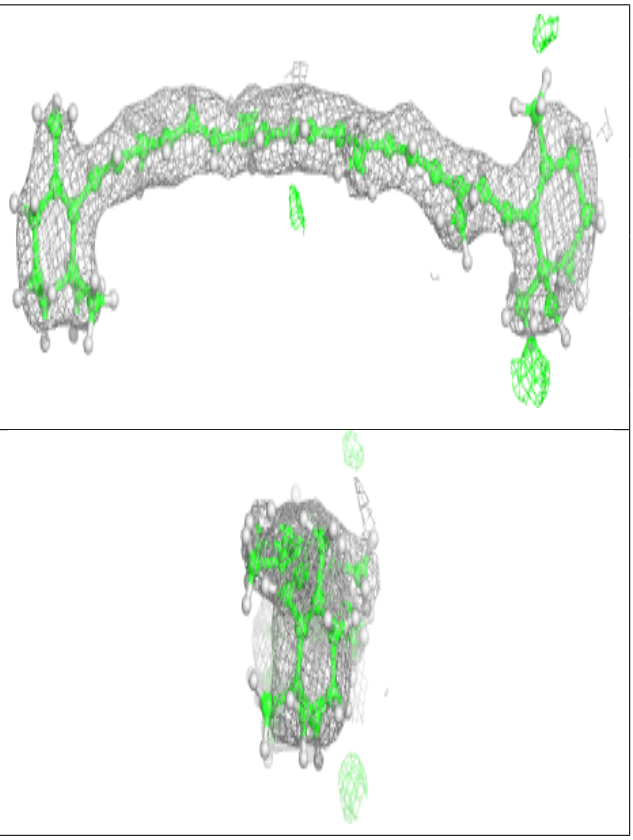
Electron density around BCR b 618:

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



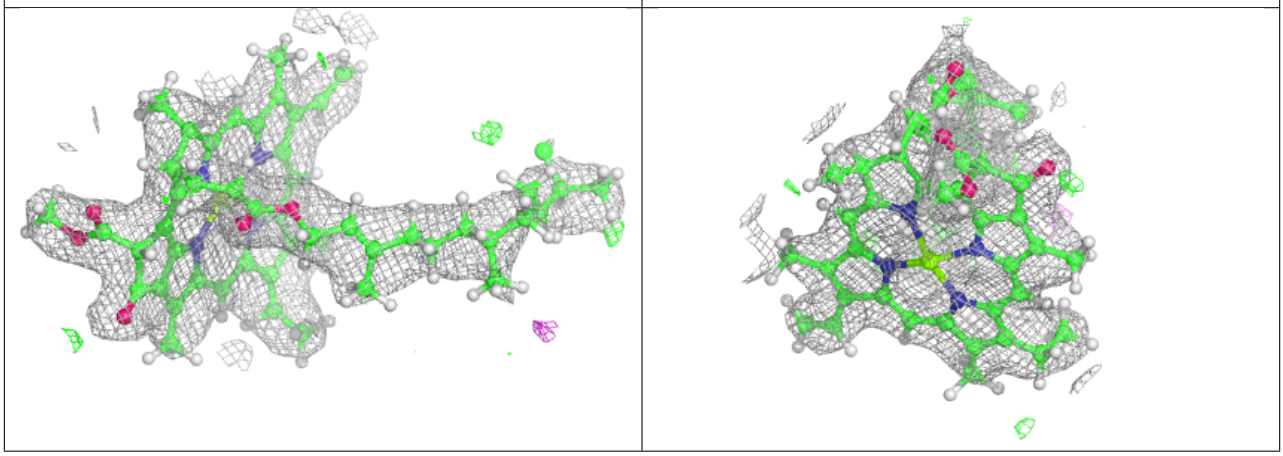
Electron density around BCR c 521:

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



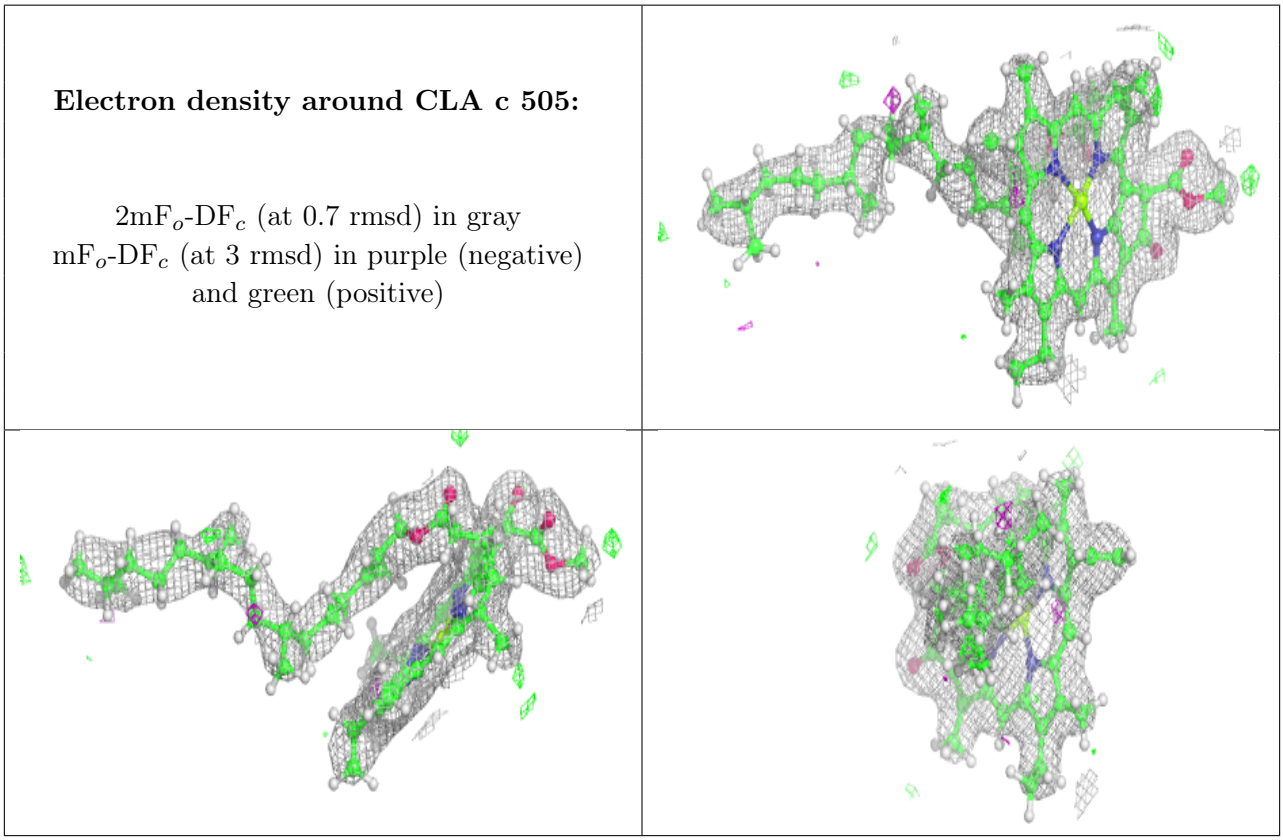
Electron density around CLA c 504:

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



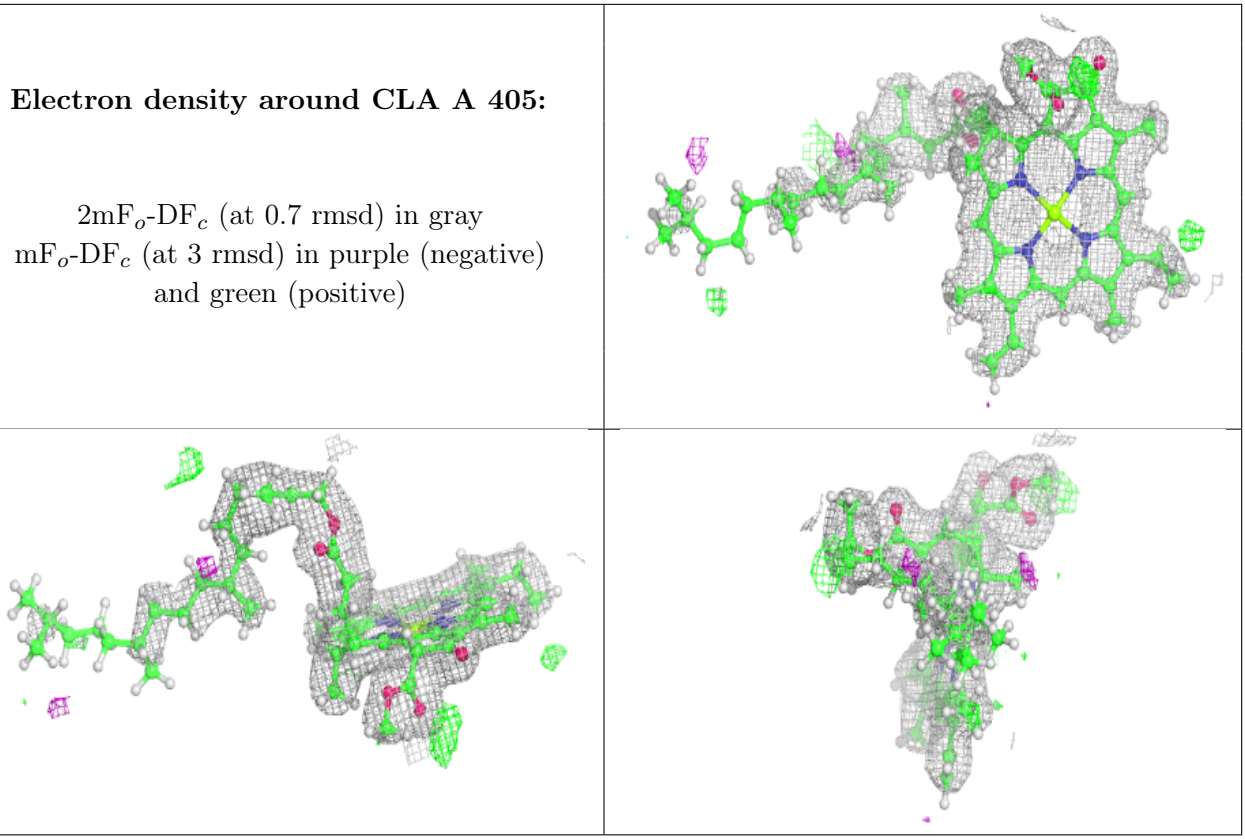
Electron density around CLA c 505:

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



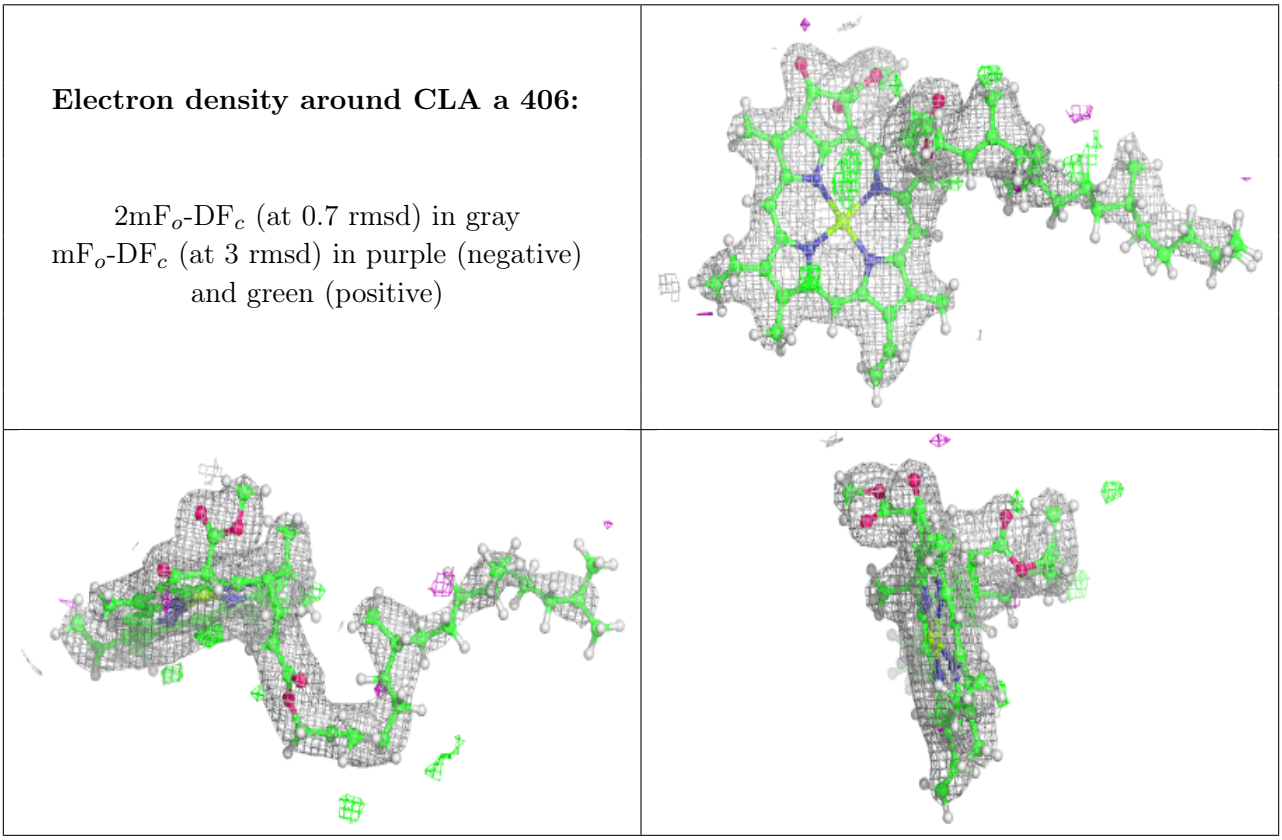
Electron density around CLA A 405:

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



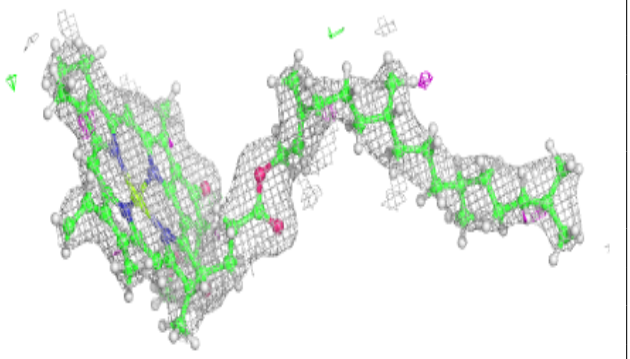
Electron density around CLA a 406:

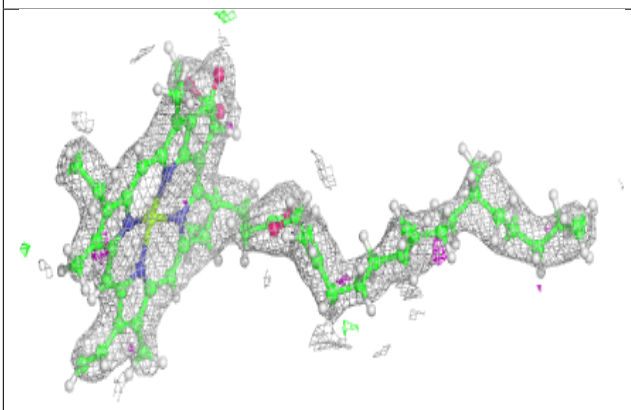
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

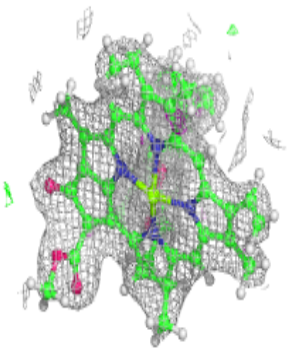


Electron density around CLA C 502:

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

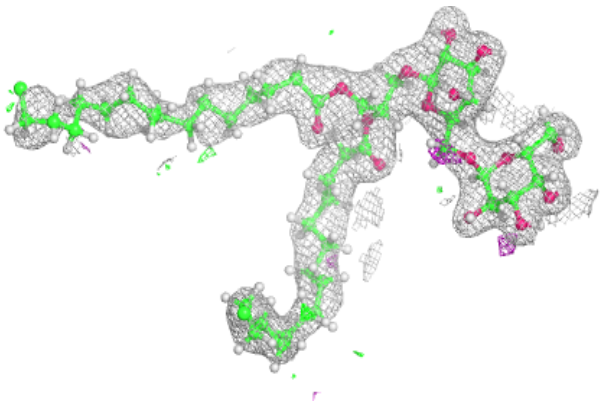


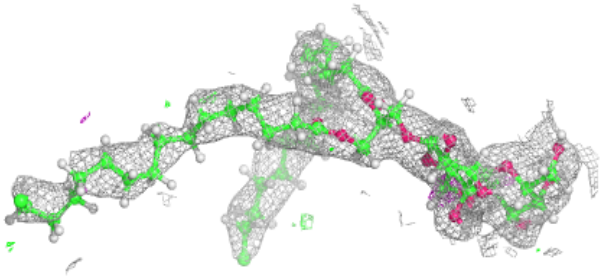


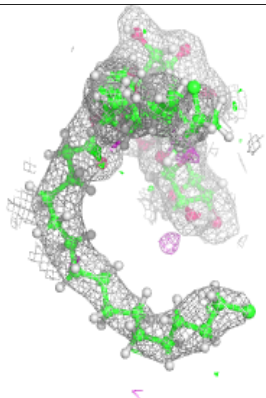


Electron density around DGD c 517:

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

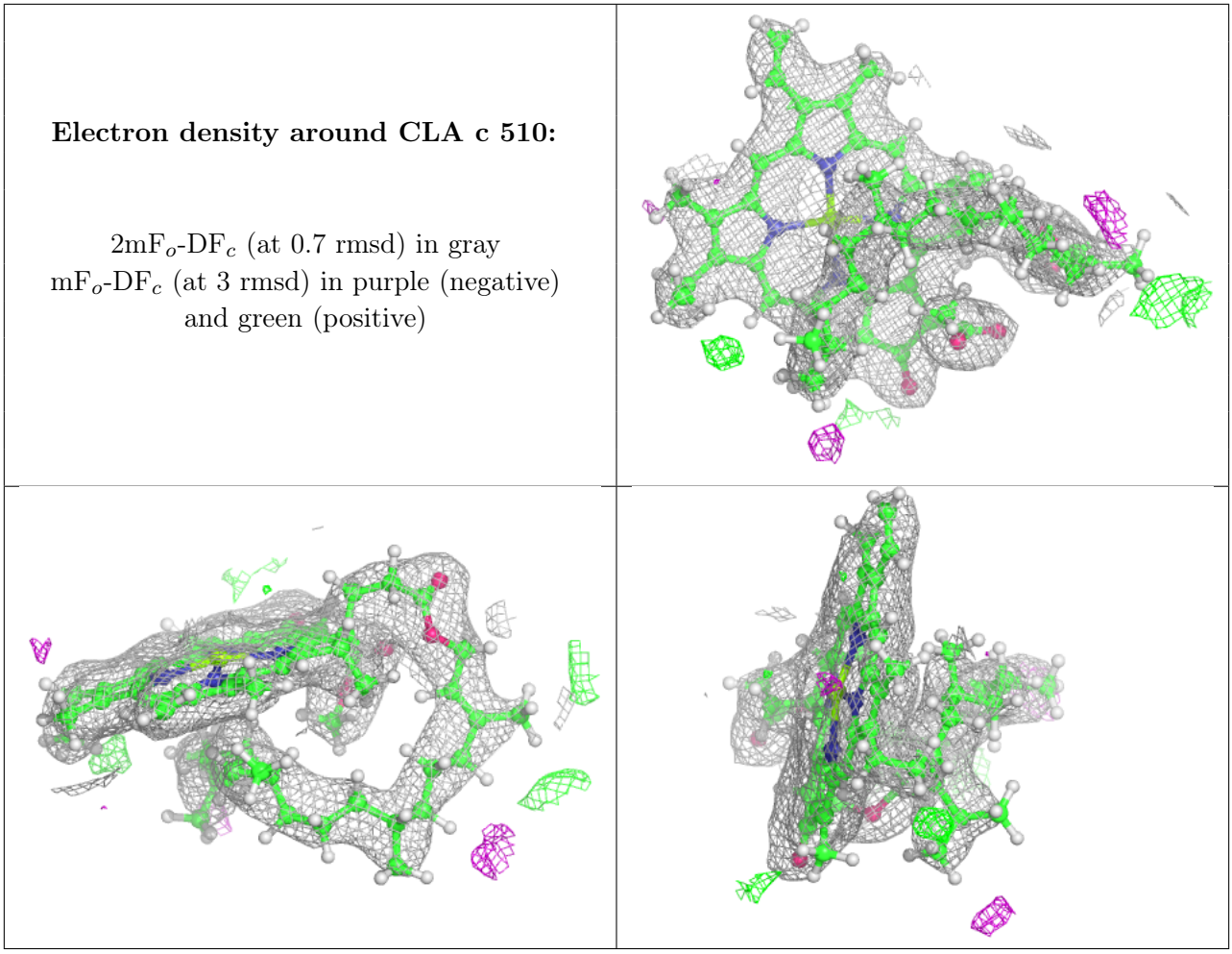






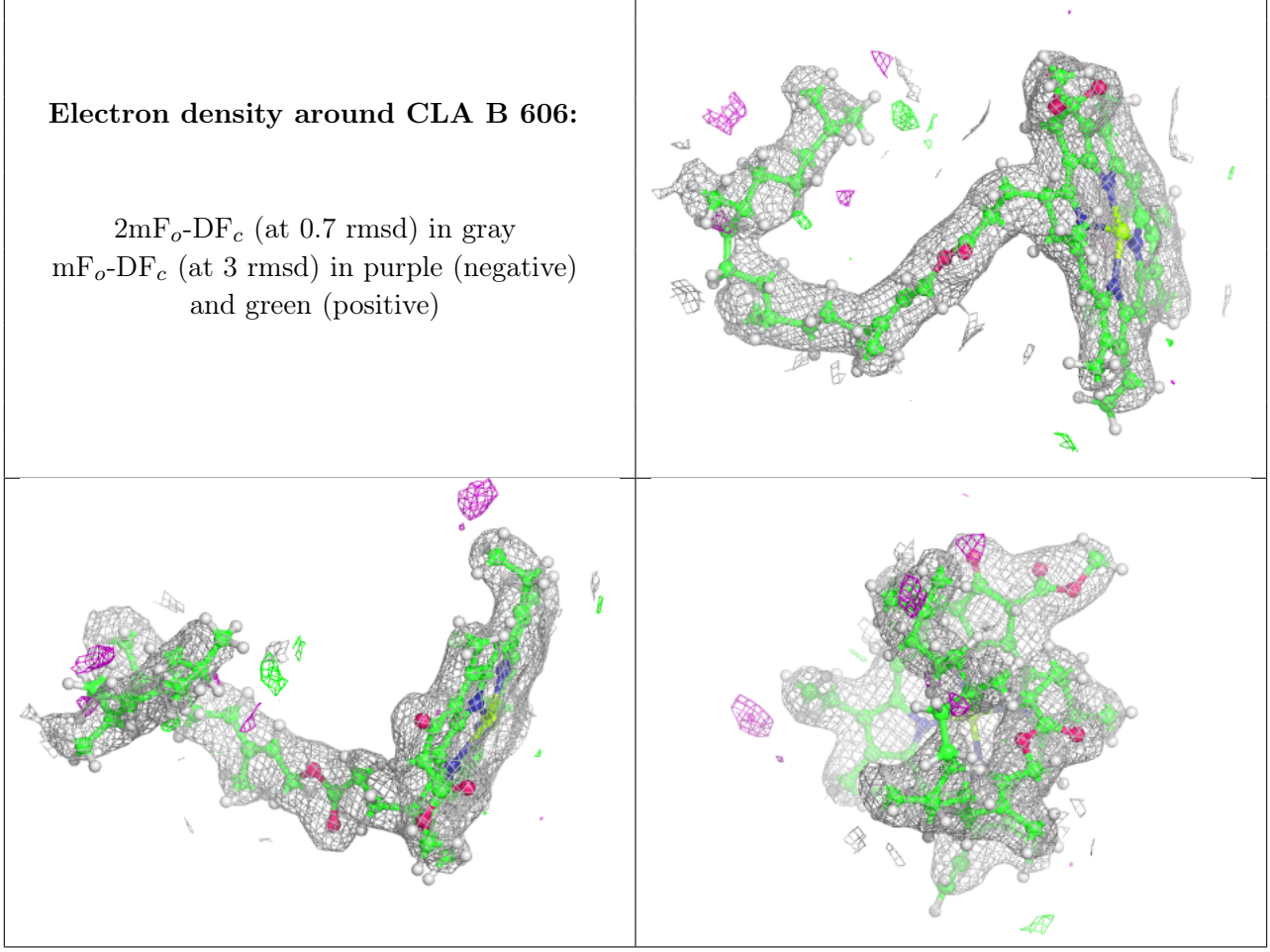
Electron density around CLA c 510:

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



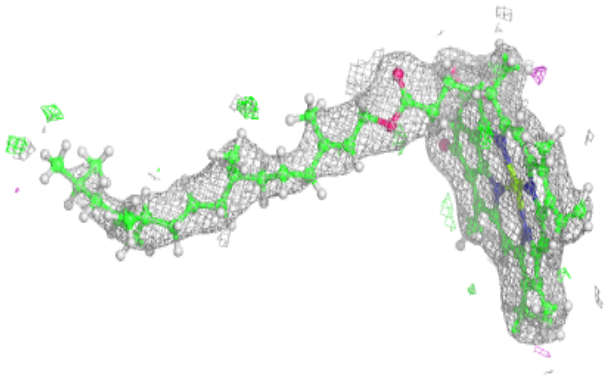
Electron density around CLA B 606:

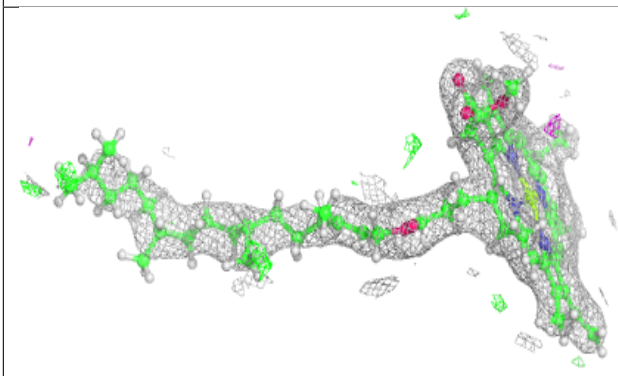
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

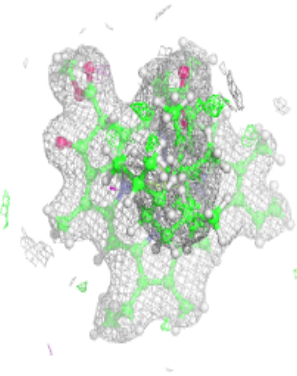


Electron density around CLA b 605:

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

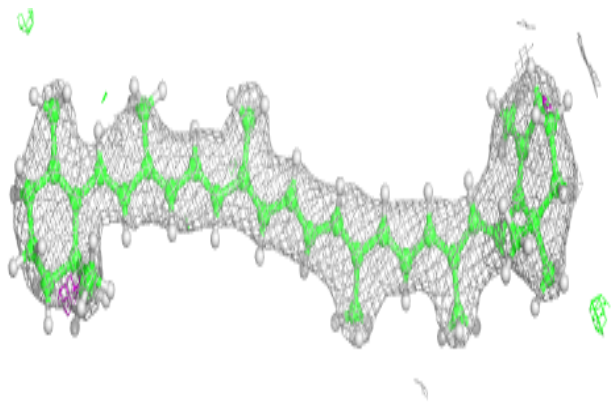


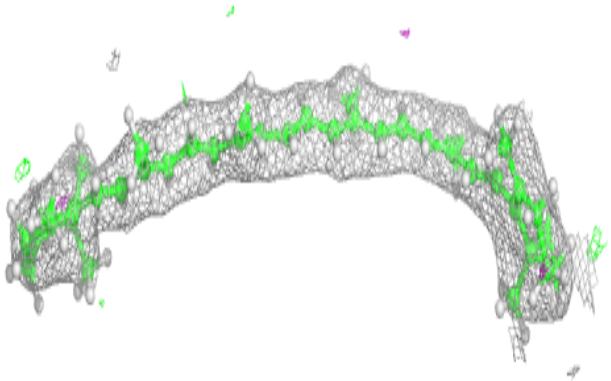


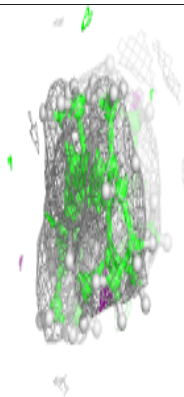


Electron density around BCR T 101:

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

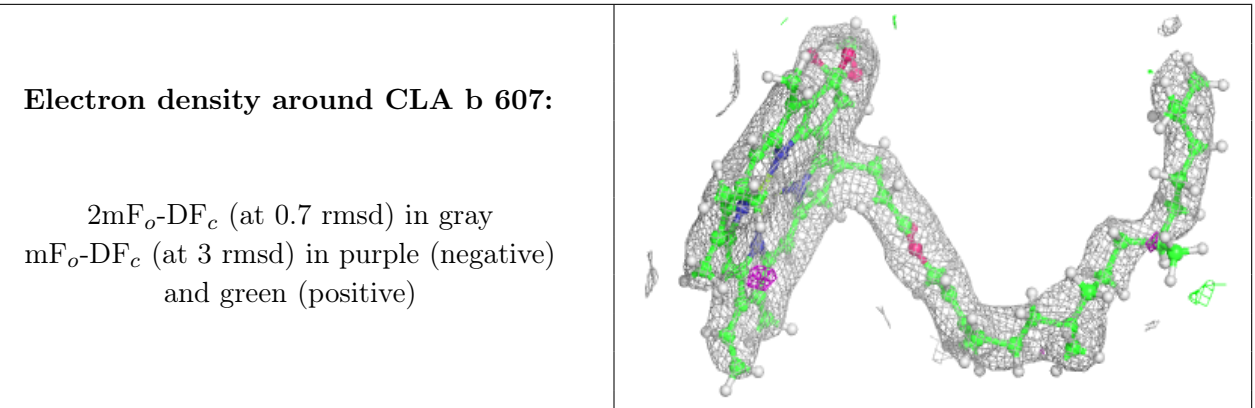






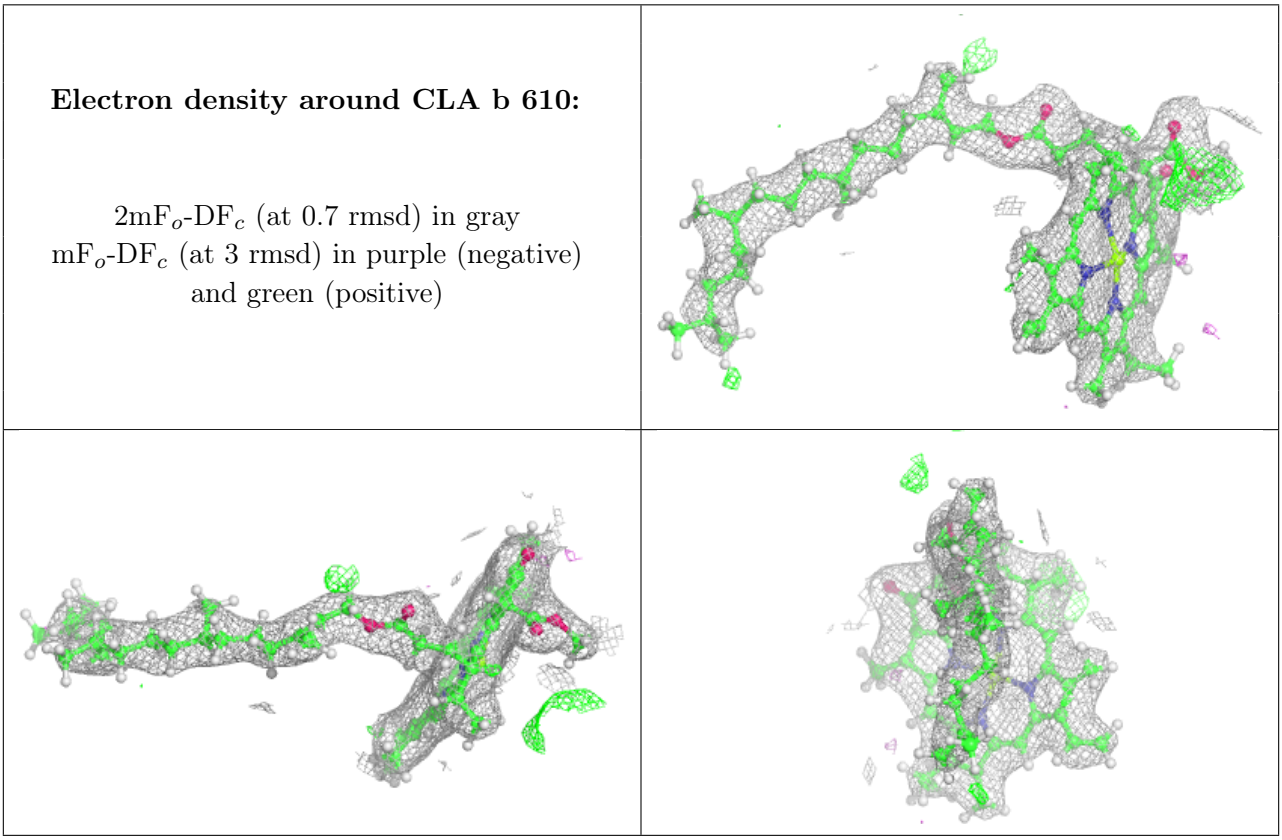
Electron density around CLA b 607:

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



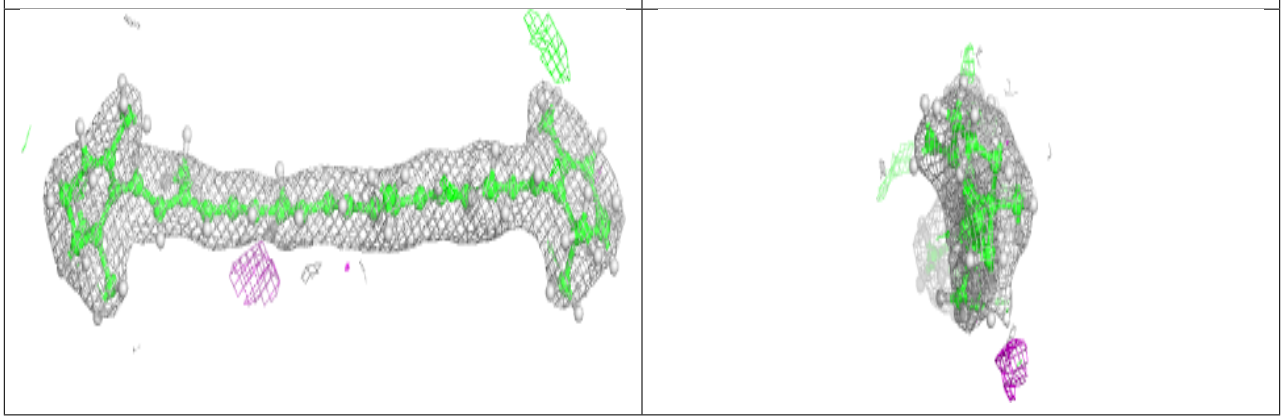
Electron density around CLA b 610:

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



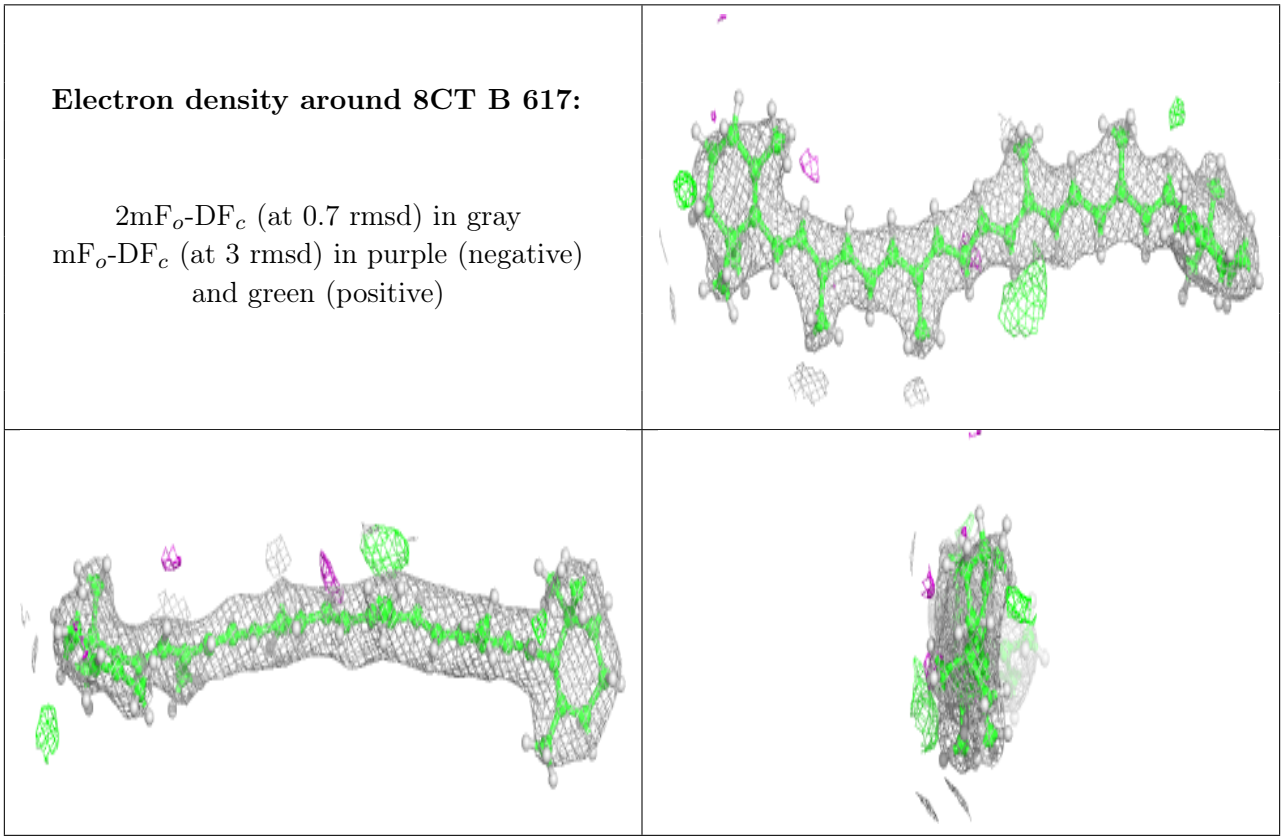
Electron density around BCR b 619:

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



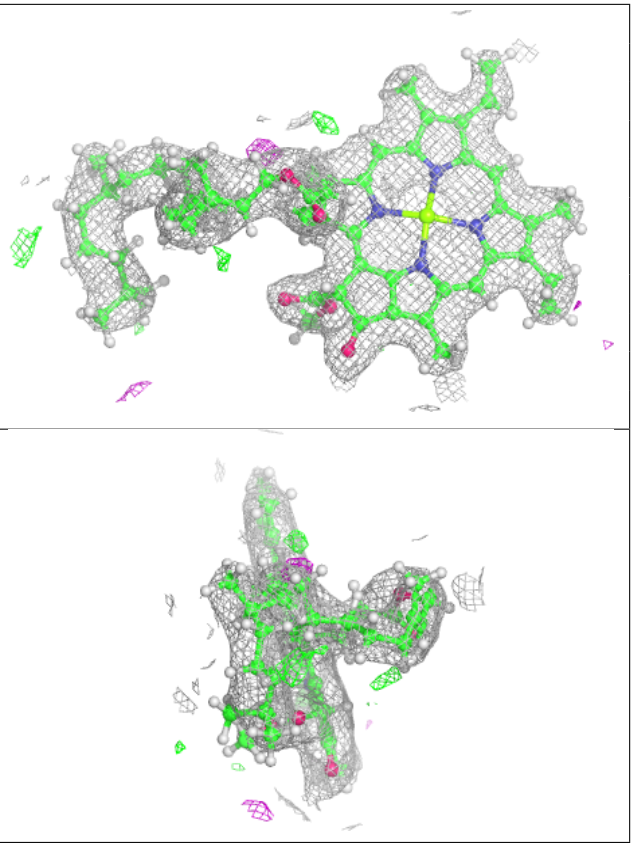
Electron density around 8CT B 617:

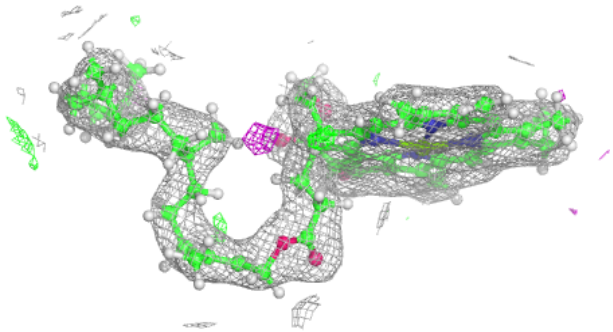
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 613:

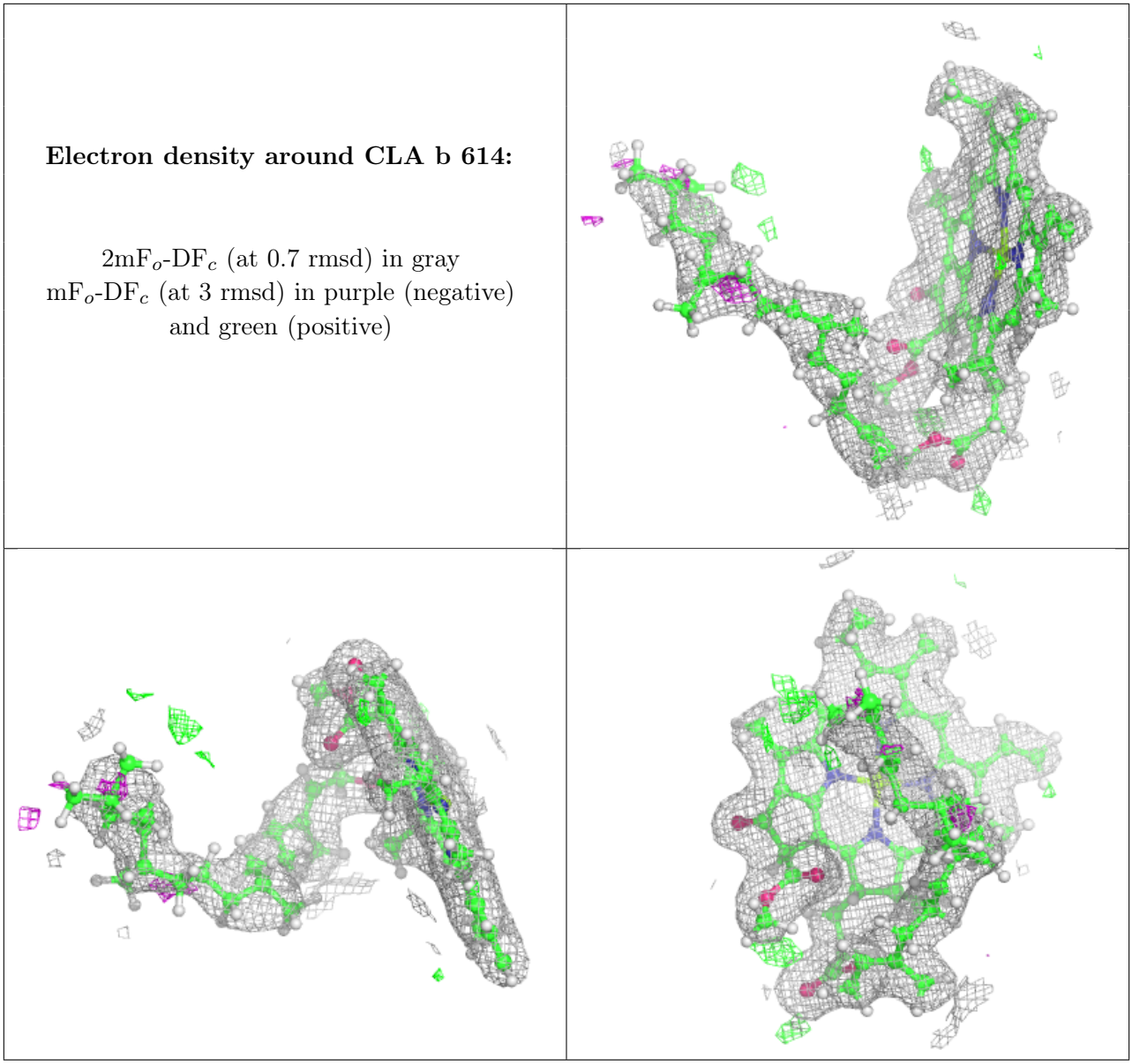
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





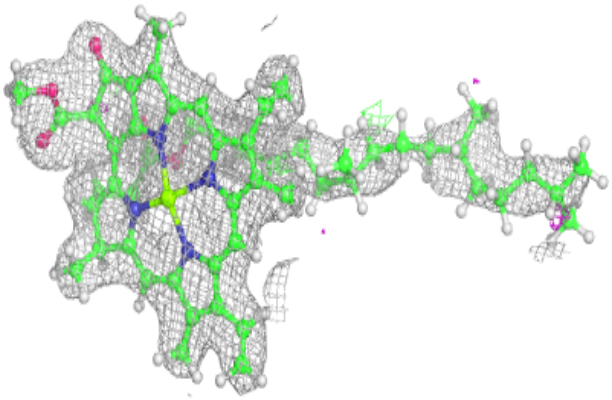
Electron density around CLA b 614:

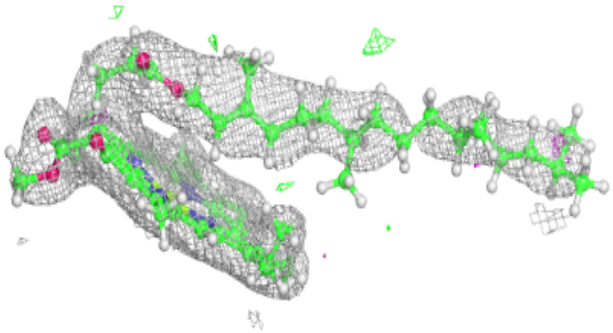
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

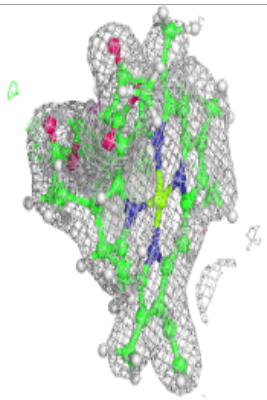


Electron density around CLA b 615:

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

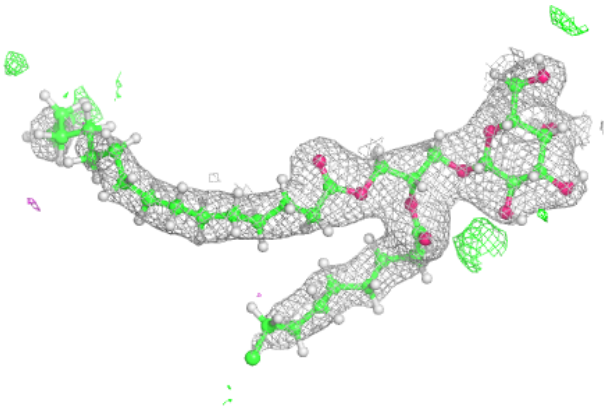


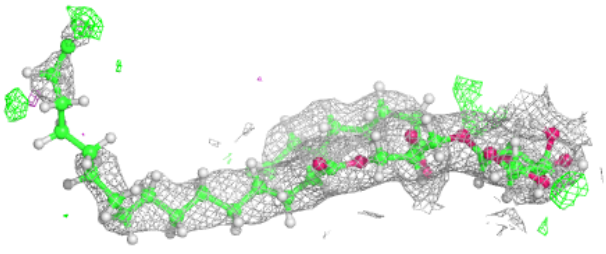


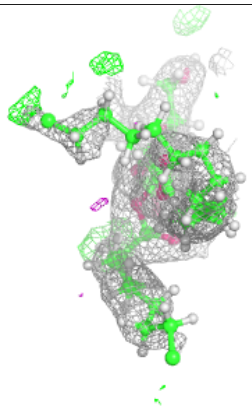


Electron density around LMG d 410:

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

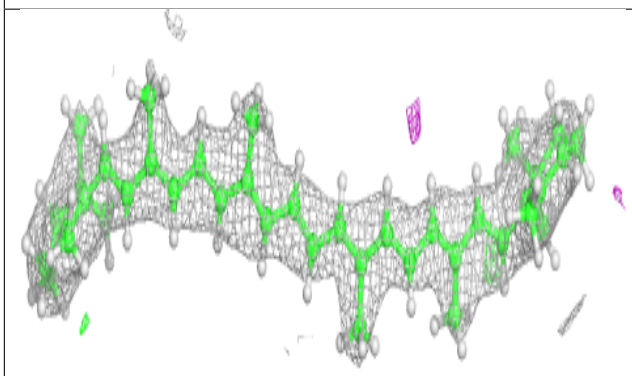


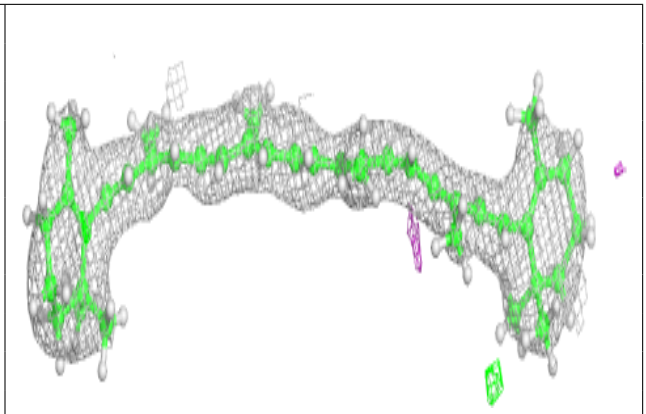


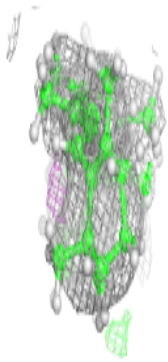


Electron density around 8CT C 520:

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

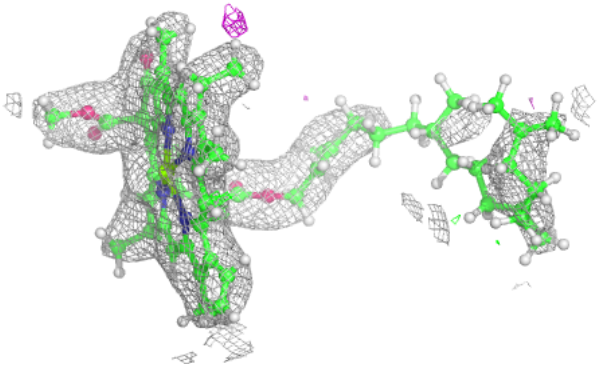


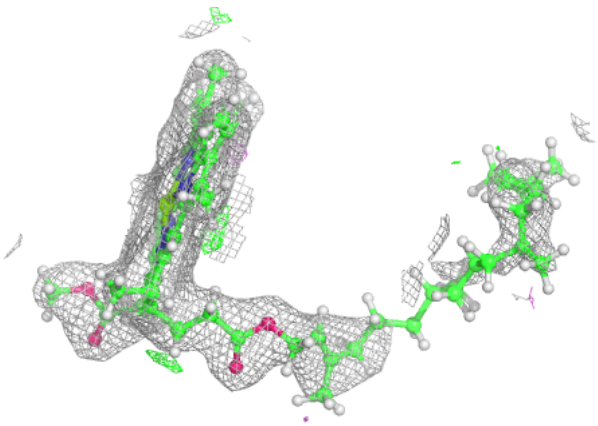


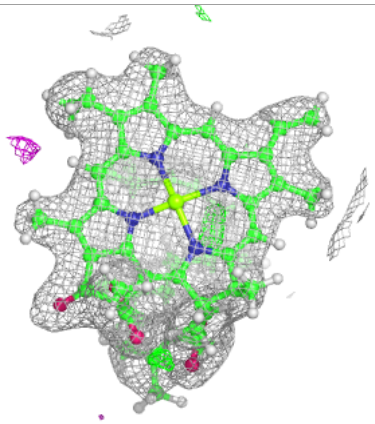


Electron density around CLA C 506:

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

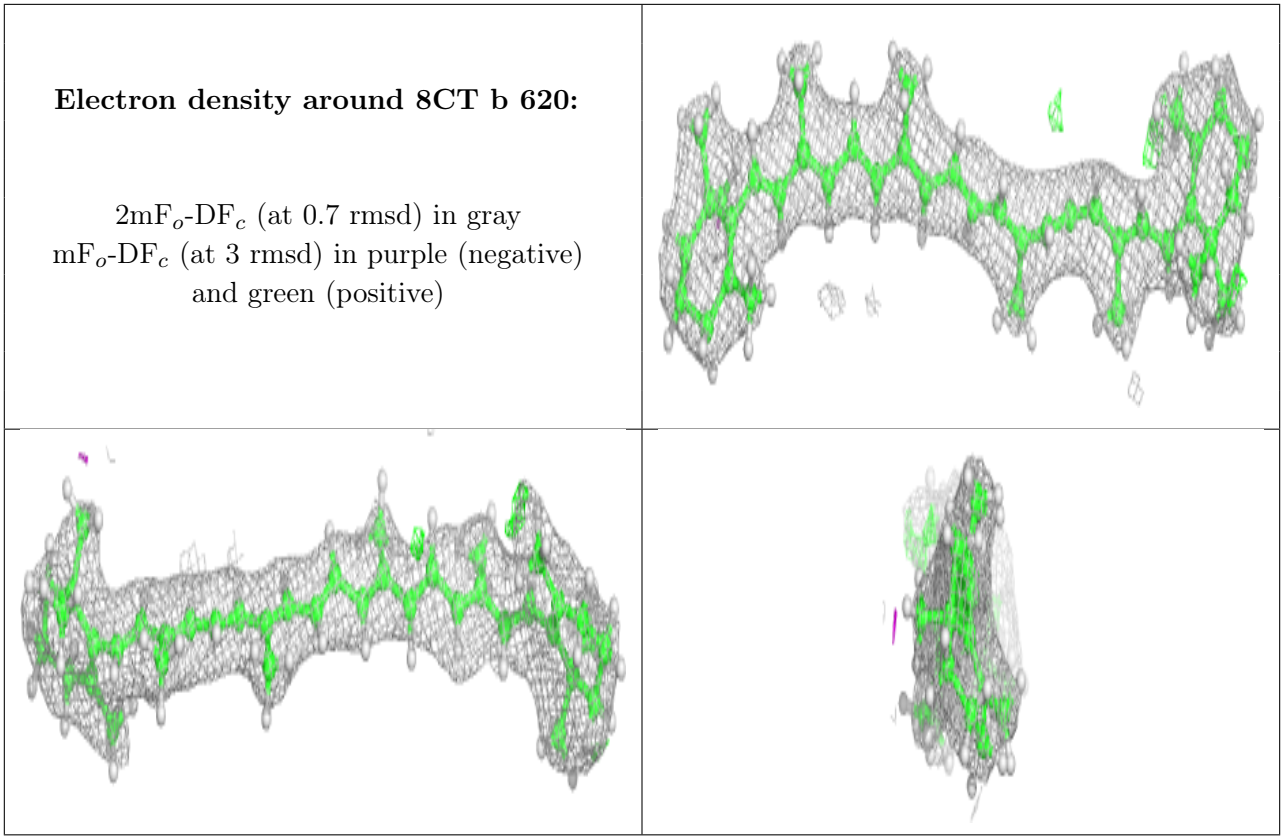






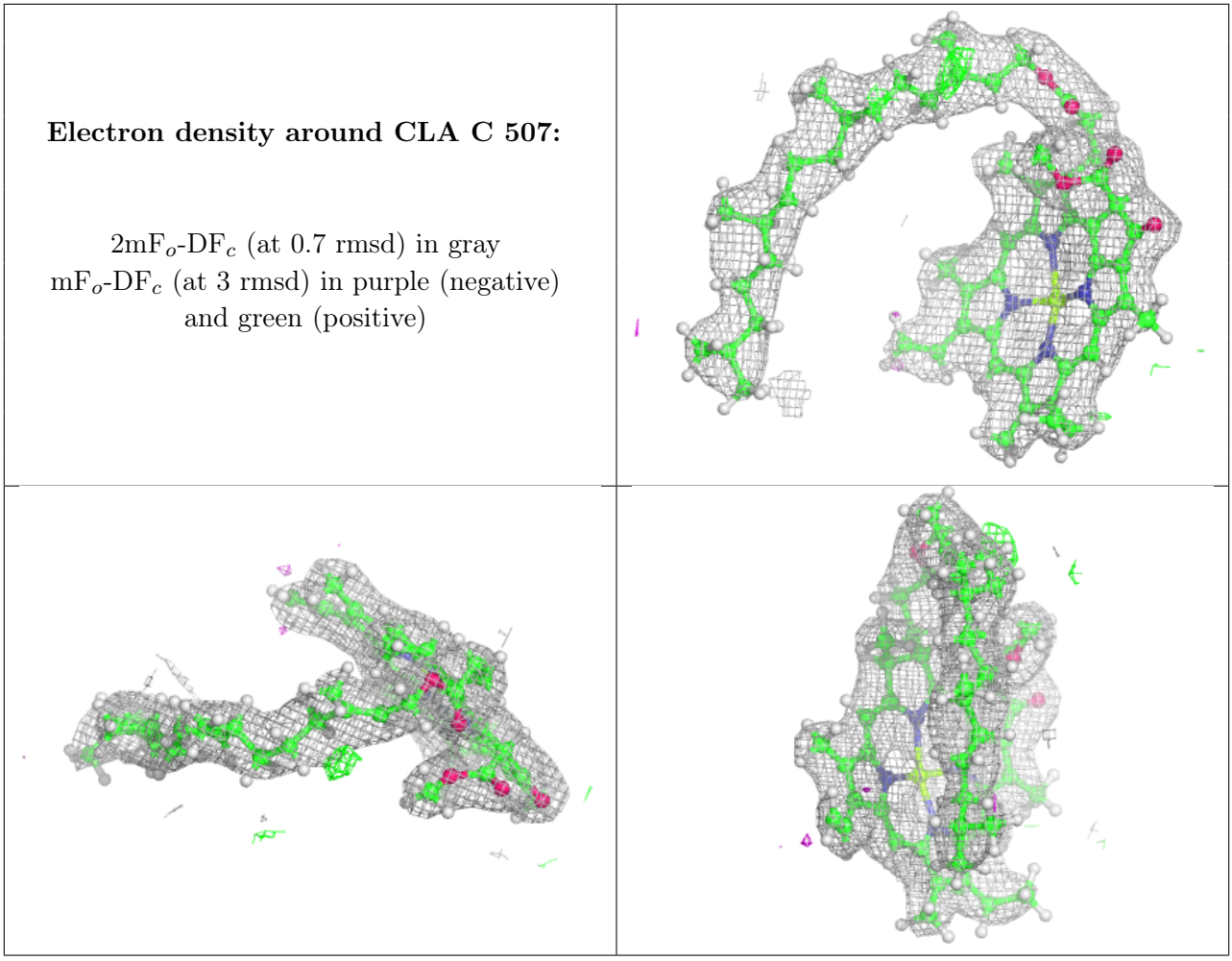
Electron density around 8CT b 620:

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



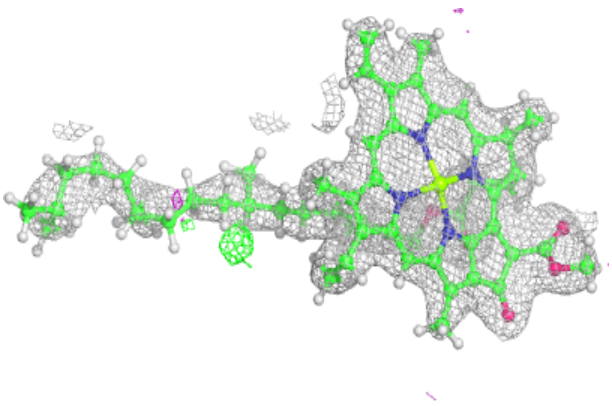
Electron density around CLA C 507:

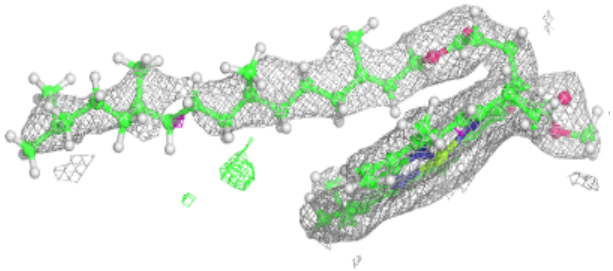
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

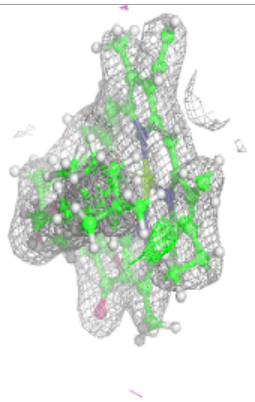


Electron density around CLA B 614:

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

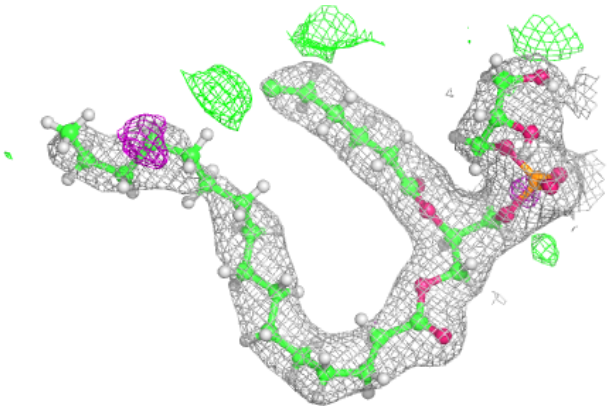


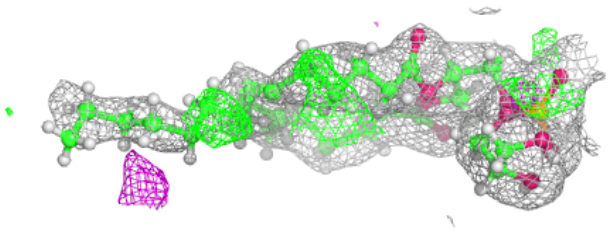


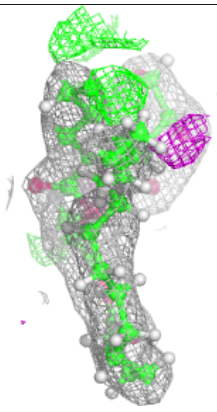


Electron density around LHG d 409:

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

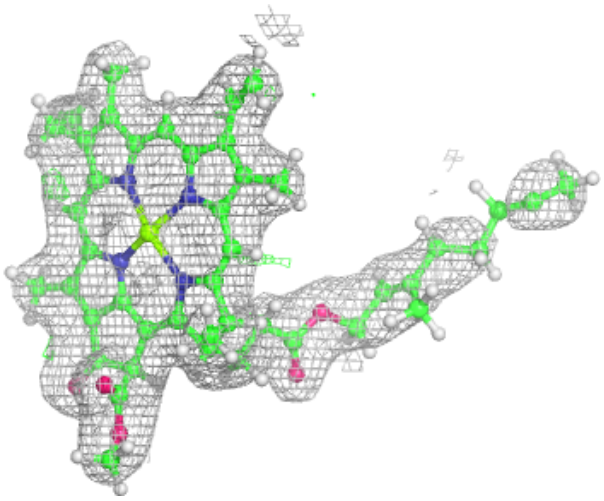


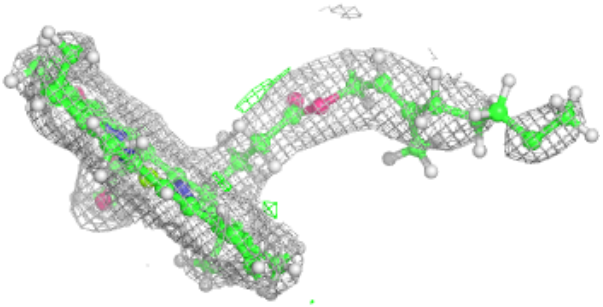


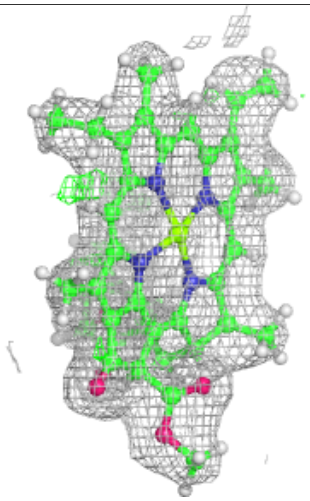


Electron density around CLA A 407:

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

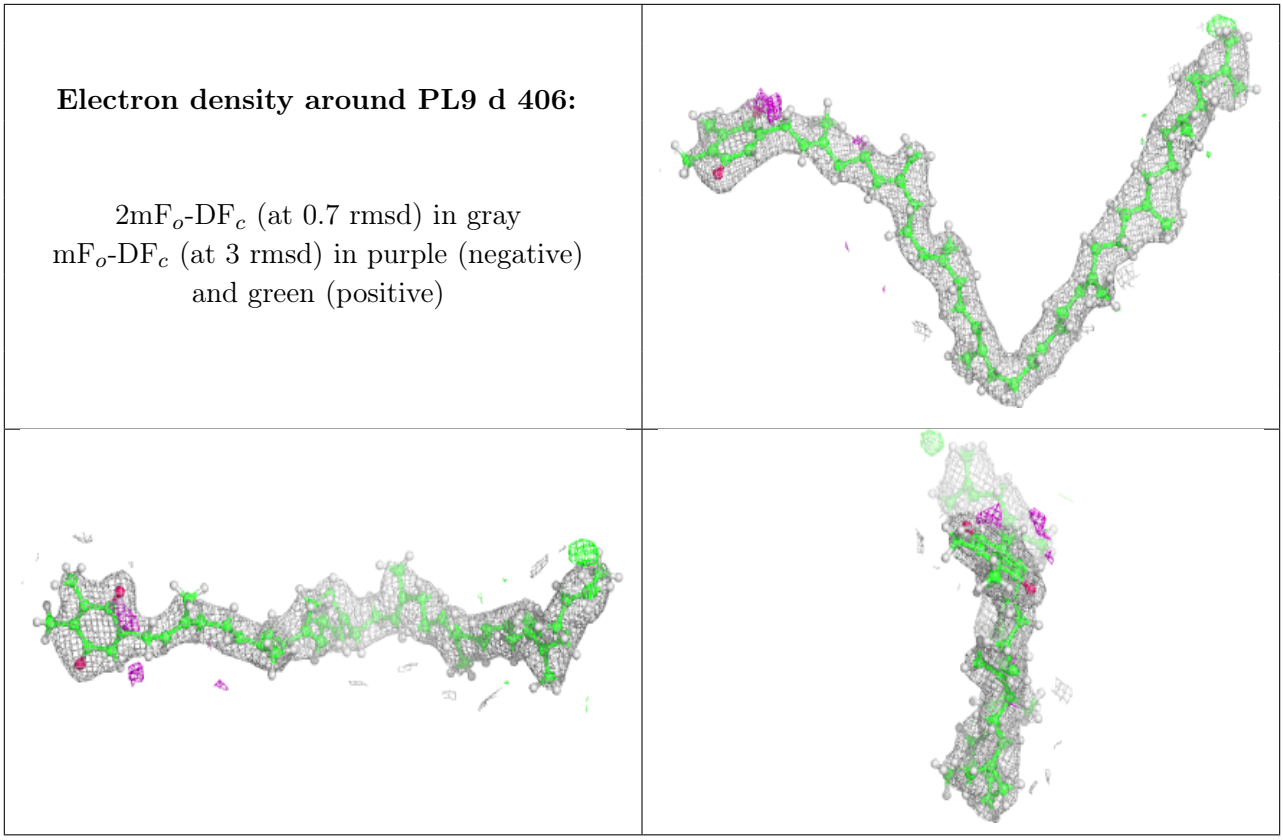






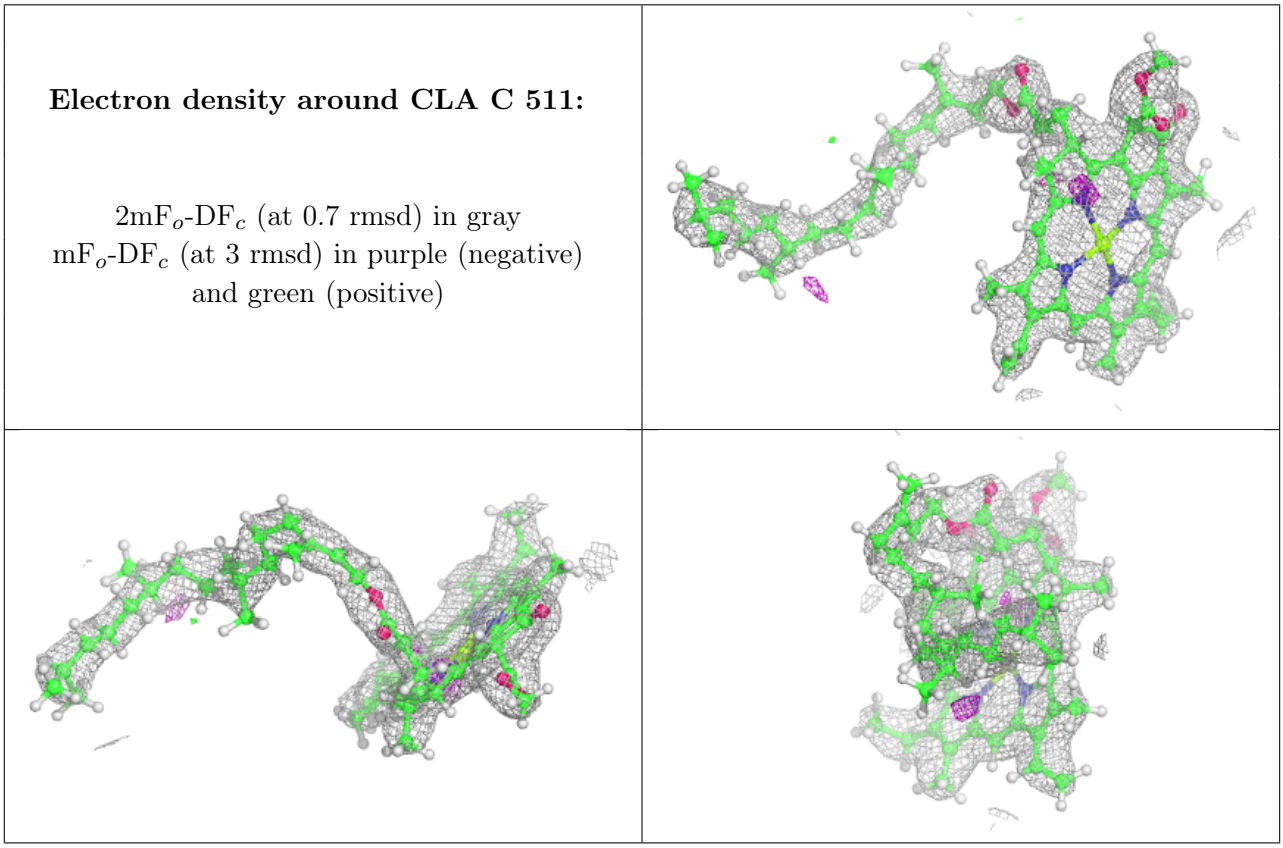
Electron density around PL9 d 406:

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



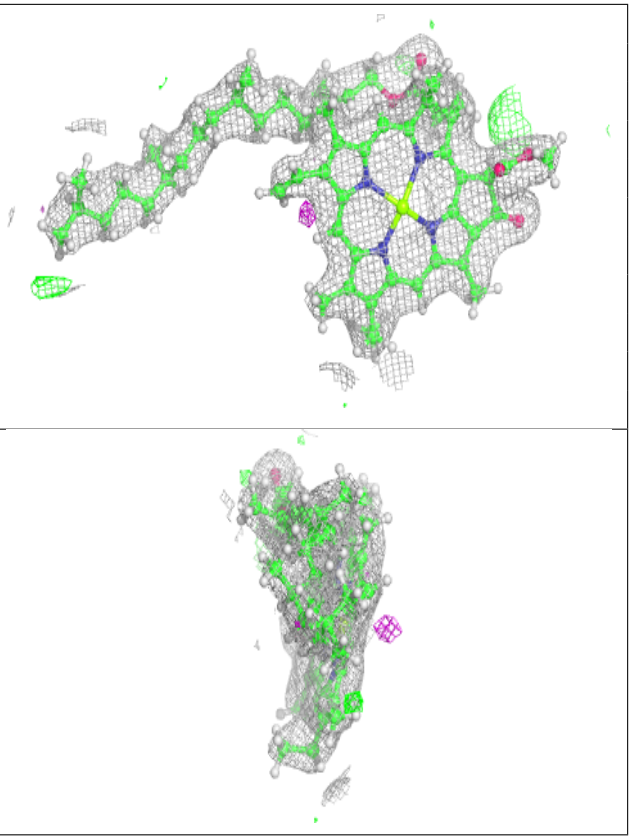
Electron density around CLA C 511:

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



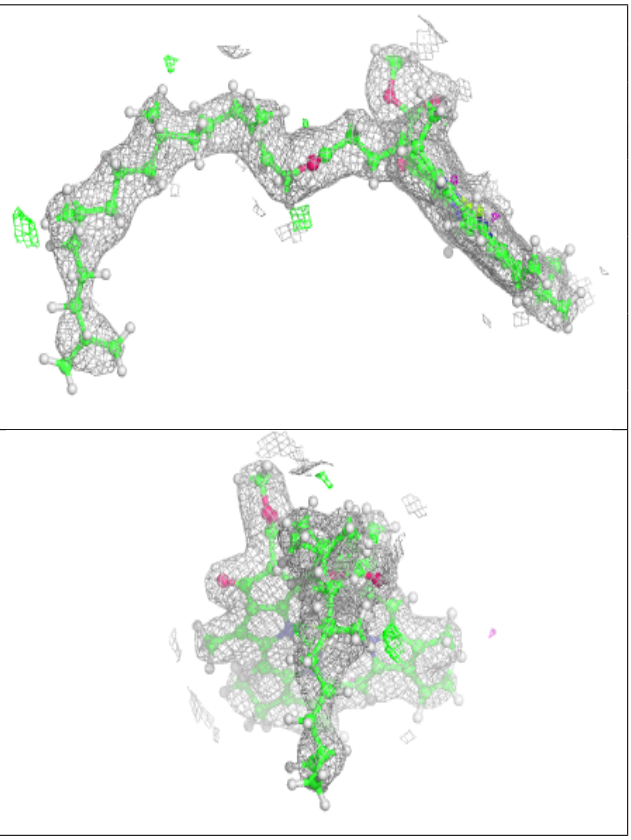
Electron density around CLA C 501:

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



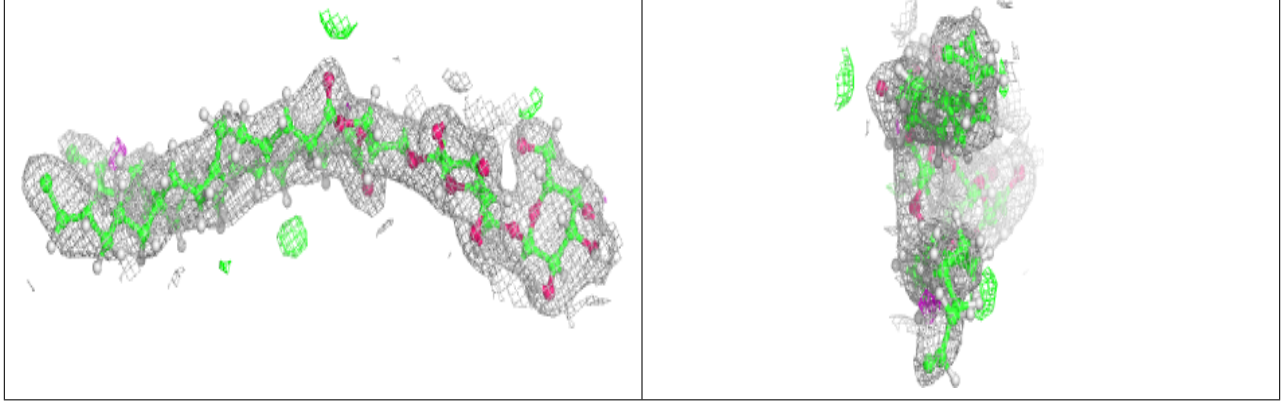
Electron density around CLA d 403:

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



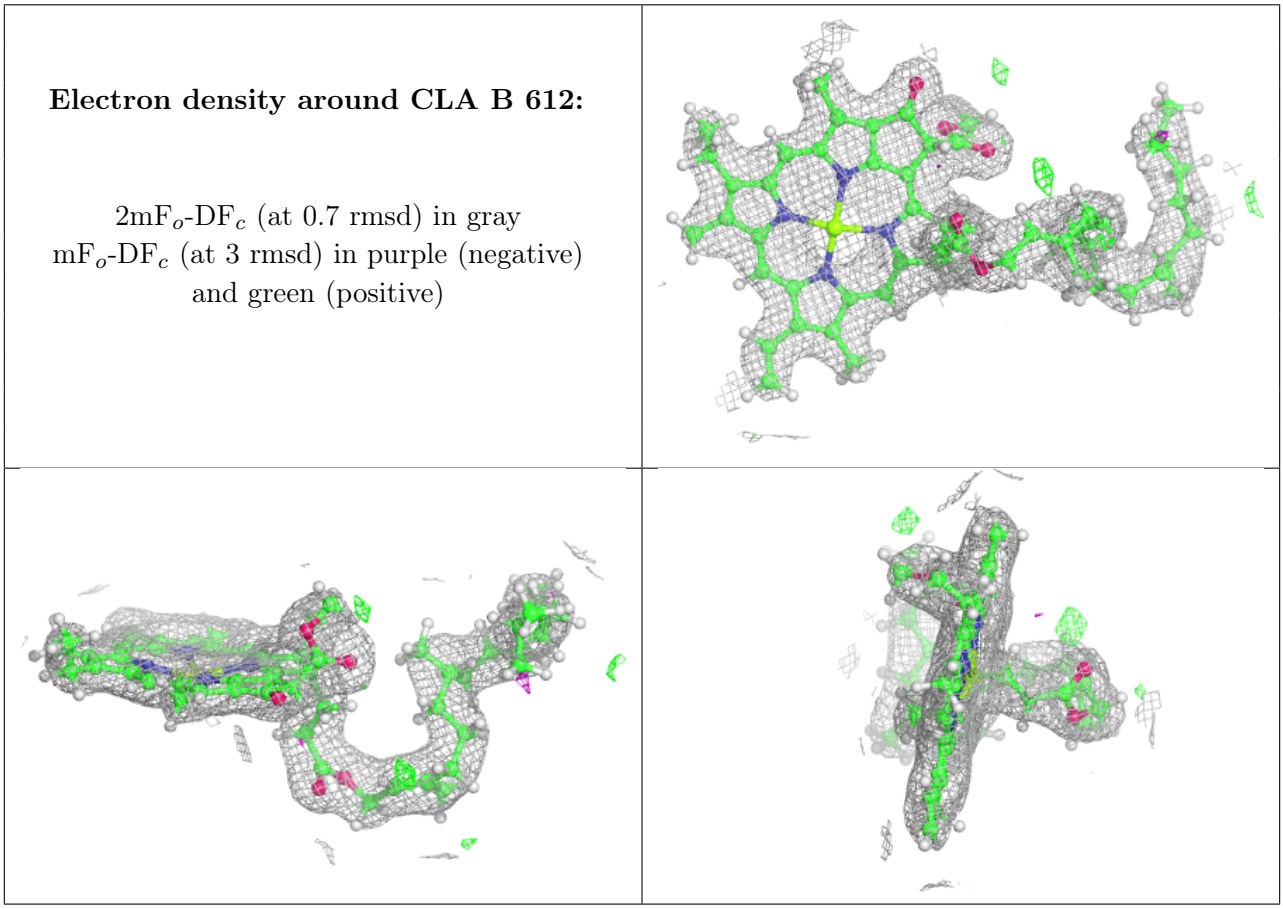
Electron density around DGD c 518:

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



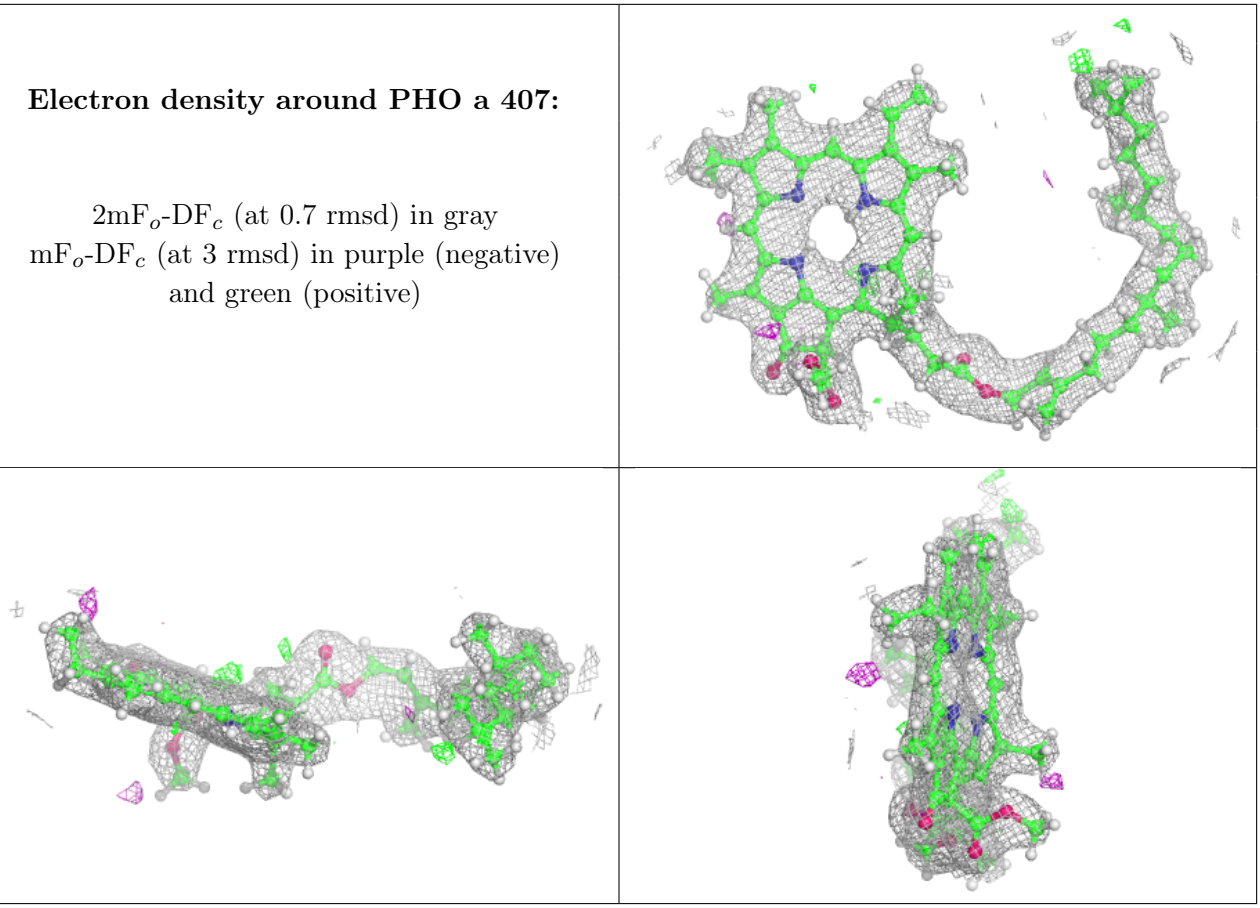
Electron density around CLA B 612:

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



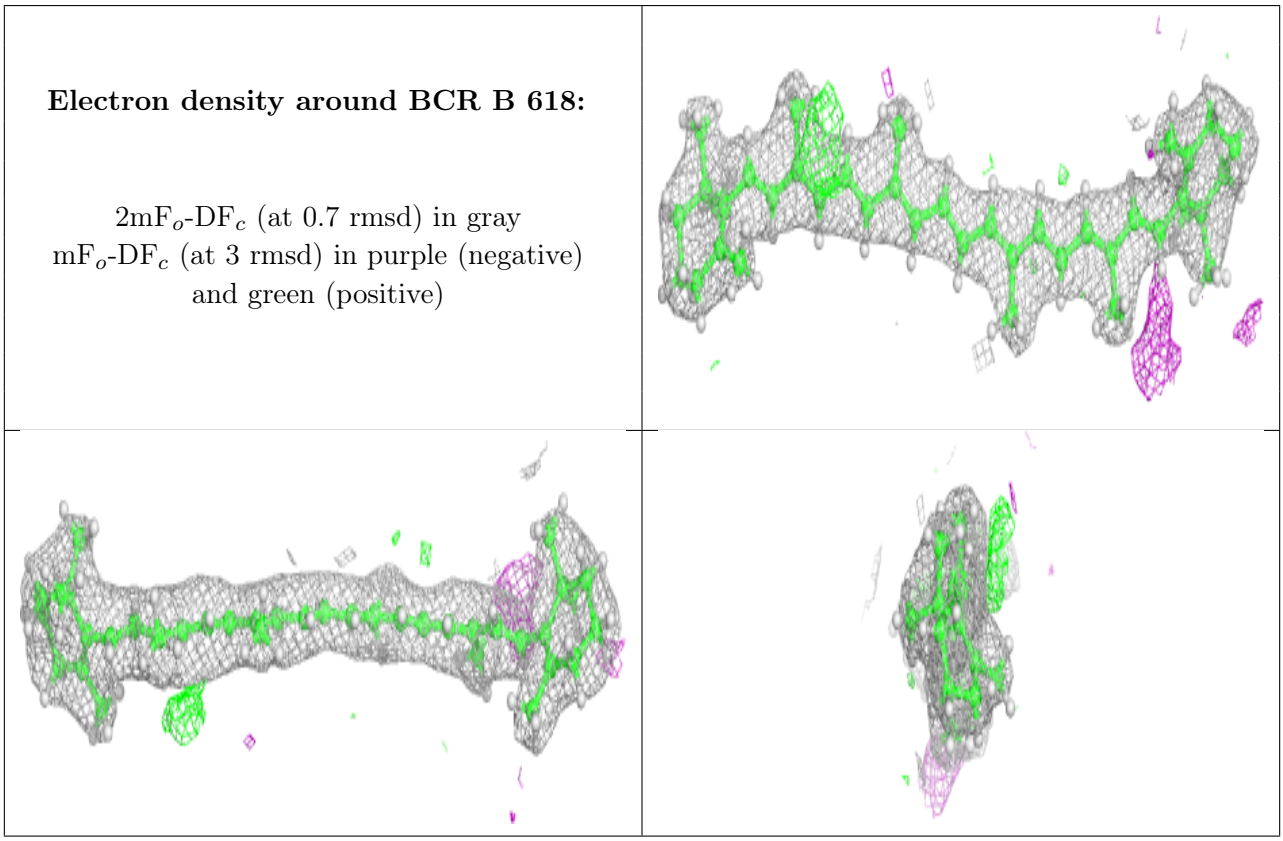
Electron density around PHO a 407:

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



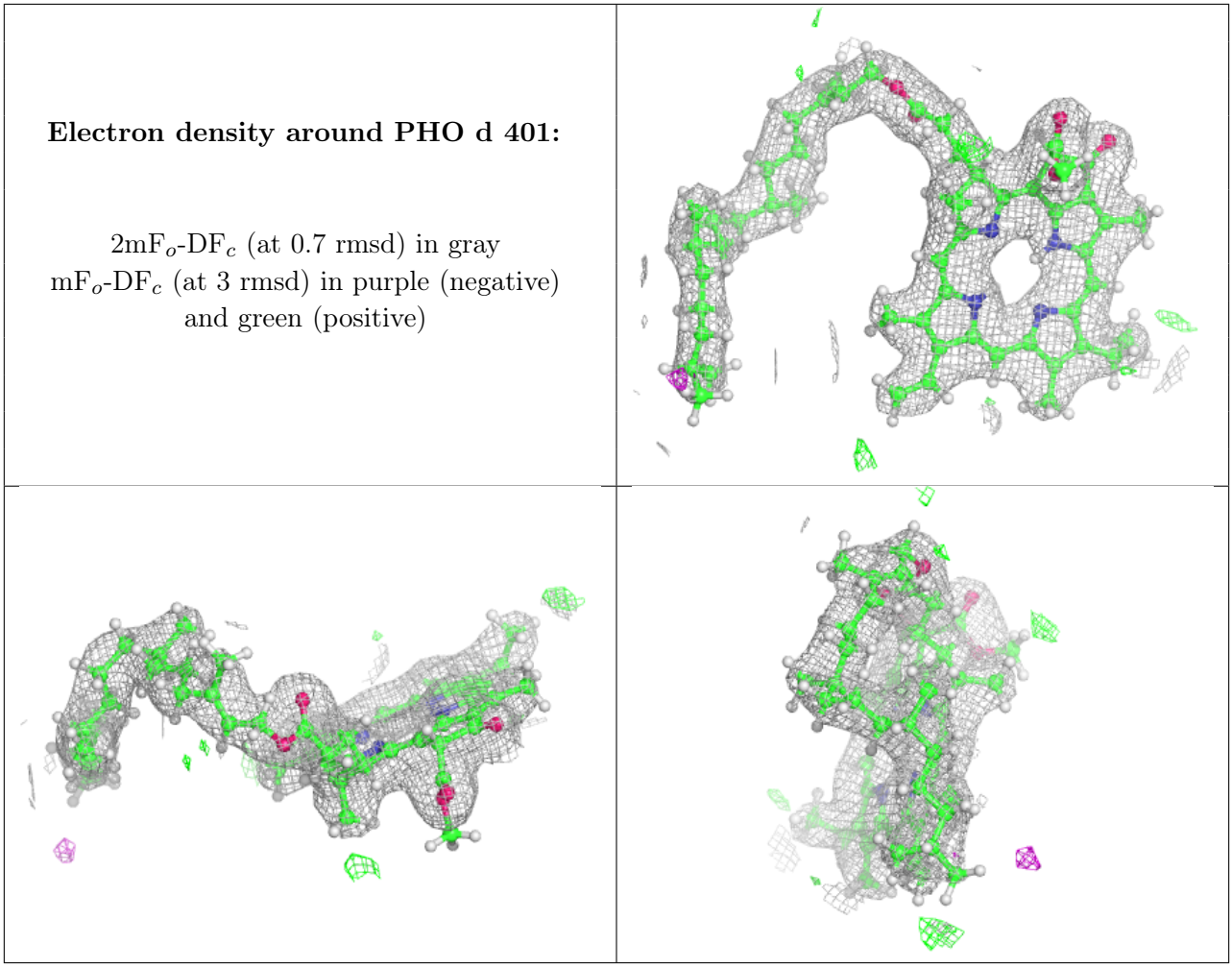
Electron density around BCR B 618:

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



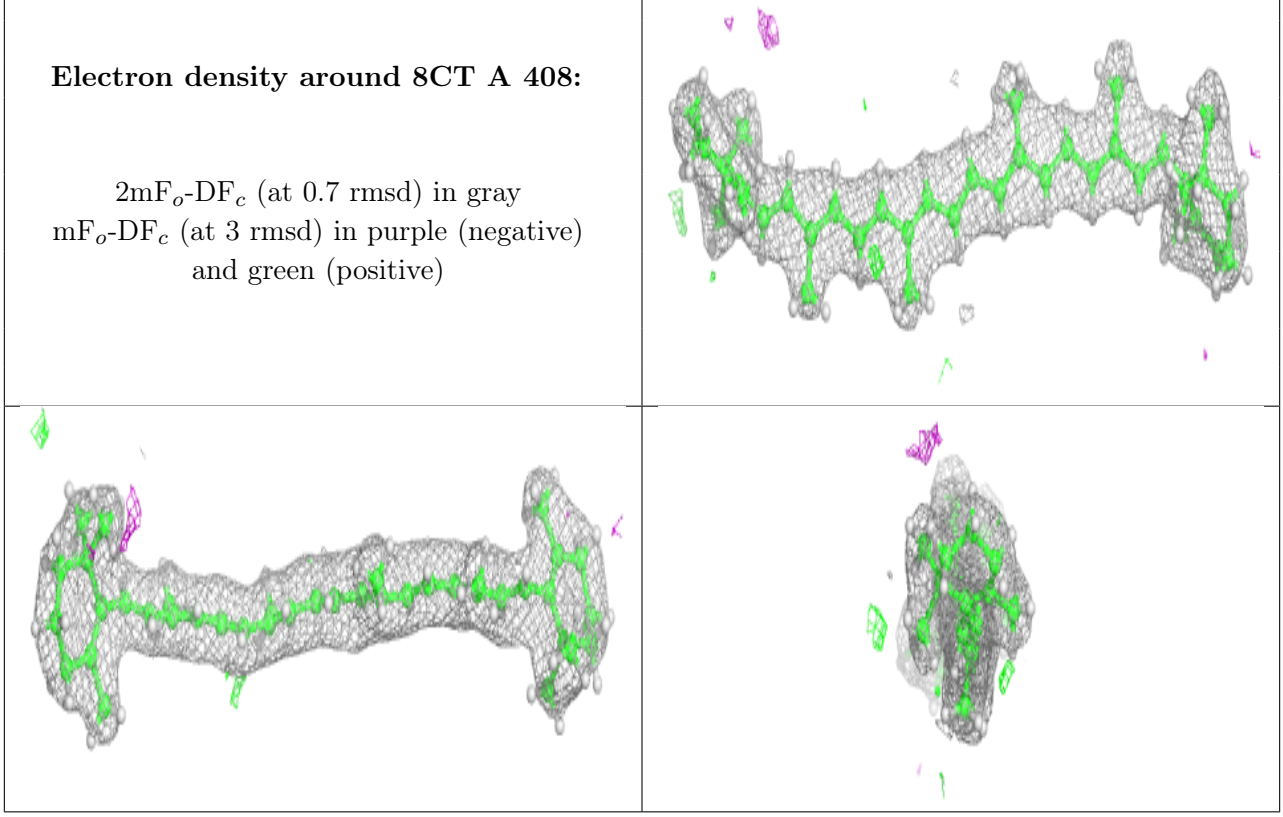
Electron density around PHO d 401:

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



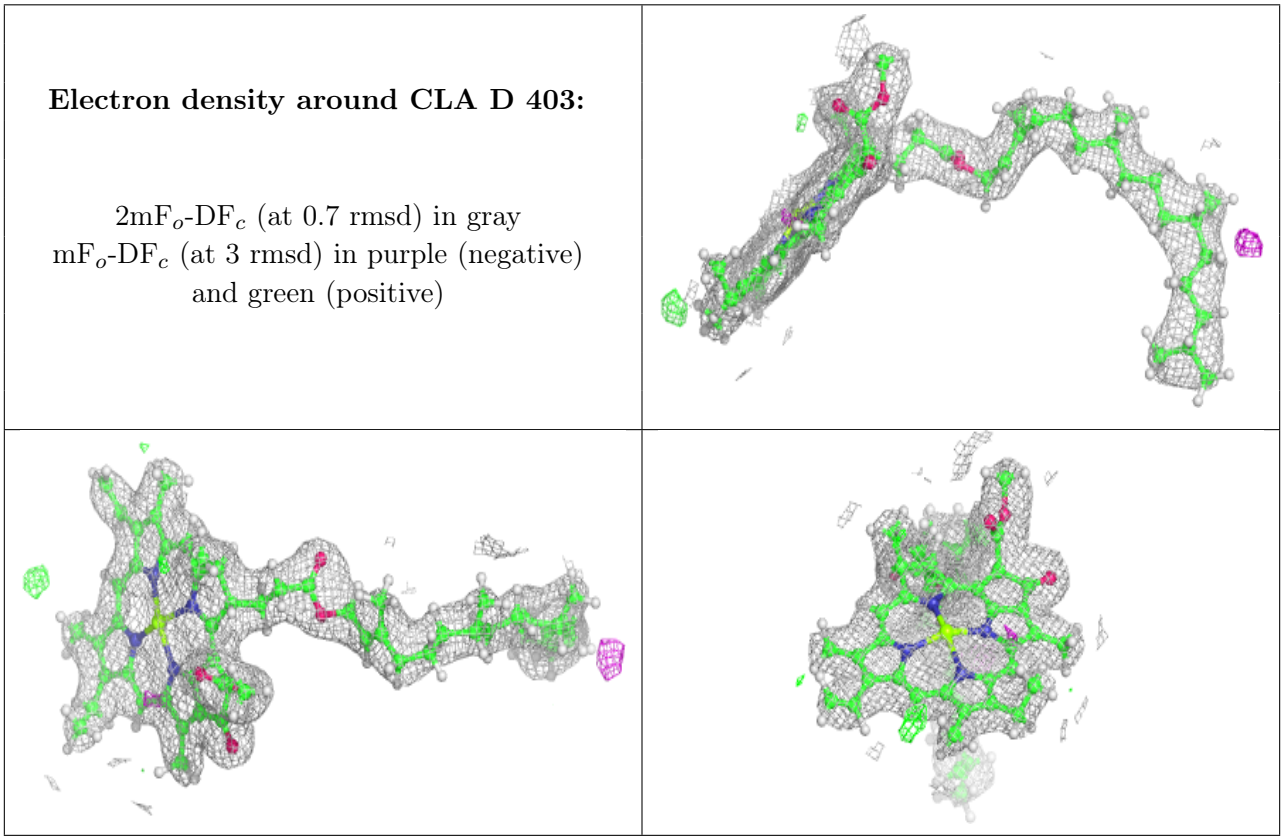
Electron density around 8CT A 408:

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



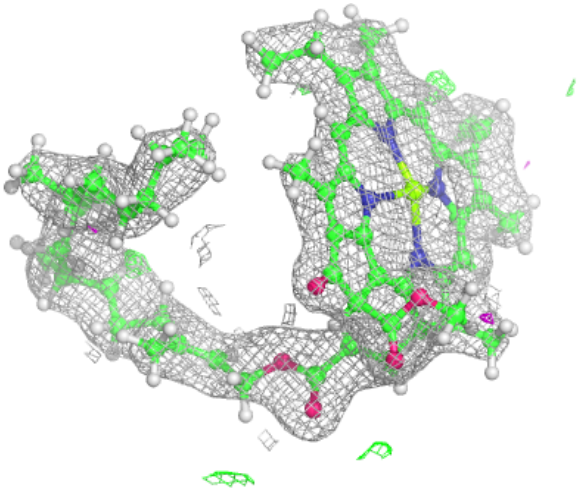
Electron density around CLA D 403:

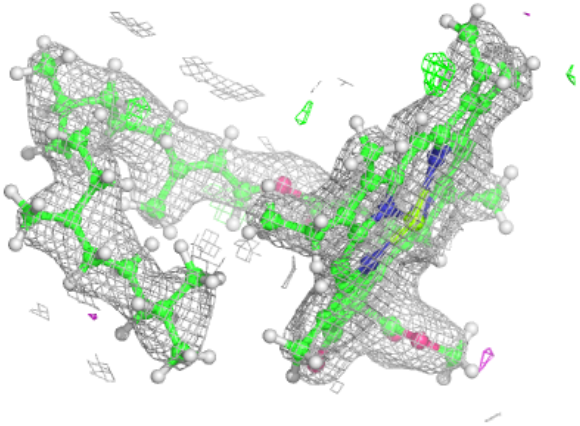
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

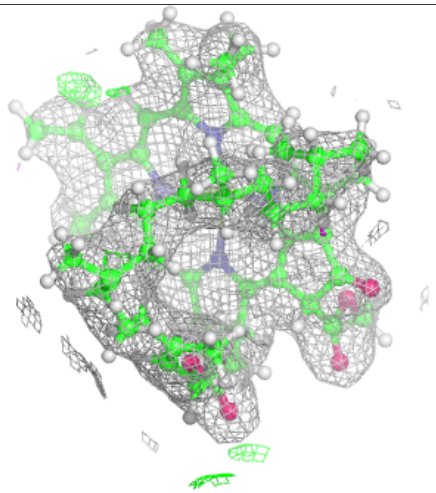


Electron density around CLA C 503:

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

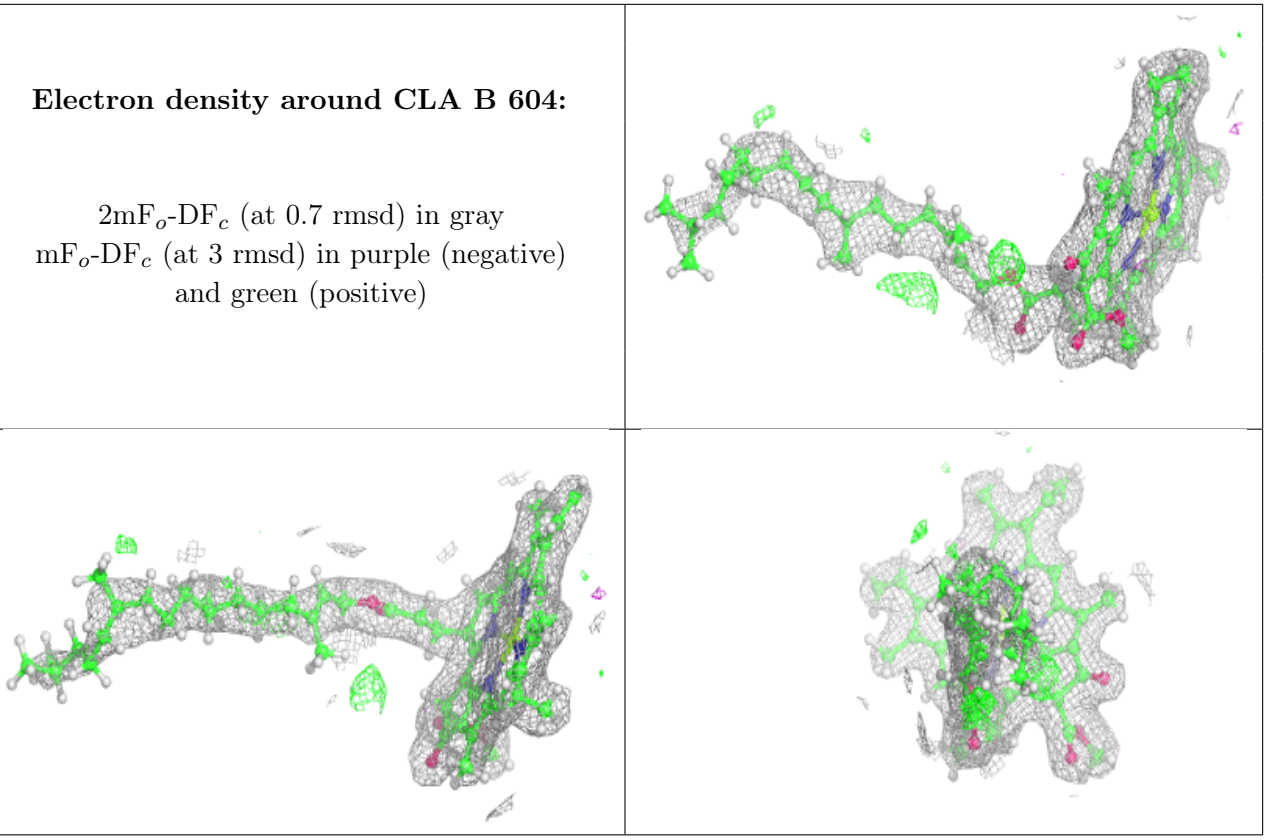






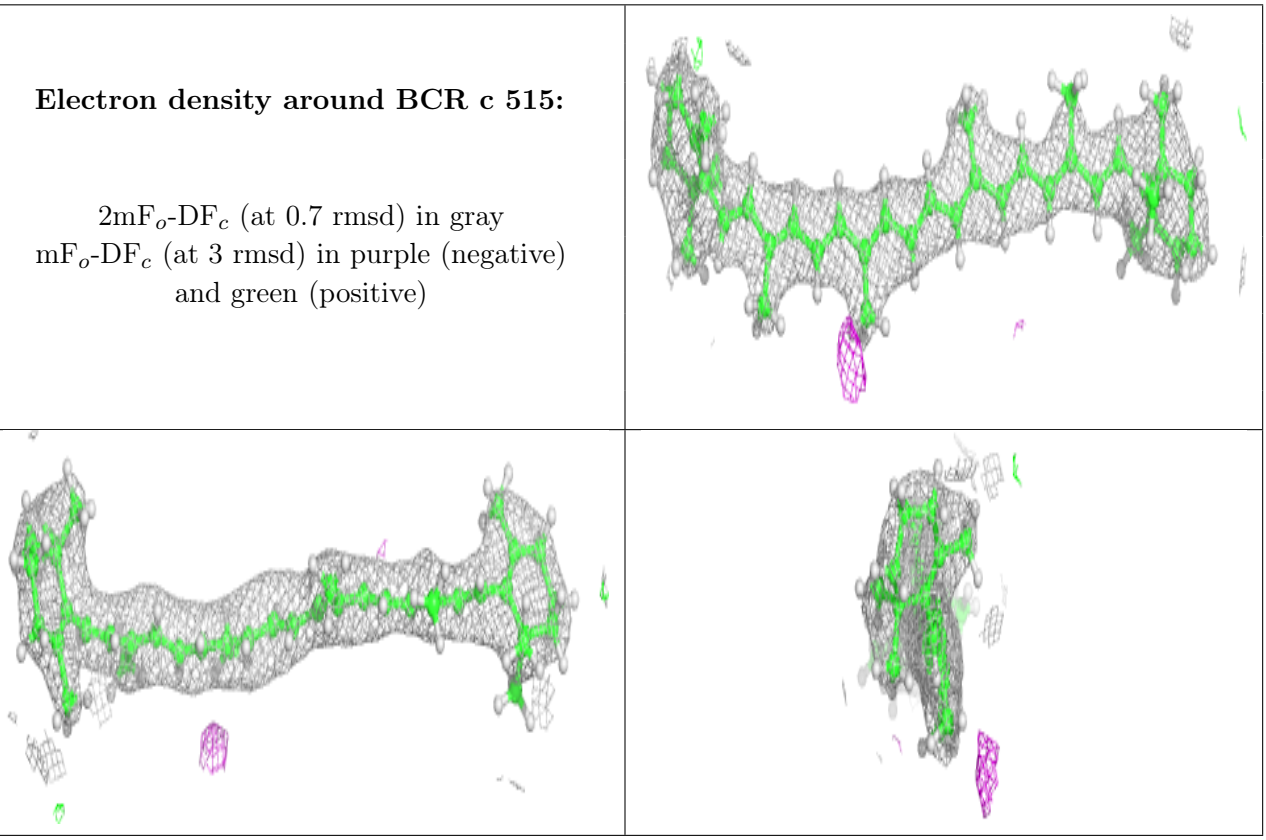
Electron density around CLA B 604:

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



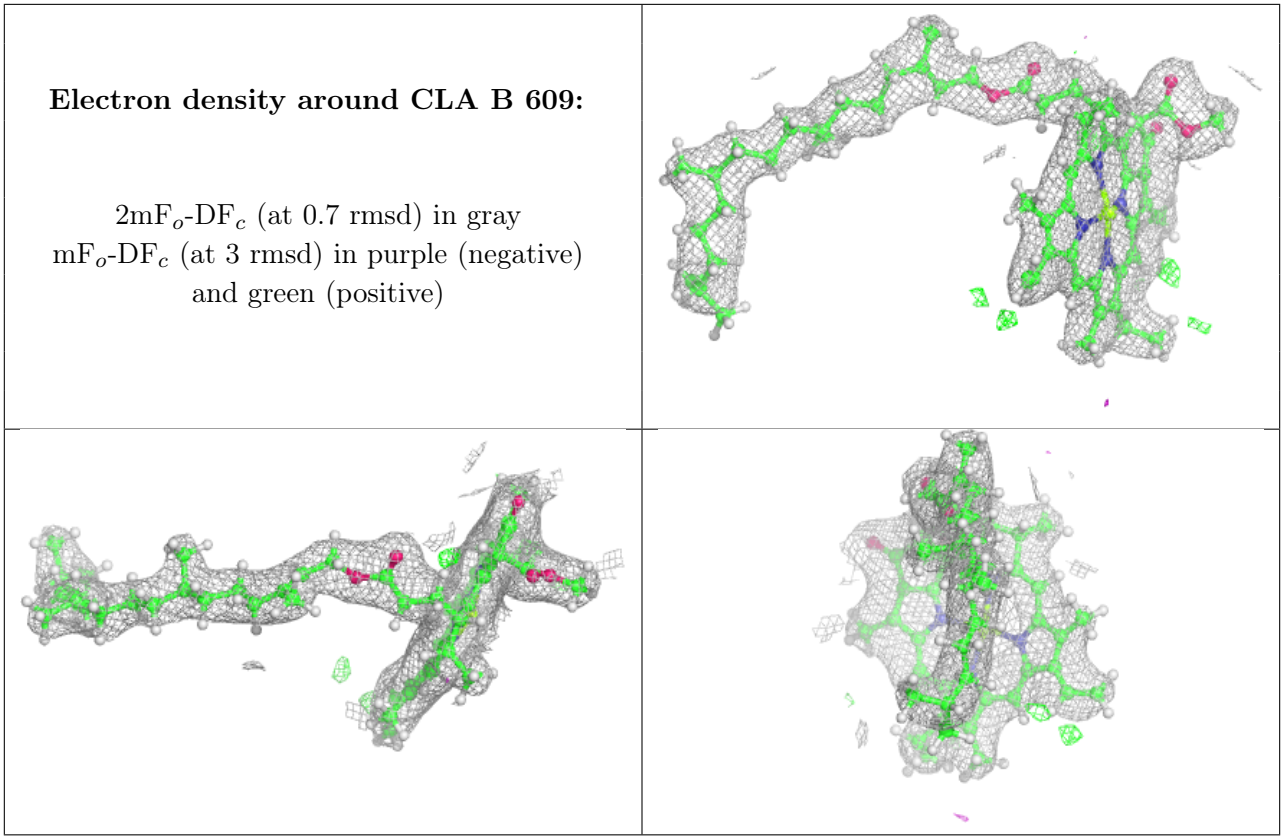
Electron density around BCR c 515:

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



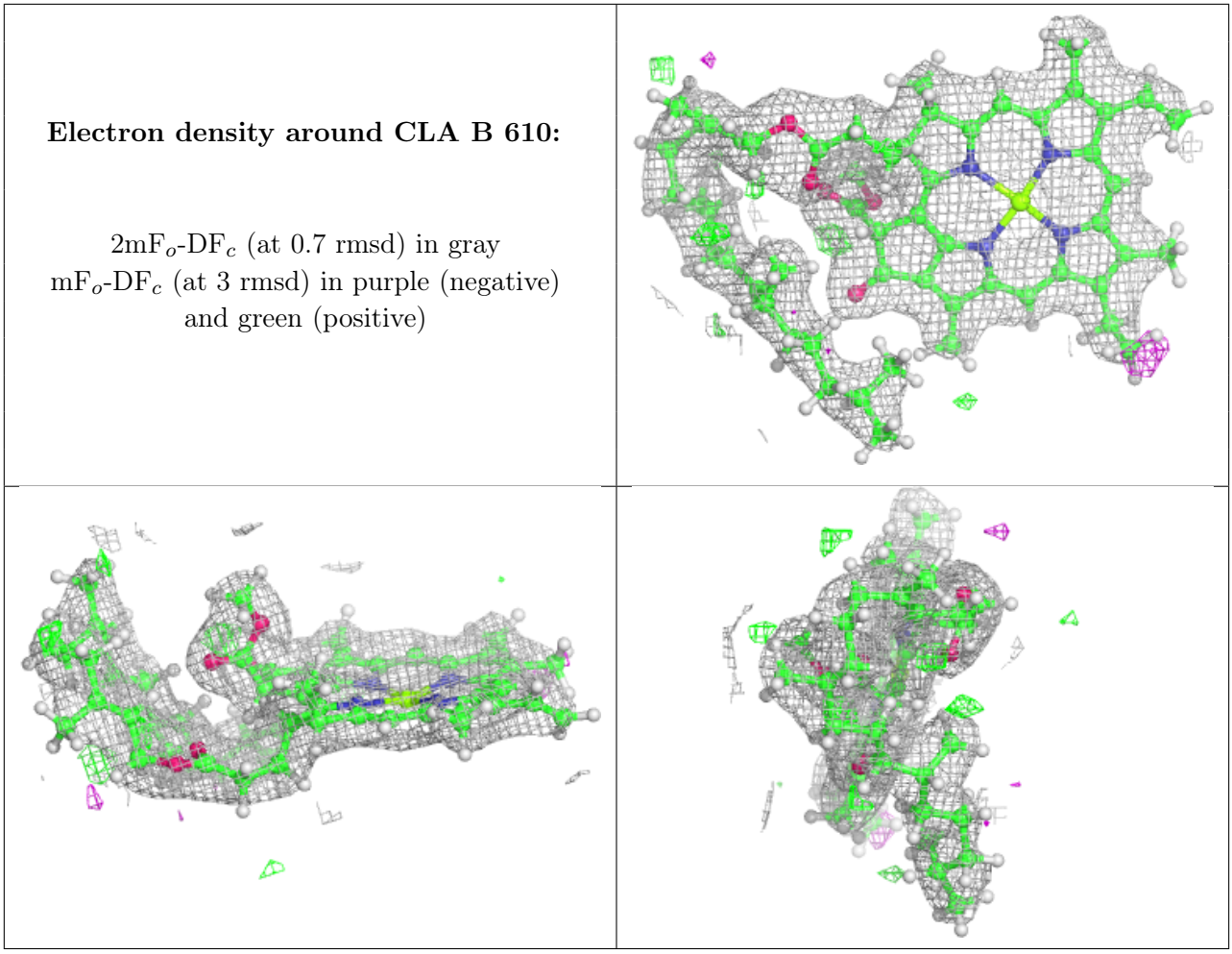
Electron density around CLA B 609:

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



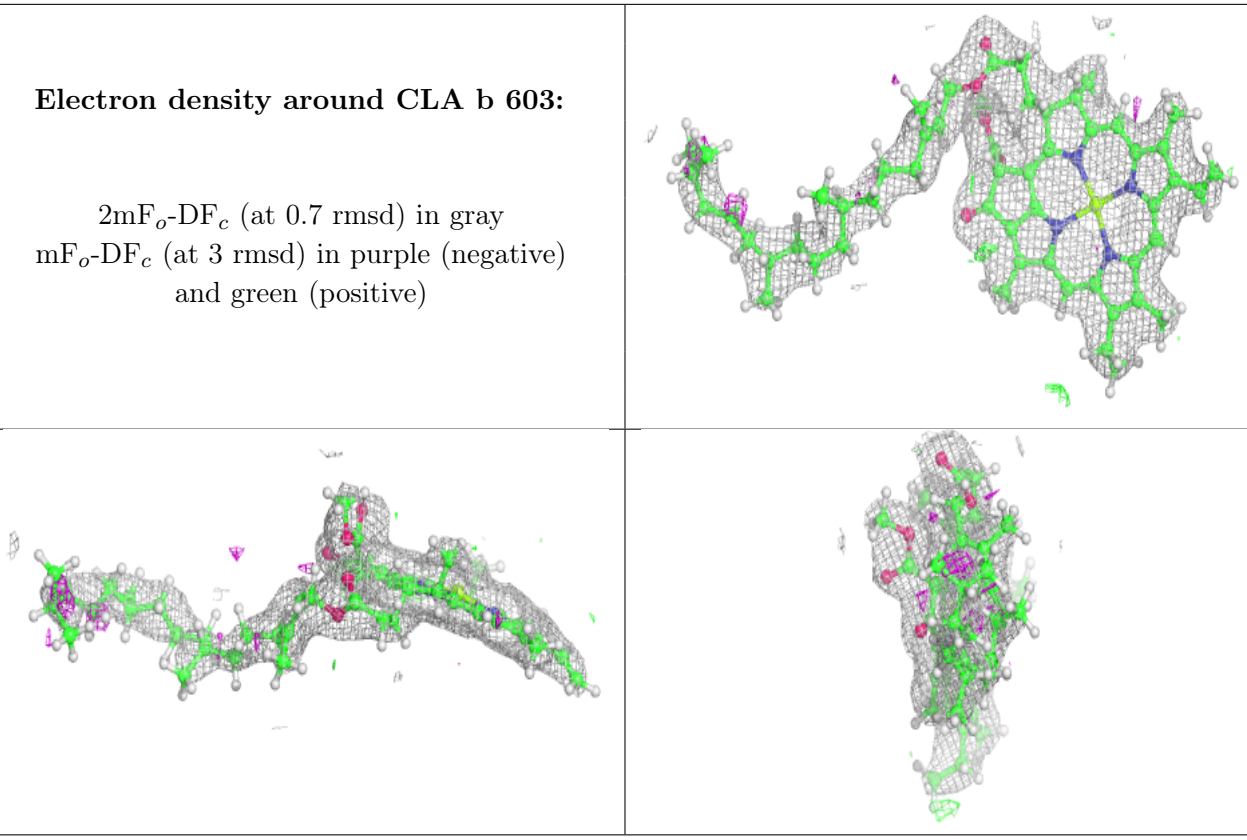
Electron density around CLA B 610:

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



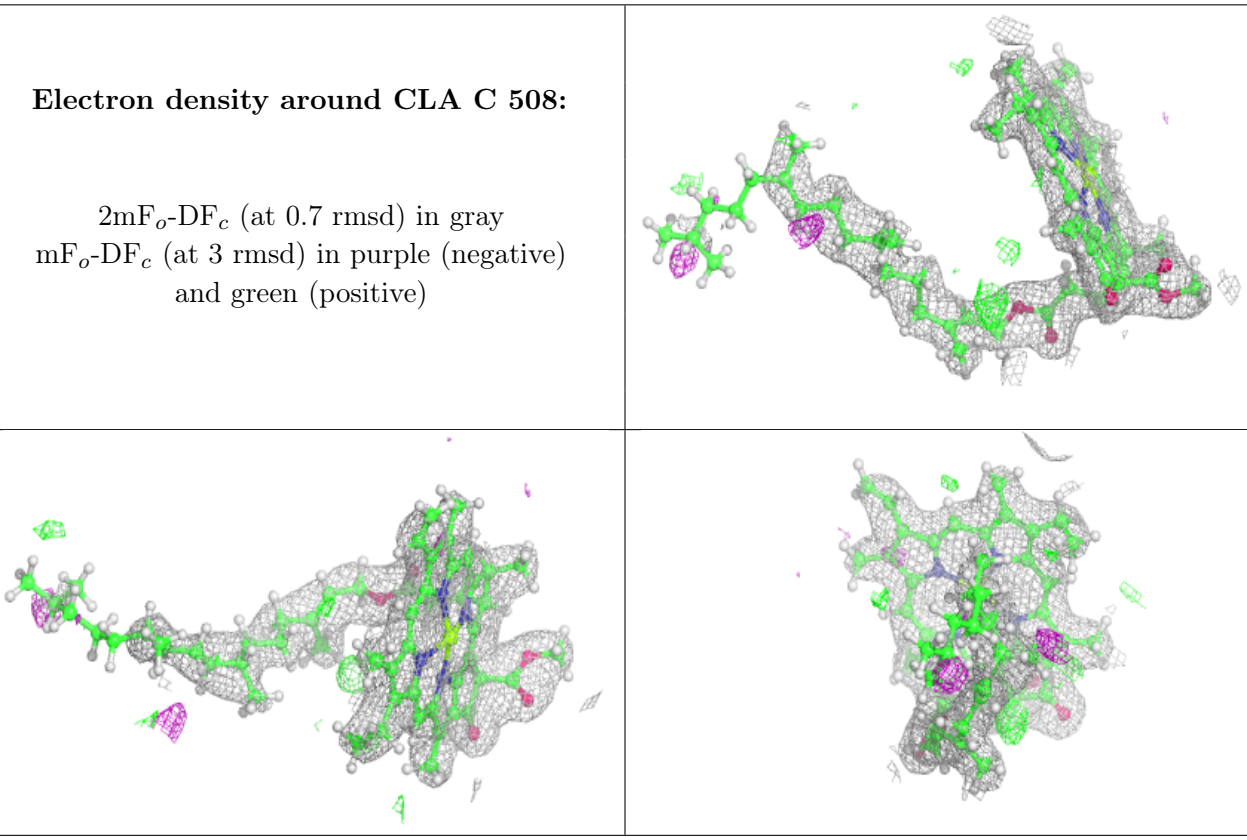
Electron density around CLA b 603:

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



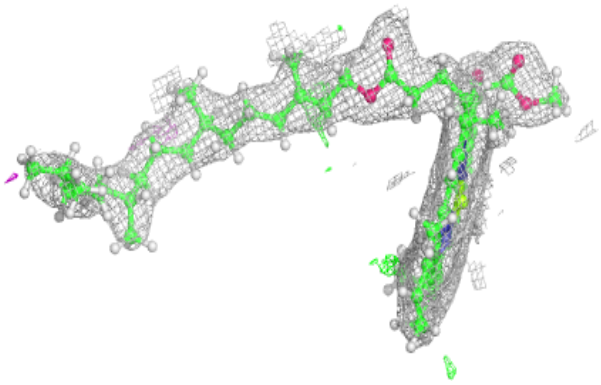
Electron density around CLA C 508:

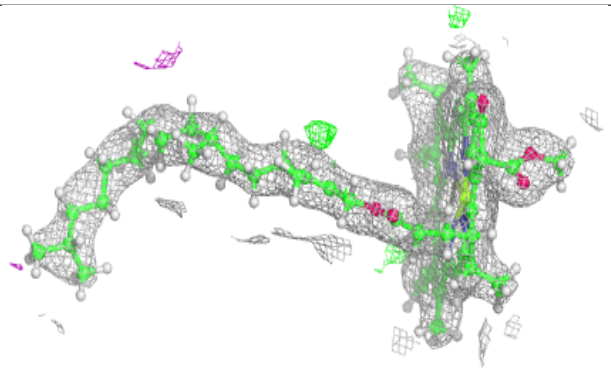
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

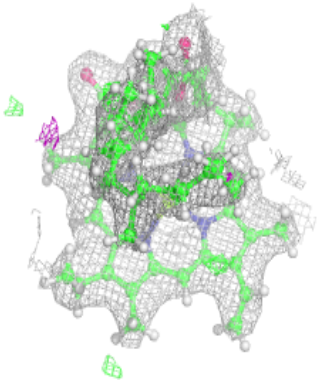


Electron density around CLA b 606:

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

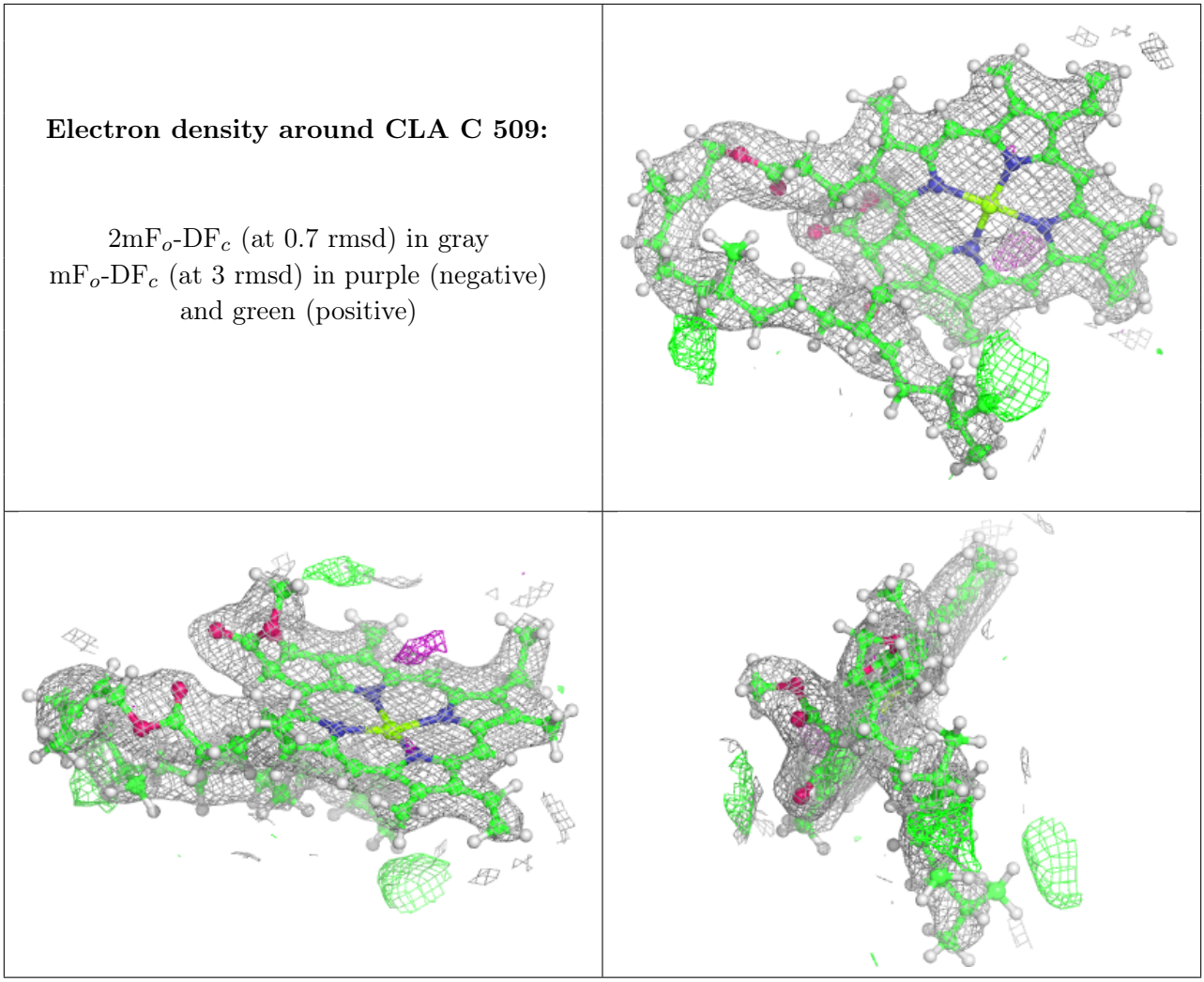






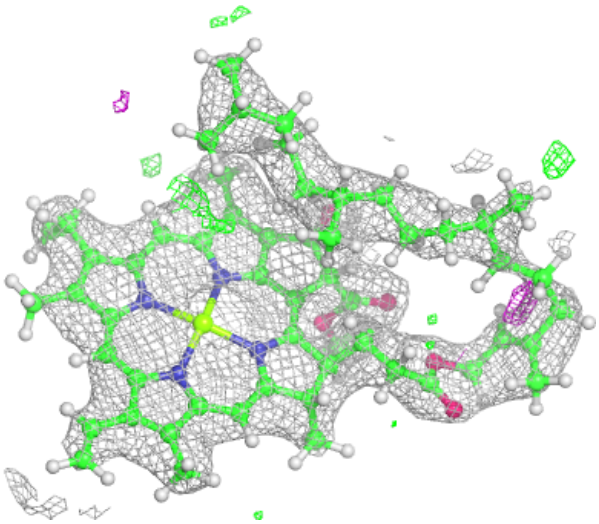
Electron density around CLA C 509:

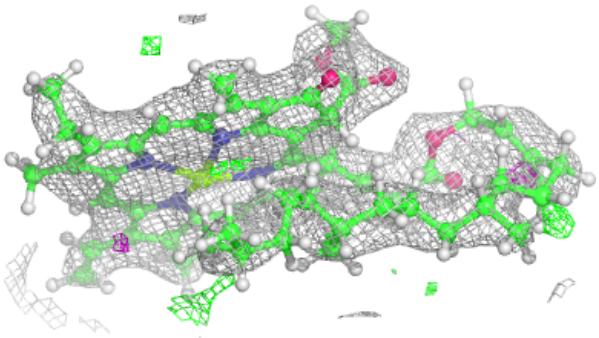
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

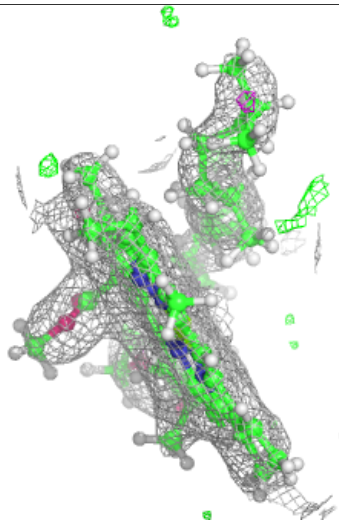


Electron density around CLA c 509:

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

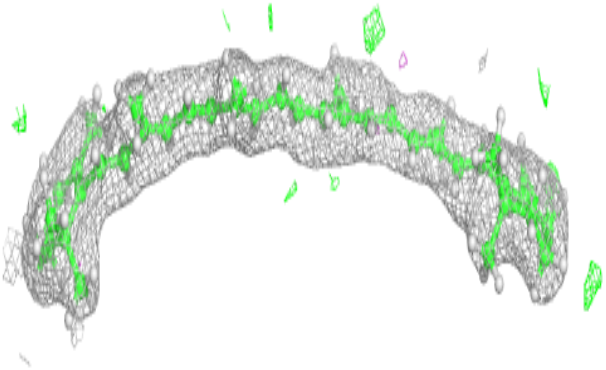


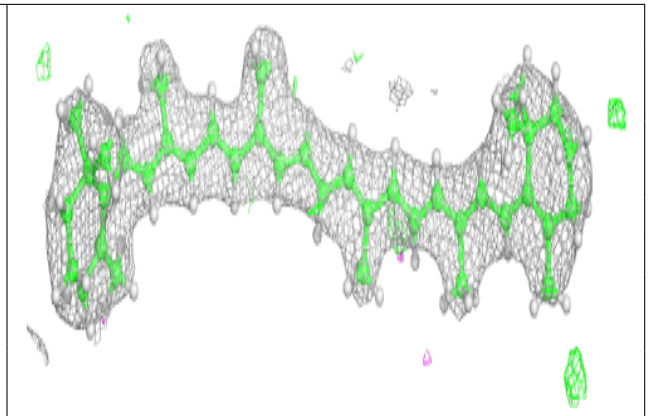


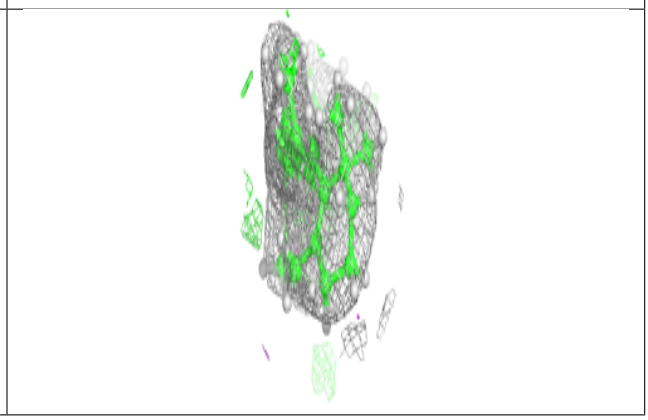


Electron density around 8CT t 101:

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

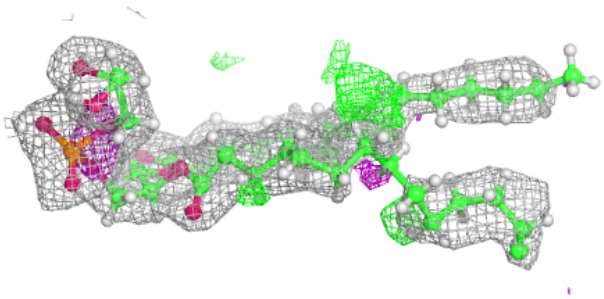


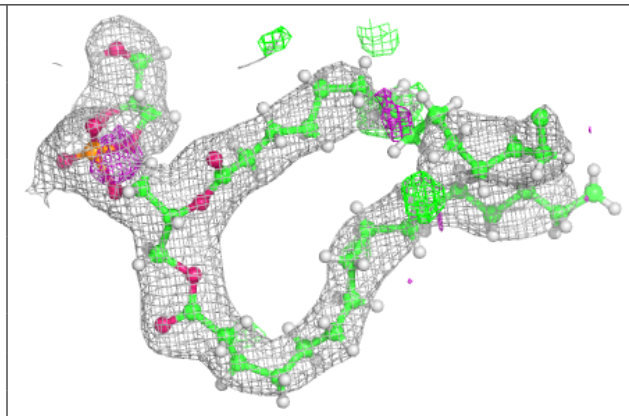


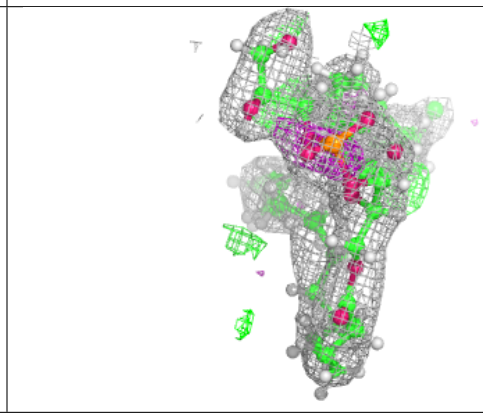


Electron density around LHG D 410:

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

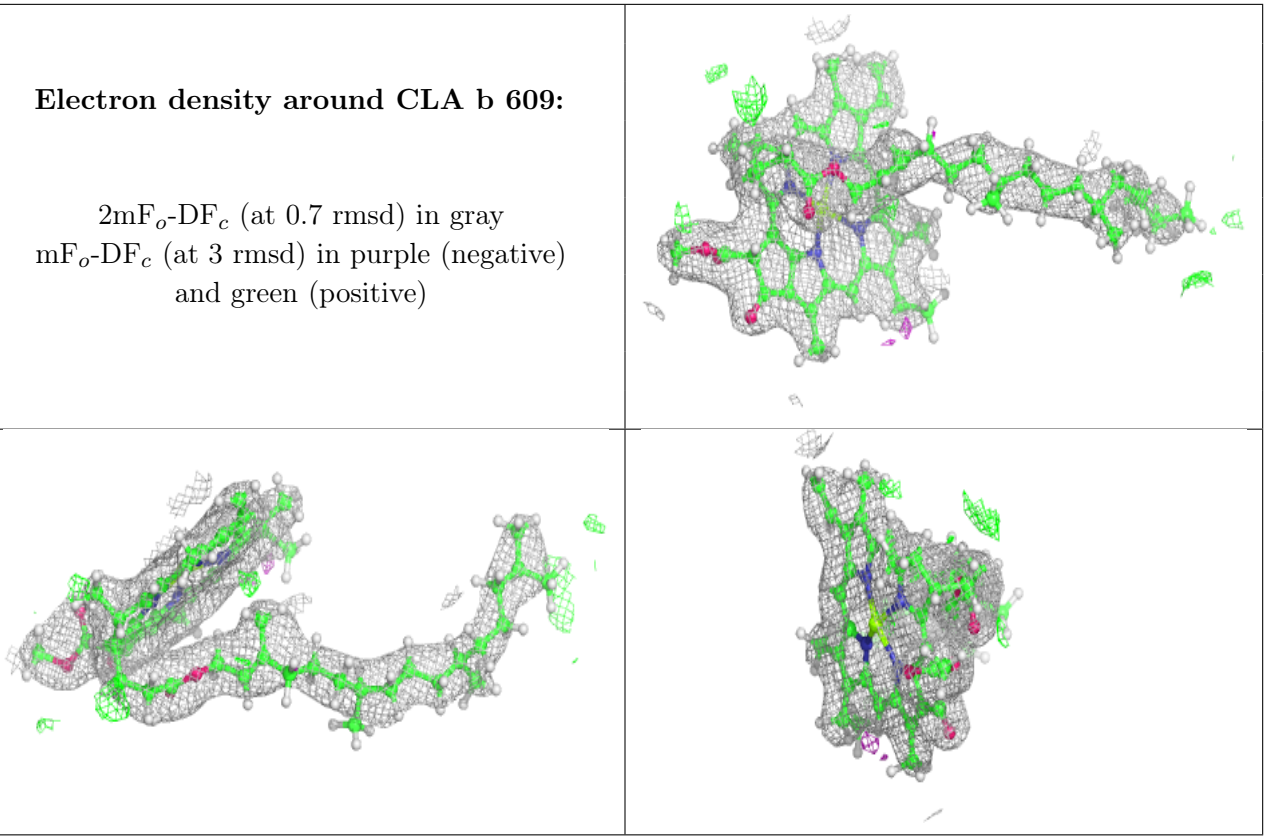






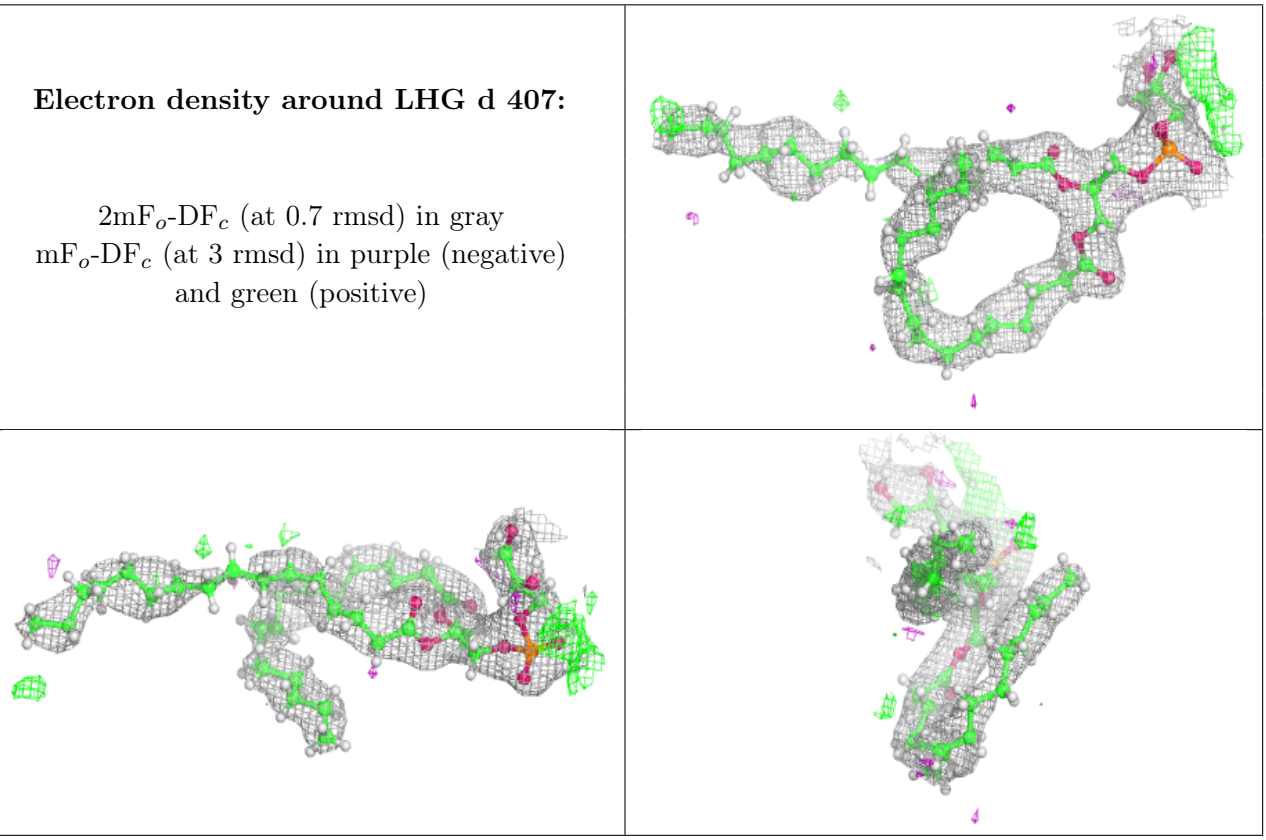
Electron density around CLA b 609:

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



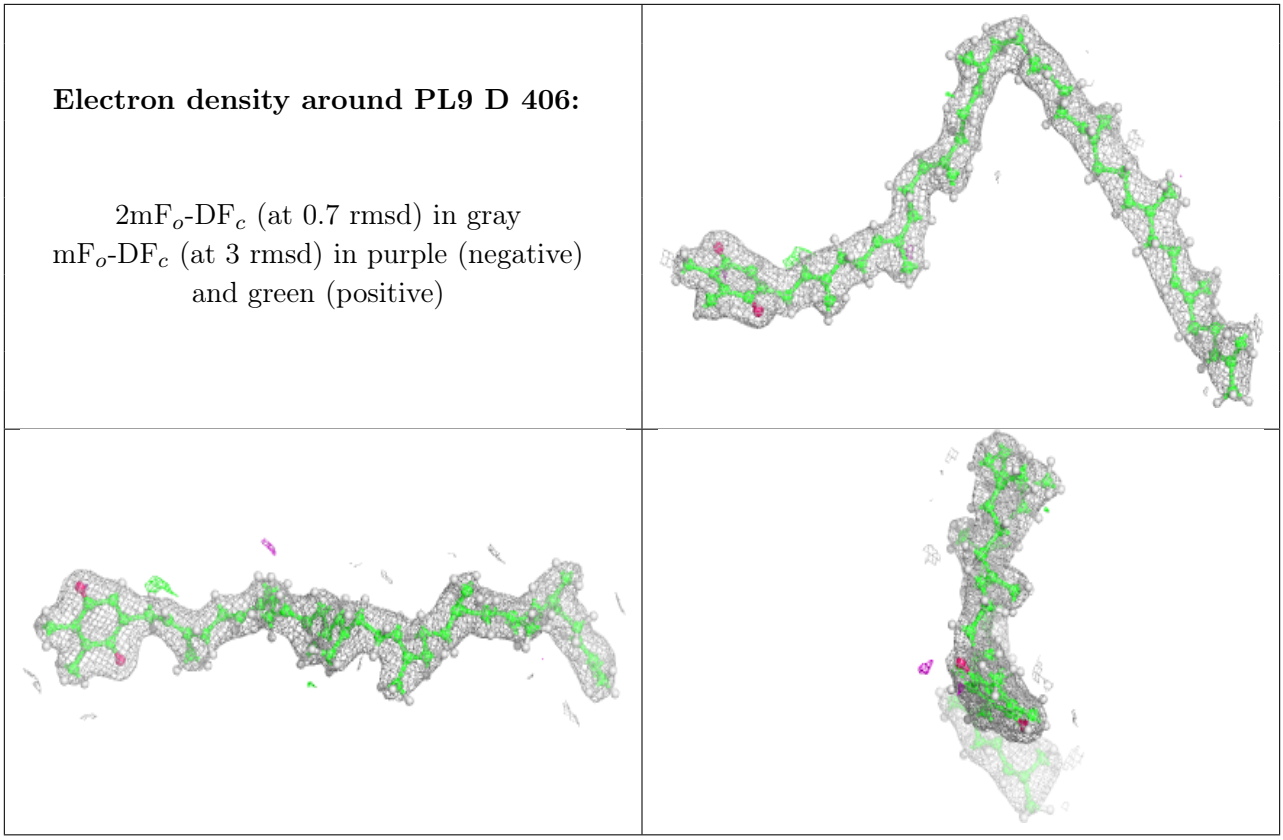
Electron density around LHG d 407:

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



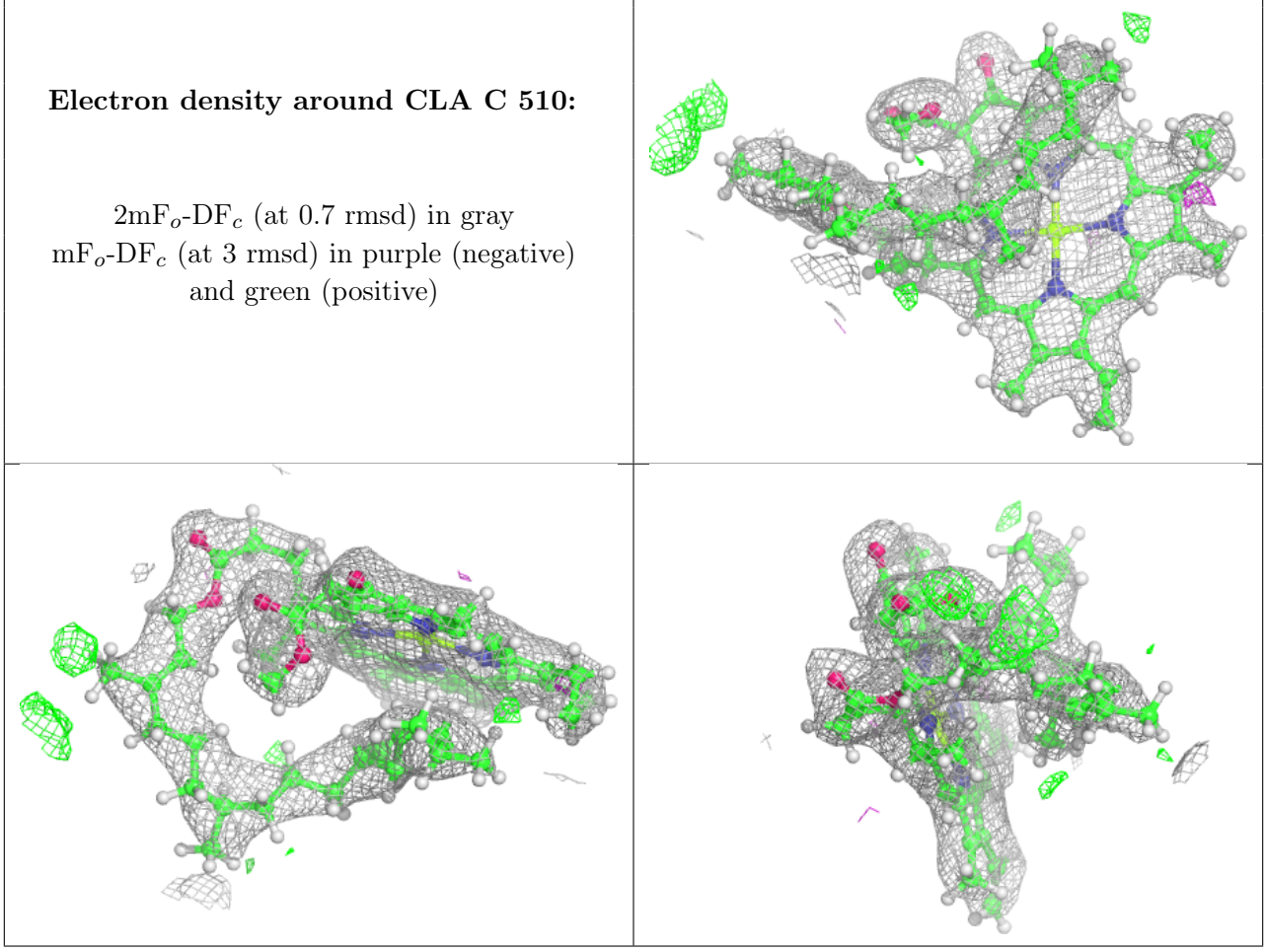
Electron density around PL9 D 406:

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



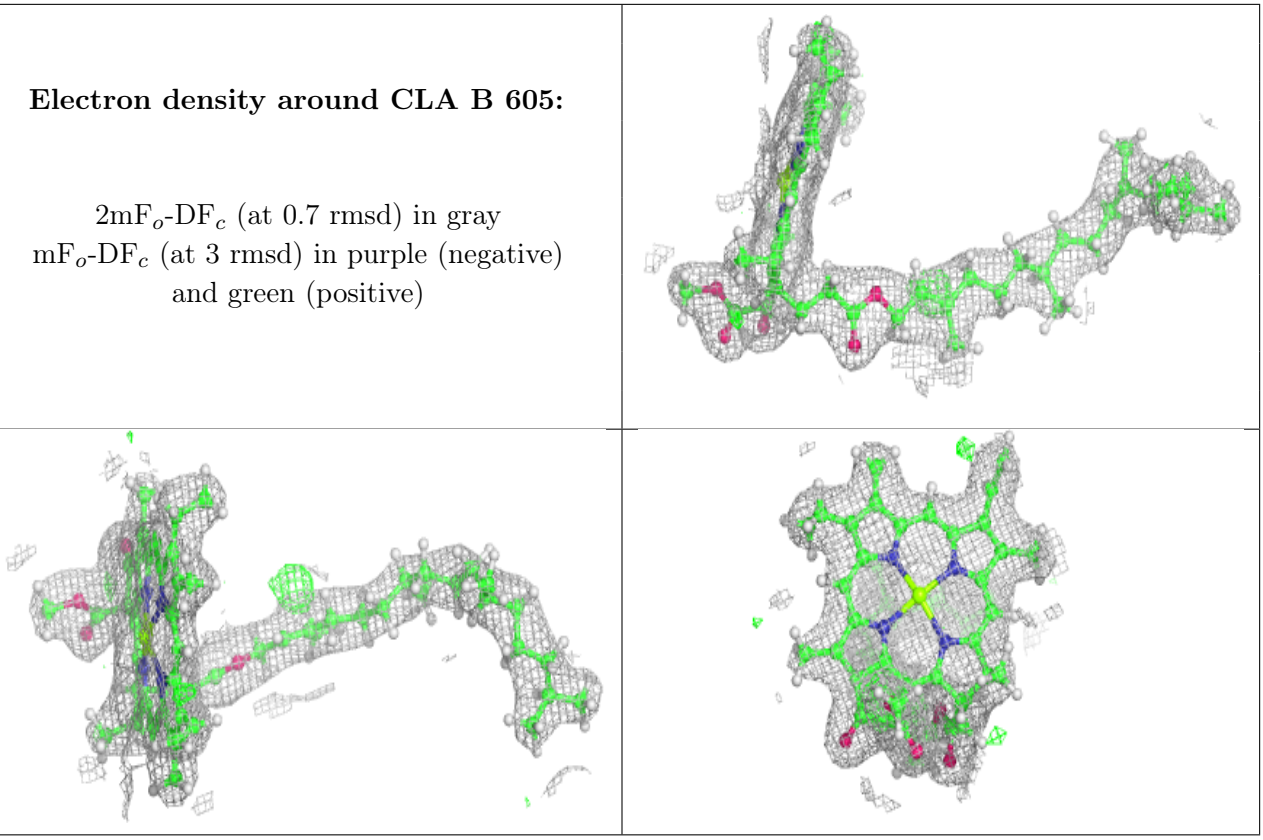
Electron density around CLA C 510:

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



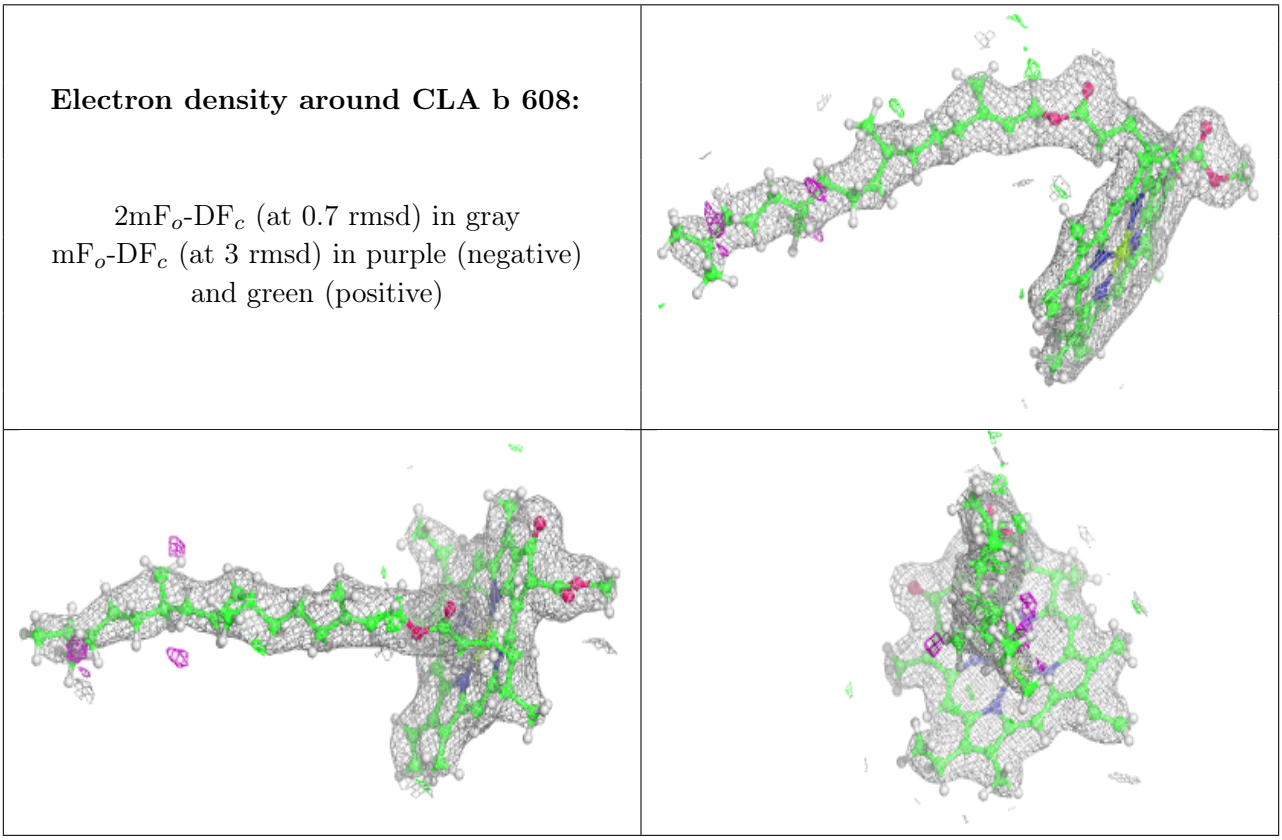
Electron density around CLA B 605:

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



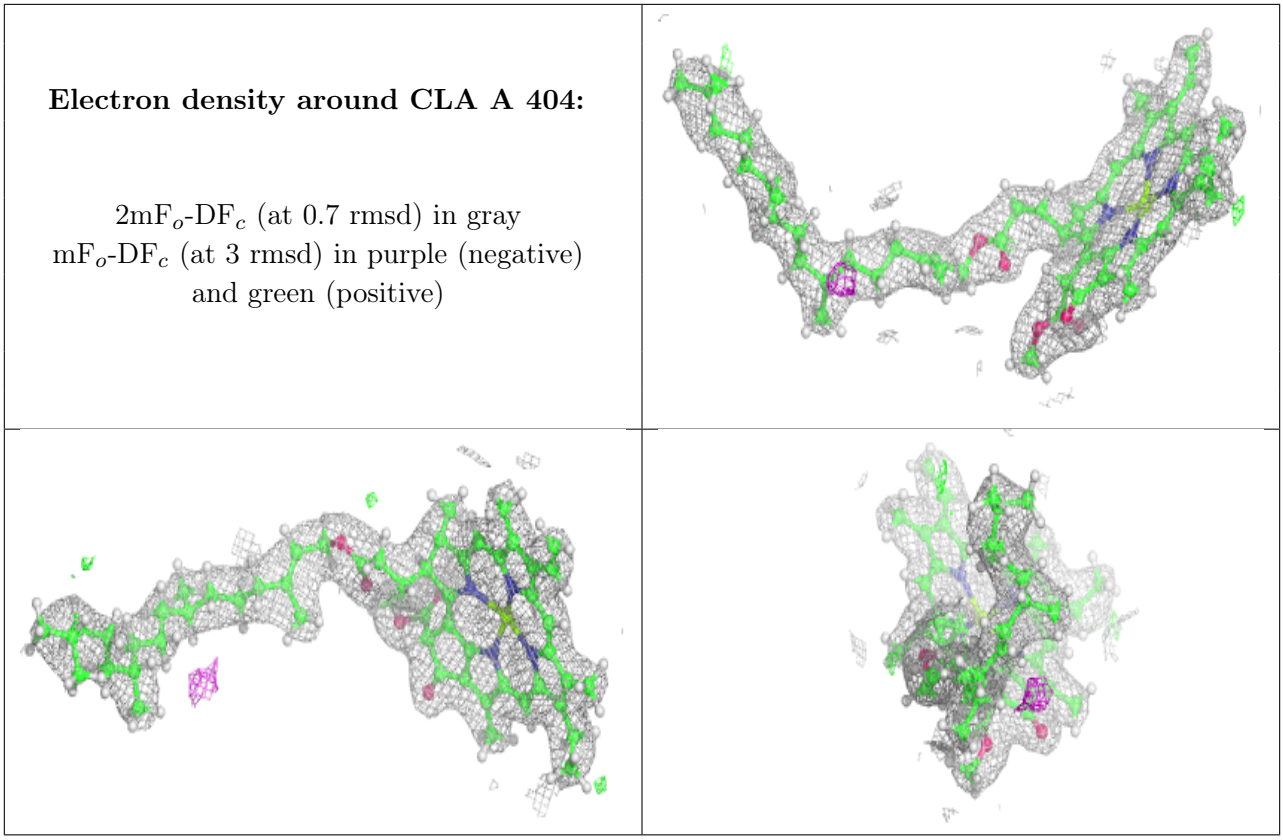
Electron density around CLA b 608:

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



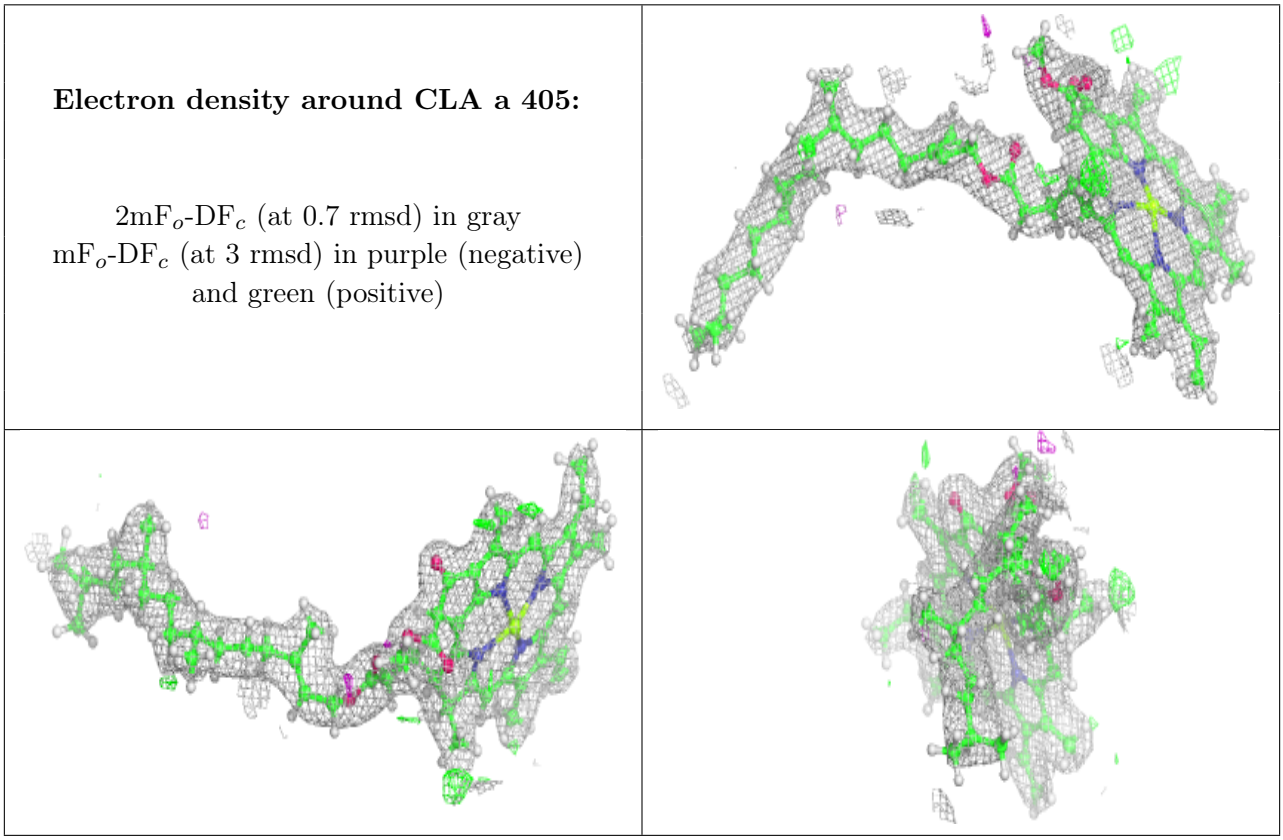
Electron density around CLA A 404:

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



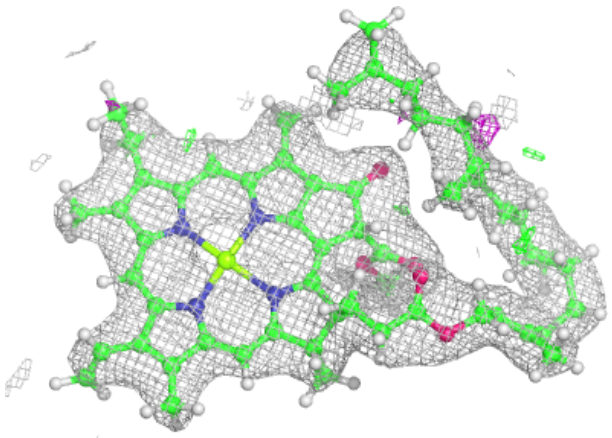
Electron density around CLA a 405:

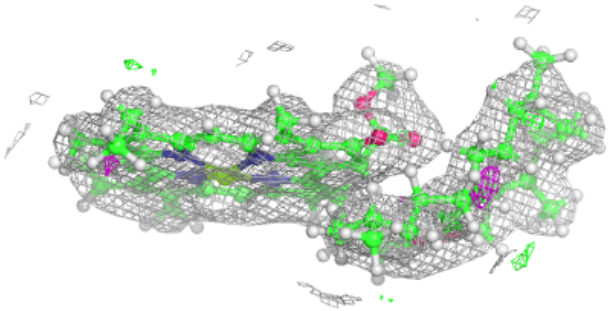
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

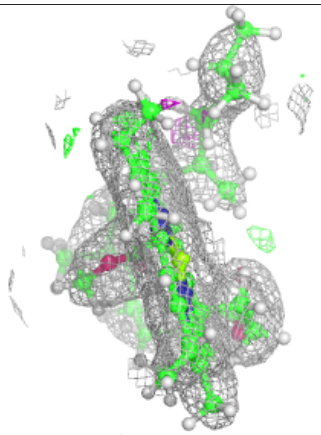


Electron density around CLA b 611:

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

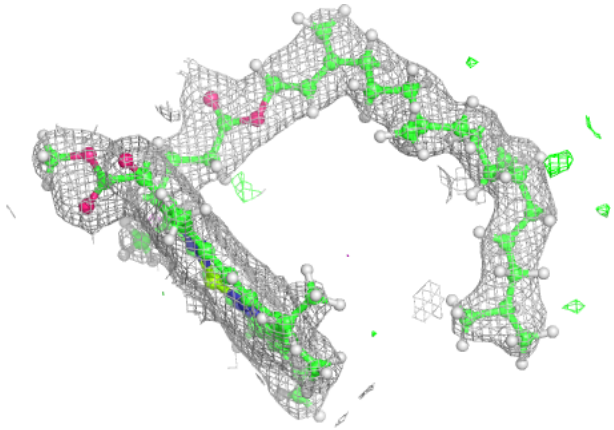


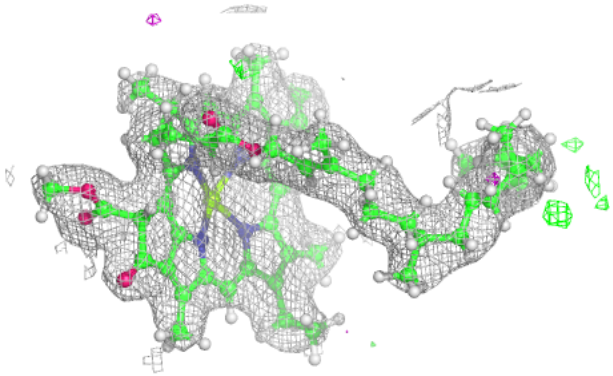


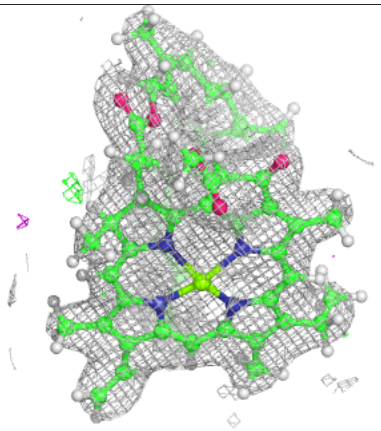


Electron density around CLA b 612:

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

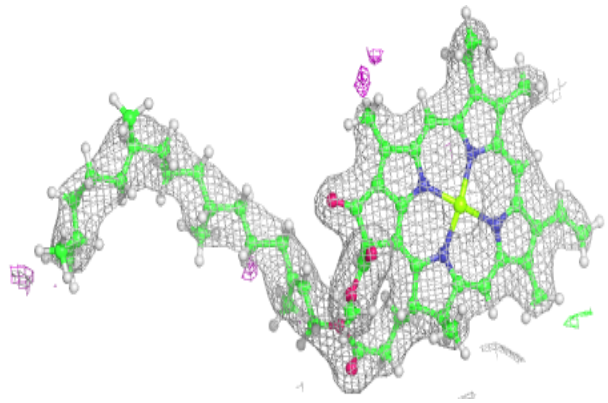


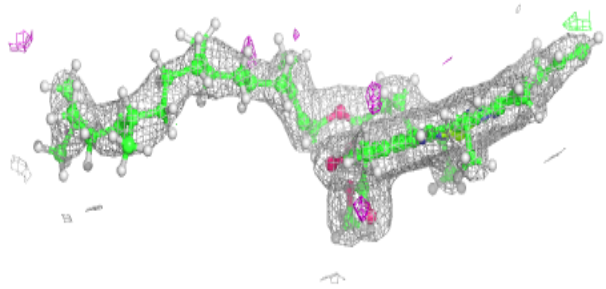


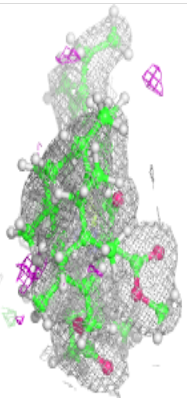


Electron density around CLA B 602:

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

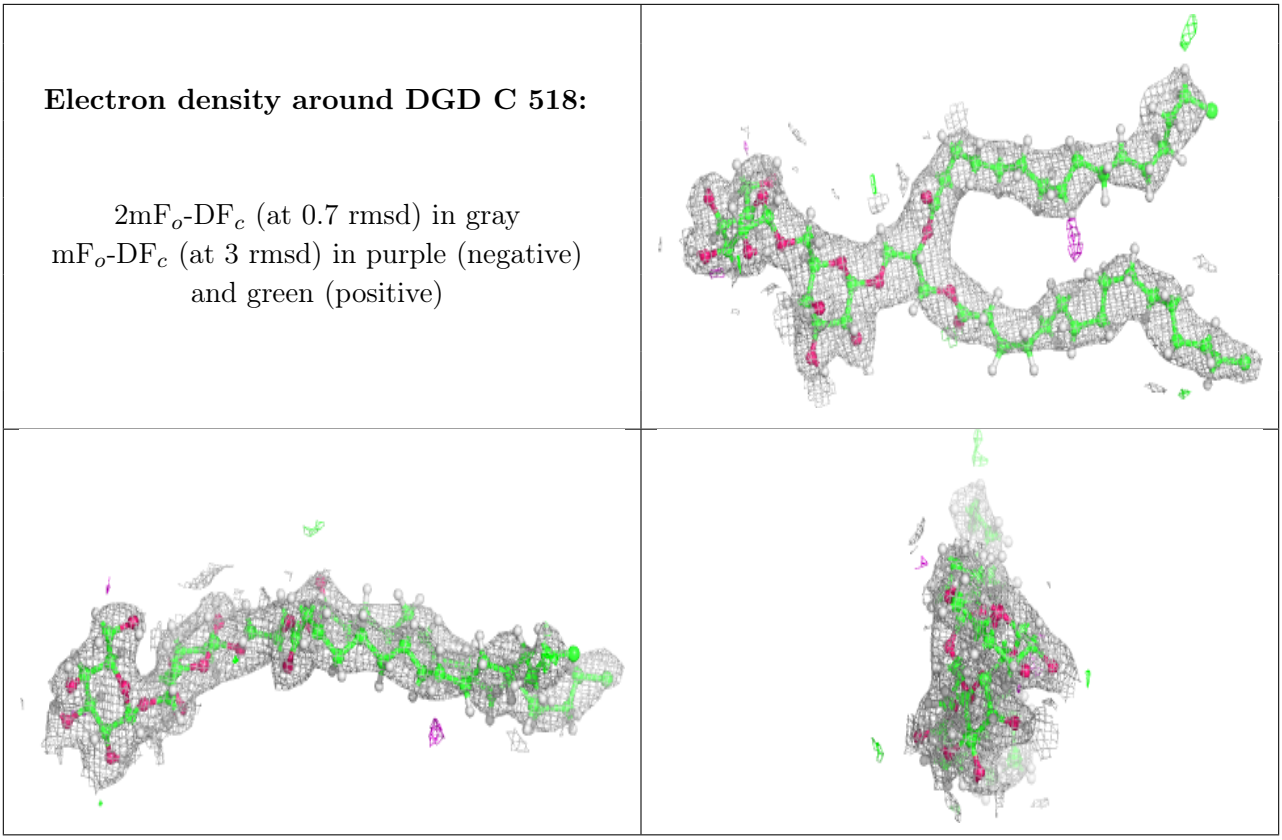






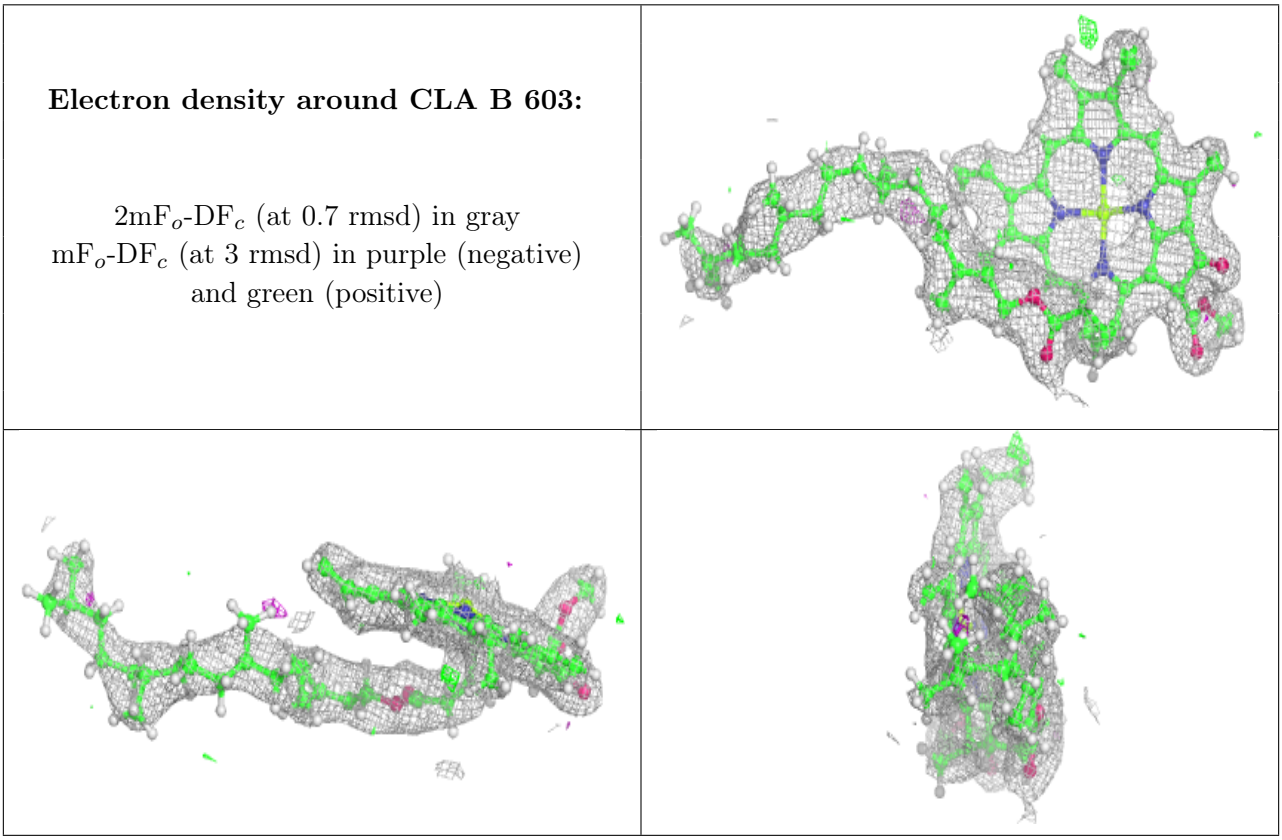
Electron density around DGD C 518:

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



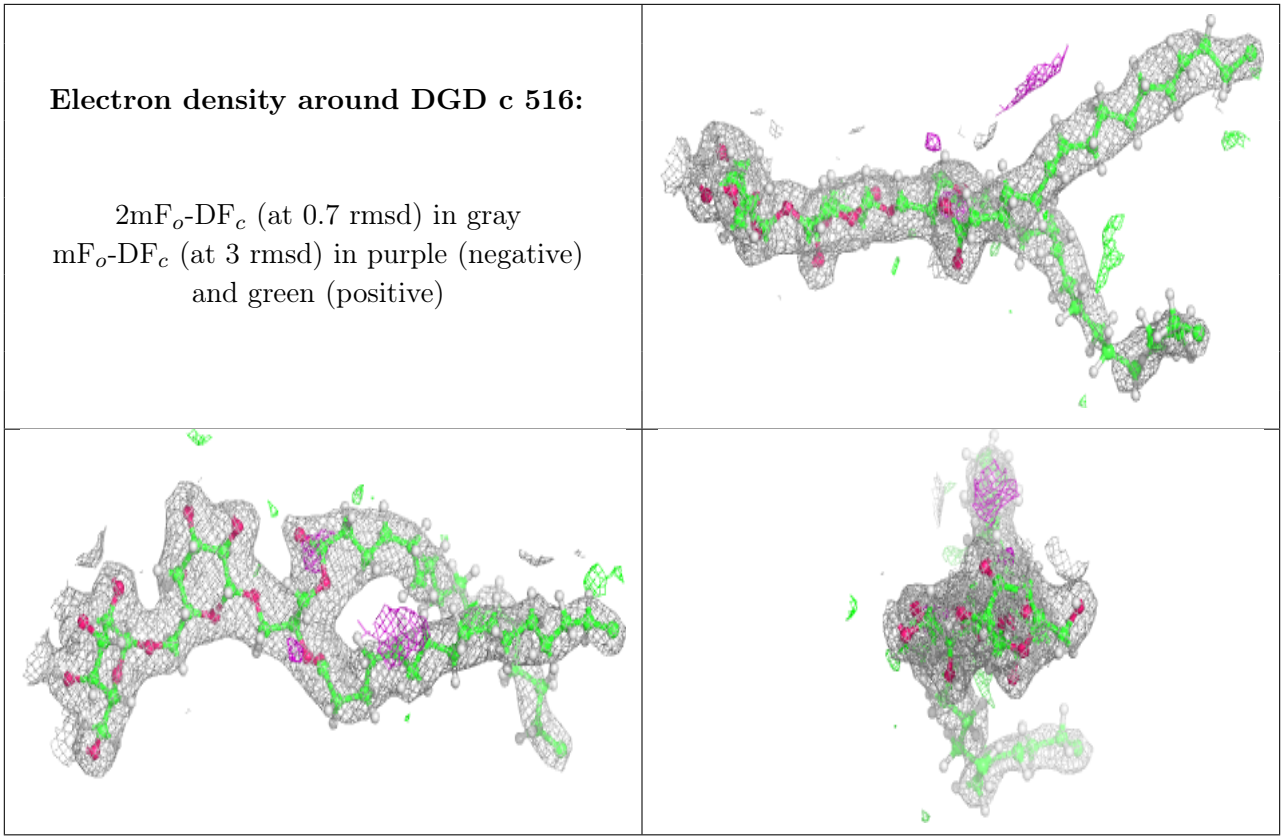
Electron density around CLA B 603:

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



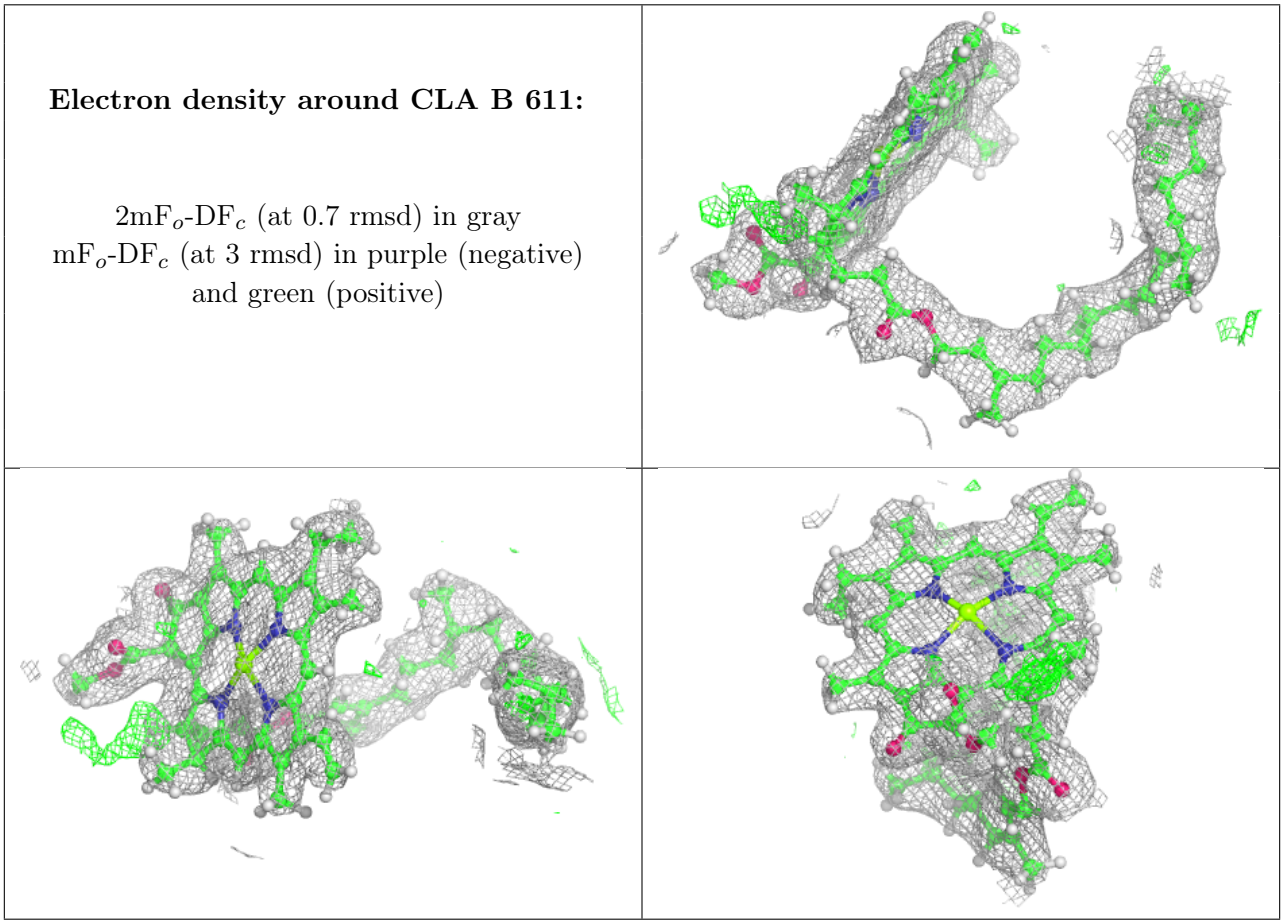
Electron density around DGD c 516:

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



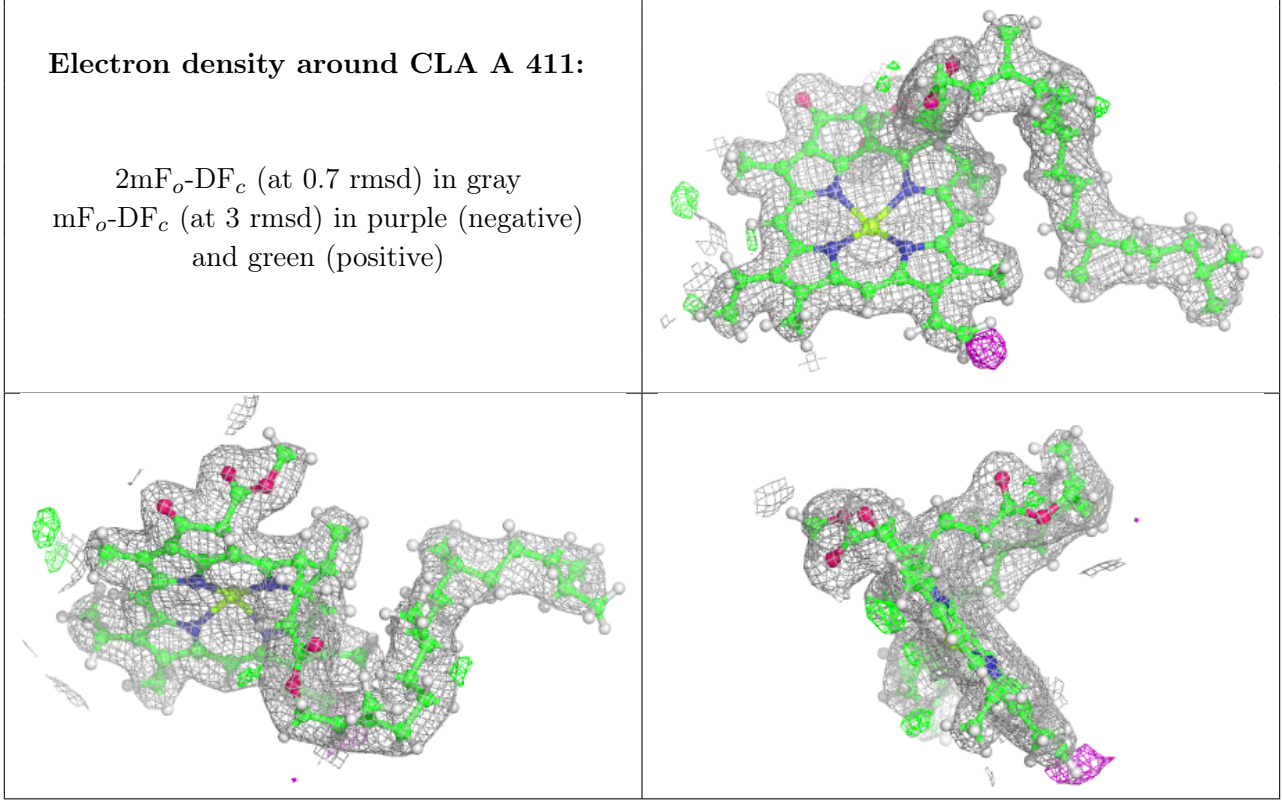
Electron density around CLA B 611:

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



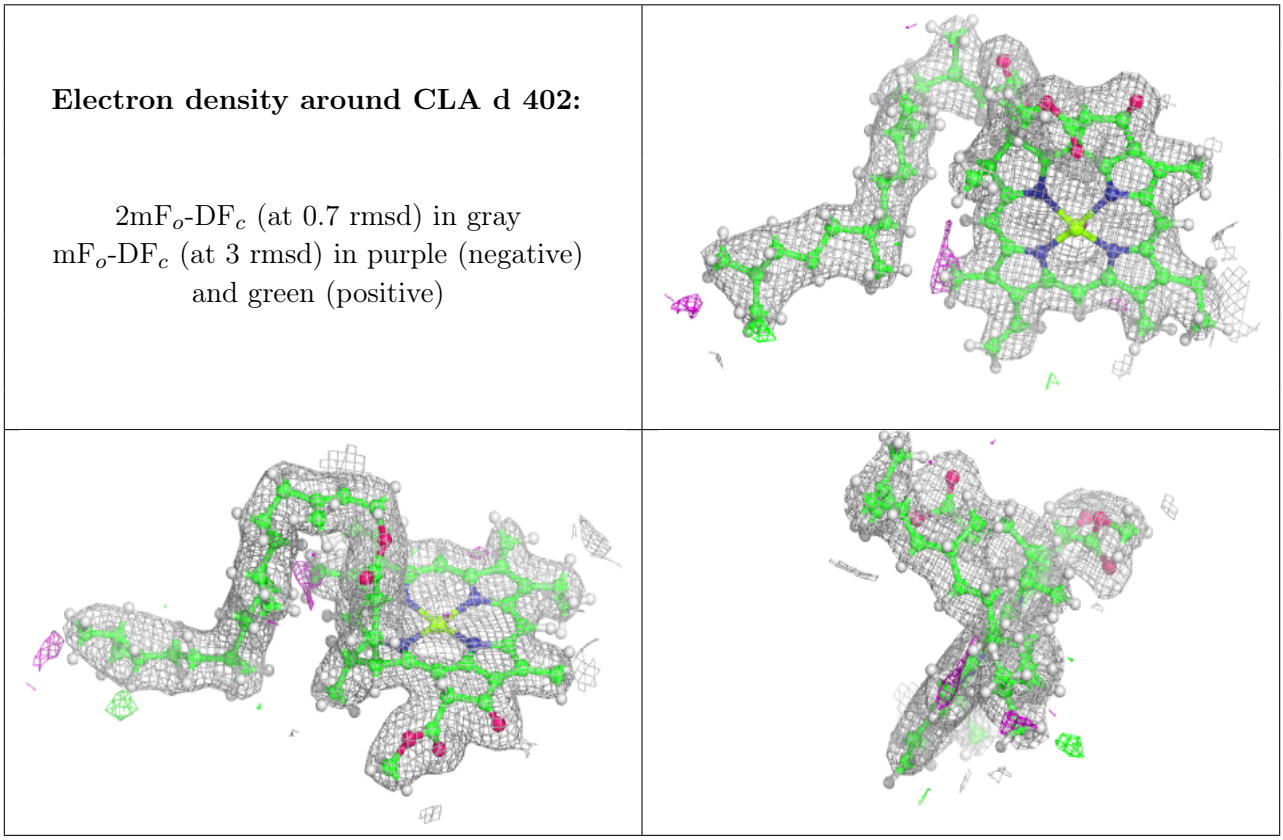
Electron density around CLA A 411:

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



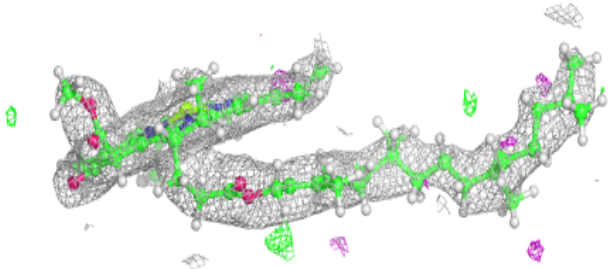
Electron density around CLA d 402:

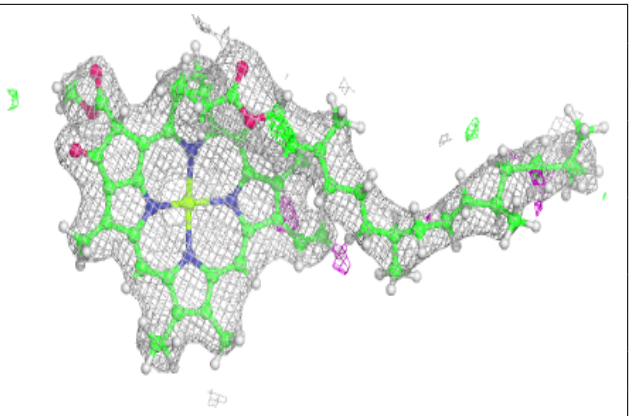
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

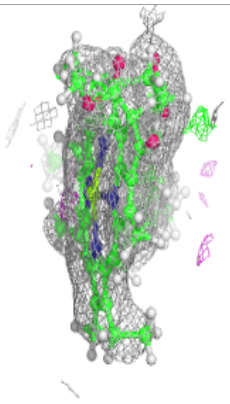


Electron density around CLA b 604:

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

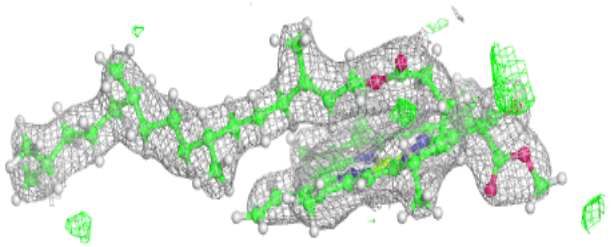


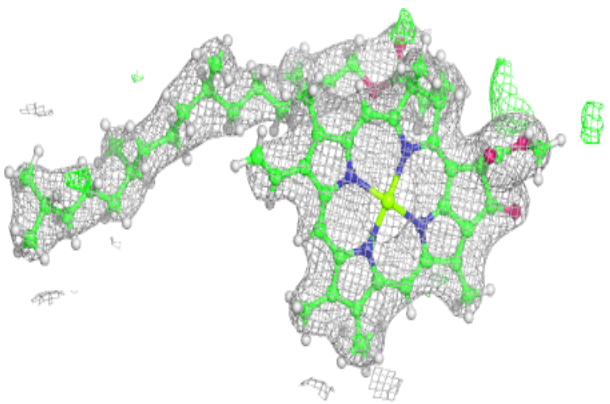


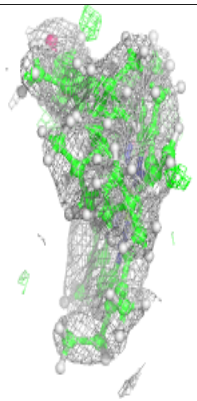


Electron density around CLA c 501:

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

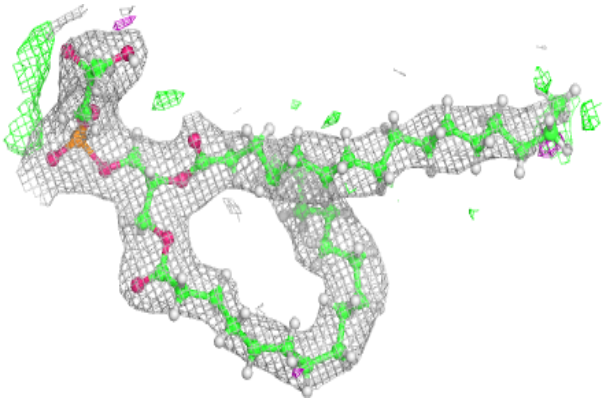


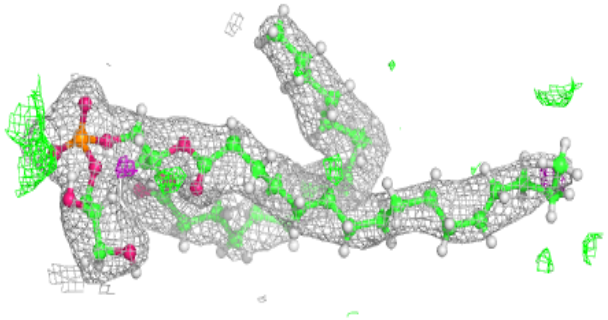


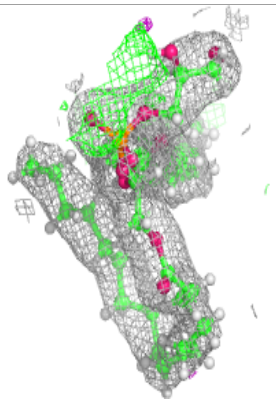


Electron density around LHG B 623:

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

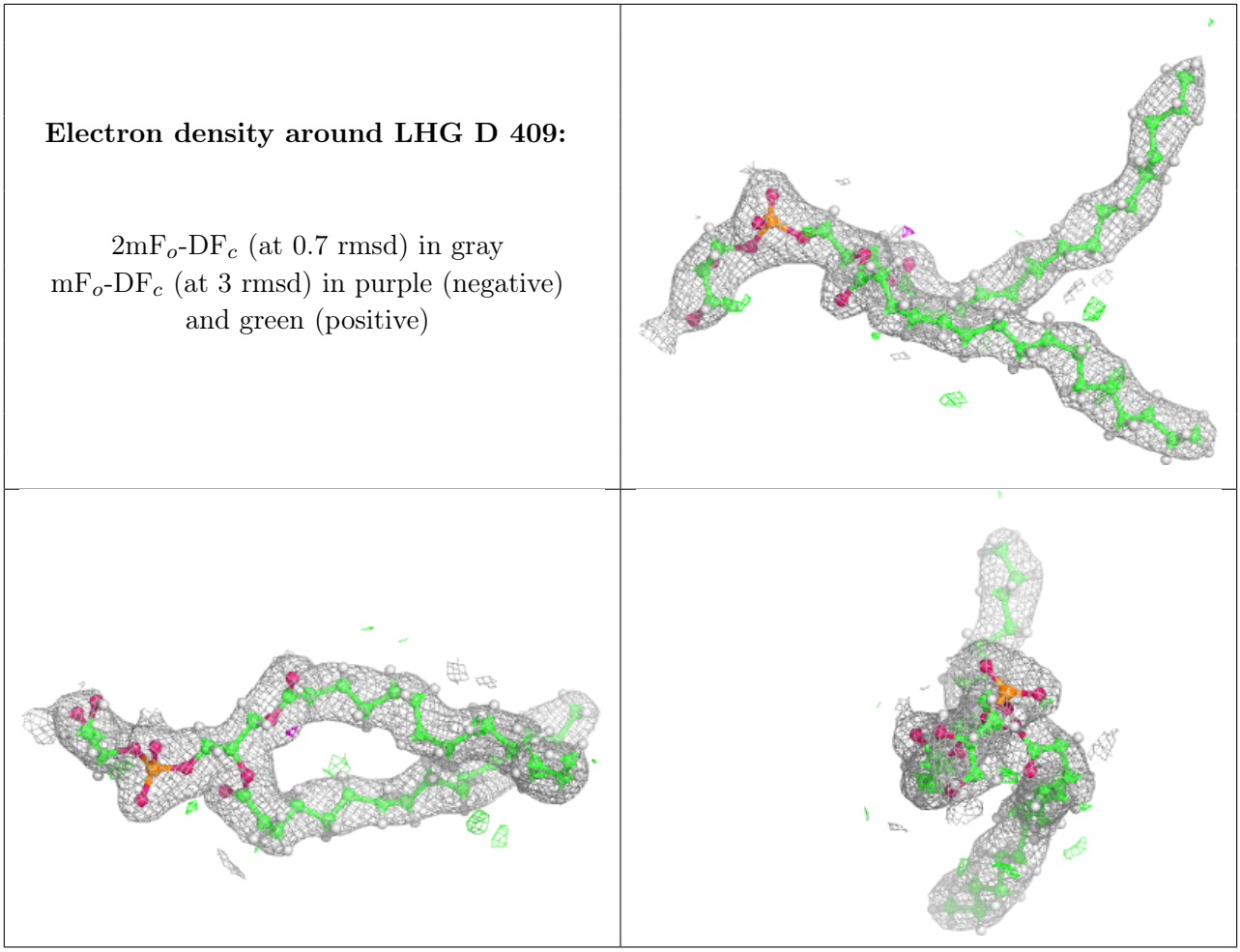






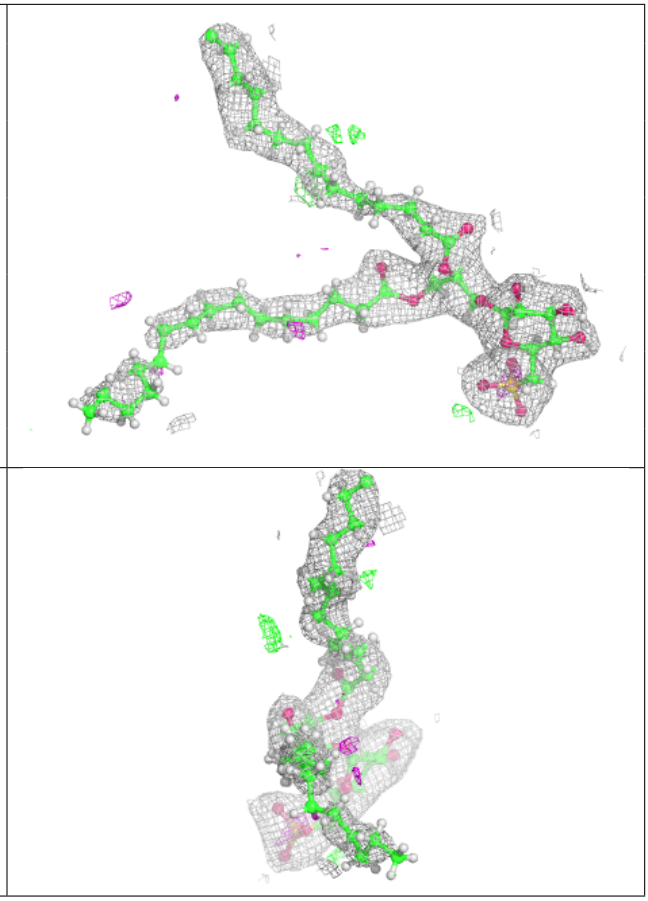
Electron density around LHG D 409:

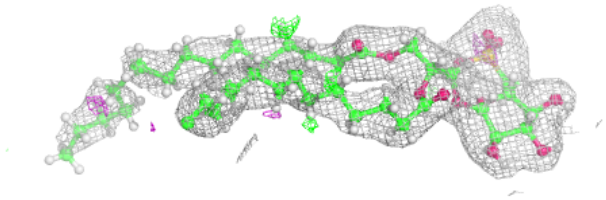
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SQD A 412:

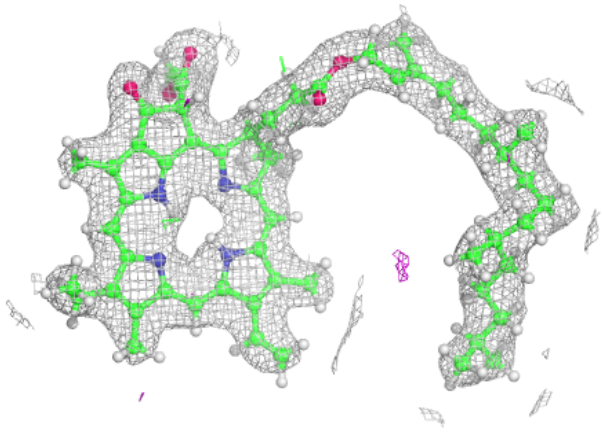
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

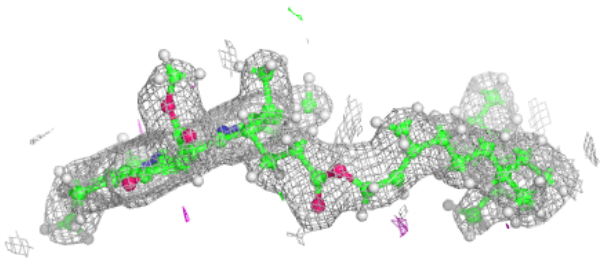


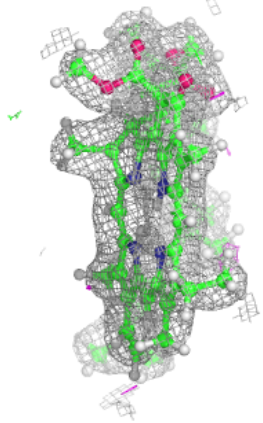


Electron density around PHO A 406:

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

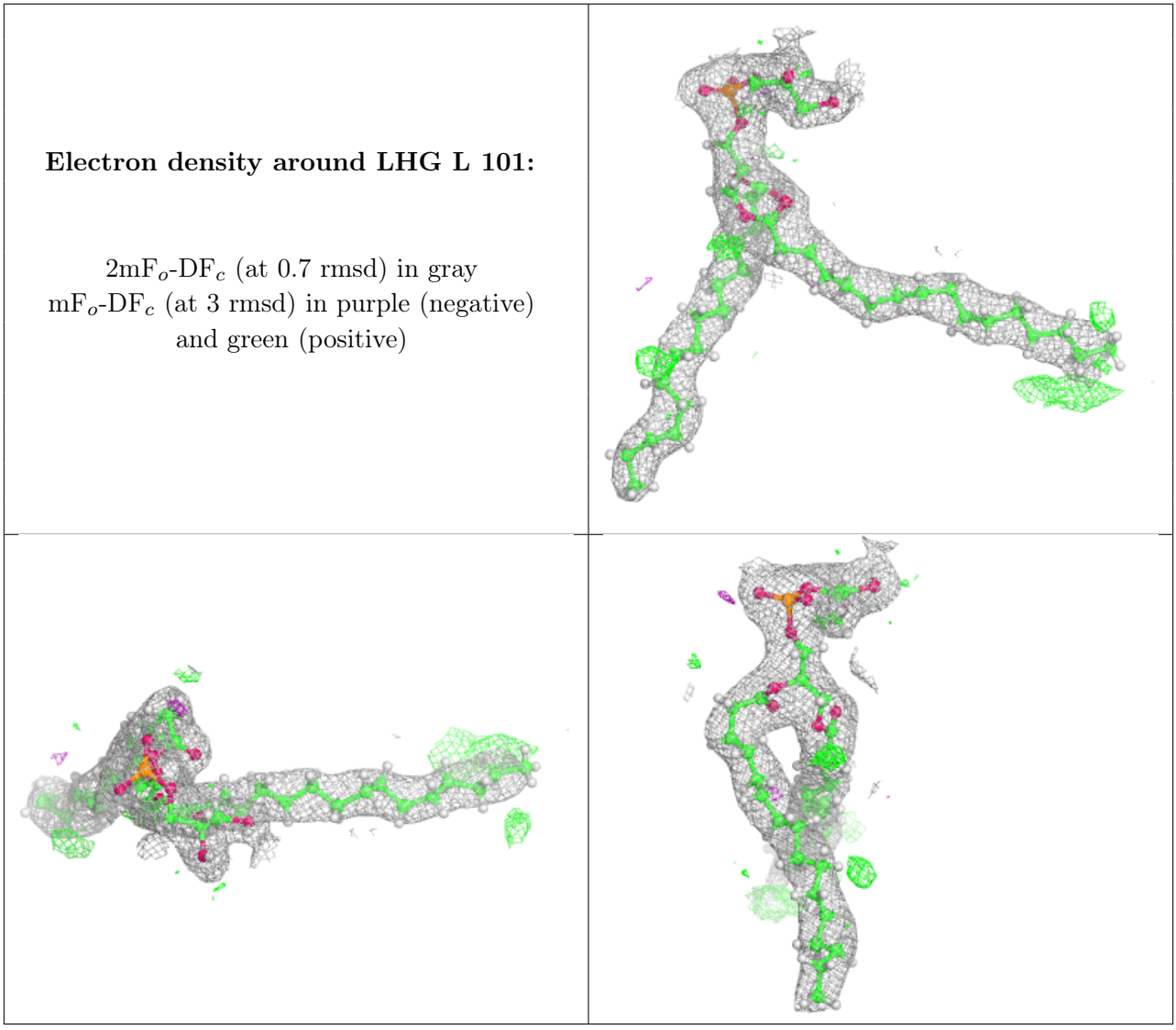






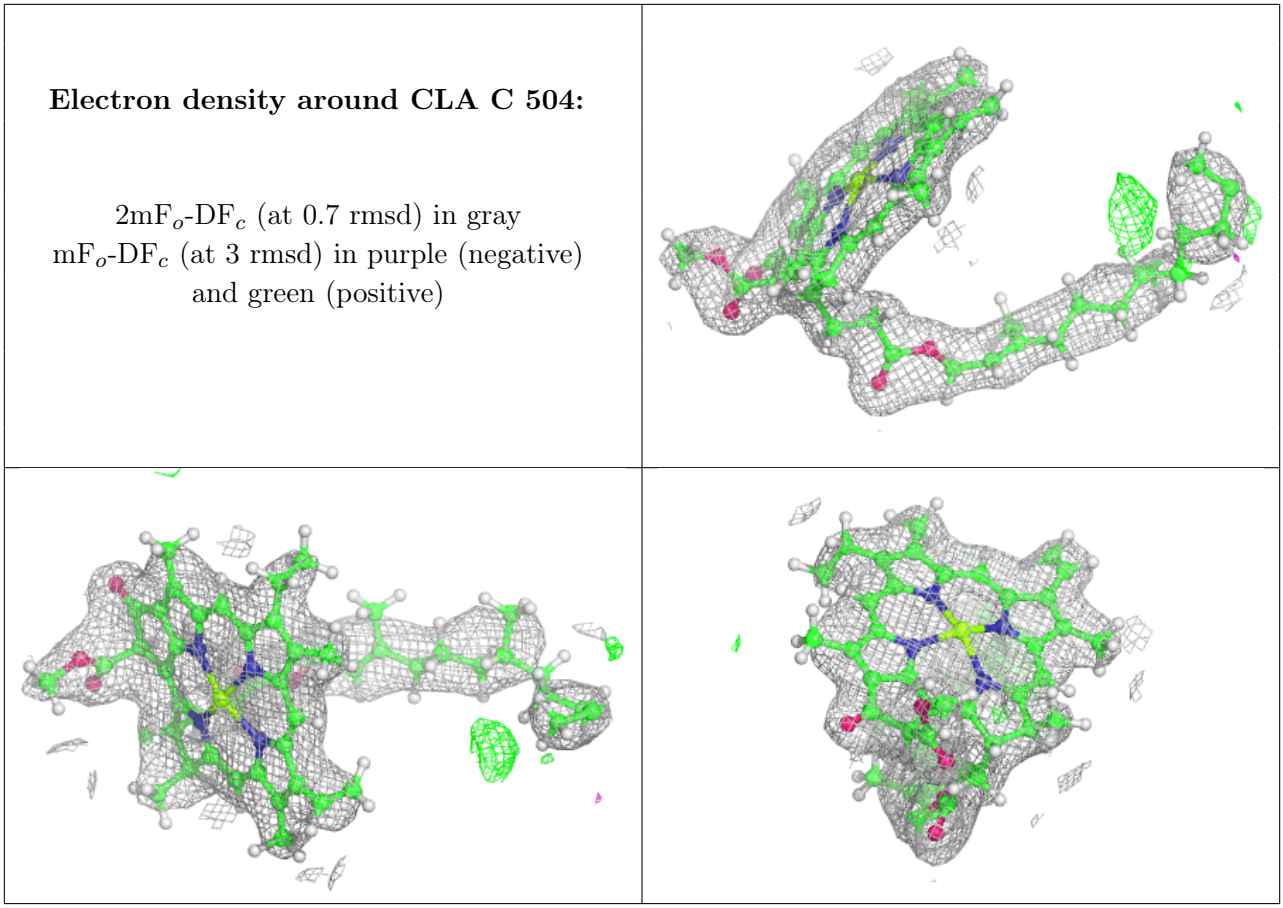
Electron density around LHG L 101:

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



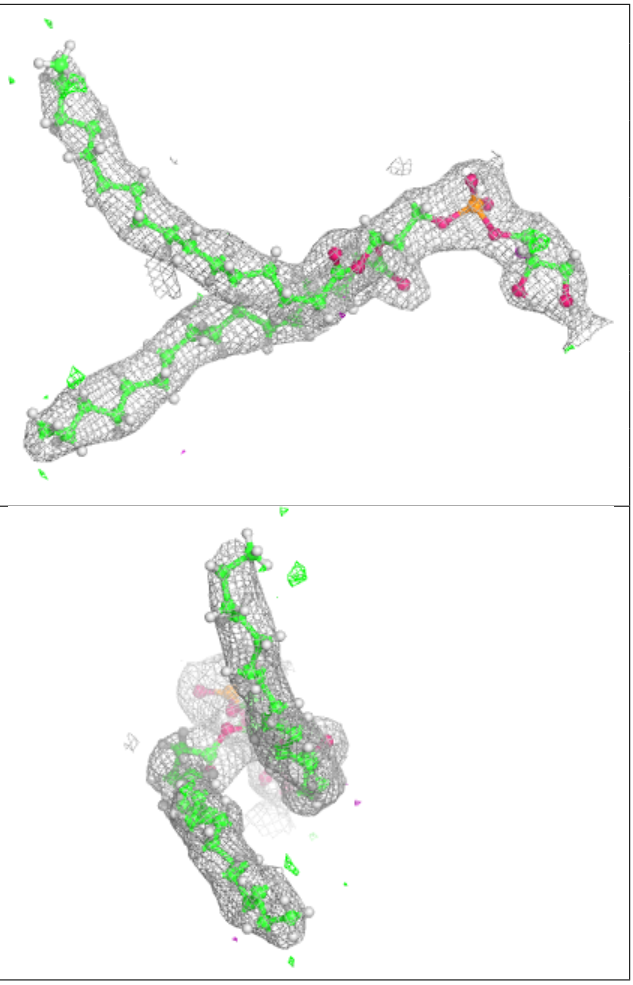
Electron density around CLA C 504:

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



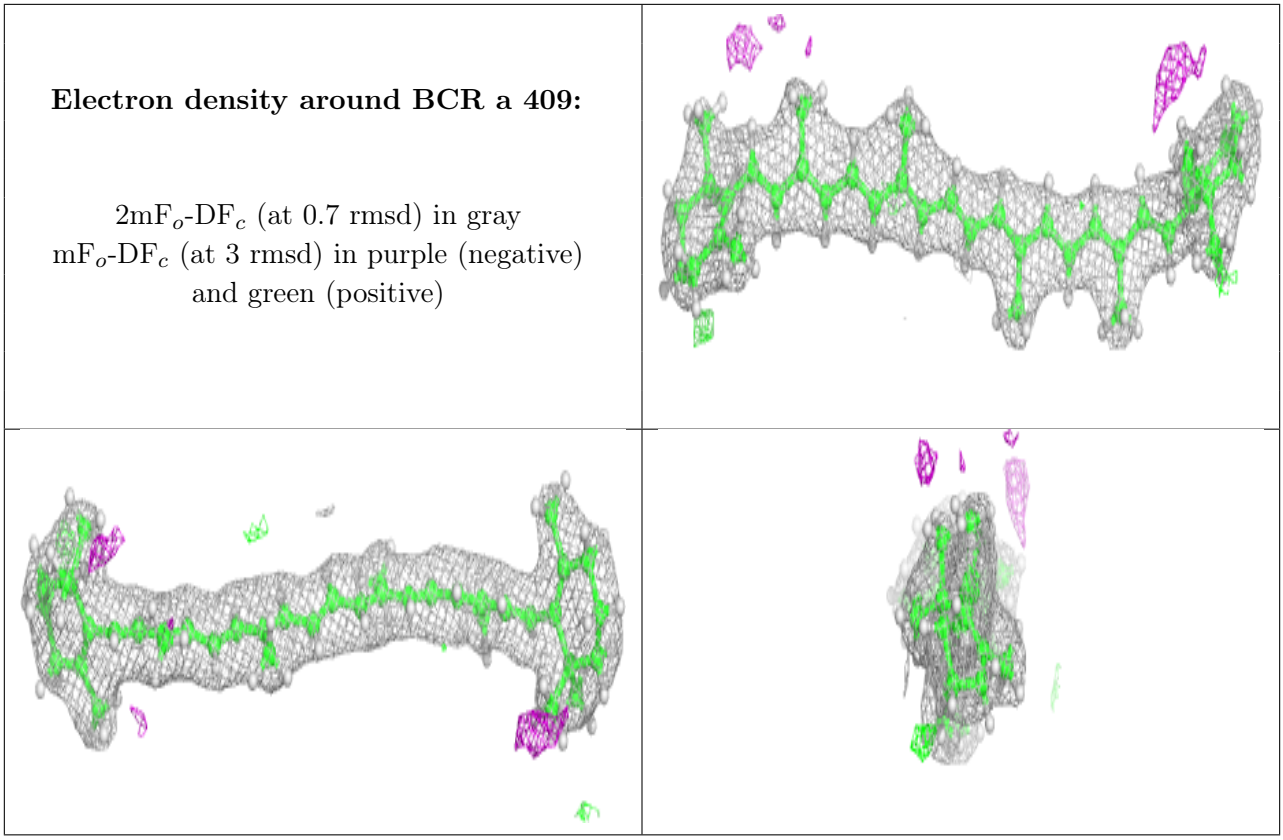
Electron density around LHG d 408:

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



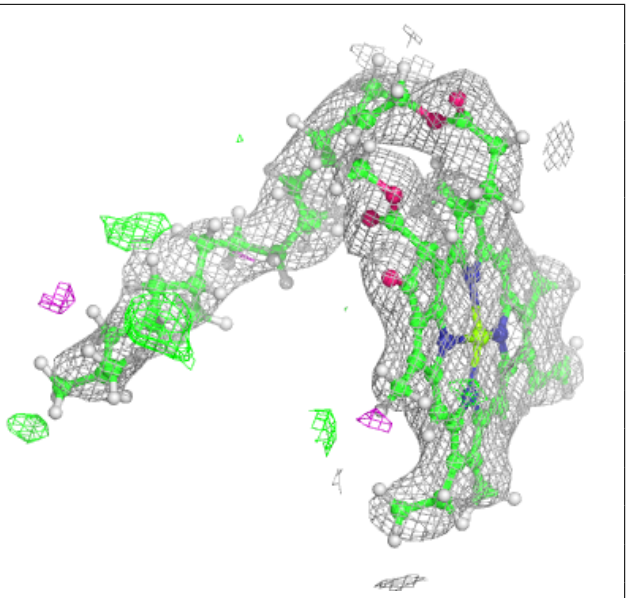
Electron density around BCR a 409:

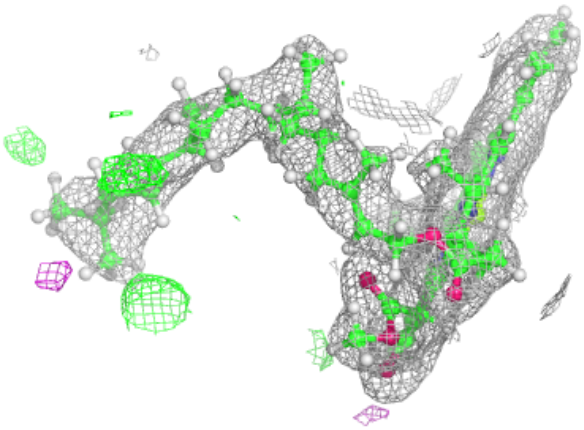
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

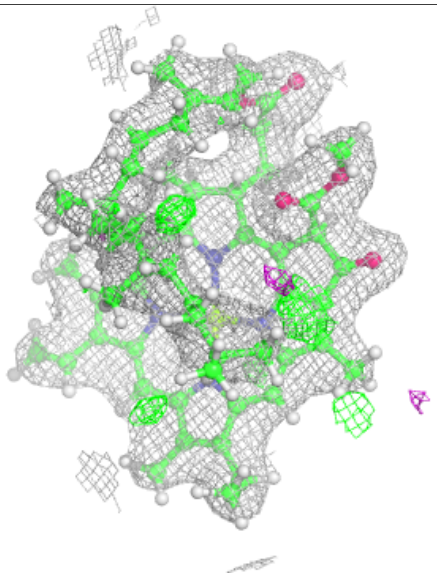


Electron density around CLA B 613:

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

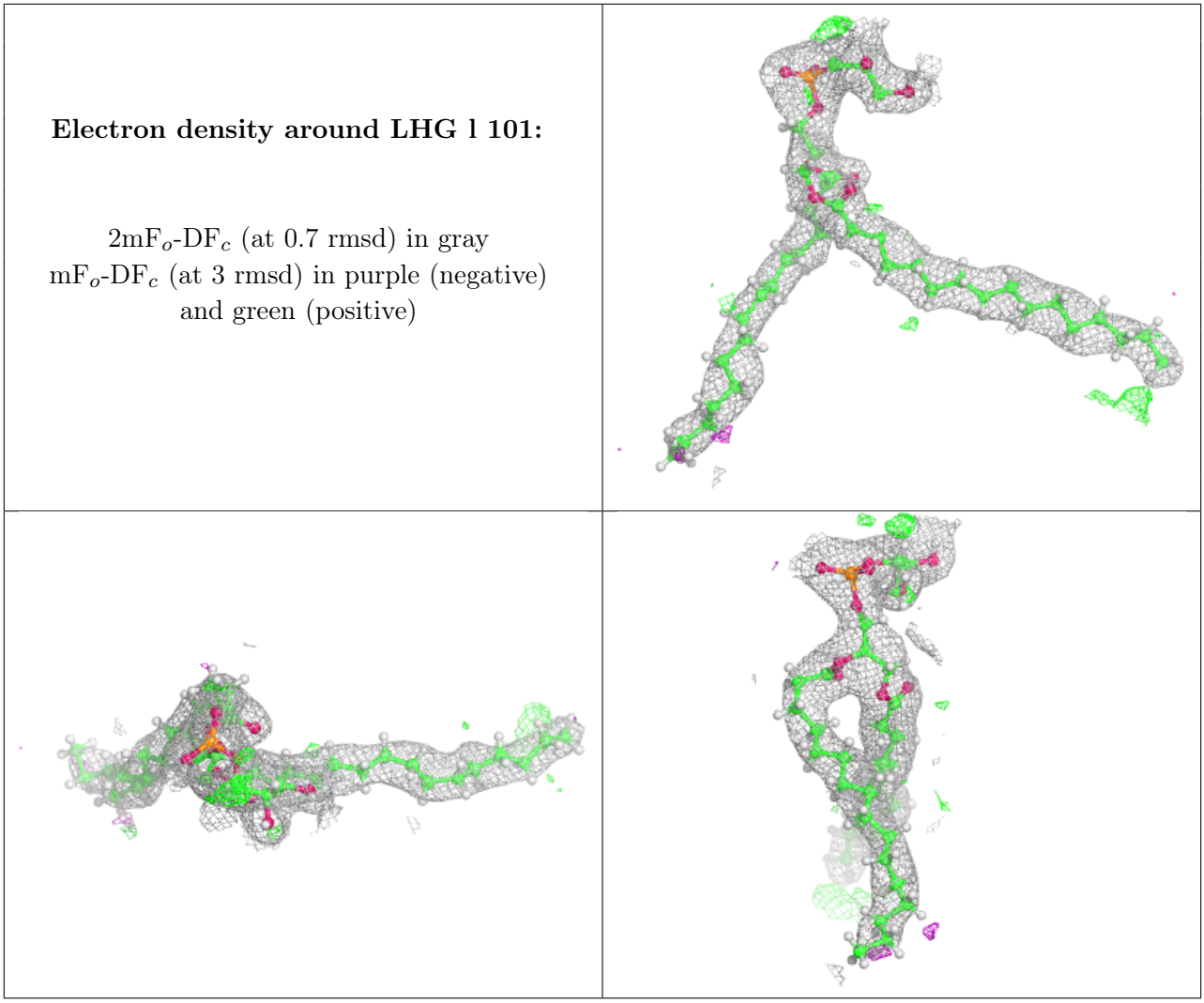






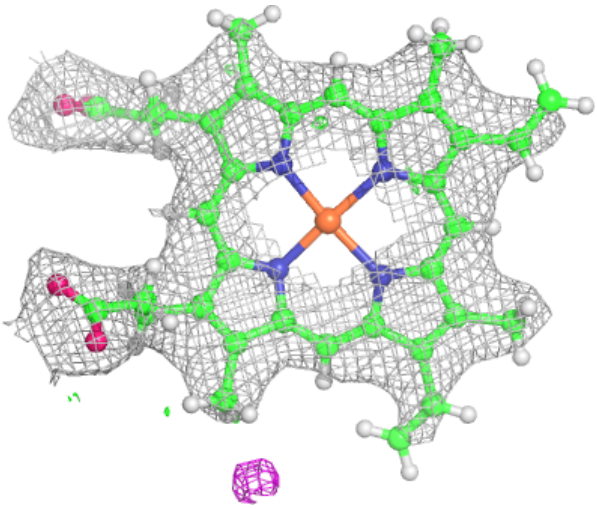
Electron density around LHG l 101:

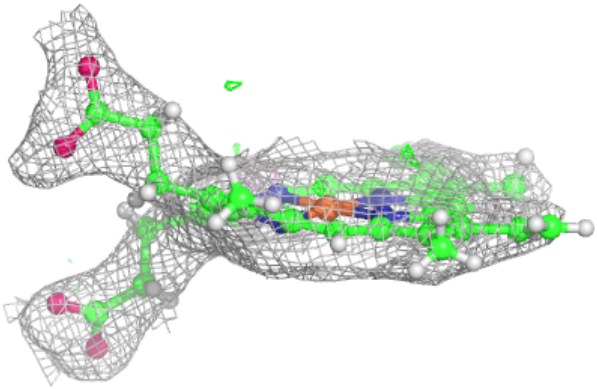
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

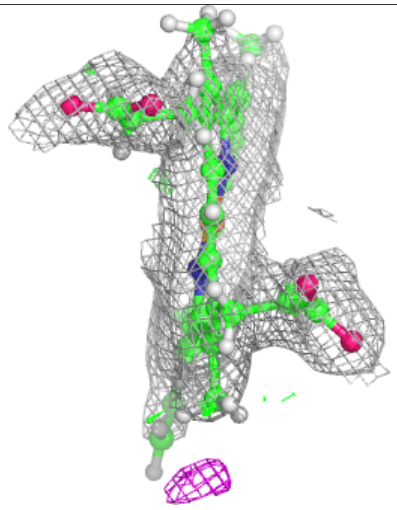


Electron density around HEM F 101:

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

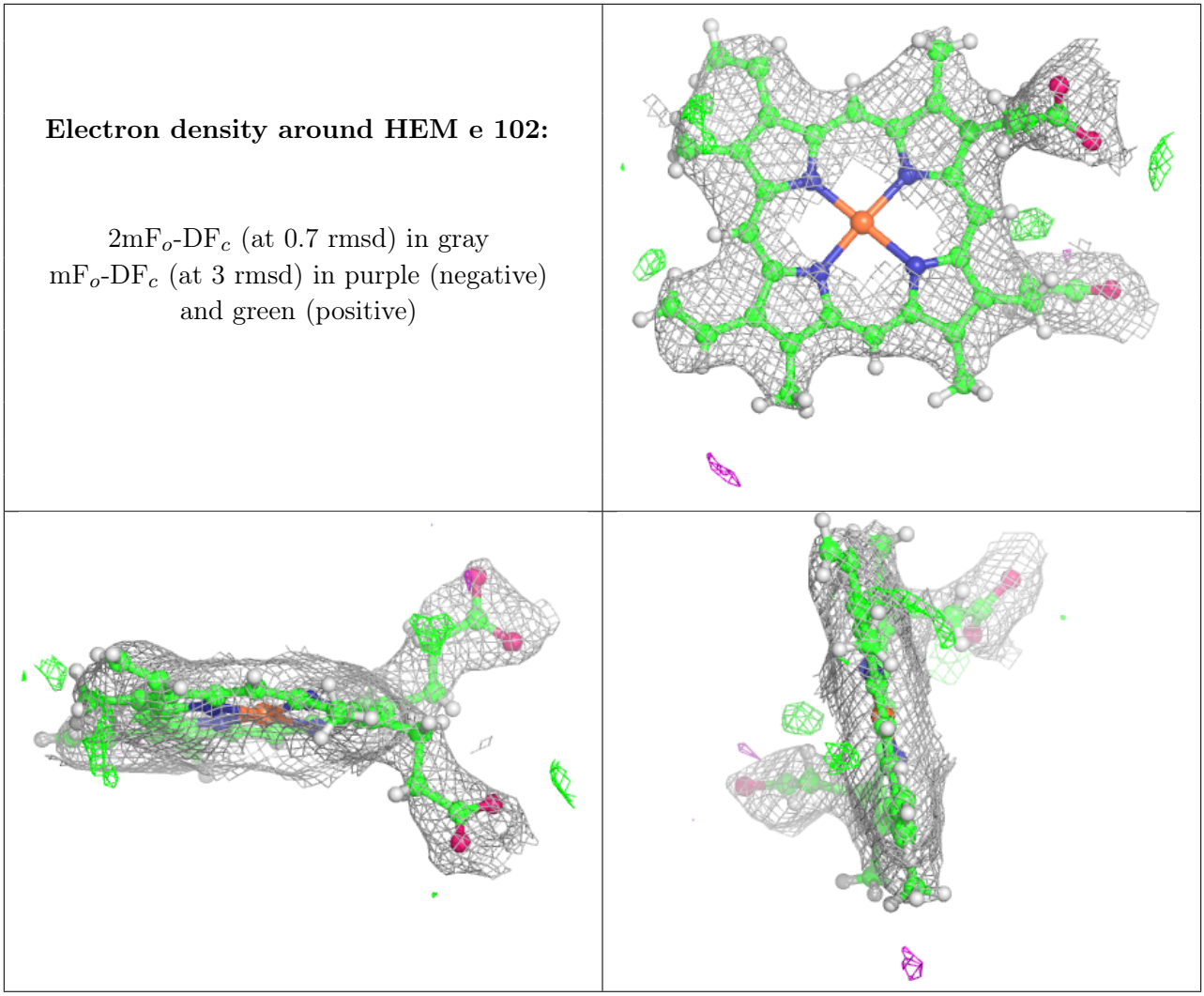






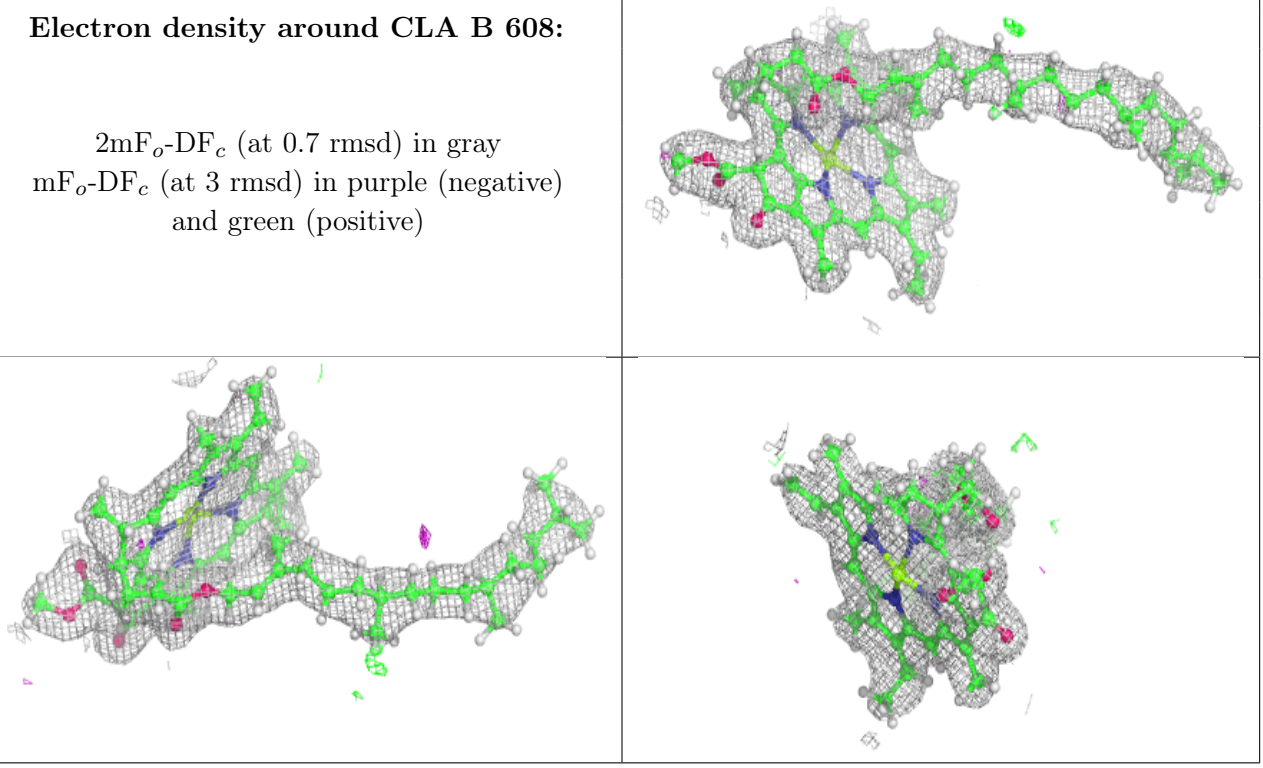
Electron density around HEM e 102:

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



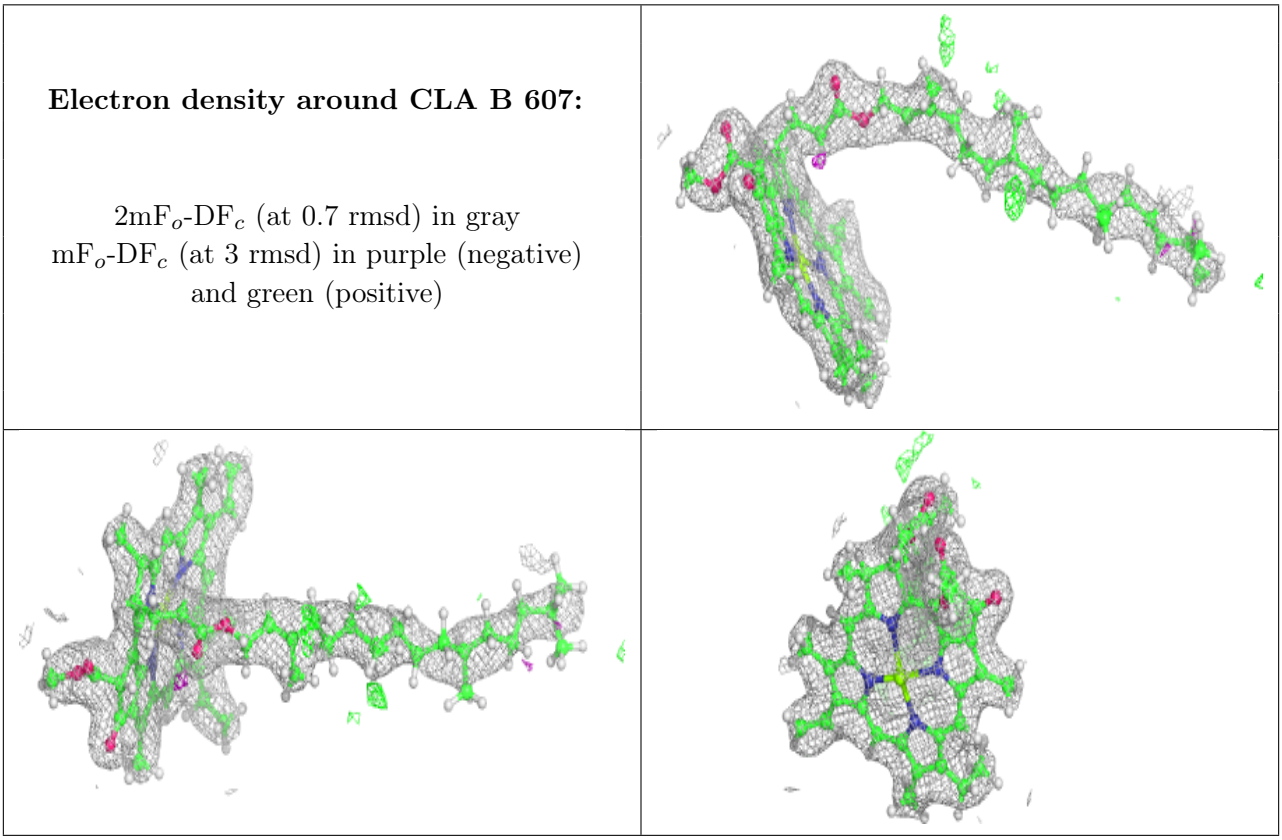
Electron density around CLA B 608:

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



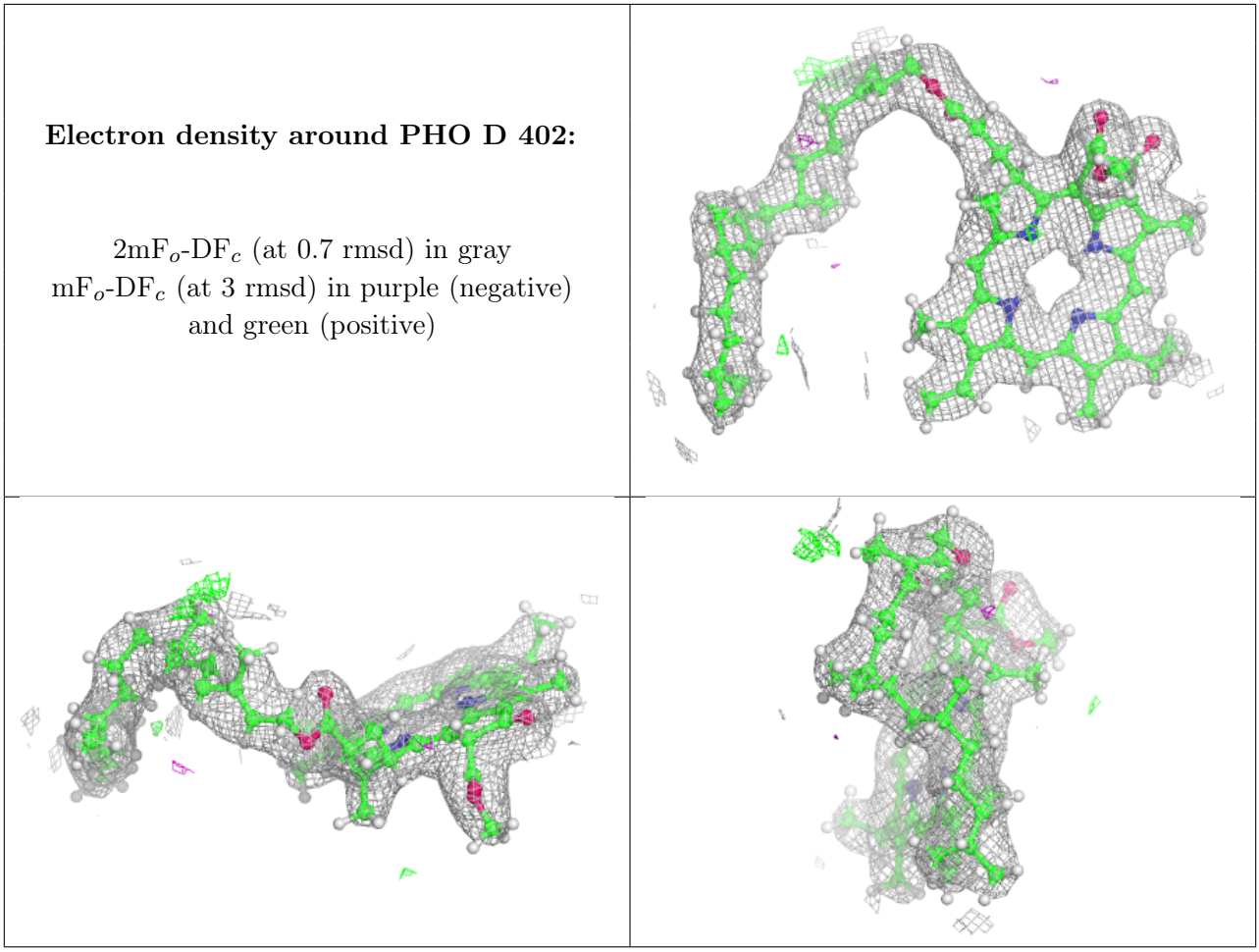
Electron density around CLA B 607:

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



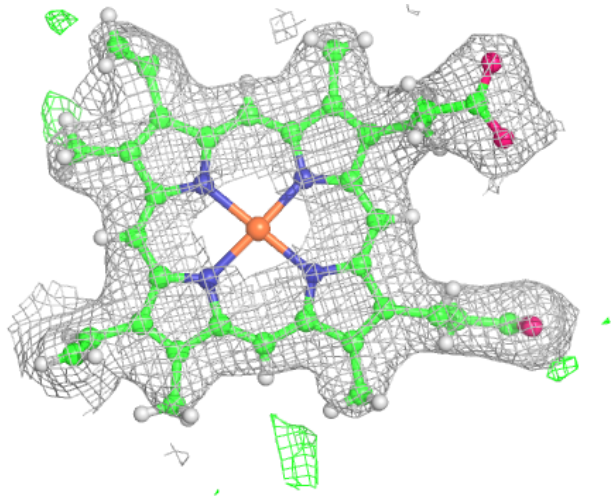
Electron density around PHO D 402:

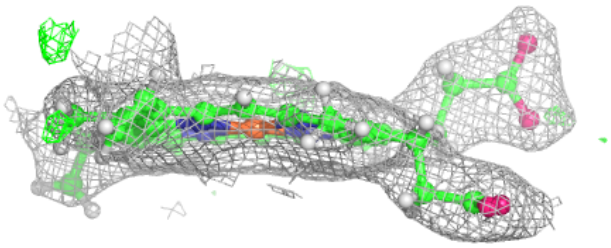
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC v 201:

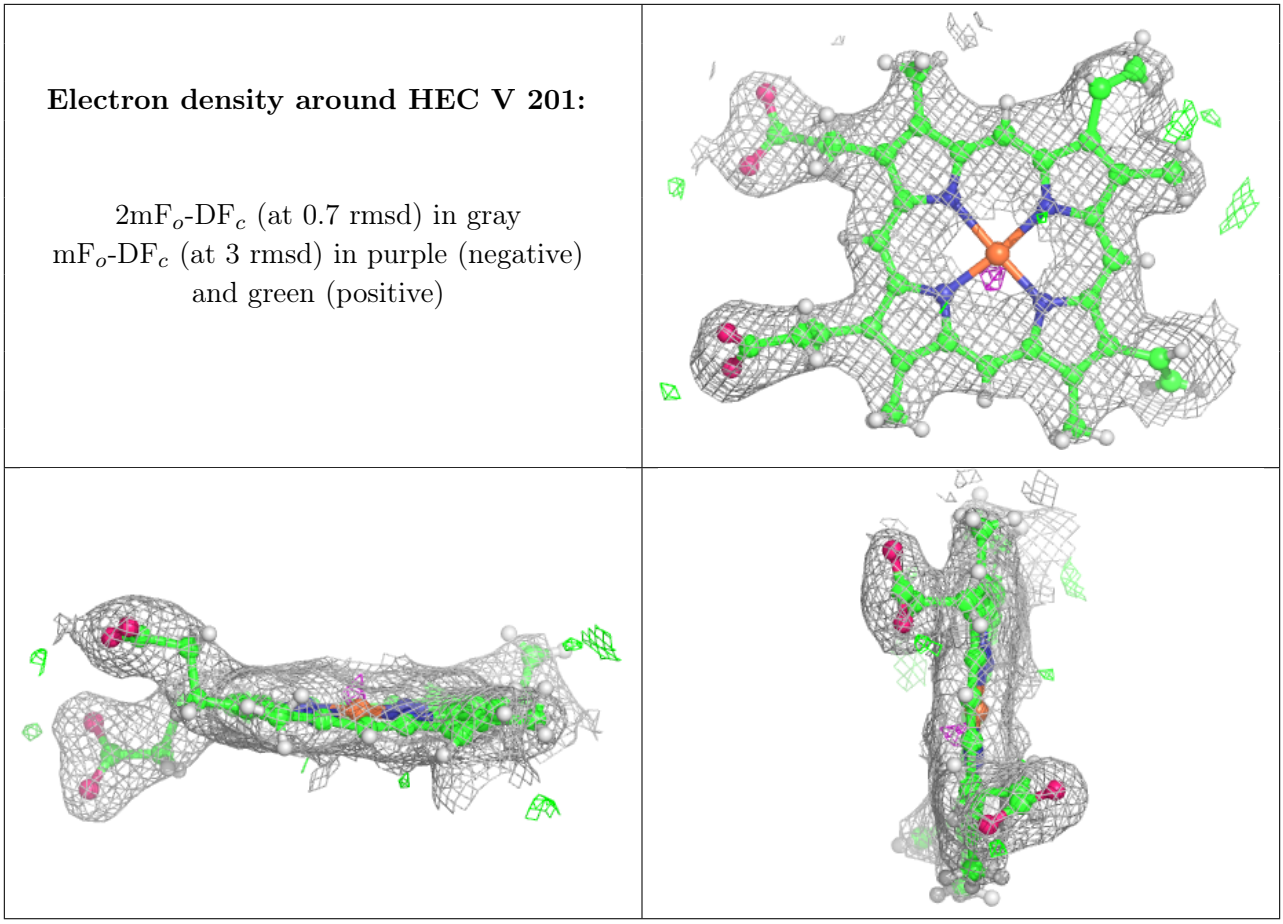
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around HEC V 201:

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



6.5 Other polymers (i)

There are no such residues in this entry.