Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 07:22 AM EST

PDB ID	:	6DHP
Title	:	RT XFEL structure of the three-flash state of Photosystem II (3F, S0-rich) at 2.04 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	:	2.04 Å(reported)

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

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

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

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

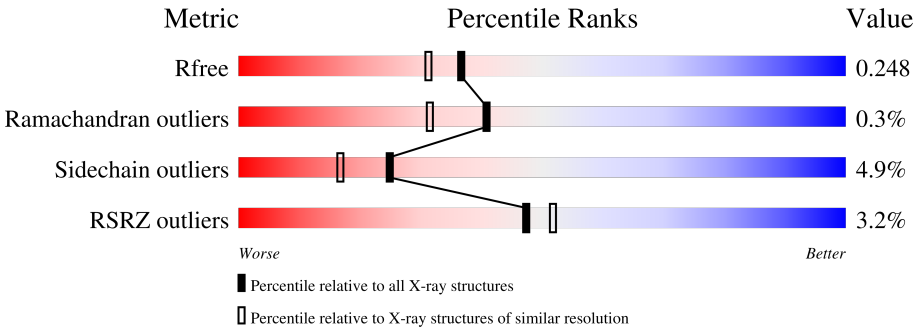
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.04 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)

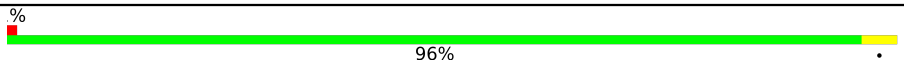
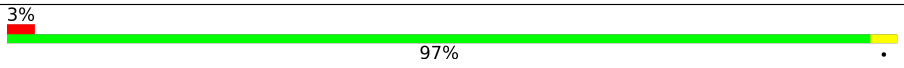
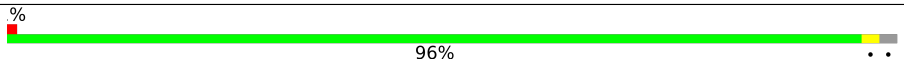
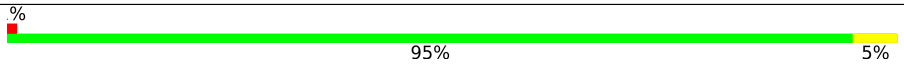
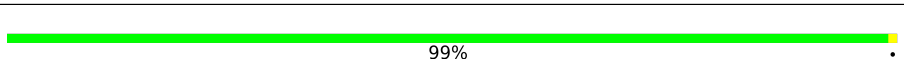
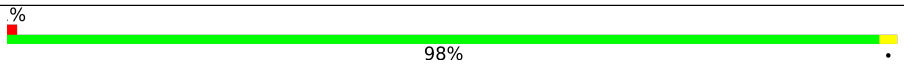
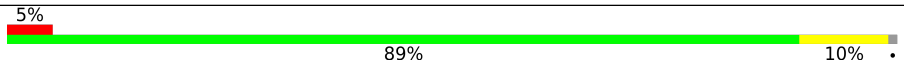
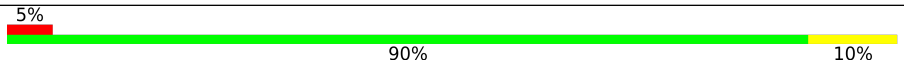
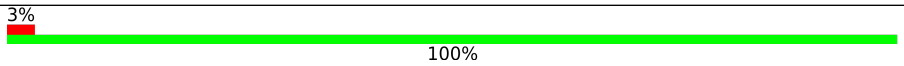
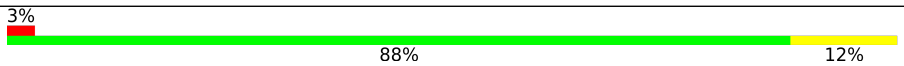
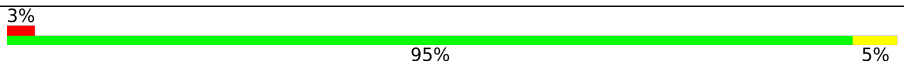
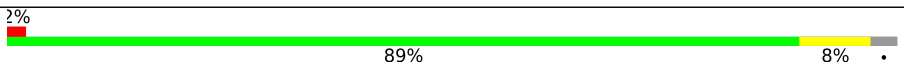
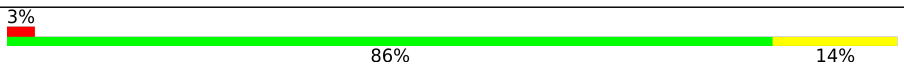
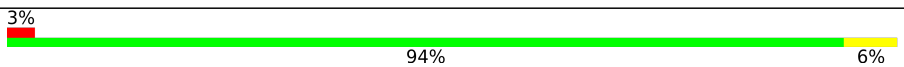
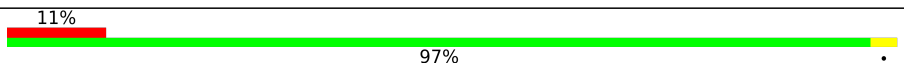
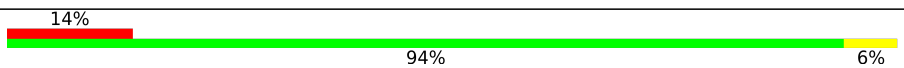
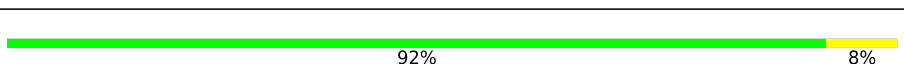
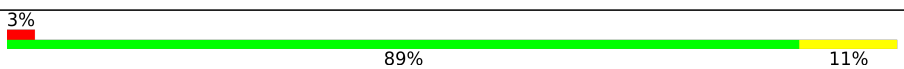
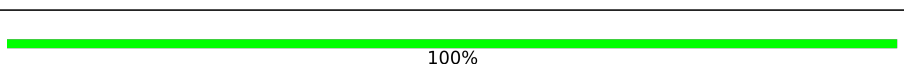
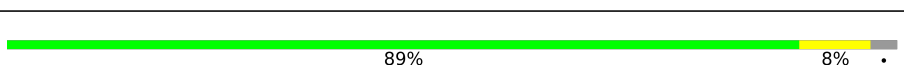
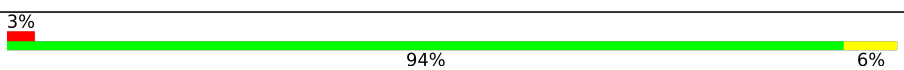
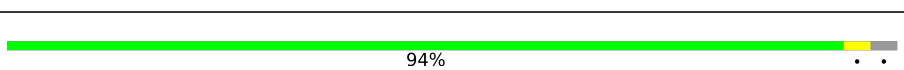
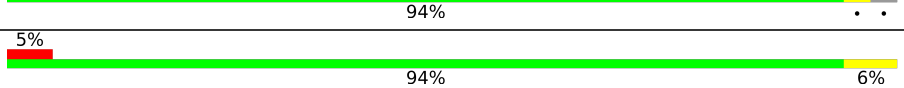
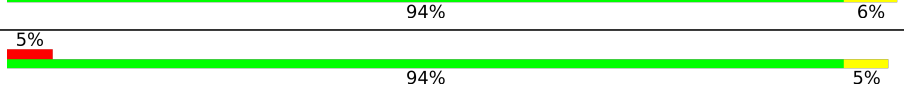
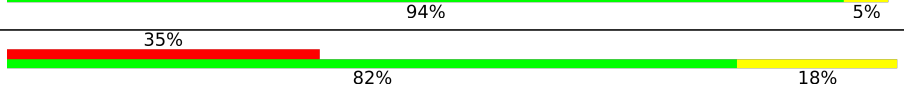
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	97%
1	a	334	96%

Continued on next page...

buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

Continued from previous page...

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	R	34	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	r	34	53% 74% 18% 9%
15	T	30	7% 83% 13%
15	t	30	7% 97%
16	U	97	3% 97%
16	u	97	% 99%
17	V	137	96%
17	v	137	% 97%
18	X	38	8% 97%
18	x	38	8% 95% 5%
19	Y	30	30% 77% 10% 10%
19	y	30	17% 87% 13%
20	Z	62	24% 82% 16%
20	z	62	19% 85% 15%

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	603	X	-	-	-
23	CLA	A	607	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	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	-	-	-
23	CLA	C	501	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	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	a	603	X	-	-	-
23	CLA	a	606	X	-	-	-
23	CLA	a	612	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	609	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	c	501	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	508	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	-	-	-
23	CLA	h	101	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 105751 atoms, of which 52470 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	59	0
			6018	2010	2937	507	545	19			
1	a	334	Total	C	H	N	O	S	0	59	0
			6006	2007	2928	507	545	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	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	7	0
			6868	2282	3392	579	601	14			
3	c	451	Total	C	H	N	O	S	0	8	0
			7017	2324	3464	596	619	14			

- 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	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	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			

Continued on next page...

Continued from previous page...

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 protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			
14	r	31	Total	C	H	N	O	0	0	0
			461	154	234	40	33			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

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

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

- 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			

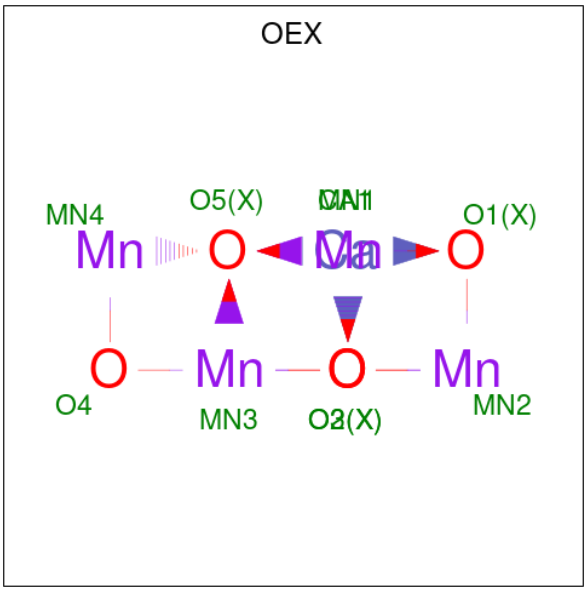
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

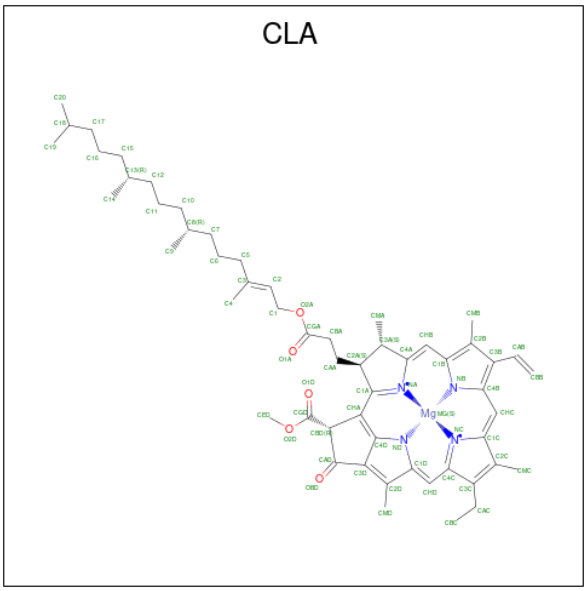


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

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

- 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	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
			102	44	48	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		

Continued on next page...

Continued from previous page...

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
			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		
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		

Continued on next page...

Continued from previous page...

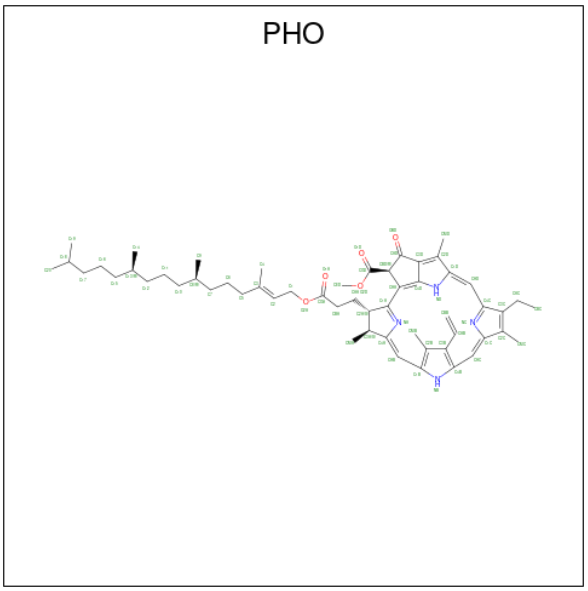
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total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

Continued on next page...

Continued from previous page...

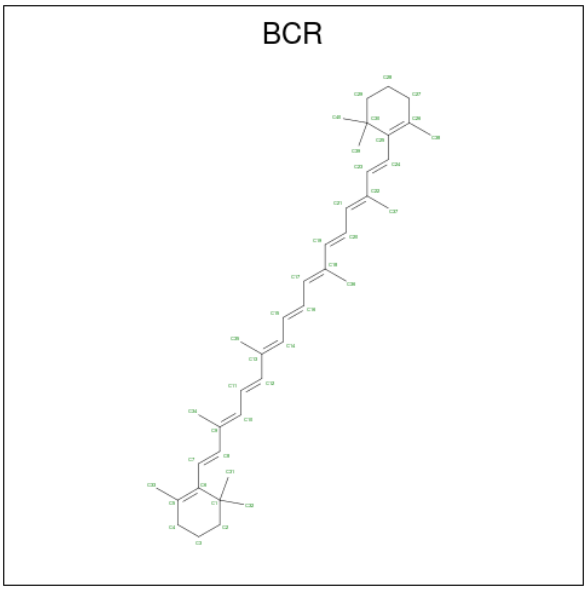
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	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		
23	h	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	A	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 BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

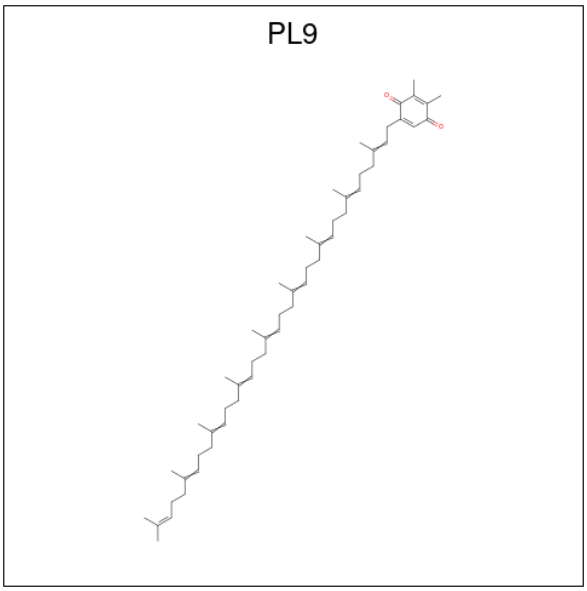


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	B	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	C	1	Total C H 96 40 56	0	0
25	D	1	Total C H 96 40 56	0	0
25	H	1	Total C H 96 40 56	0	0
25	T	1	Total C H 96 40 56	0	0
25	Y	1	Total C H 96 40 56	0	0
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	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	d	1	Total C H 96 40 56	0	0
25	h	1	Total C H 96 40 56	0	0
25	k	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 CHLORIDE ION (three-letter code: CL) (formula: Cl).

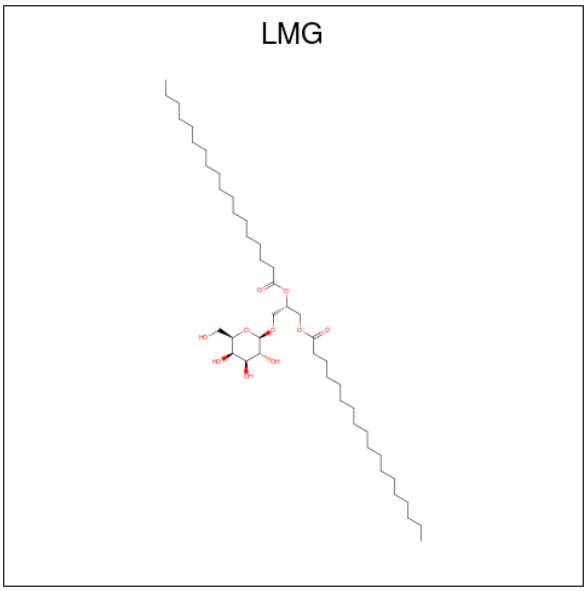
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	2	Total Cl 2 2	0	0
26	a	2	Total Cl 2 2	0	0

- Molecule 27 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
27	A	1	Total C H O 135 53 80 2	0	0
27	D	1	Total C H O 135 53 80 2	0	0
27	a	1	Total C H O 135 53 80 2	0	0
27	d	1	Total C H O 135 53 80 2	0	0

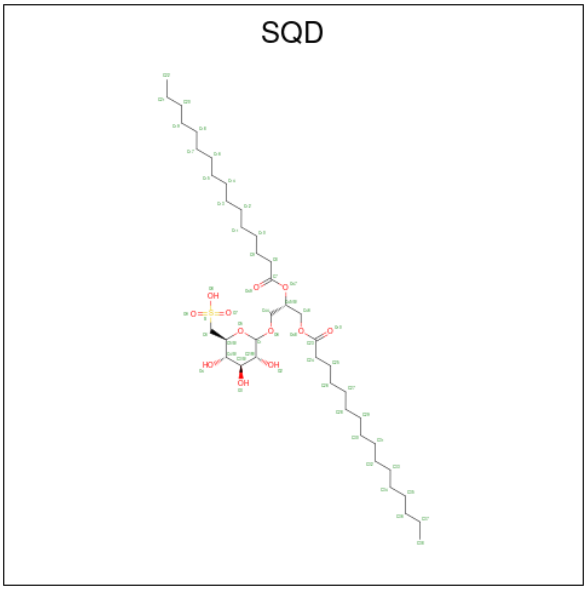
- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

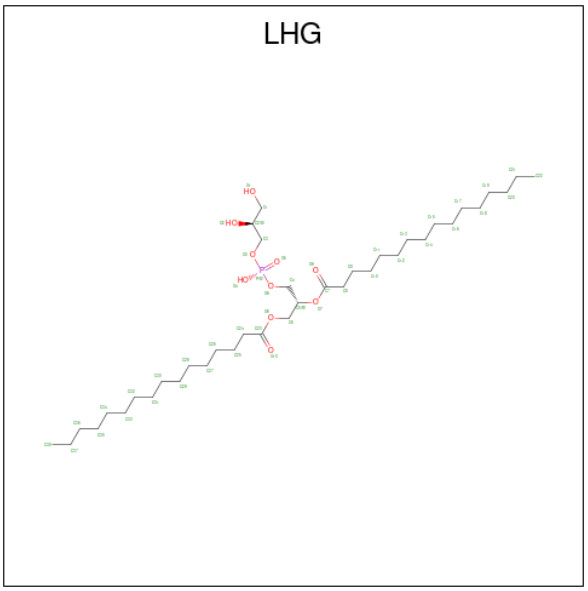
- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

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



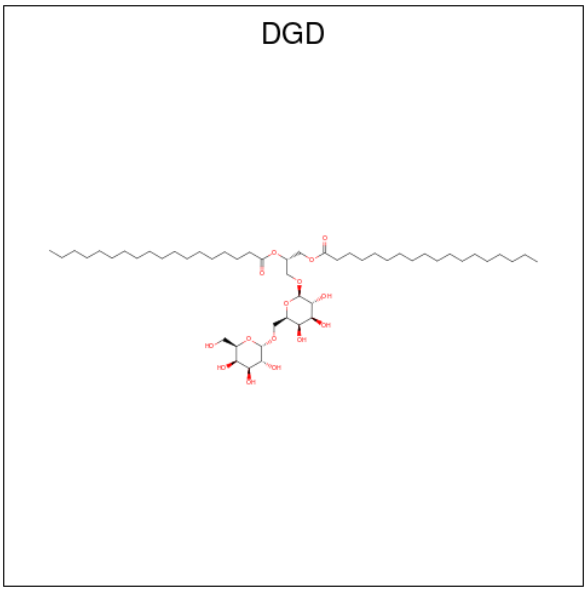
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C H O S 122 39 70 12 1	0	0
29	A	1	Total C H O 104 35 65 4	0	0
29	B	1	Total C H O S 132 41 78 12 1	0	0
29	F	1	Total C H O S 81 25 45 10 1	0	0
29	a	1	Total C H O S 132 41 78 12 1	0	0
29	a	1	Total C H O 92 31 56 5	0	0
29	b	1	Total C H O S 114 36 65 12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

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



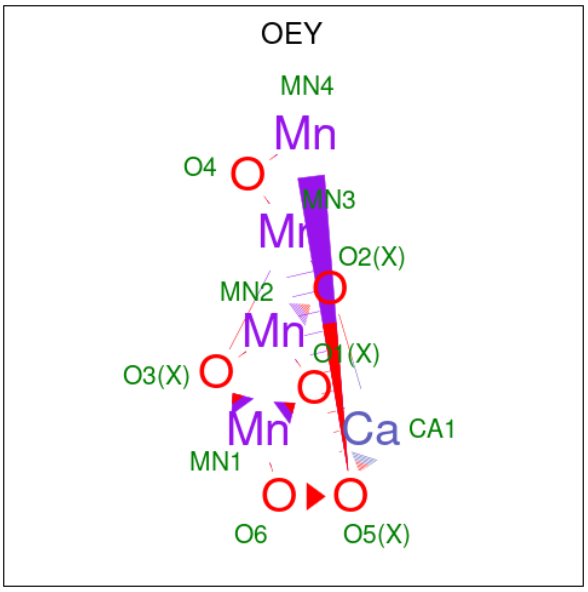
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	a	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
30	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

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



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

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: $CaMn_4O_6$).



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

- Molecule 33 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

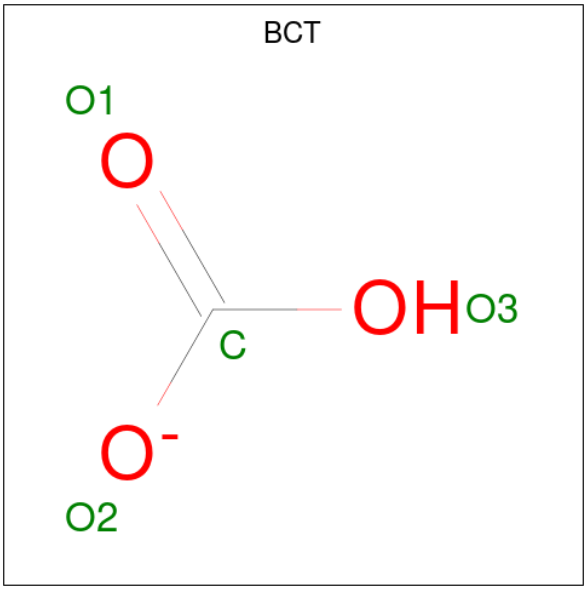
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	5	Total C H O 192 67 117 8	0	0
33	C	3	Total C H O 103 36 63 4	0	0
33	E	1	Total C H O 28 10 16 2	0	0
33	H	1	Total C H 53 18 35	0	0
33	I	1	Total C H 41 15 26	0	0
33	J	1	Total C H O 28 10 16 2	0	0
33	M	2	Total C H O 63 23 38 2	0	0
33	T	2	Total C H 91 31 60	0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

Continued on next page...

Continued from previous page...

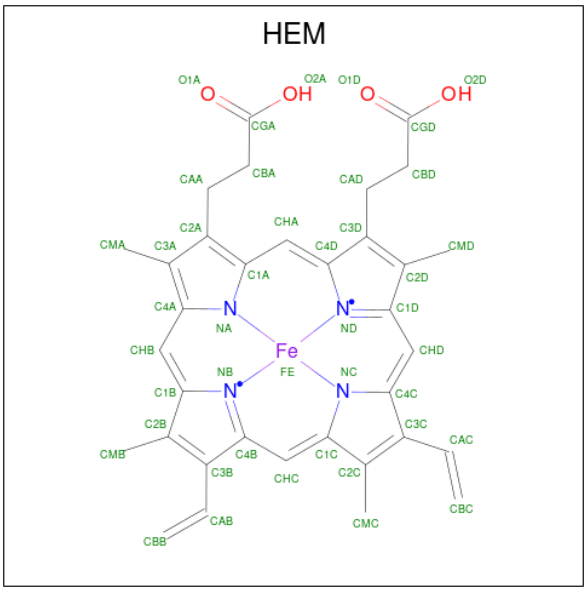
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	b	4	Total C H O 176 60 110 6	0	0
33	c	2	Total C H O 83 28 51 4	0	0
33	d	1	Total C H O 43 15 26 2	0	0
33	j	1	Total C H O 28 10 16 2	0	0
33	l	1	Total C H 53 18 35	0	0
33	m	1	Total C H O 28 10 16 2	0	0
33	t	2	Total C H O 60 22 36 2	0	0
33	x	1	Total C H O 55 18 35 2	0	0

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



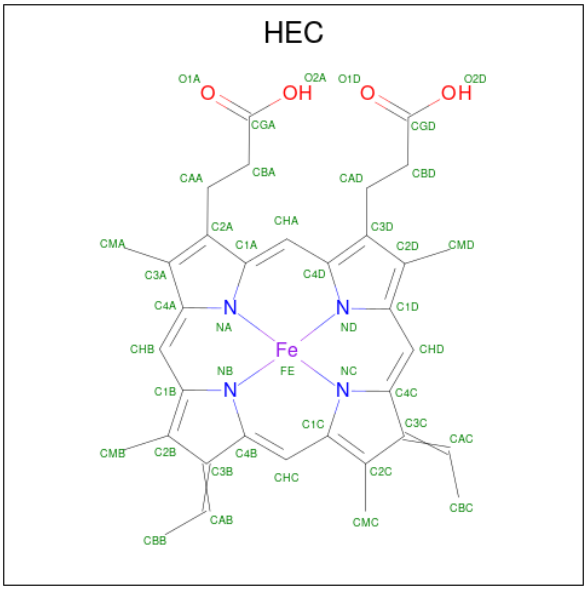
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	D	1	Total C H O 5 1 1 3	0	0
34	a	1	Total C H O 5 1 1 3	0	0

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	f	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	147	Total O 147 147	0	8
37	B	218	Total O 218 218	0	0
37	C	190	Total O 190 190	0	0
37	D	129	Total O 129 129	0	0
37	E	30	Total O 30 30	0	0
37	F	13	Total O 13 13	0	0
37	H	28	Total O 28 28	0	0
37	I	12	Total O 12 12	0	0
37	J	12	Total O 12 12	0	0
37	K	2	Total O 2 2	0	0
37	L	9	Total O 9 9	0	0
37	M	6	Total O 6 6	0	0
37	O	129	Total O 129 129	0	0
37	R	4	Total O 4 4	0	0
37	T	13	Total O 13 13	0	0
37	U	47	Total O 47 47	0	0
37	V	78	Total O 78 78	0	0
37	X	8	Total O 8 8	0	0
37	Y	5	Total O 5 5	0	0
37	Z	5	Total O 5 5	0	0
37	a	132	Total O 132 132	0	8

Continued on next page...

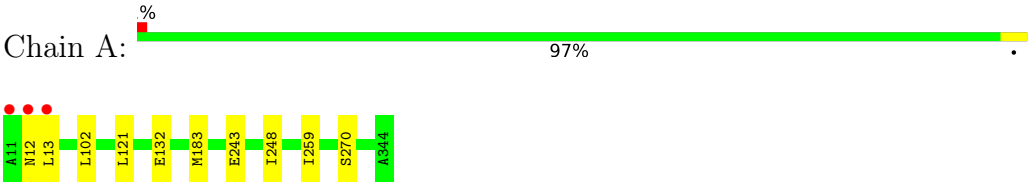
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	b	188	Total O 188 188	0	0
37	c	155	Total O 155 155	0	0
37	d	118	Total O 118 118	0	0
37	e	19	Total O 19 19	0	0
37	f	8	Total O 8 8	0	0
37	h	19	Total O 19 19	0	0
37	i	10	Total O 10 10	0	0
37	j	10	Total O 10 10	0	0
37	k	6	Total O 6 6	0	0
37	l	13	Total O 13 13	0	0
37	m	7	Total O 7 7	0	0
37	o	109	Total O 109 109	0	0
37	r	5	Total O 5 5	0	0
37	t	14	Total O 14 14	0	0
37	u	54	Total O 54 54	0	0
37	v	59	Total O 59 59	0	0
37	x	10	Total O 10 10	0	0
37	y	4	Total O 4 4	0	0
37	z	1	Total O 1 1	0	0

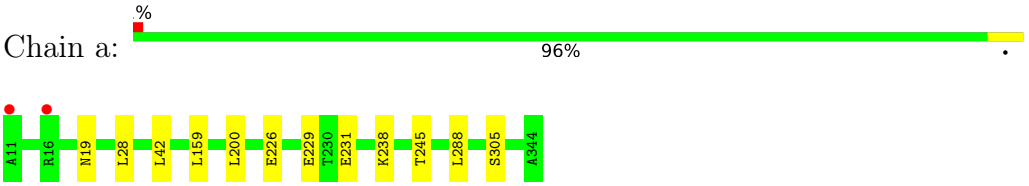
3 Residue-property plots (i)

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

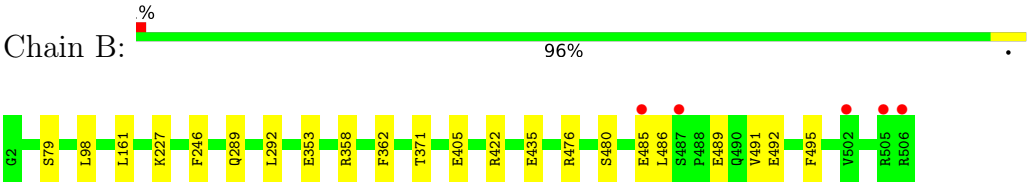
• Molecule 1: Photosystem II protein D1 1



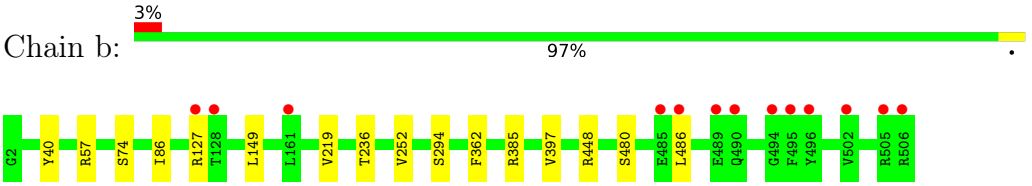
• Molecule 1: Photosystem II protein D1 1



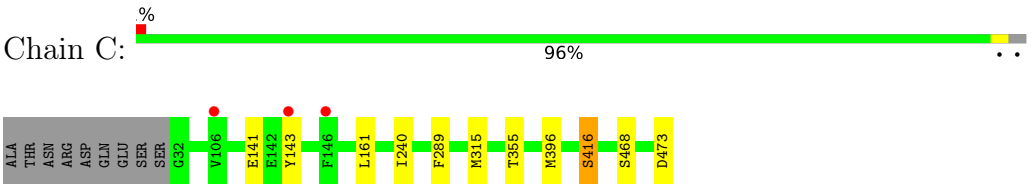
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

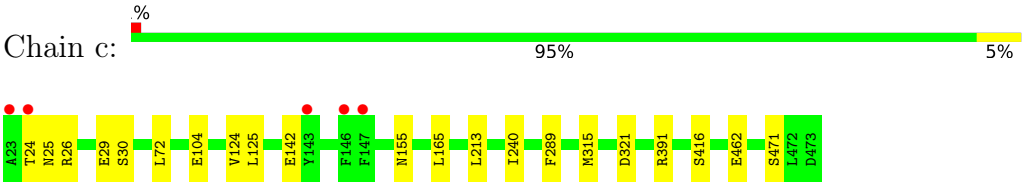


• Molecule 3: Photosystem II CP43 reaction center protein



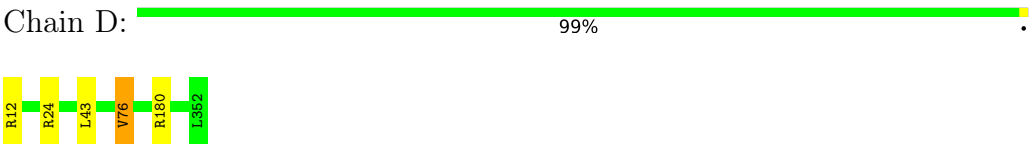
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



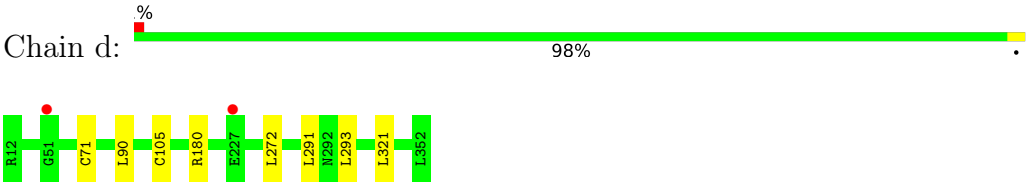
• Molecule 4: Photosystem II D2 protein

Chain D:



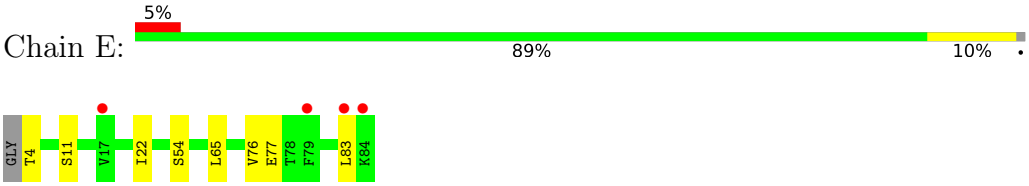
• Molecule 4: Photosystem II D2 protein

Chain d:



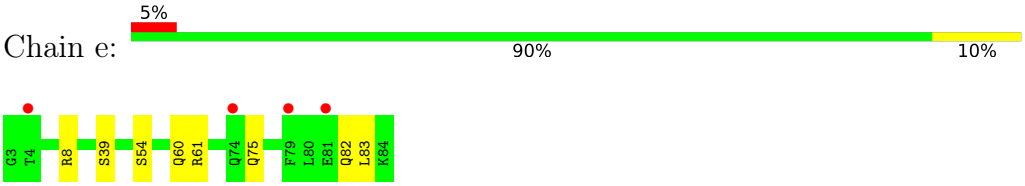
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



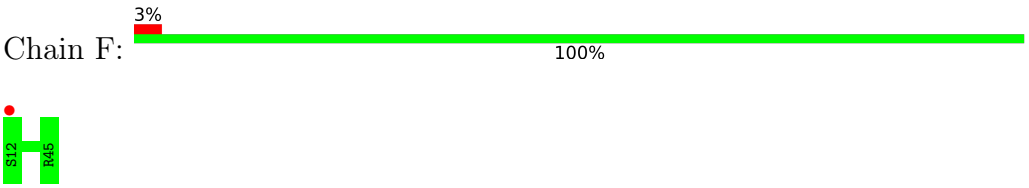
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



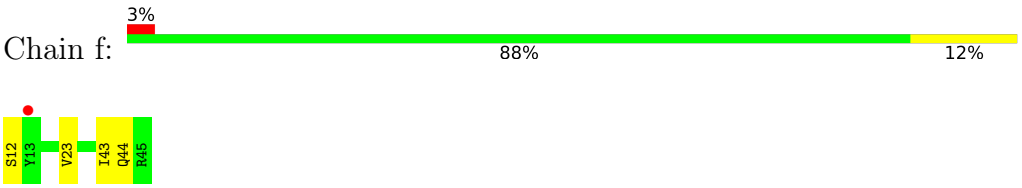
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



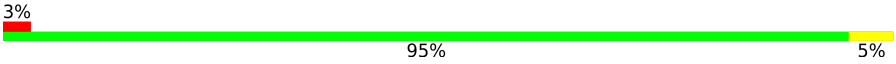
• Molecule 6: Cytochrome b559 subunit beta

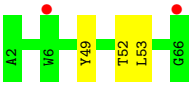
Chain f:



• Molecule 7: Photosystem II reaction center protein H

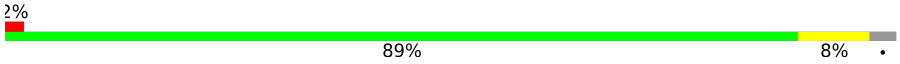
Chain H:





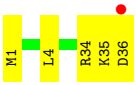
• Molecule 7: Photosystem II reaction center protein H

Chain h:



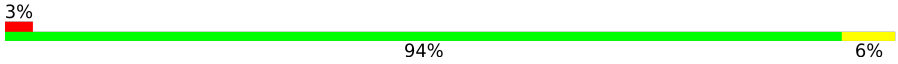
• Molecule 8: Photosystem II reaction center protein I

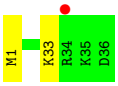
Chain I:



• Molecule 8: Photosystem II reaction center protein I

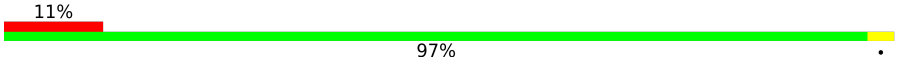
Chain i:

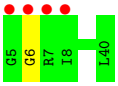




• Molecule 9: Photosystem II reaction center protein J

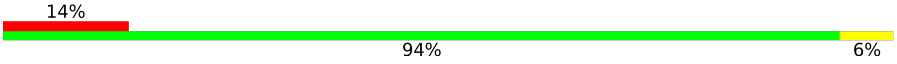
Chain J:

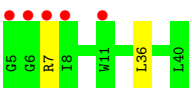




• Molecule 9: Photosystem II reaction center protein J

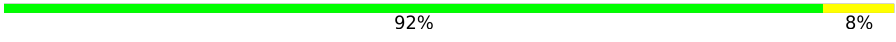
Chain j:





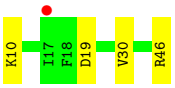
• Molecule 10: Photosystem II reaction center protein K

Chain K:



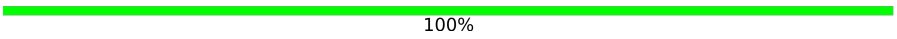
• Molecule 10: Photosystem II reaction center protein K

Chain k:



• Molecule 11: Photosystem II reaction center protein L

Chain L:



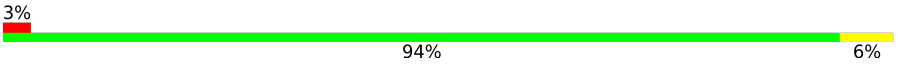
There are no outlier residues recorded for this chain.

• Molecule 11: Photosystem II reaction center protein L

Chain l:

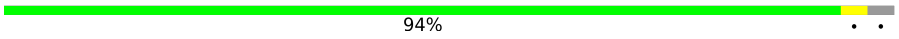
• Molecule 12: Photosystem II reaction center protein M

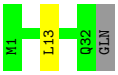
Chain M:



• Molecule 12: Photosystem II reaction center protein M

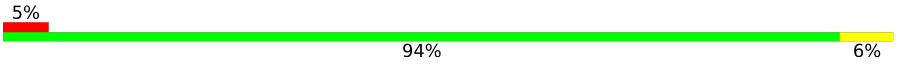
Chain m:

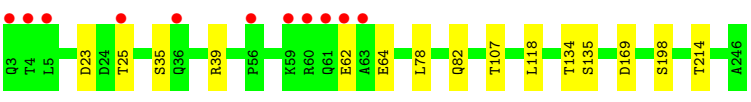




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

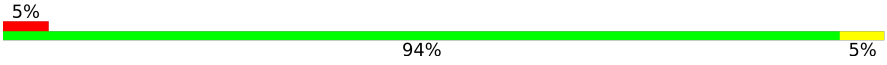
Chain O:

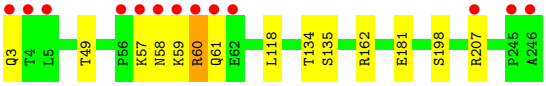




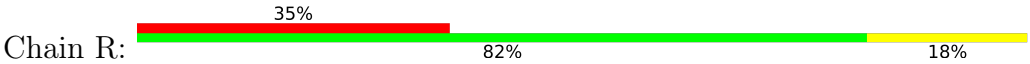
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

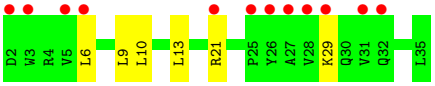
Chain o:



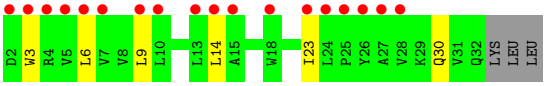


• Molecule 14: Photosystem II protein Y

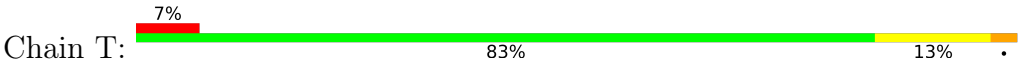


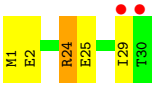


• Molecule 14: Photosystem II protein Y



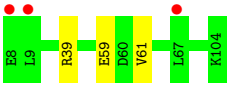
• Molecule 15: Photosystem II reaction center protein T



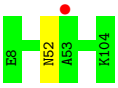


• Molecule 15: Photosystem II reaction center protein T

• Molecule 16: Photosystem II 12 kDa extrinsic protein

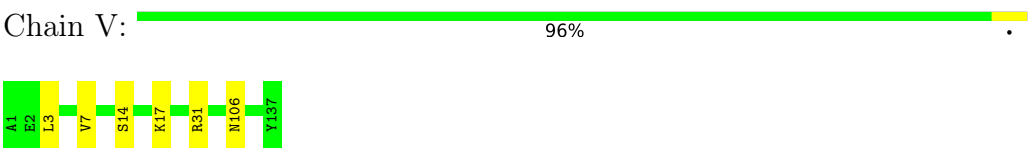


• Molecule 16: Photosystem II 12 kDa extrinsic protein



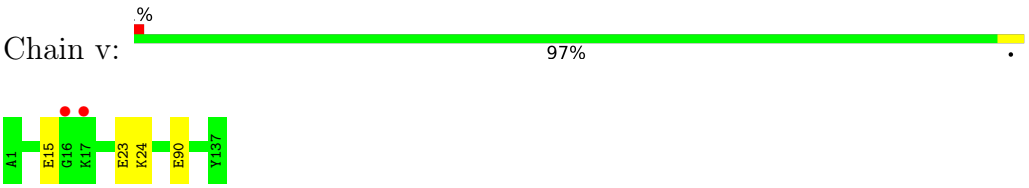
• Molecule 17: Cytochrome c-550

Chain V:



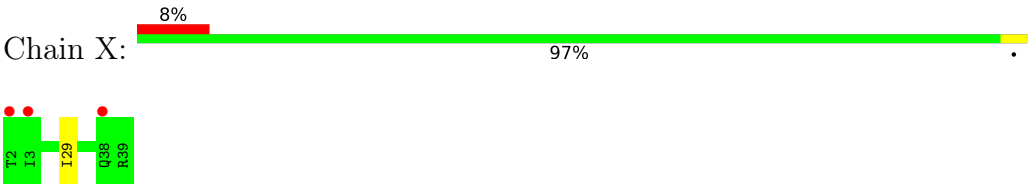
• Molecule 17: Cytochrome c-550

Chain v:



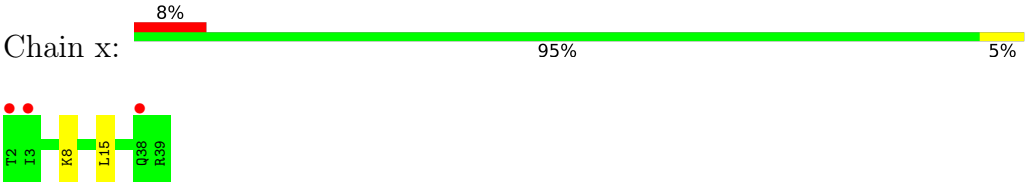
• Molecule 18: Photosystem II reaction center X protein

Chain X:



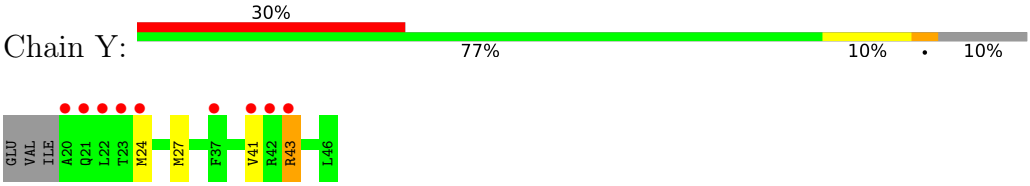
• Molecule 18: Photosystem II reaction center X protein

Chain x:



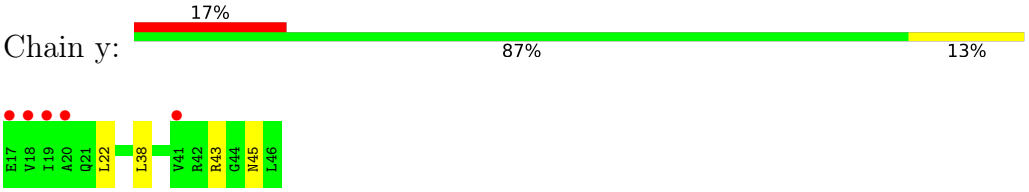
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y:



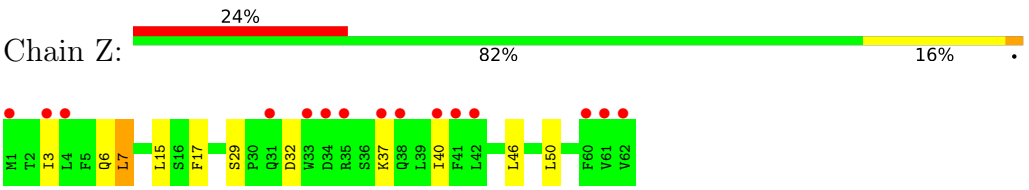
• Molecule 19: Photosystem II reaction center protein Ycf12

Chain y:



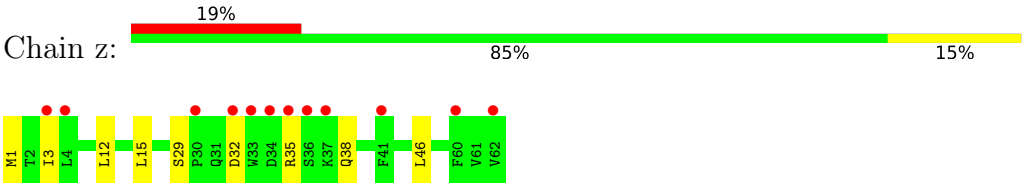
• Molecule 20: Photosystem II reaction center protein Z

Chain Z:



• Molecule 20: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	116.86Å 221.19Å 307.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.04 31.00 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.00-2.04) 88.5 (31.00-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.59 (at 2.05Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.186 , 0.248 0.186 , 0.248	Depositor DCC
R_{free} test set	4461 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	105751	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 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.69	1/3179 (0.0%)	0.74	0/4331
1	a	0.65	0/3176	0.71	0/4327
2	B	0.70	0/4160	0.73	3/5668 (0.1%)
2	b	0.69	1/4118 (0.0%)	0.73	3/5611 (0.1%)
3	C	0.67	1/3593 (0.0%)	0.71	2/4891 (0.0%)
3	c	0.62	0/3673	0.70	1/4998 (0.0%)
4	D	0.75	1/2820 (0.0%)	0.74	0/3840
4	d	0.70	2/2829 (0.1%)	0.73	2/3852 (0.1%)
5	E	0.61	0/684	0.68	0/935
5	e	0.52	0/683	0.59	0/932
6	F	0.57	0/284	0.62	0/387
6	f	0.49	0/284	0.59	0/387
7	H	0.72	0/520	0.76	0/709
7	h	0.61	0/511	0.70	0/697
8	I	0.72	0/293	0.67	0/396
8	i	0.73	0/293	0.80	0/396
9	J	0.62	0/263	0.70	0/356
9	j	0.54	0/261	0.65	0/353
10	K	0.49	0/314	0.71	0/427
10	k	0.50	0/303	0.65	0/416
11	L	0.69	0/311	0.75	0/422
11	l	0.71	0/303	0.74	0/412
12	M	0.70	0/249	0.70	0/341
12	m	0.73	0/244	0.69	0/334
13	O	0.60	0/1914	0.77	1/2596 (0.0%)
13	o	0.62	0/1905	0.75	1/2583 (0.0%)
14	R	0.44	0/277	0.64	0/380
14	r	0.37	0/233	0.49	0/323
15	T	0.80	0/257	0.90	2/349 (0.6%)
15	t	0.75	0/255	0.69	0/346
16	U	0.63	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	u	0.63	0/785	0.75	0/1064
17	V	0.65	0/1085	0.68	0/1473
17	v	0.55	0/1085	0.70	0/1473
18	X	0.56	0/284	0.68	0/384
18	x	0.39	0/284	0.56	0/384
19	Y	0.39	0/197	0.65	0/264
19	y	0.35	0/219	0.54	0/294
20	Z	0.51	0/490	0.61	0/669
20	z	0.46	0/488	0.57	0/666
All	All	0.65	6/43891 (0.0%)	0.71	15/59730 (0.0%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	105	CYS	CB-SG	-6.62	1.71	1.82
4	d	71	CYS	CB-SG	-6.40	1.71	1.82
4	D	76	VAL	CB-CG2	-5.99	1.40	1.52
1	A	132	GLU	CB-CG	5.81	1.63	1.52
3	C	468	SER	C-N	-5.57	1.21	1.34
2	b	40	TYR	CD1-CE1	-5.50	1.31	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	396	MET	CG-SD-CE	-7.82	87.69	100.20
2	b	57	ARG	NE-CZ-NH1	-7.60	116.50	120.30
15	T	24	ARG	NE-CZ-NH1	7.50	124.05	120.30
2	B	422	ARG	NE-CZ-NH1	-7.26	116.67	120.30
2	b	385	ARG	NE-CZ-NH2	-6.26	117.17	120.30
4	d	272	LEU	CB-CG-CD1	-6.26	100.36	111.00
15	T	24	ARG	NE-CZ-NH2	-5.80	117.40	120.30
4	d	293	LEU	CB-CG-CD2	5.73	120.74	111.00
3	C	473	ASP	CB-CG-OD1	5.64	123.37	118.30
2	b	448	ARG	NE-CZ-NH2	-5.61	117.50	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	169	ASP	CB-CG-OD1	5.61	123.35	118.30
3	c	321	ASP	CB-CG-OD1	5.42	123.18	118.30
2	B	292	LEU	CB-CG-CD1	-5.42	101.78	111.00
13	o	162	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	B	358	ARG	NE-CZ-NH2	-5.21	117.69	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	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	390/334 (117%)	380 (97%)	9 (2%)	1 (0%)	41	31
1	a	390/334 (117%)	383 (98%)	7 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	491 (98%)	11 (2%)	1 (0%)	47	39
3	C	447/451 (99%)	435 (97%)	10 (2%)	2 (0%)	34	24
3	c	457/451 (101%)	439 (96%)	17 (4%)	1 (0%)	47	39
4	D	339/341 (99%)	329 (97%)	10 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	78 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/82 (98%)	79 (99%)	1 (1%)	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%)	58 (92%)	5 (8%)	0	100	100
7	h	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100	100
9	J	34/36 (94%)	32 (94%)	1 (3%)	1 (3%)	4	0
9	j	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
10	K	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	4	0
10	k	35/37 (95%)	34 (97%)	1 (3%)	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%)	226 (93%)	16 (7%)	1 (0%)	34	24
13	o	242/244 (99%)	232 (96%)	8 (3%)	2 (1%)	19	10
14	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
14	r	29/34 (85%)	23 (79%)	5 (17%)	1 (3%)	3	0
15	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
16	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
17	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	v	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
18	X	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Y	25/30 (83%)	17 (68%)	6 (24%)	2 (8%)	1	0
19	y	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	3	0
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	0
20	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	9	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5365/5326 (101%)	5165 (96%)	183 (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
19	Y	41	VAL
19	Y	43	ARG
3	c	416	SER
13	o	60	ARG
14	r	30	GLN
20	Z	7	LEU
13	o	61	GLN
19	y	43	ARG
20	z	15	LEU
20	Z	6	GLN
2	b	127	ARG
3	C	143	TYR
9	J	6	GLY
1	A	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	319/270 (118%)	310 (97%)	9 (3%)	43 37
1	a	318/270 (118%)	306 (96%)	12 (4%)	33 26
2	B	407/403 (101%)	387 (95%)	20 (5%)	25 17
2	b	402/403 (100%)	391 (97%)	11 (3%)	44 38
3	C	351/352 (100%)	343 (98%)	8 (2%)	50 44
3	c	360/352 (102%)	340 (94%)	20 (6%)	21 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	D	277/276 (100%)	272 (98%)	5 (2%)	59 55
4	d	278/276 (101%)	274 (99%)	4 (1%)	67 65
5	E	72/72 (100%)	63 (88%)	9 (12%)	4 1
5	e	71/72 (99%)	63 (89%)	8 (11%)	6 1
6	F	28/28 (100%)	28 (100%)	0	100 100
6	f	28/28 (100%)	24 (86%)	4 (14%)	3 1
7	H	53/54 (98%)	50 (94%)	3 (6%)	20 12
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%)	29 (94%)	2 (6%)	17 9
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%)	31 (91%)	3 (9%)	10 4
12	M	28/29 (97%)	26 (93%)	2 (7%)	14 7
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%)	195 (94%)	12 (6%)	20 11
14	R	28/29 (97%)	22 (79%)	6 (21%)	1 0
14	r	19/29 (66%)	14 (74%)	5 (26%)	0 0
15	T	26/26 (100%)	22 (85%)	4 (15%)	2 0
15	t	25/26 (96%)	25 (100%)	0	100 100
16	U	84/84 (100%)	81 (96%)	3 (4%)	35 28
16	u	84/84 (100%)	84 (100%)	0	100 100
17	V	117/117 (100%)	111 (95%)	6 (5%)	24 15
17	v	117/117 (100%)	113 (97%)	4 (3%)	37 30
18	X	31/31 (100%)	30 (97%)	1 (3%)	39 32
18	x	31/31 (100%)	29 (94%)	2 (6%)	17 9
19	Y	19/23 (83%)	16 (84%)	3 (16%)	2 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	y	22/23 (96%)	19 (86%)	3 (14%)	3 1
20	Z	52/52 (100%)	42 (81%)	10 (19%)	1 0
20	z	51/52 (98%)	43 (84%)	8 (16%)	2 0
All	All	4435/4348 (102%)	4218 (95%)	217 (5%)	25 17

All (217) 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	121	LEU
1	A	183[A]	MET
1	A	183[B]	MET
1	A	243	GLU
1	A	248	ILE
1	A	270	SER
2	B	79	SER
2	B	98	LEU
2	B	161	LEU
2	B	227	LYS
2	B	246	PHE
2	B	289	GLN
2	B	353	GLU
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	435	GLU
2	B	476	ARG
2	B	480[A]	SER
2	B	480[B]	SER
2	B	485	GLU
2	B	486	LEU
2	B	489	GLU
2	B	491	VAL
2	B	492	GLU
2	B	495	PHE
3	C	141	GLU
3	C	161	LEU
3	C	240	ILE
3	C	289	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	315	MET
3	C	355[A]	THR
3	C	355[B]	THR
3	C	416	SER
4	D	12	ARG
4	D	24	ARG
4	D	43	LEU
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	54	SER
5	E	65	LEU
5	E	76	VAL
5	E	77	GLU
5	E	83	LEU
7	H	49	TYR
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	34	ARG
8	I	35	LYS
8	I	36	ASP
10	K	10	LYS
10	K	25	LEU
12	M	3	VAL
12	M	13	LEU
13	O	23	ASP
13	O	25	THR
13	O	35	SER
13	O	39	ARG
13	O	64	GLU
13	O	78	LEU
13	O	82	GLN
13	O	107	THR
13	O	118	LEU
13	O	134	THR
13	O	135	SER
13	O	198	SER
13	O	214	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	R	6	LEU
14	R	9	LEU
14	R	10	LEU
14	R	13	LEU
14	R	21	ARG
14	R	29	LYS
15	T	2	GLU
15	T	24	ARG
15	T	25	GLU
15	T	29	ILE
16	U	39	ARG
16	U	59	GLU
16	U	61	VAL
17	V	3	LEU
17	V	7	VAL
17	V	14	SER
17	V	17	LYS
17	V	31	ARG
17	V	106	ASN
18	X	29	ILE
19	Y	24	MET
19	Y	27	MET
19	Y	43	ARG
20	Z	3	ILE
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	29	SER
20	Z	32	ASP
20	Z	37	LYS
20	Z	40	ILE
20	Z	46	LEU
20	Z	50	LEU
1	a	19	ASN
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	226	GLU
1	a	229	GLU
1	a	231	GLU
1	a	238	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	245	THR
1	a	288	LEU
1	a	305	SER
2	b	74	SER
2	b	86	ILE
2	b	149	LEU
2	b	219	VAL
2	b	236	THR
2	b	252	VAL
2	b	294	SER
2	b	362	PHE
2	b	397	VAL
2	b	480	SER
2	b	486	LEU
3	c	24	THR
3	c	25	ASN
3	c	26	ARG
3	c	29	GLU
3	c	30	SER
3	c	72	LEU
3	c	104	GLU
3	c	124	VAL
3	c	125	LEU
3	c	142	GLU
3	c	155	ASN
3	c	165	LEU
3	c	213	LEU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	462	GLU
3	c	471	SER
4	d	90	LEU
4	d	180	ARG
4	d	291	LEU
4	d	321	LEU
5	e	8	ARG
5	e	39	SER
5	e	54	SER
5	e	60	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	e	61	ARG
5	e	75	GLN
5	e	82	GLN
5	e	83	LEU
6	f	12	SER
6	f	23	VAL
6	f	43	ILE
6	f	44	GLN
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
10	k	10	LYS
10	k	19	ASP
10	k	30	VAL
10	k	46	ARG
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
13	o	3	GLN
13	o	49	THR
13	o	57	LYS
13	o	58	ASN
13	o	59	LYS
13	o	60	ARG
13	o	118	LEU
13	o	134	THR
13	o	135	SER
13	o	181	GLU
13	o	198	SER
13	o	207	ARG
14	r	3	TRP
14	r	6	LEU
14	r	9	LEU
14	r	14	LEU
14	r	23	ILE
17	v	15	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	v	23	GLU
17	v	24	LYS
17	v	90	GLU
18	x	8	LYS
18	x	15	LEU
19	y	22	LEU
19	y	38	LEU
19	y	45	ASN
20	z	1	MET
20	z	3	ILE
20	z	12	LEU
20	z	29	SER
20	z	32	ASP
20	z	35	ARG
20	z	38	GLN
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	490	GLN
3	C	382	ASN
13	O	82	GLN
13	O	88	ASN
20	Z	6	GLN
1	a	266	ASN
2	b	395	GLN
3	c	25	ASN
3	c	418	ASN
13	o	58	ASN
13	o	80	GLN
20	z	38	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	FME	t	1	15	8,9,10	1.15	1 (12%)	7,9,11	1.08	0
12	FME	m	1	12	8,9,10	0.87	0	7,9,11	0.73	0
8	FME	i	1	8	8,9,10	1.08	0	7,9,11	1.63	2 (28%)
8	FME	I	1	8	8,9,10	0.87	0	7,9,11	1.49	1 (14%)
12	FME	M	1	12	8,9,10	0.96	0	7,9,11	0.77	0
15	FME	T	1	15	8,9,10	1.24	1 (12%)	7,9,11	1.93	3 (42%)

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
15	FME	t	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.65	1.42	1.46
15	T	1	FME	CB-CA	2.16	1.57	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	FME	C-CA-N	2.90	114.96	109.73
15	T	1	FME	CA-N-CN	-2.81	118.50	122.82
15	T	1	FME	C-CA-N	2.76	114.72	109.73
8	I	1	FME	C-CA-N	2.64	114.50	109.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	1	FME	O1-CN-N	-2.19	119.50	125.27
8	i	1	FME	CA-N-CN	-2.15	119.51	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 188 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	C	503	-	65,73,73	1.57	10 (15%)	76,113,113	1.66	13 (17%)
28	LMG	B	620	-	51,51,55	1.10	4 (7%)	59,59,63	1.48	11 (18%)
30	LHG	l	101	-	48,48,48	0.75	2 (4%)	51,54,54	1.31	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	510	-	65,73,73	1.51	7 (10%)	76,113,113	1.53	13 (17%)
25	BCR	C	514	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
25	BCR	t	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.61	13 (23%)
30	LHG	A	615	-	48,48,48	0.95	3 (6%)	51,54,54	1.15	3 (5%)
30	LHG	a	614	-	41,41,48	0.80	0	44,47,54	1.29	4 (9%)
31	DGD	A	617	-	67,67,67	1.46	9 (13%)	81,81,81	1.46	12 (14%)
21	OEX	A	601[A]	37,3,1	0,15,15	-	-	-		
31	DGD	c	518	-	63,63,67	1.11	7 (11%)	77,77,81	1.44	15 (19%)
28	LMG	b	621	-	55,55,55	0.89	2 (3%)	63,63,63	1.38	7 (11%)
23	CLA	c	504	37	60,68,73	1.67	7 (11%)	70,107,113	1.49	10 (14%)
23	CLA	B	610	37	65,73,73	1.66	8 (12%)	76,113,113	1.63	12 (15%)
23	CLA	B	601	37	65,73,73	1.98	9 (13%)	76,113,113	1.80	12 (15%)
23	CLA	B	605	-	65,73,73	1.36	7 (10%)	76,113,113	1.47	12 (15%)
23	CLA	c	508	-	64,72,73	1.47	9 (14%)	74,111,113	1.31	10 (13%)
23	CLA	a	604	37	65,73,73	1.66	9 (13%)	76,113,113	1.45	13 (17%)
23	CLA	A	613	37	65,73,73	1.72	8 (12%)	76,113,113	1.43	9 (11%)
23	CLA	b	609	-	65,73,73	1.66	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	B	613	-	65,73,73	1.60	10 (15%)	76,113,113	1.41	12 (15%)
34	BCT	D	401	22	2,3,3	1.06	0	2,3,3	3.24	2 (100%)
25	BCR	d	404	-	41,41,41	1.27	3 (7%)	56,56,56	1.24	5 (8%)
29	SQD	a	615	-	35,35,54	1.12	2 (5%)	37,37,65	1.45	7 (18%)
30	LHG	D	408	-	46,46,48	1.05	3 (6%)	49,52,54	1.35	6 (12%)
24	PHO	d	401	-	51,69,69	1.01	3 (5%)	47,99,99	1.52	10 (21%)
28	LMG	A	612	-	48,48,55	1.01	4 (8%)	56,56,63	1.42	11 (19%)
23	CLA	b	603	-	65,73,73	1.58	8 (12%)	76,113,113	1.57	11 (14%)
28	LMG	d	406	-	44,44,55	1.23	4 (9%)	52,52,63	1.34	8 (15%)
23	CLA	B	614	-	65,73,73	1.83	9 (13%)	76,113,113	1.47	9 (11%)
25	BCR	A	608	-	41,41,41	1.18	2 (4%)	56,56,56	1.48	11 (19%)
23	CLA	B	616	-	60,68,73	1.76	11 (18%)	70,107,113	1.54	13 (18%)
23	CLA	b	607	37	65,73,73	1.28	7 (10%)	76,113,113	1.45	9 (11%)
23	CLA	C	509	-	65,73,73	1.48	7 (10%)	76,113,113	1.25	7 (9%)
28	LMG	c	521	-	48,48,55	1.18	6 (12%)	56,56,63	1.33	6 (10%)
23	CLA	b	611	-	65,73,73	1.55	8 (12%)	76,113,113	1.74	21 (27%)
23	CLA	c	501	-	65,73,73	1.63	9 (13%)	76,113,113	1.78	15 (19%)
29	SQD	f	101	-	40,41,54	1.17	5 (12%)	49,52,65	1.65	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	A	603	-	65,73,73	1.56	13 (20%)	76,113,113	1.37	12 (15%)
23	CLA	b	606	-	65,73,73	1.78	11 (16%)	76,113,113	1.55	13 (17%)
23	CLA	C	502	-	65,73,73	1.52	8 (12%)	76,113,113	1.32	7 (9%)
23	CLA	B	607	37	65,73,73	1.70	13 (20%)	76,113,113	1.25	7 (9%)
31	DGD	a	616	-	43,43,67	1.29	4 (9%)	45,45,81	1.42	5 (11%)
25	BCR	B	619	-	41,41,41	1.25	2 (4%)	56,56,56	1.50	10 (17%)
31	DGD	C	518	-	63,63,67	0.89	3 (4%)	77,77,81	1.37	9 (11%)
30	LHG	d	409	-	38,38,48	0.96	1 (2%)	41,44,54	1.25	4 (9%)
23	CLA	c	506	-	65,73,73	2.06	11 (16%)	76,113,113	1.48	14 (18%)
30	LHG	D	406	-	48,48,48	0.85	1 (2%)	51,54,54	1.28	8 (15%)
23	CLA	C	504	37	59,67,73	1.65	11 (18%)	68,105,113	1.42	9 (13%)
25	BCR	H	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.50	9 (16%)
28	LMG	B	622	-	26,26,55	0.88	2 (7%)	26,26,63	1.12	2 (7%)
25	BCR	c	514	-	41,41,41	1.15	3 (7%)	56,56,56	1.36	9 (16%)
23	CLA	b	610	37	65,73,73	1.47	12 (18%)	76,113,113	1.38	11 (14%)
23	CLA	C	501	-	65,73,73	1.77	10 (15%)	76,113,113	1.59	11 (14%)
28	LMG	D	409	-	31,31,55	1.43	5 (16%)	33,33,63	1.10	4 (12%)
23	CLA	C	512	-	65,73,73	1.65	11 (16%)	76,113,113	1.50	10 (13%)
23	CLA	c	511	3	65,73,73	1.82	9 (13%)	76,113,113	1.33	10 (13%)
31	DGD	C	517	-	63,63,67	1.23	6 (9%)	77,77,81	1.60	13 (16%)
23	CLA	c	505	-	65,73,73	1.57	8 (12%)	76,113,113	1.48	14 (18%)
31	DGD	C	516	-	63,63,67	1.28	9 (14%)	77,77,81	1.33	8 (10%)
23	CLA	C	507	37	65,73,73	1.40	7 (10%)	76,113,113	1.54	10 (13%)
23	CLA	C	508	-	65,73,73	1.38	9 (13%)	76,113,113	1.45	11 (14%)
23	CLA	b	613	-	65,73,73	1.62	11 (16%)	76,113,113	1.67	14 (18%)
23	CLA	d	402	-	65,73,73	1.55	10 (15%)	76,113,113	1.42	7 (9%)
28	LMG	c	522	-	49,49,55	1.04	2 (4%)	57,57,63	1.30	4 (7%)
25	BCR	T	101	-	41,41,41	1.17	5 (12%)	56,56,56	1.40	8 (14%)
25	BCR	k	101	-	41,41,41	1.03	3 (7%)	56,56,56	1.08	4 (7%)
23	CLA	b	602	-	65,73,73	1.49	7 (10%)	76,113,113	1.68	9 (11%)
23	CLA	A	604	37	65,73,73	1.53	10 (15%)	76,113,113	1.42	12 (15%)
23	CLA	B	608	-	65,73,73	1.32	7 (10%)	76,113,113	1.54	12 (15%)
23	CLA	c	503	-	65,73,73	1.62	9 (13%)	76,113,113	1.53	14 (18%)
23	CLA	B	611	-	65,73,73	1.67	10 (15%)	76,113,113	1.52	14 (18%)
35	HEM	f	102	5,6	41,50,50	1.46	4 (9%)	45,82,82	1.48	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	b	619	-	41,41,41	1.16	3 (7%)	56,56,56	1.27	8 (14%)
23	CLA	b	608	-	65,73,73	1.47	9 (13%)	76,113,113	1.36	13 (17%)
29	SQD	b	601	-	48,49,54	0.98	4 (8%)	57,60,65	2.07	13 (22%)
23	CLA	b	614	-	65,73,73	1.50	8 (12%)	76,113,113	1.57	11 (14%)
24	PHO	A	606	-	51,69,69	1.19	6 (11%)	47,99,99	1.26	4 (8%)
23	CLA	a	606	-	65,73,73	1.64	13 (20%)	76,113,113	1.65	11 (14%)
23	CLA	B	615	-	65,73,73	1.73	15 (23%)	76,113,113	1.49	10 (13%)
35	HEM	F	102	5,6	41,50,50	1.49	4 (9%)	45,82,82	1.49	9 (20%)
23	CLA	D	403	-	65,73,73	1.83	10 (15%)	76,113,113	1.24	11 (14%)
34	BCT	a	610	22	2,3,3	1.53	0	2,3,3	2.60	1 (50%)
31	DGD	H	102	-	63,63,67	1.53	10 (15%)	77,77,81	1.54	13 (16%)
32	OEY	A	618[B]	37,3,1	0,16,16	-	-	-		
23	CLA	B	604	-	65,73,73	1.62	9 (13%)	76,113,113	1.75	10 (13%)
30	LHG	d	407	-	48,48,48	0.92	2 (4%)	51,54,54	1.15	3 (5%)
25	BCR	C	515	-	41,41,41	1.25	4 (9%)	56,56,56	1.22	5 (8%)
23	CLA	c	513	-	65,73,73	1.54	9 (13%)	76,113,113	1.11	6 (7%)
25	BCR	B	617	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	5 (8%)
23	CLA	b	615	-	65,73,73	1.98	12 (18%)	76,113,113	1.51	14 (18%)
27	PL9	a	611	-	55,55,55	1.11	6 (10%)	68,69,69	1.61	14 (20%)
23	CLA	c	509	-	65,73,73	1.43	6 (9%)	76,113,113	1.57	11 (14%)
25	BCR	C	520	-	41,41,41	1.07	4 (9%)	56,56,56	1.21	3 (5%)
25	BCR	b	617	-	41,41,41	1.14	3 (7%)	56,56,56	1.39	6 (10%)
25	BCR	D	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	5 (8%)
30	LHG	L	101	-	48,48,48	0.86	1 (2%)	51,54,54	1.12	3 (5%)
27	PL9	d	408	-	55,55,55	1.52	9 (16%)	68,69,69	1.80	20 (29%)
23	CLA	h	101	37	65,73,73	1.71	11 (16%)	76,113,113	1.58	15 (19%)
25	BCR	B	618	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	6 (10%)
23	CLA	c	507	37	65,73,73	1.59	11 (16%)	76,113,113	1.63	12 (15%)
24	PHO	a	605	-	51,69,69	1.10	5 (9%)	47,99,99	1.35	5 (10%)
27	PL9	A	611	-	55,55,55	1.01	2 (3%)	68,69,69	1.66	16 (23%)
31	DGD	c	517	-	63,63,67	1.31	11 (17%)	77,77,81	1.46	12 (15%)
29	SQD	F	101	-	35,36,54	1.08	3 (8%)	42,45,65	1.98	9 (21%)
23	CLA	b	612	-	65,73,73	1.53	8 (12%)	76,113,113	1.69	15 (19%)
36	HEC	v	201	17	32,50,50	2.04	4 (12%)	24,82,82	1.56	5 (20%)
23	CLA	B	602	-	65,73,73	1.45	9 (13%)	76,113,113	1.36	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	HEC	V	201	17	32,50,50	2.25	6 (18%)	24,82,82	1.28	3 (12%)
29	SQD	B	624	-	53,54,54	0.92	3 (5%)	62,65,65	1.78	13 (20%)
28	LMG	d	410	-	21,21,55	0.71	0	20,20,63	1.02	0
23	CLA	C	506	-	65,73,73	1.64	9 (13%)	76,113,113	1.29	9 (11%)
24	PHO	A	605	-	51,69,69	1.02	3 (5%)	47,99,99	1.44	6 (12%)
28	LMG	D	405	-	51,51,55	1.10	3 (5%)	59,59,63	1.17	5 (8%)
28	LMG	c	519	-	37,37,55	1.21	4 (10%)	45,45,63	1.21	4 (8%)
30	LHG	B	623	-	48,48,48	0.86	1 (2%)	51,54,54	1.44	9 (17%)
31	DGD	h	103	-	63,63,67	1.02	2 (3%)	77,77,81	1.42	9 (11%)
23	CLA	B	609	-	65,73,73	1.69	12 (18%)	76,113,113	1.46	8 (10%)
32	OEY	a	618[B]	37,3,1	0,16,16	-	-	-		
25	BCR	a	607	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	9 (16%)
23	CLA	C	510	-	65,73,73	1.54	13 (20%)	76,113,113	1.43	8 (10%)
23	CLA	D	402	-	65,73,73	1.48	10 (15%)	76,113,113	1.33	11 (14%)
23	CLA	C	511	3	65,73,73	1.93	8 (12%)	76,113,113	1.49	5 (6%)
28	LMG	m	101	-	51,51,55	0.84	2 (3%)	59,59,63	1.56	12 (20%)
30	LHG	d	405	-	48,48,48	0.66	0	51,54,54	1.27	4 (7%)
29	SQD	A	614	-	51,52,54	1.09	4 (7%)	60,63,65	2.46	13 (21%)
23	CLA	B	606	-	65,73,73	1.84	11 (16%)	76,113,113	1.65	12 (15%)
23	CLA	d	403	-	65,73,73	1.44	7 (10%)	76,113,113	1.35	12 (15%)
23	CLA	C	513	-	65,73,73	1.56	7 (10%)	76,113,113	1.44	8 (10%)
23	CLA	b	604	-	65,73,73	1.54	8 (12%)	76,113,113	1.57	12 (15%)
23	CLA	B	612	-	65,73,73	1.40	6 (9%)	76,113,113	1.53	11 (14%)
23	CLA	b	605	-	65,73,73	1.48	8 (12%)	76,113,113	1.76	17 (22%)
25	BCR	h	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.48	13 (23%)
25	BCR	Y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	8 (14%)
23	CLA	a	612	37	65,73,73	1.65	9 (13%)	76,113,113	1.55	10 (13%)
23	CLA	c	502	-	65,73,73	1.28	7 (10%)	76,113,113	1.79	11 (14%)
23	CLA	c	512	-	65,73,73	1.50	9 (13%)	76,113,113	1.50	10 (13%)
25	BCR	k	102	-	41,41,41	0.98	0	56,56,56	1.27	6 (10%)
25	BCR	b	618	-	41,41,41	1.37	4 (9%)	56,56,56	1.33	8 (14%)
23	CLA	A	607	-	54,62,73	1.95	8 (14%)	62,99,113	1.89	12 (19%)
23	CLA	B	603	-	65,73,73	1.42	9 (13%)	76,113,113	1.57	14 (18%)
31	DGD	c	516	-	63,63,67	1.18	6 (9%)	77,77,81	1.36	12 (15%)
27	PL9	D	407	-	55,55,55	1.70	12 (21%)	68,69,69	1.56	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	SQD	A	616	-	38,38,54	1.03	3 (7%)	40,40,65	1.63	3 (7%)
23	CLA	a	603	-	65,73,73	1.53	7 (10%)	76,113,113	1.68	13 (17%)
29	SQD	a	613	-	53,54,54	0.95	3 (5%)	62,65,65	1.93	12 (19%)
23	CLA	C	505	-	65,73,73	1.39	6 (9%)	76,113,113	1.40	10 (13%)
28	LMG	C	519	-	48,48,55	1.18	5 (10%)	56,56,63	1.29	5 (8%)
25	BCR	c	515	-	41,41,41	1.33	3 (7%)	56,56,56	1.57	14 (25%)
23	CLA	b	616	-	60,68,73	1.56	11 (18%)	70,107,113	1.63	9 (12%)
21	OEX	a	601[A]	37,3,1	0,15,15	-	-	-		

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	503	-	1/1/20/20	6/37/115/115	-
28	LMG	B	620	-	-	21/46/66/70	0/1/1/1
30	LHG	l	101	-	-	19/53/53/53	-
23	CLA	c	510	-	1/1/20/20	12/37/115/115	-
25	BCR	C	514	-	-	7/29/63/63	0/2/2/2
25	BCR	t	101	-	-	9/29/63/63	0/2/2/2
30	LHG	A	615	-	-	27/53/53/53	-
30	LHG	a	614	-	-	28/46/46/53	-
31	DGD	A	617	-	-	24/55/95/95	0/2/2/2
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
28	LMG	b	621	-	-	16/50/70/70	0/1/1/1
23	CLA	c	504	37	1/1/19/20	9/31/109/115	-
23	CLA	B	610	37	1/1/20/20	5/37/115/115	-
23	CLA	B	601	37	1/1/20/20	15/37/115/115	-
23	CLA	B	605	-	-	10/37/115/115	-
23	CLA	c	508	-	1/1/19/20	11/36/114/115	-
23	CLA	a	604	37	-	10/37/115/115	-
23	CLA	A	613	37	-	6/37/115/115	-
23	CLA	b	609	-	1/1/20/20	13/37/115/115	-
23	CLA	B	613	-	1/1/20/20	7/37/115/115	-
25	BCR	d	404	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	a	615	-	-	18/37/37/69	-
30	LHG	D	408	-	-	22/51/51/53	-
24	PHO	d	401	-	-	6/37/103/103	0/5/6/6
28	LMG	A	612	-	-	21/43/63/70	0/1/1/1
23	CLA	b	603	-	1/1/20/20	7/37/115/115	-
28	LMG	d	406	-	-	13/39/59/70	0/1/1/1
23	CLA	B	614	-	1/1/20/20	14/37/115/115	-
25	BCR	A	608	-	-	6/29/63/63	0/2/2/2
23	CLA	B	616	-	1/1/19/20	7/31/109/115	-
23	CLA	b	607	37	1/1/20/20	14/37/115/115	-
23	CLA	C	509	-	1/1/20/20	15/37/115/115	-
28	LMG	c	521	-	-	20/43/63/70	0/1/1/1
23	CLA	b	611	-	1/1/20/20	7/37/115/115	-
23	CLA	c	501	-	1/1/20/20	6/37/115/115	-
29	SQD	f	101	-	-	18/36/56/69	0/1/1/1
23	CLA	A	603	-	1/1/20/20	1/37/115/115	-
23	CLA	b	606	-	1/1/20/20	13/37/115/115	-
23	CLA	C	502	-	1/1/20/20	6/37/115/115	-
23	CLA	B	607	37	1/1/20/20	12/37/115/115	-
31	DGD	a	616	-	-	26/45/45/95	-
25	BCR	B	619	-	-	8/29/63/63	0/2/2/2
31	DGD	C	518	-	-	17/51/91/95	0/2/2/2
30	LHG	d	409	-	-	13/43/43/53	-
23	CLA	c	506	-	1/1/20/20	19/37/115/115	-
30	LHG	D	406	-	-	20/53/53/53	-
23	CLA	C	504	37	1/1/18/20	9/30/108/115	-
25	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	LMG	B	622	-	-	11/22/22/70	-
25	BCR	c	514	-	-	15/29/63/63	0/2/2/2
23	CLA	b	610	37	1/1/20/20	7/37/115/115	-
23	CLA	C	501	-	1/1/20/20	4/37/115/115	-
28	LMG	D	409	-	-	17/33/33/70	-
23	CLA	C	512	-	1/1/20/20	12/37/115/115	-
23	CLA	c	511	3	1/1/20/20	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	C	517	-	-	23/51/91/95	0/2/2/2
23	CLA	c	505	-	1/1/20/20	9/37/115/115	-
31	DGD	C	516	-	-	19/51/91/95	0/2/2/2
23	CLA	C	507	37	1/1/20/20	9/37/115/115	-
23	CLA	b	613	-	1/1/20/20	8/37/115/115	-
23	CLA	C	508	-	-	11/37/115/115	-
23	CLA	d	402	-	1/1/20/20	9/37/115/115	-
28	LMG	c	522	-	-	24/44/64/70	0/1/1/1
25	BCR	T	101	-	-	10/29/63/63	0/2/2/2
25	BCR	k	101	-	-	9/29/63/63	0/2/2/2
23	CLA	b	602	-	1/1/20/20	7/37/115/115	-
23	CLA	A	604	37	-	5/37/115/115	-
23	CLA	B	608	-	-	1/37/115/115	-
23	CLA	c	503	-	1/1/20/20	7/37/115/115	-
23	CLA	B	611	-	-	10/37/115/115	-
35	HEM	f	102	5,6	-	3/12/54/54	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	b	608	-	-	8/37/115/115	-
29	SQD	b	601	-	-	17/44/64/69	0/1/1/1
23	CLA	b	614	-	1/1/20/20	18/37/115/115	-
24	PHO	A	606	-	-	5/37/103/103	0/5/6/6
23	CLA	a	606	-	1/1/20/20	11/37/115/115	-
23	CLA	B	615	-	1/1/20/20	9/37/115/115	-
35	HEM	F	102	5,6	-	2/12/54/54	-
23	CLA	D	403	-	1/1/20/20	15/37/115/115	-
31	DGD	H	102	-	-	15/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/20/20	10/37/115/115	-
30	LHG	d	407	-	-	20/53/53/53	-
25	BCR	C	515	-	-	6/29/63/63	0/2/2/2
23	CLA	c	513	-	1/1/20/20	4/37/115/115	-
25	BCR	B	617	-	-	5/29/63/63	0/2/2/2
23	CLA	b	615	-	1/1/20/20	8/37/115/115	-
27	PL9	a	611	-	-	25/53/73/73	0/1/1/1
23	CLA	c	509	-	1/1/20/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	520	-	-	7/29/63/63	0/2/2/2
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	D	404	-	-	7/29/63/63	0/2/2/2
30	LHG	L	101	-	-	18/53/53/53	-
27	PL9	d	408	-	-	21/53/73/73	0/1/1/1
23	CLA	h	101	37	1/1/20/20	18/37/115/115	-
25	BCR	B	618	-	-	6/29/63/63	0/2/2/2
23	CLA	c	507	37	1/1/20/20	9/37/115/115	-
24	PHO	a	605	-	-	10/37/103/103	0/5/6/6
27	PL9	A	611	-	-	26/53/73/73	0/1/1/1
31	DGD	c	517	-	-	20/51/91/95	0/2/2/2
29	SQD	F	101	-	-	16/28/48/69	0/1/1/1
23	CLA	b	612	-	1/1/20/20	7/37/115/115	-
36	HEC	v	201	17	-	2/10/54/54	-
23	CLA	B	602	-	1/1/20/20	4/37/115/115	-
36	HEC	V	201	17	-	2/10/54/54	-
29	SQD	B	624	-	-	24/49/69/69	0/1/1/1
28	LMG	d	410	-	-	10/17/17/70	-
23	CLA	C	506	-	-	14/37/115/115	-
24	PHO	A	605	-	-	8/37/103/103	0/5/6/6
28	LMG	D	405	-	-	17/46/66/70	0/1/1/1
28	LMG	c	519	-	-	10/31/51/70	0/1/1/1
30	LHG	B	623	-	-	15/53/53/53	-
31	DGD	h	103	-	-	18/51/91/95	0/2/2/2
23	CLA	B	609	-	-	7/37/115/115	-
25	BCR	a	607	-	-	4/29/63/63	0/2/2/2
23	CLA	C	510	-	1/1/20/20	7/37/115/115	-
23	CLA	D	402	-	-	5/37/115/115	-
23	CLA	C	511	3	1/1/20/20	8/37/115/115	-
28	LMG	m	101	-	-	20/46/66/70	0/1/1/1
30	LHG	d	405	-	-	24/53/53/53	-
29	SQD	A	614	-	-	23/47/67/69	0/1/1/1
23	CLA	B	606	-	1/1/20/20	7/37/115/115	-
23	CLA	d	403	-	-	6/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	513	-	1/1/20/20	8/37/115/115	-
23	CLA	b	604	-	1/1/20/20	11/37/115/115	-
23	CLA	B	612	-	1/1/20/20	12/37/115/115	-
23	CLA	b	605	-	1/1/20/20	6/37/115/115	-
25	BCR	h	102	-	-	11/29/63/63	0/2/2/2
25	BCR	Y	101	-	-	12/29/63/63	0/2/2/2
23	CLA	a	612	37	1/1/20/20	3/37/115/115	-
23	CLA	c	502	-	-	6/37/115/115	-
23	CLA	c	512	-	1/1/20/20	18/37/115/115	-
25	BCR	k	102	-	-	5/29/63/63	0/2/2/2
25	BCR	b	618	-	-	7/29/63/63	0/2/2/2
23	CLA	A	607	-	1/1/17/20	3/24/102/115	-
23	CLA	B	603	-	1/1/20/20	15/37/115/115	-
31	DGD	c	516	-	-	28/51/91/95	0/2/2/2
27	PL9	D	407	-	-	10/53/73/73	0/1/1/1
29	SQD	A	616	-	-	17/39/39/69	-
23	CLA	a	603	-	1/1/20/20	1/37/115/115	-
29	SQD	a	613	-	-	25/49/69/69	0/1/1/1
23	CLA	C	505	-	1/1/20/20	11/37/115/115	-
28	LMG	C	519	-	-	17/43/63/70	0/1/1/1
25	BCR	c	515	-	-	4/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/19/20	7/31/109/115	-

All (914) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	MG-ND	-10.99	1.84	2.05
23	b	615	CLA	MG-NA	9.73	2.29	2.06
23	C	511	CLA	MG-NA	9.42	2.28	2.06
23	b	609	CLA	C4B-NB	8.45	1.42	1.35
23	B	610	CLA	C4B-NB	8.22	1.42	1.35
23	B	601	CLA	C4B-NB	8.12	1.42	1.35
23	c	511	CLA	C4B-NB	8.09	1.42	1.35
23	B	614	CLA	C4B-NB	8.08	1.42	1.35
23	C	501	CLA	C4B-NB	7.82	1.42	1.35
23	B	615	CLA	C4B-NB	7.76	1.42	1.35
23	B	613	CLA	C4B-NB	7.70	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C4B-NB	7.57	1.42	1.35
23	c	503	CLA	C4B-NB	7.54	1.41	1.35
23	C	511	CLA	C4B-NB	7.53	1.41	1.35
23	B	601	CLA	MG-ND	-7.49	1.90	2.05
23	B	614	CLA	MG-ND	-7.42	1.91	2.05
23	B	609	CLA	C4B-NB	7.41	1.41	1.35
23	c	504	CLA	C4B-NB	7.38	1.41	1.35
23	b	614	CLA	C4B-NB	7.37	1.41	1.35
23	b	604	CLA	C4B-NB	7.27	1.41	1.35
23	C	510	CLA	C4B-NB	7.26	1.41	1.35
23	c	501	CLA	C4B-NB	7.19	1.41	1.35
23	D	403	CLA	MG-ND	-7.12	1.91	2.05
23	a	606	CLA	C4B-NB	7.10	1.41	1.35
36	V	201	HEC	C2B-C3B	-7.07	1.33	1.40
23	b	603	CLA	C4B-NB	7.05	1.41	1.35
23	h	101	CLA	C4B-NB	6.97	1.41	1.35
23	C	513	CLA	C4B-NB	6.93	1.41	1.35
23	b	615	CLA	C4B-NB	6.90	1.41	1.35
23	A	607	CLA	C4B-NB	6.89	1.41	1.35
23	C	509	CLA	C4B-NB	6.89	1.41	1.35
23	c	510	CLA	C4B-NB	6.86	1.41	1.35
23	D	403	CLA	C4B-NB	6.85	1.41	1.35
23	A	607	CLA	MG-ND	-6.81	1.92	2.05
23	a	604	CLA	C4B-NB	6.80	1.41	1.35
23	B	611	CLA	C4B-NB	6.80	1.41	1.35
23	B	616	CLA	C4B-NB	6.75	1.41	1.35
23	c	505	CLA	C4B-NB	6.73	1.41	1.35
23	C	512	CLA	MG-ND	-6.72	1.92	2.05
31	A	617	DGD	C4D-C5D	6.70	1.67	1.53
23	c	512	CLA	C4B-NB	6.68	1.41	1.35
23	c	507	CLA	C4B-NB	6.67	1.41	1.35
23	b	612	CLA	C4B-NB	6.66	1.41	1.35
36	V	201	HEC	C3C-C2C	-6.64	1.33	1.40
23	b	606	CLA	MG-NA	6.63	2.22	2.06
23	a	612	CLA	MG-NA	6.61	2.22	2.06
23	B	601	CLA	MG-NA	6.61	2.22	2.06
23	c	513	CLA	C4B-NB	6.61	1.41	1.35
23	a	603	CLA	MG-NA	6.60	2.22	2.06
23	d	403	CLA	C4B-NB	6.55	1.41	1.35
23	B	602	CLA	C4B-NB	6.52	1.41	1.35
23	B	606	CLA	MG-NA	6.50	2.21	2.06
23	B	606	CLA	C4B-NB	6.49	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C4B-NB	6.49	1.41	1.35
23	B	604	CLA	MG-NA	6.45	2.21	2.06
23	b	602	CLA	C4B-NB	6.44	1.41	1.35
36	v	201	HEC	C2B-C3B	-6.42	1.34	1.40
23	A	613	CLA	C4B-NB	6.39	1.40	1.35
23	B	604	CLA	C4B-NB	6.38	1.40	1.35
23	c	509	CLA	C4B-NB	6.35	1.40	1.35
23	c	506	CLA	C4B-NB	6.28	1.40	1.35
23	A	603	CLA	C4B-NB	6.26	1.40	1.35
23	C	502	CLA	C4B-NB	6.15	1.40	1.35
23	b	606	CLA	C4B-NB	6.11	1.40	1.35
23	C	512	CLA	C4B-NB	6.10	1.40	1.35
23	B	612	CLA	C4D-ND	-6.04	1.29	1.37
23	a	612	CLA	C4B-NB	6.03	1.40	1.35
23	a	606	CLA	MG-ND	-6.01	1.93	2.05
23	C	506	CLA	MG-ND	-5.85	1.94	2.05
23	b	616	CLA	C4B-NB	5.81	1.40	1.35
31	H	102	DGD	O5D-C1E	5.79	1.50	1.40
23	b	605	CLA	C4B-NB	5.78	1.40	1.35
23	B	608	CLA	C4B-NB	5.76	1.40	1.35
23	c	511	CLA	MG-NC	5.76	2.20	2.06
23	C	503	CLA	C4B-NB	5.75	1.40	1.35
23	d	402	CLA	C4B-NB	5.74	1.40	1.35
23	b	613	CLA	C4B-NB	5.71	1.40	1.35
27	d	408	PL9	C6-C1	-5.55	1.38	1.48
23	C	505	CLA	C4B-NB	5.53	1.40	1.35
23	C	502	CLA	MG-ND	5.48	2.16	2.05
23	c	508	CLA	C4B-NB	5.48	1.40	1.35
23	C	501	CLA	MG-NA	5.48	2.19	2.06
23	A	604	CLA	C4B-NB	5.44	1.40	1.35
23	b	612	CLA	C4D-ND	-5.43	1.30	1.37
23	C	507	CLA	C4B-NB	5.40	1.40	1.35
23	A	613	CLA	C4D-ND	-5.36	1.30	1.37
23	b	609	CLA	MG-NA	5.35	2.19	2.06
23	a	604	CLA	MG-NC	5.33	2.18	2.06
23	B	612	CLA	C4B-NB	5.33	1.40	1.35
23	c	504	CLA	MG-ND	-5.30	1.95	2.05
23	C	506	CLA	C4B-NB	5.29	1.39	1.35
23	h	101	CLA	MG-NA	5.27	2.18	2.06
27	D	407	PL9	C6-C1	-5.27	1.39	1.48
23	D	402	CLA	C4B-NB	5.26	1.39	1.35
23	b	607	CLA	C4B-NB	5.24	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	604	CLA	C4D-ND	-5.24	1.30	1.37
23	a	603	CLA	C4B-NB	5.24	1.39	1.35
23	b	610	CLA	C4B-NB	5.24	1.39	1.35
23	C	508	CLA	C4B-NB	5.23	1.39	1.35
23	b	613	CLA	MG-NA	5.23	2.18	2.06
28	d	406	LMG	O7-C8	-5.23	1.33	1.46
23	c	513	CLA	MG-NA	5.11	2.18	2.06
23	A	613	CLA	MG-NA	5.11	2.18	2.06
23	B	607	CLA	C4B-NB	5.08	1.39	1.35
23	B	616	CLA	MG-NA	5.05	2.18	2.06
23	c	502	CLA	C4B-NB	5.05	1.39	1.35
23	B	603	CLA	C4B-NB	4.98	1.39	1.35
23	B	609	CLA	MG-NA	4.87	2.17	2.06
36	v	201	HEC	C3C-C2C	-4.84	1.35	1.40
23	c	505	CLA	C4D-ND	-4.84	1.31	1.37
23	b	608	CLA	C4B-NB	4.81	1.39	1.35
23	A	613	CLA	C1D-ND	4.81	1.43	1.37
23	D	403	CLA	C1D-ND	4.77	1.43	1.37
23	b	615	CLA	MG-NC	-4.77	1.94	2.06
23	B	603	CLA	C4D-ND	-4.76	1.31	1.37
23	C	504	CLA	MG-NC	-4.72	1.95	2.06
23	B	611	CLA	C4D-ND	-4.65	1.31	1.37
27	d	408	PL9	C3-C4	-4.64	1.41	1.49
35	F	102	HEM	C3C-C2C	-4.64	1.33	1.40
23	b	606	CLA	C1D-ND	4.64	1.43	1.37
23	b	602	CLA	C4D-ND	-4.62	1.31	1.37
23	B	611	CLA	MG-NA	4.61	2.17	2.06
23	C	513	CLA	MG-NA	4.60	2.17	2.06
23	B	607	CLA	MG-NC	4.59	2.17	2.06
25	C	515	BCR	C1-C6	-4.53	1.47	1.53
23	A	607	CLA	C1D-ND	4.50	1.43	1.37
25	d	404	BCR	C1-C6	-4.49	1.47	1.53
23	c	506	CLA	C1D-ND	4.47	1.43	1.37
23	B	616	CLA	C1D-ND	4.45	1.43	1.37
23	B	607	CLA	C1D-ND	4.44	1.43	1.37
23	c	501	CLA	C4D-ND	-4.43	1.31	1.37
27	D	407	PL9	C11-C9	-4.42	1.42	1.51
23	B	613	CLA	MG-ND	-4.41	1.97	2.05
25	H	101	BCR	C30-C25	-4.40	1.47	1.53
23	b	604	CLA	C4D-ND	-4.40	1.31	1.37
23	c	508	CLA	C4D-ND	-4.39	1.31	1.37
23	c	511	CLA	MG-NA	4.37	2.16	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	MG-NC	-4.37	1.95	2.06
23	C	509	CLA	C1D-ND	4.33	1.43	1.37
23	D	402	CLA	C1D-ND	4.29	1.43	1.37
23	B	607	CLA	C3B-C2B	-4.27	1.34	1.40
23	c	509	CLA	C1D-ND	4.27	1.43	1.37
23	c	507	CLA	MG-NA	4.24	2.16	2.06
25	B	619	BCR	C1-C6	-4.24	1.47	1.53
23	B	609	CLA	C1D-ND	4.24	1.43	1.37
31	c	516	DGD	O2E-C2E	-4.22	1.33	1.43
23	C	501	CLA	MG-ND	-4.21	1.97	2.05
25	b	618	BCR	C30-C25	-4.21	1.48	1.53
23	C	512	CLA	C4D-ND	-4.21	1.31	1.37
23	c	501	CLA	C1D-ND	4.19	1.42	1.37
23	B	607	CLA	MG-NA	4.18	2.16	2.06
23	C	506	CLA	MG-NC	-4.16	1.96	2.06
23	B	606	CLA	C4D-ND	-4.14	1.32	1.37
23	A	604	CLA	C1D-ND	4.14	1.42	1.37
25	c	515	BCR	C30-C25	-4.14	1.48	1.53
31	C	517	DGD	C4D-C3D	4.13	1.62	1.52
25	B	617	BCR	C1-C6	-4.12	1.48	1.53
23	B	605	CLA	C4B-NB	4.11	1.38	1.35
30	D	408	LHG	P-O6	4.11	1.75	1.59
23	c	504	CLA	C4D-ND	-4.10	1.32	1.37
23	c	507	CLA	C4D-ND	-4.09	1.32	1.37
23	B	610	CLA	C3B-C2B	-4.07	1.34	1.40
23	b	608	CLA	CHC-C1C	4.06	1.45	1.35
23	b	605	CLA	C4D-ND	-4.06	1.32	1.37
31	a	616	DGD	O2G-C1B	4.06	1.45	1.34
25	D	404	BCR	C30-C25	-4.04	1.48	1.53
23	a	604	CLA	C1D-ND	4.04	1.42	1.37
25	C	514	BCR	C1-C6	-4.04	1.48	1.53
27	A	611	PL9	C7-C3	-4.03	1.47	1.51
23	b	603	CLA	C1D-ND	4.03	1.42	1.37
23	c	511	CLA	CHC-C1C	4.03	1.45	1.35
23	b	606	CLA	C4D-ND	-4.02	1.32	1.37
31	C	516	DGD	O5D-C6D	-4.01	1.36	1.43
23	C	513	CLA	C4D-ND	-4.01	1.32	1.37
23	C	507	CLA	MG-NA	4.00	2.15	2.06
23	C	504	CLA	MG-NA	3.99	2.15	2.06
23	b	611	CLA	C4D-ND	-3.99	1.32	1.37
23	a	603	CLA	C1D-ND	3.98	1.42	1.37
23	b	608	CLA	C4D-ND	-3.97	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	MG-NC	-3.97	1.96	2.06
23	A	613	CLA	CHC-C1C	3.97	1.45	1.35
23	c	505	CLA	C3B-C2B	-3.97	1.34	1.40
35	f	102	HEM	C3C-C2C	-3.97	1.34	1.40
23	B	616	CLA	C4D-ND	-3.96	1.32	1.37
23	c	503	CLA	MG-NC	3.96	2.15	2.06
23	C	508	CLA	MG-ND	3.96	2.13	2.05
23	b	605	CLA	C1D-ND	3.96	1.42	1.37
27	D	407	PL9	C52-C5	-3.95	1.42	1.50
23	C	510	CLA	C4D-ND	-3.94	1.32	1.37
23	b	611	CLA	CHC-C1C	3.94	1.45	1.35
31	H	102	DGD	C4D-C5D	3.93	1.61	1.53
25	h	102	BCR	C30-C25	-3.93	1.48	1.53
23	A	607	CLA	MG-NC	-3.93	1.96	2.06
23	C	509	CLA	C4D-ND	-3.91	1.32	1.37
23	b	610	CLA	C1D-ND	3.91	1.42	1.37
23	C	501	CLA	C1D-ND	3.90	1.42	1.37
23	c	512	CLA	MG-NC	3.90	2.15	2.06
23	D	403	CLA	MG-NC	3.89	2.15	2.06
23	B	610	CLA	MG-ND	-3.88	1.98	2.05
28	D	405	LMG	C4-C3	3.85	1.62	1.52
23	c	509	CLA	C4D-ND	-3.84	1.32	1.37
23	B	605	CLA	C4D-ND	-3.84	1.32	1.37
28	c	521	LMG	O1-C1	3.84	1.46	1.40
23	C	503	CLA	C4D-ND	-3.84	1.32	1.37
25	b	619	BCR	C1-C6	-3.83	1.48	1.53
28	C	519	LMG	O7-C8	-3.82	1.37	1.46
23	b	603	CLA	C4D-ND	-3.82	1.32	1.37
28	D	409	LMG	C7-C8	3.82	1.60	1.51
23	C	502	CLA	C4D-ND	-3.81	1.32	1.37
23	b	610	CLA	C4D-ND	-3.80	1.32	1.37
23	c	501	CLA	MG-NA	3.79	2.15	2.06
31	C	517	DGD	O3D-C3D	-3.78	1.34	1.43
23	b	616	CLA	C4D-ND	-3.78	1.32	1.37
23	B	610	CLA	C1D-ND	3.78	1.42	1.37
25	B	618	BCR	C30-C25	-3.77	1.48	1.53
23	C	511	CLA	C1D-ND	3.77	1.42	1.37
23	B	616	CLA	MG-ND	3.75	2.13	2.05
29	a	615	SQD	O47-C7	3.75	1.44	1.34
23	c	503	CLA	C4D-ND	-3.75	1.32	1.37
30	L	101	LHG	O7-C5	-3.75	1.37	1.46
23	h	101	CLA	C1D-ND	3.73	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	615	SQD	O48-C23	3.72	1.44	1.33
23	C	508	CLA	C4D-ND	-3.71	1.32	1.37
23	b	602	CLA	C1D-ND	3.70	1.42	1.37
23	b	616	CLA	CMB-C2B	-3.69	1.44	1.51
23	B	614	CLA	C4D-ND	-3.68	1.32	1.37
25	A	608	BCR	C1-C6	-3.67	1.48	1.53
23	d	402	CLA	MG-NC	3.66	2.15	2.06
23	B	606	CLA	MG-ND	3.66	2.13	2.05
23	C	503	CLA	CHC-C1C	3.64	1.44	1.35
23	B	605	CLA	CHC-C1C	3.63	1.44	1.35
23	B	606	CLA	CHC-C1C	3.63	1.44	1.35
29	a	613	SQD	O48-C23	3.62	1.43	1.33
23	B	608	CLA	C4D-ND	-3.62	1.32	1.37
25	Y	101	BCR	C30-C25	-3.60	1.48	1.53
31	H	102	DGD	O2D-C2D	-3.60	1.34	1.43
31	c	517	DGD	O3G-C1D	-3.60	1.34	1.40
36	V	201	HEC	CBC-CAC	-3.59	1.36	1.49
23	c	510	CLA	MG-NC	-3.59	1.97	2.06
31	C	516	DGD	C4E-C3E	3.58	1.61	1.52
23	D	402	CLA	C3B-C2B	-3.57	1.35	1.40
23	C	506	CLA	C4D-ND	-3.57	1.32	1.37
23	C	506	CLA	MG-NA	3.56	2.14	2.06
25	b	617	BCR	C30-C25	-3.56	1.48	1.53
23	C	511	CLA	C1B-NB	3.56	1.38	1.35
36	V	201	HEC	CBB-CAB	-3.55	1.36	1.49
23	b	609	CLA	C4D-ND	-3.54	1.32	1.37
23	A	607	CLA	C4D-ND	-3.54	1.32	1.37
23	C	506	CLA	C1D-ND	3.52	1.42	1.37
23	c	502	CLA	C4D-ND	-3.52	1.32	1.37
25	c	515	BCR	C1-C6	-3.50	1.49	1.53
23	B	615	CLA	CMB-C2B	-3.50	1.44	1.51
23	a	604	CLA	CHC-C1C	3.50	1.43	1.35
25	T	101	BCR	C30-C25	-3.49	1.49	1.53
23	C	503	CLA	MG-NC	3.48	2.14	2.06
23	b	606	CLA	C1B-NB	3.48	1.38	1.35
23	d	402	CLA	C4D-ND	-3.47	1.32	1.37
23	d	402	CLA	C1D-ND	3.47	1.42	1.37
25	b	618	BCR	C1-C6	-3.47	1.49	1.53
25	Y	101	BCR	C1-C6	-3.46	1.49	1.53
23	C	505	CLA	C4D-ND	-3.46	1.32	1.37
25	A	608	BCR	C33-C5	-3.46	1.45	1.50
23	b	614	CLA	CHC-C1C	3.46	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CHC-C1C	3.45	1.43	1.35
23	b	613	CLA	C4D-ND	-3.45	1.33	1.37
25	C	520	BCR	C30-C25	-3.45	1.49	1.53
25	c	514	BCR	C1-C6	-3.44	1.49	1.53
23	A	603	CLA	MG-ND	-3.43	1.99	2.05
23	c	511	CLA	C4D-ND	-3.43	1.33	1.37
23	C	505	CLA	C1D-ND	3.43	1.42	1.37
36	v	201	HEC	CBB-CAB	-3.42	1.36	1.49
23	a	604	CLA	C4D-ND	-3.42	1.33	1.37
35	f	102	HEM	C3C-CAC	3.41	1.54	1.47
31	c	517	DGD	O5D-C1E	3.40	1.46	1.40
23	B	604	CLA	C1D-ND	3.40	1.42	1.37
23	d	402	CLA	C3B-C2B	-3.40	1.35	1.40
36	v	201	HEC	CBC-CAC	-3.40	1.36	1.49
23	B	606	CLA	C3B-C2B	-3.38	1.35	1.40
31	A	617	DGD	C4D-C3D	3.38	1.60	1.52
29	F	101	SQD	O48-C23	3.38	1.43	1.33
28	c	522	LMG	C4-C5	3.37	1.60	1.53
23	B	615	CLA	MG-NA	3.36	2.14	2.06
29	b	601	SQD	O48-C23	3.36	1.43	1.33
30	D	406	LHG	O8-C6	-3.36	1.37	1.45
29	f	101	SQD	O47-C7	3.35	1.43	1.34
23	D	403	CLA	CMD-C2D	-3.35	1.43	1.50
28	D	409	LMG	C9-C8	3.35	1.61	1.50
23	B	607	CLA	C1C-NC	-3.34	1.32	1.37
23	C	501	CLA	CHC-C1C	3.34	1.43	1.35
23	c	508	CLA	CHC-C1C	3.33	1.43	1.35
25	d	404	BCR	C30-C25	-3.33	1.49	1.53
23	C	510	CLA	C1D-ND	3.32	1.41	1.37
23	b	609	CLA	C1D-ND	3.32	1.41	1.37
27	D	407	PL9	C5-C4	-3.32	1.35	1.47
23	C	503	CLA	C1D-ND	3.32	1.41	1.37
23	C	510	CLA	CHC-C1C	3.32	1.43	1.35
23	B	602	CLA	C1D-ND	3.32	1.41	1.37
23	c	510	CLA	CMB-C2B	-3.31	1.44	1.51
23	b	607	CLA	MG-NA	3.30	2.14	2.06
23	B	611	CLA	MG-ND	3.30	2.12	2.05
31	a	616	DGD	O1G-C1A	3.29	1.43	1.33
23	B	603	CLA	C1D-ND	3.28	1.41	1.37
23	b	616	CLA	C3B-CAB	-3.28	1.41	1.47
23	B	615	CLA	C3B-C2B	-3.27	1.35	1.40
28	B	620	LMG	C9-C8	3.27	1.60	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	518	DGD	O2G-C2G	-3.27	1.38	1.46
27	a	611	PL9	C53-C6	-3.26	1.43	1.50
31	A	617	DGD	C1E-C2E	3.26	1.61	1.52
24	A	606	PHO	CAC-C3C	-3.25	1.46	1.52
29	A	616	SQD	O48-C23	3.25	1.42	1.33
23	b	616	CLA	C3B-C2B	-3.25	1.35	1.40
23	B	601	CLA	C1D-ND	3.24	1.41	1.37
23	b	604	CLA	CHC-C1C	3.24	1.43	1.35
23	c	512	CLA	C4D-ND	-3.24	1.33	1.37
23	B	614	CLA	MG-NA	3.24	2.14	2.06
23	c	503	CLA	CHC-C1C	3.23	1.43	1.35
23	B	609	CLA	C3B-C2B	-3.22	1.35	1.40
23	b	604	CLA	C1D-ND	3.22	1.41	1.37
23	B	615	CLA	C4D-ND	-3.22	1.33	1.37
29	f	101	SQD	O48-C23	3.22	1.42	1.33
31	A	617	DGD	O6D-C1D	3.21	1.50	1.41
30	D	408	LHG	O3-C3	-3.21	1.32	1.44
23	C	507	CLA	C4D-ND	-3.21	1.33	1.37
23	A	604	CLA	MG-NA	3.20	2.13	2.06
23	a	603	CLA	CHC-C1C	3.20	1.43	1.35
23	c	513	CLA	CHC-C1C	3.20	1.43	1.35
23	a	612	CLA	CMD-C2D	-3.19	1.44	1.50
23	B	610	CLA	CMB-C2B	-3.19	1.45	1.51
23	C	505	CLA	CHC-C1C	3.18	1.43	1.35
23	C	504	CLA	C4D-ND	-3.18	1.33	1.37
23	C	513	CLA	C1D-ND	3.17	1.41	1.37
23	b	602	CLA	CHC-C1C	3.17	1.43	1.35
25	C	514	BCR	C30-C25	-3.17	1.49	1.53
28	B	620	LMG	O1-C7	-3.17	1.38	1.43
31	H	102	DGD	O1G-C1G	-3.17	1.37	1.45
23	d	402	CLA	MG-ND	3.16	2.12	2.05
29	A	614	SQD	O48-C23	3.16	1.42	1.33
23	c	510	CLA	CHC-C1C	3.16	1.43	1.35
23	b	605	CLA	CMB-C2B	-3.16	1.45	1.51
23	C	501	CLA	C4D-ND	-3.16	1.33	1.37
25	B	618	BCR	C1-C6	-3.15	1.49	1.53
23	B	613	CLA	C4D-ND	-3.14	1.33	1.37
23	h	101	CLA	CHC-C1C	3.14	1.43	1.35
23	b	614	CLA	MG-NA	3.14	2.13	2.06
25	a	607	BCR	C30-C25	-3.14	1.49	1.53
25	c	515	BCR	C33-C5	-3.14	1.45	1.50
28	c	519	LMG	C4-C3	3.13	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	CMB-C2B	-3.13	1.45	1.51
23	a	612	CLA	C4D-ND	-3.12	1.33	1.37
25	b	617	BCR	C1-C6	-3.11	1.49	1.53
23	d	403	CLA	CMD-C2D	-3.11	1.44	1.50
23	b	613	CLA	MG-ND	-3.11	1.99	2.05
23	C	511	CLA	CHC-C1C	3.11	1.42	1.35
23	a	603	CLA	C4D-ND	-3.11	1.33	1.37
23	b	610	CLA	C3B-C2B	-3.10	1.36	1.40
23	a	606	CLA	C1D-ND	3.10	1.41	1.37
27	d	408	PL9	C53-C6	-3.10	1.44	1.50
23	C	507	CLA	C3B-C2B	-3.10	1.36	1.40
27	D	407	PL9	C36-C37	-3.09	1.43	1.53
23	b	603	CLA	CMC-C2C	-3.08	1.44	1.50
23	C	503	CLA	MG-NA	3.08	2.13	2.06
23	c	510	CLA	C4D-ND	-3.07	1.33	1.37
23	d	403	CLA	C3B-CAB	-3.07	1.41	1.47
27	D	407	PL9	C46-C44	-3.07	1.44	1.51
23	c	512	CLA	C1D-ND	3.06	1.41	1.37
23	c	507	CLA	MG-NC	-3.06	1.99	2.06
23	B	609	CLA	C4D-ND	-3.06	1.33	1.37
29	A	616	SQD	O47-C7	3.05	1.42	1.34
23	A	603	CLA	CHC-C1C	3.05	1.42	1.35
23	b	606	CLA	MG-ND	3.05	2.11	2.05
23	c	506	CLA	MG-NC	3.05	2.13	2.06
25	h	102	BCR	C1-C6	-3.05	1.49	1.53
30	A	615	LHG	O8-C23	3.04	1.42	1.33
23	D	403	CLA	CMB-C2B	-3.04	1.45	1.51
25	T	101	BCR	C1-C6	-3.04	1.49	1.53
31	c	516	DGD	C4E-C3E	3.03	1.60	1.52
23	A	603	CLA	C4D-ND	-3.03	1.33	1.37
23	c	506	CLA	MG-NA	3.03	2.13	2.06
23	B	605	CLA	C3B-C2B	-3.03	1.36	1.40
23	B	611	CLA	CHC-C1C	3.03	1.42	1.35
23	C	507	CLA	CHC-C1C	3.03	1.42	1.35
31	c	518	DGD	C6D-C5D	3.02	1.61	1.51
23	B	614	CLA	CHC-C1C	3.02	1.42	1.35
23	B	610	CLA	CHC-C1C	3.02	1.42	1.35
23	D	402	CLA	CMD-C2D	-3.01	1.44	1.50
23	B	604	CLA	C4D-ND	-3.01	1.33	1.37
29	b	601	SQD	O47-C7	3.00	1.42	1.34
23	b	603	CLA	CMB-C2B	-3.00	1.45	1.51
23	b	614	CLA	C1D-ND	3.00	1.41	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	605	PHO	CHA-CBD	-3.00	1.48	1.52
31	c	517	DGD	O3E-C3E	-2.99	1.35	1.43
23	a	612	CLA	CHC-C1C	2.99	1.42	1.35
23	c	506	CLA	C4D-ND	-2.99	1.33	1.37
23	b	608	CLA	C3B-C2B	-2.98	1.36	1.40
25	t	101	BCR	C1-C6	-2.98	1.49	1.53
29	B	624	SQD	O47-C7	2.98	1.42	1.34
23	b	614	CLA	C4D-ND	-2.98	1.33	1.37
23	h	101	CLA	C1B-NB	2.98	1.37	1.35
23	D	402	CLA	C4D-ND	-2.97	1.33	1.37
23	C	512	CLA	CHC-C1C	2.97	1.42	1.35
23	c	503	CLA	C1D-ND	2.96	1.41	1.37
23	b	611	CLA	CMD-C2D	-2.96	1.44	1.50
23	b	604	CLA	MG-NC	2.96	2.13	2.06
23	A	603	CLA	MG-NC	-2.94	1.99	2.06
29	B	624	SQD	O48-C23	2.94	1.41	1.33
28	C	519	LMG	C4-C5	2.93	1.59	1.53
23	c	508	CLA	C1D-ND	2.93	1.41	1.37
23	B	611	CLA	CMB-C2B	-2.93	1.45	1.51
23	c	513	CLA	C4D-ND	-2.92	1.33	1.37
31	C	516	DGD	C2A-C1A	-2.92	1.42	1.50
23	c	509	CLA	CHC-C1C	2.92	1.42	1.35
25	B	617	BCR	C33-C5	-2.92	1.46	1.50
23	A	603	CLA	C1D-ND	2.91	1.41	1.37
31	H	102	DGD	C1E-C2E	2.91	1.60	1.52
23	b	613	CLA	C1D-ND	2.91	1.41	1.37
23	b	606	CLA	CHC-C1C	2.91	1.42	1.35
23	B	613	CLA	C1D-ND	2.91	1.41	1.37
31	C	517	DGD	O2G-C2G	-2.90	1.39	1.46
23	B	601	CLA	C3B-C2B	-2.90	1.36	1.40
29	A	614	SQD	O47-C7	2.90	1.42	1.34
23	C	507	CLA	C3B-CAB	-2.90	1.42	1.47
23	b	612	CLA	CHC-C1C	2.89	1.42	1.35
35	f	102	HEM	CAB-C3B	2.89	1.55	1.47
23	b	603	CLA	CMD-C2D	-2.89	1.44	1.50
23	c	507	CLA	C3B-CAB	-2.89	1.42	1.47
25	k	101	BCR	C1-C6	-2.89	1.49	1.53
23	c	503	CLA	CMB-C2B	-2.88	1.45	1.51
23	B	615	CLA	CHC-C1C	2.88	1.42	1.35
31	c	518	DGD	C1D-C2D	2.88	1.60	1.52
31	H	102	DGD	C3E-C2E	2.87	1.59	1.52
23	B	606	CLA	CMD-C2D	-2.87	1.44	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	612	CLA	CMB-C2B	-2.86	1.45	1.51
23	B	603	CLA	MG-NA	-2.86	1.99	2.06
23	c	507	CLA	C4B-CHC	-2.86	1.33	1.41
23	B	612	CLA	CHC-C1C	2.86	1.42	1.35
23	C	504	CLA	CMB-C2B	-2.86	1.45	1.51
23	b	616	CLA	C1D-ND	2.86	1.41	1.37
23	d	402	CLA	CMB-C2B	-2.86	1.45	1.51
23	c	501	CLA	CMB-C2B	-2.85	1.45	1.51
25	a	607	BCR	C1-C6	-2.85	1.49	1.53
30	d	409	LHG	P-O6	2.84	1.70	1.59
28	c	519	LMG	O1-C1	2.84	1.45	1.40
23	b	608	CLA	C3B-CAB	-2.84	1.42	1.47
23	b	615	CLA	C3B-CAB	-2.83	1.42	1.47
28	c	519	LMG	C1-C2	2.83	1.60	1.52
23	c	505	CLA	C3B-CAB	-2.83	1.42	1.47
23	h	101	CLA	O2A-CGA	2.82	1.41	1.33
23	D	403	CLA	C3B-C2B	-2.82	1.36	1.40
23	b	605	CLA	MG-NA	2.82	2.13	2.06
23	d	402	CLA	CHC-C1C	2.82	1.42	1.35
23	b	612	CLA	MG-NC	-2.82	1.99	2.06
31	C	517	DGD	C1E-C2E	2.82	1.60	1.52
28	A	612	LMG	C4-C5	2.81	1.59	1.53
31	C	517	DGD	O5D-C6D	-2.81	1.38	1.43
35	F	102	HEM	C3C-CAC	2.81	1.53	1.47
23	c	512	CLA	CHC-C1C	2.80	1.42	1.35
23	B	614	CLA	C1B-NB	2.79	1.37	1.35
28	D	409	LMG	O8-C28	2.79	1.41	1.33
23	C	507	CLA	C1D-ND	2.79	1.41	1.37
23	d	403	CLA	CHC-C1C	2.78	1.42	1.35
23	b	612	CLA	CMB-C2B	-2.78	1.45	1.51
23	B	602	CLA	C4D-ND	-2.78	1.33	1.37
24	d	401	PHO	CAC-C3C	-2.78	1.47	1.52
23	C	502	CLA	CHC-C1C	2.77	1.42	1.35
23	C	506	CLA	CHC-C1C	2.77	1.42	1.35
23	h	101	CLA	C4D-ND	-2.77	1.33	1.37
23	c	513	CLA	CMB-C2B	-2.77	1.45	1.51
29	a	613	SQD	O47-C7	2.77	1.42	1.34
28	B	622	LMG	O8-C28	2.77	1.40	1.30
23	B	611	CLA	MG-NC	-2.76	1.99	2.06
23	b	603	CLA	CHC-C1C	2.76	1.42	1.35
29	A	614	SQD	O2-C2	-2.76	1.36	1.43
23	c	511	CLA	MG-ND	2.76	2.11	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	517	DGD	O2E-C2E	-2.76	1.36	1.43
31	h	103	DGD	C4D-C3D	2.76	1.59	1.52
28	m	101	LMG	C4-C3	2.75	1.59	1.52
25	c	514	BCR	C30-C25	-2.74	1.50	1.53
31	H	102	DGD	C4E-C5E	2.73	1.58	1.53
23	B	607	CLA	C4D-ND	-2.72	1.33	1.37
23	B	608	CLA	CMD-C2D	-2.72	1.45	1.50
23	a	612	CLA	MG-ND	2.72	2.11	2.05
23	B	606	CLA	C1B-NB	2.72	1.37	1.35
23	B	601	CLA	CHC-C1C	2.71	1.41	1.35
23	a	606	CLA	CMA-C3A	-2.71	1.47	1.53
28	c	521	LMG	C1-C2	2.71	1.60	1.52
23	c	508	CLA	CMD-C2D	-2.70	1.45	1.50
23	C	501	CLA	CMB-C2B	-2.70	1.46	1.51
23	B	602	CLA	CHC-C1C	2.69	1.41	1.35
23	C	508	CLA	CHC-C1C	2.69	1.41	1.35
23	B	602	CLA	CMB-C2B	-2.69	1.46	1.51
23	B	614	CLA	CMC-C2C	-2.69	1.45	1.50
29	F	101	SQD	O2-C2	-2.69	1.36	1.43
23	c	511	CLA	CMB-C2B	-2.68	1.46	1.51
31	C	516	DGD	C4D-C3D	2.68	1.59	1.52
23	c	508	CLA	MG-ND	2.68	2.11	2.05
23	c	504	CLA	CMB-C2B	-2.68	1.46	1.51
23	b	612	CLA	CMC-C2C	-2.68	1.45	1.50
23	c	505	CLA	MG-NA	-2.67	1.99	2.06
24	A	605	PHO	CMC-C2C	-2.67	1.45	1.51
25	C	515	BCR	C30-C25	-2.67	1.50	1.53
23	B	602	CLA	MG-NA	2.66	2.12	2.06
25	b	617	BCR	C33-C5	-2.66	1.46	1.50
23	C	513	CLA	CMB-C2B	-2.66	1.46	1.51
23	C	508	CLA	C1D-ND	2.65	1.41	1.37
23	C	513	CLA	CHC-C1C	2.65	1.41	1.35
30	A	615	LHG	P-O6	2.65	1.70	1.59
31	c	517	DGD	O5D-C6D	2.65	1.48	1.43
23	c	504	CLA	CHC-C1C	2.65	1.41	1.35
28	c	521	LMG	C7-C8	2.65	1.58	1.50
23	D	402	CLA	MG-NC	2.64	2.12	2.06
27	D	407	PL9	C41-C39	-2.64	1.45	1.51
23	c	502	CLA	CMD-C2D	-2.64	1.45	1.50
23	B	612	CLA	CMB-C2B	-2.64	1.46	1.51
23	B	607	CLA	CMB-C2B	-2.64	1.46	1.51
23	b	609	CLA	CHC-C1C	2.64	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C3B-C2B	-2.63	1.36	1.40
23	b	602	CLA	CMD-C2D	-2.63	1.45	1.50
23	b	610	CLA	CHC-C1C	2.63	1.41	1.35
24	a	605	PHO	CAC-C3C	-2.63	1.47	1.52
23	C	503	CLA	C1D-C2D	2.62	1.50	1.45
31	c	517	DGD	O3D-C3D	-2.62	1.36	1.43
31	c	516	DGD	C4D-C3D	2.61	1.59	1.52
23	B	615	CLA	C3B-CAB	-2.61	1.42	1.47
28	C	519	LMG	C7-C8	2.61	1.58	1.50
23	B	604	CLA	CHC-C1C	2.61	1.41	1.35
23	B	615	CLA	CMD-C2D	-2.61	1.45	1.50
23	b	605	CLA	CHC-C1C	2.61	1.41	1.35
23	b	615	CLA	C3B-C2B	-2.60	1.36	1.40
31	c	518	DGD	O4D-C4D	-2.60	1.36	1.43
31	C	518	DGD	C6D-C5D	2.60	1.59	1.51
23	A	607	CLA	C3D-C4D	2.60	1.50	1.44
23	c	511	CLA	C1D-ND	2.59	1.41	1.37
31	H	102	DGD	O2G-C2G	-2.59	1.40	1.46
29	A	616	SQD	O47-C45	-2.59	1.42	1.47
25	b	619	BCR	C30-C25	-2.59	1.50	1.53
23	b	604	CLA	CMB-C2B	-2.58	1.46	1.51
23	b	605	CLA	C4B-CHC	-2.57	1.33	1.41
28	c	522	LMG	O8-C9	-2.57	1.39	1.45
23	b	614	CLA	CMC-C2C	-2.57	1.45	1.50
23	B	605	CLA	MG-ND	-2.57	2.00	2.05
24	A	606	PHO	C3B-C2B	-2.56	1.36	1.40
23	A	607	CLA	C4B-CHC	-2.56	1.33	1.41
29	B	624	SQD	O2-C2	-2.56	1.36	1.43
23	D	403	CLA	CHC-C1C	2.56	1.41	1.35
23	B	609	CLA	C3B-CAB	-2.56	1.42	1.47
23	b	615	CLA	C4D-ND	-2.56	1.34	1.37
23	b	615	CLA	CMB-C2B	-2.56	1.46	1.51
23	A	613	CLA	CAC-C3C	-2.55	1.44	1.51
23	B	609	CLA	CHC-C1C	2.55	1.41	1.35
23	b	615	CLA	CMD-C2D	-2.55	1.45	1.50
23	B	601	CLA	CMC-C2C	-2.55	1.45	1.50
23	C	509	CLA	CMD-C2D	-2.55	1.45	1.50
23	C	501	CLA	C3B-C2B	-2.54	1.36	1.40
23	B	611	CLA	C1D-ND	2.54	1.40	1.37
23	c	508	CLA	CMB-C2B	-2.54	1.46	1.51
23	C	511	CLA	CMC-C2C	-2.54	1.45	1.50
23	C	512	CLA	C1D-ND	2.54	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	CMB-C2B	-2.54	1.46	1.51
23	A	604	CLA	MG-ND	-2.54	2.00	2.05
23	A	604	CLA	C3B-C2B	-2.53	1.36	1.40
23	a	604	CLA	C3B-C2B	-2.53	1.36	1.40
29	f	101	SQD	O2-C2	-2.53	1.37	1.43
23	c	502	CLA	CHC-C1C	2.53	1.41	1.35
24	a	605	PHO	CMC-C2C	-2.53	1.45	1.51
23	B	613	CLA	CHC-C1C	2.52	1.41	1.35
29	f	101	SQD	O3-C3	-2.52	1.37	1.43
23	b	607	CLA	CMD-C2D	-2.52	1.45	1.50
23	C	502	CLA	C3B-C2B	-2.51	1.36	1.40
31	A	617	DGD	C3G-C2G	2.51	1.58	1.50
31	c	517	DGD	C1D-C2D	2.51	1.59	1.52
23	C	504	CLA	CHC-C1C	2.51	1.41	1.35
27	d	408	PL9	C15-C14	-2.51	1.44	1.50
23	c	513	CLA	C1D-ND	2.51	1.40	1.37
24	d	401	PHO	C3B-CAB	-2.50	1.42	1.47
23	D	402	CLA	C4B-CHC	-2.50	1.34	1.41
23	b	613	CLA	CAA-C2A	-2.50	1.49	1.54
35	F	102	HEM	CAB-C3B	2.50	1.54	1.47
25	D	404	BCR	C1-C6	-2.50	1.50	1.53
23	A	604	CLA	CHC-C1C	2.50	1.41	1.35
31	A	617	DGD	O2G-C1B	2.50	1.41	1.34
23	B	601	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	613	CLA	C3B-CAB	-2.49	1.42	1.47
23	a	606	CLA	C4D-ND	-2.49	1.34	1.37
31	c	516	DGD	C6D-C5D	2.49	1.59	1.51
23	c	505	CLA	MG-NC	2.49	2.12	2.06
24	A	606	PHO	CMB-C2B	-2.47	1.45	1.51
23	c	507	CLA	CHC-C1C	2.47	1.41	1.35
28	C	519	LMG	C1-C2	2.47	1.59	1.52
24	a	605	PHO	O2D-CGD	2.47	1.39	1.33
23	c	513	CLA	MG-NC	-2.47	2.00	2.06
23	b	603	CLA	C3B-C2B	-2.46	1.37	1.40
28	B	620	LMG	O7-C8	-2.46	1.40	1.46
23	h	101	CLA	C1D-C2D	2.46	1.50	1.45
31	H	102	DGD	O3E-C3E	-2.45	1.37	1.43
28	d	406	LMG	O6-C5	-2.45	1.38	1.44
23	B	613	CLA	CMB-C2B	-2.45	1.46	1.51
23	b	616	CLA	CAA-C2A	-2.45	1.49	1.54
29	a	613	SQD	O2-C2	-2.44	1.37	1.43
23	D	402	CLA	CHC-C1C	2.44	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	MG-ND	-2.44	2.00	2.05
23	b	615	CLA	CMC-C2C	-2.44	1.45	1.50
28	D	409	LMG	C30-C29	2.44	1.61	1.52
23	B	609	CLA	CMD-C2D	-2.44	1.45	1.50
23	b	615	CLA	CHC-C1C	2.43	1.41	1.35
23	B	615	CLA	C5-C3	-2.43	1.46	1.51
23	a	604	CLA	CMB-C2B	-2.43	1.46	1.51
23	A	603	CLA	CMD-C2D	-2.42	1.45	1.50
23	a	606	CLA	C1C-NC	-2.42	1.34	1.37
23	d	403	CLA	C4D-ND	-2.42	1.34	1.37
23	B	616	CLA	CHC-C1C	2.42	1.41	1.35
23	d	403	CLA	CMC-C2C	-2.41	1.45	1.50
25	k	101	BCR	C30-C25	-2.41	1.50	1.53
23	A	613	CLA	C3C-C2C	2.41	1.41	1.36
23	b	611	CLA	MG-NA	2.40	2.12	2.06
31	c	516	DGD	O6D-C1D	2.40	1.48	1.41
23	C	510	CLA	CMD-C2D	-2.40	1.45	1.50
25	B	619	BCR	C30-C25	-2.40	1.50	1.53
23	c	505	CLA	CMB-C2B	-2.39	1.46	1.51
23	D	403	CLA	C3B-CAB	-2.39	1.43	1.47
27	D	407	PL9	C20-C19	-2.39	1.44	1.50
23	b	612	CLA	C1D-ND	2.39	1.40	1.37
23	b	608	CLA	CMB-C2B	-2.38	1.46	1.51
23	C	511	CLA	C4D-ND	-2.38	1.34	1.37
23	c	510	CLA	C1D-ND	2.38	1.40	1.37
23	B	607	CLA	CHC-C1C	2.38	1.41	1.35
23	C	510	CLA	MG-NC	2.38	2.11	2.06
23	C	511	CLA	CMB-C2B	-2.37	1.46	1.51
23	B	607	CLA	CMC-C2C	-2.37	1.45	1.50
23	b	610	CLA	C4B-CHC	-2.37	1.34	1.41
29	b	601	SQD	O2-C2	-2.37	1.37	1.43
24	A	605	PHO	O2D-CGD	2.37	1.39	1.33
25	T	101	BCR	C27-C26	-2.36	1.46	1.51
23	c	512	CLA	CMD-C2D	-2.36	1.45	1.50
31	h	103	DGD	C1E-C2E	2.36	1.59	1.52
23	b	607	CLA	C3B-C2B	-2.36	1.37	1.40
27	d	408	PL9	C23-C24	2.36	1.38	1.33
23	B	608	CLA	C1D-ND	2.35	1.40	1.37
23	b	615	CLA	C1D-ND	2.35	1.40	1.37
28	D	409	LMG	O8-C9	2.35	1.50	1.45
27	d	408	PL9	C46-C44	-2.35	1.46	1.51
23	B	606	CLA	CMC-C2C	-2.35	1.45	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	516	DGD	O3E-C3E	-2.34	1.37	1.43
23	c	513	CLA	C3B-C2B	-2.34	1.37	1.40
35	f	102	HEM	C3B-C2B	-2.34	1.32	1.37
23	C	512	CLA	C1A-CHA	-2.34	1.33	1.43
30	d	407	LHG	P-O3	2.34	1.68	1.59
25	t	101	BCR	C30-C25	-2.34	1.50	1.53
23	A	603	CLA	CMC-C2C	-2.34	1.45	1.50
23	B	605	CLA	O2D-CED	-2.33	1.39	1.45
23	C	501	CLA	CMD-C2D	-2.33	1.45	1.50
23	B	607	CLA	CAC-C3C	-2.33	1.45	1.51
25	t	101	BCR	C27-C26	-2.32	1.46	1.51
23	B	604	CLA	CMB-C2B	-2.32	1.46	1.51
23	C	504	CLA	CMD-C2D	-2.32	1.45	1.50
23	b	604	CLA	CMC-C2C	-2.32	1.45	1.50
23	B	603	CLA	MG-NC	2.32	2.11	2.06
25	C	515	BCR	C36-C18	-2.32	1.46	1.50
31	c	517	DGD	O1G-C1A	2.32	1.40	1.33
27	D	407	PL9	C45-C44	-2.31	1.44	1.50
23	B	609	CLA	CMB-C2B	-2.31	1.46	1.51
23	B	614	CLA	C3B-CAB	-2.31	1.43	1.47
28	c	521	LMG	C4-C3	2.31	1.58	1.52
23	C	504	CLA	CMA-C3A	-2.31	1.48	1.53
25	C	515	BCR	C33-C5	-2.31	1.47	1.50
23	C	505	CLA	MG-ND	-2.30	2.01	2.05
23	b	613	CLA	CMD-C2D	-2.30	1.45	1.50
23	c	503	CLA	C1D-C2D	2.30	1.49	1.45
27	a	611	PL9	C6-C1	-2.29	1.44	1.48
23	a	612	CLA	C3B-C2B	-2.29	1.37	1.40
23	c	503	CLA	CMC-C2C	-2.28	1.46	1.50
23	c	507	CLA	CMB-C2B	-2.28	1.46	1.51
23	C	509	CLA	O2D-CGD	2.28	1.38	1.33
31	C	517	DGD	C6D-C5D	2.28	1.58	1.51
23	b	613	CLA	CMC-C2C	-2.28	1.46	1.50
23	B	611	CLA	C3B-CAB	-2.28	1.43	1.47
23	A	603	CLA	C1D-C2D	2.28	1.49	1.45
23	c	507	CLA	C1D-ND	2.28	1.40	1.37
31	C	516	DGD	C2B-C1B	-2.28	1.44	1.50
23	c	508	CLA	CMC-C2C	-2.28	1.46	1.50
23	a	606	CLA	CMB-C2B	-2.28	1.46	1.51
28	B	620	LMG	C1-C2	2.28	1.59	1.52
23	B	604	CLA	C3B-C2B	-2.27	1.37	1.40
30	d	407	LHG	C6-C5	2.27	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CMB-C2B	-2.27	1.46	1.51
23	a	606	CLA	MG-NC	-2.27	2.00	2.06
23	C	509	CLA	CMC-C2C	-2.27	1.46	1.50
23	a	603	CLA	C3B-C2B	-2.27	1.37	1.40
27	D	407	PL9	C27-C28	-2.26	1.43	1.50
23	B	616	CLA	C4B-CHC	-2.26	1.34	1.41
23	b	608	CLA	C1C-C2C	2.26	1.48	1.44
23	B	615	CLA	C1D-ND	2.26	1.40	1.37
27	a	611	PL9	C7-C3	-2.26	1.49	1.51
23	a	606	CLA	C4B-CHC	-2.26	1.34	1.41
23	b	606	CLA	CAC-C3C	-2.26	1.45	1.51
23	C	506	CLA	C3B-C2B	-2.25	1.37	1.40
23	B	615	CLA	C3D-C4D	2.25	1.49	1.44
25	k	101	BCR	C33-C5	-2.25	1.47	1.50
30	l	101	LHG	P-O6	2.25	1.68	1.59
23	B	603	CLA	CMB-C2B	-2.25	1.47	1.51
29	F	101	SQD	O3-C3	-2.24	1.37	1.43
23	B	616	CLA	CMB-C2B	-2.24	1.47	1.51
23	b	607	CLA	CHC-C1C	2.24	1.40	1.35
23	a	606	CLA	MG-NA	2.24	2.11	2.06
23	C	508	CLA	CMD-C2D	-2.24	1.46	1.50
23	C	510	CLA	O2A-CGA	2.24	1.39	1.33
31	c	517	DGD	C3E-C2E	2.24	1.58	1.52
31	H	102	DGD	O6E-C1E	2.24	1.47	1.41
28	b	621	LMG	O8-C28	2.23	1.39	1.33
23	C	504	CLA	O2D-CGD	2.23	1.38	1.33
23	C	512	CLA	CMD-C2D	-2.23	1.46	1.50
23	b	604	CLA	C3B-C2B	-2.23	1.37	1.40
23	c	506	CLA	CAC-C3C	-2.23	1.45	1.51
23	c	503	CLA	C3B-CAB	-2.23	1.43	1.47
24	a	605	PHO	C1C-NC	-2.23	1.31	1.38
23	b	610	CLA	C3D-C4D	2.22	1.49	1.44
23	c	501	CLA	CMD-C2D	-2.22	1.46	1.50
30	D	408	LHG	C6-C5	2.22	1.57	1.50
23	b	610	CLA	CMD-C2D	-2.22	1.46	1.50
23	c	506	CLA	CHC-C1C	2.22	1.40	1.35
23	D	402	CLA	C1A-CHA	-2.22	1.33	1.43
28	d	406	LMG	O3-C3	-2.22	1.37	1.43
23	B	602	CLA	C1B-NB	2.21	1.37	1.35
23	b	611	CLA	C1D-C2D	2.21	1.49	1.45
25	c	514	BCR	C33-C5	-2.21	1.47	1.50
23	C	512	CLA	C3D-C4D	2.21	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	601	SQD	O3-C3	-2.21	1.37	1.43
23	B	607	CLA	MG-ND	-2.21	2.01	2.05
23	B	602	CLA	MG-ND	-2.21	2.01	2.05
24	A	606	PHO	CHA-CBD	-2.21	1.49	1.52
27	a	611	PL9	C46-C44	-2.20	1.46	1.51
23	B	611	CLA	C3B-C2B	-2.20	1.37	1.40
23	A	603	CLA	C1A-CHA	-2.20	1.34	1.43
23	c	507	CLA	MG-ND	-2.20	2.01	2.05
23	c	501	CLA	CHC-C1C	2.20	1.40	1.35
23	B	616	CLA	C3B-C2B	-2.20	1.37	1.40
30	A	615	LHG	P-O3	2.19	1.68	1.59
23	h	101	CLA	CMC-C2C	-2.19	1.46	1.50
25	C	520	BCR	C33-C5	-2.19	1.47	1.50
23	C	503	CLA	CMB-C2B	-2.19	1.47	1.51
23	B	609	CLA	CMC-C2C	-2.19	1.46	1.50
23	b	611	CLA	C3B-C2B	-2.19	1.37	1.40
28	B	622	LMG	O7-C10	2.19	1.38	1.30
23	B	614	CLA	CMD-C2D	-2.19	1.46	1.50
23	C	512	CLA	CMB-C2B	-2.18	1.47	1.51
27	d	408	PL9	C16-C14	-2.18	1.46	1.51
23	c	504	CLA	CMD-C2D	-2.18	1.46	1.50
23	b	612	CLA	C4C-C3C	2.18	1.48	1.45
23	C	502	CLA	C1D-ND	2.18	1.40	1.37
31	A	617	DGD	C4E-C5E	2.17	1.57	1.53
23	C	509	CLA	CHC-C1C	2.17	1.40	1.35
23	A	607	CLA	CHC-C1C	2.17	1.40	1.35
23	b	616	CLA	O2D-CED	-2.17	1.40	1.45
23	C	503	CLA	C3D-C4D	2.17	1.49	1.44
36	V	201	HEC	C2A-C3A	-2.17	1.31	1.37
23	B	604	CLA	CMA-C3A	-2.17	1.48	1.53
23	b	614	CLA	C1A-CHA	-2.17	1.34	1.43
28	D	405	LMG	C4-C5	2.17	1.57	1.53
31	C	516	DGD	O6E-C1E	2.17	1.47	1.41
23	B	605	CLA	CMC-C2C	-2.16	1.46	1.50
23	b	616	CLA	CAC-C3C	-2.16	1.45	1.51
31	c	517	DGD	O2G-C2G	-2.16	1.41	1.46
25	T	101	BCR	C33-C5	-2.16	1.47	1.50
36	V	201	HEC	C3D-C2D	-2.16	1.31	1.37
23	c	513	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	618	BCR	C29-C30	-2.15	1.49	1.54
23	C	502	CLA	CMB-C2B	-2.15	1.47	1.51
23	a	604	CLA	CMD-C2D	-2.15	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	611	PL9	C3-C4	-2.15	1.46	1.49
23	c	502	CLA	CMB-C2B	-2.15	1.47	1.51
23	B	609	CLA	C4B-CHC	-2.14	1.35	1.41
31	c	518	DGD	O5D-C1E	2.14	1.43	1.40
31	C	518	DGD	O6E-C1E	2.14	1.47	1.41
31	A	617	DGD	O4D-C4D	-2.14	1.37	1.43
23	b	608	CLA	CMD-C2D	-2.14	1.46	1.50
23	A	603	CLA	CAC-C3C	-2.14	1.45	1.51
23	b	616	CLA	CHC-C1C	2.13	1.40	1.35
31	c	518	DGD	C2A-C1A	-2.13	1.44	1.50
23	c	504	CLA	C1D-ND	2.13	1.40	1.37
23	B	603	CLA	C1A-CHA	-2.13	1.34	1.43
28	A	612	LMG	O1-C7	-2.13	1.39	1.43
23	B	602	CLA	C4B-CHC	-2.13	1.35	1.41
23	C	501	CLA	C3D-C4D	2.13	1.49	1.44
31	a	616	DGD	C2B-C1B	2.13	1.56	1.50
31	a	616	DGD	CFA-CEA	2.12	1.63	1.51
28	C	519	LMG	O1-C1	2.12	1.43	1.40
23	B	603	CLA	CMA-C3A	-2.12	1.48	1.53
23	D	402	CLA	C1C-NC	-2.12	1.34	1.37
23	B	601	CLA	CAC-C3C	-2.12	1.45	1.51
23	B	615	CLA	O2D-CED	-2.12	1.40	1.45
31	C	516	DGD	C6D-C5D	2.12	1.58	1.51
23	c	511	CLA	C3B-CAB	-2.12	1.43	1.47
23	B	615	CLA	C1D-C2D	2.12	1.49	1.45
23	C	506	CLA	C3B-CAB	-2.12	1.43	1.47
23	b	609	CLA	CAC-C3C	-2.12	1.45	1.51
31	C	516	DGD	C3D-C2D	2.12	1.57	1.52
23	B	613	CLA	C3B-C2B	-2.12	1.37	1.40
23	B	613	CLA	CMC-C2C	-2.12	1.46	1.50
23	b	609	CLA	C3D-C4D	2.11	1.48	1.44
23	c	506	CLA	C4B-CHC	-2.11	1.35	1.41
23	C	503	CLA	C3B-CAB	-2.11	1.43	1.47
23	C	510	CLA	C3B-CAB	-2.11	1.43	1.47
23	C	502	CLA	O2D-CGD	2.11	1.38	1.33
23	b	606	CLA	C3B-C2B	-2.11	1.37	1.40
25	T	101	BCR	C38-C26	-2.11	1.47	1.50
25	b	618	BCR	C4-C5	-2.11	1.46	1.51
28	m	101	LMG	O1-C7	-2.11	1.39	1.43
28	A	612	LMG	O2-C2	-2.11	1.38	1.43
23	b	610	CLA	CMC-C2C	-2.11	1.46	1.50
23	d	403	CLA	C1D-ND	2.11	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	CMC-C2C	-2.11	1.46	1.50
27	A	611	PL9	C6-C1	-2.11	1.44	1.48
28	c	521	LMG	O6-C5	-2.11	1.39	1.44
31	C	516	DGD	C1D-C2D	2.11	1.58	1.52
27	d	408	PL9	C7-C8	-2.10	1.47	1.50
23	B	616	CLA	C3B-CAB	-2.10	1.43	1.47
23	B	610	CLA	CAC-C3C	-2.10	1.45	1.51
30	l	101	LHG	O8-C23	2.10	1.39	1.33
29	f	101	SQD	O4-C4	-2.10	1.38	1.43
25	b	619	BCR	C33-C5	-2.10	1.47	1.50
23	b	606	CLA	MG-NC	2.10	2.11	2.06
23	b	607	CLA	CMB-C2B	-2.10	1.47	1.51
23	A	604	CLA	C3B-CAB	-2.10	1.43	1.47
23	b	607	CLA	C1D-C2D	2.10	1.49	1.45
23	c	506	CLA	CMD-C2D	-2.10	1.46	1.50
23	C	510	CLA	C3C-C2C	2.10	1.41	1.36
23	d	402	CLA	O2D-CED	-2.10	1.40	1.45
23	B	607	CLA	C4B-CHC	-2.09	1.35	1.41
24	a	605	PHO	CMB-C2B	-2.09	1.46	1.51
23	B	613	CLA	MG-NA	2.09	2.11	2.06
23	b	613	CLA	C4B-CHC	-2.09	1.35	1.41
27	D	407	PL9	C10-C9	-2.09	1.45	1.50
28	A	612	LMG	C1-C2	2.09	1.58	1.52
23	a	606	CLA	CMD-C2D	-2.09	1.46	1.50
23	b	610	CLA	C1C-NC	-2.09	1.34	1.37
23	D	403	CLA	C4B-CHC	-2.08	1.35	1.41
31	c	518	DGD	C2B-C1B	-2.08	1.44	1.50
25	d	404	BCR	C33-C5	-2.08	1.47	1.50
23	c	509	CLA	O2D-CED	-2.08	1.40	1.45
30	B	623	LHG	P-O4	-2.08	1.45	1.55
23	b	615	CLA	CAC-C3C	-2.08	1.45	1.51
23	c	512	CLA	C1D-C2D	2.08	1.49	1.45
23	C	508	CLA	C1B-NB	2.08	1.37	1.35
31	c	518	DGD	C4D-C5D	2.08	1.57	1.53
24	A	606	PHO	CMD-C2D	-2.07	1.46	1.51
23	B	606	CLA	C1D-ND	2.07	1.40	1.37
23	C	504	CLA	C4B-CHC	-2.07	1.35	1.41
29	A	614	SQD	O4-C4	-2.07	1.38	1.43
23	A	613	CLA	C3D-C4D	2.07	1.48	1.44
23	b	614	CLA	O2D-CED	-2.07	1.40	1.45
23	B	610	CLA	C3D-C4D	2.07	1.48	1.44
23	C	510	CLA	C3B-C2B	-2.07	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	603	CLA	CMC-C2C	-2.07	1.46	1.50
23	B	608	CLA	C4B-CHC	-2.07	1.35	1.41
23	c	512	CLA	C3B-CAB	-2.07	1.43	1.47
23	B	603	CLA	C3B-C2B	-2.07	1.37	1.40
24	A	606	PHO	CMC-C2C	-2.06	1.46	1.51
24	d	401	PHO	CMD-C2D	-2.06	1.46	1.51
23	C	513	CLA	C4B-CHC	-2.06	1.35	1.41
23	B	609	CLA	O2D-CGD	2.06	1.38	1.33
23	C	510	CLA	C3D-C4D	2.06	1.48	1.44
27	d	408	PL9	O2-C1	-2.06	1.19	1.24
23	B	612	CLA	C1A-CHA	-2.06	1.34	1.43
23	c	506	CLA	C3B-CAB	-2.06	1.43	1.47
23	C	508	CLA	C3B-CAB	-2.05	1.43	1.47
25	C	520	BCR	C38-C26	-2.05	1.47	1.50
23	B	604	CLA	C1B-NB	2.05	1.37	1.35
23	b	605	CLA	MG-ND	-2.05	2.01	2.05
23	b	602	CLA	C4B-CHC	-2.05	1.35	1.41
23	c	510	CLA	CMD-C2D	-2.05	1.46	1.50
31	A	617	DGD	C6E-C5E	2.05	1.58	1.51
23	c	502	CLA	C4B-CHC	-2.05	1.35	1.41
23	C	504	CLA	C1D-ND	2.05	1.40	1.37
23	C	508	CLA	CMC-C2C	-2.05	1.46	1.50
23	B	615	CLA	CAC-C3C	-2.05	1.45	1.51
23	c	508	CLA	C3B-CAB	-2.05	1.43	1.47
23	A	603	CLA	C4B-CHC	-2.04	1.35	1.41
23	b	608	CLA	O2A-CGA	2.04	1.39	1.33
23	h	101	CLA	C3B-CAB	-2.04	1.43	1.47
23	b	606	CLA	C4B-CHC	-2.04	1.35	1.41
28	c	519	LMG	C7-C8	2.04	1.57	1.50
23	a	606	CLA	O1D-CGD	2.04	1.26	1.21
23	c	502	CLA	CMC-C2C	-2.04	1.46	1.50
23	C	510	CLA	CMB-C2B	-2.04	1.47	1.51
35	F	102	HEM	CMA-C3A	2.04	1.55	1.51
28	b	621	LMG	O1-C7	-2.04	1.40	1.43
23	c	501	CLA	CAC-C3C	-2.04	1.45	1.51
23	a	612	CLA	O2D-CED	-2.04	1.40	1.45
27	a	611	PL9	C52-C5	-2.03	1.46	1.50
23	a	604	CLA	C3B-CAB	-2.03	1.43	1.47
28	d	406	LMG	O1-C7	-2.03	1.40	1.43
23	B	608	CLA	C3B-CAB	-2.03	1.43	1.47
27	D	407	PL9	C3-C4	-2.03	1.46	1.49
23	b	613	CLA	CHC-C1C	2.03	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C4B-CHC	-2.02	1.35	1.41
31	c	517	DGD	C6D-C5D	2.02	1.57	1.51
23	C	512	CLA	C3B-C2B	-2.02	1.37	1.40
23	d	402	CLA	MG-NA	2.02	2.11	2.06
23	h	101	CLA	C3D-C4D	2.02	1.48	1.44
23	C	510	CLA	CMC-C2C	-2.02	1.46	1.50
23	c	501	CLA	MG-ND	-2.02	2.01	2.05
23	A	604	CLA	C4B-CHC	-2.02	1.35	1.41
23	c	509	CLA	C3C-C2C	2.02	1.41	1.36
23	C	512	CLA	CAA-C2A	-2.02	1.50	1.54
23	a	606	CLA	C3B-C2B	-2.02	1.37	1.40
23	A	603	CLA	C5-C3	-2.02	1.47	1.51
28	c	521	LMG	C4-C5	2.01	1.57	1.53
23	B	616	CLA	CMD-C2D	-2.01	1.46	1.50
23	B	615	CLA	C4B-CHC	-2.01	1.35	1.41
23	c	507	CLA	C3B-C2B	-2.01	1.37	1.40
23	A	604	CLA	CAC-C3C	-2.01	1.46	1.51
23	b	616	CLA	CMD-C2D	-2.01	1.46	1.50
28	D	405	LMG	C34-C33	2.01	1.62	1.51
25	C	520	BCR	C1-C6	-2.00	1.51	1.53
23	C	505	CLA	C4B-CHC	-2.00	1.35	1.41

All (1395) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C4A-NA-C1A	11.08	111.69	106.71
23	B	601	CLA	C4A-NA-C1A	10.09	111.24	106.71
29	A	614	SQD	O6-C1-C2	9.95	123.84	108.30
29	A	614	SQD	O7-S-C6	9.86	118.66	106.94
23	c	502	CLA	C4A-NA-C1A	9.67	111.05	106.71
29	b	601	SQD	O6-C1-C2	9.52	123.17	108.30
23	a	606	CLA	C4A-NA-C1A	8.89	110.70	106.71
23	C	511	CLA	C4A-NA-C1A	8.47	110.52	106.71
29	a	613	SQD	O6-C1-C2	8.41	121.44	108.30
23	C	510	CLA	C4A-NA-C1A	8.35	110.46	106.71
23	a	603	CLA	C4A-NA-C1A	8.33	110.45	106.71
23	c	507	CLA	C4A-NA-C1A	8.16	110.38	106.71
29	A	616	SQD	C45-O47-C7	7.61	127.67	117.88
23	C	507	CLA	C4A-NA-C1A	7.60	110.12	106.71
23	C	501	CLA	C4A-NA-C1A	7.48	110.07	106.71
23	a	612	CLA	C4A-NA-C1A	7.47	110.06	106.71
23	b	604	CLA	C4A-NA-C1A	7.40	110.03	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	C4A-NA-C1A	7.00	109.85	106.71
23	C	513	CLA	C4A-NA-C1A	6.99	109.85	106.71
23	b	606	CLA	C4A-NA-C1A	6.81	109.77	106.71
23	B	609	CLA	C4A-NA-C1A	6.79	109.76	106.71
29	F	101	SQD	O8-S-C6	6.59	116.24	105.74
23	B	612	CLA	C4A-NA-C1A	6.56	109.66	106.71
23	c	501	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	C	503	CLA	C4A-NA-C1A	6.49	109.62	106.71
23	d	402	CLA	C4A-NA-C1A	6.39	109.58	106.71
23	B	614	CLA	O2D-CGD-O1D	-6.13	111.85	123.84
23	c	509	CLA	C4A-NA-C1A	6.13	109.46	106.71
23	b	602	CLA	C4A-NA-C1A	6.05	109.43	106.71
23	A	613	CLA	C4A-NA-C1A	5.93	109.37	106.71
23	B	610	CLA	C4A-NA-C1A	5.93	109.37	106.71
27	a	611	PL9	C7-C3-C4	5.90	121.68	116.88
23	b	615	CLA	C4A-NA-C1A	5.84	109.33	106.71
23	b	607	CLA	C4A-NA-C1A	5.81	109.32	106.71
23	c	501	CLA	O2D-CGD-O1D	-5.65	112.80	123.84
23	c	511	CLA	C4A-NA-C1A	5.63	109.24	106.71
27	A	611	PL9	C7-C3-C4	5.60	121.43	116.88
23	b	605	CLA	C4A-NA-C1A	5.57	109.21	106.71
29	a	613	SQD	O8-S-C6	5.50	114.51	105.74
23	B	615	CLA	CMB-C2B-C1B	-5.49	120.02	128.46
23	b	612	CLA	CMB-C2B-C1B	-5.47	120.06	128.46
29	F	101	SQD	O6-C1-C2	5.42	116.77	108.30
31	C	517	DGD	O3G-C3G-C2G	-5.34	98.00	110.90
23	b	613	CLA	CMB-C2B-C1B	-5.32	120.29	128.46
23	b	613	CLA	C4A-NA-C1A	5.32	109.10	106.71
23	B	616	CLA	C4A-NA-C1A	5.28	109.08	106.71
23	b	609	CLA	CMB-C2B-C1B	-5.27	120.36	128.46
31	H	102	DGD	O3G-C3G-C2G	-5.25	98.23	110.90
29	B	624	SQD	O7-S-C6	5.23	113.16	106.94
23	B	608	CLA	C4A-NA-C1A	5.19	109.04	106.71
23	b	602	CLA	CMB-C2B-C1B	-5.17	120.51	128.46
27	D	407	PL9	C7-C3-C4	5.14	121.05	116.88
23	B	606	CLA	CHD-C1D-ND	-5.14	119.73	124.45
23	B	613	CLA	C4A-NA-C1A	5.08	108.99	106.71
23	b	602	CLA	O2D-CGD-O1D	-5.04	113.99	123.84
23	b	616	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
23	b	614	CLA	C4A-NA-C1A	4.96	108.94	106.71
23	c	506	CLA	C4A-NA-C1A	4.96	108.94	106.71
23	A	607	CLA	O2D-CGD-O1D	-4.96	114.15	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
23	b	614	CLA	CHD-C1D-ND	-4.91	119.94	124.45
23	B	608	CLA	O2D-CGD-O1D	-4.91	114.23	123.84
29	f	101	SQD	O9-S-C6	4.88	112.74	106.94
24	A	605	PHO	O2D-CGD-CBD	4.84	117.13	111.00
27	d	408	PL9	C7-C3-C4	4.83	120.80	116.88
23	a	604	CLA	C4A-NA-C1A	4.82	108.87	106.71
23	C	503	CLA	C7-C6-C5	-4.81	100.30	113.36
23	b	603	CLA	CMB-C2B-C1B	-4.79	121.11	128.46
23	h	101	CLA	C4A-NA-C1A	4.76	108.85	106.71
29	f	101	SQD	O6-C1-C2	4.76	115.73	108.30
23	b	614	CLA	CMB-C2B-C1B	-4.75	121.17	128.46
23	b	612	CLA	C4A-NA-C1A	4.73	108.83	106.71
29	a	615	SQD	O47-C7-C8	4.72	121.67	111.50
23	b	616	CLA	O2D-CGD-O1D	-4.68	114.68	123.84
23	c	512	CLA	C4A-NA-C1A	4.68	108.81	106.71
23	c	501	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
23	C	505	CLA	CAC-C3C-C4C	4.66	130.85	124.81
31	a	616	DGD	C2G-O2G-C1B	4.64	129.21	117.79
23	C	504	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
23	B	603	CLA	CHD-C1D-ND	-4.63	120.20	124.45
23	h	101	CLA	CHD-C1D-ND	-4.60	120.23	124.45
23	b	603	CLA	O2D-CGD-O1D	-4.59	114.86	123.84
29	B	624	SQD	O6-C1-C2	4.58	115.45	108.30
23	B	611	CLA	O2D-CGD-O1D	-4.57	114.91	123.84
23	c	502	CLA	CMB-C2B-C1B	-4.57	121.45	128.46
23	b	612	CLA	CMB-C2B-C3B	4.55	133.18	124.68
23	b	616	CLA	CMB-C2B-C3B	4.47	133.03	124.68
28	m	101	LMG	O7-C10-O9	-4.46	112.91	123.70
23	A	607	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
23	b	611	CLA	CHD-C1D-ND	-4.45	120.37	124.45
30	D	408	LHG	O4-P-O5	4.44	134.20	112.24
23	c	503	CLA	C4A-NA-C1A	4.42	108.69	106.71
23	C	512	CLA	O2D-CGD-O1D	-4.42	115.20	123.84
23	c	510	CLA	CHB-C4A-NA	4.40	130.60	124.51
23	B	610	CLA	O2D-CGD-O1D	-4.38	115.28	123.84
23	b	613	CLA	CMB-C2B-C3B	4.38	132.87	124.68
29	A	614	SQD	O47-C7-C8	4.37	120.93	111.50
23	B	612	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
23	b	609	CLA	CMB-C2B-C3B	4.34	132.80	124.68
23	c	501	CLA	C2C-C1C-NC	4.33	114.03	109.97
23	b	615	CLA	CMB-C2B-C1B	-4.30	121.86	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	CHD-C1D-ND	-4.29	120.51	124.45
23	b	614	CLA	CMB-C2B-C3B	4.28	132.69	124.68
25	H	101	BCR	C38-C26-C25	-4.25	119.75	124.53
24	d	401	PHO	O1D-CGD-CBD	4.24	131.81	124.74
23	C	501	CLA	O2D-CGD-CBD	4.23	118.79	111.27
23	c	509	CLA	O2A-CGA-O1A	-4.23	112.92	123.59
30	a	614	LHG	O4-P-O5	4.22	133.11	112.24
29	b	601	SQD	C1-C2-C3	-4.22	101.21	110.00
23	C	508	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
23	A	607	CLA	CHD-C1D-ND	-4.21	120.58	124.45
23	C	512	CLA	CHB-C4A-NA	4.20	130.32	124.51
31	A	617	DGD	C3G-C2G-C1G	-4.20	101.86	111.79
23	b	602	CLA	CHB-C4A-NA	4.19	130.30	124.51
29	A	614	SQD	C1-C2-C3	-4.19	101.28	110.00
23	b	605	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
23	C	513	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
23	C	501	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
28	c	521	LMG	O6-C1-O1	-4.15	100.14	109.97
29	A	614	SQD	O9-S-O7	-4.15	99.58	113.95
23	A	607	CLA	C4A-NA-C1A	4.15	108.57	106.71
23	C	505	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
23	B	603	CLA	C4A-NA-C1A	4.13	108.56	106.71
23	D	403	CLA	C1B-CHB-C4A	-4.12	121.96	130.12
31	H	102	DGD	C1D-O6D-C5D	-4.12	105.60	113.69
25	B	619	BCR	C37-C22-C21	-4.12	117.16	122.92
23	b	602	CLA	O2D-CGD-CBD	4.11	118.57	111.27
31	c	516	DGD	O3G-C3G-C2G	-4.10	101.01	110.90
30	d	405	LHG	O4-P-O5	4.10	132.50	112.24
23	B	607	CLA	C4A-NA-C1A	4.09	108.55	106.71
23	D	402	CLA	C1B-CHB-C4A	-4.08	122.03	130.12
30	B	623	LHG	O4-P-O5	4.08	132.40	112.24
23	b	607	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
23	b	611	CLA	O2D-CGD-O1D	-4.05	115.91	123.84
23	a	604	CLA	CMA-C3A-C4A	-4.05	100.88	111.77
27	a	611	PL9	C7-C3-C2	-4.04	117.98	123.30
31	C	518	DGD	O3G-C3G-C2G	-4.03	101.17	110.90
30	d	407	LHG	O4-P-O5	4.03	132.17	112.24
23	b	611	CLA	C2D-C1D-ND	-4.02	107.14	110.10
23	c	501	CLA	O2D-CGD-CBD	4.02	118.41	111.27
23	c	508	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
23	B	611	CLA	CHD-C1D-ND	-4.01	120.77	124.45
31	C	516	DGD	O1G-C1A-C2A	-4.00	99.35	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	CMB-C2B-C3B	4.00	132.16	124.68
23	c	507	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
23	C	512	CLA	CMB-C2B-C3B	3.98	132.12	124.68
29	B	624	SQD	O8-S-C6	3.98	112.08	105.74
29	A	614	SQD	C3-C4-C5	3.97	117.31	110.24
23	b	602	CLA	CMB-C2B-C3B	3.96	132.09	124.68
23	B	611	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
30	A	615	LHG	O4-P-O5	3.95	131.79	112.24
23	A	603	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
23	B	614	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
23	c	502	CLA	CMB-C2B-C3B	3.93	132.04	124.68
23	B	614	CLA	CMB-C2B-C3B	3.93	132.03	124.68
23	c	509	CLA	C1B-CHB-C4A	-3.93	122.34	130.12
23	C	504	CLA	CHD-C1D-ND	-3.91	120.86	124.45
23	b	603	CLA	C1B-CHB-C4A	-3.91	122.38	130.12
23	B	610	CLA	CED-O2D-CGD	-3.90	107.11	115.94
23	c	510	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
23	c	504	CLA	CMB-C2B-C3B	3.89	131.96	124.68
24	d	401	PHO	CMC-C2C-C3C	3.88	132.26	124.94
30	d	409	LHG	O4-P-O5	3.88	131.41	112.24
31	C	517	DGD	C1D-C2D-C3D	-3.88	101.92	110.00
23	b	605	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
23	A	607	CLA	CMB-C2B-C3B	3.88	131.93	124.68
23	b	605	CLA	CHD-C1D-ND	-3.87	120.90	124.45
23	B	601	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
30	D	406	LHG	O4-P-O5	3.86	131.33	112.24
34	D	401	BCT	O2-C-O1	3.86	129.55	119.55
23	C	512	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
23	B	602	CLA	CHB-C4A-NA	3.83	129.81	124.51
23	c	512	CLA	CHB-C4A-NA	3.81	129.78	124.51
23	C	508	CLA	CMB-C2B-C3B	3.81	131.80	124.68
29	a	613	SQD	O9-S-C6	3.80	111.46	106.94
29	a	613	SQD	C1-O5-C5	-3.79	106.25	113.69
23	h	101	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
23	B	606	CLA	C4D-CHA-C1A	3.77	125.84	121.25
29	F	101	SQD	O9-S-C6	3.77	111.42	106.94
29	F	101	SQD	C46-C45-C44	-3.77	101.17	113.70
23	B	603	CLA	CHB-C4A-NA	3.76	129.71	124.51
23	B	607	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
29	b	601	SQD	O2-C2-C1	3.75	119.16	110.05
23	C	508	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
23	B	616	CLA	CMB-C2B-C1B	-3.74	122.71	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	CMB-C2B-C3B	3.74	131.68	124.68
30	l	101	LHG	O4-P-O5	3.74	130.71	112.24
23	B	601	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
23	B	614	CLA	O1D-CGD-CBD	3.71	132.07	124.48
23	c	505	CLA	CHD-C1D-ND	-3.71	121.05	124.45
23	B	615	CLA	C1B-CHB-C4A	-3.69	122.80	130.12
23	c	512	CLA	C1-C2-C3	-3.69	119.66	126.04
25	B	617	BCR	C2-C1-C6	3.69	116.16	110.48
24	A	606	PHO	C1-C2-C3	-3.69	119.66	126.04
31	h	103	DGD	O3G-C3G-C2G	-3.68	102.01	110.90
23	A	613	CLA	CMB-C2B-C3B	3.68	131.57	124.68
23	A	603	CLA	CMB-C2B-C3B	3.68	131.56	124.68
23	C	509	CLA	C4A-NA-C1A	3.66	108.35	106.71
29	B	624	SQD	C1-O5-C5	-3.66	106.51	113.69
23	a	604	CLA	CHB-C4A-NA	3.65	129.56	124.51
25	A	608	BCR	C11-C10-C9	-3.65	122.10	127.31
29	b	601	SQD	O5-C5-C4	3.64	116.31	109.69
23	b	603	CLA	CMB-C2B-C3B	3.64	131.49	124.68
23	a	606	CLA	C1B-CHB-C4A	-3.63	122.93	130.12
24	A	605	PHO	CMA-C3A-C4A	-3.62	106.45	114.38
23	A	604	CLA	CMB-C2B-C3B	3.62	131.45	124.68
29	B	624	SQD	O47-C7-C8	3.62	119.30	111.50
25	T	101	BCR	C38-C26-C27	-3.62	106.67	113.62
31	A	617	DGD	C1D-C2D-C3D	-3.61	102.48	110.00
23	c	510	CLA	C4A-NA-C1A	3.61	108.33	106.71
23	C	502	CLA	CHD-C1D-ND	-3.60	121.14	124.45
35	F	102	HEM	CBA-CAA-C2A	-3.60	106.48	112.62
23	b	612	CLA	C11-C12-C13	-3.60	104.29	115.92
30	d	409	LHG	O8-C23-O10	-3.60	114.51	123.59
23	C	509	CLA	CMB-C2B-C3B	3.59	131.40	124.68
23	C	505	CLA	CMB-C2B-C3B	3.59	131.40	124.68
23	b	611	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	c	511	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
31	h	103	DGD	C1E-O6E-C5E	3.58	120.72	113.69
23	c	504	CLA	C4A-NA-C1A	3.58	108.31	106.71
25	t	101	BCR	C34-C9-C10	-3.57	117.92	122.92
23	B	609	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
23	b	605	CLA	C1-C2-C3	-3.57	119.87	126.04
23	a	606	CLA	CHB-C4A-NA	3.57	129.45	124.51
31	c	517	DGD	C1D-C2D-C3D	-3.57	102.57	110.00
36	v	201	HEC	CBD-CAD-C3D	-3.56	106.55	112.62
25	c	515	BCR	C36-C18-C17	-3.56	117.94	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	O2A-C1-C2	-3.56	99.29	108.64
30	B	623	LHG	O8-C23-O10	-3.55	114.62	123.59
23	b	612	CLA	CHD-C1D-ND	-3.55	121.19	124.45
23	b	610	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
23	a	612	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
23	c	509	CLA	CHB-C4A-NA	3.54	129.41	124.51
23	B	615	CLA	C4A-NA-C1A	3.54	108.30	106.71
23	C	506	CLA	CHB-C4A-NA	3.54	129.41	124.51
23	d	402	CLA	C4-C3-C5	3.53	121.22	115.27
35	f	102	HEM	CBD-CAD-C3D	-3.53	102.81	112.63
23	C	507	CLA	CHD-C1D-ND	-3.53	121.21	124.45
23	B	611	CLA	O2D-CGD-CBD	3.53	117.53	111.27
23	b	610	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
23	b	613	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
31	C	516	DGD	O3G-C3G-C2G	-3.51	102.42	110.90
23	b	606	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
23	A	604	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
23	b	608	CLA	CMB-C2B-C3B	3.51	131.24	124.68
23	C	503	CLA	CHD-C1D-ND	-3.50	121.23	124.45
25	T	101	BCR	C27-C26-C25	3.50	127.81	122.73
23	c	503	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
25	t	101	BCR	C38-C26-C27	-3.49	106.90	113.62
23	c	502	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
25	t	101	BCR	C15-C16-C17	-3.49	116.32	123.47
23	c	512	CLA	CMB-C2B-C3B	3.49	131.21	124.68
23	B	605	CLA	CHD-C1D-ND	-3.49	121.25	124.45
29	B	624	SQD	O9-S-O7	-3.49	101.88	113.95
23	h	101	CLA	O2D-CGD-CBD	3.48	117.46	111.27
23	C	503	CLA	O2A-C1-C2	-3.48	99.49	108.64
23	c	512	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	b	605	CLA	CBC-CAC-C3C	-3.48	102.85	112.43
23	b	605	CLA	C16-C15-C13	-3.48	104.69	115.92
23	B	614	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
23	B	610	CLA	CHD-C1D-ND	-3.47	121.27	124.45
23	c	509	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
25	C	514	BCR	C34-C9-C10	-3.46	118.07	122.92
23	b	616	CLA	CHD-C1D-ND	-3.46	121.27	124.45
35	F	102	HEM	C2C-C3C-C4C	3.46	109.31	106.90
24	a	605	PHO	O2A-CGA-O1A	-3.46	114.87	123.59
23	b	603	CLA	CHD-C1D-ND	-3.46	121.28	124.45
23	B	604	CLA	CHB-C4A-NA	3.46	129.29	124.51
23	B	610	CLA	O2A-CGA-O1A	-3.45	114.89	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	f	101	SQD	O8-S-C6	3.45	111.23	105.74
27	a	611	PL9	C35-C34-C36	3.44	121.07	115.27
31	C	517	DGD	O3G-C1D-C2D	-3.44	102.93	108.30
23	C	513	CLA	CMB-C2B-C3B	3.44	131.11	124.68
25	c	515	BCR	C35-C13-C14	-3.44	118.11	122.92
29	B	624	SQD	C3-C4-C5	3.43	116.36	110.24
23	b	616	CLA	C1B-CHB-C4A	-3.42	123.34	130.12
23	C	512	CLA	O2D-CGD-CBD	3.42	117.35	111.27
28	c	522	LMG	C1-O6-C5	-3.42	106.97	113.69
23	B	610	CLA	CHB-C4A-NA	3.42	129.24	124.51
23	c	510	CLA	CHD-C1D-ND	-3.42	121.31	124.45
28	b	621	LMG	C1-O6-C5	-3.41	106.99	113.69
23	C	503	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
24	A	605	PHO	CMB-C2B-C3B	3.41	131.06	124.68
23	A	604	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
29	A	614	SQD	O4-C4-C3	-3.41	102.48	110.35
23	c	502	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
25	C	520	BCR	C27-C26-C25	3.39	127.66	122.73
23	b	609	CLA	CHD-C1D-ND	-3.39	121.34	124.45
31	h	103	DGD	O3E-C3E-C2E	-3.39	102.52	110.35
30	L	101	LHG	O4-P-O5	3.39	128.98	112.24
23	b	603	CLA	C4A-NA-C1A	3.38	108.23	106.71
23	A	603	CLA	CHB-C4A-NA	3.38	129.18	124.51
23	c	510	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
23	B	612	CLA	CHB-C4A-NA	3.37	129.17	124.51
23	B	612	CLA	C11-C12-C13	-3.37	105.03	115.92
23	C	506	CLA	C4A-NA-C1A	3.37	108.22	106.71
23	A	607	CLA	C1D-ND-C4D	-3.37	103.94	106.33
31	A	617	DGD	C6D-O5D-C1E	3.36	120.30	113.74
27	d	408	PL9	C40-C39-C41	3.36	120.92	115.27
30	D	408	LHG	O8-C23-O10	-3.35	115.13	123.59
23	A	607	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
23	c	503	CLA	C1D-ND-C4D	3.35	108.71	106.33
23	d	403	CLA	CMB-C2B-C3B	3.34	130.92	124.68
23	c	512	CLA	C2D-C1D-ND	-3.34	107.64	110.10
24	a	605	PHO	C1-C2-C3	-3.33	120.28	126.04
23	b	611	CLA	CHD-C1D-C2D	3.33	132.47	125.48
23	h	101	CLA	CHB-C4A-NA	3.33	129.12	124.51
27	d	408	PL9	C45-C44-C46	-3.33	109.67	115.27
23	A	604	CLA	O2A-CGA-O1A	-3.33	115.20	123.59
31	a	616	DGD	O1G-C1A-O1A	-3.33	115.20	123.59
23	b	611	CLA	CHD-C4C-NC	3.32	129.44	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	102	BCR	C27-C26-C25	3.32	127.55	122.73
23	d	402	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
23	c	508	CLA	CHB-C4A-NA	3.32	129.10	124.51
23	C	502	CLA	C4A-NA-C1A	3.32	108.20	106.71
27	A	611	PL9	C40-C39-C38	-3.31	115.18	123.68
25	b	617	BCR	C11-C10-C9	-3.31	122.58	127.31
23	D	402	CLA	CED-O2D-CGD	3.30	123.40	115.94
23	a	603	CLA	CAC-C3C-C4C	3.29	129.08	124.81
23	b	615	CLA	CMB-C2B-C3B	3.29	130.84	124.68
23	B	616	CLA	CMB-C2B-C3B	3.28	130.82	124.68
23	C	509	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
34	a	610	BCT	O2-C-O1	3.28	128.06	119.55
23	c	512	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
23	b	613	CLA	CHB-C4A-NA	3.28	129.04	124.51
23	B	606	CLA	CHD-C4C-NC	3.28	129.36	124.20
29	F	101	SQD	O7-S-C6	-3.27	103.05	106.94
23	B	601	CLA	CAA-C2A-C3A	-3.27	103.81	112.78
23	b	607	CLA	CMB-C2B-C3B	3.27	130.80	124.68
36	v	201	HEC	CMC-C2C-C1C	-3.27	123.43	128.46
23	b	614	CLA	C1-C2-C3	-3.27	120.39	126.04
31	c	518	DGD	O6D-C1D-O3G	-3.26	102.25	109.97
23	B	610	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
23	A	607	CLA	O2D-CGD-CBD	3.26	117.06	111.27
23	a	603	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
23	b	612	CLA	O1D-CGD-CBD	3.26	131.15	124.48
23	b	603	CLA	O2D-CGD-CBD	3.25	117.04	111.27
23	A	613	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
27	D	407	PL9	C37-C38-C39	-3.24	119.86	127.66
23	C	503	CLA	CMB-C2B-C3B	3.24	130.74	124.68
28	B	620	LMG	O1-C1-C2	-3.24	103.25	108.30
25	b	617	BCR	C33-C5-C6	-3.23	120.90	124.53
23	b	610	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	b	611	CLA	CMB-C2B-C3B	3.23	130.71	124.68
23	b	608	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
23	h	101	CLA	CBA-CAA-C2A	3.22	123.37	113.86
25	c	515	BCR	C34-C9-C10	-3.22	118.41	122.92
25	H	101	BCR	C35-C13-C14	-3.22	118.42	122.92
23	B	605	CLA	O2A-CGA-O1A	-3.22	115.47	123.59
23	C	506	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
23	C	508	CLA	CHD-C1D-ND	-3.21	121.50	124.45
24	d	401	PHO	CMB-C2B-C3B	3.21	130.69	124.68
23	c	505	CLA	O2D-CGD-CBD	3.21	116.97	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	b	611	CLA	CHB-C4A-NA	3.20	128.94	124.51
23	b	613	CLA	C7-C6-C5	-3.20	104.68	113.36
27	d	408	PL9	C7-C3-C2	-3.20	119.10	123.30
27	d	408	PL9	C35-C34-C36	3.19	120.64	115.27
23	C	512	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
23	B	616	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
23	c	503	CLA	C2D-C1D-ND	-3.18	107.76	110.10
27	A	611	PL9	C20-C19-C21	3.18	120.62	115.27
25	C	515	BCR	C36-C18-C17	-3.18	118.47	122.92
23	c	508	CLA	CMB-C2B-C3B	3.17	130.62	124.68
23	B	607	CLA	CMB-C2B-C3B	3.17	130.61	124.68
27	d	408	PL9	C7-C8-C9	-3.16	121.53	126.79
23	b	616	CLA	O2D-CGD-CBD	3.16	116.88	111.27
23	A	607	CLA	C2C-C1C-NC	3.16	112.93	109.97
23	b	612	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
23	c	505	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
25	t	101	BCR	C27-C26-C25	3.15	127.31	122.73
27	D	407	PL9	C22-C23-C24	-3.15	120.07	127.66
23	B	606	CLA	CHD-C4C-C3C	-3.15	120.21	124.84
25	a	607	BCR	C35-C13-C14	-3.15	118.52	122.92
29	A	616	SQD	O47-C45-C46	3.15	113.42	106.13
23	C	511	CLA	CHB-C4A-NA	3.14	128.86	124.51
23	b	605	CLA	C4D-CHA-C1A	3.14	125.07	121.25
23	b	610	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
35	F	102	HEM	CBD-CAD-C3D	-3.14	103.91	112.63
28	c	522	LMG	O8-C28-O10	-3.14	115.68	123.59
27	A	611	PL9	C7-C3-C2	-3.14	119.18	123.30
28	b	621	LMG	O1-C1-C2	-3.13	103.42	108.30
23	B	605	CLA	C16-C15-C13	-3.13	105.81	115.92
25	B	619	BCR	C33-C5-C6	-3.13	121.02	124.53
23	c	505	CLA	O2A-CGA-O1A	-3.12	115.71	123.59
23	b	604	CLA	CHB-C4A-NA	3.12	128.83	124.51
28	m	101	LMG	O8-C28-O10	-3.12	115.72	123.59
25	Y	101	BCR	C15-C16-C17	-3.12	117.09	123.47
25	b	619	BCR	C29-C30-C25	3.12	115.28	110.48
23	B	608	CLA	CMB-C2B-C1B	-3.10	123.69	128.46
23	B	605	CLA	CHB-C4A-NA	3.10	128.81	124.51
23	B	608	CLA	C2C-C1C-NC	3.10	112.88	109.97
23	b	611	CLA	O2D-CGD-CBD	3.10	116.78	111.27
23	c	503	CLA	CHD-C1D-ND	-3.10	121.60	124.45
23	c	508	CLA	O2D-CGD-O1D	-3.10	117.78	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	O2D-CGD-CBD	3.10	116.77	111.27
23	B	603	CLA	CMB-C2B-C3B	3.09	130.45	124.68
27	D	407	PL9	C36-C34-C33	-3.08	114.88	121.12
23	b	604	CLA	C11-C10-C8	-3.08	105.95	115.92
29	b	601	SQD	O9-S-C6	3.08	110.60	106.94
28	d	406	LMG	C3-C4-C5	-3.08	104.74	110.24
23	c	505	CLA	CHB-C4A-NA	3.08	128.77	124.51
31	c	517	DGD	O3D-C3D-C4D	-3.08	103.24	110.35
25	C	514	BCR	C27-C26-C25	3.07	127.19	122.73
29	A	614	SQD	O2-C2-C1	3.07	117.51	110.05
28	B	620	LMG	O6-C1-O1	-3.07	102.70	109.97
29	a	613	SQD	O47-C7-C8	3.07	118.12	111.50
25	B	619	BCR	C38-C26-C25	-3.07	121.08	124.53
29	b	601	SQD	C3-C4-C5	3.07	115.71	110.24
23	B	612	CLA	CMB-C2B-C3B	3.07	130.42	124.68
23	C	506	CLA	CHD-C1D-ND	-3.06	121.64	124.45
29	B	624	SQD	O5-C5-C4	3.06	115.25	109.69
25	d	404	BCR	C27-C26-C25	3.06	127.18	122.73
23	B	612	CLA	C7-C6-C5	-3.06	105.06	113.36
23	B	611	CLA	CMB-C2B-C3B	3.05	130.39	124.68
23	B	613	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
23	b	604	CLA	CMB-C2B-C1B	-3.04	123.78	128.46
23	A	607	CLA	C4-C3-C5	3.04	120.39	115.27
31	C	517	DGD	O5D-C6D-C5D	-3.04	103.42	109.05
25	C	514	BCR	C33-C5-C6	-3.03	121.12	124.53
29	A	614	SQD	C1-O5-C5	-3.03	107.74	113.69
31	H	102	DGD	O5D-C1E-C2E	3.03	113.03	108.30
23	c	504	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
29	a	615	SQD	O49-C7-C8	-3.02	111.93	123.73
23	c	501	CLA	CMB-C2B-C3B	3.02	130.33	124.68
27	d	408	PL9	C22-C23-C24	-3.02	120.39	127.66
30	B	623	LHG	O3-P-O5	-3.02	97.28	109.07
31	C	518	DGD	O3D-C3D-C4D	-3.02	103.37	110.35
23	b	605	CLA	O1D-CGD-CBD	3.01	130.65	124.48
25	d	404	BCR	C38-C26-C25	-3.01	121.14	124.53
27	d	408	PL9	C20-C19-C21	3.01	120.34	115.27
23	c	506	CLA	CMB-C2B-C3B	3.01	130.31	124.68
23	c	505	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
25	a	607	BCR	C38-C26-C27	-3.01	107.84	113.62
31	c	517	DGD	C3G-O3G-C1D	3.00	119.61	113.74
23	B	602	CLA	O2D-CGD-CBD	3.00	116.60	111.27
23	B	607	CLA	C1-C2-C3	-3.00	120.86	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	C4A-NA-C1A	3.00	108.05	106.71
23	a	612	CLA	CHB-C4A-NA	2.99	128.65	124.51
30	A	615	LHG	O8-C23-C24	2.99	121.28	111.91
25	B	618	BCR	C35-C13-C14	-2.99	118.74	122.92
23	b	611	CLA	C3C-C4C-NC	-2.99	107.22	110.57
29	A	614	SQD	O47-C7-O49	-2.98	116.50	123.70
29	b	601	SQD	O48-C23-C24	2.98	121.25	111.91
24	a	605	PHO	CMC-C2C-C3C	2.98	130.55	124.94
23	b	612	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	B	613	CLA	CHB-C4A-NA	2.97	128.62	124.51
25	A	608	BCR	C34-C9-C10	-2.97	118.76	122.92
23	B	606	CLA	O2A-CGA-O1A	-2.97	116.10	123.59
23	B	601	CLA	C2A-C1A-CHA	2.97	129.04	123.86
25	H	101	BCR	C16-C15-C14	-2.97	117.40	123.47
29	b	601	SQD	O7-S-C6	2.96	110.46	106.94
23	a	603	CLA	C4D-CHA-C1A	2.96	124.85	121.25
23	b	606	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
29	F	101	SQD	O9-S-O7	-2.95	103.73	113.95
31	c	517	DGD	C3E-C4E-C5E	-2.95	104.98	110.24
29	b	601	SQD	O47-C7-C8	2.95	117.86	111.50
23	b	608	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
25	c	515	BCR	C27-C26-C25	2.95	127.01	122.73
31	C	518	DGD	O3E-C3E-C2E	-2.95	103.54	110.35
23	B	615	CLA	CHD-C1D-ND	-2.94	121.75	124.45
25	B	619	BCR	C29-C30-C25	2.94	115.01	110.48
23	c	503	CLA	CMB-C2B-C3B	2.94	130.17	124.68
23	A	604	CLA	C4A-NA-C1A	2.93	108.02	106.71
23	C	502	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
23	b	614	CLA	CMD-C2D-C1D	2.93	129.88	124.71
25	b	619	BCR	C38-C26-C25	-2.93	121.24	124.53
23	D	402	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
30	l	101	LHG	O8-C23-O10	-2.93	116.20	123.59
23	b	605	CLA	C11-C12-C13	-2.92	106.47	115.92
23	B	615	CLA	CHB-C4A-NA	2.92	128.55	124.51
31	C	516	DGD	O5D-C6D-C5D	-2.92	103.65	109.05
23	C	511	CLA	CAC-C3C-C4C	2.92	128.59	124.81
23	B	604	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
35	f	102	HEM	CHB-C1B-NB	2.91	127.98	124.38
28	c	519	LMG	O6-C1-O1	-2.91	103.08	109.97
23	d	402	CLA	CHD-C1D-ND	-2.91	121.78	124.45
23	C	501	CLA	CMB-C2B-C1B	-2.91	124.00	128.46
23	C	501	CLA	CHD-C1D-ND	-2.90	121.78	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	612	LMG	C38-C37-C36	-2.90	99.69	114.42
23	d	403	CLA	O2A-C1-C2	-2.90	101.01	108.64
23	A	613	CLA	O2D-CGD-CBD	2.90	116.42	111.27
29	A	614	SQD	O8-S-C6	2.90	110.36	105.74
23	C	508	CLA	O2D-CGD-CBD	2.90	116.42	111.27
31	A	617	DGD	C4E-C3E-C2E	-2.90	105.76	110.82
23	C	512	CLA	CAA-CBA-CGA	-2.90	104.79	113.25
23	b	607	CLA	O1D-CGD-CBD	2.90	130.41	124.48
29	a	613	SQD	O9-S-O7	-2.89	103.94	113.95
25	H	101	BCR	C27-C26-C25	2.89	126.92	122.73
23	D	402	CLA	O2A-CGA-O1A	-2.89	116.31	123.59
31	h	103	DGD	O6E-C5E-C4E	2.88	114.93	109.69
23	a	604	CLA	C2D-C1D-ND	-2.88	107.98	110.10
23	B	602	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	C	503	CLA	C5-C3-C2	-2.88	115.30	121.12
25	h	102	BCR	C27-C26-C25	2.87	126.91	122.73
23	c	508	CLA	CHD-C1D-ND	-2.87	121.82	124.45
23	a	603	CLA	CMB-C2B-C3B	2.87	130.04	124.68
23	B	602	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
25	h	102	BCR	C34-C9-C8	-2.86	113.56	118.08
23	h	101	CLA	O2A-C1-C2	2.86	116.16	108.64
23	b	602	CLA	CHC-C1C-NC	2.86	128.55	124.20
23	A	613	CLA	C3C-C4C-NC	-2.86	107.36	110.57
23	C	513	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	A	604	CLA	CED-O2D-CGD	-2.86	109.48	115.94
28	d	406	LMG	O6-C1-O1	-2.85	103.22	109.97
23	a	612	CLA	C2D-C1D-ND	-2.85	108.00	110.10
23	d	403	CLA	CHA-C1A-NA	-2.85	119.87	126.40
23	B	603	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	B	617	BCR	C29-C30-C25	2.85	114.86	110.48
23	b	605	CLA	CMB-C2B-C3B	2.85	130.00	124.68
25	c	514	BCR	C27-C26-C25	2.84	126.86	122.73
25	c	515	BCR	C2-C1-C6	2.84	114.86	110.48
31	C	517	DGD	O5D-C1E-C2E	2.84	112.74	108.30
23	d	402	CLA	CMB-C2B-C3B	2.84	130.00	124.68
29	f	101	SQD	O47-C7-C8	2.84	118.71	110.80
23	B	605	CLA	CED-O2D-CGD	2.83	122.35	115.94
27	d	408	PL9	C8-C7-C3	2.83	119.99	111.98
28	B	622	LMG	O7-C10-O9	-2.83	116.25	123.30
29	b	601	SQD	O8-S-C6	2.83	110.25	105.74
24	a	605	PHO	CMB-C2B-C3B	2.83	129.97	124.68
36	V	201	HEC	CMB-C2B-C1B	-2.83	124.12	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	101	SQD	C1-C2-C3	-2.83	104.11	110.00
30	a	614	LHG	O8-C23-C24	2.82	120.77	111.91
23	d	403	CLA	CHB-C4A-NA	2.82	128.41	124.51
27	a	611	PL9	C22-C23-C24	-2.82	120.87	127.66
25	H	101	BCR	C2-C1-C6	2.82	114.82	110.48
25	a	607	BCR	C27-C26-C25	2.82	126.82	122.73
35	f	102	HEM	C3B-C2B-C1B	2.82	108.58	106.49
23	B	603	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
31	h	103	DGD	C3D-C4D-C5D	-2.81	105.22	110.24
23	C	501	CLA	C1D-ND-C4D	-2.81	104.34	106.33
25	A	608	BCR	C37-C22-C21	-2.81	118.99	122.92
27	A	611	PL9	O2-C1-C2	-2.81	115.35	121.78
28	D	405	LMG	O8-C28-O10	-2.81	116.51	123.59
31	c	518	DGD	O1G-C1A-O1A	-2.80	116.51	123.59
30	D	406	LHG	C20-C19-C18	-2.80	100.20	114.42
31	C	516	DGD	C3D-C4D-C5D	-2.80	105.24	110.24
23	c	507	CLA	C2C-C1C-NC	2.80	112.60	109.97
23	b	613	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
23	b	608	CLA	CHA-C1A-NA	-2.79	120.01	126.40
25	b	617	BCR	C27-C26-C25	2.79	126.78	122.73
23	c	501	CLA	CHD-C1D-ND	-2.79	121.89	124.45
28	C	519	LMG	O7-C10-O9	-2.79	116.97	123.70
23	B	603	CLA	CHD-C4C-NC	2.79	128.59	124.20
31	A	617	DGD	O5D-C6D-C5D	-2.79	103.89	109.05
30	d	407	LHG	C20-C19-C18	-2.78	100.30	114.42
23	c	508	CLA	C2D-C1D-ND	-2.78	108.05	110.10
29	a	613	SQD	C3-C4-C5	2.78	115.20	110.24
23	b	611	CLA	C1-C2-C3	-2.78	121.24	126.04
28	m	101	LMG	O3-C3-C2	-2.78	103.93	110.35
23	B	602	CLA	O2A-CGA-O1A	-2.77	116.59	123.59
35	F	102	HEM	C4C-CHD-C1D	2.77	126.22	122.56
23	d	402	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
30	l	101	LHG	C29-C28-C27	-2.77	100.37	114.42
23	C	510	CLA	CHD-C1D-ND	-2.77	121.91	124.45
25	b	618	BCR	C15-C14-C13	-2.76	123.36	127.31
23	h	101	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
31	C	518	DGD	O3G-C1D-C2D	-2.76	103.99	108.30
29	B	624	SQD	O48-C23-C24	2.76	120.57	111.91
23	c	506	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
29	A	616	SQD	O47-C7-C8	2.76	117.45	111.50
23	C	506	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
28	A	612	LMG	O6-C1-O1	-2.75	103.45	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	C4A-NA-C1A	2.75	107.94	106.71
27	D	407	PL9	C42-C43-C44	-2.75	121.03	127.66
25	a	607	BCR	C30-C25-C26	-2.75	118.74	122.61
30	L	101	LHG	O8-C23-O10	-2.75	116.66	123.59
31	c	518	DGD	O3G-C3G-C2G	-2.75	104.27	110.90
23	c	511	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	C	514	BCR	C11-C10-C9	-2.75	123.39	127.31
23	a	603	CLA	O1D-CGD-CBD	2.75	130.10	124.48
23	C	507	CLA	C3A-C2A-C1A	2.74	105.45	101.34
23	c	501	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
31	C	516	DGD	O6D-C1D-O3G	-2.74	103.49	109.97
31	C	517	DGD	O6D-C1D-O3G	-2.74	103.49	109.97
23	b	604	CLA	CMC-C2C-C1C	-2.74	120.87	125.04
23	b	613	CLA	C2C-C1C-NC	2.73	112.53	109.97
23	a	612	CLA	CMB-C2B-C3B	2.73	129.78	124.68
23	b	608	CLA	CHD-C1D-ND	-2.73	121.95	124.45
25	k	101	BCR	C33-C5-C6	-2.72	121.47	124.53
24	A	605	PHO	O2D-CGD-O1D	-2.72	118.52	123.84
23	b	606	CLA	C4D-CHA-C1A	2.72	124.56	121.25
25	d	404	BCR	C1-C6-C5	-2.72	118.78	122.61
23	B	608	CLA	O2D-CGD-CBD	2.72	116.10	111.27
25	C	514	BCR	C15-C14-C13	-2.72	123.44	127.31
28	C	519	LMG	O8-C28-O10	-2.71	116.74	123.59
25	c	515	BCR	C30-C25-C26	-2.71	118.79	122.61
28	c	521	LMG	O3-C3-C2	-2.71	104.08	110.35
30	l	101	LHG	O8-C23-C24	2.71	120.42	111.91
25	b	618	BCR	C37-C22-C21	-2.71	119.13	122.92
23	a	604	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
28	d	406	LMG	O2-C2-C1	-2.71	103.47	110.05
25	Y	101	BCR	C39-C30-C25	-2.71	105.91	110.30
23	c	503	CLA	O1D-CGD-CBD	2.71	130.03	124.48
23	c	502	CLA	CHD-C1D-ND	-2.71	121.97	124.45
23	A	603	CLA	O1D-CGD-CBD	2.71	130.03	124.48
31	a	616	DGD	C1G-C2G-C3G	-2.71	105.47	111.80
27	d	408	PL9	C31-C32-C33	-2.71	102.99	111.88
23	C	504	CLA	CMB-C2B-C3B	2.71	129.74	124.68
23	B	613	CLA	C1-C2-C3	-2.70	121.37	126.04
23	B	614	CLA	O2D-CGD-CBD	2.70	116.07	111.27
23	c	504	CLA	O2D-CGD-CBD	2.70	116.07	111.27
25	T	101	BCR	C2-C1-C6	2.70	114.64	110.48
25	b	617	BCR	C2-C1-C6	2.70	114.63	110.48
23	a	606	CLA	CMB-C2B-C1B	-2.70	124.32	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	m	101	LMG	C1-C2-C3	-2.70	104.38	110.00
31	c	517	DGD	O3G-C3G-C2G	-2.69	104.40	110.90
31	H	102	DGD	C3E-C4E-C5E	-2.69	105.43	110.24
23	C	508	CLA	C4A-NA-C1A	2.69	107.92	106.71
23	C	505	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
25	B	618	BCR	C27-C26-C25	2.69	126.64	122.73
24	a	605	PHO	CMD-C2D-C3D	2.69	129.71	124.68
23	b	613	CLA	O1D-CGD-CBD	2.69	129.99	124.48
23	D	402	CLA	CMB-C2B-C3B	2.68	129.70	124.68
23	c	502	CLA	C3A-C2A-C1A	2.68	105.36	101.34
23	C	506	CLA	O1D-CGD-CBD	2.68	129.97	124.48
23	c	510	CLA	O2A-C1-C2	-2.68	101.59	108.64
23	C	503	CLA	C4D-CHA-C1A	2.68	124.51	121.25
23	b	608	CLA	C6-C7-C8	-2.68	107.26	115.92
28	D	405	LMG	O2-C2-C1	-2.68	103.54	110.05
25	c	514	BCR	C34-C9-C10	-2.68	119.17	122.92
31	c	518	DGD	O3E-C3E-C2E	-2.68	104.16	110.35
31	h	103	DGD	C1D-C2D-C3D	-2.67	104.43	110.00
23	b	616	CLA	CHB-C4A-NA	2.67	128.21	124.51
29	F	101	SQD	C1-O5-C5	-2.67	108.44	113.69
25	D	404	BCR	C2-C1-C6	2.67	114.59	110.48
25	k	101	BCR	C27-C26-C25	2.67	126.61	122.73
27	D	407	PL9	C7-C3-C2	-2.67	119.79	123.30
28	B	622	LMG	O8-C28-O10	-2.67	116.65	123.30
25	C	515	BCR	C15-C16-C17	-2.67	118.01	123.47
25	t	101	BCR	C35-C13-C12	2.67	122.28	118.08
25	c	515	BCR	C8-C9-C10	2.67	123.03	118.94
25	h	102	BCR	C30-C25-C26	-2.66	118.86	122.61
28	c	519	LMG	O8-C28-O10	-2.66	116.88	123.59
30	B	623	LHG	C11-C10-C9	-2.66	100.92	114.42
25	C	515	BCR	C33-C5-C6	-2.66	121.54	124.53
23	C	508	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
23	b	605	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
23	a	604	CLA	CED-O2D-CGD	-2.66	109.93	115.94
23	b	610	CLA	CAA-CBA-CGA	-2.66	105.49	113.25
25	c	515	BCR	C33-C5-C6	-2.66	121.54	124.53
23	b	608	CLA	CHD-C4C-C3C	-2.66	120.94	124.84
25	T	101	BCR	C15-C14-C13	-2.65	123.52	127.31
25	h	102	BCR	C2-C1-C6	2.65	114.57	110.48
23	C	501	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
25	b	617	BCR	C29-C30-C25	2.65	114.56	110.48
23	c	513	CLA	CMB-C2B-C1B	-2.65	124.39	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	603	CLA	C9-C8-C7	-2.65	101.70	111.29
23	A	613	CLA	CAA-C2A-C1A	-2.65	103.30	111.97
30	d	405	LHG	O8-C6-C5	-2.65	100.73	108.43
23	C	509	CLA	CHB-C4A-NA	2.64	128.17	124.51
23	b	614	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
23	B	606	CLA	C6-C5-C3	-2.64	106.53	113.45
23	B	601	CLA	C1-C2-C3	-2.64	121.47	126.04
30	d	405	LHG	C11-C10-C9	-2.64	101.02	114.42
31	c	517	DGD	CDB-CCB-CBB	-2.64	101.03	114.42
28	A	612	LMG	O8-C28-O10	-2.64	116.93	123.59
23	B	604	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
23	B	614	CLA	C1-C2-C3	-2.64	121.48	126.04
23	b	606	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
31	C	518	DGD	CDB-CCB-CBB	-2.63	101.05	114.42
23	b	609	CLA	O1D-CGD-CBD	2.63	129.87	124.48
29	a	613	SQD	O48-C23-C24	2.63	120.16	111.91
23	A	603	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
25	C	514	BCR	C38-C26-C25	-2.63	121.58	124.53
23	b	609	CLA	CHD-C4C-NC	2.63	128.35	124.20
31	c	517	DGD	C8B-C7B-C6B	-2.63	101.08	114.42
23	b	611	CLA	C1D-ND-C4D	2.63	108.20	106.33
23	b	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	B	624	SQD	O9-S-C6	2.63	110.06	106.94
23	B	603	CLA	CHD-C1D-C2D	2.63	130.99	125.48
31	c	518	DGD	C3D-C4D-C5D	-2.62	105.56	110.24
23	c	505	CLA	C3B-C4B-NB	-2.62	105.82	109.21
25	T	101	BCR	C1-C6-C5	-2.62	118.92	122.61
29	a	613	SQD	O47-C7-O49	-2.62	117.36	123.70
29	b	601	SQD	O10-C23-C24	-2.62	113.51	123.73
30	a	614	LHG	O8-C23-O10	-2.62	116.98	123.59
31	c	517	DGD	O2E-C2E-C1E	-2.62	103.69	110.05
25	b	618	BCR	C15-C16-C17	-2.62	118.11	123.47
31	c	516	DGD	O3E-C3E-C2E	-2.61	104.32	110.35
23	b	608	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
23	A	604	CLA	O2D-CGD-CBD	2.61	115.90	111.27
28	c	519	LMG	O7-C10-O9	-2.60	117.79	122.96
23	B	613	CLA	CAC-C3C-C4C	2.60	128.19	124.81
25	A	608	BCR	C27-C26-C25	2.60	126.50	122.73
23	c	509	CLA	CMD-C2D-C3D	2.60	133.59	127.61
23	a	612	CLA	CHD-C1D-ND	-2.60	122.07	124.45
23	C	509	CLA	C1-C2-C3	-2.60	121.55	126.04
25	Y	101	BCR	C27-C26-C25	2.59	126.49	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	CHD-C1D-ND	-2.59	122.07	124.45
25	a	607	BCR	C33-C5-C6	-2.59	121.62	124.53
23	B	603	CLA	C7-C6-C5	-2.59	106.33	113.36
31	H	102	DGD	O2D-C2D-C1D	-2.59	103.76	110.05
29	a	615	SQD	O48-C23-C24	2.59	120.02	111.91
23	b	605	CLA	CHA-C1A-NA	-2.59	120.48	126.40
35	F	102	HEM	O2D-CGD-CBD	2.58	122.33	114.03
27	A	611	PL9	C41-C39-C38	-2.58	115.89	121.12
23	C	512	CLA	C4A-NA-C1A	2.58	107.87	106.71
23	D	402	CLA	C1D-CHD-C4C	-2.58	120.49	126.06
27	d	408	PL9	C36-C34-C33	-2.57	115.91	121.12
31	H	102	DGD	O2G-C1B-O1B	-2.57	117.48	123.70
28	D	405	LMG	O1-C7-C8	-2.57	104.69	110.90
28	A	612	LMG	C36-C35-C34	-2.57	101.36	114.42
23	c	503	CLA	CAC-C3C-C4C	2.57	128.15	124.81
23	b	606	CLA	CHD-C1D-ND	-2.57	122.09	124.45
23	c	502	CLA	C1-C2-C3	-2.57	121.59	126.04
23	B	606	CLA	CHD-C1D-C2D	2.57	130.87	125.48
23	B	601	CLA	CMB-C2B-C3B	2.57	129.48	124.68
27	a	611	PL9	C11-C12-C13	-2.57	103.44	111.88
23	C	505	CLA	CAC-C3C-C2C	-2.57	123.14	127.53
23	b	612	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
23	B	602	CLA	CMB-C2B-C3B	2.56	129.47	124.68
25	b	618	BCR	C34-C9-C10	-2.56	119.34	122.92
23	c	513	CLA	C4A-NA-C1A	2.56	107.86	106.71
31	A	617	DGD	CDB-CCB-CBB	-2.55	101.46	114.42
31	c	518	DGD	O1G-C1A-C2A	-2.55	103.89	111.91
23	c	506	CLA	CGD-CBD-CAD	-2.55	102.47	110.73
30	D	408	LHG	O8-C23-C24	2.55	119.91	111.91
23	b	611	CLA	C4-C3-C2	-2.55	117.14	123.68
23	a	604	CLA	O2D-CGD-CBD	2.55	115.80	111.27
23	c	503	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	c	505	CLA	C6-C7-C8	-2.55	107.68	115.92
29	f	101	SQD	O9-S-O7	-2.55	105.13	113.95
36	V	201	HEC	CMC-C2C-C1C	-2.55	124.55	128.46
28	c	521	LMG	O8-C28-O10	-2.55	117.17	123.59
23	c	506	CLA	CAC-C3C-C4C	2.54	128.11	124.81
25	h	102	BCR	C38-C26-C25	-2.54	121.67	124.53
23	B	605	CLA	O1D-CGD-CBD	2.54	129.69	124.48
23	B	608	CLA	CHD-C1D-ND	-2.54	122.12	124.45
27	d	408	PL9	C37-C38-C39	-2.54	121.54	127.66
23	c	501	CLA	CED-O2D-CGD	-2.54	110.19	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CAC-C3C-C4C	2.54	128.11	124.81
25	H	101	BCR	C35-C13-C12	2.54	122.08	118.08
23	A	603	CLA	C6-C5-C3	2.54	120.11	113.45
29	a	613	SQD	C1-C2-C3	-2.54	104.71	110.00
23	a	603	CLA	C2A-C1A-CHA	2.54	128.29	123.86
31	C	518	DGD	O6D-C1D-O3G	-2.54	103.97	109.97
27	D	407	PL9	C20-C19-C21	2.54	119.54	115.27
23	B	608	CLA	O1D-CGD-CBD	2.53	129.66	124.48
31	c	518	DGD	C7B-C6B-C5B	-2.53	101.57	114.42
23	B	608	CLA	CMB-C2B-C3B	2.53	129.41	124.68
30	D	408	LHG	C25-C24-C23	2.53	122.82	113.62
23	d	403	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
25	a	607	BCR	C29-C30-C25	2.53	114.37	110.48
28	d	406	LMG	O1-C7-C8	-2.53	104.80	110.90
23	b	611	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
31	c	516	DGD	C3D-C4D-C5D	-2.52	105.74	110.24
25	B	617	BCR	C11-C10-C9	-2.52	123.71	127.31
23	c	510	CLA	O2D-CGD-CBD	2.52	115.75	111.27
25	a	607	BCR	C37-C22-C21	-2.52	119.39	122.92
23	C	507	CLA	C2A-C1A-CHA	2.52	128.26	123.86
23	B	607	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
25	c	514	BCR	C11-C10-C9	-2.51	123.72	127.31
28	A	612	LMG	O7-C10-O9	-2.51	117.62	123.70
36	v	201	HEC	CMC-C2C-C3C	2.51	128.78	125.82
28	d	406	LMG	C1-C2-C3	-2.51	104.76	110.00
23	b	604	CLA	CHC-C1C-NC	2.51	128.01	124.20
23	B	613	CLA	C4-C3-C5	2.51	119.50	115.27
25	c	514	BCR	C15-C14-C13	-2.51	123.72	127.31
25	C	514	BCR	C35-C13-C14	-2.51	119.41	122.92
23	D	402	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	B	606	CLA	CGD-CBD-CAD	-2.51	102.62	110.73
23	B	602	CLA	CHA-C1A-NA	-2.51	120.66	126.40
23	B	613	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	C	501	CLA	CAC-C3C-C4C	2.50	128.05	124.81
23	B	609	CLA	C7-C6-C5	-2.50	106.58	113.36
23	A	603	CLA	O2D-CGD-CBD	-2.49	106.84	111.27
31	A	617	DGD	C3E-C4E-C5E	-2.49	105.79	110.24
23	c	506	CLA	C6-C5-C3	-2.49	106.93	113.45
23	B	611	CLA	CHD-C1D-C2D	2.49	130.70	125.48
23	D	403	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
23	C	506	CLA	CMB-C2B-C3B	2.49	129.33	124.68
23	B	615	CLA	C4-C3-C2	2.48	130.05	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	CHD-C4C-C3C	-2.48	121.19	124.84
25	h	102	BCR	C35-C13-C14	-2.48	119.45	122.92
34	D	401	BCT	O3-C-O1	-2.48	113.12	119.55
28	A	612	LMG	C40-C39-C38	-2.48	101.84	114.42
27	A	611	PL9	C22-C23-C24	-2.48	121.69	127.66
23	A	613	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
23	c	508	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
28	B	620	LMG	O3-C3-C2	-2.48	104.62	110.35
30	B	623	LHG	O8-C23-C24	2.48	119.67	111.91
23	C	504	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	D	407	PL9	C27-C28-C29	-2.47	121.70	127.66
23	b	609	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
25	C	520	BCR	C11-C10-C9	-2.47	123.78	127.31
23	c	509	CLA	C4D-C3D-CAD	-2.47	105.18	108.10
23	c	510	CLA	C2A-C3A-C4A	2.47	105.86	101.87
23	C	502	CLA	CMB-C2B-C3B	2.47	129.30	124.68
23	b	615	CLA	C3B-C4B-NB	-2.47	106.02	109.21
28	m	101	LMG	O1-C7-C8	-2.47	104.94	110.90
23	C	507	CLA	CHD-C4C-NC	2.47	128.09	124.20
31	H	102	DGD	C1E-O6E-C5E	2.47	118.53	113.69
23	B	605	CLA	C4A-NA-C1A	2.47	107.81	106.71
23	C	510	CLA	CHB-C4A-NA	2.47	127.92	124.51
25	A	608	BCR	C33-C5-C6	-2.46	121.76	124.53
23	c	503	CLA	C4-C3-C5	2.46	119.42	115.27
27	A	611	PL9	O2-C1-C6	2.46	124.85	120.59
24	d	401	PHO	CMA-C3A-C4A	-2.46	108.99	114.38
23	C	508	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
25	A	608	BCR	C19-C18-C17	-2.46	115.17	118.94
23	c	510	CLA	CMB-C2B-C3B	2.46	129.28	124.68
25	h	102	BCR	C16-C17-C18	-2.46	123.80	127.31
23	B	616	CLA	CHA-C1A-NA	-2.46	120.77	126.40
29	f	101	SQD	O5-C5-C4	2.46	114.16	109.69
23	C	511	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
23	b	613	CLA	CHD-C1D-ND	-2.46	122.20	124.45
27	A	611	PL9	C31-C32-C33	-2.46	103.81	111.88
30	d	405	LHG	O8-C23-O10	-2.45	117.40	123.59
29	a	615	SQD	O48-C23-O10	-2.45	117.40	123.59
23	C	507	CLA	CMB-C2B-C3B	2.45	129.27	124.68
23	a	606	CLA	O2D-CGD-CBD	2.45	115.62	111.27
23	C	508	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	A	608	BCR	C2-C1-C6	2.45	114.25	110.48
23	c	506	CLA	CHA-C1A-NA	-2.45	120.79	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	CHD-C1D-C2D	2.45	130.61	125.48
23	b	611	CLA	C5-C3-C2	2.45	126.07	121.12
23	b	607	CLA	C2C-C1C-NC	2.45	112.26	109.97
23	c	502	CLA	C4D-CHA-C1A	2.45	124.23	121.25
23	b	602	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	B	613	CLA	CHA-C1A-NA	-2.44	120.80	126.40
23	C	503	CLA	O1D-CGD-CBD	2.44	129.49	124.48
27	d	408	PL9	C50-C49-C48	-2.44	115.58	122.65
25	c	515	BCR	C15-C14-C13	-2.44	123.82	127.31
23	b	612	CLA	O2D-CGD-CBD	-2.44	106.93	111.27
23	B	608	CLA	CED-O2D-CGD	-2.44	110.41	115.94
29	a	613	SQD	O5-C5-C4	2.44	114.13	109.69
24	A	606	PHO	CMB-C2B-C3B	2.44	129.25	124.68
28	b	621	LMG	C8-O7-C10	2.44	123.80	117.79
25	D	404	BCR	C16-C15-C14	-2.44	118.48	123.47
31	H	102	DGD	C1D-C2D-C3D	-2.44	104.92	110.00
23	c	511	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
24	d	401	PHO	C1B-NB-C4B	2.44	112.10	107.09
23	C	504	CLA	C6-C5-C3	2.44	119.84	113.45
23	c	509	CLA	O2A-CGA-CBA	2.44	119.56	111.91
23	B	616	CLA	O2A-C1-C2	2.44	115.04	108.64
23	C	507	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
29	F	101	SQD	O48-C23-O10	-2.43	117.45	123.59
25	c	514	BCR	C24-C23-C22	-2.43	122.56	126.23
23	B	611	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
23	A	613	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	A	604	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
23	C	507	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	C	504	CLA	CHD-C4C-NC	2.43	128.03	124.20
27	A	611	PL9	C36-C37-C38	-2.43	103.90	111.88
23	A	603	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	c	506	CLA	C1B-CHB-C4A	-2.42	125.31	130.12
23	A	613	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	b	619	BCR	C11-C10-C9	-2.42	123.85	127.31
23	a	606	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
31	a	616	DGD	C1G-O1G-C1A	2.42	126.09	117.12
23	B	612	CLA	CED-O2D-CGD	-2.42	110.46	115.94
25	h	102	BCR	C11-C10-C9	-2.42	123.85	127.31
30	d	407	LHG	O8-C23-C24	2.42	119.51	111.91
23	b	605	CLA	C2C-C1C-NC	2.42	112.24	109.97
23	D	403	CLA	O2D-CGD-CBD	2.42	115.57	111.27
25	B	618	BCR	C2-C1-C6	2.42	114.20	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
35	f	102	HEM	CAB-C3B-C2B	-2.42	120.64	128.60
25	b	619	BCR	C2-C1-C6	2.42	114.20	110.48
27	A	611	PL9	C11-C9-C8	-2.41	116.23	121.12
23	h	101	CLA	CMB-C2B-C3B	2.41	129.19	124.68
25	b	619	BCR	C27-C26-C25	2.41	126.23	122.73
28	A	612	LMG	C4-C3-C2	-2.41	106.61	110.82
25	B	619	BCR	C2-C1-C6	2.41	114.19	110.48
23	B	606	CLA	CHC-C1C-NC	2.41	127.86	124.20
28	m	101	LMG	O6-C1-O1	-2.41	104.27	109.97
23	b	606	CLA	C6-C5-C3	2.41	119.77	113.45
23	c	513	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
25	c	514	BCR	C30-C25-C26	-2.41	119.23	122.61
23	B	601	CLA	CHA-C4D-ND	2.40	137.53	132.50
23	c	507	CLA	O1D-CGD-CBD	2.40	129.40	124.48
23	A	607	CLA	CHC-C1C-C2C	-2.40	120.08	126.72
23	B	602	CLA	C2D-C1D-ND	-2.40	108.33	110.10
23	b	604	CLA	CHD-C1D-ND	-2.40	122.25	124.45
23	B	616	CLA	C1-O2A-CGA	2.40	122.74	116.44
25	D	404	BCR	C27-C26-C25	2.40	126.21	122.73
28	d	406	LMG	O1-C1-C2	-2.39	104.56	108.30
28	A	612	LMG	C9-C8-C7	-2.39	106.13	111.79
23	C	510	CLA	O2D-CGD-CBD	2.39	115.52	111.27
23	C	503	CLA	C4-C3-C5	2.39	119.30	115.27
23	D	403	CLA	CAA-CBA-CGA	-2.39	106.26	113.25
23	B	613	CLA	C2A-C1A-CHA	2.39	128.04	123.86
23	B	601	CLA	O1D-CGD-CBD	2.39	129.38	124.48
31	C	517	DGD	O6E-C1E-O5D	-2.39	104.31	109.97
23	D	403	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
25	D	404	BCR	C24-C23-C22	-2.39	122.62	126.23
23	b	608	CLA	C3B-C4B-NB	-2.39	106.12	109.21
23	b	610	CLA	CHA-C1A-NA	-2.39	120.93	126.40
23	B	605	CLA	C3A-C2A-C1A	2.38	104.90	101.34
31	c	516	DGD	O6E-C5E-C4E	2.38	114.01	109.69
23	b	611	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
27	D	407	PL9	C31-C32-C33	-2.38	104.07	111.88
25	c	515	BCR	C11-C10-C9	-2.37	123.92	127.31
23	c	508	CLA	O2D-CGD-CBD	2.37	115.49	111.27
23	C	505	CLA	CHD-C1D-ND	-2.37	122.27	124.45
23	a	603	CLA	CMC-C2C-C1C	2.37	128.65	125.04
23	a	612	CLA	C1-O2A-CGA	2.37	122.66	116.44
27	a	611	PL9	C27-C28-C29	-2.37	121.95	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	407	PL9	C50-C49-C48	-2.37	115.80	122.65
23	h	101	CLA	CMB-C2B-C1B	-2.37	124.83	128.46
29	B	624	SQD	O48-C23-O10	-2.37	117.62	123.59
31	C	516	DGD	CCB-CBB-CAB	-2.36	102.42	114.42
23	A	604	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	B	602	CLA	C1-C2-C3	-2.36	121.95	126.04
29	A	614	SQD	O8-S-O7	-2.36	105.50	111.27
28	B	620	LMG	O1-C7-C8	-2.36	105.20	110.90
31	c	518	DGD	O2D-C2D-C3D	-2.36	104.89	110.35
25	A	608	BCR	C4-C5-C6	2.36	126.16	122.73
30	D	406	LHG	C27-C26-C25	-2.36	102.45	114.42
25	B	619	BCR	C12-C13-C14	-2.36	115.33	118.94
23	b	615	CLA	CHD-C4C-C3C	-2.36	121.38	124.84
23	B	603	CLA	C6-C5-C3	2.36	119.63	113.45
23	a	603	CLA	C14-C13-C15	-2.35	102.77	111.29
23	B	613	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	c	514	BCR	C15-C16-C17	-2.35	118.66	123.47
23	b	612	CLA	C2C-C1C-NC	2.35	112.17	109.97
23	B	609	CLA	CHD-C1D-ND	-2.35	122.30	124.45
23	c	506	CLA	C2A-C1A-CHA	2.35	127.96	123.86
25	t	101	BCR	C7-C8-C9	-2.35	122.69	126.23
28	b	621	LMG	O6-C5-C6	2.34	112.26	106.44
23	c	501	CLA	CHA-C1A-NA	-2.34	121.03	126.40
23	c	507	CLA	CHD-C1D-ND	-2.34	122.30	124.45
23	c	503	CLA	C11-C12-C13	-2.34	108.35	115.92
23	b	606	CLA	C3C-C4C-NC	-2.34	107.94	110.57
35	f	102	HEM	CHC-C4B-C3B	2.34	128.15	124.57
31	A	617	DGD	C1E-O6E-C5E	2.34	118.28	113.69
28	b	621	LMG	C6-C5-C4	-2.34	107.53	113.00
25	b	619	BCR	C36-C18-C17	-2.34	119.65	122.92
30	D	406	LHG	O8-C23-O10	-2.34	117.69	123.59
23	B	616	CLA	CHD-C1D-ND	-2.34	122.31	124.45
23	B	616	CLA	CED-O2D-CGD	2.34	121.22	115.94
31	H	102	DGD	C8B-C7B-C6B	-2.33	102.57	114.42
24	d	401	PHO	O2A-CGA-O1A	-2.33	117.70	123.59
23	C	508	CLA	C2D-C1D-ND	-2.33	108.38	110.10
23	B	610	CLA	O2D-CGD-CBD	2.33	115.42	111.27
23	b	611	CLA	C4A-NA-C1A	2.33	107.75	106.71
29	b	601	SQD	O9-S-O7	-2.33	105.88	113.95
27	A	611	PL9	C46-C47-C48	-2.33	104.22	111.88
25	h	102	BCR	C36-C18-C17	-2.33	119.66	122.92
25	c	514	BCR	C33-C5-C6	-2.33	121.91	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
27	a	611	PL9	C36-C34-C33	-2.33	116.40	121.12
23	b	607	CLA	C2D-C1D-ND	-2.33	108.39	110.10
23	b	605	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
31	C	518	DGD	O1G-C1A-C2A	-2.33	104.61	111.91
24	d	401	PHO	O2D-CGD-CBD	-2.33	108.05	111.00
23	B	616	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
23	c	508	CLA	C1D-ND-C4D	2.32	107.99	106.33
25	d	404	BCR	C16-C15-C14	-2.32	118.71	123.47
29	B	624	SQD	O47-C7-O49	-2.32	118.09	123.70
25	c	515	BCR	C1-C6-C5	-2.32	119.34	122.61
23	D	403	CLA	CMB-C2B-C3B	2.32	129.02	124.68
31	c	517	DGD	O6D-C1D-O3G	-2.32	104.48	109.97
23	b	608	CLA	O2D-CGD-CBD	2.32	115.39	111.27
23	c	511	CLA	CHA-C1A-NA	-2.32	121.09	126.40
36	v	201	HEC	O2D-CGD-CBD	2.32	121.48	114.03
25	C	514	BCR	C15-C16-C17	-2.32	118.72	123.47
35	f	102	HEM	CMC-C2C-C3C	2.32	129.02	124.68
35	f	102	HEM	CMA-C3A-C4A	-2.32	124.90	128.46
23	B	605	CLA	CAC-C3C-C4C	2.32	127.81	124.81
28	C	519	LMG	O6-C1-O1	-2.32	104.49	109.97
28	B	620	LMG	C40-C39-C38	-2.32	102.67	114.42
24	A	605	PHO	C5-C3-C2	2.31	125.80	121.12
23	c	513	CLA	CMB-C2B-C3B	2.31	129.01	124.68
28	c	522	LMG	O6-C1-O1	-2.31	104.49	109.97
23	d	403	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
23	a	606	CLA	O2A-C1-C2	-2.31	102.56	108.64
23	c	507	CLA	CHD-C4C-NC	2.31	127.85	124.20
23	C	510	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	a	603	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
30	D	406	LHG	O8-C23-C24	2.31	119.15	111.91
31	h	103	DGD	O5E-C6E-C5E	-2.31	103.38	111.29
28	B	620	LMG	O8-C28-O10	-2.31	117.77	123.59
23	C	512	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
25	Y	101	BCR	C11-C10-C9	-2.30	124.02	127.31
25	T	101	BCR	C7-C8-C9	-2.30	122.76	126.23
28	m	101	LMG	O8-C9-C8	-2.30	101.73	108.43
23	c	501	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
28	B	620	LMG	C38-C37-C36	-2.30	102.74	114.42
28	b	621	LMG	O2-C2-C1	-2.30	104.46	110.05
35	F	102	HEM	C4D-ND-C1D	2.30	107.45	105.07
23	C	503	CLA	CHA-C1A-NA	-2.30	121.13	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	CMB-C2B-C3B	2.30	128.98	124.68
23	b	615	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
25	Y	101	BCR	C23-C24-C25	-2.30	120.75	127.20
28	m	101	LMG	O1-C1-C2	-2.30	104.72	108.30
27	d	408	PL9	C26-C27-C28	-2.30	104.33	111.88
23	b	615	CLA	O2D-CGD-CBD	2.30	115.35	111.27
25	a	607	BCR	C19-C18-C17	-2.29	115.42	118.94
31	h	103	DGD	O2D-C2D-C1D	-2.29	104.48	110.05
23	B	610	CLA	O1D-CGD-CBD	2.29	129.17	124.48
25	H	101	BCR	C30-C25-C26	-2.29	119.39	122.61
23	B	614	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
23	a	606	CLA	CMB-C2B-C3B	2.29	128.96	124.68
28	A	612	LMG	O3-C3-C2	-2.29	105.06	110.35
31	c	517	DGD	O3G-C1D-C2D	-2.29	104.73	108.30
23	B	608	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
27	A	611	PL9	C27-C28-C29	-2.28	122.16	127.66
23	B	608	CLA	C11-C12-C13	-2.28	108.54	115.92
23	b	610	CLA	O2D-CGD-CBD	2.28	115.32	111.27
23	A	603	CLA	CHA-C1A-NA	-2.28	121.18	126.40
23	B	602	CLA	CHA-C4D-ND	2.28	137.26	132.50
23	c	501	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
30	a	614	LHG	C11-C10-C9	-2.28	102.86	114.42
27	d	408	PL9	C11-C9-C8	-2.28	116.51	121.12
23	c	510	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
25	A	608	BCR	C16-C15-C14	-2.28	118.81	123.47
31	c	518	DGD	C3G-C2G-C1G	-2.28	106.41	111.79
23	a	603	CLA	C1D-ND-C4D	2.27	107.95	106.33
23	c	507	CLA	CHB-C4A-NA	2.27	127.66	124.51
27	a	611	PL9	C21-C19-C18	-2.27	116.52	121.12
27	A	611	PL9	C36-C34-C33	-2.27	116.52	121.12
27	a	611	PL9	C30-C29-C28	-2.27	117.85	123.68
23	A	604	CLA	O2A-C1-C2	-2.27	102.67	108.64
25	H	101	BCR	C24-C23-C22	-2.27	122.81	126.23
35	f	102	HEM	CBA-CAA-C2A	-2.27	108.75	112.62
23	c	504	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	h	101	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
28	C	519	LMG	O1-C7-C8	-2.26	105.43	110.90
25	k	101	BCR	C38-C26-C25	-2.26	121.98	124.53
23	c	503	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	c	506	CLA	O1A-CGA-CBA	2.26	132.56	123.73
23	B	612	CLA	CHD-C1D-ND	-2.26	122.37	124.45
25	c	515	BCR	C15-C16-C17	-2.26	118.85	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	CHA-C1A-NA	-2.26	121.23	126.40
23	b	604	CLA	C1-C2-C3	-2.26	122.14	126.04
23	C	501	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
25	B	619	BCR	C15-C16-C17	-2.25	118.86	123.47
23	B	615	CLA	C6-C7-C8	-2.25	108.65	115.92
25	Y	101	BCR	C40-C30-C25	2.25	113.95	110.30
23	C	504	CLA	C1-O2A-CGA	2.25	122.34	116.44
35	F	102	HEM	CHC-C4B-NB	2.25	126.87	124.43
31	A	617	DGD	O6D-C1D-O3G	-2.25	104.65	109.97
23	B	616	CLA	CAA-CBA-CGA	-2.25	106.68	113.25
27	a	611	PL9	C12-C13-C14	-2.25	122.25	127.66
31	c	517	DGD	CBB-CAB-C9B	-2.25	103.02	114.42
23	b	616	CLA	C4A-NA-C1A	2.25	107.72	106.71
27	a	611	PL9	C40-C39-C38	-2.25	117.92	123.68
23	B	604	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
25	b	618	BCR	C30-C25-C26	-2.24	119.45	122.61
23	B	608	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
25	C	514	BCR	C7-C8-C9	-2.24	122.85	126.23
23	C	506	CLA	CMC-C2C-C1C	2.24	128.45	125.04
23	b	614	CLA	CHD-C1D-C2D	2.24	130.18	125.48
23	A	603	CLA	C7-C6-C5	-2.24	107.27	113.36
25	C	515	BCR	C35-C13-C14	-2.24	119.78	122.92
23	B	604	CLA	O2A-C1-C2	2.24	114.52	108.64
23	B	602	CLA	C2A-C1A-CHA	2.24	127.78	123.86
30	D	408	LHG	C11-C10-C9	-2.24	103.06	114.42
25	b	619	BCR	C37-C22-C21	-2.24	119.79	122.92
31	c	516	DGD	O5D-C6D-C5D	-2.24	104.91	109.05
28	A	612	LMG	C3-C4-C5	-2.24	106.25	110.24
23	c	512	CLA	O1D-CGD-CBD	2.23	129.06	124.48
25	B	618	BCR	C15-C14-C13	-2.23	124.12	127.31
31	c	517	DGD	O2G-C1B-O1B	-2.23	118.31	123.70
31	H	102	DGD	CDB-CCB-CBB	-2.23	103.11	114.42
23	A	604	CLA	C2C-C1C-NC	2.23	112.06	109.97
27	A	611	PL9	C7-C8-C9	-2.23	123.08	126.79
31	C	517	DGD	CDB-CCB-CBB	-2.23	103.11	114.42
25	k	102	BCR	C11-C10-C9	-2.23	124.13	127.31
23	a	604	CLA	CHA-C1A-NA	-2.23	121.30	126.40
36	v	201	HEC	CBA-CAA-C2A	-2.23	108.85	112.60
25	t	101	BCR	C4-C5-C6	2.22	125.96	122.73
23	a	612	CLA	C3A-C2A-C1A	2.22	104.67	101.34
31	H	102	DGD	O3E-C3E-C2E	-2.22	105.21	110.35
23	D	403	CLA	CHB-C4A-NA	2.22	127.59	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	408	PL9	C41-C42-C43	-2.22	104.58	111.88
30	l	101	LHG	C20-C19-C18	-2.22	103.15	114.42
23	B	605	CLA	OBD-CAD-C3D	2.22	133.87	128.52
23	b	604	CLA	CMB-C2B-C3B	2.22	128.83	124.68
23	d	403	CLA	O1D-CGD-CBD	2.22	129.02	124.48
25	H	101	BCR	C36-C18-C17	-2.22	119.81	122.92
23	B	601	CLA	C3C-C4C-NC	-2.22	108.08	110.57
23	A	604	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
23	d	403	CLA	CHD-C1D-C2D	2.22	130.13	125.48
23	b	605	CLA	CHD-C1D-C2D	2.22	130.13	125.48
23	c	508	CLA	CHD-C1D-C2D	2.22	130.13	125.48
23	b	615	CLA	CHA-C4D-ND	2.22	137.13	132.50
23	B	612	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
25	t	101	BCR	C1-C6-C5	-2.21	119.50	122.61
25	h	102	BCR	C37-C22-C21	-2.21	119.82	122.92
25	B	617	BCR	C3-C4-C5	-2.21	110.13	114.08
23	C	504	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
24	A	605	PHO	CMC-C2C-C3C	2.21	129.11	124.94
23	B	604	CLA	C11-C10-C8	-2.21	108.77	115.92
23	C	508	CLA	CHD-C1D-C2D	2.21	130.11	125.48
23	b	612	CLA	CHD-C4C-C3C	-2.21	121.59	124.84
31	H	102	DGD	O6E-C5E-C4E	2.21	113.70	109.69
31	c	518	DGD	C9B-C8B-C7B	-2.21	103.22	114.42
30	d	409	LHG	C27-C26-C25	-2.21	103.22	114.42
28	m	101	LMG	C6-C5-C4	-2.21	107.84	113.00
23	c	505	CLA	CAC-C3C-C4C	2.21	127.67	124.81
31	h	103	DGD	CDB-CCB-CBB	-2.20	103.24	114.42
23	B	605	CLA	C1-O2A-CGA	-2.20	110.66	116.44
31	c	516	DGD	CBB-CAB-C9B	-2.20	103.24	114.42
28	c	521	LMG	C9-C8-C7	-2.20	106.58	111.79
25	B	619	BCR	C16-C15-C14	-2.20	118.97	123.47
31	C	518	DGD	C4A-C3A-C2A	-2.20	105.28	113.19
30	B	623	LHG	C20-C19-C18	-2.20	103.26	114.42
23	b	606	CLA	O2D-CGD-CBD	2.20	115.17	111.27
27	D	407	PL9	C12-C13-C14	-2.20	122.37	127.66
25	k	102	BCR	C16-C15-C14	-2.20	118.97	123.47
23	b	609	CLA	CHA-C1A-NA	-2.20	121.37	126.40
25	b	618	BCR	C27-C26-C25	2.20	125.92	122.73
25	t	101	BCR	C36-C18-C19	2.20	121.54	118.08
28	c	519	LMG	O3-C3-C2	-2.19	105.28	110.35
25	b	618	BCR	C11-C10-C9	-2.19	124.18	127.31
35	F	102	HEM	C3C-C4C-NC	-2.19	106.80	110.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	409	LMG	O7-C10-O9	-2.19	118.41	123.70
25	B	617	BCR	C33-C5-C6	-2.19	122.07	124.53
23	B	610	CLA	C3C-C4C-NC	-2.19	108.11	110.57
24	A	606	PHO	CMC-C2C-C3C	2.19	129.07	124.94
23	a	603	CLA	CAA-C2A-C1A	-2.19	104.80	111.97
23	a	612	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	b	604	CLA	C11-C12-C13	-2.19	108.85	115.92
27	d	408	PL9	C40-C39-C38	-2.19	118.07	123.68
30	l	101	LHG	C27-C26-C25	-2.18	103.33	114.42
25	B	619	BCR	C35-C13-C14	-2.18	119.86	122.92
23	c	506	CLA	C2D-C1D-ND	-2.18	108.50	110.10
23	b	611	CLA	C11-C10-C8	-2.18	108.87	115.92
28	D	409	LMG	O1-C7-C8	-2.18	106.00	111.78
23	B	610	CLA	CHA-C1A-NA	-2.18	121.40	126.40
23	b	611	CLA	C11-C12-C13	-2.18	108.87	115.92
23	D	402	CLA	C2D-C1D-ND	-2.18	108.50	110.10
23	c	511	CLA	C4D-CHA-C1A	2.18	123.90	121.25
23	b	604	CLA	CMC-C2C-C3C	2.18	132.03	126.12
27	a	611	PL9	O2-C1-C6	2.18	124.36	120.59
28	B	620	LMG	C1-O6-C5	-2.18	109.41	113.69
25	Y	101	BCR	C8-C7-C6	-2.18	121.09	127.20
23	C	505	CLA	OBD-CAD-C3D	2.18	133.76	128.52
29	a	615	SQD	C10-C9-C8	-2.18	105.36	113.19
30	l	101	LHG	O10-C23-C24	-2.18	115.24	123.73
25	A	608	BCR	C1-C6-C5	-2.18	119.55	122.61
23	B	605	CLA	CHA-C1A-NA	-2.18	121.42	126.40
23	b	613	CLA	C2D-C1D-ND	2.18	111.71	110.10
23	a	604	CLA	C4D-C3D-CAD	-2.17	105.53	108.10
31	a	616	DGD	O3G-C3G-C2G	-2.17	106.02	111.78
24	A	606	PHO	O1D-CGD-CBD	2.17	128.35	124.74
23	C	502	CLA	CAC-C3C-C4C	2.17	127.63	124.81
27	D	407	PL9	C11-C9-C8	-2.17	116.73	121.12
23	b	606	CLA	C2C-C1C-NC	2.17	112.00	109.97
23	B	609	CLA	CHA-C1A-NA	-2.17	121.44	126.40
25	c	515	BCR	C29-C30-C25	2.16	113.81	110.48
24	d	401	PHO	C6-C7-C8	-2.16	108.93	115.92
23	b	610	CLA	C4A-NA-C1A	2.16	107.68	106.71
25	k	102	BCR	C2-C1-C6	2.16	113.81	110.48
23	B	611	CLA	C2C-C1C-NC	2.16	111.99	109.97
23	D	403	CLA	CHA-C1A-NA	-2.16	121.46	126.40
23	b	612	CLA	CAC-C3C-C4C	2.15	127.61	124.81
23	b	615	CLA	C6-C5-C3	-2.15	107.81	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	C4D-CHA-C1A	2.15	123.87	121.25
23	b	608	CLA	CHB-C4A-NA	2.15	127.49	124.51
27	a	611	PL9	C37-C38-C39	-2.15	122.48	127.66
30	D	406	LHG	C18-C17-C16	-2.15	103.50	114.42
23	c	507	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	B	609	CLA	C4-C3-C5	-2.15	111.66	115.27
23	b	606	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
23	c	505	CLA	CED-O2D-CGD	-2.15	111.08	115.94
23	b	614	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
28	m	101	LMG	C40-C39-C38	-2.15	103.52	114.42
25	t	101	BCR	C15-C14-C13	-2.15	124.24	127.31
23	a	604	CLA	O1A-CGA-CBA	2.15	132.10	123.73
23	b	613	CLA	C16-C15-C13	-2.14	108.99	115.92
23	c	504	CLA	CHB-C4A-NA	2.14	127.48	124.51
23	C	510	CLA	O2D-CGD-O1D	-2.14	119.64	123.84
23	B	611	CLA	CHD-C4C-NC	2.14	127.58	124.20
23	b	616	CLA	CHD-C4C-NC	2.14	127.58	124.20
23	B	610	CLA	O1A-CGA-CBA	2.14	132.10	123.73
23	C	501	CLA	OBD-CAD-C3D	2.14	133.68	128.52
23	B	611	CLA	C9-C8-C10	-2.14	103.54	111.29
23	c	501	CLA	C4D-CHA-C1A	2.14	123.85	121.25
23	b	604	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
31	A	617	DGD	CAB-C9B-C8B	-2.14	103.57	114.42
30	D	406	LHG	O2-C2-C3	-2.14	102.06	109.56
31	C	517	DGD	C4E-C3E-C2E	-2.14	107.09	110.82
25	k	101	BCR	C16-C15-C14	-2.13	119.10	123.47
25	T	101	BCR	C33-C5-C6	-2.13	122.13	124.53
27	D	407	PL9	C7-C8-C9	-2.13	123.24	126.79
23	h	101	CLA	C2A-C3A-C4A	2.13	105.31	101.87
30	l	101	LHG	C11-C10-C9	-2.13	103.60	114.42
28	B	620	LMG	C37-C36-C35	-2.13	103.60	114.42
31	c	516	DGD	O2D-C2D-C1D	-2.13	104.87	110.05
23	B	611	CLA	C2D-C1D-ND	-2.13	108.53	110.10
23	c	507	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
23	b	607	CLA	C3A-C2A-C1A	2.13	104.53	101.34
23	a	604	CLA	C2A-C1A-CHA	2.13	127.58	123.86
23	C	507	CLA	O2D-CGD-CBD	2.13	115.05	111.27
23	b	603	CLA	O2A-C1-C2	-2.13	103.04	108.64
25	b	617	BCR	C15-C16-C17	-2.13	119.11	123.47
31	C	517	DGD	C7B-C6B-C5B	-2.13	103.62	114.42
23	C	513	CLA	O2D-CGD-CBD	2.13	115.05	111.27
23	c	507	CLA	C2A-C1A-CHA	2.13	127.58	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C2C-C1C-NC	2.13	111.97	109.97
23	b	610	CLA	CBC-CAC-C3C	2.13	118.30	112.43
28	m	101	LMG	C9-C8-C7	-2.13	106.76	111.79
23	c	512	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
23	b	607	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
23	b	603	CLA	CHD-C1D-C2D	2.12	129.94	125.48
31	C	517	DGD	CAB-C9B-C8B	-2.12	103.64	114.42
27	D	407	PL9	O2-C1-C2	-2.12	116.91	121.78
23	h	101	CLA	C3C-C4C-NC	-2.12	108.19	110.57
23	B	607	CLA	CHA-C1A-NA	-2.12	121.54	126.40
25	B	618	BCR	C8-C7-C6	-2.12	121.24	127.20
23	c	502	CLA	CHB-C4A-NA	2.12	127.44	124.51
25	b	618	BCR	C7-C8-C9	-2.12	123.03	126.23
23	B	612	CLA	C16-C15-C13	-2.12	109.07	115.92
23	D	403	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	B	603	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
23	C	505	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	d	401	PHO	CED-O2D-CGD	2.11	120.72	115.94
23	b	608	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
23	c	510	CLA	CED-O2D-CGD	2.11	120.72	115.94
25	k	102	BCR	C24-C23-C22	-2.11	123.04	126.23
23	C	501	CLA	CBA-CAA-C2A	2.11	120.09	113.86
23	d	402	CLA	CBA-CAA-C2A	-2.11	107.64	113.86
27	D	407	PL9	C41-C39-C38	-2.11	116.85	121.12
25	T	101	BCR	C35-C13-C14	-2.11	119.97	122.92
25	t	101	BCR	C35-C13-C14	-2.11	119.97	122.92
23	c	505	CLA	CHC-C1C-NC	2.11	127.40	124.20
31	c	518	DGD	C3E-C4E-C5E	-2.11	106.48	110.24
31	c	516	DGD	CDB-CCB-CBB	-2.11	103.73	114.42
23	c	509	CLA	CMD-C2D-C1D	-2.11	121.00	124.71
23	b	615	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	A	603	CLA	C1D-ND-C4D	-2.10	104.84	106.33
23	B	615	CLA	C4-C3-C5	-2.10	111.73	115.27
29	a	615	SQD	C45-O47-C7	2.10	122.97	117.79
23	C	505	CLA	C11-C10-C8	-2.10	109.12	115.92
23	B	606	CLA	OBD-CAD-C3D	2.10	133.58	128.52
23	a	603	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
23	D	403	CLA	C1D-ND-C4D	-2.10	104.84	106.33
23	b	614	CLA	CAC-C3C-C4C	2.10	127.53	124.81
31	A	617	DGD	C7B-C6B-C5B	-2.10	103.77	114.42
23	C	513	CLA	C3A-C2A-C1A	2.10	104.48	101.34
23	d	403	CLA	CGD-CBD-CAD	-2.10	103.94	110.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	516	DGD	C3G-O3G-C1D	-2.10	109.64	113.74
23	c	510	CLA	C4-C3-C5	2.10	118.80	115.27
31	C	517	DGD	O3D-C3D-C4D	-2.10	105.50	110.35
23	C	512	CLA	C1-C2-C3	-2.09	122.42	126.04
23	b	613	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
25	Y	101	BCR	C33-C5-C6	-2.09	122.18	124.53
23	d	403	CLA	C1-C2-C3	-2.09	122.42	126.04
25	C	515	BCR	C27-C26-C25	2.09	125.77	122.73
23	b	611	CLA	CHA-C1A-NA	-2.09	121.61	126.40
23	c	504	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
24	d	401	PHO	C1-C2-C3	-2.09	122.43	126.04
23	B	613	CLA	CMB-C2B-C3B	2.09	128.59	124.68
28	D	405	LMG	O3-C3-C2	-2.09	105.52	110.35
23	h	101	CLA	CHD-C1D-C2D	2.09	129.86	125.48
28	d	406	LMG	C6-C5-C4	-2.09	108.12	113.00
23	c	513	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
29	f	101	SQD	C1-C2-C3	-2.08	105.65	110.00
23	C	509	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
25	c	515	BCR	C4-C5-C6	2.08	125.76	122.73
25	a	607	BCR	C8-C9-C10	2.08	122.14	118.94
23	c	504	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
23	b	608	CLA	CAC-C3C-C4C	2.08	127.51	124.81
25	c	514	BCR	C7-C8-C9	-2.08	123.09	126.23
25	C	514	BCR	C12-C13-C14	2.08	122.13	118.94
23	b	613	CLA	C2A-C3A-C4A	2.08	105.23	101.87
28	D	409	LMG	C8-O7-C10	2.08	122.91	117.79
29	A	614	SQD	O2-C2-C3	-2.08	105.54	110.35
29	f	101	SQD	C45-O47-C7	2.08	122.91	117.79
23	b	614	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	c	509	CLA	OBD-CAD-C3D	2.08	133.52	128.52
28	D	409	LMG	C38-C37-C36	-2.08	103.88	114.42
31	C	518	DGD	C1D-C2D-C3D	-2.08	105.67	110.00
23	c	501	CLA	O1D-CGD-CBD	2.08	128.73	124.48
28	D	405	LMG	O6-C1-O1	-2.08	105.06	109.97
25	k	102	BCR	C40-C30-C25	2.08	113.67	110.30
25	B	619	BCR	C34-C9-C10	-2.07	120.02	122.92
23	D	402	CLA	C1-C2-C3	-2.07	122.46	126.04
25	h	102	BCR	C7-C8-C9	-2.07	123.10	126.23
25	t	101	BCR	C11-C10-C9	-2.07	124.35	127.31
25	h	102	BCR	C35-C13-C12	2.07	121.34	118.08
23	B	604	CLA	CHD-C1D-ND	-2.07	122.55	124.45
28	A	612	LMG	C1-O6-C5	-2.07	109.62	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	521	LMG	C42-C41-C40	-2.07	103.92	114.42
23	b	602	CLA	CHD-C4C-NC	2.07	127.47	124.20
27	d	408	PL9	C41-C39-C38	-2.07	116.93	121.12
25	C	520	BCR	C37-C22-C21	-2.07	120.03	122.92
23	b	603	CLA	CMD-C2D-C1D	2.07	128.36	124.71
23	a	612	CLA	CHD-C1D-C2D	2.07	129.82	125.48
23	b	615	CLA	C2A-C1A-CHA	2.07	127.48	123.86
23	C	510	CLA	C3A-C2A-C1A	2.07	104.44	101.34
31	c	518	DGD	O5D-C6D-C5D	-2.07	105.22	109.05
23	a	604	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
29	b	601	SQD	O48-C23-O10	-2.06	118.39	123.59
28	c	521	LMG	O7-C10-O9	-2.06	118.72	123.70
30	B	623	LHG	C9-C8-C7	-2.06	106.13	113.62
23	b	606	CLA	C1-O2A-CGA	2.06	121.85	116.44
36	V	201	HEC	CBD-CAD-C3D	-2.06	109.11	112.62
23	C	503	CLA	CHD-C1D-C2D	2.06	129.80	125.48
23	C	509	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
23	c	502	CLA	O2D-CGD-CBD	2.06	114.93	111.27
23	b	607	CLA	CMA-C3A-C4A	2.06	117.30	111.77
23	B	611	CLA	C3C-C4C-NC	-2.06	108.27	110.57
23	c	505	CLA	C4D-C3D-CAD	-2.05	105.67	108.10
23	B	604	CLA	C2A-C3A-C4A	2.05	105.19	101.87
30	D	408	LHG	O3-P-O5	-2.05	101.04	109.07
23	B	603	CLA	C2D-C1D-ND	-2.05	108.59	110.10
23	C	511	CLA	C3C-C4C-NC	-2.05	108.27	110.57
23	c	510	CLA	C16-C15-C13	-2.05	109.28	115.92
23	a	606	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
23	B	602	CLA	C6-C5-C3	-2.05	108.08	113.45
23	B	604	CLA	CHA-C4D-ND	2.05	136.79	132.50
23	A	607	CLA	O1D-CGD-CBD	2.05	128.68	124.48
23	B	606	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	c	501	CLA	C11-C10-C8	-2.05	109.30	115.92
31	A	617	DGD	C6D-C5D-C4D	2.05	116.37	112.09
23	c	513	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	c	511	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
31	c	516	DGD	C5B-C4B-C3B	-2.05	104.03	114.42
23	a	606	CLA	C2C-C1C-NC	2.05	111.89	109.97
23	h	101	CLA	O2A-CGA-CBA	2.05	118.33	111.91
29	a	615	SQD	C9-C8-C7	-2.05	106.18	113.62
28	B	620	LMG	C22-C21-C20	-2.05	104.04	114.42
23	C	502	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
31	C	517	DGD	O4D-C4D-C3D	2.04	115.07	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	518	DGD	CDB-CCB-CBB	-2.04	104.05	114.42
23	b	611	CLA	CMD-C2D-C1D	2.04	128.31	124.71
29	a	613	SQD	O10-C23-C24	-2.04	115.77	123.73
23	B	613	CLA	O1D-CGD-CBD	2.04	128.66	124.48
27	d	408	PL9	C36-C37-C38	-2.04	105.18	111.88
28	c	522	LMG	O5-C6-C5	-2.04	104.30	111.29
23	b	612	CLA	CMD-C2D-C3D	2.04	132.30	127.61
23	b	615	CLA	CHA-C1A-NA	-2.04	121.73	126.40
23	b	603	CLA	C7-C6-C5	-2.04	107.83	113.36
31	c	516	DGD	C3G-C2G-C1G	-2.04	106.97	111.79
31	C	516	DGD	O3D-C3D-C4D	-2.04	105.64	110.35
23	b	609	CLA	C1C-C2C-C3C	-2.04	104.82	106.96
30	D	406	LHG	C11-C10-C9	-2.04	104.09	114.42
25	A	608	BCR	C40-C30-C39	-2.03	102.28	108.53
23	b	605	CLA	CHC-C1C-NC	2.03	127.29	124.20
23	c	507	CLA	C3A-C2A-C1A	2.03	104.38	101.34
27	A	611	PL9	O1-C4-C3	-2.03	118.48	120.72
25	d	404	BCR	C30-C25-C26	-2.03	119.75	122.61
23	B	612	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
30	B	623	LHG	C18-C17-C16	-2.03	104.12	114.42
23	b	610	CLA	C11-C12-C13	-2.03	109.36	115.92
25	D	404	BCR	C38-C26-C25	-2.03	122.25	124.53
28	m	101	LMG	C19-C18-C17	-2.03	104.12	114.42
23	c	511	CLA	O1A-CGA-CBA	2.03	131.64	123.73
23	b	615	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
30	A	615	LHG	C27-C26-C25	-2.03	104.14	114.42
23	C	513	CLA	C2A-C1A-CHA	2.03	127.40	123.86
28	b	621	LMG	C42-C41-C40	-2.03	104.14	114.42
31	C	516	DGD	C9B-C8B-C7B	-2.03	104.14	114.42
23	c	511	CLA	C3B-C4B-NB	-2.03	106.59	109.21
23	C	507	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
23	c	504	CLA	CMC-C2C-C1C	2.02	128.12	125.04
31	c	518	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
23	C	505	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	a	606	CLA	C4-C3-C5	2.02	118.67	115.27
25	B	618	BCR	C15-C16-C17	-2.02	119.34	123.47
27	a	611	PL9	O2-C1-C2	-2.02	117.15	121.78
23	d	403	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
31	c	516	DGD	O6D-C1D-O3G	-2.02	105.19	109.97
23	B	603	CLA	C3C-C4C-NC	-2.02	108.31	110.57
28	C	519	LMG	O3-C3-C2	-2.02	105.68	110.35
29	B	624	SQD	O47-C45-C46	2.02	115.71	108.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	H	102	DGD	O4E-C4E-C5E	2.02	114.31	109.30
27	d	408	PL9	C12-C13-C14	-2.02	122.80	127.66
23	B	614	CLA	CAC-C3C-C4C	2.02	127.43	124.81
23	B	615	CLA	C7-C6-C5	-2.02	107.88	113.36
23	c	511	CLA	C2A-C1A-CHA	2.02	127.39	123.86
35	F	102	HEM	O2D-CGD-O1D	-2.02	118.27	123.30
30	d	409	LHG	O7-C7-O9	-2.02	118.83	123.70
23	C	504	CLA	CHD-C1D-C2D	2.01	129.70	125.48
23	D	402	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
23	a	604	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	C	510	CLA	CHD-C4C-NC	2.01	127.37	124.20
25	b	619	BCR	C16-C15-C14	-2.01	119.36	123.47
23	C	513	CLA	C6-C7-C8	-2.01	109.43	115.92
23	c	506	CLA	CHD-C4C-C3C	2.01	127.79	124.84
23	C	503	CLA	C4D-C3D-CAD	-2.01	105.73	108.10
23	c	512	CLA	CHA-C1A-NA	-2.01	121.80	126.40
23	c	506	CLA	CAC-C3C-C2C	-2.01	124.10	127.53
25	h	102	BCR	C15-C14-C13	-2.01	124.45	127.31
29	f	101	SQD	O47-C45-C46	2.01	115.67	108.40
30	L	101	LHG	C12-C11-C10	-2.01	104.24	114.42
23	B	611	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
28	d	406	LMG	O3-C3-C2	-2.01	105.71	110.35
23	A	603	CLA	CHD-C1D-ND	-2.00	122.61	124.45
30	B	623	LHG	O10-C23-C24	-2.00	115.91	123.73
23	b	612	CLA	C11-C10-C8	-2.00	109.44	115.92
23	B	607	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
28	B	620	LMG	C8-O7-C10	2.00	122.72	117.79
23	D	403	CLA	C3D-C4D-ND	2.00	113.48	110.24
25	t	101	BCR	C40-C30-C25	2.00	113.55	110.30
23	D	402	CLA	CAC-C3C-C2C	2.00	130.95	127.53
23	c	503	CLA	O2D-CGD-O1D	-2.00	119.93	123.84
23	B	616	CLA	C4D-CHA-C1A	2.00	123.68	121.25
23	B	611	CLA	C1-C2-C3	-2.00	122.58	126.04
31	c	518	DGD	CAB-C9B-C8B	-2.00	104.27	114.42

All (57) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	603	CLA	ND
23	A	607	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	B	603	CLA	ND
23	B	604	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	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	a	603	CLA	ND
23	a	606	CLA	ND
23	a	612	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	609	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	c	501	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	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	h	101	CLA	ND

All (1698) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	C11-C12-C13-C14
23	C	504	CLA	C2-C3-C5-C6
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	O2A-C1-C2-C3
23	a	604	CLA	CHA-CBD-CGD-O1D
23	b	603	CLA	C2-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	604	CLA	C6-C7-C8-C9
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CBD-CGD-O2D-CED
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	C2-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	CBD-CGD-O2D-CED
23	d	403	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	h	101	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	CAD-CBD-CGD-O1D
23	h	101	CLA	CAD-CBD-CGD-O2D
25	A	608	BCR	C7-C8-C9-C34
25	B	617	BCR	C1-C6-C7-C8
25	B	618	BCR	C7-C8-C9-C34
25	B	619	BCR	C11-C12-C13-C35
25	B	619	BCR	C35-C13-C14-C15
25	C	514	BCR	C7-C8-C9-C34
25	C	514	BCR	C11-C12-C13-C35
25	C	514	BCR	C16-C17-C18-C19
25	C	514	BCR	C16-C17-C18-C36
25	C	515	BCR	C7-C8-C9-C34
25	C	515	BCR	C21-C22-C23-C24
25	C	515	BCR	C37-C22-C23-C24
25	C	520	BCR	C7-C8-C9-C10
25	C	520	BCR	C7-C8-C9-C34
25	C	520	BCR	C20-C21-C22-C37
25	D	404	BCR	C16-C17-C18-C36
25	D	404	BCR	C22-C23-C24-C25
25	D	404	BCR	C23-C24-C25-C26
25	H	101	BCR	C11-C12-C13-C14
25	H	101	BCR	C11-C12-C13-C35
25	T	101	BCR	C11-C12-C13-C14
25	Y	101	BCR	C5-C6-C7-C8
25	Y	101	BCR	C11-C10-C9-C34
25	Y	101	BCR	C20-C21-C22-C37
25	Y	101	BCR	C37-C22-C23-C24
25	b	619	BCR	C11-C12-C13-C14
25	b	619	BCR	C11-C12-C13-C35
25	c	514	BCR	C7-C8-C9-C10
25	c	514	BCR	C11-C10-C9-C34
25	c	514	BCR	C11-C12-C13-C14
25	c	514	BCR	C11-C12-C13-C35
25	c	514	BCR	C13-C14-C15-C16
25	c	514	BCR	C15-C16-C17-C18
25	c	514	BCR	C18-C19-C20-C21
25	c	515	BCR	C21-C22-C23-C24
25	c	515	BCR	C37-C22-C23-C24
25	h	102	BCR	C7-C8-C9-C34
25	h	102	BCR	C20-C21-C22-C37
25	k	101	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	k	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C37-C22-C23-C24
25	t	101	BCR	C11-C10-C9-C34
25	t	101	BCR	C10-C11-C12-C13
25	t	101	BCR	C17-C18-C19-C20
25	t	101	BCR	C36-C18-C19-C20
25	t	101	BCR	C20-C21-C22-C37
25	t	101	BCR	C37-C22-C23-C24
27	A	611	PL9	C11-C12-C13-C14
27	A	611	PL9	C12-C13-C14-C15
27	A	611	PL9	C12-C13-C14-C16
27	A	611	PL9	C15-C14-C16-C17
27	A	611	PL9	C17-C18-C19-C20
27	A	611	PL9	C17-C18-C19-C21
27	A	611	PL9	C22-C23-C24-C25
27	A	611	PL9	C22-C23-C24-C26
27	A	611	PL9	C32-C33-C34-C36
27	A	611	PL9	C37-C38-C39-C40
27	A	611	PL9	C37-C38-C39-C41
27	D	407	PL9	C32-C33-C34-C36
27	D	407	PL9	C47-C48-C49-C51
27	a	611	PL9	C16-C17-C18-C19
27	a	611	PL9	C17-C18-C19-C21
27	a	611	PL9	C22-C23-C24-C25
27	a	611	PL9	C22-C23-C24-C26
27	a	611	PL9	C24-C26-C27-C28
27	a	611	PL9	C32-C33-C34-C35
27	a	611	PL9	C35-C34-C36-C37
27	a	611	PL9	C34-C36-C37-C38
27	a	611	PL9	C42-C43-C44-C46
27	d	408	PL9	C12-C13-C14-C15
27	d	408	PL9	C32-C33-C34-C35
27	d	408	PL9	C32-C33-C34-C36
27	d	408	PL9	C37-C38-C39-C41
27	d	408	PL9	C40-C39-C41-C42
27	d	408	PL9	C42-C43-C44-C46
27	d	408	PL9	C47-C48-C49-C51
28	A	612	LMG	O9-C10-O7-C8
28	A	612	LMG	C11-C10-O7-C8
28	C	519	LMG	C11-C10-O7-C8
28	D	409	LMG	O1-C7-C8-C9
28	D	409	LMG	O1-C7-C8-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	409	LMG	C11-C10-O7-C8
28	b	621	LMG	O9-C10-O7-C8
28	c	519	LMG	C11-C10-O7-C8
28	c	522	LMG	O6-C1-O1-C7
28	c	522	LMG	O10-C28-O8-C9
28	c	522	LMG	C29-C28-O8-C9
29	A	616	SQD	C44-C45-C46-O48
29	A	616	SQD	C46-C45-O47-C7
29	B	624	SQD	C2-C1-O6-C44
29	B	624	SQD	O5-C1-O6-C44
29	B	624	SQD	O6-C44-C45-O47
29	B	624	SQD	O49-C7-O47-C45
29	B	624	SQD	C8-C7-O47-C45
29	F	101	SQD	C45-C44-O6-C1
29	a	613	SQD	O47-C45-C46-O48
29	a	613	SQD	C5-C6-S-O8
29	b	601	SQD	C8-C7-O47-C45
29	b	601	SQD	C24-C23-O48-C46
29	f	101	SQD	O5-C1-O6-C44
30	A	615	LHG	O10-C23-O8-C6
30	B	623	LHG	O1-C1-C2-C3
30	B	623	LHG	C3-O3-P-O4
30	D	406	LHG	O1-C1-C2-C3
30	D	406	LHG	C3-O3-P-O5
30	D	406	LHG	C4-O6-P-O4
30	D	408	LHG	C3-O3-P-O5
30	D	408	LHG	C3-O3-P-O6
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O4
30	a	614	LHG	C3-O3-P-O5
30	a	614	LHG	C4-O6-P-O5
30	a	614	LHG	O10-C23-O8-C6
30	d	405	LHG	O1-C1-C2-C3
30	d	407	LHG	O1-C1-C2-C3
30	d	407	LHG	C4-O6-P-O4
30	l	101	LHG	C4-O6-P-O3
30	l	101	LHG	C4-O6-P-O4
30	l	101	LHG	C4-O6-P-O5
31	A	617	DGD	O1B-C1B-O2G-C2G
31	A	617	DGD	O2G-C2G-C3G-O3G
31	a	616	DGD	C2A-C1A-O1G-C1G
31	a	616	DGD	O1A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	a	616	DGD	O1G-C1G-C2G-O2G
23	c	513	CLA	O1D-CGD-O2D-CED
23	h	101	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	CBD-CGD-O2D-CED
29	b	601	SQD	O10-C23-O48-C46
23	B	604	CLA	C13-C15-C16-C17
23	B	601	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
30	A	615	LHG	C24-C23-O8-C6
30	a	614	LHG	C24-C23-O8-C6
27	d	408	PL9	C47-C48-C49-C50
23	C	508	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	CBD-CGD-O2D-CED
23	b	614	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	d	403	CLA	CBD-CGD-O2D-CED
29	a	615	SQD	O10-C23-O48-C46
23	B	607	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED
28	D	409	LMG	O9-C10-O7-C8
29	a	615	SQD	O49-C7-O47-C45
31	a	616	DGD	O1B-C1B-O2G-C2G
23	C	506	CLA	C3-C5-C6-C7
23	b	602	CLA	C3-C5-C6-C7
23	h	101	CLA	C3-C5-C6-C7
28	b	621	LMG	C11-C10-O7-C8
29	a	615	SQD	C8-C7-O47-C45
31	A	617	DGD	C2B-C1B-O2G-C2G
27	D	407	PL9	C47-C48-C49-C50
23	C	504	CLA	C4-C3-C5-C6
27	A	611	PL9	C23-C24-C26-C27
23	B	606	CLA	C2A-CAA-CBA-CGA
23	h	101	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C3-C5-C6-C7
23	B	616	CLA	CBA-CGA-O2A-C1
29	f	101	SQD	C24-C23-O48-C46
27	a	611	PL9	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	d	408	PL9	C37-C38-C39-C40
23	c	511	CLA	CBD-CGD-O2D-CED
23	d	403	CLA	O1D-CGD-O2D-CED
28	B	620	LMG	O6-C5-C6-O5
27	a	611	PL9	C27-C28-C29-C31
27	a	611	PL9	C32-C33-C34-C36
28	c	521	LMG	C4-C5-C6-O5
28	A	612	LMG	O10-C28-O8-C9
28	c	521	LMG	O10-C28-O8-C9
29	F	101	SQD	O10-C23-O48-C46
29	a	613	SQD	O10-C23-O48-C46
31	h	103	DGD	O6E-C5E-C6E-O5E
30	D	408	LHG	O2-C2-C3-O3
23	B	601	CLA	CBA-CGA-O2A-C1
31	c	518	DGD	O1A-C1A-O1G-C1G
28	B	620	LMG	C4-C5-C6-O5
28	c	522	LMG	C4-C5-C6-O5
23	c	509	CLA	C13-C15-C16-C17
27	A	611	PL9	C47-C48-C49-C50
29	a	613	SQD	C24-C23-O48-C46
29	a	615	SQD	C24-C23-O48-C46
23	B	616	CLA	O1A-CGA-O2A-C1
28	B	620	LMG	O10-C28-O8-C9
23	A	607	CLA	C4-C3-C5-C6
27	A	611	PL9	C20-C19-C21-C22
27	A	611	PL9	C40-C39-C41-C42
23	A	607	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
27	A	611	PL9	C13-C14-C16-C17
27	A	611	PL9	C18-C19-C21-C22
27	a	611	PL9	C28-C29-C31-C32
27	a	611	PL9	C33-C34-C36-C37
27	d	408	PL9	C38-C39-C41-C42
28	c	521	LMG	O6-C5-C6-O5
28	c	522	LMG	O6-C5-C6-O5
23	B	601	CLA	O1A-CGA-O2A-C1
27	A	611	PL9	C24-C26-C27-C28
27	A	611	PL9	C44-C46-C47-C48
27	a	611	PL9	C14-C16-C17-C18
27	a	611	PL9	C19-C21-C22-C23
27	d	408	PL9	C9-C11-C12-C13
28	C	519	LMG	C29-C28-O8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	O1D-CGD-O2D-CED
23	C	508	CLA	O1D-CGD-O2D-CED
23	C	512	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
28	A	612	LMG	C29-C28-O8-C9
28	c	521	LMG	C29-C28-O8-C9
29	F	101	SQD	C24-C23-O48-C46
23	c	504	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	C15-C16-C17-C18
23	b	613	CLA	O1D-CGD-O2D-CED
29	B	624	SQD	C29-C30-C31-C32
31	h	103	DGD	C4E-C5E-C6E-O5E
23	B	611	CLA	C13-C15-C16-C17
23	C	513	CLA	C13-C15-C16-C17
30	D	406	LHG	O2-C2-C3-O3
28	c	522	LMG	C2-C1-O1-C7
29	f	101	SQD	C2-C1-O6-C44
29	A	614	SQD	O6-C44-C45-O47
29	a	613	SQD	O6-C44-C45-O47
29	a	613	SQD	C12-C13-C14-C15
23	B	605	CLA	C11-C10-C8-C9
23	B	614	CLA	C14-C13-C15-C16
23	C	507	CLA	C11-C10-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	D	402	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C12-C13-C14
23	b	613	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
23	c	511	CLA	C14-C13-C15-C16
24	A	605	PHO	C14-C13-C15-C16
25	c	514	BCR	C36-C18-C19-C20
25	d	404	BCR	C37-C22-C23-C24
28	A	612	LMG	C4-C5-C6-O5
29	A	614	SQD	C7-C8-C9-C10
29	B	624	SQD	C23-C24-C25-C26
30	d	405	LHG	C23-C24-C25-C26
23	b	606	CLA	C15-C16-C17-C18
23	b	604	CLA	C3-C5-C6-C7
28	m	101	LMG	C29-C28-O8-C9
23	B	607	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C8-C10-C11-C12
23	C	512	CLA	C10-C11-C12-C13
23	c	506	CLA	C10-C11-C12-C13
28	c	519	LMG	O6-C5-C6-O5
29	F	101	SQD	C23-C24-C25-C26
31	a	616	DGD	C1A-C2A-C3A-C4A
23	C	501	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	C5-C6-C7-C8
23	C	505	CLA	C5-C6-C7-C8
23	b	607	CLA	C10-C11-C12-C13
23	b	608	CLA	C13-C15-C16-C17
23	b	614	CLA	C8-C10-C11-C12
23	c	510	CLA	C15-C16-C17-C18
27	d	408	PL9	C27-C28-C29-C30
28	D	409	LMG	C10-C11-C12-C13
28	c	522	LMG	C28-C29-C30-C31
28	d	406	LMG	C28-C29-C30-C31
30	a	614	LHG	C7-C8-C9-C10
31	C	517	DGD	C1B-C2B-C3B-C4B
31	c	518	DGD	C1A-C2A-C3A-C4A
23	B	605	CLA	C10-C11-C12-C13
23	B	612	CLA	C10-C11-C12-C13
23	C	511	CLA	C8-C10-C11-C12
23	b	614	CLA	C15-C16-C17-C18
23	c	506	CLA	CBA-CGA-O2A-C1
28	B	620	LMG	C29-C28-O8-C9
30	A	615	LHG	O9-C7-O7-C5
23	B	604	CLA	C10-C11-C12-C13
23	a	606	CLA	C10-C11-C12-C13
23	a	606	CLA	C13-C15-C16-C17
23	c	513	CLA	C5-C6-C7-C8
30	D	408	LHG	C7-C8-C9-C10
23	b	614	CLA	C5-C6-C7-C8
31	C	517	DGD	O6E-C5E-C6E-O5E
23	B	614	CLA	O1D-CGD-O2D-CED
23	b	602	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	B	605	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
23	c	505	CLA	C15-C16-C17-C18
23	c	507	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	512	CLA	C5-C6-C7-C8
23	b	609	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
28	A	612	LMG	O6-C1-O1-C7
27	A	611	PL9	C9-C11-C12-C13
27	A	611	PL9	C34-C36-C37-C38
27	d	408	PL9	C44-C46-C47-C48
28	B	622	LMG	C28-C29-C30-C31
30	A	615	LHG	C7-C8-C9-C10
25	B	619	BCR	C10-C11-C12-C13
25	C	514	BCR	C18-C19-C20-C21
25	C	520	BCR	C18-C19-C20-C21
25	d	404	BCR	C10-C11-C12-C13
30	d	405	LHG	O2-C2-C3-O3
23	b	611	CLA	C8-C10-C11-C12
23	c	504	CLA	C5-C6-C7-C8
23	c	506	CLA	C5-C6-C7-C8
23	h	101	CLA	C8-C10-C11-C12
29	f	101	SQD	O10-C23-O48-C46
31	C	518	DGD	O1A-C1A-O1G-C1G
23	B	612	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
23	c	506	CLA	C13-C15-C16-C17
23	A	603	CLA	C15-C16-C17-C18
23	B	607	CLA	C13-C15-C16-C17
23	a	603	CLA	C15-C16-C17-C18
23	a	604	CLA	C8-C10-C11-C12
23	b	607	CLA	C5-C6-C7-C8
23	b	616	CLA	C10-C11-C12-C13
23	c	503	CLA	C8-C10-C11-C12
30	D	406	LHG	C3-O3-P-O6
30	L	101	LHG	C4-O6-P-O3
30	a	614	LHG	C4-O6-P-O3
30	d	405	LHG	C3-O3-P-O6
30	d	407	LHG	C4-O6-P-O3
28	c	519	LMG	O9-C10-O7-C8
23	c	512	CLA	C13-C15-C16-C17
23	B	607	CLA	O1D-CGD-O2D-CED
29	f	101	SQD	O49-C7-O47-C45
27	a	611	PL9	C30-C29-C31-C32
27	A	611	PL9	C43-C44-C46-C47
23	B	611	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	504	CLA	C8-C10-C11-C12
23	C	507	CLA	C10-C11-C12-C13
23	b	606	CLA	C2A-CAA-CBA-CGA
29	B	624	SQD	C24-C23-O48-C46
29	b	601	SQD	C11-C10-C9-C8
30	A	615	LHG	C27-C28-C29-C30
25	c	514	BCR	C9-C10-C11-C12
30	a	614	LHG	C23-C24-C25-C26
29	a	613	SQD	C24-C25-C26-C27
30	B	623	LHG	C14-C15-C16-C17
23	a	606	CLA	C5-C6-C7-C8
25	A	608	BCR	C20-C21-C22-C37
25	B	617	BCR	C16-C17-C18-C36
25	B	618	BCR	C20-C21-C22-C37
25	B	619	BCR	C11-C10-C9-C34
25	C	514	BCR	C20-C21-C22-C37
25	C	520	BCR	C11-C10-C9-C34
25	D	404	BCR	C20-C21-C22-C37
25	T	101	BCR	C11-C10-C9-C34
25	T	101	BCR	C20-C21-C22-C37
25	Y	101	BCR	C35-C13-C14-C15
25	a	607	BCR	C35-C13-C14-C15
25	a	607	BCR	C16-C17-C18-C36
25	b	618	BCR	C16-C17-C18-C36
25	b	619	BCR	C16-C17-C18-C36
25	c	514	BCR	C16-C17-C18-C36
25	d	404	BCR	C35-C13-C14-C15
25	h	102	BCR	C16-C17-C18-C36
25	k	101	BCR	C35-C13-C14-C15
25	k	101	BCR	C20-C21-C22-C37
25	k	102	BCR	C35-C13-C14-C15
25	k	102	BCR	C20-C21-C22-C37
25	t	101	BCR	C16-C17-C18-C36
23	C	512	CLA	C3-C5-C6-C7
23	b	612	CLA	C3-C5-C6-C7
28	A	612	LMG	C16-C17-C18-C19
28	B	620	LMG	C13-C14-C15-C16
28	C	519	LMG	C11-C12-C13-C14
28	D	405	LMG	C30-C31-C32-C33
28	b	621	LMG	C16-C17-C18-C19
28	c	521	LMG	C41-C42-C43-C44
28	c	522	LMG	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	615	SQD	C12-C13-C14-C15
30	B	623	LHG	C29-C30-C31-C32
30	d	405	LHG	C30-C31-C32-C33
30	d	407	LHG	C34-C35-C36-C37
30	d	409	LHG	C30-C31-C32-C33
31	A	617	DGD	C5B-C6B-C7B-C8B
23	B	610	CLA	C16-C17-C18-C20
23	C	502	CLA	C16-C17-C18-C19
28	B	622	LMG	C16-C17-C18-C19
28	c	521	LMG	C32-C33-C34-C35
28	c	522	LMG	C35-C36-C37-C38
29	B	624	SQD	C11-C12-C13-C14
30	A	615	LHG	C28-C29-C30-C31
30	d	405	LHG	C10-C11-C12-C13
30	l	101	LHG	C16-C17-C18-C19
31	c	516	DGD	C9A-CAA-CBA-CCA
28	D	409	LMG	C9-C8-O7-C10
29	b	601	SQD	C46-C45-O47-C7
28	c	521	LMG	O9-C10-O7-C8
23	b	611	CLA	C13-C15-C16-C17
29	A	614	SQD	C23-C24-C25-C26
28	c	521	LMG	C11-C12-C13-C14
29	A	616	SQD	C14-C15-C16-C17
29	f	101	SQD	C28-C29-C30-C31
31	A	617	DGD	C9B-CAB-CBB-CCB
31	c	518	DGD	C9A-CAA-CBA-CCA
28	B	620	LMG	C16-C17-C18-C19
28	B	622	LMG	C14-C15-C16-C17
30	a	614	LHG	C13-C14-C15-C16
30	a	614	LHG	C17-C18-C19-C20
30	d	407	LHG	C33-C34-C35-C36
30	l	101	LHG	C28-C29-C30-C31
31	C	517	DGD	C5A-C6A-C7A-C8A
31	c	518	DGD	CCA-CDA-CEA-CFA
23	c	511	CLA	O1D-CGD-O2D-CED
28	A	612	LMG	C30-C31-C32-C33
29	F	101	SQD	C27-C28-C29-C30
29	a	613	SQD	C34-C35-C36-C37
30	L	101	LHG	C31-C32-C33-C34
30	d	405	LHG	C32-C33-C34-C35
30	l	101	LHG	C9-C10-C11-C12
31	A	617	DGD	C2B-C3B-C4B-C5B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	619	BCR	C11-C10-C9-C8
25	C	520	BCR	C20-C21-C22-C23
25	H	101	BCR	C11-C10-C9-C8
25	Y	101	BCR	C11-C10-C9-C8
25	Y	101	BCR	C12-C13-C14-C15
25	h	102	BCR	C11-C10-C9-C8
25	h	102	BCR	C20-C21-C22-C23
25	k	101	BCR	C11-C10-C9-C8
31	C	517	DGD	C2E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
28	B	622	LMG	C29-C30-C31-C32
28	b	621	LMG	C34-C35-C36-C37
28	c	519	LMG	C36-C37-C38-C39
28	d	410	LMG	C31-C32-C33-C34
29	A	614	SQD	C31-C32-C33-C34
29	f	101	SQD	C32-C33-C34-C35
30	B	623	LHG	C25-C26-C27-C28
30	d	407	LHG	C31-C32-C33-C34
31	A	617	DGD	C4A-C5A-C6A-C7A
31	C	517	DGD	CCB-CDB-CEB-CFB
31	H	102	DGD	C3B-C4B-C5B-C6B
23	c	503	CLA	C5-C6-C7-C8
23	c	506	CLA	O1A-CGA-O2A-C1
23	A	604	CLA	C16-C17-C18-C19
28	A	612	LMG	O6-C5-C6-O5
23	c	512	CLA	C4-C3-C5-C6
27	A	611	PL9	C42-C43-C44-C45
27	D	407	PL9	C7-C8-C9-C10
28	B	620	LMG	C36-C37-C38-C39
28	b	621	LMG	C11-C12-C13-C14
28	c	522	LMG	C12-C13-C14-C15
29	A	614	SQD	C30-C31-C32-C33
29	f	101	SQD	C31-C32-C33-C34
30	D	408	LHG	C11-C12-C13-C14
30	D	408	LHG	C27-C28-C29-C30
31	c	517	DGD	C6A-C7A-C8A-C9A
23	B	611	CLA	C11-C12-C13-C14
23	C	513	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	a	604	CLA	C6-C7-C8-C9
23	h	101	CLA	C11-C10-C8-C9
28	D	405	LMG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	522	LMG	C29-C30-C31-C32
28	d	410	LMG	C11-C12-C13-C14
29	A	616	SQD	C28-C29-C30-C31
29	F	101	SQD	C33-C34-C35-C36
29	F	101	SQD	C34-C35-C36-C37
30	d	409	LHG	C26-C27-C28-C29
30	l	101	LHG	C14-C15-C16-C17
30	l	101	LHG	C24-C25-C26-C27
31	C	518	DGD	C2A-C3A-C4A-C5A
31	c	518	DGD	C8A-C9A-CAA-CBA
31	h	103	DGD	C5B-C6B-C7B-C8B
23	B	613	CLA	C8-C10-C11-C12
23	c	512	CLA	C2A-CAA-CBA-CGA
25	c	514	BCR	C7-C8-C9-C34
28	D	405	LMG	C18-C19-C20-C21
28	c	522	LMG	C34-C35-C36-C37
28	d	406	LMG	C13-C14-C15-C16
31	A	617	DGD	C8B-C9B-CAB-CBB
31	A	617	DGD	CDB-CEB-CFB-CGB
30	d	409	LHG	O1-C1-C2-C3
23	C	509	CLA	C10-C11-C12-C13
31	a	616	DGD	C2B-C1B-O2G-C2G
28	c	522	LMG	C11-C12-C13-C14
29	A	614	SQD	C32-C33-C34-C35
29	B	624	SQD	C9-C10-C11-C12
29	a	613	SQD	C26-C27-C28-C29
29	f	101	SQD	C24-C25-C26-C27
30	a	614	LHG	C16-C17-C18-C19
30	d	405	LHG	C7-C8-C9-C10
28	D	405	LMG	C17-C18-C19-C20
28	D	405	LMG	C20-C21-C22-C23
28	D	405	LMG	C39-C40-C41-C42
28	b	621	LMG	C18-C19-C20-C21
28	c	521	LMG	C15-C16-C17-C18
29	A	616	SQD	C26-C27-C28-C29
29	a	615	SQD	C10-C11-C12-C13
30	d	407	LHG	C11-C12-C13-C14
31	A	617	DGD	CBA-CCA-CDA-CEA
31	C	517	DGD	C6B-C7B-C8B-C9B
31	a	616	DGD	C2A-C3A-C4A-C5A
23	A	604	CLA	C16-C17-C18-C20
23	C	502	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C16-C17-C18-C19
23	b	609	CLA	C16-C17-C18-C19
23	b	609	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
31	C	517	DGD	O6E-C1E-O5D-C6D
31	c	517	DGD	O6E-C1E-O5D-C6D
28	C	519	LMG	C32-C33-C34-C35
28	b	621	LMG	C31-C32-C33-C34
28	c	522	LMG	C19-C20-C21-C22
29	A	616	SQD	C12-C13-C14-C15
30	D	406	LHG	C11-C10-C9-C8
31	C	517	DGD	C7A-C8A-C9A-CAA
31	h	103	DGD	C2B-C3B-C4B-C5B
28	c	521	LMG	C34-C35-C36-C37
31	C	517	DGD	CAA-CBA-CCA-CDA
31	H	102	DGD	CBB-CCB-CDB-CEB
31	c	516	DGD	C5B-C6B-C7B-C8B
28	m	101	LMG	C10-C11-C12-C13
23	B	614	CLA	C8-C10-C11-C12
28	B	620	LMG	C39-C40-C41-C42
31	c	516	DGD	C4B-C5B-C6B-C7B
29	f	101	SQD	C33-C34-C35-C36
30	A	615	LHG	C16-C17-C18-C19
31	C	518	DGD	CAA-CBA-CCA-CDA
31	h	103	DGD	C9A-CAA-CBA-CCA
23	c	504	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
23	C	513	CLA	C10-C11-C12-C13
27	A	611	PL9	C47-C48-C49-C51
28	c	521	LMG	C38-C39-C40-C41
28	d	410	LMG	C38-C39-C40-C41
29	A	614	SQD	C14-C15-C16-C17
31	C	516	DGD	CBA-CCA-CDA-CEA
31	c	516	DGD	C8B-C9B-CAB-CBB
28	D	409	LMG	C14-C15-C16-C17
29	F	101	SQD	C25-C26-C27-C28
30	a	614	LHG	C14-C15-C16-C17
23	B	603	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	C2C-C3C-CAC-CBC
30	d	405	LHG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	C	518	DGD	C9A-CAA-CBA-CCA
31	c	516	DGD	O6D-C5D-C6D-O5D
25	T	101	BCR	C14-C15-C16-C17
28	c	519	LMG	C29-C28-O8-C9
23	c	512	CLA	C2-C3-C5-C6
30	a	614	LHG	C8-C7-O7-C5
28	b	621	LMG	C37-C38-C39-C40
31	a	616	DGD	C5B-C6B-C7B-C8B
30	B	623	LHG	O1-C1-C2-O2
28	d	406	LMG	C34-C35-C36-C37
29	A	614	SQD	C11-C10-C9-C8
29	A	614	SQD	C28-C29-C30-C31
30	d	405	LHG	C24-C25-C26-C27
31	a	616	DGD	CEA-CFA-CGA-CHA
31	c	516	DGD	CCB-CDB-CEB-CFB
30	a	614	LHG	C26-C27-C28-C29
31	C	518	DGD	C6A-C7A-C8A-C9A
31	h	103	DGD	CAB-CBB-CCB-CDB
28	D	405	LMG	C37-C38-C39-C40
30	A	615	LHG	C11-C10-C9-C8
31	C	517	DGD	C6A-C7A-C8A-C9A
29	b	601	SQD	O49-C7-O47-C45
23	B	616	CLA	C2-C1-O2A-CGA
23	b	616	CLA	C2-C1-O2A-CGA
23	c	507	CLA	C2-C1-O2A-CGA
28	c	521	LMG	C40-C41-C42-C43
28	d	410	LMG	C36-C37-C38-C39
30	D	408	LHG	C32-C33-C34-C35
30	d	409	LHG	C27-C28-C29-C30
31	C	516	DGD	C9A-CAA-CBA-CCA
31	c	516	DGD	C4D-C5D-C6D-O5D
30	L	101	LHG	O10-C23-O8-C6
28	A	612	LMG	C14-C15-C16-C17
28	m	101	LMG	C17-C18-C19-C20
30	L	101	LHG	C18-C19-C20-C21
31	a	616	DGD	C4A-C5A-C6A-C7A
31	a	616	DGD	CDA-CEA-CFA-CGA
31	c	517	DGD	C7B-C8B-C9B-CAB
31	c	518	DGD	C3A-C4A-C5A-C6A
31	h	103	DGD	C7B-C8B-C9B-CAB
31	C	516	DGD	C1B-C2B-C3B-C4B
25	B	617	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	515	BCR	C5-C6-C7-C8
25	D	404	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	c	514	BCR	C5-C6-C7-C8
25	h	102	BCR	C23-C24-C25-C26
25	h	102	BCR	C23-C24-C25-C30
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
30	L	101	LHG	C12-C13-C14-C15
23	B	602	CLA	C13-C15-C16-C17
23	D	403	CLA	C15-C16-C17-C18
23	c	509	CLA	C10-C11-C12-C13
28	c	521	LMG	C10-C11-C12-C13
28	m	101	LMG	C28-C29-C30-C31
28	d	410	LMG	C32-C33-C34-C35
29	A	614	SQD	C10-C11-C12-C13
31	a	616	DGD	C5A-C6A-C7A-C8A
27	a	611	PL9	C47-C48-C49-C50
23	B	610	CLA	C8-C10-C11-C12
23	b	603	CLA	C5-C6-C7-C8
23	b	615	CLA	C8-C10-C11-C12
28	D	409	LMG	C16-C17-C18-C19
28	D	409	LMG	C34-C35-C36-C37
23	C	506	CLA	C4-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
23	C	506	CLA	C12-C13-C15-C16
23	C	511	CLA	C6-C7-C8-C10
23	C	513	CLA	C11-C10-C8-C7
23	D	403	CLA	C11-C10-C8-C7
23	a	604	CLA	C6-C7-C8-C10
23	a	606	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C12-C13-C15
23	b	612	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
27	D	407	PL9	C28-C29-C31-C32
27	a	611	PL9	C38-C39-C41-C42
28	c	519	LMG	C39-C40-C41-C42
31	c	517	DGD	CAB-CBB-CCB-CDB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C8-C10-C11-C12
23	h	101	CLA	C15-C16-C17-C18
23	c	507	CLA	C16-C17-C18-C20
28	C	519	LMG	O9-C10-O7-C8
29	A	616	SQD	O49-C7-O47-C45
31	C	516	DGD	C5B-C6B-C7B-C8B
23	d	403	CLA	C15-C16-C17-C18
28	b	621	LMG	C39-C40-C41-C42
31	c	518	DGD	C5B-C6B-C7B-C8B
23	C	503	CLA	C5-C6-C7-C8
23	C	506	CLA	C15-C16-C17-C18
28	m	101	LMG	C19-C20-C21-C22
29	a	613	SQD	C30-C31-C32-C33
30	a	614	LHG	C11-C10-C9-C8
31	a	616	DGD	CBA-CCA-CDA-CEA
29	a	615	SQD	C18-C19-C20-C21
30	l	101	LHG	C32-C33-C34-C35
31	c	516	DGD	C4A-C5A-C6A-C7A
23	D	403	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	CBD-CGD-O2D-CED
31	c	518	DGD	C2A-C1A-O1G-C1G
23	B	603	CLA	C16-C17-C18-C20
23	c	506	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C19
30	D	406	LHG	C25-C26-C27-C28
30	L	101	LHG	C11-C12-C13-C14
28	c	521	LMG	C11-C10-O7-C8
29	f	101	SQD	C8-C7-O47-C45
30	A	615	LHG	C8-C7-O7-C5
25	c	514	BCR	C10-C11-C12-C13
25	h	102	BCR	C14-C15-C16-C17
29	A	614	SQD	C24-C25-C26-C27
29	a	615	SQD	C11-C12-C13-C14
28	c	519	LMG	C35-C36-C37-C38
23	B	603	CLA	C10-C11-C12-C13
23	h	101	CLA	C10-C11-C12-C13
29	b	601	SQD	O47-C45-C46-O48
28	D	405	LMG	C11-C12-C13-C14
28	D	405	LMG	C33-C34-C35-C36
29	a	615	SQD	C11-C10-C9-C8
27	a	611	PL9	C15-C14-C16-C17
27	d	408	PL9	C15-C14-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	616	SQD	C7-C8-C9-C10
23	b	614	CLA	C2-C3-C5-C6
28	d	410	LMG	C37-C38-C39-C40
31	C	518	DGD	CBA-CCA-CDA-CEA
23	C	511	CLA	C6-C7-C8-C9
23	b	602	CLA	C6-C7-C8-C9
23	b	605	CLA	C11-C12-C13-C14
23	b	606	CLA	C6-C7-C8-C9
23	b	607	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	612	CLA	C6-C7-C8-C9
23	b	612	CLA	C14-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	c	508	CLA	C14-C13-C15-C16
24	A	606	PHO	C6-C7-C8-C9
28	c	521	LMG	C36-C37-C38-C39
29	a	613	SQD	C18-C19-C20-C21
31	h	103	DGD	CBA-CCA-CDA-CEA
23	b	606	CLA	C10-C11-C12-C13
28	C	519	LMG	O10-C28-O8-C9
23	a	606	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C16-C17-C18-C19
23	C	509	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C20
30	a	614	LHG	O9-C7-O7-C5
31	c	516	DGD	O1B-C1B-O2G-C2G
28	d	406	LMG	C35-C36-C37-C38
30	L	101	LHG	C27-C28-C29-C30
23	B	606	CLA	C15-C16-C17-C18
28	c	519	LMG	C33-C34-C35-C36
29	f	101	SQD	C30-C31-C32-C33
31	C	517	DGD	C8B-C9B-CAB-CBB
23	B	601	CLA	C3-C5-C6-C7
23	B	613	CLA	C13-C15-C16-C17
23	c	512	CLA	CBA-CGA-O2A-C1
28	c	522	LMG	C16-C17-C18-C19
28	b	621	LMG	O6-C5-C6-O5
23	c	510	CLA	C16-C17-C18-C19
28	m	101	LMG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	B	624	SQD	C34-C35-C36-C37
29	a	613	SQD	C16-C17-C18-C19
30	B	623	LHG	C24-C25-C26-C27
31	A	617	DGD	C6B-C7B-C8B-C9B
30	d	407	LHG	C14-C15-C16-C17
30	d	405	LHG	C1-C2-C3-O3
23	B	614	CLA	C4-C3-C5-C6
27	d	408	PL9	C43-C44-C46-C47
28	D	405	LMG	C35-C36-C37-C38
28	d	406	LMG	C14-C15-C16-C17
29	a	613	SQD	C11-C10-C9-C8
30	D	408	LHG	C25-C26-C27-C28
23	b	610	CLA	C15-C16-C17-C18
28	A	612	LMG	C12-C13-C14-C15
28	B	620	LMG	C15-C16-C17-C18
28	B	622	LMG	C11-C12-C13-C14
30	d	405	LHG	C25-C26-C27-C28
30	A	615	LHG	C15-C16-C17-C18
30	B	623	LHG	C12-C13-C14-C15
23	B	615	CLA	C16-C17-C18-C20
28	D	405	LMG	O6-C5-C6-O5
28	d	406	LMG	O6-C5-C6-O5
28	D	409	LMG	C7-C8-C9-O8
29	B	624	SQD	O6-C44-C45-C46
29	a	613	SQD	C44-C45-C46-O48
29	a	615	SQD	C13-C14-C15-C16
31	A	617	DGD	C1G-C2G-C3G-O3G
31	H	102	DGD	CBA-CCA-CDA-CEA
31	c	516	DGD	O1G-C1G-C2G-C3G
30	A	615	LHG	C33-C34-C35-C36
31	c	516	DGD	CAB-CBB-CCB-CDB
31	C	517	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C2G-C3G-O3G-C1D
31	c	517	DGD	C5D-C6D-O5D-C1E
28	C	519	LMG	C29-C30-C31-C32
30	D	406	LHG	C30-C31-C32-C33
30	d	409	LHG	C29-C30-C31-C32
28	D	409	LMG	C15-C16-C17-C18
31	H	102	DGD	C9B-CAB-CBB-CCB
31	H	102	DGD	CDB-CEB-CFB-CGB
28	D	409	LMG	C28-C29-C30-C31
31	A	617	DGD	C1A-C2A-C3A-C4A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	512	CLA	O1A-CGA-O2A-C1
30	d	405	LHG	O10-C23-O8-C6
28	c	521	LMG	C13-C14-C15-C16
29	B	624	SQD	C13-C14-C15-C16
30	D	406	LHG	C15-C16-C17-C18
31	c	517	DGD	CAA-CBA-CCA-CDA
23	C	504	CLA	C11-C12-C13-C14
23	c	508	CLA	C16-C17-C18-C19
30	d	405	LHG	C27-C28-C29-C30
30	d	405	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
31	c	516	DGD	C3B-C4B-C5B-C6B
30	A	615	LHG	C24-C25-C26-C27
25	T	101	BCR	C35-C13-C14-C15
31	c	516	DGD	O6E-C5E-C6E-O5E
23	C	505	CLA	C4-C3-C5-C6
29	B	624	SQD	C35-C36-C37-C38
30	A	615	LHG	C31-C32-C33-C34
31	h	103	DGD	CDA-CEA-CFA-CGA
23	B	614	CLA	C2-C3-C5-C6
30	d	409	LHG	C24-C23-O8-C6
23	B	610	CLA	C15-C16-C17-C18
23	b	613	CLA	C13-C15-C16-C17
23	b	614	CLA	C13-C15-C16-C17
28	B	622	LMG	C30-C31-C32-C33
30	d	405	LHG	C15-C16-C17-C18
31	C	516	DGD	O6E-C5E-C6E-O5E
23	d	402	CLA	C2-C1-O2A-CGA
30	D	406	LHG	C12-C13-C14-C15
31	A	617	DGD	C3B-C4B-C5B-C6B
30	D	406	LHG	C11-C12-C13-C14
30	L	101	LHG	C19-C20-C21-C22
31	h	103	DGD	CCA-CDA-CEA-CFA
23	C	507	CLA	C13-C15-C16-C17
30	A	615	LHG	C29-C30-C31-C32
30	a	614	LHG	O6-C4-C5-O7
23	B	607	CLA	C16-C17-C18-C20
23	C	509	CLA	C16-C17-C18-C19
30	a	614	LHG	C19-C20-C21-C22
31	C	516	DGD	CCA-CDA-CEA-CFA
31	c	517	DGD	C8B-C9B-CAB-CBB
23	c	511	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	617	DGD	CEB-CFB-CGB-CHB
23	b	605	CLA	C15-C16-C17-C18
23	c	513	CLA	C8-C10-C11-C12
25	Y	101	BCR	C20-C21-C22-C23
28	D	405	LMG	C34-C35-C36-C37
28	D	409	LMG	C33-C34-C35-C36
28	c	522	LMG	C40-C41-C42-C43
29	a	615	SQD	O47-C45-C46-O48
31	c	518	DGD	CBB-CCB-CDB-CEB
23	B	611	CLA	C15-C16-C17-C18
28	m	101	LMG	C29-C30-C31-C32
29	A	614	SQD	C11-C12-C13-C14
31	h	103	DGD	CBB-CCB-CDB-CEB
23	b	614	CLA	C4-C3-C5-C6
27	D	407	PL9	C30-C29-C31-C32
28	c	522	LMG	C13-C14-C15-C16
23	C	503	CLA	C8-C10-C11-C12
23	B	604	CLA	C11-C10-C8-C7
23	B	605	CLA	C11-C10-C8-C7
23	B	607	CLA	C11-C10-C8-C7
23	B	614	CLA	C11-C12-C13-C15
23	B	615	CLA	C6-C7-C8-C10
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C10-C8-C7
23	C	509	CLA	C11-C10-C8-C7
23	a	604	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
23	b	607	CLA	C6-C7-C8-C10
23	b	609	CLA	C12-C13-C15-C16
23	b	612	CLA	C6-C7-C8-C10
23	c	505	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C10-C8-C7
23	c	506	CLA	C6-C7-C8-C10
23	c	508	CLA	C12-C13-C15-C16
31	H	102	DGD	O2G-C1B-C2B-C3B
23	B	601	CLA	C6-C7-C8-C9
23	B	604	CLA	C11-C10-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	B	615	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	a	604	CLA	C11-C10-C8-C9
23	a	604	CLA	C14-C13-C15-C16
23	a	606	CLA	C11-C10-C8-C9
23	b	603	CLA	C11-C12-C13-C14
23	b	604	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C10-C8-C9
23	b	606	CLA	C14-C13-C15-C16
23	b	609	CLA	C11-C12-C13-C14
23	b	615	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C9
23	c	509	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C10-C8-C9
31	A	617	DGD	O6D-C5D-C6D-O5D
31	h	103	DGD	C6A-C7A-C8A-C9A
25	c	515	BCR	C36-C18-C19-C20
23	B	601	CLA	C16-C17-C18-C20
25	h	102	BCR	C21-C22-C23-C24
30	A	615	LHG	C19-C20-C21-C22
30	D	408	LHG	C17-C18-C19-C20
30	L	101	LHG	C15-C16-C17-C18
31	h	103	DGD	C3A-C4A-C5A-C6A
30	D	406	LHG	C1-C2-C3-O3
23	c	507	CLA	C8-C10-C11-C12
31	A	617	DGD	CFA-CGA-CHA-CIA
23	B	602	CLA	C8-C10-C11-C12
23	B	603	CLA	C8-C10-C11-C12
31	H	102	DGD	CCA-CDA-CEA-CFA
31	H	102	DGD	C4B-C5B-C6B-C7B
31	a	616	DGD	CDB-CEB-CFB-CGB
30	d	407	LHG	C26-C27-C28-C29
31	a	616	DGD	CEB-CFB-CGB-CHB
23	C	507	CLA	C15-C16-C17-C18
30	A	615	LHG	O6-C4-C5-C6
28	d	410	LMG	C28-C29-C30-C31
31	C	517	DGD	CCA-CDA-CEA-CFA
30	D	408	LHG	C30-C31-C32-C33
30	d	409	LHG	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C13-C15-C16-C17
23	b	609	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	B	606	CLA	C16-C17-C18-C19
23	c	506	CLA	C16-C17-C18-C19
30	l	101	LHG	C19-C20-C21-C22
23	b	607	CLA	C8-C10-C11-C12
23	b	607	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CAA-CBA-CGA-O2A
31	C	516	DGD	O6D-C5D-C6D-O5D
30	D	408	LHG	C23-C24-C25-C26
28	c	521	LMG	C16-C17-C18-C19
25	h	102	BCR	C9-C10-C11-C12
28	B	620	LMG	C12-C13-C14-C15
29	a	615	SQD	C15-C16-C17-C18
31	c	518	DGD	C8B-C9B-CAB-CBB
30	l	101	LHG	C7-C8-C9-C10
23	c	509	CLA	C15-C16-C17-C18
23	B	610	CLA	C16-C17-C18-C19
23	c	503	CLA	CBA-CGA-O2A-C1
28	B	620	LMG	C7-C8-C9-O8
28	C	519	LMG	O1-C7-C8-C9
28	c	521	LMG	C7-C8-C9-O8
29	A	614	SQD	O6-C44-C45-C46
29	a	613	SQD	O6-C44-C45-C46
30	a	614	LHG	C28-C29-C30-C31
30	l	101	LHG	C30-C31-C32-C33
23	D	403	CLA	O2A-C1-C2-C3
24	a	605	PHO	O2A-C1-C2-C3
23	c	506	CLA	C3-C5-C6-C7
23	C	501	CLA	O1D-CGD-O2D-CED
30	l	101	LHG	C23-C24-C25-C26
28	d	406	LMG	C33-C34-C35-C36
31	a	616	DGD	CFA-CGA-CHA-CIA
31	c	518	DGD	C6B-C7B-C8B-C9B
23	D	403	CLA	C4-C3-C5-C6
28	A	612	LMG	C32-C33-C34-C35
29	a	615	SQD	C9-C10-C11-C12
30	D	408	LHG	C11-C10-C9-C8
23	B	615	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C10-C11-C12-C13
30	d	407	LHG	C3-O3-P-O6
28	D	405	LMG	C13-C14-C15-C16
29	a	613	SQD	C10-C11-C12-C13
31	A	617	DGD	CAA-CBA-CCA-CDA
30	A	615	LHG	O6-C4-C5-O7
23	b	606	CLA	CBA-CGA-O2A-C1
30	B	623	LHG	C31-C32-C33-C34
23	B	607	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
23	c	507	CLA	C16-C17-C18-C19
23	C	510	CLA	C15-C16-C17-C18
28	m	101	LMG	C37-C38-C39-C40
28	d	406	LMG	C40-C41-C42-C43
29	f	101	SQD	C25-C26-C27-C28
31	A	617	DGD	CCA-CDA-CEA-CFA
23	B	604	CLA	C2C-C3C-CAC-CBC
31	h	103	DGD	C7A-C8A-C9A-CAA
29	A	616	SQD	O47-C45-C46-O48
31	c	517	DGD	CDA-CEA-CFA-CGA
28	A	612	LMG	O1-C7-C8-O7
28	B	620	LMG	O7-C8-C9-O8
29	A	614	SQD	O47-C45-C46-O48
24	d	401	PHO	O1D-CGD-O2D-CED
31	C	517	DGD	C4B-C5B-C6B-C7B
23	B	615	CLA	C16-C17-C18-C19
24	a	605	PHO	C16-C17-C18-C20
27	A	611	PL9	C19-C21-C22-C23
30	D	408	LHG	C1-C2-C3-O3
30	a	614	LHG	C1-C2-C3-O3
30	d	405	LHG	C28-C29-C30-C31
23	B	615	CLA	C2-C3-C5-C6
27	d	408	PL9	C13-C14-C16-C17
30	D	408	LHG	C31-C32-C33-C34
29	F	101	SQD	O48-C23-C24-C25
23	B	611	CLA	C14-C13-C15-C16
23	B	613	CLA	C6-C7-C8-C9
23	C	506	CLA	C6-C7-C8-C9
23	b	604	CLA	C14-C13-C15-C16
31	c	516	DGD	CBB-CCB-CDB-CEB
31	a	616	DGD	CAA-CBA-CCA-CDA
23	B	603	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C10-C11-C12-C13
30	d	409	LHG	C2-C3-O3-P
30	D	406	LHG	C10-C11-C12-C13
23	B	601	CLA	C16-C17-C18-C19
23	B	616	CLA	C11-C12-C13-C14
25	A	608	BCR	C5-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C26
25	B	618	BCR	C23-C24-C25-C30
25	C	515	BCR	C1-C6-C7-C8
25	b	618	BCR	C23-C24-C25-C30
25	c	514	BCR	C1-C6-C7-C8
23	b	613	CLA	C8-C10-C11-C12
31	C	518	DGD	C5A-C6A-C7A-C8A
25	C	520	BCR	C11-C12-C13-C14
23	C	506	CLA	C8-C10-C11-C12
23	c	512	CLA	C8-C10-C11-C12
30	a	614	LHG	C18-C19-C20-C21
31	c	516	DGD	C6B-C7B-C8B-C9B
31	c	518	DGD	CDB-CEB-CFB-CGB
25	t	101	BCR	C14-C15-C16-C17
28	m	101	LMG	C35-C36-C37-C38
28	m	101	LMG	C39-C40-C41-C42
30	D	406	LHG	C29-C30-C31-C32
23	D	403	CLA	C16-C17-C18-C20
30	d	407	LHG	C23-C24-C25-C26
30	d	405	LHG	C33-C34-C35-C36
28	D	409	LMG	C11-C12-C13-C14
28	d	406	LMG	C29-C30-C31-C32
30	d	407	LHG	C10-C11-C12-C13
23	B	607	CLA	C15-C16-C17-C18
30	l	101	LHG	O6-C4-C5-C6
23	B	601	CLA	C4-C3-C5-C6
23	B	613	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C12-C13-C15
23	B	616	CLA	C6-C7-C8-C10
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	509	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	604	CLA	C11-C10-C8-C7
23	b	603	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C10-C8-C7
23	b	604	CLA	C12-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C10-C8-C7
23	c	509	CLA	C12-C13-C15-C16
23	c	511	CLA	C12-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C15
24	a	605	PHO	C6-C7-C8-C10
28	C	519	LMG	C34-C35-C36-C37
25	k	101	BCR	C19-C20-C21-C22
23	b	602	CLA	C16-C17-C18-C19
28	C	519	LMG	O6-C5-C6-O5
31	C	517	DGD	CDA-CEA-CFA-CGA
30	d	407	LHG	C18-C19-C20-C21
31	A	617	DGD	CCB-CDB-CEB-CFB
31	C	517	DGD	C3A-C4A-C5A-C6A
25	B	619	BCR	C20-C21-C22-C37
25	H	101	BCR	C11-C10-C9-C34
25	b	618	BCR	C11-C10-C9-C34
25	d	404	BCR	C16-C17-C18-C36
25	d	404	BCR	C20-C21-C22-C37
29	B	624	SQD	C45-C46-O48-C23
29	A	614	SQD	C33-C34-C35-C36
29	B	624	SQD	C11-C10-C9-C8
30	l	101	LHG	C24-C23-O8-C6
23	A	607	CLA	C6-C7-C8-C9
30	L	101	LHG	C24-C25-C26-C27
28	c	519	LMG	C4-C5-C6-O5
30	D	408	LHG	C9-C10-C11-C12
29	A	616	SQD	C10-C11-C12-C13
29	F	101	SQD	C29-C30-C31-C32
29	F	101	SQD	C31-C32-C33-C34
23	C	501	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	A	605	PHO	CAD-CBD-CGD-O2D
24	A	606	PHO	CAD-CBD-CGD-O2D
24	a	605	PHO	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	d	401	PHO	CAD-CBD-CGD-O2D
31	a	616	DGD	C1G-C2G-O2G-C1B
23	B	607	CLA	C10-C11-C12-C13
28	b	621	LMG	C41-C42-C43-C44
28	d	410	LMG	C29-C30-C31-C32
25	d	404	BCR	C22-C23-C24-C25
23	c	510	CLA	C4-C3-C5-C6
28	m	101	LMG	C15-C16-C17-C18
29	B	624	SQD	C33-C34-C35-C36
28	C	519	LMG	O6-C1-O1-C7
23	B	601	CLA	C2-C3-C5-C6
27	a	611	PL9	C44-C46-C47-C48
30	D	406	LHG	C34-C35-C36-C37
28	b	621	LMG	C7-C8-C9-O8
29	a	615	SQD	C44-C45-C46-O48
31	C	516	DGD	O1G-C1G-C2G-C3G
31	a	616	DGD	O1G-C1G-C2G-C3G
23	c	503	CLA	O1A-CGA-O2A-C1
31	a	616	DGD	C4B-C5B-C6B-C7B
23	D	403	CLA	C5-C6-C7-C8
23	d	403	CLA	C5-C6-C7-C8
23	C	509	CLA	C3-C5-C6-C7
29	A	614	SQD	C26-C27-C28-C29
29	b	601	SQD	C25-C26-C27-C28
35	f	102	HEM	C4B-C3B-CAB-CBB
23	B	606	CLA	C16-C17-C18-C20
30	A	615	LHG	O2-C2-C3-O3
23	A	613	CLA	CHA-CBD-CGD-O1D
23	A	613	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	CHA-CBD-CGD-O1D
23	B	612	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	a	604	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-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-O2D
23	b	606	CLA	O1A-CGA-O2A-C1
23	b	607	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	516	DGD	O1A-C1A-O1G-C1G
31	c	517	DGD	O1A-C1A-O1G-C1G
31	C	517	DGD	C3B-C4B-C5B-C6B
25	T	101	BCR	C16-C17-C18-C19
25	b	618	BCR	C16-C17-C18-C19
31	C	518	DGD	CBB-CCB-CDB-CEB
28	C	519	LMG	O1-C7-C8-O7
28	D	409	LMG	O7-C8-C9-O8
29	b	601	SQD	O6-C44-C45-O47
31	C	516	DGD	O1G-C1G-C2G-O2G
30	l	101	LHG	C35-C36-C37-C38
31	C	518	DGD	C7B-C8B-C9B-CAB
23	A	613	CLA	C16-C17-C18-C19
30	d	409	LHG	O1-C1-C2-O2
30	l	101	LHG	C11-C12-C13-C14
23	C	505	CLA	C11-C12-C13-C14
23	b	615	CLA	C11-C10-C8-C9
28	B	620	LMG	C32-C33-C34-C35
30	a	614	LHG	C12-C13-C14-C15
30	d	405	LHG	C16-C17-C18-C19
23	B	604	CLA	O1D-CGD-O2D-CED
23	c	508	CLA	O1D-CGD-O2D-CED
31	c	517	DGD	C3B-C4B-C5B-C6B
28	c	521	LMG	C31-C32-C33-C34
25	C	515	BCR	C7-C8-C9-C10
25	T	101	BCR	C7-C8-C9-C10
25	Y	101	BCR	C7-C8-C9-C10
31	c	517	DGD	C2B-C3B-C4B-C5B
23	B	614	CLA	C16-C17-C18-C20
23	C	501	CLA	C16-C17-C18-C20
31	C	516	DGD	C4D-C5D-C6D-O5D
28	A	612	LMG	C33-C34-C35-C36
31	C	516	DGD	C3A-C4A-C5A-C6A
27	A	611	PL9	C38-C39-C41-C42
30	B	623	LHG	O10-C23-O8-C6
30	D	406	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O5
30	a	614	LHG	C4-O6-P-O4
30	d	405	LHG	C3-O3-P-O5
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C4-O6-P-O5
31	A	617	DGD	C6A-C7A-C8A-C9A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	L	101	LHG	C11-C10-C9-C8
31	c	518	DGD	CCB-CDB-CEB-CFB
30	A	615	LHG	C13-C14-C15-C16
31	a	616	DGD	C7B-C8B-C9B-CAB
29	A	614	SQD	C12-C13-C14-C15
23	B	612	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
29	A	614	SQD	C5-C6-S-O7
29	a	613	SQD	C5-C6-S-O7
29	a	613	SQD	C5-C6-S-O9
29	f	101	SQD	C5-C6-S-O7
28	A	612	LMG	C28-C29-C30-C31
31	A	617	DGD	C4D-C5D-C6D-O5D
23	a	606	CLA	O1A-CGA-O2A-C1
30	D	408	LHG	C35-C36-C37-C38
30	L	101	LHG	C26-C27-C28-C29
31	H	102	DGD	C7A-C8A-C9A-CAA
23	a	606	CLA	CBA-CGA-O2A-C1
29	a	615	SQD	C19-C20-C21-C22
23	B	612	CLA	C16-C17-C18-C19
23	B	612	CLA	C11-C10-C8-C7
23	C	505	CLA	C6-C7-C8-C10
23	C	508	CLA	C12-C13-C15-C16
23	C	512	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C12-C13-C15
23	b	607	CLA	C11-C12-C13-C15
23	b	608	CLA	C11-C10-C8-C7
23	b	614	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C10-C8-C7
23	c	501	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	c	512	CLA	C12-C13-C15-C16
23	d	402	CLA	C6-C7-C8-C10
23	h	101	CLA	C11-C12-C13-C15
24	A	605	PHO	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	c	522	LMG	C31-C32-C33-C34
29	B	624	SQD	C14-C15-C16-C17
31	C	516	DGD	C4B-C5B-C6B-C7B
31	C	518	DGD	CCA-CDA-CEA-CFA
23	C	508	CLA	C13-C15-C16-C17
28	d	410	LMG	C34-C35-C36-C37
30	A	615	LHG	C30-C31-C32-C33
28	m	101	LMG	C31-C32-C33-C34
23	C	512	CLA	C16-C17-C18-C19
29	A	616	SQD	C32-C33-C34-C35
30	B	623	LHG	C19-C20-C21-C22
29	f	101	SQD	C44-C45-C46-O48
28	c	521	LMG	O7-C8-C9-O8
29	f	101	SQD	O47-C45-C46-O48
30	A	615	LHG	O7-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-O2G
31	H	102	DGD	CCB-CDB-CEB-CFB
31	h	103	DGD	O2G-C1B-C2B-C3B
23	B	616	CLA	C11-C12-C13-C15
29	a	613	SQD	C13-C14-C15-C16
30	d	407	LHG	C25-C26-C27-C28
30	A	615	LHG	C9-C10-C11-C12
23	C	510	CLA	C4-C3-C5-C6
23	c	506	CLA	C8-C10-C11-C12
23	B	607	CLA	C11-C10-C8-C9
23	B	608	CLA	C6-C7-C8-C9
23	B	612	CLA	C11-C10-C8-C9
23	B	616	CLA	C6-C7-C8-C9
23	C	504	CLA	C11-C10-C8-C9
23	C	506	CLA	C11-C12-C13-C14
23	C	509	CLA	C14-C13-C15-C16
23	D	403	CLA	C14-C13-C15-C16
23	b	602	CLA	C11-C10-C8-C9
23	b	604	CLA	C11-C10-C8-C9
23	c	509	CLA	C14-C13-C15-C16
24	a	605	PHO	C6-C7-C8-C9
25	c	514	BCR	C22-C23-C24-C25
25	h	102	BCR	C22-C23-C24-C25
25	k	102	BCR	C6-C7-C8-C9
31	C	516	DGD	O1A-C1A-O1G-C1G
24	a	605	PHO	C16-C17-C18-C19
28	D	405	LMG	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	d	406	LMG	C30-C31-C32-C33
31	c	516	DGD	C8A-C9A-CAA-CBA
25	A	608	BCR	C36-C18-C19-C20
25	B	617	BCR	C7-C8-C9-C34
25	T	101	BCR	C11-C12-C13-C35
25	T	101	BCR	C36-C18-C19-C20
30	A	615	LHG	C10-C11-C12-C13
31	c	516	DGD	C2A-C3A-C4A-C5A
30	d	409	LHG	C33-C34-C35-C36
28	A	612	LMG	C9-C8-O7-C10
29	B	624	SQD	C44-C45-O47-C7
30	a	614	LHG	O6-C4-C5-C6
30	D	408	LHG	C16-C17-C18-C19
23	B	613	CLA	C2-C1-O2A-CGA
23	C	512	CLA	C2-C1-O2A-CGA
23	D	402	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
29	F	101	SQD	C24-C25-C26-C27
31	a	616	DGD	C8B-C9B-CAB-CBB
31	a	616	DGD	O2G-C1B-C2B-C3B
28	A	612	LMG	C19-C20-C21-C22
28	D	405	LMG	C31-C32-C33-C34
28	B	620	LMG	C28-C29-C30-C31
30	l	101	LHG	O6-C4-C5-O7
29	A	616	SQD	C11-C12-C13-C14
31	C	516	DGD	O1G-C1A-C2A-C3A
23	a	604	CLA	C15-C16-C17-C18
23	c	505	CLA	C4-C3-C5-C6
28	b	621	LMG	C23-C24-C25-C26
25	A	608	BCR	C1-C6-C7-C8
25	Y	101	BCR	C23-C24-C25-C30
25	a	607	BCR	C1-C6-C7-C8
25	b	618	BCR	C23-C24-C25-C26
23	c	510	CLA	C2-C3-C5-C6
30	L	101	LHG	C30-C31-C32-C33
31	C	518	DGD	C2A-C1A-O1G-C1G
31	c	516	DGD	O6E-C1E-O5D-C6D
25	A	608	BCR	C20-C21-C22-C23
25	T	101	BCR	C20-C21-C22-C23
27	d	408	PL9	C34-C36-C37-C38
31	a	616	DGD	CFB-CGB-CHB-CIB
29	a	613	SQD	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	D	406	LHG	C14-C15-C16-C17
28	m	101	LMG	C11-C12-C13-C14
29	b	601	SQD	O6-C44-C45-C46
30	A	615	LHG	C4-C5-C6-O8
23	D	403	CLA	C13-C15-C16-C17
23	B	601	CLA	C6-C7-C8-C10
23	B	611	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	511	CLA	C11-C12-C13-C15
23	b	605	CLA	C12-C13-C15-C16
23	b	613	CLA	C6-C7-C8-C10
23	c	505	CLA	C2-C3-C5-C6
31	C	517	DGD	C8A-C9A-CAA-CBA
29	A	614	SQD	C15-C16-C17-C18
23	C	503	CLA	C6-C7-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	513	CLA	C14-C13-C15-C16
23	b	607	CLA	C11-C12-C13-C14
23	b	609	CLA	C14-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C10-C8-C9
23	d	402	CLA	C6-C7-C8-C9
24	A	606	PHO	C14-C13-C15-C16
24	A	605	PHO	C15-C16-C17-C18
23	C	512	CLA	C16-C17-C18-C20
28	m	101	LMG	C22-C23-C24-C25
29	a	615	SQD	C17-C18-C19-C20
30	a	614	LHG	C25-C26-C27-C28
23	C	502	CLA	C10-C11-C12-C13
25	b	618	BCR	C37-C22-C23-C24
23	D	402	CLA	C15-C16-C17-C18
29	A	614	SQD	C17-C18-C19-C20
29	F	101	SQD	C45-C46-O48-C23
28	d	410	LMG	C39-C40-C41-C42
30	A	615	LHG	C1-C2-C3-O3
23	h	101	CLA	C13-C15-C16-C17
29	F	101	SQD	O6-C44-C45-C46
30	L	101	LHG	C23-C24-C25-C26
23	b	609	CLA	C2-C3-C5-C6
29	a	615	SQD	C26-C27-C28-C29
23	B	612	CLA	CBA-CGA-O2A-C1
31	h	103	DGD	C8B-C9B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	616	SQD	C30-C31-C32-C33
29	A	616	SQD	C16-C17-C18-C19
29	B	624	SQD	C10-C11-C12-C13
23	d	402	CLA	C2C-C3C-CAC-CBC
28	d	406	LMG	C32-C33-C34-C35
31	a	616	DGD	C9B-CAB-CBB-CCB
23	b	610	CLA	C2A-CAA-CBA-CGA
31	C	517	DGD	O6D-C1D-O3G-C3G
25	d	404	BCR	C9-C10-C11-C12
31	c	517	DGD	O1B-C1B-O2G-C2G
27	D	407	PL9	C44-C46-C47-C48
29	b	601	SQD	C15-C16-C17-C18
36	V	201	HEC	CAD-CBD-CGD-O2D
25	D	404	BCR	C18-C19-C20-C21
24	d	401	PHO	CBD-CGD-O2D-CED
29	a	615	SQD	C27-C28-C29-C30
29	a	613	SQD	C7-C8-C9-C10
23	c	506	CLA	C4-C3-C5-C6
23	c	502	CLA	C15-C16-C17-C18
23	B	604	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	C2-C3-C5-C6
23	B	611	CLA	C2-C3-C5-C6
27	D	407	PL9	C13-C14-C16-C17
27	a	611	PL9	C13-C14-C16-C17
23	B	609	CLA	C13-C15-C16-C17
23	C	506	CLA	C10-C11-C12-C13
23	b	615	CLA	C16-C17-C18-C20
28	B	620	LMG	C35-C36-C37-C38
30	B	623	LHG	C18-C19-C20-C21
23	c	508	CLA	C13-C15-C16-C17
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C2A-CAA-CBA-CGA
28	D	409	LMG	C31-C32-C33-C34
30	d	405	LHG	C18-C19-C20-C21
23	c	506	CLA	C4C-C3C-CAC-CBC
28	c	522	LMG	C33-C34-C35-C36
31	c	518	DGD	CBA-CCA-CDA-CEA
23	B	609	CLA	C3A-C2A-CAA-CBA
35	f	102	HEM	CAD-CBD-CGD-O1D
23	c	501	CLA	O1D-CGD-O2D-CED
28	B	622	LMG	O9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	609	CLA	C4-C3-C5-C6
27	a	611	PL9	C40-C39-C41-C42
27	d	408	PL9	C30-C29-C31-C32
23	C	510	CLA	C2-C3-C5-C6
27	a	611	PL9	C4-C3-C7-C8
31	c	516	DGD	O1G-C1A-C2A-C3A
23	C	508	CLA	C11-C12-C13-C14
23	b	610	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	c	509	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
29	a	613	SQD	C15-C16-C17-C18
30	a	614	LHG	C27-C28-C29-C30
23	c	508	CLA	O1A-CGA-O2A-C1
25	c	515	BCR	C35-C13-C14-C15
31	C	516	DGD	C6A-C7A-C8A-C9A
23	c	510	CLA	C10-C11-C12-C13
31	C	518	DGD	C4A-C5A-C6A-C7A
23	C	508	CLA	C16-C17-C18-C19
23	c	504	CLA	C11-C12-C13-C15
23	c	508	CLA	CBA-CGA-O2A-C1
29	a	613	SQD	C29-C30-C31-C32
28	A	612	LMG	C39-C40-C41-C42
29	b	601	SQD	C13-C14-C15-C16
23	b	603	CLA	C8-C10-C11-C12
29	F	101	SQD	C26-C27-C28-C29
28	c	522	LMG	C9-C8-O7-C10
29	B	624	SQD	C46-C45-O47-C7
29	f	101	SQD	C46-C45-O47-C7
23	B	603	CLA	C5-C6-C7-C8
23	B	609	CLA	C10-C11-C12-C13
27	a	611	PL9	C25-C24-C26-C27
23	B	602	CLA	C1A-C2A-CAA-CBA
23	A	613	CLA	C11-C12-C13-C15
23	B	603	CLA	C6-C7-C8-C10
23	B	605	CLA	C12-C13-C15-C16
29	A	616	SQD	C33-C34-C35-C36
36	v	201	HEC	CAD-CBD-CGD-O2D
24	d	401	PHO	C3-C5-C6-C7
23	b	610	CLA	O1D-CGD-O2D-CED
23	c	501	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C10-C11-C12-C13
23	D	402	CLA	C10-C11-C12-C13
31	h	103	DGD	C3B-C4B-C5B-C6B
30	d	409	LHG	C24-C25-C26-C27
31	C	517	DGD	O1B-C1B-O2G-C2G
28	b	621	LMG	C29-C28-O8-C9
23	d	402	CLA	C3-C5-C6-C7
23	b	615	CLA	C16-C17-C18-C19
28	B	622	LMG	O8-C28-C29-C30
36	v	201	HEC	CAD-CBD-CGD-O1D
28	A	612	LMG	C17-C18-C19-C20
28	B	620	LMG	C40-C41-C42-C43
30	d	405	LHG	C31-C32-C33-C34
31	c	516	DGD	C1A-C2A-C3A-C4A
23	b	611	CLA	C2-C3-C5-C6
23	B	605	CLA	C5-C6-C7-C8
28	m	101	LMG	C32-C33-C34-C35
31	H	102	DGD	C8B-C9B-CAB-CBB
28	B	620	LMG	C10-C11-C12-C13
31	A	617	DGD	C4E-C5E-C6E-O5E
30	D	408	LHG	C24-C25-C26-C27
25	C	514	BCR	C11-C10-C9-C8
25	B	619	BCR	C15-C16-C17-C18
25	D	404	BCR	C9-C10-C11-C12
25	d	404	BCR	C13-C14-C15-C16
28	d	406	LMG	C10-C11-C12-C13
30	B	623	LHG	C32-C33-C34-C35
35	f	102	HEM	CAD-CBD-CGD-O2D
36	V	201	HEC	CAD-CBD-CGD-O1D
23	B	603	CLA	C4-C3-C5-C6
28	D	405	LMG	C40-C41-C42-C43
23	c	502	CLA	C11-C12-C13-C14
31	C	518	DGD	C3A-C4A-C5A-C6A
28	m	101	LMG	O10-C28-O8-C9
30	d	409	LHG	C9-C10-C11-C12
25	a	607	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	k	102	BCR	C1-C6-C7-C8
28	m	101	LMG	C30-C31-C32-C33
30	d	407	LHG	C16-C17-C18-C19
31	c	517	DGD	C5B-C6B-C7B-C8B
29	b	601	SQD	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	605	PHO	C4-C3-C5-C6
25	B	618	BCR	C7-C8-C9-C10
23	D	403	CLA	C2-C3-C5-C6
31	C	517	DGD	C2G-C3G-O3G-C1D
31	c	516	DGD	C5D-C6D-O5D-C1E
23	B	603	CLA	C13-C15-C16-C17
28	B	622	LMG	O7-C10-C11-C12
28	C	519	LMG	C14-C15-C16-C17
31	C	518	DGD	C3B-C4B-C5B-C6B
30	d	405	LHG	O6-C4-C5-O7
31	c	516	DGD	C3A-C4A-C5A-C6A
27	d	408	PL9	C35-C34-C36-C37
31	h	103	DGD	O1B-C1B-C2B-C3B
23	C	503	CLA	C6-C7-C8-C10
24	a	605	PHO	C2-C3-C5-C6
28	C	519	LMG	C37-C38-C39-C40
30	D	406	LHG	O1-C1-C2-O2
25	t	101	BCR	C13-C14-C15-C16
28	C	519	LMG	C2-C1-O1-C7
31	c	516	DGD	C2E-C1E-O5D-C6D
28	b	621	LMG	C42-C43-C44-C45
28	b	621	LMG	O7-C8-C9-O8
31	H	102	DGD	CDA-CEA-CFA-CGA
23	C	507	CLA	C5-C6-C7-C8
28	c	522	LMG	C37-C38-C39-C40
35	F	102	HEM	CAD-CBD-CGD-O1D
23	C	511	CLA	CBA-CGA-O2A-C1
30	d	407	LHG	C19-C20-C21-C22
31	c	517	DGD	C9A-CAA-CBA-CCA
23	b	608	CLA	C2C-C3C-CAC-CBC
31	c	517	DGD	CCB-CDB-CEB-CFB
23	d	402	CLA	C16-C17-C18-C20
23	B	603	CLA	C6-C7-C8-C9
23	C	508	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C10-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	b	608	CLA	C11-C10-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	h	101	CLA	C11-C12-C13-C14
23	B	602	CLA	C3A-C2A-CAA-CBA
30	A	615	LHG	C14-C15-C16-C17
23	B	612	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	612	CLA	CAA-CBA-CGA-O2A
23	b	608	CLA	CBD-CGD-O2D-CED
31	C	517	DGD	C9A-CAA-CBA-CCA
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	603	CLA	CAD-CBD-CGD-O2D
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	C	506	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	C11-C12-C13-C14
23	h	101	CLA	C16-C17-C18-C20
31	c	518	DGD	C2A-C3A-C4A-C5A
23	b	609	CLA	C3-C5-C6-C7
31	H	102	DGD	C5B-C6B-C7B-C8B
28	c	522	LMG	O8-C28-C29-C30
28	B	620	LMG	C14-C15-C16-C17
31	c	517	DGD	CCA-CDA-CEA-CFA
30	d	407	LHG	C32-C33-C34-C35
31	C	518	DGD	C4B-C5B-C6B-C7B
23	b	610	CLA	C13-C15-C16-C17
23	d	402	CLA	C10-C11-C12-C13
29	a	613	SQD	O47-C7-C8-C9
25	B	617	BCR	C11-C12-C13-C14
31	A	617	DGD	C2A-C3A-C4A-C5A
31	H	102	DGD	C7B-C8B-C9B-CAB
28	c	522	LMG	O1-C7-C8-C9
29	A	614	SQD	C44-C45-C46-O48
29	b	601	SQD	C44-C45-C46-O48
31	C	518	DGD	C8A-C9A-CAA-CBA
23	c	509	CLA	CAA-CBA-CGA-O1A
28	A	612	LMG	C38-C39-C40-C41
29	b	601	SQD	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	B	620	LMG	C18-C19-C20-C21
23	B	604	CLA	O2A-C1-C2-C3
23	C	509	CLA	O2A-C1-C2-C3
23	h	101	CLA	O2A-C1-C2-C3
24	A	605	PHO	O2A-C1-C2-C3
28	m	101	LMG	C38-C39-C40-C41
30	D	408	LHG	C24-C23-O8-C6
28	m	101	LMG	O8-C28-C29-C30
23	A	613	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C19
24	a	605	PHO	O1D-CGD-O2D-CED
30	d	405	LHG	O9-C7-O7-C5
23	A	604	CLA	CHA-CBD-CGD-O1D
23	A	604	CLA	CHA-CBD-CGD-O2D
23	C	503	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	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	a	612	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	609	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	512	CLA	CHA-CBD-CGD-O2D
25	Y	101	BCR	C13-C14-C15-C16
25	b	618	BCR	C9-C10-C11-C12
29	B	624	SQD	C16-C17-C18-C19
23	B	614	CLA	C16-C17-C18-C19
28	B	622	LMG	C31-C32-C33-C34
23	b	607	CLA	C13-C15-C16-C17
29	A	614	SQD	O47-C7-C8-C9
30	L	101	LHG	O7-C7-C8-C9
31	C	516	DGD	O2G-C1B-C2B-C3B
31	c	518	DGD	C7B-C8B-C9B-CAB
24	A	606	PHO	CHA-CBD-CGD-O1D
24	a	605	PHO	CHA-CBD-CGD-O1D
30	a	614	LHG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	511	CLA	CBA-CGA-O2A-C1
23	B	611	CLA	O1A-CGA-O2A-C1
28	B	622	LMG	C13-C14-C15-C16
23	b	613	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
23	B	603	CLA	C12-C13-C15-C16
23	b	614	CLA	C12-C13-C15-C16
24	A	606	PHO	C12-C13-C15-C16
27	d	408	PL9	C28-C29-C31-C32
23	b	607	CLA	C16-C17-C18-C20
29	b	601	SQD	C16-C17-C18-C19
23	A	613	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C12-C13-C14
23	B	611	CLA	C6-C7-C8-C9
23	C	505	CLA	C6-C7-C8-C9
23	b	602	CLA	C14-C13-C15-C16
23	b	614	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C9
31	c	517	DGD	C1A-C2A-C3A-C4A
25	b	619	BCR	C9-C10-C11-C12
30	B	623	LHG	C27-C28-C29-C30
25	B	619	BCR	C14-C15-C16-C17
29	A	616	SQD	C24-C23-O48-C46
29	A	614	SQD	C5-C6-S-O8
23	b	607	CLA	C16-C17-C18-C19
29	F	101	SQD	C35-C36-C37-C38
31	C	518	DGD	C8B-C9B-CAB-CBB
23	B	603	CLA	C2-C3-C5-C6
35	F	102	HEM	CAD-CBD-CGD-O2D
23	C	509	CLA	C5-C6-C7-C8
23	B	609	CLA	C1A-C2A-CAA-CBA
29	a	613	SQD	C19-C20-C21-C22
23	C	513	CLA	C15-C16-C17-C18
30	B	623	LHG	C16-C17-C18-C19
27	D	407	PL9	C21-C22-C23-C24
28	d	406	LMG	C12-C13-C14-C15
28	B	620	LMG	O1-C7-C8-C9
31	c	516	DGD	C1G-C2G-C3G-O3G
23	D	402	CLA	C4C-C3C-CAC-CBC
23	h	101	CLA	C16-C17-C18-C19
23	c	510	CLA	CAA-CBA-CGA-O1A
31	c	516	DGD	O1B-C1B-C2B-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C8-C10-C11-C12
31	a	616	DGD	C7A-C8A-C9A-CAA
23	C	511	CLA	O1A-CGA-O2A-C1
23	B	611	CLA	C4-C3-C5-C6
23	B	613	CLA	CAA-CBA-CGA-O2A
30	D	408	LHG	C2-C3-O3-P
30	D	406	LHG	C33-C34-C35-C36
23	c	504	CLA	C8-C10-C11-C12
28	c	522	LMG	C32-C33-C34-C35
30	D	408	LHG	C4-O6-P-O4
28	m	101	LMG	O9-C10-C11-C12
30	d	409	LHG	O10-C23-C24-C25
25	B	618	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	k	102	BCR	C5-C6-C7-C8
23	B	612	CLA	CAA-CBA-CGA-O1A
30	a	614	LHG	O10-C23-C24-C25
30	D	406	LHG	C16-C17-C18-C19
31	C	516	DGD	O1B-C1B-C2B-C3B
24	d	401	PHO	C8-C10-C11-C12
24	A	605	PHO	C4-C3-C5-C6
28	B	620	LMG	C38-C39-C40-C41
23	b	613	CLA	C16-C17-C18-C19
29	b	601	SQD	C10-C11-C12-C13
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
29	f	101	SQD	C44-C45-O47-C7
23	B	605	CLA	C14-C13-C15-C16
23	a	612	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C12-C13-C14
23	b	611	CLA	C6-C7-C8-C9
23	c	512	CLA	C11-C12-C13-C14
24	A	605	PHO	C6-C7-C8-C9
28	c	519	LMG	C34-C35-C36-C37
23	a	606	CLA	CAA-CBA-CGA-O2A
29	B	624	SQD	O47-C7-C8-C9
27	D	407	PL9	C37-C38-C39-C40
28	D	409	LMG	C35-C36-C37-C38
29	A	616	SQD	C34-C35-C36-C37
31	c	517	DGD	C8A-C9A-CAA-CBA
29	B	624	SQD	O48-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	516	DGD	O2G-C1B-C2B-C3B
28	C	519	LMG	C17-C18-C19-C20
31	c	518	DGD	O1B-C1B-C2B-C3B
23	C	507	CLA	C4-C3-C5-C6
24	d	401	PHO	C5-C6-C7-C8
23	B	601	CLA	C3A-C2A-CAA-CBA
23	B	601	CLA	C12-C13-C15-C16
23	a	606	CLA	C12-C13-C15-C16
23	b	608	CLA	C6-C7-C8-C10
23	b	610	CLA	C12-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C15
24	A	605	PHO	C6-C7-C8-C10
27	d	408	PL9	C33-C34-C36-C37
31	C	517	DGD	O1G-C1A-C2A-C3A
23	A	604	CLA	C15-C16-C17-C18
31	H	102	DGD	C5A-C6A-C7A-C8A
31	C	516	DGD	CDB-CEB-CFB-CGB
23	a	612	CLA	C2C-C3C-CAC-CBC
30	l	101	LHG	C33-C34-C35-C36
28	D	405	LMG	C19-C20-C21-C22
31	C	516	DGD	O6E-C1E-O5D-C6D
23	c	507	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
28	A	612	LMG	C37-C38-C39-C40
23	a	606	CLA	CAA-CBA-CGA-O1A
28	C	519	LMG	O10-C28-C29-C30
30	D	408	LHG	O10-C23-C24-C25
30	a	614	LHG	O2-C2-C3-O3
23	b	612	CLA	C8-C10-C11-C12
30	A	615	LHG	C12-C13-C14-C15
23	B	613	CLA	CAA-CBA-CGA-O1A
23	b	611	CLA	C4-C3-C5-C6

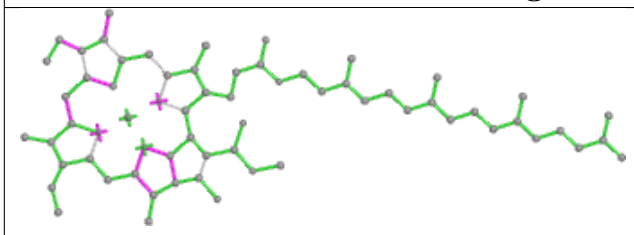
There are no ring outliers.

No monomer is involved in short contacts.

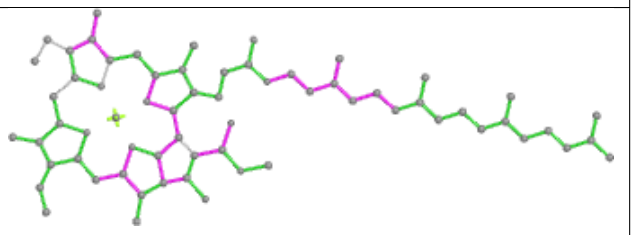
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

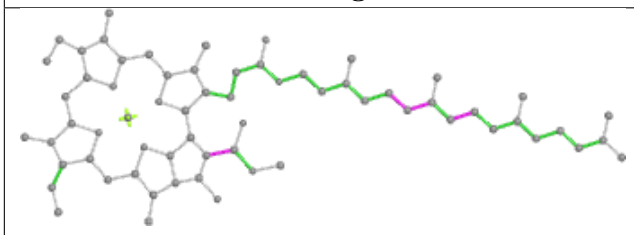
Ligand CLA C 503



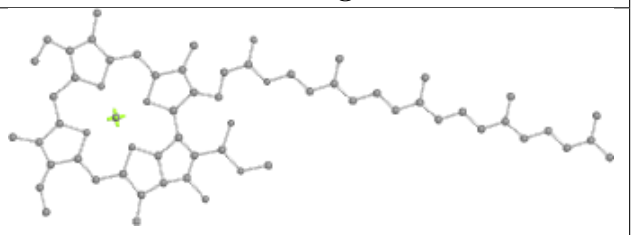
Bond lengths



Bond angles

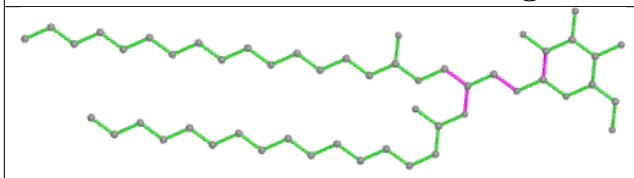


Torsions

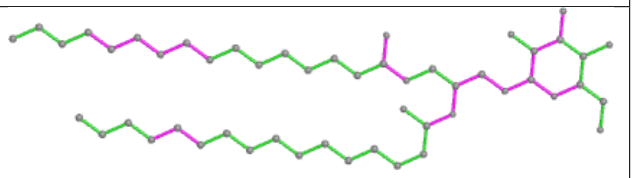


Rings

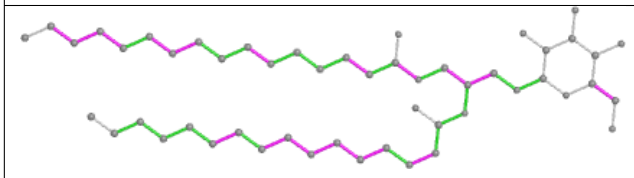
Ligand LMG B 620



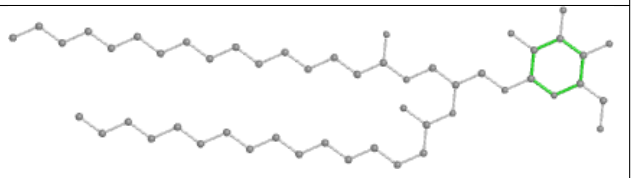
Bond lengths



Bond angles

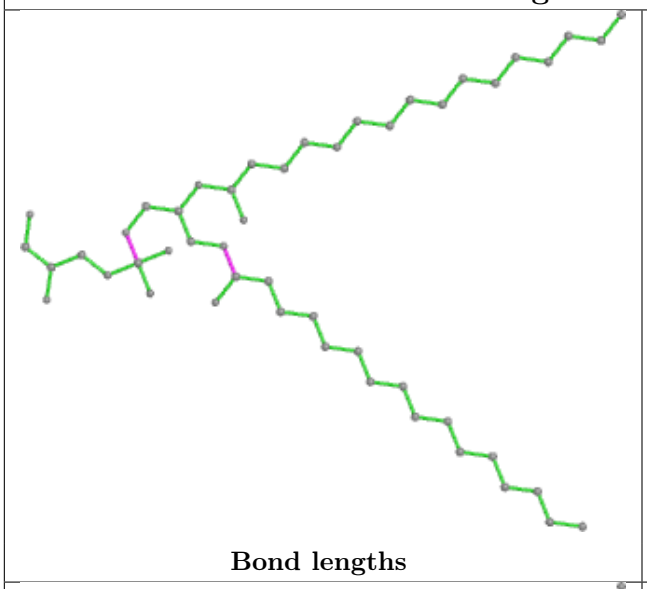


Torsions

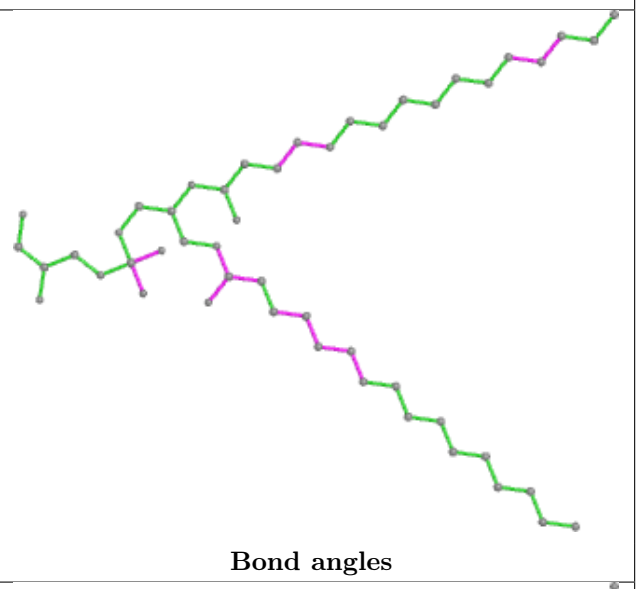


Rings

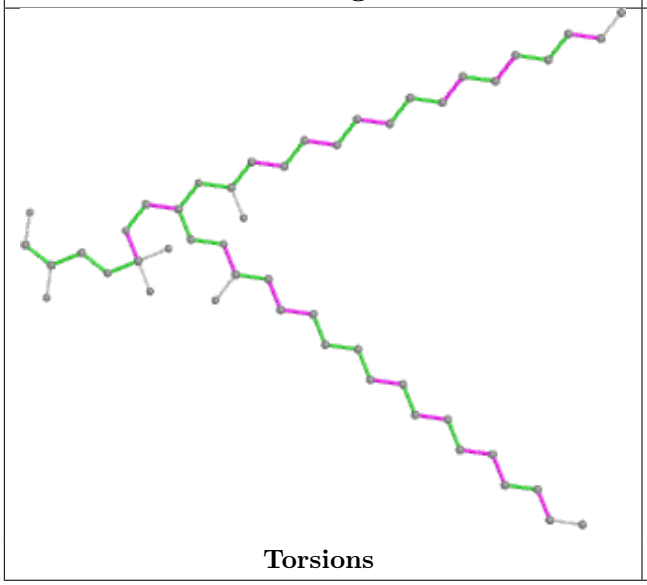
Ligand LHG l 101



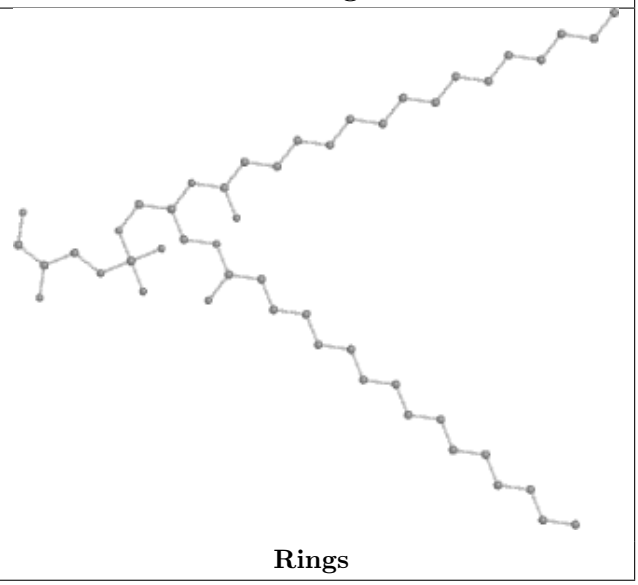
Bond lengths



Bond angles

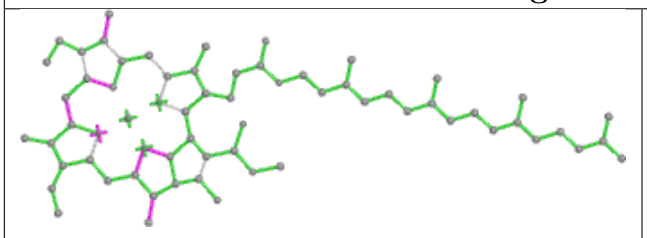


Torsions

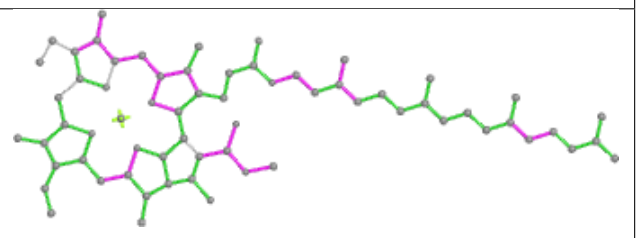


Rings

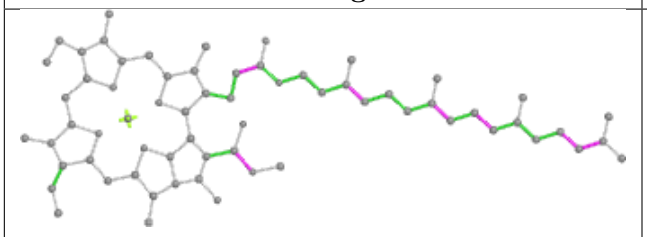
Ligand CLA c 510



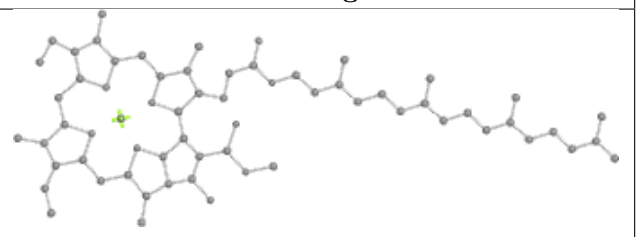
Bond lengths



Bond angles

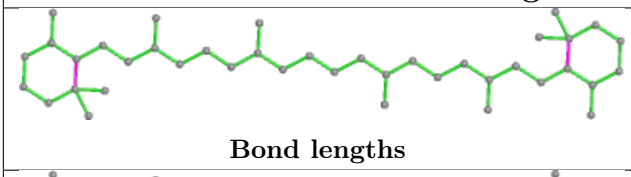


Torsions

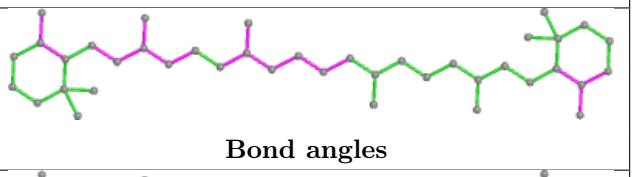


Rings

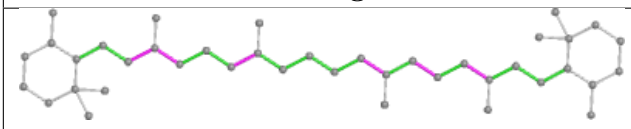
Ligand BCR C 514



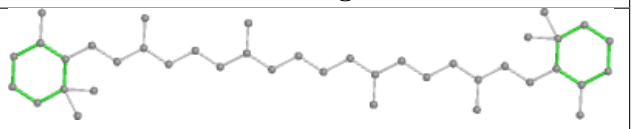
Bond lengths



Bond angles

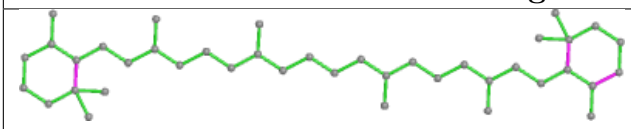


Torsions

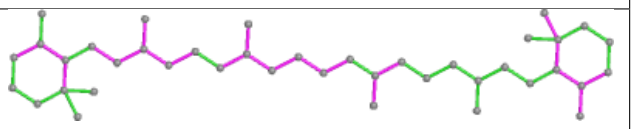


Rings

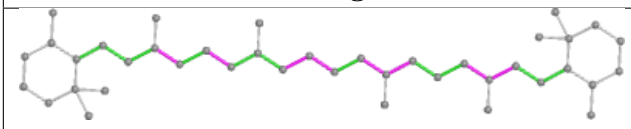
Ligand BCR t 101



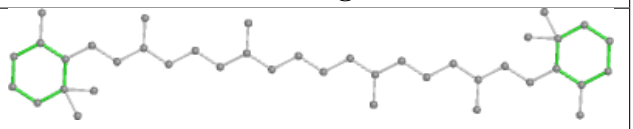
Bond lengths



Bond angles

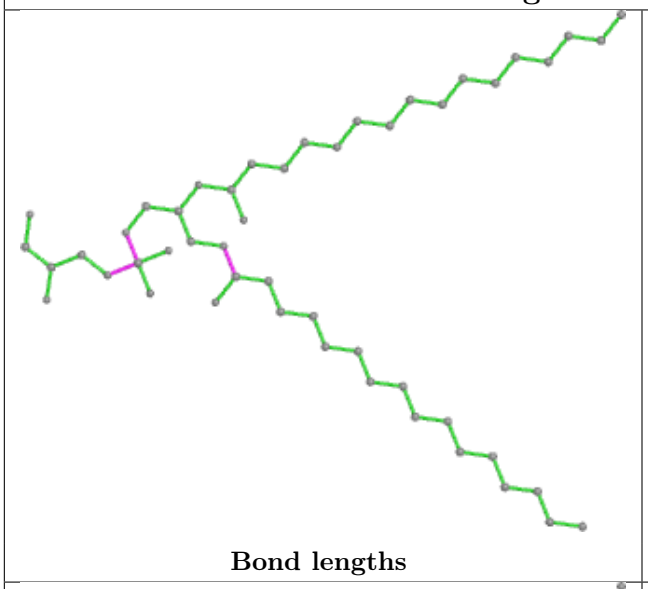


Torsions

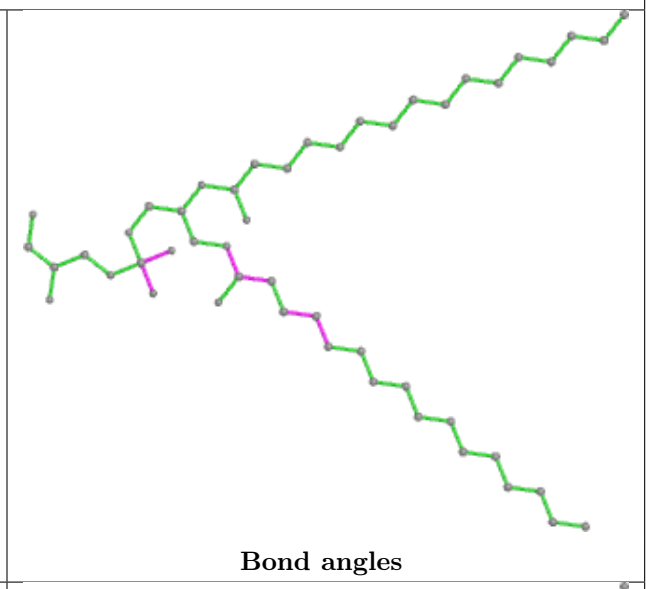


Rings

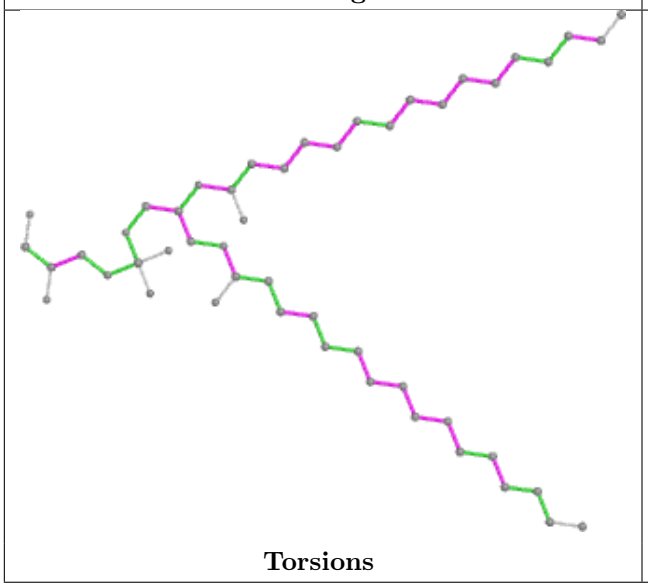
Ligand LHG A 615



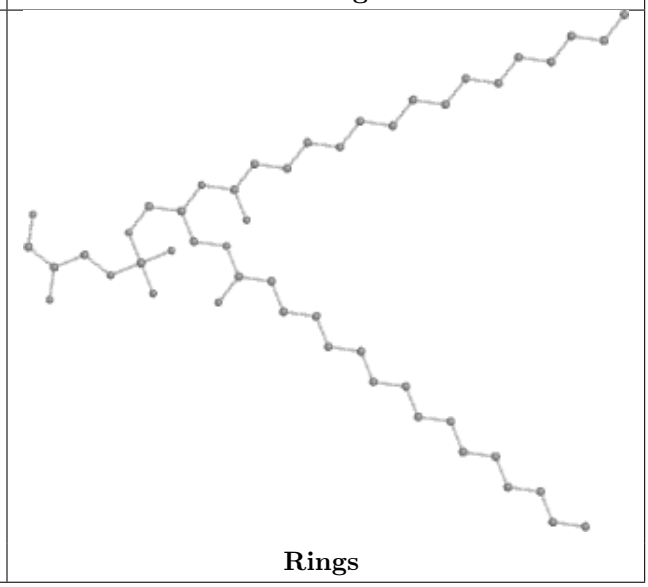
Bond lengths



Bond angles

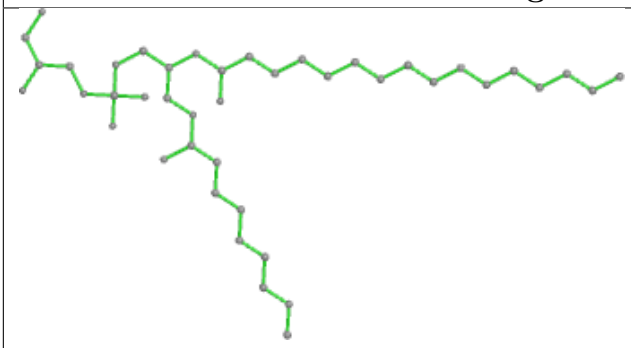


Torsions

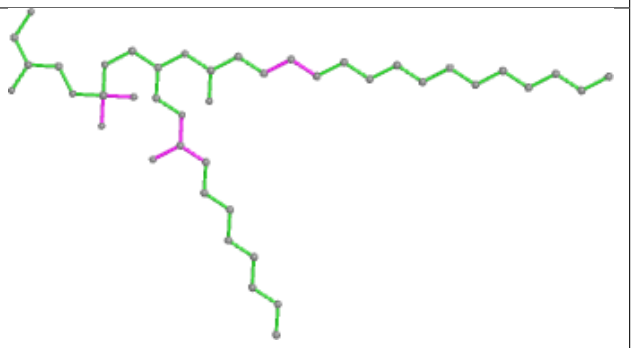


Rings

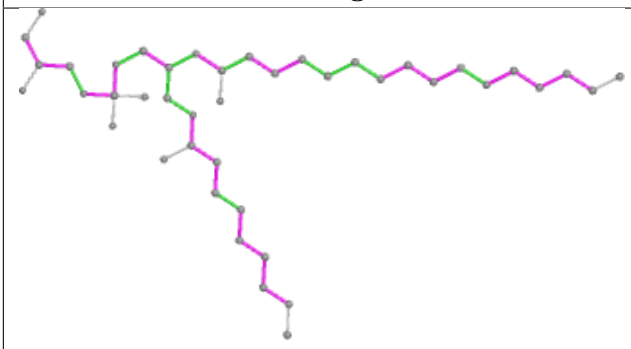
Ligand LHG a 614



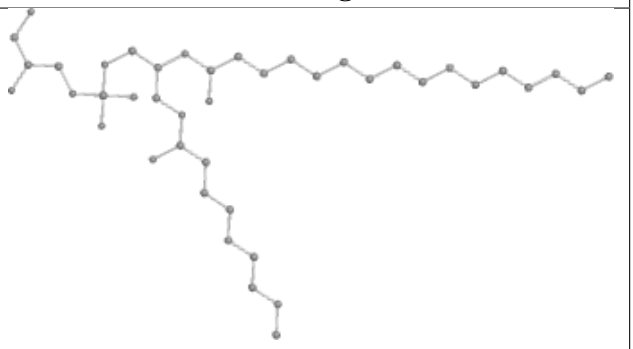
Bond lengths



Bond angles

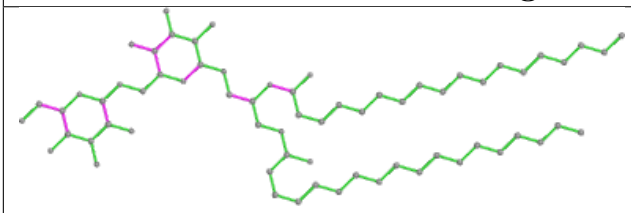


Torsions

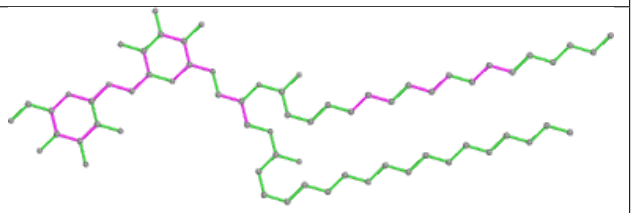


Rings

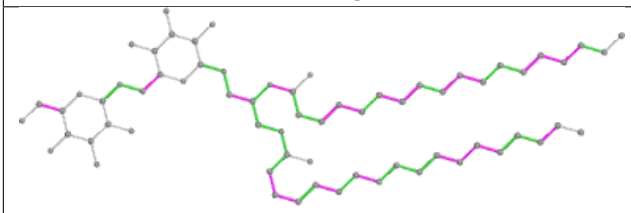
Ligand DGD A 617



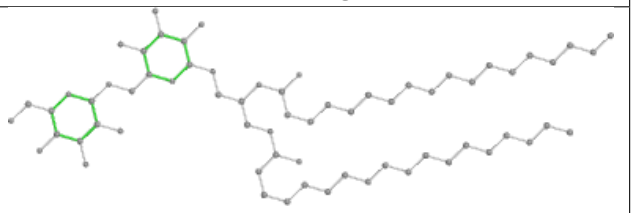
Bond lengths



Bond angles

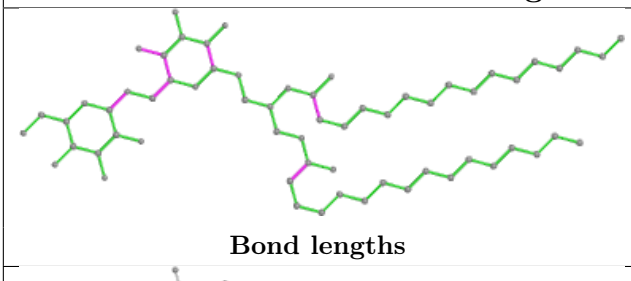


Torsions

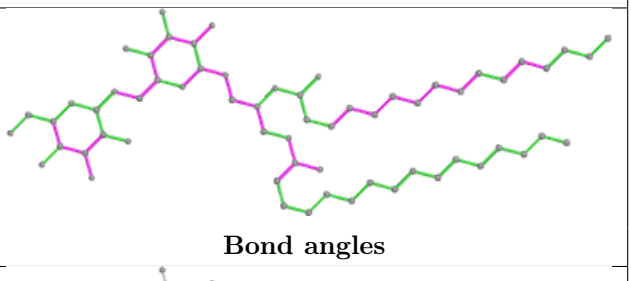


Rings

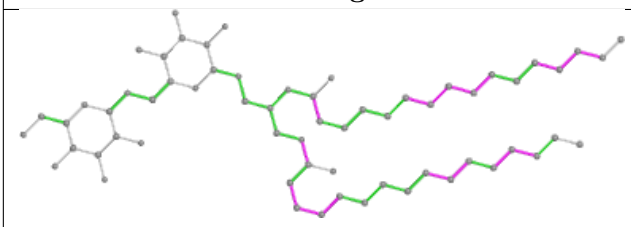
Ligand DGD c 518



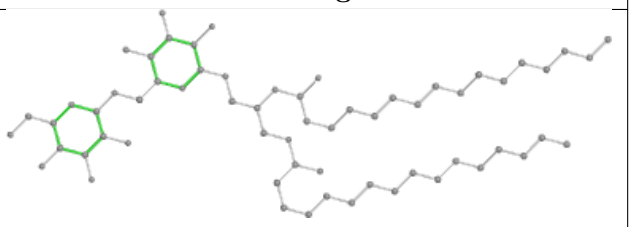
Bond lengths



Bond angles

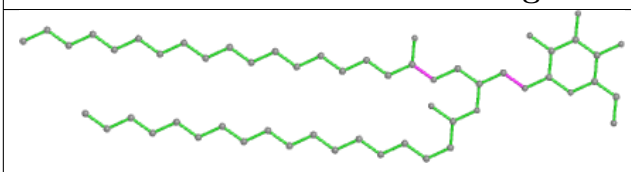


Torsions

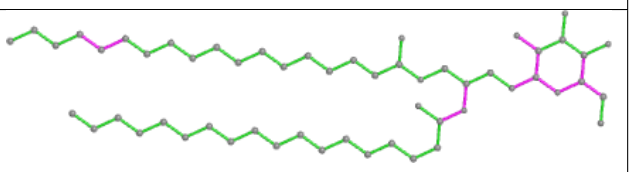


Rings

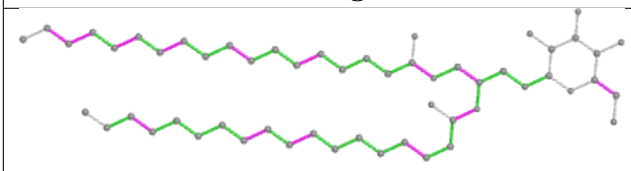
Ligand LMG b 621



Bond lengths



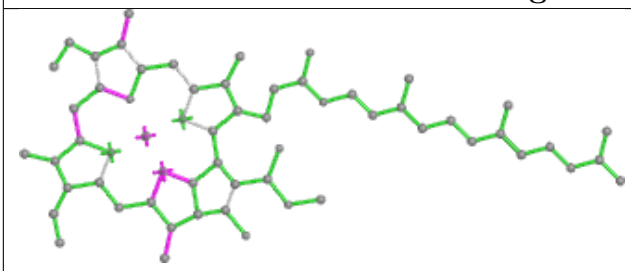
Bond angles



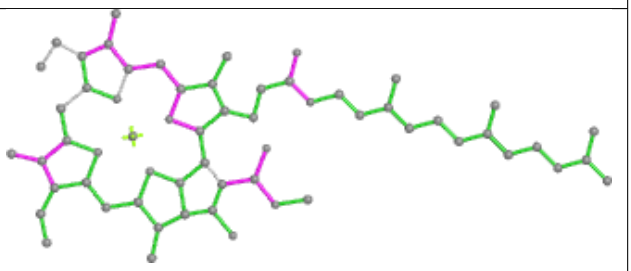
Torsions

Rings

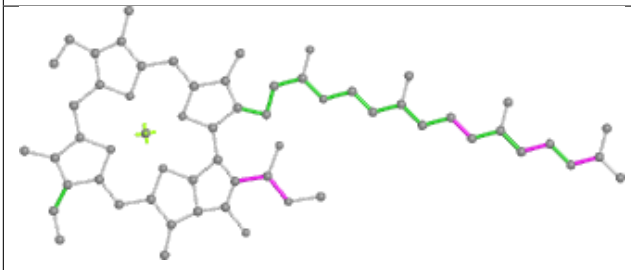
Ligand CLA c 504



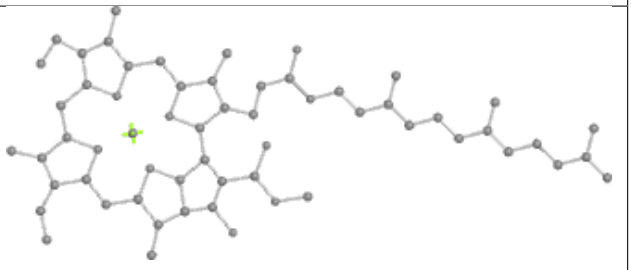
Bond lengths



Bond angles

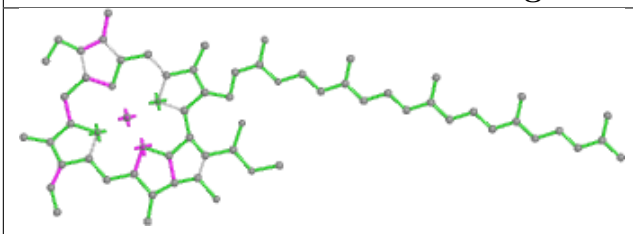


Torsions

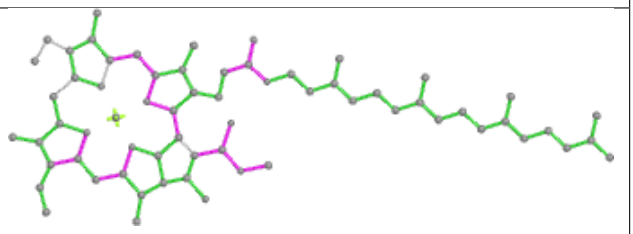


Rings

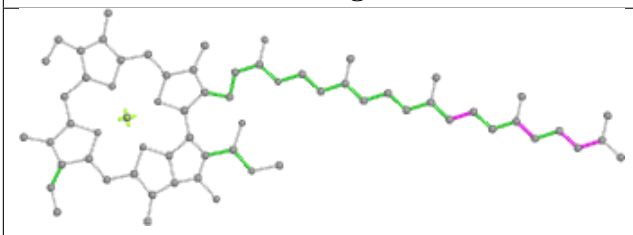
Ligand CLA B 610



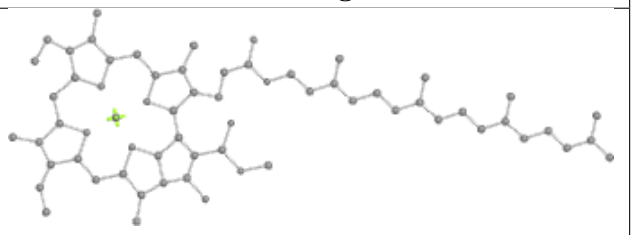
Bond lengths



Bond angles

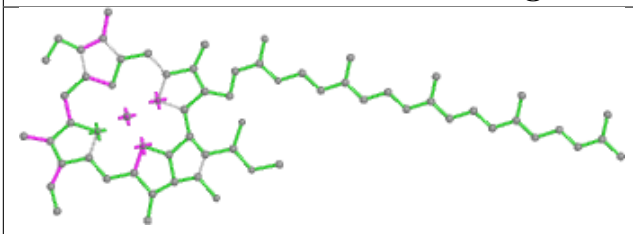


Torsions

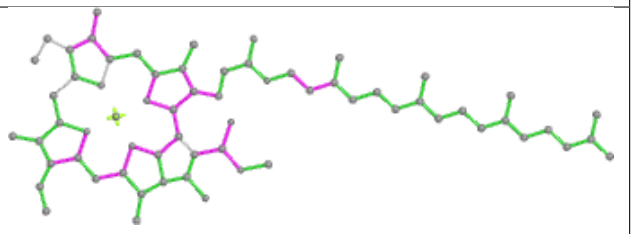


Rings

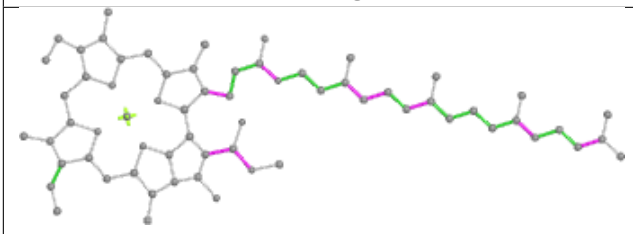
Ligand CLA B 601



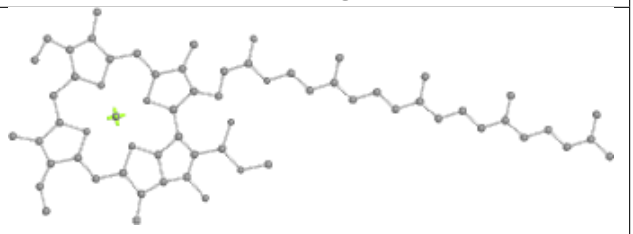
Bond lengths



Bond angles

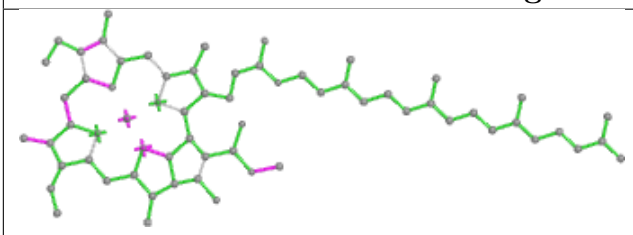


Torsions

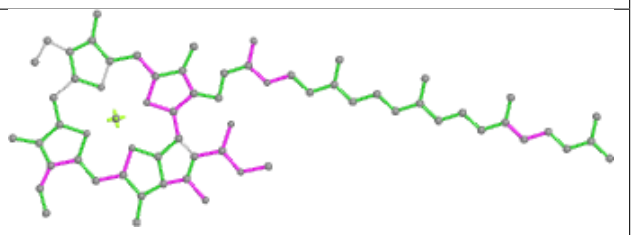


Rings

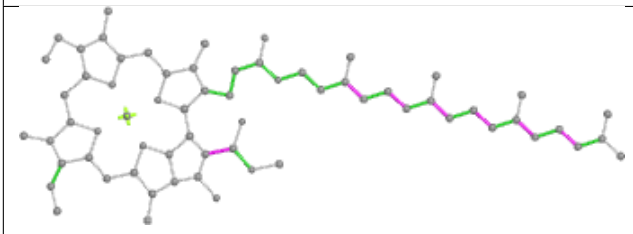
Ligand CLA B 605



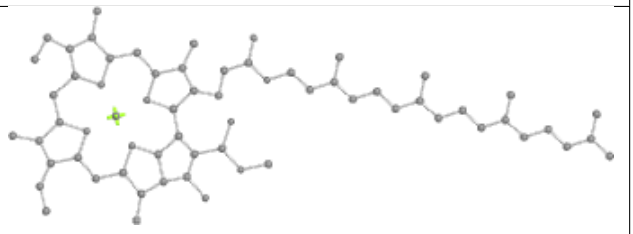
Bond lengths



Bond angles

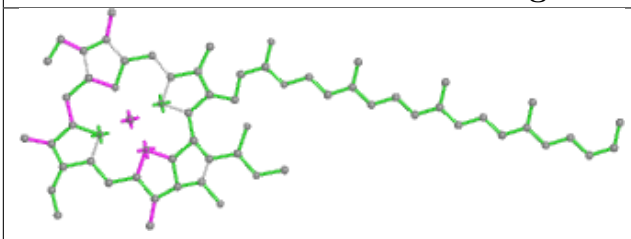


Torsions

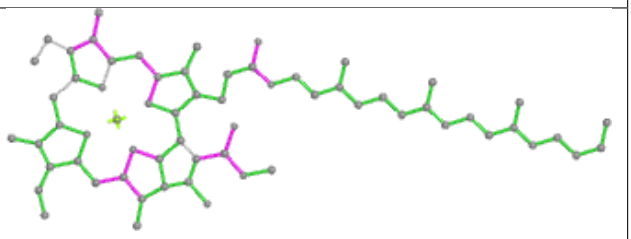


Rings

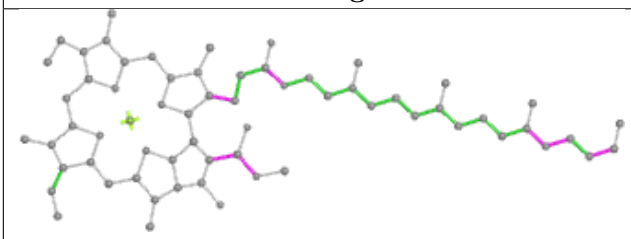
Ligand CLA c 508



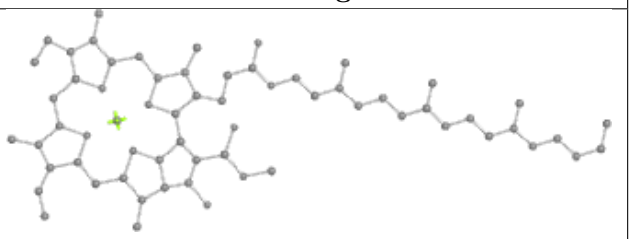
Bond lengths



Bond angles

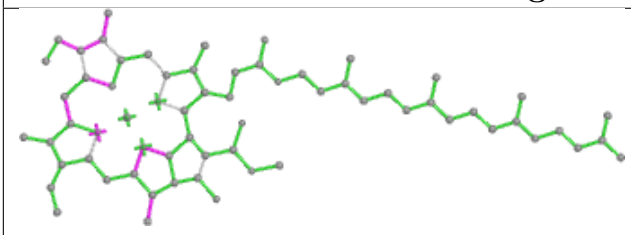


Torsions

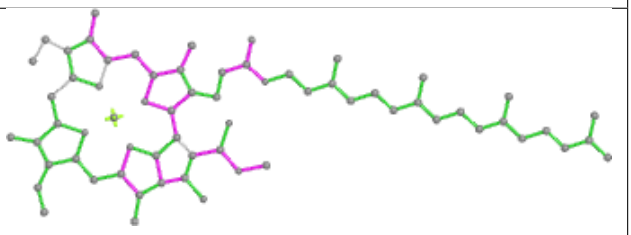


Rings

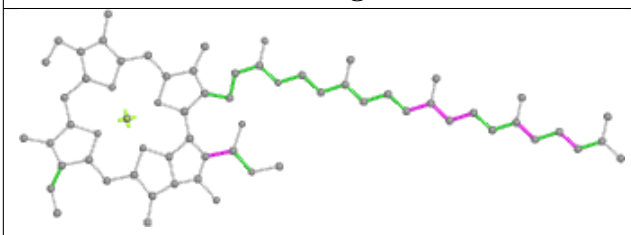
Ligand CLA a 604



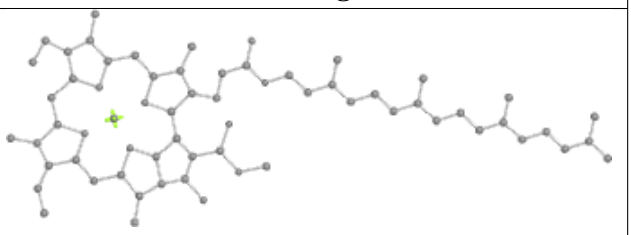
Bond lengths



Bond angles

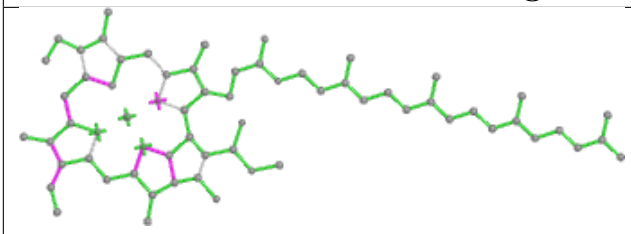


Torsions

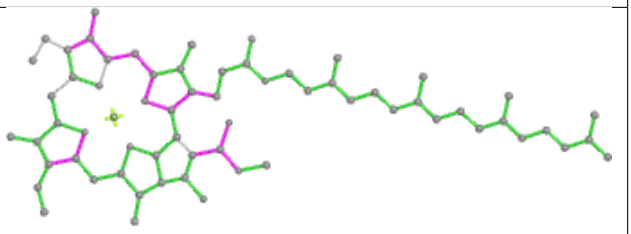


Rings

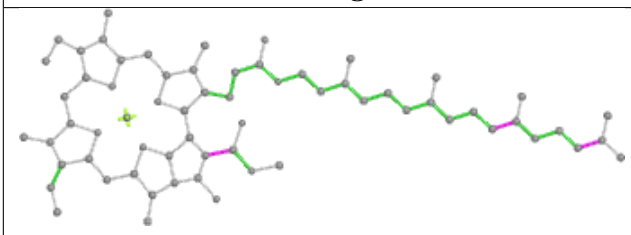
Ligand CLA A 613



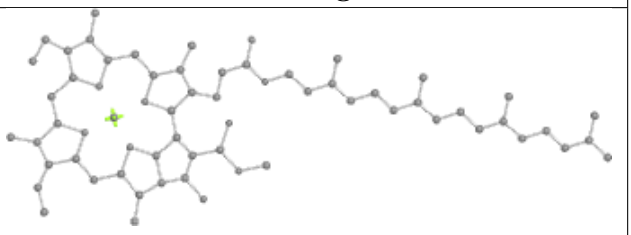
Bond lengths



Bond angles

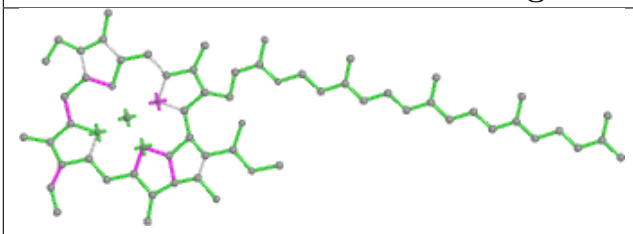


Torsions

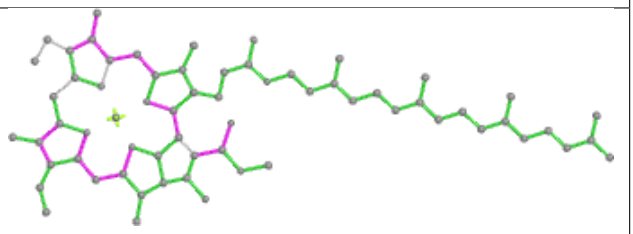


Rings

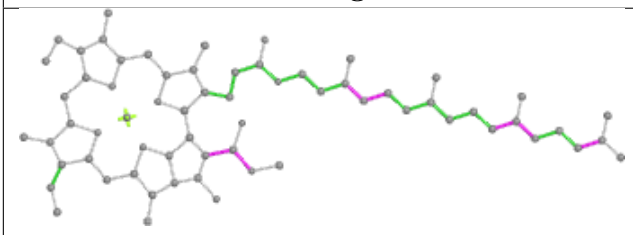
Ligand CLA b 609



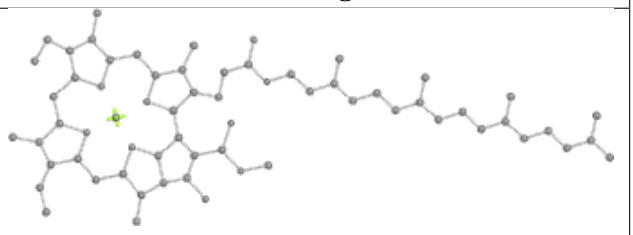
Bond lengths



Bond angles

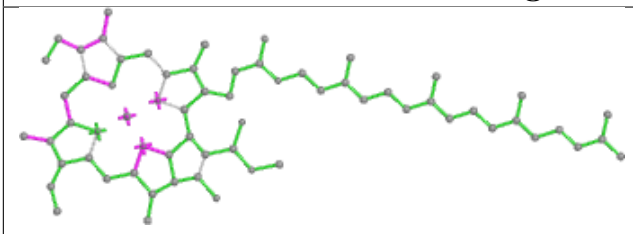


Torsions

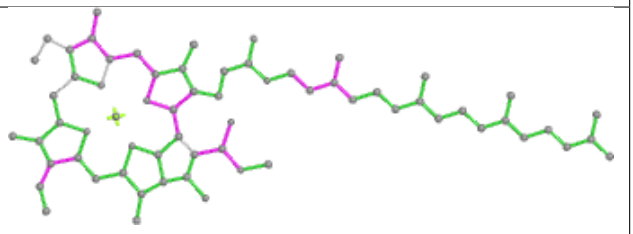


Rings

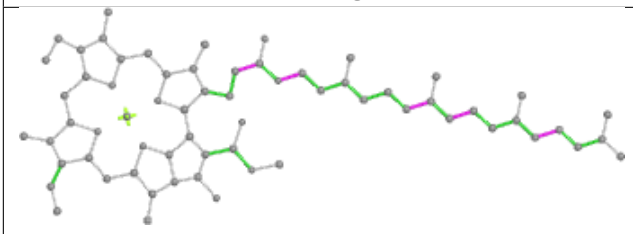
Ligand CLA B 613



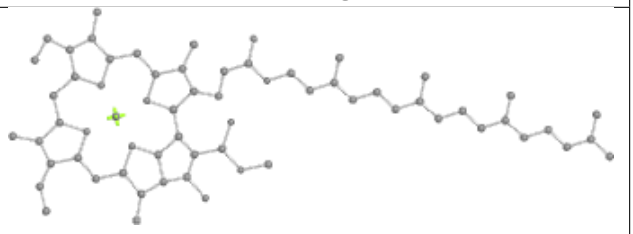
Bond lengths



Bond angles

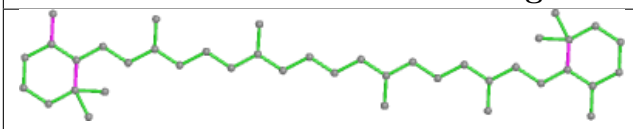


Torsions

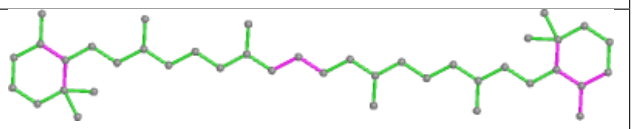


Rings

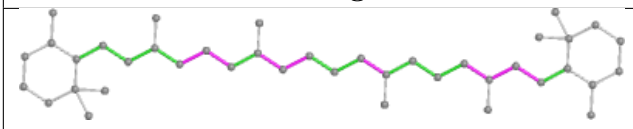
Ligand BCR d 404



Bond lengths



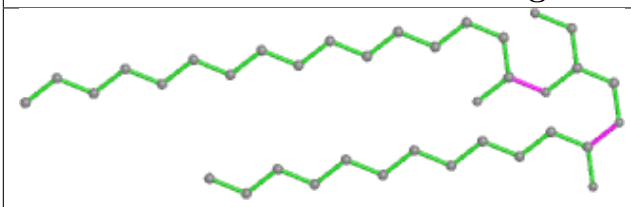
Bond angles



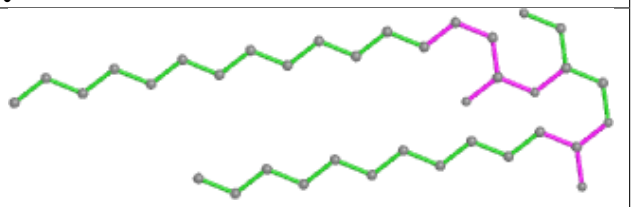
Torsions

Rings

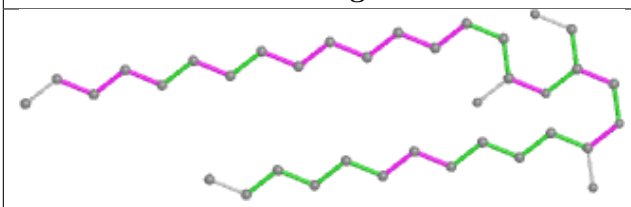
Ligand SQD a 615



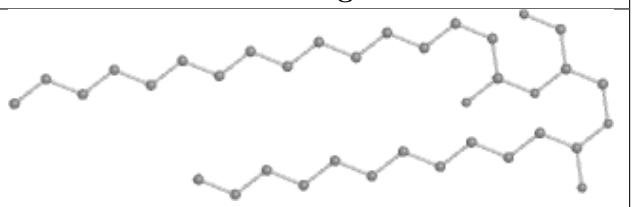
Bond lengths



Bond angles

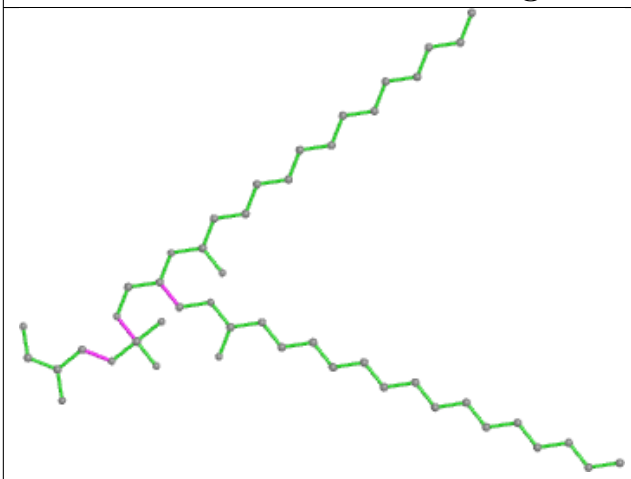


Torsions

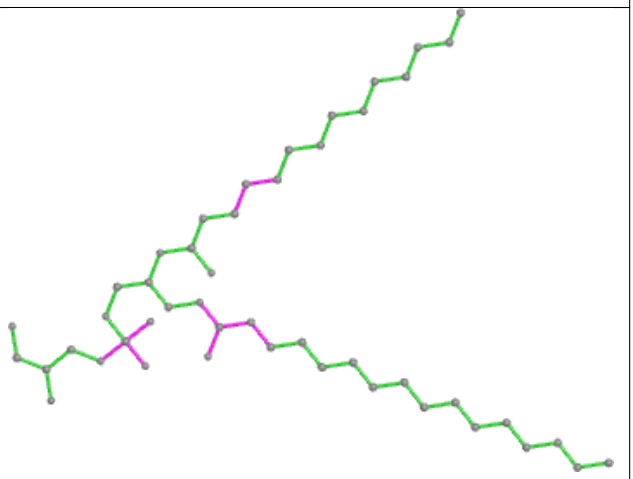


Rings

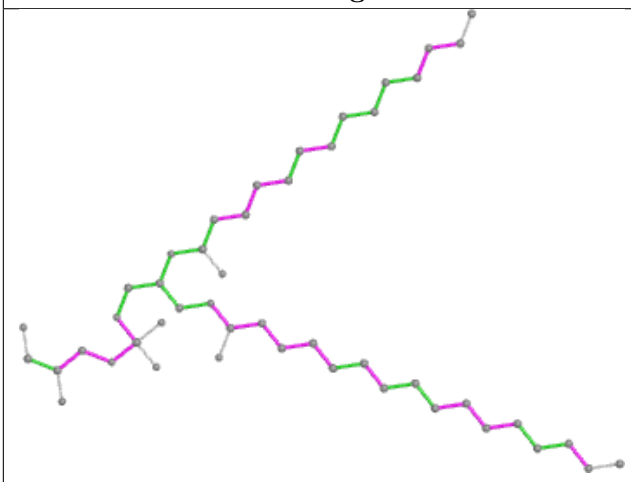
Ligand LHG D 408



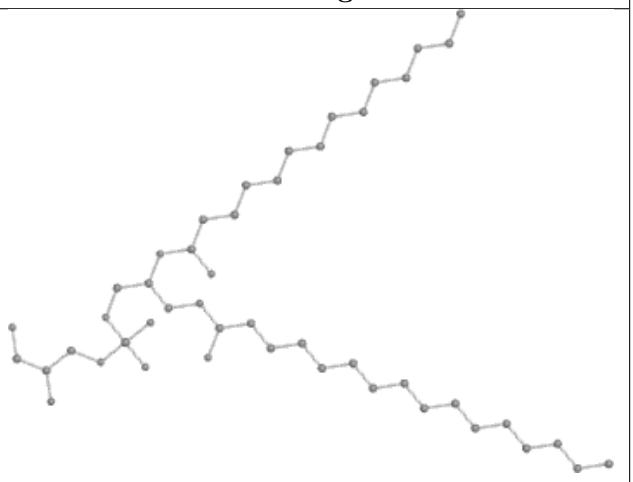
Bond lengths



Bond angles

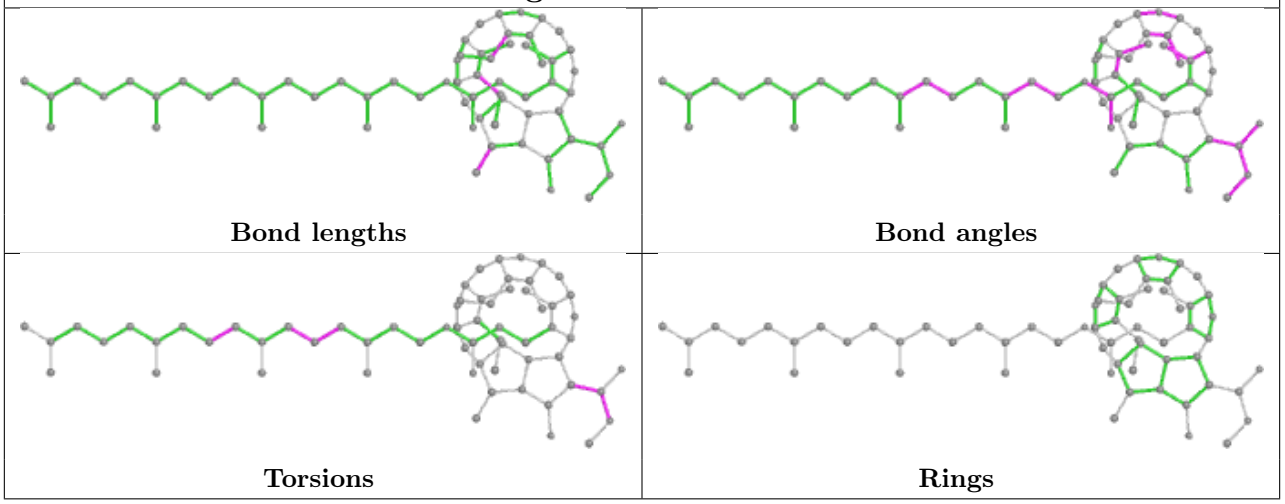


Torsions

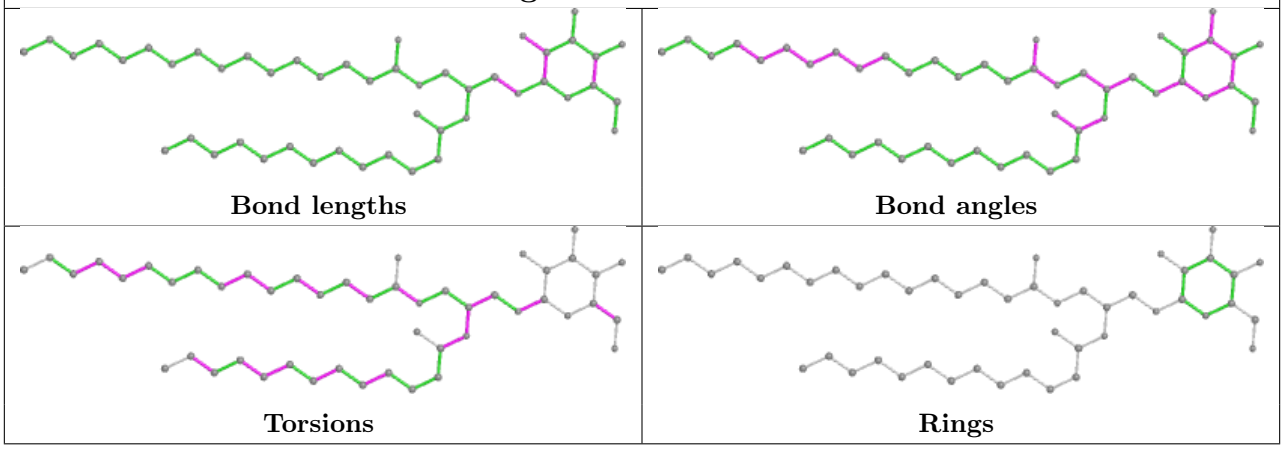


Rings

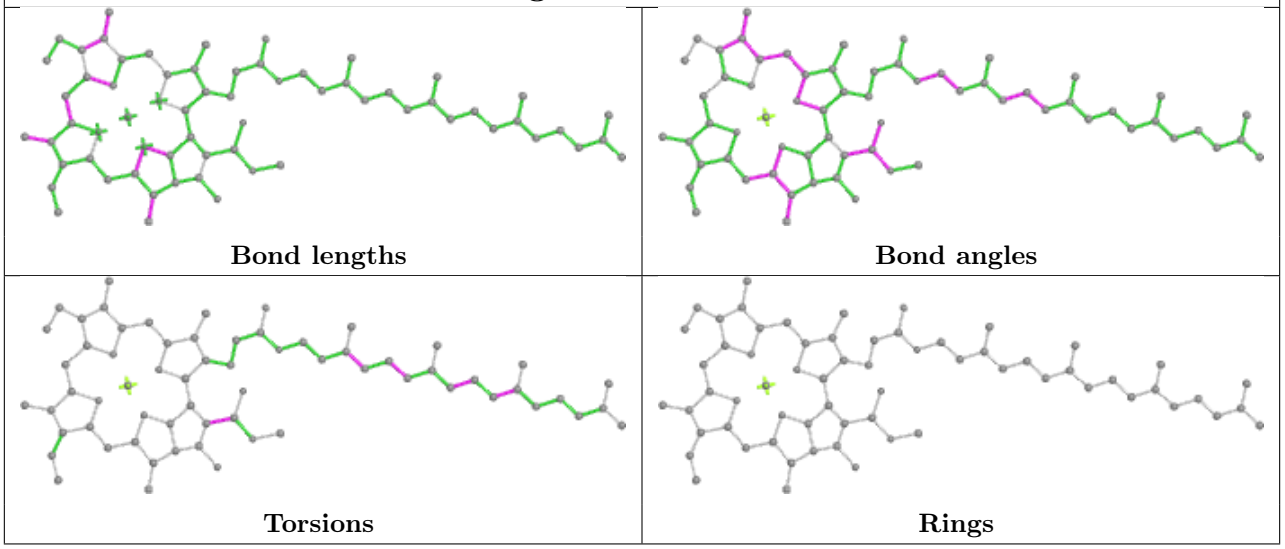
Ligand PHO d 401



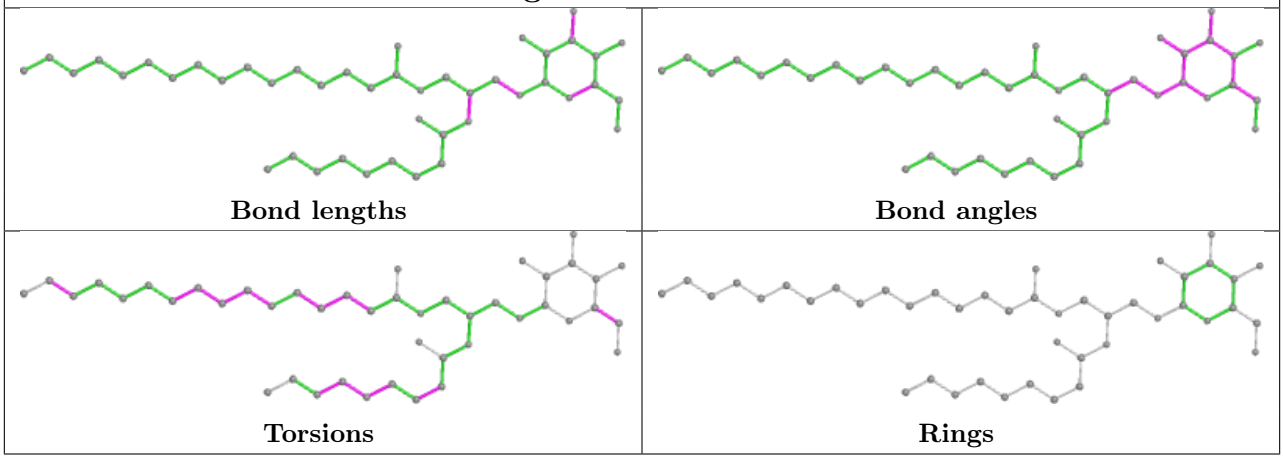
Ligand LMG A 612



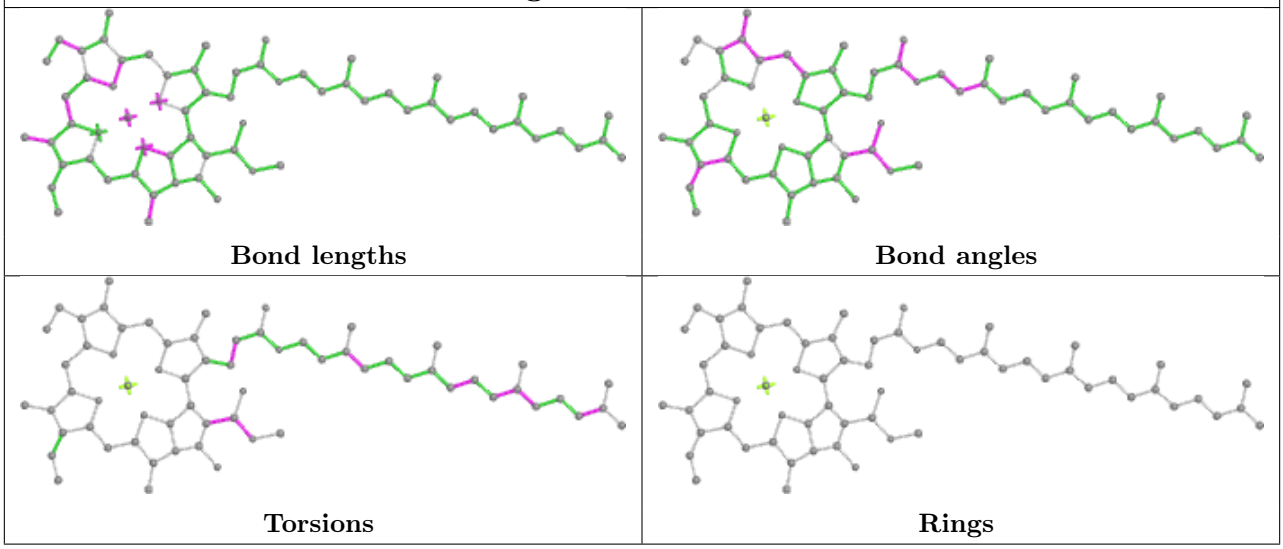
Ligand CLA b 603



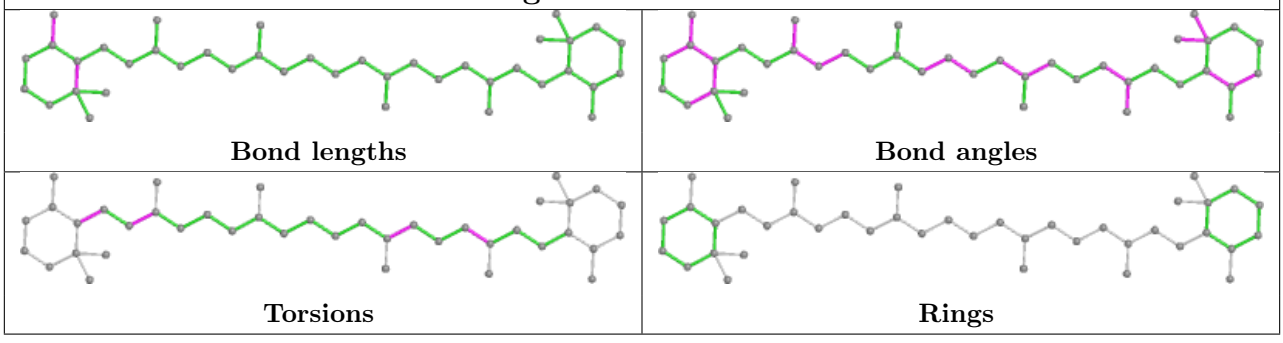
Ligand LMG d 406



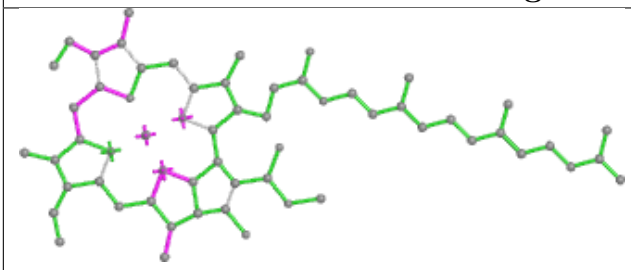
Ligand CLA B 614



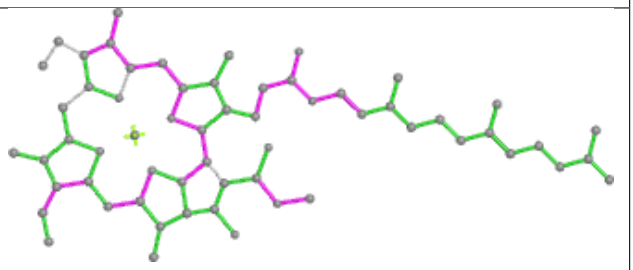
Ligand BCR A 608



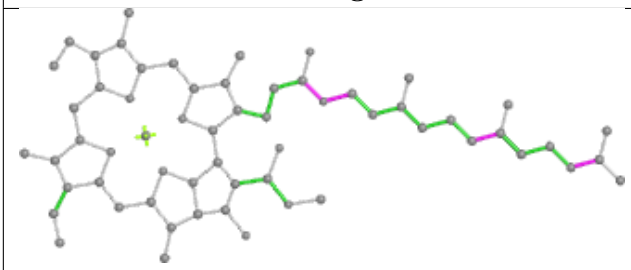
Ligand CLA B 616



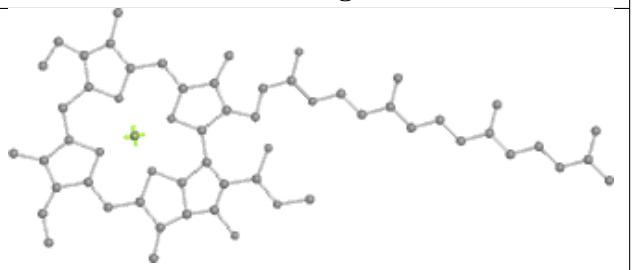
Bond lengths



Bond angles

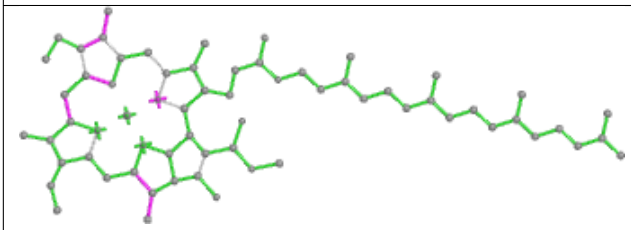


Torsions

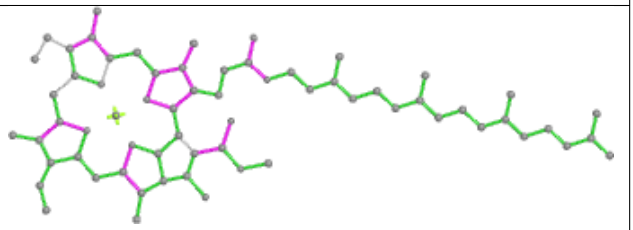


Rings

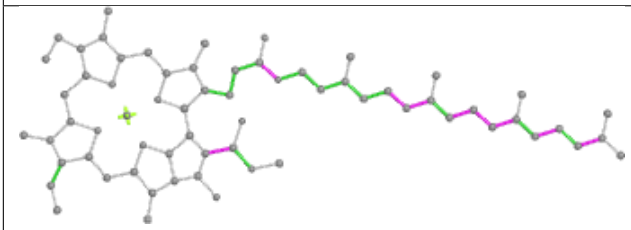
Ligand CLA b 607



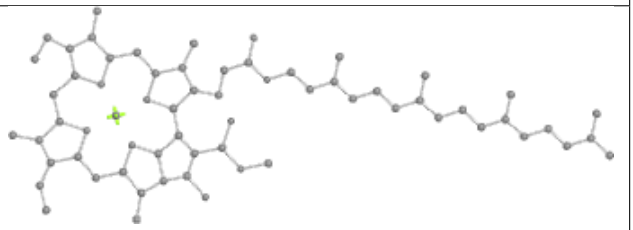
Bond lengths



Bond angles

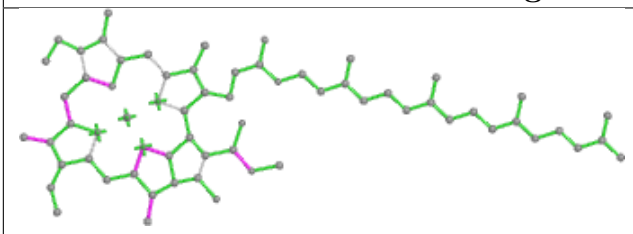


Torsions

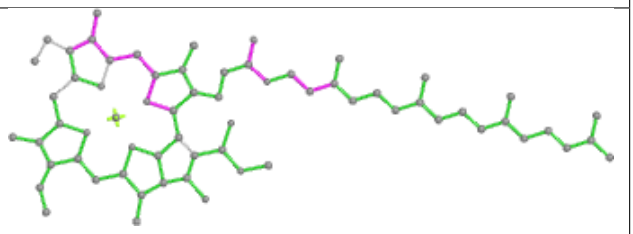


Rings

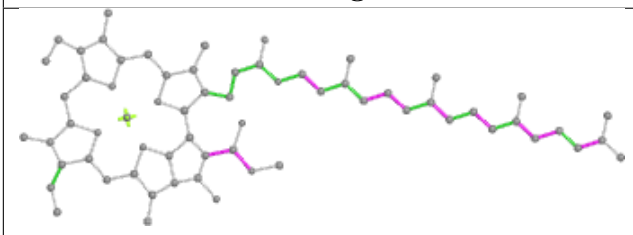
Ligand CLA C 509



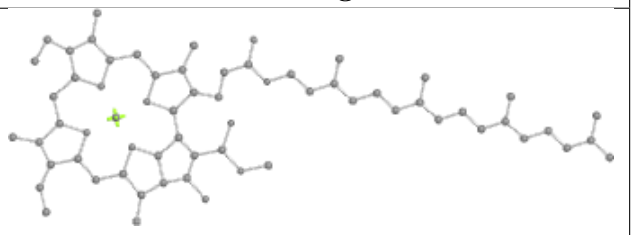
Bond lengths



Bond angles

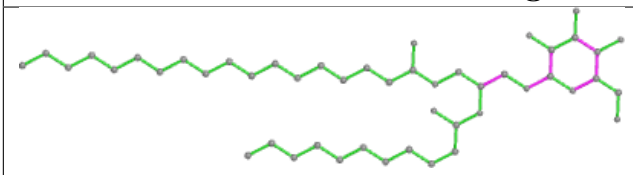


Torsions

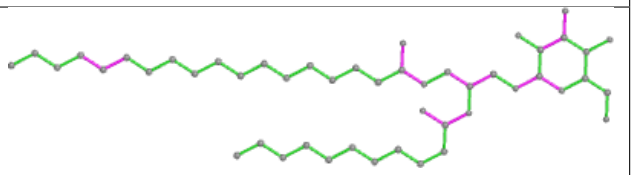


Rings

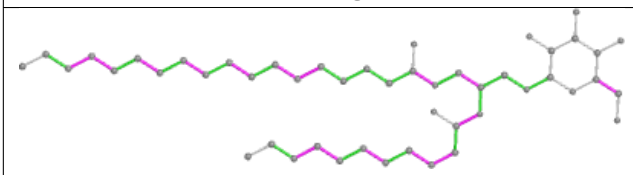
Ligand LMG c 521



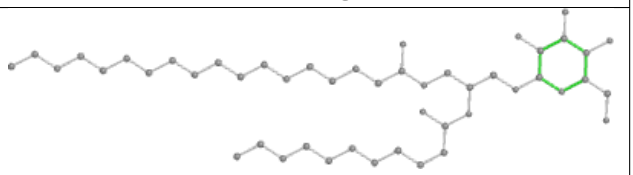
Bond lengths



Bond angles

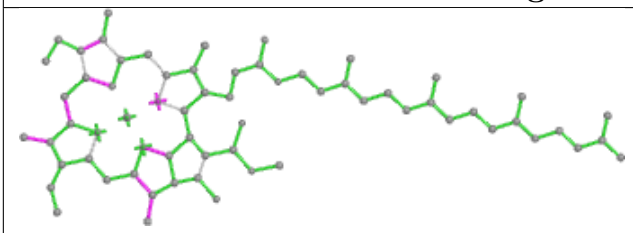


Torsions

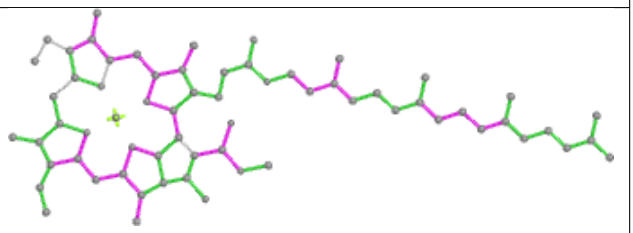


Rings

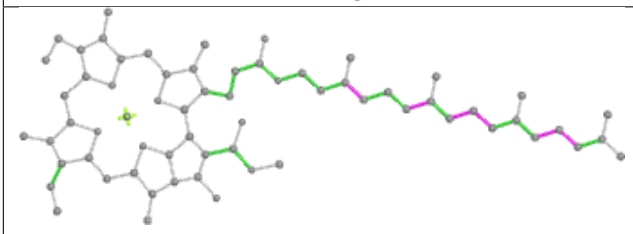
Ligand CLA b 611



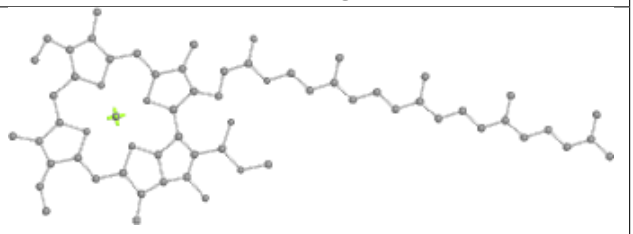
Bond lengths



Bond angles

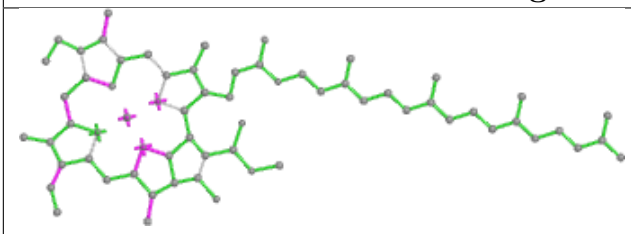


Torsions

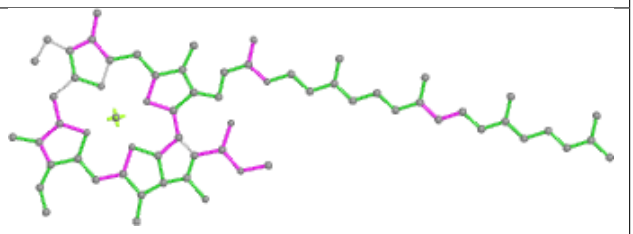


Rings

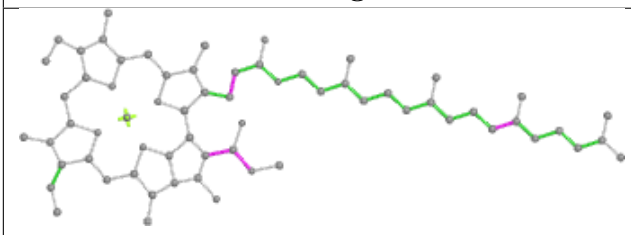
Ligand CLA c 501



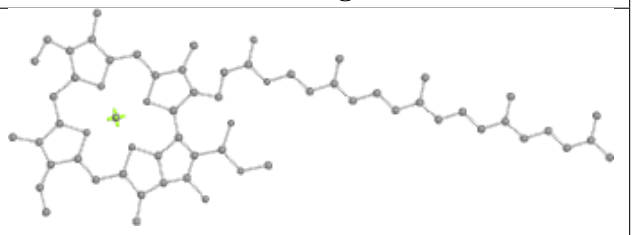
Bond lengths



Bond angles

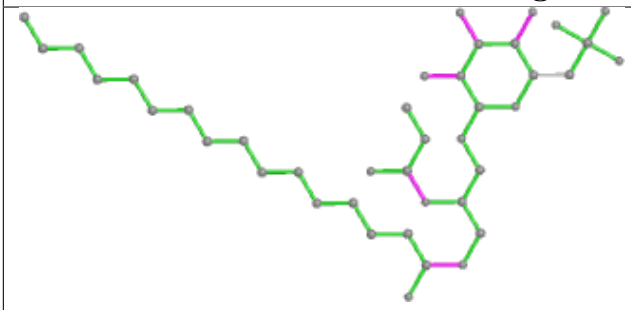


Torsions

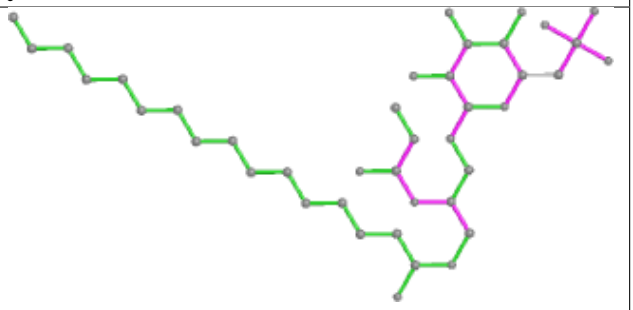


Rings

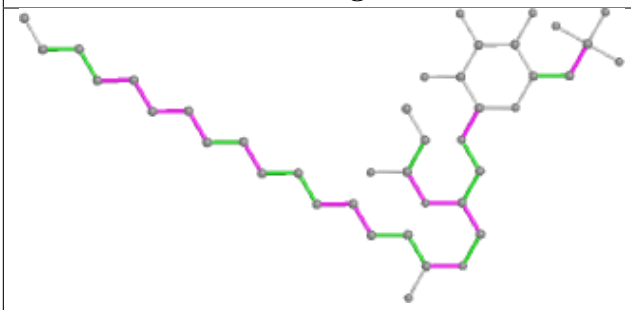
Ligand SQD f 101



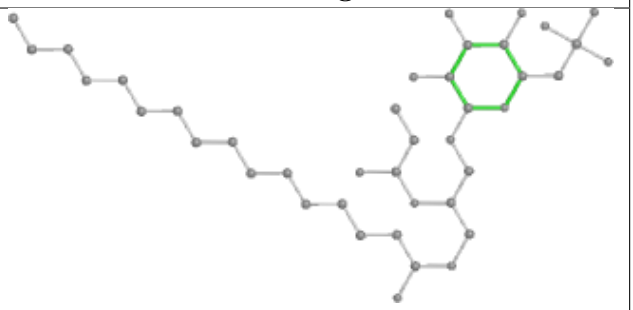
Bond lengths



Bond angles

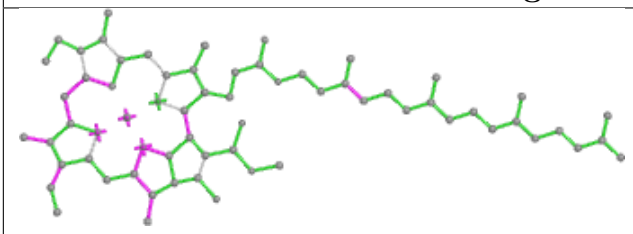


Torsions

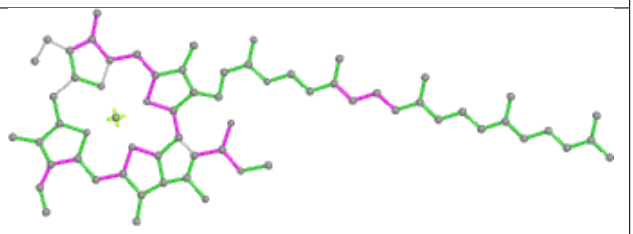


Rings

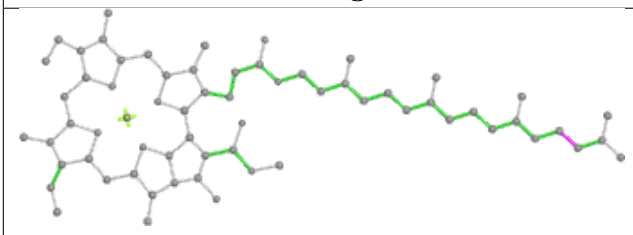
Ligand CLA A 603



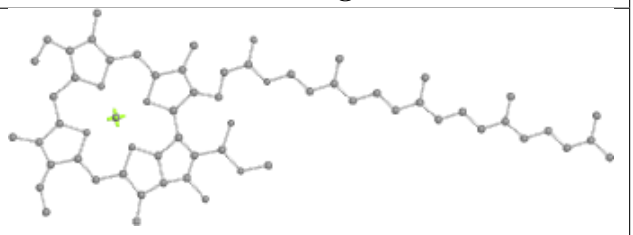
Bond lengths



Bond angles

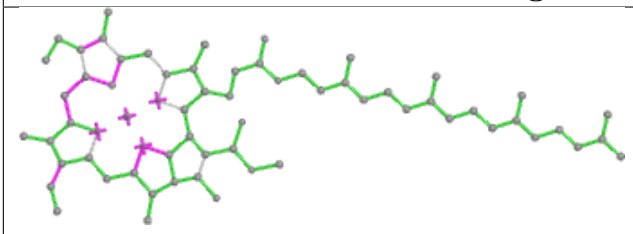


Torsions

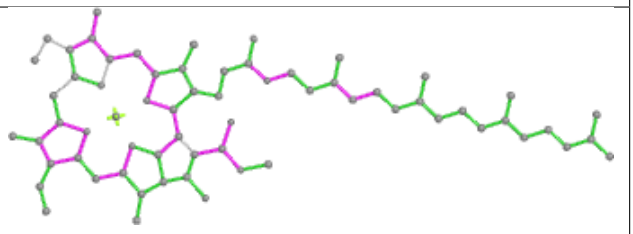


Rings

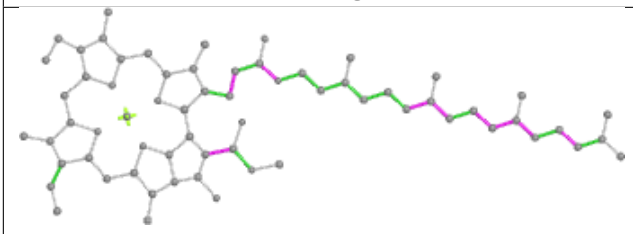
Ligand CLA b 606



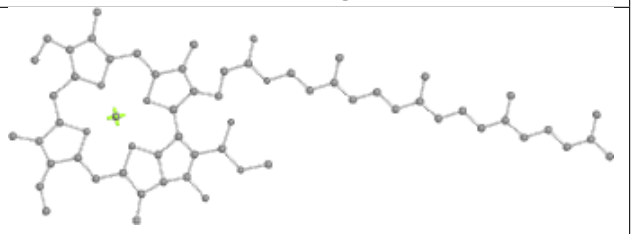
Bond lengths



Bond angles

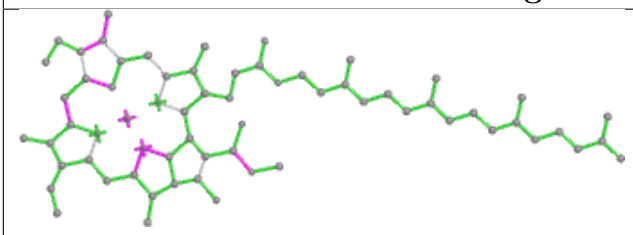


Torsions

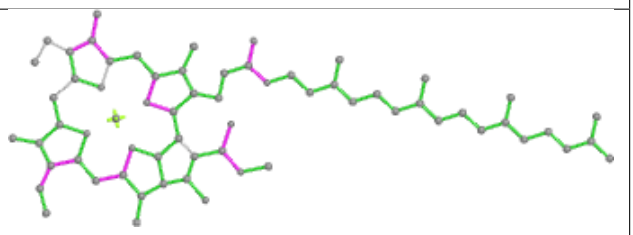


Rings

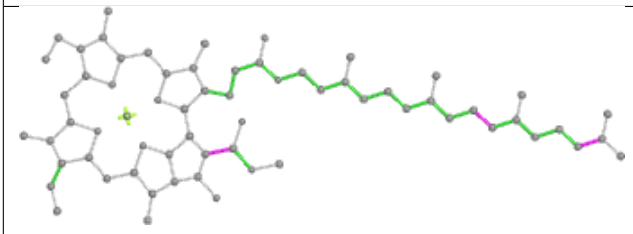
Ligand CLA C 502



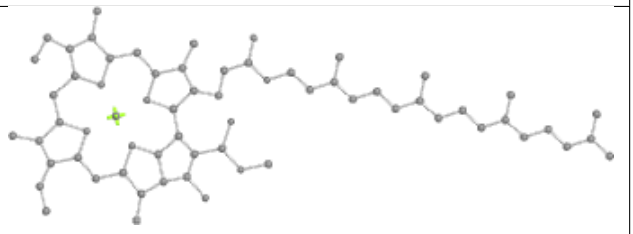
Bond lengths



Bond angles

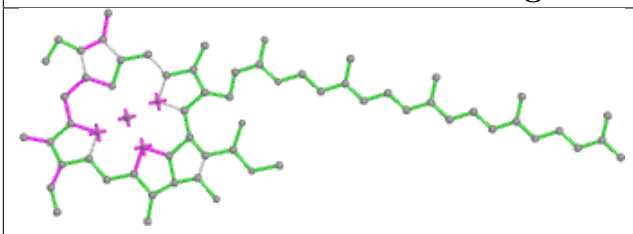


Torsions

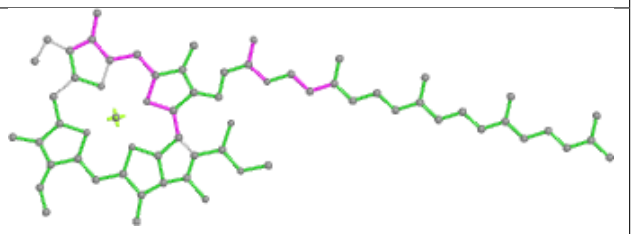


Rings

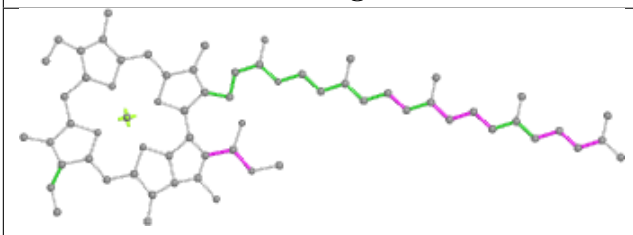
Ligand CLA B 607



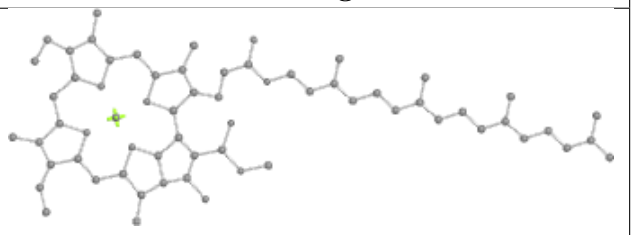
Bond lengths



Bond angles

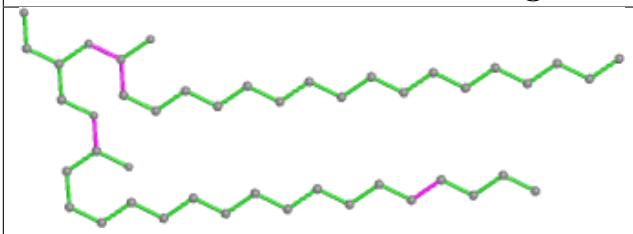


Torsions

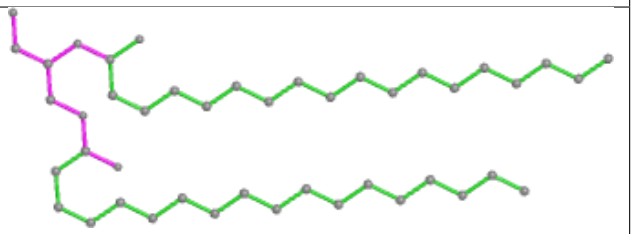


Rings

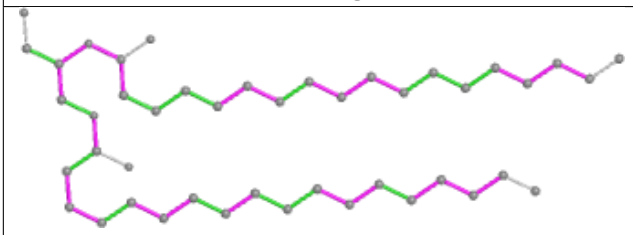
Ligand DGD a 616



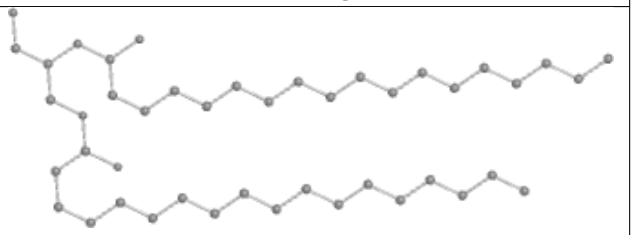
Bond lengths



Bond angles

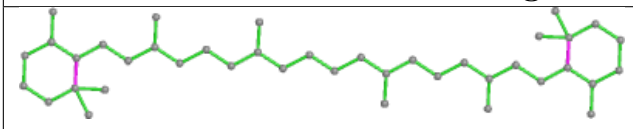


Torsions

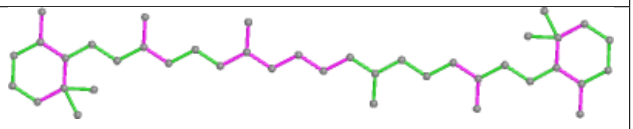


Rings

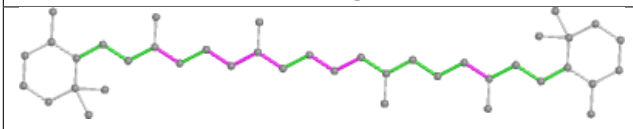
Ligand BCR B 619



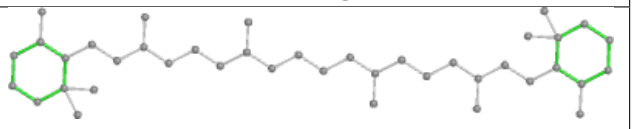
Bond lengths



Bond angles

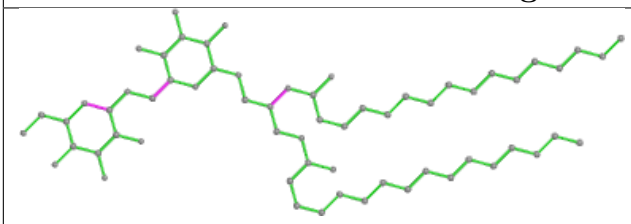


Torsions

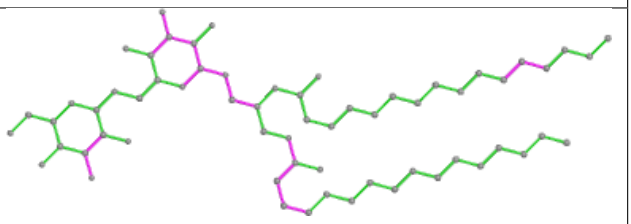


Rings

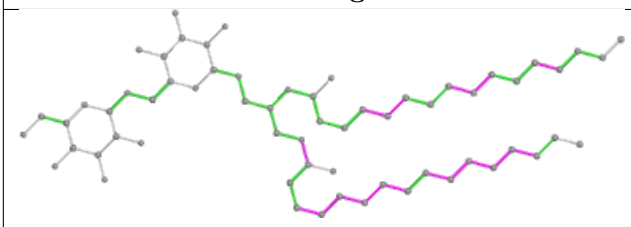
Ligand DGD C 518



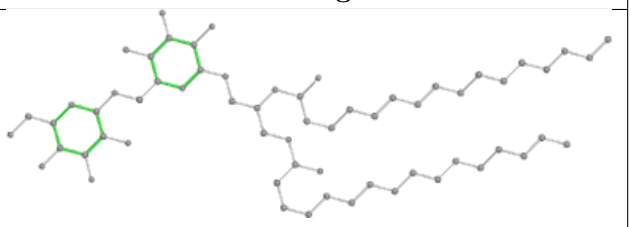
Bond lengths



Bond angles

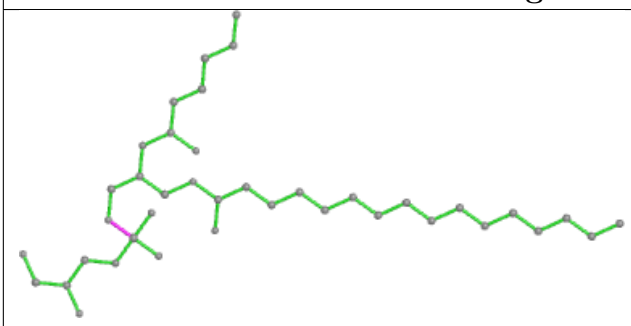


Torsions

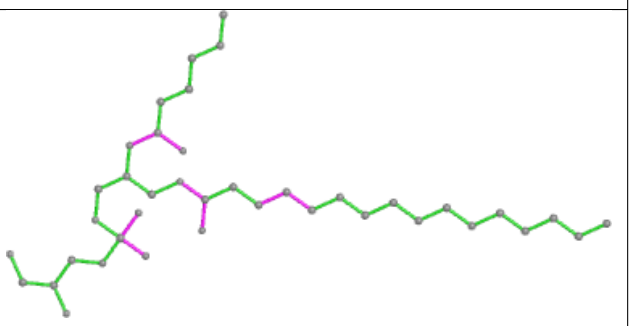


Rings

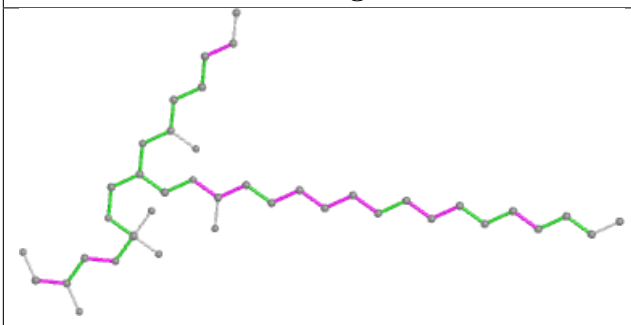
Ligand LHG d 409



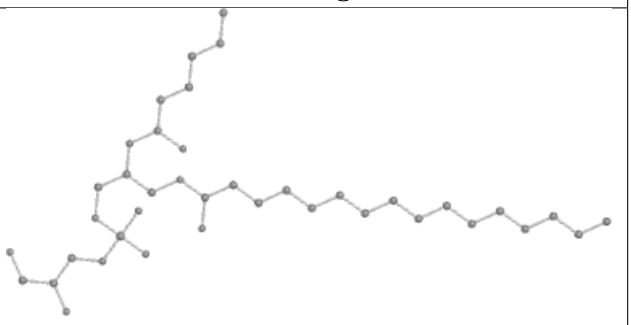
Bond lengths



Bond angles

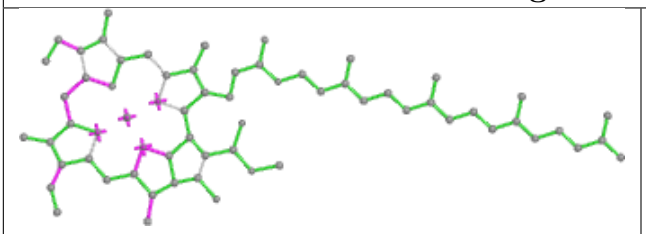


Torsions

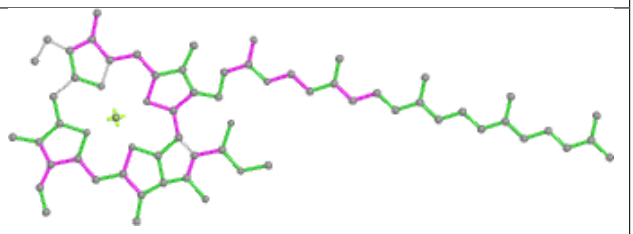


Rings

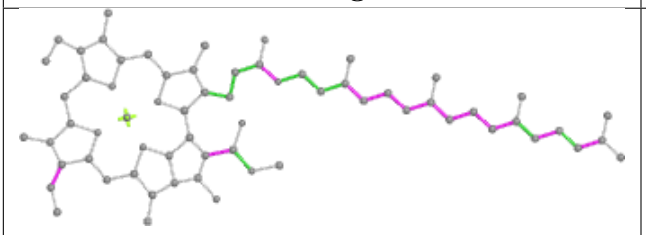
Ligand CLA c 506



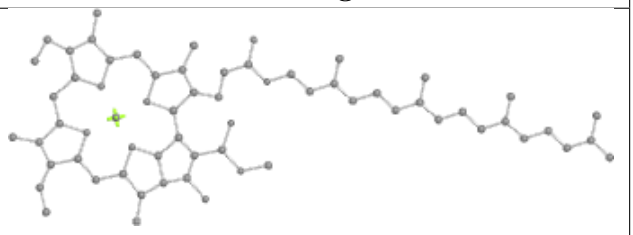
Bond lengths



Bond angles

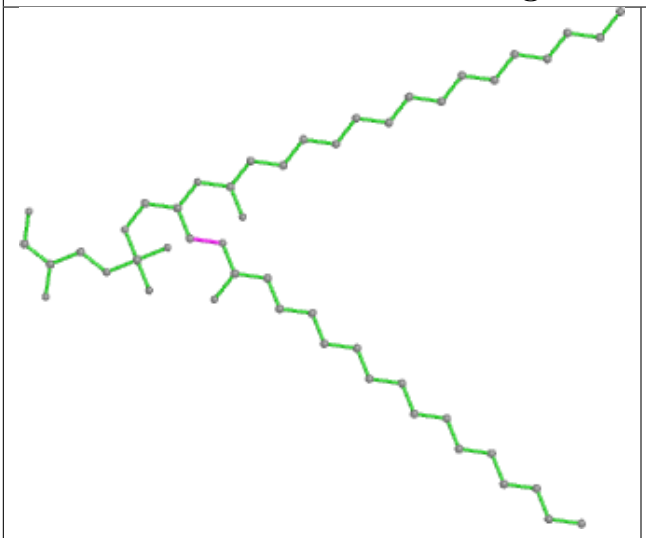


Torsions

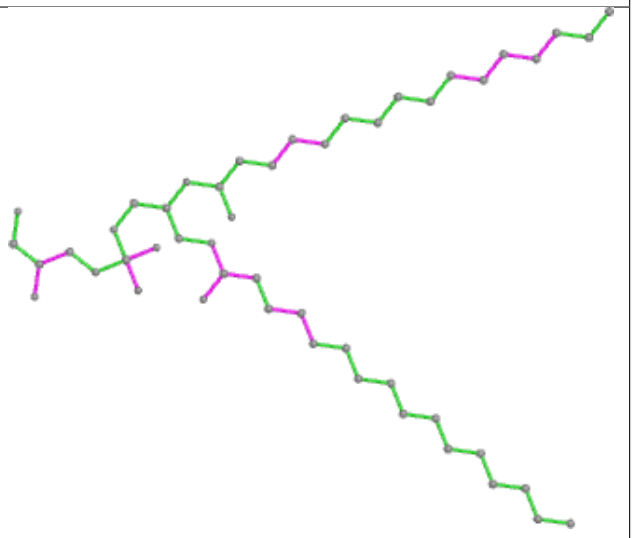


Rings

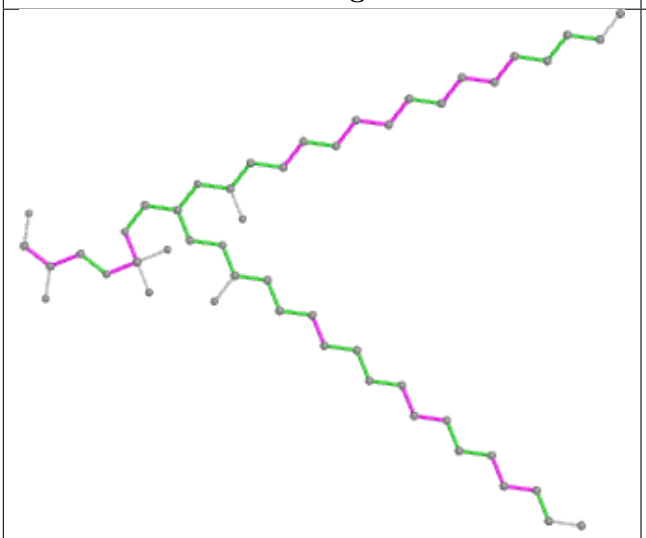
Ligand LHG D 406



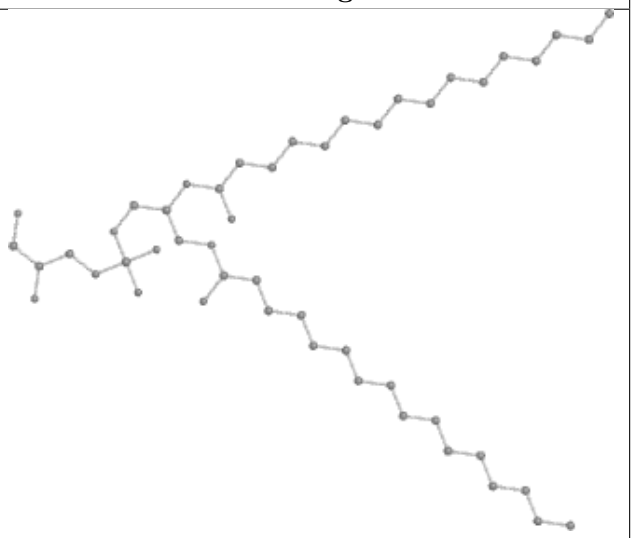
Bond lengths



Bond angles

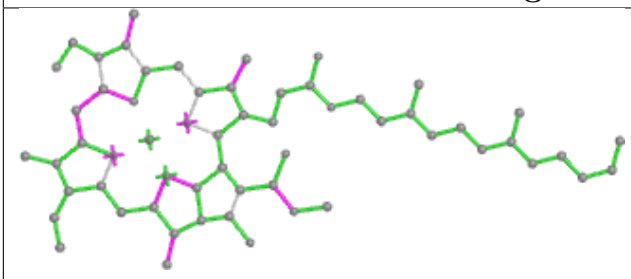


Torsions

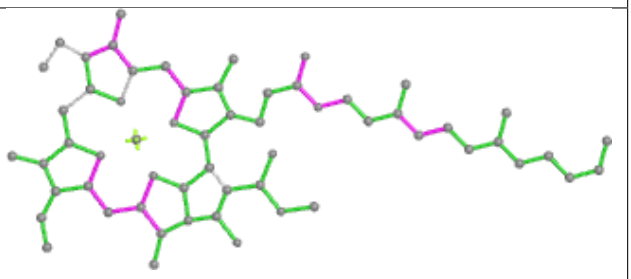


Rings

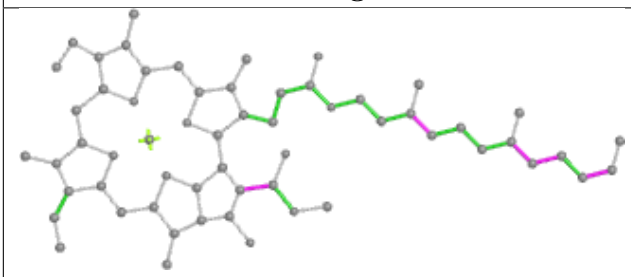
Ligand CLA C 504



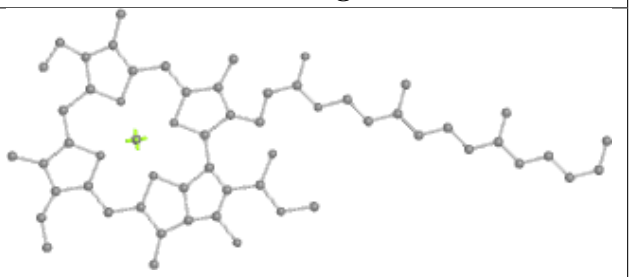
Bond lengths



Bond angles

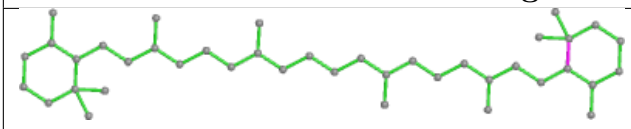


Torsions

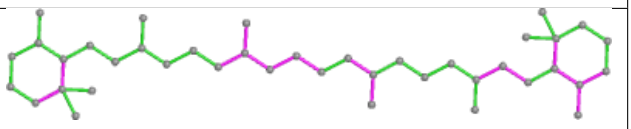


Rings

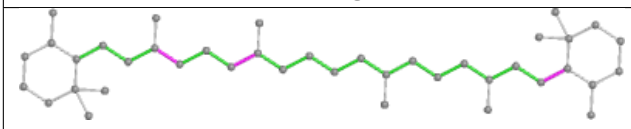
Ligand BCR H 101



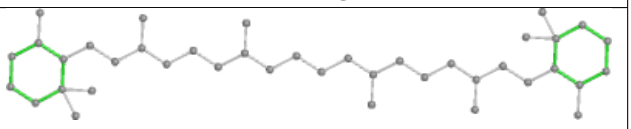
Bond lengths



Bond angles



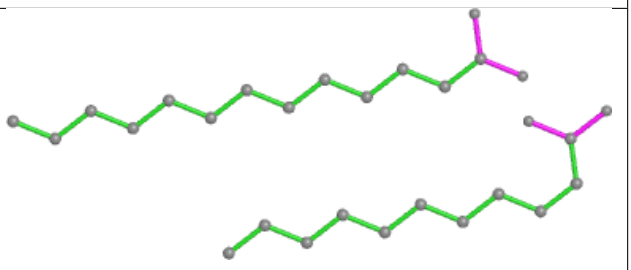
Torsions



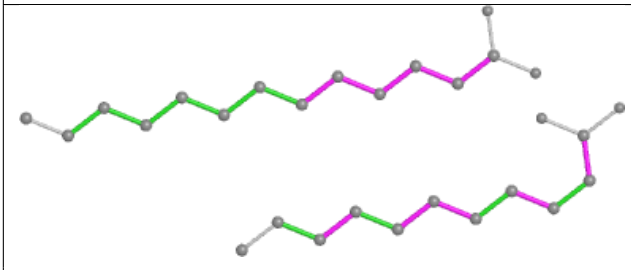
Rings

Ligand LMG B 622

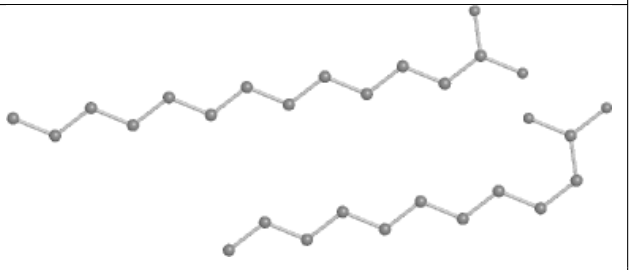
Bond lengths



Bond angles

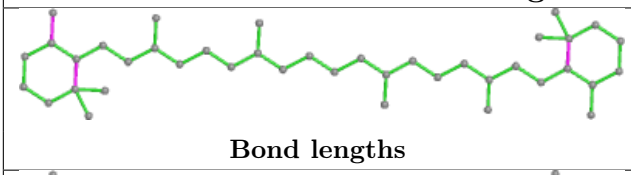


Torsions

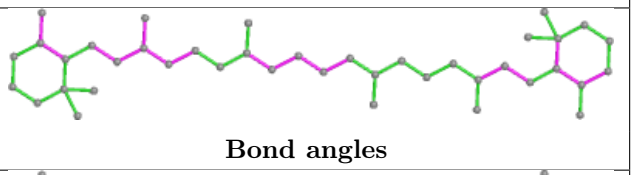


Rings

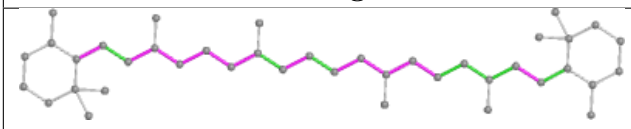
Ligand BCR c 514



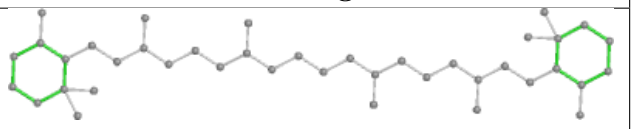
Bond lengths



Bond angles

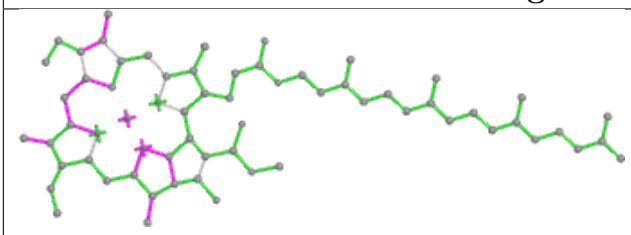


Torsions

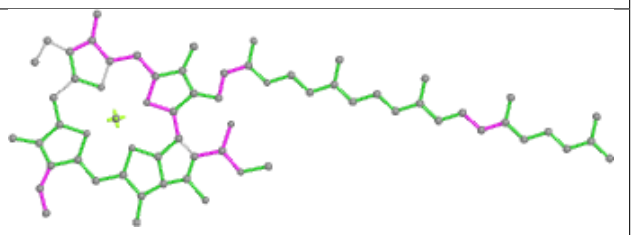


Rings

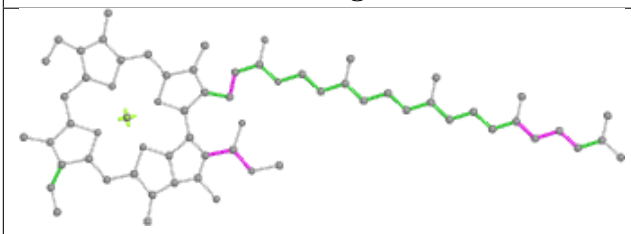
Ligand CLA b 610



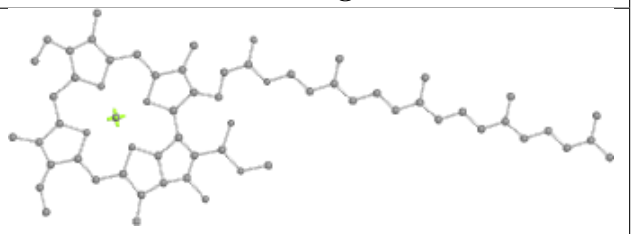
Bond lengths



Bond angles

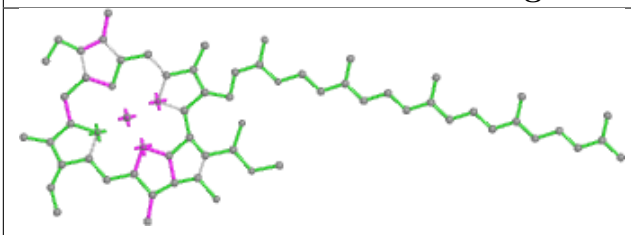


Torsions

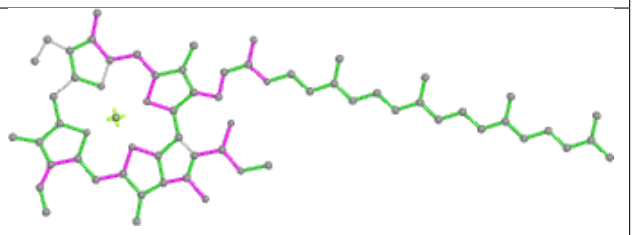


Rings

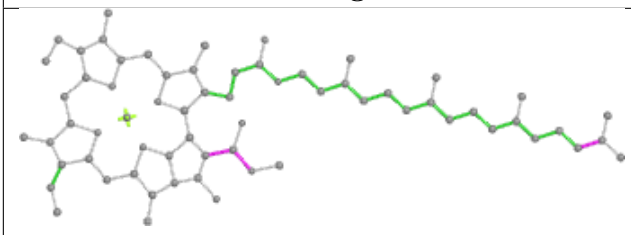
Ligand CLA C 501



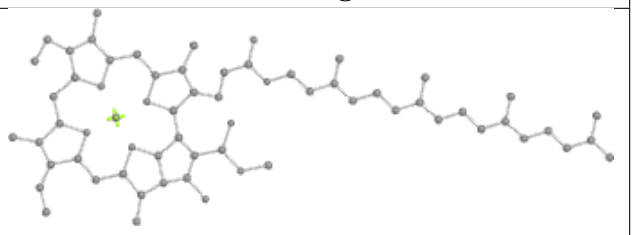
Bond lengths



Bond angles

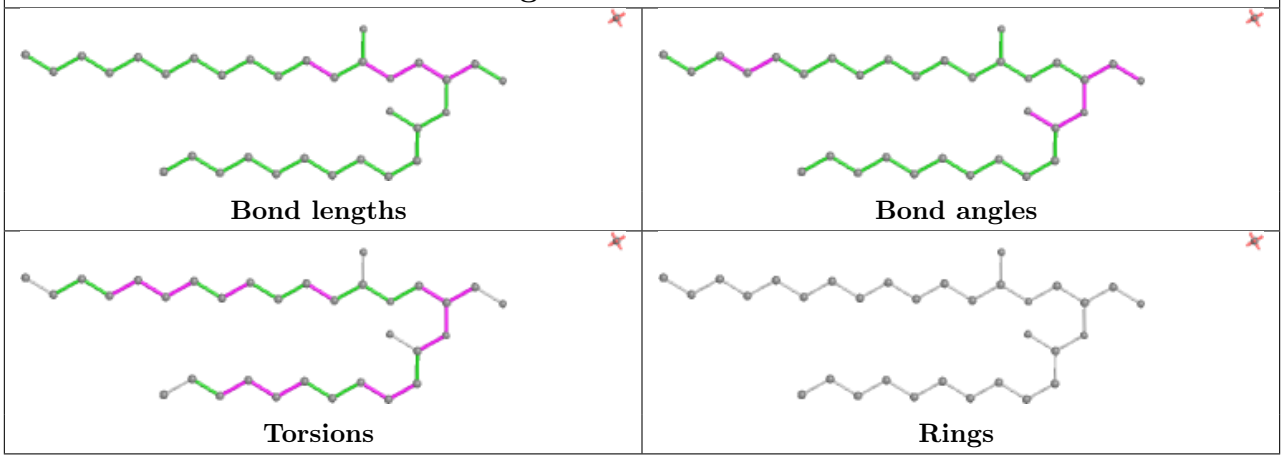


Torsions

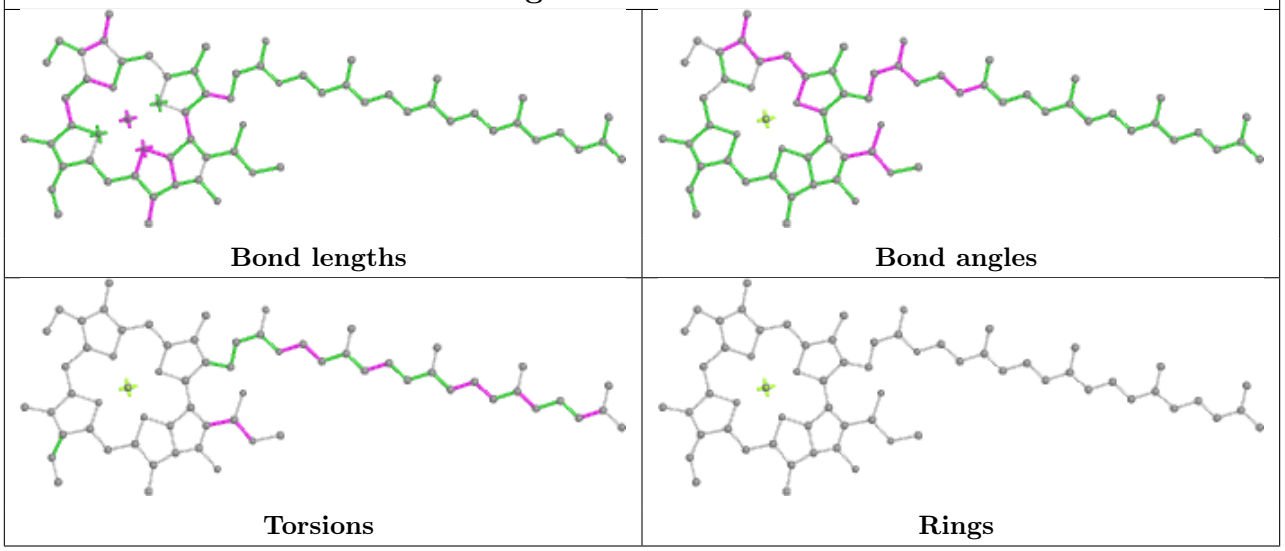


Rings

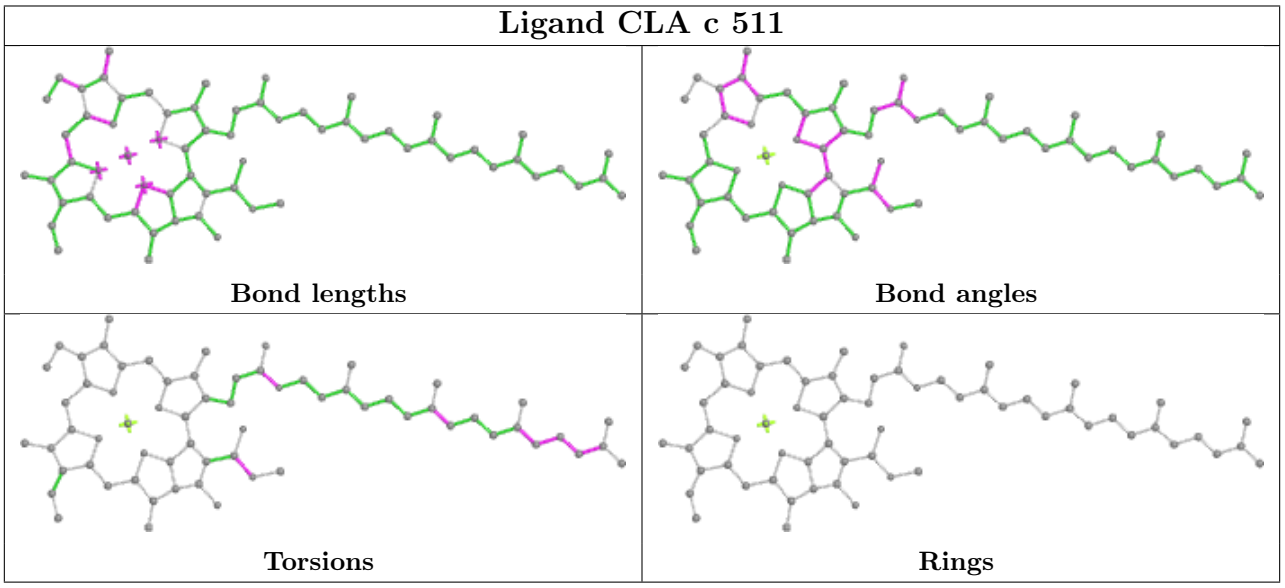
Ligand LMG D 409



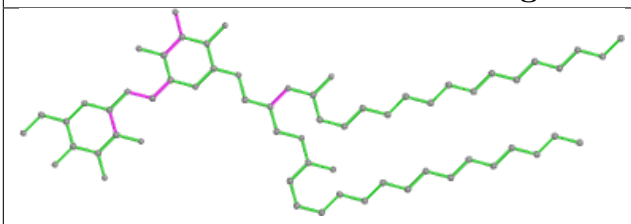
Ligand CLA C 512



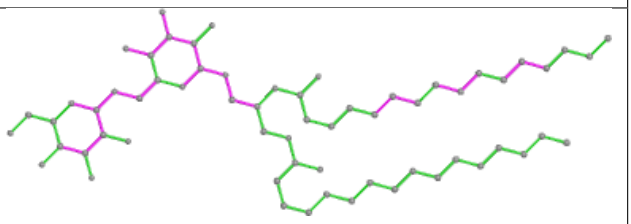
Ligand CLA c 511



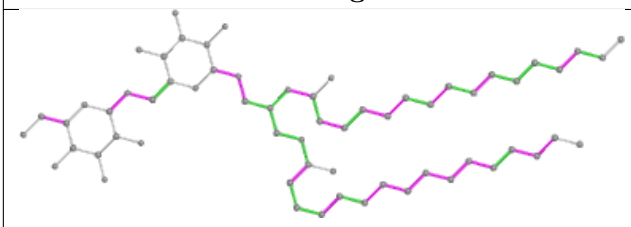
Ligand DGD C 517



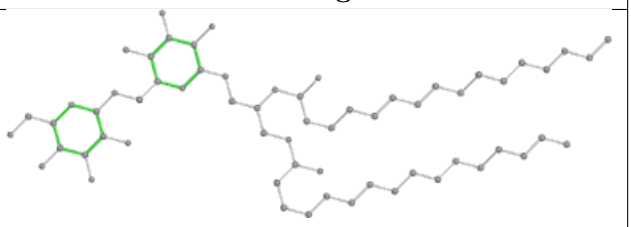
Bond lengths



Bond angles

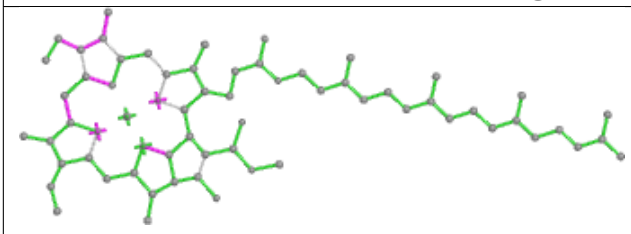


Torsions

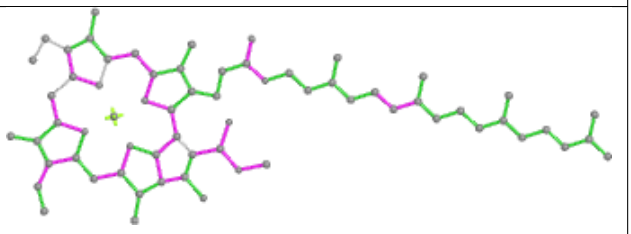


Rings

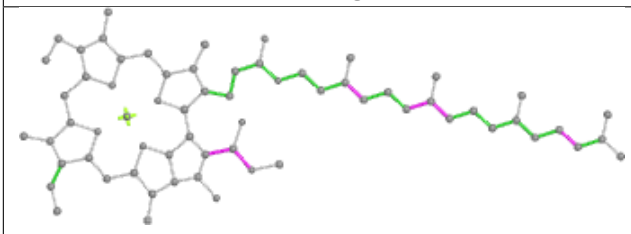
Ligand CLA c 505



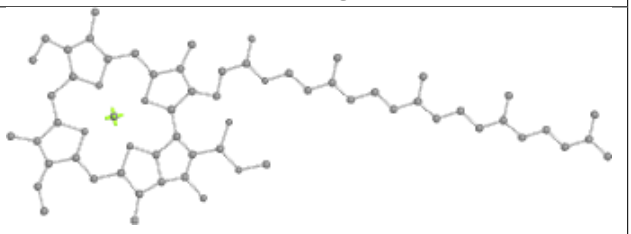
Bond lengths



Bond angles

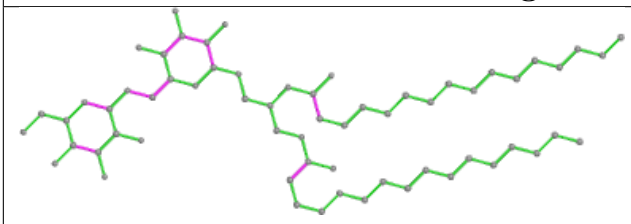


Torsions

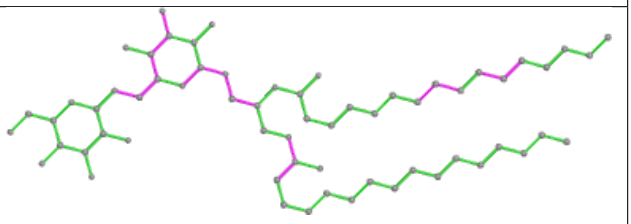


Rings

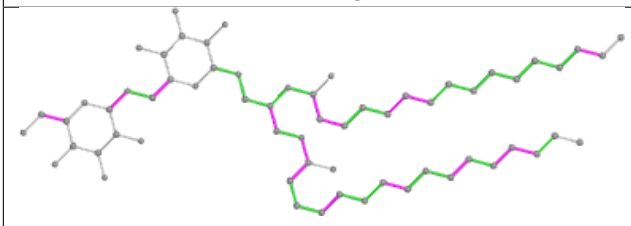
Ligand DGD C 516



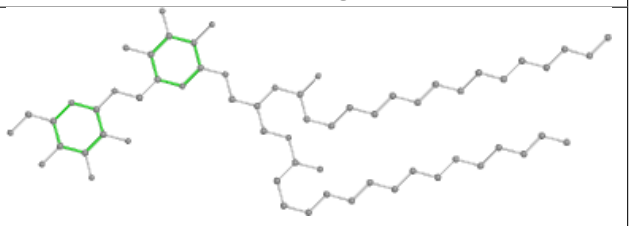
Bond lengths



Bond angles

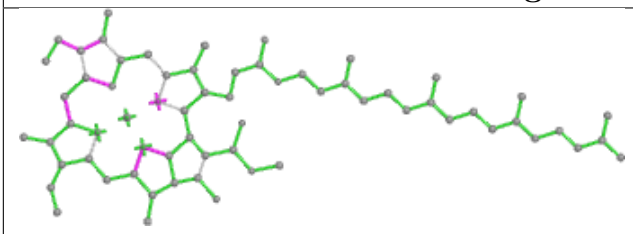


Torsions

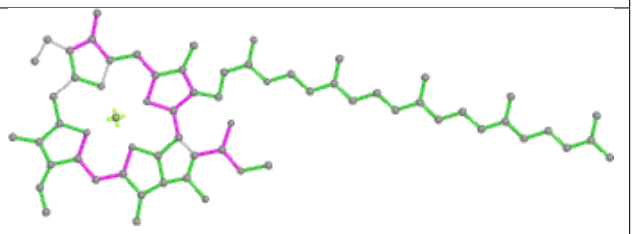


Rings

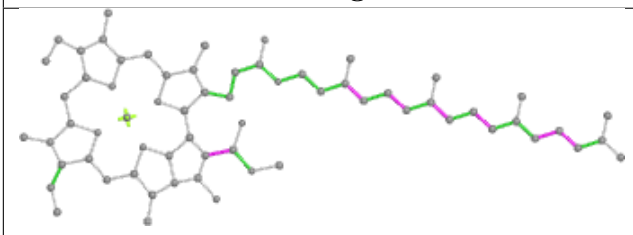
Ligand CLA C 507



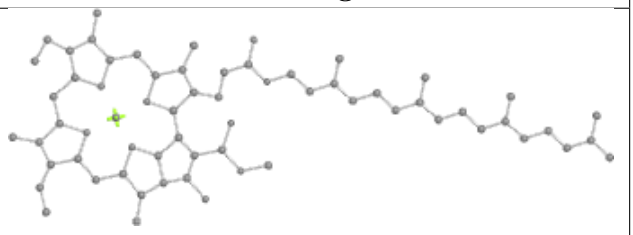
Bond lengths



Bond angles

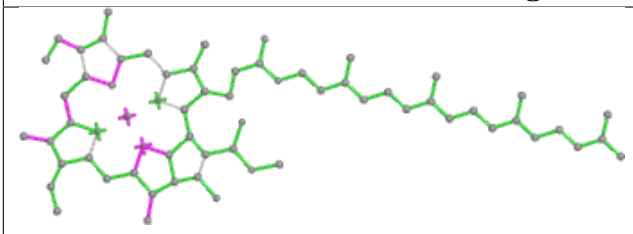


Torsions

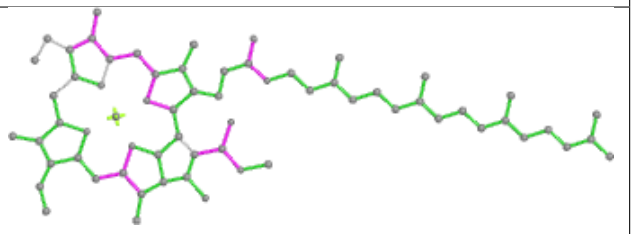


Rings

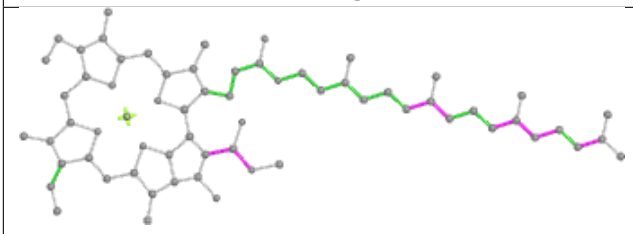
Ligand CLA C 508



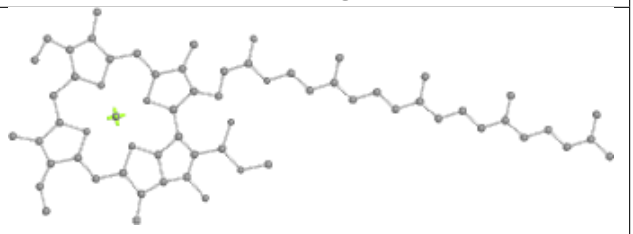
Bond lengths



Bond angles

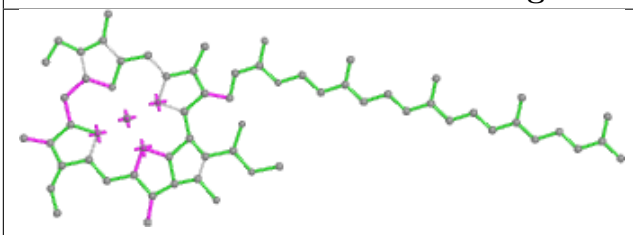


Torsions

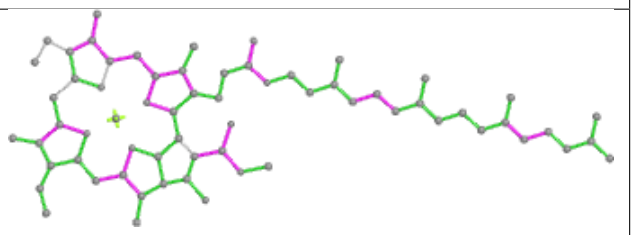


Rings

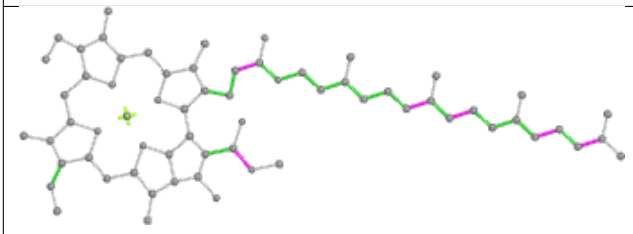
Ligand CLA b 613



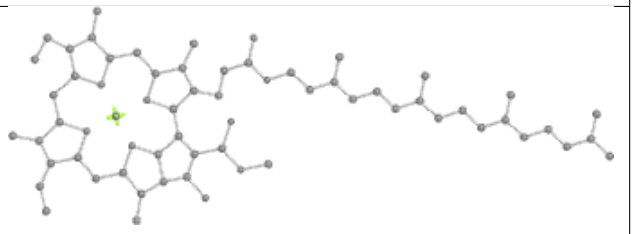
Bond lengths



Bond angles

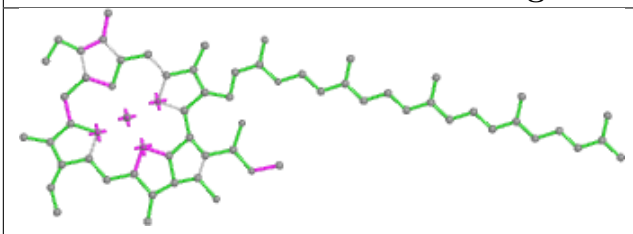


Torsions

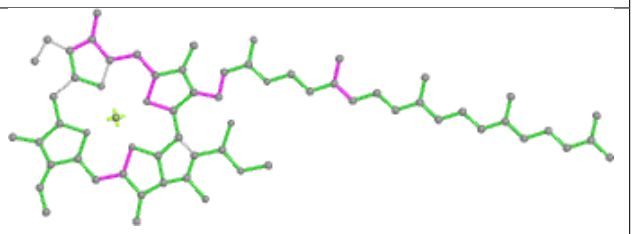


Rings

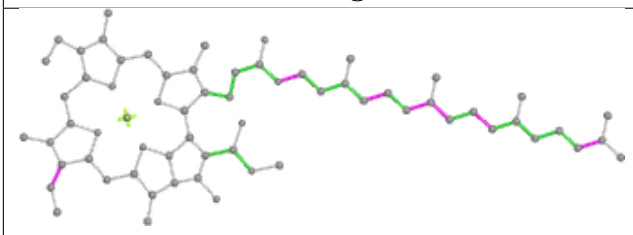
Ligand CLA d 402



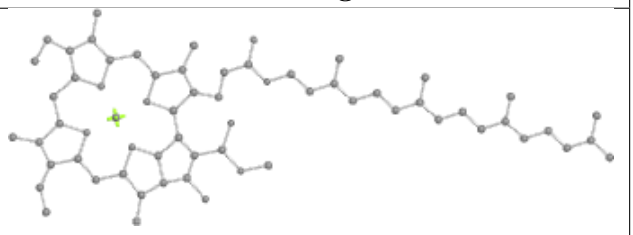
Bond lengths



Bond angles

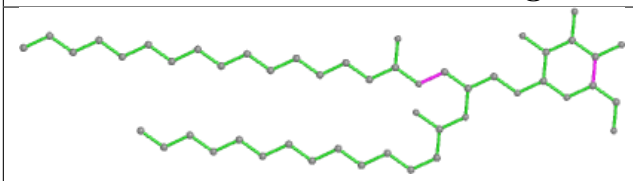


Torsions

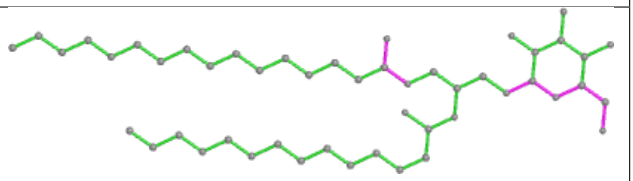


Rings

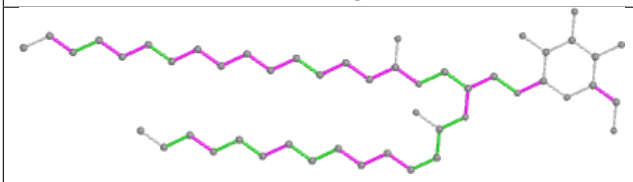
Ligand LMG c 522



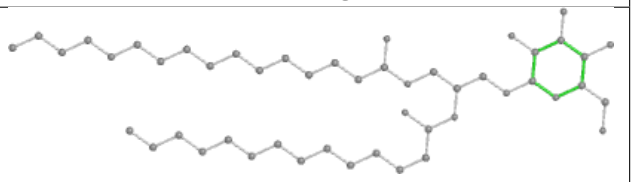
Bond lengths



Bond angles

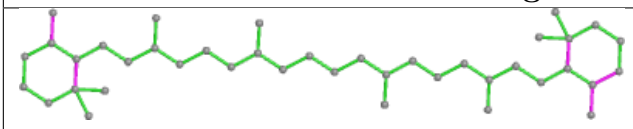


Torsions

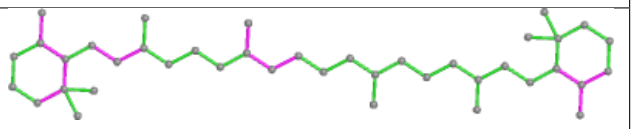


Rings

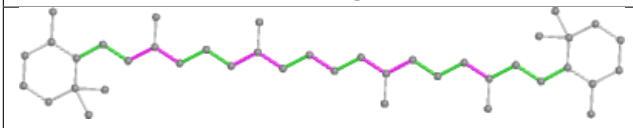
Ligand BCR T 101



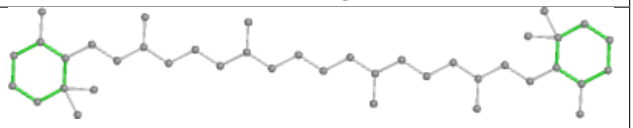
Bond lengths



Bond angles

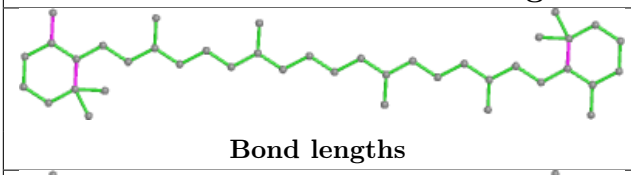


Torsions

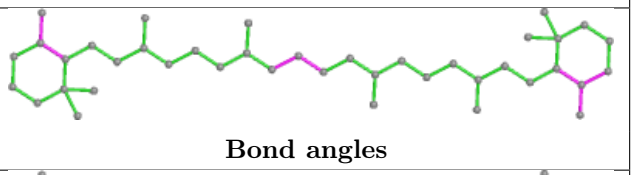


Rings

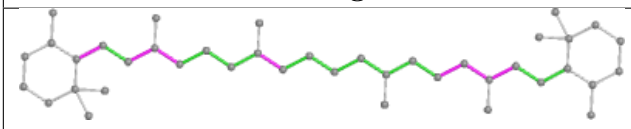
Ligand BCR k 101



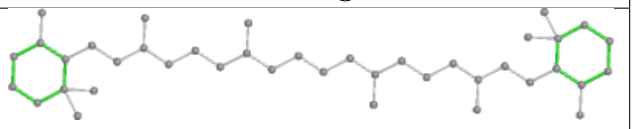
Bond lengths



Bond angles

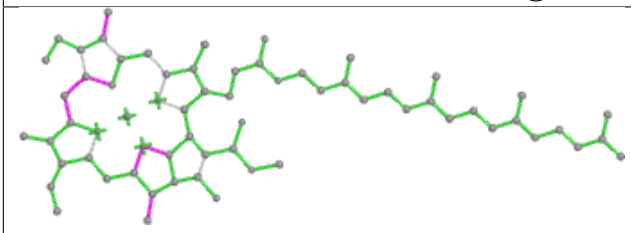


Torsions

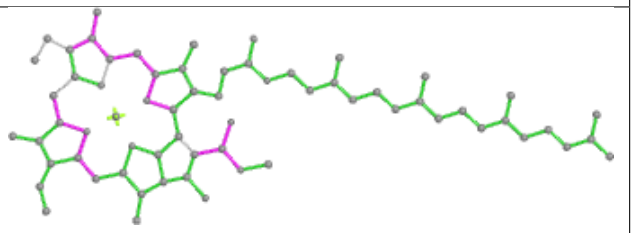


Rings

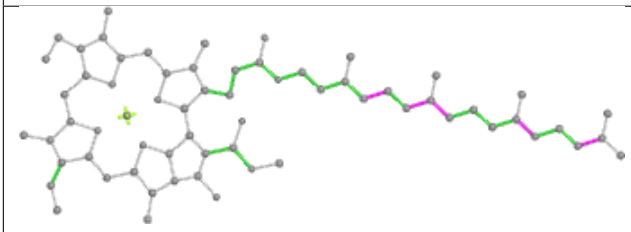
Ligand CLA b 602



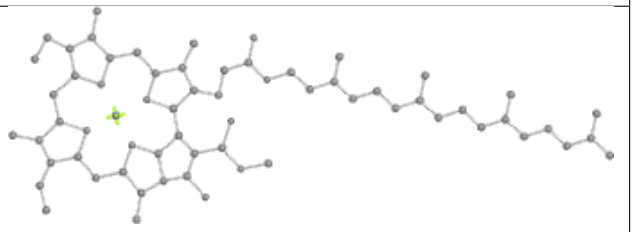
Bond lengths



Bond angles

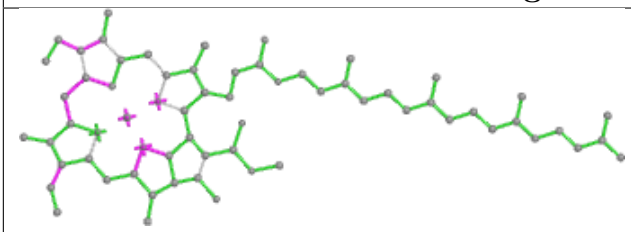


Torsions

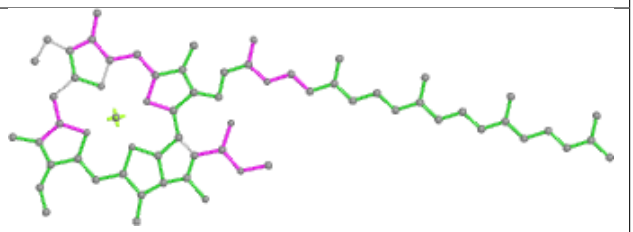


Rings

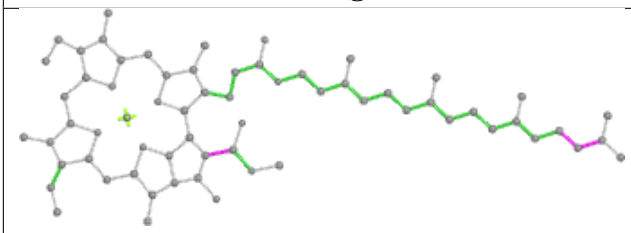
Ligand CLA A 604



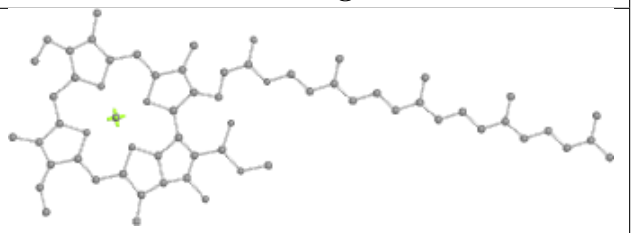
Bond lengths



Bond angles

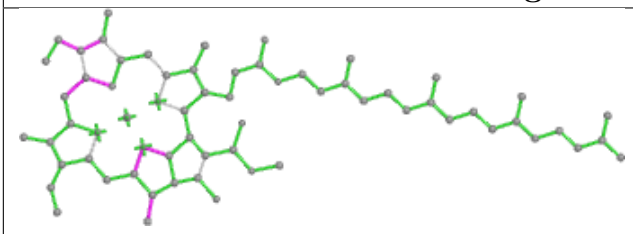


Torsions

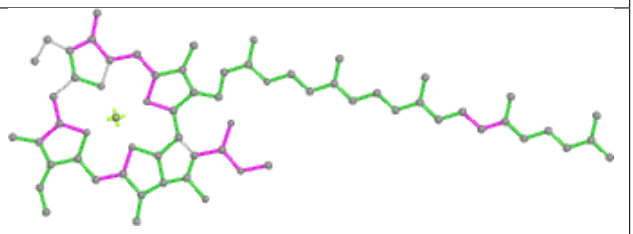


Rings

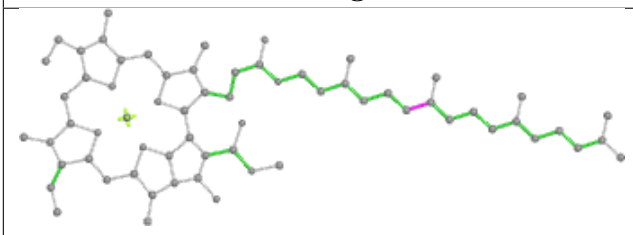
Ligand CLA B 608



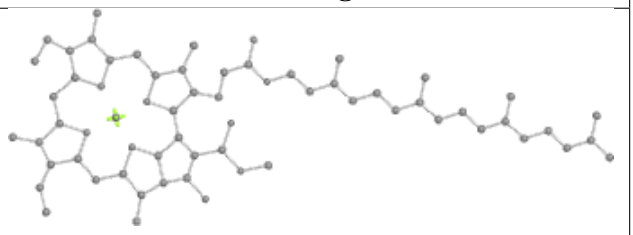
Bond lengths



Bond angles

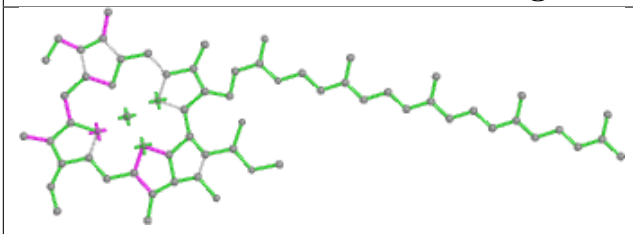


Torsions

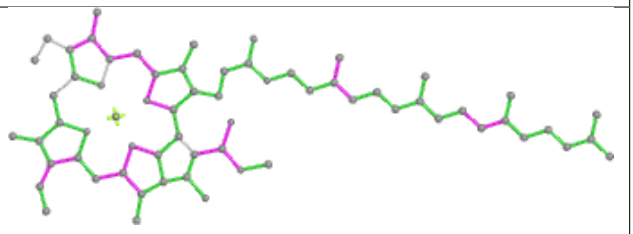


Rings

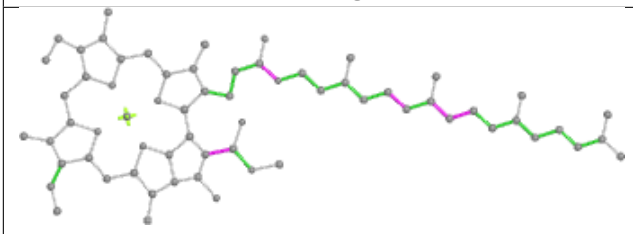
Ligand CLA c 503



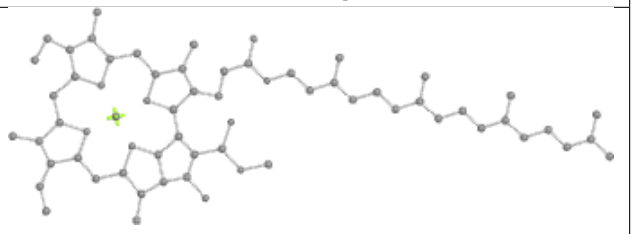
Bond lengths



Bond angles

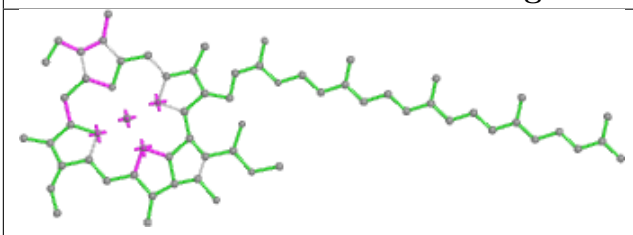


Torsions

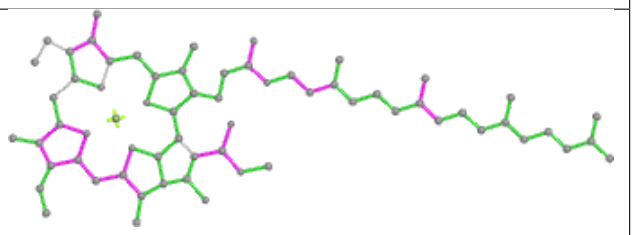


Rings

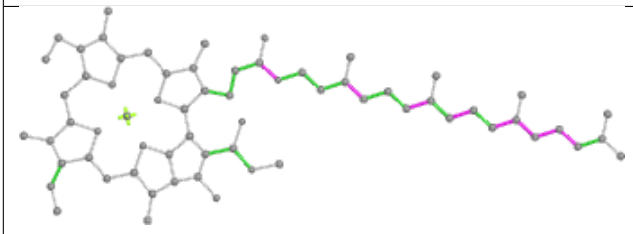
Ligand CLA B 611



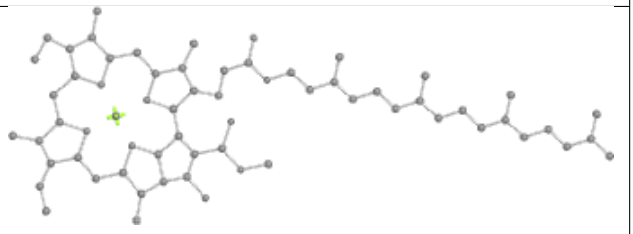
Bond lengths



Bond angles

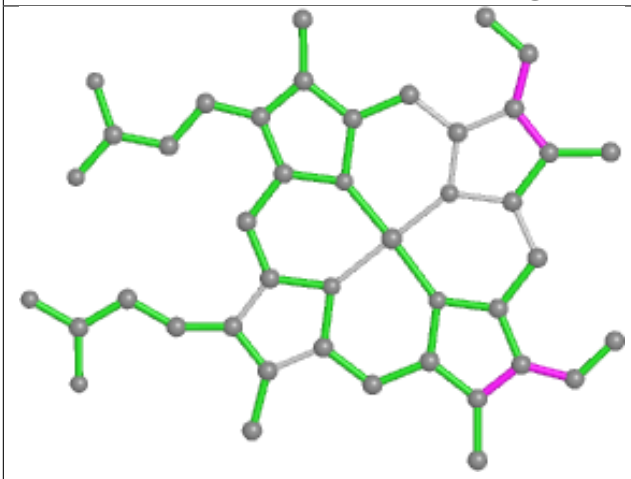


Torsions

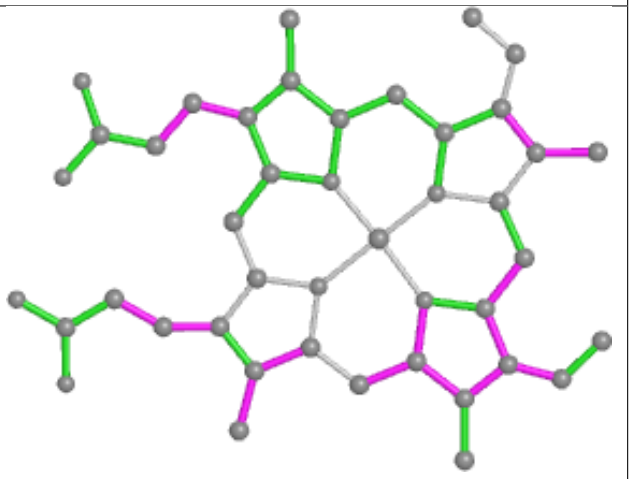


Rings

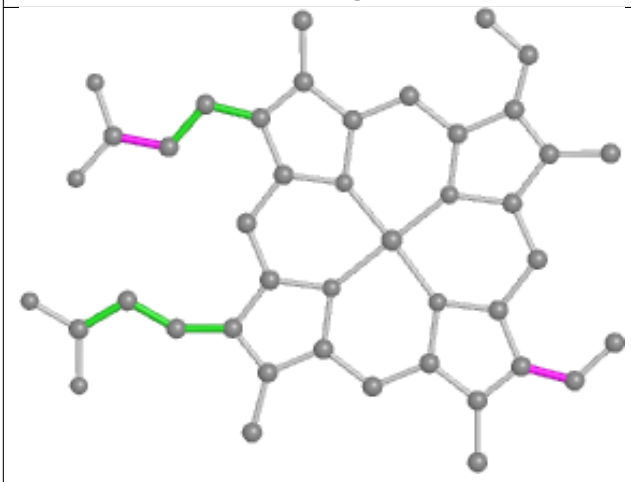
Ligand HEM f 102



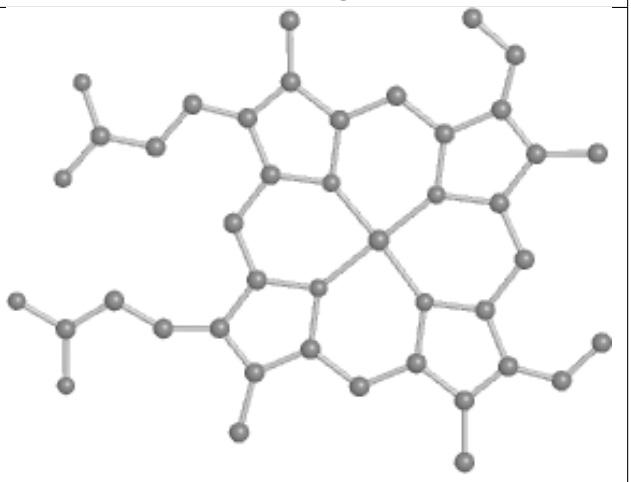
Bond lengths



Bond angles

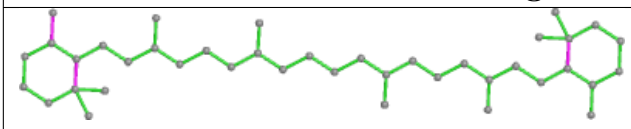


Torsions

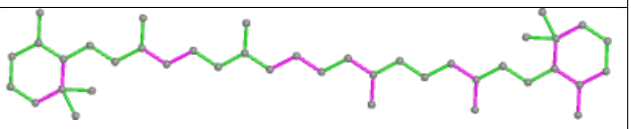


Rings

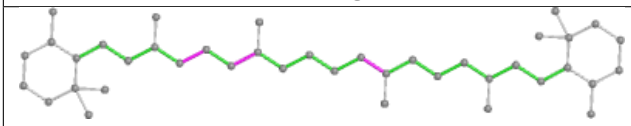
Ligand BCR b 619



Bond lengths



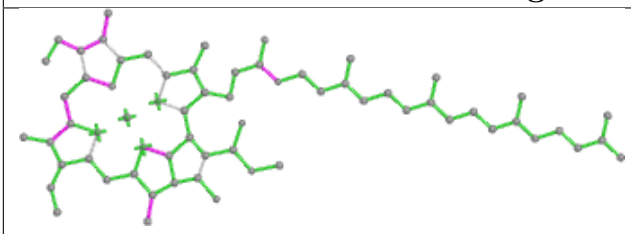
Bond angles



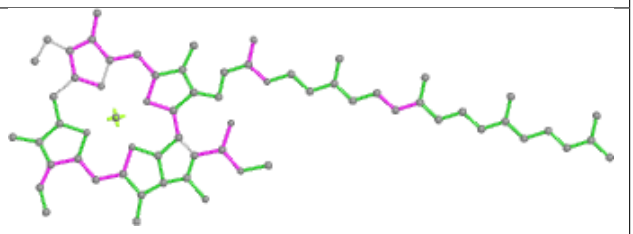
Torsions

Rings

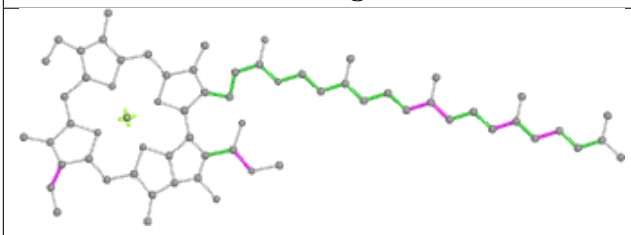
Ligand CLA b 608



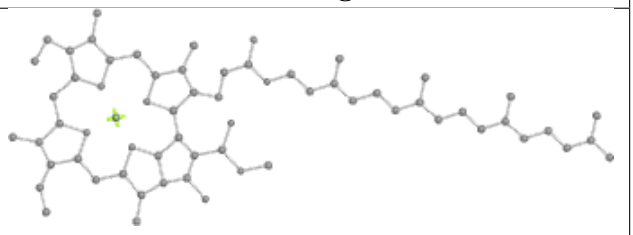
Bond lengths



Bond angles

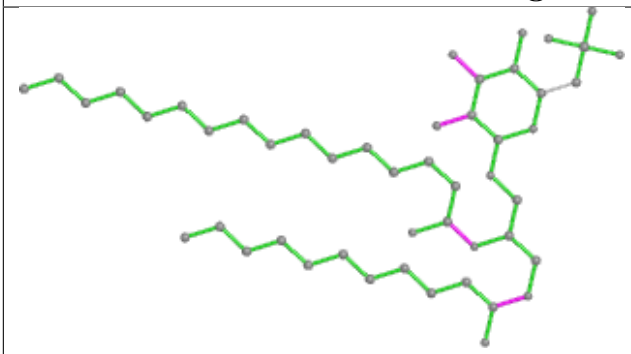


Torsions

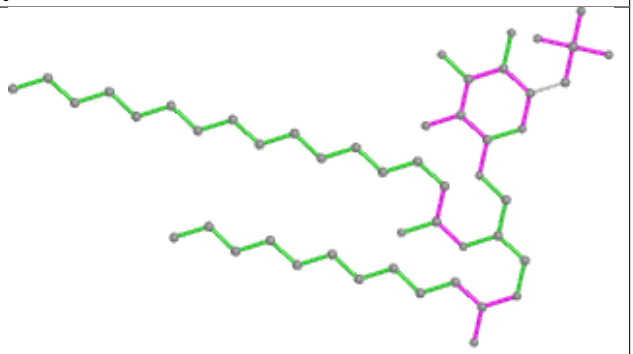


Rings

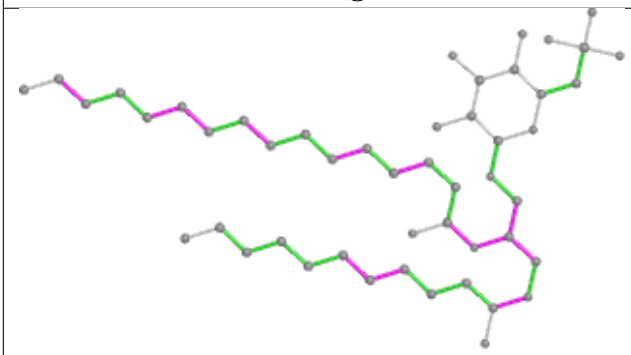
Ligand SQD b 601



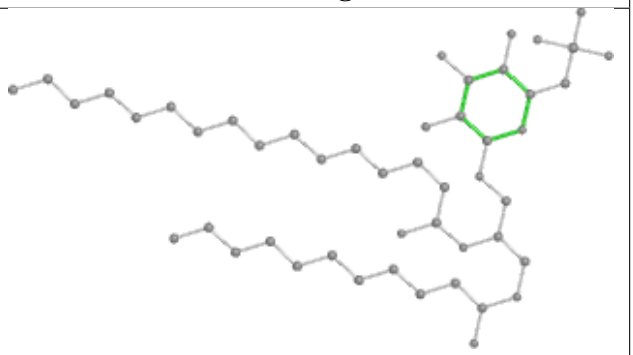
Bond lengths



Bond angles

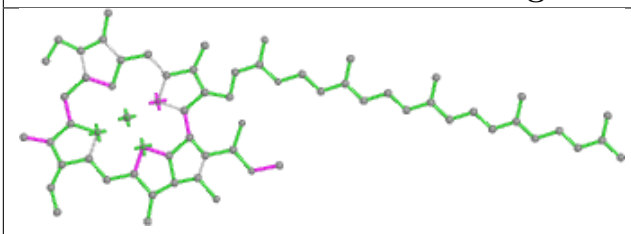


Torsions

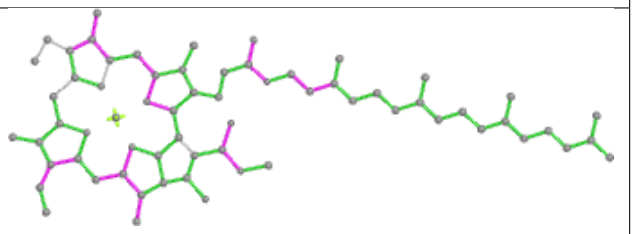


Rings

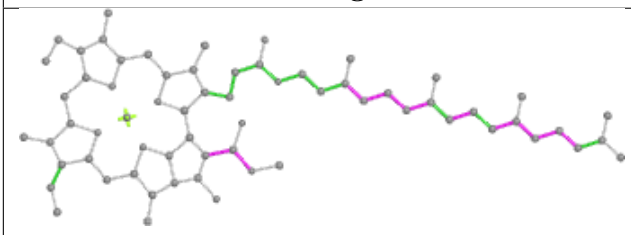
Ligand CLA b 614



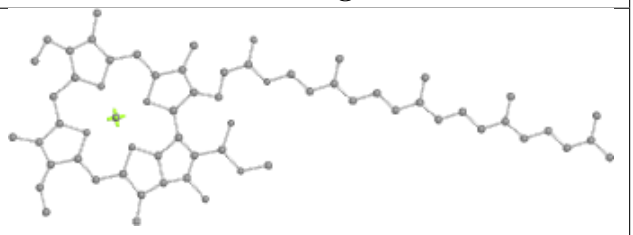
Bond lengths



Bond angles

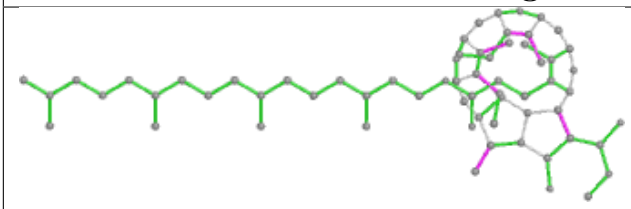


Torsions

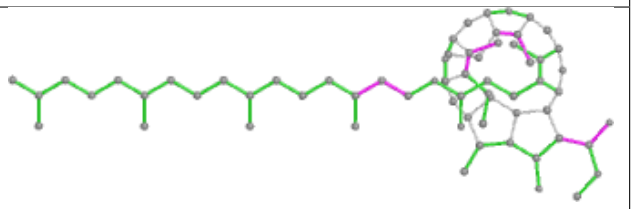


Rings

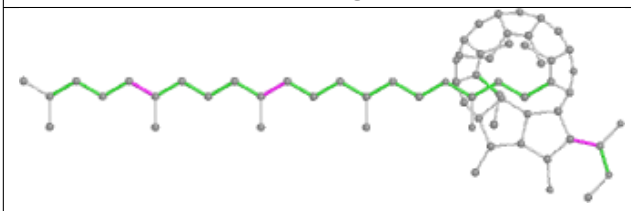
Ligand PHO A 606



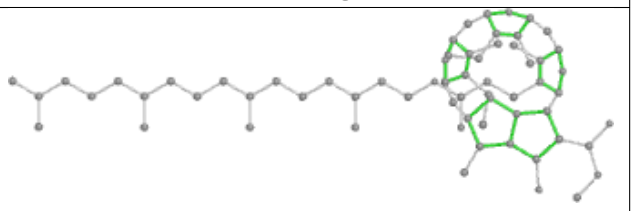
Bond lengths



Bond angles

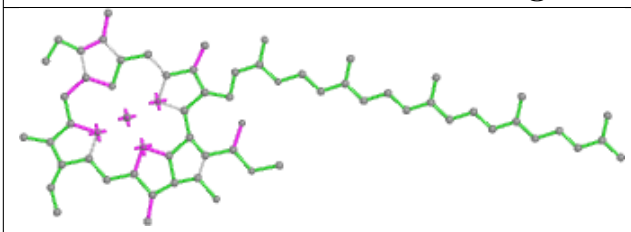


Torsions

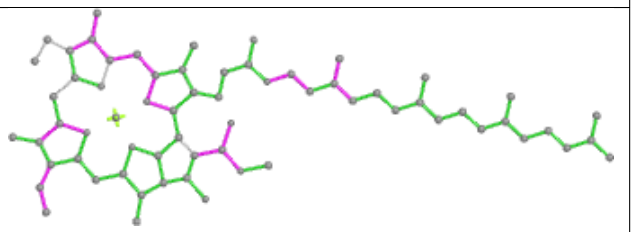


Rings

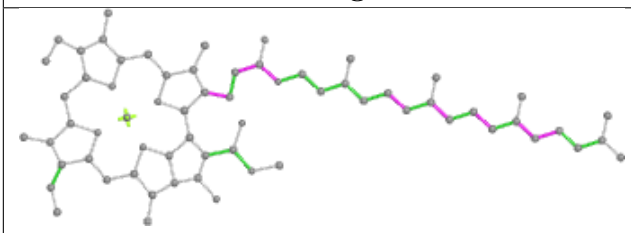
Ligand CLA a 606



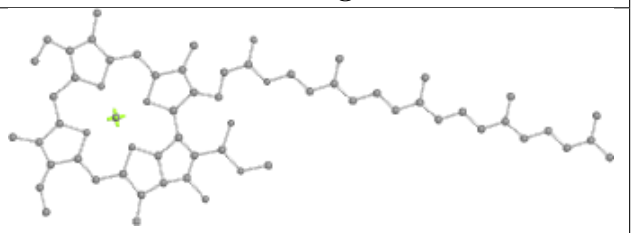
Bond lengths



Bond angles

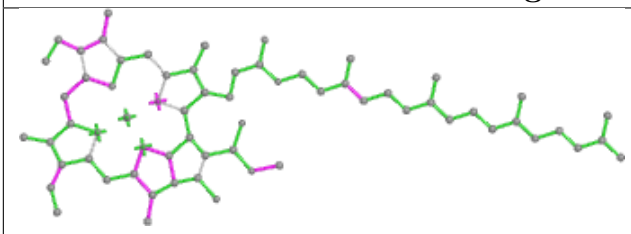


Torsions

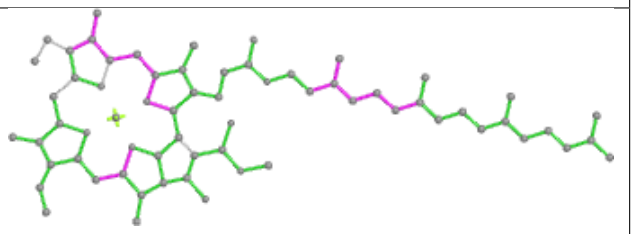


Rings

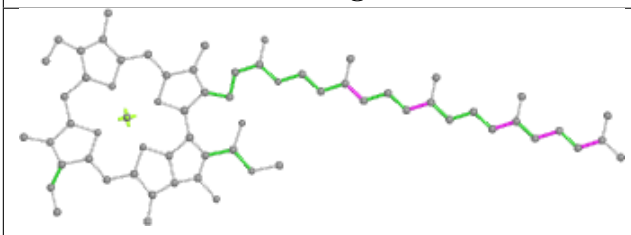
Ligand CLA B 615



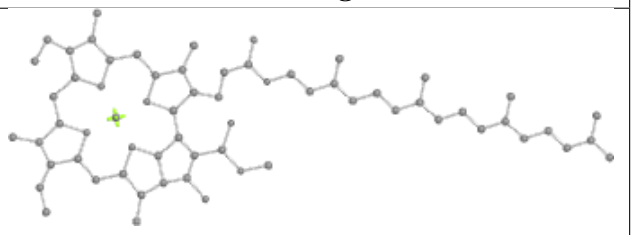
Bond lengths



Bond angles

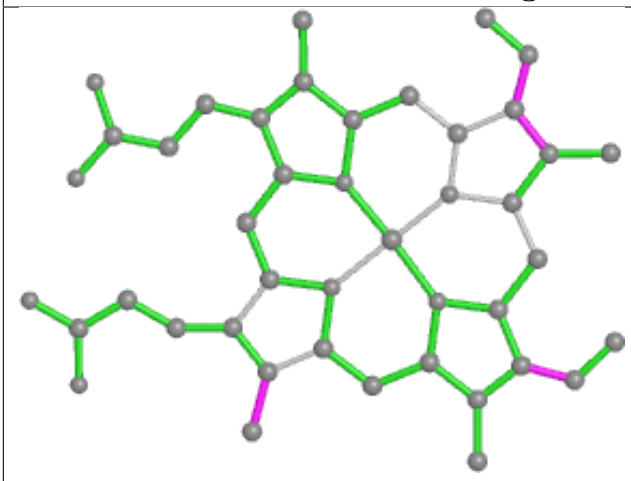


Torsions

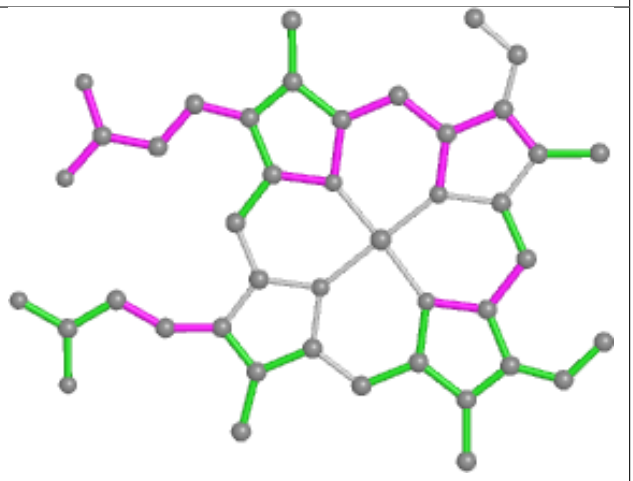


Rings

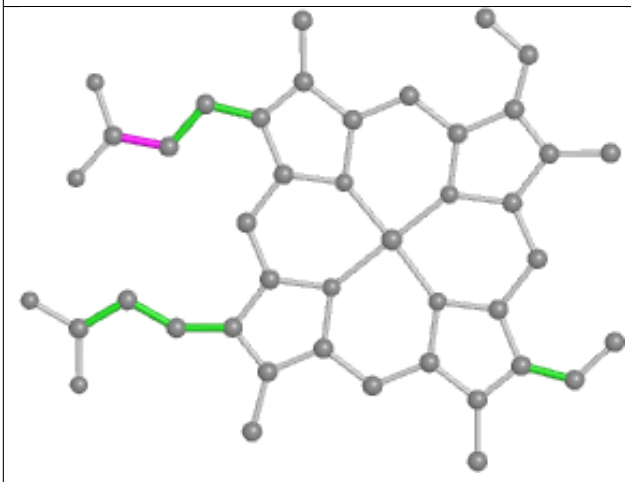
Ligand HEM F 102



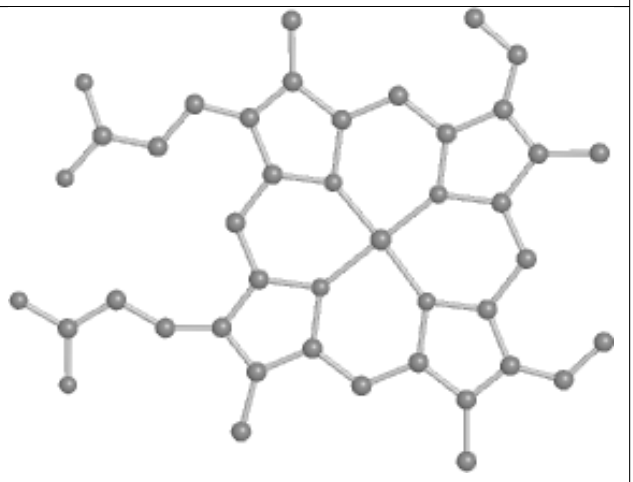
Bond lengths



Bond angles

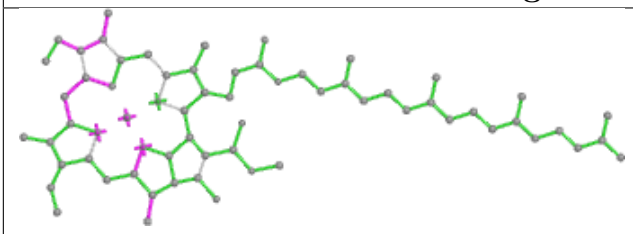


Torsions

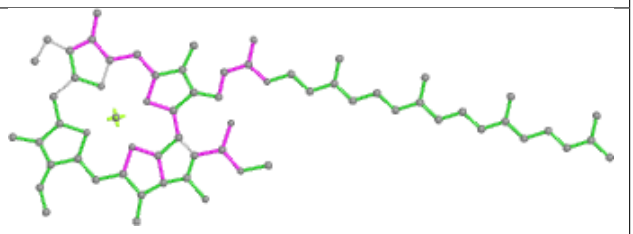


Rings

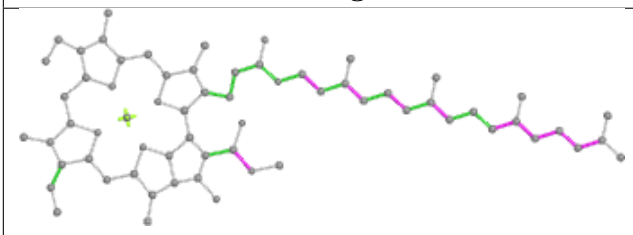
Ligand CLA D 403



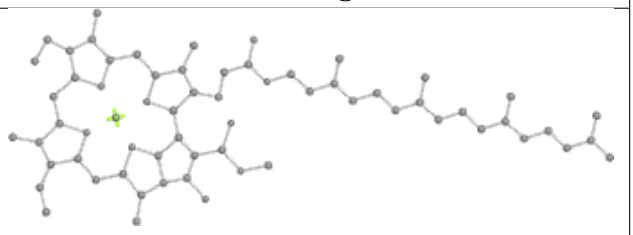
Bond lengths



Bond angles

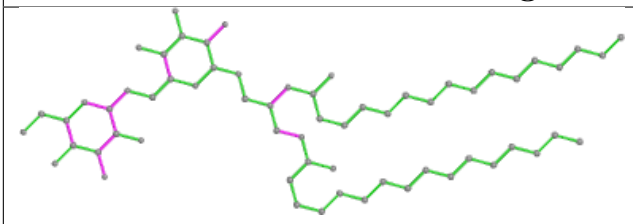


Torsions

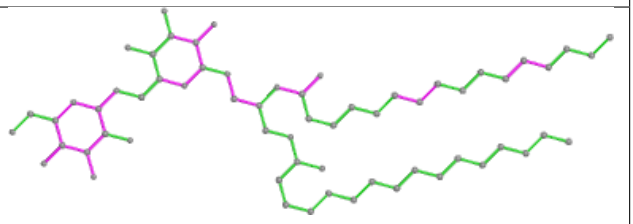


Rings

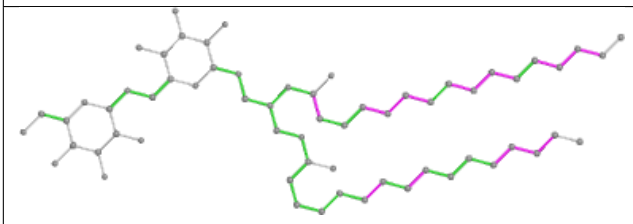
Ligand DGD H 102



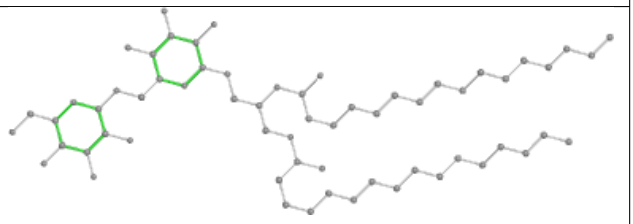
Bond lengths



Bond angles

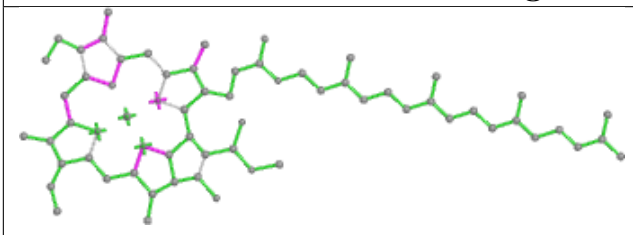


Torsions

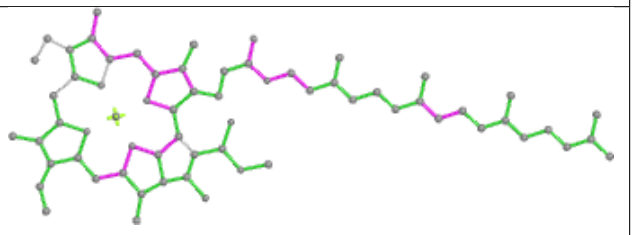


Rings

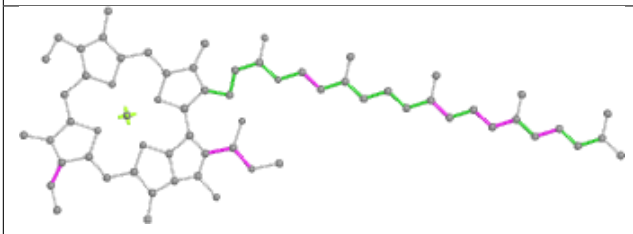
Ligand CLA B 604



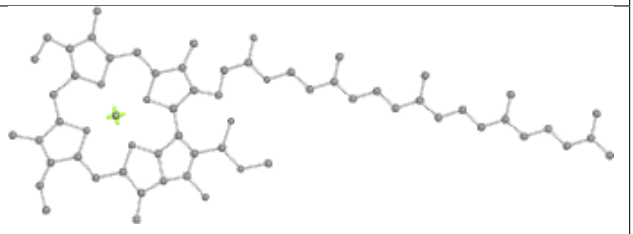
Bond lengths



Bond angles

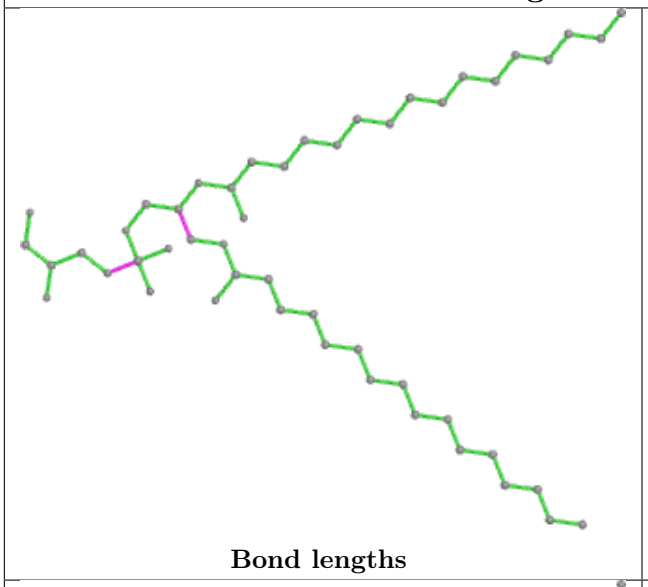


Torsions

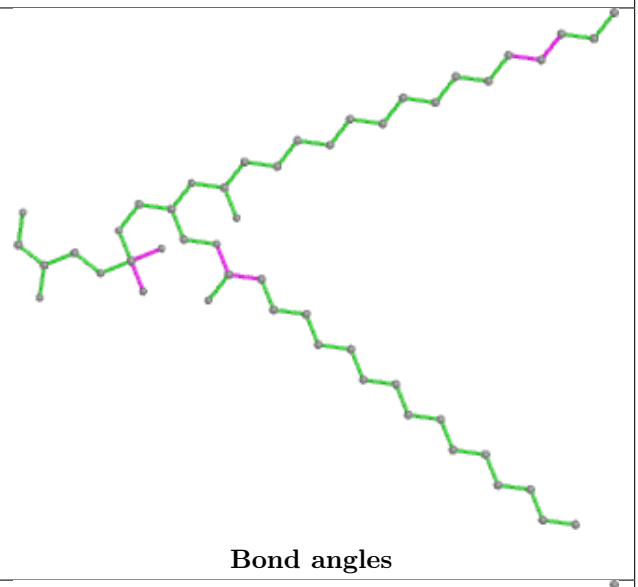


Rings

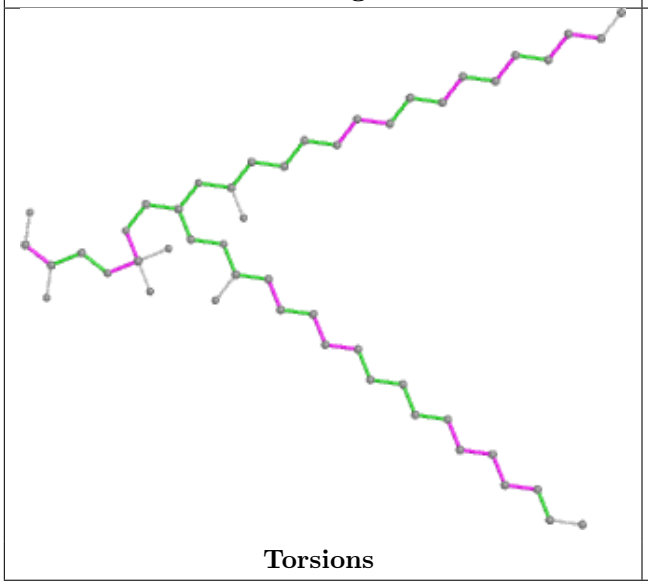
Ligand LHG d 407



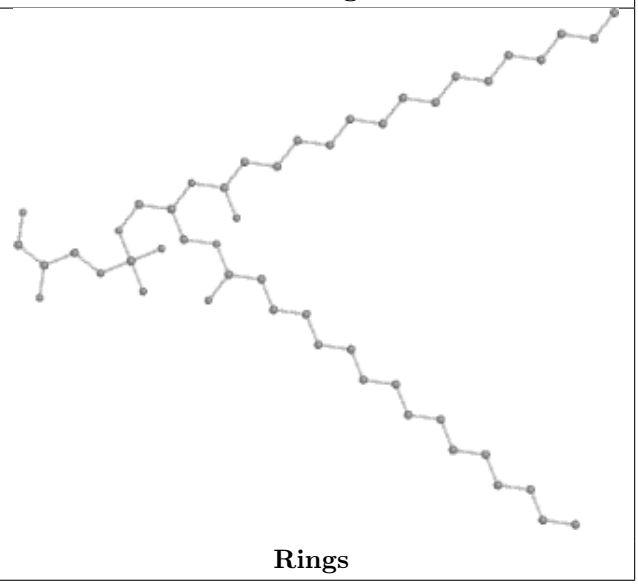
Bond lengths



Bond angles

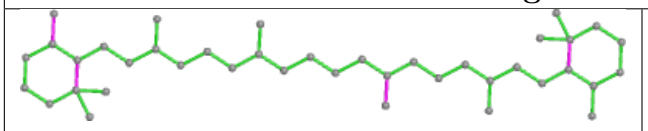


Torsions

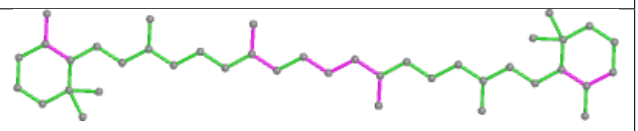


Rings

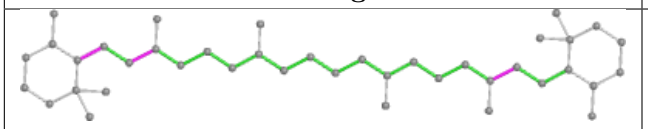
Ligand BCR C 515



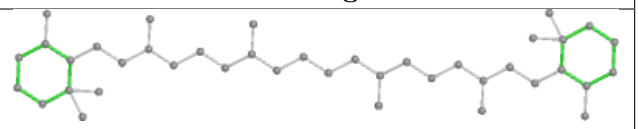
Bond lengths



Bond angles

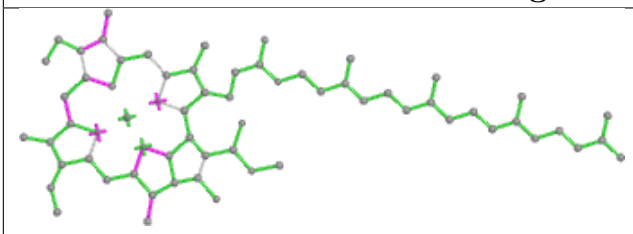


Torsions

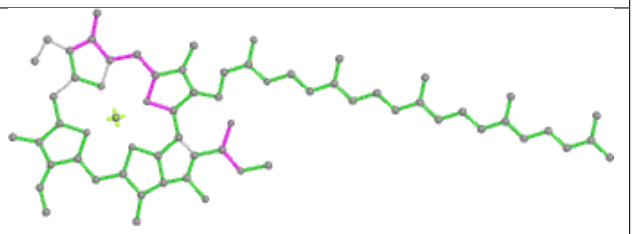


Rings

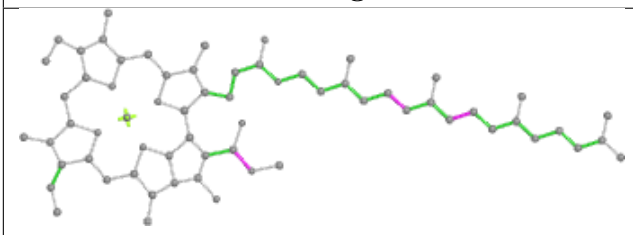
Ligand CLA c 513



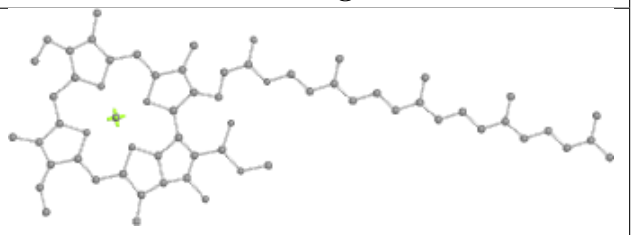
Bond lengths



Bond angles

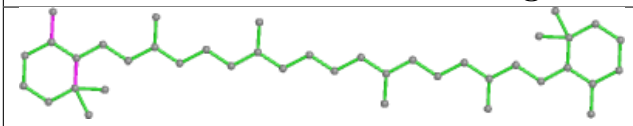


Torsions

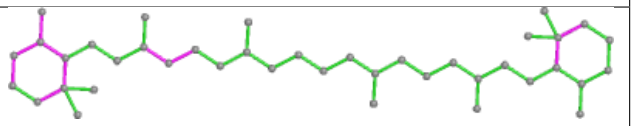


Rings

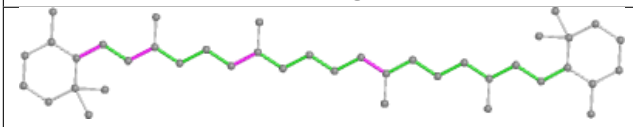
Ligand BCR B 617



Bond lengths



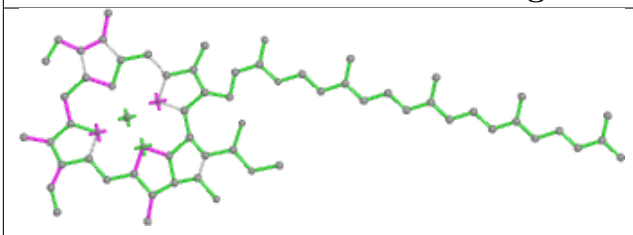
Bond angles



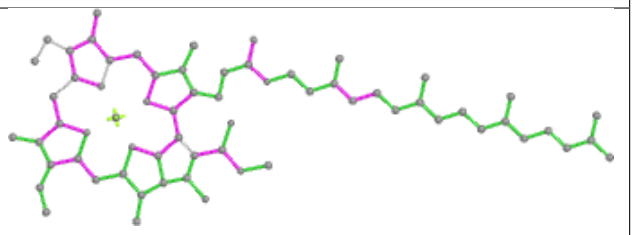
Torsions

Rings

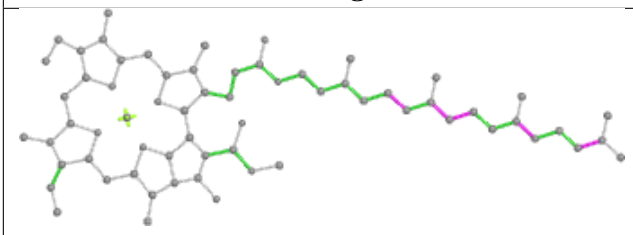
Ligand CLA b 615



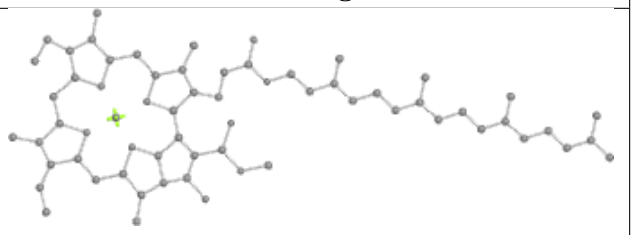
Bond lengths



Bond angles

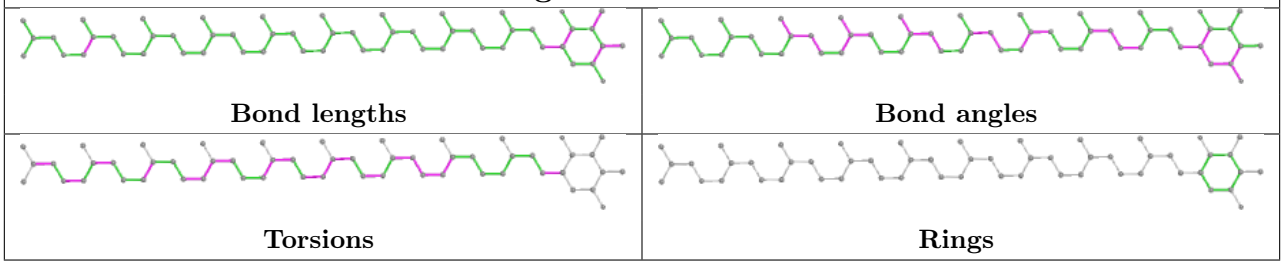


Torsions

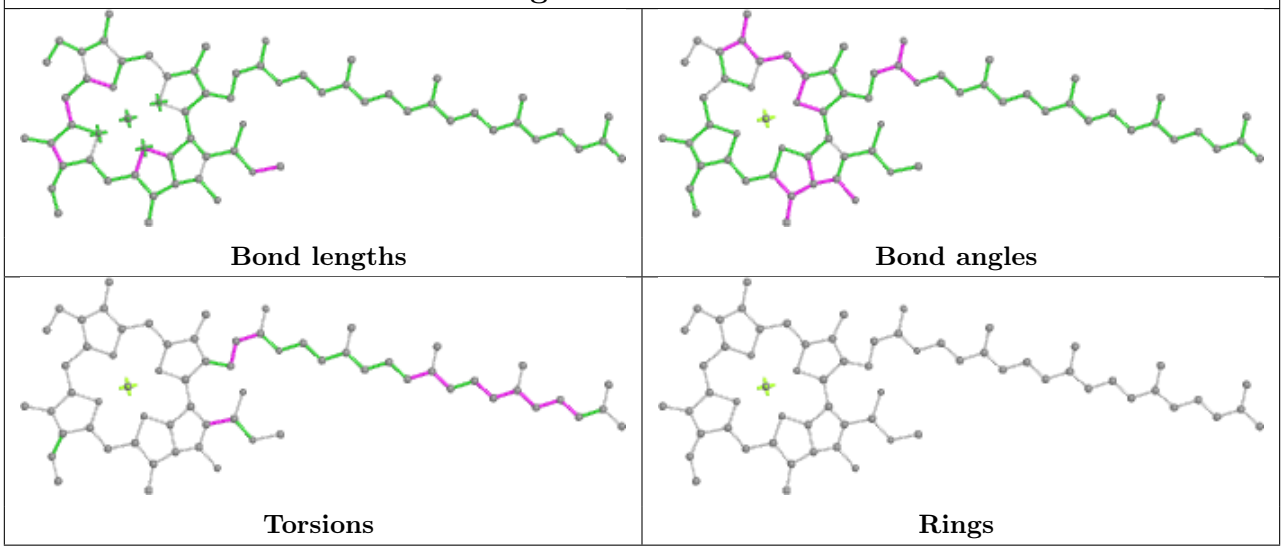


Rings

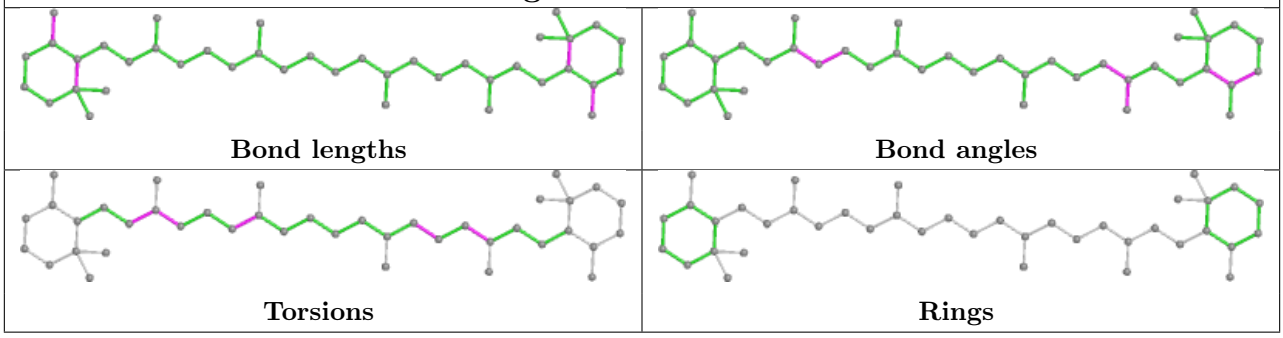
Ligand PL9 a 611



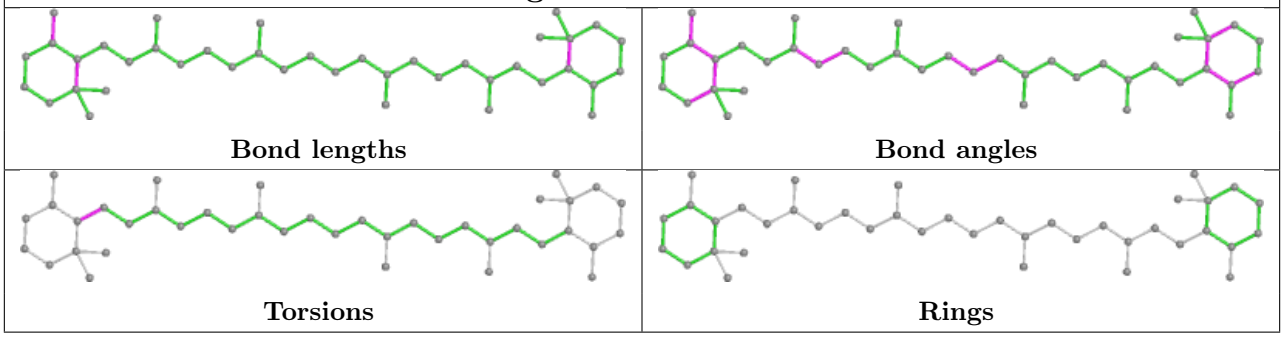
Ligand CLA c 509



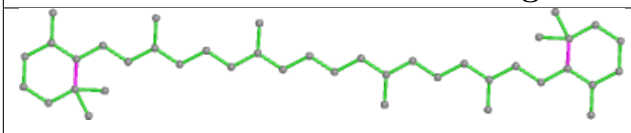
Ligand BCR C 520



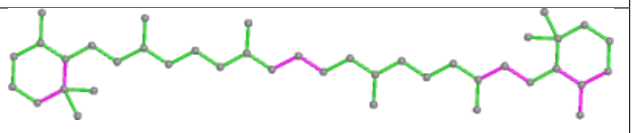
Ligand BCR b 617



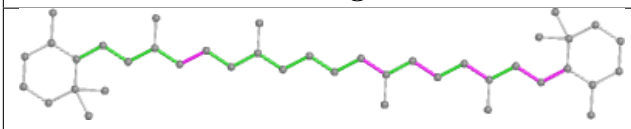
Ligand BCR D 404



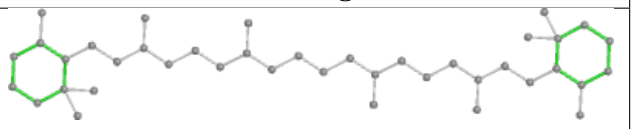
Bond lengths



Bond angles

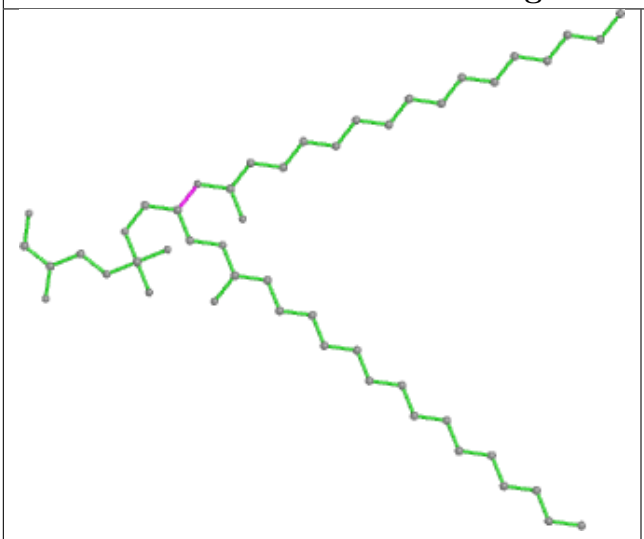


Torsions

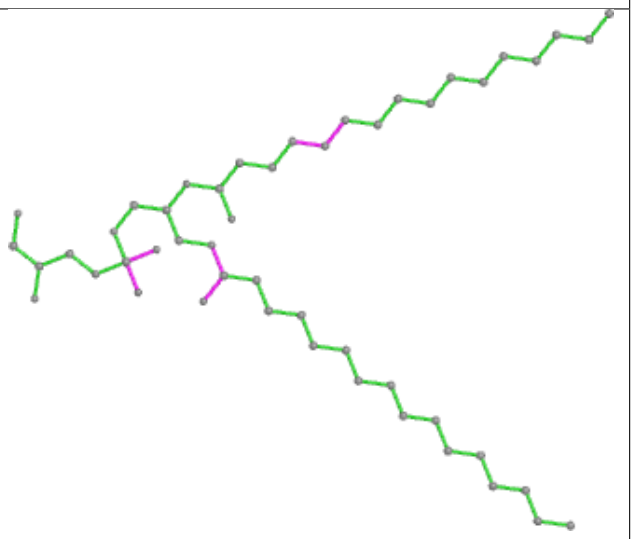


Rings

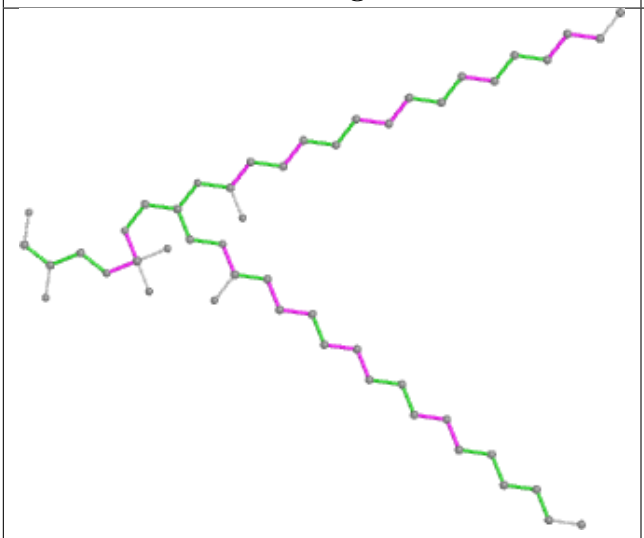
Ligand LHG L 101



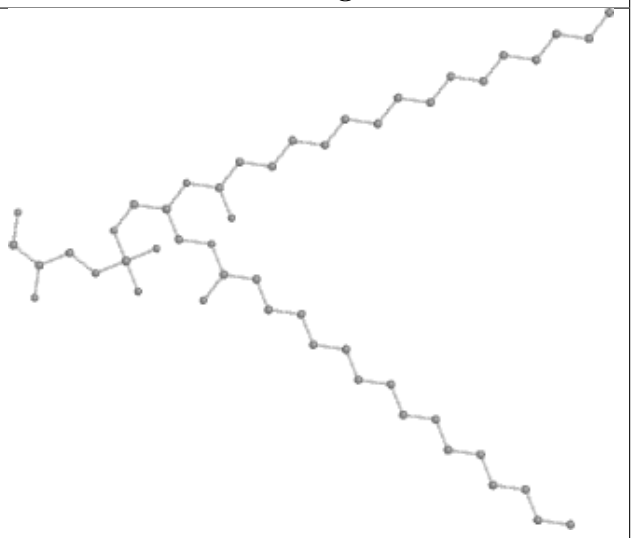
Bond lengths



Bond angles

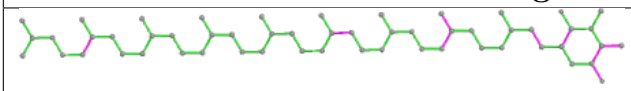


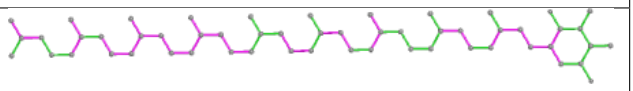
Torsions

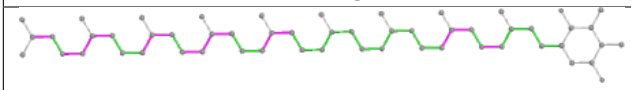


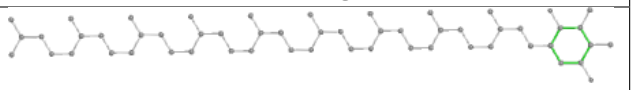
Rings

Ligand PL9 d 408

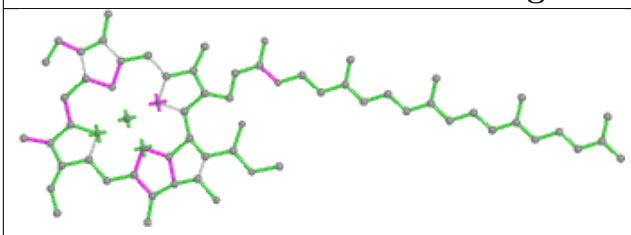

Bond lengths

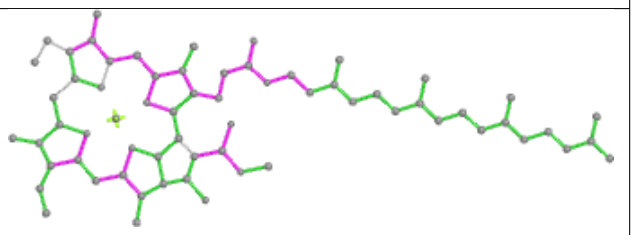

Bond angles

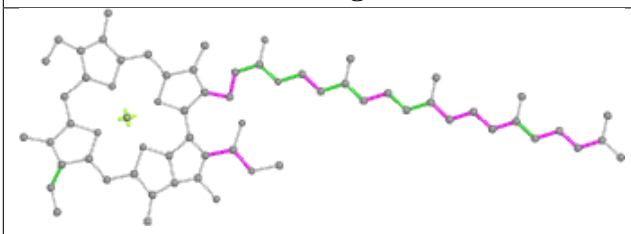

Torsions

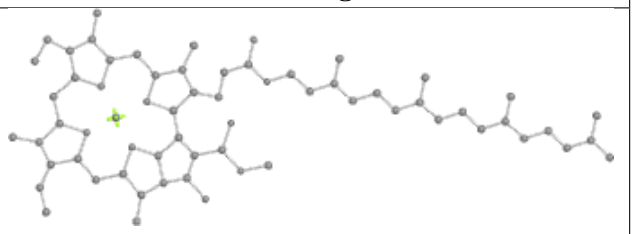

Rings

Ligand CLA h 101

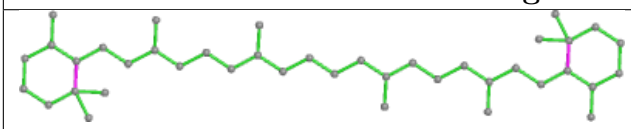

Bond lengths

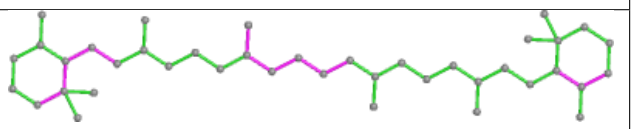

Bond angles

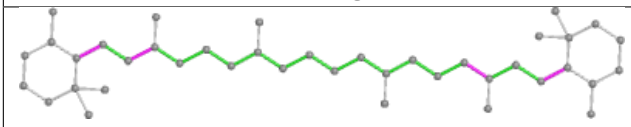

Torsions

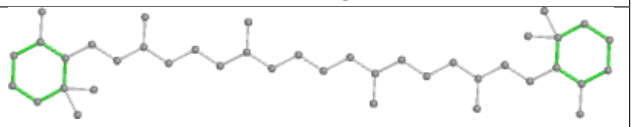

Rings

Ligand BCR B 618

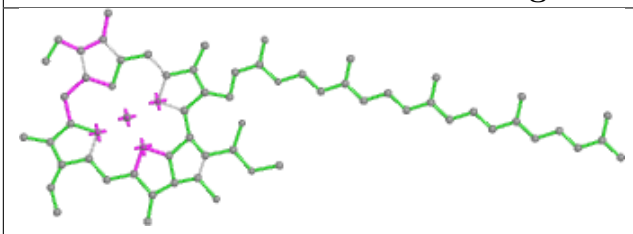

Bond lengths


Bond angles

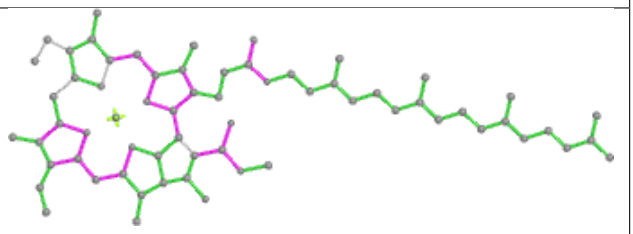

Torsions


Rings

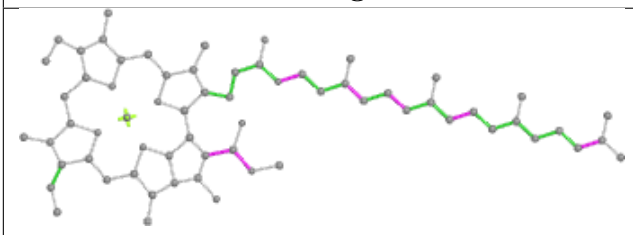
Ligand CLA c 507



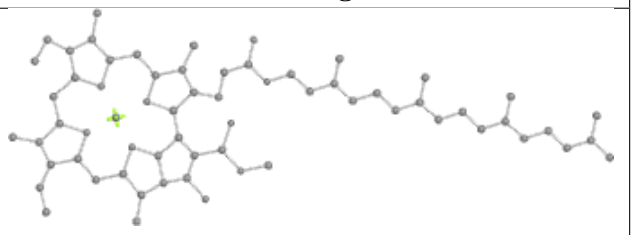
Bond lengths



Bond angles

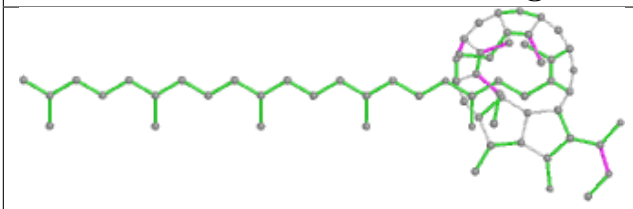


Torsions

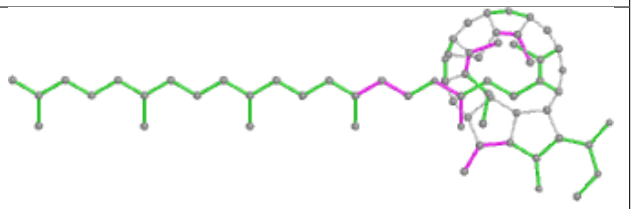


Rings

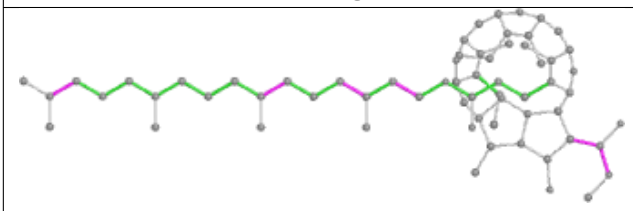
Ligand PHO a 605



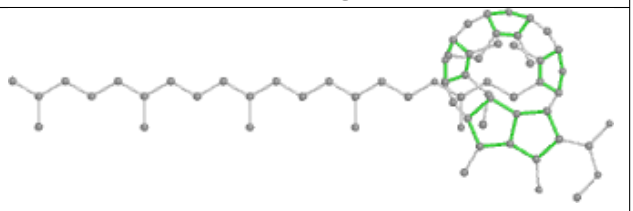
Bond lengths



Bond angles

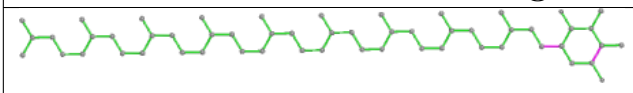


Torsions

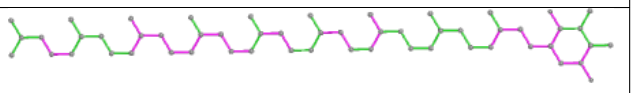


Rings

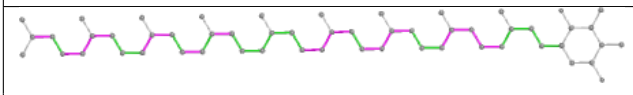
Ligand PL9 A 611



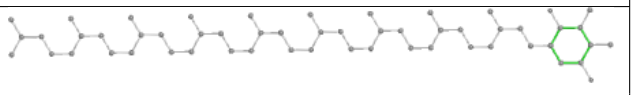
Bond lengths



Bond angles

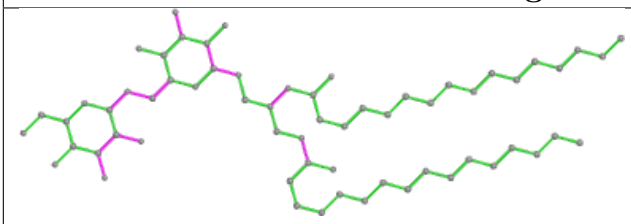


Torsions

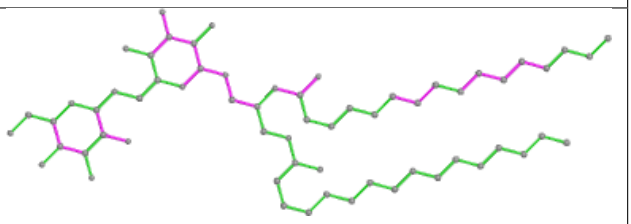


Rings

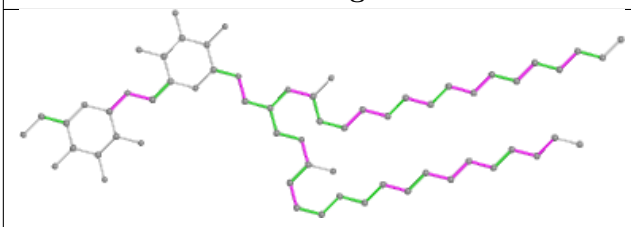
Ligand DGD c 517



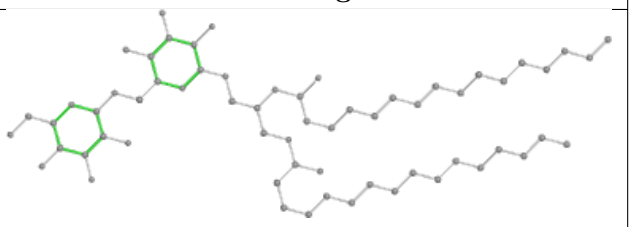
Bond lengths



Bond angles

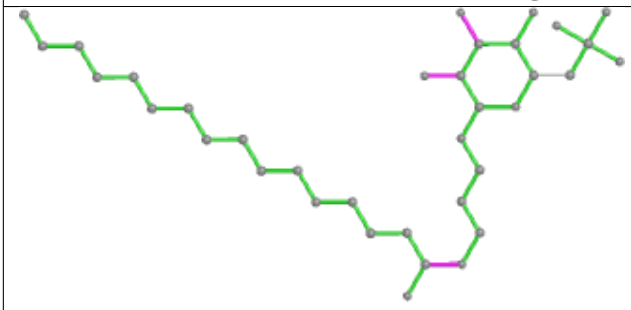


Torsions

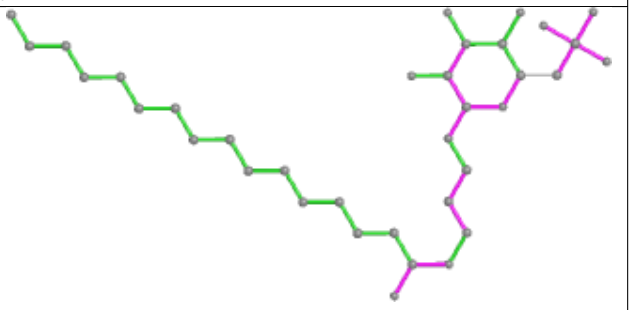


Rings

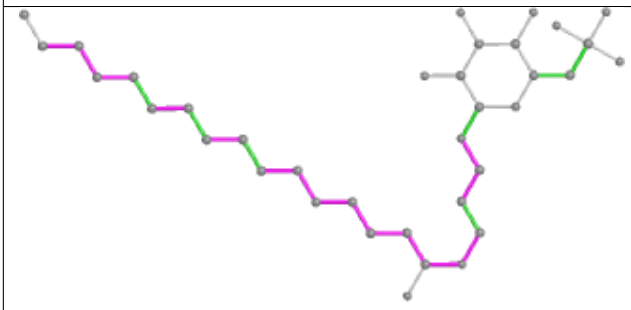
Ligand SQD F 101



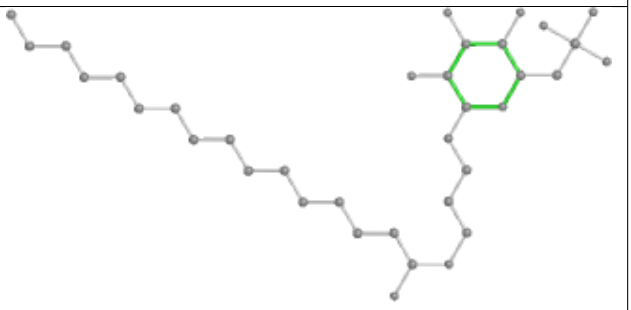
Bond lengths



Bond angles

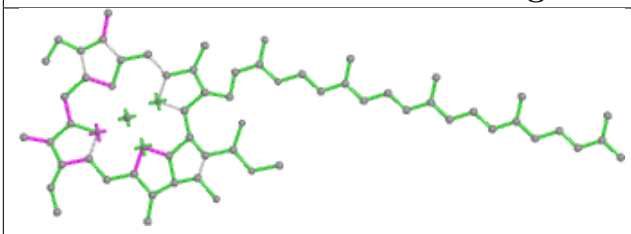


Torsions

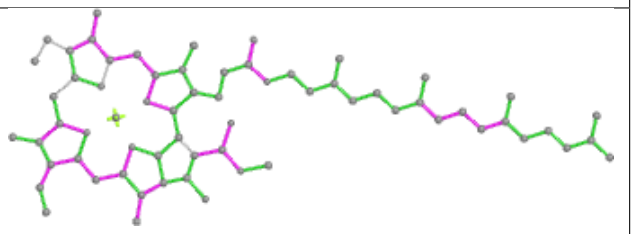


Rings

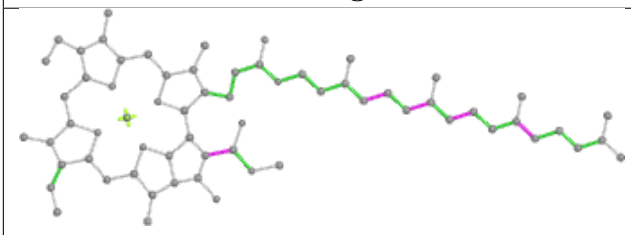
Ligand CLA b 612



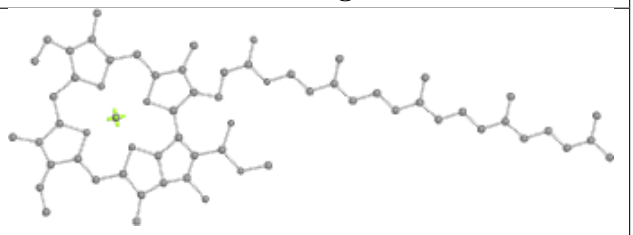
Bond lengths



Bond angles

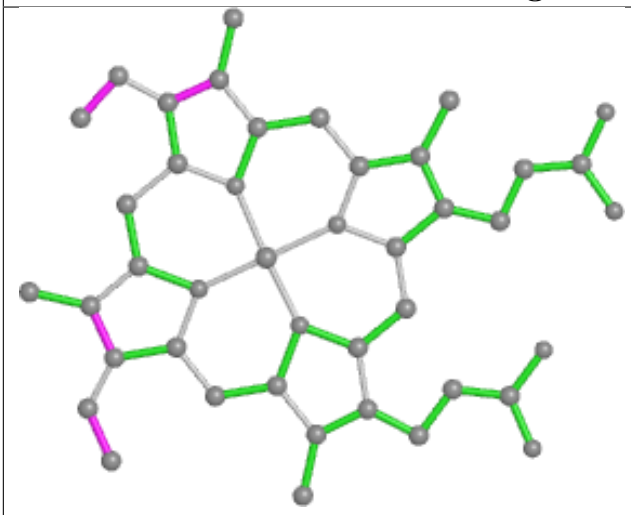


Torsions

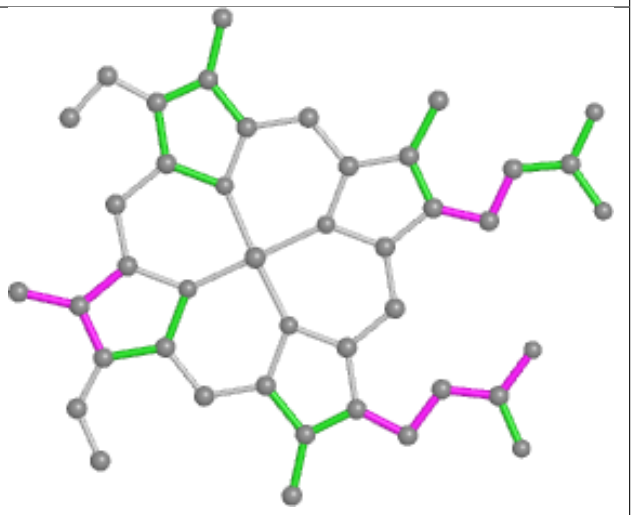


Rings

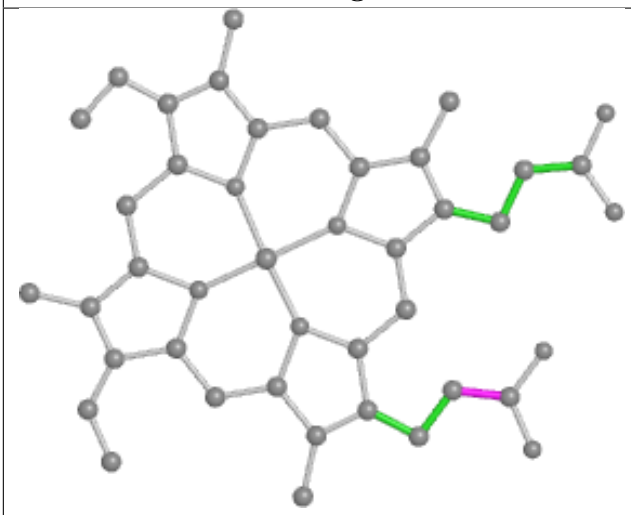
Ligand HEC v 201



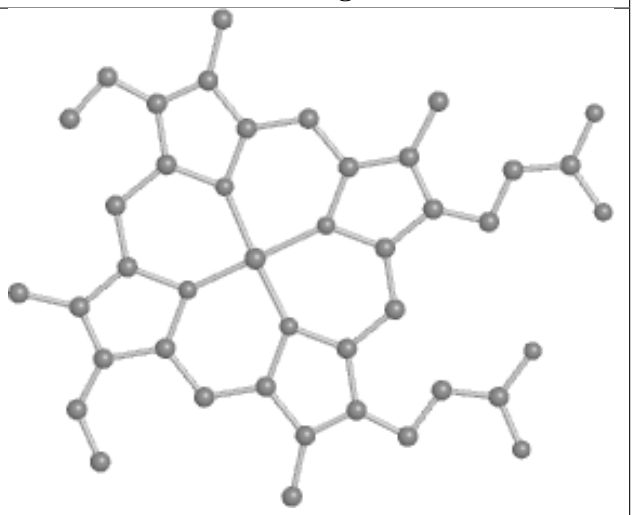
Bond lengths



Bond angles

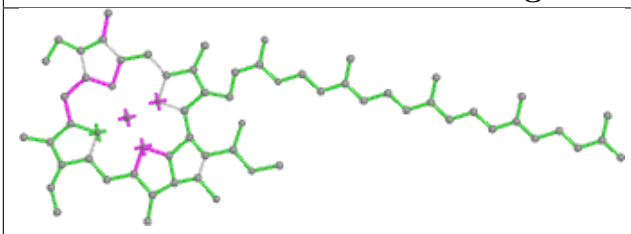


Torsions

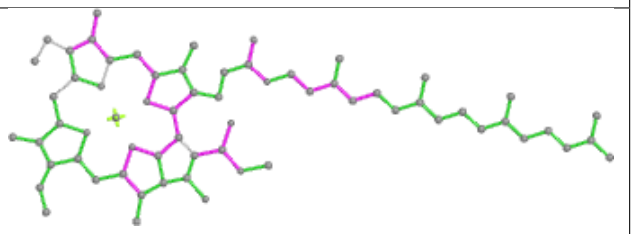


Rings

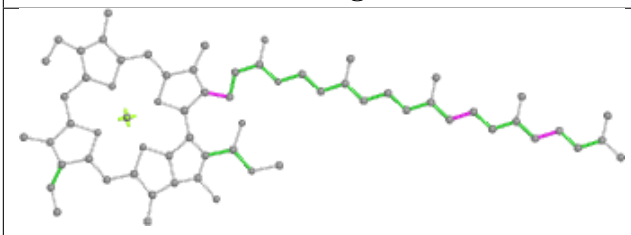
Ligand CLA B 602



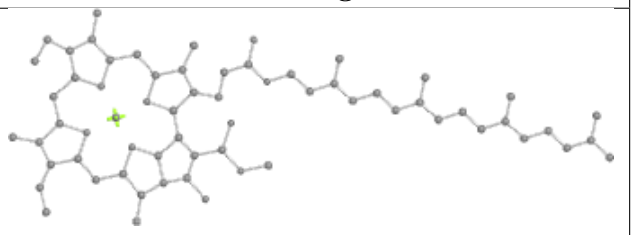
Bond lengths



Bond angles

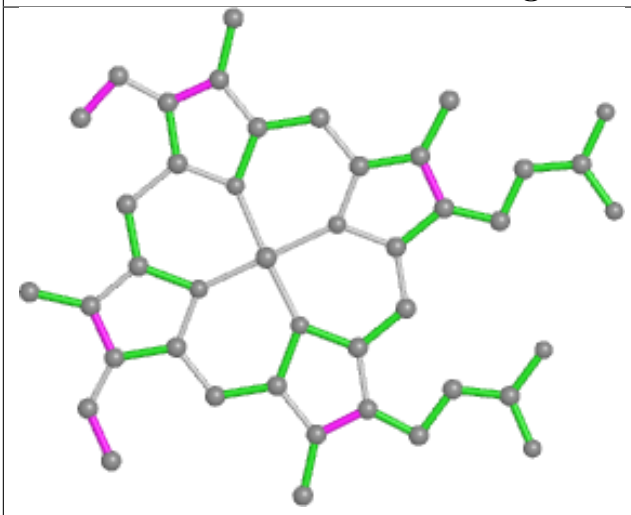


Torsions

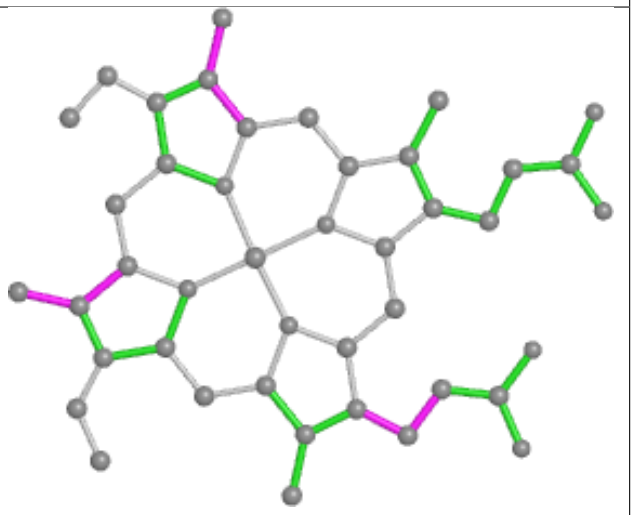


Rings

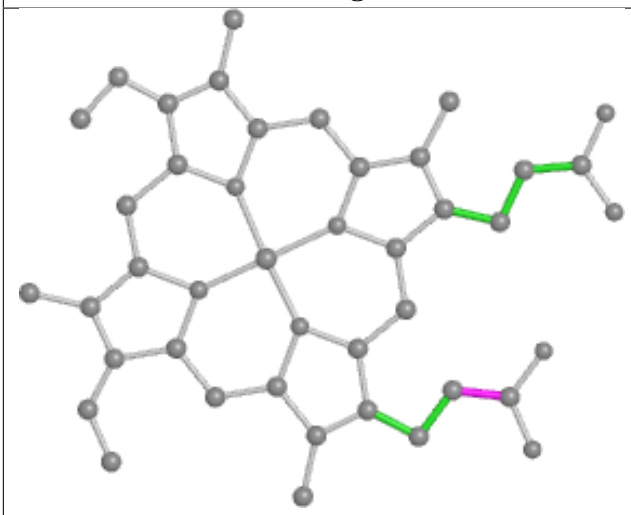
Ligand HEC V 201



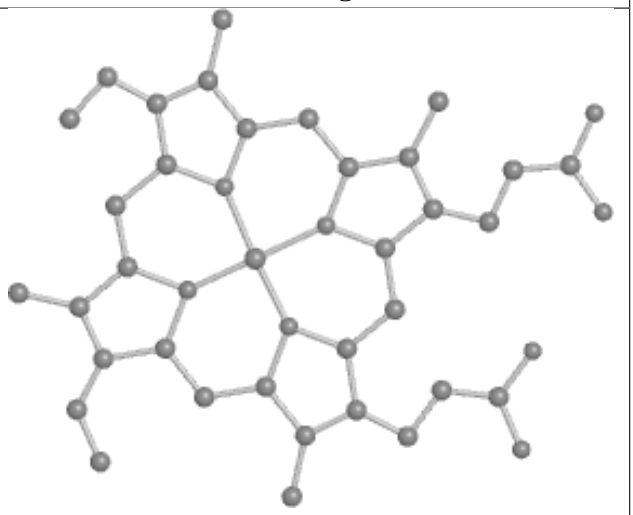
Bond lengths



Bond angles

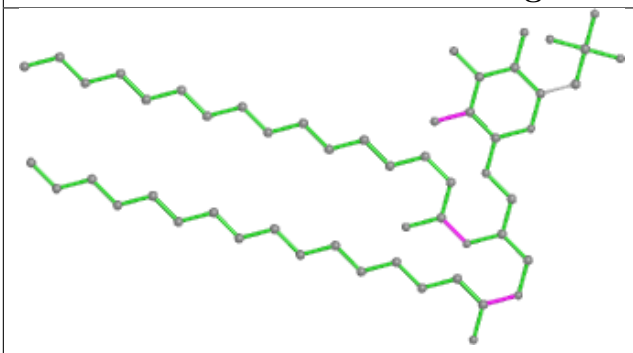


Torsions

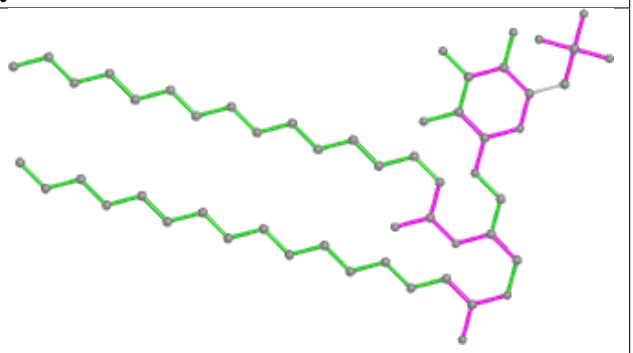


Rings

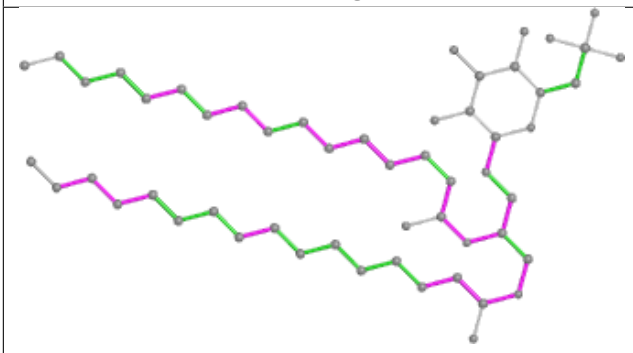
Ligand SQD B 624



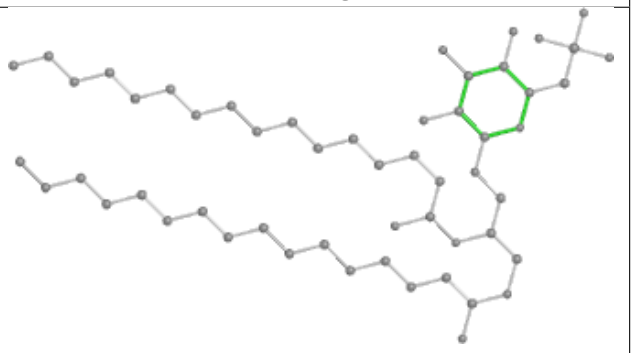
Bond lengths



Bond angles

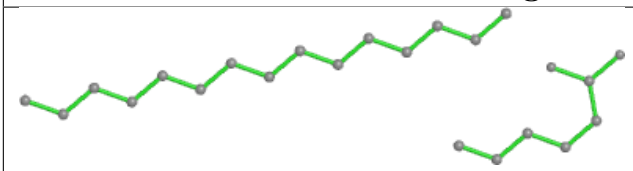


Torsions

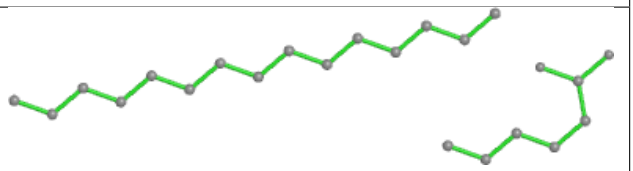


Rings

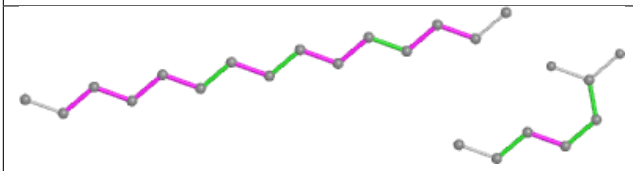
Ligand LMG d 410



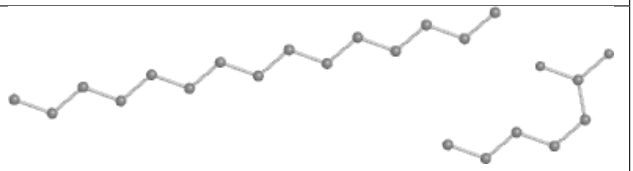
Bond lengths



Bond angles

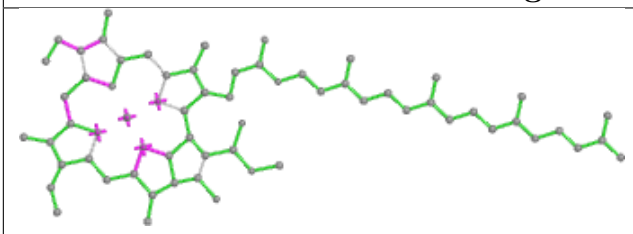


Torsions

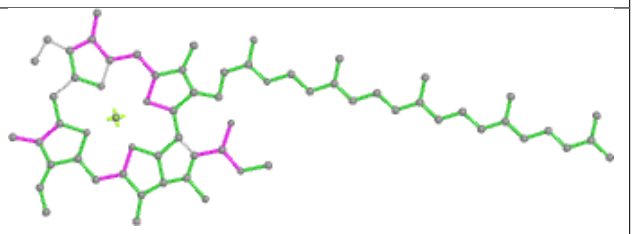


Rings

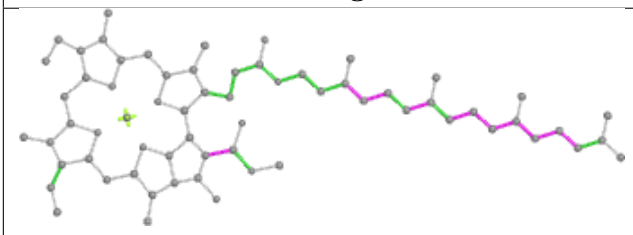
Ligand CLA C 506



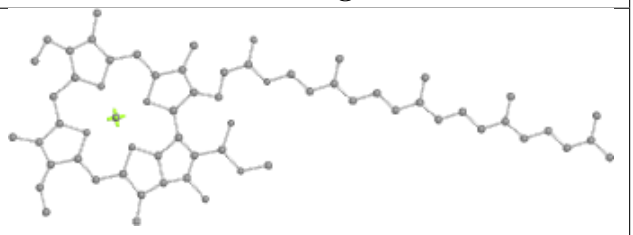
Bond lengths



Bond angles

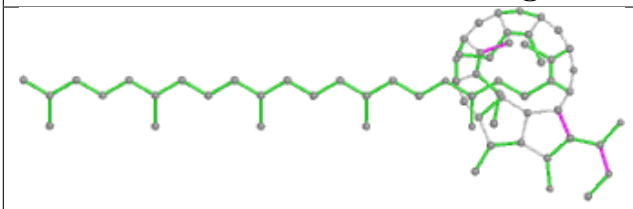


Torsions

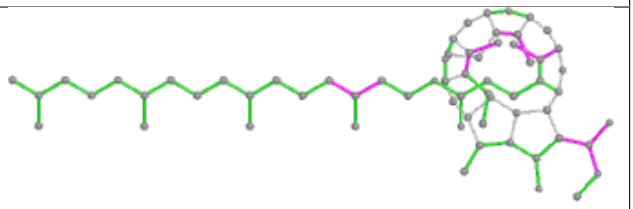


Rings

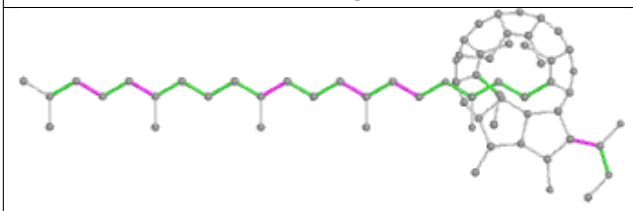
Ligand PHO A 605



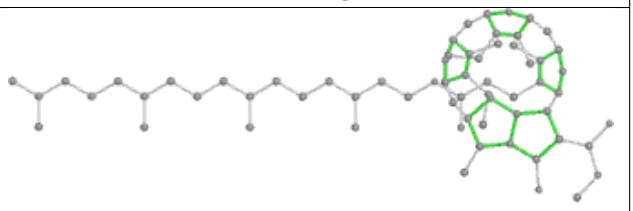
Bond lengths



Bond angles

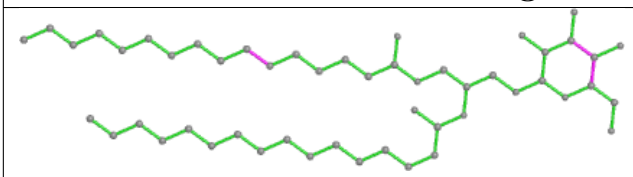


Torsions

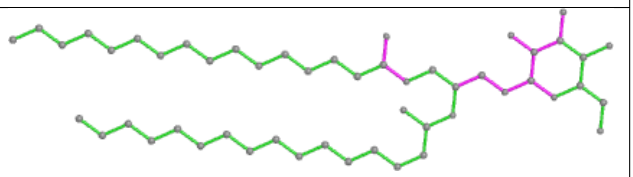


Rings

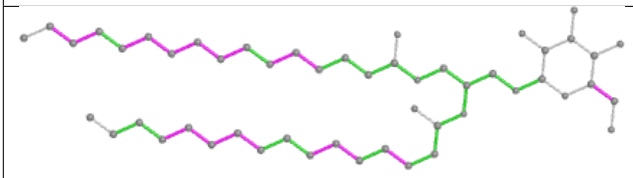
Ligand LMG D 405



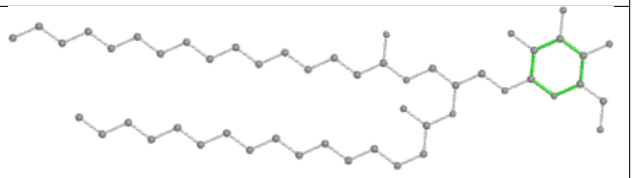
Bond lengths



Bond angles

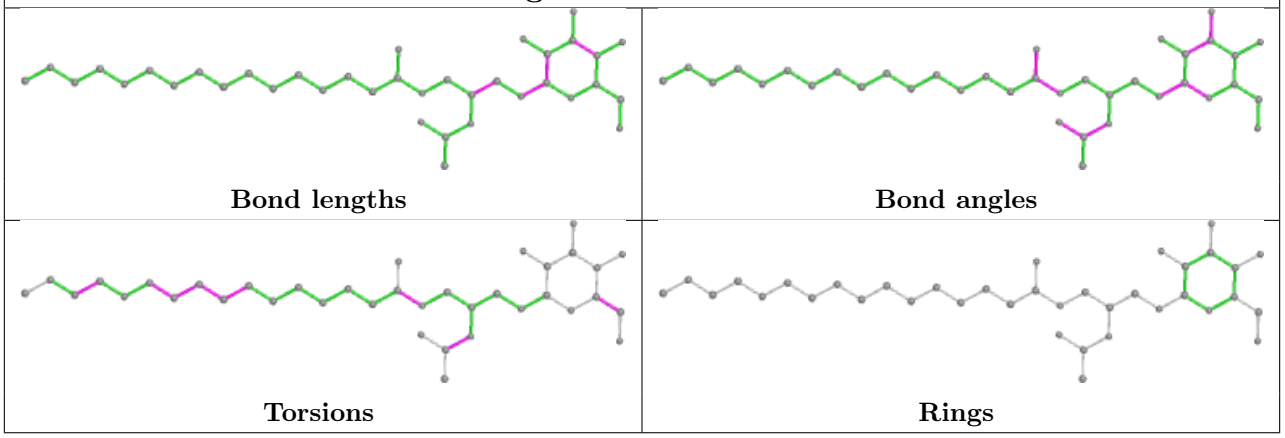


Torsions

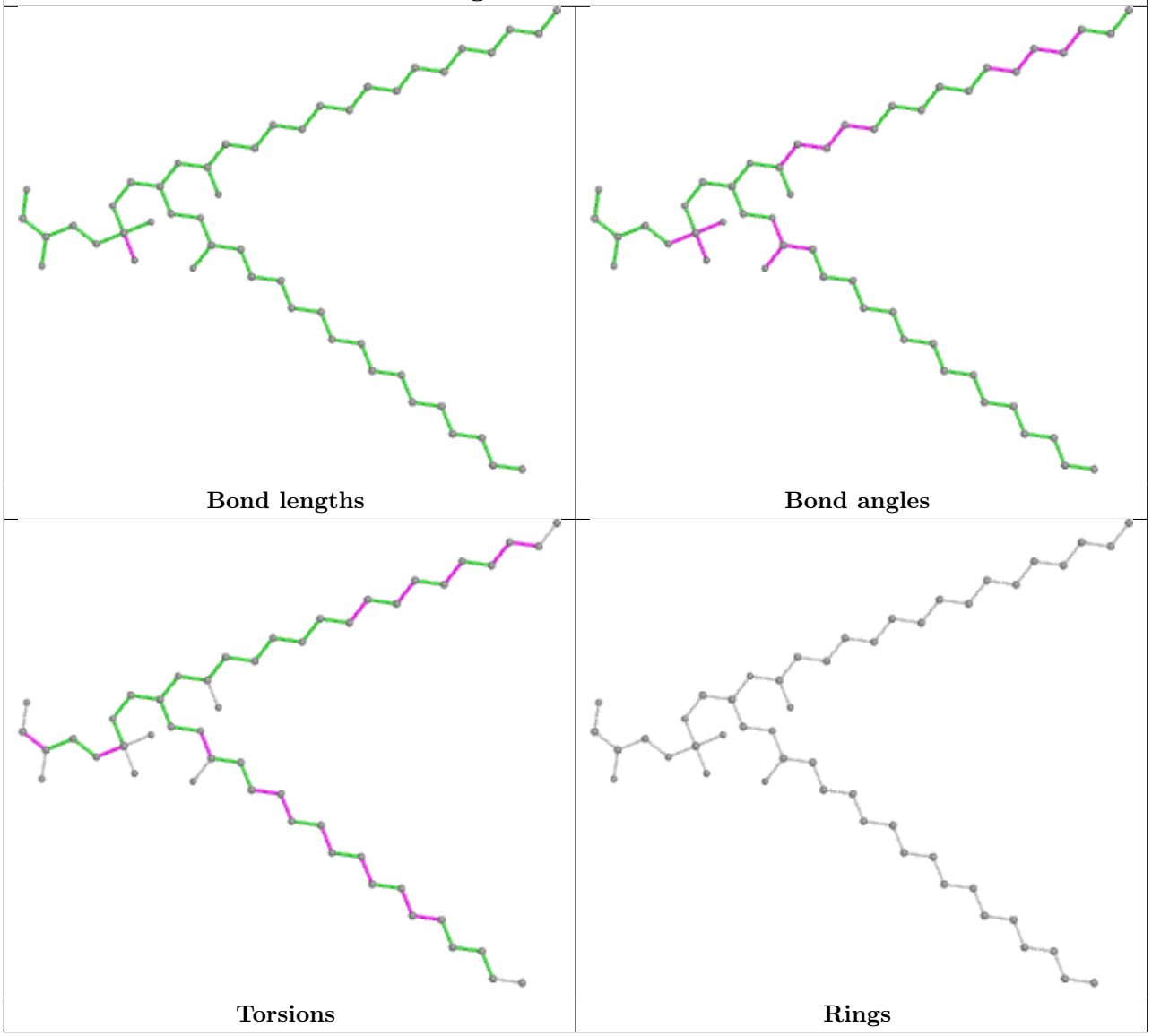


Rings

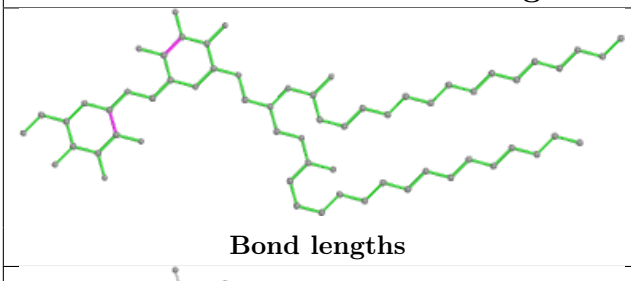
Ligand LMG c 519



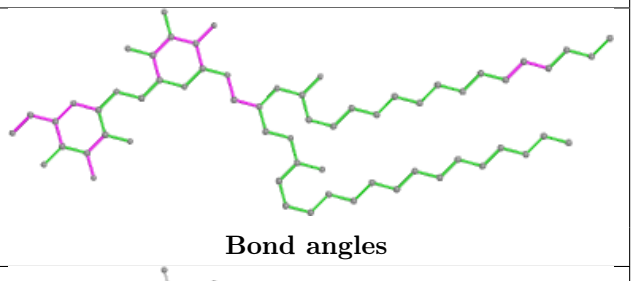
Ligand LHG B 623



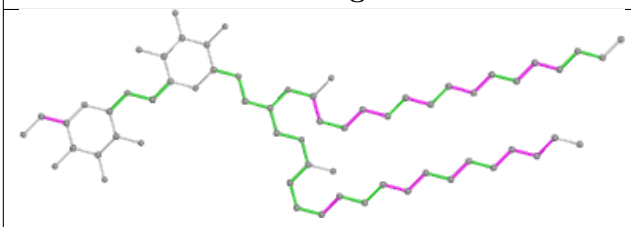
Ligand DGD h 103



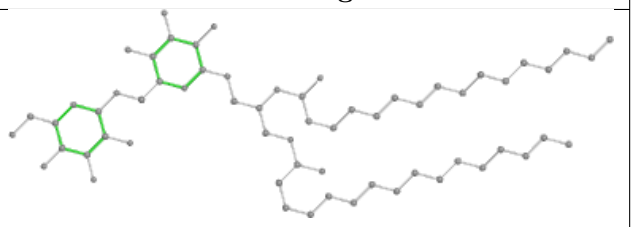
Bond lengths



Bond angles

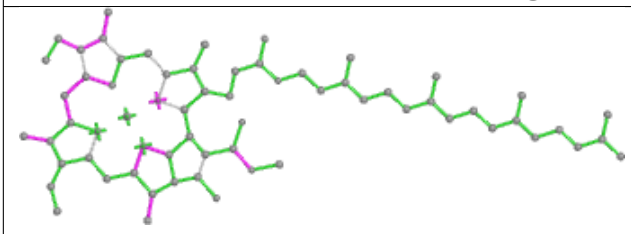


Torsions

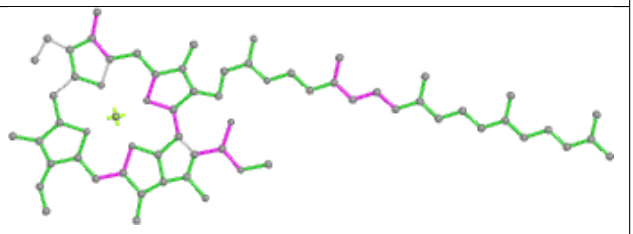


Rings

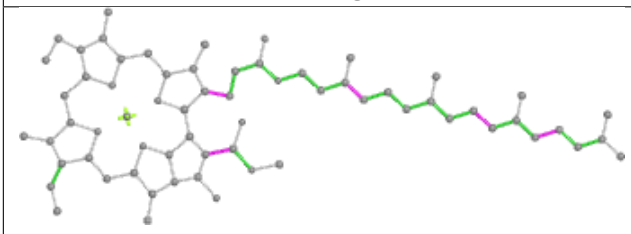
Ligand CLA B 609



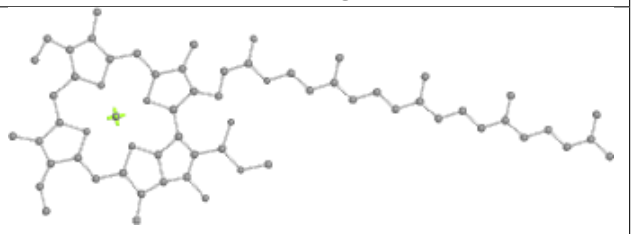
Bond lengths



Bond angles

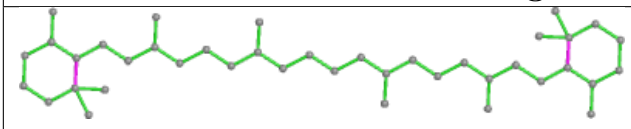


Torsions

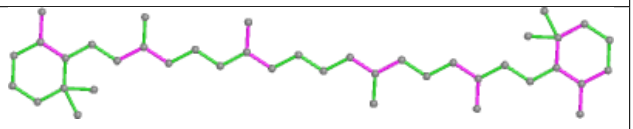


Rings

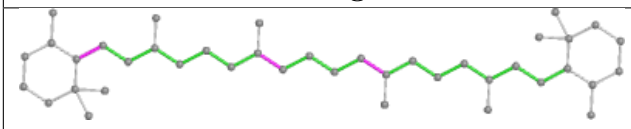
Ligand BCR a 607



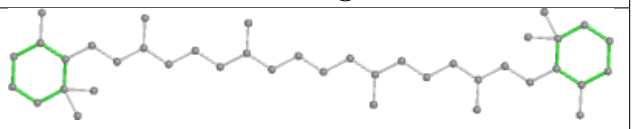
Bond lengths



Bond angles

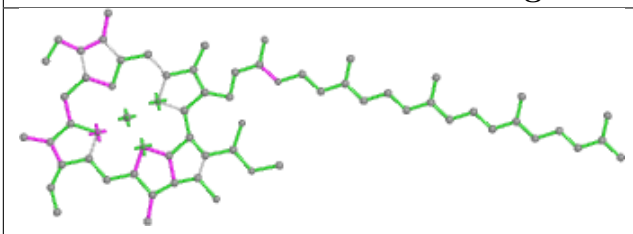


Torsions

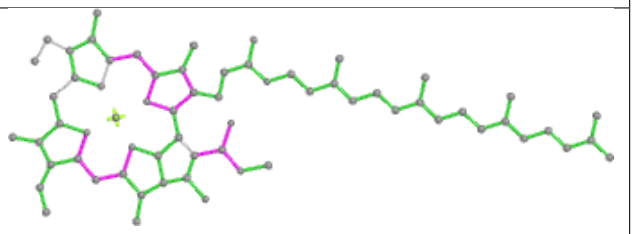


Rings

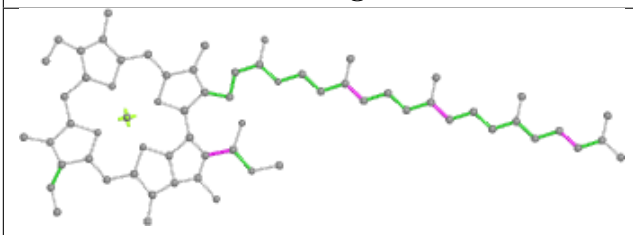
Ligand CLA C 510



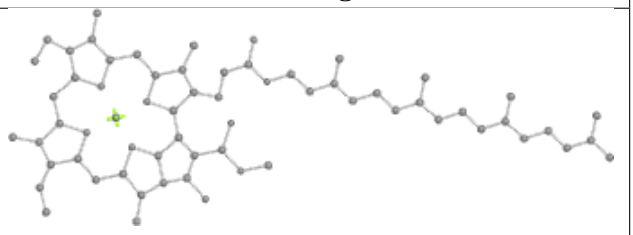
Bond lengths



Bond angles

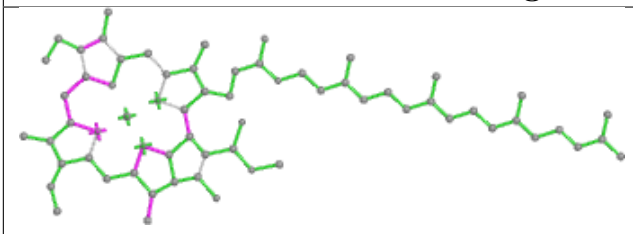


Torsions

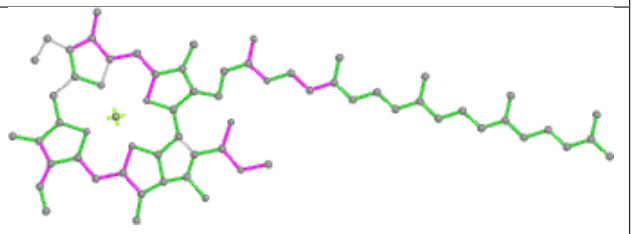


Rings

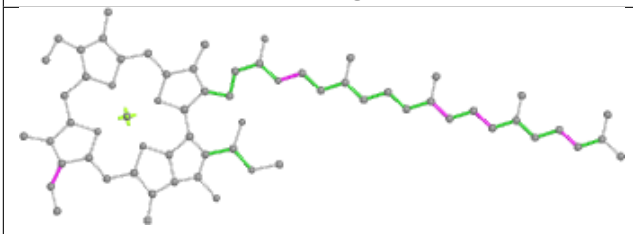
Ligand CLA D 402



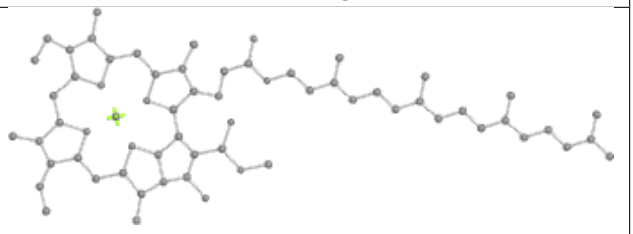
Bond lengths



Bond angles

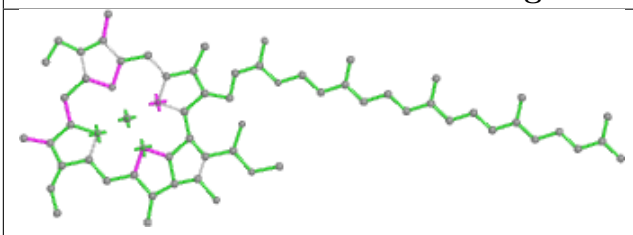


Torsions

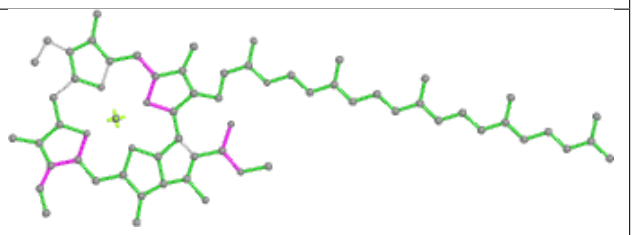


Rings

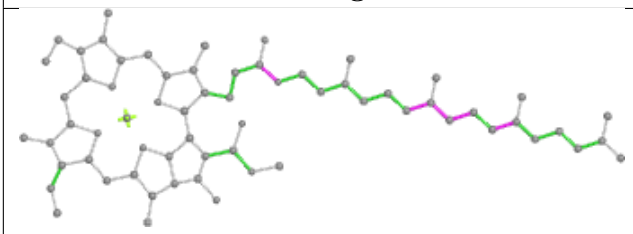
Ligand CLA C 511



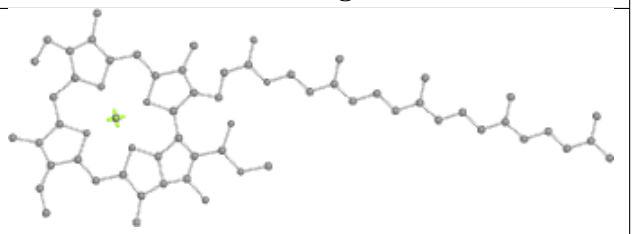
Bond lengths



Bond angles

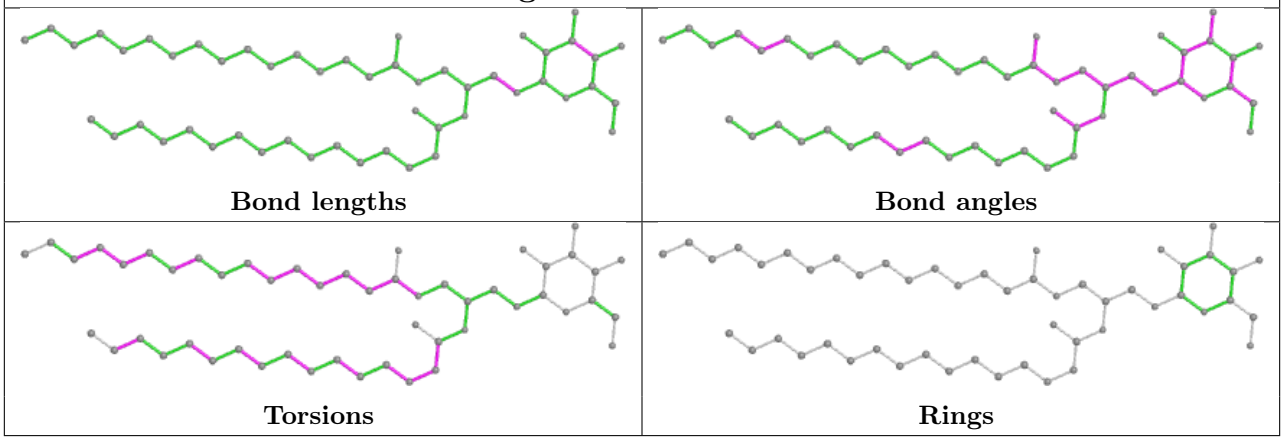


Torsions

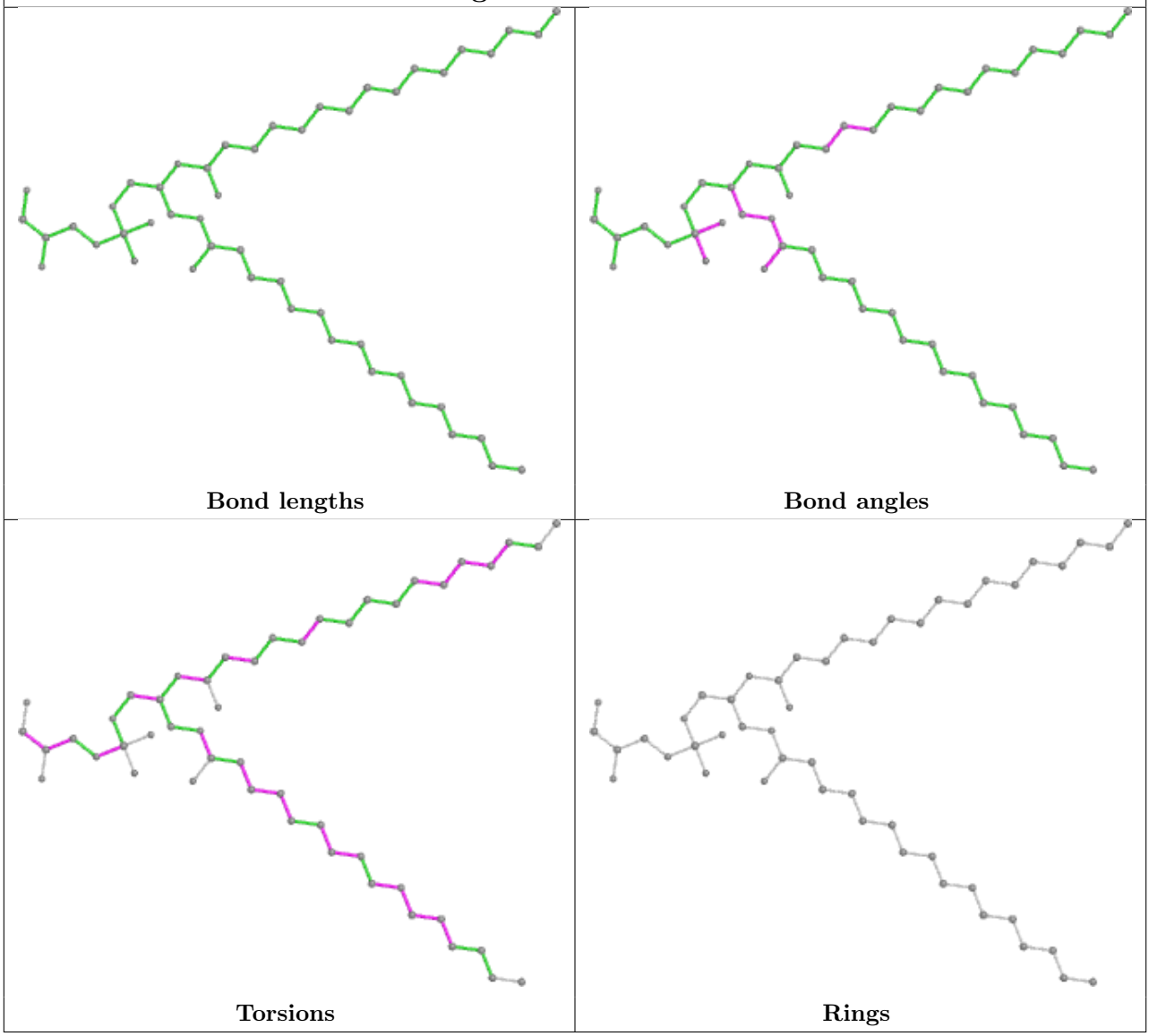


Rings

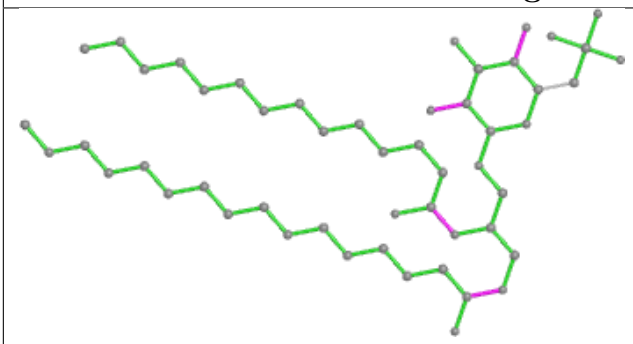
Ligand LMG m 101



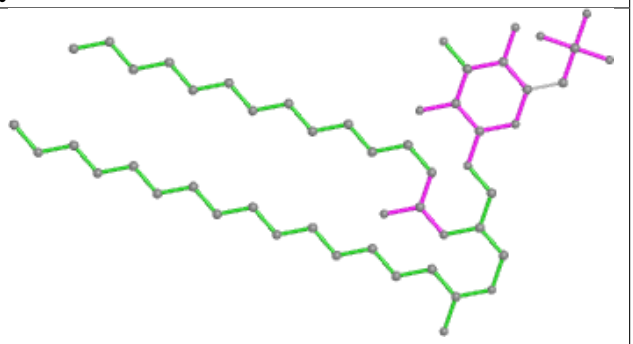
Ligand LHG d 405



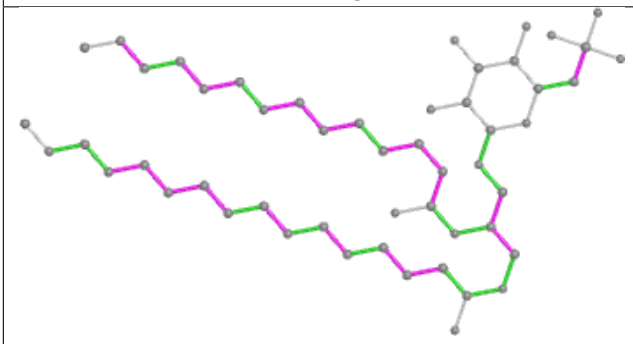
Ligand SQD A 614



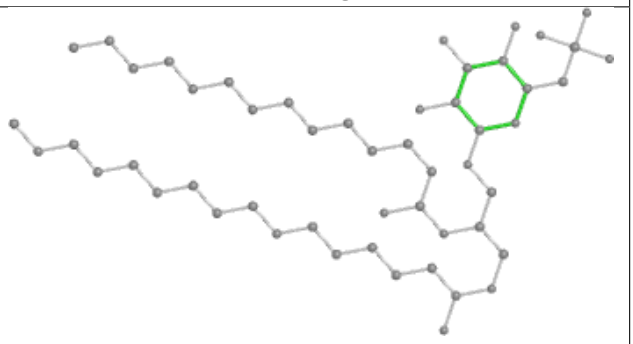
Bond lengths



Bond angles

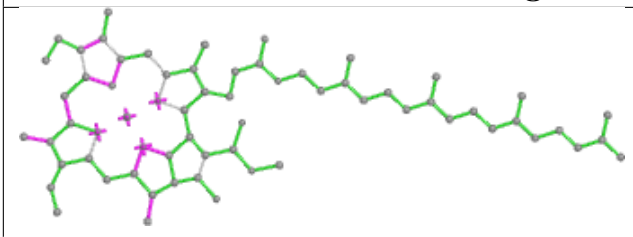


Torsions

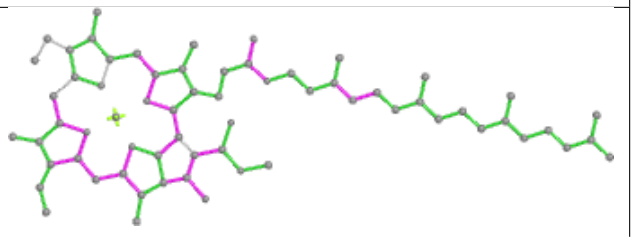


Rings

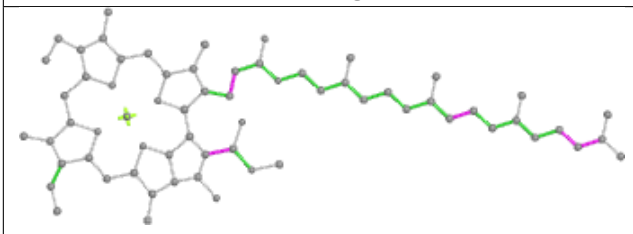
Ligand CLA B 606



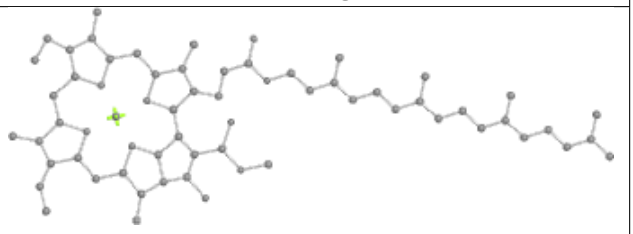
Bond lengths



Bond angles

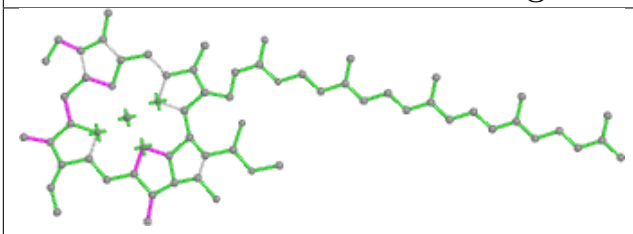


Torsions

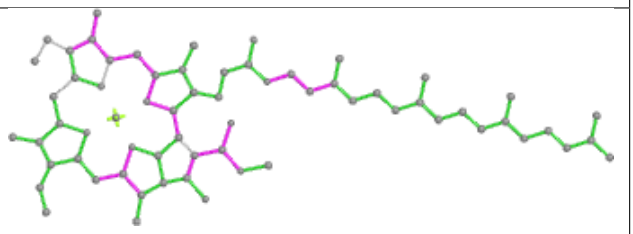


Rings

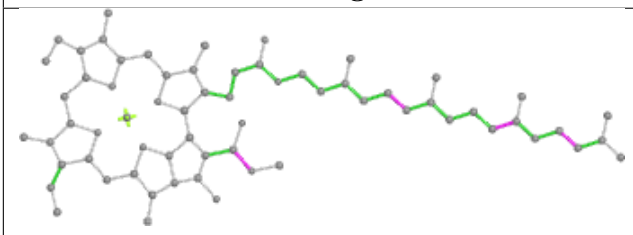
Ligand CLA d 403



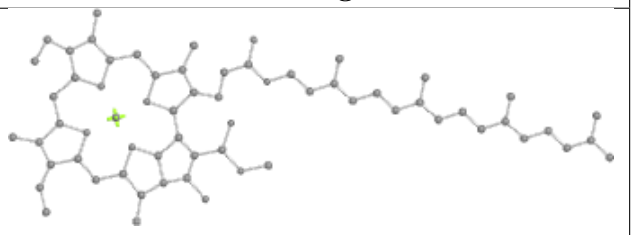
Bond lengths



Bond angles

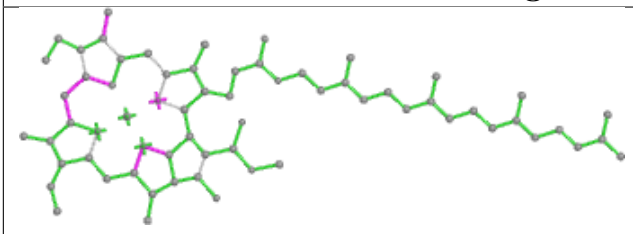


Torsions

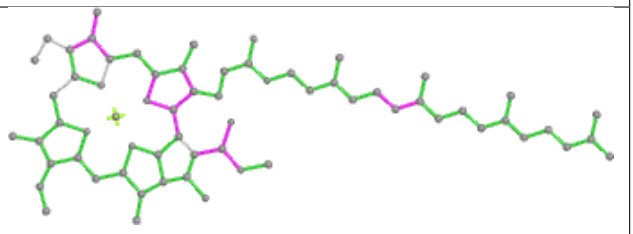


Rings

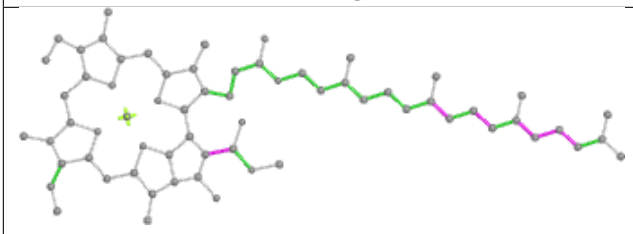
Ligand CLA C 513



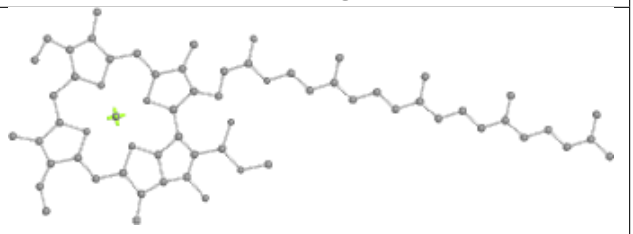
Bond lengths



Bond angles

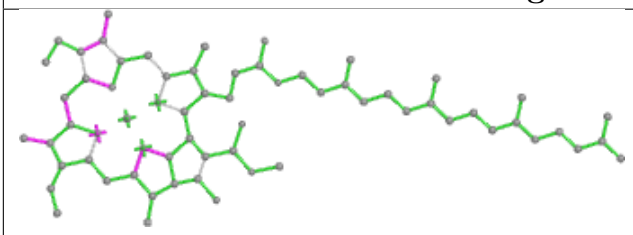


Torsions

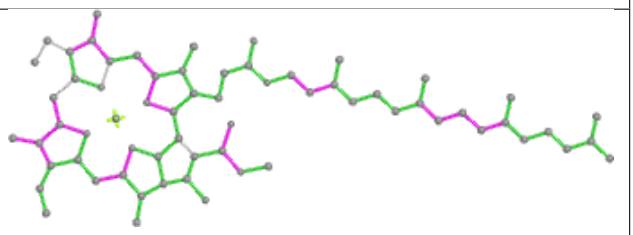


Rings

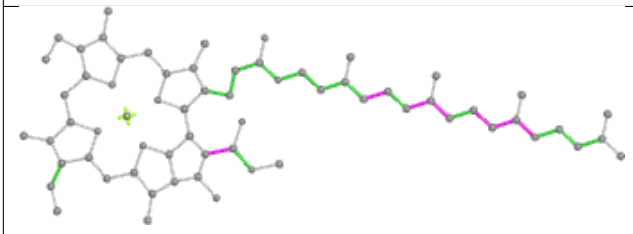
Ligand CLA b 604



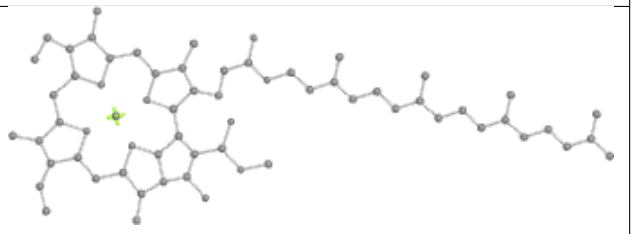
Bond lengths



Bond angles

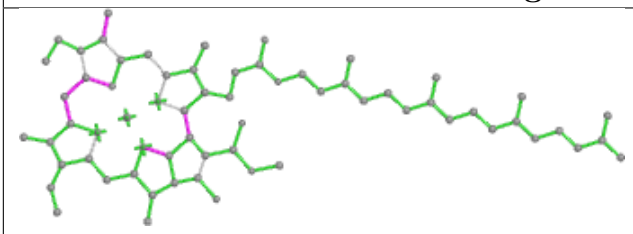


Torsions

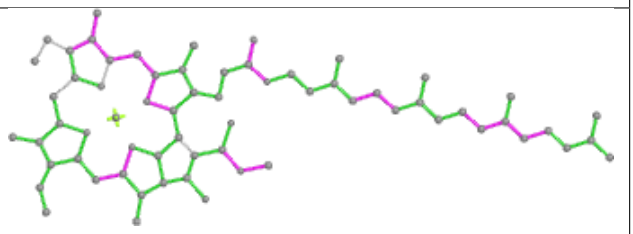


Rings

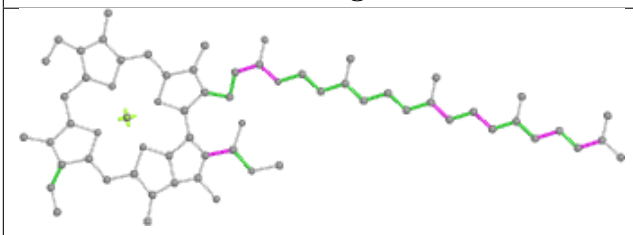
Ligand CLA B 612



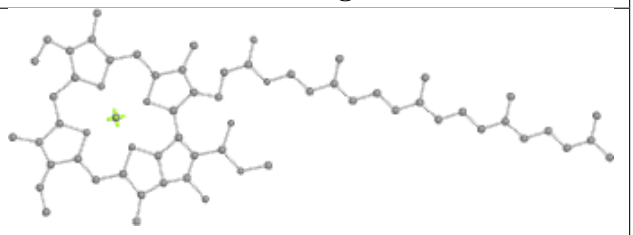
Bond lengths



Bond angles

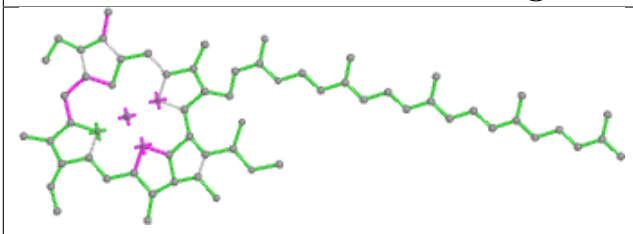


Torsions

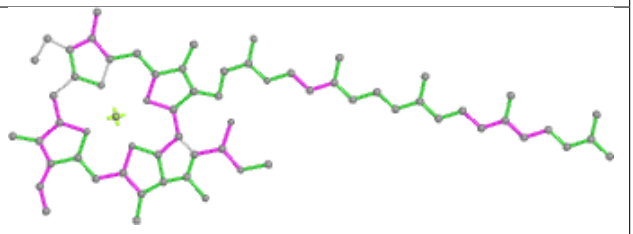


Rings

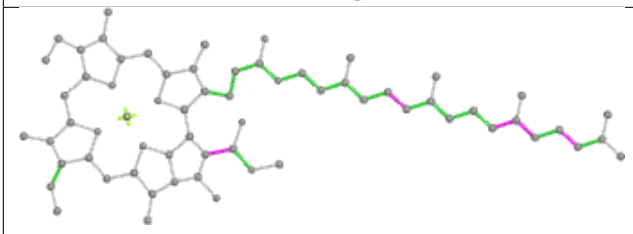
Ligand CLA b 605



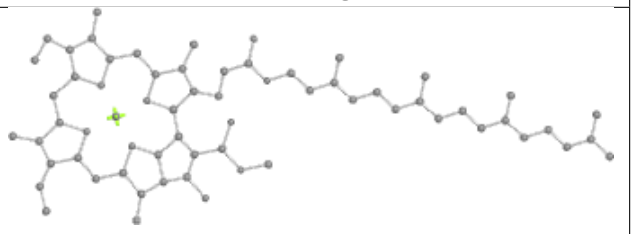
Bond lengths



Bond angles

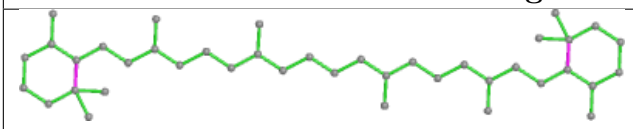


Torsions

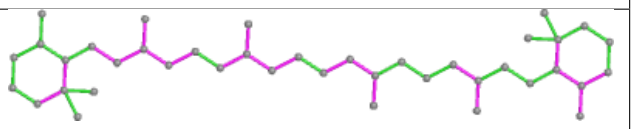


Rings

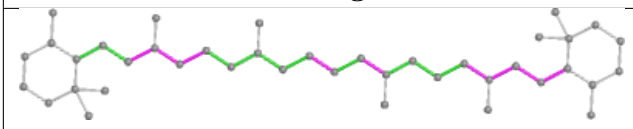
Ligand BCR h 102



Bond lengths



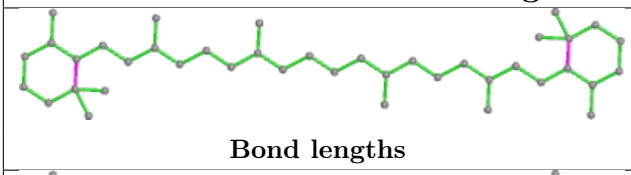
Bond angles



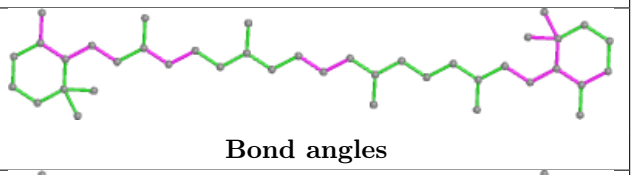
Torsions

Rings

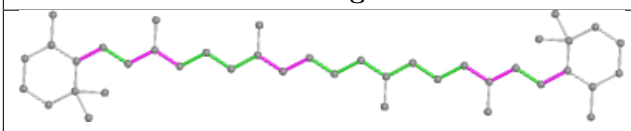
Ligand BCR Y 101



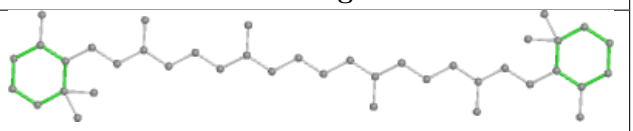
Bond lengths



Bond angles

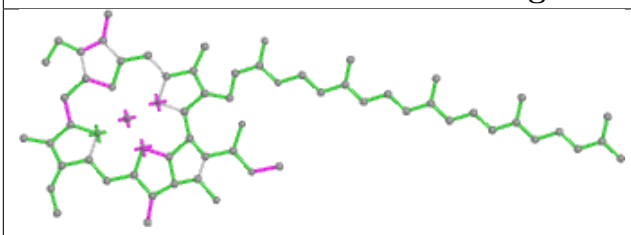


Torsions

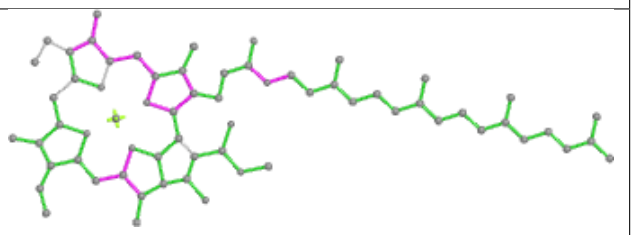


Rings

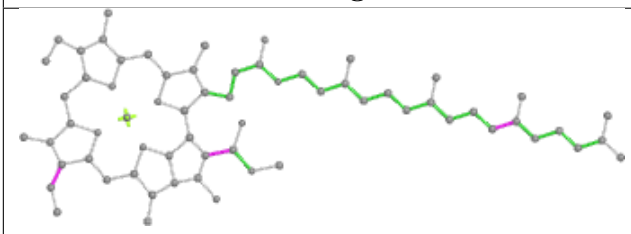
Ligand CLA a 612



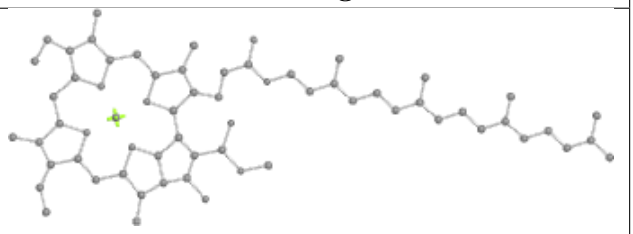
Bond lengths



Bond angles

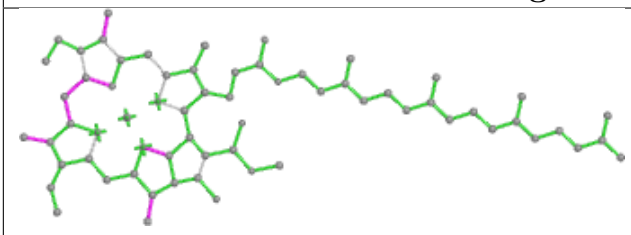


Torsions

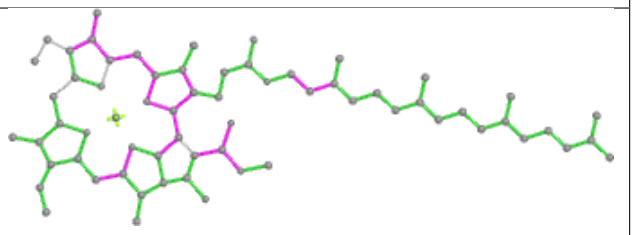


Rings

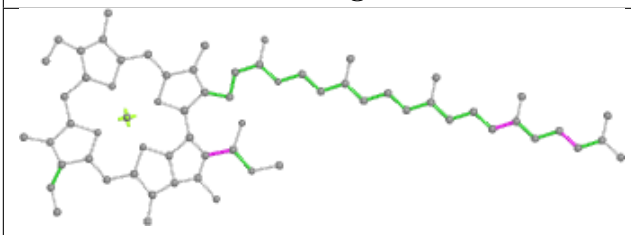
Ligand CLA c 502



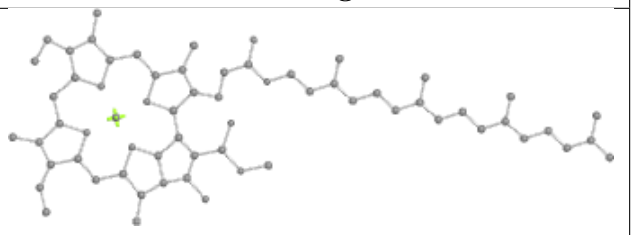
Bond lengths



Bond angles

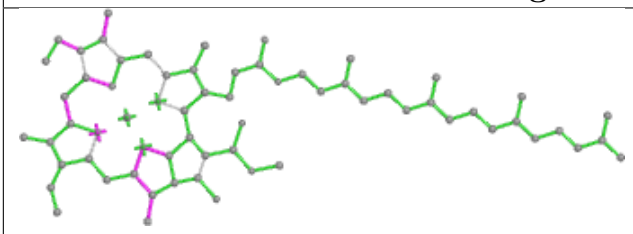


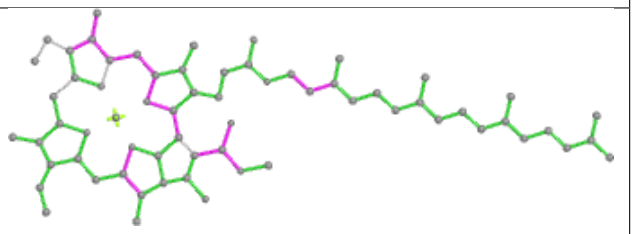
Torsions

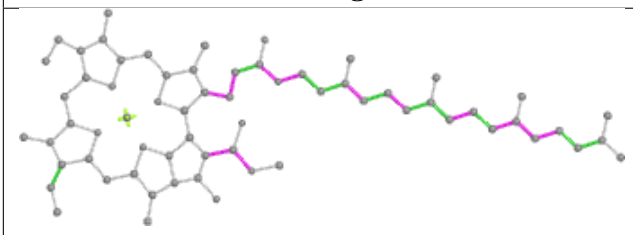


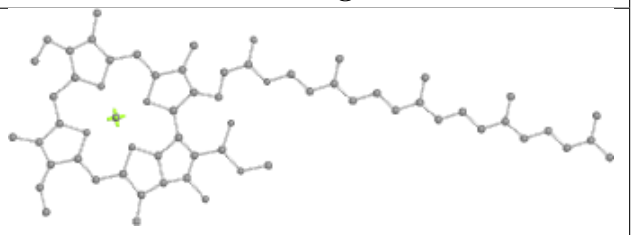
Rings

Ligand CLA c 512

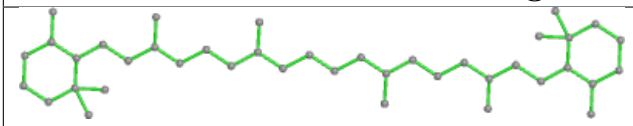

Bond lengths

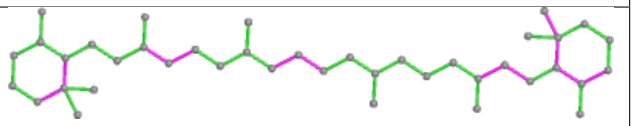

Bond angles

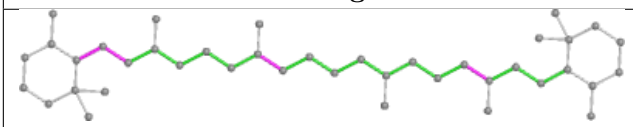

Torsions

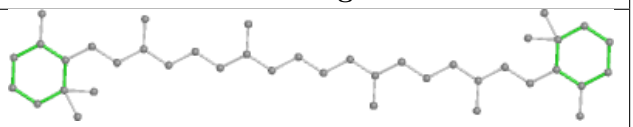

Rings

Ligand BCR k 102

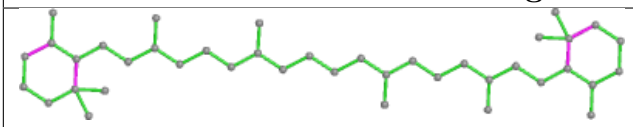

Bond lengths

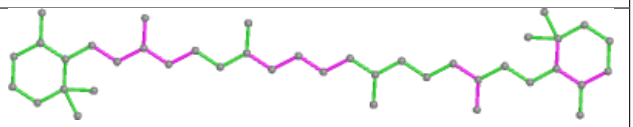

Bond angles

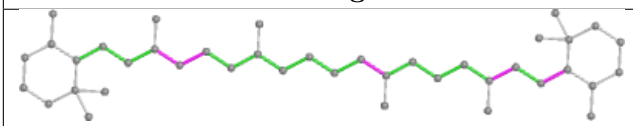

Torsions


Rings

Ligand BCR b 618

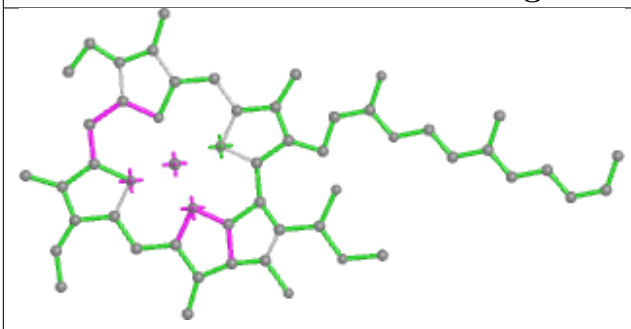

Bond lengths


Bond angles

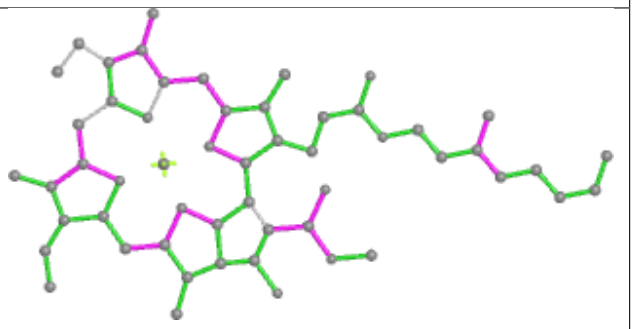

Torsions

Rings

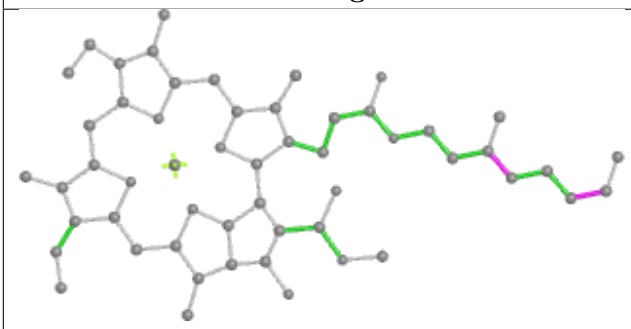
Ligand CLA A 607



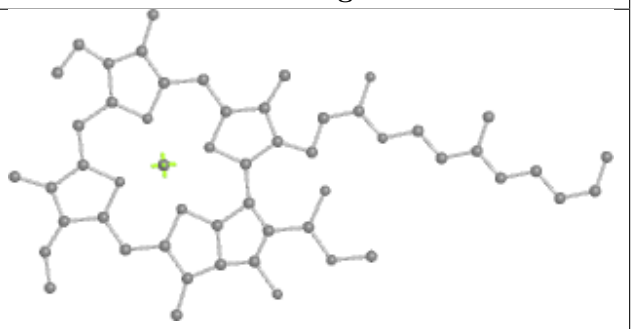
Bond lengths



Bond angles

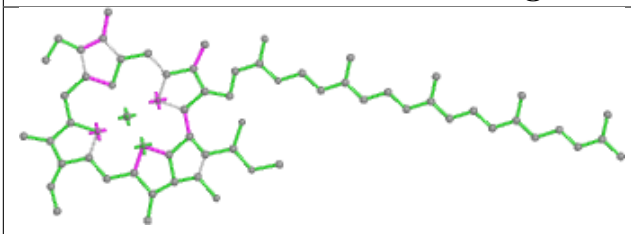


Torsions

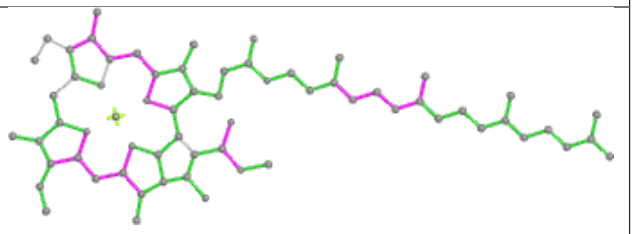


Rings

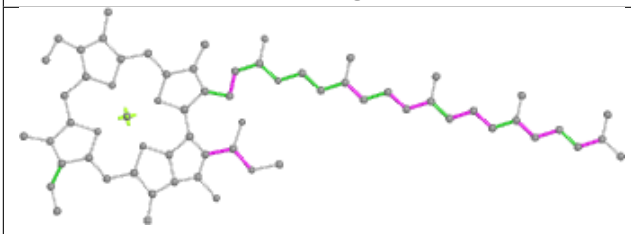
Ligand CLA B 603



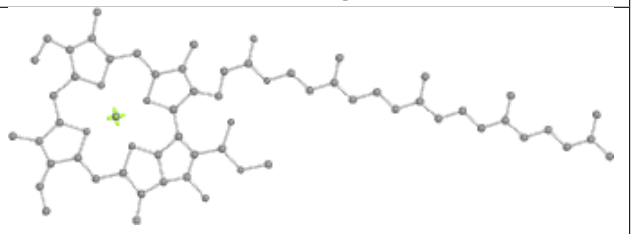
Bond lengths



Bond angles

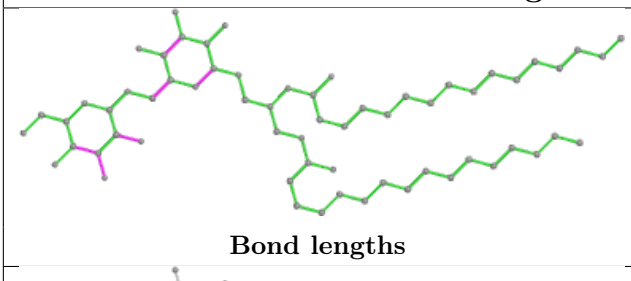


Torsions

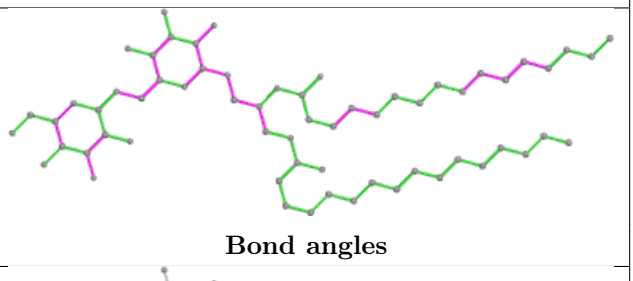


Rings

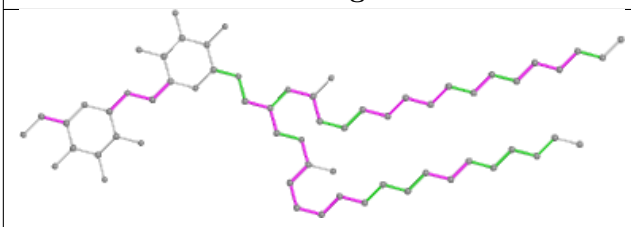
Ligand DGD c 516



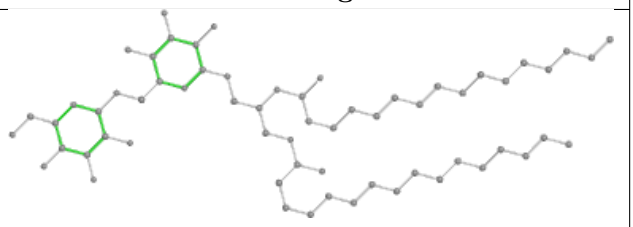
Bond lengths



Bond angles

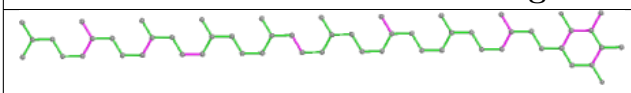


Torsions

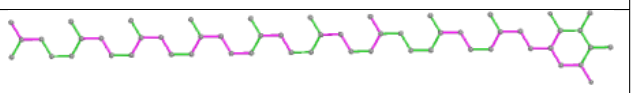


Rings

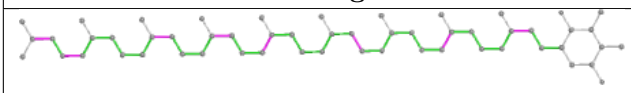
Ligand PL9 D 407



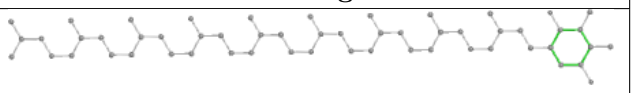
Bond lengths



Bond angles

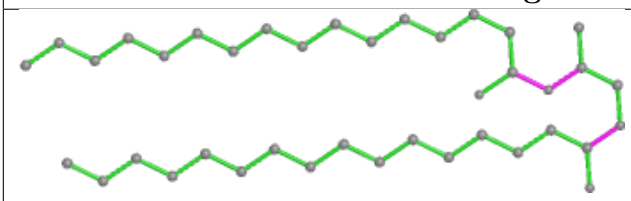


Torsions

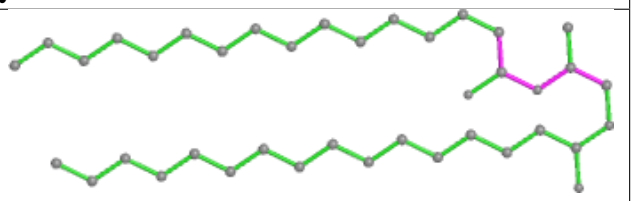


Rings

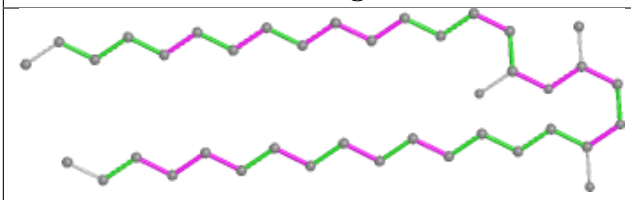
Ligand SQD A 616



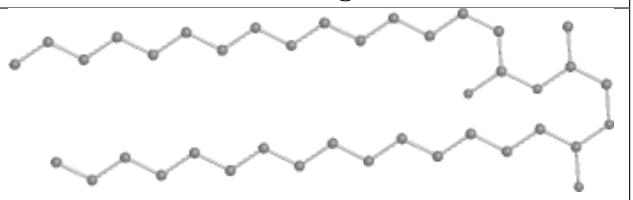
Bond lengths



Bond angles

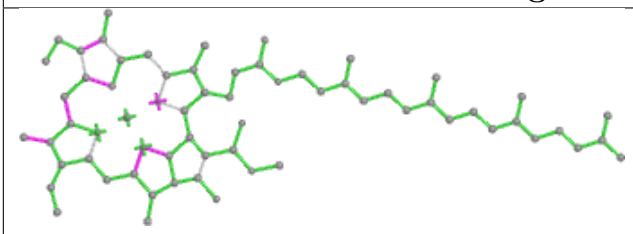


Torsions

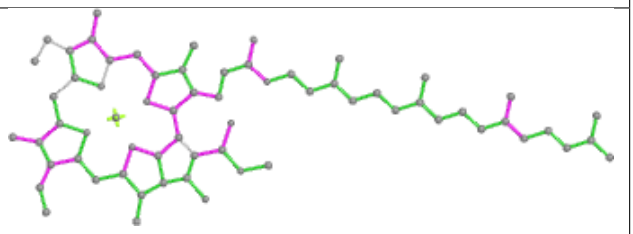


Rings

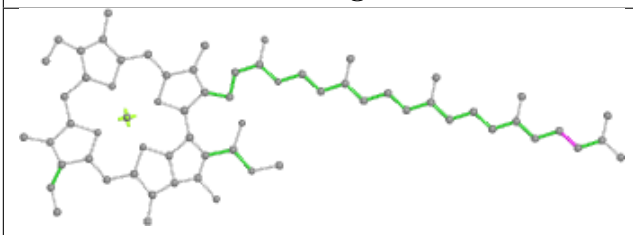
Ligand CLA a 603



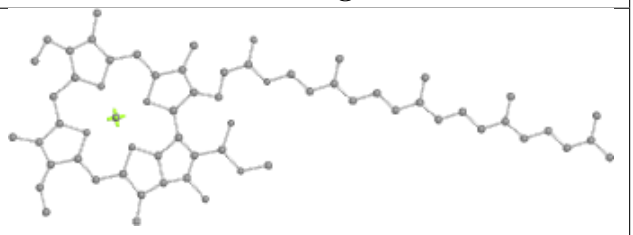
Bond lengths



Bond angles

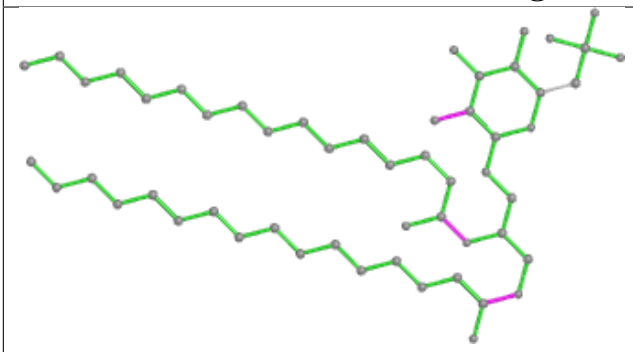


Torsions

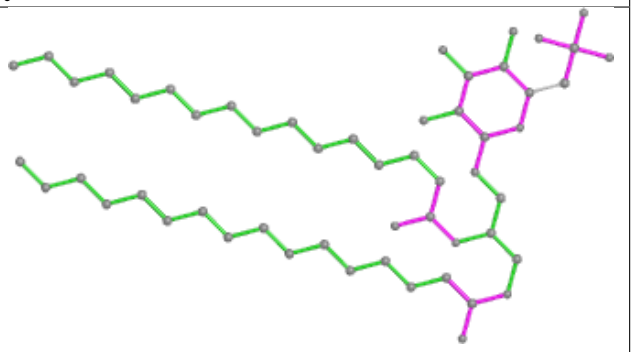


Rings

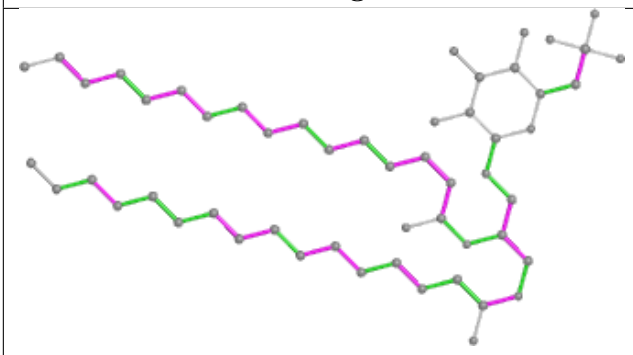
Ligand SQD a 613



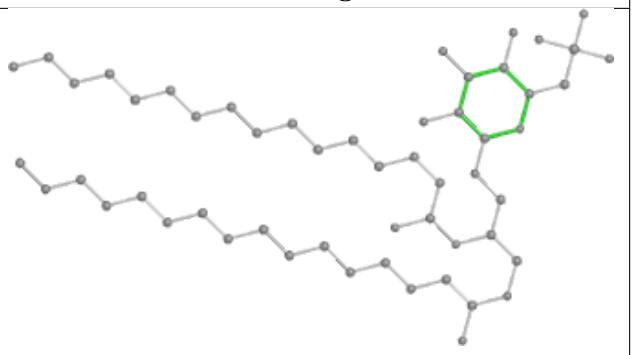
Bond lengths



Bond angles

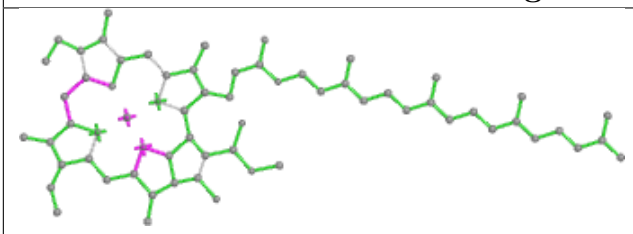


Torsions

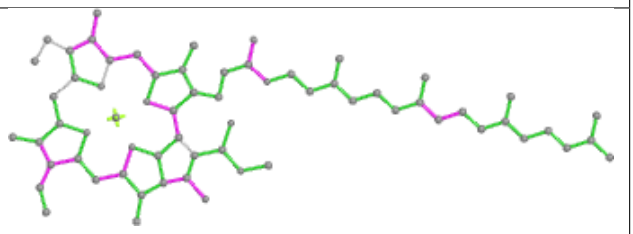


Rings

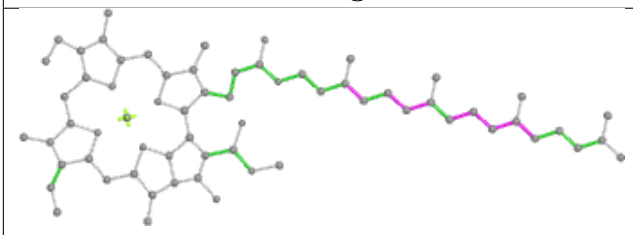
Ligand CLA C 505



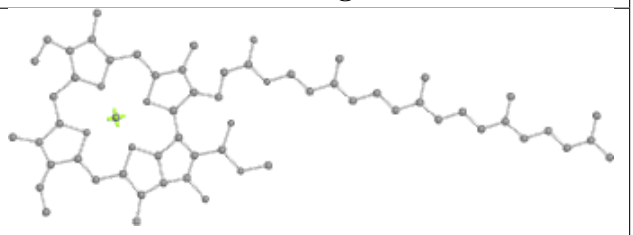
Bond lengths



Bond angles

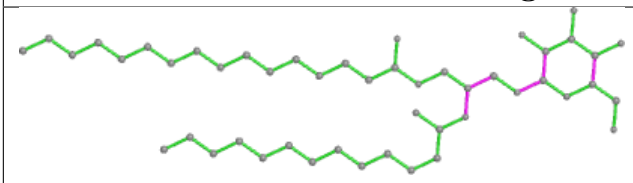


Torsions

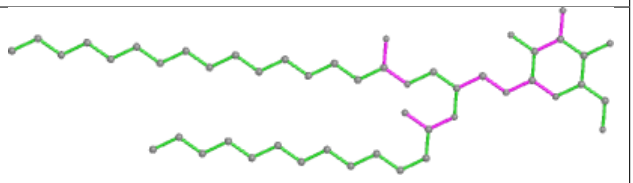


Rings

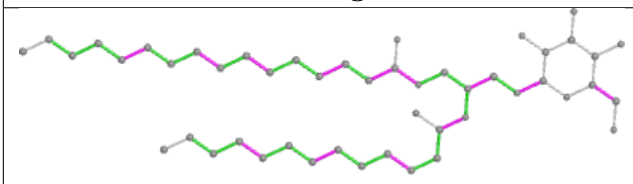
Ligand LMG C 519



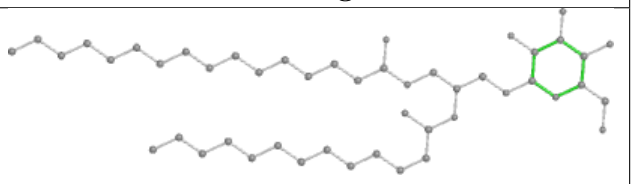
Bond lengths



Bond angles

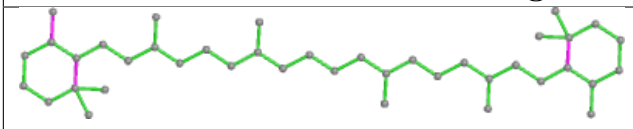


Torsions

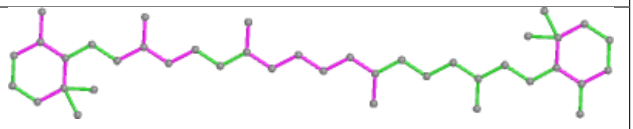


Rings

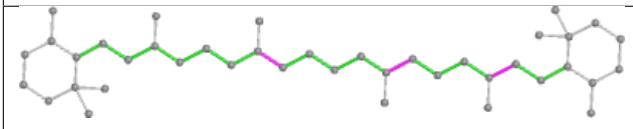
Ligand BCR c 515



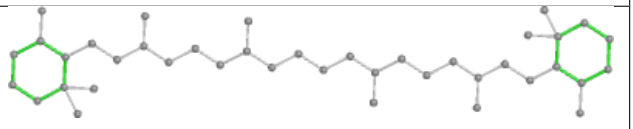
Bond lengths



Bond angles

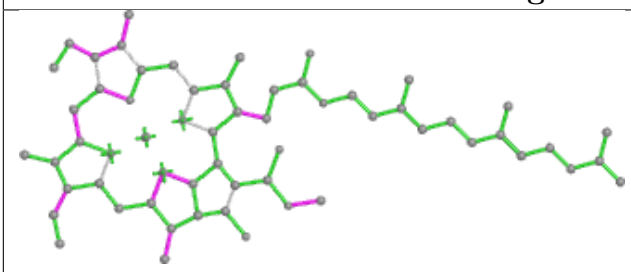


Torsions

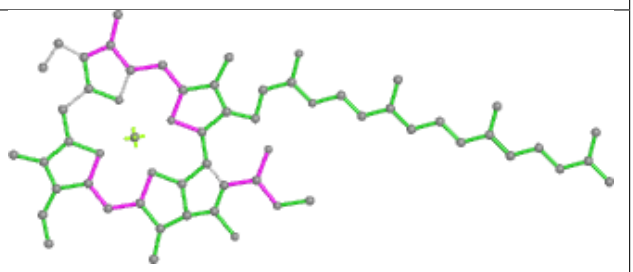


Rings

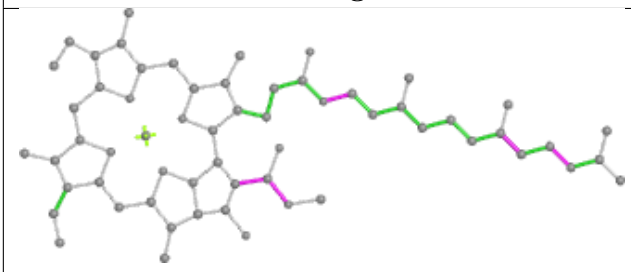
Ligand CLA b 616



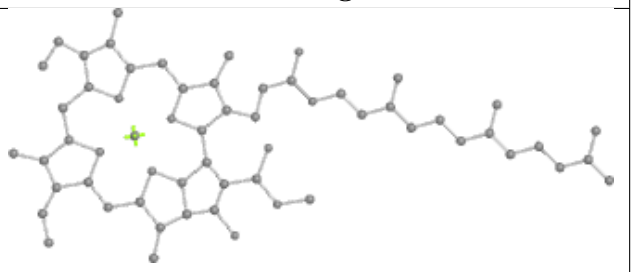
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/334 (100%)	-0.49	3 (0%) 84 86	19, 26, 44, 75	0
1	a	334/334 (100%)	-0.45	2 (0%) 89 91	20, 28, 55, 78	0
2	B	505/505 (100%)	-0.42	5 (0%) 82 84	20, 30, 60, 94	0
2	b	505/505 (100%)	-0.30	13 (2%) 56 60	22, 34, 72, 106	0
3	C	442/451 (98%)	-0.36	3 (0%) 87 89	23, 34, 51, 75	0
3	c	451/451 (100%)	-0.31	5 (1%) 80 82	23, 38, 60, 101	0
4	D	341/341 (100%)	-0.39	0 100 100	20, 28, 44, 84	0
4	d	341/341 (100%)	-0.38	2 (0%) 89 91	20, 32, 57, 76	0
5	E	81/82 (98%)	0.06	4 (4%) 29 31	30, 48, 69, 87	0
5	e	82/82 (100%)	0.24	4 (4%) 29 31	36, 57, 81, 89	0
6	F	34/34 (100%)	-0.38	1 (2%) 51 56	33, 40, 57, 80	0
6	f	34/34 (100%)	-0.20	1 (2%) 51 56	41, 49, 80, 86	0
7	H	65/65 (100%)	-0.08	2 (3%) 49 53	30, 37, 58, 71	0
7	h	63/65 (96%)	0.07	1 (1%) 72 74	38, 48, 56, 70	0
8	I	35/36 (97%)	-0.28	1 (2%) 51 56	28, 35, 68, 73	0
8	i	35/36 (97%)	-0.25	1 (2%) 51 56	30, 38, 68, 73	0
9	J	36/36 (100%)	0.23	4 (11%) 5 5	32, 46, 77, 91	0
9	j	36/36 (100%)	0.31	5 (13%) 2 2	36, 49, 85, 89	0
10	K	37/37 (100%)	-0.23	0 100 100	39, 49, 63, 69	0
10	k	37/37 (100%)	0.10	1 (2%) 54 59	45, 54, 70, 75	0
11	L	37/37 (100%)	-0.42	0 100 100	22, 26, 63, 70	0
11	l	36/37 (97%)	-0.39	0 100 100	23, 27, 66, 79	0
12	M	32/33 (96%)	-0.28	1 (3%) 49 53	24, 31, 64, 72	0
12	m	31/33 (93%)	-0.29	0 100 100	26, 32, 45, 66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	-0.09	11 (4%) 33 35	22, 40, 79, 136	0
13	o	244/244 (100%)	-0.18	13 (5%) 26 28	22, 38, 78, 134	0
14	R	34/34 (100%)	1.73	12 (35%) 0 0	58, 68, 84, 92	0
14	r	31/34 (91%)	2.51	18 (58%) 0 0	66, 85, 99, 104	0
15	T	29/30 (96%)	-0.67	2 (6%) 16 18	24, 28, 58, 70	0
15	t	29/30 (96%)	-0.51	2 (6%) 16 18	23, 28, 75, 90	0
16	U	97/97 (100%)	-0.29	3 (3%) 49 53	28, 40, 67, 94	0
16	u	97/97 (100%)	-0.49	1 (1%) 82 84	28, 37, 56, 88	0
17	V	137/137 (100%)	-0.57	0 100 100	25, 38, 54, 80	0
17	v	137/137 (100%)	-0.23	2 (1%) 73 76	31, 44, 67, 81	0
18	X	38/38 (100%)	0.05	3 (7%) 12 13	35, 49, 74, 82	0
18	x	38/38 (100%)	0.44	3 (7%) 12 13	45, 58, 83, 98	0
19	Y	27/30 (90%)	1.72	9 (33%) 0 0	51, 74, 114, 117	0
19	y	30/30 (100%)	0.88	5 (16%) 1 1	54, 72, 96, 103	0
20	Z	62/62 (100%)	0.74	15 (24%) 0 0	48, 62, 114, 126	0
20	z	62/62 (100%)	0.94	12 (19%) 1 0	54, 70, 109, 121	0
All	All	5300/5326 (99%)	-0.24	170 (3%) 47 52	19, 35, 72, 136	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	z	33	TRP	8.8
13	o	3	GLN	8.1
13	O	3	GLN	8.0
18	X	2	THR	7.1
19	Y	20	ALA	7.1
1	A	13	LEU	6.4
13	O	4	THR	6.2
9	J	5	GLY	6.1
13	O	60	ARG	5.7
14	r	14	LEU	5.7
13	O	59	LYS	5.4
13	o	58	ASN	5.4
14	r	26	TYR	5.0
14	r	3	TRP	5.0
19	Y	37	PHE	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	o	4	THR	4.8
19	Y	23	THR	4.8
19	Y	22	LEU	4.7
3	c	23	ALA	4.7
13	o	56	PRO	4.7
14	r	13	LEU	4.6
20	z	35	ARG	4.6
13	o	61	GLN	4.5
19	Y	41	VAL	4.5
19	Y	21	GLN	4.5
9	J	7	ARG	4.5
14	R	3	TRP	4.5
2	b	127	ARG	4.4
9	J	8	ILE	4.4
13	o	57	LYS	4.4
18	x	2	THR	4.4
14	R	6	LEU	4.4
9	J	6	GLY	4.4
19	Y	43	ARG	4.4
20	Z	33	TRP	4.3
19	y	19	ILE	4.3
5	E	79	PHE	4.2
2	b	506	ARG	4.2
5	e	79	PHE	4.1
14	r	6	LEU	4.0
9	j	8	ILE	4.0
14	r	24	LEU	4.0
3	c	24	THR	3.9
2	B	505	ARG	3.9
6	F	12	SER	3.9
14	r	5	VAL	3.8
14	R	26	TYR	3.7
9	j	5	GLY	3.7
14	r	10	LEU	3.7
20	z	30	PRO	3.6
13	O	56	PRO	3.6
20	z	34	ASP	3.5
2	b	495	PHE	3.5
18	X	3	ILE	3.5
20	Z	38	GLN	3.5
9	j	7	ARG	3.4
20	Z	62	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	r	23	ILE	3.4
14	r	18	TRP	3.4
14	r	2	ASP	3.4
14	r	9	LEU	3.4
20	Z	42	LEU	3.4
20	Z	35	ARG	3.3
20	Z	34	ASP	3.3
13	O	63	ALA	3.3
16	U	8	GLU	3.3
20	z	60	PHE	3.3
13	o	5	LEU	3.3
20	Z	3	ILE	3.3
20	z	41	PHE	3.3
14	R	32	GLN	3.2
14	R	21	ARG	3.2
13	O	61	GLN	3.2
6	f	13	TYR	3.2
3	c	143	TYR	3.2
20	z	3	ILE	3.2
2	B	506	ARG	3.1
13	O	62	GLU	3.1
19	y	18	VAL	3.1
5	E	83	LEU	3.1
19	Y	42	ARG	3.1
20	z	4	LEU	3.1
8	i	34	ARG	3.1
15	t	29	ILE	3.1
1	A	11	ALA	3.0
20	z	62	VAL	3.0
2	b	128	THR	3.0
14	R	28	VAL	3.0
7	H	66	GLY	3.0
14	r	25	PRO	3.0
16	U	67	LEU	3.0
20	Z	4	LEU	2.9
14	R	5	VAL	2.8
5	e	4	THR	2.8
14	R	27	ALA	2.8
18	x	3	ILE	2.8
20	Z	60	PHE	2.8
14	R	25	PRO	2.8
19	y	41	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	k	17	ILE	2.8
13	O	5	LEU	2.8
2	B	487	SER	2.8
19	y	17	GLU	2.8
8	I	36	ASP	2.7
20	Z	41	PHE	2.7
2	b	490	GLN	2.7
13	O	36	GLN	2.7
13	o	62	GLU	2.7
7	h	6	TRP	2.7
2	b	494	GLY	2.7
2	b	505	ARG	2.6
2	B	502	VAL	2.6
5	e	74	GLN	2.6
13	o	59	LYS	2.6
3	c	146	PHE	2.6
1	a	11	ALA	2.5
14	r	4	ARG	2.5
16	U	9	LEU	2.5
16	u	53	ALA	2.5
14	r	28	VAL	2.5
3	c	147	PHE	2.5
20	Z	1	MET	2.5
5	E	84	LYS	2.5
13	O	25	THR	2.4
14	r	7	VAL	2.4
19	y	20	ALA	2.4
5	E	17	VAL	2.4
7	H	6	TRP	2.4
1	A	12	ASN	2.4
2	b	502	VAL	2.4
20	Z	61	VAL	2.4
19	Y	24	MET	2.4
2	b	485	GLU	2.4
13	o	60	ARG	2.4
12	M	33	GLN	2.4
20	Z	31	GLN	2.4
20	z	37	LYS	2.4
9	j	11	TRP	2.3
17	v	16	GLY	2.3
20	Z	37	LYS	2.3
2	b	496	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	R	29	LYS	2.3
3	C	143	TYR	2.3
14	r	27	ALA	2.3
13	o	245	PRO	2.3
9	j	6	GLY	2.3
5	e	81	GLU	2.3
2	b	161	LEU	2.2
3	C	146	PHE	2.2
14	R	2	ASP	2.2
14	R	31	VAL	2.2
15	T	30	THR	2.2
2	B	485	GLU	2.2
1	a	16	ARG	2.2
13	o	207	ARG	2.2
4	d	51	GLY	2.2
3	C	106	VAL	2.2
20	z	32	ASP	2.2
13	o	246	ALA	2.2
15	t	28	ARG	2.1
20	z	36	SER	2.1
4	d	227[A]	GLU	2.1
2	b	489	GLU	2.1
18	X	38	GLN	2.1
17	v	17	LYS	2.1
2	b	486	LEU	2.1
14	r	15	ALA	2.0
15	T	29	ILE	2.0
20	Z	40	ILE	2.0
18	x	38	GLN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	FME	M	1	10/11	0.94	0.12	36,45,71,81	0
15	FME	T	1	10/11	0.94	0.12	27,45,71,71	0
8	FME	i	1	10/11	0.95	0.12	35,43,56,58	0
8	FME	I	1	10/11	0.96	0.12	34,47,61,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	FME	t	1	10/11	0.96	0.08	19,33,65,69	0
12	FME	m	1	10/11	0.97	0.12	26,49,72,73	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	UNL	c	523	28/-	0.72	0.20	45,67,86,88	0
33	UNL	a	617	28/-	0.75	0.30	42,65,78,78	0
33	UNL	H	103	53/-	0.78	0.22	45,74,95,103	0
30	LHG	A	615	49/49	0.78	0.22	48,80,108,117	0
33	UNL	c	520	55/-	0.78	0.17	34,54,93,94	0
33	UNL	E	101	28/-	0.78	0.31	45,71,88,95	0
33	UNL	B	628	28/-	0.80	0.39	52,70,102,107	0
28	LMG	c	521	48/55	0.80	0.25	39,81,114,121	0
28	LMG	D	409	33/55	0.80	0.16	34,53,93,95	0
29	SQD	a	615	36/54	0.81	0.18	30,66,85,87	0
33	UNL	B	627	47/-	0.81	0.32	44,63,79,79	0
33	UNL	b	620	55/-	0.82	0.20	37,60,83,90	0
33	UNL	b	623	55/-	0.82	0.17	42,64,85,85	0
33	UNL	m	102	28/-	0.82	0.16	42,63,77,78	0
33	UNL	x	101	55/-	0.82	0.19	39,58,75,75	0
27	PL9	a	611	55/55	0.83	0.20	38,69,88,94	0
28	LMG	d	410	23/55	0.83	0.19	31,71,94,98	0
33	UNL	t	103	26/-	0.83	0.20	35,59,76,83	0
28	LMG	b	621	55/55	0.83	0.27	40,76,103,112	0
31	DGD	A	617	66/66	0.84	0.18	42,64,85,111	0
33	UNL	C	523	47/-	0.84	0.11	37,53,71,75	0
27	PL9	A	611	55/55	0.84	0.23	35,58,81,84	135
23	CLA	c	513	65/65	0.85	0.19	44,69,104,112	0
31	DGD	a	616	44/66	0.85	0.15	33,56,77,89	0
33	UNL	B	621	43/-	0.85	0.13	31,50,71,76	0
25	BCR	h	102	40/40	0.85	0.14	35,54,74,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	512	65/65	0.86	0.14	38,55,94,108	0
33	UNL	b	622	40/-	0.86	0.14	43,59,81,83	0
30	LHG	a	614	42/49	0.86	0.26	58,86,109,122	0
23	CLA	C	513	65/65	0.86	0.16	43,62,88,97	0
23	CLA	h	101	65/65	0.86	0.15	41,62,91,97	0
25	BCR	H	101	40/40	0.86	0.11	29,45,59,68	0
33	UNL	T	102	47/-	0.86	0.17	35,51,66,74	0
33	UNL	B	626	46/-	0.86	0.14	39,59,72,77	0
29	SQD	b	601	49/54	0.87	0.13	39,58,99,111	0
25	BCR	Y	101	40/40	0.87	0.13	33,53,73,76	0
33	UNL	b	624	26/-	0.87	0.22	39,54,65,72	0
33	UNL	I	101	41/-	0.87	0.15	36,53,72,79	0
29	SQD	B	624	54/54	0.88	0.14	37,59,97,109	0
28	LMG	c	519	37/55	0.88	0.16	38,69,88,92	0
25	BCR	k	101	40/40	0.88	0.12	44,63,75,80	0
29	SQD	f	101	41/54	0.88	0.19	45,84,111,119	0
33	UNL	J	101	28/-	0.88	0.13	48,62,68,70	0
28	LMG	B	622	28/55	0.88	0.15	31,48,58,63	0
33	UNL	d	411	43/-	0.88	0.16	39,55,66,70	0
33	UNL	l	102	53/-	0.88	0.15	25,48,87,99	0
33	UNL	T	103	44/-	0.88	0.18	38,57,79,84	0
33	UNL	X	101	55/-	0.88	0.21	33,52,73,79	0
29	SQD	A	616	39/54	0.88	0.16	41,65,88,92	0
33	UNL	j	101	28/-	0.89	0.12	46,61,70,74	0
23	CLA	C	512	65/65	0.89	0.15	31,53,103,112	0
28	LMG	c	522	49/55	0.89	0.14	32,56,91,110	0
33	UNL	t	102	34/-	0.89	0.13	35,50,56,63	0
23	CLA	B	616	60/65	0.89	0.15	21,39,94,99	0
28	LMG	C	519	48/55	0.89	0.16	46,73,95,106	0
28	LMG	A	612	48/55	0.90	0.15	31,56,74,91	0
33	UNL	M	102	26/-	0.91	0.14	30,50,60,62	0
23	CLA	D	403	65/65	0.91	0.13	19,39,104,113	0
33	UNL	C	521	28/-	0.91	0.09	28,40,53,66	0
33	UNL	C	522	28/-	0.91	0.12	43,54,64,66	0
28	LMG	B	620	51/55	0.91	0.11	25,49,73,87	0
28	LMG	m	101	51/55	0.91	0.12	33,51,81,98	0
33	UNL	B	625	28/-	0.91	0.11	26,48,64,71	0
23	CLA	a	606	65/65	0.91	0.14	17,34,86,104	0
23	CLA	b	616	60/65	0.91	0.14	25,42,90,95	0
23	CLA	b	615	65/65	0.92	0.11	25,40,55,65	0
23	CLA	d	403	65/65	0.92	0.14	31,48,100,105	0
25	BCR	k	102	40/40	0.92	0.15	36,51,72,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	615	65/65	0.92	0.12	22,37,67,83	0
25	BCR	C	515	40/40	0.92	0.11	21,35,50,54	0
31	DGD	h	103	62/66	0.92	0.11	31,48,61,74	0
25	BCR	D	404	40/40	0.92	0.10	28,43,98,109	0
23	CLA	c	508	64/65	0.92	0.12	28,44,83,104	0
23	CLA	B	601	65/65	0.92	0.14	25,60,104,130	0
29	SQD	a	613	54/54	0.92	0.13	39,67,93,101	0
25	BCR	c	514	40/40	0.92	0.15	39,60,71,72	0
25	BCR	d	404	40/40	0.92	0.11	32,51,90,97	0
23	CLA	b	604	65/65	0.93	0.15	20,34,80,90	0
30	LHG	d	409	39/49	0.93	0.12	27,47,66,70	0
25	BCR	C	514	40/40	0.93	0.11	35,54,66,68	0
31	DGD	C	517	62/66	0.93	0.12	32,51,107,118	0
31	DGD	H	102	62/66	0.93	0.11	30,48,61,73	0
23	CLA	c	510	65/65	0.93	0.13	33,49,67,74	0
28	LMG	D	405	51/55	0.93	0.14	26,54,98,102	0
33	UNL	M	101	37/-	0.93	0.11	31,43,63,70	0
23	CLA	b	606	65/65	0.93	0.11	20,38,69,74	0
23	CLA	c	503	65/65	0.93	0.14	32,44,57,62	0
23	CLA	c	507	65/65	0.93	0.14	23,42,57,66	0
25	BCR	b	617	40/40	0.93	0.10	24,42,54,58	0
25	BCR	b	618	40/40	0.93	0.09	25,37,53,60	0
23	CLA	C	510	65/65	0.94	0.12	28,45,67,73	0
23	CLA	C	511	65/65	0.94	0.11	28,50,68,68	0
23	CLA	c	502	65/65	0.94	0.13	28,41,65,67	0
28	LMG	d	406	44/55	0.94	0.13	31,54,94,113	0
23	CLA	A	604	65/65	0.94	0.12	14,33,101,121	0
23	CLA	c	504	60/65	0.94	0.12	31,45,79,90	0
25	BCR	b	619	40/40	0.94	0.11	25,47,58,64	0
23	CLA	c	505	65/65	0.94	0.14	22,41,66,73	0
29	SQD	F	101	36/54	0.94	0.12	45,67,87,92	0
23	CLA	c	506	65/65	0.94	0.13	31,52,107,111	0
23	CLA	B	606	65/65	0.94	0.10	17,32,74,80	0
23	CLA	C	503	65/65	0.94	0.09	24,39,51,63	0
23	CLA	a	604	65/65	0.94	0.12	26,40,89,107	0
25	BCR	t	101	40/40	0.94	0.08	24,36,57,63	0
23	CLA	c	511	65/65	0.94	0.13	36,54,72,75	0
27	PL9	D	407	55/55	0.94	0.11	20,31,40,48	0
23	CLA	C	505	65/65	0.94	0.16	20,39,71,83	0
31	DGD	C	516	62/66	0.94	0.11	21,41,76,90	0
23	CLA	b	602	65/65	0.94	0.14	23,41,65,75	0
31	DGD	C	518	62/66	0.94	0.10	25,44,75,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	506	65/65	0.94	0.12	25,40,101,113	0
23	CLA	C	507	65/65	0.94	0.12	20,38,60,68	0
31	DGD	c	517	62/66	0.94	0.11	29,50,83,96	0
31	DGD	c	518	62/66	0.94	0.11	27,50,77,91	0
25	BCR	A	608	40/40	0.94	0.09	20,32,40,46	0
25	BCR	B	618	40/40	0.94	0.08	21,37,56,56	0
23	CLA	b	609	65/65	0.94	0.13	27,45,69,79	0
23	CLA	b	613	65/65	0.94	0.12	18,32,65,75	0
23	CLA	C	501	65/65	0.95	0.11	23,35,49,60	0
27	PL9	d	408	55/55	0.95	0.10	21,33,43,47	0
25	BCR	C	520	40/40	0.95	0.15	36,51,66,69	0
30	LHG	B	623	49/49	0.95	0.11	25,42,70,73	0
23	CLA	C	502	65/65	0.95	0.10	26,40,54,61	0
30	LHG	d	405	49/49	0.95	0.12	35,50,72,88	0
23	CLA	b	612	65/65	0.95	0.13	16,33,47,56	0
25	BCR	T	101	40/40	0.95	0.08	25,42,61,68	0
23	CLA	c	509	65/65	0.95	0.15	28,46,64,68	0
25	BCR	a	607	40/40	0.95	0.08	15,31,41,49	0
23	CLA	A	607	54/65	0.95	0.12	15,28,62,69	0
23	CLA	b	614	65/65	0.95	0.13	22,36,77,87	0
23	CLA	D	402	65/65	0.95	0.10	16,30,56,64	0
31	DGD	c	516	62/66	0.95	0.11	19,41,75,84	0
23	CLA	B	609	65/65	0.95	0.10	23,35,58,66	0
25	BCR	c	515	40/40	0.95	0.10	28,41,52,71	0
23	CLA	c	501	65/65	0.95	0.12	27,38,49,55	0
23	CLA	B	614	65/65	0.95	0.12	20,34,82,95	0
29	SQD	A	614	52/54	0.95	0.13	31,58,84,89	0
23	CLA	A	603	65/65	0.95	0.10	13,25,44,57	0
25	BCR	B	617	40/40	0.95	0.09	25,39,53,56	0
23	CLA	C	508	65/65	0.95	0.10	23,40,100,118	0
25	BCR	B	619	40/40	0.95	0.09	20,39,59,66	0
23	CLA	B	604	65/65	0.95	0.11	18,31,82,93	0
24	PHO	a	605	64/64	0.96	0.11	18,29,38,43	0
24	PHO	d	401	64/64	0.96	0.11	25,38,46,65	0
23	CLA	C	504	59/65	0.96	0.12	24,42,80,85	0
23	CLA	B	612	65/65	0.96	0.12	19,30,44,44	0
23	CLA	a	603	65/65	0.96	0.09	16,29,43,51	0
30	LHG	D	406	49/49	0.96	0.11	22,38,54,65	0
23	CLA	B	613	65/65	0.96	0.11	17,30,68,73	0
23	CLA	A	613	65/65	0.96	0.10	14,26,48,58	0
30	LHG	d	407	49/49	0.96	0.10	25,42,60,64	0
23	CLA	a	612	65/65	0.96	0.10	18,28,38,44	0

Continued on next page...

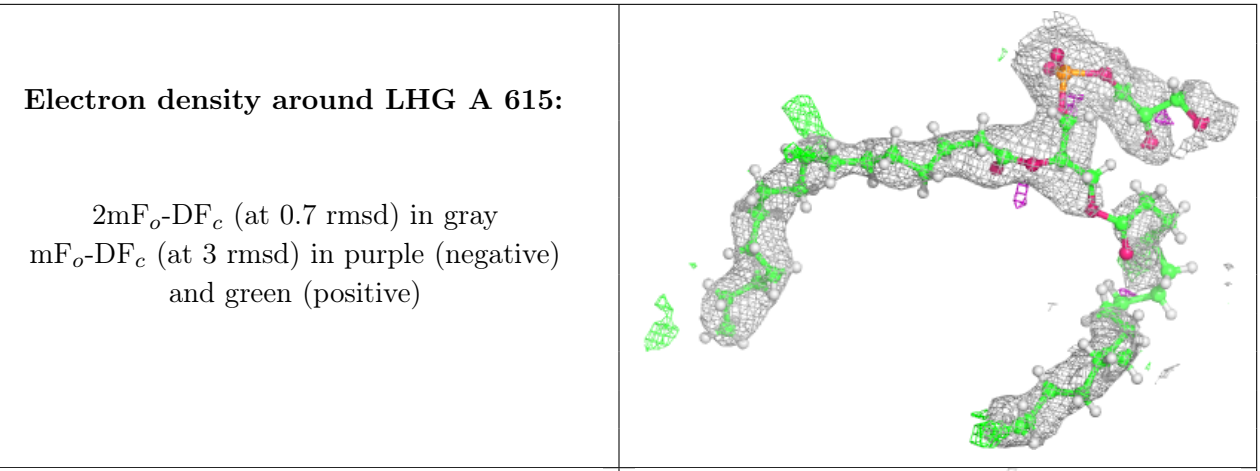
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LHG	l	101	49/49	0.96	0.11	29,43,59,64	0
23	CLA	B	605	65/65	0.96	0.14	17,29,47,49	0
23	CLA	b	603	65/65	0.96	0.13	21,36,69,76	0
23	CLA	C	509	65/65	0.96	0.13	22,41,63,64	0
23	CLA	b	605	65/65	0.96	0.12	19,33,47,56	0
23	CLA	B	602	65/65	0.96	0.11	22,34,59,63	0
23	CLA	b	607	65/65	0.96	0.11	19,36,61,68	0
23	CLA	b	608	65/65	0.96	0.10	24,39,61,64	0
23	CLA	B	607	65/65	0.96	0.10	15,31,59,67	0
23	CLA	b	610	65/65	0.96	0.13	22,36,53,55	0
23	CLA	b	611	65/65	0.96	0.10	20,34,51,55	0
23	CLA	d	402	65/65	0.96	0.09	20,34,64,70	0
23	CLA	B	603	65/65	0.96	0.12	14,31,62,69	0
23	CLA	B	610	65/65	0.96	0.13	18,30,43,47	0
24	PHO	A	605	64/64	0.96	0.09	12,27,36,40	0
24	PHO	A	606	64/64	0.96	0.08	19,30,44,50	0
35	HEM	F	102	43/43	0.96	0.12	34,48,68,69	0
30	LHG	L	101	49/49	0.97	0.11	24,39,54,65	0
23	CLA	B	611	65/65	0.97	0.11	18,30,47,53	0
23	CLA	B	608	65/65	0.97	0.10	20,33,52,64	0
30	LHG	D	408	47/49	0.97	0.09	23,46,81,103	0
35	HEM	f	102	43/43	0.97	0.11	41,55,76,78	0
36	HEC	v	201	43/43	0.97	0.13	27,36,49,53	0
36	HEC	V	201	43/43	0.98	0.12	21,31,42,46	0
22	FE2	A	602	1/1	0.99	0.07	25,25,25,25	0
22	FE2	a	602	1/1	0.99	0.06	30,30,30,30	0
26	CL	A	609	1/1	0.99	0.05	27,27,27,27	0
32	OEY	A	618[B]	11/11	0.99	0.10	23,27,30,31	11
32	OEY	a	618[B]	11/11	0.99	0.11	22,28,30,31	11
26	CL	A	610	1/1	0.99	0.04	24,24,24,24	0
34	BCT	D	401	4/4	0.99	0.15	26,27,32,37	0
34	BCT	a	610	4/4	0.99	0.17	26,32,41,50	0
26	CL	a	608	1/1	0.99	0.06	25,25,25,25	0
26	CL	a	609	1/1	0.99	0.05	25,25,25,25	0
21	OEX	A	601[A]	10/10	0.99	0.10	21,25,28,32	10
21	OEX	a	601[A]	10/10	0.99	0.10	19,22,28,28	10

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.

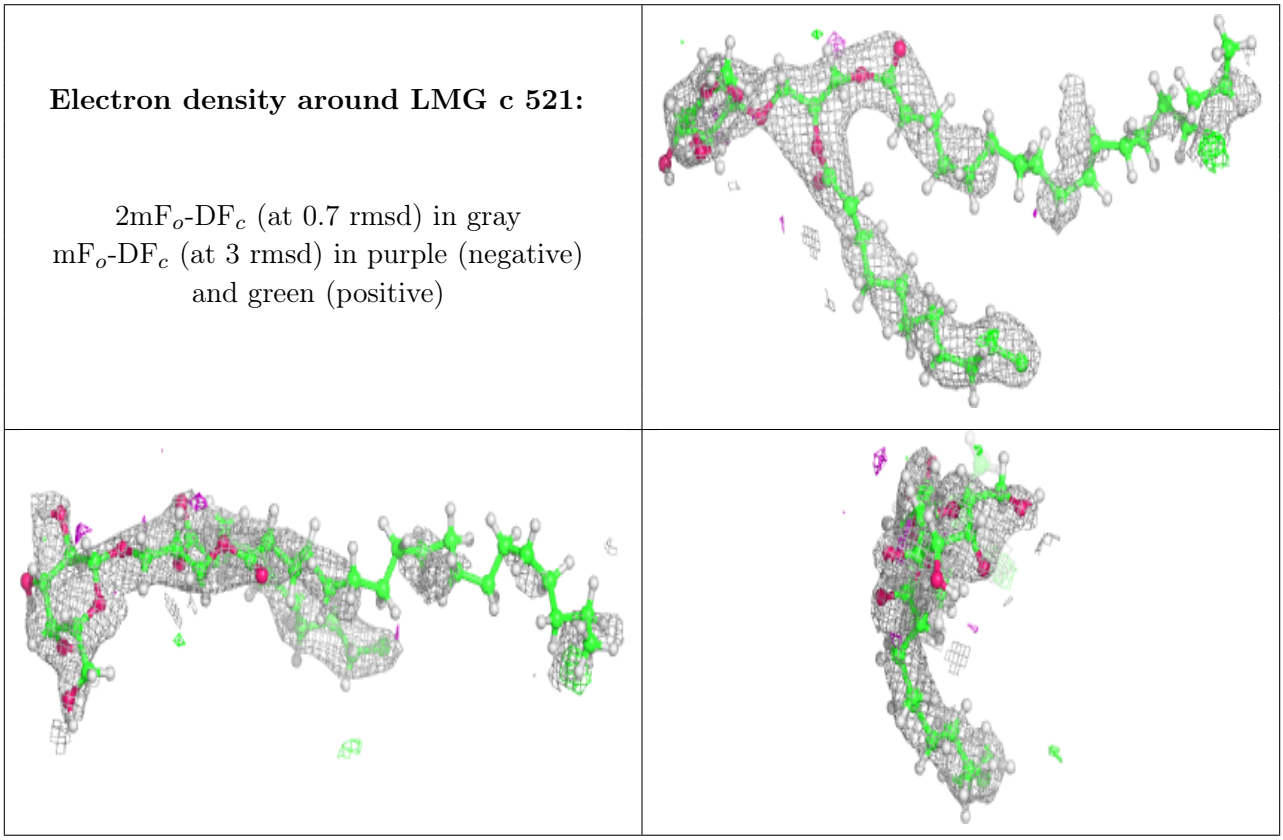
Electron density around LHG A 615:

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



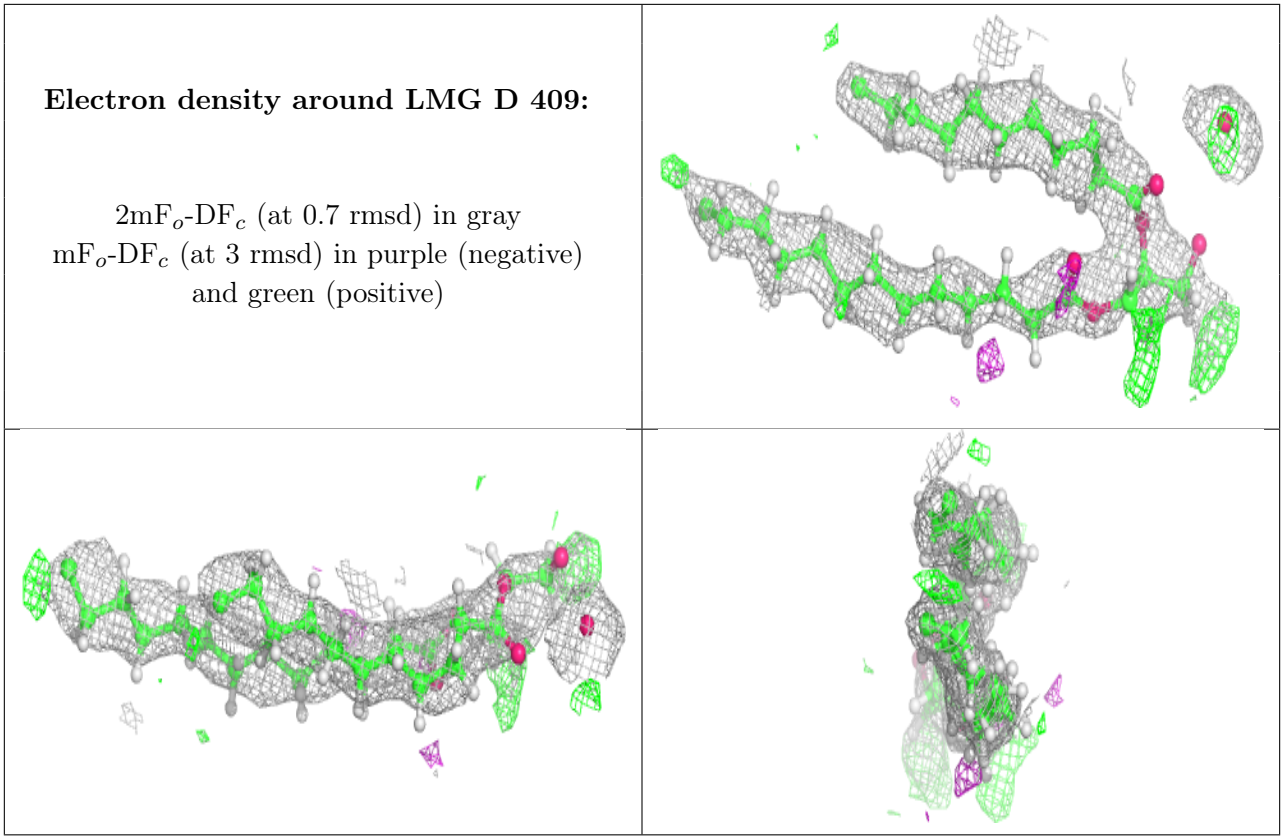
Electron density around LMG c 521:

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



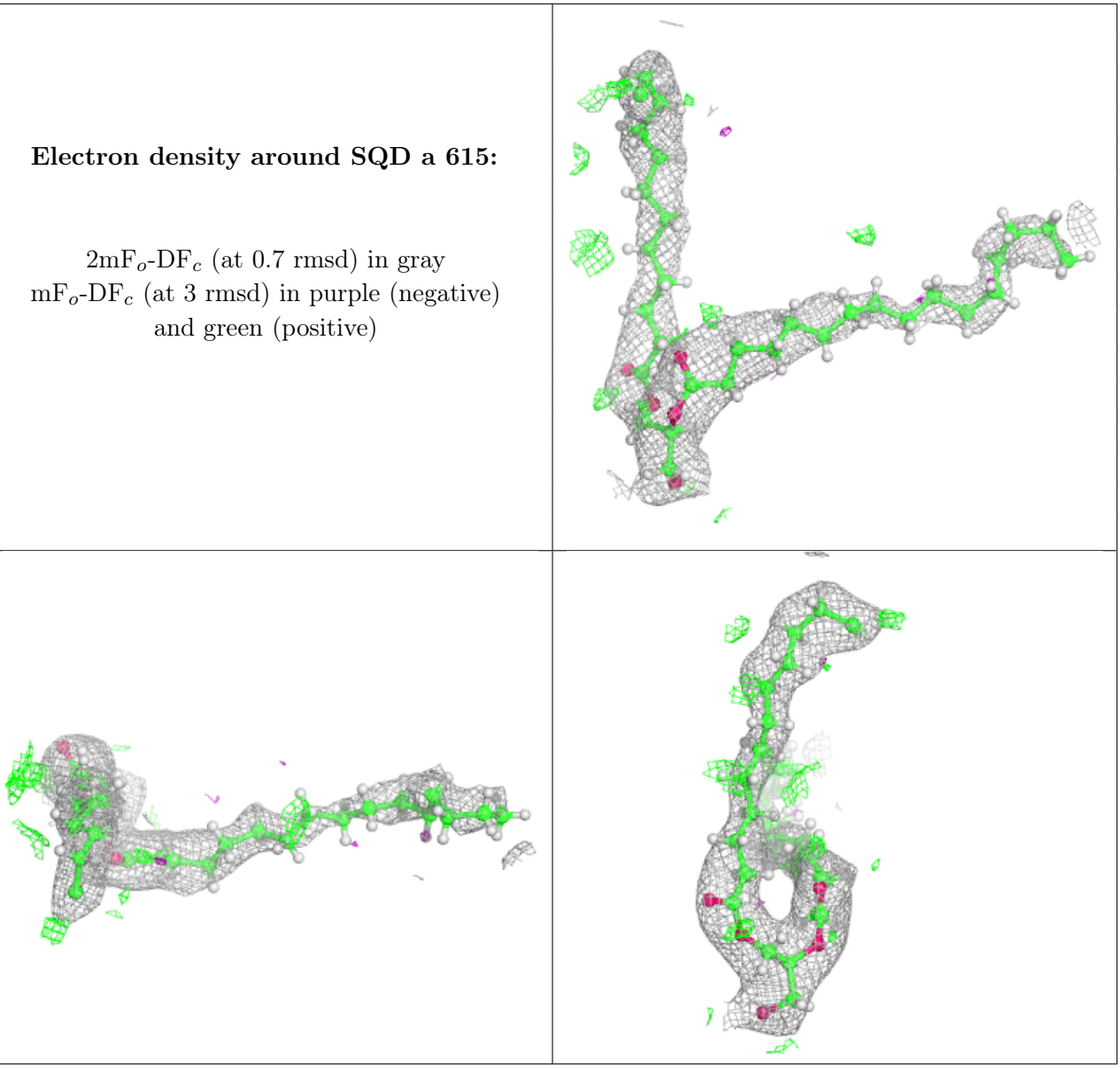
Electron density around LMG D 409:

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



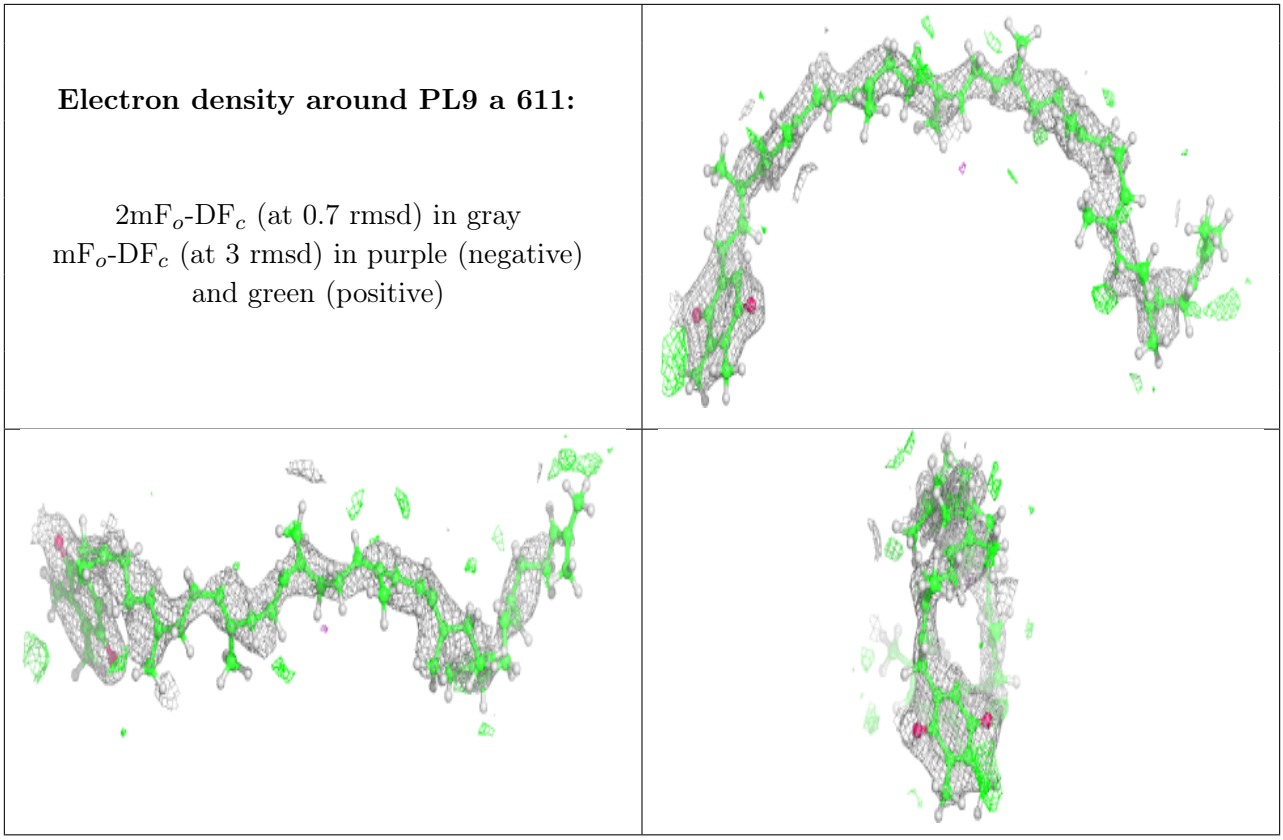
Electron density around SQD a 615:

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



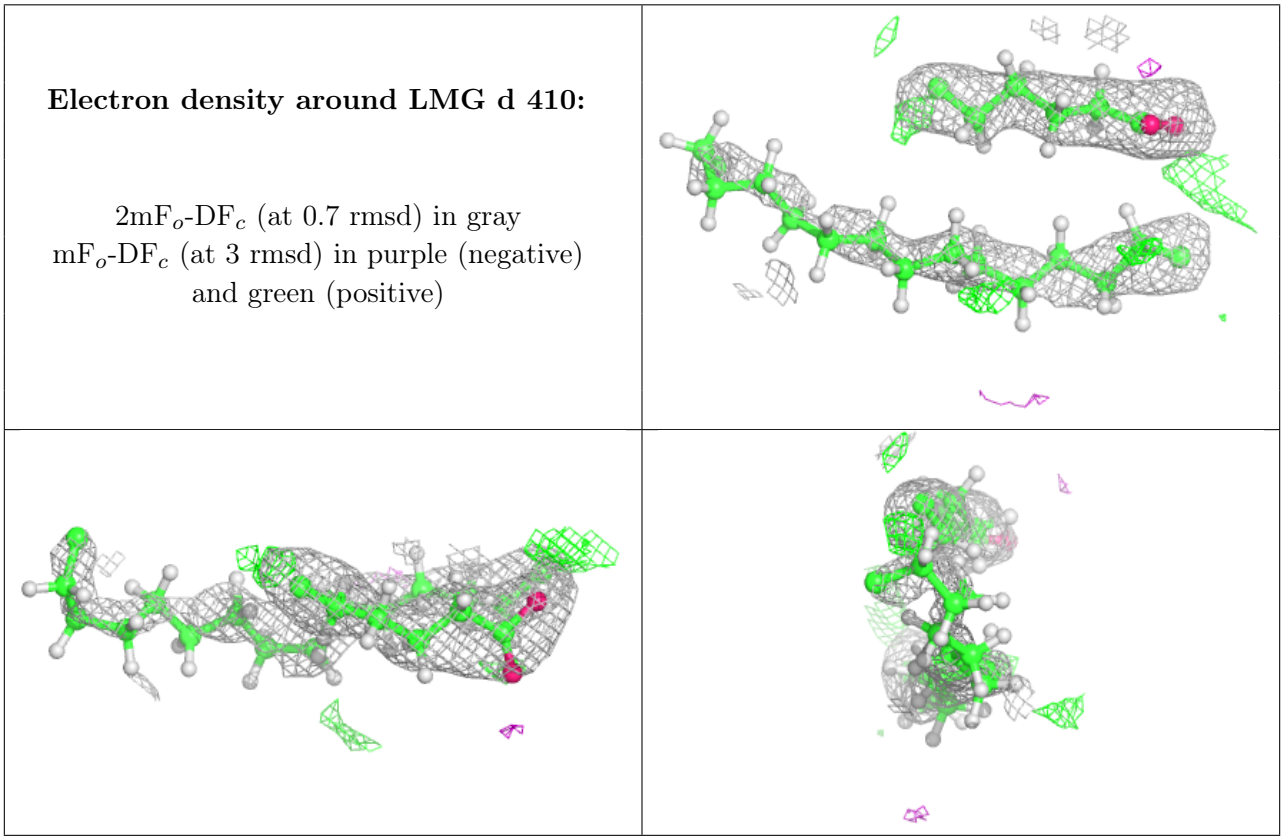
Electron density around PL9 a 611:

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



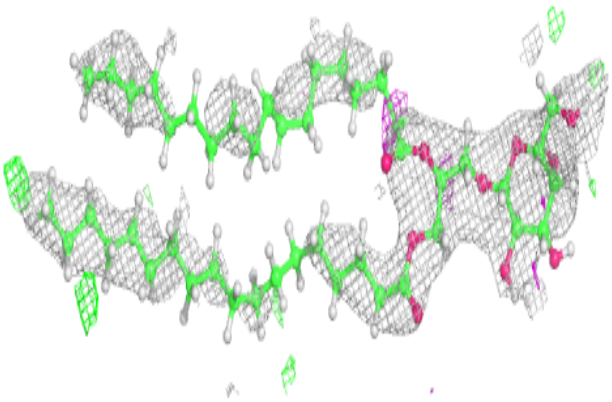
Electron density around LMG d 410:

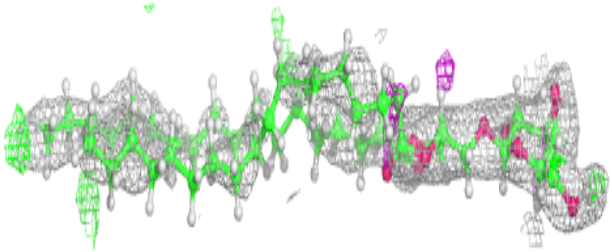
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

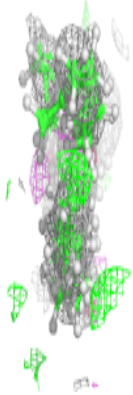


Electron density around LMG b 621:

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

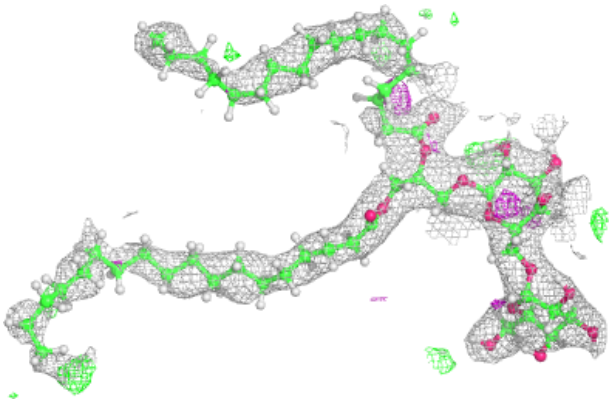


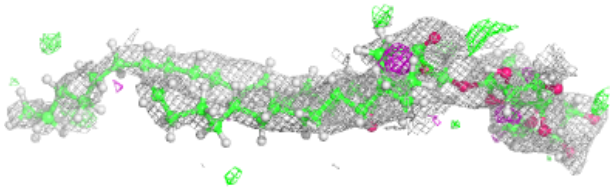




Electron density around DGD A 617:

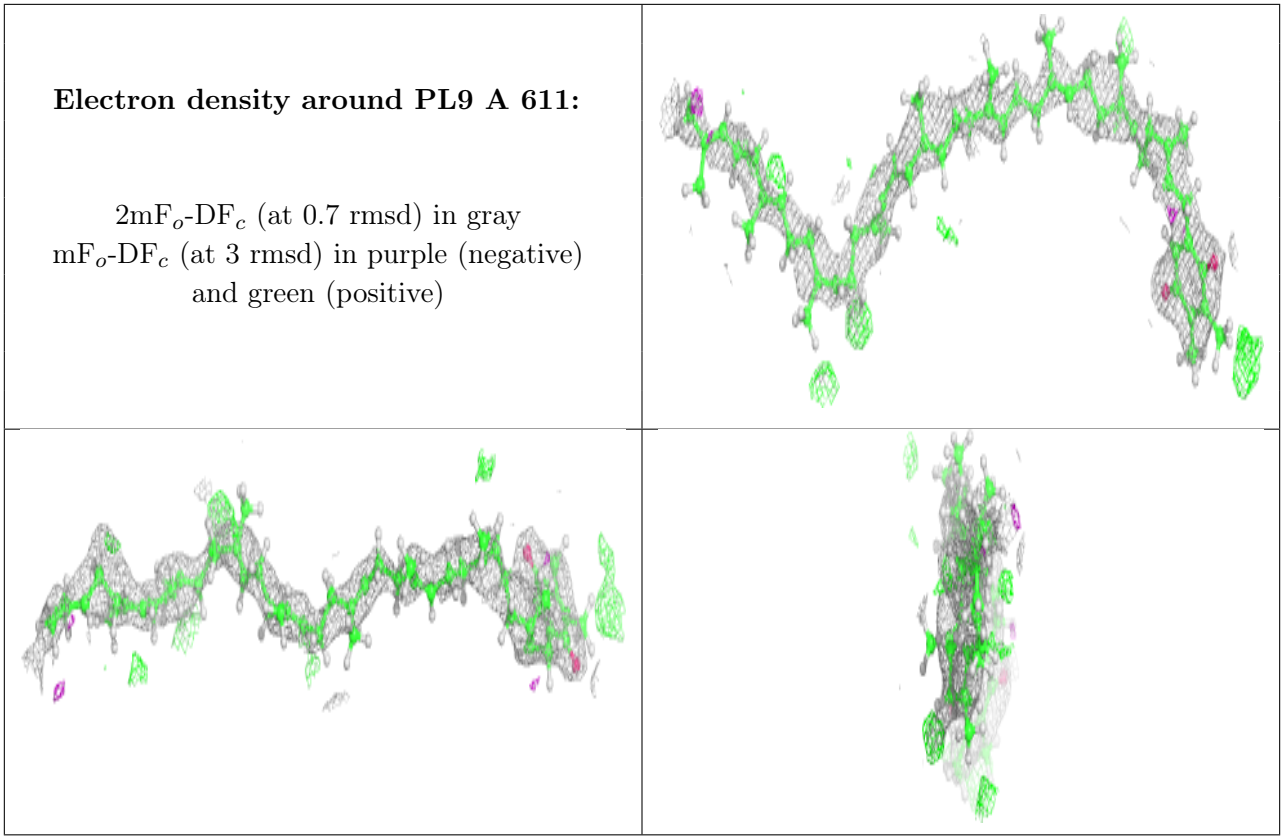
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





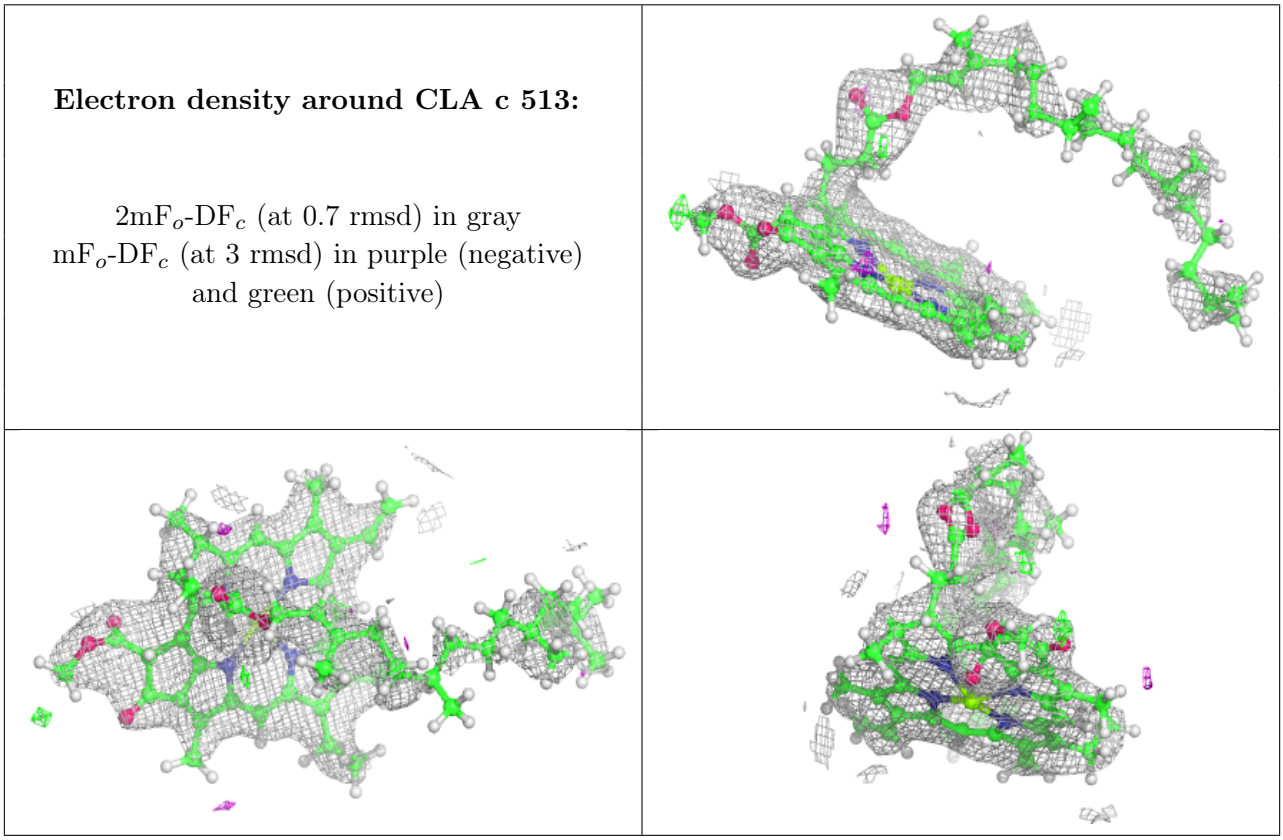
Electron density around PL9 A 611:

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



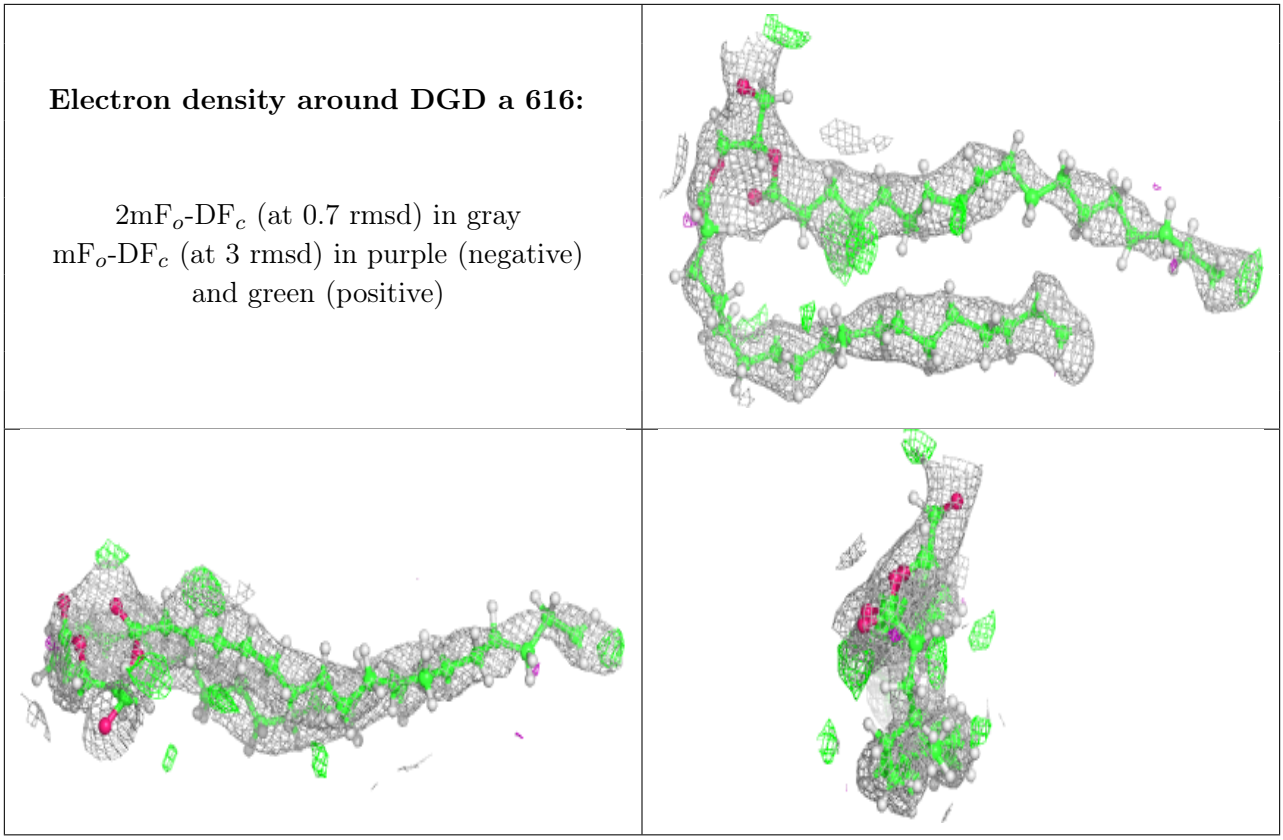
Electron density around CLA c 513:

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



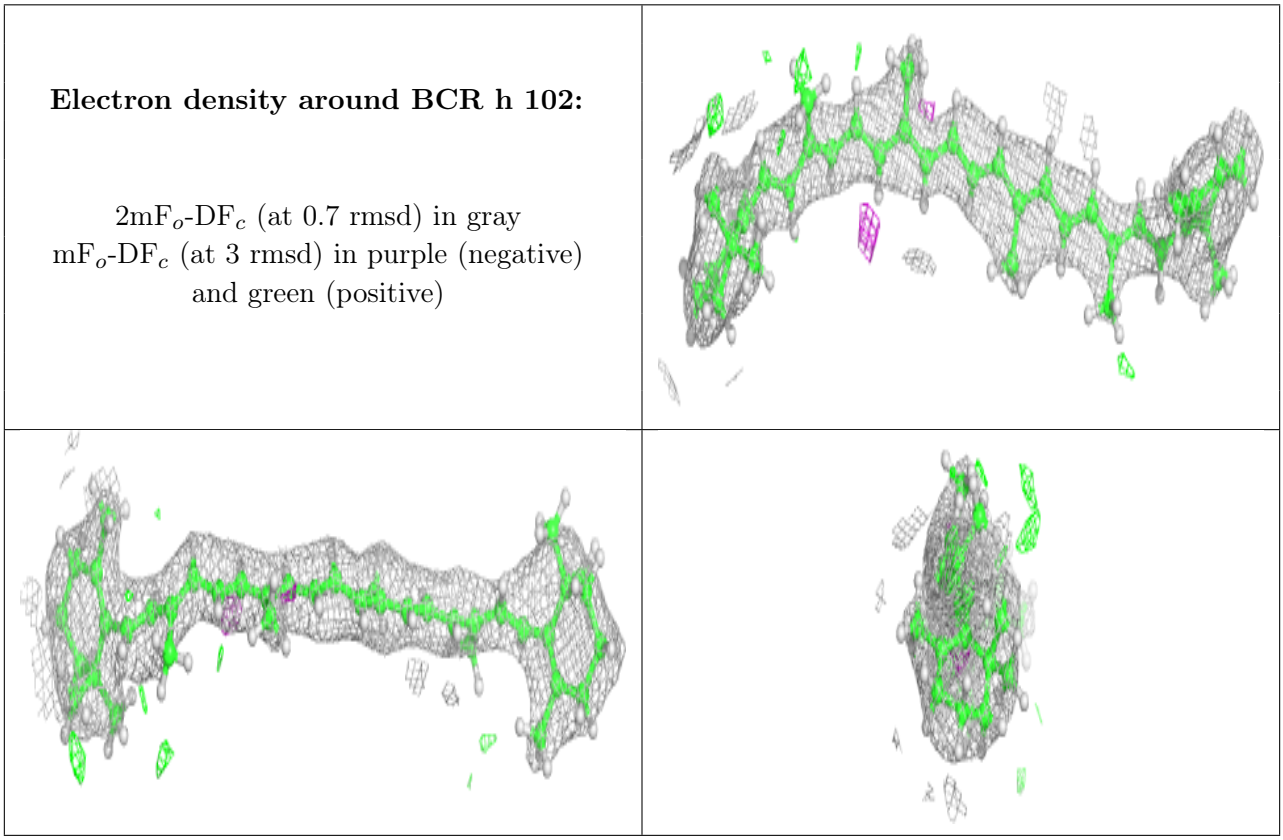
Electron density around DGD a 616:

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



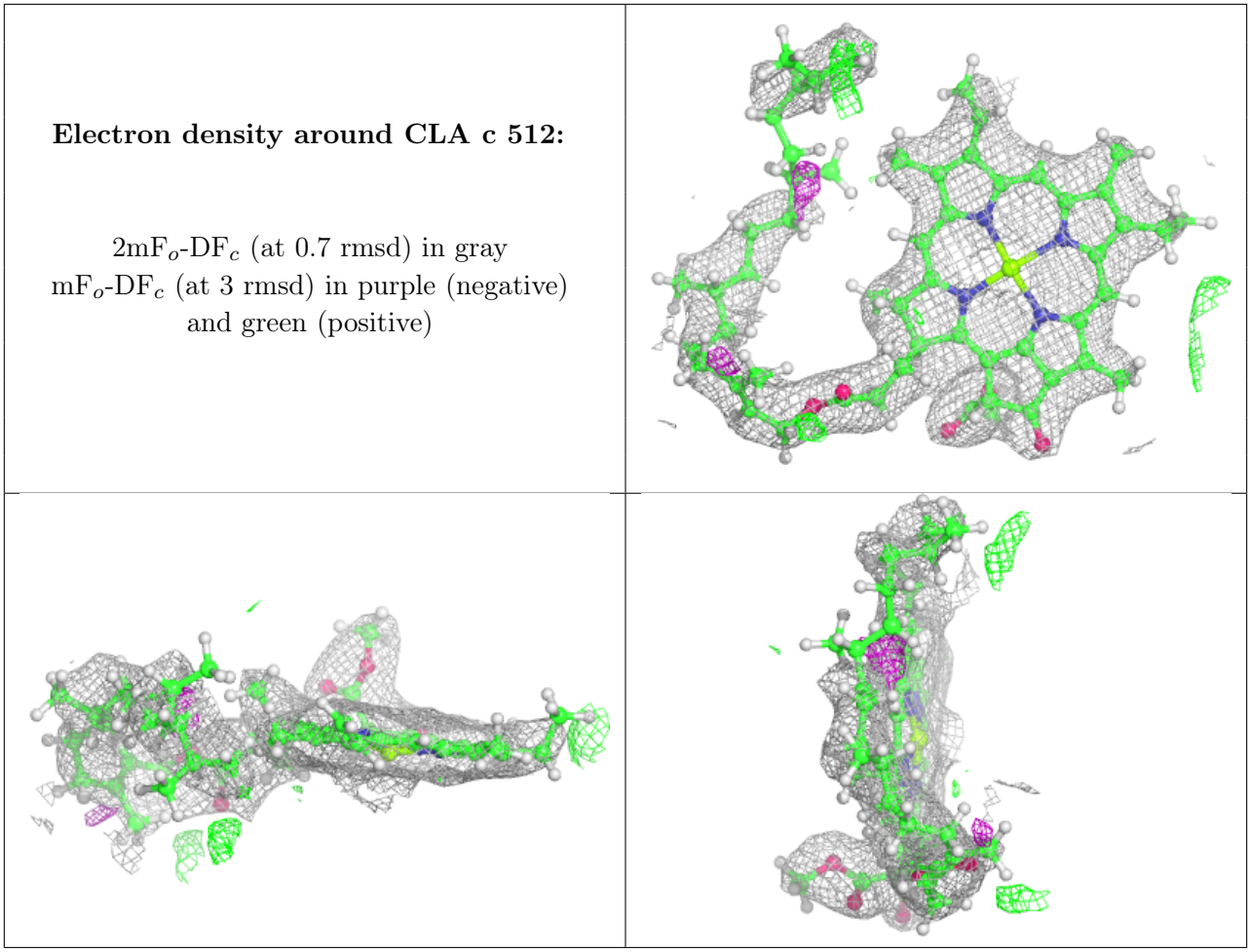
Electron density around BCR h 102:

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



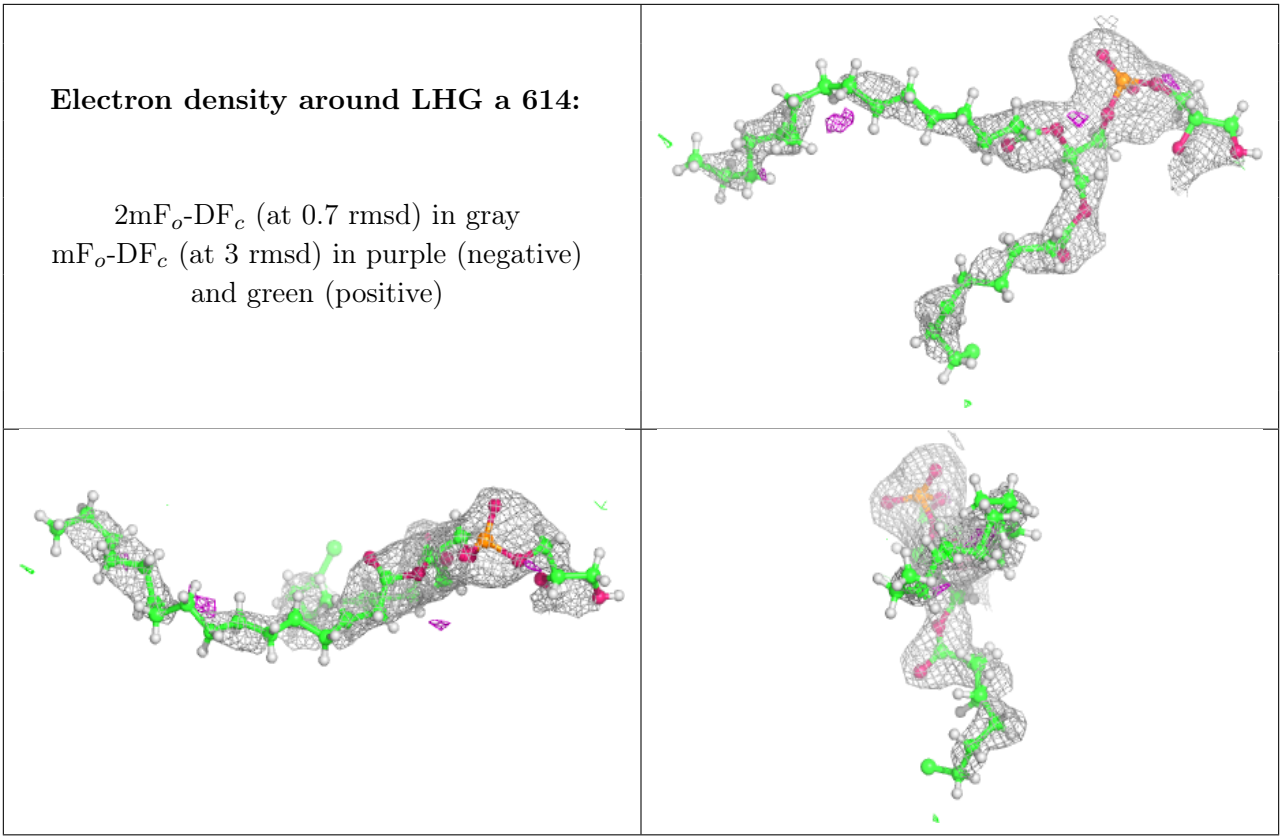
Electron density around CLA c 512:

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



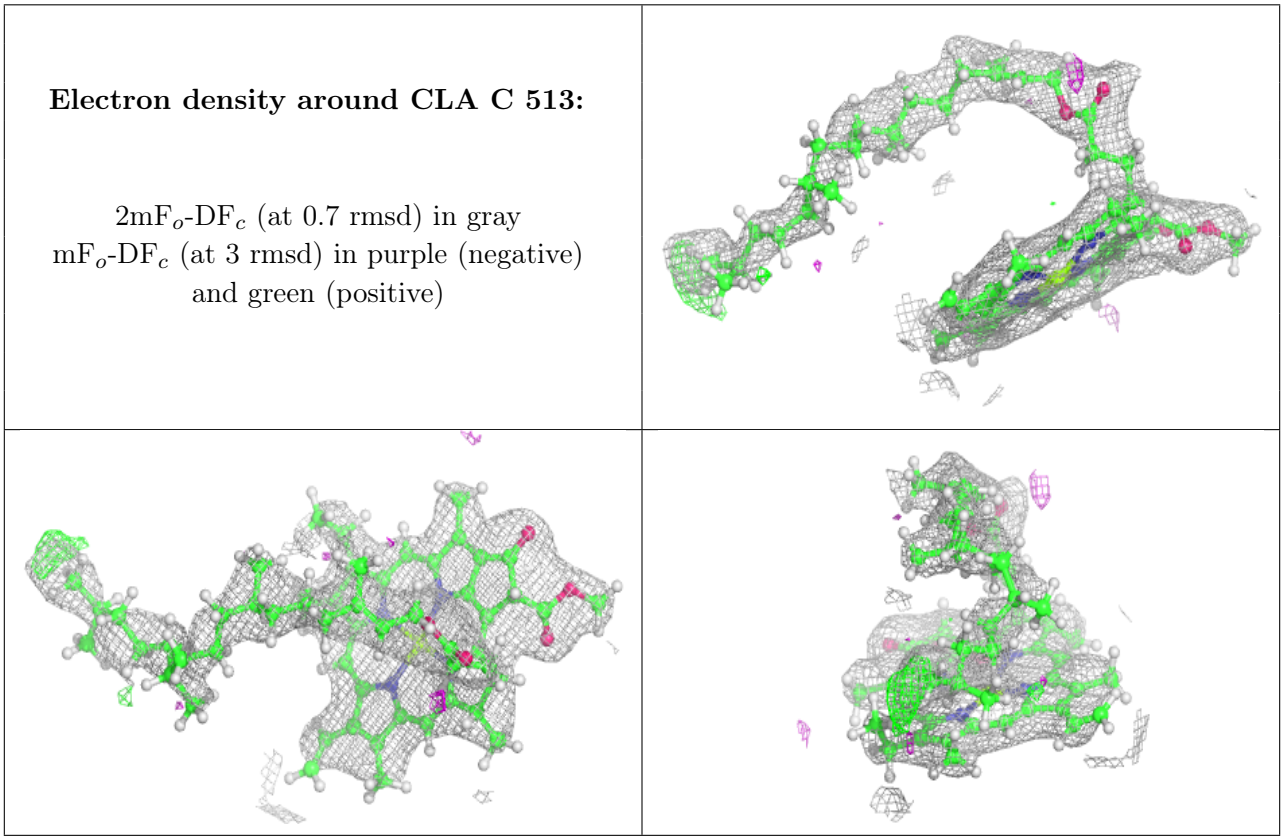
Electron density around LHG a 614:

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



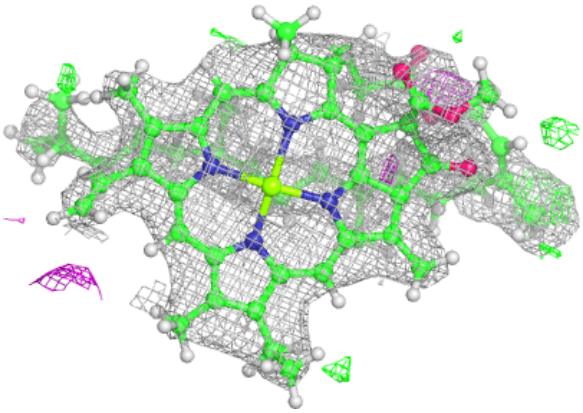
Electron density around CLA C 513:

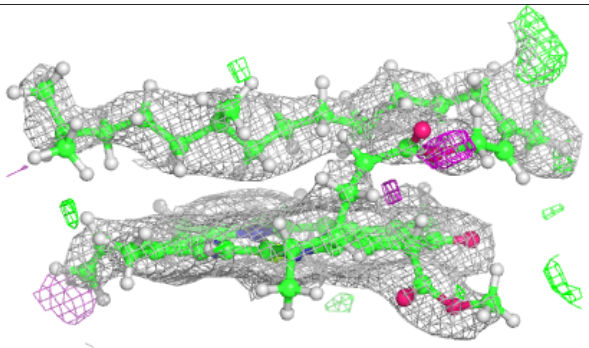
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA h 101:

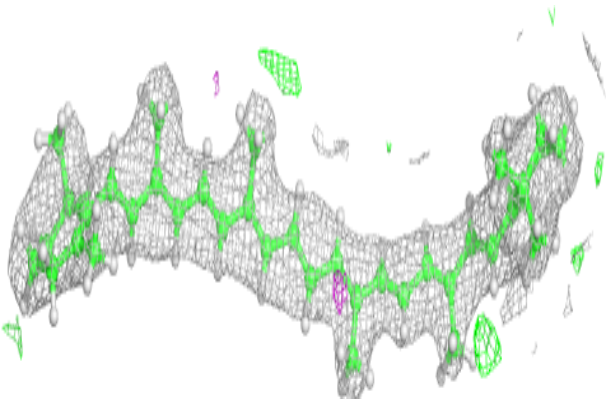
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

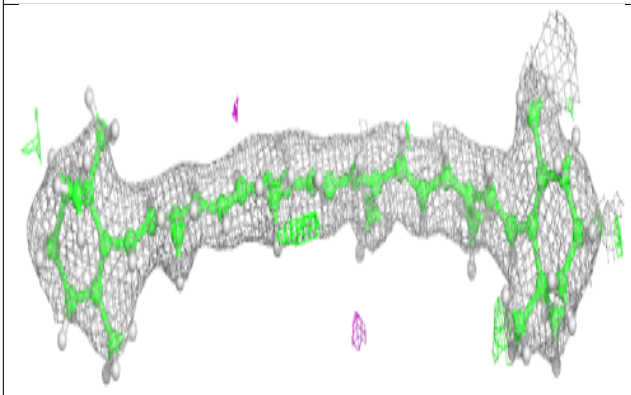


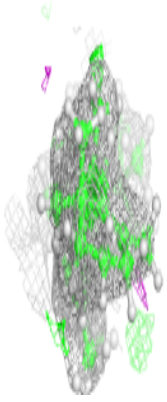


Electron density around BCR H 101:

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

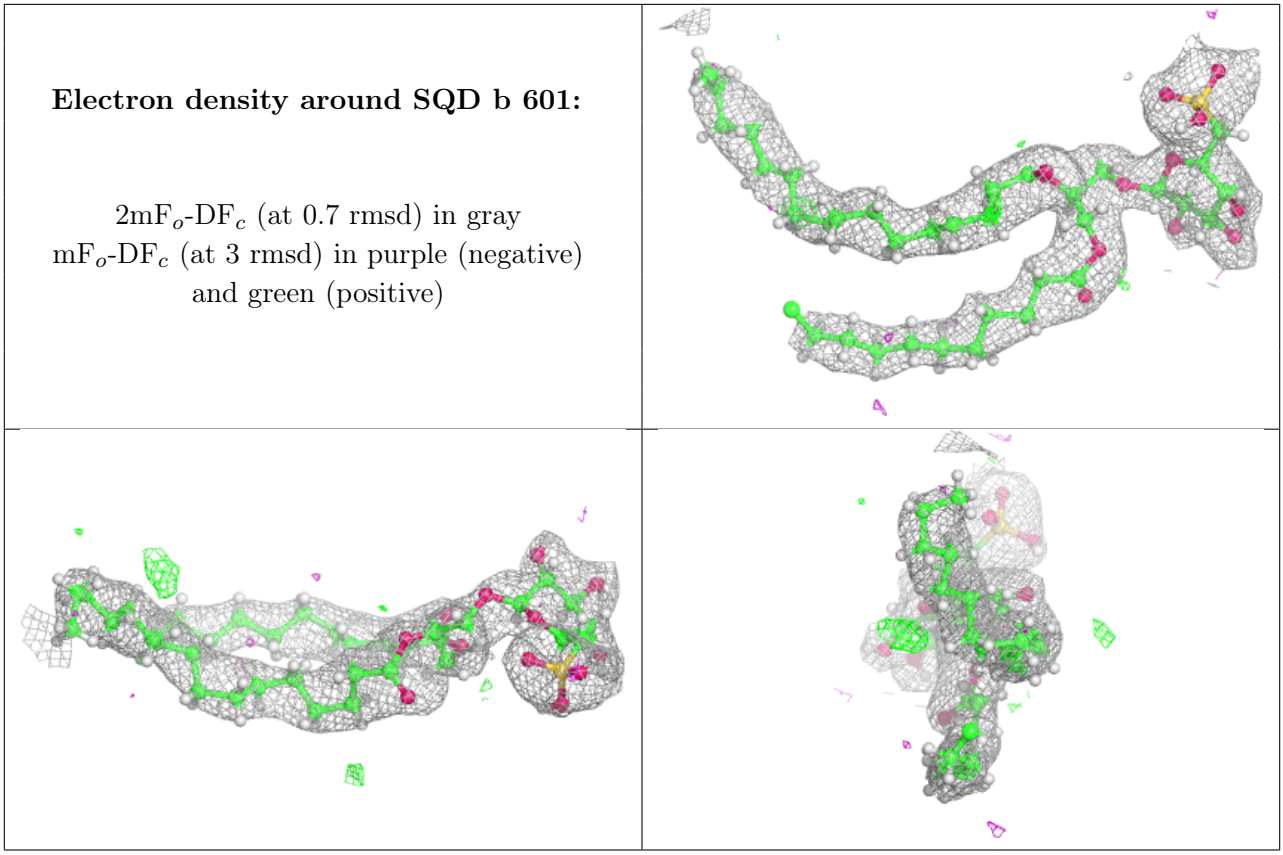






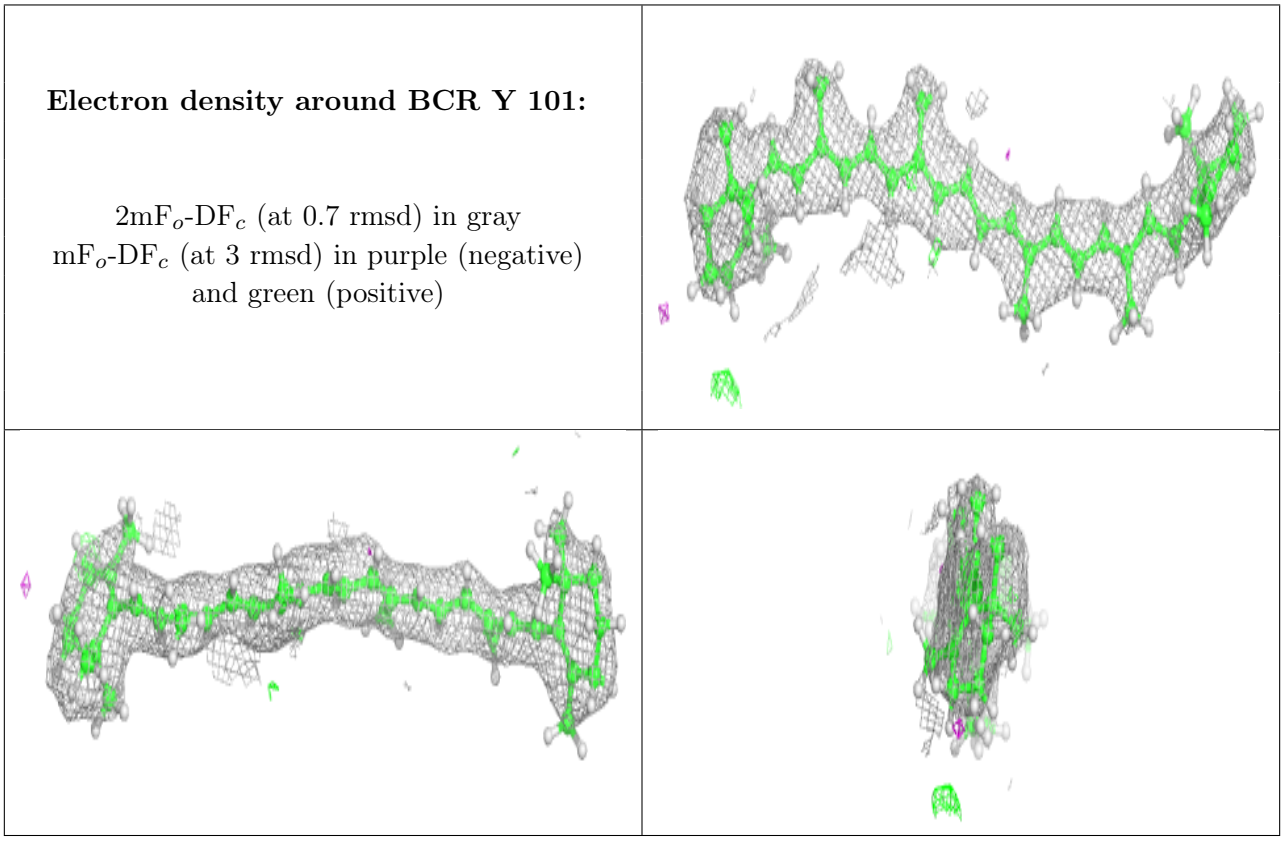
Electron density around SQD b 601:

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



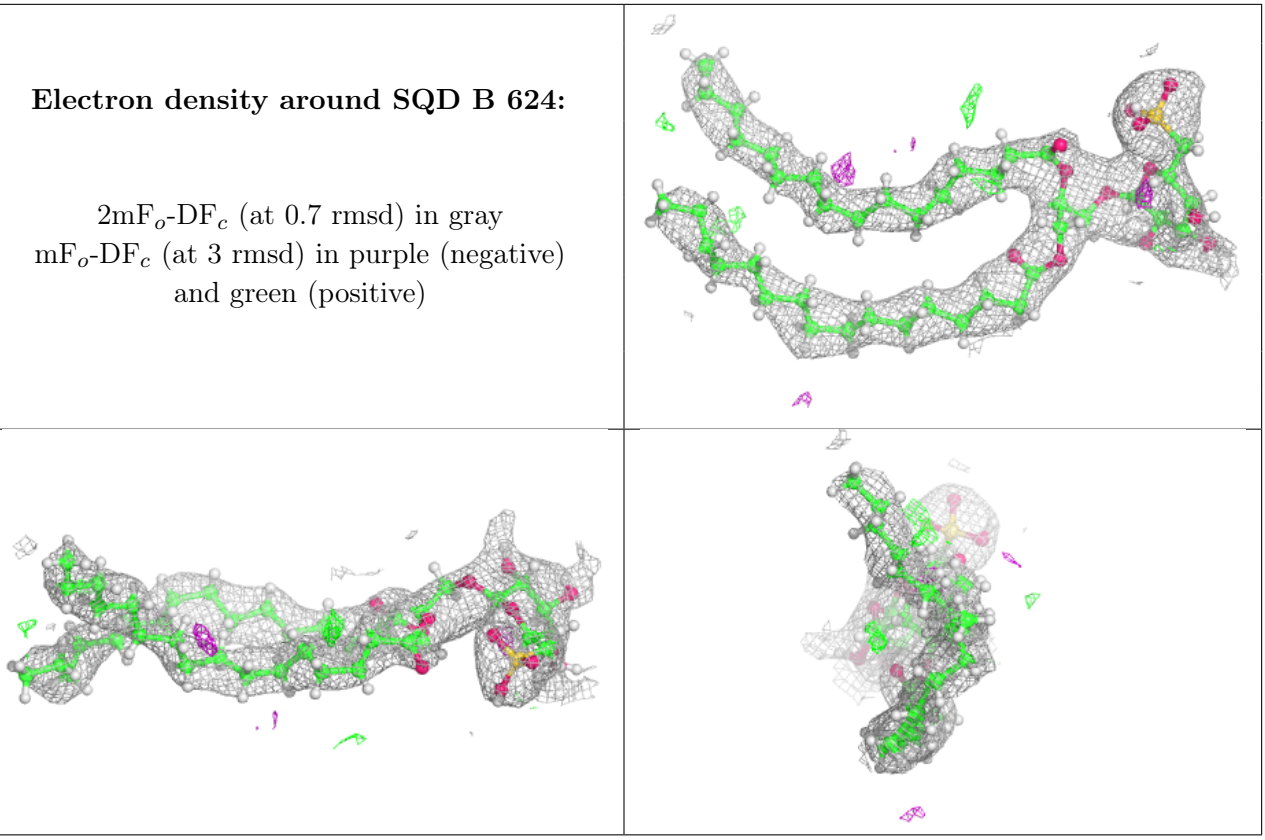
Electron density around BCR Y 101:

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



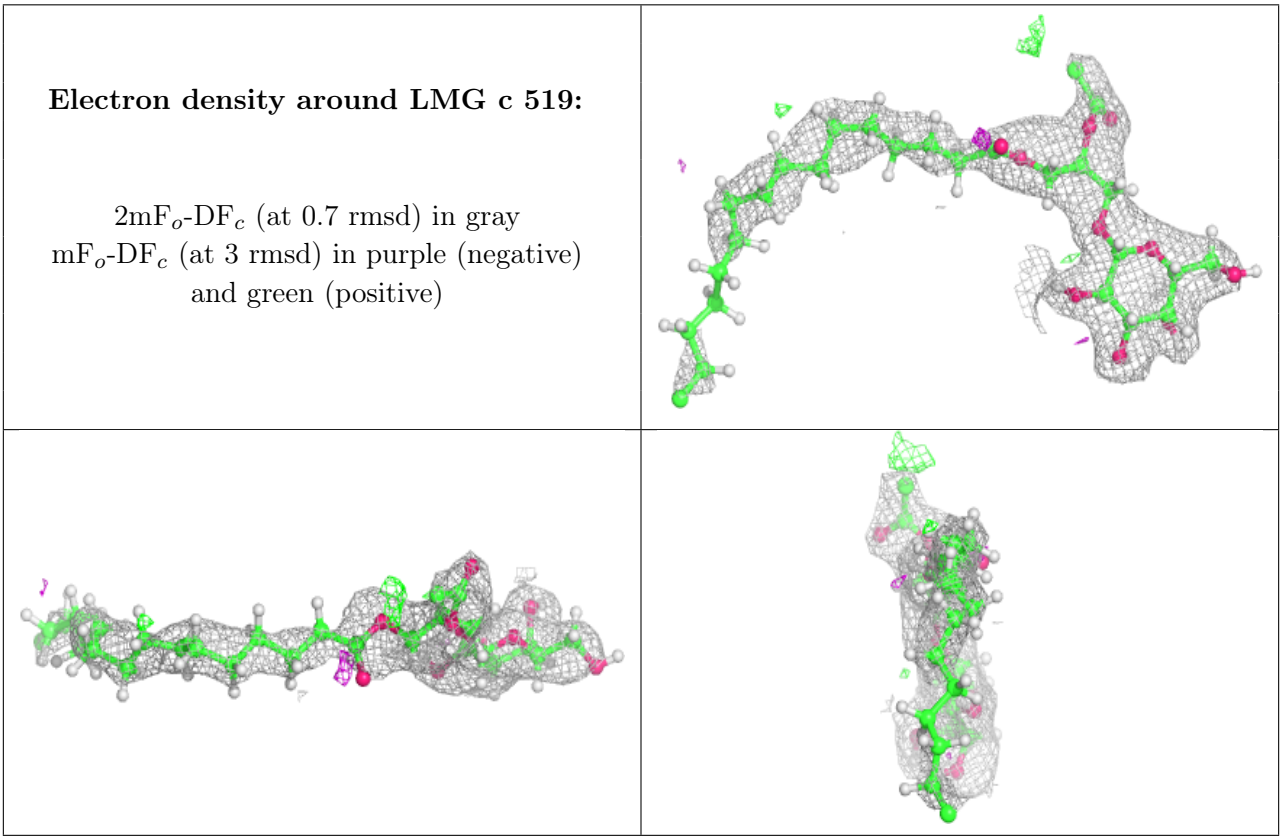
Electron density around SQD B 624:

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



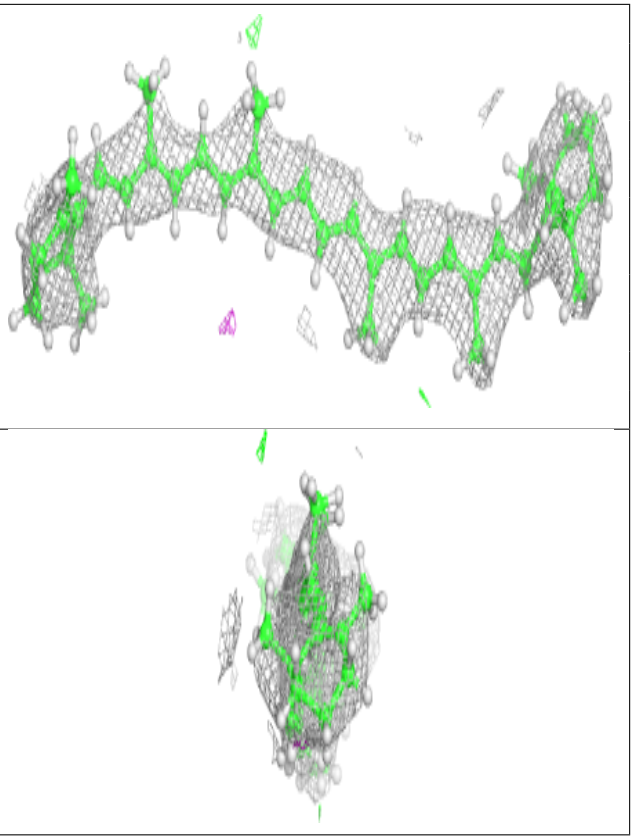
Electron density around LMG c 519:

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



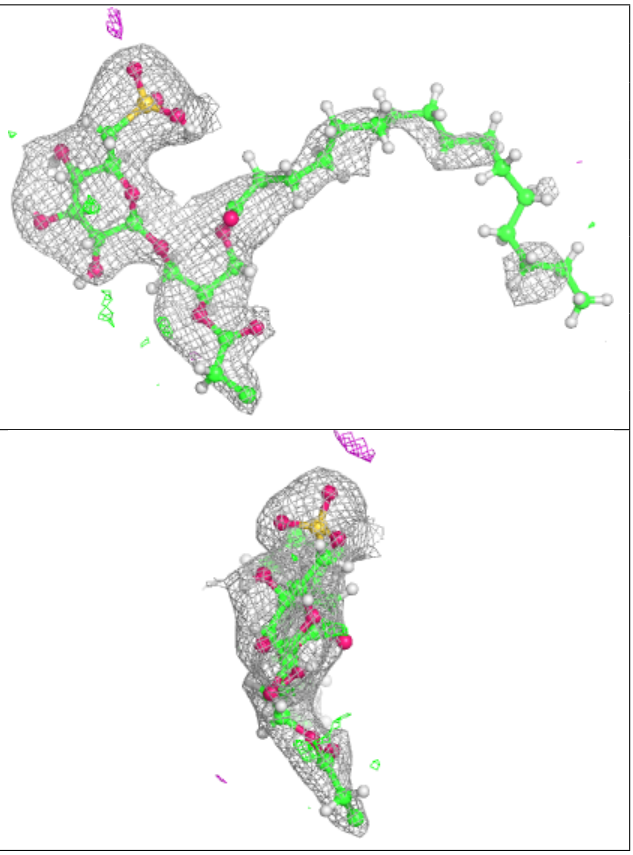
Electron density around BCR k 101:

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



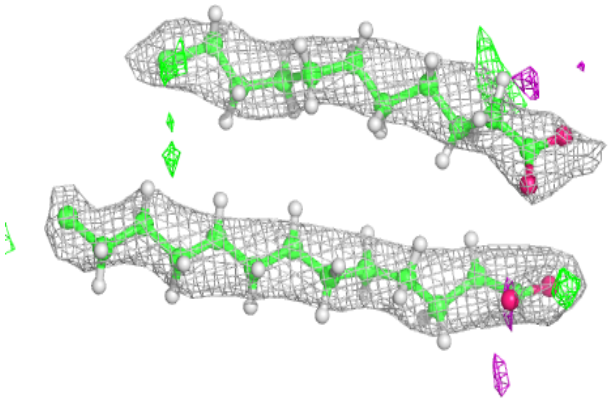
Electron density around SQD f 101:

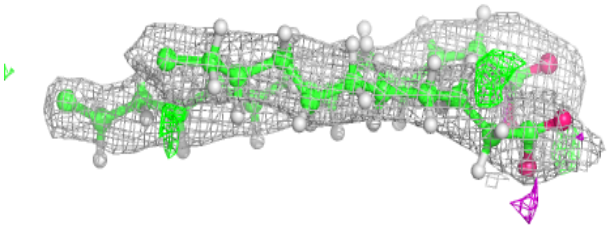
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

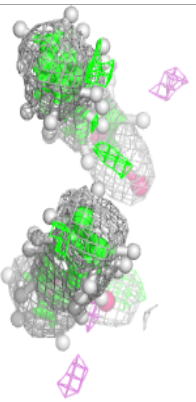


Electron density around LMG B 622:

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

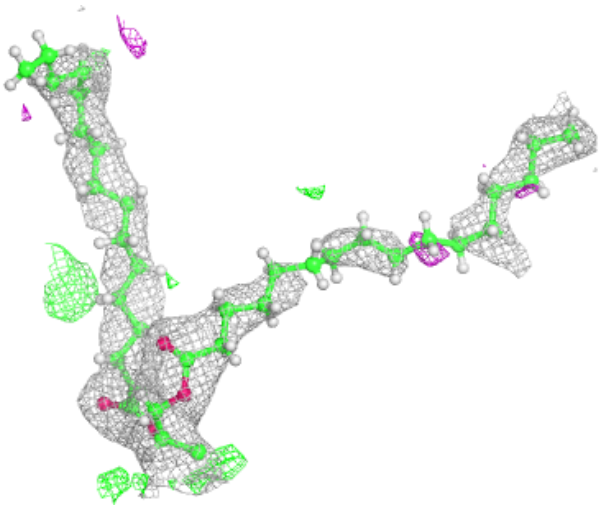


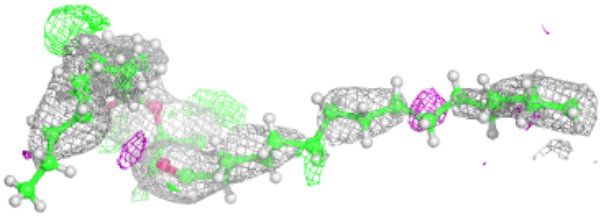


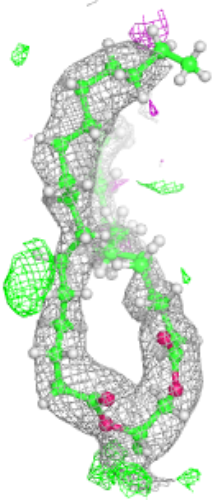


Electron density around SQD A 616:

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

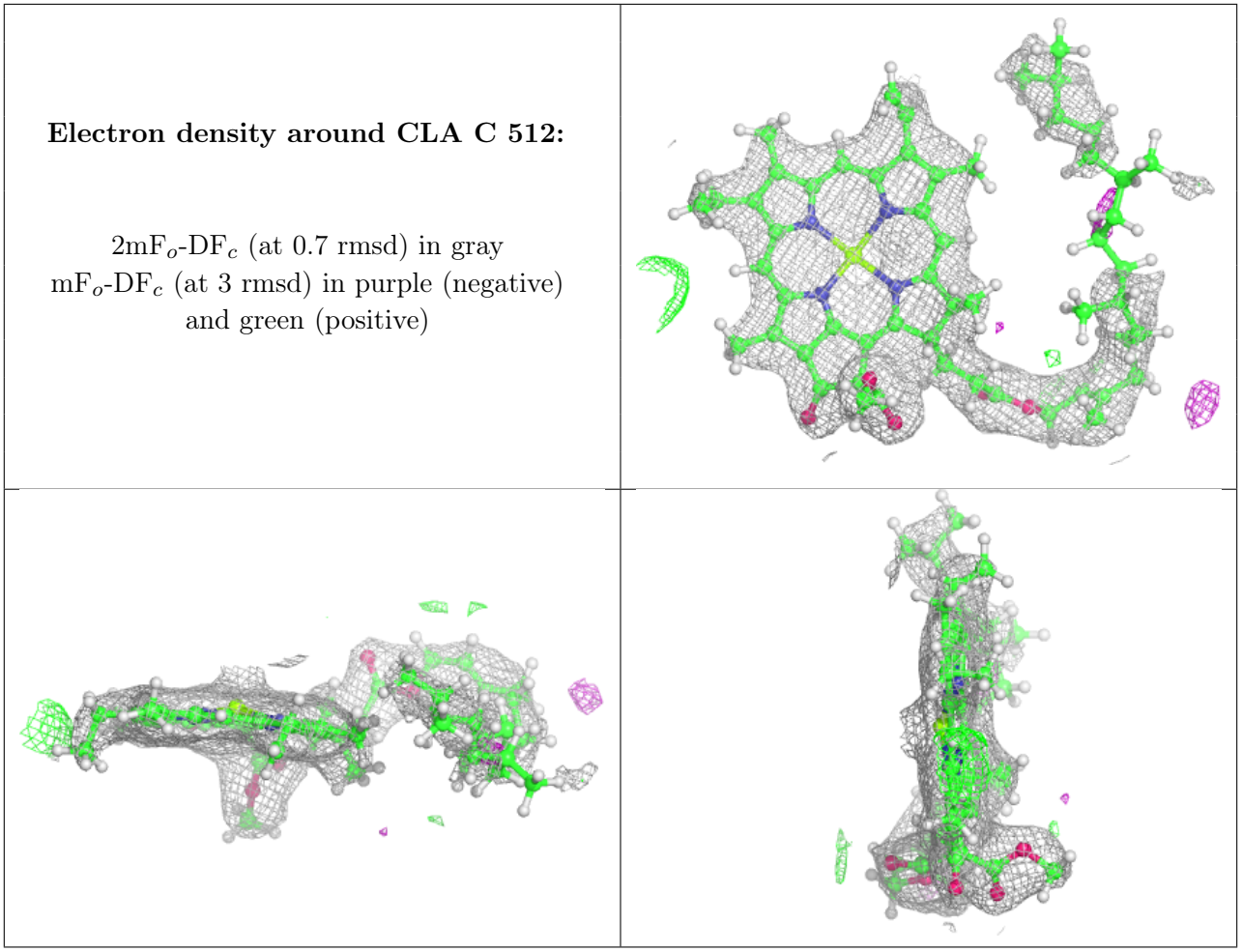






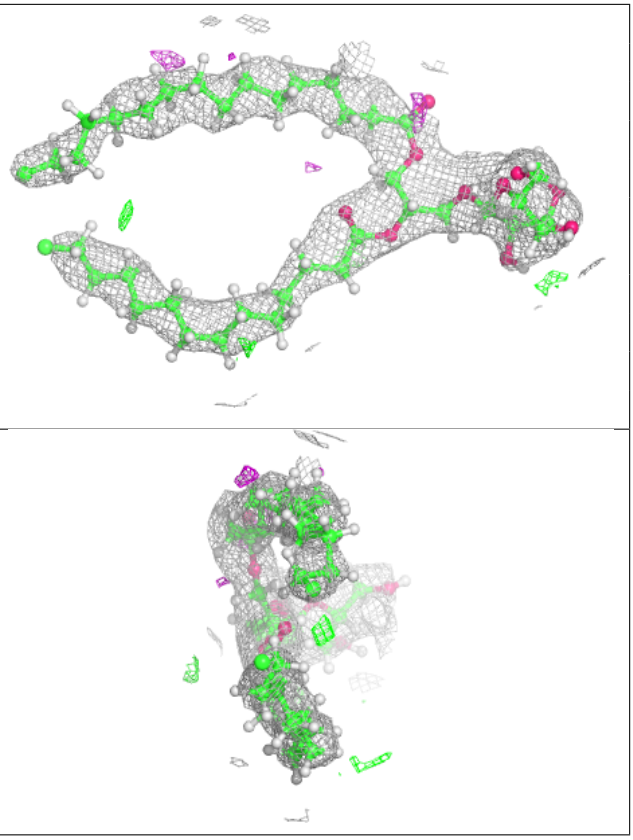
Electron density around CLA C 512:

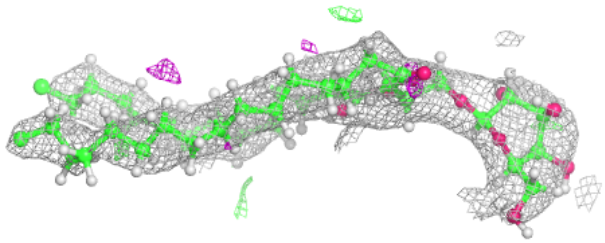
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG c 522:

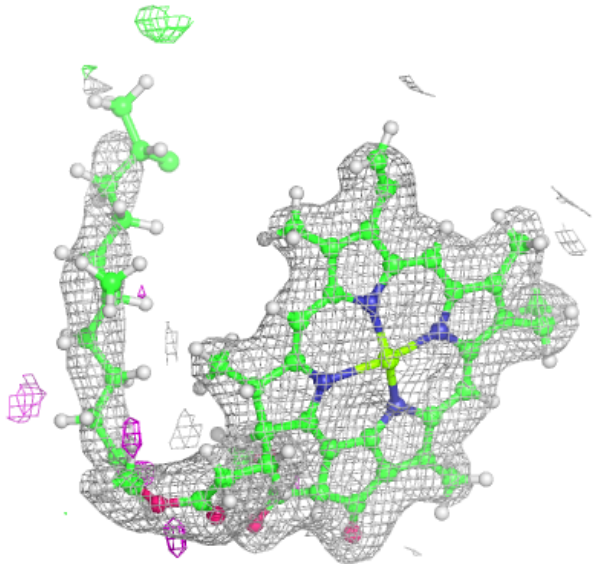
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

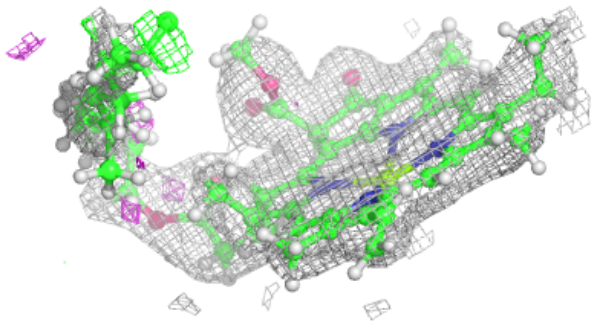


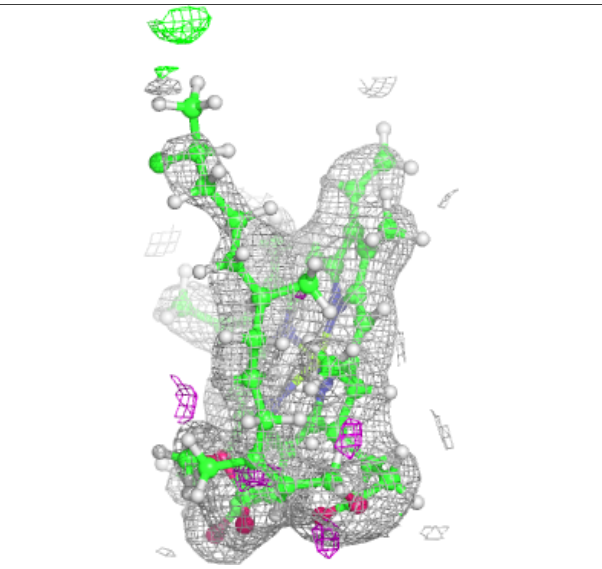


Electron density around CLA B 616:

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

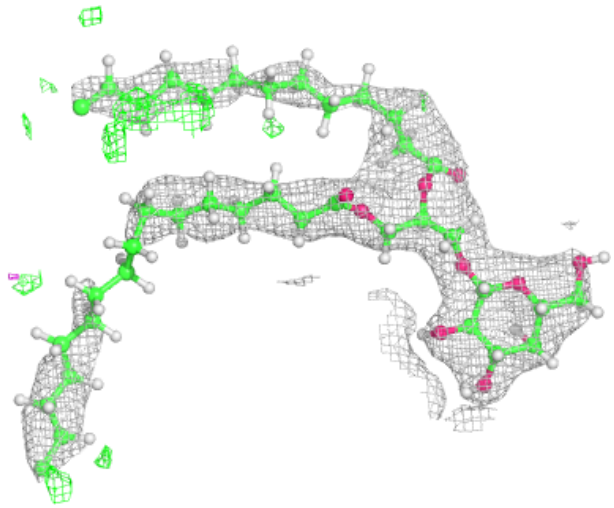


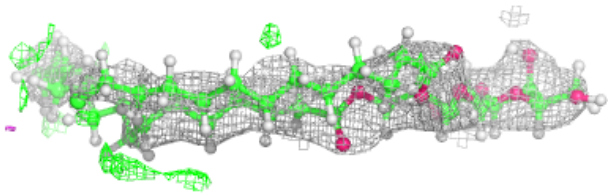


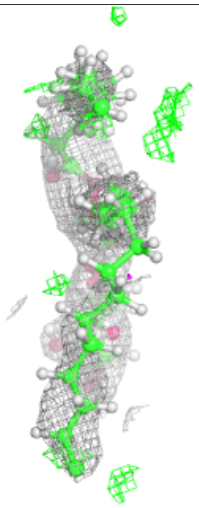


Electron density around LMG C 519:

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

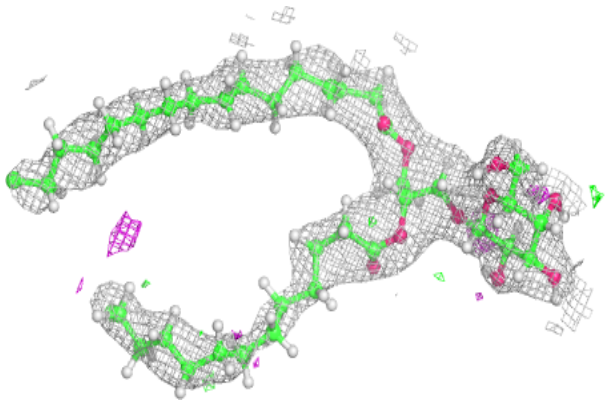


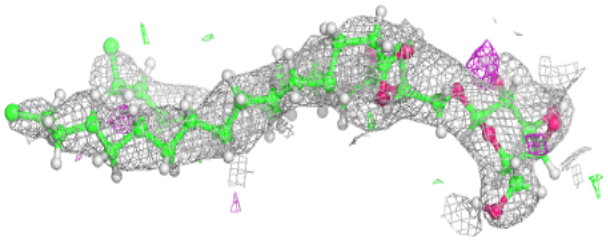


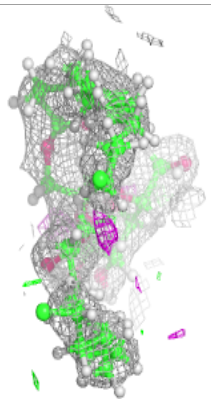


Electron density around LMG A 612:

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

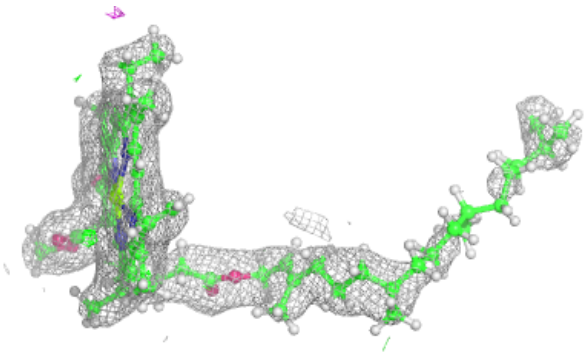


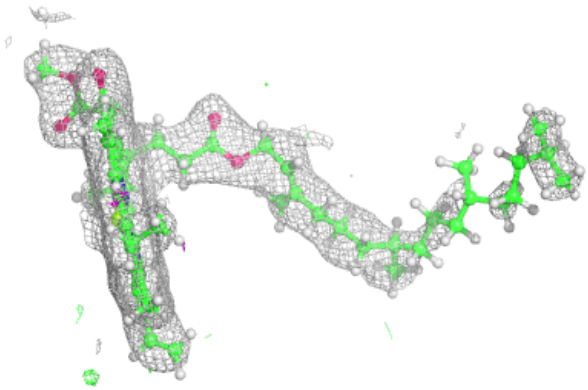


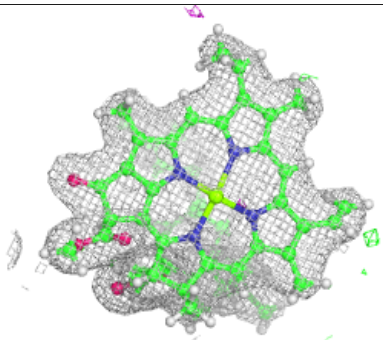


Electron density around CLA D 403:

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

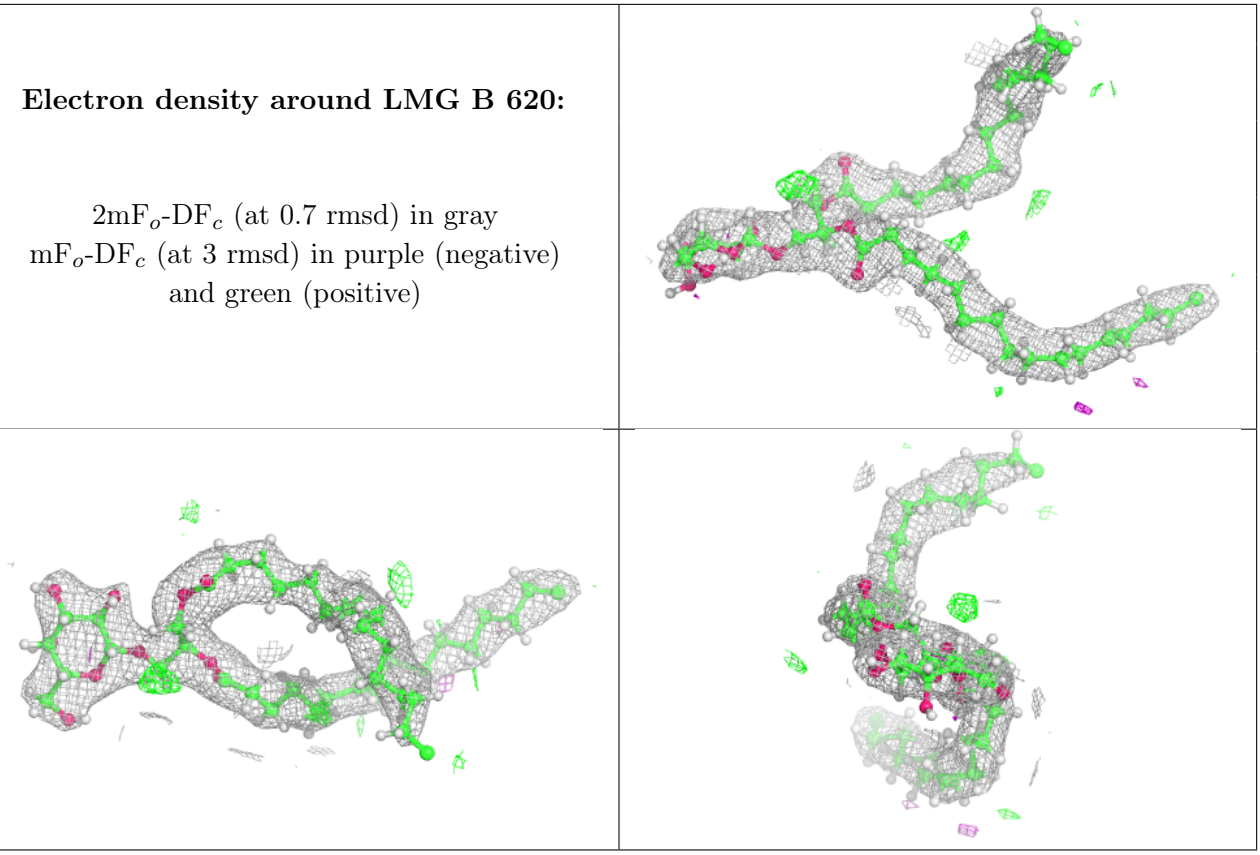






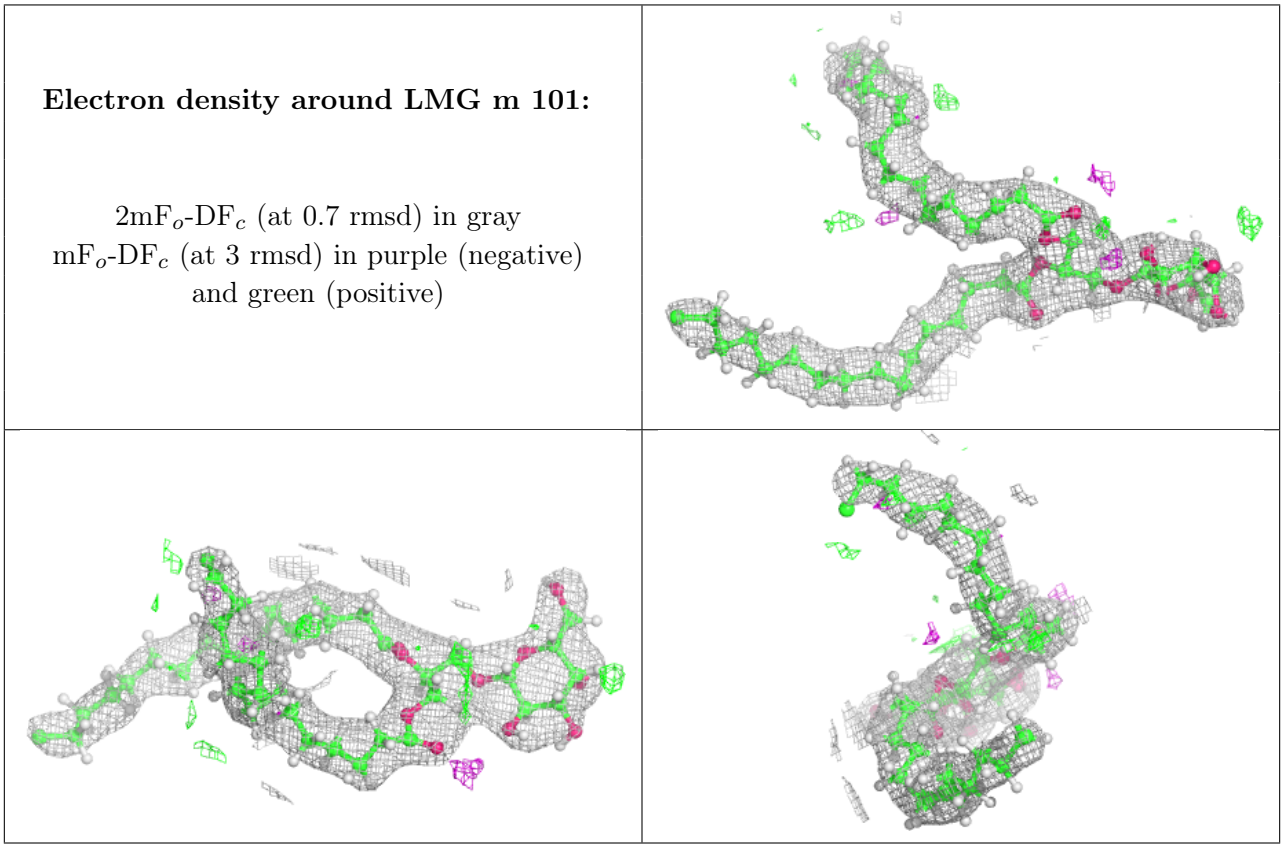
Electron density around LMG B 620:

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



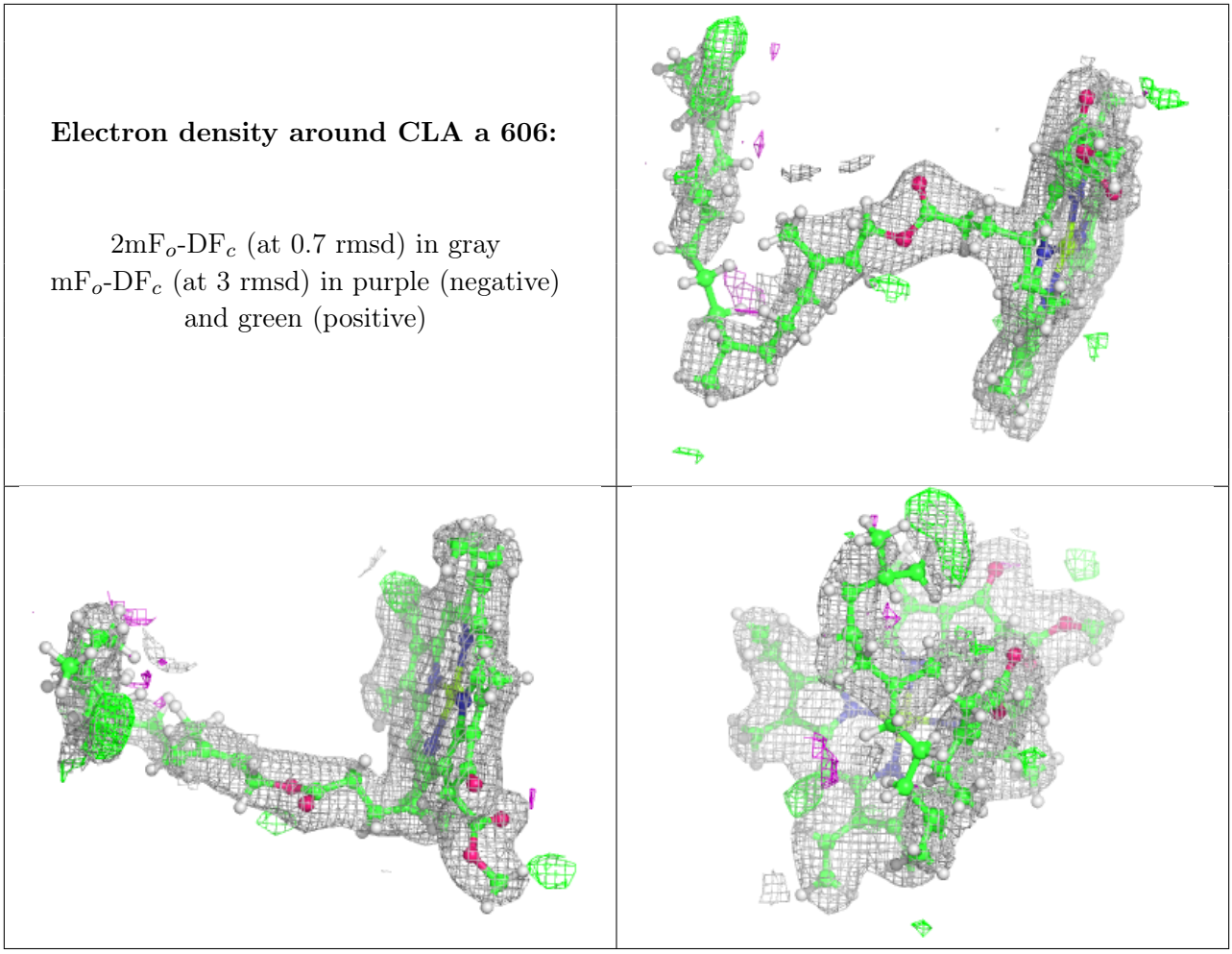
Electron density around LMG m 101:

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



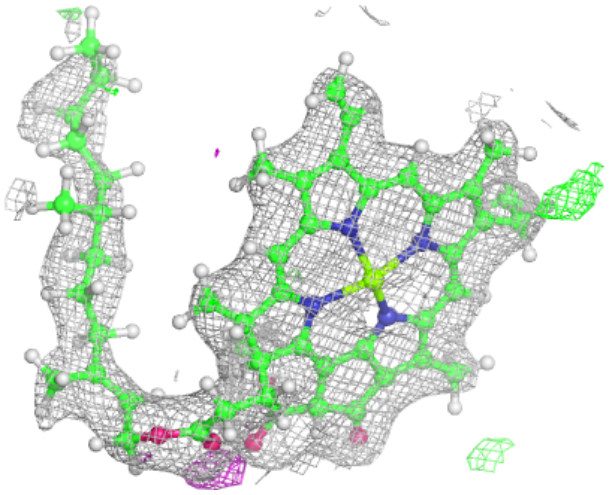
Electron density around CLA a 606:

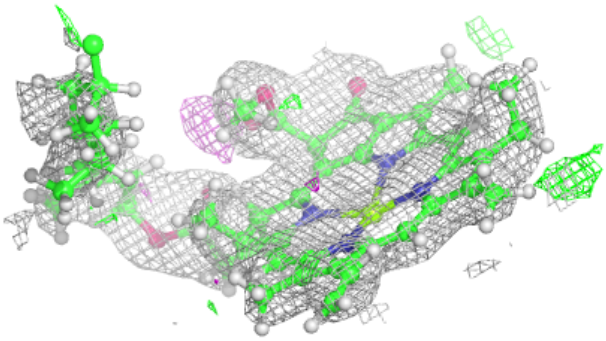
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

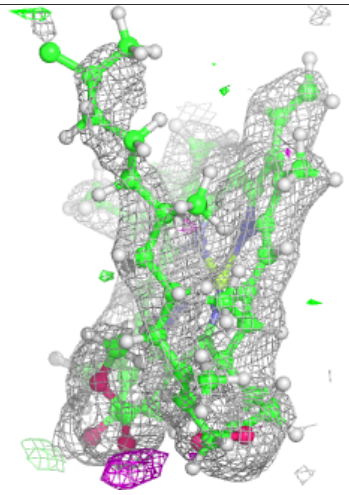


Electron density around CLA b 616:

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

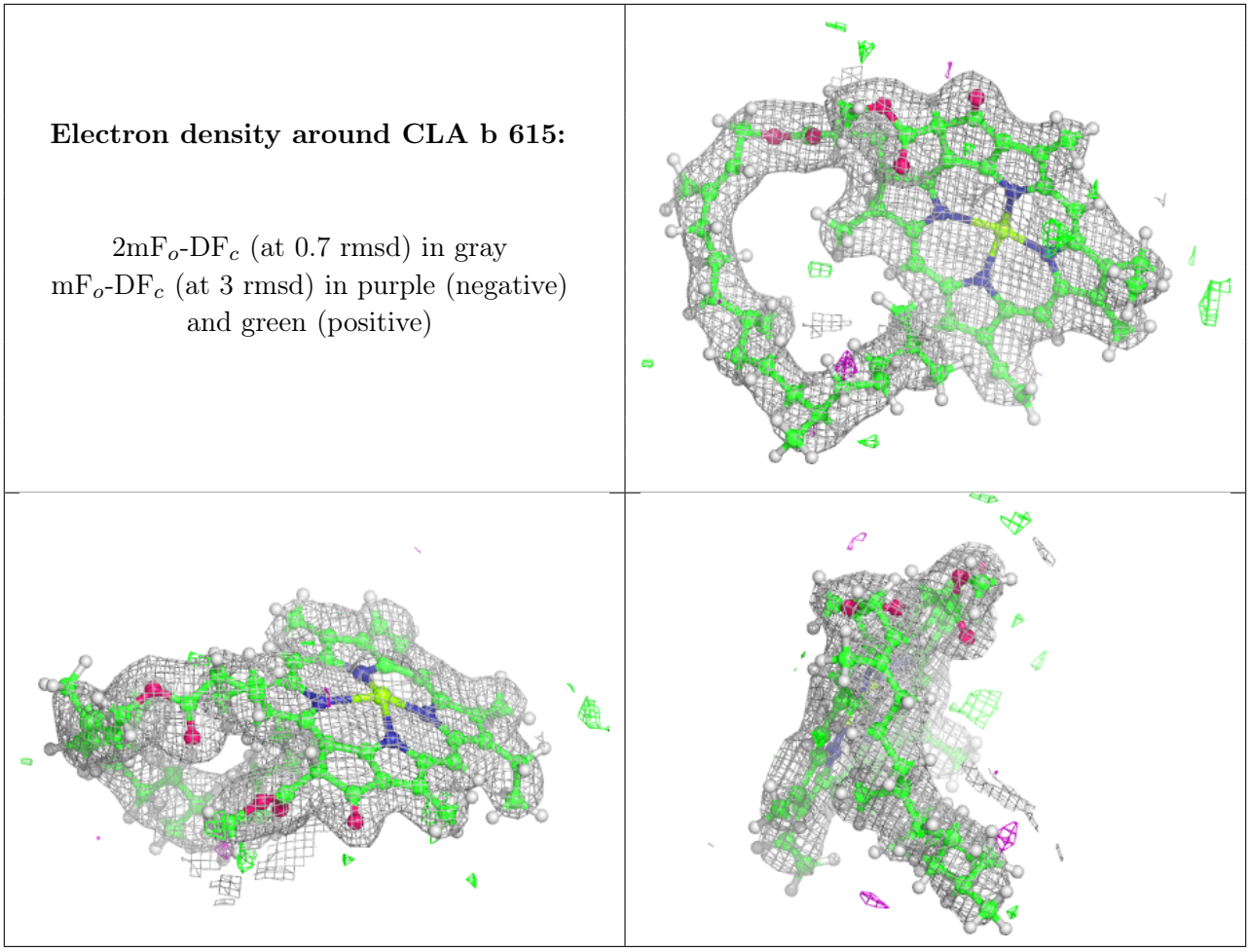






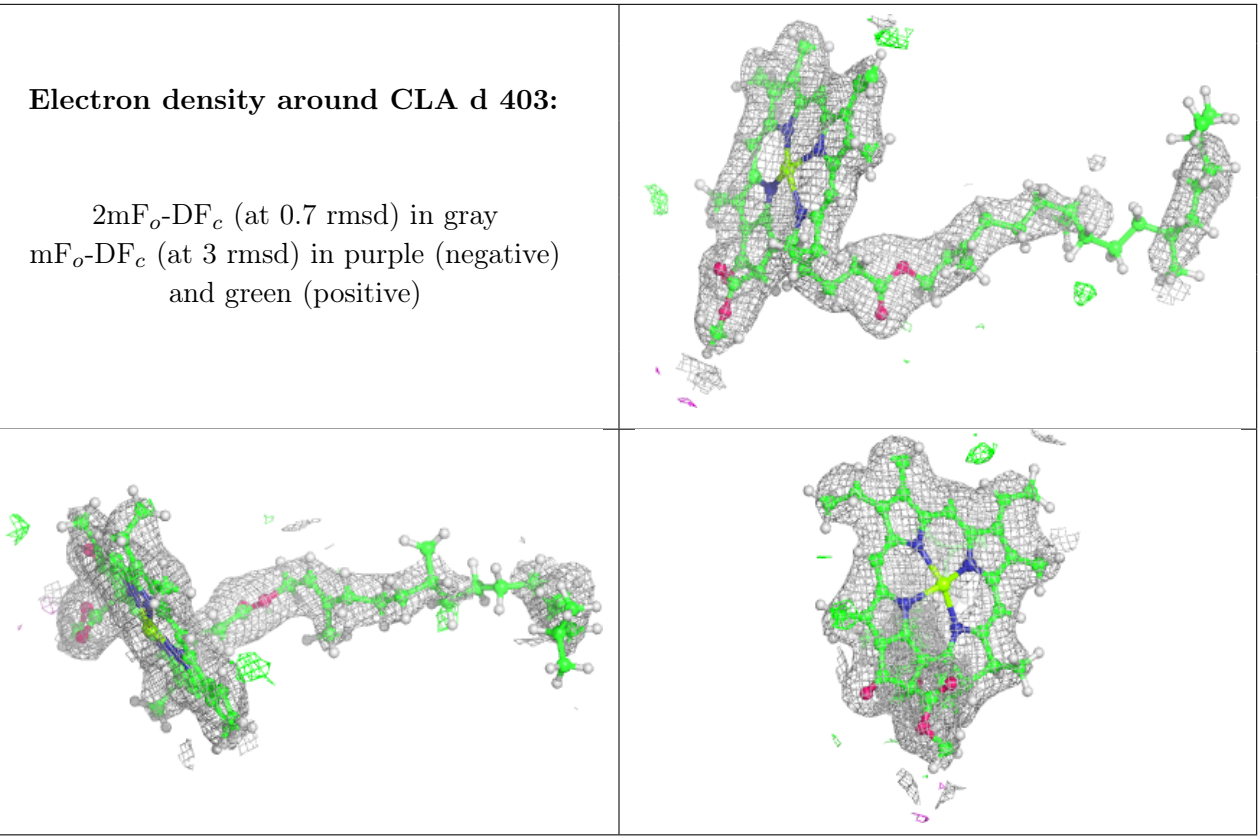
Electron density around CLA b 615:

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



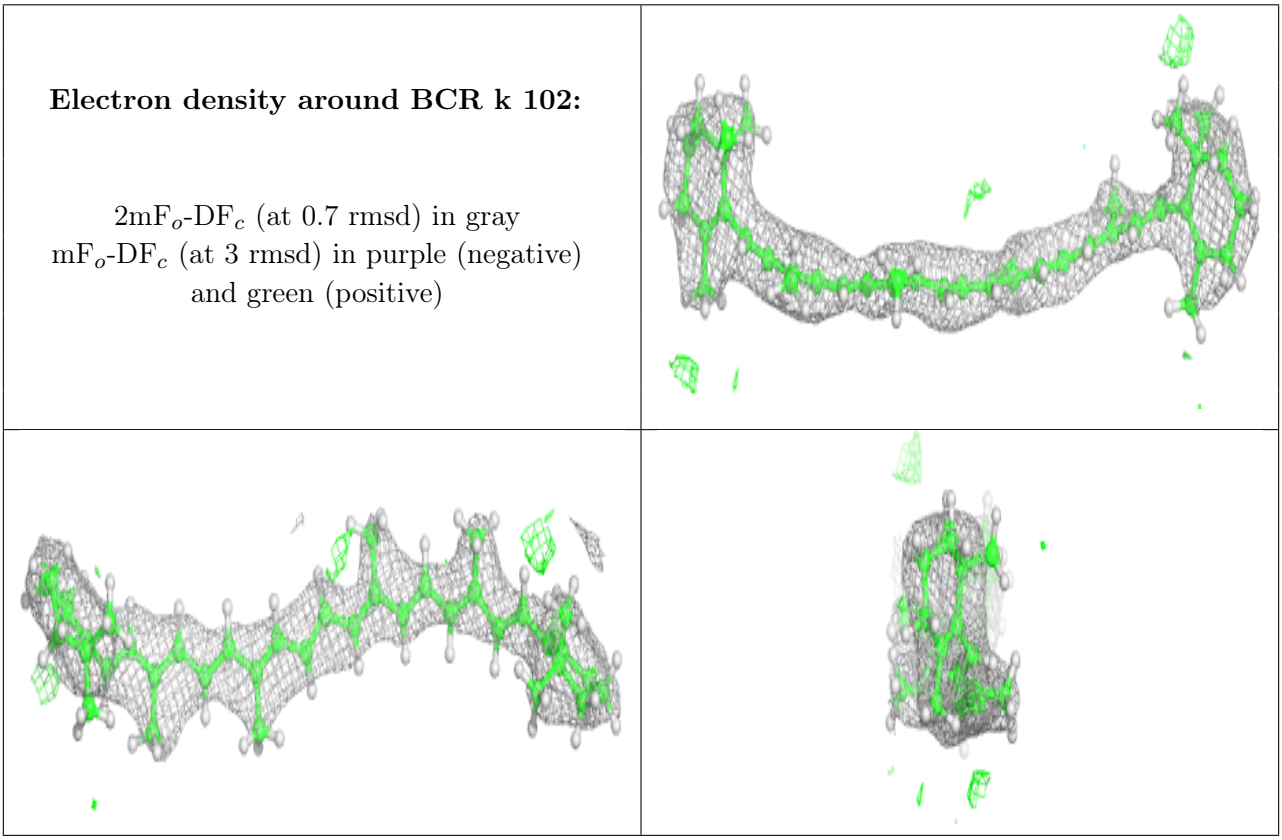
Electron density around CLA d 403:

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



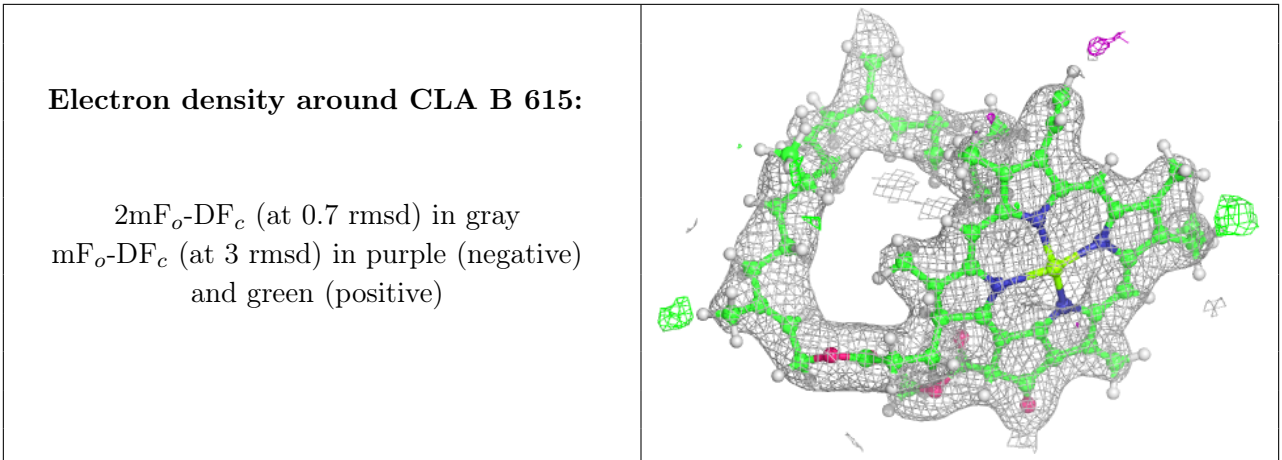
Electron density around BCR k 102:

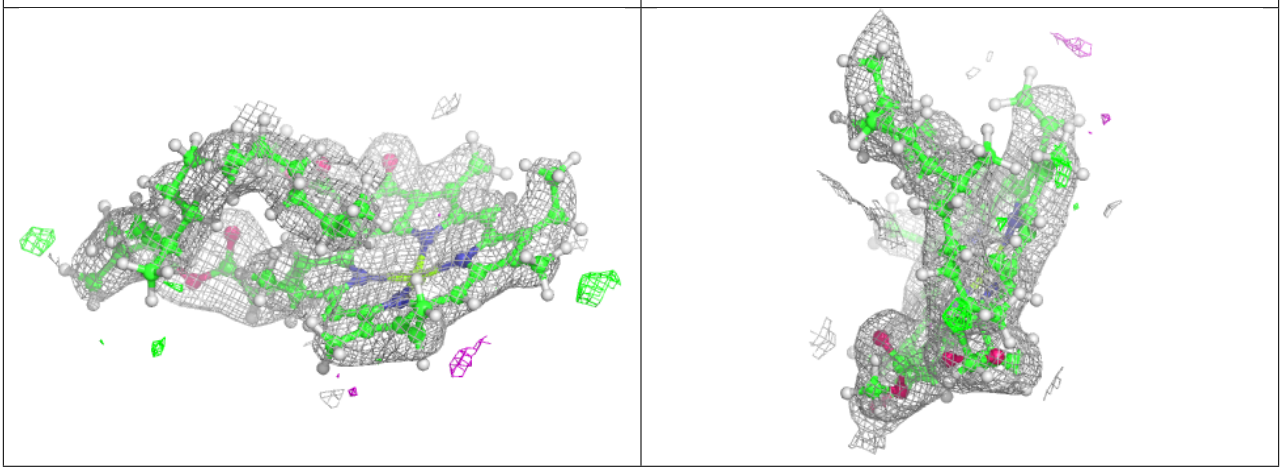
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 615:

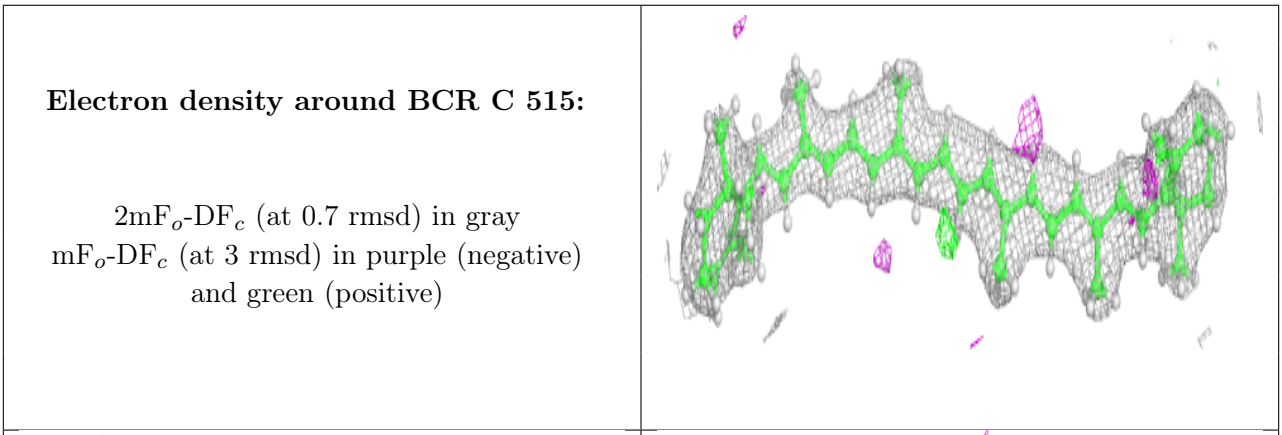
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

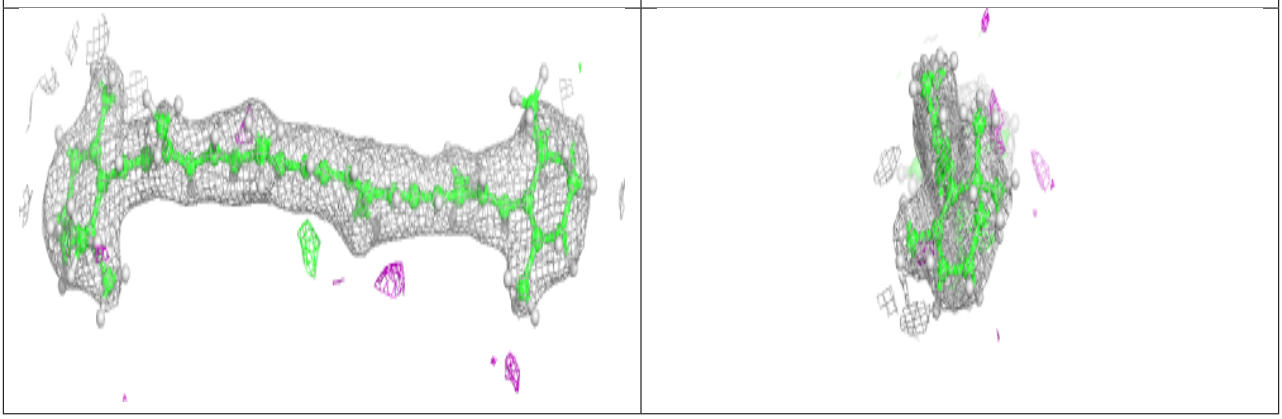




Electron density around BCR C 515:

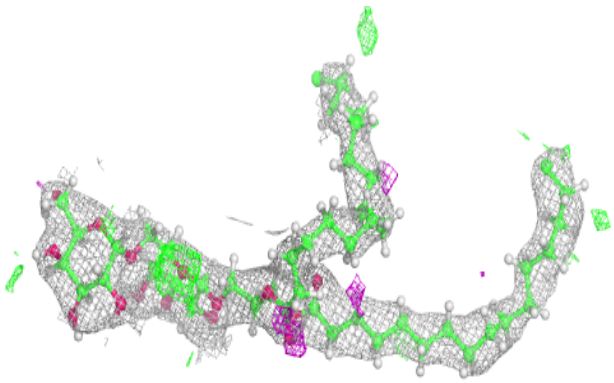
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

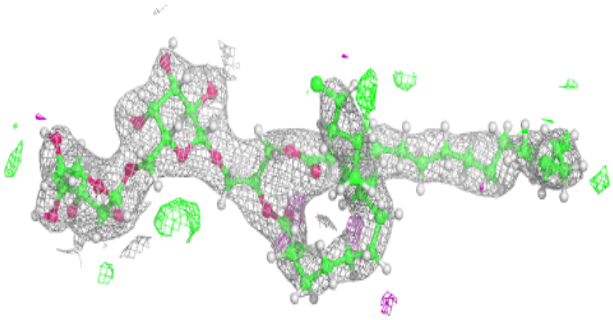




Electron density around DGD h 103:

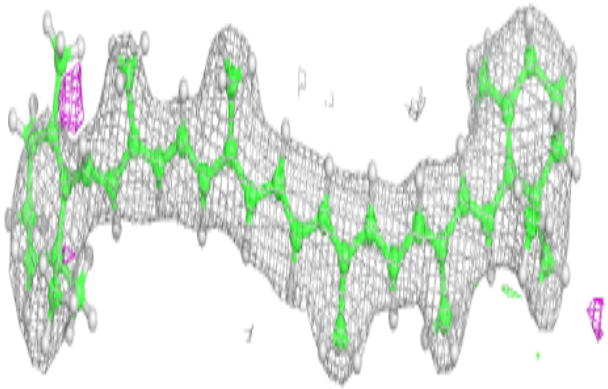
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

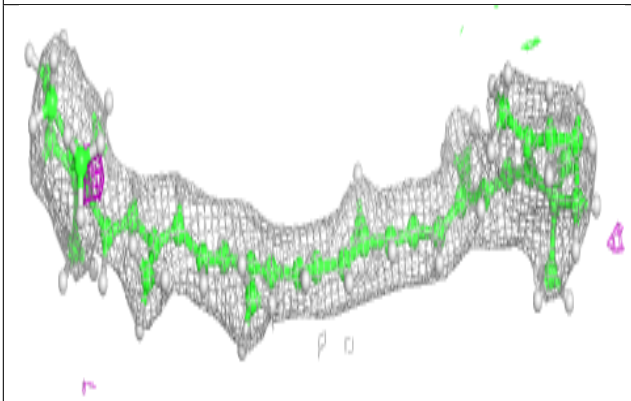


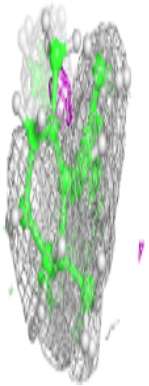


Electron density around BCR D 404:

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

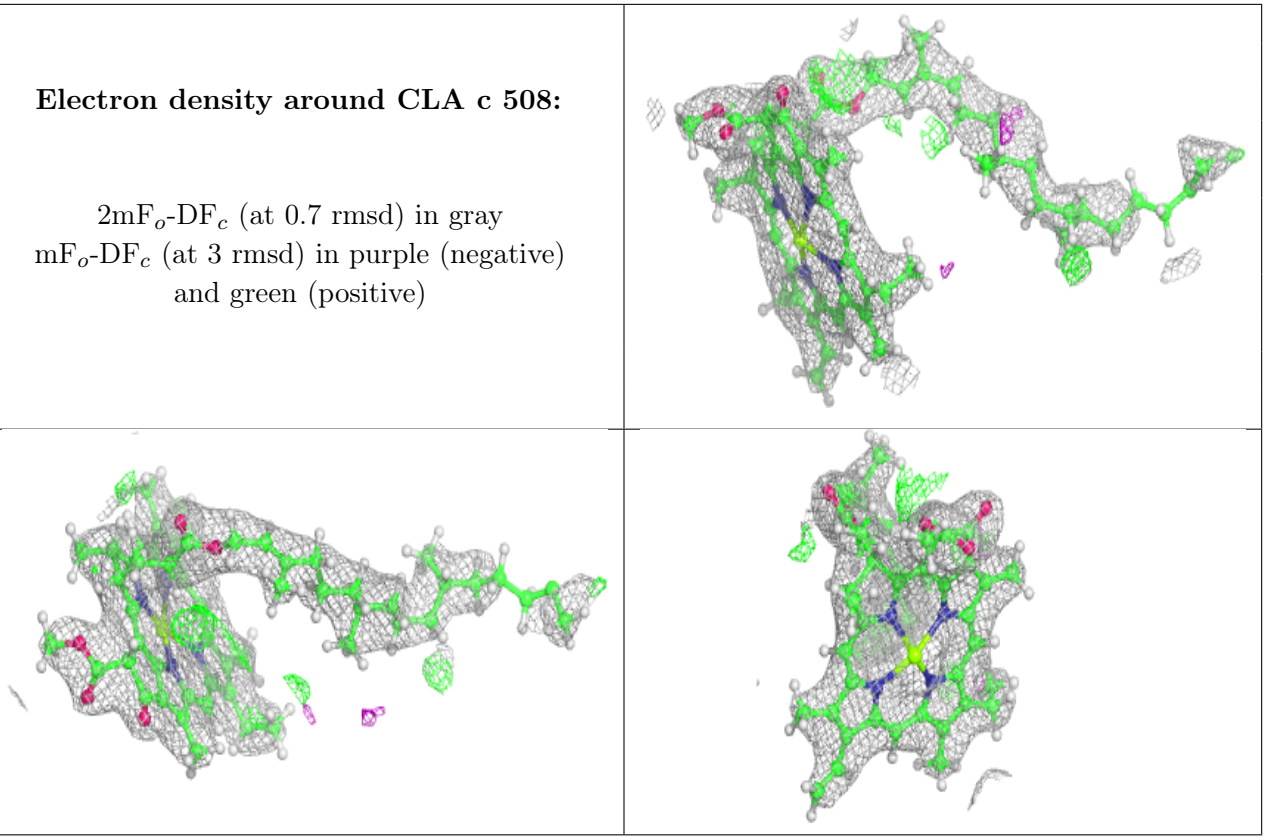






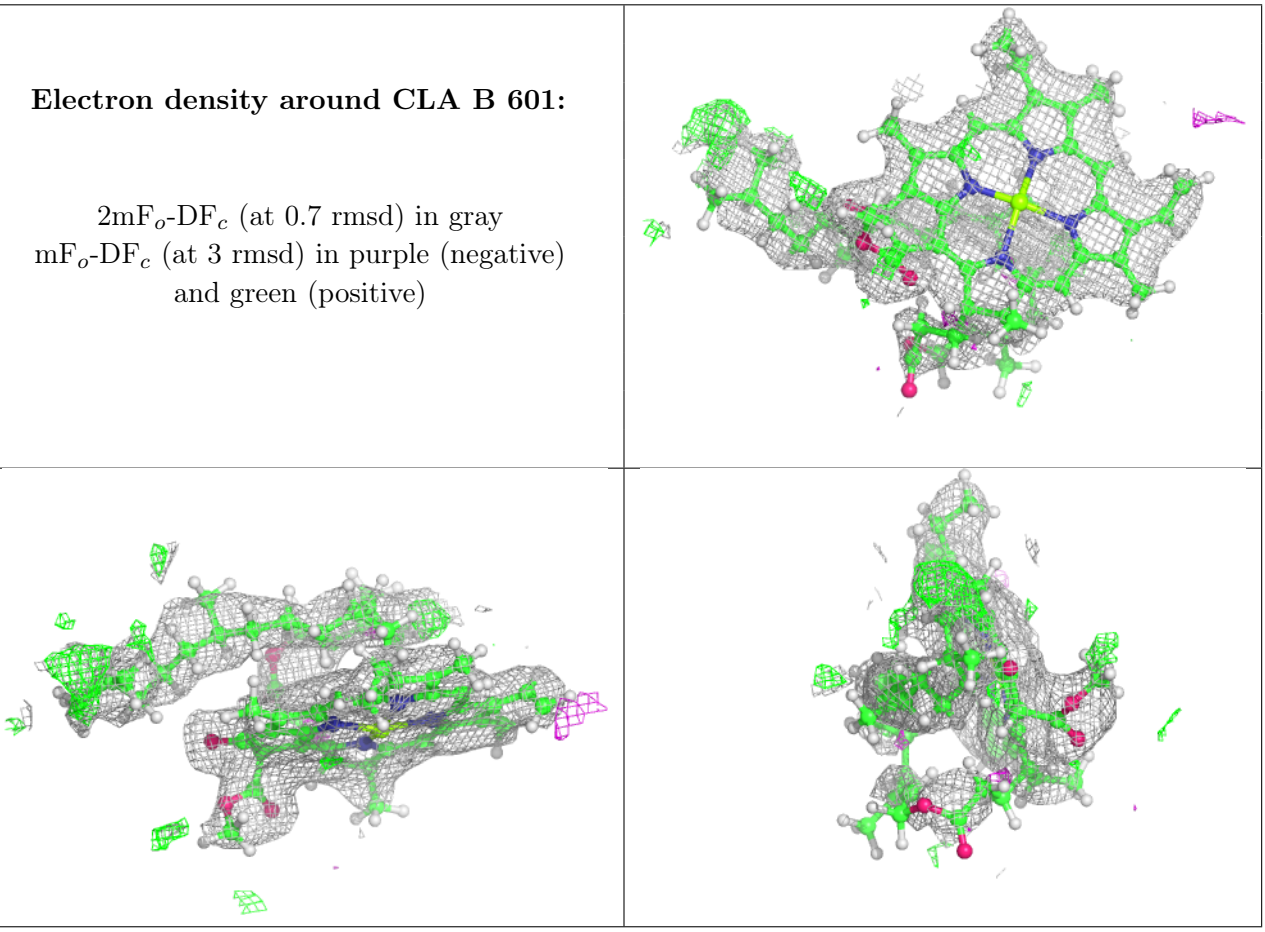
Electron density around CLA c 508:

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



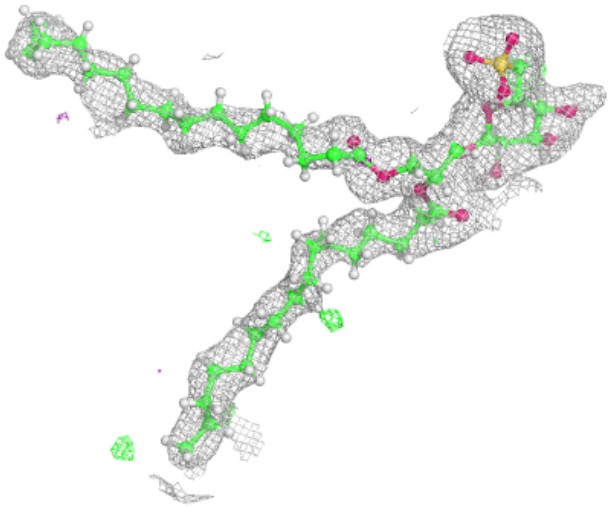
Electron density around CLA B 601:

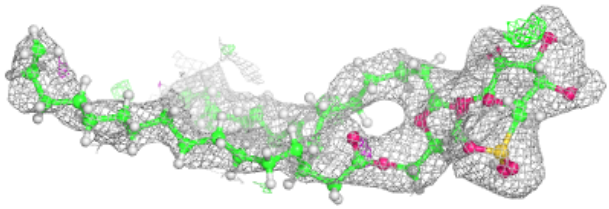
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

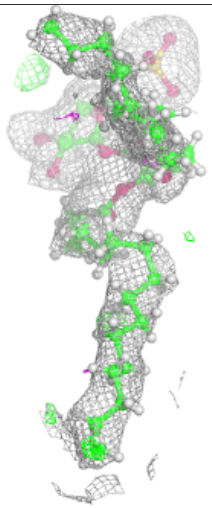


Electron density around SQD a 613:

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

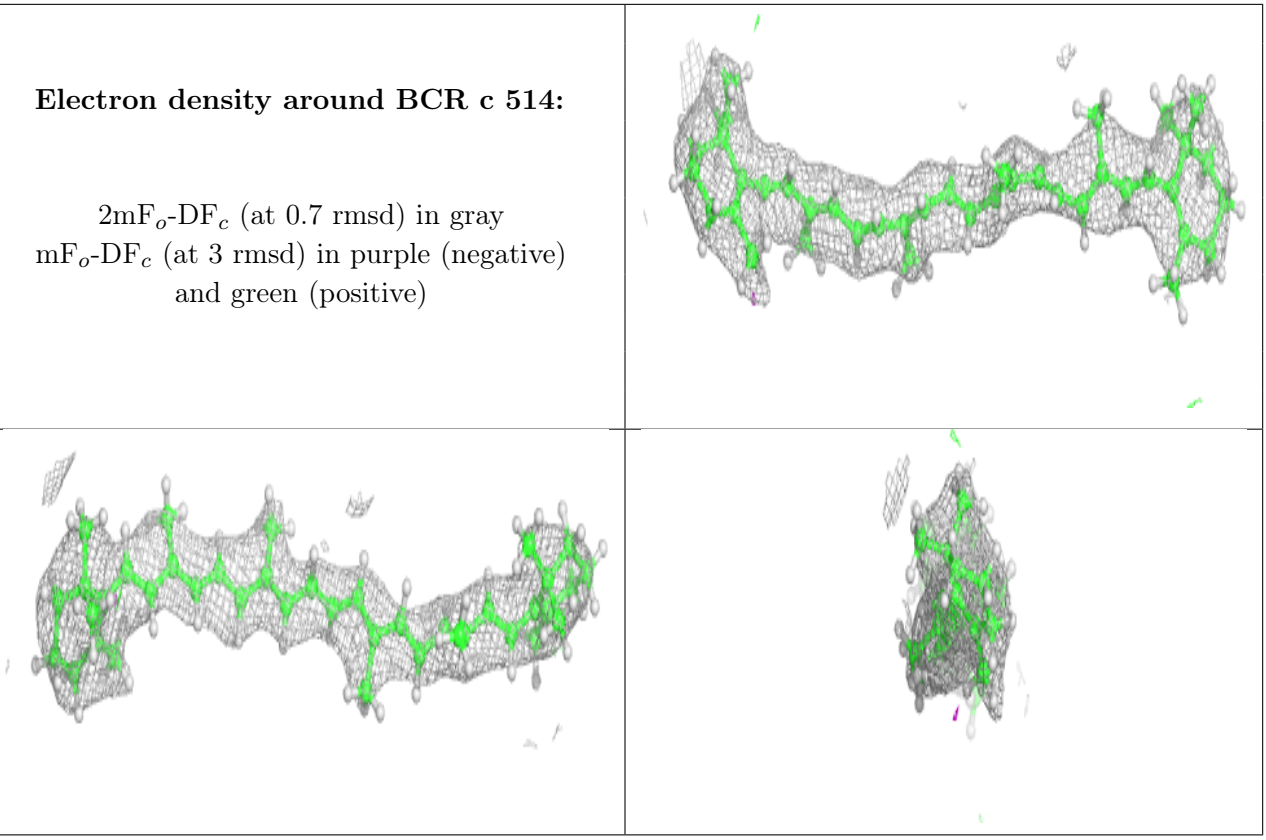






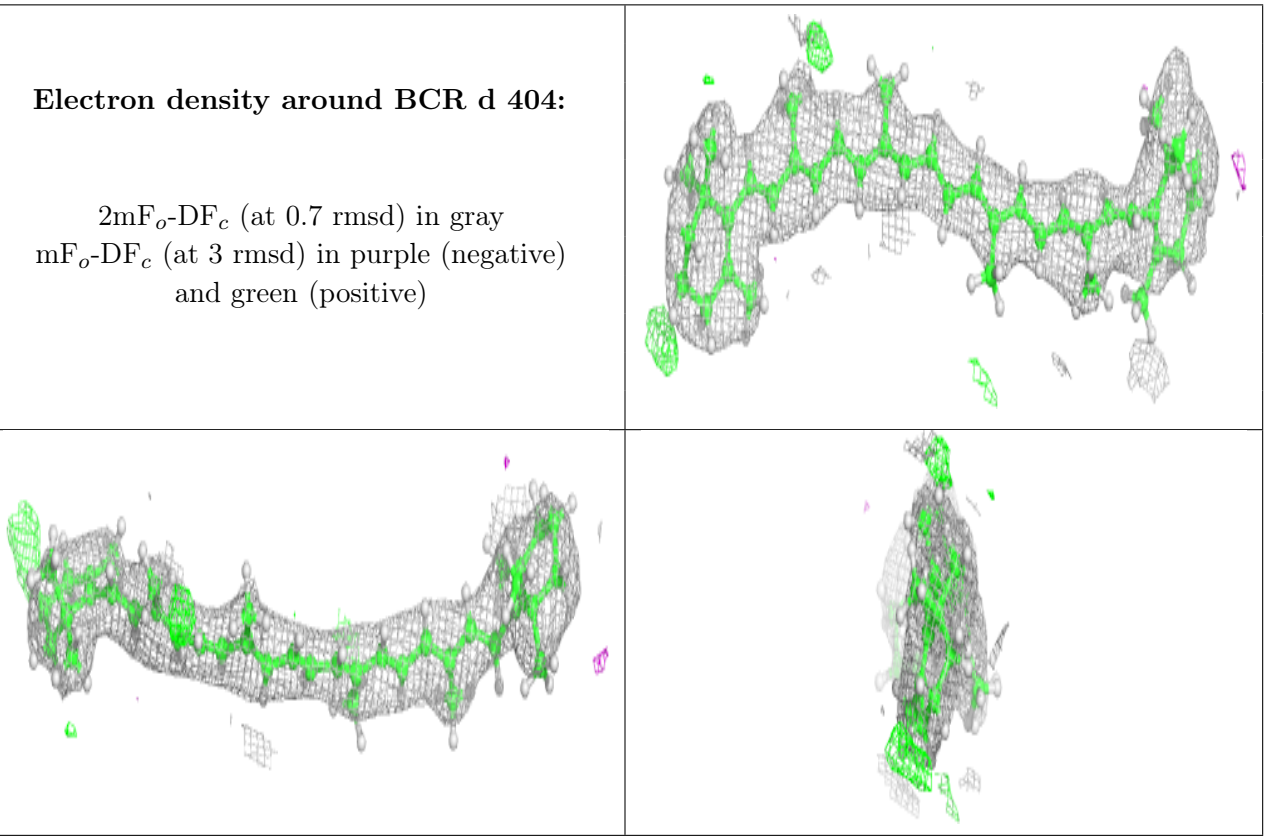
Electron density around BCR c 514:

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



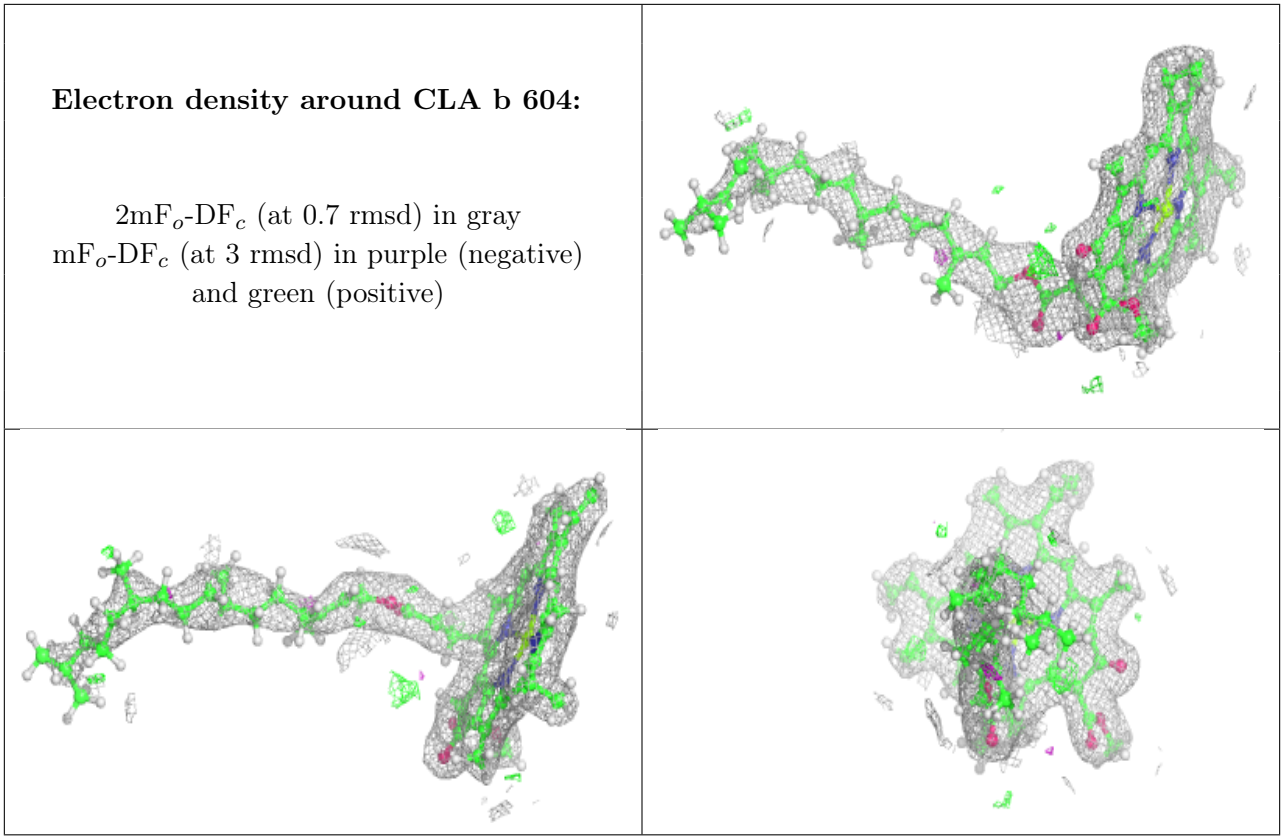
Electron density around BCR d 404:

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



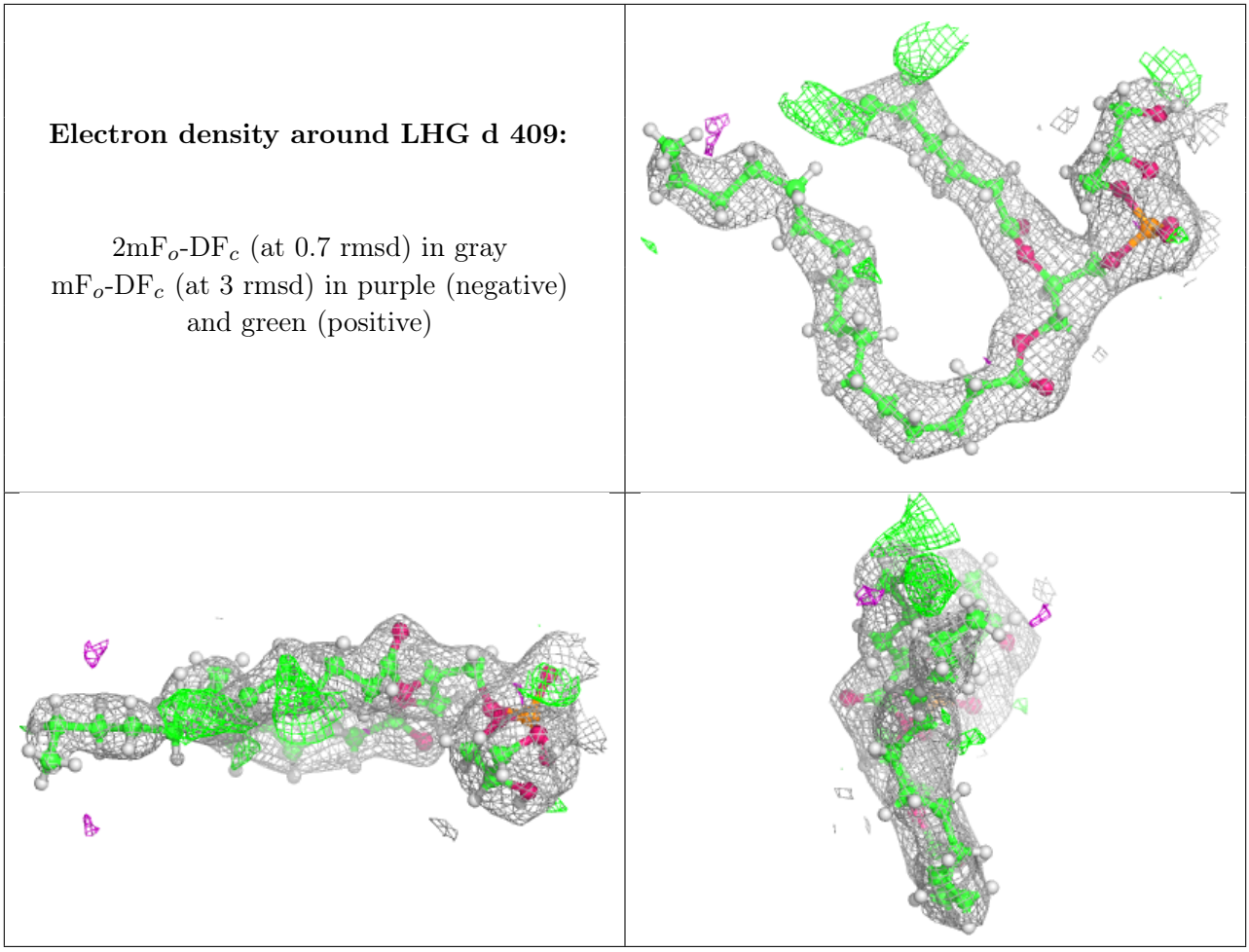
Electron density around CLA b 604:

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



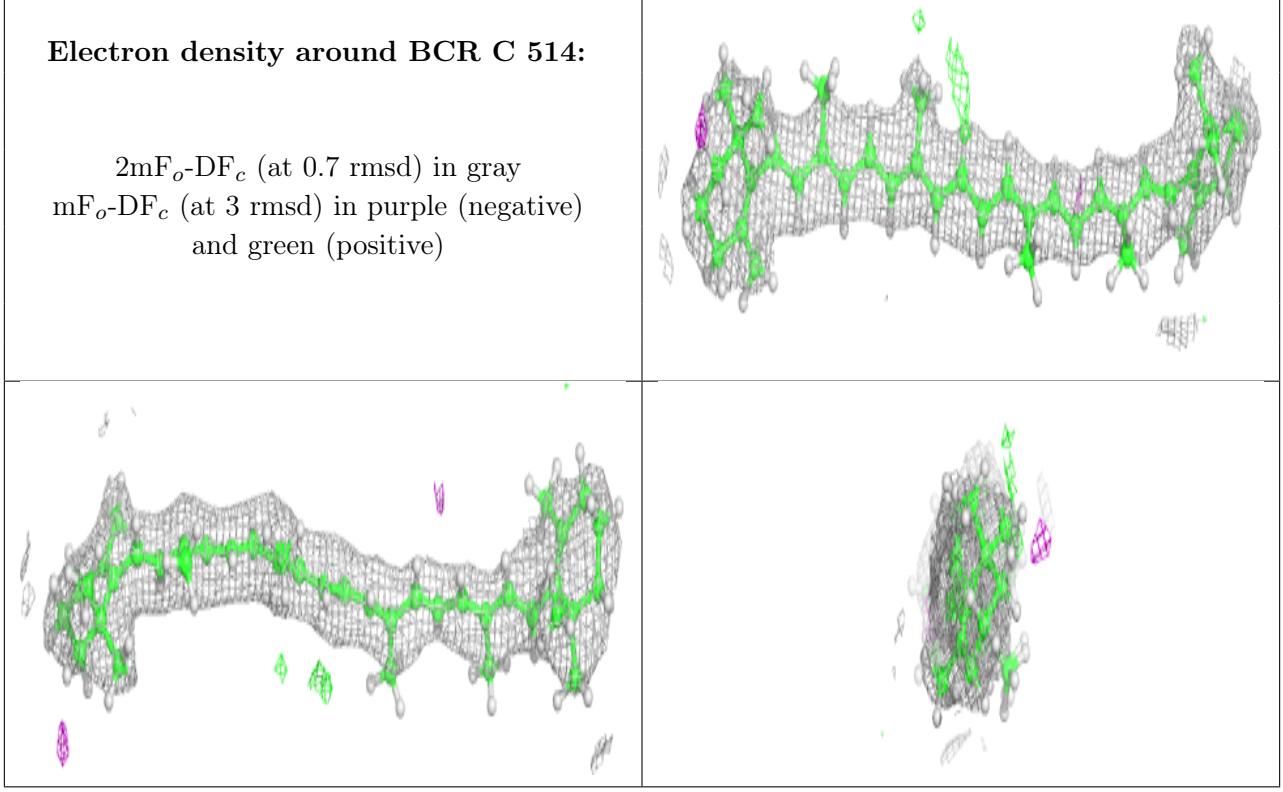
Electron density around LHG d 409:

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



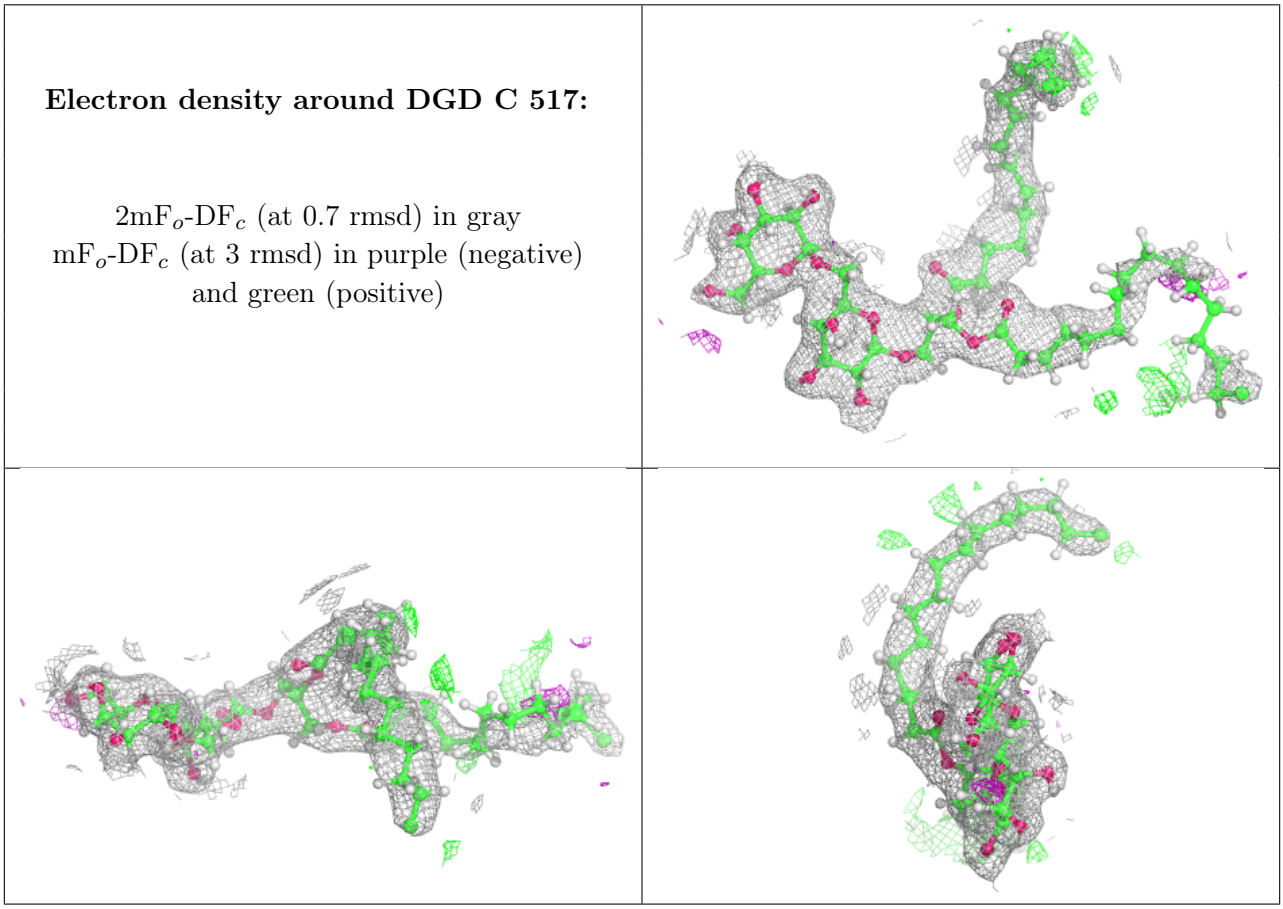
Electron density around BCR C 514:

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



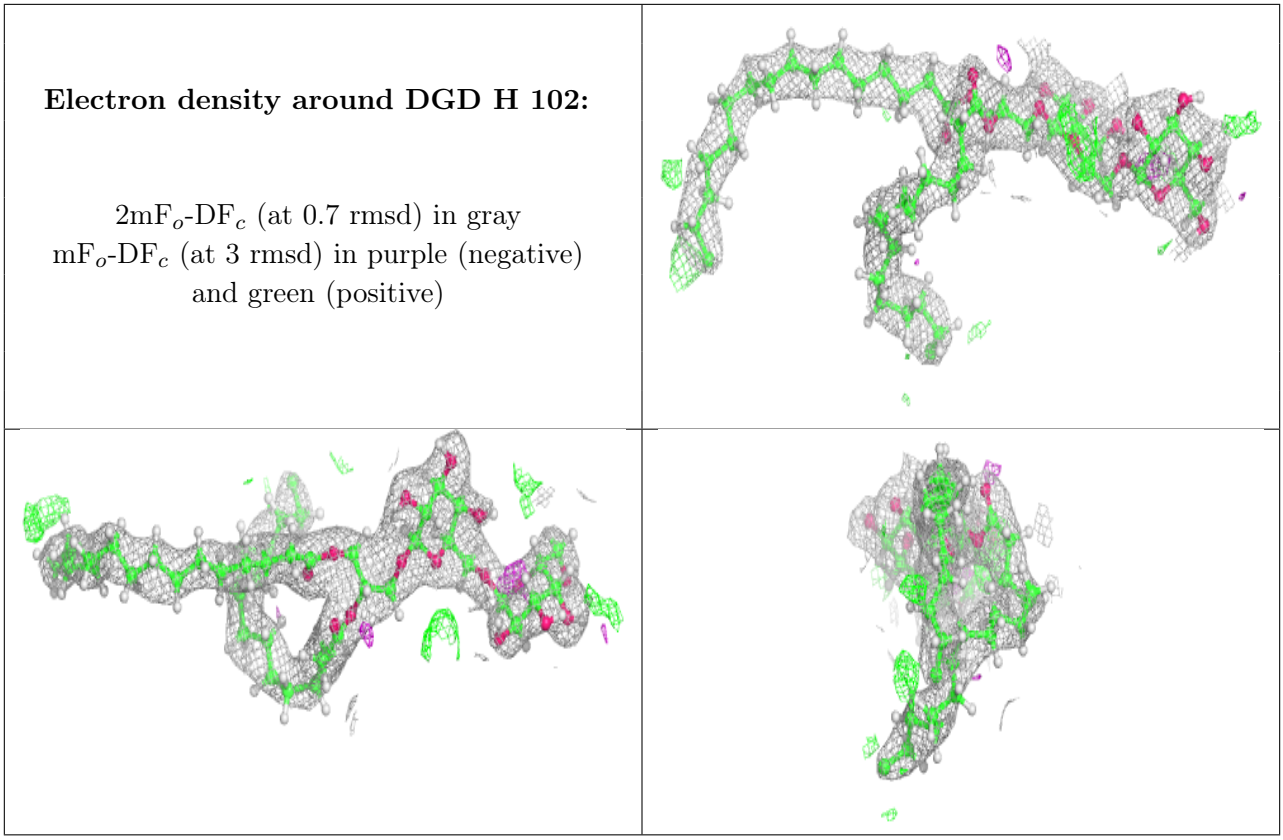
Electron density around DGD C 517:

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



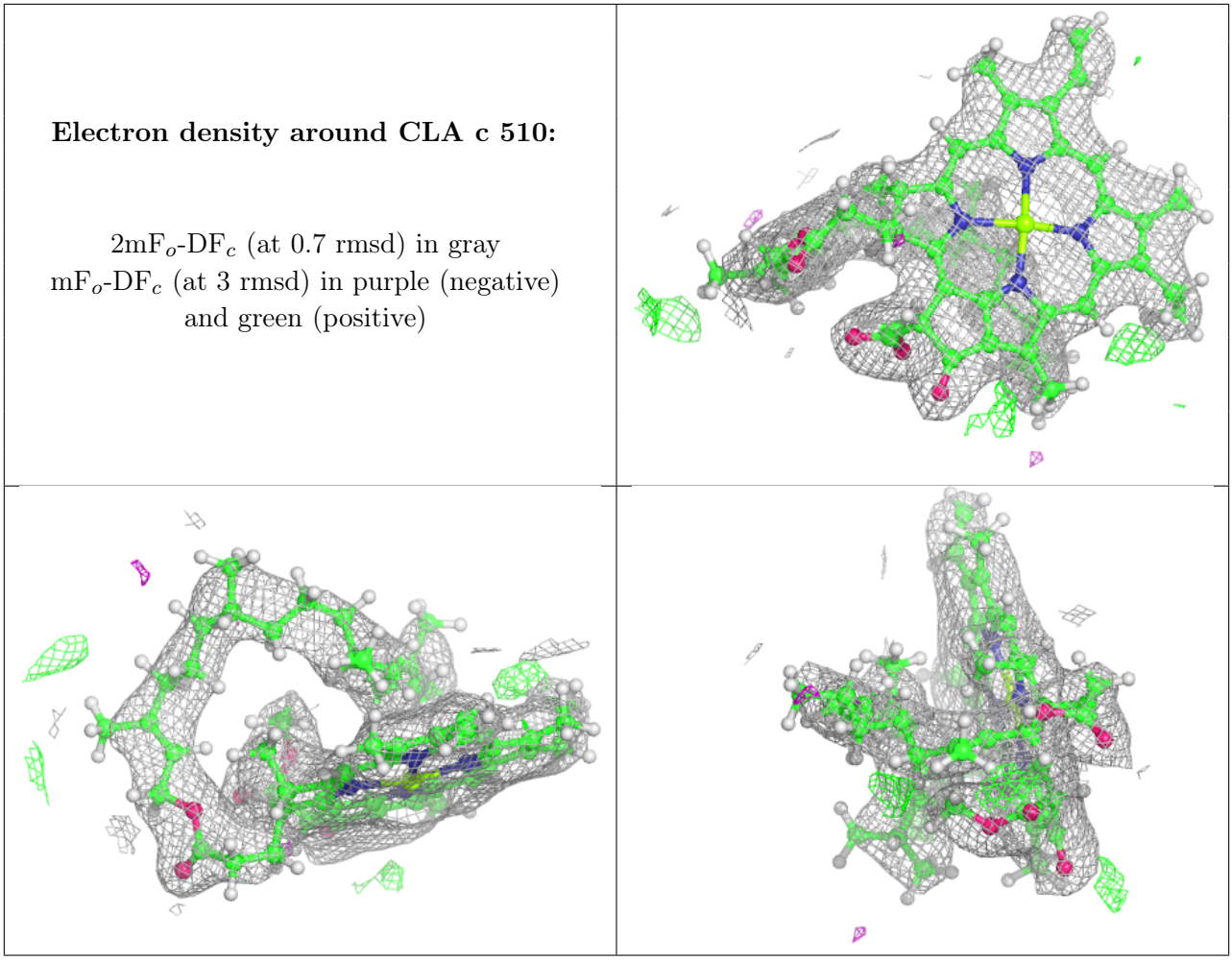
Electron density around DGD H 102:

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



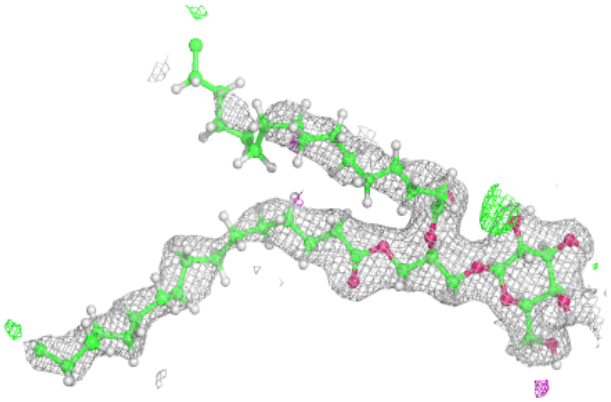
Electron density around CLA c 510:

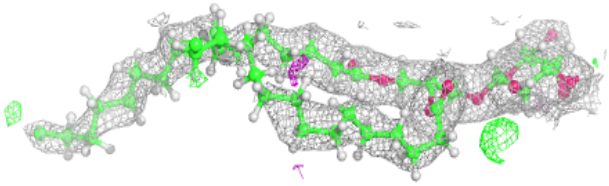
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

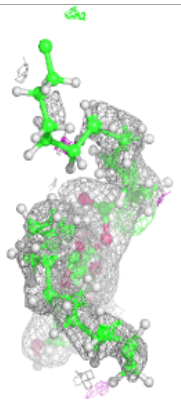


Electron density around LMG D 405:

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

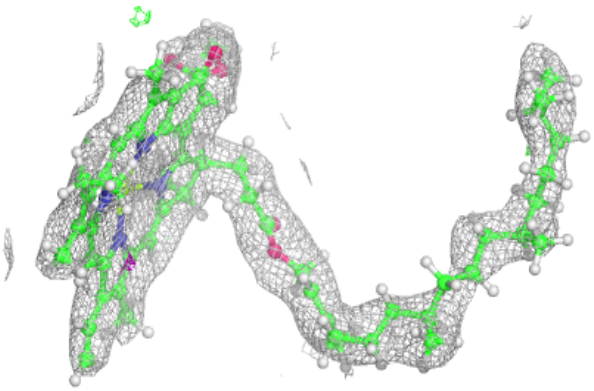


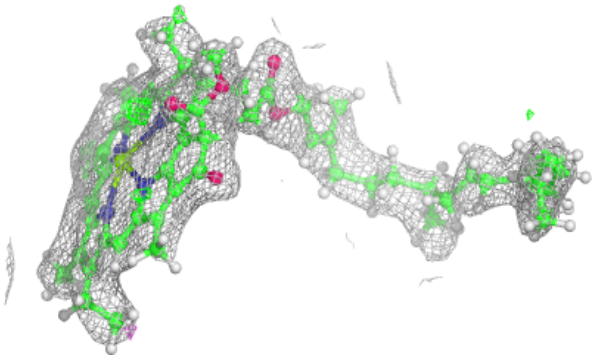


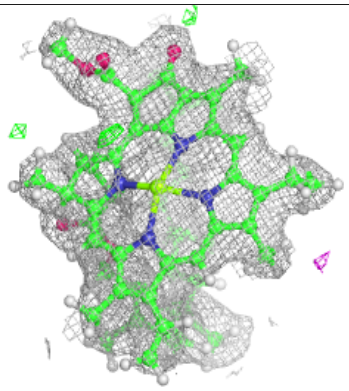


Electron density around CLA b 606:

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

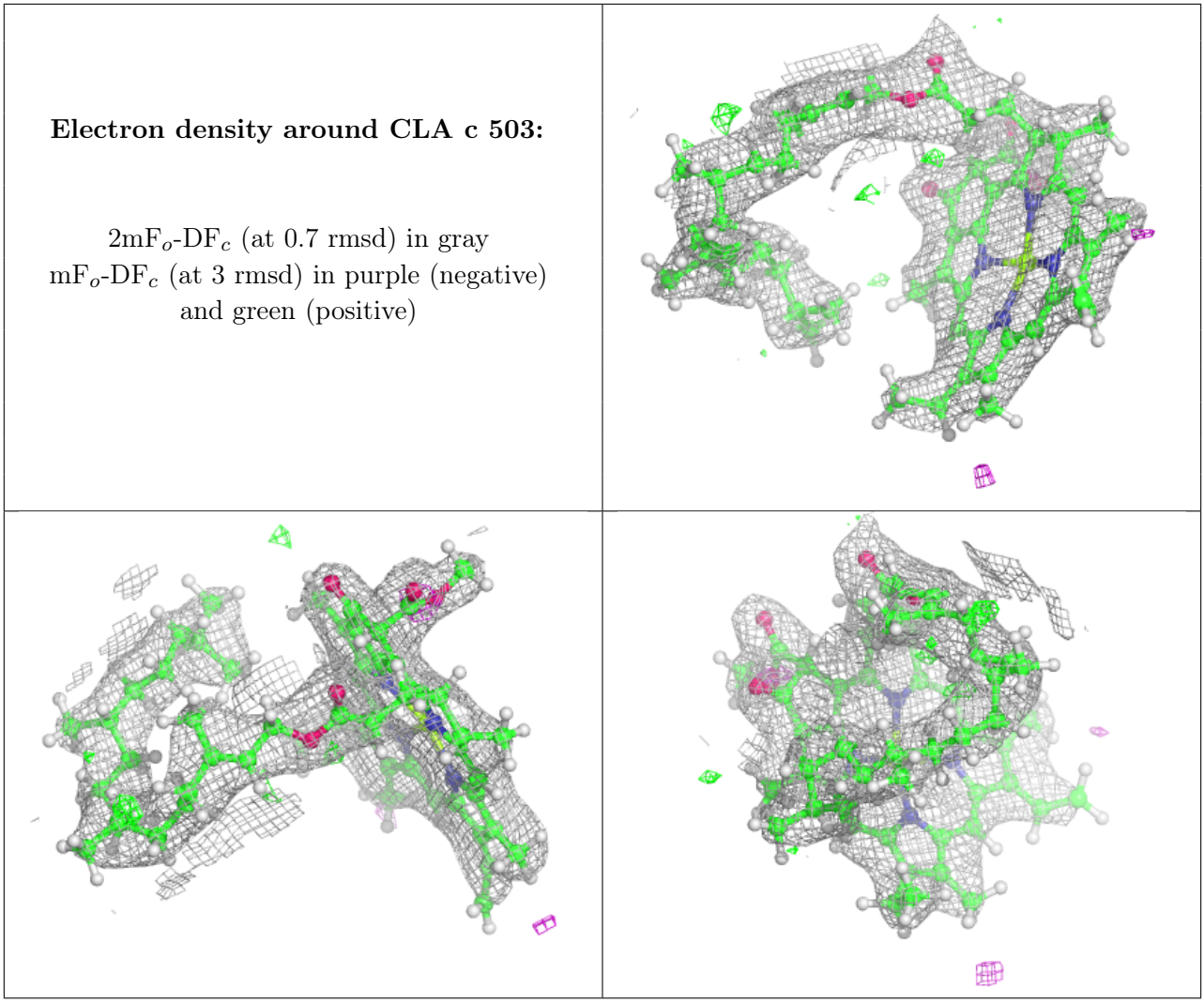






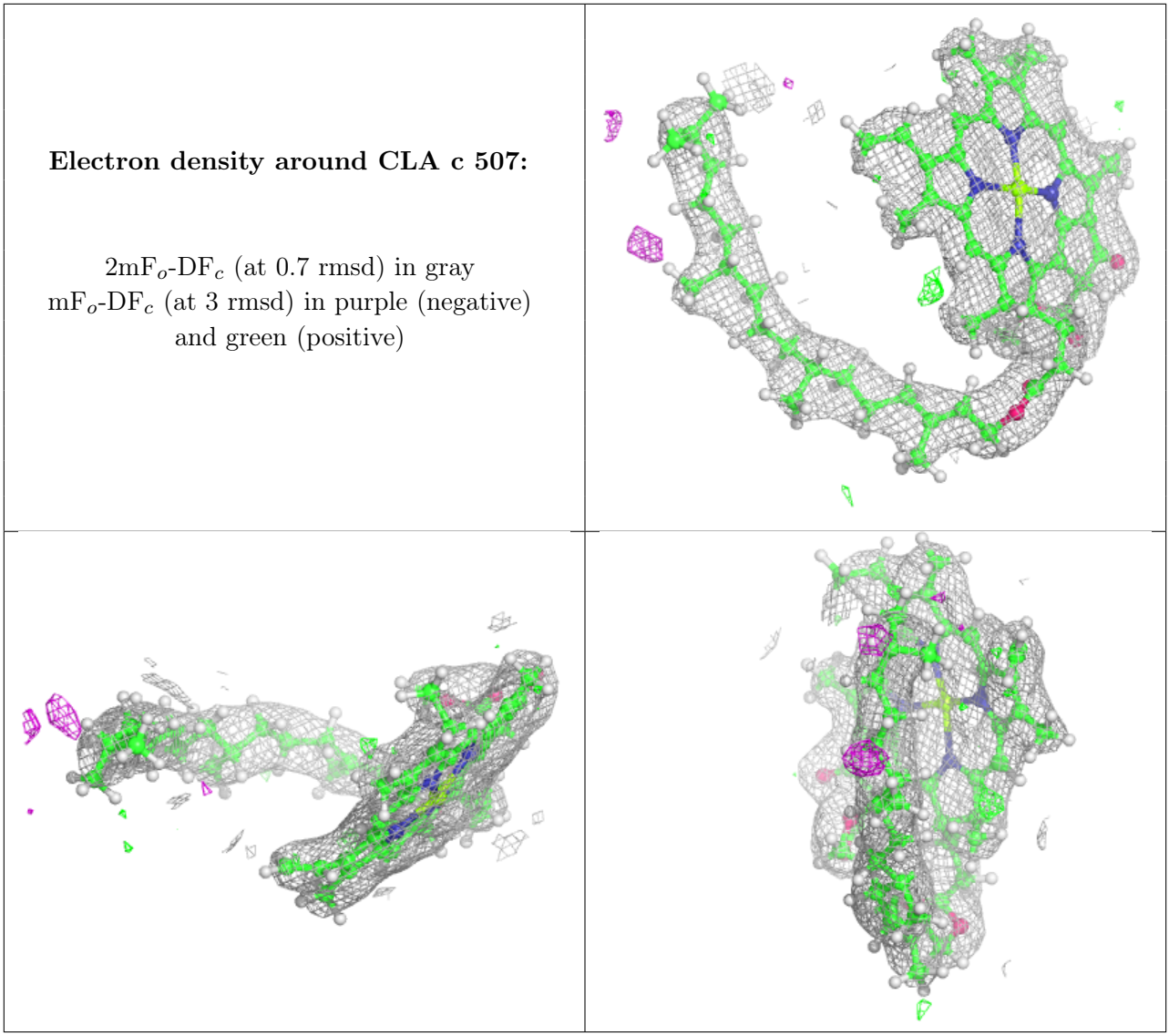
Electron density around CLA c 503:

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



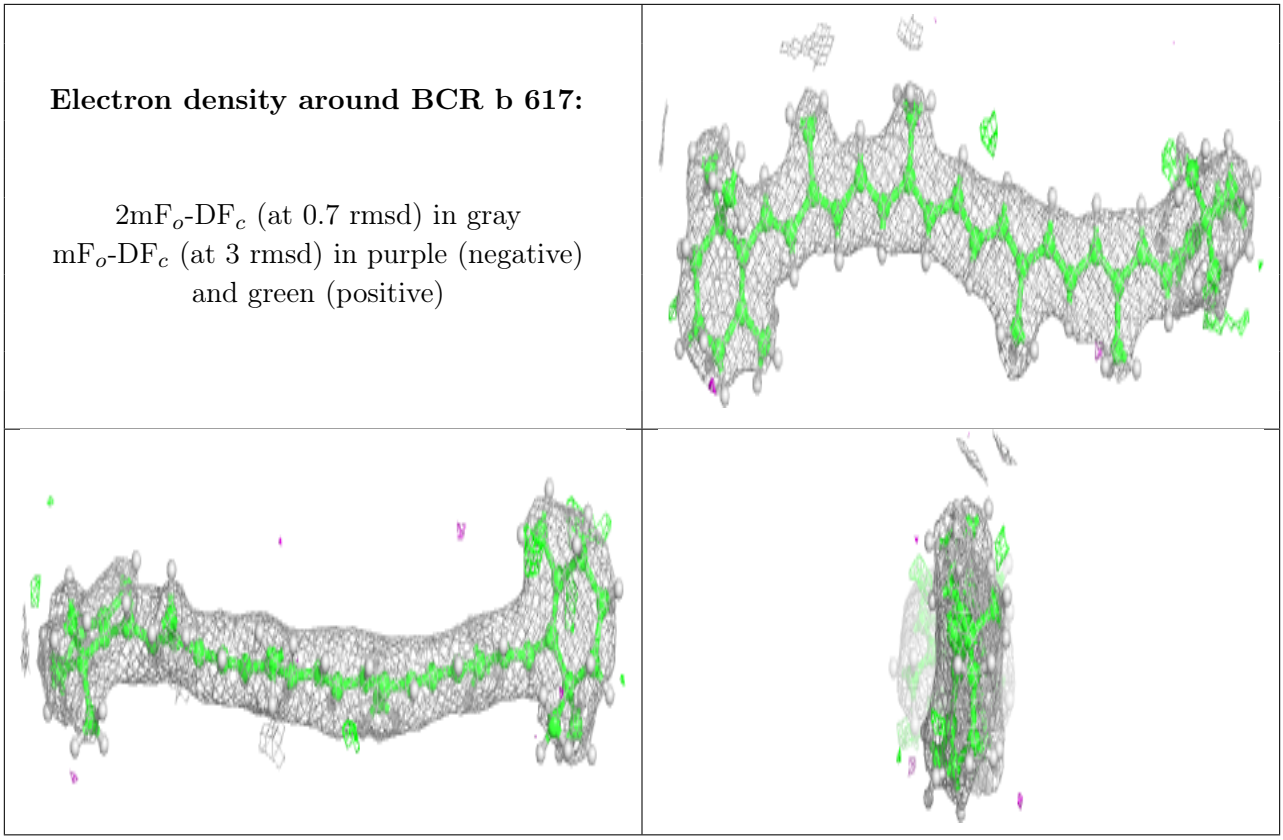
Electron density around CLA c 507:

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



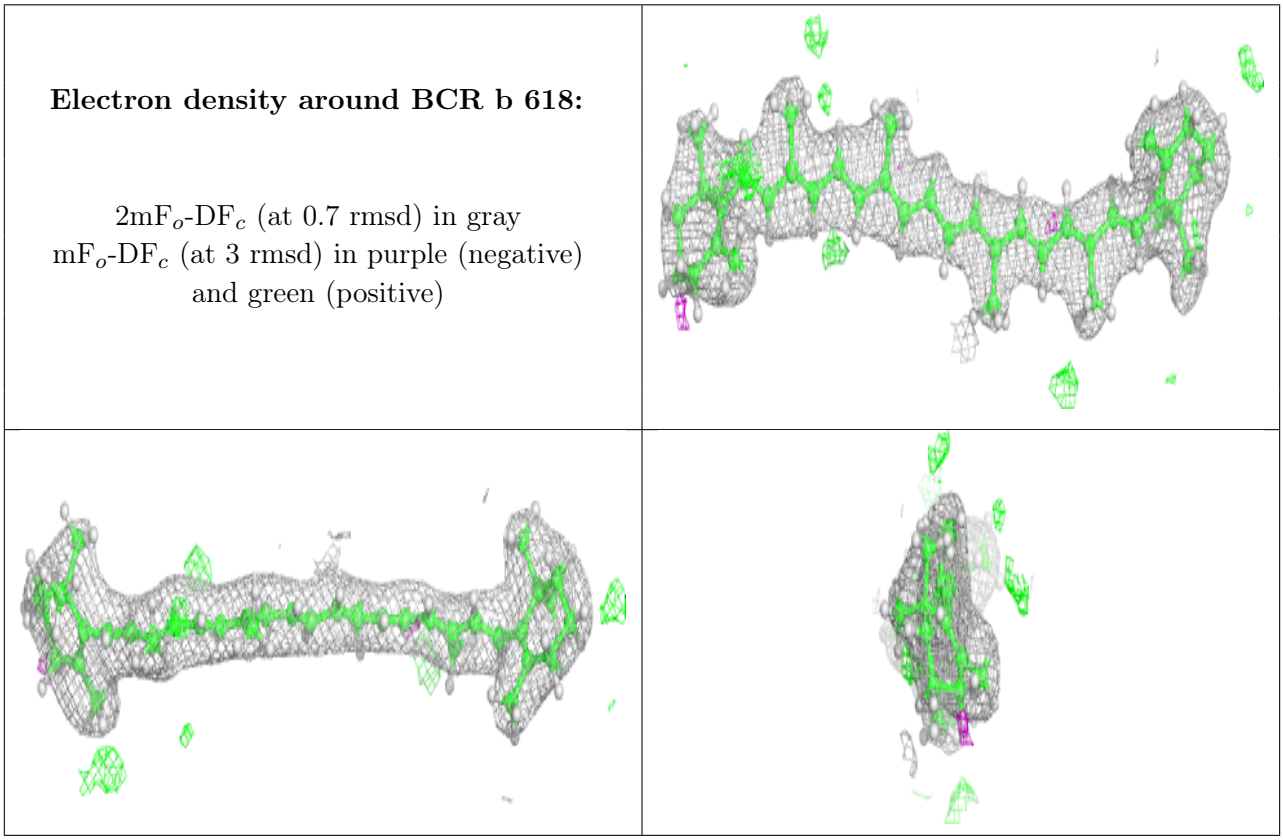
Electron density around BCR b 617:

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



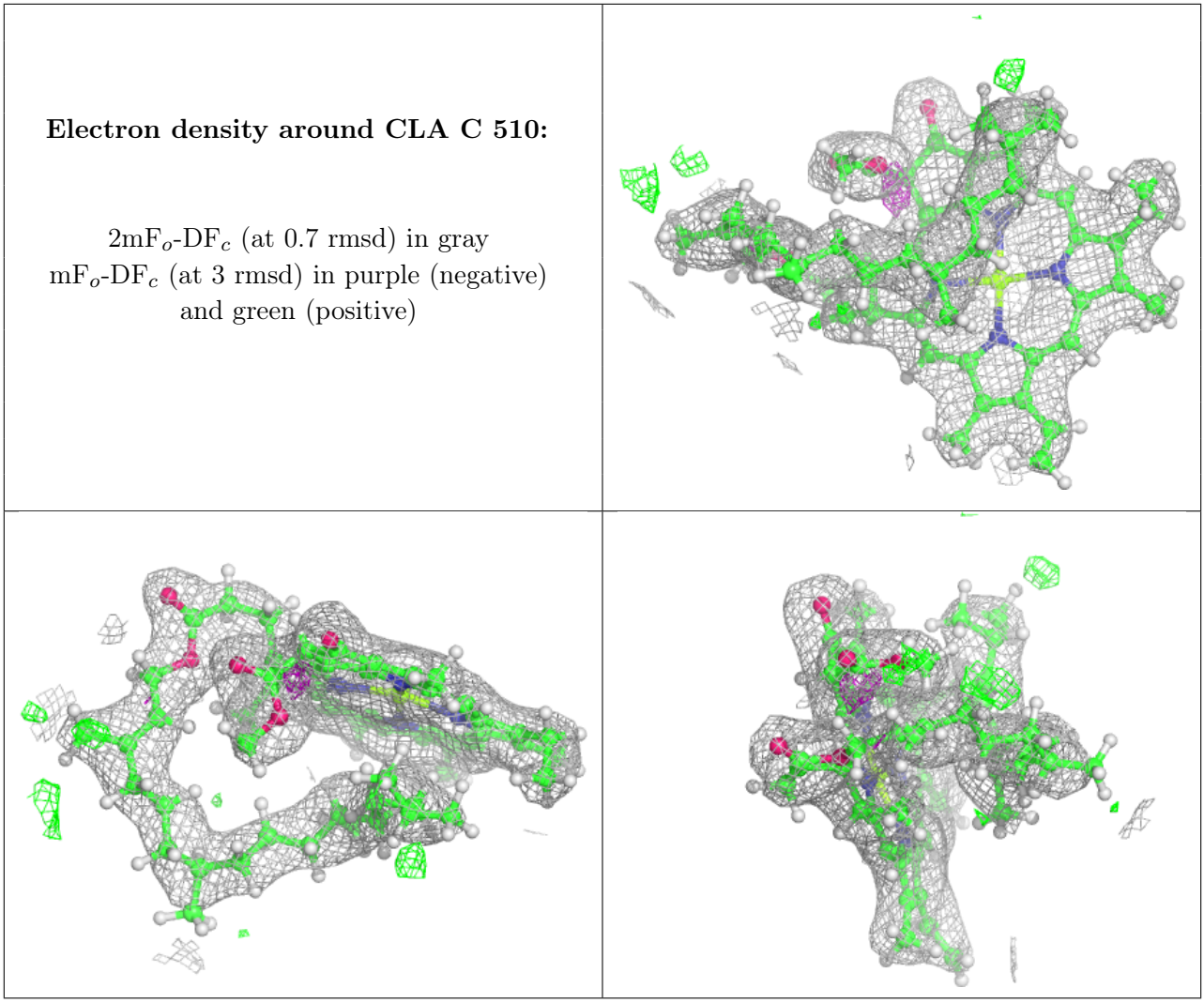
Electron density around BCR b 618:

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



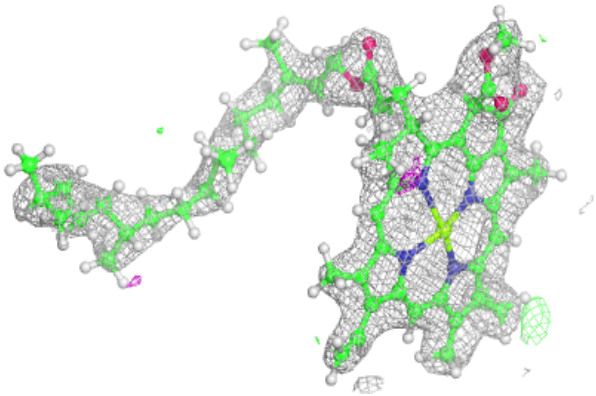
Electron density around CLA C 510:

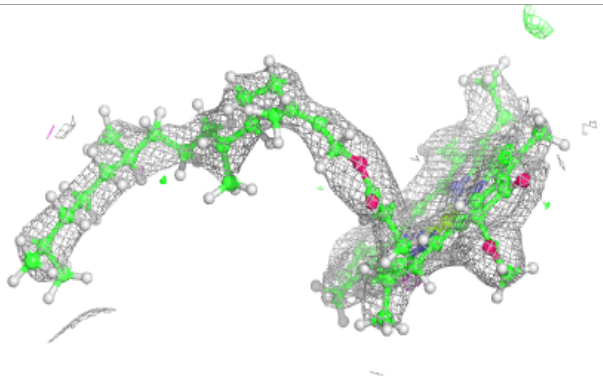
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

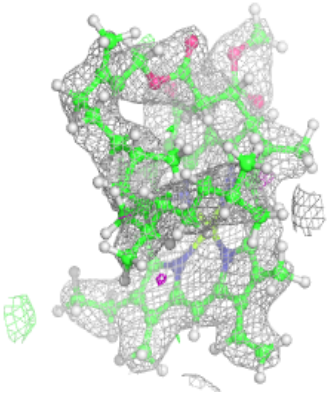


Electron density around CLA C 511:

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

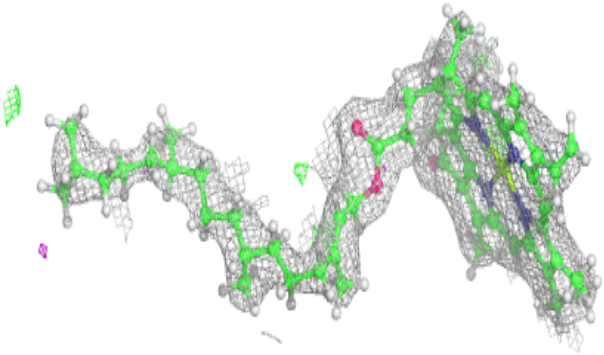


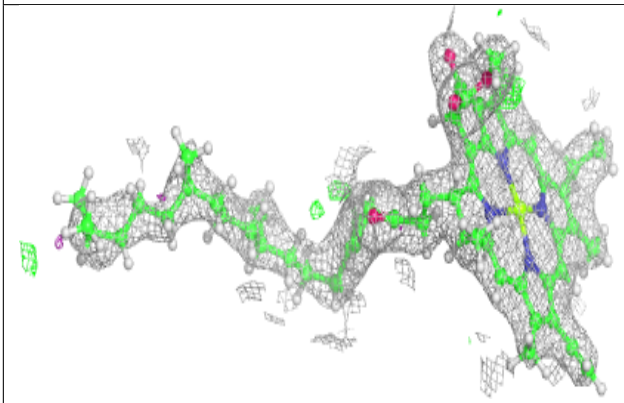


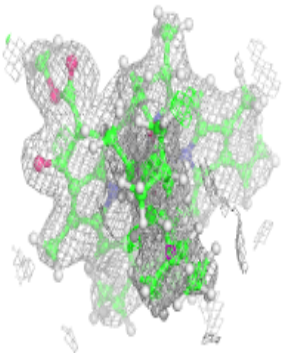


Electron density around CLA c 502:

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

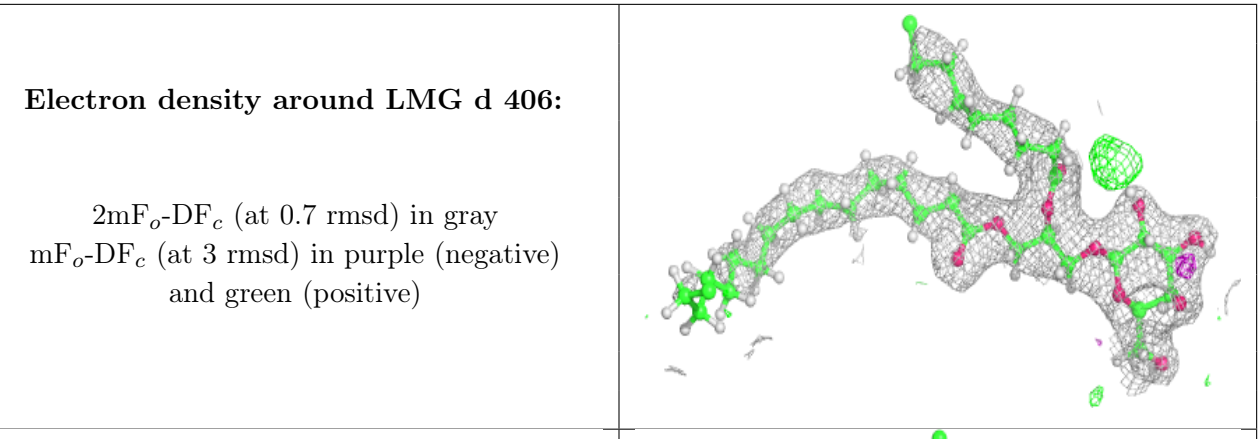






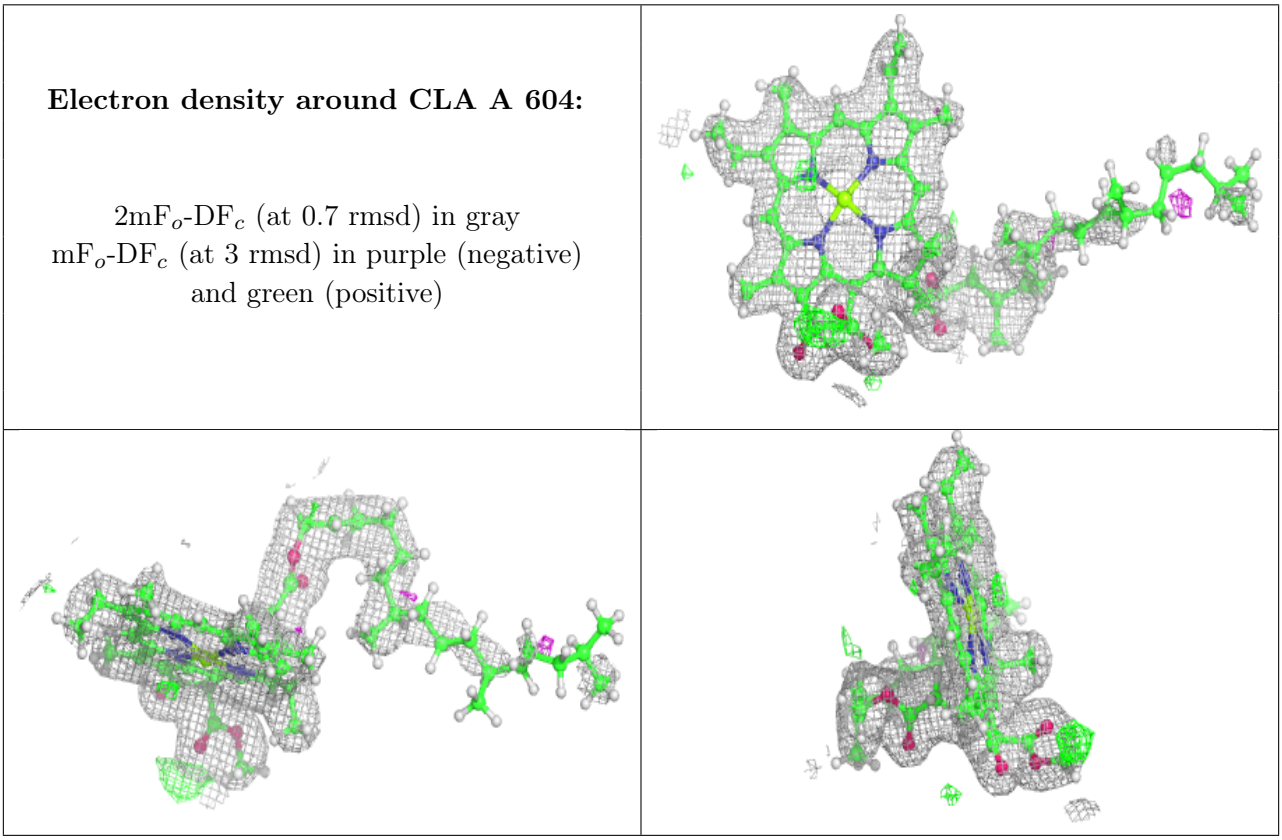
Electron density around LMG d 406:

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



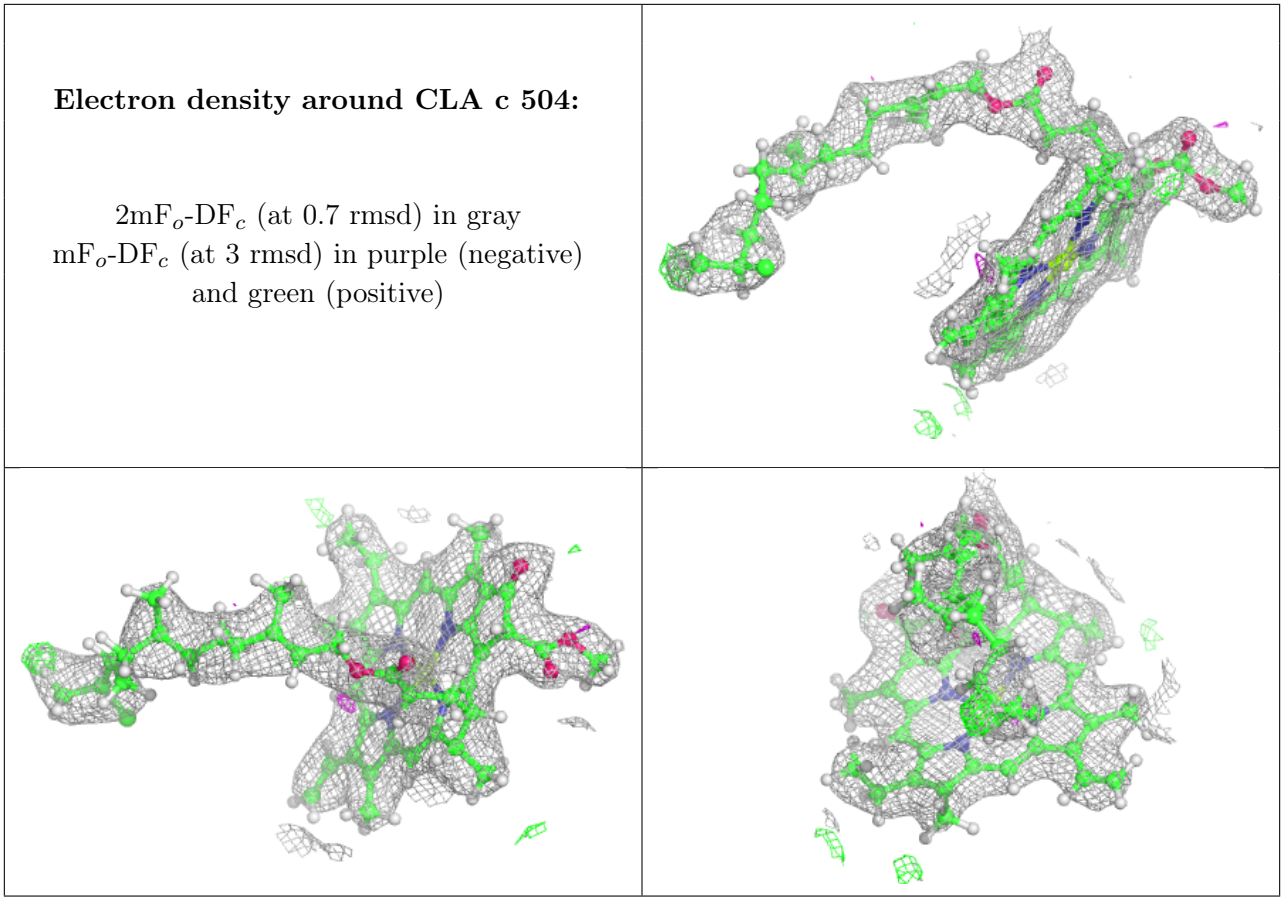
Electron density around CLA A 604:

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



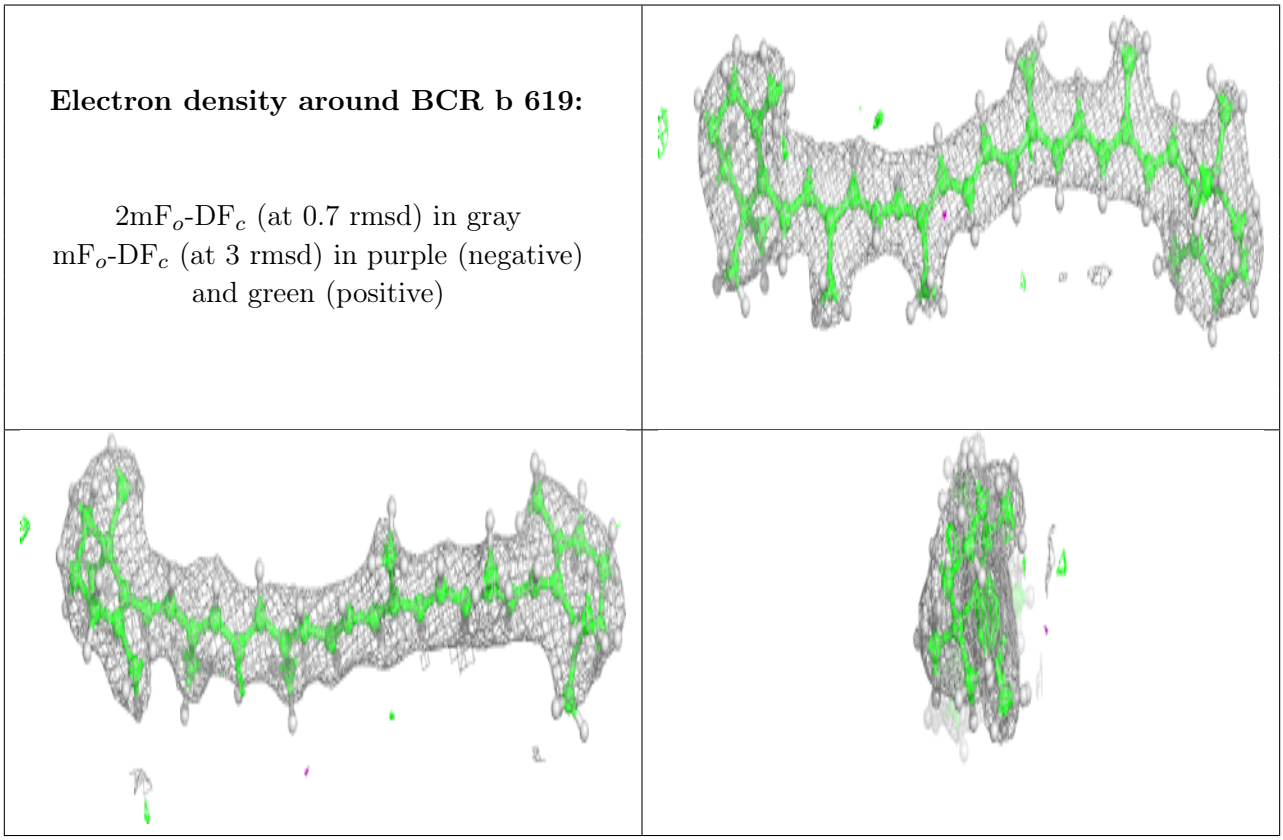
Electron density around CLA c 504:

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



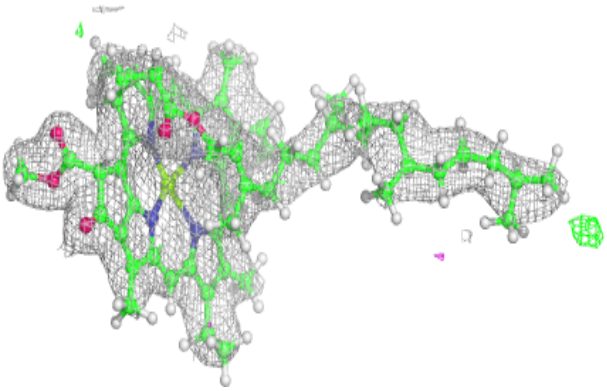
Electron density around BCR b 619:

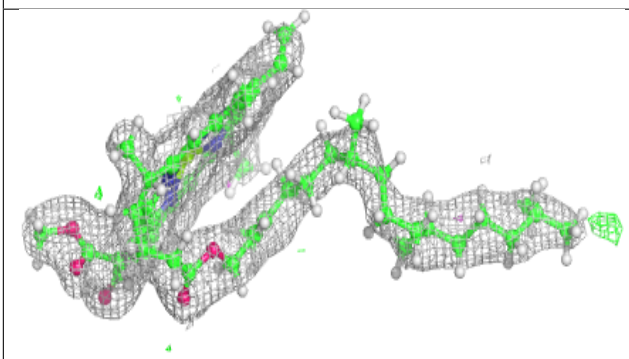
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

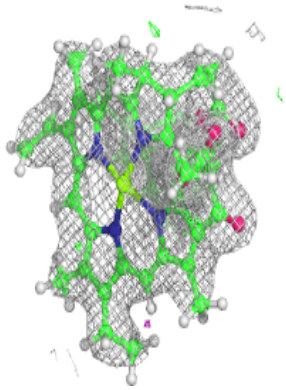


Electron density around CLA c 505:

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

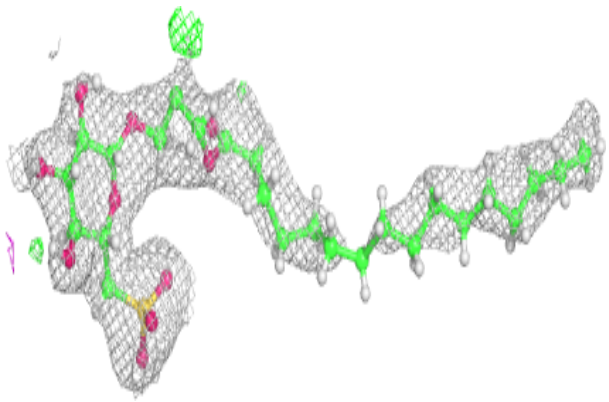


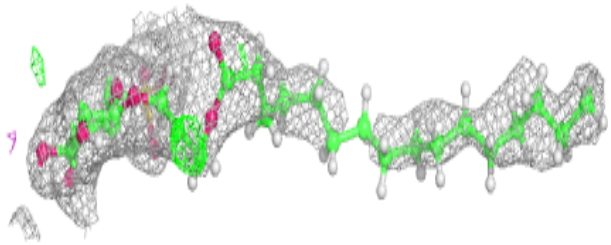


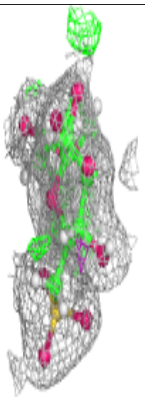


Electron density around SQD F 101:

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

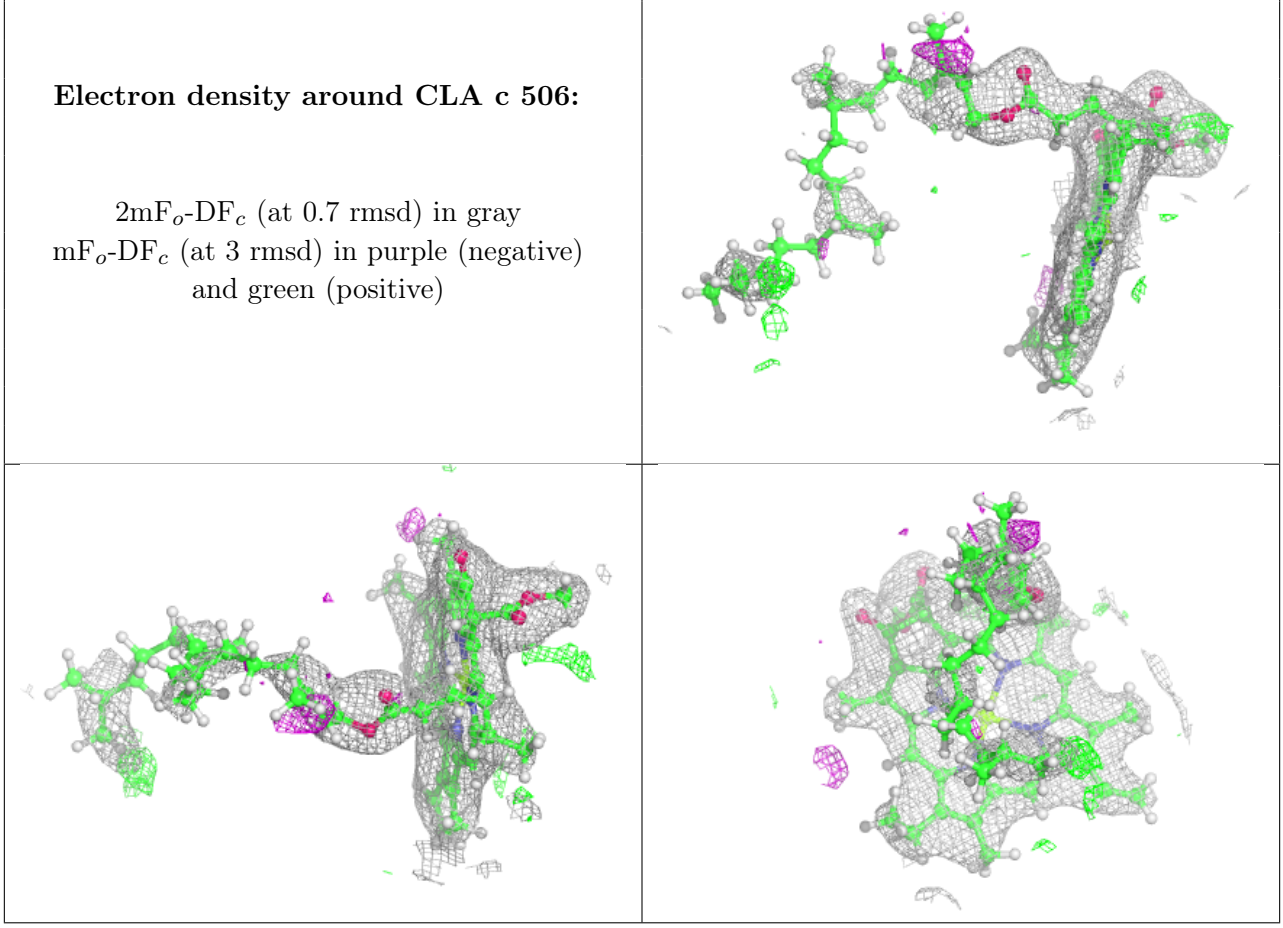






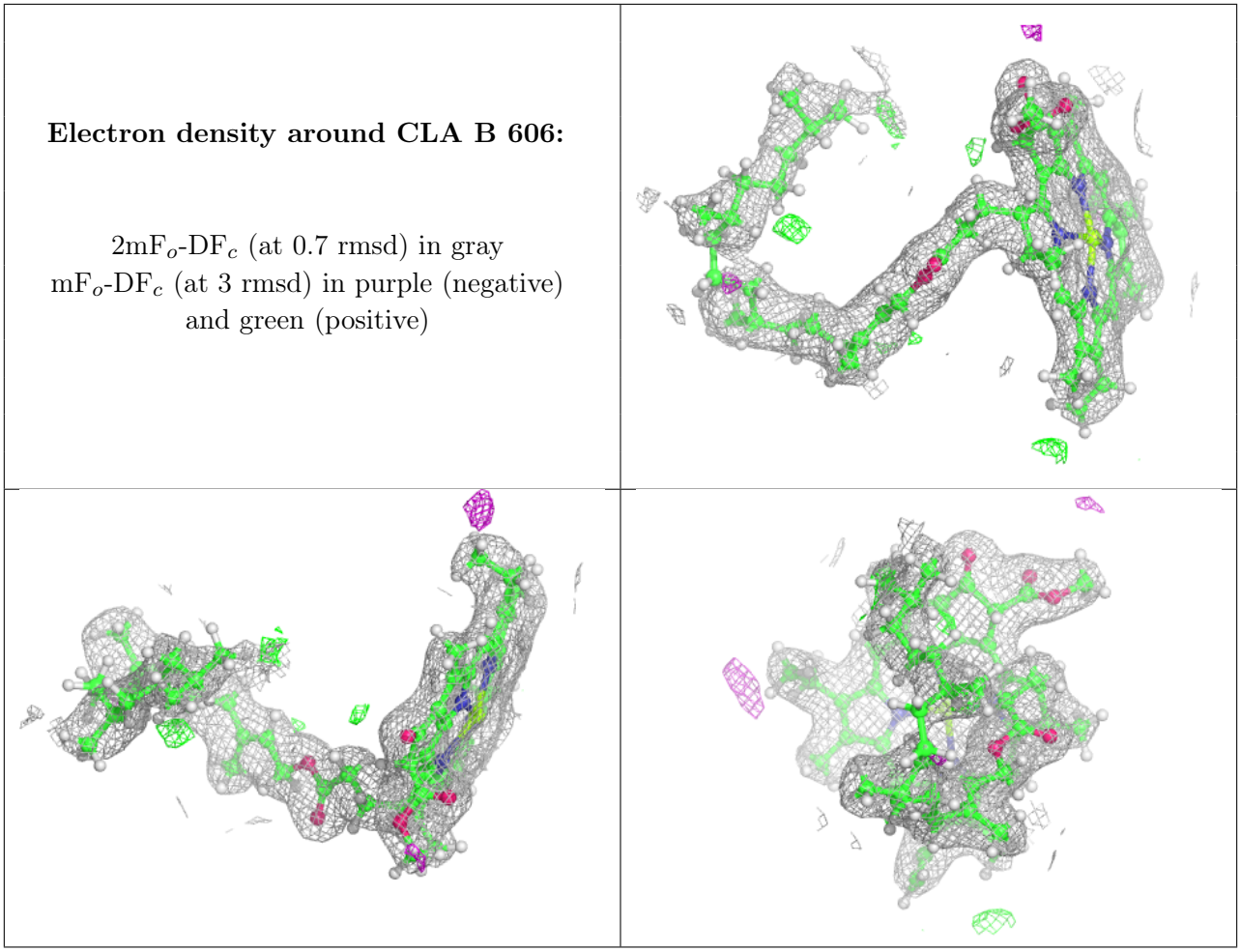
Electron density around CLA c 506:

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



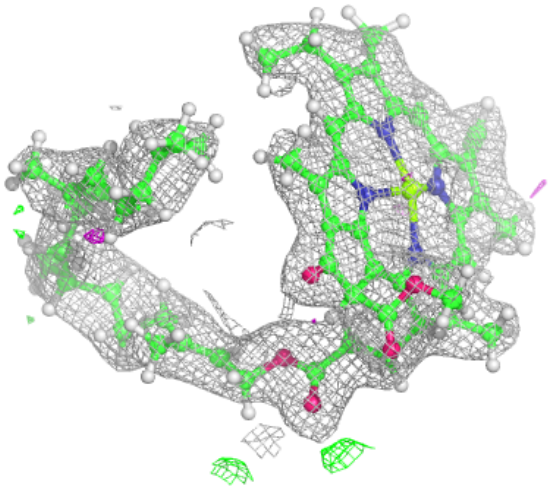
Electron density around CLA B 606:

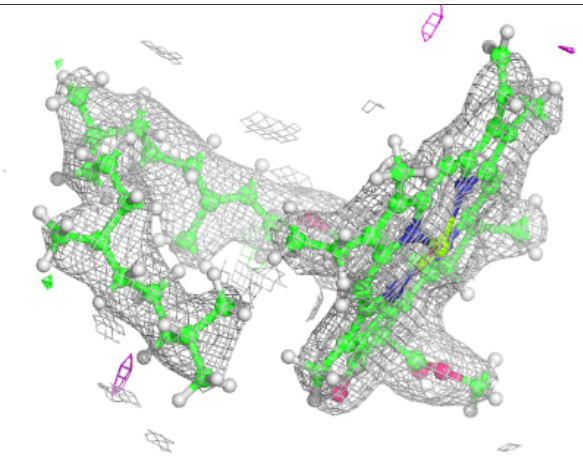
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

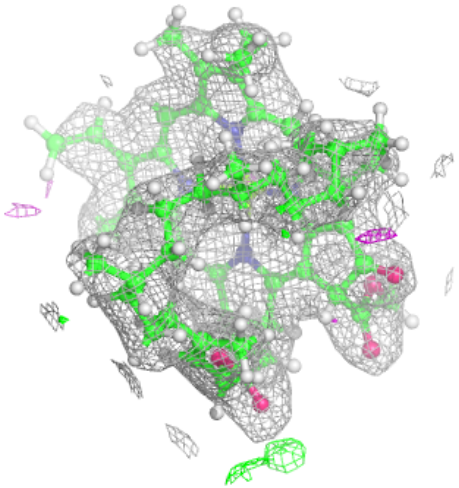


Electron density around CLA C 503:

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

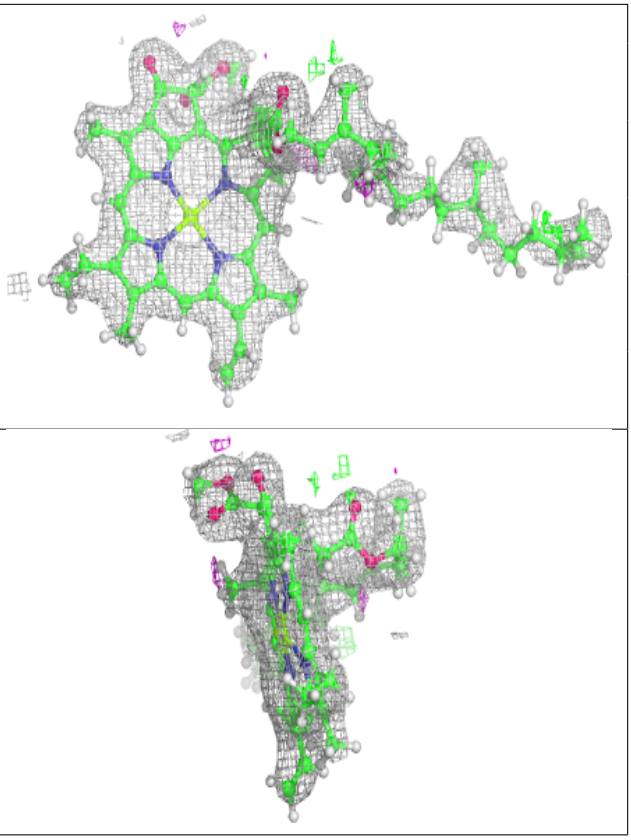






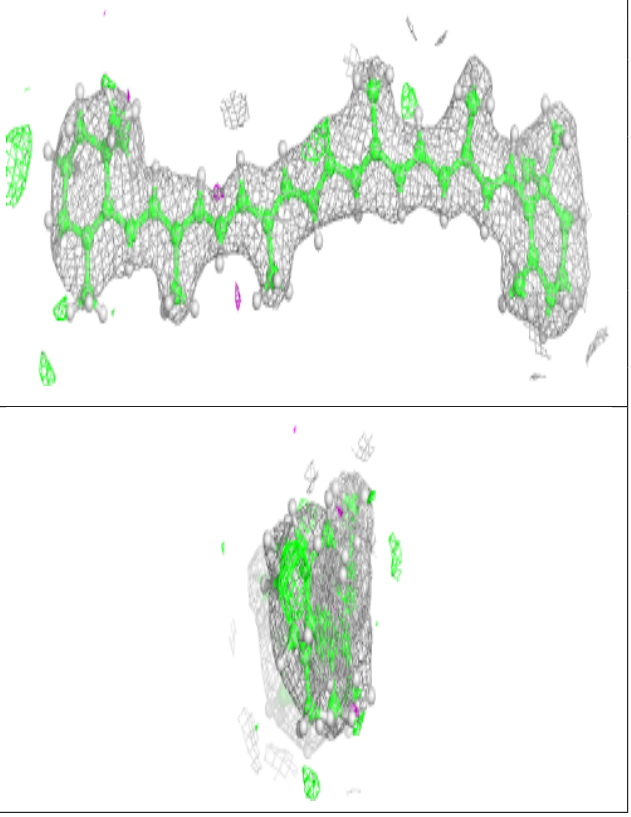
Electron density around CLA a 604:

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



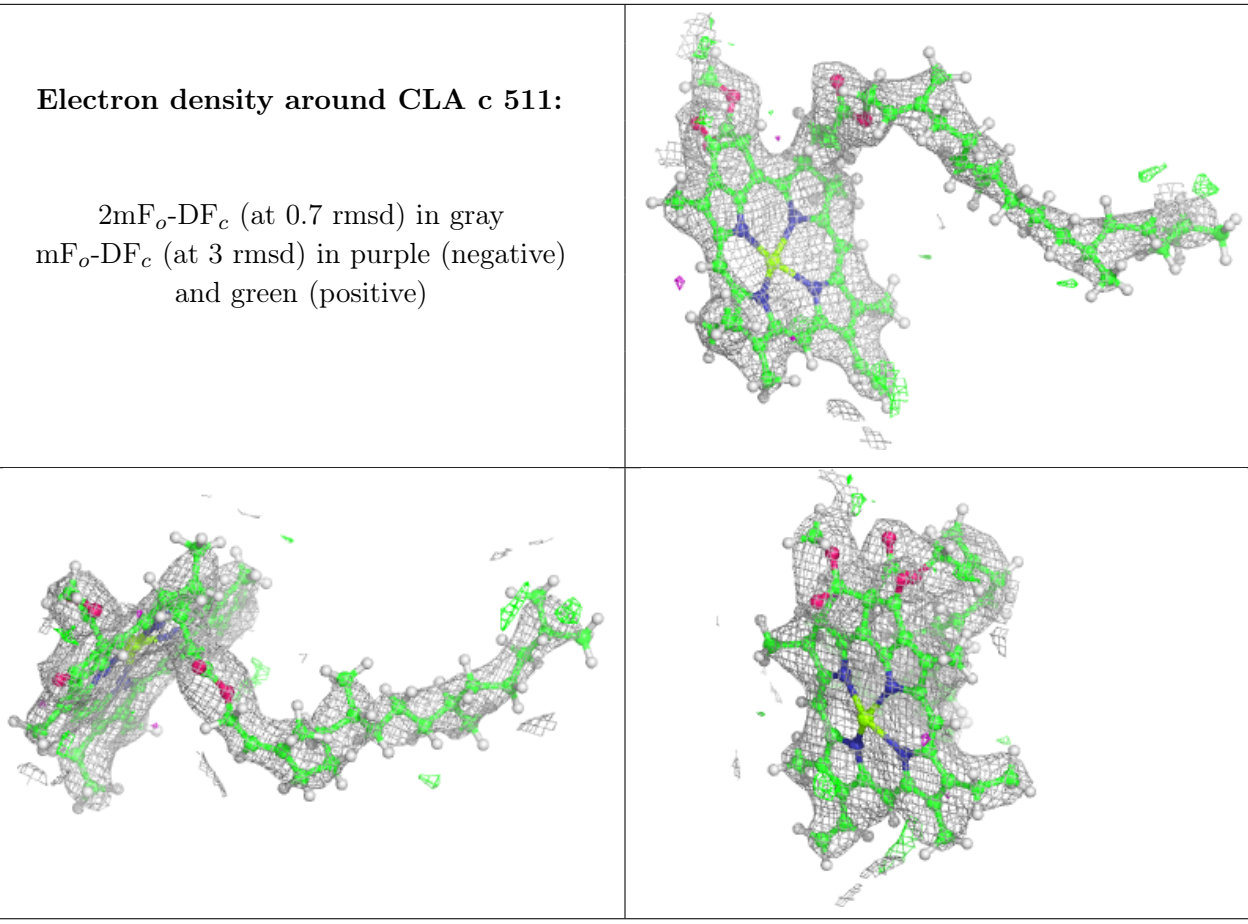
Electron density around BCR t 101:

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



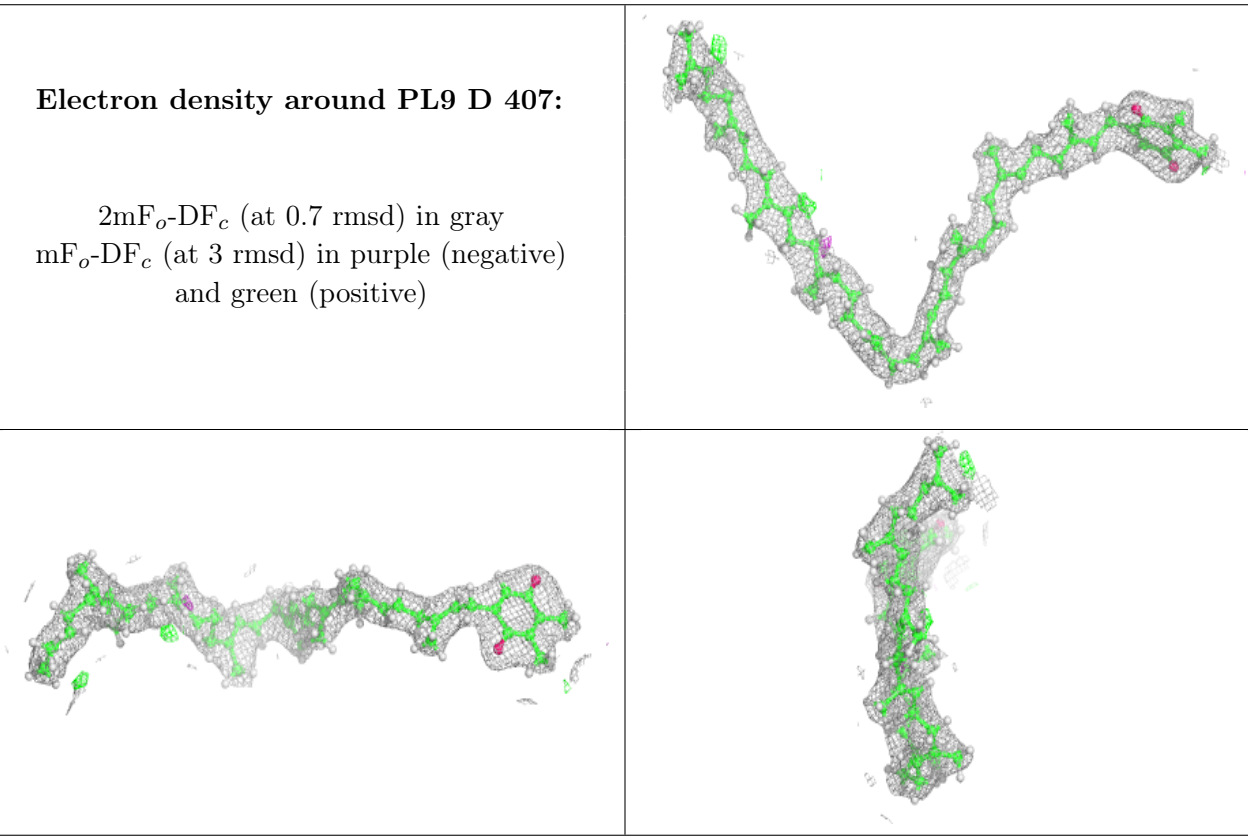
Electron density around CLA c 511:

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



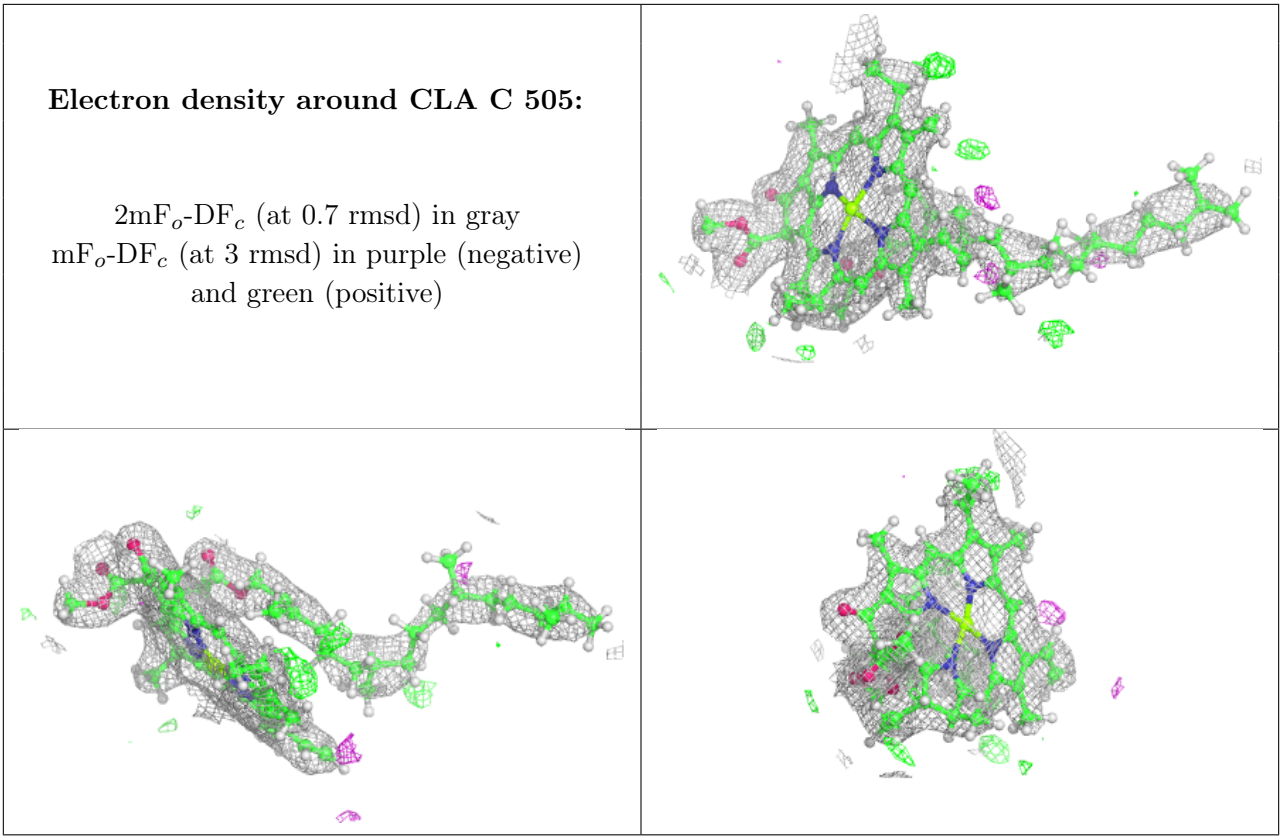
Electron density around PL9 D 407:

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



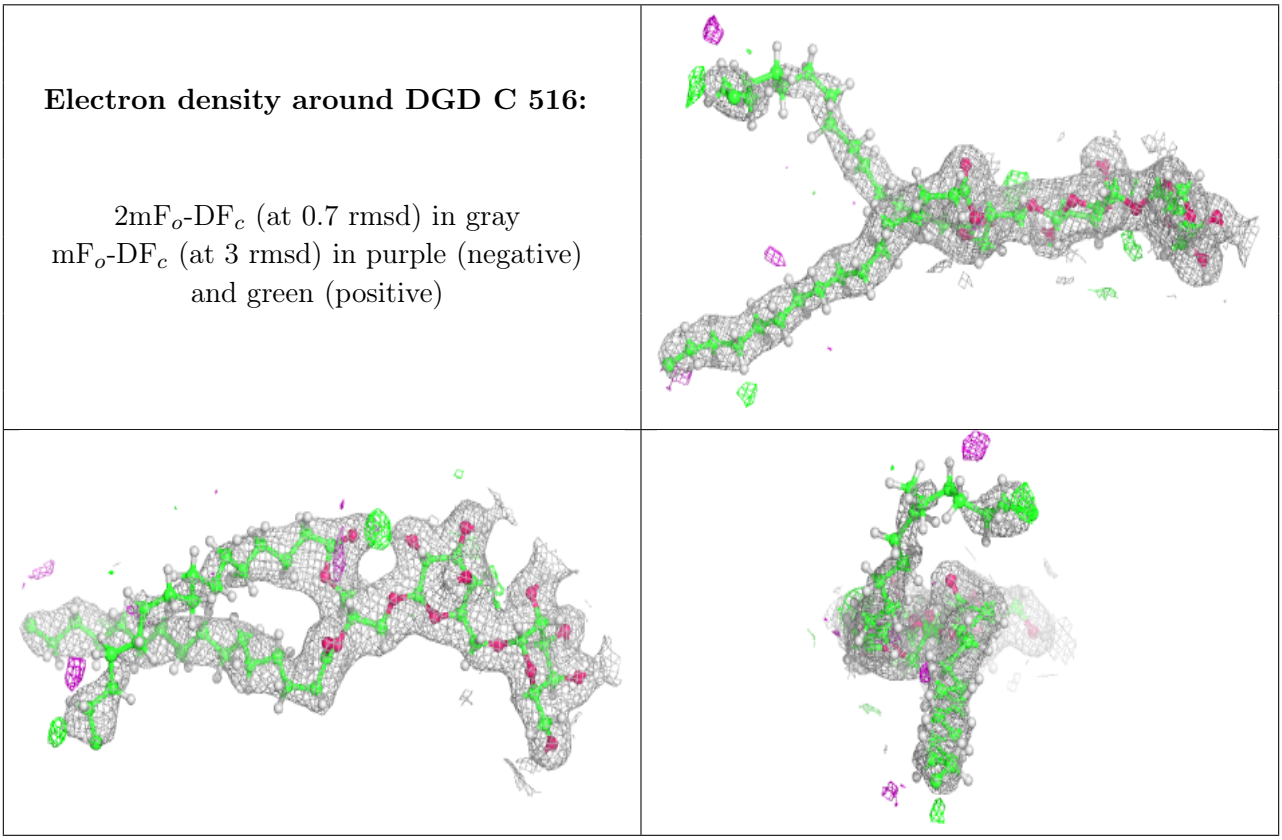
Electron density around CLA C 505:

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



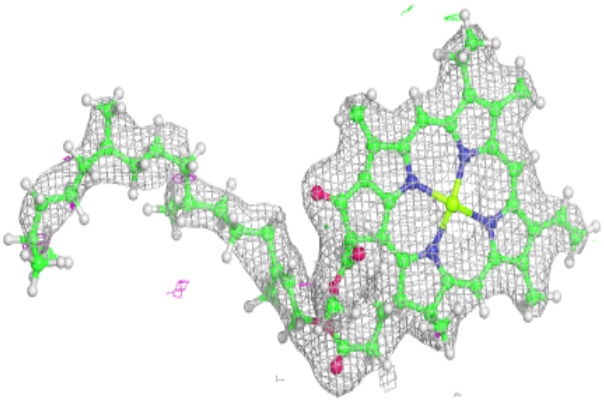
Electron density around DGD C 516:

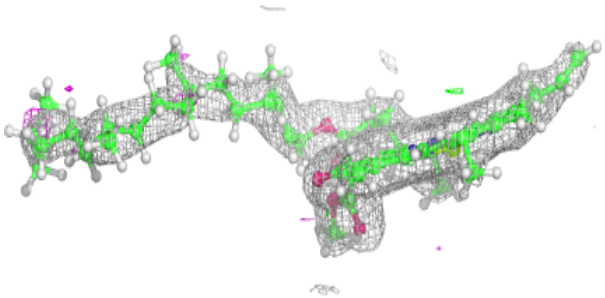
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

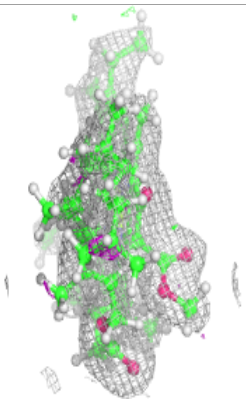


Electron density around CLA b 602:

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

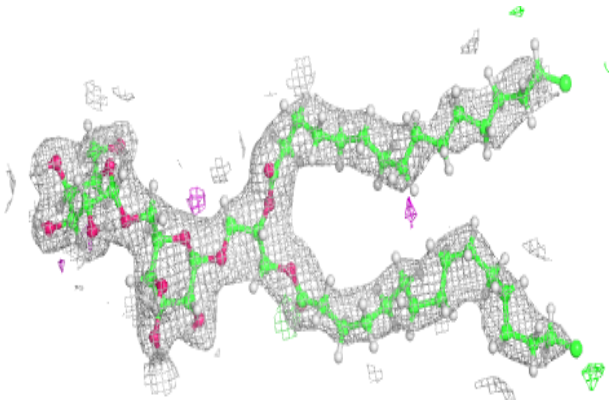


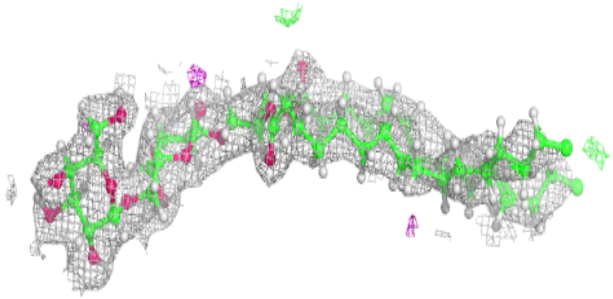


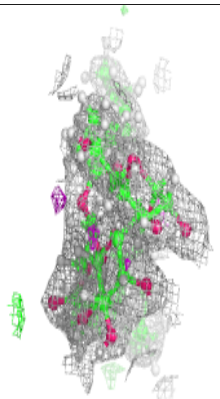


Electron density around DGD C 518:

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

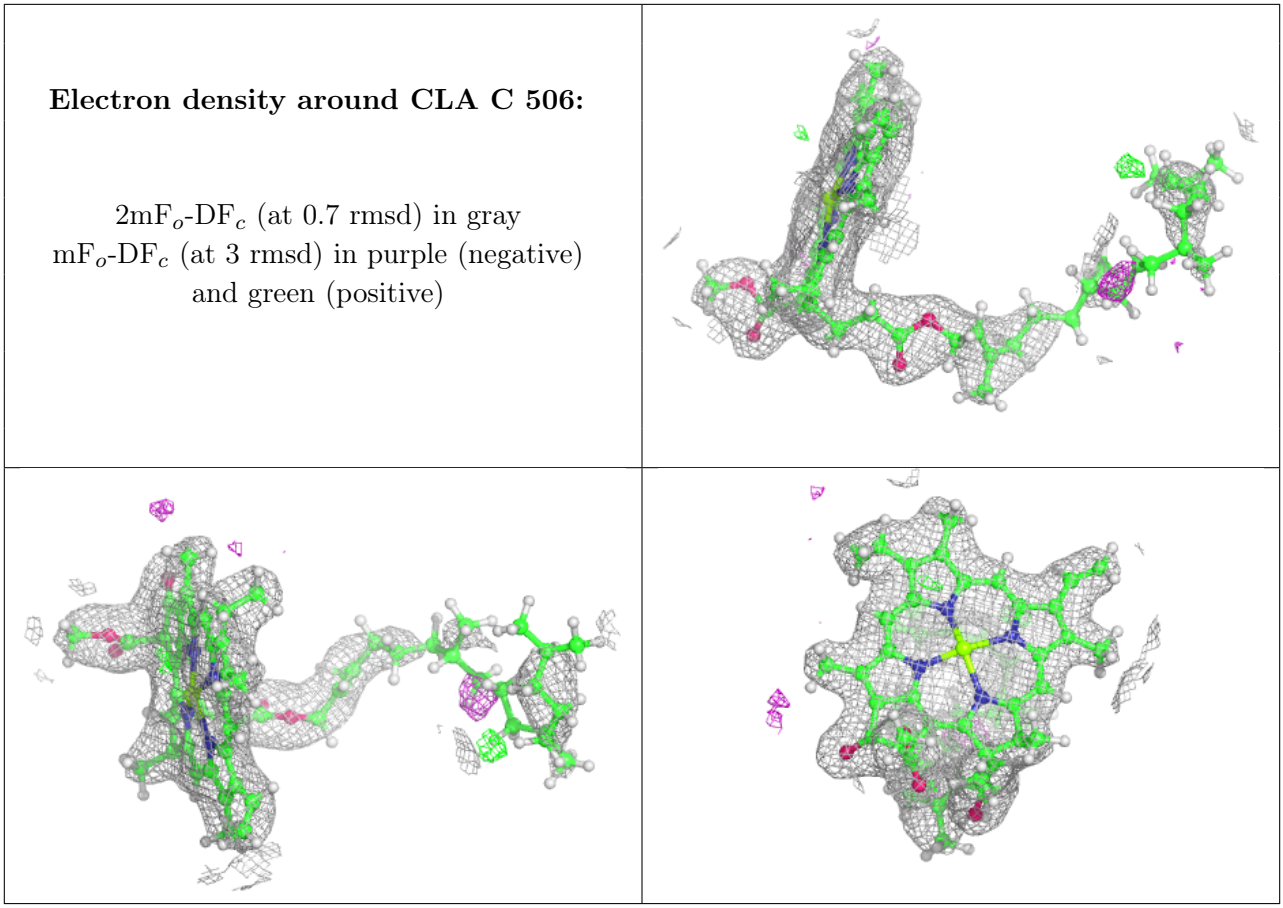






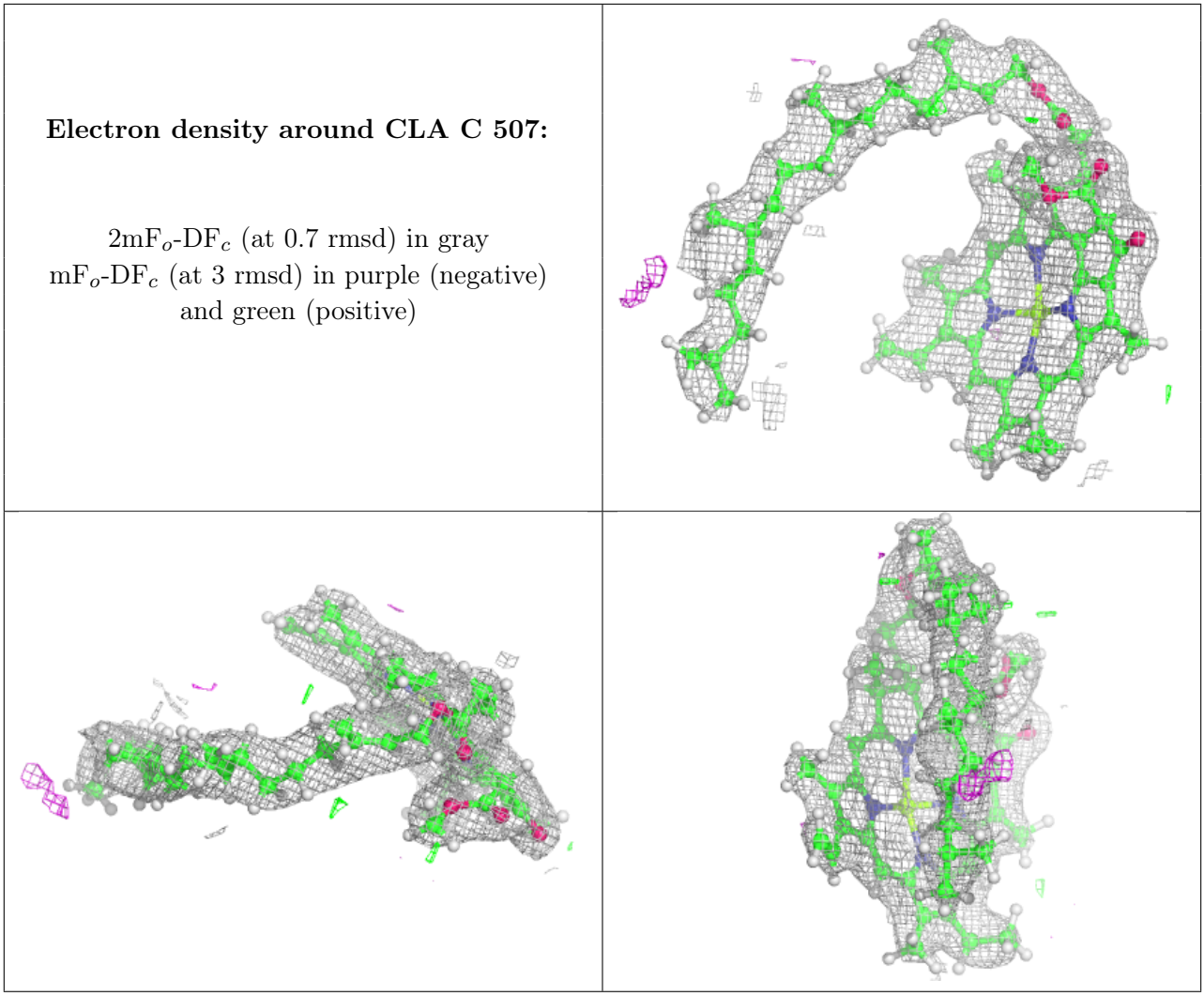
Electron density around CLA C 506:

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



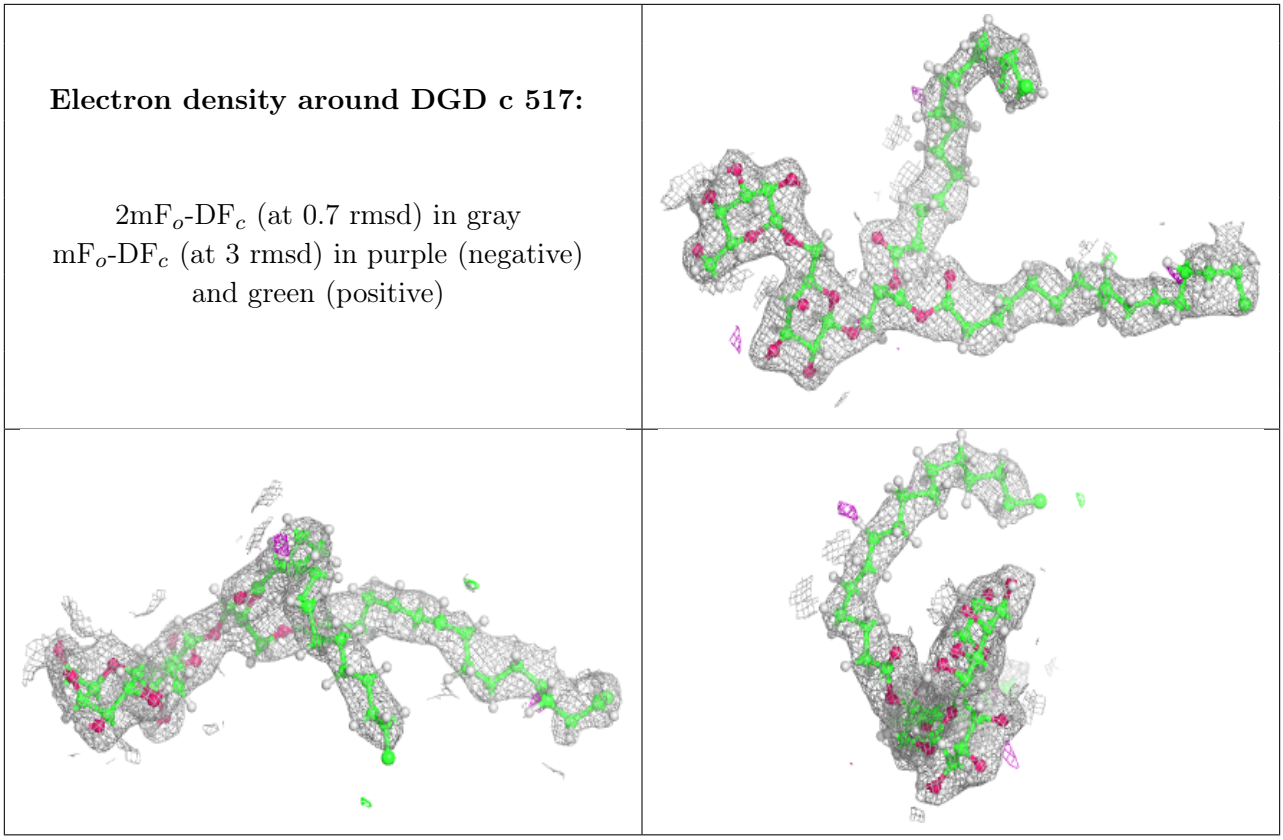
Electron density around CLA C 507:

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



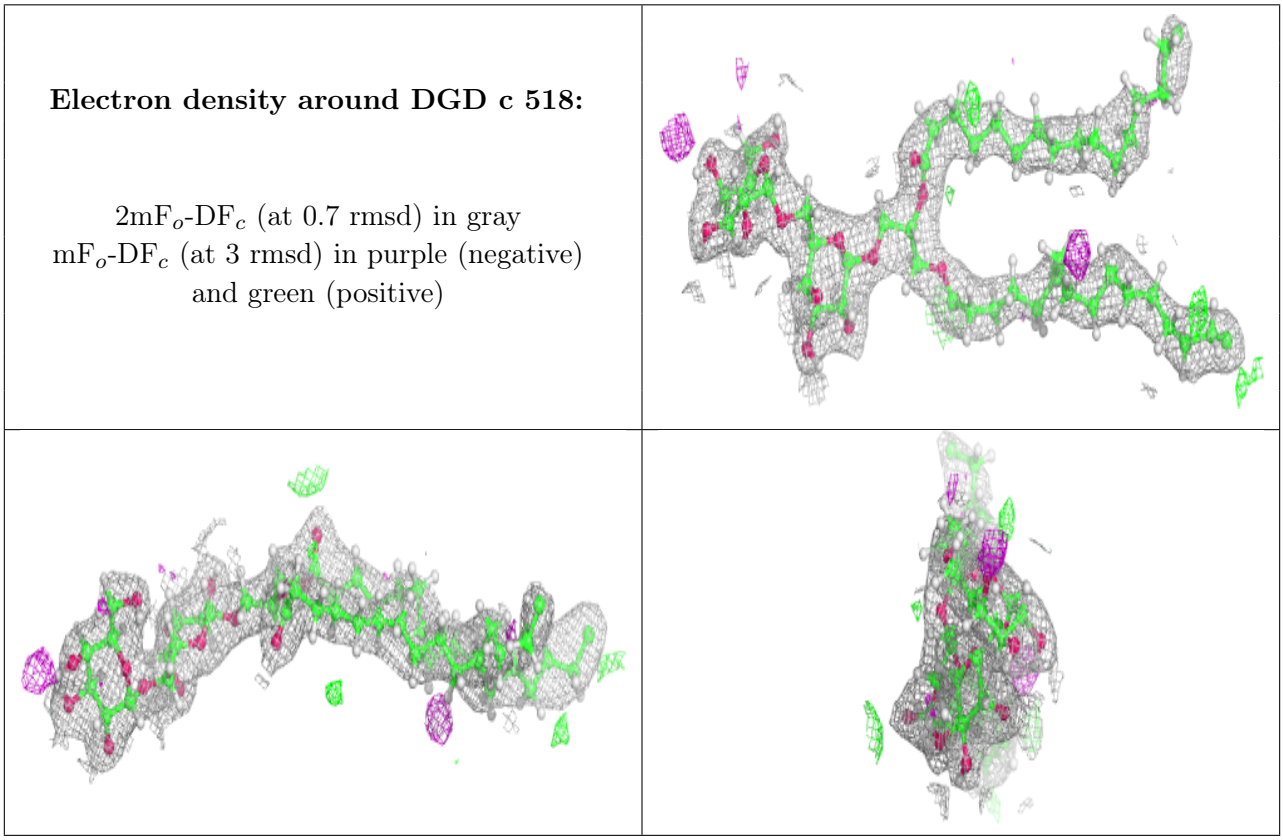
Electron density around DGD c 517:

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



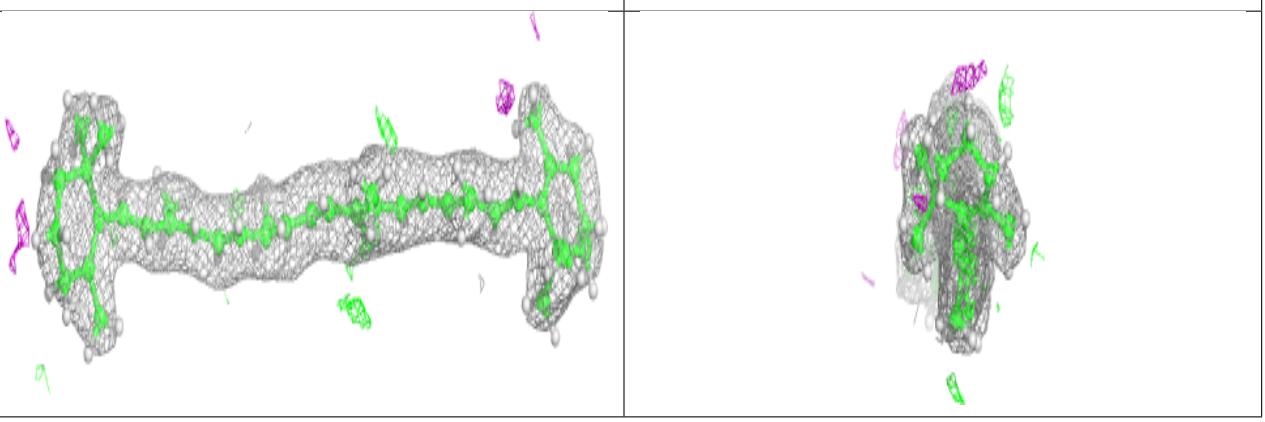
Electron density around DGD c 518:

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



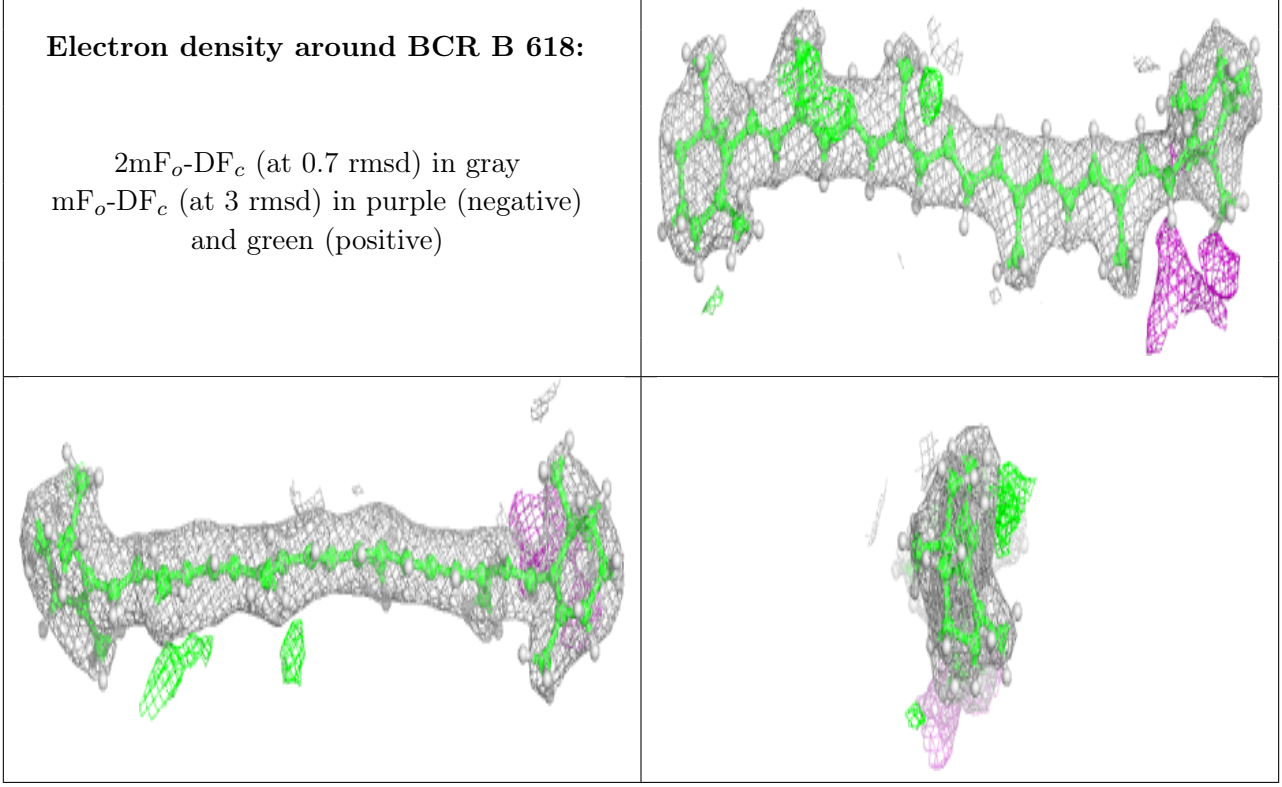
Electron density around BCR A 608:

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



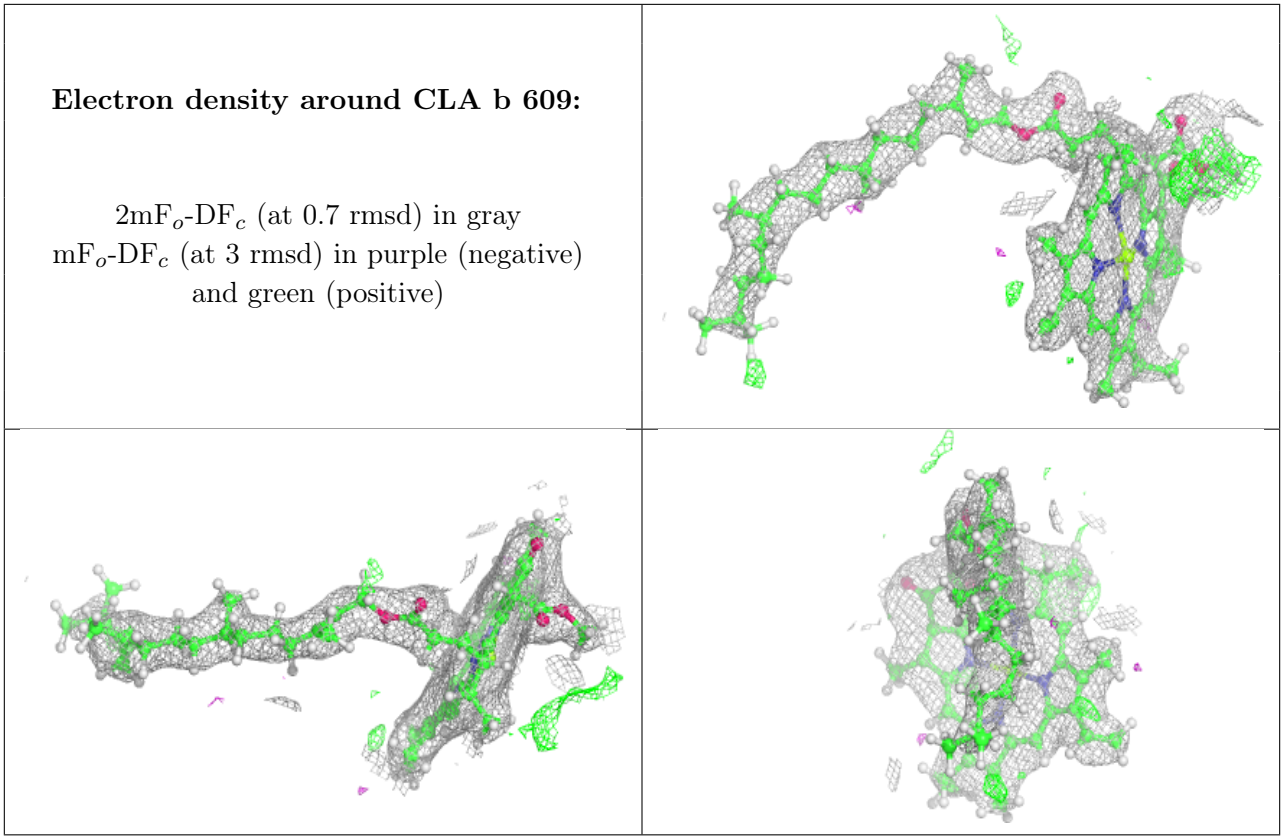
Electron density around BCR B 618:

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



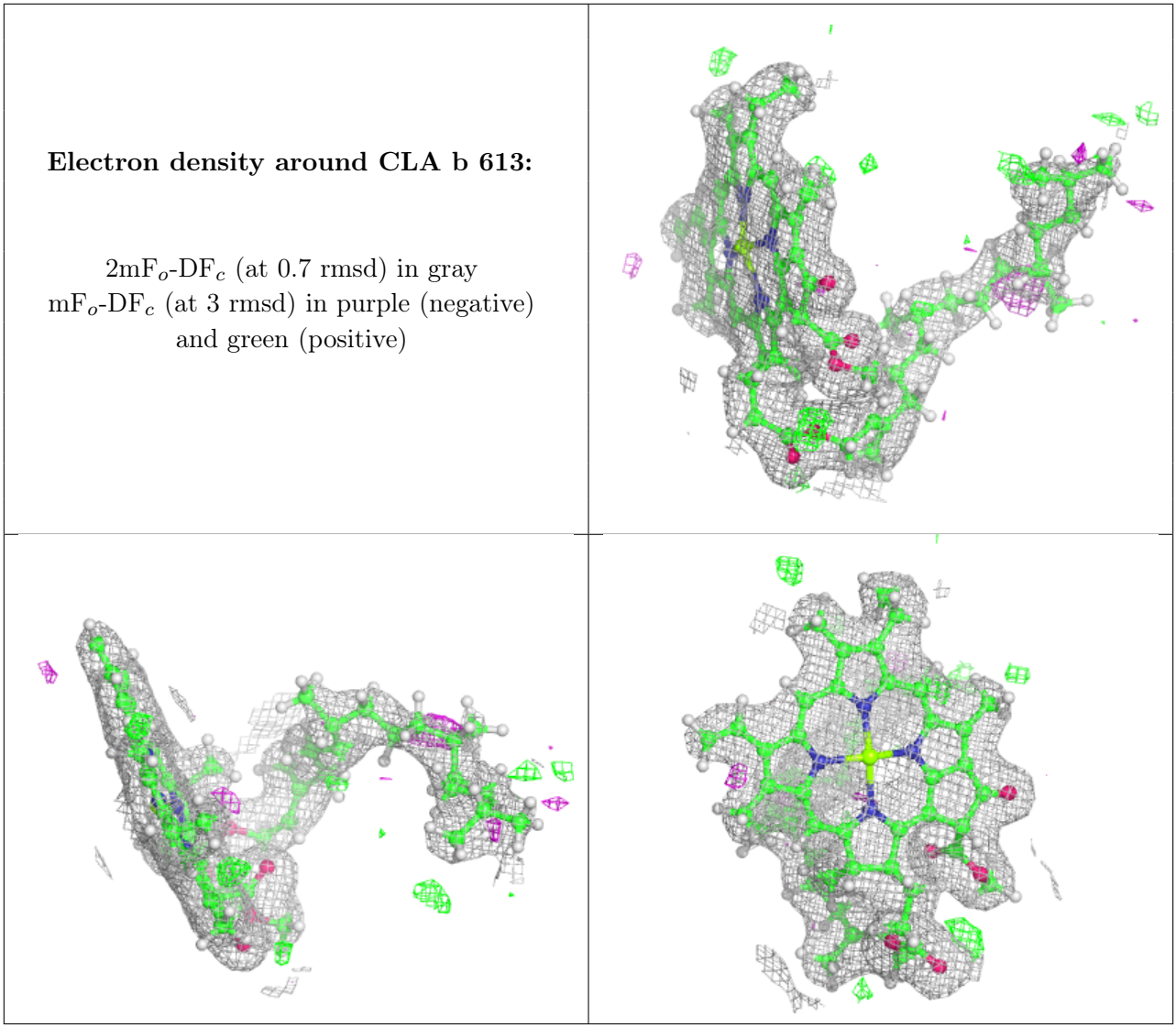
Electron density around CLA b 609:

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



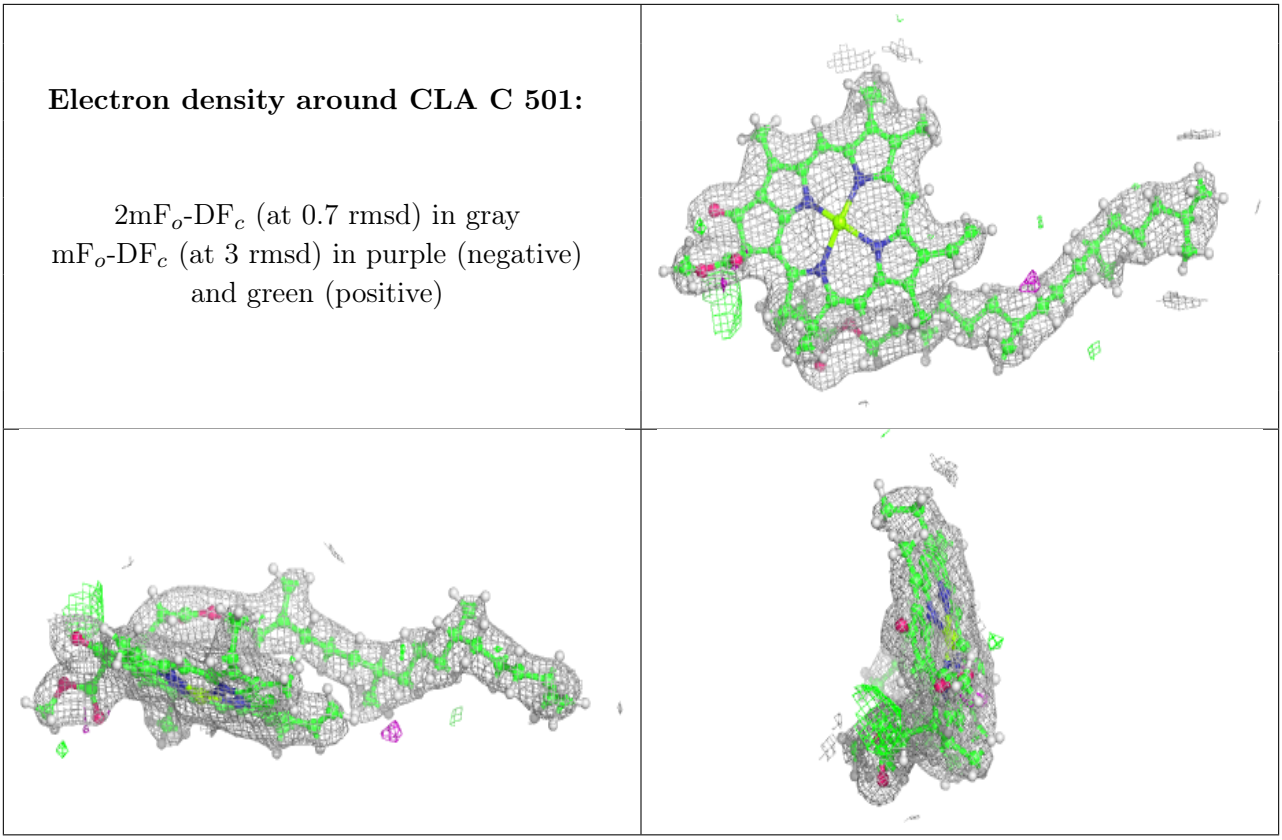
Electron density around CLA b 613:

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



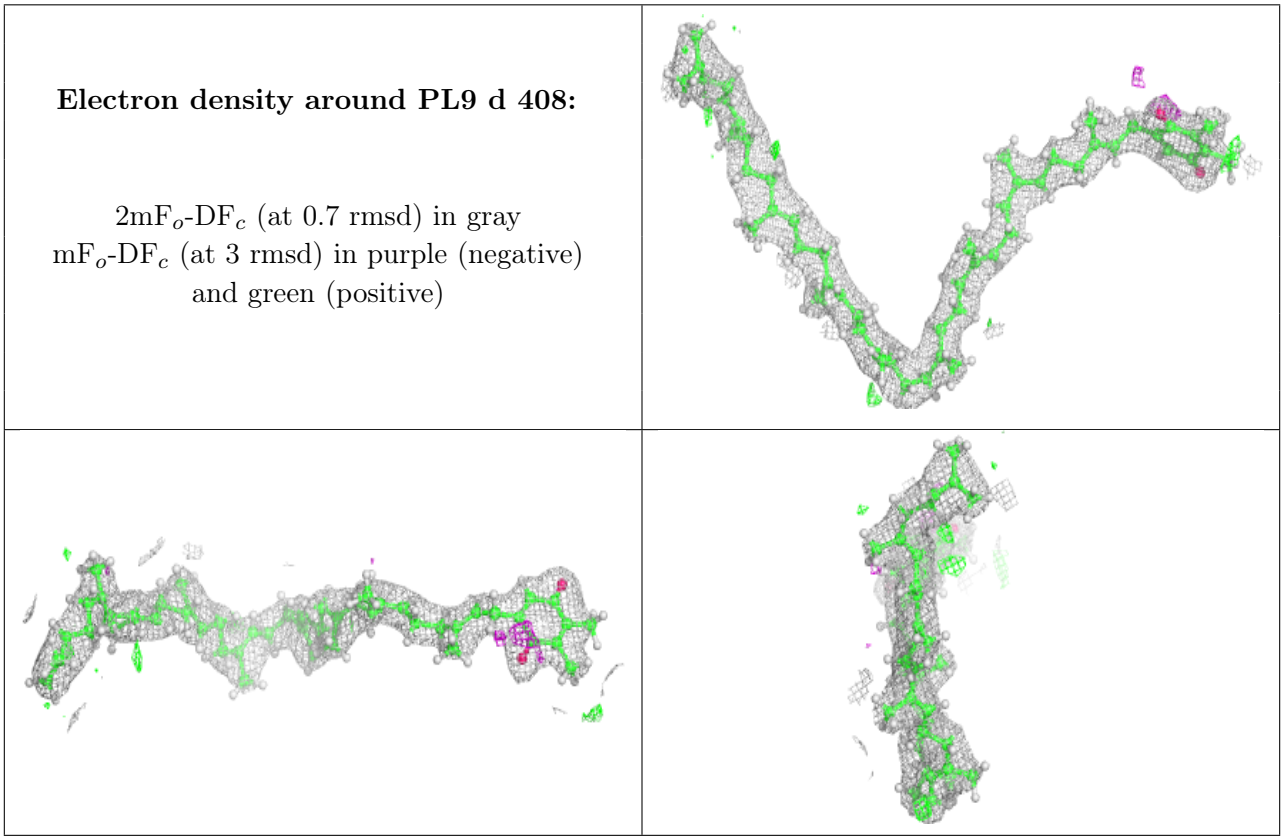
Electron density around CLA C 501:

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



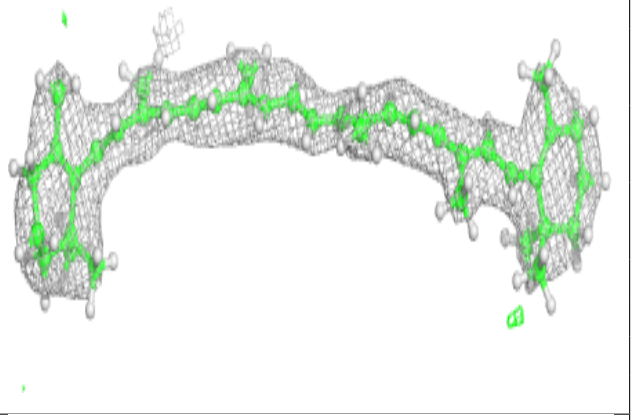
Electron density around PL9 d 408:

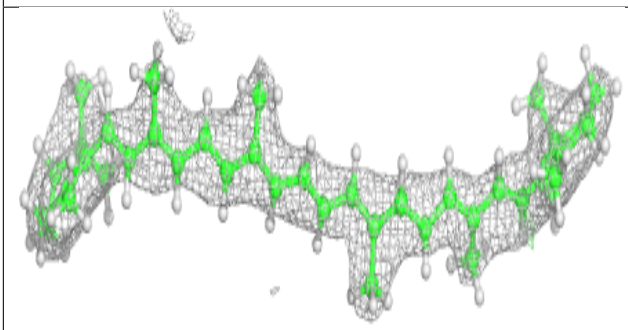
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

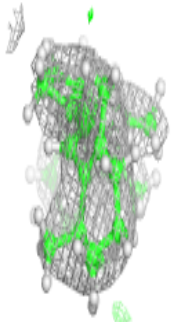


Electron density around BCR C 520:

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

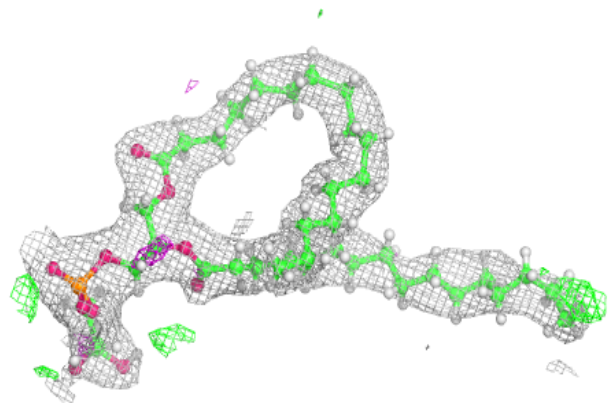


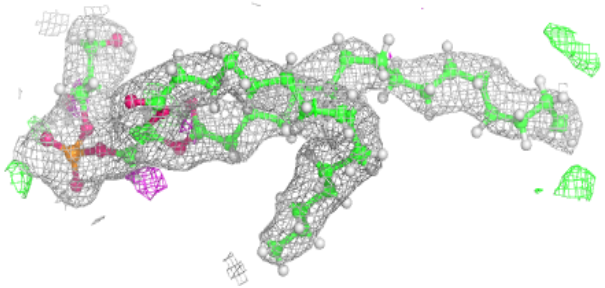




Electron density around LHG B 623:

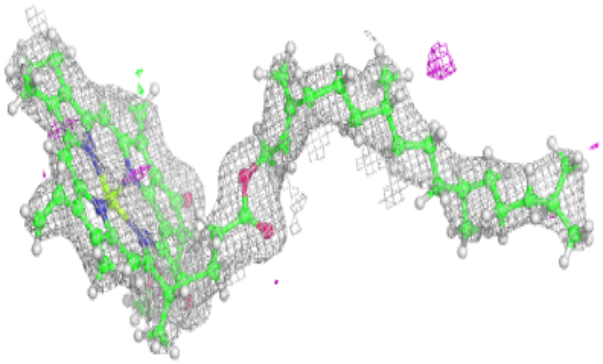
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

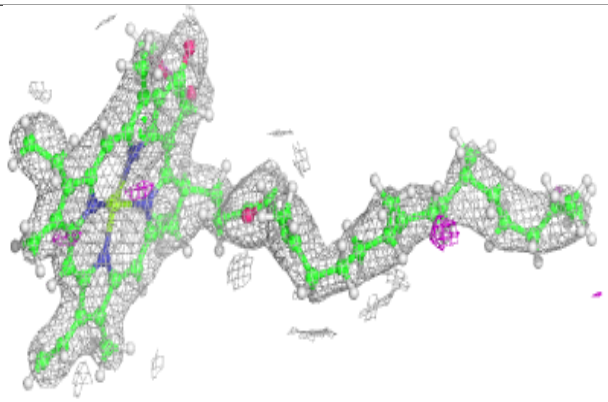


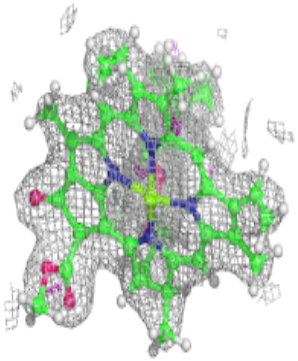


Electron density around CLA C 502:

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

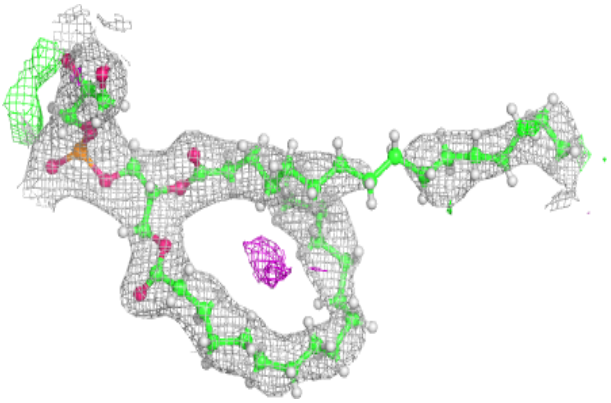


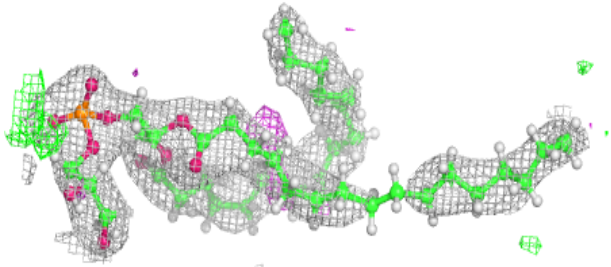


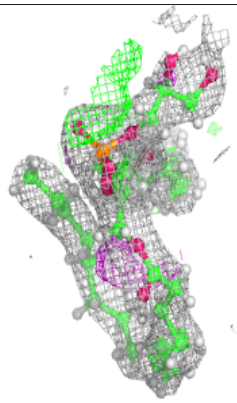


Electron density around LHG d 405:

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

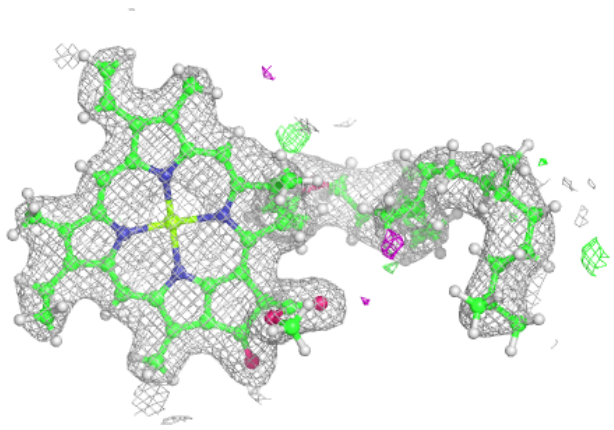


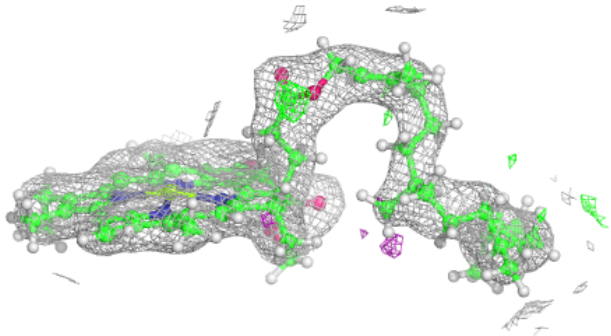


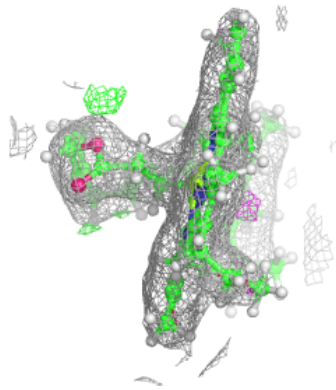


Electron density around CLA b 612:

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

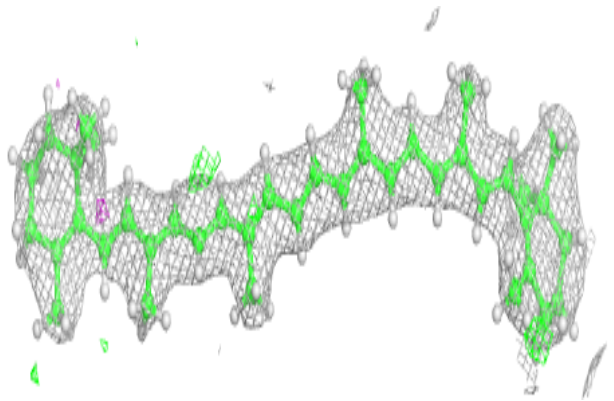


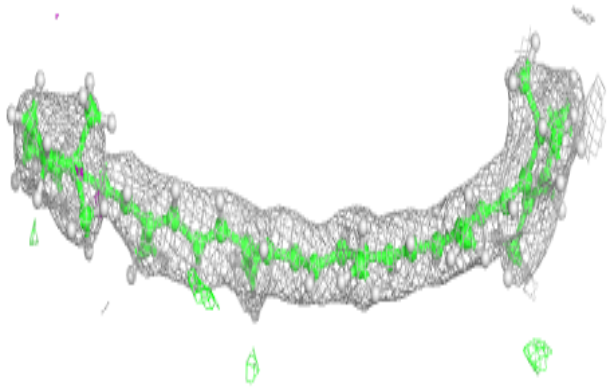


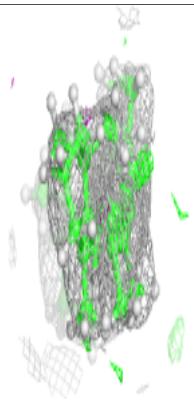


Electron density around BCR T 101:

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

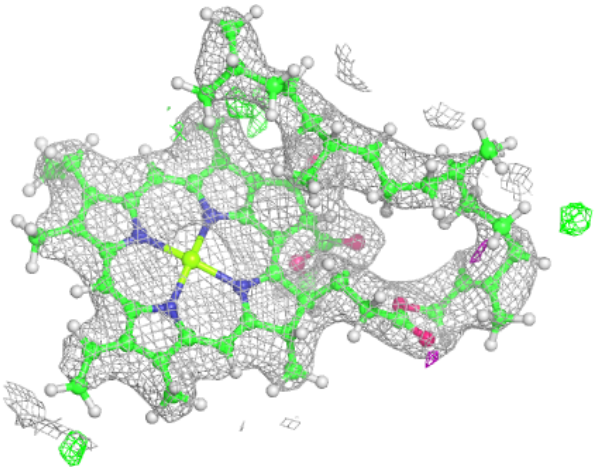


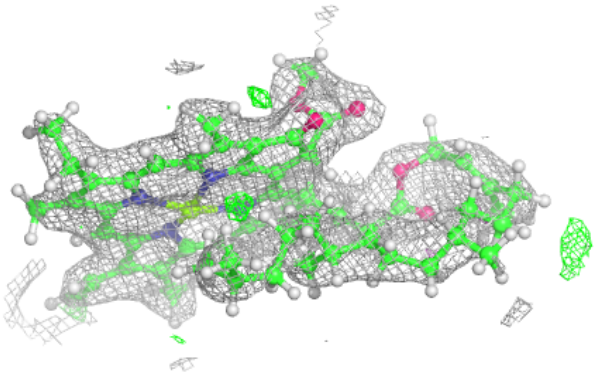


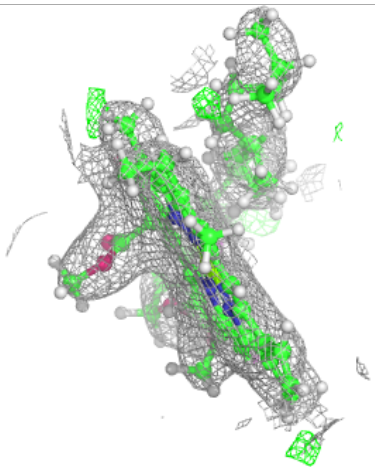


Electron density around CLA c 509:

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

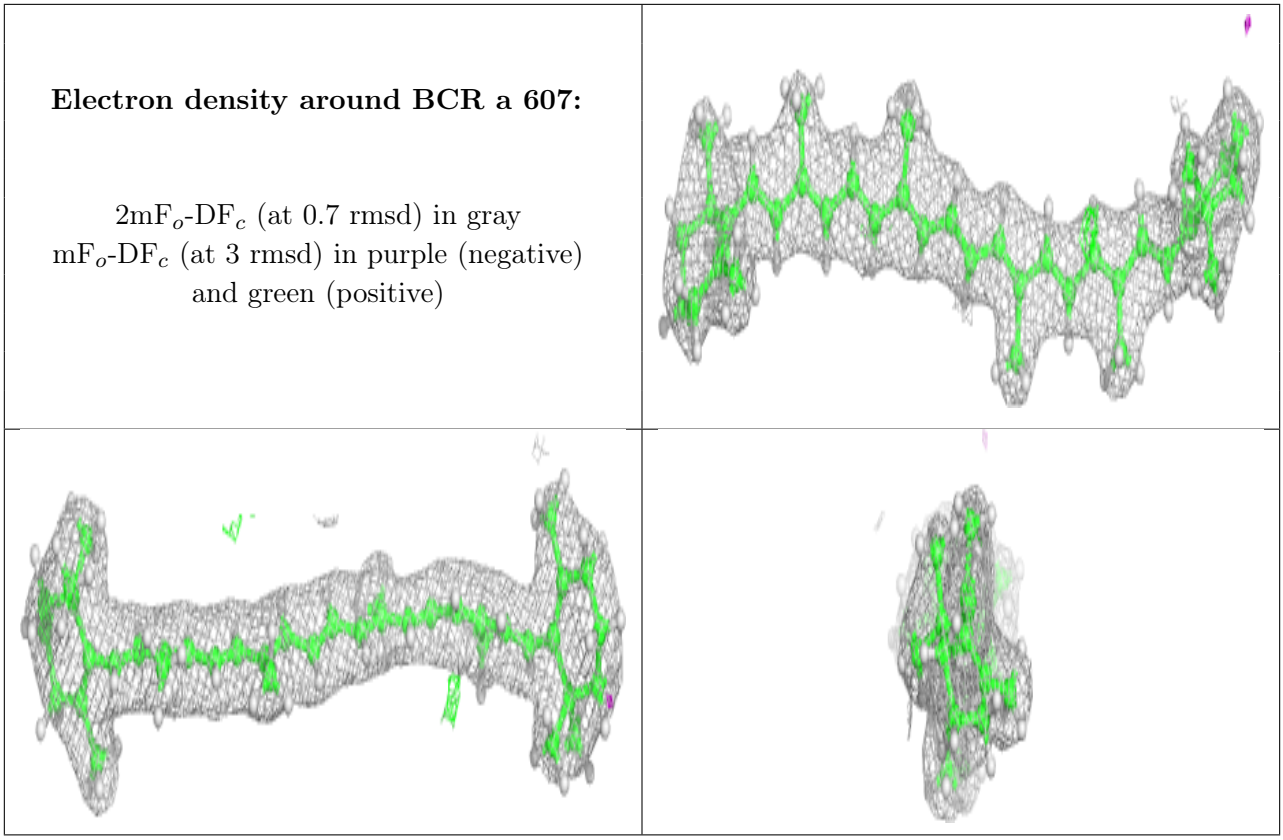






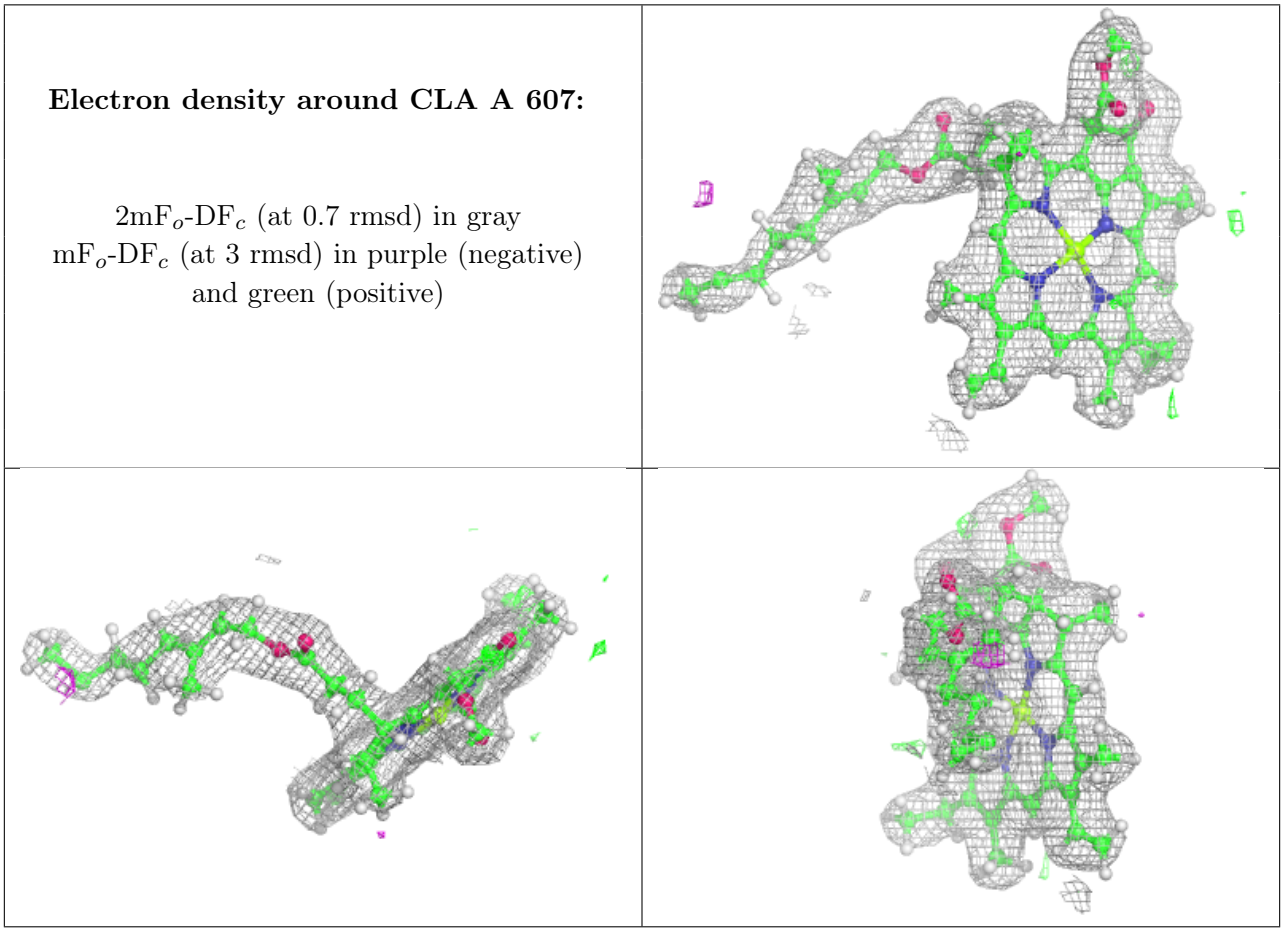
Electron density around BCR a 607:

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



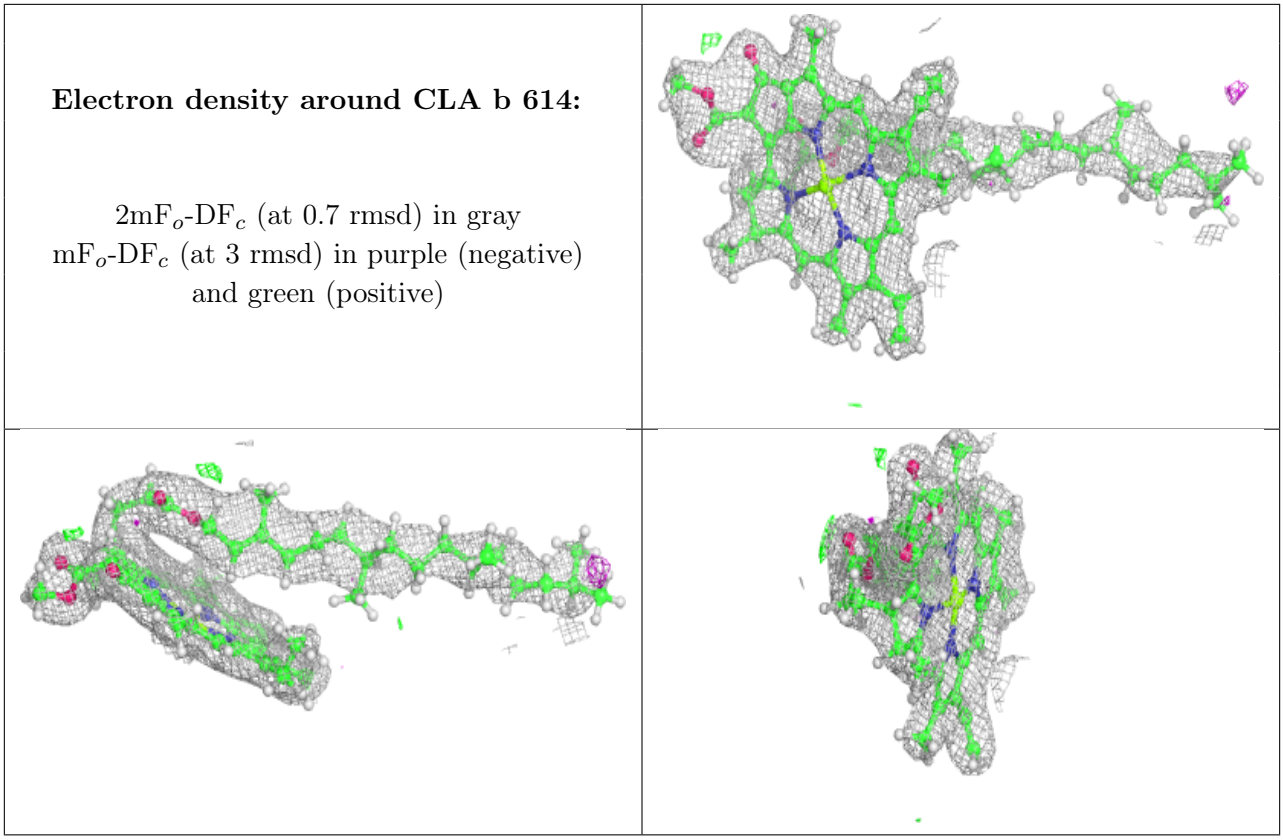
Electron density around CLA A 607:

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



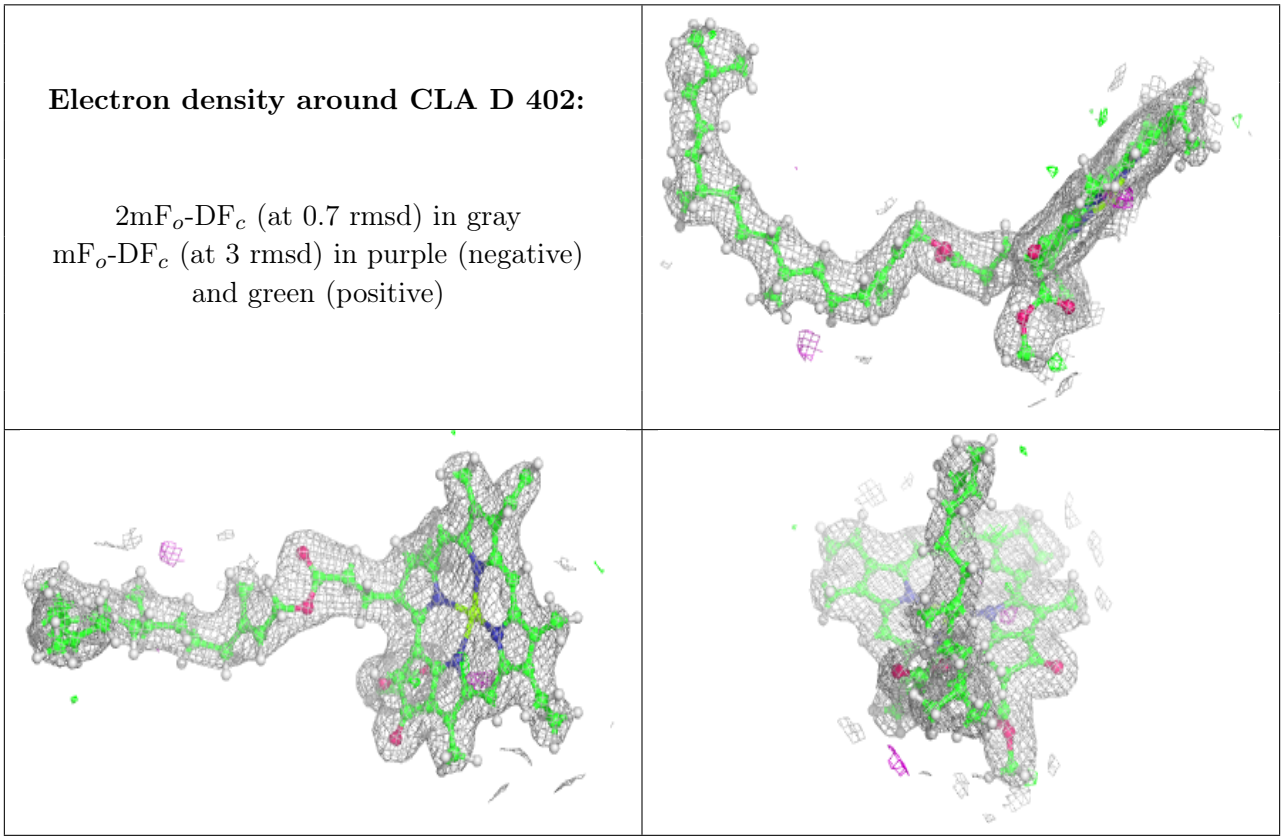
Electron density around CLA b 614:

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



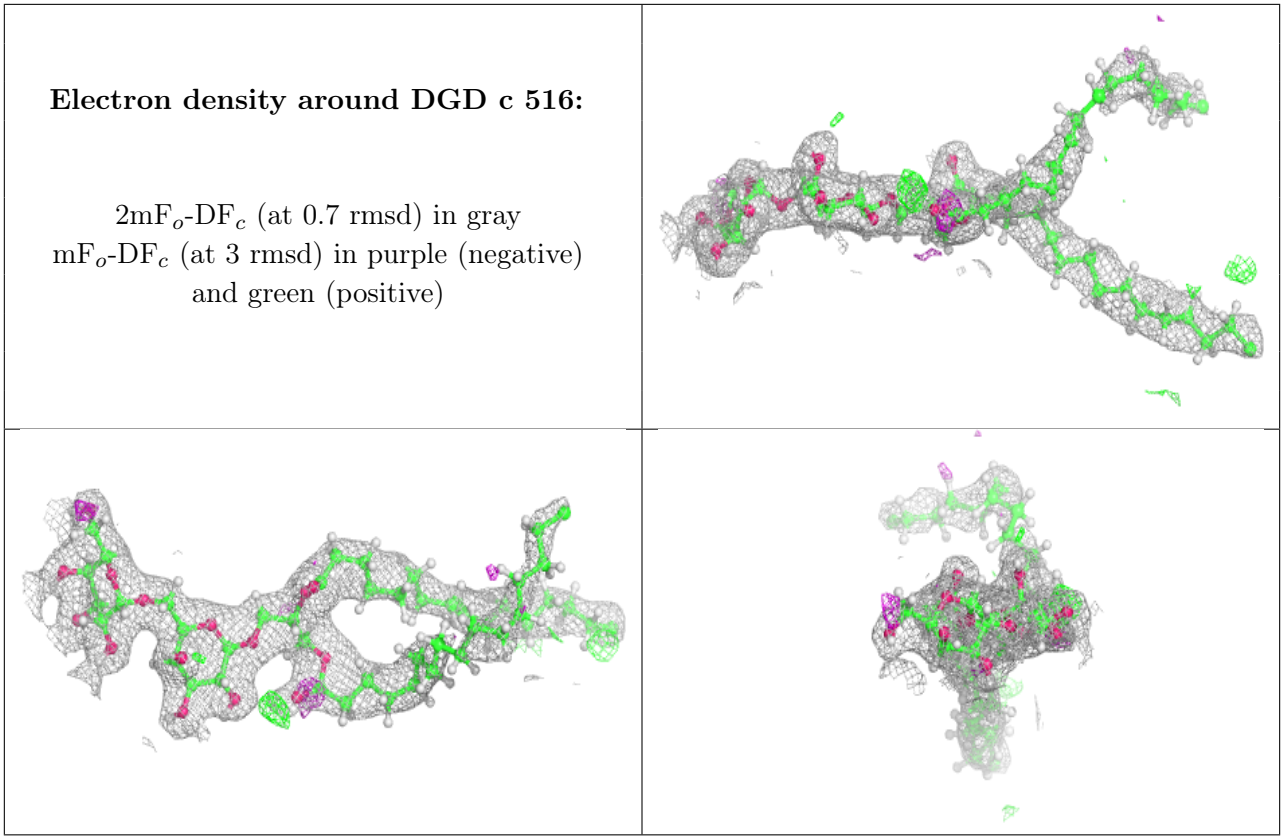
Electron density around CLA D 402:

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



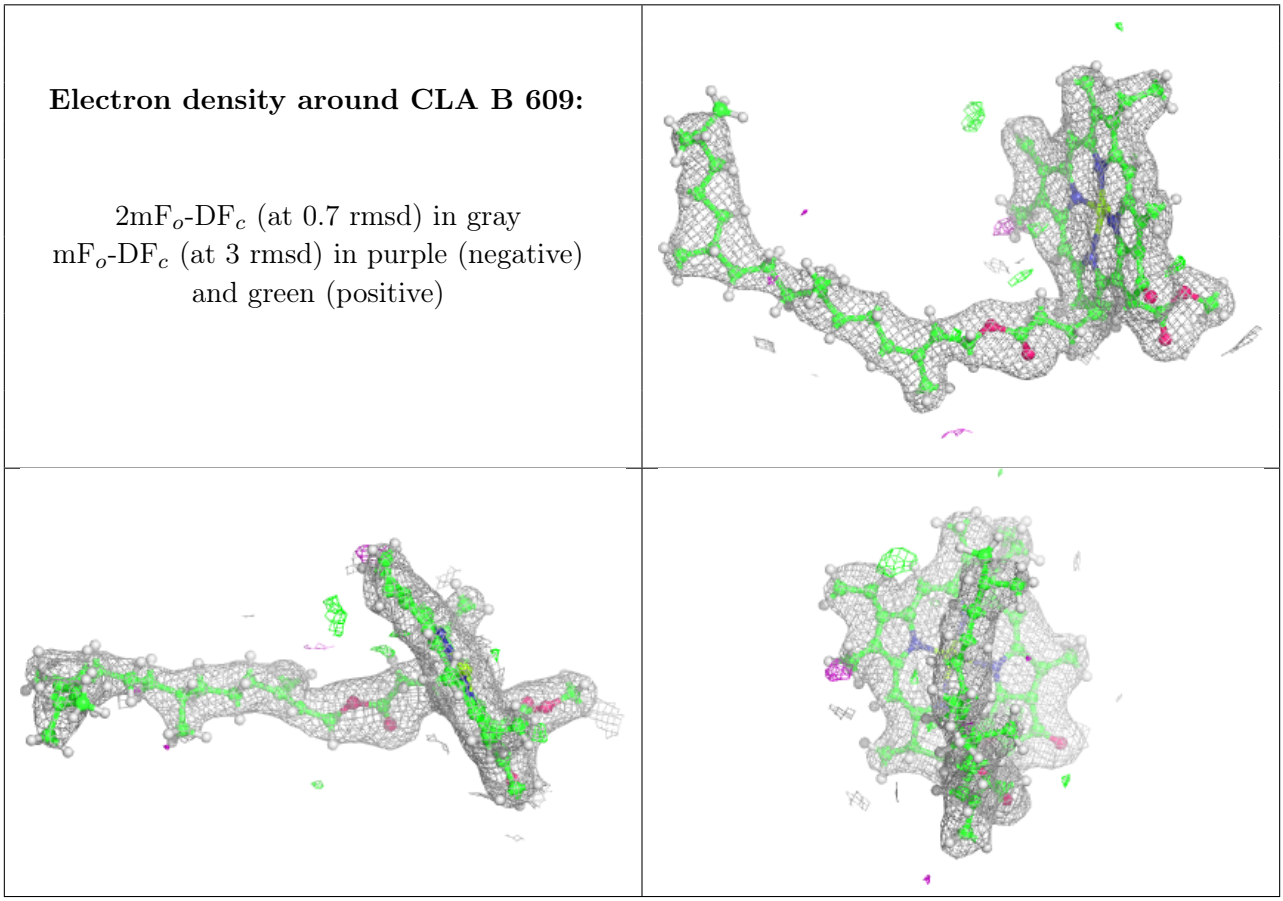
Electron density around DGD c 516:

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



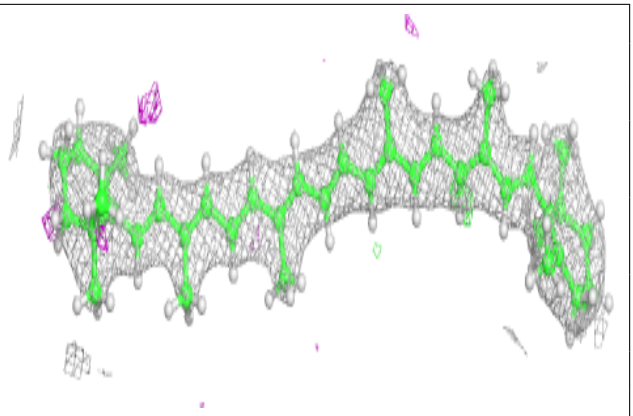
Electron density around CLA B 609:

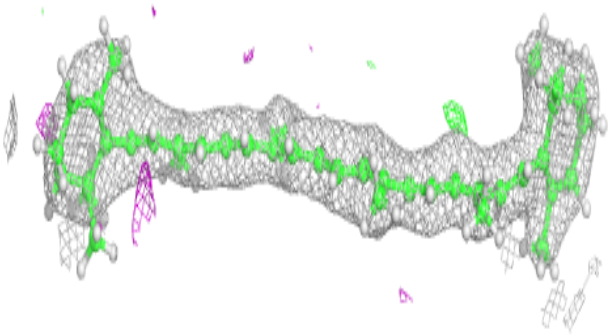
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

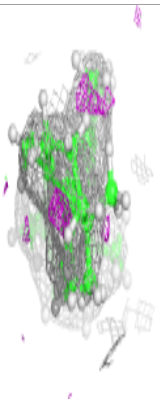


Electron density around BCR c 515:

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

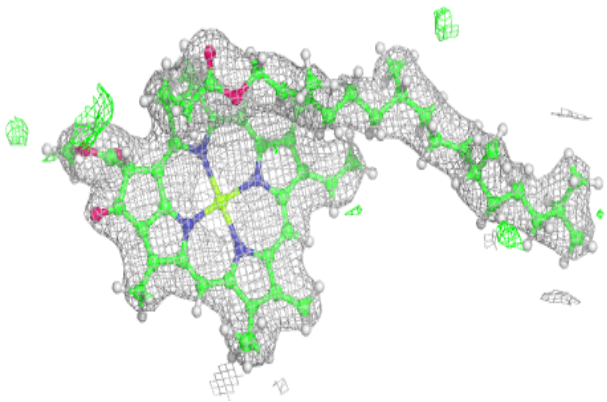


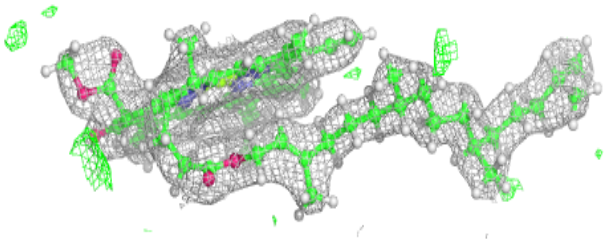


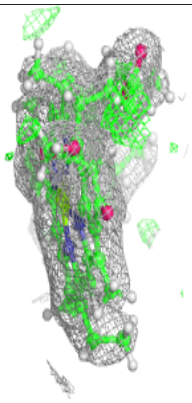


Electron density around CLA c 501:

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

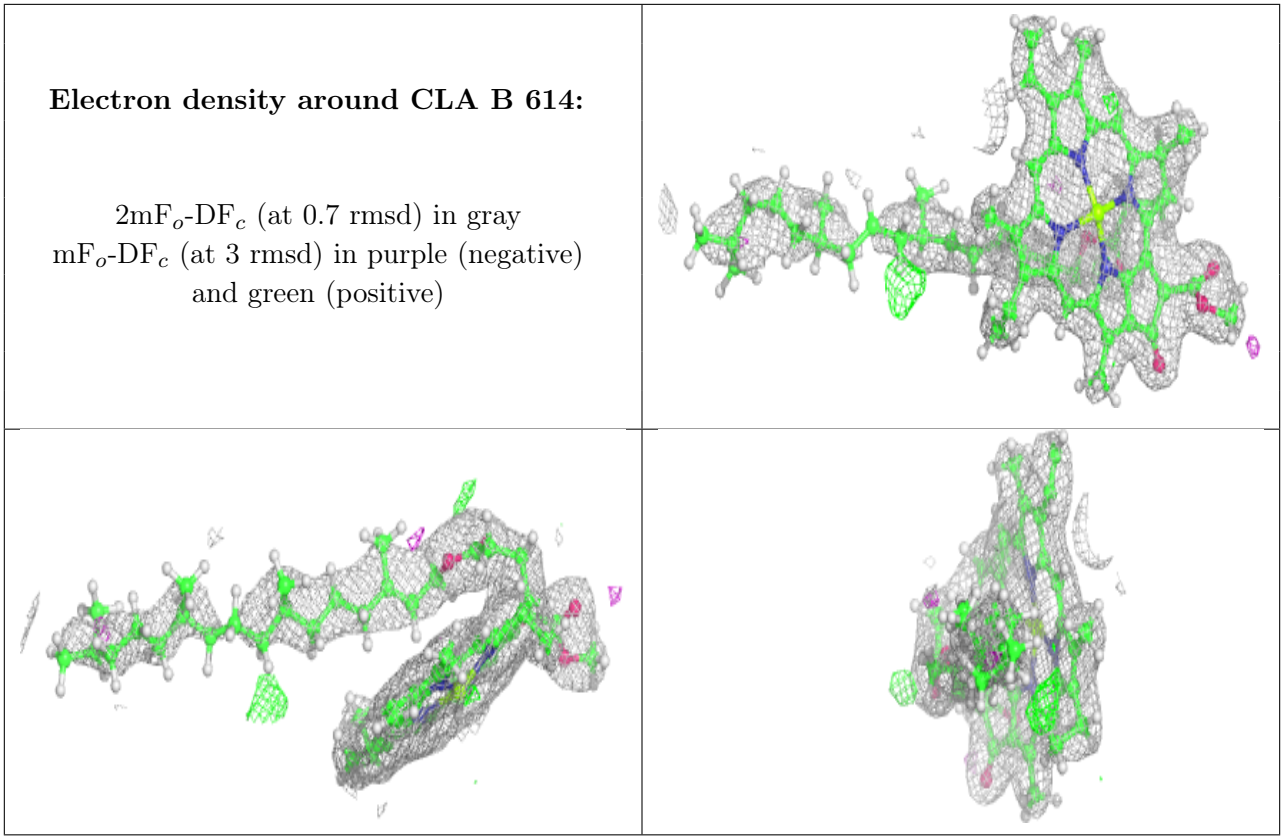






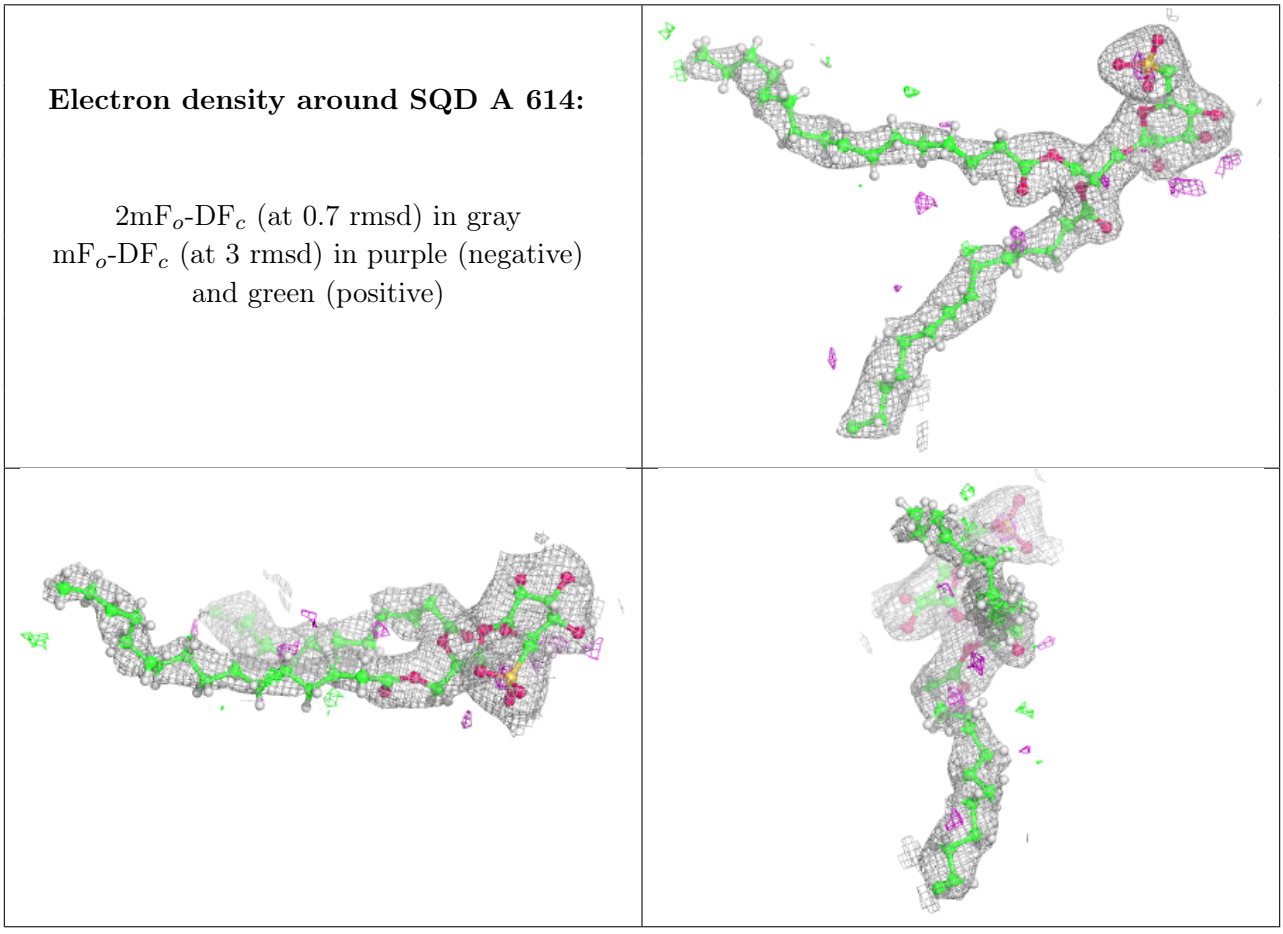
Electron density around CLA B 614:

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



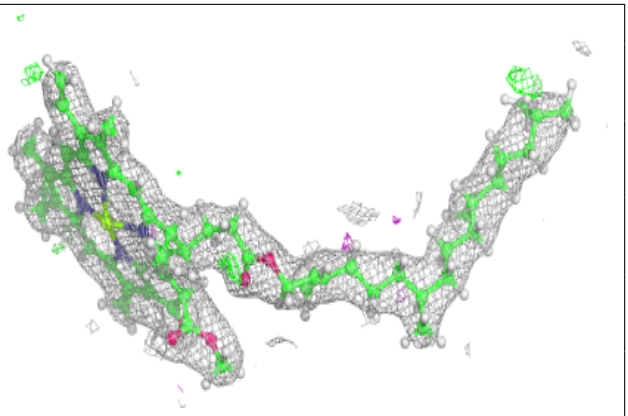
Electron density around SQD A 614:

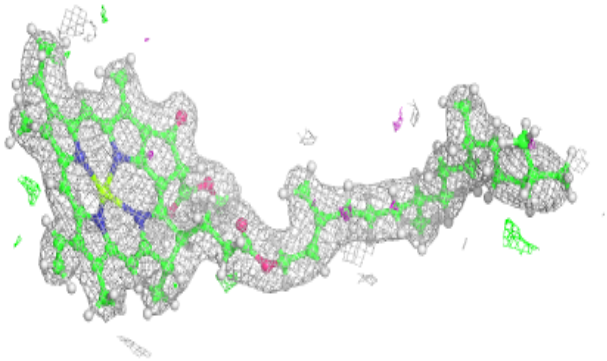
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

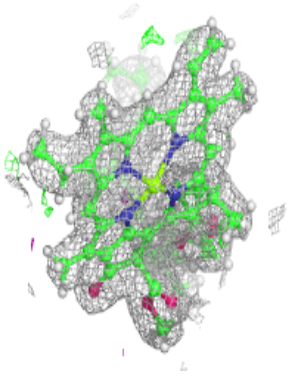


Electron density around CLA A 603:

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

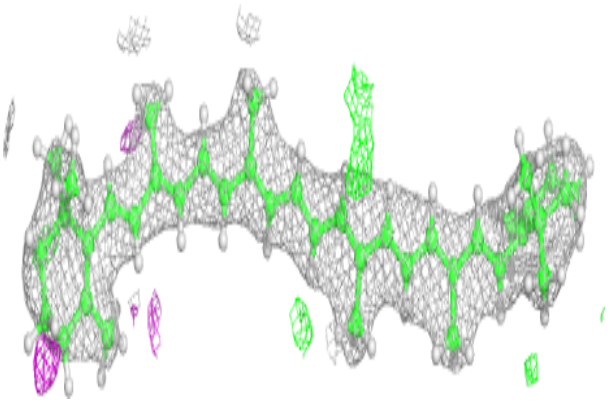


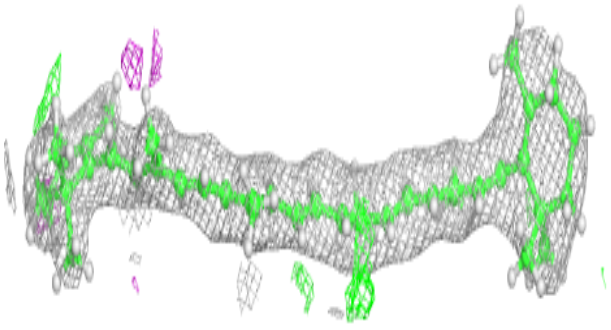


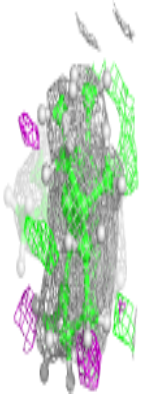


Electron density around BCR B 617:

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

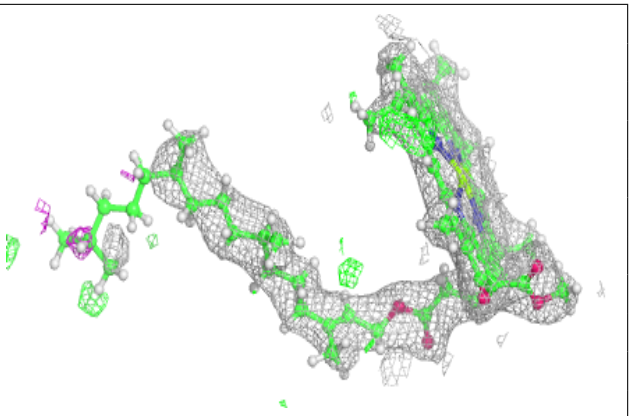


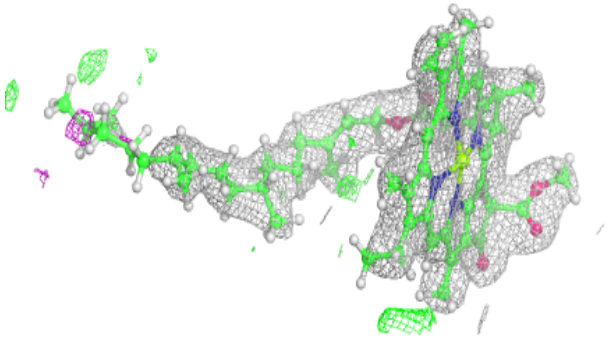


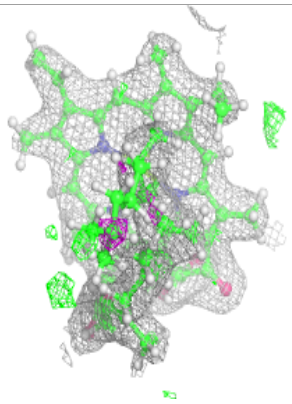


Electron density around CLA C 508:

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

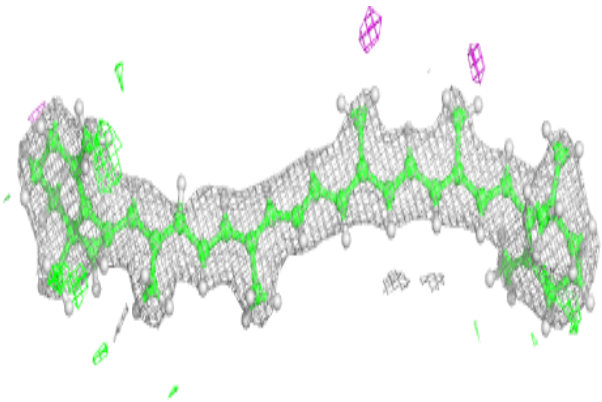


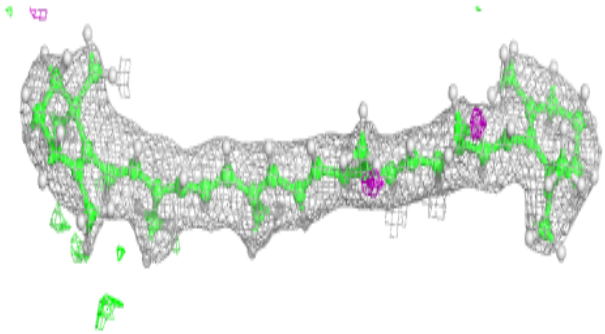


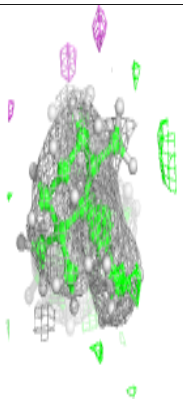


Electron density around BCR B 619:

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

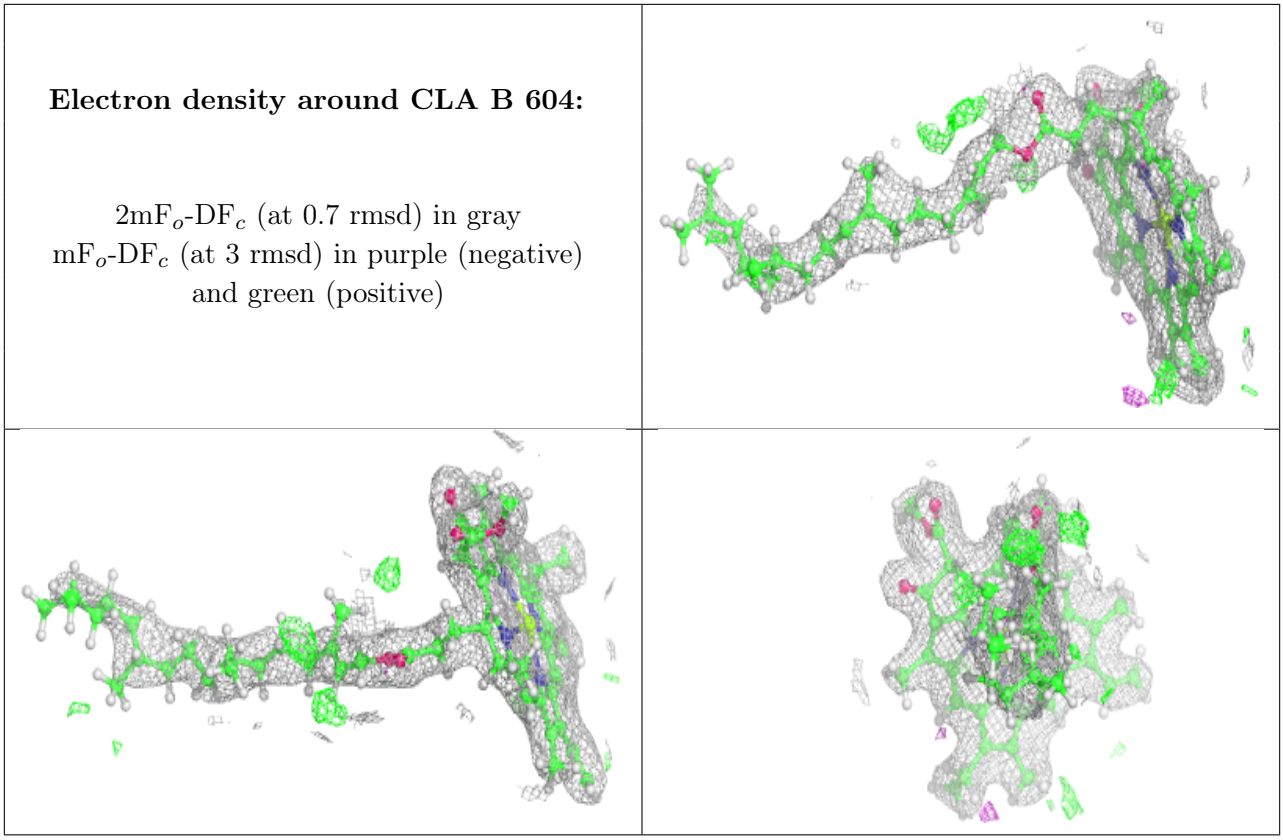






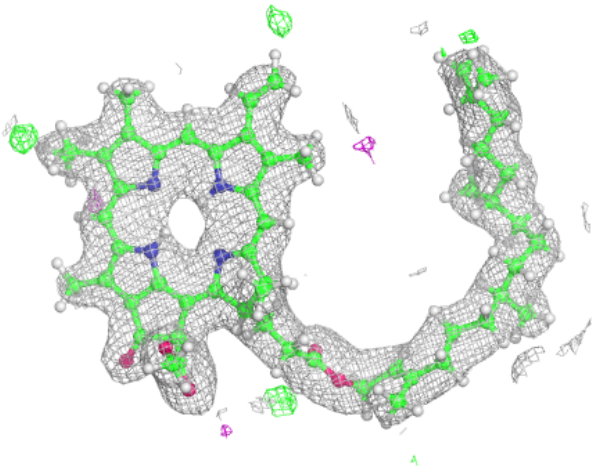
Electron density around CLA B 604:

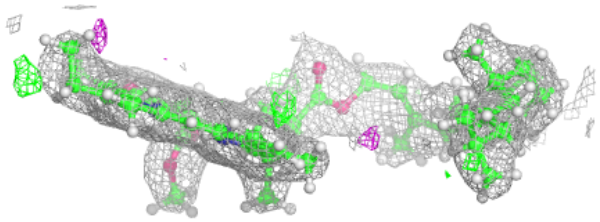
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

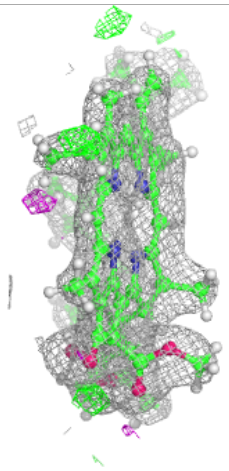


Electron density around PHO a 605:

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

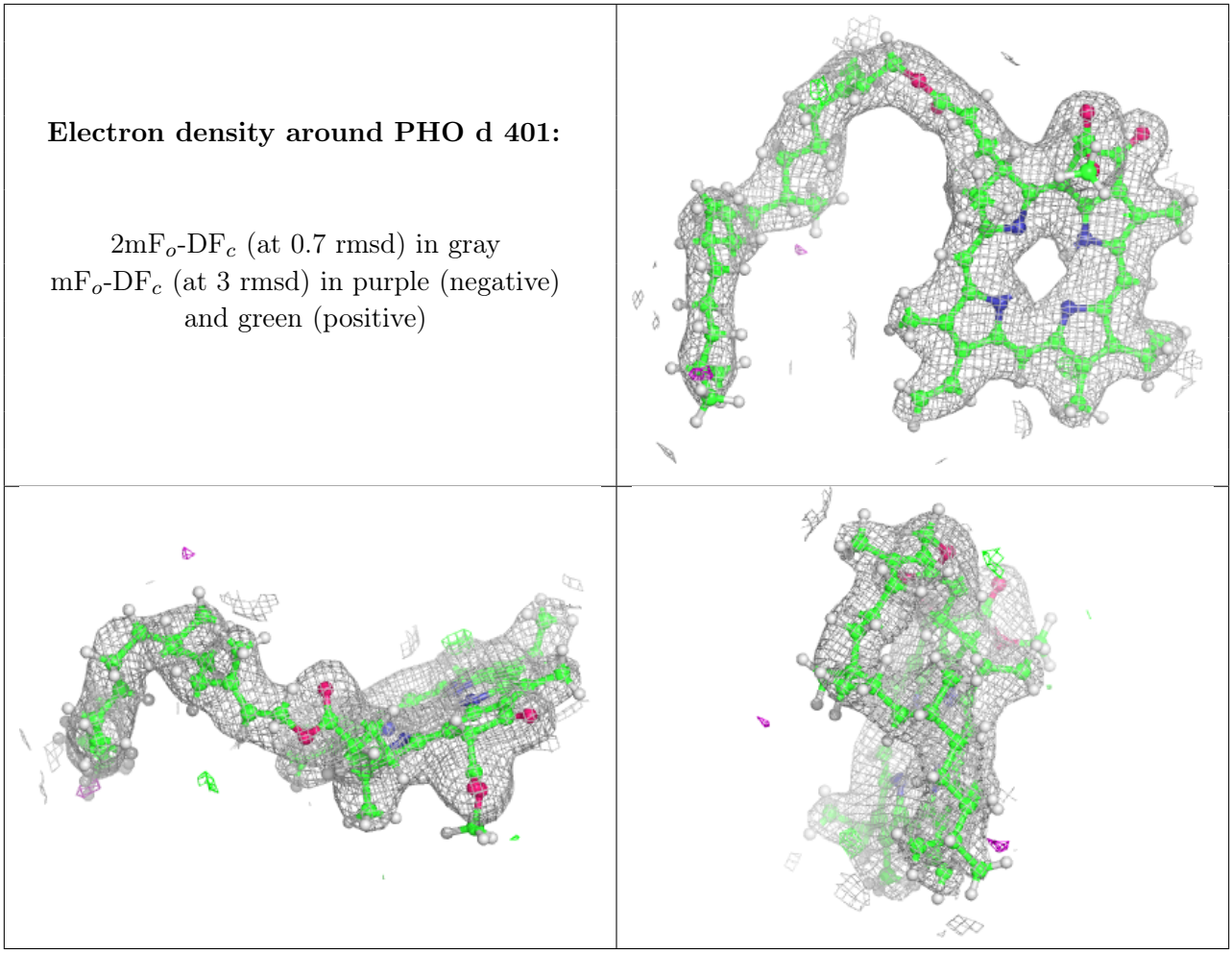






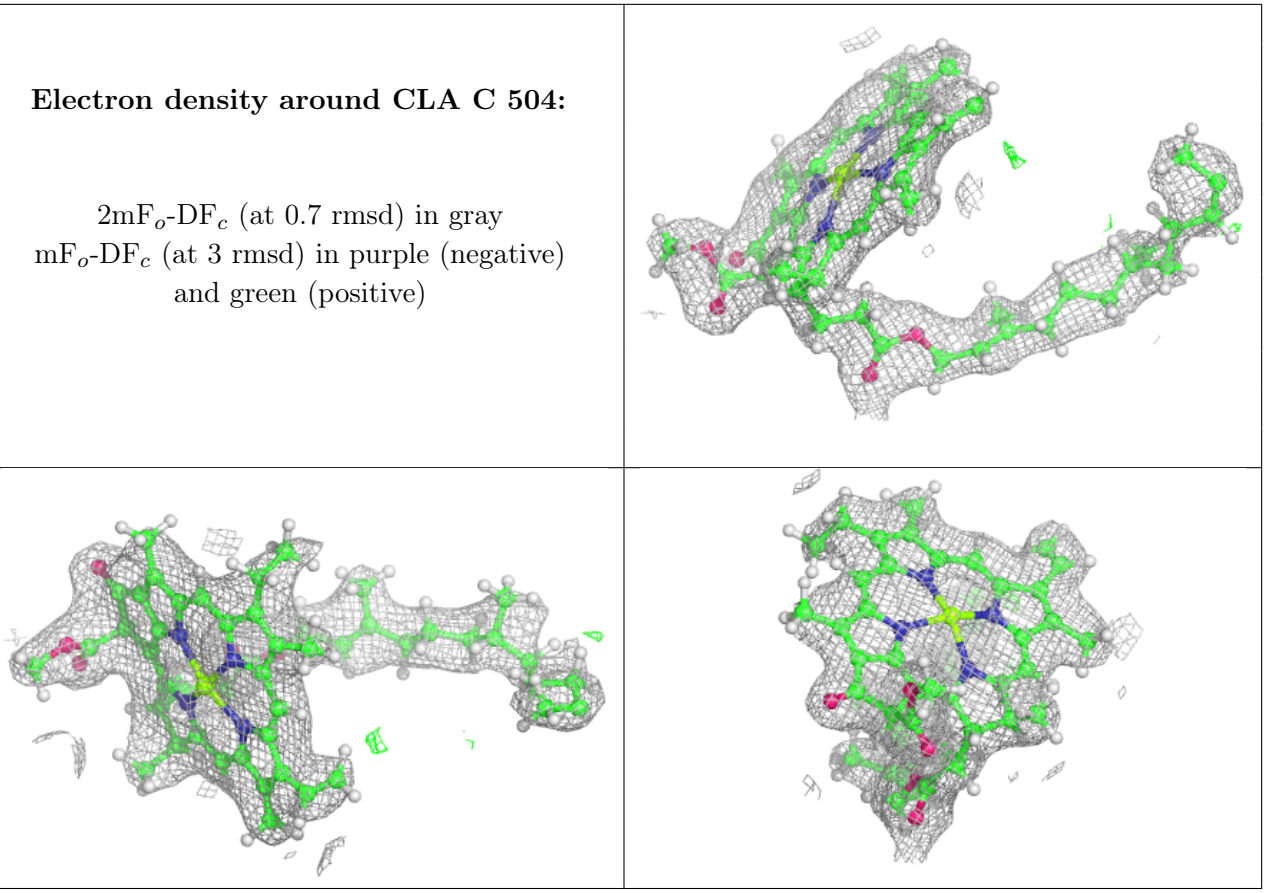
Electron density around PHO d 401:

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



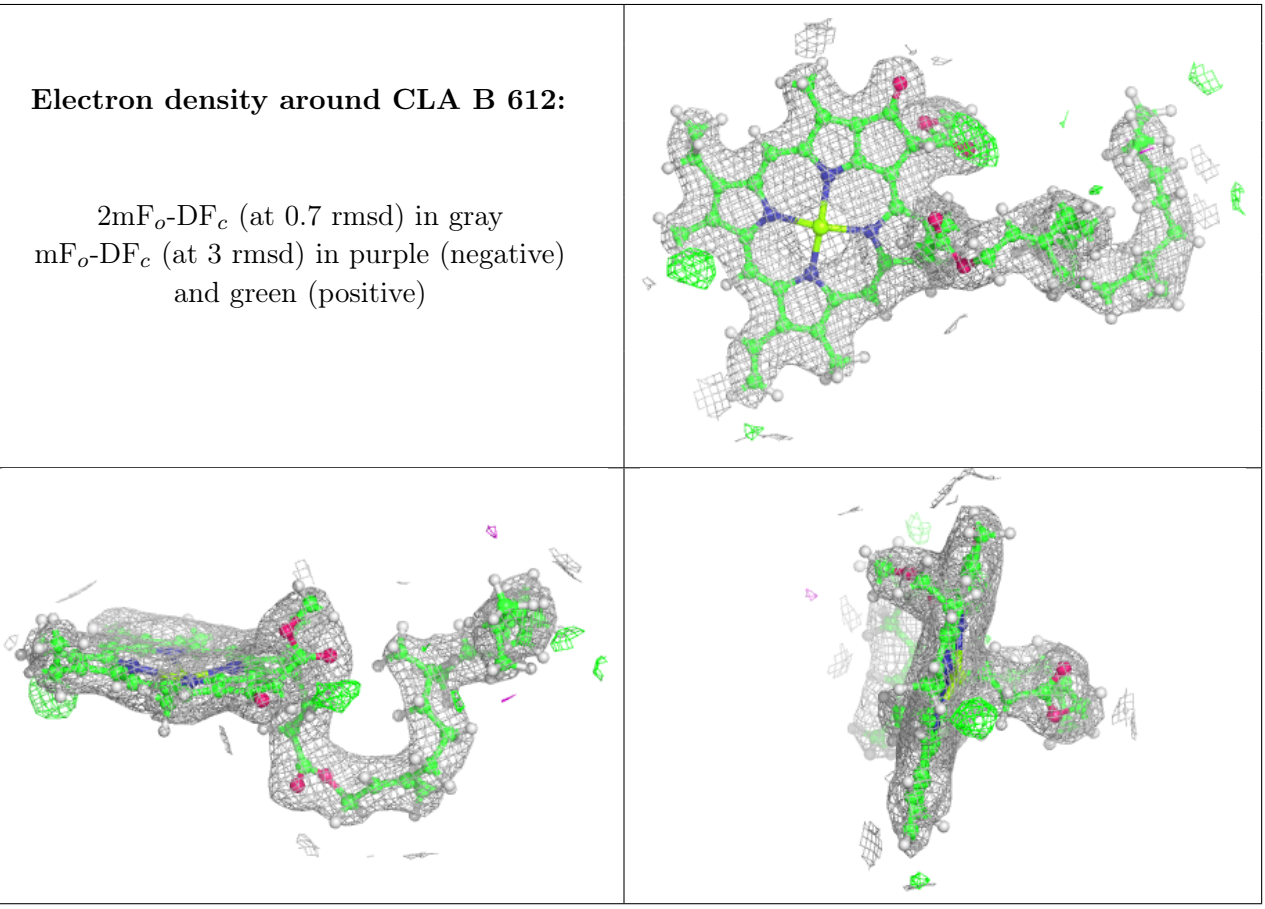
Electron density around CLA C 504:

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



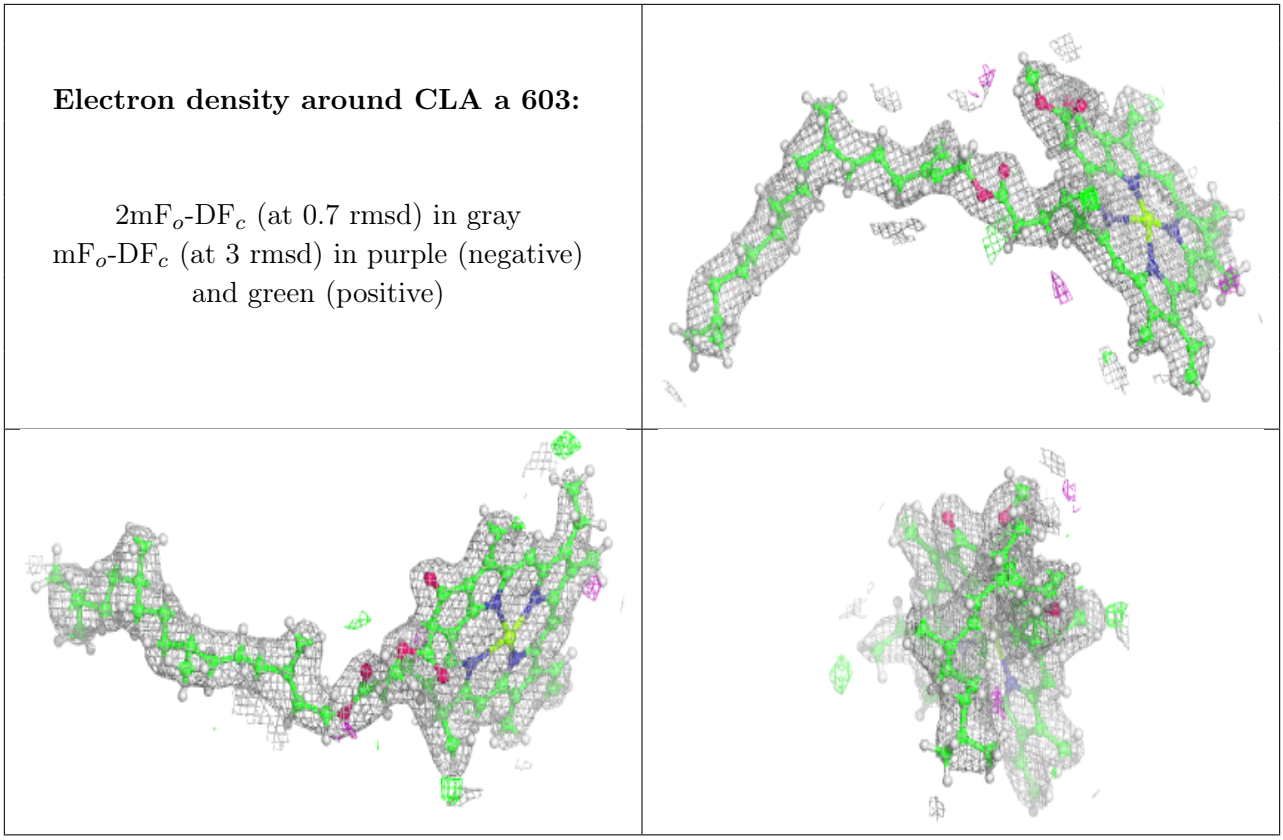
Electron density around CLA B 612:

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



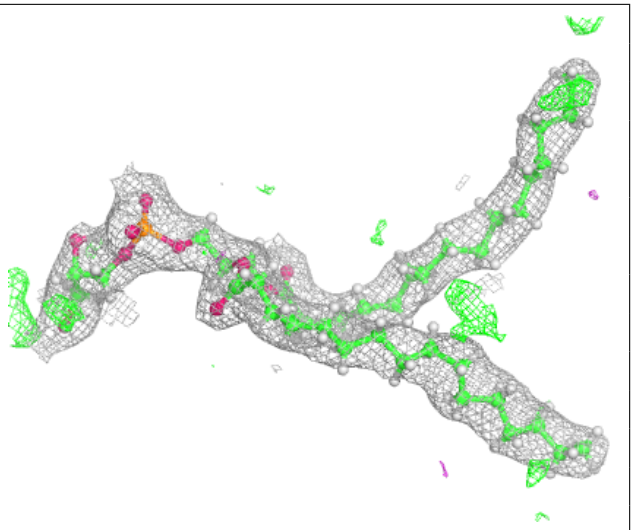
Electron density around CLA a 603:

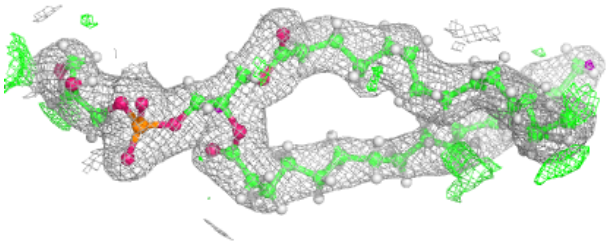
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

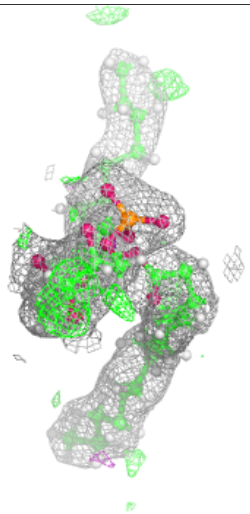


Electron density around LHG D 406:

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

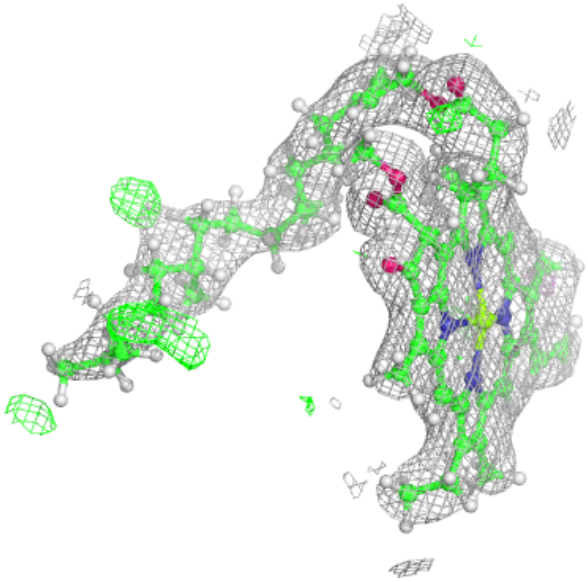


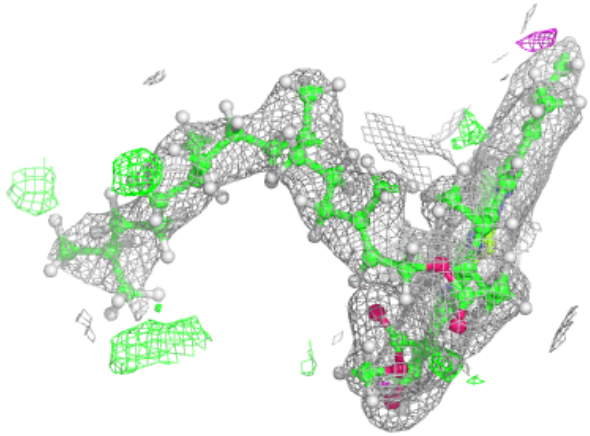


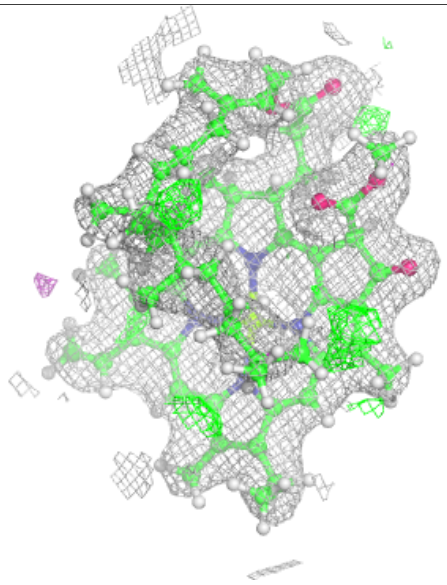


Electron density around CLA B 613:

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

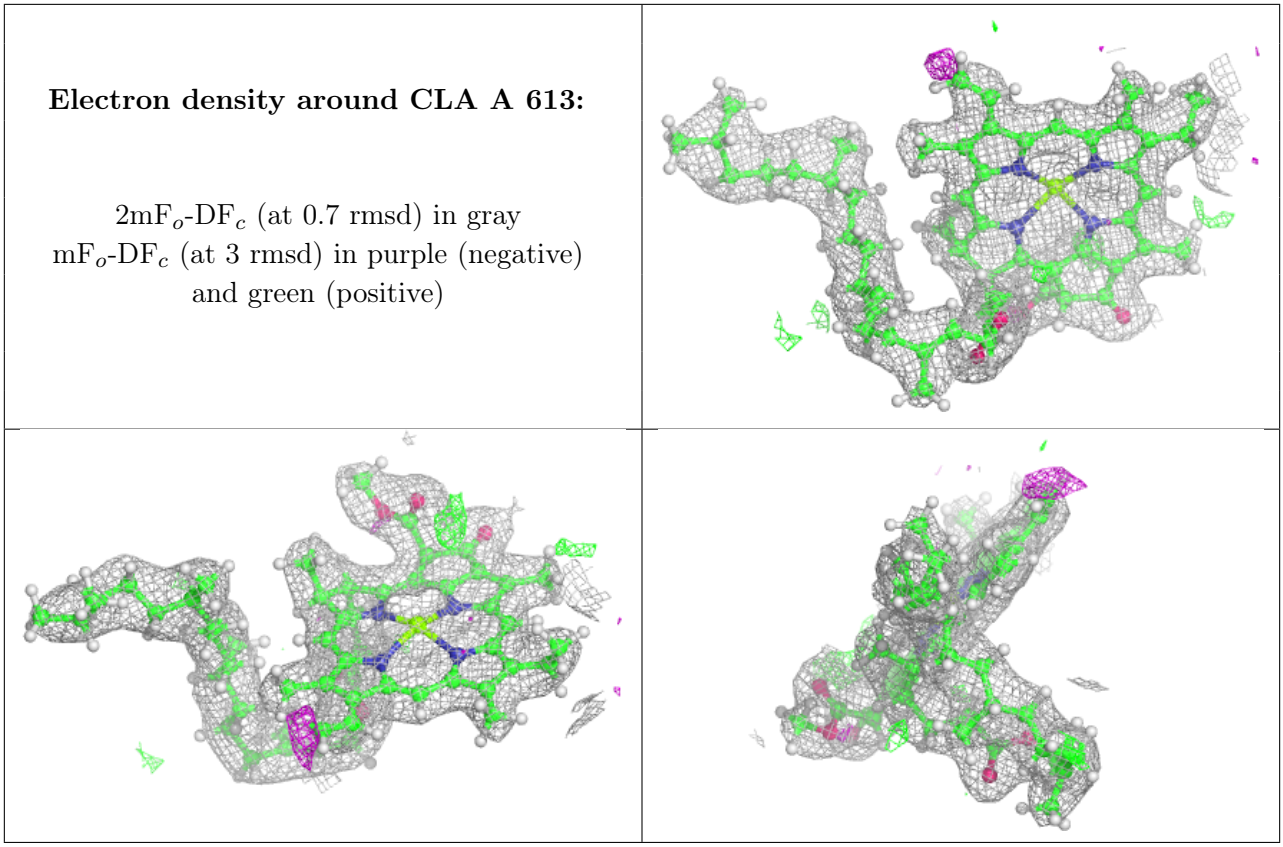






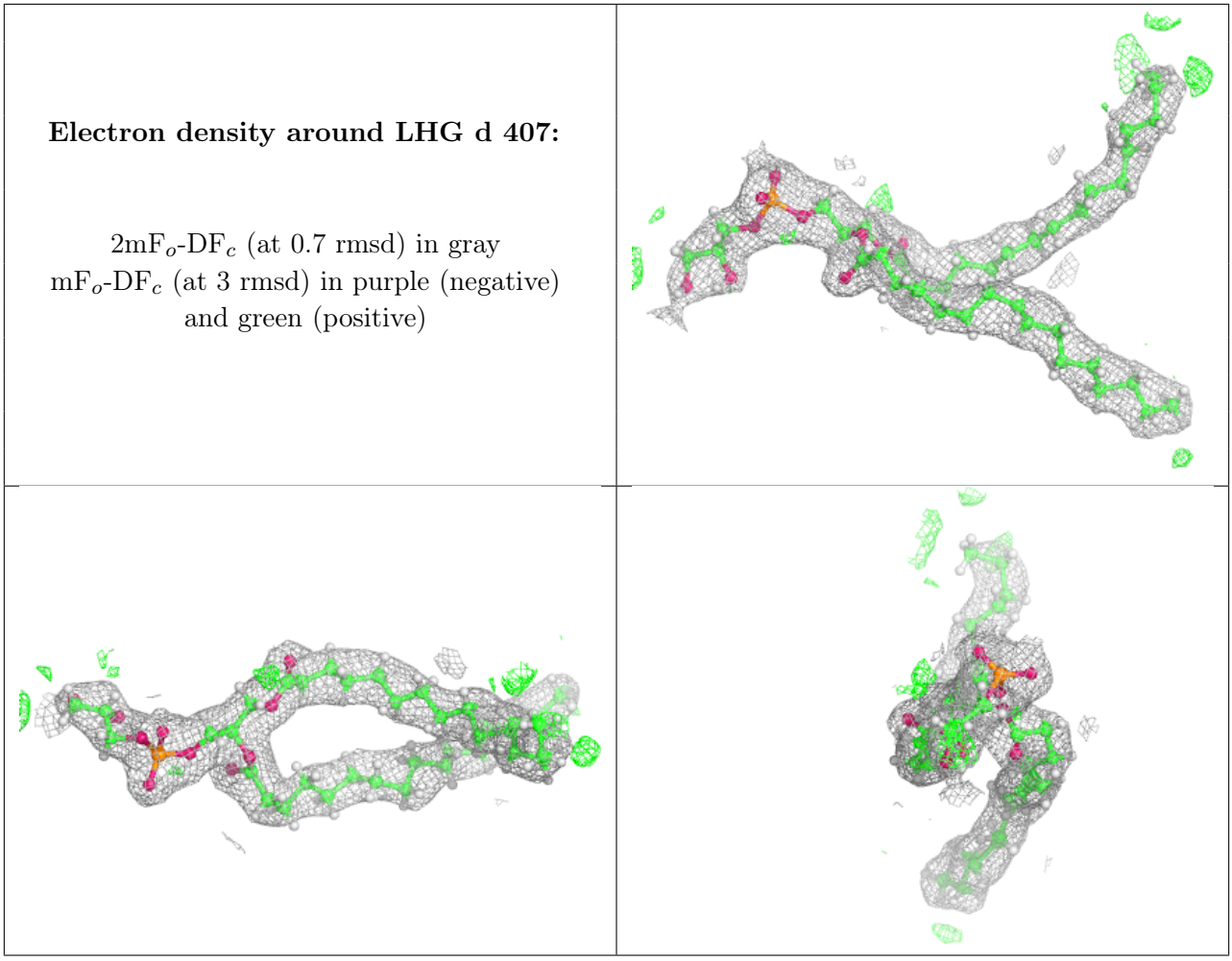
Electron density around CLA A 613:

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



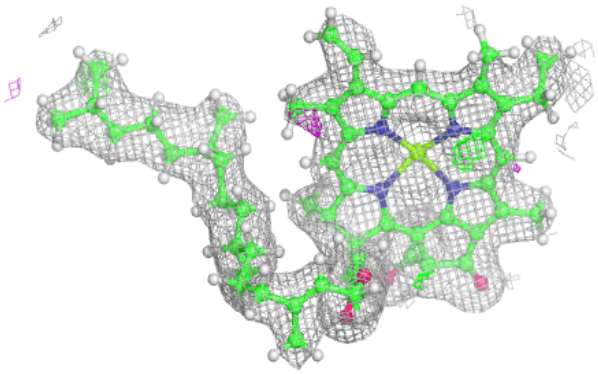
Electron density around LHG d 407:

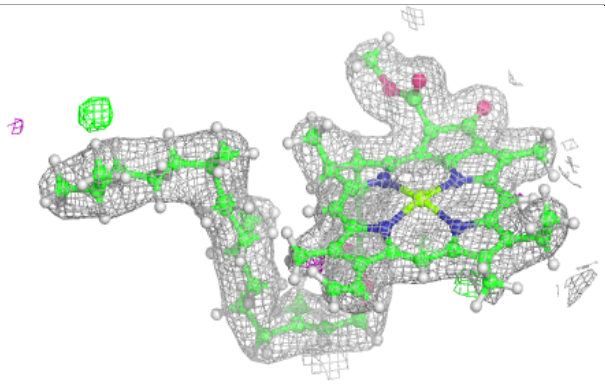
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

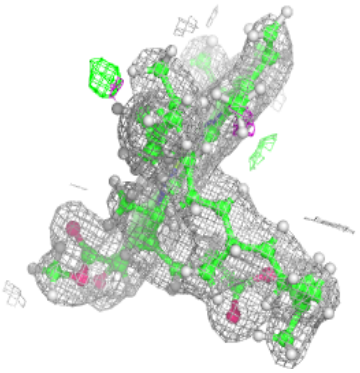


Electron density around CLA a 612:

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

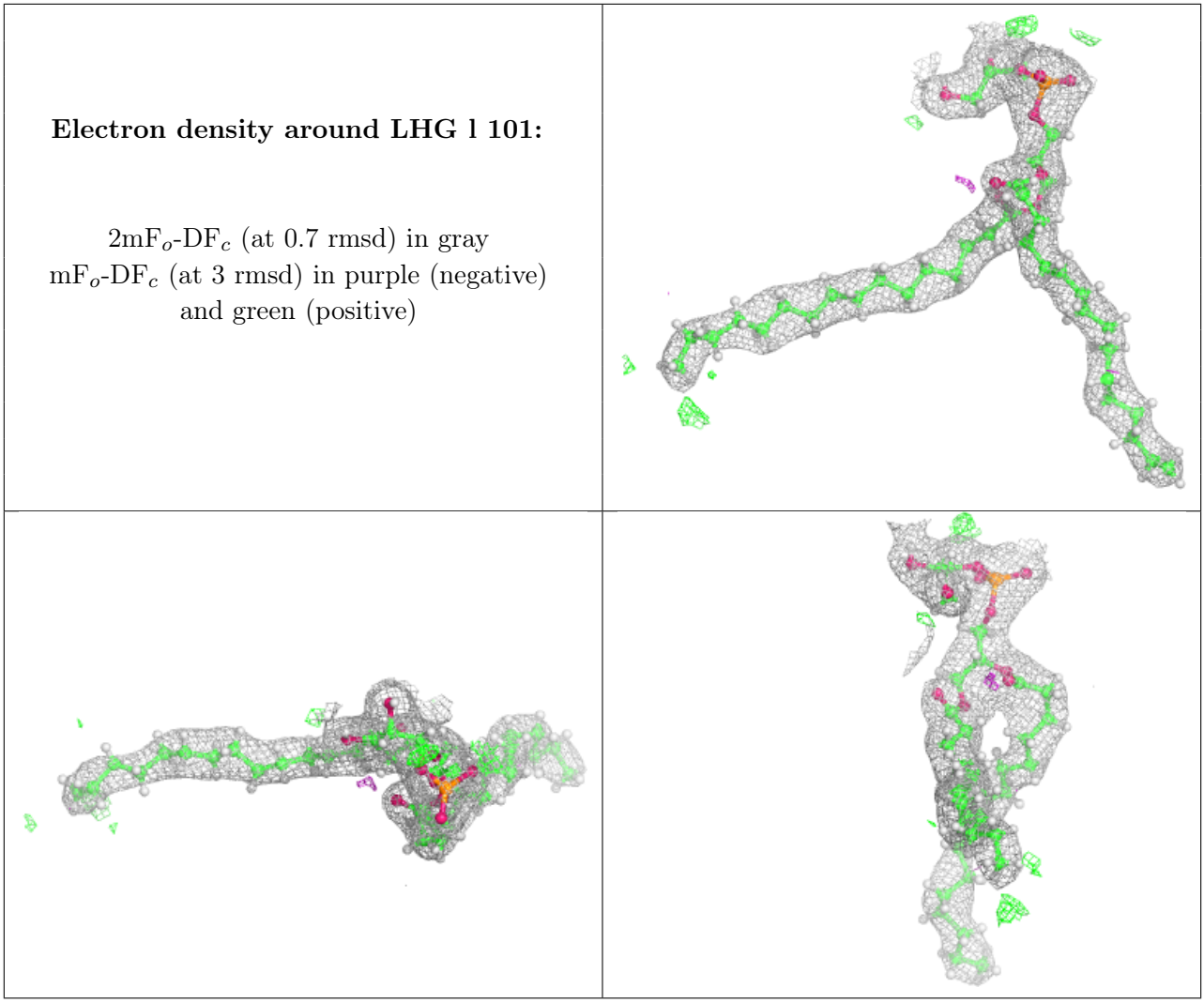






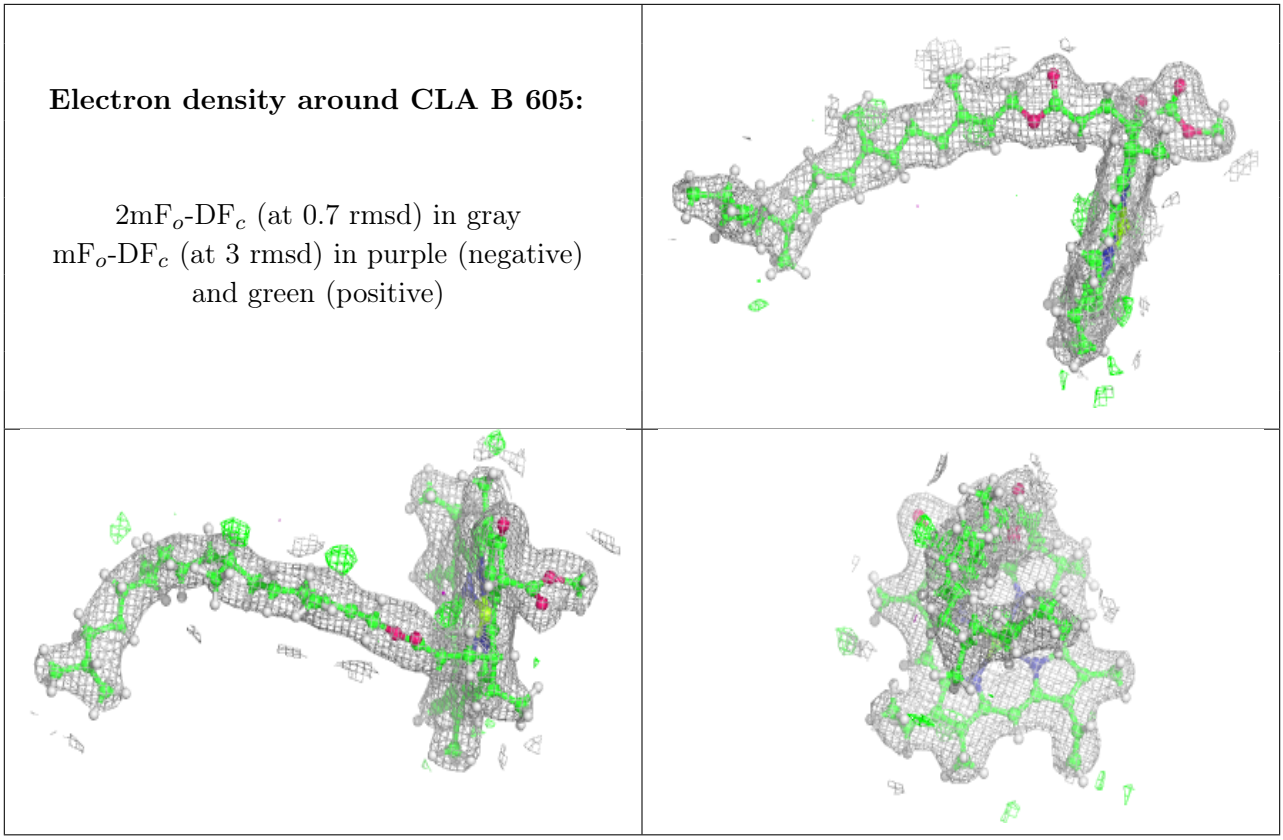
Electron density around LHG l 101:

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



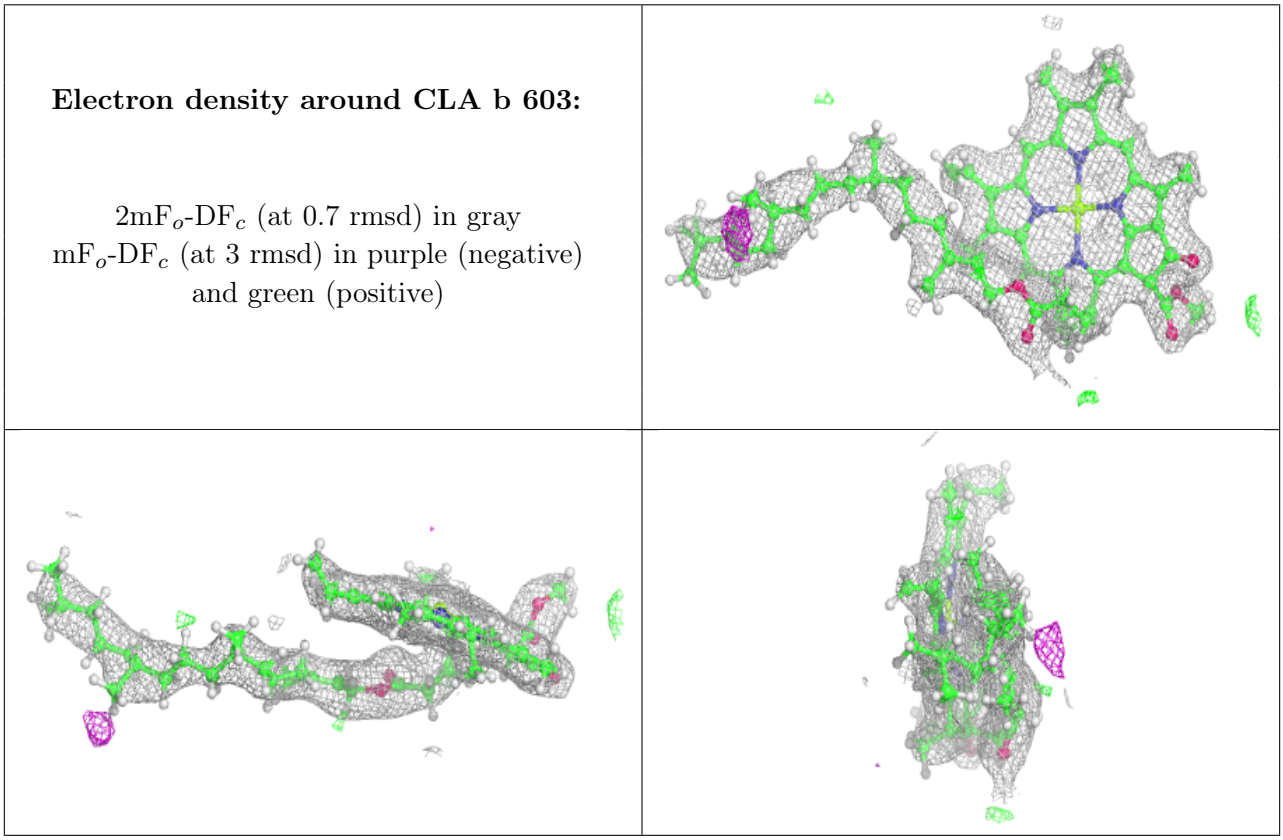
Electron density around CLA B 605:

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



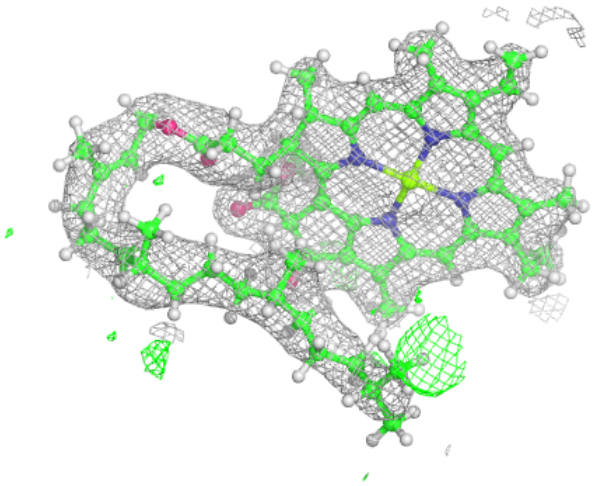
Electron density around CLA b 603:

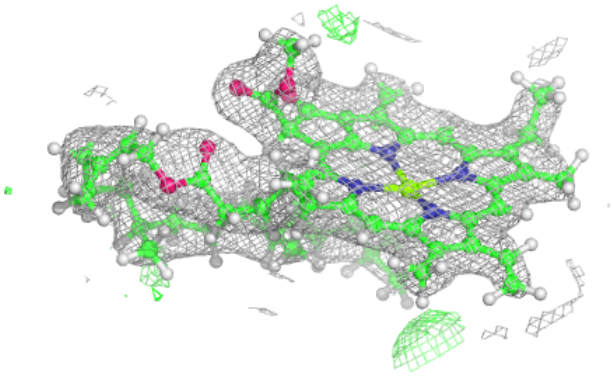
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

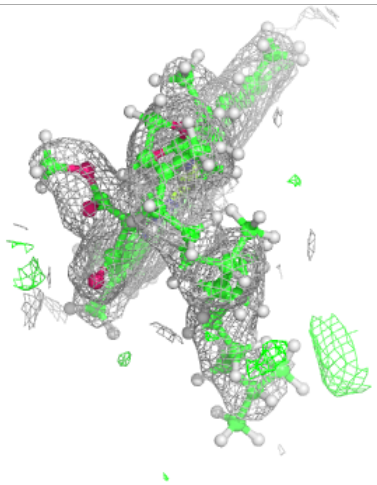


Electron density around CLA C 509:

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

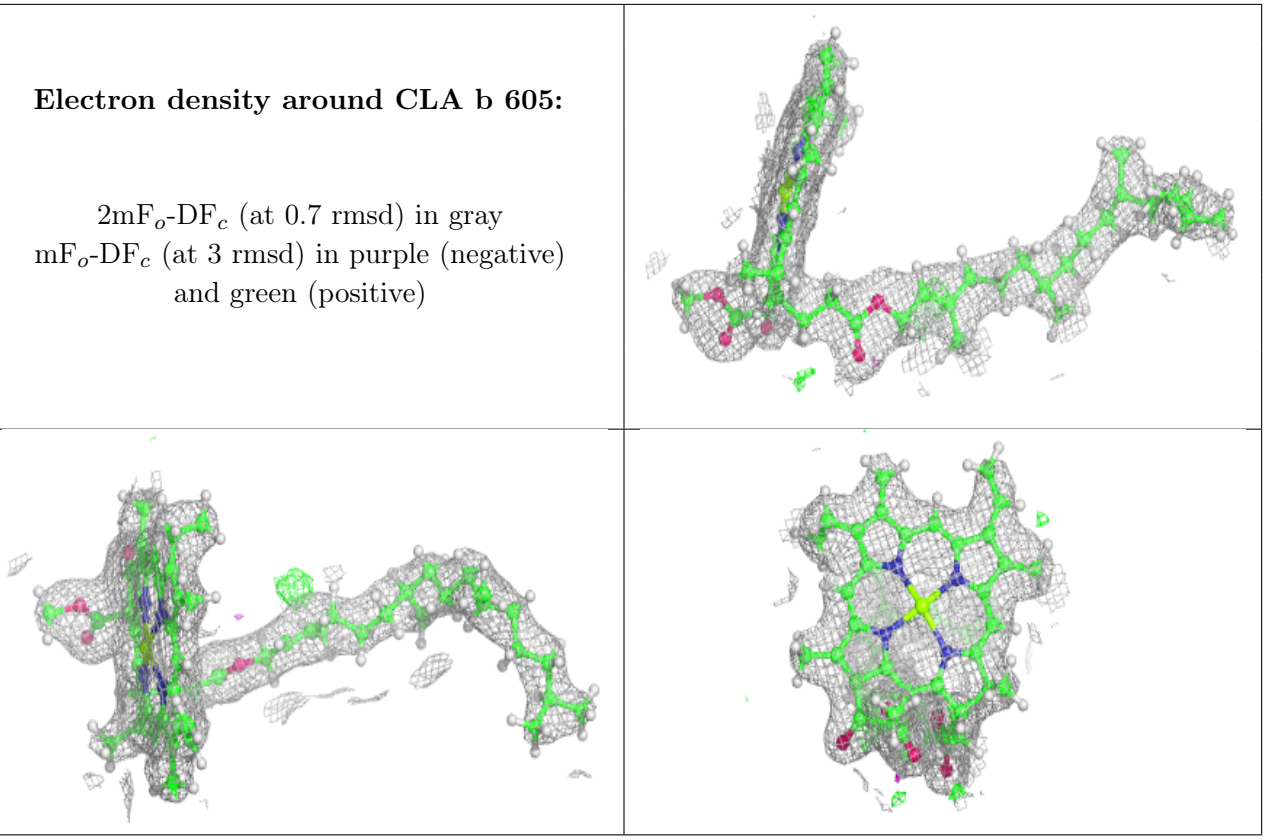






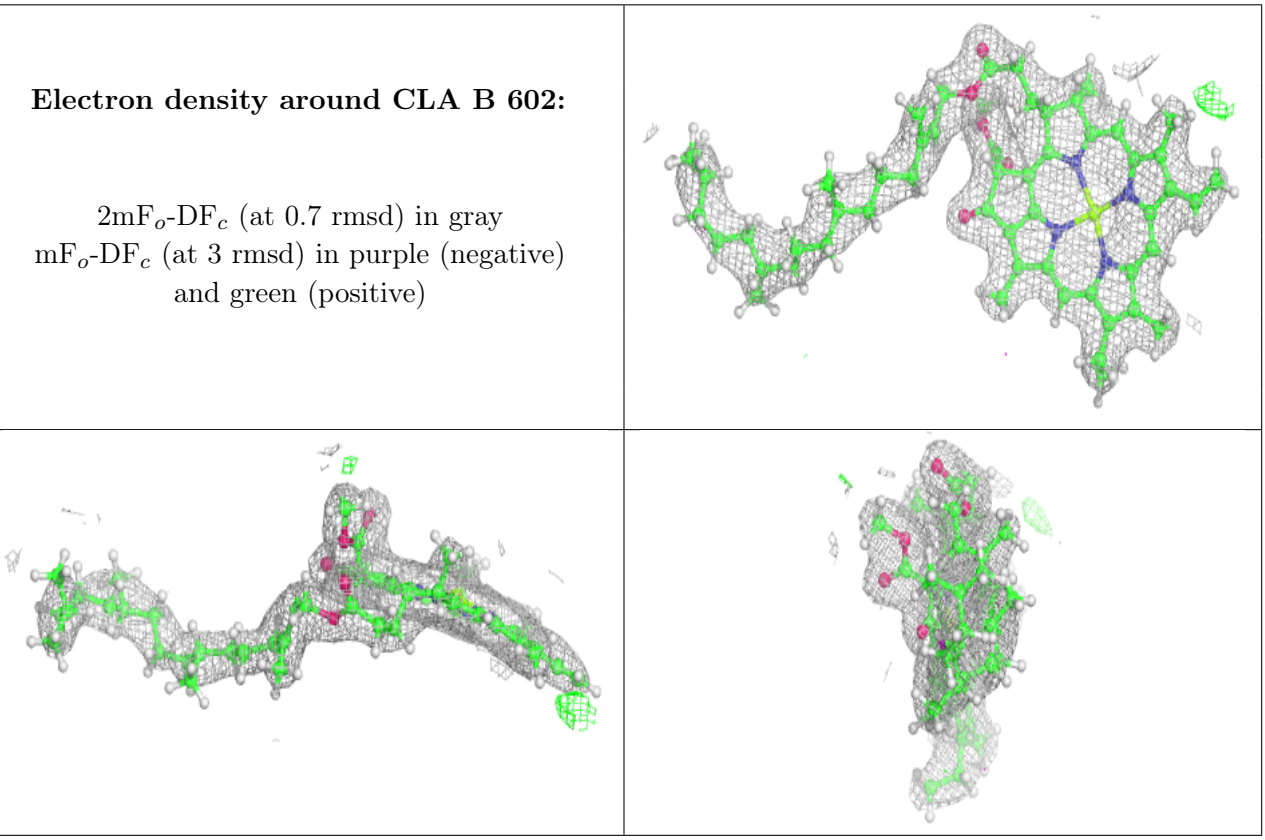
Electron density around CLA b 605:

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



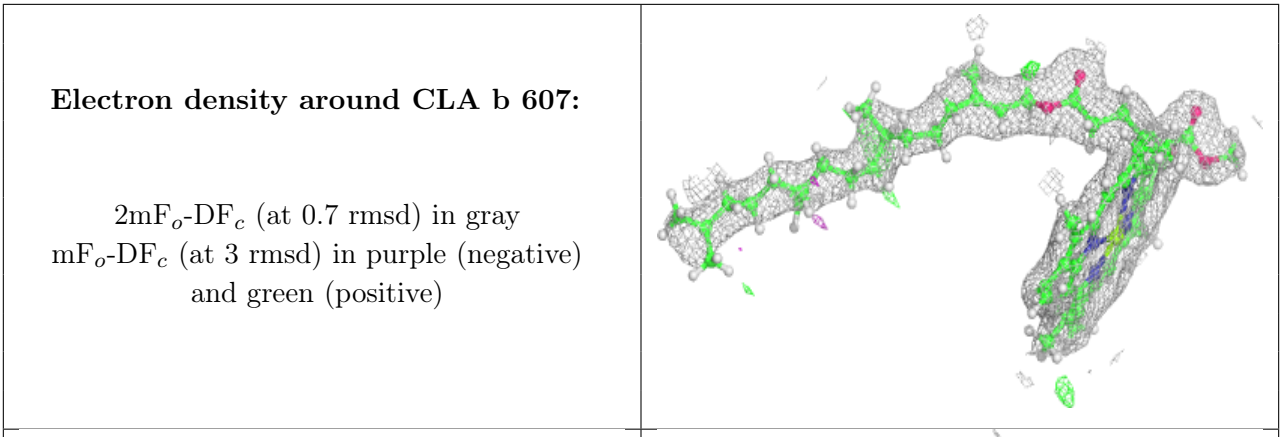
Electron density around CLA B 602:

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



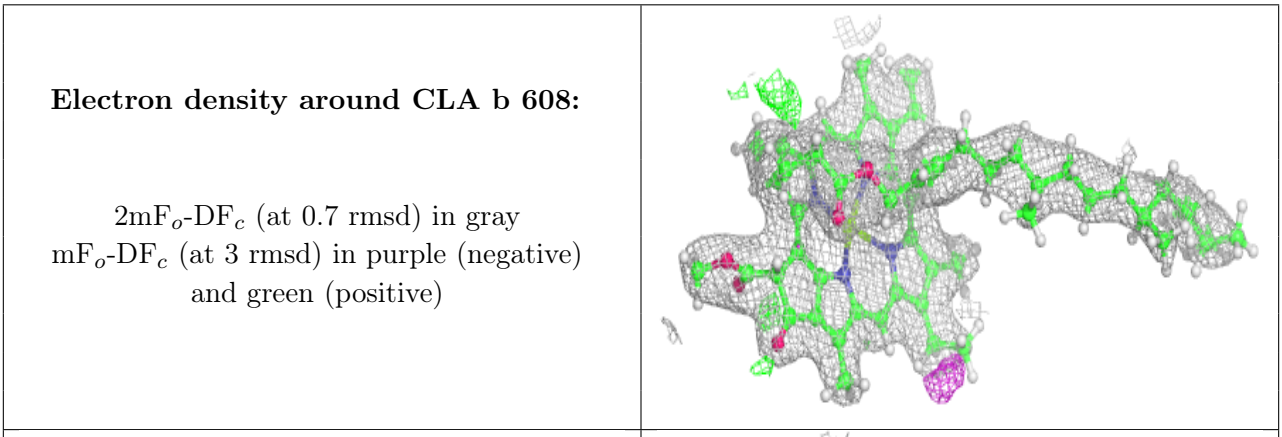
Electron density around CLA b 607:

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



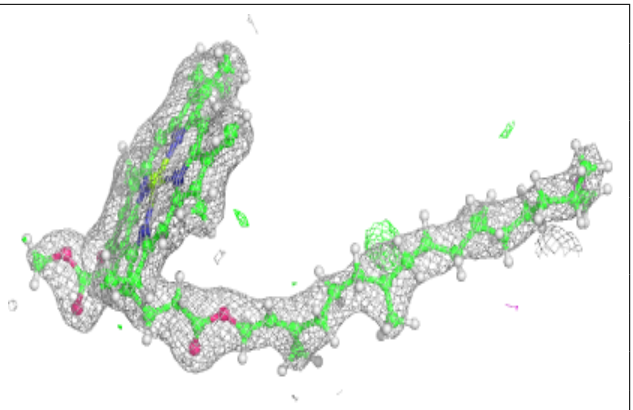
Electron density around CLA b 608:

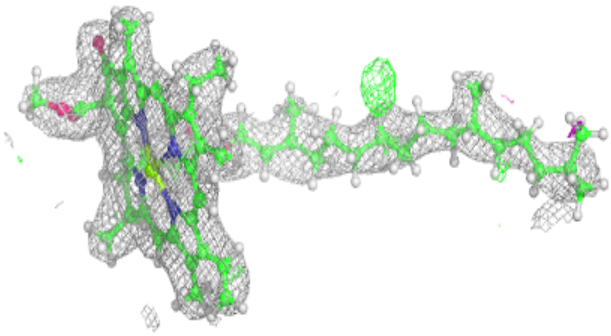
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

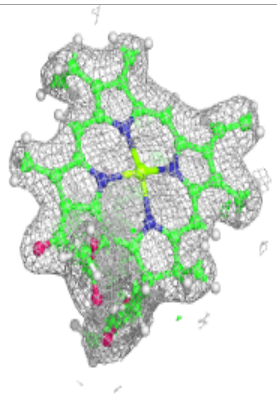


Electron density around CLA B 607:

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

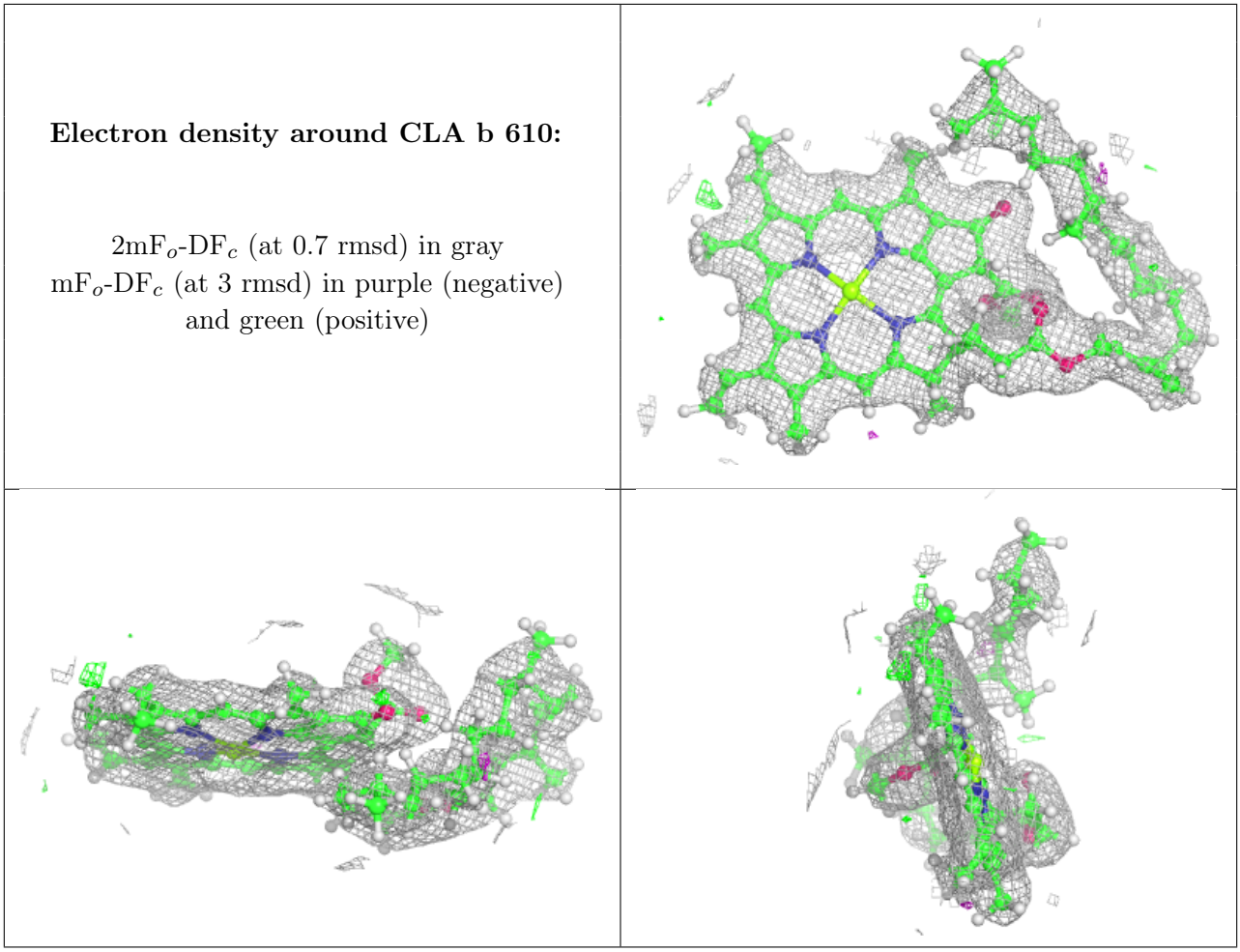






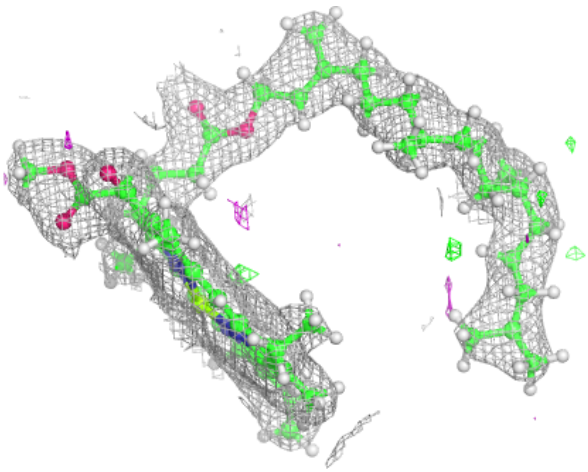
Electron density around CLA b 610:

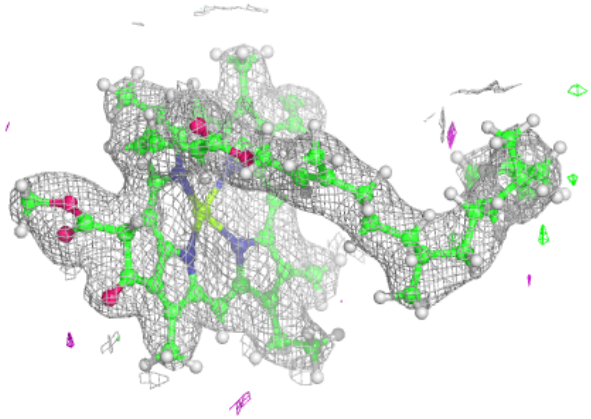
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

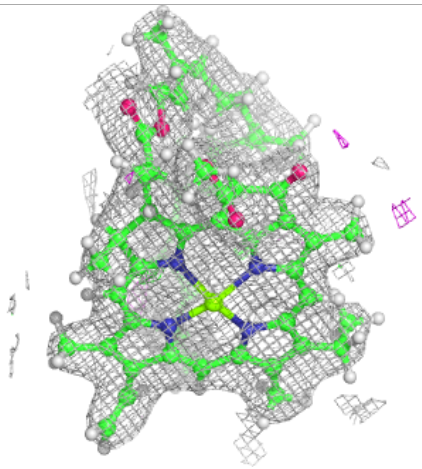


Electron density around CLA b 611:

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

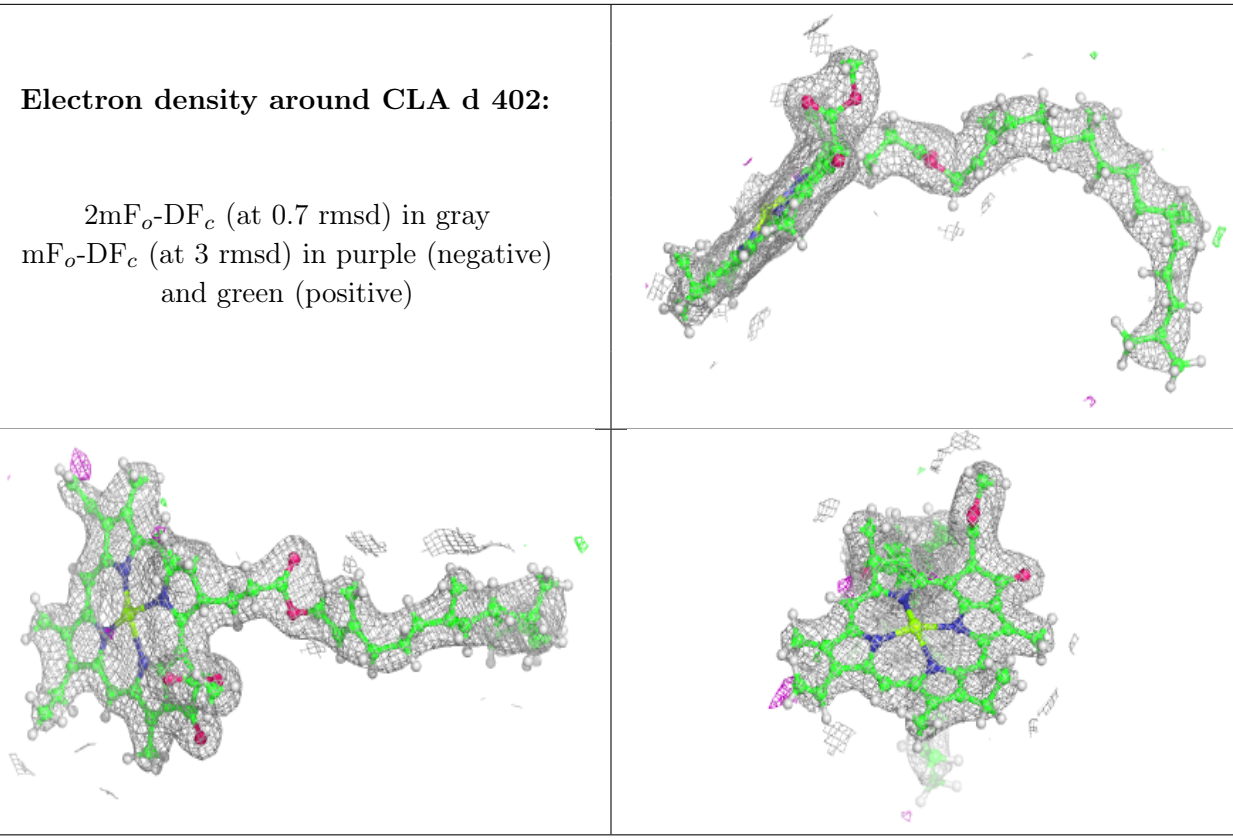






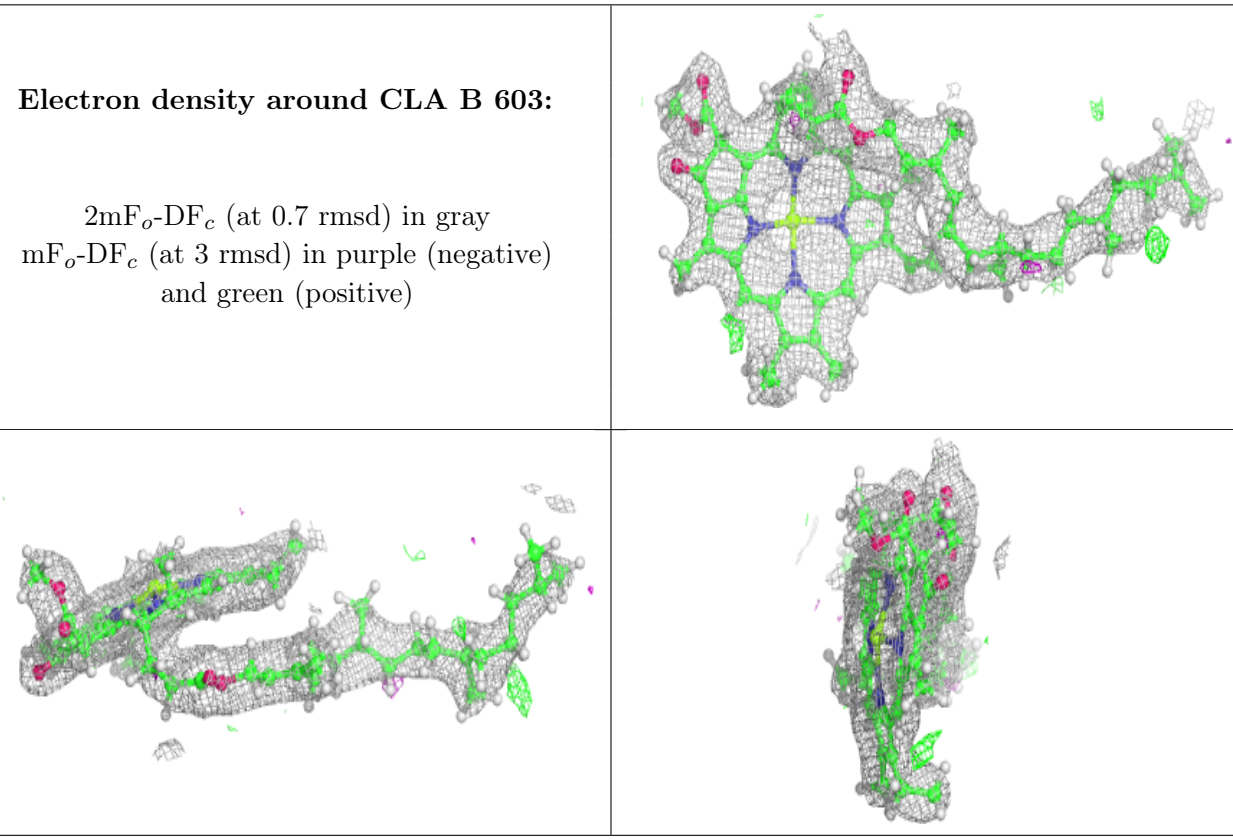
Electron density around CLA d 402:

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



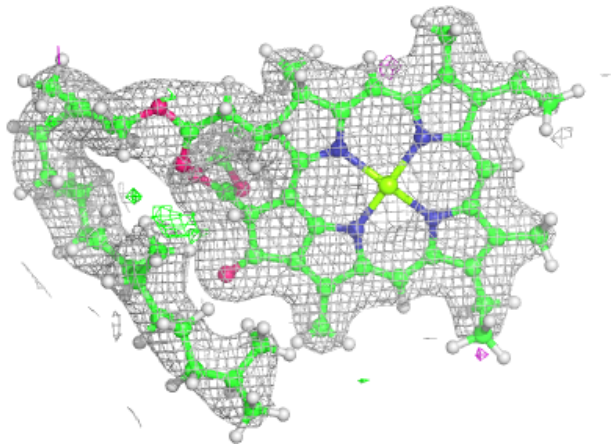
Electron density around CLA B 603:

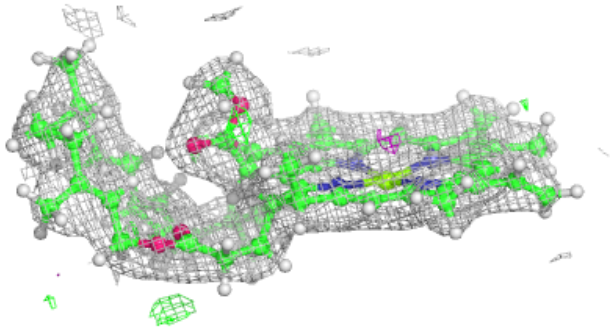
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

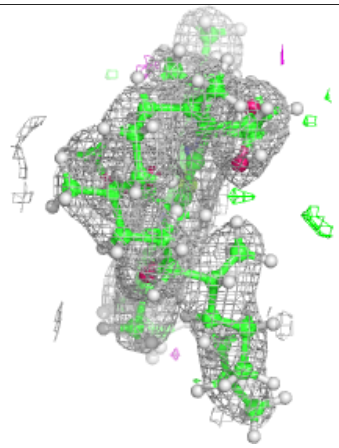


Electron density around CLA B 610:

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

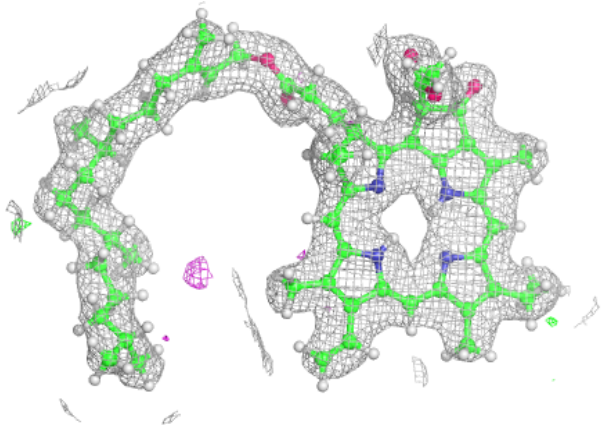


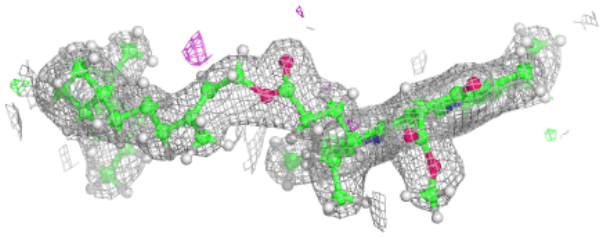




Electron density around PHO A 605:

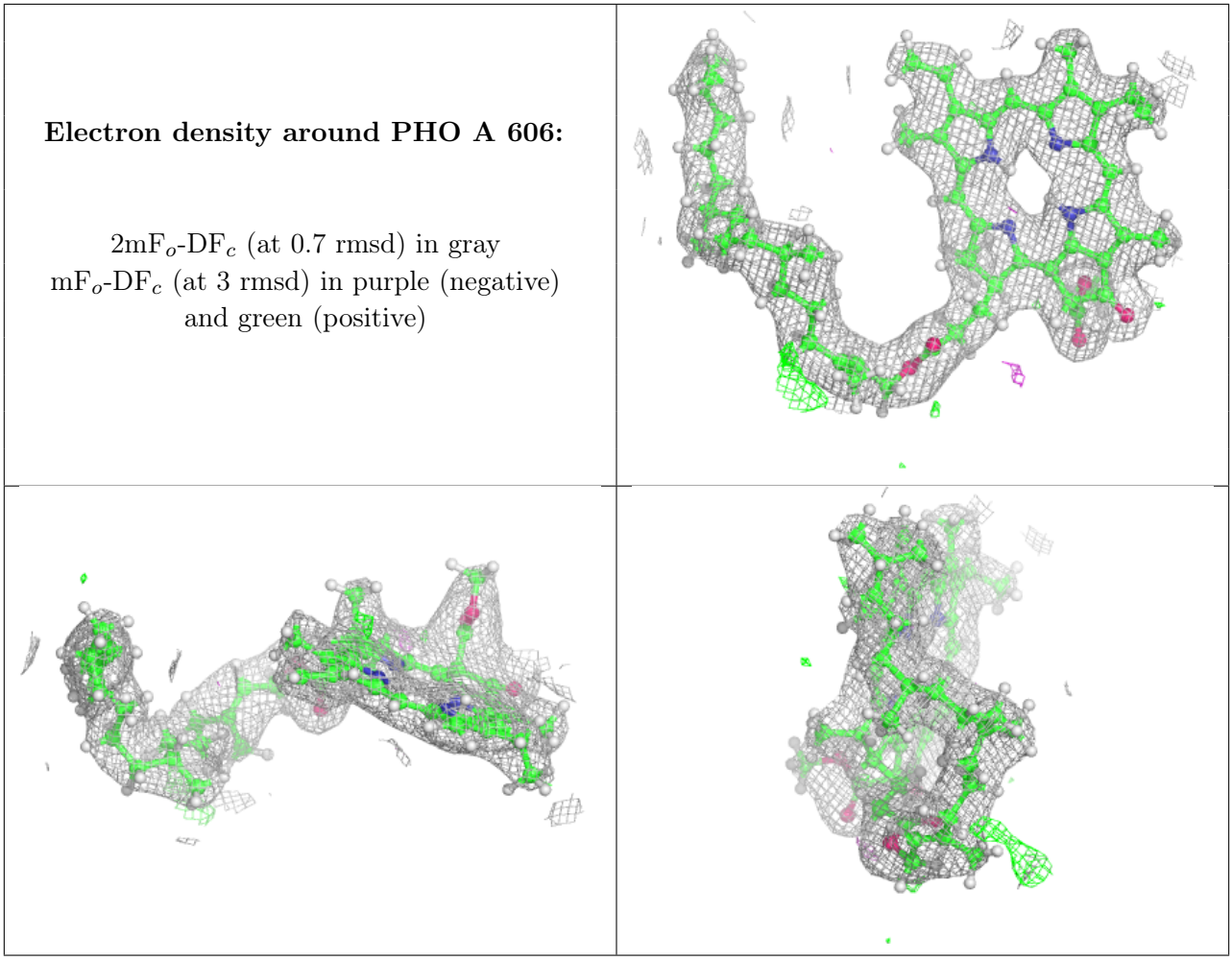
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





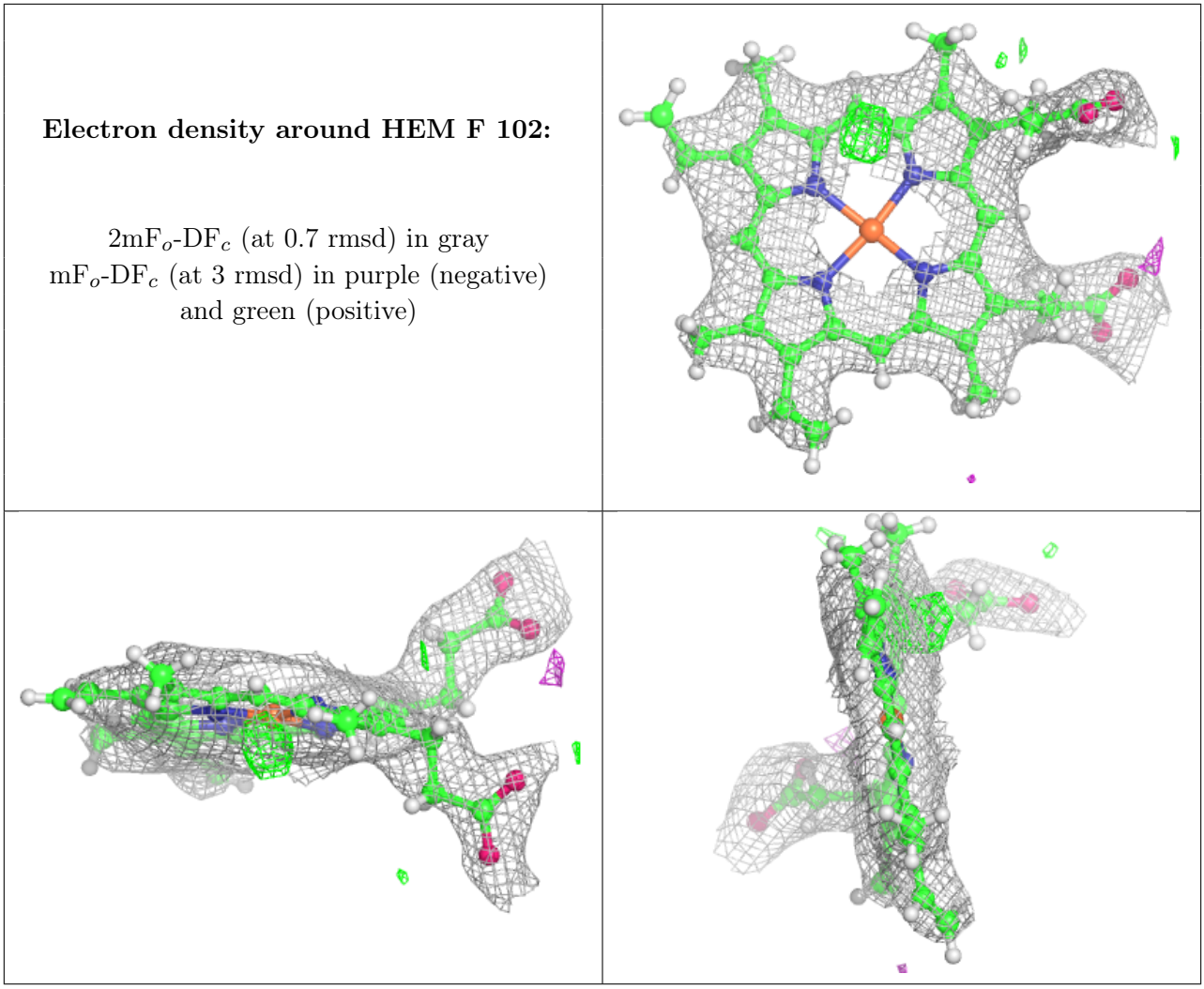
Electron density around PHO A 606:

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



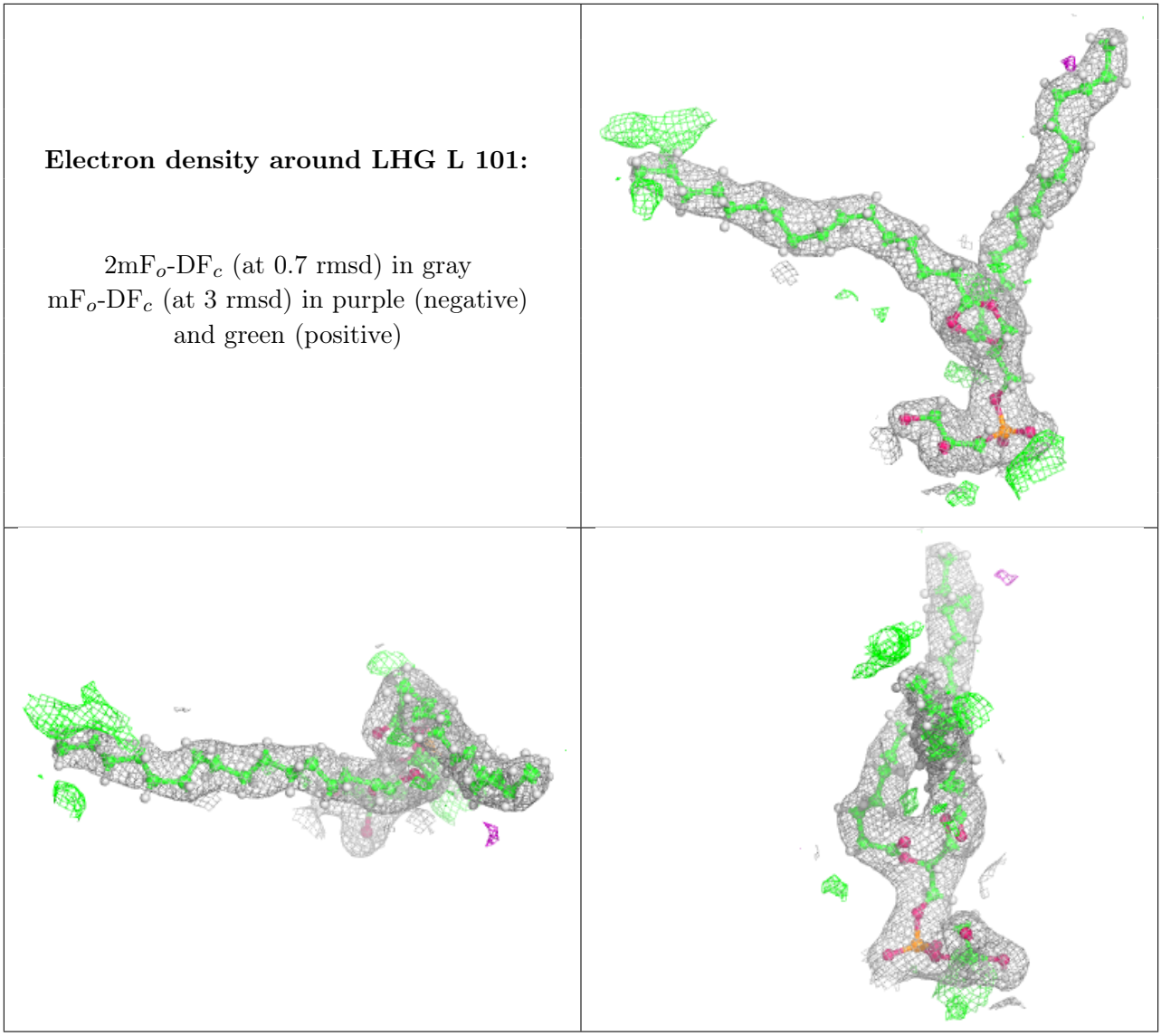
Electron density around HEM F 102:

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



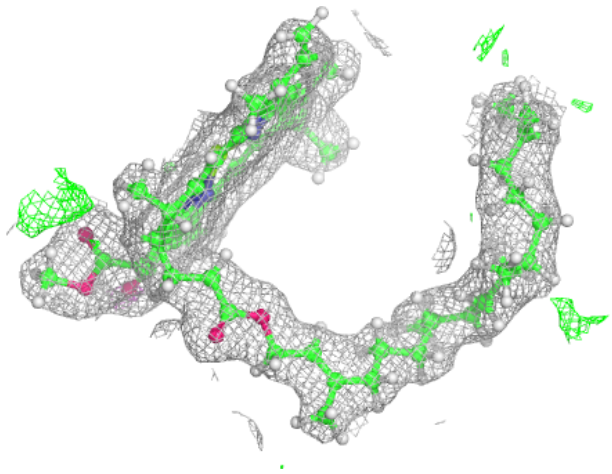
Electron density around LHG L 101:

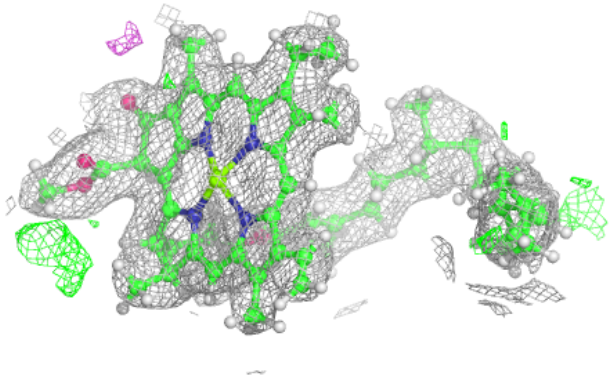
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

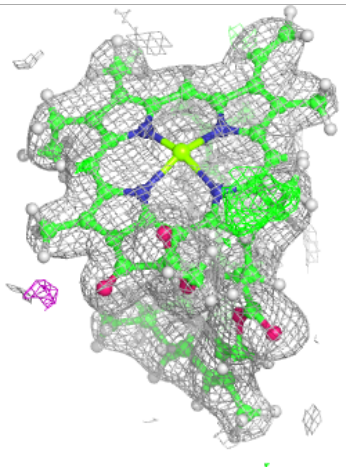


Electron density around CLA B 611:

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

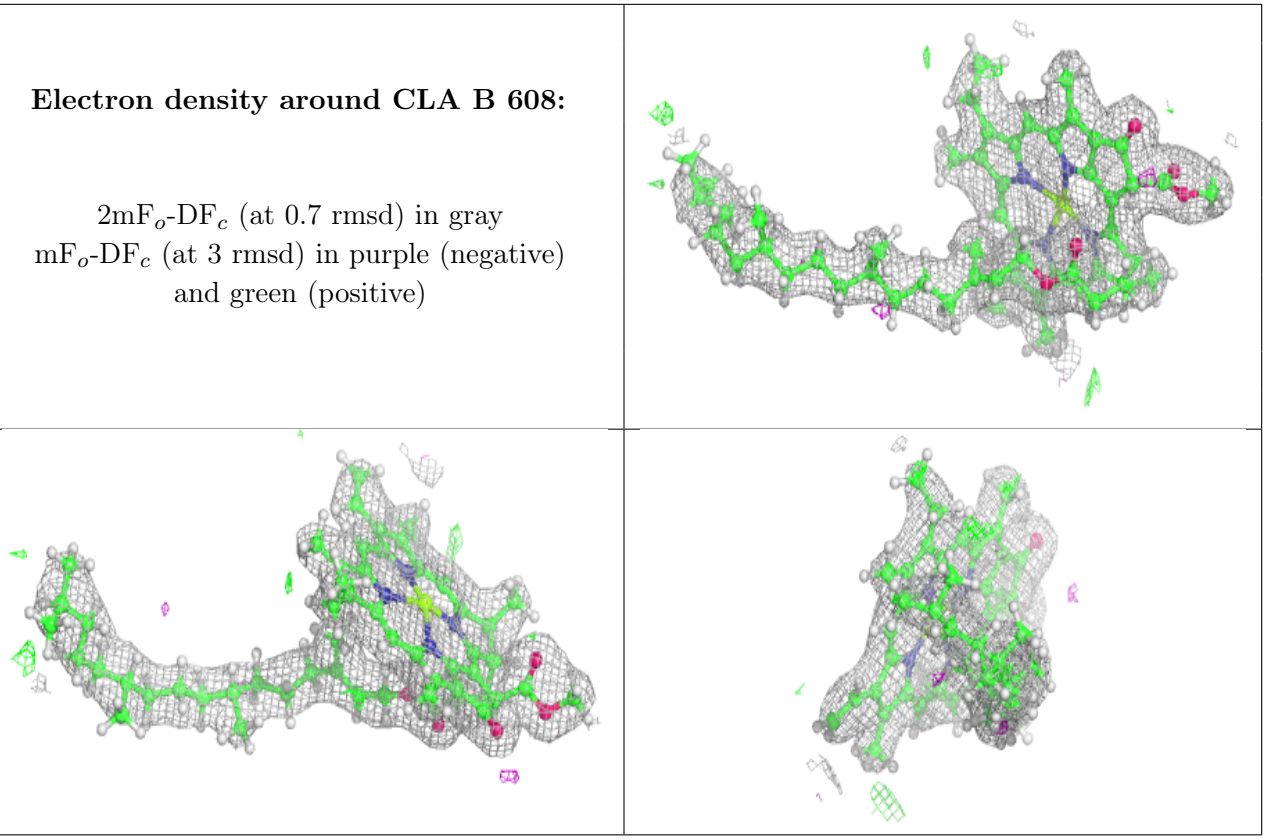






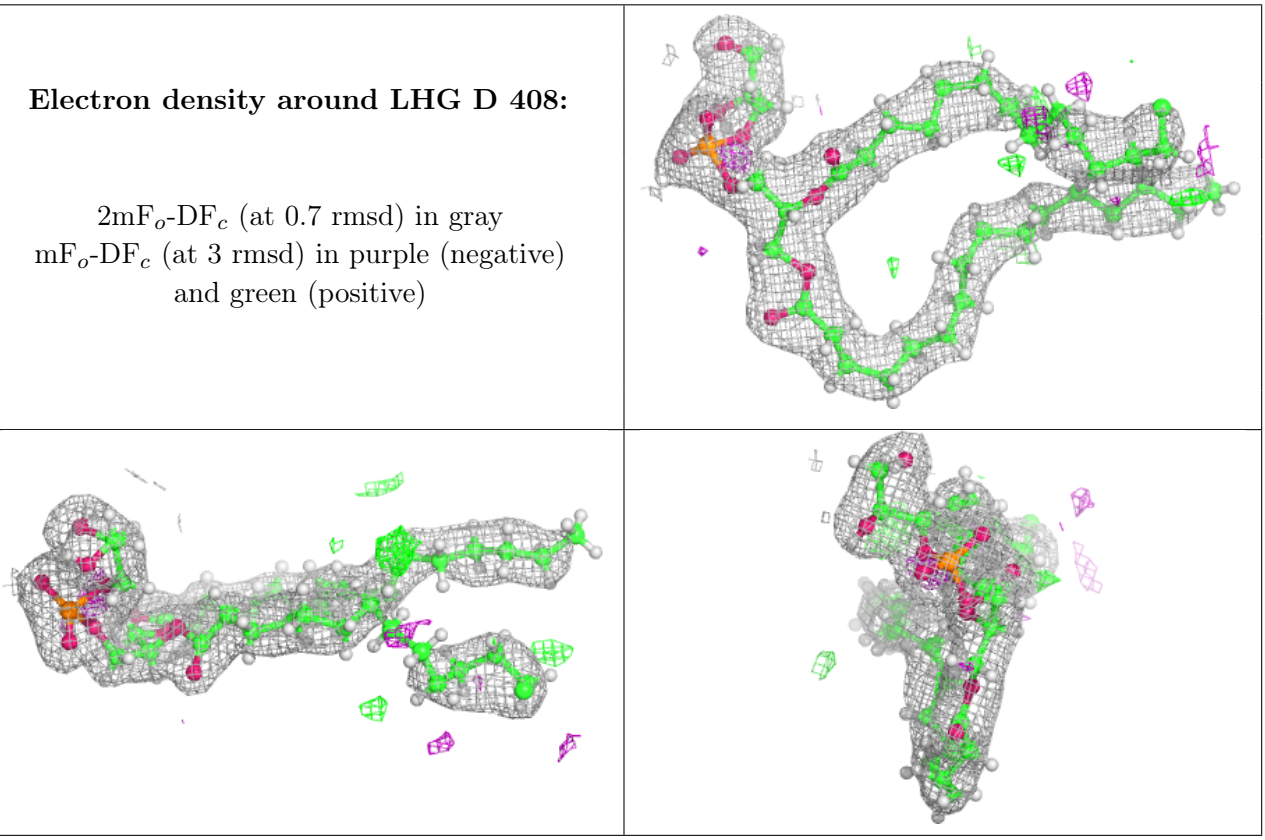
Electron density around CLA B 608:

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



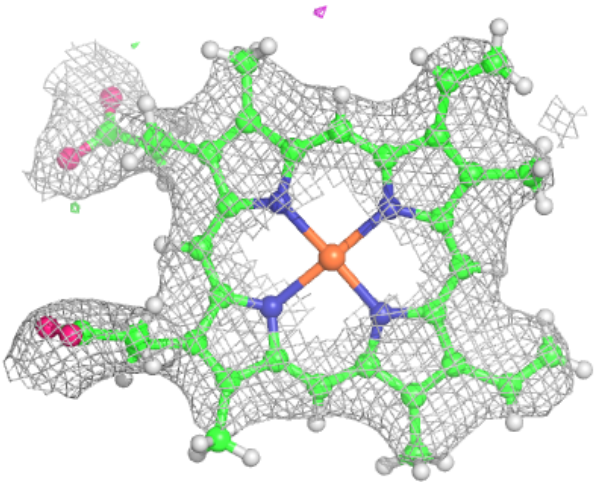
Electron density around LHG D 408:

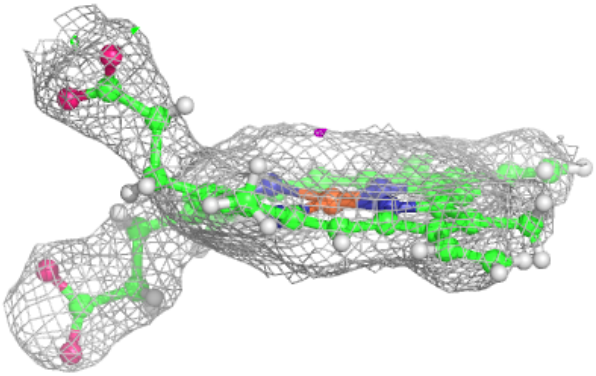
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

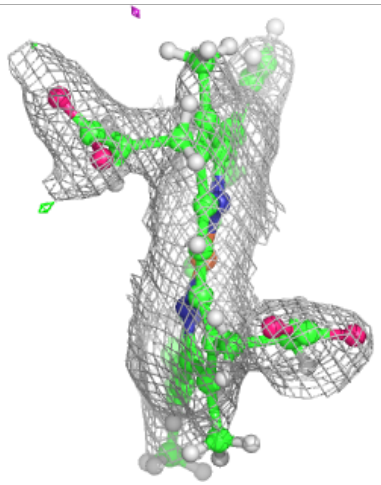


Electron density around HEM f 102:

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

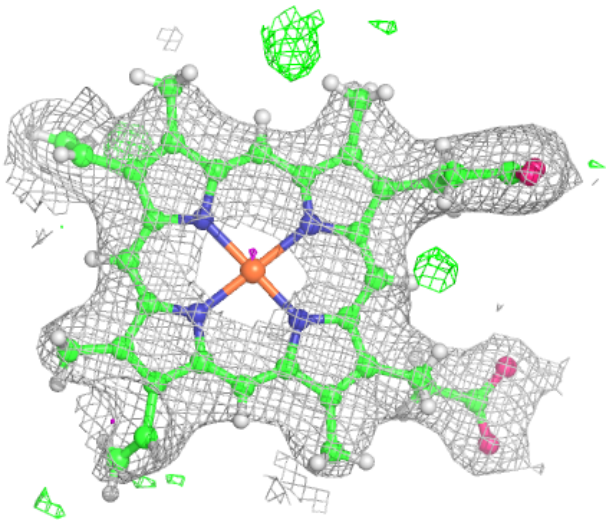


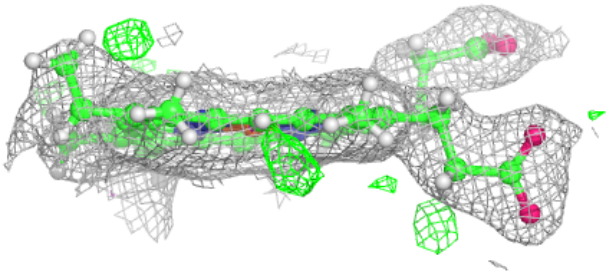


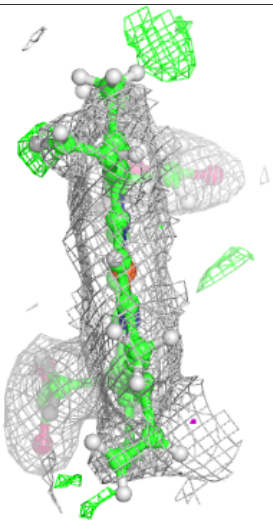


Electron density around HEC v 201:

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

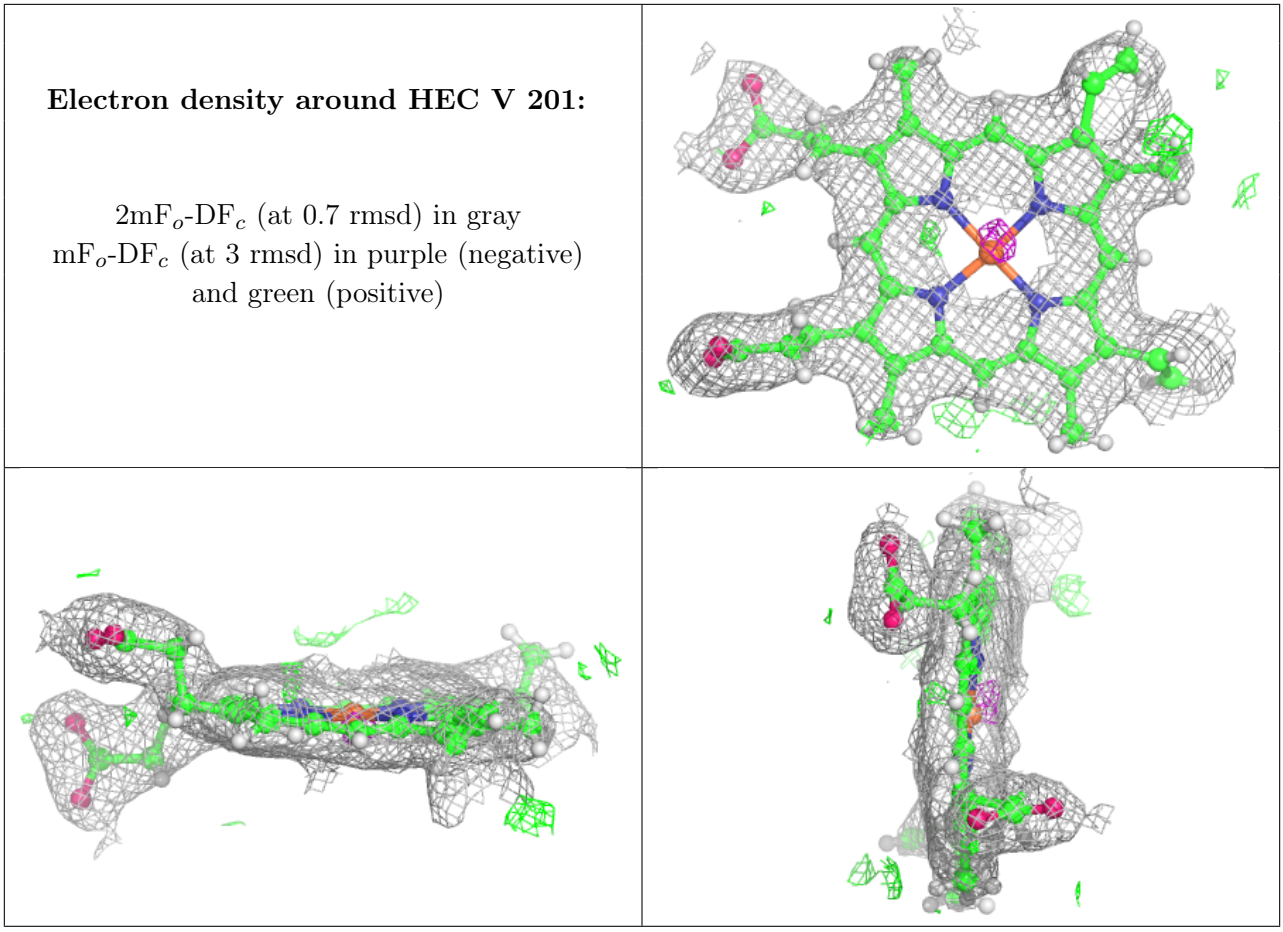






Electron density around HEC V 201:

$2mF_o$-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.