Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 11:34 PM EDT

PDB ID	:	5KAF
Title	:	RT XFEL structure of Photosystem II in the dark state at 3.0 A resolution
Authors	:	Young, I.D.; Ibrahim, M.; Chatterjee, R.; Gul, S.; Koroidov, S.; Brewster, A.S.; Tran, R.; Alonso-Mori, R.; Fuller, F.; Kroll, T.; Michels-Clark, T.; Laksmono, H.; Sierra, R.G.; Stan, C.A.; Saracini, C.; Bean, M.A.; Seuffert, I.; Sokaras, D.; Weng, T.-C.; Hunter, M.S.; Aquila, A.; Koglin, J.E.; Robinson, J.; Liang, M.; Boutet, S.; Lyubimov, A.Y.; Uervirojnangkoorn, M.; Moriarty, N.W.; Liebschner, D.; Afonine, P.V.; Waterman, D.G.; Evans, G.; Dobbek, H.; Weis, W.I.; Brunger, A.T.; Zwart, P.H.; Adams, P.D.; Zouni, A.; Messinger, J.; Bergmann, U.; Sauter, N.K.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on	:	2016-06-01
Resolution	:	3.00 Å(reported)

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

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

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

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

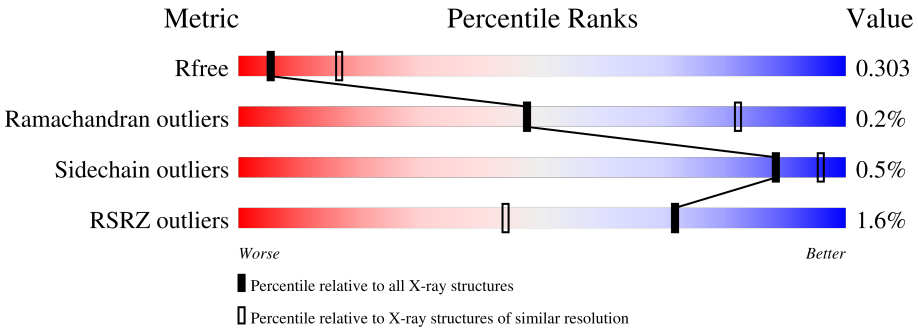
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

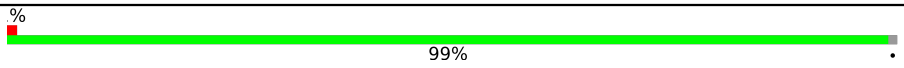
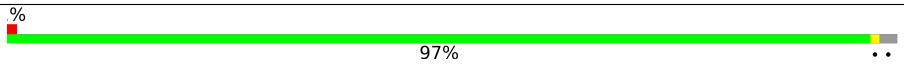
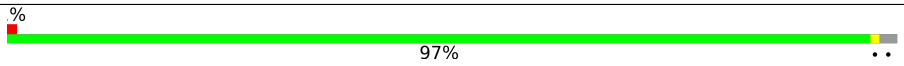
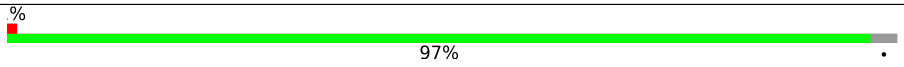
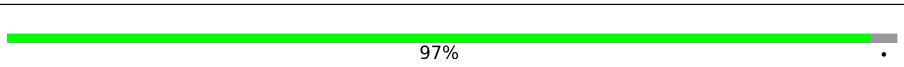
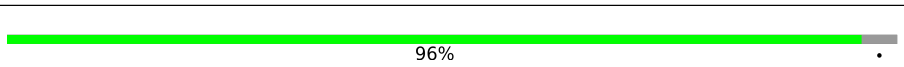
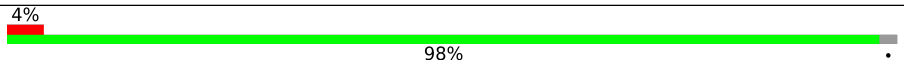
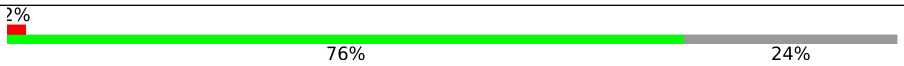
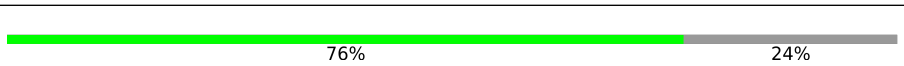
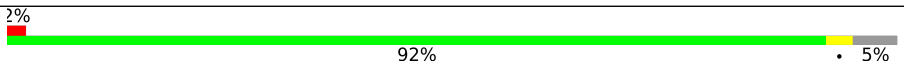
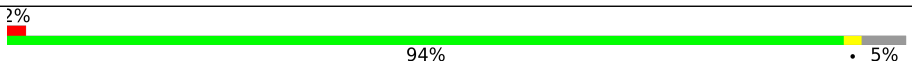
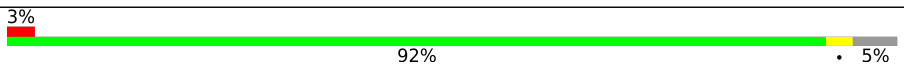
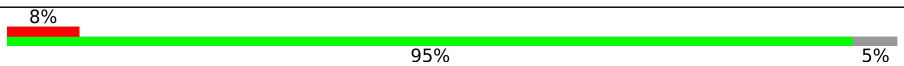
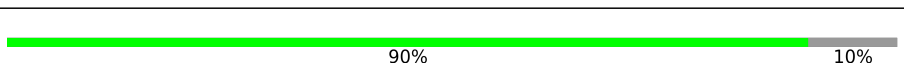
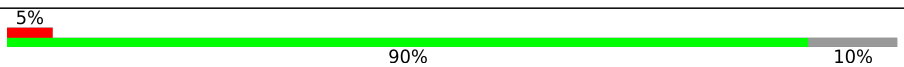
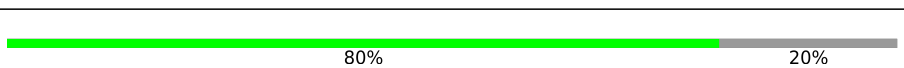
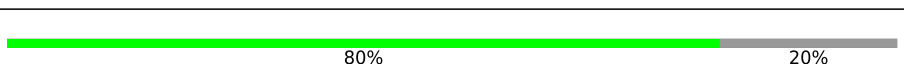
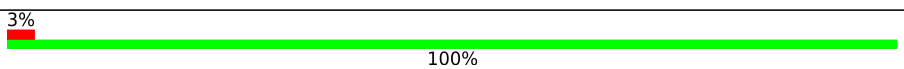
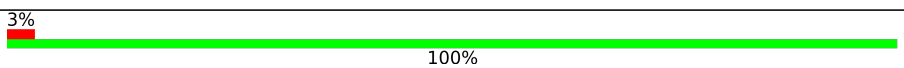
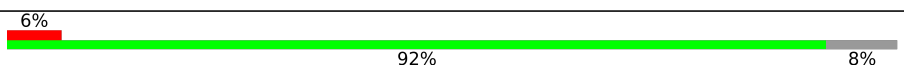
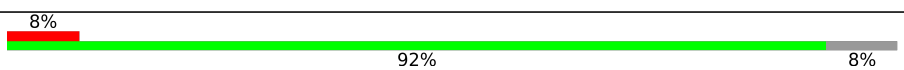
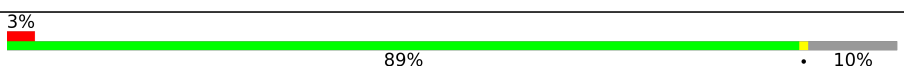
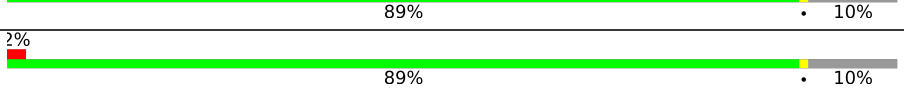
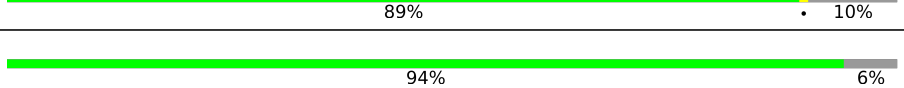
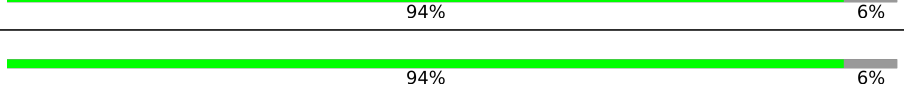
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	97%
1	a	344	97%
2	B	510	2% 99%

Continued on next page...

Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	U	134	72% 28%
15	u	134	72% 28%
16	V	163	84% 16%
16	v	163	% 83% 16%
17	Y	46	7% 63% 35%
17	y	46	4% 65% 35%
18	X	41	5% 93% 7%
18	x	41	5% 93% 7%
19	Z	62	8% 95% 5%
19	z	62	13% 98%
20	R	41	7% 83% 17%
20	r	41	80% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	A	606	X	-	-	-
25	CLA	A	607	X	-	-	-
25	CLA	A	609	X	-	-	-
25	CLA	A	615	X	-	-	-
25	CLA	B	601	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	B	616	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	a	606	X	-	-	-
25	CLA	a	607	X	-	-	-
25	CLA	a	609	X	-	-	-
25	CLA	a	612	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	b	618	X	-	-	-
25	CLA	b	619	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	c	514	X	-	-	-
25	CLA	c	515	X	-	-	-
25	CLA	d	404	X	-	-	-
29	LMG	b	625	-	-	-	X

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 50162 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2618	1715	431	457	15			
1	a	334	Total	C	N	O	S	0	0	0
			2613	1713	428	457	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3953	2596	658	686	13			
2	b	504	Total	C	N	O	S	3	1	0
			3960	2600	658	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	0	0
			2716	1800	444	460	12			
4	d	341	Total	C	N	O	S	0	0	0
			2709	1798	441	458	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total 657	C 429	N 106	O 122	0	0	0
5	e	82	Total 665	C 434	N 108	O 123	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total 274	C 187	N 45	O 41	S 1	0	0	0
6	f	34	Total 274	C 187	N 45	O 41	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total 498	C 333	N 80	O 83	S 2	0	0	0
7	h	63	Total 498	C 333	N 80	O 83	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total 296	C 200	N 46	O 49	S 1	0	0	0
8	i	36	Total 296	C 200	N 46	O 49	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	expression tag	UNP Q8DJZ6
i	1	FME	-	expression tag	UNP Q8DJZ6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total 257	C 174	N 40	O 42	S 1	0	0	0
9	j	36	Total 257	C 174	N 40	O 42	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	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	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			
12	m	33	Total	C	N	O	S	0	0	0
			256	171	37	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	expression tag	UNP Q8DHA7
m	1	FME	-	expression tag	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	0	0
			1845	1154	309	378	4			
13	o	244	Total	C	N	O	S	0	0	0
			1853	1160	312	377	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	expression tag	UNP Q8DIQ0
t	1	FME	-	expression tag	UNP Q8DIQ0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O	0	0	0
			279	187	45	47			
18	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

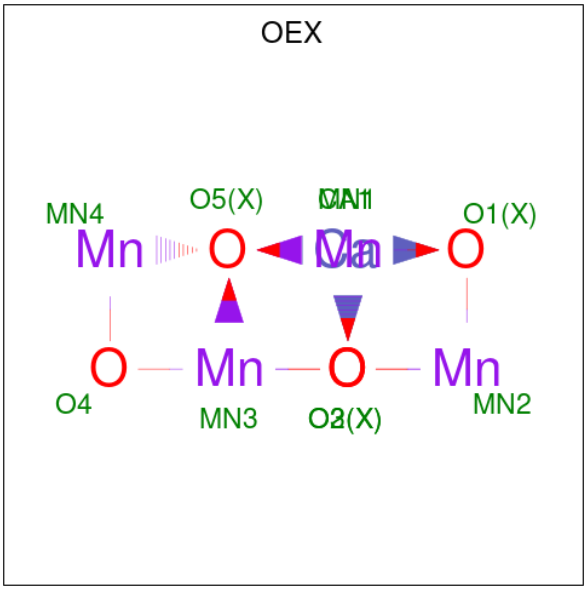
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			
20	r	34	Total	C	N	O	0	0	0
			273	186	47	40			

- 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	0
			10	1	4	5		
21	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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

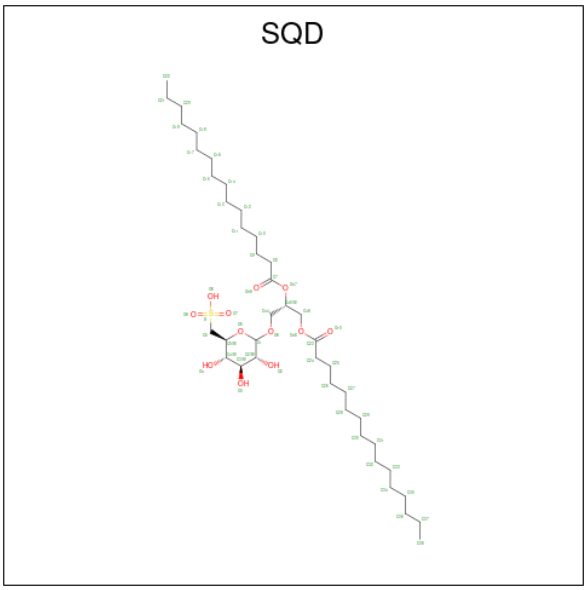
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

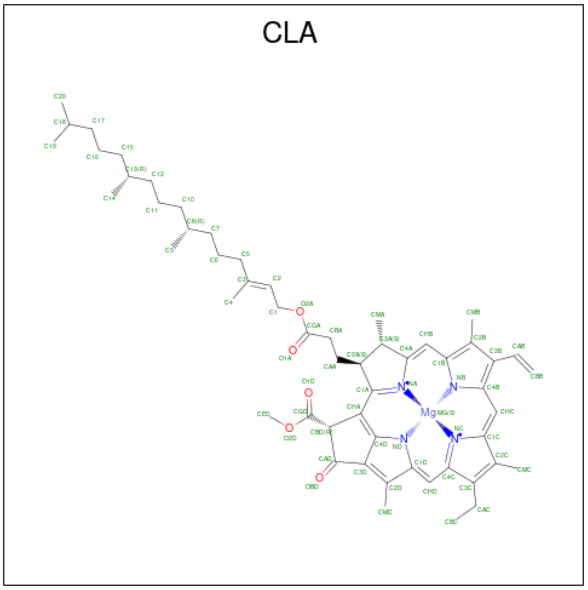


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 52 39 12 1	0	0
23	A	1	Total C O 40 35 5	0	0
23	B	1	Total C O S 54 41 12 1	0	0
23	D	1	Total C O S 47 34 12 1	0	0
23	D	1	Total C O S 43 30 12 1	0	0
23	I	1	Total C O 40 35 5	0	0
23	b	1	Total C O S 54 41 12 1	0	0
23	c	1	Total C O S 54 41 12 1	0	0
23	f	1	Total C O S 43 30 12 1	0	0

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

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 57 47 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	A	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0
25	B	1	Total C Mg N O 65 55 1 4 5	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

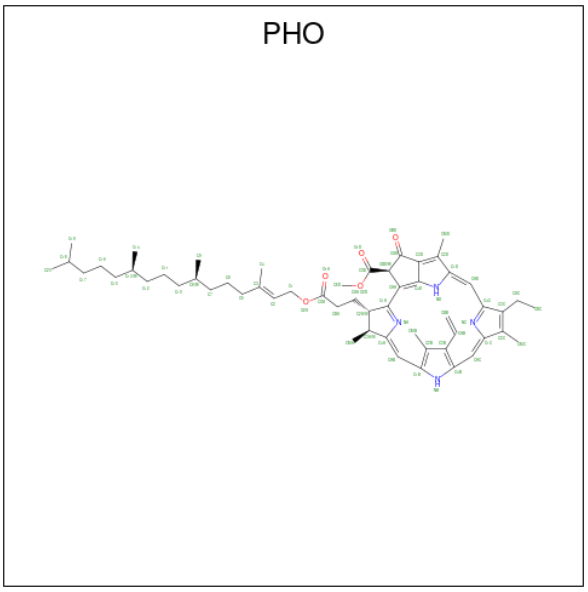
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

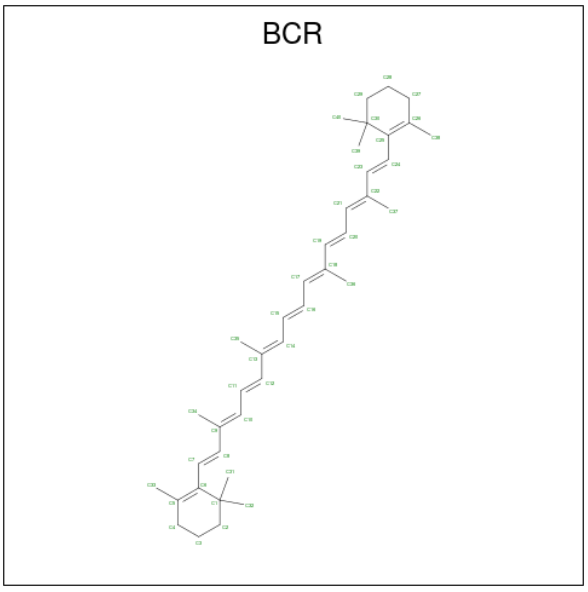
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
25	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



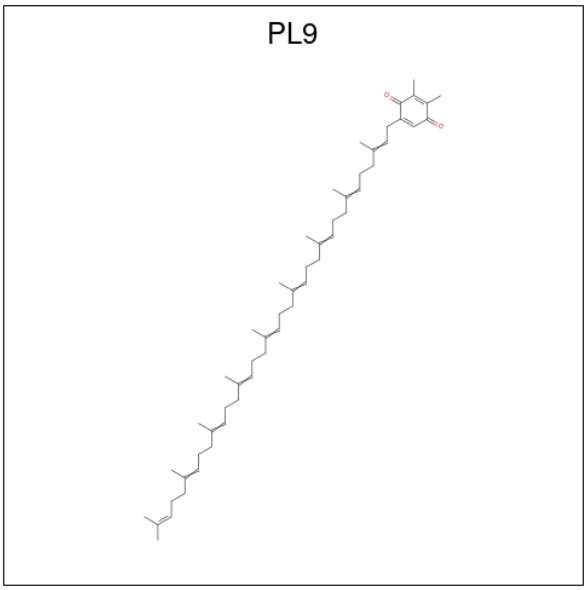
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			64	55	4	5		
26	D	1	Total	C	N	O	0	0
			64	55	4	5		
26	a	1	Total	C	N	O	0	0
			64	55	4	5		
26	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



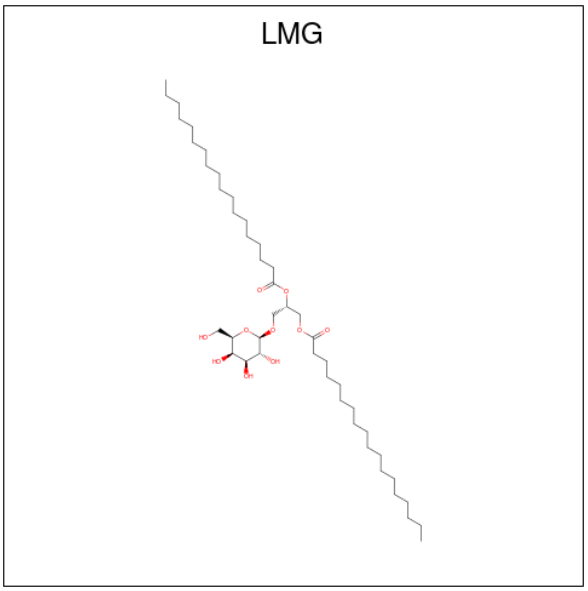
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	K	1	Total C 40 40	0	0
27	T	1	Total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

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



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	A	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	D	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	b	1	Total C 9 9	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0

Continued on next page...

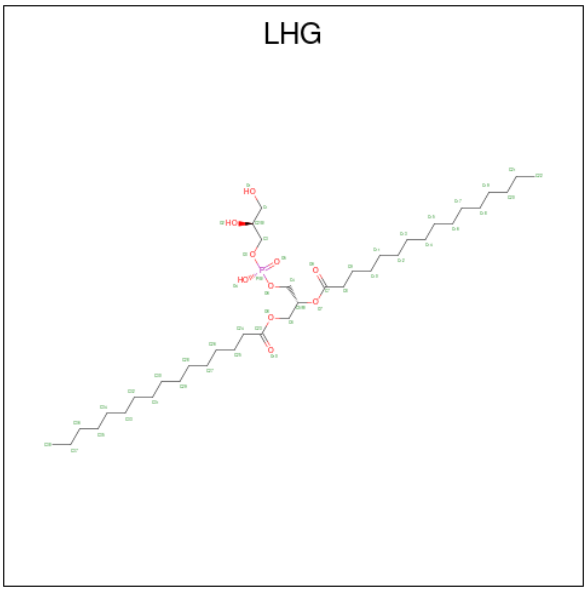
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	d	1	Total C O 42 32 10	0	0
29	d	1	Total C O 40 35 5	0	0

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

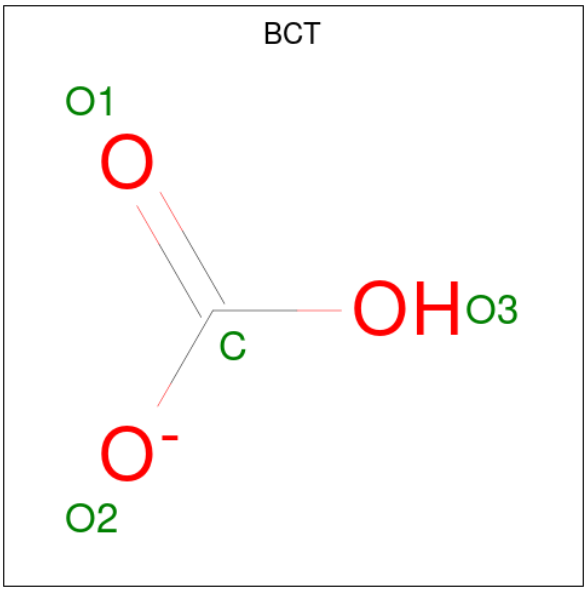
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C 7 7	0	0
30	B	3	Total C 28 28	0	0
30	C	1	Total C 9 9	0	0
30	H	1	Total C 8 8	0	0
30	M	2	Total C 23 23	0	0
30	b	2	Total C 26 26	0	0
30	d	1	Total C 22 22	0	0
30	i	1	Total C 12 12	0	0
30	j	1	Total C 9 9	0	0
30	m	2	Total C 21 21	0	0
30	t	1	Total C 10 10	0	0
30	z	1	Total C 11 11	0	0

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



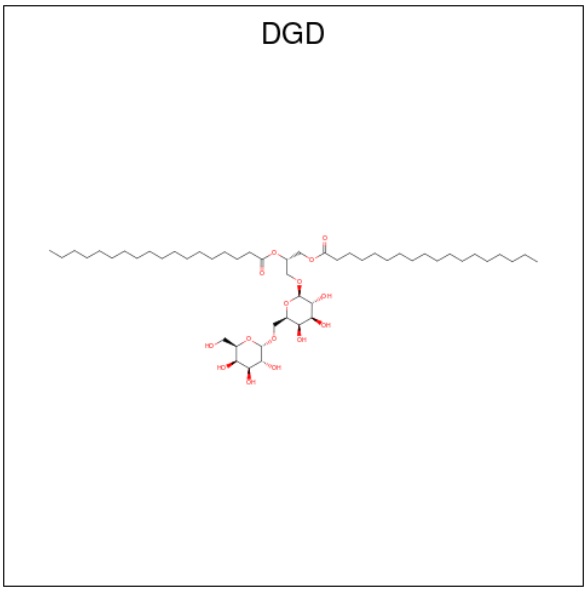
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			35	24	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 4 1 3	0	0
32	a	1	Total C O 4 1 3	0	0

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



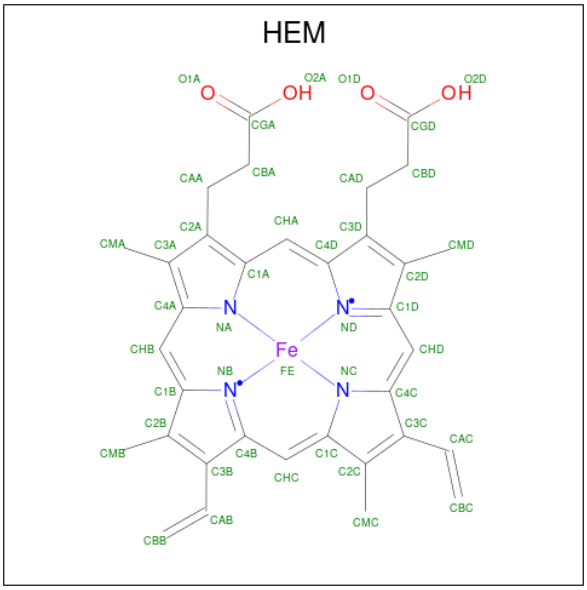
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0

Continued on next page...

Continued from previous page...

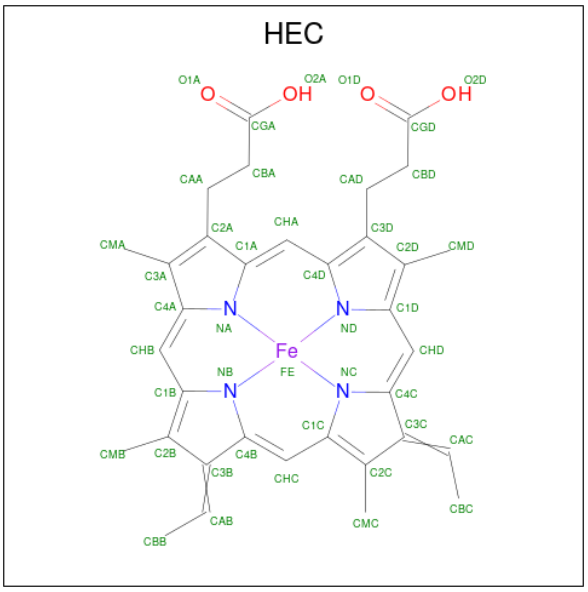
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 62 47 15	0	0
33	C	1	Total C O 62 47 15	0	0
33	H	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	c	1	Total C O 62 47 15	0	0
33	h	1	Total C O 62 47 15	0	0

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



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

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	10	Total	O	0	0
			10	10		
36	B	17	Total	O	0	0
			17	17		
36	C	11	Total	O	0	0
			11	11		
36	D	9	Total	O	0	0
			9	9		
36	E	3	Total	O	0	0
			3	3		
36	L	2	Total	O	0	0
			2	2		
36	M	2	Total	O	0	0
			2	2		
36	O	5	Total	O	0	0
			5	5		
36	T	1	Total	O	0	0
			1	1		
36	V	2	Total	O	0	0
			2	2		

Continued on next page...

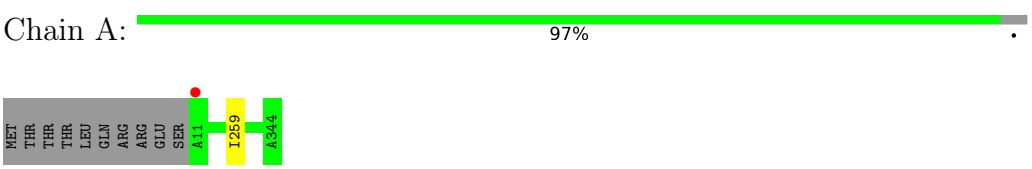
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	X	1	Total O 1 1	0	0
36	Z	1	Total O 1 1	0	0
36	a	11	Total O 11 11	0	0
36	b	12	Total O 12 12	0	0
36	c	11	Total O 11 11	0	0
36	d	9	Total O 9 9	0	0
36	i	1	Total O 1 1	0	0
36	l	2	Total O 2 2	0	0
36	o	9	Total O 9 9	0	0
36	u	2	Total O 2 2	0	0
36	v	3	Total O 3 3	0	0

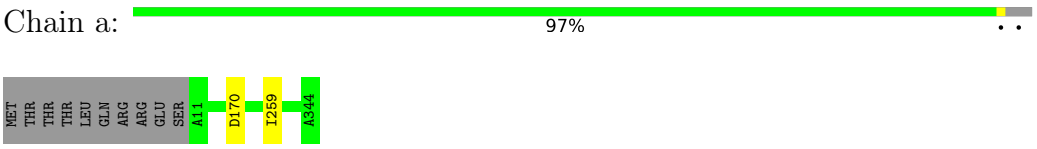
3 Residue-property plots (i)

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

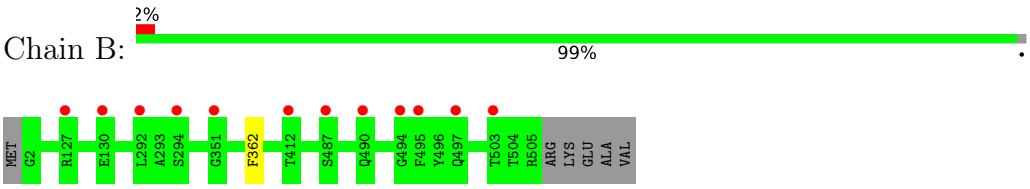
• Molecule 1: Photosystem II protein D1 1



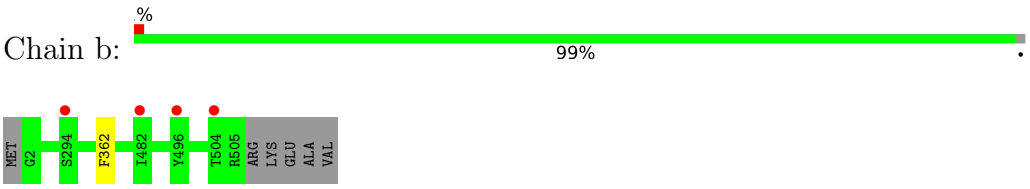
• Molecule 1: Photosystem II protein D1 1



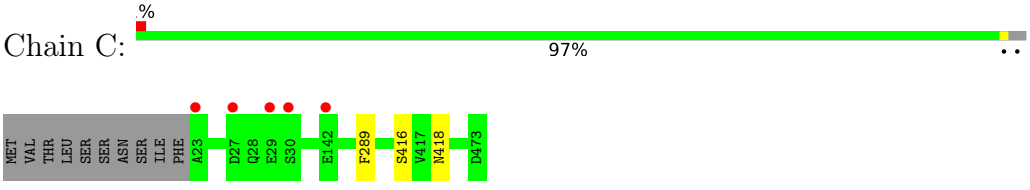
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 2: Photosystem II CP47 reaction center protein

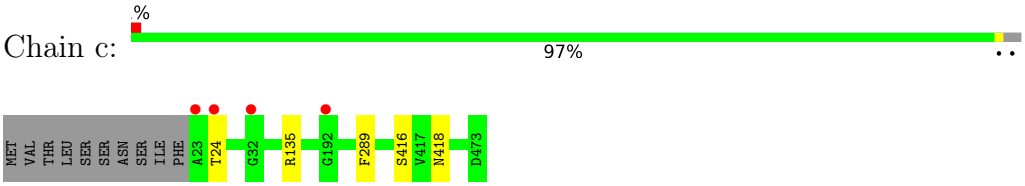


• Molecule 3: Photosystem II CP43 reaction center protein



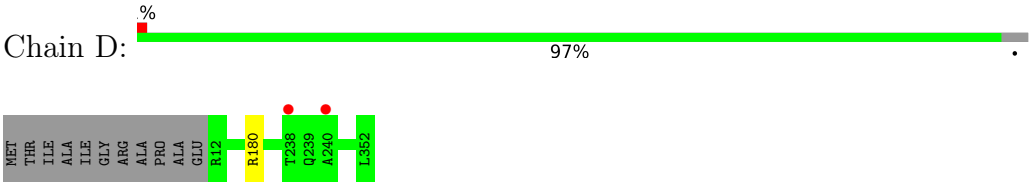
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



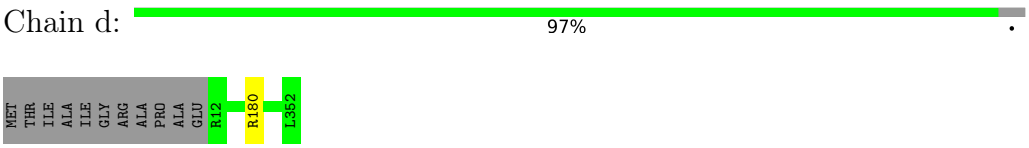
• Molecule 4: Photosystem II D2 protein

Chain D:



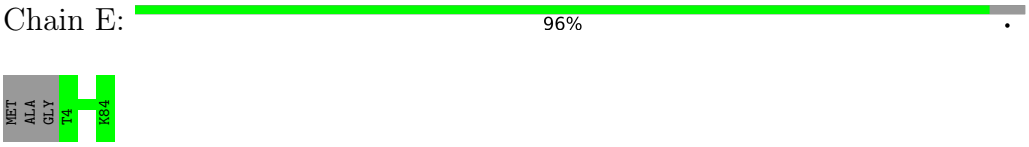
• Molecule 4: Photosystem II D2 protein

Chain d:



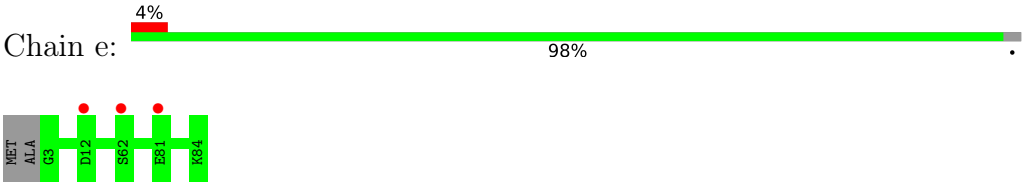
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



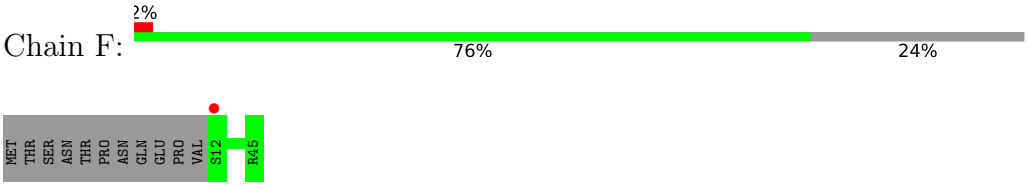
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



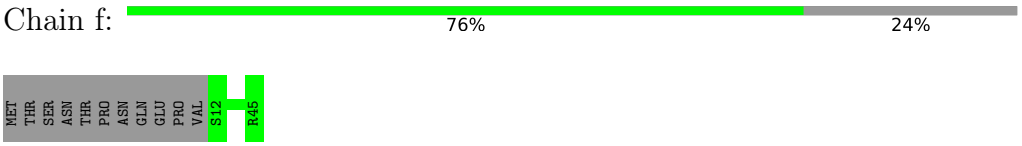
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



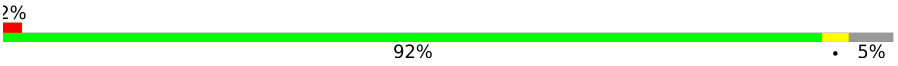
• Molecule 6: Cytochrome b559 subunit beta

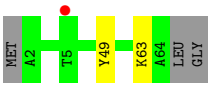
Chain f:



• Molecule 7: Photosystem II reaction center protein H

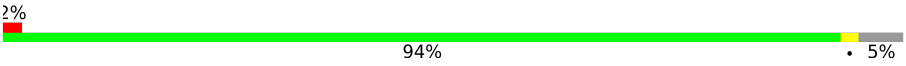
Chain H:

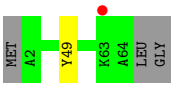




• Molecule 7: Photosystem II reaction center protein H

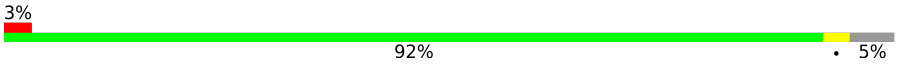
Chain h:

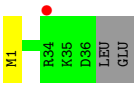




• Molecule 8: Photosystem II reaction center protein I

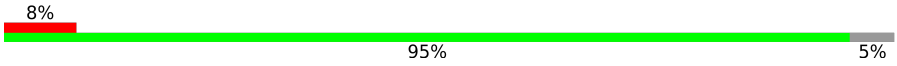
Chain I:

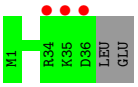




• Molecule 8: Photosystem II reaction center protein I

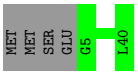
Chain i:





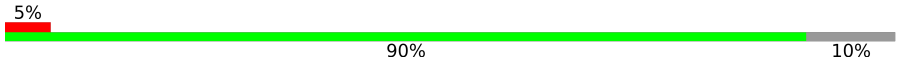
• Molecule 9: Photosystem II reaction center protein J

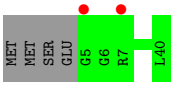
Chain J:



• Molecule 9: Photosystem II reaction center protein J

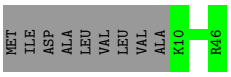
Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

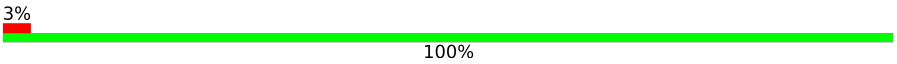


• Molecule 10: Photosystem II reaction center protein K

Chain k:

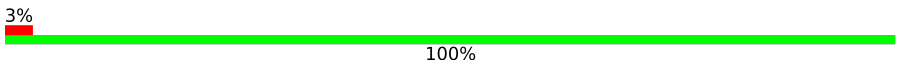
• Molecule 11: Photosystem II reaction center protein L

Chain L:



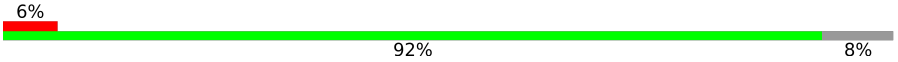
• Molecule 11: Photosystem II reaction center protein L

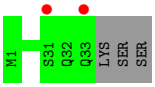
Chain l:



• Molecule 12: Photosystem II reaction center protein M

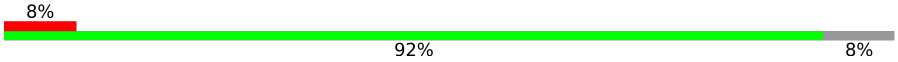
Chain M:

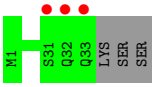




• Molecule 12: Photosystem II reaction center protein M

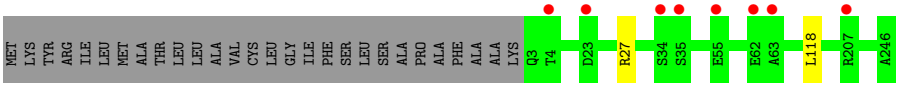
Chain m:





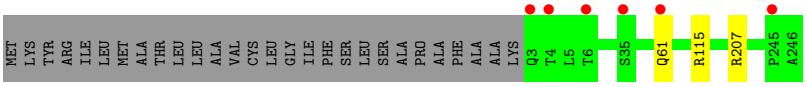
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



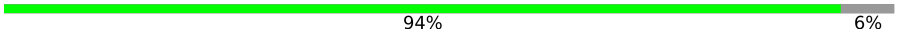
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



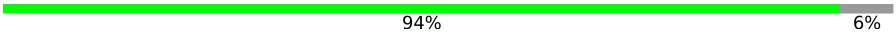
• Molecule 14: Photosystem II reaction center protein T

Chain T:



• Molecule 14: Photosystem II reaction center protein T

Chain t:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

• Molecule 15: Photosystem II 12 kDa extrinsic protein

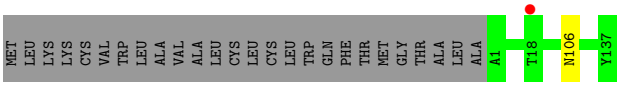
Chain u:

• Molecule 16: Cytochrome c-550

Chain V:

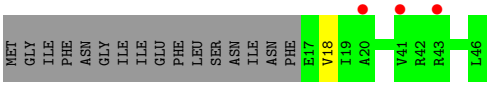
• Molecule 16: Cytochrome c-550

Chain v:

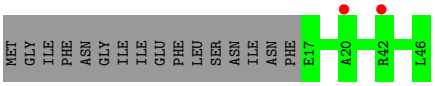


• Molecule 17: Photosystem II reaction center protein Ycf12

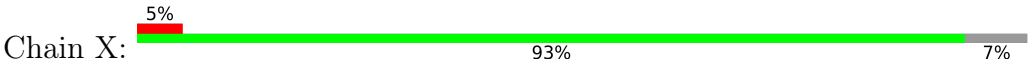
Chain Y:

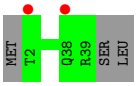


• Molecule 17: Photosystem II reaction center protein Ycf12

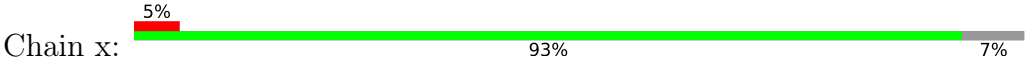


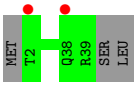
• Molecule 18: Photosystem II reaction center X protein



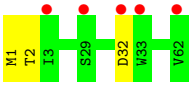


• Molecule 18: Photosystem II reaction center X protein

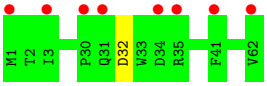




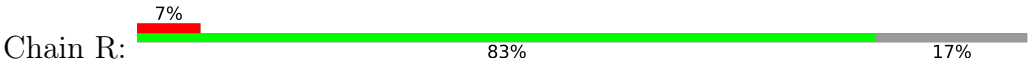
• Molecule 19: Photosystem II reaction center protein Z

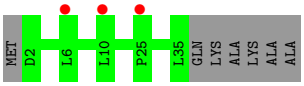


• Molecule 19: Photosystem II reaction center protein Z



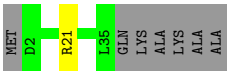
• Molecule 20: Photosystem II protein Y





• Molecule 20: Photosystem II protein Y

Chain r:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.73Å 223.81Å 330.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.12 – 3.00 43.12 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.12-3.00) 86.3 (43.12-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX dev_2411	Depositor
R, R_{free}	0.264 , 0.303 0.264 , 0.303	Depositor DCC
R_{free} test set	1446 reflections (0.85%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 56.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	50162	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/2703	0.39	0/3687
1	a	0.24	0/2698	0.39	0/3681
2	B	0.25	0/4093	0.39	0/5580
2	b	0.25	0/4103	0.39	0/5593
3	C	0.24	0/3599	0.39	0/4900
3	c	0.24	0/3599	0.38	0/4900
4	D	0.25	0/2811	0.39	0/3830
4	d	0.25	0/2804	0.39	0/3821
5	E	0.30	0/676	0.39	0/924
5	e	0.23	0/684	0.39	0/933
6	F	0.24	0/283	0.37	0/386
6	f	0.24	0/283	0.37	0/386
7	H	0.24	0/511	0.41	0/697
7	h	0.24	0/511	0.40	0/697
8	I	0.24	0/293	0.37	0/396
8	i	0.25	0/293	0.38	0/396
9	J	0.24	0/263	0.37	0/356
9	j	0.24	0/263	0.38	0/356
10	K	0.25	0/303	0.40	0/416
10	k	0.25	0/303	0.37	0/416
11	L	0.24	0/308	0.37	0/419
11	l	0.23	0/308	0.36	0/419
12	M	0.24	0/249	0.35	0/341
12	m	0.24	0/249	0.35	0/341
13	O	0.24	0/1876	0.45	0/2549
13	o	0.24	0/1884	0.45	0/2557
14	T	0.26	0/257	0.35	0/349
14	t	0.26	0/257	0.36	0/349
15	U	0.23	0/785	0.40	0/1064
15	u	0.24	0/785	0.41	0/1064
16	V	0.23	0/1085	0.40	0/1473
16	v	0.22	0/1085	0.41	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Y	0.27	0/225	0.54	0/301
17	y	0.24	0/225	0.37	0/301
18	X	0.23	0/282	0.35	0/381
18	x	0.24	0/284	0.37	0/384
19	Z	0.23	0/490	0.34	0/669
19	z	0.24	0/490	0.36	0/669
20	R	0.21	0/279	0.36	0/383
20	r	0.22	0/279	0.39	0/383
All	All	0.24	0/42758	0.39	0/58220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	41	76
1	a	332/344 (96%)	320 (96%)	11 (3%)	1 (0%)	41	76
2	B	502/510 (98%)	483 (96%)	19 (4%)	0	100	100
2	b	503/510 (99%)	486 (97%)	17 (3%)	0	100	100
3	C	449/461 (97%)	436 (97%)	12 (3%)	1 (0%)	47	82
3	c	449/461 (97%)	430 (96%)	17 (4%)	2 (0%)	34	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	339/352 (96%)	328 (97%)	11 (3%)	0	100	100
4	d	339/352 (96%)	324 (96%)	15 (4%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	9	40
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
13	O	242/272 (89%)	228 (94%)	14 (6%)	0	100	100
13	o	242/272 (89%)	232 (96%)	9 (4%)	1 (0%)	34	72
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
15	u	95/134 (71%)	90 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	128 (95%)	7 (5%)	0	100	100
16	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
17	Y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	3	19
17	y	28/46 (61%)	28 (100%)	0	0	100	100
18	X	36/41 (88%)	36 (100%)	0	0	100	100
18	x	36/41 (88%)	32 (89%)	4 (11%)	0	100	100
19	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	z	60/62 (97%)	57 (95%)	3 (5%)	0	100 100
20	R	32/41 (78%)	32 (100%)	0	0	100 100
20	r	32/41 (78%)	32 (100%)	0	0	100 100
All	All	5240/5700 (92%)	5040 (96%)	190 (4%)	10 (0%)	47 82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Y	18	VAL
19	Z	32	ASP
13	o	61	GLN
3	C	416	SER
7	H	63	LYS
3	c	24	THR
3	c	416	SER
19	Z	2	THR
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	269/280 (96%)	269 (100%)	0	100 100
1	a	268/280 (96%)	267 (100%)	1 (0%)	91 97
2	B	398/407 (98%)	397 (100%)	1 (0%)	92 97
2	b	400/407 (98%)	399 (100%)	1 (0%)	92 97
3	C	352/362 (97%)	350 (99%)	2 (1%)	86 95
3	c	352/362 (97%)	349 (99%)	3 (1%)	78 92
4	D	276/283 (98%)	275 (100%)	1 (0%)	91 97
4	d	274/283 (97%)	273 (100%)	1 (0%)	91 97
5	E	71/73 (97%)	71 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	72/73 (99%)	72 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	27 (100%)	0	100	100
7	H	53/55 (96%)	52 (98%)	1 (2%)	57	84
7	h	53/55 (96%)	52 (98%)	1 (2%)	57	84
8	I	32/34 (94%)	32 (100%)	0	100	100
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	28 (100%)	0	100	100
13	O	200/228 (88%)	198 (99%)	2 (1%)	76	91
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	91
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	84/112 (75%)	84 (100%)	0	100	100
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	90
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	116 (99%)	1 (1%)	78	92
17	Y	23/37 (62%)	23 (100%)	0	100	100
17	y	23/37 (62%)	23 (100%)	0	100	100
18	X	30/34 (88%)	30 (100%)	0	100	100
18	x	31/34 (91%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	84
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	84
20	R	29/33 (88%)	29 (100%)	0	100	100
20	r	29/33 (88%)	28 (97%)	1 (3%)	37	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4313/4654 (93%)	4292 (100%)	21 (0%)	88 96

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
3	C	289	PHE
3	C	418	ASN
4	D	180	ARG
7	H	49	TYR
13	O	27	ARG
13	O	118	LEU
19	Z	1	MET
1	a	170	ASP
2	b	362	PHE
3	c	135	ARG
3	c	289	PHE
3	c	418	ASN
4	d	180	ARG
7	h	49	TYR
13	o	115	ARG
13	o	207	ARG
15	u	86	GLU
16	v	106	ASN
19	z	32	ASP
20	r	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	216	HIS
2	B	223	GLN
2	B	289	GLN
4	D	332	GLN
13	O	196	GLN
19	Z	31	GLN
2	b	216	HIS
2	b	289	GLN
2	b	374	ASN
4	d	332	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	m	5	GLN
13	o	104	GLN
16	v	118	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	FME	t	1	14	8,9,10	0.94	0	7,9,11	0.87	0
8	FME	I	1	8	8,9,10	0.85	0	7,9,11	1.74	2 (28%)
8	FME	i	1	8	8,9,10	0.93	0	7,9,11	0.86	0
12	FME	m	1	12	8,9,10	0.93	0	7,9,11	0.87	0
14	FME	T	1	14	8,9,10	0.93	0	7,9,11	0.94	0
12	FME	M	1	12	8,9,10	0.94	0	7,9,11	0.81	0

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	1	FME	C-CA-N	3.53	116.10	109.73
8	I	1	FME	CA-N-CN	2.44	126.57	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
8	i	1	FME	CB-CA-N-CN
12	m	1	FME	N-CA-CB-CG
12	m	1	FME	C-CA-CB-CG
14	T	1	FME	CA-CB-CG-SD
12	M	1	FME	CA-CB-CG-SD
8	i	1	FME	CB-CG-SD-CE
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 174 ligands modelled in this entry, 6 are monoatomic and 17 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	$\#\|Z\|>2$
25	CLA	c	508	-	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)
35	HEC	V	201	16	32,50,50	2.10	5 (15%)	24,82,82	1.56	4 (16%)
29	LMG	B	621	-	51,51,55	0.73	0	59,59,63	1.39	6 (10%)
27	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
25	CLA	B	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.26	8 (10%)
25	CLA	B	602	-	65,73,73	1.48	5 (7%)	76,113,113	1.25	8 (10%)
33	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.43	9 (11%)
25	CLA	B	601	36	65,73,73	1.47	5 (7%)	76,113,113	1.32	8 (10%)
25	CLA	D	402	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	7 (9%)
26	PHO	a	608	-	51,69,69	1.00	4 (7%)	47,99,99	1.12	4 (8%)
25	CLA	A	609	-	65,73,73	1.48	5 (7%)	76,113,113	1.34	9 (11%)
25	CLA	b	618	-	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
29	LMG	B	625	-	51,51,55	0.83	3 (5%)	59,59,63	1.40	8 (13%)
31	LHG	l	101	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	C	501	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	8 (10%)
29	LMG	C	519	-	51,51,55	0.72	1 (1%)	59,59,63	1.33	6 (10%)
27	BCR	c	516	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
27	BCR	b	621	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	4 (7%)
23	SQD	f	101	-	42,43,54	1.07	5 (11%)	51,54,65	1.65	11 (21%)
27	BCR	H	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	7 (12%)
27	BCR	K	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
33	DGD	H	103	-	63,63,67	0.87	1 (1%)	77,77,81	1.34	7 (9%)
27	BCR	C	514	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	7 (12%)
26	PHO	d	401	-	51,69,69	0.99	3 (5%)	47,99,99	1.13	4 (8%)
29	LMG	c	522	-	51,51,55	0.79	1 (1%)	59,59,63	1.37	6 (10%)
25	CLA	a	607	36	59,67,73	1.55	6 (10%)	68,105,113	1.34	8 (11%)
26	PHO	A	608	-	51,69,69	1.00	4 (7%)	47,99,99	1.10	4 (8%)
25	CLA	c	511	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	8 (10%)
27	BCR	C	515	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	7 (12%)
25	CLA	B	608	-	65,73,73	1.48	5 (7%)	76,113,113	1.29	8 (10%)
27	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	8 (14%)
23	SQD	A	603	-	51,52,54	0.97	5 (9%)	60,63,65	1.59	11 (18%)
31	LHG	A	618	-	48,48,48	0.65	1 (2%)	51,54,54	1.24	7 (13%)
25	CLA	b	610	36	65,73,73	1.47	5 (7%)	76,113,113	1.28	7 (9%)
27	BCR	b	620	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LHG	a	614	-	34,34,48	0.72	0	37,40,54	1.19	3 (8%)
25	CLA	c	514	-	65,73,73	1.46	5 (7%)	76,113,113	1.39	8 (10%)
25	CLA	c	509	36	65,73,73	1.49	5 (7%)	76,113,113	1.35	7 (9%)
25	CLA	B	610	36	65,73,73	1.48	5 (7%)	76,113,113	1.22	8 (10%)
23	SQD	B	626	-	53,54,54	0.95	4 (7%)	62,65,65	1.65	12 (19%)
25	CLA	b	617	-	65,73,73	1.48	6 (9%)	76,113,113	1.29	7 (9%)
27	BCR	Y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	4 (7%)
25	CLA	C	507	36	65,73,73	1.47	5 (7%)	76,113,113	1.36	7 (9%)
25	CLA	C	506	-	65,73,73	1.50	5 (7%)	76,113,113	1.30	9 (11%)
25	CLA	c	515	-	65,73,73	1.47	5 (7%)	76,113,113	1.30	8 (10%)
29	LMG	C	520	-	51,51,55	0.78	1 (1%)	59,59,63	1.36	7 (11%)
33	DGD	h	102	-	63,63,67	0.87	1 (1%)	77,77,81	1.32	8 (10%)
33	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	10 (12%)
25	CLA	b	619	-	65,73,73	1.45	6 (9%)	76,113,113	1.32	7 (9%)
32	BCT	a	605	22	2,3,3	1.24	0	2,3,3	2.55	1 (50%)
25	CLA	c	507	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	7 (9%)
25	CLA	C	502	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	b	606	-	65,73,73	1.49	6 (9%)	76,113,113	1.25	8 (10%)
29	LMG	A	613	-	51,51,55	0.70	0	59,59,63	1.48	9 (15%)
25	CLA	b	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.33	9 (11%)
25	CLA	B	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.28	8 (10%)
29	LMG	B	620	-	51,51,55	0.73	0	59,59,63	1.34	6 (10%)
23	SQD	D	408	-	46,47,54	1.00	4 (8%)	55,58,65	1.78	11 (20%)
33	DGD	c	519	-	63,63,67	0.89	2 (3%)	77,77,81	1.38	8 (10%)
25	CLA	b	604	36	65,73,73	1.47	5 (7%)	76,113,113	1.33	8 (10%)
25	CLA	c	505	-	65,73,73	1.48	5 (7%)	76,113,113	1.34	8 (10%)
29	LMG	b	623	-	51,51,55	0.72	0	59,59,63	1.35	7 (11%)
25	CLA	B	614	-	65,73,73	1.47	6 (9%)	76,113,113	1.28	7 (9%)
27	BCR	D	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	7 (12%)
25	CLA	A	607	36	57,65,73	1.56	6 (10%)	66,103,113	1.38	9 (13%)
27	BCR	T	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)
28	PL9	D	407	-	55,55,55	0.99	4 (7%)	68,69,69	1.53	13 (19%)
25	CLA	B	605	-	65,73,73	1.49	6 (9%)	76,113,113	1.28	7 (9%)
27	BCR	y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	5 (8%)
25	CLA	B	607	36	65,73,73	1.47	5 (7%)	76,113,113	1.24	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	a	606	-	65,73,73	1.46	6 (9%)	76,113,113	1.30	8 (10%)
23	SQD	b	601	-	53,54,54	0.96	5 (9%)	62,65,65	1.45	9 (14%)
29	LMG	d	409	-	39,39,55	0.56	0	41,41,63	1.29	3 (7%)
25	CLA	b	616	-	65,73,73	1.47	5 (7%)	76,113,113	1.33	8 (10%)
33	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	1.40	8 (10%)
35	HEC	v	201	16	32,50,50	2.12	4 (12%)	24,82,82	1.55	3 (12%)
25	CLA	C	504	36	65,73,73	1.46	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	a	612	36	65,73,73	1.47	5 (7%)	76,113,113	1.30	7 (9%)
25	CLA	b	609	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	7 (9%)
27	BCR	b	622	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	7 (12%)
31	LHG	A	617	-	48,48,48	0.61	0	51,54,54	1.24	6 (11%)
25	CLA	C	508	-	65,73,73	1.48	5 (7%)	76,113,113	1.31	9 (11%)
31	LHG	D	406	-	48,48,48	0.62	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	c	503	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	9 (11%)
31	LHG	a	615	-	41,41,48	0.67	1 (2%)	44,47,54	1.30	6 (13%)
23	SQD	A	619	-	39,39,54	0.88	2 (5%)	41,41,65	1.17	2 (4%)
27	BCR	k	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
32	BCT	A	620	22	2,3,3	1.26	0	2,3,3	2.67	2 (100%)
25	CLA	C	511	3	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
26	PHO	D	401	-	51,69,69	0.98	3 (5%)	47,99,99	1.13	4 (8%)
25	CLA	c	513	3	65,73,73	1.47	5 (7%)	76,113,113	1.37	8 (10%)
29	LMG	b	624	-	51,51,55	0.75	0	59,59,63	1.30	6 (10%)
29	LMG	b	625	-	8,8,55	0.14	0	7,7,63	0.92	0
25	CLA	B	616	-	65,73,73	1.46	6 (9%)	76,113,113	1.35	8 (10%)
25	CLA	B	615	-	65,73,73	1.49	5 (7%)	76,113,113	1.33	8 (10%)
27	BCR	B	627	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	7 (12%)
29	LMG	d	406	-	42,42,55	0.79	0	50,50,63	1.31	6 (12%)
25	CLA	C	509	-	65,73,73	1.45	5 (7%)	76,113,113	1.34	7 (9%)
28	PL9	d	408	-	55,55,55	0.99	4 (7%)	68,69,69	1.51	13 (19%)
25	CLA	b	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	c	510	-	58,66,73	1.56	5 (8%)	67,104,113	1.38	9 (13%)
31	LHG	a	613	-	48,48,48	0.62	1 (2%)	51,54,54	1.28	6 (11%)
21	OEX	A	601	3,36,1	0,15,15	-	-	-		
23	SQD	D	409	-	42,43,54	1.07	5 (11%)	51,54,65	1.62	11 (21%)
31	LHG	A	616	-	48,48,48	0.62	2 (4%)	51,54,54	1.27	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	CLA	b	612	-	65,73,73	1.49	5 (7%)	76,113,113	1.30	8 (10%)
25	CLA	c	504	-	65,73,73	1.47	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	A	615	36	65,73,73	1.46	5 (7%)	76,113,113	1.29	7 (9%)
25	CLA	b	608	-	65,73,73	1.49	6 (9%)	76,113,113	1.29	8 (10%)
25	CLA	C	510	-	65,73,73	1.47	6 (9%)	76,113,113	1.28	8 (10%)
25	CLA	a	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.27	9 (11%)
25	CLA	C	505	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	c	512	-	65,73,73	1.46	5 (7%)	76,113,113	1.32	8 (10%)
25	CLA	B	611	-	65,73,73	1.48	5 (7%)	76,113,113	1.33	9 (11%)
27	BCR	B	617	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)
34	HEM	e	101	6,5	41,50,50	1.47	4 (9%)	45,82,82	1.41	7 (15%)
25	CLA	B	612	-	65,73,73	1.45	6 (9%)	76,113,113	1.34	9 (11%)
21	OEX	a	601	3,36,1	0,15,15	-	-	-		
28	PL9	a	611	-	55,55,55	0.94	3 (5%)	68,69,69	1.52	12 (17%)
27	BCR	d	405	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
33	DGD	C	517	-	63,63,67	0.90	2 (3%)	77,77,81	1.36	8 (10%)
23	SQD	I	101	-	39,39,54	0.86	2 (5%)	41,41,65	1.19	2 (4%)
25	CLA	b	613	36	65,73,73	1.47	5 (7%)	76,113,113	1.24	8 (10%)
25	CLA	b	607	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
25	CLA	b	615	-	65,73,73	1.47	7 (10%)	76,113,113	1.33	8 (10%)
25	CLA	d	404	-	65,73,73	1.46	5 (7%)	76,113,113	1.33	8 (10%)
25	CLA	B	604	-	65,73,73	1.47	5 (7%)	76,113,113	1.38	8 (10%)
25	CLA	c	506	36	65,73,73	1.46	5 (7%)	76,113,113	1.32	7 (9%)
29	LMG	c	521	-	51,51,55	0.71	0	59,59,63	1.33	6 (10%)
25	CLA	B	606	-	65,73,73	1.48	5 (7%)	76,113,113	1.33	9 (11%)
27	BCR	A	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	6 (10%)
25	CLA	D	403	-	65,73,73	1.48	5 (7%)	76,113,113	1.31	8 (10%)
25	CLA	b	605	-	65,73,73	1.49	5 (7%)	76,113,113	1.26	8 (10%)
25	CLA	C	503	-	65,73,73	1.47	6 (9%)	76,113,113	1.34	8 (10%)
29	LMG	A	612	-	51,51,55	0.72	0	59,59,63	1.31	4 (6%)
29	LMG	c	502	-	51,51,55	0.77	1 (1%)	59,59,63	1.33	6 (10%)
33	DGD	c	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.42	8 (10%)
25	CLA	C	512	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
25	CLA	d	403	-	65,73,73	1.49	5 (7%)	76,113,113	1.28	7 (9%)
25	CLA	C	513	-	65,73,73	1.46	5 (7%)	76,113,113	1.28	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	BCR	c	517	-	41,41,41	1.11	2 (4%)	56,56,56	1.19	6 (10%)
28	PL9	A	611	-	55,55,55	1.02	3 (5%)	68,69,69	1.53	13 (19%)
29	LMG	D	405	-	51,51,55	0.73	0	59,59,63	1.32	6 (10%)
27	BCR	a	610	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	5 (8%)
31	LHG	L	101	-	48,48,48	0.63	1 (2%)	51,54,54	1.24	6 (11%)
25	CLA	A	606	-	65,73,73	1.46	5 (7%)	76,113,113	1.30	8 (10%)
23	SQD	c	501	-	53,54,54	0.95	5 (9%)	62,65,65	1.51	9 (14%)
34	HEM	E	101	6,5	41,50,50	1.47	5 (12%)	45,82,82	1.36	7 (15%)
27	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	5 (8%)
25	CLA	B	613	-	65,73,73	1.46	5 (7%)	76,113,113	1.35	8 (10%)
31	LHG	d	407	-	48,48,48	0.62	1 (2%)	51,54,54	1.26	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	508	-	1/1/15/20	19/37/115/115	-
35	HEC	V	201	16	-	1/10/54/54	-
29	LMG	B	621	-	-	18/46/66/70	0/1/1/1
27	BCR	h	101	-	-	5/29/63/63	0/2/2/2
25	CLA	B	603	-	1/1/15/20	8/37/115/115	-
25	CLA	B	602	-	1/1/15/20	12/37/115/115	-
33	DGD	C	516	-	-	12/51/91/95	0/2/2/2
25	CLA	B	601	36	1/1/15/20	14/37/115/115	-
25	CLA	D	402	-	-	8/37/115/115	-
26	PHO	a	608	-	-	8/37/103/103	0/5/6/6
25	CLA	A	609	-	1/1/15/20	7/37/115/115	-
25	CLA	b	618	-	1/1/15/20	10/37/115/115	-
29	LMG	B	625	-	-	21/46/66/70	0/1/1/1
31	LHG	l	101	-	-	20/53/53/53	-
25	CLA	C	501	-	1/1/15/20	5/37/115/115	-
29	LMG	C	519	-	-	21/46/66/70	0/1/1/1
27	BCR	c	516	-	-	7/29/63/63	0/2/2/2
27	BCR	b	621	-	-	6/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	SQD	f	101	-	-	19/38/58/69	0/1/1/1
27	BCR	H	102	-	-	5/29/63/63	0/2/2/2
27	BCR	K	101	-	-	6/29/63/63	0/2/2/2
33	DGD	H	103	-	-	13/51/91/95	0/2/2/2
27	BCR	C	514	-	-	4/29/63/63	0/2/2/2
26	PHO	d	401	-	-	6/37/103/103	0/5/6/6
29	LMG	c	522	-	-	15/46/66/70	0/1/1/1
25	CLA	a	607	36	1/1/13/20	8/30/108/115	-
26	PHO	A	608	-	-	9/37/103/103	0/5/6/6
25	CLA	c	511	-	1/1/15/20	8/37/115/115	-
27	BCR	C	515	-	-	6/29/63/63	0/2/2/2
25	CLA	B	608	-	1/1/15/20	2/37/115/115	-
27	BCR	B	619	-	-	4/29/63/63	0/2/2/2
23	SQD	A	603	-	-	15/47/67/69	0/1/1/1
31	LHG	A	618	-	-	24/53/53/53	-
25	CLA	b	610	36	1/1/15/20	10/37/115/115	-
27	BCR	b	620	-	-	5/29/63/63	0/2/2/2
31	LHG	a	614	-	-	16/39/39/53	-
25	CLA	c	514	-	1/1/15/20	10/37/115/115	-
25	CLA	c	509	36	1/1/15/20	10/37/115/115	-
25	CLA	B	610	36	1/1/15/20	8/37/115/115	-
25	CLA	b	617	-	1/1/15/20	8/37/115/115	-
23	SQD	B	626	-	-	26/49/69/69	0/1/1/1
27	BCR	Y	101	-	-	10/29/63/63	0/2/2/2
25	CLA	C	507	36	1/1/15/20	5/37/115/115	-
25	CLA	C	506	-	-	17/37/115/115	-
25	CLA	c	515	-	1/1/15/20	4/37/115/115	-
29	LMG	C	520	-	-	16/46/66/70	0/1/1/1
33	DGD	h	102	-	-	10/51/91/95	0/2/2/2
33	DGD	c	520	-	-	12/51/91/95	0/2/2/2
25	CLA	b	619	-	1/1/15/20	15/37/115/115	-
25	CLA	c	507	-	-	13/37/115/115	-
25	CLA	C	502	-	-	6/37/115/115	-
25	CLA	b	606	-	1/1/15/20	7/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	A	613	-	-	15/46/66/70	0/1/1/1
25	CLA	b	614	-	1/1/15/20	5/37/115/115	-
25	CLA	B	609	-	-	12/37/115/115	-
29	LMG	B	620	-	-	16/46/66/70	0/1/1/1
23	SQD	D	408	-	-	20/42/62/69	0/1/1/1
33	DGD	c	519	-	-	19/51/91/95	0/2/2/2
25	CLA	b	604	36	1/1/15/20	18/37/115/115	-
25	CLA	c	505	-	1/1/15/20	5/37/115/115	-
29	LMG	b	623	-	-	11/46/66/70	0/1/1/1
25	CLA	B	614	-	1/1/15/20	19/37/115/115	-
27	BCR	D	404	-	-	6/29/63/63	0/2/2/2
25	CLA	A	607	36	1/1/13/20	9/28/106/115	-
27	BCR	T	101	-	-	11/29/63/63	0/2/2/2
28	PL9	D	407	-	-	9/53/73/73	0/1/1/1
27	BCR	y	101	-	-	6/29/63/63	0/2/2/2
25	CLA	B	607	36	1/1/15/20	11/37/115/115	-
25	CLA	a	606	-	1/1/15/20	3/37/115/115	-
23	SQD	b	601	-	-	18/49/69/69	0/1/1/1
29	LMG	d	409	-	-	22/41/41/70	-
25	CLA	b	616	-	1/1/15/20	9/37/115/115	-
33	DGD	C	518	-	-	15/51/91/95	0/2/2/2
35	HEC	v	201	16	-	2/10/54/54	-
25	CLA	C	504	36	1/1/15/20	7/37/115/115	-
25	CLA	a	612	36	1/1/15/20	2/37/115/115	-
25	CLA	b	609	-	1/1/15/20	8/37/115/115	-
27	BCR	b	622	-	-	6/29/63/63	0/2/2/2
31	LHG	A	617	-	-	16/53/53/53	-
25	CLA	C	508	-	1/1/15/20	6/37/115/115	-
31	LHG	D	406	-	-	20/53/53/53	-
25	CLA	c	503	-	1/1/15/20	6/37/115/115	-
31	LHG	a	615	-	-	21/46/46/53	-
23	SQD	A	619	-	-	28/41/41/69	-
27	BCR	k	101	-	-	5/29/63/63	0/2/2/2
25	CLA	C	511	3	-	4/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PHO	D	401	-	-	7/37/103/103	0/5/6/6
25	CLA	c	513	3	1/1/15/20	4/37/115/115	-
29	LMG	b	624	-	-	23/46/66/70	0/1/1/1
29	LMG	b	625	-	-	1/6/6/70	-
25	CLA	B	616	-	1/1/15/20	15/37/115/115	-
25	CLA	B	615	-	1/1/15/20	4/37/115/115	-
27	BCR	B	627	-	-	10/29/63/63	0/2/2/2
29	LMG	d	406	-	-	4/37/57/70	0/1/1/1
25	CLA	C	509	-	1/1/15/20	11/37/115/115	-
28	PL9	d	408	-	-	10/53/73/73	0/1/1/1
25	CLA	b	611	-	1/1/15/20	3/37/115/115	-
25	CLA	c	510	-	1/1/13/20	6/29/107/115	-
31	LHG	a	613	-	-	19/53/53/53	-
23	SQD	D	409	-	-	17/38/58/69	0/1/1/1
31	LHG	A	616	-	-	17/53/53/53	-
25	CLA	b	612	-	-	10/37/115/115	-
25	CLA	c	504	-	-	5/37/115/115	-
25	CLA	A	615	36	1/1/15/20	3/37/115/115	-
25	CLA	b	608	-	-	7/37/115/115	-
25	CLA	C	510	-	1/1/15/20	7/37/115/115	-
25	CLA	a	609	-	1/1/15/20	9/37/115/115	-
25	CLA	c	512	-	1/1/15/20	9/37/115/115	-
25	CLA	C	505	-	-	14/37/115/115	-
25	CLA	B	611	-	1/1/15/20	4/37/115/115	-
27	BCR	B	617	-	-	5/29/63/63	0/2/2/2
34	HEM	e	101	6,5	-	3/12/54/54	-
25	CLA	B	612	-	1/1/15/20	8/37/115/115	-
28	PL9	a	611	-	-	15/53/73/73	0/1/1/1
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2
33	DGD	C	517	-	-	17/51/91/95	0/2/2/2
23	SQD	I	101	-	-	22/41/41/69	-
25	CLA	b	613	36	1/1/15/20	8/37/115/115	-
25	CLA	b	607	-	1/1/15/20	8/37/115/115	-
25	CLA	b	615	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	d	404	-	1/1/15/20	6/37/115/115	-
25	CLA	B	604	-	1/1/15/20	8/37/115/115	-
25	CLA	c	506	36	1/1/15/20	7/37/115/115	-
29	LMG	c	521	-	-	24/46/66/70	0/1/1/1
25	CLA	B	606	-	1/1/15/20	7/37/115/115	-
25	CLA	B	613	-	1/1/15/20	3/37/115/115	-
27	BCR	A	610	-	-	5/29/63/63	0/2/2/2
25	CLA	D	403	-	1/1/15/20	5/37/115/115	-
25	CLA	b	605	-	1/1/15/20	8/37/115/115	-
25	CLA	C	503	-	1/1/15/20	1/37/115/115	-
29	LMG	A	612	-	-	17/46/66/70	0/1/1/1
29	LMG	c	502	-	-	27/46/66/70	0/1/1/1
33	DGD	c	518	-	-	15/51/91/95	0/2/2/2
25	CLA	C	512	-	1/1/15/20	14/37/115/115	-
25	CLA	d	403	-	-	8/37/115/115	-
25	CLA	C	513	-	1/1/15/20	5/37/115/115	-
27	BCR	c	517	-	-	6/29/63/63	0/2/2/2
28	PL9	A	611	-	-	10/53/73/73	0/1/1/1
29	LMG	D	405	-	-	14/46/66/70	0/1/1/1
27	BCR	a	610	-	-	5/29/63/63	0/2/2/2
31	LHG	L	101	-	-	19/53/53/53	-
25	CLA	A	606	-	1/1/15/20	3/37/115/115	-
23	SQD	c	501	-	-	19/49/69/69	0/1/1/1
34	HEM	E	101	6,5	-	5/12/54/54	-
27	BCR	B	618	-	-	4/29/63/63	0/2/2/2
25	CLA	B	605	-	-	9/37/115/115	-
31	LHG	d	407	-	-	15/53/53/53	-

All (528) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	609	CLA	C4B-NB	7.81	1.42	1.35
25	C	512	CLA	C4B-NB	7.70	1.42	1.35
25	D	402	CLA	C4B-NB	7.70	1.42	1.35
25	C	506	CLA	C4B-NB	7.67	1.42	1.35
25	d	403	CLA	C4B-NB	7.66	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	C4B-NB	7.64	1.42	1.35
25	c	507	CLA	C4B-NB	7.64	1.42	1.35
25	B	605	CLA	C4B-NB	7.63	1.42	1.35
25	c	508	CLA	C4B-NB	7.61	1.42	1.35
25	b	612	CLA	C4B-NB	7.61	1.42	1.35
25	C	505	CLA	C4B-NB	7.61	1.42	1.35
25	a	609	CLA	C4B-NB	7.59	1.42	1.35
25	b	606	CLA	C4B-NB	7.57	1.42	1.35
25	b	617	CLA	C4B-NB	7.55	1.41	1.35
25	b	605	CLA	C4B-NB	7.54	1.41	1.35
25	b	608	CLA	C4B-NB	7.54	1.41	1.35
25	A	609	CLA	C4B-NB	7.53	1.41	1.35
25	B	614	CLA	C4B-NB	7.52	1.41	1.35
25	D	403	CLA	C4B-NB	7.52	1.41	1.35
25	b	611	CLA	C4B-NB	7.52	1.41	1.35
25	B	615	CLA	C4B-NB	7.51	1.41	1.35
25	b	618	CLA	C4B-NB	7.49	1.41	1.35
25	c	509	CLA	C4B-NB	7.48	1.41	1.35
25	B	606	CLA	C4B-NB	7.47	1.41	1.35
25	C	508	CLA	C4B-NB	7.45	1.41	1.35
25	B	607	CLA	C4B-NB	7.45	1.41	1.35
25	d	404	CLA	C4B-NB	7.44	1.41	1.35
25	B	608	CLA	C4B-NB	7.44	1.41	1.35
25	b	604	CLA	C4B-NB	7.43	1.41	1.35
25	c	505	CLA	C4B-NB	7.43	1.41	1.35
25	C	507	CLA	C4B-NB	7.43	1.41	1.35
25	B	611	CLA	C4B-NB	7.43	1.41	1.35
25	b	607	CLA	C4B-NB	7.42	1.41	1.35
25	c	513	CLA	C4B-NB	7.42	1.41	1.35
25	B	610	CLA	C4B-NB	7.42	1.41	1.35
25	C	502	CLA	C4B-NB	7.42	1.41	1.35
25	B	602	CLA	C4B-NB	7.41	1.41	1.35
25	b	615	CLA	C4B-NB	7.40	1.41	1.35
25	B	601	CLA	C4B-NB	7.40	1.41	1.35
25	a	612	CLA	C4B-NB	7.40	1.41	1.35
25	B	616	CLA	C4B-NB	7.40	1.41	1.35
25	a	606	CLA	C4B-NB	7.40	1.41	1.35
25	b	610	CLA	C4B-NB	7.40	1.41	1.35
25	c	512	CLA	C4B-NB	7.39	1.41	1.35
25	C	503	CLA	C4B-NB	7.38	1.41	1.35
25	B	604	CLA	C4B-NB	7.38	1.41	1.35
25	c	510	CLA	C4B-NB	7.37	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	606	CLA	C4B-NB	7.37	1.41	1.35
25	C	511	CLA	C4B-NB	7.37	1.41	1.35
25	b	616	CLA	C4B-NB	7.36	1.41	1.35
25	b	613	CLA	C4B-NB	7.36	1.41	1.35
25	b	609	CLA	C4B-NB	7.36	1.41	1.35
25	B	613	CLA	C4B-NB	7.35	1.41	1.35
25	c	504	CLA	C4B-NB	7.35	1.41	1.35
25	C	510	CLA	C4B-NB	7.35	1.41	1.35
25	A	607	CLA	C4B-NB	7.34	1.41	1.35
25	c	514	CLA	C4B-NB	7.33	1.41	1.35
25	c	515	CLA	C4B-NB	7.32	1.41	1.35
25	b	614	CLA	C4B-NB	7.32	1.41	1.35
25	a	607	CLA	C4B-NB	7.32	1.41	1.35
25	c	503	CLA	C4B-NB	7.30	1.41	1.35
25	C	504	CLA	C4B-NB	7.30	1.41	1.35
25	B	612	CLA	C4B-NB	7.28	1.41	1.35
25	C	501	CLA	C4B-NB	7.28	1.41	1.35
25	c	506	CLA	C4B-NB	7.26	1.41	1.35
25	c	511	CLA	C4B-NB	7.25	1.41	1.35
25	C	513	CLA	C4B-NB	7.24	1.41	1.35
25	A	615	CLA	C4B-NB	7.24	1.41	1.35
25	b	619	CLA	C4B-NB	7.23	1.41	1.35
25	C	509	CLA	C4B-NB	7.13	1.41	1.35
35	v	201	HEC	C3C-C2C	-6.41	1.34	1.40
35	V	201	HEC	C3C-C2C	-6.35	1.34	1.40
35	v	201	HEC	C2B-C3B	-5.29	1.35	1.40
35	V	201	HEC	C2B-C3B	-5.18	1.35	1.40
35	v	201	HEC	CBC-CAC	-4.08	1.34	1.49
35	V	201	HEC	CBB-CAB	-4.06	1.34	1.49
35	v	201	HEC	CBB-CAB	-4.05	1.34	1.49
35	V	201	HEC	CBC-CAC	-4.04	1.34	1.49
25	B	610	CLA	C1D-ND	3.94	1.42	1.37
25	b	613	CLA	C1D-ND	3.93	1.42	1.37
25	b	619	CLA	C1D-ND	3.91	1.42	1.37
25	c	509	CLA	C1D-ND	3.90	1.42	1.37
25	b	616	CLA	C1D-ND	3.89	1.42	1.37
25	B	616	CLA	C1D-ND	3.88	1.42	1.37
25	b	607	CLA	C1D-ND	3.87	1.42	1.37
25	C	509	CLA	C1D-ND	3.86	1.42	1.37
25	C	507	CLA	C1D-ND	3.86	1.42	1.37
25	b	615	CLA	C1D-ND	3.86	1.42	1.37
25	c	511	CLA	C1D-ND	3.85	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	514	CLA	C1D-ND	3.85	1.42	1.37
25	B	615	CLA	C1D-ND	3.84	1.42	1.37
25	C	511	CLA	C1D-ND	3.83	1.42	1.37
34	E	101	HEM	C3C-CAC	3.83	1.55	1.47
25	b	605	CLA	C1D-ND	3.83	1.42	1.37
25	C	502	CLA	C1D-ND	3.83	1.42	1.37
25	C	512	CLA	C1D-ND	3.83	1.42	1.37
34	e	101	HEM	C3C-CAC	3.82	1.55	1.47
25	B	604	CLA	C1D-ND	3.82	1.42	1.37
25	C	506	CLA	C1D-ND	3.81	1.42	1.37
25	b	604	CLA	C1D-ND	3.81	1.42	1.37
25	c	504	CLA	C1D-ND	3.81	1.42	1.37
25	B	613	CLA	C1D-ND	3.81	1.42	1.37
25	b	618	CLA	C1D-ND	3.80	1.42	1.37
25	A	609	CLA	C1D-ND	3.80	1.42	1.37
25	b	614	CLA	C1D-ND	3.80	1.42	1.37
25	c	513	CLA	C1D-ND	3.79	1.42	1.37
25	c	512	CLA	C1D-ND	3.79	1.42	1.37
25	B	601	CLA	C1D-ND	3.79	1.42	1.37
25	B	606	CLA	C1D-ND	3.78	1.42	1.37
25	b	610	CLA	C1D-ND	3.78	1.42	1.37
25	b	612	CLA	C1D-ND	3.78	1.42	1.37
25	B	609	CLA	C1D-ND	3.78	1.42	1.37
25	D	402	CLA	C1D-ND	3.78	1.42	1.37
25	B	602	CLA	C1D-ND	3.77	1.42	1.37
25	C	503	CLA	C1D-ND	3.77	1.42	1.37
25	d	404	CLA	C1D-ND	3.77	1.42	1.37
25	D	403	CLA	C1D-ND	3.76	1.42	1.37
25	B	605	CLA	C1D-ND	3.76	1.42	1.37
28	A	611	PL9	C7-C3	-3.75	1.47	1.51
25	b	608	CLA	C1D-ND	3.75	1.42	1.37
25	C	508	CLA	C1D-ND	3.75	1.42	1.37
25	c	508	CLA	C1D-ND	3.75	1.42	1.37
25	a	607	CLA	C1D-ND	3.75	1.42	1.37
25	a	612	CLA	C1D-ND	3.74	1.42	1.37
25	C	510	CLA	C1D-ND	3.74	1.42	1.37
25	A	615	CLA	C1D-ND	3.74	1.42	1.37
25	b	617	CLA	C1D-ND	3.73	1.42	1.37
25	c	510	CLA	C1D-ND	3.73	1.42	1.37
25	c	505	CLA	C1D-ND	3.73	1.42	1.37
25	B	608	CLA	C1D-ND	3.73	1.42	1.37
25	d	403	CLA	C1D-ND	3.72	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	507	CLA	C1D-ND	3.72	1.42	1.37
25	B	603	CLA	C1D-ND	3.71	1.42	1.37
25	C	513	CLA	C1D-ND	3.71	1.42	1.37
25	c	515	CLA	C1D-ND	3.70	1.42	1.37
25	a	609	CLA	C1D-ND	3.70	1.42	1.37
25	a	606	CLA	C1D-ND	3.70	1.42	1.37
25	B	611	CLA	C1D-ND	3.70	1.42	1.37
25	A	606	CLA	C1D-ND	3.69	1.42	1.37
34	E	101	HEM	C3C-C2C	-3.69	1.35	1.40
25	c	506	CLA	C1D-ND	3.69	1.42	1.37
25	B	607	CLA	C1D-ND	3.68	1.42	1.37
25	C	505	CLA	C1D-ND	3.68	1.42	1.37
34	e	101	HEM	C3C-C2C	-3.68	1.35	1.40
25	A	607	CLA	C1D-ND	3.68	1.42	1.37
25	C	501	CLA	C1D-ND	3.68	1.42	1.37
25	b	611	CLA	C1D-ND	3.67	1.42	1.37
25	b	609	CLA	C1D-ND	3.67	1.42	1.37
25	B	612	CLA	C1D-ND	3.66	1.42	1.37
25	B	614	CLA	C1D-ND	3.66	1.42	1.37
25	c	503	CLA	C1D-ND	3.65	1.42	1.37
25	C	504	CLA	C1D-ND	3.64	1.42	1.37
25	b	606	CLA	C1D-ND	3.61	1.42	1.37
27	B	627	BCR	C1-C6	-3.57	1.48	1.53
27	C	515	BCR	C1-C6	-3.50	1.49	1.53
27	C	514	BCR	C1-C6	-3.48	1.49	1.53
27	B	617	BCR	C1-C6	-3.47	1.49	1.53
27	T	101	BCR	C1-C6	-3.47	1.49	1.53
27	D	404	BCR	C1-C6	-3.45	1.49	1.53
27	b	620	BCR	C1-C6	-3.42	1.49	1.53
27	y	101	BCR	C1-C6	-3.42	1.49	1.53
28	D	407	PL9	C7-C3	-3.39	1.47	1.51
27	c	517	BCR	C1-C6	-3.37	1.49	1.53
27	B	618	BCR	C1-C6	-3.37	1.49	1.53
27	b	621	BCR	C1-C6	-3.32	1.49	1.53
27	a	610	BCR	C1-C6	-3.30	1.49	1.53
27	B	617	BCR	C30-C25	-3.30	1.49	1.53
27	A	610	BCR	C1-C6	-3.29	1.49	1.53
27	b	620	BCR	C30-C25	-3.28	1.49	1.53
27	Y	101	BCR	C1-C6	-3.27	1.49	1.53
23	A	619	SQD	O48-C23	3.27	1.42	1.33
25	A	609	CLA	CHC-C1C	3.26	1.43	1.35
25	c	515	CLA	CHC-C1C	3.26	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	617	CLA	CHC-C1C	3.24	1.43	1.35
27	B	619	BCR	C1-C6	-3.24	1.49	1.53
25	c	512	CLA	CHC-C1C	3.24	1.43	1.35
28	d	408	PL9	C7-C3	-3.24	1.48	1.51
27	k	101	BCR	C1-C6	-3.24	1.49	1.53
27	B	619	BCR	C30-C25	-3.23	1.49	1.53
25	C	508	CLA	CHC-C1C	3.22	1.43	1.35
25	C	510	CLA	CHC-C1C	3.22	1.43	1.35
28	a	611	PL9	C7-C3	-3.22	1.48	1.51
25	C	513	CLA	CHC-C1C	3.22	1.43	1.35
25	a	606	CLA	CHC-C1C	3.22	1.43	1.35
25	c	510	CLA	CHC-C1C	3.21	1.43	1.35
25	a	607	CLA	CHC-C1C	3.21	1.43	1.35
25	b	615	CLA	CHC-C1C	3.21	1.43	1.35
25	B	612	CLA	CHC-C1C	3.21	1.43	1.35
23	I	101	SQD	O48-C23	3.21	1.42	1.33
25	B	615	CLA	CHC-C1C	3.21	1.43	1.35
25	b	613	CLA	CHC-C1C	3.21	1.43	1.35
25	d	403	CLA	CHC-C1C	3.21	1.43	1.35
25	C	511	CLA	CHC-C1C	3.20	1.43	1.35
25	b	611	CLA	CHC-C1C	3.20	1.43	1.35
25	d	404	CLA	CHC-C1C	3.20	1.43	1.35
25	b	606	CLA	CHC-C1C	3.20	1.43	1.35
25	C	503	CLA	CHC-C1C	3.20	1.43	1.35
25	B	602	CLA	CHC-C1C	3.20	1.43	1.35
25	C	504	CLA	CHC-C1C	3.20	1.43	1.35
25	B	606	CLA	CHC-C1C	3.20	1.43	1.35
25	c	505	CLA	CHC-C1C	3.20	1.43	1.35
25	c	513	CLA	CHC-C1C	3.20	1.43	1.35
25	c	506	CLA	CHC-C1C	3.20	1.43	1.35
25	B	607	CLA	CHC-C1C	3.19	1.43	1.35
25	b	605	CLA	CHC-C1C	3.19	1.43	1.35
25	A	606	CLA	CHC-C1C	3.19	1.43	1.35
25	B	608	CLA	CHC-C1C	3.19	1.43	1.35
25	b	610	CLA	CHC-C1C	3.19	1.43	1.35
25	B	614	CLA	CHC-C1C	3.19	1.43	1.35
25	b	608	CLA	CHC-C1C	3.19	1.43	1.35
25	c	511	CLA	CHC-C1C	3.19	1.43	1.35
25	B	605	CLA	CHC-C1C	3.19	1.43	1.35
25	B	603	CLA	CHC-C1C	3.19	1.43	1.35
25	c	503	CLA	CHC-C1C	3.19	1.43	1.35
25	A	607	CLA	CHC-C1C	3.18	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	502	CLA	CHC-C1C	3.18	1.43	1.35
25	A	615	CLA	CHC-C1C	3.18	1.43	1.35
25	B	610	CLA	CHC-C1C	3.18	1.43	1.35
27	K	101	BCR	C30-C25	-3.18	1.49	1.53
25	C	501	CLA	CHC-C1C	3.18	1.43	1.35
25	b	609	CLA	CHC-C1C	3.17	1.43	1.35
25	D	402	CLA	CHC-C1C	3.17	1.43	1.35
25	B	613	CLA	CHC-C1C	3.17	1.43	1.35
25	b	616	CLA	CHC-C1C	3.17	1.43	1.35
25	B	611	CLA	CHC-C1C	3.17	1.43	1.35
25	b	612	CLA	CHC-C1C	3.17	1.43	1.35
25	b	614	CLA	CHC-C1C	3.17	1.43	1.35
23	c	501	SQD	O48-C23	3.17	1.42	1.33
25	B	609	CLA	CHC-C1C	3.17	1.43	1.35
25	a	609	CLA	CHC-C1C	3.17	1.43	1.35
25	c	514	CLA	CHC-C1C	3.16	1.43	1.35
25	D	403	CLA	CHC-C1C	3.16	1.43	1.35
25	C	509	CLA	CHC-C1C	3.16	1.43	1.35
25	B	604	CLA	CHC-C1C	3.16	1.43	1.35
23	B	626	SQD	O48-C23	3.16	1.42	1.33
23	f	101	SQD	O48-C23	3.16	1.42	1.33
25	B	601	CLA	CHC-C1C	3.16	1.43	1.35
25	c	504	CLA	CHC-C1C	3.15	1.43	1.35
25	C	504	CLA	C4D-ND	-3.15	1.33	1.37
23	D	409	SQD	O48-C23	3.15	1.42	1.33
23	A	603	SQD	O48-C23	3.15	1.42	1.33
25	c	510	CLA	C4D-ND	-3.15	1.33	1.37
25	c	507	CLA	CHC-C1C	3.15	1.43	1.35
27	y	101	BCR	C30-C25	-3.15	1.49	1.53
25	C	505	CLA	CHC-C1C	3.14	1.43	1.35
25	b	604	CLA	CHC-C1C	3.14	1.43	1.35
25	d	404	CLA	C4D-ND	-3.14	1.33	1.37
25	C	506	CLA	CHC-C1C	3.14	1.43	1.35
25	a	612	CLA	CHC-C1C	3.14	1.43	1.35
25	B	616	CLA	CHC-C1C	3.13	1.43	1.35
25	b	618	CLA	CHC-C1C	3.13	1.43	1.35
25	b	607	CLA	CHC-C1C	3.13	1.43	1.35
25	c	503	CLA	C4D-ND	-3.13	1.33	1.37
25	C	508	CLA	C4D-ND	-3.13	1.33	1.37
25	A	606	CLA	C4D-ND	-3.13	1.33	1.37
25	A	609	CLA	C4D-ND	-3.13	1.33	1.37
27	c	516	BCR	C30-C25	-3.13	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	508	CLA	CHC-C1C	3.12	1.43	1.35
25	A	615	CLA	C4D-ND	-3.12	1.33	1.37
27	b	621	BCR	C30-C25	-3.12	1.49	1.53
25	b	619	CLA	CHC-C1C	3.12	1.43	1.35
27	b	622	BCR	C30-C25	-3.12	1.49	1.53
25	C	513	CLA	C4D-ND	-3.11	1.33	1.37
25	C	512	CLA	CHC-C1C	3.11	1.42	1.35
25	c	509	CLA	CHC-C1C	3.11	1.42	1.35
27	c	517	BCR	C30-C25	-3.11	1.49	1.53
25	c	504	CLA	C4D-ND	-3.11	1.33	1.37
25	c	515	CLA	C4D-ND	-3.11	1.33	1.37
25	b	608	CLA	C4D-ND	-3.11	1.33	1.37
23	b	601	SQD	O48-C23	3.11	1.42	1.33
25	b	614	CLA	C4D-ND	-3.10	1.33	1.37
23	D	408	SQD	O48-C23	3.10	1.42	1.33
25	C	507	CLA	CHC-C1C	3.10	1.42	1.35
25	C	510	CLA	C4D-ND	-3.09	1.33	1.37
25	a	612	CLA	C4D-ND	-3.09	1.33	1.37
27	Y	101	BCR	C30-C25	-3.09	1.49	1.53
25	C	501	CLA	C4D-ND	-3.08	1.33	1.37
25	B	605	CLA	C4D-ND	-3.08	1.33	1.37
27	c	516	BCR	C1-C6	-3.08	1.49	1.53
27	d	405	BCR	C1-C6	-3.08	1.49	1.53
25	b	610	CLA	C4D-ND	-3.07	1.33	1.37
25	b	616	CLA	C4D-ND	-3.07	1.33	1.37
27	C	514	BCR	C30-C25	-3.07	1.49	1.53
25	C	502	CLA	C4D-ND	-3.07	1.33	1.37
25	B	602	CLA	C4D-ND	-3.06	1.33	1.37
25	a	607	CLA	C4D-ND	-3.06	1.33	1.37
27	h	101	BCR	C30-C25	-3.06	1.49	1.53
27	A	610	BCR	C30-C25	-3.06	1.49	1.53
25	c	506	CLA	C4D-ND	-3.06	1.33	1.37
27	C	515	BCR	C30-C25	-3.06	1.49	1.53
25	B	601	CLA	C4D-ND	-3.06	1.33	1.37
27	K	101	BCR	C1-C6	-3.06	1.49	1.53
27	D	404	BCR	C30-C25	-3.06	1.49	1.53
25	b	615	CLA	C4D-ND	-3.05	1.33	1.37
27	h	101	BCR	C1-C6	-3.05	1.49	1.53
27	d	405	BCR	C30-C25	-3.05	1.49	1.53
25	a	606	CLA	C4D-ND	-3.05	1.33	1.37
25	D	403	CLA	C4D-ND	-3.05	1.33	1.37
25	b	606	CLA	C4D-ND	-3.05	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	622	BCR	C1-C6	-3.04	1.49	1.53
25	b	609	CLA	C4D-ND	-3.04	1.33	1.37
25	b	617	CLA	C4D-ND	-3.04	1.33	1.37
27	B	618	BCR	C30-C25	-3.04	1.49	1.53
25	b	611	CLA	C4D-ND	-3.04	1.33	1.37
25	B	607	CLA	C4D-ND	-3.04	1.33	1.37
25	B	612	CLA	C4D-ND	-3.04	1.33	1.37
25	D	402	CLA	C4D-ND	-3.04	1.33	1.37
25	A	607	CLA	C4D-ND	-3.04	1.33	1.37
34	e	101	HEM	CAB-C3B	3.03	1.55	1.47
25	C	509	CLA	C4D-ND	-3.03	1.33	1.37
25	a	609	CLA	C4D-ND	-3.03	1.33	1.37
25	B	603	CLA	C4D-ND	-3.03	1.33	1.37
25	b	619	CLA	C4D-ND	-3.03	1.33	1.37
25	b	618	CLA	C4D-ND	-3.02	1.33	1.37
25	B	616	CLA	C4D-ND	-3.02	1.33	1.37
25	B	614	CLA	C4D-ND	-3.02	1.33	1.37
25	c	514	CLA	C4D-ND	-3.01	1.33	1.37
25	c	513	CLA	C4D-ND	-3.01	1.33	1.37
25	c	508	CLA	C4D-ND	-3.01	1.33	1.37
25	B	606	CLA	C4D-ND	-3.01	1.33	1.37
25	B	611	CLA	C4D-ND	-3.01	1.33	1.37
25	b	613	CLA	C4D-ND	-3.01	1.33	1.37
25	b	604	CLA	C4D-ND	-3.00	1.33	1.37
25	C	511	CLA	C4D-ND	-3.00	1.33	1.37
34	E	101	HEM	CAB-C3B	3.00	1.55	1.47
25	c	511	CLA	C4D-ND	-3.00	1.33	1.37
25	C	503	CLA	C4D-ND	-2.99	1.33	1.37
25	B	608	CLA	C4D-ND	-2.99	1.33	1.37
27	a	610	BCR	C30-C25	-2.99	1.49	1.53
25	b	605	CLA	C4D-ND	-2.98	1.33	1.37
25	c	512	CLA	C4D-ND	-2.98	1.33	1.37
25	c	505	CLA	C4D-ND	-2.98	1.33	1.37
25	B	613	CLA	C4D-ND	-2.97	1.33	1.37
25	b	612	CLA	C4D-ND	-2.97	1.33	1.37
25	d	403	CLA	C4D-ND	-2.97	1.33	1.37
23	A	619	SQD	O47-C7	2.96	1.42	1.34
25	c	509	CLA	C4D-ND	-2.96	1.33	1.37
27	B	627	BCR	C30-C25	-2.96	1.49	1.53
25	B	609	CLA	C4D-ND	-2.94	1.33	1.37
25	C	506	CLA	C4D-ND	-2.94	1.33	1.37
25	C	507	CLA	C4D-ND	-2.94	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	512	CLA	C4D-ND	-2.94	1.33	1.37
25	B	604	CLA	C4D-ND	-2.94	1.33	1.37
27	H	102	BCR	C1-C6	-2.94	1.49	1.53
25	B	615	CLA	C4D-ND	-2.93	1.33	1.37
27	k	101	BCR	C30-C25	-2.93	1.49	1.53
27	H	102	BCR	C30-C25	-2.93	1.49	1.53
25	c	507	CLA	C4D-ND	-2.93	1.33	1.37
23	D	408	SQD	O47-C7	2.90	1.42	1.34
23	B	626	SQD	O47-C7	2.90	1.42	1.34
25	B	610	CLA	C4D-ND	-2.90	1.33	1.37
23	D	409	SQD	O47-C7	2.88	1.42	1.34
25	C	505	CLA	C4D-ND	-2.88	1.33	1.37
23	I	101	SQD	O47-C7	2.85	1.42	1.34
23	c	501	SQD	O47-C7	2.84	1.42	1.34
23	A	603	SQD	O47-C7	2.84	1.42	1.34
27	T	101	BCR	C30-C25	-2.84	1.49	1.53
23	f	101	SQD	O47-C7	2.83	1.42	1.34
25	b	607	CLA	C4D-ND	-2.80	1.33	1.37
23	b	601	SQD	O47-C7	2.79	1.42	1.34
28	d	408	PL9	C3-C4	-2.74	1.45	1.49
28	D	407	PL9	C3-C4	-2.71	1.45	1.49
28	A	611	PL9	C3-C4	-2.70	1.45	1.49
26	a	608	PHO	CAC-C3C	-2.65	1.47	1.52
26	D	401	PHO	CAC-C3C	-2.62	1.47	1.52
25	c	508	CLA	CMB-C2B	-2.60	1.46	1.51
25	C	506	CLA	CMB-C2B	-2.59	1.46	1.51
26	d	401	PHO	CAC-C3C	-2.59	1.47	1.52
26	A	608	PHO	CAC-C3C	-2.52	1.47	1.52
29	c	522	LMG	C1-C2	2.51	1.59	1.52
25	b	614	CLA	CMB-C2B	-2.50	1.46	1.51
28	a	611	PL9	C3-C4	-2.50	1.45	1.49
25	B	611	CLA	CMB-C2B	-2.48	1.46	1.51
25	c	504	CLA	CMB-C2B	-2.46	1.46	1.51
25	B	604	CLA	CMB-C2B	-2.45	1.46	1.51
25	c	511	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	604	CLA	CMB-C2B	-2.45	1.46	1.51
25	b	611	CLA	CMB-C2B	-2.44	1.46	1.51
25	A	615	CLA	CMB-C2B	-2.44	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	606	CLA	CMB-C2B	-2.43	1.46	1.51
25	c	510	CLA	CMB-C2B	-2.43	1.46	1.51
29	C	520	LMG	C1-C2	2.43	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	507	CLA	CMB-C2B	-2.43	1.46	1.51
25	a	609	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	618	CLA	CMB-C2B	-2.43	1.46	1.51
25	c	506	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	608	CLA	CMB-C2B	-2.42	1.46	1.51
25	a	607	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	609	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	610	CLA	CMB-C2B	-2.42	1.46	1.51
25	C	504	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	612	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	607	CLA	CMB-C2B	-2.41	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.41	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	601	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	608	CLA	CMB-C2B	-2.40	1.46	1.51
25	a	612	CLA	CMB-C2B	-2.40	1.46	1.51
25	C	508	CLA	CMB-C2B	-2.40	1.46	1.51
25	B	605	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	606	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	612	CLA	CMB-C2B	-2.40	1.46	1.51
25	b	615	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	509	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	507	CLA	CMB-C2B	-2.39	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.39	1.46	1.51
25	A	607	CLA	CMB-C2B	-2.39	1.46	1.51
25	D	403	CLA	CMB-C2B	-2.39	1.46	1.51
25	D	402	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	607	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	617	CLA	CMB-C2B	-2.39	1.46	1.51
25	d	403	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	505	CLA	CMB-C2B	-2.39	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.39	1.46	1.51
25	B	615	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.38	1.46	1.51
25	c	503	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	613	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	605	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	614	CLA	CMB-C2B	-2.38	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.38	1.46	1.51
25	b	610	CLA	CMB-C2B	-2.38	1.46	1.51
25	A	609	CLA	CMB-C2B	-2.38	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	513	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.37	1.46	1.51
25	C	501	CLA	CMB-C2B	-2.37	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.37	1.46	1.51
25	b	613	CLA	CMB-C2B	-2.37	1.46	1.51
25	a	606	CLA	CMB-C2B	-2.37	1.46	1.51
25	c	513	CLA	CMB-C2B	-2.37	1.46	1.51
25	C	502	CLA	CMB-C2B	-2.36	1.46	1.51
25	c	515	CLA	CMB-C2B	-2.35	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.34	1.46	1.51
25	c	514	CLA	CMB-C2B	-2.34	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.34	1.46	1.51
25	A	606	CLA	CMB-C2B	-2.32	1.46	1.51
25	d	404	CLA	CMB-C2B	-2.31	1.46	1.51
29	B	625	LMG	O6-C5	-2.31	1.38	1.44
25	b	619	CLA	CMB-C2B	-2.31	1.46	1.51
31	l	101	LHG	O7-C5	-2.22	1.41	1.46
33	c	518	DGD	O2G-C2G	-2.21	1.41	1.46
23	c	501	SQD	O2-C2	-2.21	1.37	1.43
29	B	625	LMG	C3-C2	2.20	1.57	1.52
25	C	505	CLA	CMD-C2D	-2.18	1.46	1.50
23	A	603	SQD	O2-C2	-2.18	1.37	1.43
23	f	101	SQD	O2-C2	-2.18	1.37	1.43
23	D	409	SQD	O2-C2	-2.18	1.37	1.43
33	c	519	DGD	O2G-C2G	-2.17	1.41	1.46
25	c	507	CLA	CMD-C2D	-2.17	1.46	1.50
33	C	516	DGD	O1G-C1G	-2.17	1.40	1.45
33	C	517	DGD	O1G-C1G	-2.16	1.40	1.45
33	c	519	DGD	O1G-C1G	-2.16	1.40	1.45
23	B	626	SQD	O2-C2	-2.15	1.37	1.43
33	c	518	DGD	O1G-C1G	-2.15	1.40	1.45
31	L	101	LHG	O7-C5	-2.13	1.41	1.46
23	b	601	SQD	O2-C2	-2.13	1.38	1.43
31	D	406	LHG	O7-C5	-2.13	1.41	1.46
33	c	520	DGD	O1G-C1G	-2.12	1.40	1.45
25	b	619	CLA	CMC-C2C	-2.12	1.46	1.50
33	H	103	DGD	O2G-C2G	-2.11	1.41	1.46
35	V	201	HEC	CAD-C3D	2.11	1.55	1.52
31	d	407	LHG	O7-C5	-2.10	1.41	1.46
33	c	520	DGD	O2G-C2G	-2.10	1.41	1.46
31	A	618	LHG	P-O6	2.10	1.67	1.59
28	D	407	PL9	C6-C1	-2.10	1.44	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	408	PL9	C53-C6	-2.09	1.46	1.50
23	D	408	SQD	O2-C2	-2.09	1.38	1.43
28	d	408	PL9	C6-C1	-2.08	1.44	1.48
26	A	608	PHO	CMC-C2C	-2.08	1.46	1.51
25	B	616	CLA	CMC-C2C	-2.08	1.46	1.50
25	b	606	CLA	CMD-C2D	-2.08	1.46	1.50
33	C	518	DGD	O1G-C1G	-2.08	1.40	1.45
31	A	616	LHG	O7-C5	-2.08	1.41	1.46
29	c	502	LMG	C4-C5	2.07	1.57	1.53
26	a	608	PHO	CMB-C2B	-2.06	1.46	1.51
23	c	501	SQD	O3-C3	-2.06	1.38	1.43
25	D	402	CLA	CMD-C2D	-2.06	1.46	1.50
23	b	601	SQD	O3-C3	-2.06	1.38	1.43
23	b	601	SQD	O4-C4	-2.06	1.38	1.43
28	a	611	PL9	C53-C6	-2.05	1.46	1.50
28	A	611	PL9	C53-C6	-2.05	1.46	1.50
23	D	409	SQD	O4-C4	-2.05	1.38	1.43
31	a	613	LHG	O7-C5	-2.05	1.41	1.46
26	d	401	PHO	CMC-C2C	-2.05	1.46	1.51
26	D	401	PHO	CMC-C2C	-2.05	1.46	1.51
26	A	608	PHO	CMD-C2D	-2.05	1.46	1.51
23	D	409	SQD	O3-C3	-2.04	1.38	1.43
34	E	101	HEM	CMB-C2B	2.04	1.55	1.50
26	d	401	PHO	CMD-C2D	-2.04	1.46	1.51
26	a	608	PHO	CMC-C2C	-2.03	1.46	1.51
25	B	612	CLA	CMD-C2D	-2.03	1.46	1.50
28	D	407	PL9	C53-C6	-2.03	1.46	1.50
25	B	603	CLA	CMD-C2D	-2.03	1.46	1.50
25	C	503	CLA	CMD-C2D	-2.03	1.46	1.50
23	D	408	SQD	O3-C3	-2.03	1.38	1.43
29	C	519	LMG	O7-C8	-2.02	1.41	1.46
25	A	607	CLA	CMD-C2D	-2.02	1.46	1.50
33	C	516	DGD	O2G-C2G	-2.02	1.41	1.46
29	B	625	LMG	O7-C8	-2.02	1.41	1.46
26	a	608	PHO	CMD-C2D	-2.02	1.46	1.51
34	E	101	HEM	CMD-C2D	2.02	1.55	1.50
23	A	603	SQD	O3-C3	-2.02	1.38	1.43
33	h	102	DGD	O2G-C2G	-2.02	1.41	1.46
25	B	614	CLA	CMD-C2D	-2.02	1.46	1.50
33	C	518	DGD	O2G-C2G	-2.02	1.41	1.46
26	A	608	PHO	CMB-C2B	-2.02	1.46	1.51
34	e	101	HEM	CMB-C2B	2.02	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	607	CLA	CMD-C2D	-2.02	1.46	1.50
25	C	512	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	607	CLA	CMD-C2D	-2.02	1.46	1.50
25	a	606	CLA	CMD-C2D	-2.02	1.46	1.50
25	b	615	CLA	CMC-C2C	-2.02	1.46	1.50
23	f	101	SQD	O3-C3	-2.01	1.38	1.43
25	B	605	CLA	CMD-C2D	-2.01	1.46	1.50
31	a	615	LHG	P-O6	2.01	1.67	1.59
23	B	626	SQD	O3-C3	-2.01	1.38	1.43
23	c	501	SQD	O4-C4	-2.01	1.38	1.43
25	b	615	CLA	CMD-C2D	-2.01	1.46	1.50
26	D	401	PHO	CMD-C2D	-2.01	1.46	1.51
33	C	517	DGD	O2G-C2G	-2.01	1.41	1.46
25	b	617	CLA	CMD-C2D	-2.01	1.46	1.50
23	A	603	SQD	O4-C4	-2.01	1.38	1.43
25	C	510	CLA	CMD-C2D	-2.01	1.46	1.50
25	b	608	CLA	CMD-C2D	-2.00	1.46	1.50
23	f	101	SQD	O4-C4	-2.00	1.38	1.43
31	A	616	LHG	P-O6	2.00	1.67	1.59

All (1077) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	507	CLA	C4A-NA-C1A	6.39	109.58	106.71
25	C	503	CLA	C4A-NA-C1A	6.28	109.53	106.71
25	B	604	CLA	C4A-NA-C1A	6.28	109.53	106.71
25	b	607	CLA	C4A-NA-C1A	6.26	109.52	106.71
25	c	513	CLA	C4A-NA-C1A	6.25	109.51	106.71
25	C	512	CLA	C4A-NA-C1A	6.19	109.49	106.71
25	C	511	CLA	C4A-NA-C1A	6.08	109.44	106.71
25	c	514	CLA	C4A-NA-C1A	6.08	109.44	106.71
25	c	509	CLA	C4A-NA-C1A	6.01	109.41	106.71
25	c	505	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	c	504	CLA	C4A-NA-C1A	5.99	109.40	106.71
25	B	615	CLA	C4A-NA-C1A	5.96	109.39	106.71
25	c	511	CLA	C4A-NA-C1A	5.96	109.39	106.71
25	b	618	CLA	C4A-NA-C1A	5.93	109.37	106.71
25	b	604	CLA	C4A-NA-C1A	5.90	109.36	106.71
25	b	612	CLA	C4A-NA-C1A	5.86	109.34	106.71
25	b	616	CLA	C4A-NA-C1A	5.86	109.34	106.71
25	B	613	CLA	C4A-NA-C1A	5.84	109.33	106.71
25	B	601	CLA	C4A-NA-C1A	5.81	109.32	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	502	CLA	C4A-NA-C1A	5.79	109.31	106.71
25	C	509	CLA	C4A-NA-C1A	5.77	109.30	106.71
25	B	616	CLA	C4A-NA-C1A	5.64	109.24	106.71
25	C	505	CLA	C4A-NA-C1A	5.64	109.24	106.71
25	B	612	CLA	C4A-NA-C1A	5.63	109.23	106.71
25	C	506	CLA	C4A-NA-C1A	5.58	109.21	106.71
25	B	609	CLA	C4A-NA-C1A	5.56	109.20	106.71
25	c	507	CLA	C4A-NA-C1A	5.56	109.20	106.71
25	B	606	CLA	C4A-NA-C1A	5.51	109.18	106.71
25	C	501	CLA	C4A-NA-C1A	5.48	109.17	106.71
28	a	611	PL9	C7-C3-C4	5.46	121.32	116.88
25	b	615	CLA	C4A-NA-C1A	5.44	109.15	106.71
25	c	512	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	B	605	CLA	C4A-NA-C1A	5.39	109.13	106.71
25	b	614	CLA	C4A-NA-C1A	5.37	109.12	106.71
25	d	403	CLA	C4A-NA-C1A	5.36	109.11	106.71
25	B	611	CLA	C4A-NA-C1A	5.35	109.11	106.71
28	D	407	PL9	C7-C3-C4	5.28	121.17	116.88
25	D	403	CLA	C4A-NA-C1A	5.27	109.08	106.71
25	D	402	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	d	404	CLA	C4A-NA-C1A	5.26	109.07	106.71
25	b	608	CLA	C4A-NA-C1A	5.22	109.05	106.71
25	c	503	CLA	C4A-NA-C1A	5.21	109.05	106.71
25	A	607	CLA	C4A-NA-C1A	5.19	109.04	106.71
25	b	609	CLA	C4A-NA-C1A	5.19	109.04	106.71
25	b	617	CLA	C4A-NA-C1A	5.19	109.04	106.71
28	d	408	PL9	C7-C3-C4	5.18	121.09	116.88
28	A	611	PL9	C7-C3-C4	5.17	121.08	116.88
25	c	506	CLA	C4A-NA-C1A	5.17	109.03	106.71
25	c	510	CLA	C4A-NA-C1A	5.14	109.02	106.71
25	C	504	CLA	C4A-NA-C1A	5.13	109.01	106.71
25	A	609	CLA	C4A-NA-C1A	5.13	109.01	106.71
25	B	614	CLA	C4A-NA-C1A	5.12	109.01	106.71
25	C	508	CLA	C4A-NA-C1A	5.10	109.00	106.71
25	a	612	CLA	C4A-NA-C1A	5.04	108.97	106.71
25	c	508	CLA	C4A-NA-C1A	4.95	108.93	106.71
25	c	515	CLA	C4A-NA-C1A	4.92	108.92	106.71
25	B	608	CLA	C4A-NA-C1A	4.89	108.91	106.71
23	D	408	SQD	O5-C5-C4	4.86	118.52	109.69
25	b	619	CLA	C4A-NA-C1A	4.78	108.86	106.71
25	A	615	CLA	C4A-NA-C1A	4.76	108.85	106.71
23	D	408	SQD	C1-O5-C5	4.70	122.92	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	611	CLA	C4A-NA-C1A	4.63	108.79	106.71
25	B	602	CLA	C4A-NA-C1A	4.62	108.78	106.71
25	b	605	CLA	C4A-NA-C1A	4.56	108.75	106.71
25	C	510	CLA	C4A-NA-C1A	4.54	108.75	106.71
25	C	513	CLA	C4A-NA-C1A	4.52	108.74	106.71
25	b	610	CLA	C4A-NA-C1A	4.48	108.72	106.71
25	a	607	CLA	C4A-NA-C1A	4.47	108.71	106.71
25	a	609	CLA	C4A-NA-C1A	4.47	108.71	106.71
33	c	518	DGD	O3G-C3G-C2G	-4.46	100.14	110.90
25	b	613	CLA	C4A-NA-C1A	4.45	108.71	106.71
25	a	606	CLA	C4A-NA-C1A	4.44	108.70	106.71
25	B	603	CLA	C4A-NA-C1A	4.43	108.70	106.71
33	C	516	DGD	O3G-C3G-C2G	-4.43	100.21	110.90
33	C	518	DGD	O3G-C3G-C2G	-4.24	100.66	110.90
25	A	606	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
23	B	626	SQD	O5-C5-C4	4.24	117.39	109.69
31	a	614	LHG	O4-P-O5	4.23	133.16	112.24
33	c	520	DGD	O3G-C3G-C2G	-4.23	100.69	110.90
25	c	514	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
31	L	101	LHG	O4-P-O5	4.20	133.02	112.24
31	A	617	LHG	O4-P-O5	4.20	133.01	112.24
31	a	613	LHG	O4-P-O5	4.19	132.97	112.24
31	A	616	LHG	O4-P-O5	4.19	132.96	112.24
31	l	101	LHG	O4-P-O5	4.19	132.95	112.24
31	D	406	LHG	O4-P-O5	4.19	132.93	112.24
31	d	407	LHG	O4-P-O5	4.18	132.93	112.24
23	A	603	SQD	O9-S-C6	4.18	111.91	106.94
31	a	615	LHG	O4-P-O5	4.17	132.86	112.24
33	c	519	DGD	O3G-C3G-C2G	-4.16	100.85	110.90
31	A	618	LHG	O4-P-O5	4.13	132.66	112.24
25	B	610	CLA	C4A-NA-C1A	4.05	108.53	106.71
25	d	404	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
25	b	619	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
25	a	606	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
23	c	501	SQD	O7-S-C6	4.02	111.71	106.94
23	f	101	SQD	O9-S-C6	4.01	111.71	106.94
23	B	626	SQD	O9-S-C6	4.01	111.70	106.94
25	C	509	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
23	b	601	SQD	O7-S-C6	3.99	111.68	106.94
23	D	409	SQD	O9-S-C6	3.96	111.64	106.94
23	B	626	SQD	O47-C7-C8	3.95	120.02	111.50
25	B	616	CLA	CMB-C2B-C1B	-3.89	122.48	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	409	SQD	O7-S-C6	3.89	111.56	106.94
25	b	606	CLA	C4A-NA-C1A	3.86	108.44	106.71
29	A	613	LMG	O1-C1-C2	-3.86	102.28	108.30
25	B	612	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
29	c	522	LMG	O6-C1-O1	-3.84	100.88	109.97
25	c	512	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
29	C	520	LMG	O6-C1-O1	-3.83	100.90	109.97
33	H	103	DGD	O3G-C3G-C2G	-3.83	101.66	110.90
23	A	603	SQD	O9-S-O7	-3.80	100.79	113.95
23	f	101	SQD	O7-S-C6	3.79	111.44	106.94
23	A	603	SQD	O7-S-C6	3.77	111.42	106.94
25	B	613	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
23	f	101	SQD	O47-C7-C8	3.76	119.60	111.50
25	c	508	CLA	CMB-C2B-C1B	-3.75	122.69	128.46
23	c	501	SQD	O9-S-C6	3.74	111.39	106.94
23	D	408	SQD	O9-S-O7	-3.72	101.08	113.95
25	C	508	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
23	B	626	SQD	O9-S-O7	-3.71	101.11	113.95
33	C	517	DGD	O3G-C3G-C2G	-3.71	101.95	110.90
23	I	101	SQD	O47-C7-C8	3.71	119.49	111.50
33	h	102	DGD	O3G-C3G-C2G	-3.70	101.96	110.90
25	A	609	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
25	b	615	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
23	D	408	SQD	O9-S-C6	3.69	111.33	106.94
23	A	619	SQD	O47-C7-C8	3.68	119.44	111.50
23	f	101	SQD	O9-S-O7	-3.68	101.22	113.95
23	D	409	SQD	O9-S-O7	-3.67	101.24	113.95
25	c	510	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
23	c	501	SQD	O9-S-O7	-3.65	101.31	113.95
25	C	510	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
23	A	603	SQD	O5-C5-C4	3.64	116.31	109.69
25	B	611	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
25	D	403	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
23	b	601	SQD	O47-C7-C8	3.63	119.33	111.50
25	B	607	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
25	b	614	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
25	C	504	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
23	b	601	SQD	O9-S-O7	-3.62	101.40	113.95
25	b	606	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
23	D	408	SQD	O47-C7-C8	3.62	119.30	111.50
29	B	621	LMG	O6-C1-O1	-3.58	101.48	109.97
23	A	603	SQD	O47-C7-C8	3.58	119.22	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	611	PL9	C7-C3-C2	-3.58	118.59	123.30
25	c	506	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
35	V	201	HEC	CMB-C2B-C1B	-3.57	122.98	128.46
25	c	515	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	c	513	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
27	c	516	BCR	C2-C1-C6	3.56	115.97	110.48
25	c	514	CLA	CMB-C2B-C3B	3.56	131.33	124.68
23	b	601	SQD	O9-S-C6	3.54	111.15	106.94
25	A	606	CLA	CMB-C2B-C3B	3.54	131.30	124.68
28	D	407	PL9	C7-C3-C2	-3.54	118.64	123.30
28	A	611	PL9	C7-C3-C2	-3.54	118.65	123.30
25	c	511	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
25	B	603	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
25	b	611	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
25	B	606	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
25	B	614	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
25	b	616	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
25	b	609	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
23	D	408	SQD	O7-S-C6	3.49	111.09	106.94
23	D	409	SQD	O47-C7-C8	3.49	119.02	111.50
25	b	619	CLA	CMB-C2B-C3B	3.48	131.19	124.68
25	a	607	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
25	b	607	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
25	c	503	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
28	d	408	PL9	C7-C3-C2	-3.47	118.74	123.30
25	b	610	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
25	C	512	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
25	B	608	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
25	d	403	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
25	c	505	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
33	C	517	DGD	O6D-C1D-O3G	-3.44	101.82	109.97
23	c	501	SQD	O47-C7-C8	3.44	118.92	111.50
33	c	518	DGD	O6D-C1D-O3G	-3.44	101.83	109.97
25	C	513	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	c	509	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	b	617	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
25	C	511	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
25	C	501	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
35	v	201	HEC	CMB-C2B-C1B	-3.41	123.22	128.46
25	C	505	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
33	c	520	DGD	O6D-C1D-O3G	-3.40	101.92	109.97
25	C	507	CLA	CMB-C2B-C1B	-3.40	123.24	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	606	CLA	CMB-C2B-C3B	3.40	131.04	124.68
25	A	606	CLA	C4A-NA-C1A	3.39	108.23	106.71
23	c	501	SQD	O5-C5-C4	3.39	115.85	109.69
33	C	516	DGD	O6D-C1D-O3G	-3.39	101.94	109.97
25	b	605	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
25	A	607	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
33	C	518	DGD	O6D-C1D-O3G	-3.38	101.96	109.97
23	B	626	SQD	O6-C1-C2	3.38	113.58	108.30
25	B	607	CLA	C4A-NA-C1A	3.38	108.22	106.71
25	d	404	CLA	CMB-C2B-C3B	3.38	130.99	124.68
25	A	615	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
25	B	605	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
29	A	613	LMG	O6-C1-O1	-3.37	101.99	109.97
25	b	613	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
25	a	609	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
25	C	503	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
25	C	509	CLA	CMB-C2B-C3B	3.36	130.96	124.68
25	b	608	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
25	C	506	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
25	B	610	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
25	B	604	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
25	B	601	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
25	D	402	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
25	C	502	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
33	c	519	DGD	O6D-C1D-O3G	-3.31	102.14	109.97
25	c	507	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	B	602	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
23	f	101	SQD	O6-C1-C2	3.27	113.41	108.30
25	B	616	CLA	CMB-C2B-C3B	3.27	130.80	124.68
25	a	612	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
25	B	615	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
25	b	604	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
23	B	626	SQD	O8-S-C6	3.25	110.91	105.74
23	D	409	SQD	O5-C5-C4	3.24	115.57	109.69
25	b	618	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
25	B	609	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
25	b	612	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
23	B	626	SQD	O7-S-C6	3.20	110.75	106.94
23	D	409	SQD	O6-C1-C2	3.20	113.29	108.30
25	B	612	CLA	CMB-C2B-C3B	3.19	130.64	124.68
25	c	504	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
25	c	512	CLA	CMB-C2B-C3B	3.18	130.62	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	H	103	DGD	O6D-C1D-O3G	-3.17	102.47	109.97
32	A	620	BCT	O2-C-O1	-3.17	111.33	119.55
26	d	401	PHO	CMB-C2B-C3B	3.15	130.58	124.68
23	B	626	SQD	C3-C4-C5	3.15	115.86	110.24
25	B	613	CLA	CMB-C2B-C3B	3.14	130.56	124.68
25	A	609	CLA	CMB-C2B-C3B	3.13	130.53	124.68
25	b	610	CLA	CHB-C4A-NA	3.12	128.83	124.51
26	D	401	PHO	CMB-C2B-C3B	3.12	130.51	124.68
23	D	408	SQD	O8-S-C6	3.11	110.69	105.74
25	b	607	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
29	A	613	LMG	O1-C7-C8	-3.09	103.45	110.90
32	a	605	BCT	O2-C-O1	-3.08	111.56	119.55
25	b	615	CLA	CMB-C2B-C3B	3.07	130.43	124.68
25	A	615	CLA	CHB-C4A-NA	3.07	128.76	124.51
25	a	612	CLA	CHB-C4A-NA	3.06	128.74	124.51
23	f	101	SQD	O5-C5-C4	3.05	115.23	109.69
25	C	508	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	B	607	CLA	CMB-C2B-C3B	3.05	130.38	124.68
25	b	617	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
33	h	102	DGD	O6D-C1D-O3G	-3.04	102.77	109.97
25	b	606	CLA	CMB-C2B-C3B	3.04	130.37	124.68
23	b	601	SQD	C44-O6-C1	3.04	119.68	113.74
25	b	606	CLA	CHB-C4A-NA	3.04	128.71	124.51
25	D	403	CLA	CMB-C2B-C3B	3.03	130.35	124.68
34	e	101	HEM	C4B-CHC-C1C	3.03	126.55	122.56
28	D	407	PL9	C40-C39-C41	3.03	120.36	115.27
25	b	609	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
34	E	101	HEM	C4B-CHC-C1C	3.02	126.55	122.56
25	B	606	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	B	607	CLA	CHB-C4A-NA	3.02	128.69	124.51
27	c	516	BCR	C15-C16-C17	-3.02	117.30	123.47
25	c	510	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	c	510	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
25	C	510	CLA	CMB-C2B-C3B	2.99	130.27	124.68
25	C	504	CLA	CMB-C2B-C3B	2.99	130.27	124.68
29	B	625	LMG	O6-C1-O1	-2.99	102.90	109.97
25	b	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	A	606	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	c	509	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	d	404	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
25	C	512	CLA	CMB-C2B-C3B	2.97	130.24	124.68
25	B	601	CLA	O2D-CGD-O1D	-2.97	118.03	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	501	SQD	O6-C1-C2	2.96	112.93	108.30
25	C	507	CLA	CHB-C4A-NA	2.96	128.60	124.51
25	c	506	CLA	CMB-C2B-C3B	2.96	130.21	124.68
25	b	611	CLA	CMB-C2B-C3B	2.96	130.21	124.68
25	c	509	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
29	b	624	LMG	O6-C1-O1	-2.95	102.98	109.97
25	a	607	CLA	CHB-C4A-NA	2.95	128.60	124.51
25	c	515	CLA	CMB-C2B-C3B	2.95	130.20	124.68
25	A	609	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	B	603	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
25	B	603	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	b	619	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	A	603	SQD	O6-C1-C2	2.94	112.90	108.30
34	e	101	HEM	C4D-ND-C1D	2.94	108.11	105.07
25	B	604	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
25	B	603	CLA	CMB-C2B-C3B	2.94	130.17	124.68
25	b	616	CLA	CMB-C2B-C3B	2.93	130.17	124.68
25	C	507	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	b	610	CLA	CMB-C2B-C3B	2.93	130.16	124.68
25	b	606	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	c	511	CLA	CMB-C2B-C3B	2.93	130.16	124.68
25	c	513	CLA	CMB-C2B-C3B	2.93	130.16	124.68
25	B	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	d	403	CLA	CMB-C2B-C3B	2.93	130.16	124.68
27	H	102	BCR	C2-C1-C6	2.93	114.99	110.48
25	C	507	CLA	CMB-C2B-C3B	2.93	130.15	124.68
26	a	608	PHO	CMB-C2B-C3B	2.93	130.15	124.68
25	c	506	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	C	505	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
27	B	627	BCR	C15-C14-C13	-2.92	123.14	127.31
25	C	513	CLA	CHB-C4A-NA	2.92	128.55	124.51
27	C	515	BCR	C15-C16-C17	-2.91	117.50	123.47
25	b	618	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	c	509	CLA	CMB-C2B-C3B	2.91	130.13	124.68
25	c	506	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	C	508	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	C	505	CLA	CMB-C2B-C3B	2.91	130.12	124.68
25	c	503	CLA	CMB-C2B-C3B	2.91	130.12	124.68
25	b	607	CLA	CHB-C4A-NA	2.91	128.53	124.51
25	C	504	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	c	508	CLA	CMB-C2B-C3B	2.91	130.12	124.68
25	c	503	CLA	O2D-CGD-O1D	-2.91	118.16	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	614	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	B	614	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	B	611	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	b	609	CLA	CMB-C2B-C3B	2.90	130.10	124.68
25	c	505	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	a	606	CLA	CHB-C4A-NA	2.90	128.52	124.51
23	D	408	SQD	C44-O6-C1	2.90	119.40	113.74
25	B	602	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
25	b	609	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	b	605	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
25	B	613	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
23	A	603	SQD	C3-C4-C5	2.88	115.38	110.24
25	C	504	CLA	CHB-C4A-NA	2.88	128.50	124.51
25	B	606	CLA	CMB-C2B-C3B	2.88	130.07	124.68
27	T	101	BCR	C33-C5-C6	-2.88	121.30	124.53
25	b	615	CLA	CHB-C4A-NA	2.88	128.49	124.51
27	h	101	BCR	C24-C23-C22	-2.88	121.89	126.23
25	B	610	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
25	c	507	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	a	609	CLA	CHB-C4A-NA	2.87	128.49	124.51
25	c	515	CLA	CHB-C4A-NA	2.87	128.49	124.51
23	D	408	SQD	C3-C4-C5	2.87	115.36	110.24
25	B	615	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	D	403	CLA	CHB-C4A-NA	2.87	128.48	124.51
25	a	612	CLA	CHD-C1D-ND	-2.87	121.82	124.45
25	a	609	CLA	CMB-C2B-C3B	2.87	130.05	124.68
25	C	501	CLA	CMB-C2B-C3B	2.87	130.04	124.68
23	B	626	SQD	C44-O6-C1	2.87	119.34	113.74
25	a	607	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	b	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	c	514	CLA	CHB-C4A-NA	2.87	128.47	124.51
25	a	612	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
27	b	622	BCR	C2-C1-C6	2.86	114.89	110.48
25	B	608	CLA	CMB-C2B-C3B	2.86	130.03	124.68
28	d	408	PL9	C22-C23-C24	-2.86	120.78	127.66
25	C	513	CLA	CMB-C2B-C3B	2.86	130.02	124.68
25	B	602	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	c	505	CLA	CMB-C2B-C3B	2.85	130.02	124.68
25	b	615	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	b	605	CLA	CMB-C2B-C3B	2.85	130.01	124.68
27	B	627	BCR	C33-C5-C6	-2.85	121.33	124.53
25	A	607	CLA	O2D-CGD-O1D	-2.85	118.27	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	402	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	B	601	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	A	615	CLA	CHD-C1D-ND	-2.85	121.84	124.45
25	B	616	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	C	509	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	c	515	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	B	617	BCR	C15-C16-C17	-2.85	117.64	123.47
25	b	607	CLA	CMB-C2B-C3B	2.85	130.00	124.68
25	b	614	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	B	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	B	612	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
25	A	609	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	b	616	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
27	C	514	BCR	C15-C16-C17	-2.84	117.66	123.47
25	c	513	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	C	502	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	C	511	CLA	CMB-C2B-C3B	2.84	129.99	124.68
25	A	607	CLA	CHB-C4A-NA	2.84	128.43	124.51
25	b	617	CLA	CMB-C2B-C3B	2.84	129.98	124.68
34	E	101	HEM	C4D-ND-C1D	2.84	108.00	105.07
25	C	501	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
25	C	508	CLA	CHB-C4A-NA	2.83	128.43	124.51
25	C	503	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	c	504	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
25	C	506	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	C	510	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
29	B	621	LMG	O1-C7-C8	-2.82	104.09	110.90
25	c	508	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	c	511	CLA	CHB-C4A-NA	2.82	128.41	124.51
29	b	623	LMG	O6-C1-O1	-2.82	103.30	109.97
25	c	510	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	B	612	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	a	609	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	T	101	BCR	C15-C14-C13	-2.81	123.29	127.31
26	D	401	PHO	O2D-CGD-O1D	-2.81	118.34	123.84
23	b	601	SQD	O8-S-C6	2.81	110.22	105.74
25	B	607	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	c	517	BCR	C15-C16-C17	-2.81	117.72	123.47
25	C	509	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	c	512	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	A	609	CLA	CHD-C1D-ND	-2.81	121.88	124.45
25	B	605	CLA	CMB-C2B-C3B	2.80	129.92	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	507	CLA	CMB-C2B-C3B	2.80	129.92	124.68
25	b	605	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	B	602	CLA	CMB-C2B-C3B	2.80	129.92	124.68
25	C	512	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
25	B	611	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
25	b	608	CLA	CMB-C2B-C3B	2.79	129.90	124.68
33	h	102	DGD	CDB-CCB-CBB	-2.79	100.25	114.42
25	a	607	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	A	607	CLA	CMB-C2B-C3B	2.79	129.90	124.68
28	A	611	PL9	C7-C8-C9	-2.79	122.15	126.79
25	C	513	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	c	514	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	B	610	CLA	CMB-C2B-C3B	2.79	129.89	124.68
31	A	616	LHG	O8-C23-C24	2.79	120.66	111.91
25	A	615	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	B	608	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	B	615	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	b	604	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	A	608	PHO	O2D-CGD-O1D	-2.79	118.39	123.84
31	a	614	LHG	O8-C23-C24	2.79	120.65	111.91
25	c	506	CLA	CHD-C1D-ND	-2.78	121.89	124.45
25	D	403	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
27	D	404	BCR	C27-C26-C25	2.78	126.77	122.73
27	K	101	BCR	C15-C16-C17	-2.78	117.77	123.47
26	A	608	PHO	O1D-CGD-CBD	2.78	129.38	124.74
25	a	607	CLA	CHD-C1D-ND	-2.78	121.90	124.45
25	b	612	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
26	d	401	PHO	O2D-CGD-O1D	-2.78	118.40	123.84
25	A	615	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	D	402	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
25	B	613	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	c	503	CLA	CHD-C1D-ND	-2.77	121.90	124.45
26	a	608	PHO	O1D-CGD-CBD	2.77	129.36	124.74
33	C	518	DGD	CDB-CCB-CBB	-2.77	100.34	114.42
26	d	401	PHO	O1D-CGD-CBD	2.77	129.36	124.74
25	C	512	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	d	404	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	b	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
33	c	518	DGD	CDB-CCB-CBB	-2.77	100.36	114.42
25	b	611	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	C	506	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
31	A	618	LHG	O8-C23-C24	2.77	120.60	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	405	BCR	C27-C26-C25	2.77	126.75	122.73
25	c	513	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	B	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
26	D	401	PHO	O1D-CGD-CBD	2.77	129.35	124.74
25	B	607	CLA	CHD-C1D-ND	-2.77	121.91	124.45
27	B	627	BCR	C15-C16-C17	-2.76	117.81	123.47
28	A	611	PL9	C40-C39-C41	2.76	119.92	115.27
25	b	617	CLA	CHB-C4A-NA	2.76	128.33	124.51
27	c	516	BCR	C15-C14-C13	-2.76	123.37	127.31
25	b	618	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	C	503	CLA	CMB-C2B-C3B	2.76	129.84	124.68
25	C	504	CLA	CHD-C1D-ND	-2.76	121.92	124.45
25	a	609	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
27	h	101	BCR	C29-C30-C25	2.75	114.72	110.48
25	C	501	CLA	CHB-C4A-NA	2.75	128.32	124.51
27	b	620	BCR	C15-C16-C17	-2.75	117.84	123.47
27	b	621	BCR	C27-C26-C25	2.75	126.73	122.73
25	c	511	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
25	D	403	CLA	CHD-C1D-ND	-2.75	121.93	124.45
33	c	519	DGD	CDB-CCB-CBB	-2.75	100.48	114.42
25	b	613	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	B	616	CLA	CHB-C4A-NA	2.75	128.31	124.51
27	B	619	BCR	C27-C26-C25	2.75	126.72	122.73
35	V	201	HEC	CMB-C2B-C3B	2.75	129.05	125.82
25	B	606	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	B	611	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	C	502	CLA	CMB-C2B-C3B	2.75	129.81	124.68
25	b	613	CLA	CHB-C4A-NA	2.74	128.31	124.51
25	a	612	CLA	CMB-C2B-C3B	2.74	129.81	124.68
25	B	601	CLA	CMB-C2B-C3B	2.74	129.81	124.68
25	c	503	CLA	CHB-C4A-NA	2.74	128.30	124.51
27	b	620	BCR	C33-C5-C6	-2.74	121.45	124.53
25	C	513	CLA	CHD-C1D-ND	-2.74	121.94	124.45
25	B	603	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
27	B	618	BCR	C27-C26-C25	2.74	126.70	122.73
25	b	618	CLA	CMB-C2B-C3B	2.74	129.80	124.68
27	K	101	BCR	C24-C23-C22	-2.73	122.10	126.23
33	H	103	DGD	CDB-CCB-CBB	-2.73	100.57	114.42
25	b	619	CLA	CHB-C4A-NA	2.73	128.29	124.51
33	c	520	DGD	CDB-CCB-CBB	-2.73	100.59	114.42
25	c	505	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	a	606	CLA	CHD-C1D-ND	-2.72	121.95	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	506	CLA	CMB-C2B-C3B	2.72	129.77	124.68
23	f	101	SQD	O8-S-C6	2.72	110.08	105.74
25	C	503	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
31	d	407	LHG	O8-C23-C24	2.72	120.45	111.91
25	C	511	CLA	CHB-C4A-NA	2.72	128.28	124.51
27	B	617	BCR	C33-C5-C6	-2.72	121.47	124.53
25	C	511	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	c	515	CLA	CHD-C1D-ND	-2.72	121.96	124.45
29	C	519	LMG	O6-C1-O1	-2.71	103.55	109.97
27	C	514	BCR	C33-C5-C6	-2.71	121.48	124.53
25	B	604	CLA	CMB-C2B-C3B	2.71	129.75	124.68
25	b	613	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
25	B	610	CLA	CHB-C4A-NA	2.71	128.25	124.51
34	e	101	HEM	C1B-NB-C4B	2.71	107.87	105.07
23	c	501	SQD	C44-O6-C1	2.71	119.03	113.74
28	a	611	PL9	C40-C39-C41	2.70	119.82	115.27
25	d	403	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
25	A	606	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
27	C	514	BCR	C15-C14-C13	-2.70	123.46	127.31
25	b	610	CLA	CHD-C1D-ND	-2.70	121.97	124.45
31	A	617	LHG	O8-C23-C24	2.70	120.37	111.91
25	b	608	CLA	CHD-C1D-ND	-2.70	121.98	124.45
25	C	510	CLA	CHB-C4A-NA	2.70	128.24	124.51
26	A	608	PHO	CMB-C2B-C3B	2.69	129.72	124.68
25	c	507	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
25	A	607	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	d	403	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
27	b	622	BCR	C27-C26-C25	2.69	126.63	122.73
25	B	615	CLA	CMB-C2B-C3B	2.69	129.71	124.68
25	C	502	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	a	609	CLA	CHD-C1D-ND	-2.69	121.98	124.45
25	B	602	CLA	CHD-C1D-ND	-2.69	121.99	124.45
27	d	405	BCR	C2-C1-C6	2.68	114.61	110.48
25	c	504	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	b	612	CLA	CMB-C2B-C3B	2.68	129.69	124.68
25	C	501	CLA	CHD-C1D-ND	-2.68	121.99	124.45
25	a	606	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	C	505	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
25	b	609	CLA	CHD-C1D-ND	-2.68	121.99	124.45
23	A	603	SQD	O8-S-C6	2.68	110.01	105.74
25	b	608	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	b	612	CLA	CHB-C4A-NA	2.68	128.21	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	614	CLA	CHB-C4A-NA	2.68	128.21	124.51
25	A	609	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
25	b	614	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	d	404	CLA	CHD-C1D-ND	-2.67	122.00	124.45
25	b	617	CLA	CHD-C1D-ND	-2.67	122.00	124.45
25	b	605	CLA	CHD-C1D-ND	-2.67	122.00	124.45
25	b	608	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	b	606	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
23	f	101	SQD	C44-O6-C1	2.67	118.95	113.74
25	D	402	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
23	D	409	SQD	O8-S-C6	2.66	109.98	105.74
25	B	609	CLA	CMB-C2B-C3B	2.66	129.66	124.68
25	d	403	CLA	CHD-C1D-ND	-2.66	122.01	124.45
25	B	608	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	a	608	PHO	O2D-CGD-O1D	-2.66	118.64	123.84
25	c	512	CLA	CHB-C4A-NA	2.66	128.19	124.51
34	E	101	HEM	C1B-NB-C4B	2.66	107.82	105.07
27	K	101	BCR	C27-C26-C25	2.66	126.59	122.73
25	B	605	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	b	616	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	C	512	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
25	b	604	CLA	CMB-C2B-C3B	2.65	129.64	124.68
27	C	515	BCR	C15-C14-C13	-2.65	123.53	127.31
27	B	619	BCR	C24-C23-C22	-2.65	122.23	126.23
25	b	619	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
25	c	510	CLA	CHD-C1D-ND	-2.65	122.02	124.45
27	H	102	BCR	C27-C26-C25	2.65	126.58	122.73
25	B	607	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
33	C	517	DGD	CDB-CCB-CBB	-2.65	100.99	114.42
28	A	611	PL9	C22-C23-C24	-2.64	121.30	127.66
31	D	406	LHG	O8-C23-C24	2.64	120.19	111.91
25	B	605	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
25	A	606	CLA	CHD-C1D-ND	-2.64	122.03	124.45
23	c	501	SQD	O8-S-C6	2.64	109.94	105.74
25	b	614	CLA	CHD-C1D-ND	-2.63	122.03	124.45
31	L	101	LHG	O8-C23-C24	2.63	120.17	111.91
25	b	611	CLA	CHD-C1D-ND	-2.63	122.04	124.45
25	c	508	CLA	CHB-C4A-NA	2.62	128.14	124.51
29	B	625	LMG	O1-C7-C8	-2.62	104.58	110.90
31	a	613	LHG	O8-C23-C24	2.62	120.13	111.91
25	C	508	CLA	CHD-C1D-ND	-2.62	122.05	124.45
33	C	517	DGD	O5D-C6D-C5D	-2.62	104.21	109.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	611	CLA	CHD-C1D-ND	-2.61	122.05	124.45
25	B	614	CLA	CHD-C1D-ND	-2.61	122.05	124.45
25	b	611	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
29	B	620	LMG	O6-C1-O1	-2.60	103.81	109.97
33	C	516	DGD	CDB-CCB-CBB	-2.60	101.23	114.42
25	B	608	CLA	CHD-C1D-ND	-2.60	122.07	124.45
25	b	605	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
27	c	517	BCR	C15-C14-C13	-2.60	123.60	127.31
25	A	609	CLA	C1-C2-C3	-2.60	121.55	126.04
35	v	201	HEC	CBD-CAD-C3D	-2.60	108.19	112.62
25	c	508	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
27	D	404	BCR	C33-C5-C6	-2.59	121.61	124.53
29	A	613	LMG	C40-C39-C38	-2.59	101.27	114.42
25	b	610	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
29	A	612	LMG	O6-C1-O1	-2.59	103.84	109.97
31	a	615	LHG	O8-C23-C24	2.59	120.02	111.91
23	B	626	SQD	C1-O5-C5	2.58	118.76	113.69
25	b	604	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	B	609	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	B	605	CLA	CHD-C1D-ND	-2.58	122.08	124.45
25	A	606	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
25	b	608	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
25	c	504	CLA	CMB-C2B-C3B	2.58	129.51	124.68
27	B	617	BCR	C27-C26-C25	2.58	126.48	122.73
33	C	518	DGD	C3G-C2G-C1G	-2.58	105.68	111.79
25	B	611	CLA	C1-C2-C3	-2.58	121.58	126.04
25	d	403	CLA	CHB-C4A-NA	2.58	128.08	124.51
31	A	616	LHG	C11-C10-C9	-2.58	101.34	114.42
29	c	521	LMG	O6-C1-O1	-2.58	103.87	109.97
29	d	406	LMG	O6-C1-O1	-2.58	103.87	109.97
27	B	617	BCR	C24-C23-C22	-2.57	122.35	126.23
27	B	627	BCR	C24-C23-C22	-2.57	122.35	126.23
27	B	619	BCR	C33-C5-C6	-2.57	121.64	124.53
25	c	509	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
27	b	620	BCR	C15-C14-C13	-2.57	123.64	127.31
25	B	610	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
25	C	506	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	C	510	CLA	CHD-C1D-ND	-2.57	122.09	124.45
23	I	101	SQD	O48-C23-C24	2.57	119.96	111.91
27	b	620	BCR	C27-C26-C25	2.57	126.46	122.73
33	c	519	DGD	O5D-C6D-C5D	-2.56	104.30	109.05
27	B	619	BCR	C15-C16-C17	-2.56	118.23	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	y	101	BCR	C33-C5-C6	-2.56	121.66	124.53
25	B	601	CLA	CHD-C1D-ND	-2.56	122.11	124.45
25	B	606	CLA	CHD-C1D-ND	-2.56	122.11	124.45
25	B	609	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
28	d	408	PL9	C7-C8-C9	-2.55	122.54	126.79
35	v	201	HEC	CMB-C2B-C3B	2.55	128.82	125.82
27	B	617	BCR	C15-C14-C13	-2.55	123.67	127.31
25	D	402	CLA	CHB-C4A-NA	2.55	128.04	124.51
31	a	613	LHG	C11-C10-C9	-2.55	101.48	114.42
25	c	505	CLA	CHD-C1D-ND	-2.55	122.11	124.45
25	B	603	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	b	619	CLA	CHD-C1D-ND	-2.54	122.12	124.45
27	T	101	BCR	C15-C16-C17	-2.54	118.27	123.47
33	C	516	DGD	O5D-C6D-C5D	-2.54	104.35	109.05
25	b	606	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	c	511	CLA	CHD-C1D-ND	-2.54	122.12	124.45
25	a	612	CLA	C1B-CHB-C4A	-2.54	125.10	130.12
33	c	520	DGD	O5D-C6D-C5D	-2.53	104.36	109.05
29	B	625	LMG	O1-C1-C2	-2.53	104.35	108.30
29	B	625	LMG	O3-C3-C2	-2.53	104.50	110.35
28	a	611	PL9	C22-C23-C24	-2.53	121.57	127.66
27	B	617	BCR	C11-C10-C9	-2.53	123.70	127.31
29	A	613	LMG	C3-C4-C5	-2.53	105.73	110.24
25	B	605	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
27	T	101	BCR	C24-C23-C22	-2.52	122.43	126.23
23	B	626	SQD	O48-C23-C24	2.51	119.80	111.91
31	a	613	LHG	C20-C19-C18	-2.51	101.67	114.42
29	B	625	LMG	C40-C39-C38	-2.51	101.68	114.42
25	b	612	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
28	A	611	PL9	C27-C28-C29	-2.51	121.62	127.66
25	C	507	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
29	B	620	LMG	C40-C39-C38	-2.51	101.69	114.42
31	l	101	LHG	C11-C10-C9	-2.50	101.73	114.42
25	B	616	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
31	a	615	LHG	C11-C10-C9	-2.50	101.74	114.42
27	y	101	BCR	C27-C26-C25	2.50	126.36	122.73
25	b	617	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
27	A	610	BCR	C15-C16-C17	-2.50	118.36	123.47
25	A	615	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
25	B	602	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
28	D	407	PL9	C22-C23-C24	-2.49	121.66	127.66
29	B	625	LMG	O2-C2-C1	-2.49	103.99	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	101	BCR	C24-C23-C22	-2.49	122.47	126.23
25	D	403	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
25	C	509	CLA	CHD-C1D-ND	-2.49	122.17	124.45
27	B	618	BCR	C15-C16-C17	-2.49	118.38	123.47
25	c	508	CLA	CHD-C1D-ND	-2.48	122.17	124.45
25	b	614	CLA	C1-C2-C3	-2.48	121.76	126.04
28	D	407	PL9	C7-C8-C9	-2.48	122.67	126.79
29	c	502	LMG	O6-C1-O1	-2.48	104.11	109.97
23	A	603	SQD	C44-O6-C1	2.47	118.57	113.74
28	a	611	PL9	C7-C8-C9	-2.47	122.68	126.79
27	K	101	BCR	C15-C14-C13	-2.47	123.79	127.31
25	a	606	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
28	d	408	PL9	C27-C28-C29	-2.47	121.72	127.66
25	b	613	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
27	C	514	BCR	C11-C10-C9	-2.46	123.79	127.31
31	D	406	LHG	C20-C19-C18	-2.46	101.92	114.42
31	L	101	LHG	C11-C10-C9	-2.46	101.93	114.42
23	b	601	SQD	O48-C23-C24	2.46	119.62	111.91
28	d	408	PL9	C36-C34-C33	-2.45	116.15	121.12
27	C	515	BCR	C33-C5-C6	-2.45	121.77	124.53
25	B	614	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	C	508	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
33	c	518	DGD	O5D-C6D-C5D	-2.45	104.52	109.05
25	C	503	CLA	CHD-C1D-ND	-2.45	122.21	124.45
25	B	611	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
29	D	405	LMG	C40-C39-C38	-2.44	102.02	114.42
29	c	521	LMG	C40-C39-C38	-2.44	102.03	114.42
29	b	623	LMG	C40-C39-C38	-2.44	102.04	114.42
25	C	506	CLA	CHD-C1D-ND	-2.44	122.21	124.45
25	c	513	CLA	CHD-C1D-ND	-2.44	122.21	124.45
27	B	618	BCR	C15-C14-C13	-2.44	123.83	127.31
27	c	517	BCR	C33-C5-C6	-2.44	121.79	124.53
28	a	611	PL9	C27-C28-C29	-2.44	121.80	127.66
33	C	516	DGD	C3G-C2G-C1G	-2.43	106.03	111.79
29	b	624	LMG	C38-C37-C36	-2.43	102.09	114.42
29	b	623	LMG	C38-C37-C36	-2.43	102.09	114.42
25	B	606	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
31	A	617	LHG	C11-C10-C9	-2.43	102.10	114.42
25	C	505	CLA	CHB-C4A-NA	2.43	127.87	124.51
31	l	101	LHG	O8-C23-C24	2.43	119.52	111.91
25	B	609	CLA	CHD-C1D-ND	-2.43	122.22	124.45
27	a	610	BCR	C27-C26-C25	2.43	126.25	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	512	CLA	CHD-C1D-ND	-2.43	122.22	124.45
25	D	402	CLA	CHD-C1D-ND	-2.42	122.23	124.45
29	c	521	LMG	C38-C37-C36	-2.42	102.12	114.42
25	b	609	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
25	C	511	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	c	516	BCR	C27-C26-C25	2.42	126.25	122.73
23	A	603	SQD	C4-C3-C2	2.42	115.05	110.82
29	B	620	LMG	C38-C37-C36	-2.42	102.13	114.42
27	B	618	BCR	C33-C5-C6	-2.42	121.81	124.53
31	d	407	LHG	C20-C19-C18	-2.42	102.13	114.42
27	a	610	BCR	C15-C16-C17	-2.42	118.52	123.47
25	b	615	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
25	b	612	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	A	610	BCR	C15-C14-C13	-2.42	123.86	127.31
31	a	615	LHG	C20-C19-C18	-2.42	102.15	114.42
25	b	618	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
23	A	619	SQD	O48-C23-C24	2.42	119.49	111.91
34	e	101	HEM	C4C-CHD-C1D	2.42	125.75	122.56
23	A	603	SQD	O48-C23-C24	2.42	119.49	111.91
29	C	520	LMG	C40-C39-C38	-2.41	102.17	114.42
27	C	515	BCR	C27-C26-C25	2.41	126.24	122.73
29	C	519	LMG	C38-C37-C36	-2.41	102.17	114.42
27	a	610	BCR	C33-C5-C6	-2.41	121.82	124.53
25	B	608	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
29	A	612	LMG	C40-C39-C38	-2.41	102.19	114.42
25	b	618	CLA	CHD-C1D-ND	-2.41	122.24	124.45
25	c	507	CLA	CHB-C4A-NA	2.41	127.84	124.51
27	k	101	BCR	C33-C5-C6	-2.41	121.83	124.53
25	a	607	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
25	C	502	CLA	CHD-C1D-ND	-2.40	122.24	124.45
29	D	405	LMG	O6-C1-O1	-2.40	104.28	109.97
28	D	407	PL9	C27-C28-C29	-2.40	121.87	127.66
25	C	502	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
27	C	514	BCR	C27-C26-C25	2.40	126.22	122.73
25	b	604	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
31	d	407	LHG	C11-C10-C9	-2.40	102.24	114.42
29	c	502	LMG	C40-C39-C38	-2.40	102.24	114.42
25	B	601	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	b	615	CLA	CHD-C1D-ND	-2.40	122.25	124.45
33	C	518	DGD	O5D-C6D-C5D	-2.40	104.61	109.05
29	C	519	LMG	C40-C39-C38	-2.40	102.26	114.42
27	a	610	BCR	C15-C14-C13	-2.40	123.89	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	517	BCR	C27-C26-C25	2.40	126.21	122.73
27	b	621	BCR	C33-C5-C6	-2.39	121.84	124.53
25	A	607	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
25	B	615	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	d	404	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
33	c	520	DGD	C3G-C2G-C1G	-2.39	106.14	111.79
31	l	101	LHG	C20-C19-C18	-2.39	102.31	114.42
33	h	102	DGD	C3G-C2G-C1G	-2.39	106.15	111.79
28	D	407	PL9	C20-C19-C21	2.38	119.28	115.27
28	d	408	PL9	C40-C39-C41	2.38	119.28	115.27
27	Y	101	BCR	C33-C5-C6	-2.38	121.85	124.53
27	k	101	BCR	C29-C30-C25	2.38	114.15	110.48
33	c	518	DGD	C3G-C2G-C1G	-2.38	106.15	111.79
27	A	610	BCR	C27-C26-C25	2.38	126.19	122.73
29	B	625	LMG	C38-C37-C36	-2.38	102.34	114.42
29	c	502	LMG	C38-C37-C36	-2.38	102.34	114.42
29	c	522	LMG	C40-C39-C38	-2.38	102.35	114.42
34	E	101	HEM	CMC-C2C-C3C	2.38	129.13	124.68
29	A	612	LMG	C38-C37-C36	-2.38	102.36	114.42
23	D	409	SQD	O48-C23-C24	2.37	119.36	111.91
31	L	101	LHG	C20-C19-C18	-2.37	102.38	114.42
25	B	616	CLA	CHD-C1D-ND	-2.37	122.28	124.45
27	C	515	BCR	C11-C10-C9	-2.37	123.93	127.31
29	B	621	LMG	C40-C39-C38	-2.37	102.40	114.42
25	c	514	CLA	CHD-C1D-ND	-2.37	122.28	124.45
27	H	102	BCR	C15-C14-C13	-2.37	123.93	127.31
35	V	201	HEC	CMD-C2D-C1D	-2.36	124.83	128.46
31	A	617	LHG	C20-C19-C18	-2.36	102.42	114.42
27	A	610	BCR	C33-C5-C6	-2.36	121.87	124.53
29	b	623	LMG	O1-C7-C8	-2.36	105.20	110.90
23	c	501	SQD	O48-C23-C24	2.36	119.32	111.91
29	d	406	LMG	C40-C39-C38	-2.36	102.44	114.42
31	A	616	LHG	C20-C19-C18	-2.36	102.45	114.42
27	h	101	BCR	C15-C14-C13	-2.36	123.95	127.31
29	b	624	LMG	C40-C39-C38	-2.36	102.46	114.42
31	A	618	LHG	C11-C10-C9	-2.36	102.47	114.42
25	C	513	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
25	c	510	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
25	b	614	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
27	c	516	BCR	C11-C10-C9	-2.35	123.95	127.31
27	y	101	BCR	C24-C23-C22	-2.35	122.68	126.23
25	b	613	CLA	CHD-C1D-ND	-2.35	122.29	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	504	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	B	604	CLA	CHD-C1D-ND	-2.35	122.30	124.45
25	B	610	CLA	CHD-C1D-ND	-2.35	122.30	124.45
25	B	613	CLA	CHD-C1D-ND	-2.35	122.30	124.45
29	C	520	LMG	C38-C37-C36	-2.35	102.51	114.42
27	Y	101	BCR	C27-C26-C25	2.34	126.13	122.73
25	C	510	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	B	615	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
27	h	101	BCR	C11-C10-C9	-2.34	123.97	127.31
25	C	509	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	c	511	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
34	E	101	HEM	CBA-CAA-C2A	-2.34	108.63	112.62
31	a	613	LHG	C18-C17-C16	-2.34	102.56	114.42
25	c	506	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	b	616	CLA	CHD-C1D-ND	-2.34	122.31	124.45
25	c	515	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
34	e	101	HEM	CMC-C2C-C3C	2.34	129.05	124.68
25	C	501	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
25	c	504	CLA	CHD-C1D-ND	-2.33	122.31	124.45
25	c	504	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
31	D	406	LHG	C11-C10-C9	-2.33	102.61	114.42
28	A	611	PL9	C20-C19-C21	2.33	119.19	115.27
33	H	103	DGD	C3G-C2G-C1G	-2.33	106.29	111.79
29	c	522	LMG	C38-C37-C36	-2.32	102.63	114.42
27	k	101	BCR	C27-C26-C25	2.32	126.10	122.73
25	B	612	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
25	C	511	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
27	b	621	BCR	C15-C16-C17	-2.31	118.74	123.47
25	c	505	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
27	b	620	BCR	C24-C23-C22	-2.31	122.74	126.23
27	d	405	BCR	C33-C5-C6	-2.31	121.93	124.53
27	H	102	BCR	C11-C10-C9	-2.31	124.01	127.31
25	B	612	CLA	CHD-C1D-ND	-2.30	122.34	124.45
25	b	607	CLA	O2D-CGD-CBD	2.30	115.36	111.27
25	c	510	CLA	C1-C2-C3	-2.30	122.06	126.04
29	d	409	LMG	C40-C39-C38	-2.30	102.75	114.42
25	C	503	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	D	404	BCR	C11-C10-C9	-2.30	124.03	127.31
33	c	519	DGD	C3G-C2G-C1G	-2.30	106.35	111.79
31	A	618	LHG	C20-C19-C18	-2.30	102.77	114.42
25	c	509	CLA	CHD-C1D-ND	-2.29	122.34	124.45
29	B	625	LMG	C1-O6-C5	-2.29	109.19	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	514	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
28	A	611	PL9	C37-C38-C39	-2.29	122.16	127.66
29	B	621	LMG	O3-C3-C2	-2.29	105.06	110.35
25	b	607	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
29	d	406	LMG	C38-C37-C36	-2.28	102.83	114.42
25	c	503	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
27	H	102	BCR	C24-C23-C22	-2.28	122.79	126.23
29	D	405	LMG	C38-C37-C36	-2.28	102.85	114.42
27	B	627	BCR	C27-C26-C25	2.28	126.04	122.73
28	d	408	PL9	C31-C32-C33	-2.27	104.41	111.88
28	a	611	PL9	C20-C19-C21	2.27	119.09	115.27
33	c	519	DGD	CBB-CAB-C9B	-2.27	102.92	114.42
27	h	101	BCR	C2-C1-C6	2.27	113.97	110.48
27	c	516	BCR	C3-C4-C5	-2.26	110.03	114.08
29	A	613	LMG	O3-C3-C2	-2.25	105.14	110.35
31	A	617	LHG	C27-C26-C25	-2.25	103.00	114.42
29	d	409	LMG	C38-C37-C36	-2.25	103.01	114.42
27	A	610	BCR	C24-C23-C22	-2.25	122.84	126.23
27	C	514	BCR	C24-C23-C22	-2.24	122.85	126.23
27	K	101	BCR	C33-C5-C6	-2.24	122.01	124.53
29	c	502	LMG	O3-C3-C2	-2.24	105.17	110.35
29	C	520	LMG	O3-C3-C2	-2.24	105.17	110.35
25	b	612	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
25	B	604	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
27	y	101	BCR	C15-C16-C17	-2.24	118.89	123.47
29	B	621	LMG	C38-C37-C36	-2.24	103.07	114.42
25	b	616	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
25	c	512	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
34	E	101	HEM	C4C-CHD-C1D	2.23	125.51	122.56
25	B	613	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
25	C	508	CLA	C1-C2-C3	-2.23	122.18	126.04
27	B	619	BCR	C2-C1-C6	2.23	113.92	110.48
29	c	502	LMG	C1-C2-C3	-2.23	105.35	110.00
29	B	621	LMG	C3-C4-C5	-2.23	106.26	110.24
25	b	607	CLA	CHD-C1D-ND	-2.23	122.41	124.45
29	B	620	LMG	O3-C3-C2	-2.23	105.20	110.35
28	A	611	PL9	C36-C34-C33	-2.23	116.61	121.12
29	d	409	LMG	O1-C7-C8	-2.23	105.88	111.78
27	b	622	BCR	C33-C5-C6	-2.22	122.03	124.53
25	a	609	CLA	C1-C2-C3	-2.22	122.20	126.04
25	C	505	CLA	CHD-C1D-ND	-2.22	122.41	124.45
25	B	609	CLA	O2A-CGA-O1A	-2.22	117.99	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	404	BCR	C24-C23-C22	-2.22	122.88	126.23
28	a	611	PL9	C37-C38-C39	-2.22	122.33	127.66
29	b	624	LMG	O3-C3-C2	-2.21	105.23	110.35
29	c	522	LMG	O3-C3-C2	-2.21	105.23	110.35
25	c	513	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
31	d	407	LHG	C27-C26-C25	-2.21	103.22	114.42
26	D	401	PHO	CMC-C2C-C3C	2.21	129.10	124.94
27	a	610	BCR	C24-C23-C22	-2.21	122.90	126.23
25	c	507	CLA	CHD-C1D-ND	-2.20	122.43	124.45
31	a	614	LHG	C27-C26-C25	-2.20	103.24	114.42
26	A	608	PHO	CMC-C2C-C3C	2.20	129.10	124.94
31	l	101	LHG	C18-C17-C16	-2.20	103.25	114.42
29	c	522	LMG	C3-C4-C5	-2.20	106.31	110.24
31	A	616	LHG	C27-C26-C25	-2.20	103.25	114.42
23	D	408	SQD	O5-C1-C2	2.20	115.01	110.35
33	C	516	DGD	CAB-C9B-C8B	-2.20	103.26	114.42
29	b	623	LMG	O3-C3-C2	-2.20	105.26	110.35
25	c	508	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
28	A	611	PL9	O2-C1-C6	2.20	124.40	120.59
27	h	101	BCR	C15-C16-C17	-2.20	118.97	123.47
33	C	517	DGD	C1D-C2D-C3D	-2.20	105.42	110.00
27	d	405	BCR	C15-C16-C17	-2.20	118.97	123.47
29	A	612	LMG	O3-C3-C2	-2.20	105.27	110.35
25	c	515	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	b	601	SQD	O5-C5-C4	2.19	113.67	109.69
27	B	619	BCR	C15-C14-C13	-2.19	124.18	127.31
31	a	613	LHG	C27-C26-C25	-2.19	103.30	114.42
27	Y	101	BCR	C15-C16-C17	-2.19	118.99	123.47
25	C	510	CLA	C1-C2-C3	-2.18	122.27	126.04
23	D	409	SQD	C3-C4-C5	2.18	114.14	110.24
31	a	615	LHG	C18-C17-C16	-2.18	103.34	114.42
26	d	401	PHO	CMC-C2C-C3C	2.18	129.06	124.94
29	A	613	LMG	C38-C37-C36	-2.18	103.34	114.42
27	K	101	BCR	C8-C7-C6	-2.18	121.07	127.20
23	B	626	SQD	C4-C3-C2	2.18	114.63	110.82
29	d	406	LMG	O1-C7-C8	-2.18	105.64	110.90
23	f	101	SQD	C4-C3-C2	2.18	114.63	110.82
33	c	518	DGD	CBB-CAB-C9B	-2.18	103.36	114.42
23	f	101	SQD	C3-C4-C5	2.18	114.12	110.24
27	B	627	BCR	C35-C13-C14	-2.18	119.87	122.92
31	d	407	LHG	C18-C17-C16	-2.18	103.38	114.42
25	B	603	CLA	O2A-CGA-O1A	-2.17	118.11	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	407	PL9	C37-C38-C39	-2.17	122.43	127.66
23	b	601	SQD	O6-C1-C2	2.17	111.70	108.30
25	C	513	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
33	C	518	DGD	CAB-C9B-C8B	-2.17	103.40	114.42
27	d	405	BCR	C11-C10-C9	-2.17	124.21	127.31
31	A	618	LHG	C27-C26-C25	-2.17	103.41	114.42
26	a	608	PHO	CMC-C2C-C3C	2.17	129.03	124.94
35	V	201	HEC	CBA-CAA-C2A	-2.17	108.95	112.60
29	C	519	LMG	O3-C3-C2	-2.17	105.34	110.35
25	c	503	CLA	C1-C2-C3	-2.17	122.30	126.04
28	D	407	PL9	O1-C4-C3	-2.17	118.33	120.72
29	c	521	LMG	O3-C3-C2	-2.16	105.34	110.35
29	b	623	LMG	O2-C2-C1	-2.16	104.79	110.05
31	L	101	LHG	C18-C17-C16	-2.16	103.44	114.42
27	D	404	BCR	C15-C16-C17	-2.16	119.05	123.47
27	T	101	BCR	C27-C26-C25	2.16	125.86	122.73
25	a	607	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
25	c	511	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
28	d	408	PL9	O1-C4-C3	-2.16	118.34	120.72
25	c	510	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
25	C	507	CLA	CHD-C1D-ND	-2.15	122.47	124.45
25	B	604	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
27	B	618	BCR	C11-C10-C9	-2.15	124.24	127.31
33	H	103	DGD	CBB-CAB-C9B	-2.15	103.50	114.42
27	b	622	BCR	C15-C16-C17	-2.15	119.07	123.47
29	c	521	LMG	O2-C2-C1	-2.15	104.83	110.05
31	a	615	LHG	C27-C26-C25	-2.15	103.52	114.42
23	D	409	SQD	C44-O6-C1	2.15	117.93	113.74
27	B	617	BCR	C7-C8-C9	-2.15	122.99	126.23
27	b	622	BCR	C24-C23-C22	-2.15	122.99	126.23
29	C	520	LMG	O2-C2-C3	-2.15	105.39	110.35
25	B	606	CLA	C1-C2-C3	-2.14	122.34	126.04
25	a	609	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
27	C	515	BCR	C24-C23-C22	-2.14	123.00	126.23
25	b	614	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
31	D	406	LHG	C18-C17-C16	-2.14	103.57	114.42
29	b	624	LMG	O1-C7-C8	-2.14	105.74	110.90
27	D	404	BCR	C15-C14-C13	-2.14	124.26	127.31
28	a	611	PL9	O2-C1-C6	2.13	124.29	120.59
33	c	520	DGD	CBB-CAB-C9B	-2.13	103.59	114.42
27	K	101	BCR	C2-C1-C6	2.13	113.76	110.48
34	e	101	HEM	CBA-CAA-C2A	-2.13	108.98	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	h	101	BCR	C33-C5-C6	-2.13	122.14	124.53
31	A	616	LHG	C18-C17-C16	-2.13	103.63	114.42
27	T	101	BCR	C11-C10-C9	-2.13	124.28	127.31
27	B	627	BCR	C11-C10-C9	-2.13	124.28	127.31
34	e	101	HEM	C3D-C4D-ND	-2.12	107.80	110.17
33	h	102	DGD	CBB-CAB-C9B	-2.12	103.65	114.42
33	c	518	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
25	B	611	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	b	611	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	B	612	CLA	C1-C2-C3	-2.12	122.38	126.04
28	a	611	PL9	O2-C1-C2	-2.12	116.93	121.78
27	Y	101	BCR	C8-C7-C6	-2.11	121.26	127.20
25	b	618	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	k	101	BCR	C15-C16-C17	-2.11	119.14	123.47
29	c	502	LMG	O2-C2-C1	-2.11	104.91	110.05
25	B	608	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
28	d	408	PL9	C42-C43-C44	-2.11	122.57	127.66
27	D	404	BCR	C7-C8-C9	-2.11	123.04	126.23
25	b	607	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	C	514	BCR	C7-C8-C9	-2.11	123.05	126.23
33	c	520	DGD	CAB-C9B-C8B	-2.11	103.72	114.42
23	D	409	SQD	C4-C3-C2	2.11	114.50	110.82
25	b	606	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
28	D	407	PL9	O2-C1-C2	-2.11	116.95	121.78
31	l	101	LHG	C27-C26-C25	-2.11	103.72	114.42
25	A	609	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
33	c	520	DGD	C3D-C4D-C5D	-2.11	106.48	110.24
31	A	617	LHG	C18-C17-C16	-2.10	103.74	114.42
25	B	602	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
28	D	407	PL9	O2-C1-C6	2.10	124.23	120.59
31	D	406	LHG	C27-C26-C25	-2.10	103.75	114.42
29	A	613	LMG	C6-C5-C4	-2.10	108.08	113.00
27	c	517	BCR	C11-C10-C9	-2.10	124.31	127.31
31	L	101	LHG	C27-C26-C25	-2.10	103.76	114.42
31	A	618	LHG	C5-O7-C7	-2.10	112.62	117.79
29	b	623	LMG	O1-C1-C2	-2.10	105.03	108.30
27	b	621	BCR	C15-C14-C13	-2.10	124.32	127.31
29	C	519	LMG	O2-C2-C1	-2.10	104.95	110.05
25	C	508	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	B	613	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
28	A	611	PL9	O2-C1-C2	-2.09	116.98	121.78
27	B	619	BCR	C38-C26-C25	-2.09	122.18	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	406	LMG	O3-C3-C2	-2.09	105.51	110.35
31	A	618	LHG	C18-C17-C16	-2.09	103.80	114.42
23	D	408	SQD	O48-C23-C24	2.09	118.48	111.91
28	A	611	PL9	O1-C4-C3	-2.09	118.42	120.72
28	d	408	PL9	O2-C1-C6	2.09	124.20	120.59
29	D	405	LMG	C1-C2-C3	-2.09	105.65	110.00
25	C	512	CLA	CHD-C1D-ND	-2.09	122.54	124.45
25	b	616	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
29	c	521	LMG	O1-C7-C8	-2.08	105.87	110.90
25	C	511	CLA	C1-C2-C3	-2.08	122.44	126.04
33	C	518	DGD	C5B-C4B-C3B	-2.08	103.86	114.42
33	C	517	DGD	CBB-CAB-C9B	-2.08	103.86	114.42
25	A	607	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
29	B	620	LMG	O1-C7-C8	-2.08	105.88	110.90
25	C	505	CLA	C1-C2-C3	-2.08	122.45	126.04
25	c	503	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
29	B	620	LMG	O2-C2-C1	-2.08	105.00	110.05
25	C	506	CLA	C1-C2-C3	-2.07	122.46	126.04
33	C	518	DGD	CBB-CAB-C9B	-2.07	103.92	114.42
33	h	102	DGD	C5B-C4B-C3B	-2.07	103.92	114.42
29	A	613	LMG	O2-C2-C1	-2.07	105.02	110.05
28	a	611	PL9	C36-C34-C33	-2.07	116.93	121.12
32	A	620	BCT	O3-C-O1	-2.07	114.18	119.55
27	H	102	BCR	C15-C16-C17	-2.07	119.24	123.47
33	c	519	DGD	O3E-C3E-C2E	-2.07	105.57	110.35
29	C	519	LMG	O1-C7-C8	-2.06	105.92	110.90
29	c	522	LMG	O2-C2-C3	-2.06	105.58	110.35
33	c	520	DGD	C5B-C4B-C3B	-2.06	103.96	114.42
33	h	102	DGD	C1D-C2D-C3D	-2.06	105.70	110.00
25	B	615	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	f	101	SQD	O48-C23-C24	2.06	118.37	111.91
25	A	606	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
28	a	611	PL9	O1-C4-C3	-2.06	118.45	120.72
27	B	619	BCR	C8-C7-C6	-2.06	121.42	127.20
29	C	520	LMG	C3-C4-C5	-2.06	106.57	110.24
25	c	512	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
29	D	405	LMG	O3-C3-C2	-2.06	105.59	110.35
27	b	620	BCR	C11-C10-C9	-2.06	124.38	127.31
28	d	408	PL9	O2-C1-C2	-2.05	117.07	121.78
33	C	516	DGD	C4E-C3E-C2E	-2.05	107.24	110.82
28	D	407	PL9	C32-C33-C34	-2.05	122.72	127.66
29	D	405	LMG	O2-C2-C1	-2.05	105.06	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c	518	DGD	C5B-C4B-C3B	-2.05	104.02	114.42
25	B	610	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
25	B	612	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
29	b	624	LMG	O1-C1-C2	-2.05	105.11	108.30
25	b	613	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
33	C	517	DGD	O3E-C3E-C2E	-2.05	105.62	110.35
27	C	515	BCR	C7-C8-C9	-2.04	123.15	126.23
25	C	501	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
33	H	103	DGD	CAB-C9B-C8B	-2.04	104.05	114.42
25	C	512	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	B	616	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	C	503	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
25	b	604	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
29	d	406	LMG	O2-C2-C1	-2.04	105.10	110.05
25	C	506	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
29	C	520	LMG	C6-C5-C4	-2.03	108.24	113.00
25	D	403	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
33	h	102	DGD	CAB-C9B-C8B	-2.03	104.11	114.42
25	c	504	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	B	606	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
27	k	101	BCR	C8-C7-C6	-2.03	121.51	127.20
33	c	519	DGD	CAB-C9B-C8B	-2.03	104.13	114.42
25	A	607	CLA	C1-C2-C3	-2.03	122.54	126.04
27	b	622	BCR	C38-C26-C25	-2.02	122.25	124.53
33	C	516	DGD	C5B-C4B-C3B	-2.02	104.15	114.42
25	b	605	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
28	d	408	PL9	C20-C19-C21	2.02	118.67	115.27
27	b	622	BCR	C15-C14-C13	-2.02	124.42	127.31
27	c	517	BCR	C24-C23-C22	-2.02	123.18	126.23
25	d	404	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	b	608	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	c	505	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
33	C	517	DGD	CAB-C9B-C8B	-2.02	104.18	114.42
33	c	520	DGD	O2D-C2D-C1D	-2.02	105.15	110.05
25	c	513	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
25	B	601	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
28	D	407	PL9	C36-C34-C33	-2.02	117.04	121.12
25	B	607	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
27	y	101	BCR	C8-C7-C6	-2.01	121.55	127.20
25	b	615	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	C	502	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
33	C	516	DGD	CBB-CAB-C9B	-2.01	104.23	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	H	103	DGD	C3D-C4D-C5D	-2.01	106.66	110.24
27	A	610	BCR	C8-C7-C6	-2.01	121.56	127.20
27	H	102	BCR	C33-C5-C6	-2.01	122.28	124.53
34	E	101	HEM	C3D-C4D-ND	-2.00	107.94	110.17
25	c	514	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
28	A	611	PL9	C31-C32-C33	-2.00	105.30	111.88
25	a	606	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
27	h	101	BCR	C27-C26-C25	2.00	125.64	122.73

All (58) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	606	CLA	ND
25	A	607	CLA	ND
25	A	609	CLA	ND
25	A	615	CLA	ND
25	B	601	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	606	CLA	ND
25	B	607	CLA	ND
25	B	608	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	C	501	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	403	CLA	ND
25	a	606	CLA	ND
25	a	607	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
25	a	609	CLA	ND
25	a	612	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND
25	b	607	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	b	617	CLA	ND
25	b	618	CLA	ND
25	b	619	CLA	ND
25	c	503	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	511	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	c	514	CLA	ND
25	c	515	CLA	ND
25	d	404	CLA	ND

All (1536) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	603	SQD	C5-C6-S-O7
23	A	603	SQD	C5-C6-S-O8
23	A	603	SQD	C5-C6-S-O9
23	A	619	SQD	O6-C44-C45-C46
23	B	626	SQD	C2-C1-O6-C44
23	B	626	SQD	O5-C1-O6-C44
23	B	626	SQD	O6-C44-C45-O47
23	B	626	SQD	O49-C7-O47-C45
23	B	626	SQD	C8-C7-O47-C45
23	D	408	SQD	C2-C1-O6-C44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	408	SQD	O5-C1-O6-C44
23	D	408	SQD	O49-C7-O47-C45
23	D	408	SQD	C5-C6-S-O7
23	D	408	SQD	C5-C6-S-O8
23	D	408	SQD	C5-C6-S-O9
23	I	101	SQD	O6-C44-C45-O47
23	I	101	SQD	C8-C7-O47-C45
23	b	601	SQD	O5-C1-O6-C44
23	b	601	SQD	C8-C7-O47-C45
23	b	601	SQD	O5-C5-C6-S
23	c	501	SQD	C5-C6-S-O7
23	f	101	SQD	C2-C1-O6-C44
23	f	101	SQD	O5-C1-O6-C44
25	B	601	CLA	CHA-CBD-CGD-O1D
25	B	601	CLA	CHA-CBD-CGD-O2D
25	B	601	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	CHA-CBD-CGD-O1D
25	B	607	CLA	CHA-CBD-CGD-O2D
25	B	607	CLA	CBD-CGD-O2D-CED
25	B	609	CLA	CHA-CBD-CGD-O1D
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	610	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CHA-CBD-CGD-O1D
25	B	614	CLA	CHA-CBD-CGD-O2D
25	B	614	CLA	C2-C3-C5-C6
25	B	614	CLA	C4-C3-C5-C6
25	C	504	CLA	CHA-CBD-CGD-O1D
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	508	CLA	CHA-CBD-CGD-O1D
25	C	508	CLA	CHA-CBD-CGD-O2D
25	C	512	CLA	C6-C7-C8-C9
25	D	402	CLA	C1A-C2A-CAA-CBA
25	a	606	CLA	CBD-CGD-O2D-CED
25	a	609	CLA	C2-C3-C5-C6
25	a	609	CLA	C4-C3-C5-C6
25	a	612	CLA	CHA-CBD-CGD-O1D
25	a	612	CLA	CHA-CBD-CGD-O2D
25	b	604	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	604	CLA	CHA-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O1D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CBD-CGD-O2D-CED
25	b	604	CLA	C14-C13-C15-C16
25	b	608	CLA	C14-C13-C15-C16
25	b	609	CLA	CHA-CBD-CGD-O1D
25	b	609	CLA	CHA-CBD-CGD-O2D
25	b	610	CLA	CHA-CBD-CGD-O1D
25	b	610	CLA	CAD-CBD-CGD-O1D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	C1A-C2A-CAA-CBA
25	b	615	CLA	C3A-C2A-CAA-CBA
25	b	617	CLA	CAD-CBD-CGD-O1D
25	b	617	CLA	C2-C3-C5-C6
25	b	617	CLA	C4-C3-C5-C6
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	506	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	c	508	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	CBD-CGD-O2D-CED
25	d	404	CLA	C1A-C2A-CAA-CBA
25	d	404	CLA	C3A-C2A-CAA-CBA
27	B	619	BCR	C1-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C30
27	B	627	BCR	C7-C8-C9-C10
27	B	627	BCR	C21-C22-C23-C24
27	D	404	BCR	C7-C8-C9-C10
27	D	404	BCR	C21-C22-C23-C24
27	H	102	BCR	C7-C8-C9-C10
27	H	102	BCR	C7-C8-C9-C34
27	T	101	BCR	C21-C22-C23-C24
27	Y	101	BCR	C7-C8-C9-C34
27	b	620	BCR	C1-C6-C7-C8
27	b	622	BCR	C23-C24-C25-C30
27	d	405	BCR	C7-C8-C9-C10
27	d	405	BCR	C7-C8-C9-C34
27	d	405	BCR	C37-C22-C23-C24
27	h	101	BCR	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	h	101	BCR	C7-C8-C9-C34
27	y	101	BCR	C1-C6-C7-C8
27	y	101	BCR	C7-C8-C9-C10
27	y	101	BCR	C7-C8-C9-C34
28	A	611	PL9	C9-C11-C12-C13
28	A	611	PL9	C42-C43-C44-C46
28	D	407	PL9	C33-C34-C36-C37
28	D	407	PL9	C35-C34-C36-C37
28	a	611	PL9	C25-C24-C26-C27
28	a	611	PL9	C35-C34-C36-C37
28	d	408	PL9	C18-C19-C21-C22
28	d	408	PL9	C33-C34-C36-C37
28	d	408	PL9	C37-C38-C39-C41
29	A	612	LMG	C2-C1-O1-C7
29	A	612	LMG	O6-C1-O1-C7
29	A	613	LMG	O1-C7-C8-O7
29	B	621	LMG	O6-C1-O1-C7
29	C	520	LMG	O6-C1-O1-C7
29	b	624	LMG	C2-C1-O1-C7
29	b	624	LMG	O6-C1-O1-C7
29	c	522	LMG	O6-C1-O1-C7
29	d	409	LMG	O9-C10-O7-C8
31	A	616	LHG	O1-C1-C2-C3
31	A	618	LHG	C1-C2-C3-O3
31	A	618	LHG	C4-O6-P-O5
31	A	618	LHG	O6-C4-C5-O7
31	D	406	LHG	O1-C1-C2-C3
31	D	406	LHG	C3-O3-P-O4
31	D	406	LHG	C3-O3-P-O6
31	D	406	LHG	C4-O6-P-O3
31	D	406	LHG	C4-O6-P-O4
31	D	406	LHG	C4-O6-P-O5
31	L	101	LHG	C4-O6-P-O5
31	a	613	LHG	C3-O3-P-O5
31	a	613	LHG	C3-O3-P-O6
31	a	613	LHG	C4-O6-P-O5
31	a	614	LHG	C4-O6-P-O4
31	a	615	LHG	O1-C1-C2-C3
31	a	615	LHG	C3-O3-P-O4
31	a	615	LHG	O7-C5-C6-O8
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C4-O6-P-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C3-O3-P-O4
31	l	101	LHG	C4-O6-P-O5
33	C	517	DGD	C2E-C1E-O5D-C6D
33	C	517	DGD	O6E-C1E-O5D-C6D
33	c	519	DGD	C2E-C1E-O5D-C6D
25	b	610	CLA	O1D-CGD-O2D-CED
25	A	606	CLA	CBD-CGD-O2D-CED
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	b	610	CLA	CBD-CGD-O2D-CED
25	b	619	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
25	B	610	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	CBD-CGD-O2D-CED
25	B	604	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	c	514	CLA	CBD-CGD-O2D-CED
26	D	401	PHO	CBD-CGD-O2D-CED
23	A	619	SQD	O10-C23-O48-C46
23	B	626	SQD	O10-C23-O48-C46
25	B	607	CLA	O1D-CGD-O2D-CED
25	a	606	CLA	O1D-CGD-O2D-CED
25	c	508	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	O1D-CGD-O2D-CED
25	B	609	CLA	O1D-CGD-O2D-CED
25	b	604	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
25	c	515	CLA	CBD-CGD-O2D-CED
23	A	619	SQD	O49-C7-O47-C45
23	I	101	SQD	O49-C7-O47-C45
23	b	601	SQD	O49-C7-O47-C45
33	h	102	DGD	C4E-C5E-C6E-O5E
25	b	619	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	C3-C5-C6-C7
25	B	616	CLA	C3-C5-C6-C7
25	C	506	CLA	C3-C5-C6-C7
25	C	512	CLA	C3-C5-C6-C7
25	b	619	CLA	C3-C5-C6-C7
23	A	619	SQD	C24-C23-O48-C46
23	B	626	SQD	C24-C23-O48-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	408	SQD	C8-C7-O47-C45
29	d	409	LMG	C11-C10-O7-C8
25	A	609	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
29	B	625	LMG	C4-C5-C6-O5
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	502	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	C2A-CAA-CBA-CGA
25	b	609	CLA	C2A-CAA-CBA-CGA
23	b	601	SQD	C24-C23-O48-C46
25	b	619	CLA	CBA-CGA-O2A-C1
29	c	521	LMG	O6-C5-C6-O5
29	c	502	LMG	O6-C5-C6-O5
33	h	102	DGD	O6E-C5E-C6E-O5E
23	b	601	SQD	O10-C23-O48-C46
25	C	511	CLA	CBD-CGD-O2D-CED
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	O1D-CGD-O2D-CED
31	A	618	LHG	O2-C2-C3-O3
31	a	615	LHG	O2-C2-C3-O3
31	d	407	LHG	O2-C2-C3-O3
23	D	408	SQD	C24-C23-O48-C46
25	B	616	CLA	CBA-CGA-O2A-C1
25	b	619	CLA	O1A-CGA-O2A-C1
33	C	517	DGD	O6E-C5E-C6E-O5E
33	c	519	DGD	O6E-C5E-C6E-O5E
29	c	521	LMG	C4-C5-C6-O5
25	C	506	CLA	O1D-CGD-O2D-CED
25	b	607	CLA	CBD-CGD-O2D-CED
33	H	103	DGD	C4D-C5D-C6D-O5D
25	b	604	CLA	C3-C5-C6-C7
25	c	508	CLA	C3-C5-C6-C7
25	A	606	CLA	O1D-CGD-O2D-CED
34	E	101	HEM	C3D-CAD-CBD-CGD
34	e	101	HEM	C3D-CAD-CBD-CGD
29	C	519	LMG	O6-C5-C6-O5
29	b	624	LMG	O6-C5-C6-O5
25	B	602	CLA	C4-C3-C5-C6
25	B	605	CLA	C4-C3-C5-C6
25	b	605	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	608	CLA	C4-C3-C5-C6
25	B	602	CLA	C2-C3-C5-C6
25	B	605	CLA	C2-C3-C5-C6
25	b	605	CLA	C2-C3-C5-C6
25	b	608	CLA	C2-C3-C5-C6
28	a	611	PL9	C23-C24-C26-C27
29	B	625	LMG	O6-C5-C6-O5
25	B	616	CLA	O1A-CGA-O2A-C1
29	c	521	LMG	O6-C1-O1-C7
33	c	519	DGD	O6E-C1E-O5D-C6D
28	a	611	PL9	C9-C11-C12-C13
28	d	408	PL9	C9-C11-C12-C13
28	d	408	PL9	C39-C41-C42-C43
23	I	101	SQD	C24-C23-O48-C46
31	D	406	LHG	C28-C29-C30-C31
26	D	401	PHO	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
31	a	615	LHG	C1-C2-C3-O3
29	c	502	LMG	C4-C5-C6-O5
29	b	624	LMG	C4-C5-C6-O5
31	d	407	LHG	C32-C33-C34-C35
31	a	614	LHG	O2-C2-C3-O3
23	D	409	SQD	C2-C1-O6-C44
29	B	621	LMG	C2-C1-O1-C7
29	C	519	LMG	C4-C5-C6-O5
25	B	601	CLA	C14-C13-C15-C16
25	B	602	CLA	C6-C7-C8-C9
25	B	602	CLA	C14-C13-C15-C16
25	B	605	CLA	C14-C13-C15-C16
25	B	609	CLA	C14-C13-C15-C16
25	B	610	CLA	C11-C12-C13-C14
25	B	614	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C10-C8-C9
25	C	509	CLA	C11-C12-C13-C14
25	b	604	CLA	C11-C10-C8-C9
25	b	605	CLA	C14-C13-C15-C16
25	b	612	CLA	C14-C13-C15-C16
25	b	613	CLA	C11-C12-C13-C14
25	c	507	CLA	C14-C13-C15-C16
25	c	511	CLA	C11-C10-C8-C9
25	B	614	CLA	O1D-CGD-O2D-CED
25	c	514	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	610	CLA	C13-C15-C16-C17
27	A	610	BCR	C7-C8-C9-C34
27	B	627	BCR	C7-C8-C9-C34
27	D	404	BCR	C7-C8-C9-C34
27	T	101	BCR	C7-C8-C9-C34
27	Y	101	BCR	C37-C22-C23-C24
27	a	610	BCR	C7-C8-C9-C34
27	b	622	BCR	C37-C22-C23-C24
27	c	516	BCR	C7-C8-C9-C34
27	c	517	BCR	C7-C8-C9-C34
27	T	101	BCR	C7-C8-C9-C10
27	c	516	BCR	C7-C8-C9-C10
23	A	619	SQD	C8-C7-O47-C45
33	c	519	DGD	C4E-C5E-C6E-O5E
29	A	612	LMG	C28-C29-C30-C31
29	B	621	LMG	C10-C11-C12-C13
25	A	609	CLA	C13-C15-C16-C17
25	C	505	CLA	C5-C6-C7-C8
33	C	517	DGD	C4E-C5E-C6E-O5E
25	B	601	CLA	CBA-CGA-O2A-C1
35	V	201	HEC	C3D-CAD-CBD-CGD
25	b	619	CLA	C10-C11-C12-C13
31	A	618	LHG	C7-C8-C9-C10
33	c	519	DGD	C1B-C2B-C3B-C4B
33	c	520	DGD	O6E-C5E-C6E-O5E
25	B	613	CLA	C5-C6-C7-C8
25	B	604	CLA	O1D-CGD-O2D-CED
31	A	616	LHG	O1-C1-C2-O2
23	D	409	SQD	C23-C24-C25-C26
23	I	101	SQD	C23-C24-C25-C26
23	b	601	SQD	C7-C8-C9-C10
29	c	502	LMG	C10-C11-C12-C13
31	a	615	LHG	C23-C24-C25-C26
33	C	517	DGD	C1B-C2B-C3B-C4B
29	c	522	LMG	O6-C5-C6-O5
25	A	609	CLA	C10-C11-C12-C13
25	B	614	CLA	C13-C15-C16-C17
25	B	603	CLA	O1D-CGD-O2D-CED
25	b	619	CLA	C8-C10-C11-C12
23	A	619	SQD	C23-C24-C25-C26
29	b	623	LMG	C28-C29-C30-C31
31	A	618	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C23-C24-C25-C26
25	b	614	CLA	CBD-CGD-O2D-CED
23	D	409	SQD	C8-C7-O47-C45
25	C	506	CLA	C8-C10-C11-C12
25	b	604	CLA	C10-C11-C12-C13
25	C	506	CLA	C11-C10-C8-C7
25	B	605	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	CBD-CGD-O2D-CED
29	c	502	LMG	O6-C1-O1-C7
25	c	515	CLA	O1D-CGD-O2D-CED
28	A	611	PL9	C24-C26-C27-C28
28	D	407	PL9	C39-C41-C42-C43
28	d	408	PL9	C34-C36-C37-C38
29	d	409	LMG	C10-C11-C12-C13
31	L	101	LHG	C23-C24-C25-C26
31	a	613	LHG	C7-C8-C9-C10
27	B	627	BCR	C10-C11-C12-C13
27	T	101	BCR	C10-C11-C12-C13
25	a	609	CLA	C8-C10-C11-C12
25	b	604	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
29	B	625	LMG	C10-C11-C12-C13
31	d	407	LHG	C23-C24-C25-C26
25	A	609	CLA	O1D-CGD-O2D-CED
25	B	601	CLA	C10-C11-C12-C13
25	B	616	CLA	C10-C11-C12-C13
25	C	510	CLA	C5-C6-C7-C8
25	b	615	CLA	C13-C15-C16-C17
31	A	616	LHG	C3-O3-P-O6
31	a	614	LHG	C4-O6-P-O3
31	a	615	LHG	C3-O3-P-O6
31	d	407	LHG	C3-O3-P-O6
31	A	616	LHG	C23-C24-C25-C26
25	b	608	CLA	C13-C15-C16-C17
25	B	606	CLA	O1D-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
29	B	621	LMG	O6-C5-C6-O5
31	d	407	LHG	C1-C2-C3-O3
23	f	101	SQD	O49-C7-O47-C45
25	c	508	CLA	C10-C11-C12-C13
25	b	615	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	503	CLA	C2A-CAA-CBA-CGA
25	d	404	CLA	C16-C17-C18-C20
23	f	101	SQD	C24-C23-O48-C46
29	C	519	LMG	C29-C28-O8-C9
25	C	502	CLA	O1D-CGD-O2D-CED
23	B	626	SQD	C14-C15-C16-C17
29	B	620	LMG	C28-C29-C30-C31
29	B	625	LMG	C20-C21-C22-C23
29	D	405	LMG	C17-C18-C19-C20
31	l	101	LHG	C34-C35-C36-C37
33	C	518	DGD	C7B-C8B-C9B-CAB
23	f	101	SQD	C8-C7-O47-C45
29	A	613	LMG	C11-C10-O7-C8
23	A	619	SQD	C12-C13-C14-C15
23	B	626	SQD	C10-C11-C12-C13
23	B	626	SQD	C31-C32-C33-C34
23	b	601	SQD	C27-C28-C29-C30
23	f	101	SQD	C27-C28-C29-C30
29	A	612	LMG	C14-C15-C16-C17
29	B	625	LMG	C14-C15-C16-C17
29	B	625	LMG	C19-C20-C21-C22
29	C	519	LMG	C31-C32-C33-C34
29	b	624	LMG	C19-C20-C21-C22
29	c	521	LMG	C31-C32-C33-C34
31	A	617	LHG	C12-C13-C14-C15
31	a	615	LHG	C11-C12-C13-C14
33	C	517	DGD	C4A-C5A-C6A-C7A
33	C	517	DGD	C5A-C6A-C7A-C8A
33	C	517	DGD	C7B-C8B-C9B-CAB
33	C	518	DGD	C6B-C7B-C8B-C9B
23	A	619	SQD	C17-C18-C19-C20
23	B	626	SQD	C9-C10-C11-C12
23	b	601	SQD	C9-C10-C11-C12
23	f	101	SQD	C33-C34-C35-C36
29	A	613	LMG	C17-C18-C19-C20
29	C	519	LMG	C15-C16-C17-C18
31	d	407	LHG	C25-C26-C27-C28
31	l	101	LHG	C10-C11-C12-C13
33	h	102	DGD	C3B-C4B-C5B-C6B
25	B	614	CLA	C8-C10-C11-C12
29	c	502	LMG	C28-C29-C30-C31
29	B	625	LMG	C30-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C17-C18-C19-C20
29	C	520	LMG	C30-C31-C32-C33
23	A	619	SQD	C28-C29-C30-C31
23	I	101	SQD	C10-C11-C12-C13
23	I	101	SQD	C13-C14-C15-C16
29	A	613	LMG	C14-C15-C16-C17
29	B	621	LMG	C29-C30-C31-C32
29	b	624	LMG	C29-C30-C31-C32
29	c	502	LMG	C13-C14-C15-C16
33	c	519	DGD	C6B-C7B-C8B-C9B
23	A	603	SQD	C29-C30-C31-C32
23	A	603	SQD	C30-C31-C32-C33
23	I	101	SQD	C9-C10-C11-C12
31	L	101	LHG	C34-C35-C36-C37
29	c	502	LMG	C2-C1-O1-C7
29	c	521	LMG	C2-C1-O1-C7
25	b	610	CLA	CBA-CGA-O2A-C1
23	b	601	SQD	C11-C10-C9-C8
29	C	519	LMG	C32-C33-C34-C35
31	a	613	LHG	C25-C26-C27-C28
31	a	614	LHG	C29-C30-C31-C32
31	d	407	LHG	C34-C35-C36-C37
33	C	516	DGD	C4B-C5B-C6B-C7B
33	c	519	DGD	C9A-CAA-CBA-CCA
25	C	505	CLA	C4-C3-C5-C6
23	B	626	SQD	C12-C13-C14-C15
23	c	501	SQD	C10-C11-C12-C13
29	C	520	LMG	C12-C13-C14-C15
31	L	101	LHG	C29-C30-C31-C32
31	a	615	LHG	C9-C10-C11-C12
33	c	519	DGD	CAA-CBA-CCA-CDA
25	C	505	CLA	C2-C3-C5-C6
25	B	603	CLA	C6-C7-C8-C9
25	B	606	CLA	C14-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C12-C13-C14
25	C	506	CLA	C11-C12-C13-C14
25	b	616	CLA	C14-C13-C15-C16
25	b	618	CLA	C11-C12-C13-C14
25	b	619	CLA	C6-C7-C8-C9
25	C	511	CLA	O1D-CGD-O2D-CED
29	D	405	LMG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	603	SQD	C13-C14-C15-C16
23	I	101	SQD	C26-C27-C28-C29
23	c	501	SQD	C9-C10-C11-C12
23	c	501	SQD	C17-C18-C19-C20
23	f	101	SQD	C34-C35-C36-C37
29	B	620	LMG	C30-C31-C32-C33
29	C	519	LMG	C16-C17-C18-C19
29	D	405	LMG	C20-C21-C22-C23
29	b	623	LMG	C30-C31-C32-C33
29	c	522	LMG	C19-C20-C21-C22
31	A	617	LHG	C27-C28-C29-C30
31	a	614	LHG	C30-C31-C32-C33
31	l	101	LHG	C27-C28-C29-C30
33	C	517	DGD	C6B-C7B-C8B-C9B
33	c	518	DGD	C4B-C5B-C6B-C7B
33	c	519	DGD	C4B-C5B-C6B-C7B
25	B	601	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1
27	B	627	BCR	C37-C22-C23-C24
27	T	101	BCR	C37-C22-C23-C24
29	A	612	LMG	C13-C14-C15-C16
31	a	615	LHG	C27-C28-C29-C30
31	a	613	LHG	O1-C1-C2-C3
27	d	405	BCR	C21-C22-C23-C24
23	I	101	SQD	C14-C15-C16-C17
29	A	612	LMG	C18-C19-C20-C21
29	C	519	LMG	C11-C12-C13-C14
29	D	405	LMG	C30-C31-C32-C33
29	b	624	LMG	C37-C38-C39-C40
29	d	409	LMG	C33-C34-C35-C36
23	f	101	SQD	C26-C27-C28-C29
29	B	621	LMG	C16-C17-C18-C19
29	C	519	LMG	C19-C20-C21-C22
29	C	519	LMG	C29-C30-C31-C32
29	D	405	LMG	C15-C16-C17-C18
29	b	623	LMG	C36-C37-C38-C39
29	c	522	LMG	C17-C18-C19-C20
29	d	409	LMG	C31-C32-C33-C34
31	A	616	LHG	C32-C33-C34-C35
31	D	406	LHG	C11-C10-C9-C8
31	l	101	LHG	C14-C15-C16-C17
33	H	103	DGD	CBA-CCA-CDA-CEA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	403	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C20
25	a	609	CLA	C16-C17-C18-C19
23	D	409	SQD	O5-C1-O6-C44
25	B	602	CLA	C5-C6-C7-C8
23	I	101	SQD	C11-C12-C13-C14
29	B	621	LMG	C20-C21-C22-C23
29	C	519	LMG	C14-C15-C16-C17
29	c	502	LMG	C32-C33-C34-C35
29	c	502	LMG	C36-C37-C38-C39
33	C	518	DGD	CBA-CCA-CDA-CEA
23	I	101	SQD	C25-C26-C27-C28
23	c	501	SQD	C12-C13-C14-C15
29	B	621	LMG	C31-C32-C33-C34
29	B	625	LMG	C13-C14-C15-C16
29	B	625	LMG	C18-C19-C20-C21
29	C	519	LMG	C18-C19-C20-C21
31	l	101	LHG	C30-C31-C32-C33
33	H	103	DGD	CCA-CDA-CEA-CFA
33	c	518	DGD	C4A-C5A-C6A-C7A
23	I	101	SQD	C7-C8-C9-C10
25	B	616	CLA	C13-C15-C16-C17
23	B	626	SQD	C13-C14-C15-C16
23	B	626	SQD	C15-C16-C17-C18
29	A	613	LMG	C11-C12-C13-C14
29	b	623	LMG	C31-C32-C33-C34
25	b	609	CLA	O1D-CGD-O2D-CED
29	C	520	LMG	C19-C20-C21-C22
29	c	522	LMG	C14-C15-C16-C17
31	l	101	LHG	C16-C17-C18-C19
33	c	518	DGD	C5B-C6B-C7B-C8B
25	b	612	CLA	O1D-CGD-O2D-CED
25	D	402	CLA	C3A-C2A-CAA-CBA
26	a	608	PHO	C3A-C2A-CAA-CBA
25	B	605	CLA	C13-C15-C16-C17
29	b	623	LMG	C35-C36-C37-C38
29	c	521	LMG	C32-C33-C34-C35
33	C	517	DGD	C6A-C7A-C8A-C9A
25	a	609	CLA	C16-C17-C18-C20
23	I	101	SQD	C17-C18-C19-C20
29	C	520	LMG	C20-C21-C22-C23
31	A	616	LHG	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	L	101	LHG	C10-C11-C12-C13
26	d	401	PHO	CBD-CGD-O2D-CED
23	A	619	SQD	C18-C19-C20-C21
33	H	103	DGD	C5B-C6B-C7B-C8B
23	I	101	SQD	C27-C28-C29-C30
31	l	101	LHG	C9-C10-C11-C12
25	b	604	CLA	O1A-CGA-O2A-C1
28	a	611	PL9	C12-C11-C9-C10
25	B	609	CLA	C2-C3-C5-C6
28	a	611	PL9	C13-C14-C16-C17
29	A	612	LMG	C11-C10-O7-C8
29	c	502	LMG	C29-C30-C31-C32
31	a	615	LHG	O1-C1-C2-O2
23	D	408	SQD	C12-C13-C14-C15
31	a	615	LHG	C14-C15-C16-C17
25	d	404	CLA	C16-C17-C18-C19
25	C	505	CLA	C8-C10-C11-C12
29	C	520	LMG	C34-C35-C36-C37
29	c	521	LMG	C29-C28-O8-C9
29	C	519	LMG	C30-C31-C32-C33
29	A	613	LMG	C31-C32-C33-C34
31	A	616	LHG	C25-C26-C27-C28
25	C	505	CLA	C13-C15-C16-C17
23	D	408	SQD	O10-C23-O48-C46
25	b	610	CLA	O1A-CGA-O2A-C1
31	A	617	LHG	C32-C33-C34-C35
31	l	101	LHG	C33-C34-C35-C36
25	c	511	CLA	C3-C5-C6-C7
27	B	617	BCR	C1-C6-C7-C8
27	B	617	BCR	C5-C6-C7-C8
27	B	619	BCR	C5-C6-C7-C8
27	B	619	BCR	C23-C24-C25-C26
27	B	627	BCR	C1-C6-C7-C8
27	B	627	BCR	C5-C6-C7-C8
27	C	514	BCR	C1-C6-C7-C8
27	C	514	BCR	C5-C6-C7-C8
27	T	101	BCR	C1-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	b	620	BCR	C5-C6-C7-C8
27	b	622	BCR	C23-C24-C25-C26
27	y	101	BCR	C5-C6-C7-C8
33	H	103	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	612	LMG	C17-C18-C19-C20
33	C	518	DGD	C2A-C1A-O1G-C1G
25	a	609	CLA	C15-C16-C17-C18
23	B	626	SQD	C29-C30-C31-C32
23	B	626	SQD	C32-C33-C34-C35
29	B	625	LMG	C31-C32-C33-C34
29	c	522	LMG	C20-C21-C22-C23
31	A	618	LHG	C32-C33-C34-C35
23	I	101	SQD	O10-C23-O48-C46
23	D	408	SQD	C7-C8-C9-C10
31	a	614	LHG	C7-C8-C9-C10
29	c	502	LMG	C31-C32-C33-C34
25	b	605	CLA	C5-C6-C7-C8
23	A	619	SQD	C11-C10-C9-C8
23	b	601	SQD	C28-C29-C30-C31
29	C	519	LMG	C38-C39-C40-C41
29	c	502	LMG	C21-C22-C23-C24
31	A	618	LHG	C30-C31-C32-C33
25	B	602	CLA	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	B	606	CLA	C12-C13-C15-C16
25	B	611	CLA	C12-C13-C15-C16
25	C	502	CLA	C11-C12-C13-C15
25	C	505	CLA	C11-C12-C13-C15
25	C	506	CLA	C11-C12-C13-C15
25	b	618	CLA	C11-C12-C13-C15
25	b	618	CLA	C12-C13-C15-C16
25	b	619	CLA	C11-C12-C13-C15
25	c	514	CLA	C12-C13-C15-C16
28	A	611	PL9	C12-C11-C9-C8
25	B	614	CLA	C3-C5-C6-C7
23	I	101	SQD	C30-C31-C32-C33
23	c	501	SQD	C16-C17-C18-C19
29	d	409	LMG	C11-C12-C13-C14
25	C	513	CLA	CBD-CGD-O2D-CED
25	A	609	CLA	C16-C17-C18-C20
25	B	607	CLA	CBA-CGA-O2A-C1
29	B	620	LMG	C32-C33-C34-C35
29	B	625	LMG	C34-C35-C36-C37
25	B	603	CLA	C2A-CAA-CBA-CGA
25	b	606	CLA	C2A-CAA-CBA-CGA
25	B	608	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	613	CLA	C13-C15-C16-C17
25	c	511	CLA	C8-C10-C11-C12
33	C	516	DGD	C4A-C5A-C6A-C7A
29	A	613	LMG	C37-C38-C39-C40
31	a	613	LHG	C32-C33-C34-C35
23	A	619	SQD	C32-C33-C34-C35
29	c	502	LMG	C20-C21-C22-C23
33	C	518	DGD	C8A-C9A-CAA-CBA
29	B	620	LMG	C18-C19-C20-C21
33	c	520	DGD	C2A-C1A-O1G-C1G
25	b	619	CLA	C16-C17-C18-C19
23	c	501	SQD	C28-C29-C30-C31
31	a	614	LHG	C11-C10-C9-C8
33	c	520	DGD	CBA-CCA-CDA-CEA
31	A	617	LHG	O6-C4-C5-O7
23	A	603	SQD	C12-C13-C14-C15
29	C	519	LMG	C20-C21-C22-C23
25	C	505	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
29	b	623	LMG	C17-C18-C19-C20
33	C	518	DGD	C4B-C5B-C6B-C7B
23	D	409	SQD	O49-C7-O47-C45
29	A	613	LMG	O9-C10-O7-C8
23	D	408	SQD	C24-C25-C26-C27
23	A	619	SQD	C24-C25-C26-C27
25	b	607	CLA	O1D-CGD-O2D-CED
23	I	101	SQD	C31-C32-C33-C34
29	A	612	LMG	C15-C16-C17-C18
29	B	621	LMG	C14-C15-C16-C17
31	A	616	LHG	C30-C31-C32-C33
29	D	405	LMG	O6-C5-C6-O5
25	B	609	CLA	C4-C3-C5-C6
26	a	608	PHO	C4-C3-C5-C6
28	a	611	PL9	C15-C14-C16-C17
28	D	407	PL9	C4-C3-C7-C8
25	B	611	CLA	C14-C13-C15-C16
25	a	607	CLA	C6-C7-C8-C9
25	b	607	CLA	C6-C7-C8-C9
25	b	618	CLA	C14-C13-C15-C16
25	b	619	CLA	C14-C13-C15-C16
25	c	507	CLA	C11-C12-C13-C14
25	c	508	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	C	520	LMG	O6-C5-C6-O5
29	B	625	LMG	C37-C38-C39-C40
25	C	501	CLA	C2A-CAA-CBA-CGA
27	b	621	BCR	C7-C8-C9-C34
29	B	621	LMG	C18-C19-C20-C21
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	C	506	CLA	C16-C17-C18-C20
25	b	619	CLA	C16-C17-C18-C20
29	B	620	LMG	C17-C18-C19-C20
29	c	521	LMG	C20-C21-C22-C23
31	A	618	LHG	C17-C18-C19-C20
33	h	102	DGD	C8A-C9A-CAA-CBA
31	A	617	LHG	C4-O6-P-O3
31	L	101	LHG	C30-C31-C32-C33
25	c	512	CLA	CBD-CGD-O2D-CED
29	c	502	LMG	C37-C38-C39-C40
29	c	522	LMG	C30-C31-C32-C33
29	d	409	LMG	C17-C18-C19-C20
25	D	403	CLA	C13-C15-C16-C17
31	A	618	LHG	O6-C4-C5-C6
29	c	521	LMG	C19-C20-C21-C22
23	B	626	SQD	C11-C12-C13-C14
29	A	612	LMG	C29-C30-C31-C32
29	D	405	LMG	C16-C17-C18-C19
33	C	516	DGD	C6A-C7A-C8A-C9A
33	c	519	DGD	CCB-CDB-CEB-CFB
28	D	407	PL9	C45-C44-C46-C47
23	f	101	SQD	C25-C26-C27-C28
33	H	103	DGD	C7A-C8A-C9A-CAA
31	A	618	LHG	C28-C29-C30-C31
31	A	618	LHG	C8-C7-O7-C5
23	A	619	SQD	C44-C45-C46-O48
23	D	409	SQD	C44-C45-C46-O48
29	B	625	LMG	O1-C7-C8-C9
29	c	502	LMG	C7-C8-C9-O8
31	A	618	LHG	C4-C5-C6-O8
33	c	520	DGD	C6A-C7A-C8A-C9A
25	b	616	CLA	C5-C6-C7-C8
25	B	607	CLA	O1A-CGA-O2A-C1
33	C	517	DGD	C5D-C6D-O5D-C1E
33	c	519	DGD	C5D-C6D-O5D-C1E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	408	SQD	C10-C11-C12-C13
29	b	624	LMG	C40-C41-C42-C43
29	c	521	LMG	C29-C30-C31-C32
31	A	618	LHG	C19-C20-C21-C22
31	L	101	LHG	C27-C28-C29-C30
23	D	408	SQD	C14-C15-C16-C17
29	D	405	LMG	C19-C20-C21-C22
23	c	501	SQD	O5-C1-O6-C44
29	C	519	LMG	C17-C18-C19-C20
31	A	616	LHG	C11-C12-C13-C14
31	a	613	LHG	C10-C11-C12-C13
33	C	518	DGD	CAA-CBA-CCA-CDA
31	a	613	LHG	O1-C1-C2-O2
27	T	101	BCR	C20-C21-C22-C37
27	Y	101	BCR	C20-C21-C22-C37
33	C	516	DGD	O6E-C5E-C6E-O5E
33	c	518	DGD	O6E-C5E-C6E-O5E
29	A	612	LMG	C22-C23-C24-C25
25	b	615	CLA	CBA-CGA-O2A-C1
29	b	624	LMG	C29-C28-O8-C9
29	d	406	LMG	O6-C5-C6-O5
25	C	506	CLA	C15-C16-C17-C18
25	c	508	CLA	C8-C10-C11-C12
29	d	409	LMG	C13-C14-C15-C16
31	A	616	LHG	C29-C30-C31-C32
25	c	508	CLA	C15-C16-C17-C18
33	c	520	DGD	C4E-C5E-C6E-O5E
31	A	618	LHG	C29-C30-C31-C32
25	C	509	CLA	C10-C11-C12-C13
29	B	625	LMG	C17-C18-C19-C20
29	C	519	LMG	C34-C35-C36-C37
33	h	102	DGD	CAA-CBA-CCA-CDA
25	C	505	CLA	CBA-CGA-O2A-C1
29	B	625	LMG	C29-C28-O8-C9
29	B	620	LMG	C31-C32-C33-C34
33	h	102	DGD	C9A-CAA-CBA-CCA
23	B	626	SQD	C11-C10-C9-C8
33	C	516	DGD	C5B-C6B-C7B-C8B
33	C	517	DGD	CBB-CCB-CDB-CEB
25	b	614	CLA	O1D-CGD-O2D-CED
27	c	516	BCR	C11-C10-C9-C8
29	C	520	LMG	C2-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	c	522	LMG	C2-C1-O1-C7
33	C	516	DGD	O6D-C5D-C6D-O5D
33	c	518	DGD	O6D-C5D-C6D-O5D
29	A	612	LMG	O9-C10-O7-C8
23	D	409	SQD	C32-C33-C34-C35
29	b	624	LMG	C14-C15-C16-C17
29	c	521	LMG	C38-C39-C40-C41
25	A	607	CLA	C6-C7-C8-C10
25	B	602	CLA	C11-C12-C13-C15
25	B	605	CLA	C12-C13-C15-C16
25	B	615	CLA	C12-C13-C15-C16
25	C	509	CLA	C12-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C10
25	C	512	CLA	C6-C7-C8-C10
25	C	512	CLA	C11-C10-C8-C7
25	C	512	CLA	C12-C13-C15-C16
25	a	607	CLA	C6-C7-C8-C10
25	b	604	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C12-C13-C15
25	b	607	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C12-C13-C15
25	c	509	CLA	C11-C10-C8-C7
25	d	403	CLA	C12-C13-C15-C16
29	b	624	LMG	C32-C33-C34-C35
25	A	607	CLA	C6-C7-C8-C9
25	B	611	CLA	C11-C12-C13-C14
25	B	614	CLA	C14-C13-C15-C16
25	B	615	CLA	C14-C13-C15-C16
25	B	616	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C10-C8-C9
25	C	510	CLA	C6-C7-C8-C9
25	C	511	CLA	C6-C7-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	b	614	CLA	C14-C13-C15-C16
25	c	510	CLA	C11-C10-C8-C9
25	c	514	CLA	C14-C13-C15-C16
29	B	621	LMG	C12-C13-C14-C15
31	A	618	LHG	C33-C34-C35-C36
33	c	518	DGD	C6A-C7A-C8A-C9A
23	D	409	SQD	C24-C23-O48-C46
25	c	503	CLA	O1D-CGD-O2D-CED
33	C	516	DGD	C4D-C5D-C6D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	c	518	DGD	C4D-C5D-C6D-O5D
29	C	520	LMG	C40-C41-C42-C43
33	C	518	DGD	C2B-C3B-C4B-C5B
31	a	614	LHG	C1-C2-C3-O3
25	C	506	CLA	C13-C15-C16-C17
29	A	613	LMG	C33-C34-C35-C36
29	c	522	LMG	C32-C33-C34-C35
29	d	409	LMG	C21-C22-C23-C24
28	D	407	PL9	C2-C3-C7-C8
29	A	612	LMG	C38-C39-C40-C41
29	b	623	LMG	C18-C19-C20-C21
31	a	615	LHG	C13-C14-C15-C16
29	b	624	LMG	C16-C17-C18-C19
31	A	617	LHG	O6-C4-C5-C6
31	L	101	LHG	O6-C4-C5-C6
31	l	101	LHG	O6-C4-C5-C6
29	b	624	LMG	C15-C16-C17-C18
31	A	616	LHG	C9-C10-C11-C12
29	b	624	LMG	C30-C31-C32-C33
25	b	605	CLA	C8-C10-C11-C12
25	b	615	CLA	C10-C11-C12-C13
28	A	611	PL9	C12-C11-C9-C10
28	a	611	PL9	C20-C19-C21-C22
26	a	608	PHO	C2-C3-C5-C6
28	a	611	PL9	C12-C11-C9-C8
25	b	617	CLA	C10-C11-C12-C13
26	A	608	PHO	C13-C15-C16-C17
31	L	101	LHG	O2-C2-C3-O3
31	a	613	LHG	O2-C2-C3-O3
25	b	612	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
29	c	502	LMG	C33-C34-C35-C36
25	c	508	CLA	C3A-C2A-CAA-CBA
27	c	516	BCR	C9-C10-C11-C12
29	c	521	LMG	C30-C31-C32-C33
33	h	102	DGD	CDA-CEA-CFA-CGA
29	b	624	LMG	O10-C28-O8-C9
33	H	103	DGD	O6D-C5D-C6D-O5D
23	A	603	SQD	C25-C26-C27-C28
29	b	625	LMG	C12-C13-C14-C15
29	c	521	LMG	C14-C15-C16-C17
33	c	518	DGD	C8A-C9A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	d	404	CLA	C13-C15-C16-C17
23	B	626	SQD	O6-C44-C45-C46
29	B	621	LMG	O1-C7-C8-C9
29	b	624	LMG	O1-C7-C8-C9
29	b	624	LMG	C7-C8-C9-O8
29	c	502	LMG	O1-C7-C8-C9
29	c	521	LMG	O1-C7-C8-C9
29	d	409	LMG	C7-C8-C9-O8
31	a	615	LHG	C4-C5-C6-O8
29	c	521	LMG	C34-C35-C36-C37
29	d	409	LMG	C35-C36-C37-C38
31	L	101	LHG	C33-C34-C35-C36
23	A	619	SQD	C35-C36-C37-C38
23	I	101	SQD	C11-C10-C9-C8
29	B	621	LMG	C19-C20-C21-C22
31	A	616	LHG	C10-C11-C12-C13
25	b	607	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	A	609	CLA	C16-C17-C18-C19
33	C	518	DGD	CBB-CCB-CDB-CEB
31	a	614	LHG	C3-O3-P-O6
25	b	615	CLA	O1A-CGA-O2A-C1
26	d	401	PHO	O1D-CGD-O2D-CED
31	d	407	LHG	O6-C4-C5-O7
28	d	408	PL9	C37-C38-C39-C40
25	C	505	CLA	O1A-CGA-O2A-C1
29	c	502	LMG	O10-C28-O8-C9
33	C	517	DGD	C4B-C5B-C6B-C7B
33	c	518	DGD	C5A-C6A-C7A-C8A
29	D	405	LMG	C32-C33-C34-C35
29	c	521	LMG	C10-C11-C12-C13
23	D	409	SQD	O6-C44-C45-O47
29	A	612	LMG	O1-C7-C8-O7
29	C	520	LMG	O7-C8-C9-O8
29	b	624	LMG	O7-C8-C9-O8
29	c	502	LMG	O7-C8-C9-O8
29	c	521	LMG	O1-C7-C8-O7
29	c	522	LMG	O7-C8-C9-O8
25	B	601	CLA	C8-C10-C11-C12
25	C	513	CLA	O1D-CGD-O2D-CED
23	c	501	SQD	C11-C12-C13-C14
29	c	502	LMG	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C16-C17-C18-C19
23	I	101	SQD	O6-C44-C45-C46
23	c	501	SQD	C34-C35-C36-C37
31	a	615	LHG	C28-C29-C30-C31
25	B	604	CLA	C6-C7-C8-C9
25	C	512	CLA	C11-C10-C8-C9
25	a	609	CLA	C11-C12-C13-C14
25	b	614	CLA	C11-C12-C13-C14
25	b	617	CLA	C11-C12-C13-C14
25	c	508	CLA	C11-C10-C8-C9
25	c	512	CLA	C6-C7-C8-C9
33	C	516	DGD	C3B-C4B-C5B-C6B
25	a	609	CLA	C10-C11-C12-C13
25	b	616	CLA	C13-C15-C16-C17
26	a	608	PHO	C1A-C2A-CAA-CBA
23	D	409	SQD	C34-C35-C36-C37
29	c	502	LMG	C22-C23-C24-C25
33	C	516	DGD	C7A-C8A-C9A-CAA
33	H	103	DGD	C5A-C6A-C7A-C8A
27	A	610	BCR	C1-C6-C7-C8
27	A	610	BCR	C5-C6-C7-C8
27	A	610	BCR	C23-C24-C25-C26
27	A	610	BCR	C23-C24-C25-C30
27	B	618	BCR	C1-C6-C7-C8
27	B	618	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C26
27	C	515	BCR	C1-C6-C7-C8
27	C	515	BCR	C5-C6-C7-C8
27	C	515	BCR	C23-C24-C25-C26
27	C	515	BCR	C23-C24-C25-C30
27	D	404	BCR	C1-C6-C7-C8
27	D	404	BCR	C5-C6-C7-C8
27	H	102	BCR	C23-C24-C25-C26
27	H	102	BCR	C23-C24-C25-C30
27	K	101	BCR	C1-C6-C7-C8
27	K	101	BCR	C5-C6-C7-C8
27	K	101	BCR	C23-C24-C25-C26
27	K	101	BCR	C23-C24-C25-C30
27	Y	101	BCR	C1-C6-C7-C8
27	Y	101	BCR	C5-C6-C7-C8
27	a	610	BCR	C1-C6-C7-C8
27	a	610	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	610	BCR	C23-C24-C25-C26
27	a	610	BCR	C23-C24-C25-C30
27	b	621	BCR	C1-C6-C7-C8
27	b	621	BCR	C5-C6-C7-C8
27	b	621	BCR	C23-C24-C25-C26
27	b	621	BCR	C23-C24-C25-C30
27	b	622	BCR	C1-C6-C7-C8
27	b	622	BCR	C5-C6-C7-C8
27	c	517	BCR	C1-C6-C7-C8
27	c	517	BCR	C5-C6-C7-C8
27	c	517	BCR	C23-C24-C25-C26
27	c	517	BCR	C23-C24-C25-C30
27	d	405	BCR	C1-C6-C7-C8
27	d	405	BCR	C5-C6-C7-C8
27	h	101	BCR	C23-C24-C25-C26
27	k	101	BCR	C1-C6-C7-C8
27	k	101	BCR	C5-C6-C7-C8
27	k	101	BCR	C23-C24-C25-C26
27	k	101	BCR	C23-C24-C25-C30
31	A	617	LHG	C30-C31-C32-C33
33	H	103	DGD	O2G-C1B-C2B-C3B
27	b	621	BCR	C11-C12-C13-C35
29	c	522	LMG	C4-C5-C6-O5
29	d	409	LMG	C16-C17-C18-C19
27	Y	101	BCR	C21-C22-C23-C24
25	A	609	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
33	C	518	DGD	O1B-C1B-O2G-C2G
29	C	519	LMG	C11-C10-O7-C8
29	B	620	LMG	C34-C35-C36-C37
26	A	608	PHO	C3-C5-C6-C7
23	A	619	SQD	C16-C17-C18-C19
31	D	406	LHG	O6-C4-C5-C6
31	d	407	LHG	O6-C4-C5-C6
29	B	621	LMG	C28-C29-C30-C31
33	c	519	DGD	CCA-CDA-CEA-CFA
33	c	520	DGD	C5B-C6B-C7B-C8B
25	B	607	CLA	C12-C13-C15-C16
25	B	614	CLA	C11-C12-C13-C15
25	B	616	CLA	C6-C7-C8-C10
25	B	616	CLA	C11-C10-C8-C7
25	C	508	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	511	CLA	C6-C7-C8-C10
25	a	609	CLA	C11-C12-C13-C15
25	b	608	CLA	C12-C13-C15-C16
25	b	612	CLA	C12-C13-C15-C16
25	b	614	CLA	C12-C13-C15-C16
25	b	616	CLA	C12-C13-C15-C16
25	b	617	CLA	C11-C12-C13-C15
25	c	508	CLA	C11-C10-C8-C7
25	c	511	CLA	C11-C10-C8-C7
25	c	512	CLA	C6-C7-C8-C10
25	b	613	CLA	C16-C17-C18-C20
33	C	517	DGD	O1B-C1B-O2G-C2G
33	c	519	DGD	O1A-C1A-O1G-C1G
29	D	405	LMG	C11-C10-O7-C8
27	B	627	BCR	C20-C21-C22-C37
27	b	622	BCR	C20-C21-C22-C37
31	A	616	LHG	C33-C34-C35-C36
29	b	623	LMG	C15-C16-C17-C18
31	D	406	LHG	C25-C26-C27-C28
29	c	502	LMG	C29-C28-O8-C9
23	f	101	SQD	C44-C45-O47-C7
25	B	616	CLA	CAD-CBD-CGD-O2D
25	b	608	CLA	CAD-CBD-CGD-O2D
25	b	617	CLA	CAD-CBD-CGD-O2D
25	c	508	CLA	CAD-CBD-CGD-O2D
25	d	404	CLA	CAD-CBD-CGD-O2D
26	A	608	PHO	CAD-CBD-CGD-O2D
29	c	521	LMG	C16-C17-C18-C19
25	b	619	CLA	C13-C15-C16-C17
27	T	101	BCR	C6-C7-C8-C9
27	b	620	BCR	C22-C23-C24-C25
28	d	408	PL9	C20-C19-C21-C22
23	f	101	SQD	C28-C29-C30-C31
28	a	611	PL9	C18-C19-C21-C22
28	a	611	PL9	C24-C26-C27-C28
29	A	613	LMG	O1-C7-C8-C9
29	A	613	LMG	C7-C8-C9-O8
31	a	614	LHG	C4-C5-C6-O8
23	B	626	SQD	C24-C25-C26-C27
31	D	406	LHG	O6-C4-C5-O7
31	L	101	LHG	O6-C4-C5-O7
31	l	101	LHG	O6-C4-C5-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	612	LMG	C32-C33-C34-C35
33	H	103	DGD	O1A-C1A-O1G-C1G
23	c	501	SQD	C11-C10-C9-C8
29	b	624	LMG	C17-C18-C19-C20
25	c	512	CLA	O1D-CGD-O2D-CED
31	L	101	LHG	C1-C2-C3-O3
31	a	613	LHG	C1-C2-C3-O3
25	A	615	CLA	CHA-CBD-CGD-O1D
25	A	615	CLA	CHA-CBD-CGD-O2D
25	B	604	CLA	CHA-CBD-CGD-O1D
25	B	604	CLA	CHA-CBD-CGD-O2D
25	B	609	CLA	CHA-CBD-CGD-O2D
25	B	612	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	a	607	CLA	CHA-CBD-CGD-O1D
25	a	607	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	510	CLA	CHA-CBD-CGD-O1D
25	c	510	CLA	CHA-CBD-CGD-O2D
29	C	519	LMG	O10-C28-O8-C9
25	B	605	CLA	C15-C16-C17-C18
23	A	619	SQD	O47-C45-C46-O48
23	D	408	SQD	O47-C45-C46-O48
23	b	601	SQD	O6-C44-C45-O47
23	f	101	SQD	O6-C44-C45-O47
29	B	621	LMG	O1-C7-C8-O7
29	b	624	LMG	O1-C7-C8-O7
29	d	409	LMG	O7-C8-C9-O8
31	a	614	LHG	O7-C5-C6-O8
29	A	613	LMG	C22-C23-C24-C25
25	c	507	CLA	O1D-CGD-O2D-CED
31	D	406	LHG	O1-C1-C2-O2
31	l	101	LHG	O1-C1-C2-O2
25	C	505	CLA	O1D-CGD-O2D-CED
23	c	501	SQD	C24-C25-C26-C27
25	b	612	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
28	a	611	PL9	C4-C3-C7-C8
25	B	614	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C14-C13-C15-C16
26	A	608	PHO	C14-C13-C15-C16
23	c	501	SQD	C5-C6-S-O8
23	D	408	SQD	C11-C12-C13-C14
23	D	409	SQD	C24-C25-C26-C27
29	C	519	LMG	C40-C41-C42-C43
27	c	516	BCR	C37-C22-C23-C24
31	l	101	LHG	C32-C33-C34-C35
31	l	101	LHG	O1-C1-C2-C3
25	A	615	CLA	C1A-C2A-CAA-CBA
25	a	607	CLA	C1A-C2A-CAA-CBA
25	c	505	CLA	C1A-C2A-CAA-CBA
29	b	623	LMG	C10-C11-C12-C13
26	a	608	PHO	C16-C17-C18-C19
25	C	504	CLA	C13-C15-C16-C17
31	a	613	LHG	C12-C13-C14-C15
31	L	101	LHG	C4-O6-P-O3
31	a	613	LHG	C18-C19-C20-C21
33	C	518	DGD	CCB-CDB-CEB-CFB
31	A	618	LHG	C2-C3-O3-P
31	A	616	LHG	C3-O3-P-O5
31	A	617	LHG	C4-O6-P-O5
31	a	614	LHG	C3-O3-P-O4
31	a	614	LHG	C4-O6-P-O5
31	d	407	LHG	C4-O6-P-O5
25	B	611	CLA	C16-C17-C18-C19
23	A	619	SQD	C29-C30-C31-C32
25	B	604	CLA	C3-C5-C6-C7
29	B	620	LMG	C35-C36-C37-C38
31	D	406	LHG	C27-C28-C29-C30
23	A	603	SQD	C9-C10-C11-C12
25	B	616	CLA	C16-C17-C18-C20
23	b	601	SQD	C5-C6-S-O9
25	B	601	CLA	CAD-CBD-CGD-O1D
25	B	607	CLA	CAD-CBD-CGD-O1D
25	B	609	CLA	CAD-CBD-CGD-O1D
25	B	612	CLA	CAD-CBD-CGD-O1D
25	B	614	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	b	615	CLA	C15-C16-C17-C18
26	D	401	PHO	C3-C5-C6-C7
33	H	103	DGD	C7B-C8B-C9B-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	d	409	LMG	C28-C29-C30-C31
31	a	613	LHG	C23-C24-C25-C26
29	B	621	LMG	C15-C16-C17-C18
25	B	612	CLA	CBA-CGA-O2A-C1
25	C	508	CLA	CBA-CGA-O2A-C1
33	c	519	DGD	C5A-C6A-C7A-C8A
26	A	608	PHO	C16-C17-C18-C19
28	a	611	PL9	C30-C29-C31-C32
25	A	607	CLA	C11-C10-C8-C7
25	C	504	CLA	C12-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C7
25	C	509	CLA	C11-C12-C13-C15
25	C	510	CLA	C11-C10-C8-C7
25	D	402	CLA	C11-C12-C13-C15
25	b	610	CLA	C12-C13-C15-C16
25	b	612	CLA	C2-C3-C5-C6
25	c	506	CLA	C12-C13-C15-C16
25	c	508	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7
25	c	514	CLA	C11-C10-C8-C7
31	a	615	LHG	C17-C18-C19-C20
23	D	409	SQD	C7-C8-C9-C10
29	B	625	LMG	C16-C17-C18-C19
29	d	409	LMG	C38-C39-C40-C41
33	C	518	DGD	C3B-C4B-C5B-C6B
29	C	520	LMG	O10-C28-O8-C9
29	c	521	LMG	C37-C38-C39-C40
25	b	613	CLA	C15-C16-C17-C18
25	C	509	CLA	C16-C17-C18-C20
31	D	406	LHG	C18-C19-C20-C21
31	a	615	LHG	C11-C10-C9-C8
33	h	102	DGD	O2G-C1B-C2B-C3B
23	D	409	SQD	O6-C44-C45-C46
23	b	601	SQD	O6-C44-C45-C46
23	f	101	SQD	O6-C44-C45-C46
29	A	612	LMG	O1-C7-C8-C9
29	c	502	LMG	C17-C18-C19-C20
33	c	518	DGD	C1G-C2G-C3G-O3G
23	D	409	SQD	O47-C45-C46-O48
29	B	625	LMG	O1-C7-C8-O7
29	c	502	LMG	O1-C7-C8-O7
31	A	618	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	c	518	DGD	O2G-C2G-C3G-O3G
31	a	613	LHG	C24-C23-O8-C6
29	B	625	LMG	C15-C16-C17-C18
29	c	521	LMG	O10-C28-O8-C9
26	a	608	PHO	C13-C15-C16-C17
33	C	517	DGD	CCA-CDA-CEA-CFA
25	C	501	CLA	CBA-CGA-O2A-C1
29	b	623	LMG	C34-C35-C36-C37
25	B	603	CLA	C5-C6-C7-C8
25	B	607	CLA	C14-C13-C15-C16
25	B	609	CLA	C6-C7-C8-C9
25	B	615	CLA	C11-C12-C13-C14
25	B	616	CLA	C11-C10-C8-C9
25	b	618	CLA	C11-C10-C8-C9
25	c	509	CLA	C11-C10-C8-C9
25	c	514	CLA	C6-C7-C8-C9
27	T	101	BCR	C22-C23-C24-C25
25	C	508	CLA	O1A-CGA-O2A-C1
25	c	509	CLA	C16-C17-C18-C19
31	L	101	LHG	C9-C10-C11-C12
25	C	501	CLA	O1A-CGA-O2A-C1
33	C	517	DGD	CDA-CEA-CFA-CGA
25	B	612	CLA	O1A-CGA-O2A-C1
29	C	520	LMG	C36-C37-C38-C39
29	A	613	LMG	C35-C36-C37-C38
23	c	501	SQD	C27-C28-C29-C30
29	d	406	LMG	C38-C39-C40-C41
29	B	620	LMG	C38-C39-C40-C41
31	a	615	LHG	C10-C11-C12-C13
25	b	606	CLA	C5-C6-C7-C8
31	a	613	LHG	C11-C12-C13-C14
23	A	619	SQD	C46-C45-O47-C7
23	D	408	SQD	C46-C45-O47-C7
29	b	624	LMG	C7-C8-O7-C10
25	C	507	CLA	C2A-CAA-CBA-CGA
31	D	406	LHG	C12-C13-C14-C15
29	c	522	LMG	C29-C28-O8-C9
25	A	607	CLA	C2-C1-O2A-CGA
25	a	606	CLA	C2-C1-O2A-CGA
25	b	616	CLA	C2-C1-O2A-CGA
28	A	611	PL9	C47-C48-C49-C51
31	A	618	LHG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	506	CLA	C5-C6-C7-C8
29	A	612	LMG	C33-C34-C35-C36
29	D	405	LMG	C31-C32-C33-C34
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C30
27	h	101	BCR	C23-C24-C25-C30
27	y	101	BCR	C23-C24-C25-C26
27	y	101	BCR	C23-C24-C25-C30
23	A	619	SQD	C10-C11-C12-C13
31	d	407	LHG	C16-C17-C18-C19
25	c	509	CLA	C2A-CAA-CBA-CGA
28	a	611	PL9	C39-C41-C42-C43
31	A	618	LHG	C3-O3-P-O6
31	l	101	LHG	C4-O6-P-O3
31	D	406	LHG	C14-C15-C16-C17
26	D	401	PHO	CHA-CBD-CGD-O1D
26	D	401	PHO	CHA-CBD-CGD-O2D
29	d	406	LMG	C30-C31-C32-C33
25	B	601	CLA	C11-C12-C13-C15
25	B	604	CLA	C6-C7-C8-C10
25	c	507	CLA	C11-C12-C13-C15
25	c	510	CLA	C11-C10-C8-C7
25	c	511	CLA	C11-C12-C13-C15
31	a	613	LHG	C9-C10-C11-C12
25	C	504	CLA	C14-C13-C15-C16
25	C	507	CLA	C11-C10-C8-C9
25	C	509	CLA	C14-C13-C15-C16
25	b	604	CLA	C11-C12-C13-C14
25	B	616	CLA	C16-C17-C18-C19
26	D	401	PHO	C16-C17-C18-C20
25	c	507	CLA	CBA-CGA-O2A-C1
25	c	508	CLA	CBA-CGA-O2A-C1
23	A	619	SQD	C33-C34-C35-C36
29	B	625	LMG	C28-C29-C30-C31
29	c	522	LMG	C40-C41-C42-C43
27	D	404	BCR	C37-C22-C23-C24
25	b	604	CLA	C8-C10-C11-C12
23	A	619	SQD	C34-C35-C36-C37
31	a	614	LHG	C2-C3-O3-P
31	a	615	LHG	C5-C4-O6-P
29	C	520	LMG	C15-C16-C17-C18
29	B	620	LMG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	508	CLA	O1A-CGA-O2A-C1
25	c	506	CLA	C13-C15-C16-C17
25	c	507	CLA	O1A-CGA-O2A-C1
33	C	518	DGD	O6D-C1D-O3G-C3G
23	B	626	SQD	C19-C20-C21-C22
29	B	625	LMG	C38-C39-C40-C41
29	b	624	LMG	C31-C32-C33-C34
25	B	603	CLA	C15-C16-C17-C18
25	b	606	CLA	C15-C16-C17-C18
31	L	101	LHG	C16-C17-C18-C19
31	a	615	LHG	O10-C23-O8-C6
26	d	401	PHO	C13-C15-C16-C17
23	I	101	SQD	C12-C13-C14-C15
29	c	502	LMG	C39-C40-C41-C42
25	A	606	CLA	C2-C1-O2A-CGA
23	B	626	SQD	C18-C19-C20-C21
33	H	103	DGD	C9B-CAB-CBB-CCB
25	C	509	CLA	C16-C17-C18-C19
25	b	613	CLA	C16-C17-C18-C19
23	b	601	SQD	C12-C13-C14-C15
33	c	520	DGD	C8A-C9A-CAA-CBA
25	C	505	CLA	C2A-CAA-CBA-CGA
25	b	613	CLA	C2A-CAA-CBA-CGA
29	d	406	LMG	C34-C35-C36-C37
26	D	401	PHO	C3A-C2A-CAA-CBA
25	B	601	CLA	CAA-CBA-CGA-O2A
27	k	101	BCR	C19-C20-C21-C22
28	D	407	PL9	C43-C44-C46-C47
28	A	611	PL9	C4-C3-C7-C8
29	d	409	LMG	C36-C37-C38-C39
31	A	616	LHG	C27-C28-C29-C30
33	c	519	DGD	C8A-C9A-CAA-CBA
25	B	607	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C10-C8-C9
25	C	505	CLA	C14-C13-C15-C16
25	b	605	CLA	C6-C7-C8-C9
25	b	612	CLA	C11-C10-C8-C9
25	c	504	CLA	C6-C7-C8-C9
25	c	504	CLA	C14-C13-C15-C16
25	c	508	CLA	C14-C13-C15-C16
23	D	409	SQD	C30-C31-C32-C33
29	D	405	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	C	519	LMG	C37-C38-C39-C40
31	d	407	LHG	C26-C27-C28-C29
29	d	409	LMG	C22-C23-C24-C25
31	D	406	LHG	C26-C27-C28-C29
25	c	509	CLA	C16-C17-C18-C20
33	c	520	DGD	O6D-C1D-O3G-C3G
33	c	520	DGD	C2B-C3B-C4B-C5B
23	c	501	SQD	C26-C27-C28-C29
25	b	618	CLA	C4-C3-C5-C6
25	B	607	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	C	512	CLA	C1A-C2A-CAA-CBA
25	C	513	CLA	C1A-C2A-CAA-CBA
29	c	521	LMG	C17-C18-C19-C20
25	B	614	CLA	C11-C10-C8-C7
25	D	402	CLA	C12-C13-C15-C16
25	b	605	CLA	C11-C12-C13-C15
25	b	609	CLA	C12-C13-C15-C16
25	b	618	CLA	C11-C10-C8-C7
25	c	507	CLA	C12-C13-C15-C16
25	c	509	CLA	C11-C12-C13-C15
23	B	626	SQD	C30-C31-C32-C33
25	B	613	CLA	C13-C15-C16-C17
25	b	619	CLA	C5-C6-C7-C8
27	K	101	BCR	C19-C20-C21-C22
29	B	620	LMG	C33-C34-C35-C36
23	c	501	SQD	C15-C16-C17-C18
31	A	617	LHG	C11-C12-C13-C14
25	C	509	CLA	C5-C6-C7-C8
29	d	409	LMG	C12-C13-C14-C15
34	E	101	HEM	CAD-CBD-CGD-O2D
35	v	201	HEC	CAD-CBD-CGD-O1D
25	B	610	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
23	f	101	SQD	C35-C36-C37-C38
33	c	518	DGD	CAA-CBA-CCA-CDA
26	A	608	PHO	C15-C16-C17-C18
28	d	408	PL9	C35-C34-C36-C37
31	A	616	LHG	C7-C8-C9-C10
27	Y	101	BCR	C20-C21-C22-C23
25	B	616	CLA	C8-C10-C11-C12
35	v	201	HEC	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	D	406	LHG	C30-C31-C32-C33
33	c	519	DGD	O1G-C1G-C2G-O2G
23	I	101	SQD	C18-C19-C20-C21
27	B	627	BCR	C6-C7-C8-C9
23	B	626	SQD	C17-C18-C19-C20
23	f	101	SQD	C31-C32-C33-C34
28	A	611	PL9	C39-C41-C42-C43
25	a	607	CLA	C2-C1-O2A-CGA
25	B	614	CLA	C5-C6-C7-C8
25	c	505	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	C6-C7-C8-C9
29	D	405	LMG	C13-C14-C15-C16
31	A	617	LHG	C15-C16-C17-C18
25	b	607	CLA	C3-C5-C6-C7
26	A	608	PHO	C1A-C2A-CAA-CBA
25	b	611	CLA	C2A-CAA-CBA-CGA
25	b	617	CLA	C2A-CAA-CBA-CGA
31	A	617	LHG	C13-C14-C15-C16
27	B	617	BCR	C23-C24-C25-C30
27	B	627	BCR	C23-C24-C25-C30
27	C	514	BCR	C23-C24-C25-C26
27	H	102	BCR	C1-C6-C7-C8
27	T	101	BCR	C23-C24-C25-C30
27	Y	101	BCR	C23-C24-C25-C30
27	b	620	BCR	C23-C24-C25-C30
27	c	516	BCR	C1-C6-C7-C8
27	c	516	BCR	C23-C24-C25-C30
25	b	604	CLA	CAA-CBA-CGA-O2A
34	E	101	HEM	CAD-CBD-CGD-O1D
25	c	505	CLA	CBD-CGD-O2D-CED
31	A	617	LHG	O1-C1-C2-C3
23	A	603	SQD	C33-C34-C35-C36
23	A	619	SQD	C11-C12-C13-C14
29	d	409	LMG	C39-C40-C41-C42
28	D	407	PL9	C13-C14-C16-C17
23	A	603	SQD	C45-C44-O6-C1
23	f	101	SQD	C45-C44-O6-C1
29	c	522	LMG	C21-C22-C23-C24
31	A	618	LHG	C13-C14-C15-C16
31	A	617	LHG	C34-C35-C36-C37
25	B	614	CLA	C16-C17-C18-C19
31	A	617	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	409	SQD	O48-C23-C24-C25
28	D	407	PL9	C15-C14-C16-C17
28	d	408	PL9	C15-C14-C16-C17
25	B	615	CLA	C11-C12-C13-C15
25	C	506	CLA	C6-C7-C8-C10
25	b	607	CLA	C2-C3-C5-C6
25	b	618	CLA	C2-C3-C5-C6
23	A	619	SQD	O6-C44-C45-O47
25	c	511	CLA	C13-C15-C16-C17
29	B	620	LMG	C40-C41-C42-C43
29	A	613	LMG	O7-C8-C9-O8
25	b	615	CLA	C8-C10-C11-C12
31	a	613	LHG	C28-C29-C30-C31
31	A	616	LHG	C24-C25-C26-C27
23	A	603	SQD	C24-C23-O48-C46
27	C	515	BCR	C20-C21-C22-C37
29	B	625	LMG	C32-C33-C34-C35
28	A	611	PL9	C40-C39-C41-C42
33	c	520	DGD	C4B-C5B-C6B-C7B
28	a	611	PL9	C33-C34-C36-C37
23	D	408	SQD	C13-C14-C15-C16
31	d	407	LHG	C28-C29-C30-C31
26	d	401	PHO	C16-C17-C18-C20
25	C	510	CLA	CAA-CBA-CGA-O2A
25	b	616	CLA	CAA-CBA-CGA-O2A
31	l	101	LHG	O7-C7-C8-C9
25	A	607	CLA	C11-C10-C8-C9
25	B	601	CLA	C11-C12-C13-C14
25	C	510	CLA	C11-C10-C8-C9
25	D	402	CLA	C11-C12-C13-C14
25	b	610	CLA	C14-C13-C15-C16
25	c	506	CLA	C14-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C9
25	c	514	CLA	C11-C10-C8-C9
25	c	515	CLA	C6-C7-C8-C9
34	E	101	HEM	CAA-CBA-CGA-O2A
26	A	608	PHO	C3A-C2A-CAA-CBA
26	d	401	PHO	C3A-C2A-CAA-CBA
33	C	518	DGD	O1A-C1A-O1G-C1G
25	B	610	CLA	CAD-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	512	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	b	606	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	b	612	CLA	CAD-CBD-CGD-O2D
25	b	615	CLA	CAD-CBD-CGD-O2D
25	b	616	CLA	CAD-CBD-CGD-O2D
25	c	505	CLA	CAD-CBD-CGD-O2D
25	c	512	CLA	CAD-CBD-CGD-O2D
25	c	515	CLA	CAD-CBD-CGD-O2D
26	a	608	PHO	CAD-CBD-CGD-O2D
25	c	512	CLA	CAA-CBA-CGA-O2A
27	B	617	BCR	C22-C23-C24-C25
23	A	603	SQD	C10-C11-C12-C13
29	c	521	LMG	O7-C10-C11-C12
29	d	409	LMG	O7-C10-C11-C12
29	B	620	LMG	C19-C20-C21-C22
27	K	101	BCR	C21-C22-C23-C24
27	c	517	BCR	C7-C8-C9-C10
23	D	408	SQD	C44-C45-C46-O48
33	h	102	DGD	C1G-C2G-C3G-O3G
23	A	619	SQD	O47-C7-C8-C9
25	C	512	CLA	CAA-CBA-CGA-O2A
29	B	620	LMG	O8-C28-C29-C30
31	L	101	LHG	C17-C18-C19-C20
25	B	613	CLA	O2A-C1-C2-C3
25	C	509	CLA	O2A-C1-C2-C3
25	D	402	CLA	O2A-C1-C2-C3
25	d	403	CLA	O2A-C1-C2-C3
25	B	608	CLA	C2A-CAA-CBA-CGA
25	D	402	CLA	CAA-CBA-CGA-O2A
25	d	403	CLA	CAA-CBA-CGA-O2A
33	h	102	DGD	O1A-C1A-O1G-C1G
25	A	607	CLA	CHA-CBD-CGD-O1D
25	A	607	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	602	CLA	CHA-CBD-CGD-O2D
25	B	612	CLA	CHA-CBD-CGD-O2D
25	C	509	CLA	CHA-CBD-CGD-O1D
25	C	509	CLA	CHA-CBD-CGD-O2D
25	b	610	CLA	CHA-CBD-CGD-O2D
25	c	507	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	c	508	CLA	CHA-CBD-CGD-O2D
25	c	509	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O2D
25	c	514	CLA	CHA-CBD-CGD-O1D
23	D	409	SQD	C35-C36-C37-C38
31	A	618	LHG	C26-C27-C28-C29
29	c	502	LMG	O8-C28-C29-C30
29	c	521	LMG	O7-C8-C9-O8
31	L	101	LHG	O7-C5-C6-O8
31	L	101	LHG	O7-C7-C8-C9
31	a	614	LHG	O8-C23-C24-C25
34	e	101	HEM	CAA-CBA-CGA-O2A
26	A	608	PHO	CHA-CBD-CGD-O1D
26	a	608	PHO	CHA-CBD-CGD-O1D
25	b	609	CLA	C8-C10-C11-C12
29	D	405	LMG	C28-C29-C30-C31
25	c	508	CLA	C5-C6-C7-C8
31	D	406	LHG	C34-C35-C36-C37
33	c	518	DGD	C2A-C3A-C4A-C5A
25	C	506	CLA	C12-C13-C15-C16
25	a	607	CLA	C11-C10-C8-C7
25	b	604	CLA	C12-C13-C15-C16
29	B	621	LMG	C36-C37-C38-C39
25	B	612	CLA	CAA-CBA-CGA-O2A
23	A	619	SQD	C15-C16-C17-C18
25	c	509	CLA	C11-C12-C13-C14
25	c	511	CLA	C11-C12-C13-C14
25	d	403	CLA	C14-C13-C15-C16
29	B	620	LMG	C29-C30-C31-C32
33	H	103	DGD	C6A-C7A-C8A-C9A
33	c	518	DGD	O2G-C1B-C2B-C3B
23	b	601	SQD	C4-C5-C6-S
23	b	601	SQD	C5-C6-S-O8
31	A	618	LHG	C27-C28-C29-C30
31	l	101	LHG	C11-C12-C13-C14
34	E	101	HEM	CAA-CBA-CGA-O1A
23	c	501	SQD	C31-C32-C33-C34
25	b	618	CLA	C13-C15-C16-C17
25	c	505	CLA	C15-C16-C17-C18
25	b	618	CLA	C16-C17-C18-C19
31	a	613	LHG	C29-C30-C31-C32
25	c	509	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	d	403	CLA	CBA-CGA-O2A-C1
25	B	602	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C1A-C2A-CAA-CBA
25	d	403	CLA	C1A-C2A-CAA-CBA
29	c	502	LMG	C15-C16-C17-C18
33	c	519	DGD	C4A-C5A-C6A-C7A
28	A	611	PL9	C36-C37-C38-C39
31	a	615	LHG	C25-C26-C27-C28
25	A	607	CLA	CBA-CGA-O2A-C1
23	A	603	SQD	O49-C7-C8-C9
23	c	501	SQD	O49-C7-C8-C9
25	B	612	CLA	CAA-CBA-CGA-O1A
25	C	510	CLA	CAA-CBA-CGA-O1A
29	d	409	LMG	O9-C10-C11-C12
29	C	520	LMG	C7-C8-C9-O8
33	C	516	DGD	C1G-C2G-C3G-O3G
25	c	507	CLA	C2A-CAA-CBA-CGA
31	D	406	LHG	O2-C2-C3-O3
25	c	507	CLA	C16-C17-C18-C19
25	d	403	CLA	CAA-CBA-CGA-O1A
29	b	623	LMG	O10-C28-C29-C30
29	C	520	LMG	C21-C22-C23-C24
25	b	616	CLA	CAA-CBA-CGA-O1A
23	f	101	SQD	O10-C23-O48-C46
33	C	518	DGD	C2D-C1D-O3G-C3G
25	B	603	CLA	C13-C15-C16-C17
25	B	614	CLA	C15-C16-C17-C18
31	A	618	LHG	C3-O3-P-O5
31	a	614	LHG	C3-O3-P-O5
25	B	602	CLA	C16-C17-C18-C20
33	c	520	DGD	C2A-C3A-C4A-C5A
25	C	512	CLA	CAA-CBA-CGA-O1A
25	D	402	CLA	CAA-CBA-CGA-O1A
25	c	512	CLA	CAA-CBA-CGA-O1A
31	l	101	LHG	O9-C7-C8-C9
23	c	501	SQD	O47-C7-C8-C9
33	C	516	DGD	O6E-C1E-O5D-C6D
25	A	607	CLA	O1A-CGA-O2A-C1
27	B	617	BCR	C23-C24-C25-C26
27	Y	101	BCR	C23-C24-C25-C26
27	b	620	BCR	C23-C24-C25-C26
26	d	401	PHO	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	c	521	LMG	O9-C10-C11-C12
33	c	519	DGD	O1B-C1B-C2B-C3B
25	d	403	CLA	O1A-CGA-O2A-C1
25	B	610	CLA	C16-C17-C18-C20
27	C	515	BCR	C18-C19-C20-C21
34	e	101	HEM	CAA-CBA-CGA-O1A
31	A	617	LHG	O8-C23-C24-C25
33	c	520	DGD	C9B-CAB-CBB-CCB
29	B	620	LMG	O10-C28-C29-C30
23	B	626	SQD	O5-C5-C6-S
25	B	604	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	c	507	CLA	CAD-CBD-CGD-O1D
25	c	514	CLA	CAD-CBD-CGD-O1D
29	b	624	LMG	C9-C8-O7-C10
23	B	626	SQD	C27-C28-C29-C30
23	b	601	SQD	O47-C7-C8-C9
25	b	611	CLA	C13-C15-C16-C17
25	C	506	CLA	C6-C7-C8-C9
25	a	607	CLA	C11-C10-C8-C9
25	b	619	CLA	C11-C12-C13-C14
25	C	501	CLA	CAA-CBA-CGA-O2A
29	c	522	LMG	C37-C38-C39-C40
25	c	509	CLA	O1A-CGA-O2A-C1
25	B	612	CLA	C13-C15-C16-C17
23	A	603	SQD	O47-C7-C8-C9
23	D	408	SQD	O48-C23-C24-C25
23	f	101	SQD	O47-C7-C8-C9
25	c	514	CLA	CAA-CBA-CGA-O2A
25	c	503	CLA	CAA-CBA-CGA-O1A
23	A	619	SQD	C26-C27-C28-C29
25	B	602	CLA	C6-C7-C8-C10
25	B	609	CLA	C12-C13-C15-C16
25	B	610	CLA	C11-C10-C8-C7
25	B	614	CLA	C6-C7-C8-C10
25	C	512	CLA	C3A-C2A-CAA-CBA
25	C	513	CLA	C11-C10-C8-C7
25	D	403	CLA	C6-C7-C8-C10
25	b	605	CLA	C12-C13-C15-C16
25	b	616	CLA	C11-C10-C8-C7
25	b	615	CLA	CAA-CBA-CGA-O2A
29	B	621	LMG	O7-C10-C11-C12

Continued on next page...

Continued from previous page...

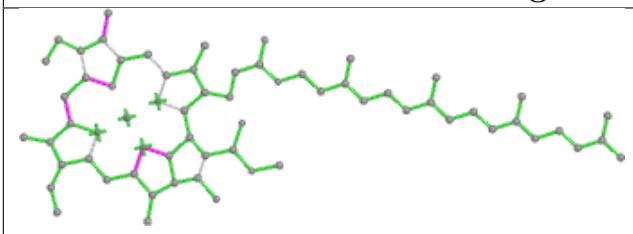
Mol	Chain	Res	Type	Atoms
33	c	519	DGD	O2G-C1B-C2B-C3B
27	Y	101	BCR	C7-C8-C9-C10
27	h	101	BCR	C17-C18-C19-C20
31	L	101	LHG	O9-C7-C8-C9
33	C	516	DGD	O1G-C1A-C2A-C3A
33	C	517	DGD	O6D-C1D-O3G-C3G
33	c	518	DGD	O6E-C1E-O5D-C6D
25	B	609	CLA	C5-C6-C7-C8
23	A	619	SQD	O49-C7-C8-C9
29	d	409	LMG	C30-C31-C32-C33
25	c	503	CLA	CAA-CBA-CGA-O2A
29	A	613	LMG	O8-C28-C29-C30
25	C	501	CLA	CAA-CBA-CGA-O1A
31	A	617	LHG	O10-C23-C24-C25

There are no ring outliers.

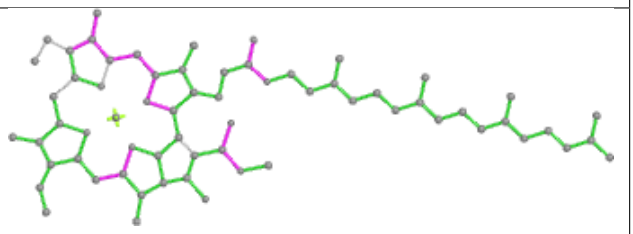
No monomer is involved in short contacts.

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.

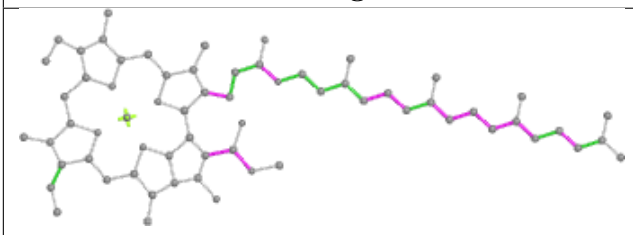
Ligand CLA c 508



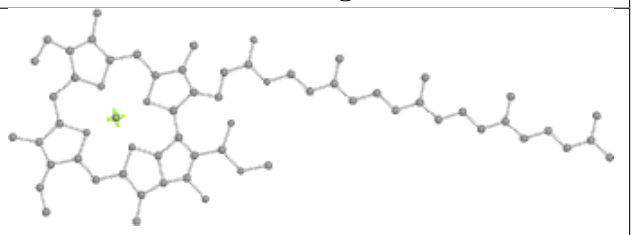
Bond lengths



Bond angles

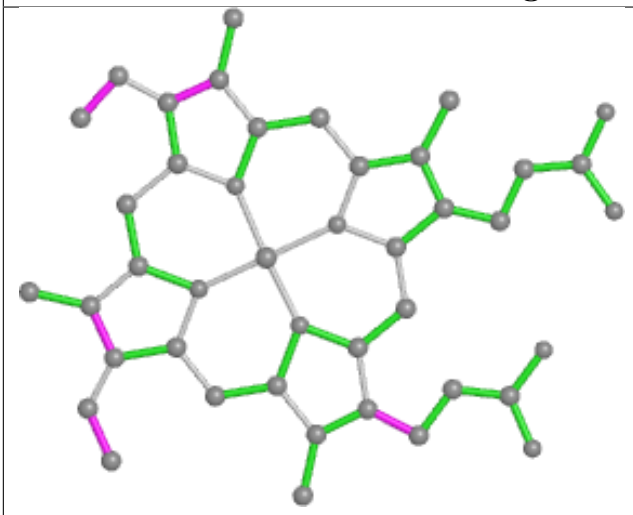


Torsions

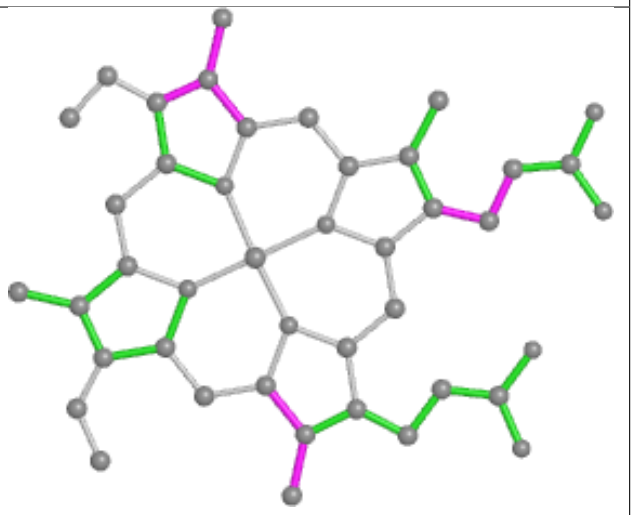


Rings

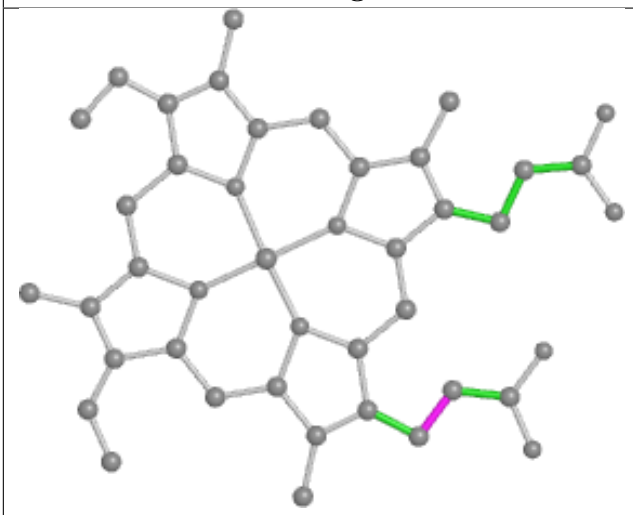
Ligand HEC V 201



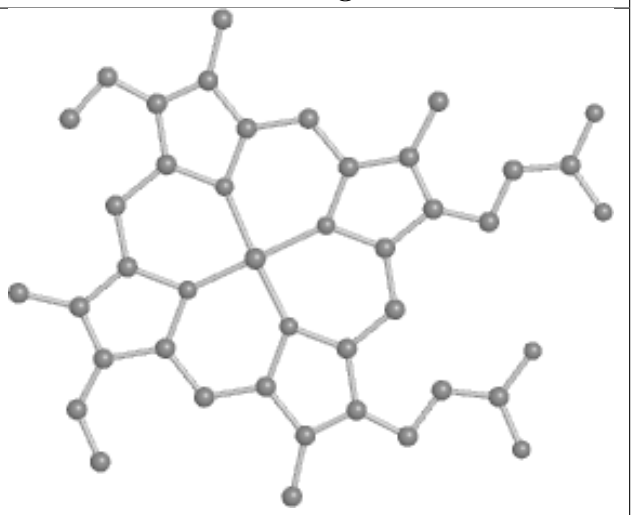
Bond lengths



Bond angles

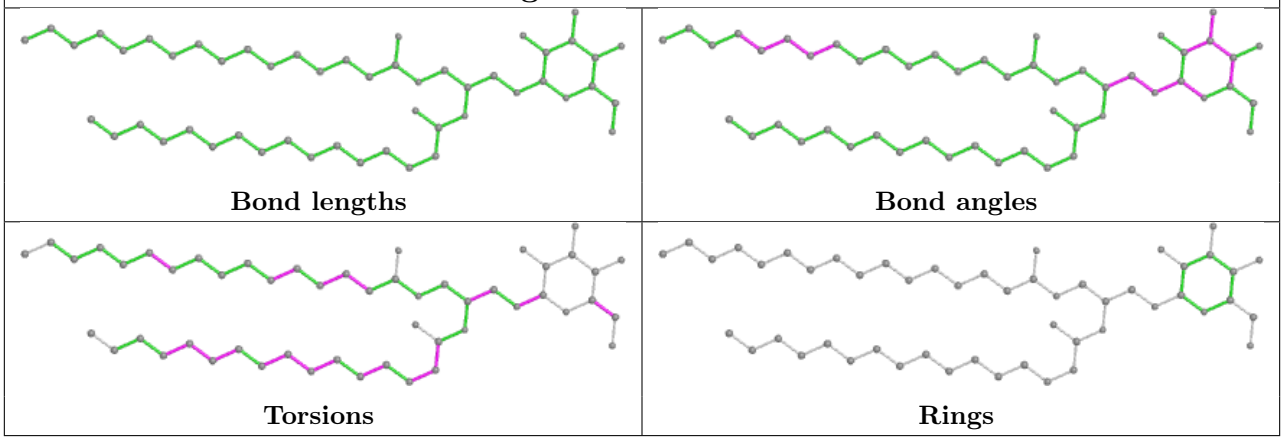


Torsions

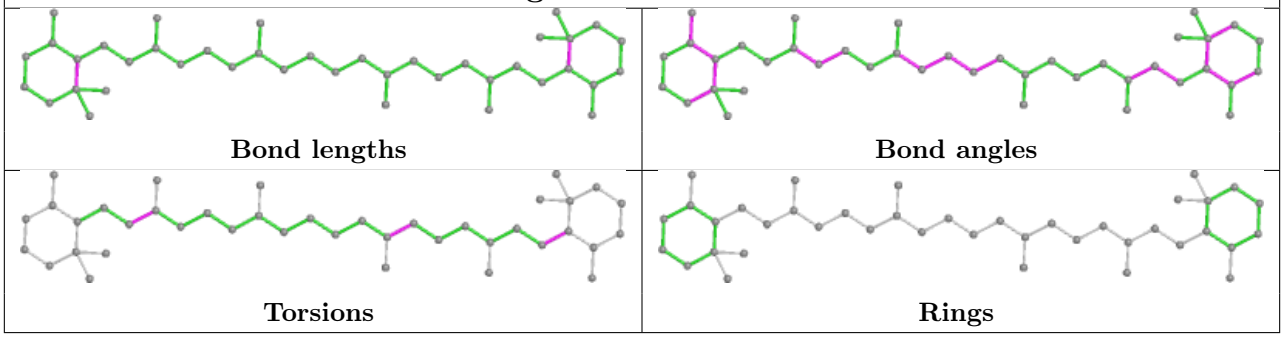


Rings

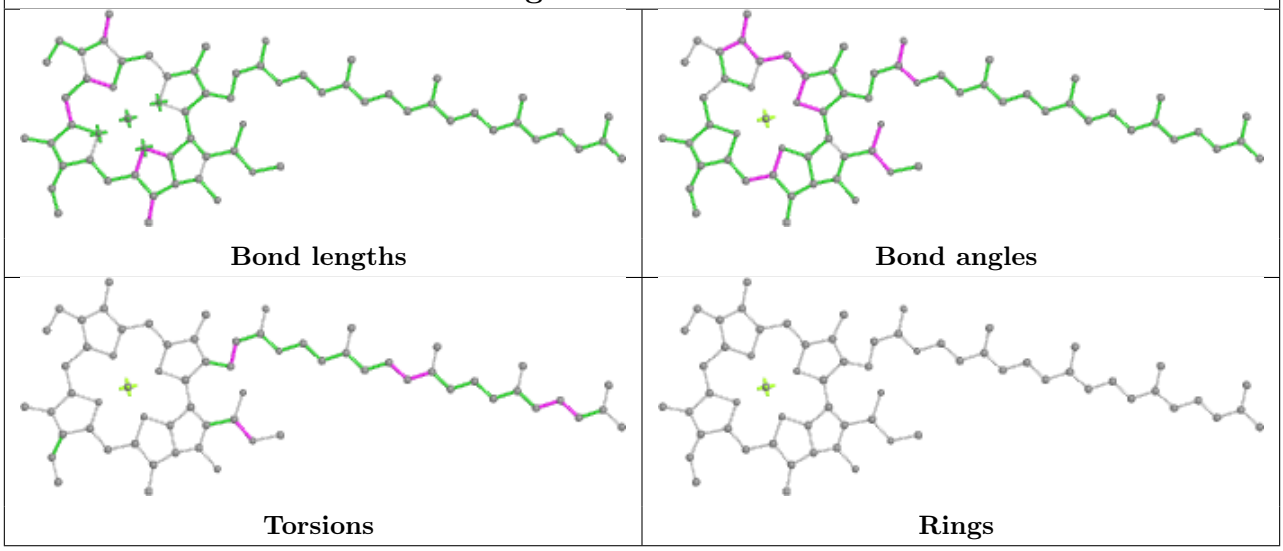
Ligand LMG B 621



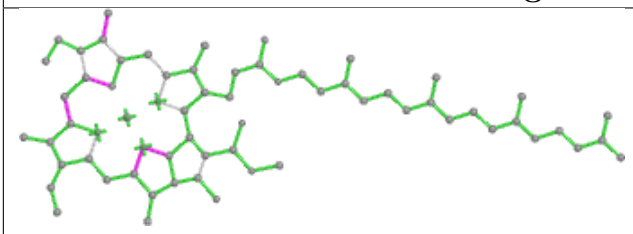
Ligand BCR h 101



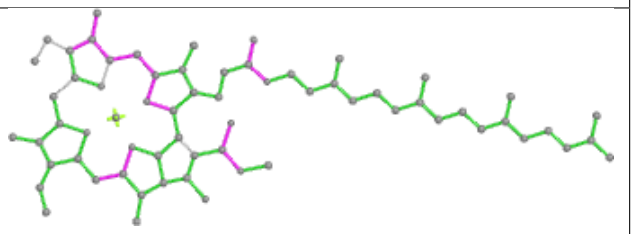
Ligand CLA B 603



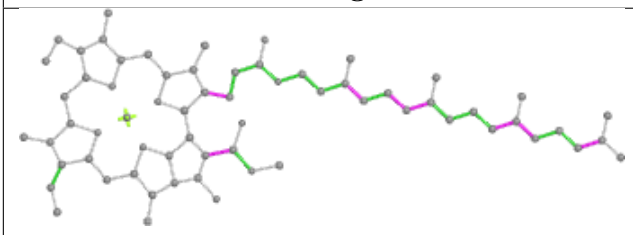
Ligand CLA B 602



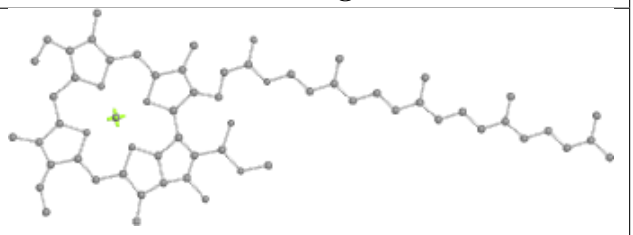
Bond lengths



Bond angles

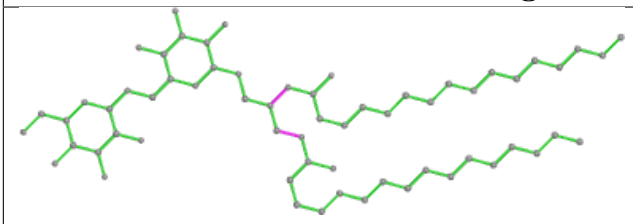


Torsions

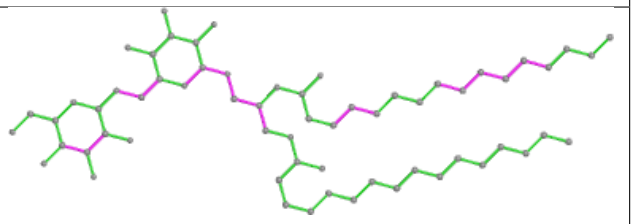


Rings

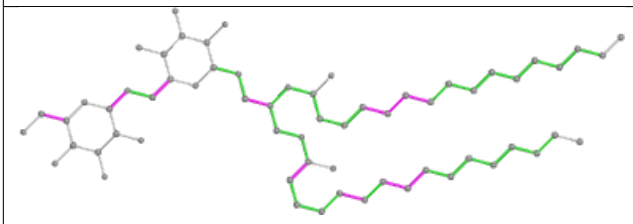
Ligand DGD C 516



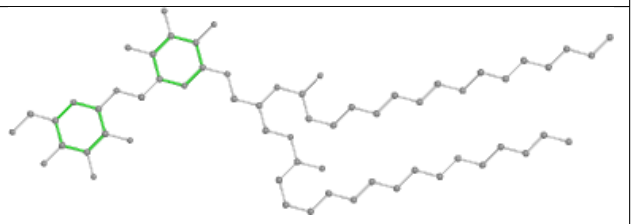
Bond lengths



Bond angles

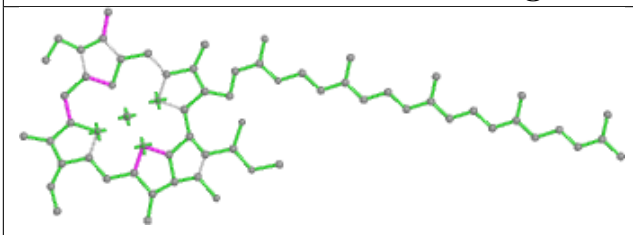


Torsions

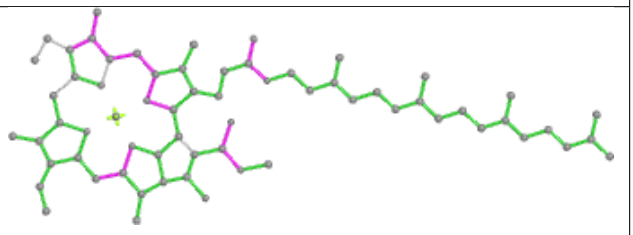


Rings

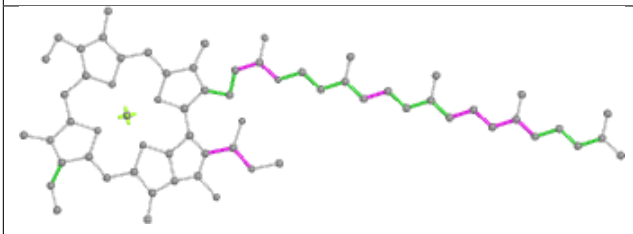
Ligand CLA B 601



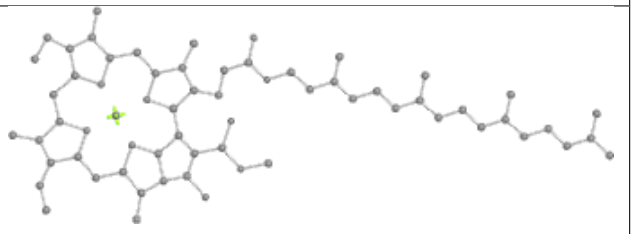
Bond lengths



Bond angles

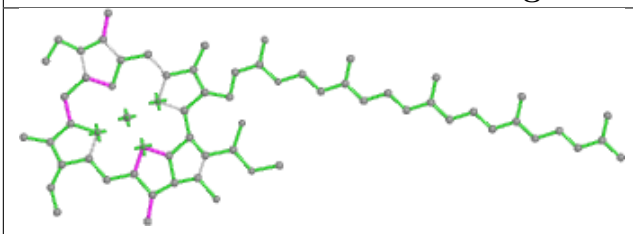


Torsions

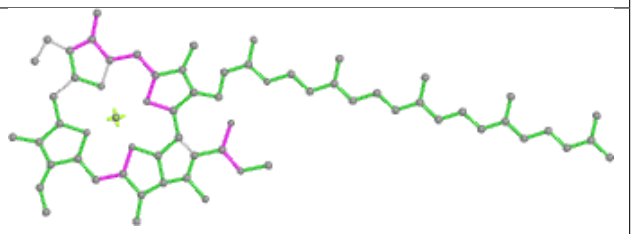


Rings

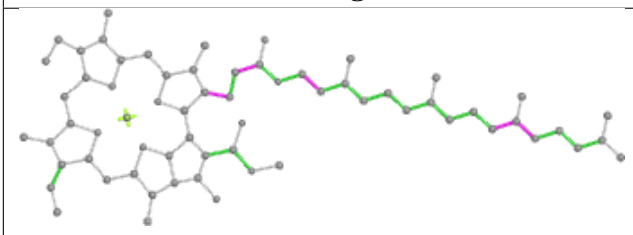
Ligand CLA D 402



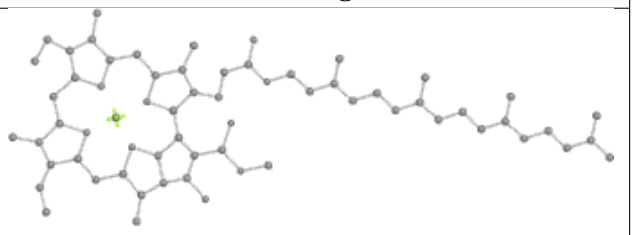
Bond lengths



Bond angles

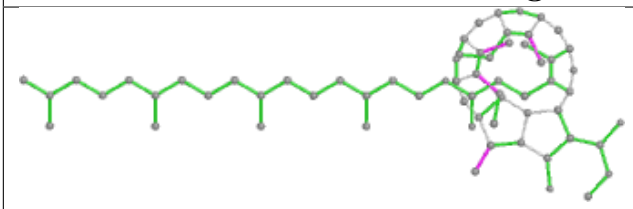


Torsions

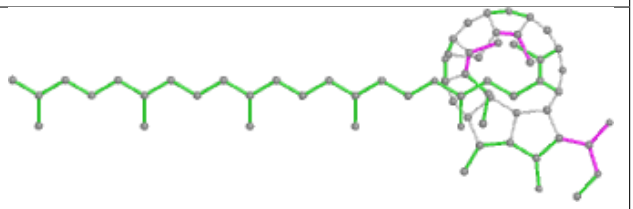


Rings

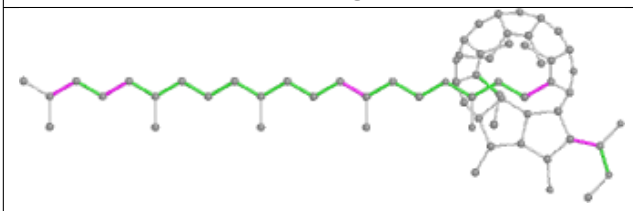
Ligand PHO a 608



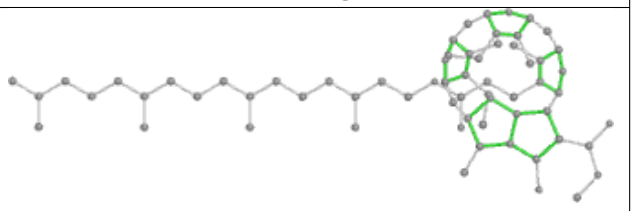
Bond lengths



Bond angles

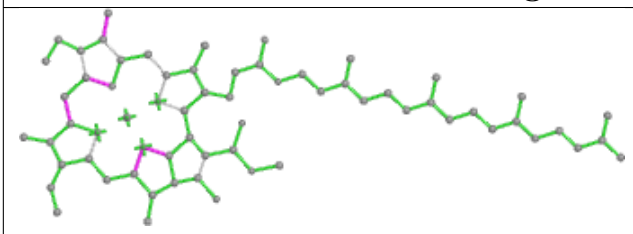


Torsions

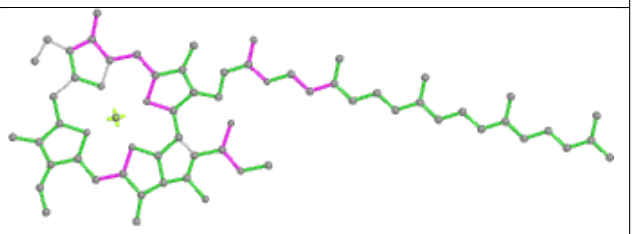


Rings

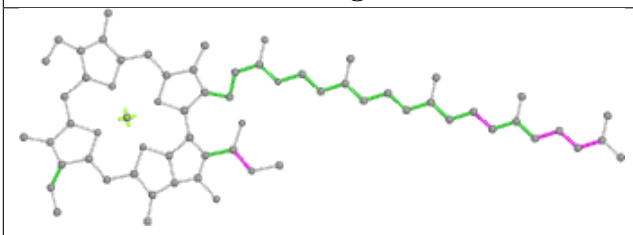
Ligand CLA A 609



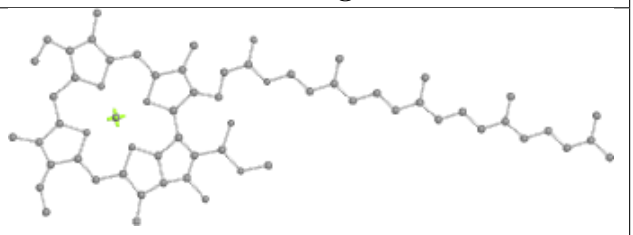
Bond lengths



Bond angles

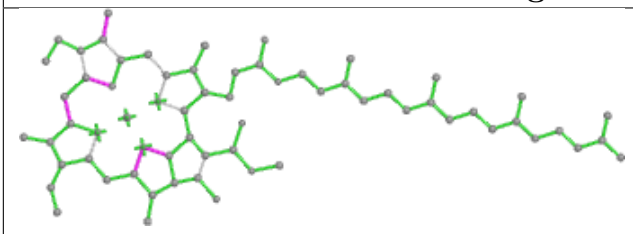


Torsions

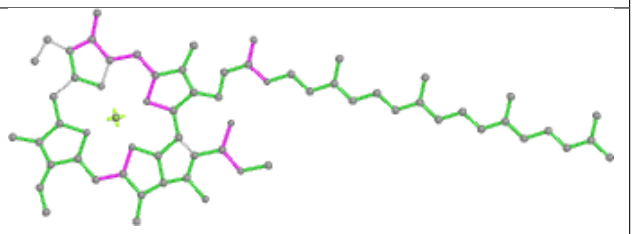


Rings

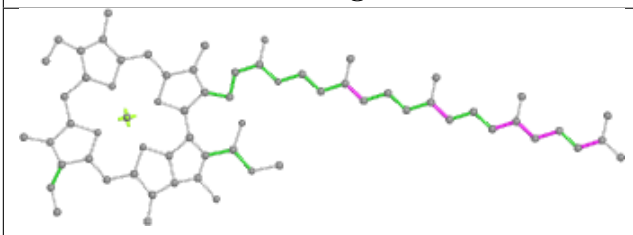
Ligand CLA b 618



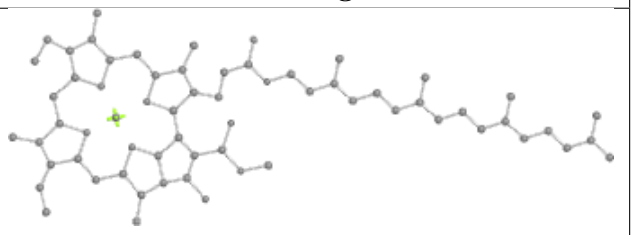
Bond lengths



Bond angles

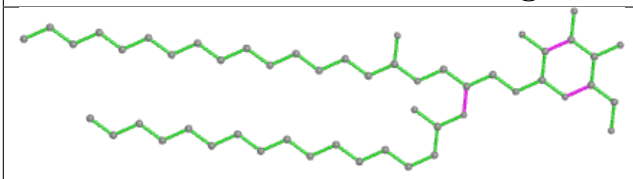


Torsions

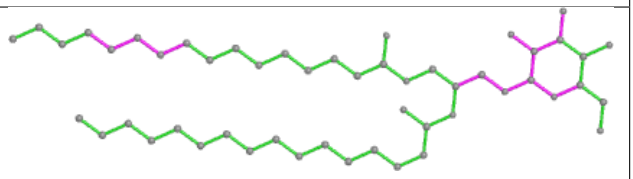


Rings

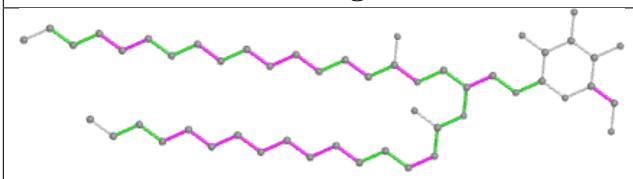
Ligand LMG B 625



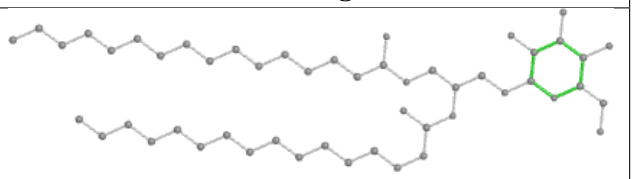
Bond lengths



Bond angles

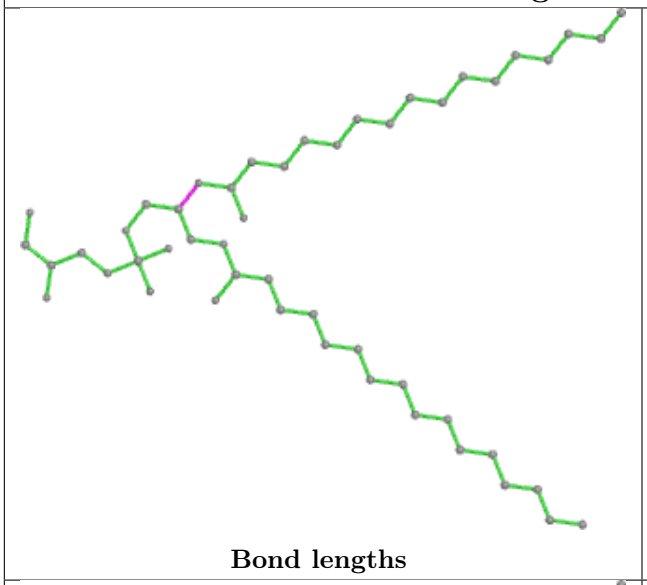


Torsions

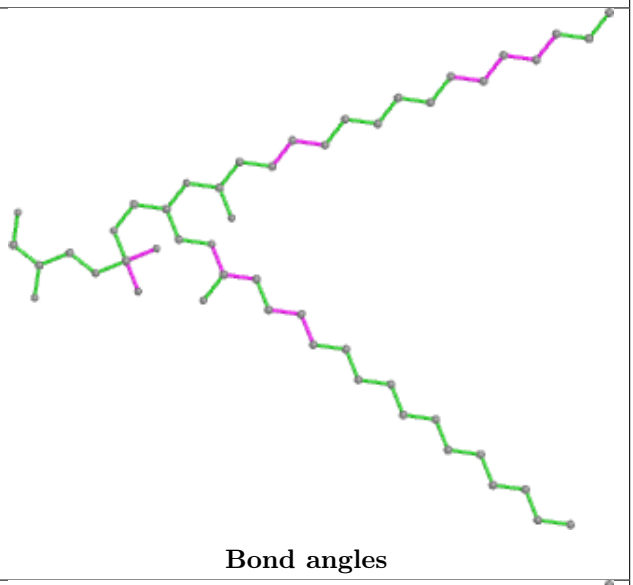


Rings

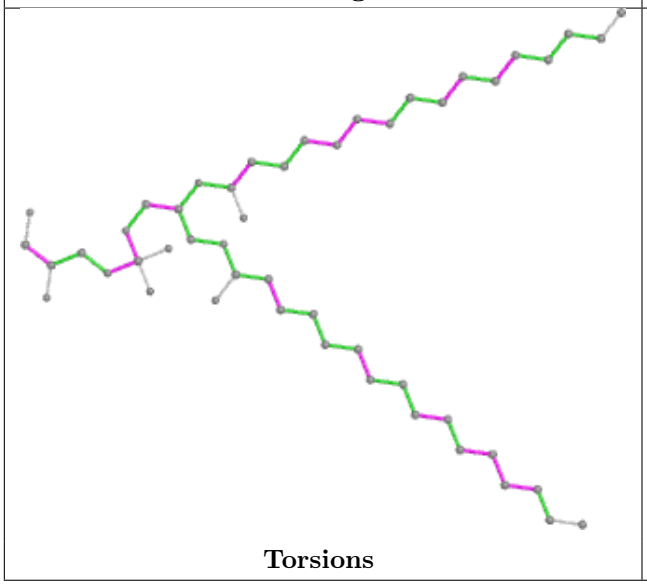
Ligand LHG l 101



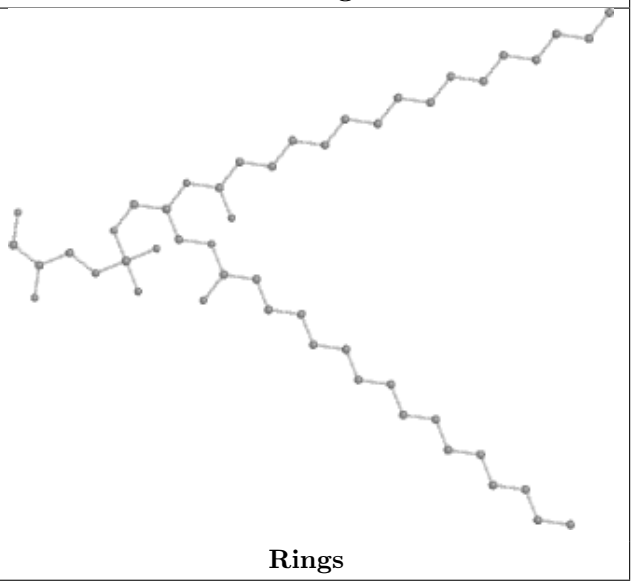
Bond lengths



Bond angles

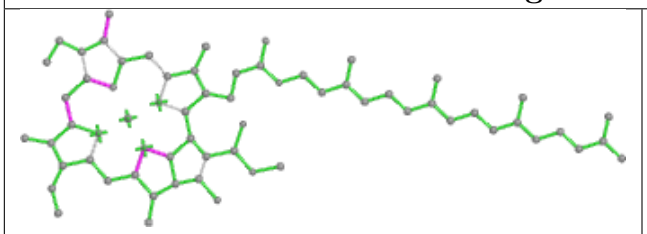


Torsions

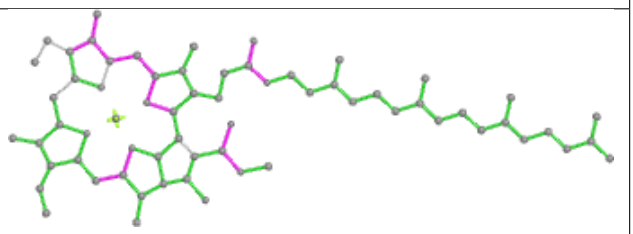


Rings

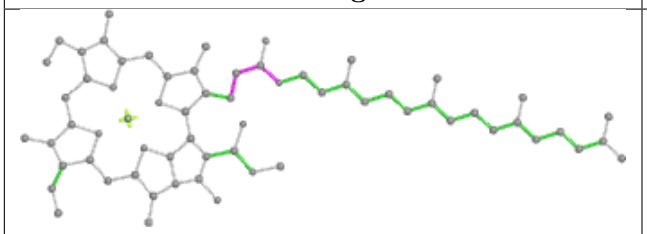
Ligand CLA C 501



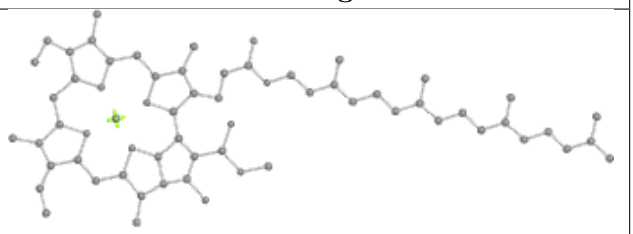
Bond lengths



Bond angles

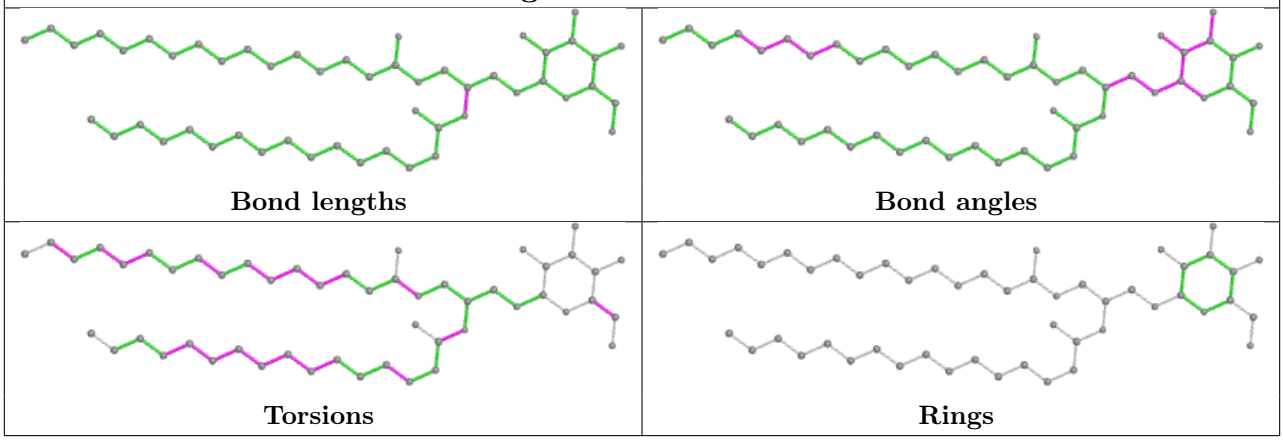


Torsions

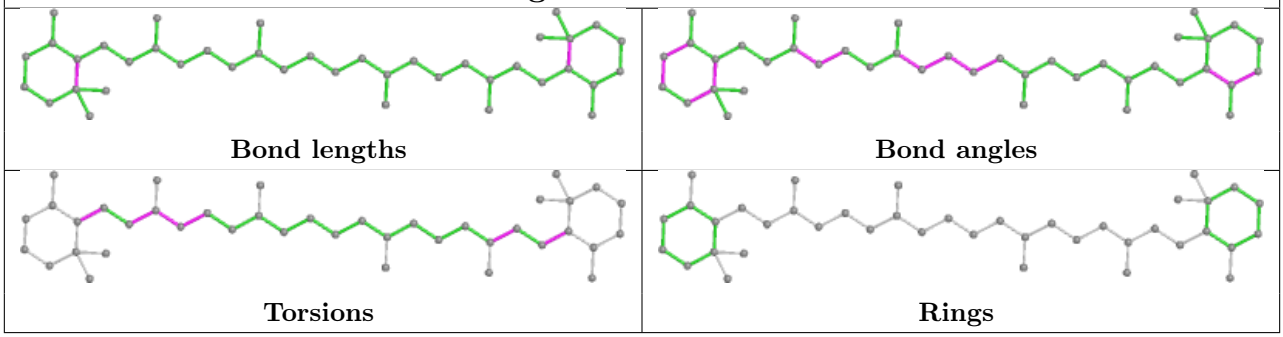


Rings

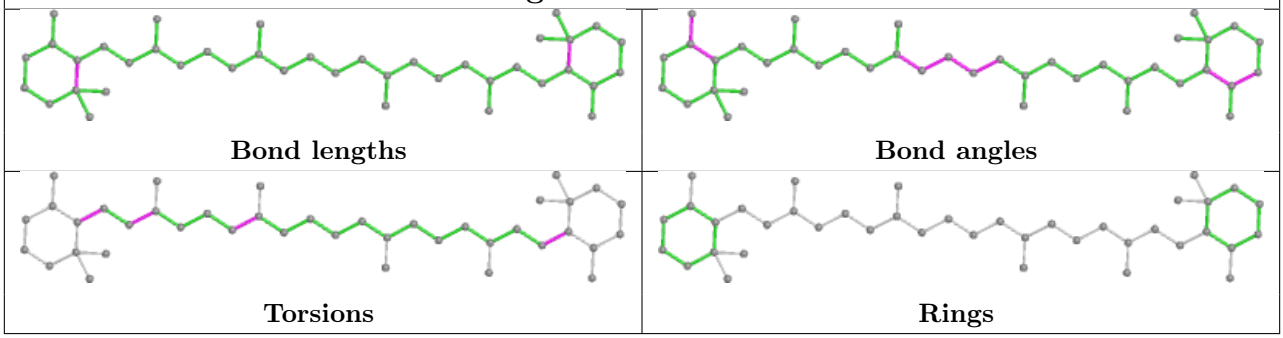
Ligand LMG C 519



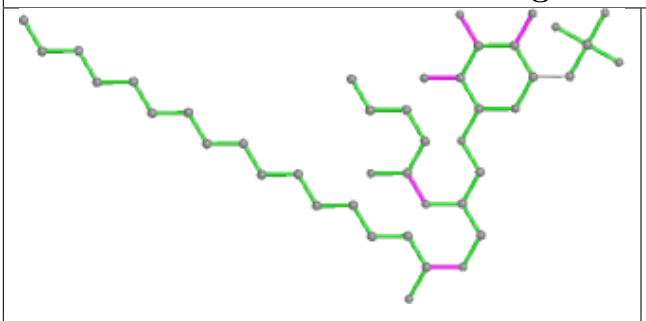
Ligand BCR c 516



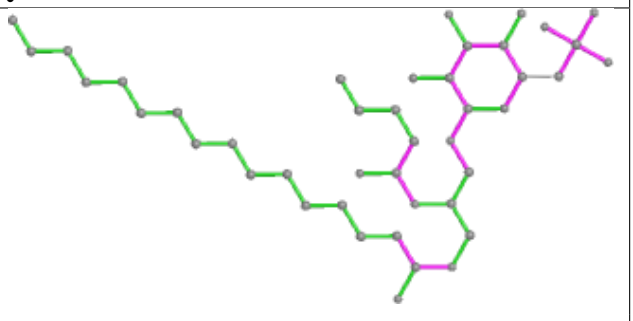
Ligand BCR b 621



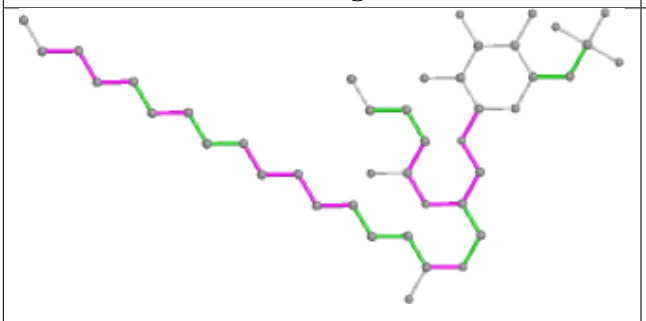
Ligand SQD f 101



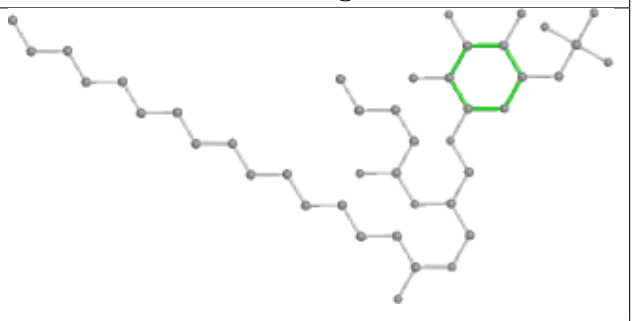
Bond lengths



Bond angles



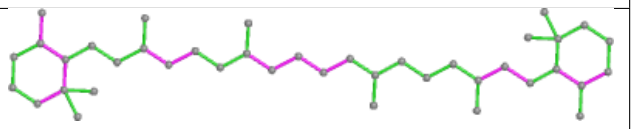
Torsions



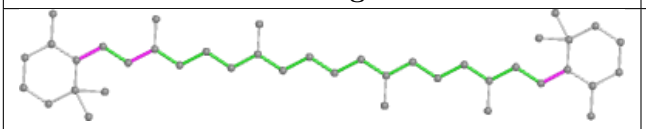
Rings

Ligand BCR H 102

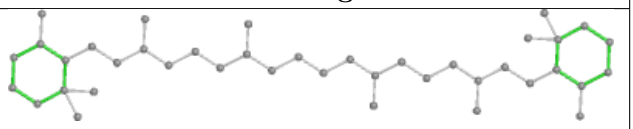
Bond lengths



Bond angles



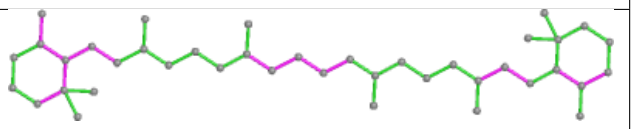
Torsions



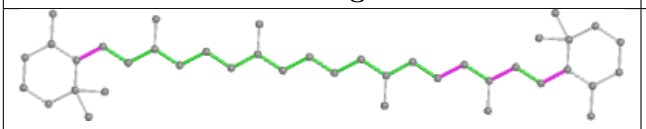
Rings

Ligand BCR K 101

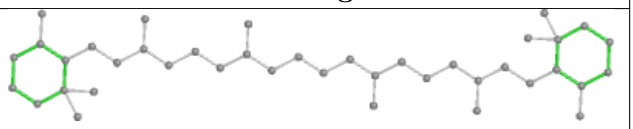
Bond lengths



Bond angles

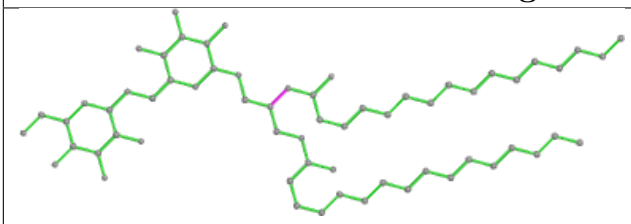


Torsions

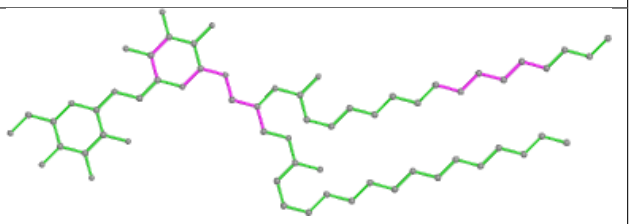


Rings

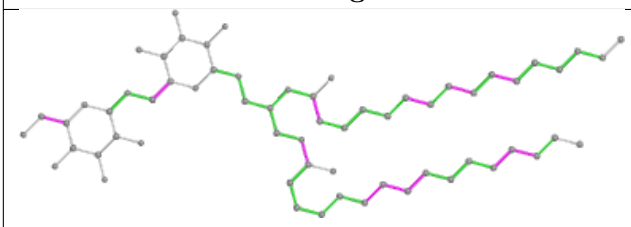
Ligand DGD H 103



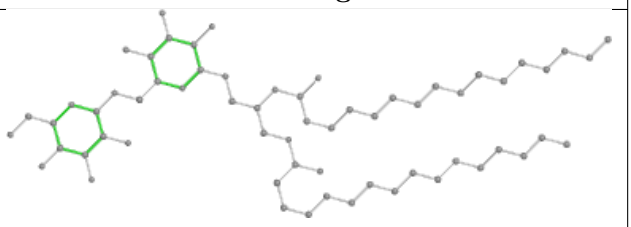
Bond lengths



Bond angles

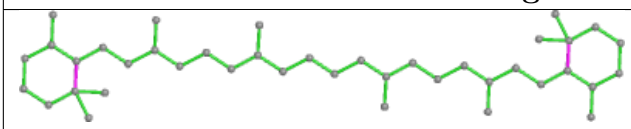


Torsions

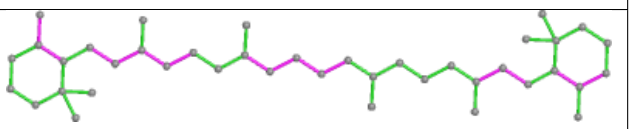


Rings

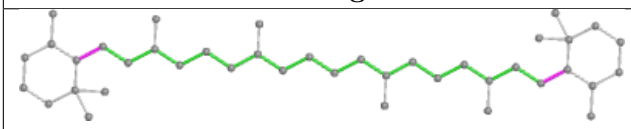
Ligand BCR C 514



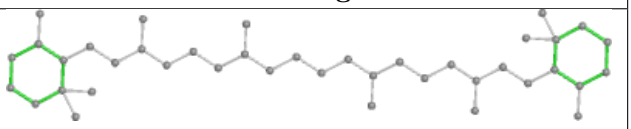
Bond lengths



Bond angles

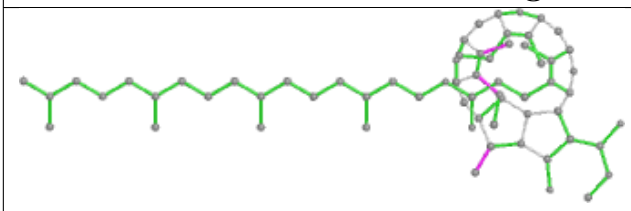


Torsions

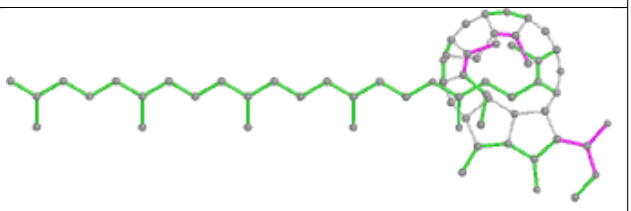


Rings

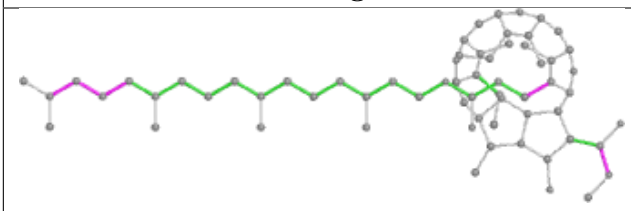
Ligand PHO d 401



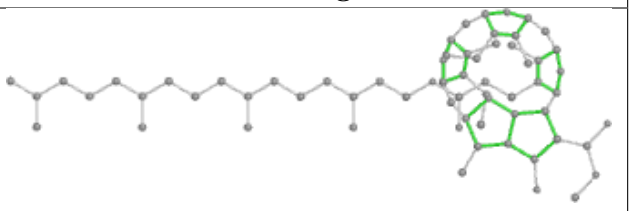
Bond lengths



Bond angles

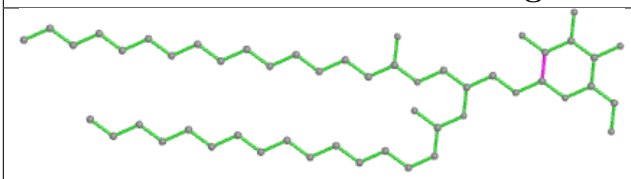


Torsions

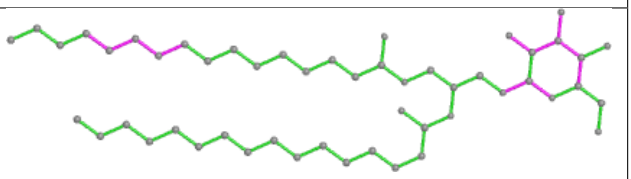


Rings

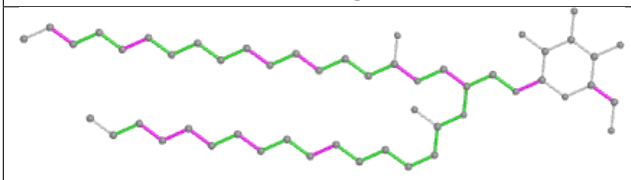
Ligand LMG c 522



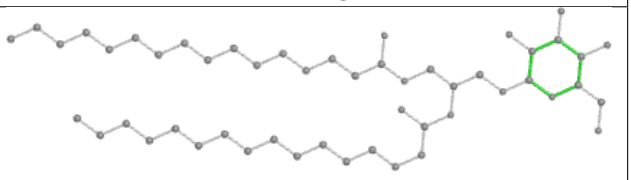
Bond lengths



Bond angles

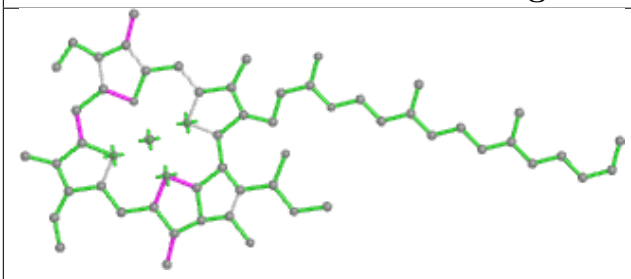


Torsions

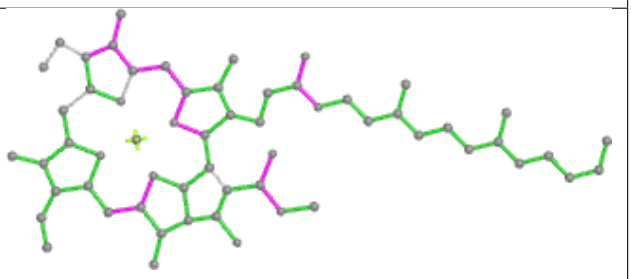


Rings

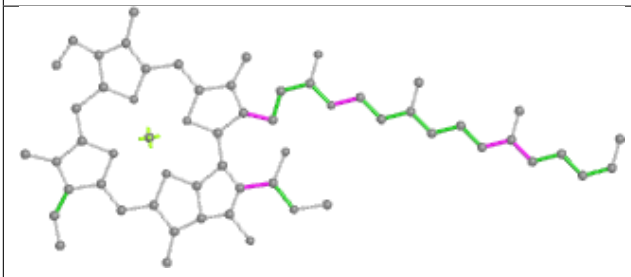
Ligand CLA a 607



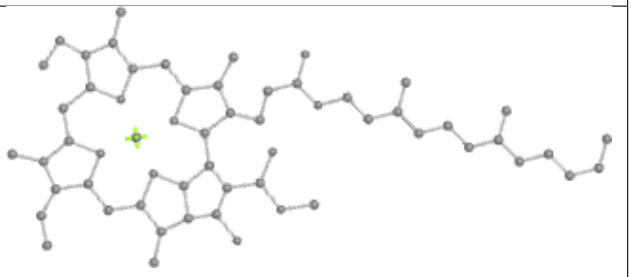
Bond lengths



Bond angles

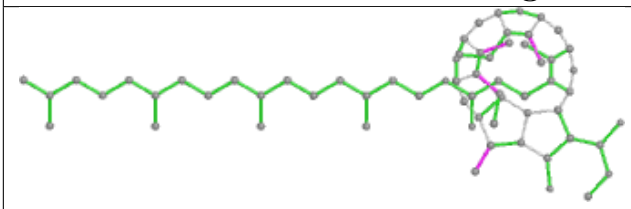


Torsions

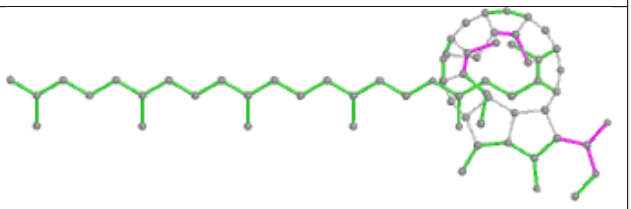


Rings

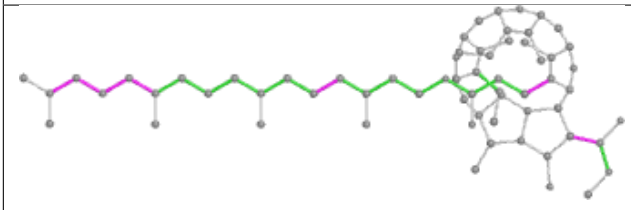
Ligand PHO A 608



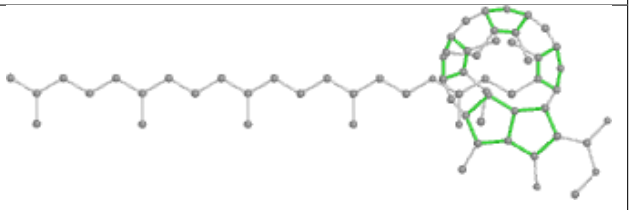
Bond lengths



Bond angles

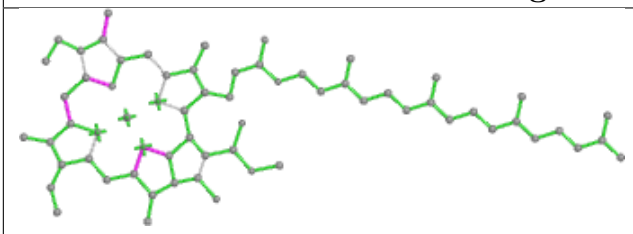


Torsions

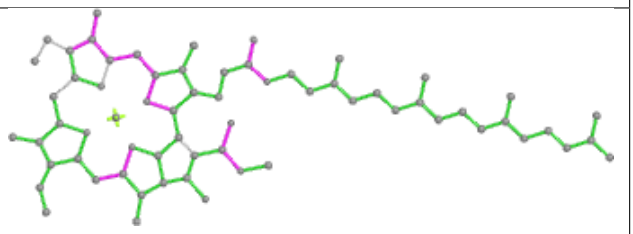


Rings

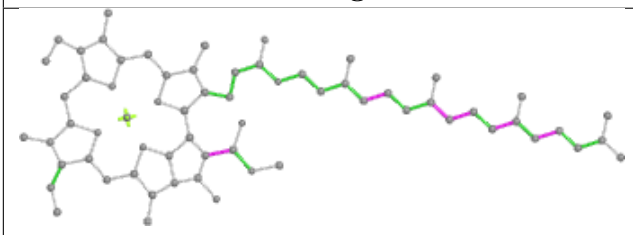
Ligand CLA c 511



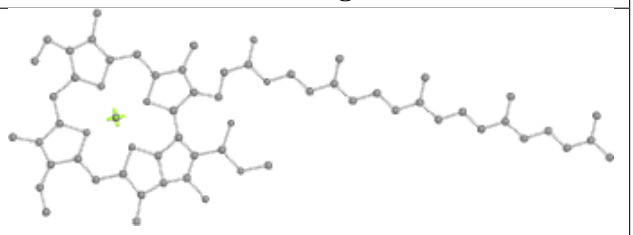
Bond lengths



Bond angles

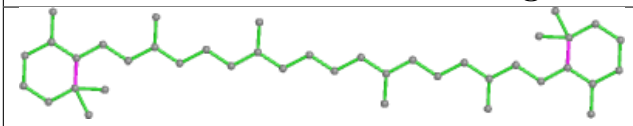


Torsions

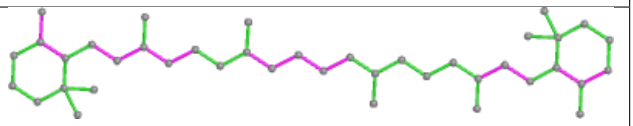


Rings

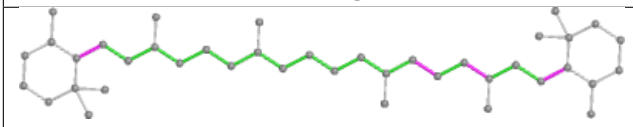
Ligand BCR C 515



Bond lengths



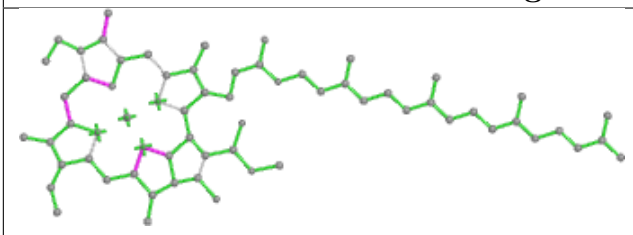
Bond angles



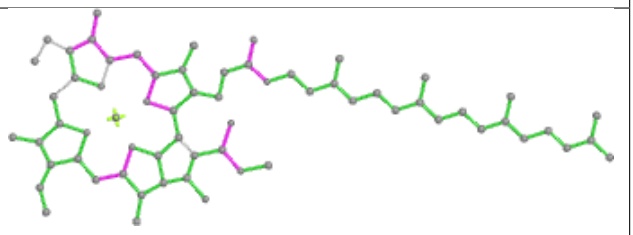
Torsions

Rings

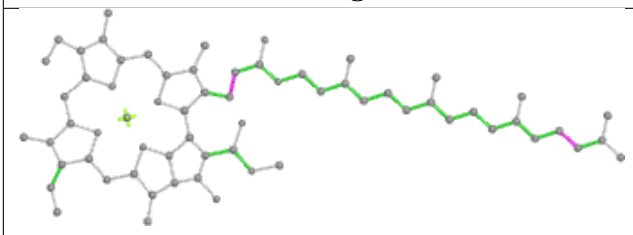
Ligand CLA B 608



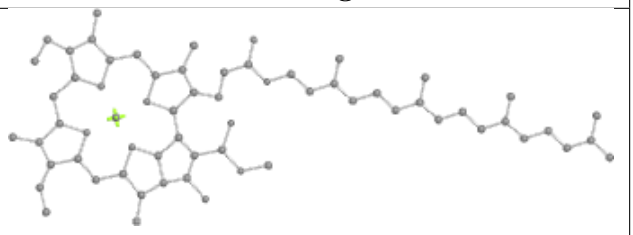
Bond lengths



Bond angles

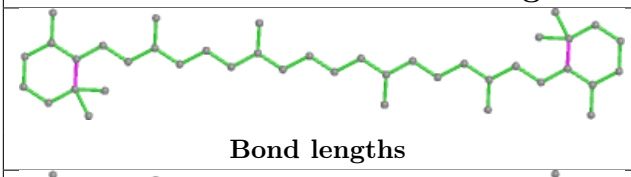


Torsions

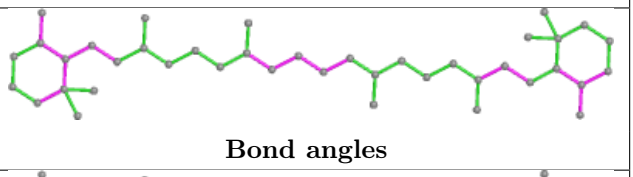


Rings

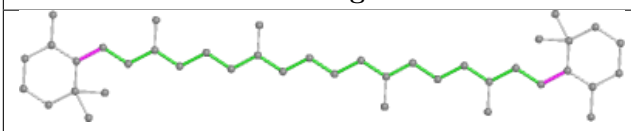
Ligand BCR B 619



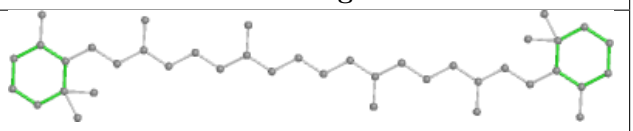
Bond lengths



Bond angles

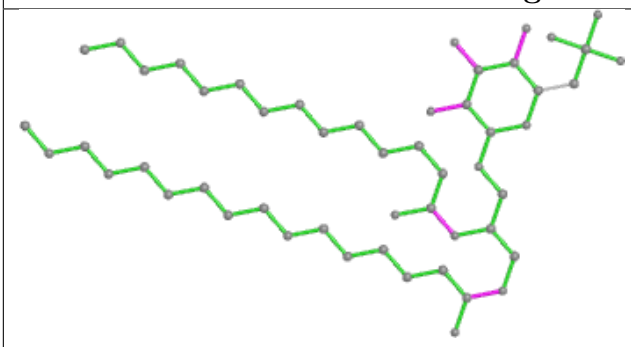


Torsions

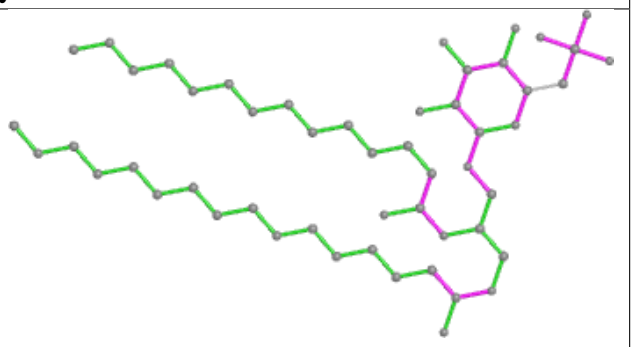


Rings

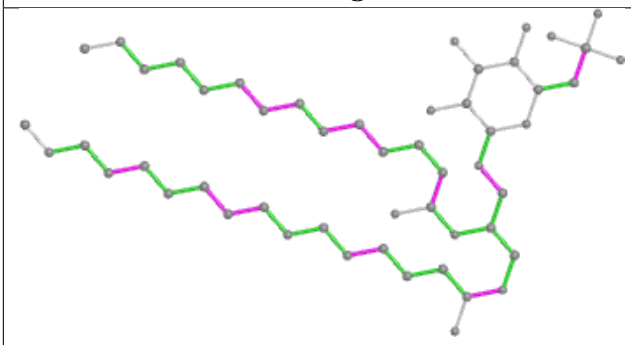
Ligand SQD A 603



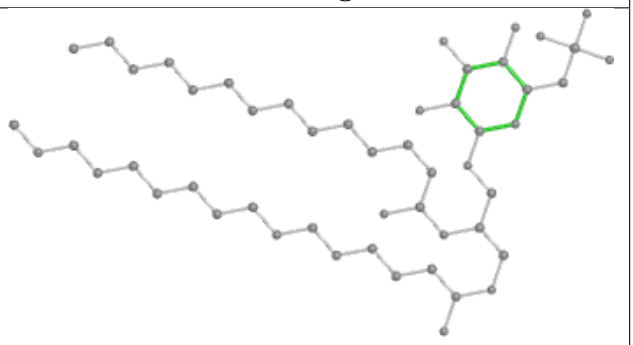
Bond lengths



Bond angles

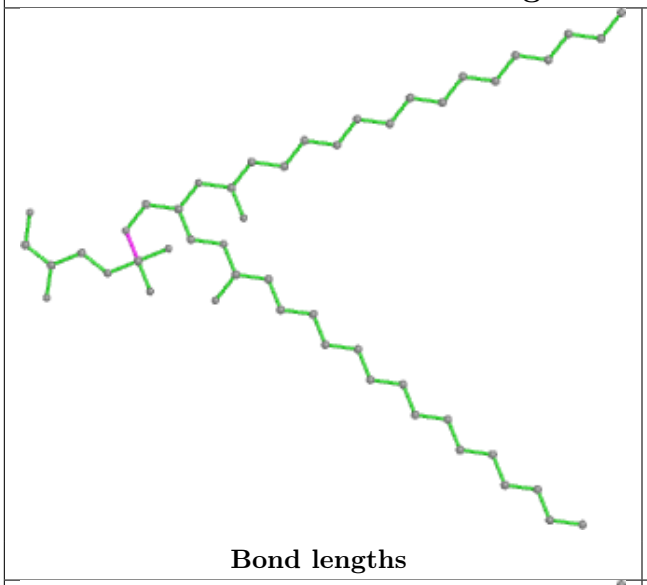


Torsions

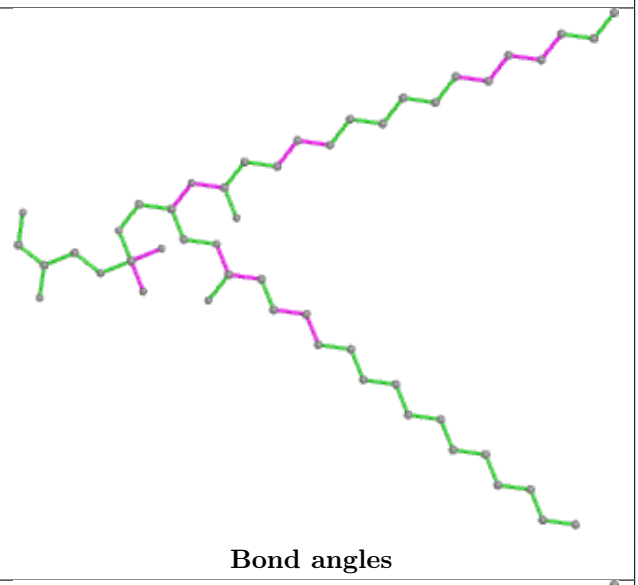


Rings

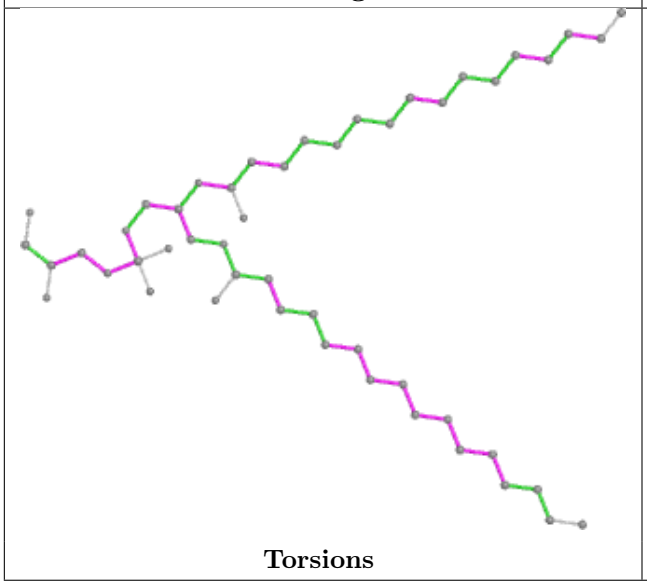
Ligand LHG A 618



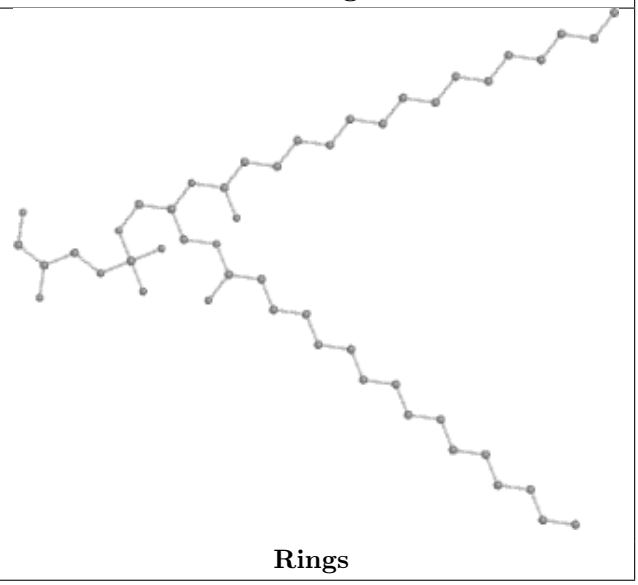
Bond lengths



Bond angles

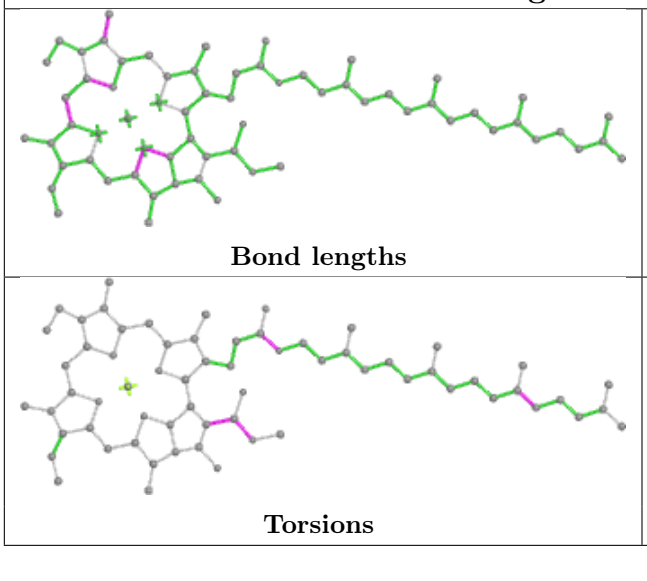


Torsions

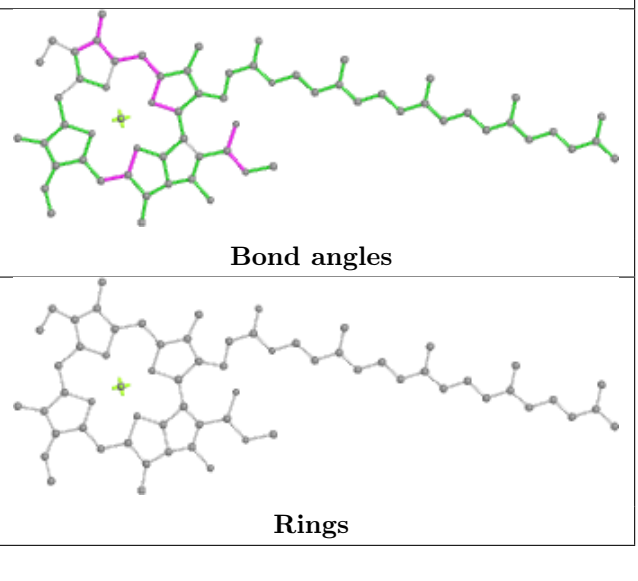


Rings

Ligand CLA b 610



Bond lengths

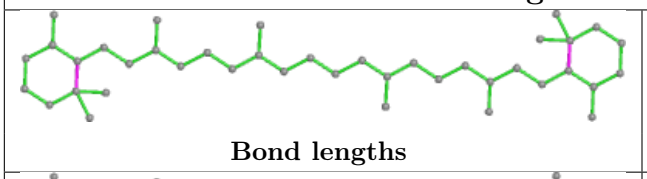


Bond angles

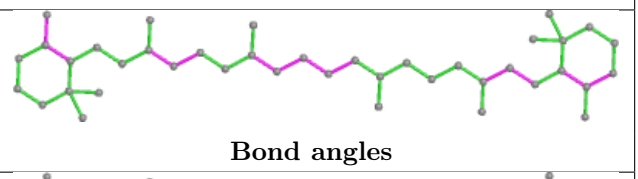
Torsions

Rings

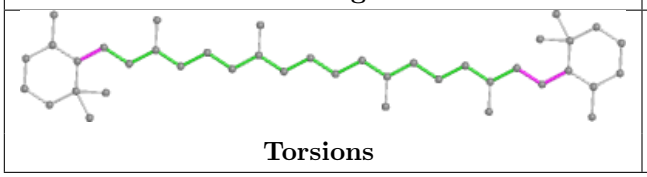
Ligand BCR b 620



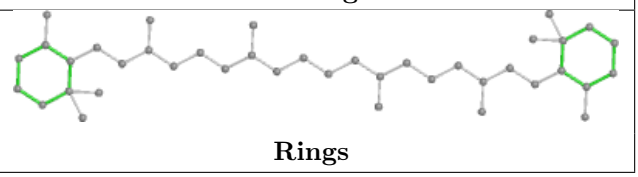
Bond lengths



Bond angles

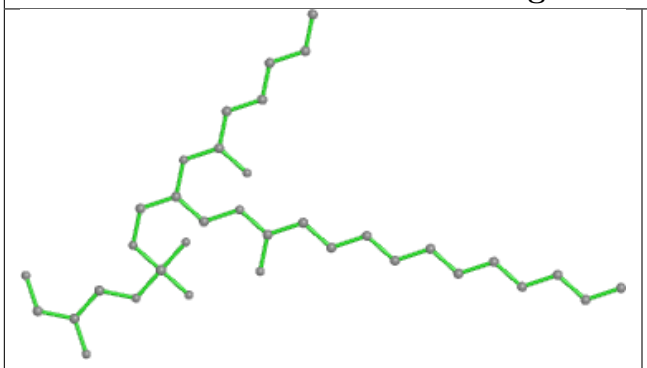


Torsions

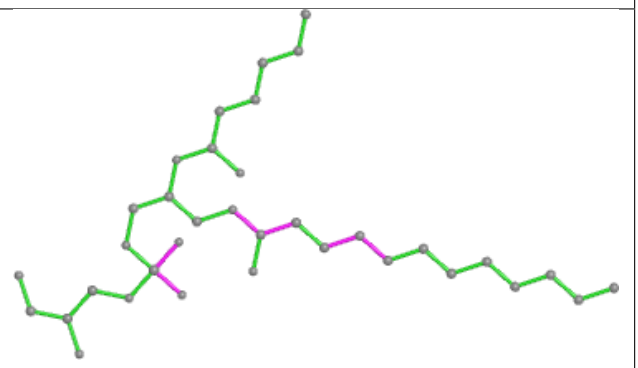


Rings

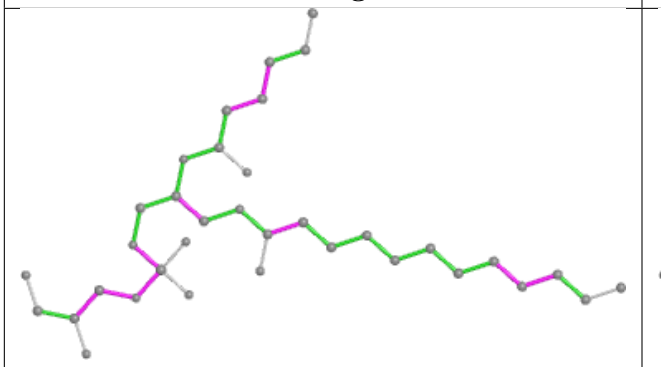
Ligand LHG a 614



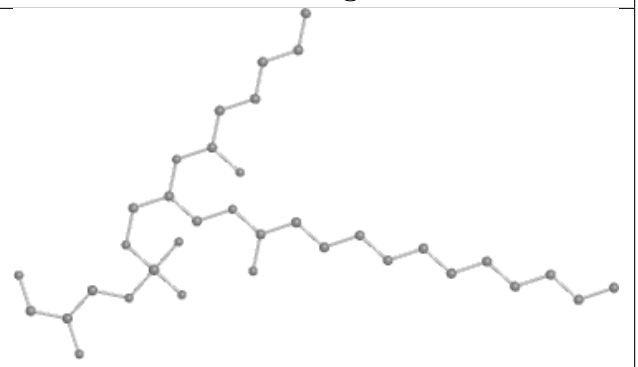
Bond lengths



Bond angles

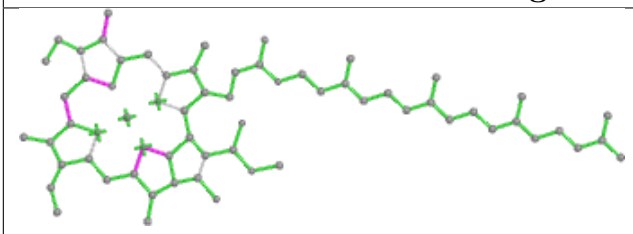


Torsions

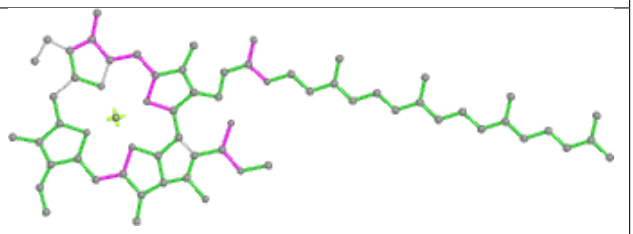


Rings

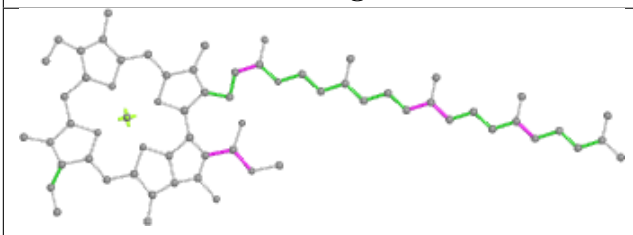
Ligand CLA c 514



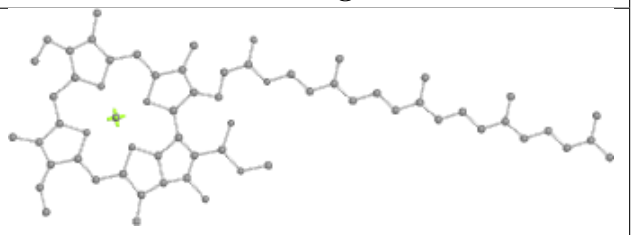
Bond lengths



Bond angles

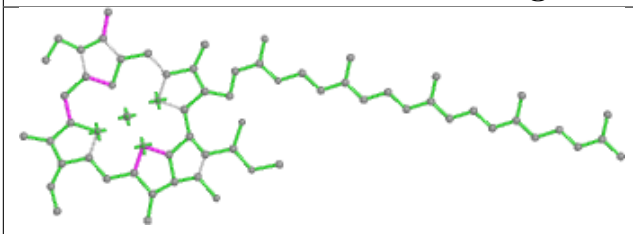


Torsions

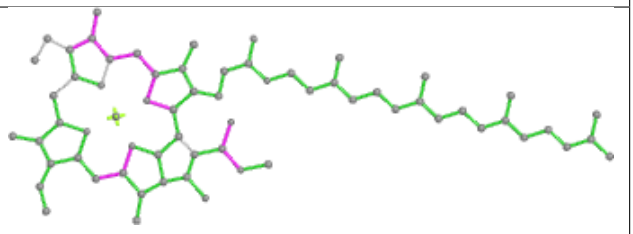


Rings

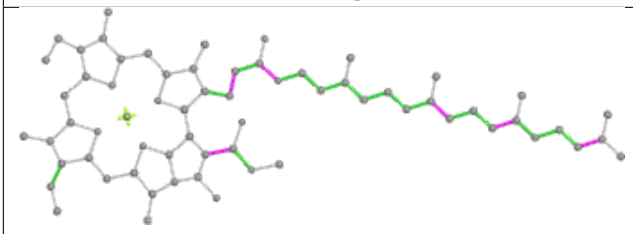
Ligand CLA c 509



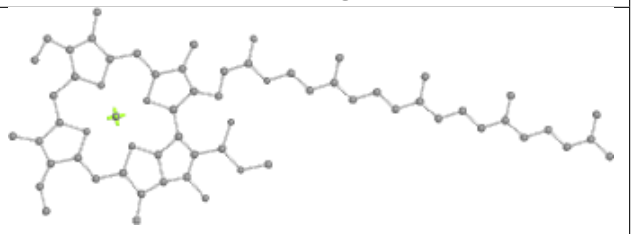
Bond lengths



Bond angles

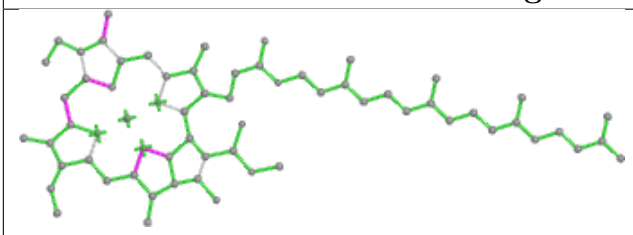


Torsions

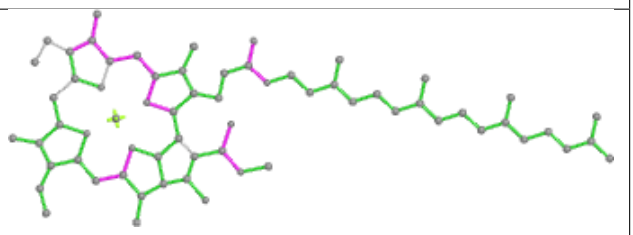


Rings

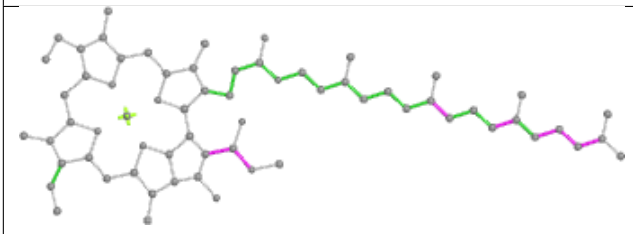
Ligand CLA B 610



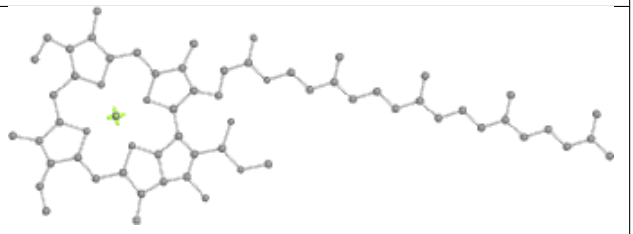
Bond lengths



Bond angles

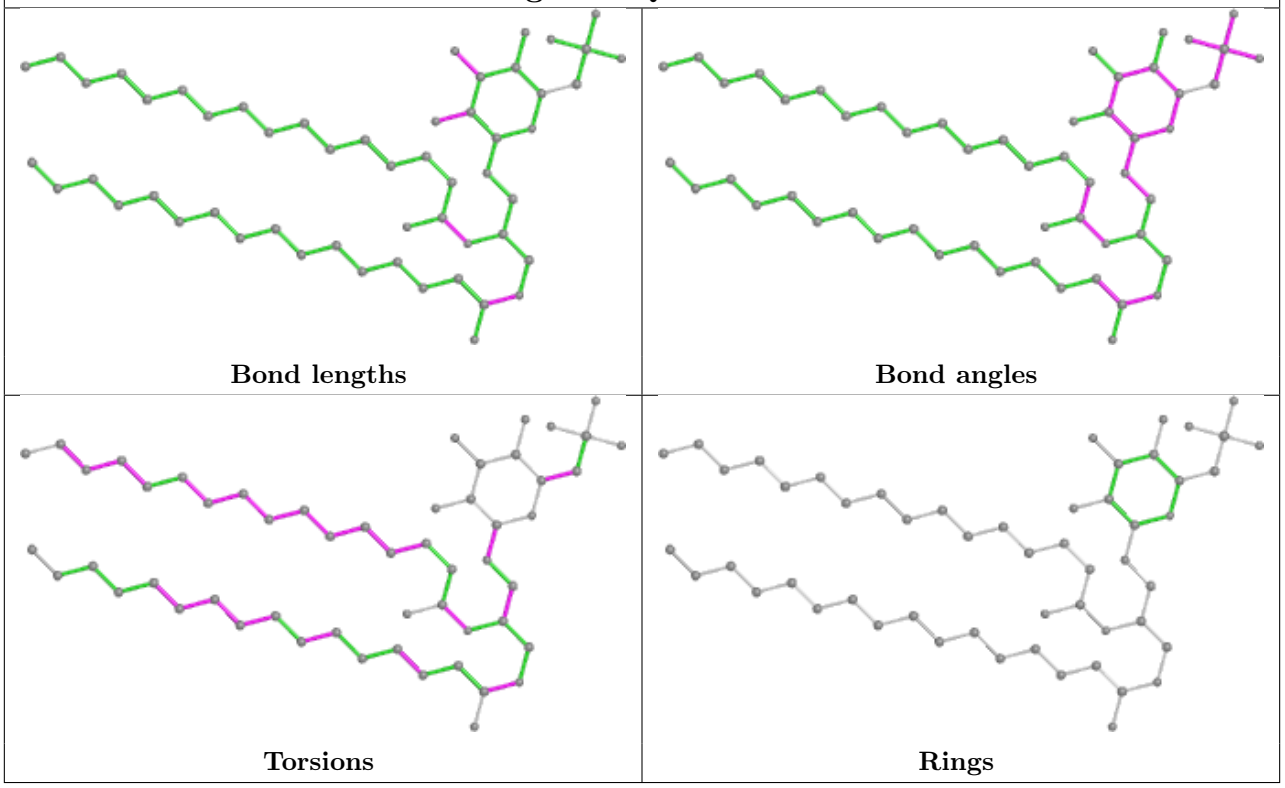


Torsions

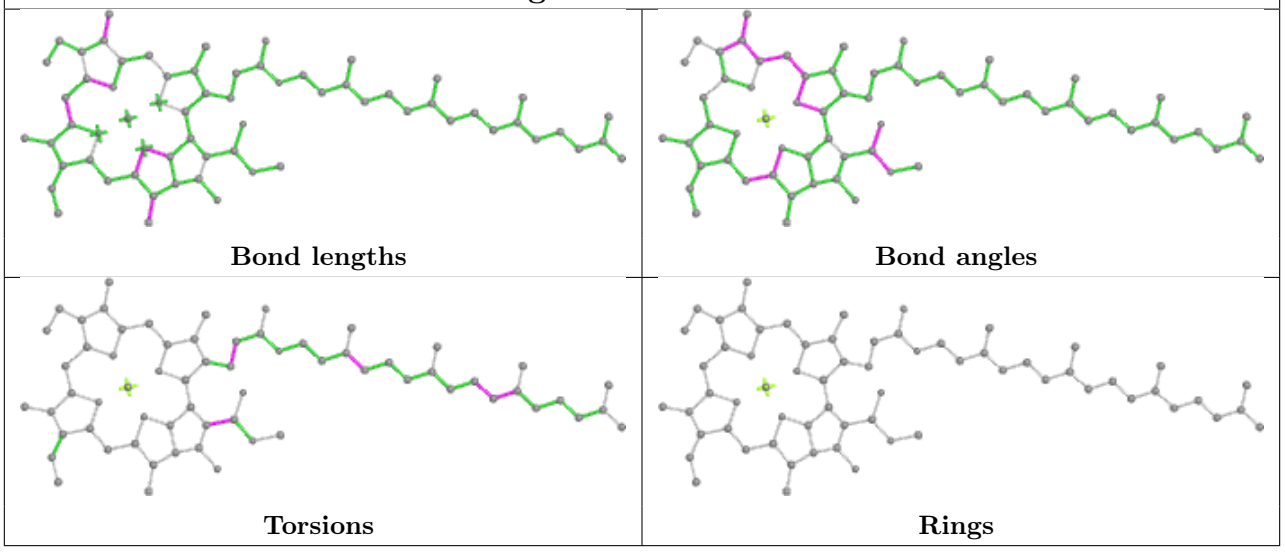


Rings

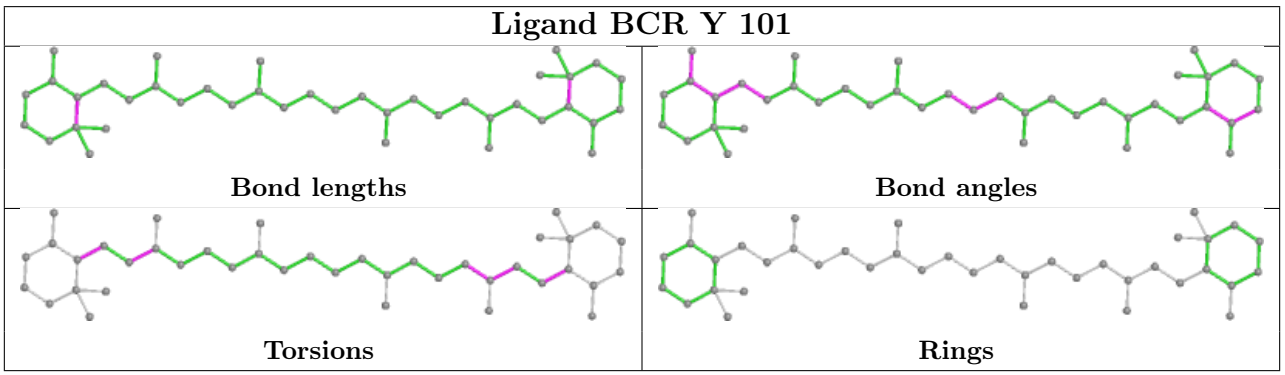
Ligand SQD B 626



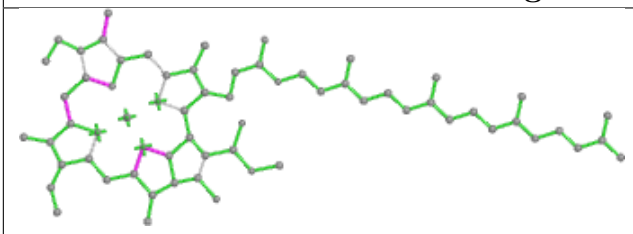
Ligand CLA b 617



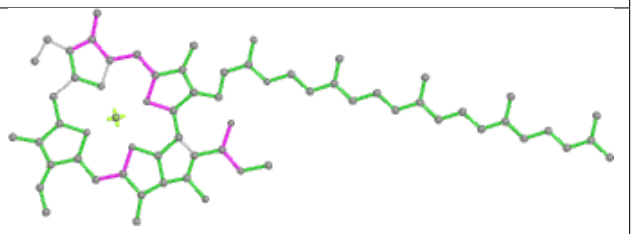
Ligand BCR Y 101



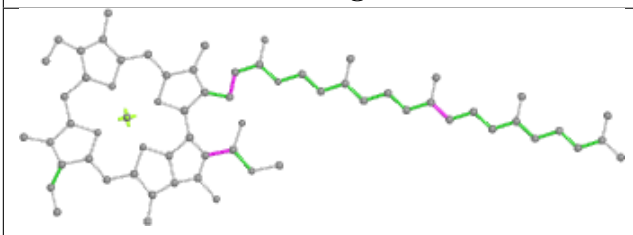
Ligand CLA C 507



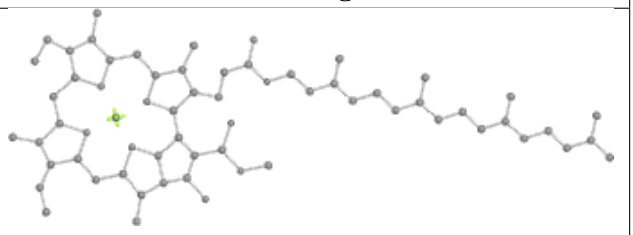
Bond lengths



Bond angles

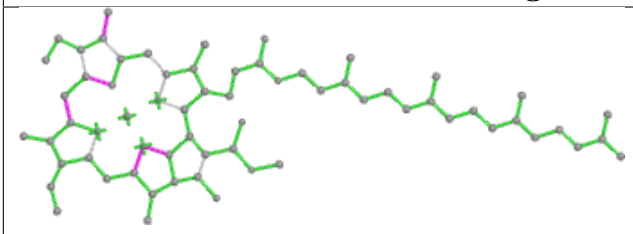


Torsions

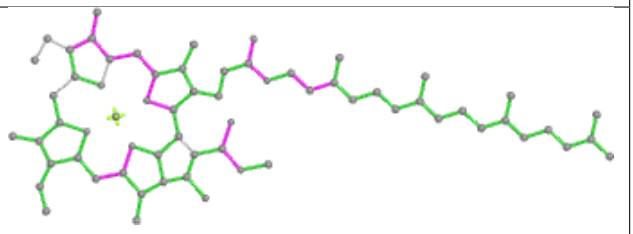


Rings

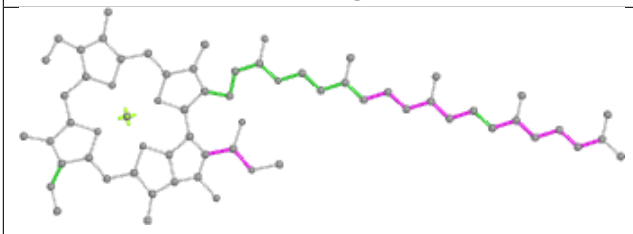
Ligand CLA C 506



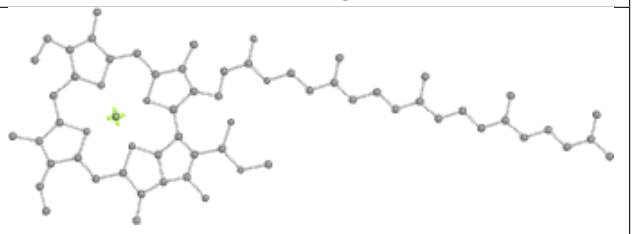
Bond lengths



Bond angles

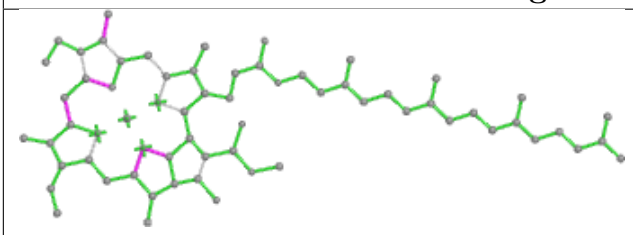


Torsions

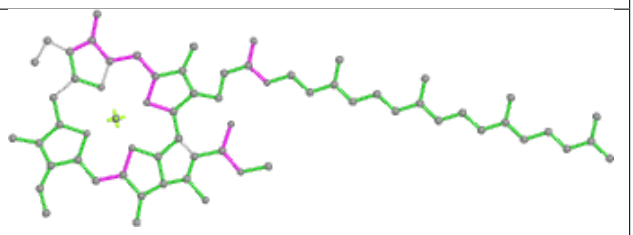


Rings

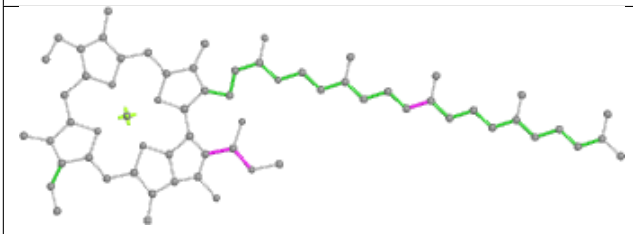
Ligand CLA c 515



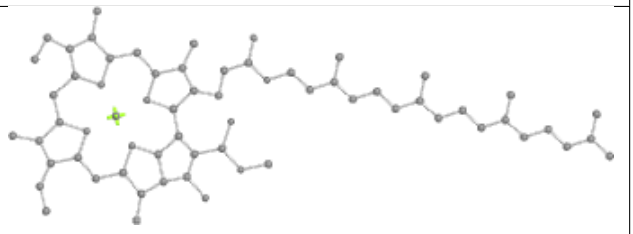
Bond lengths



Bond angles

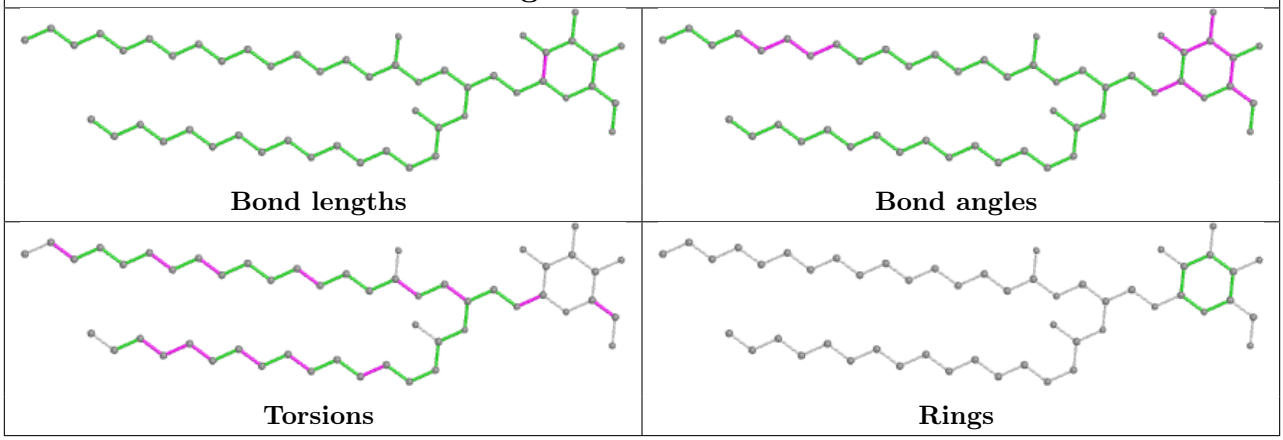


Torsions

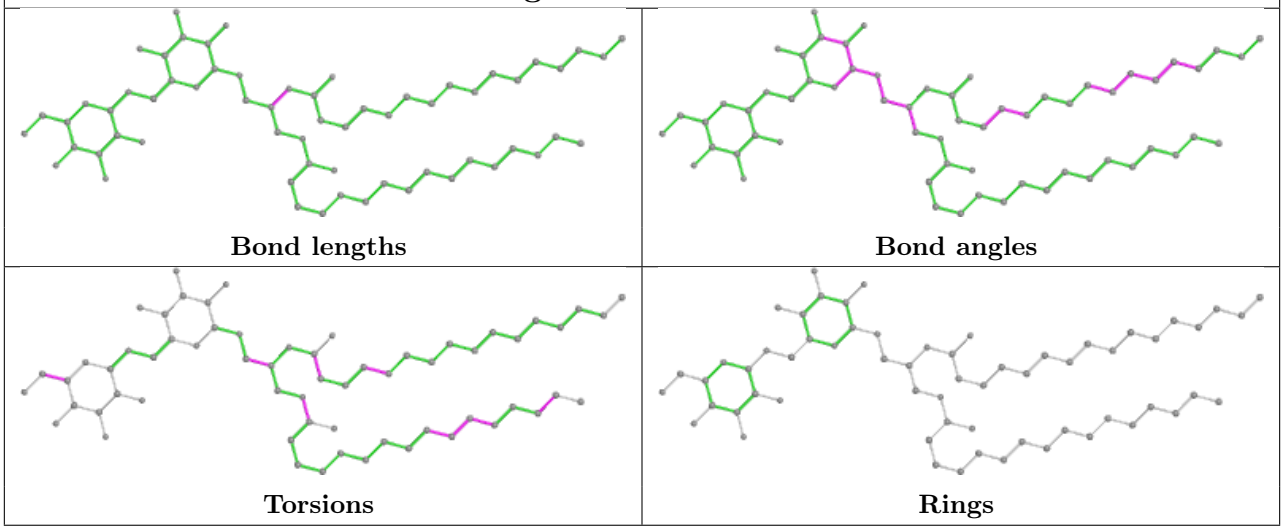


Rings

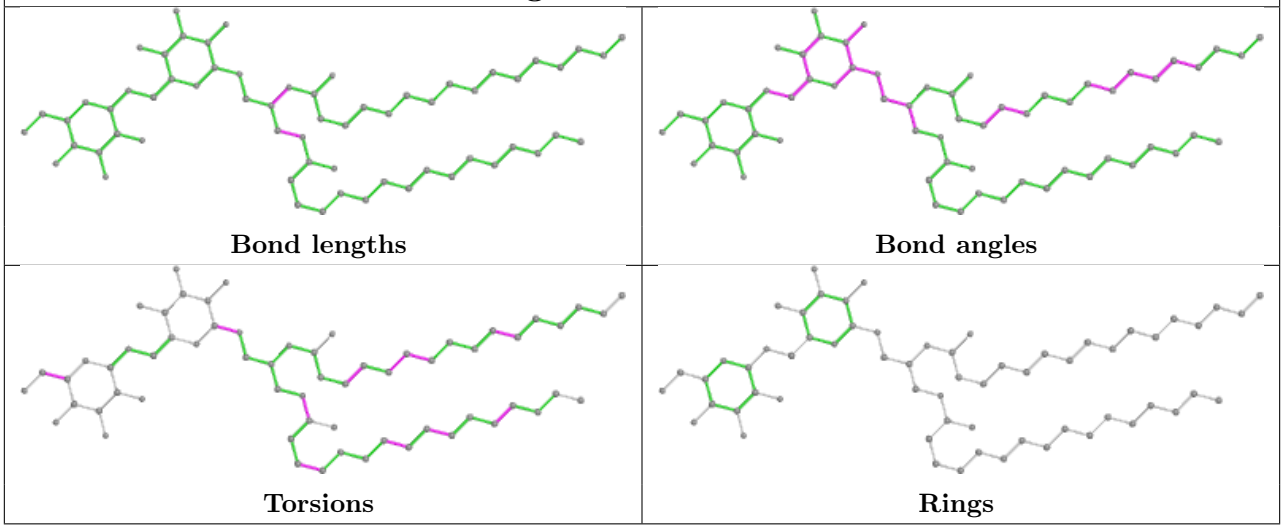
Ligand LMG C 520



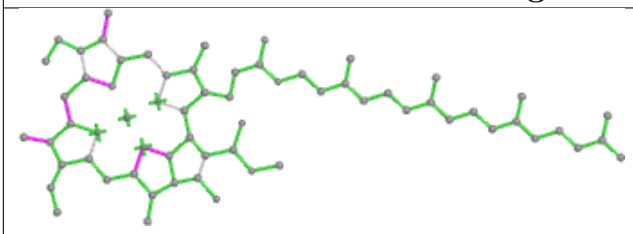
Ligand DGD h 102



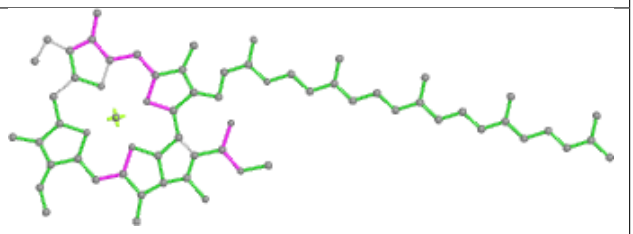
Ligand DGD c 520



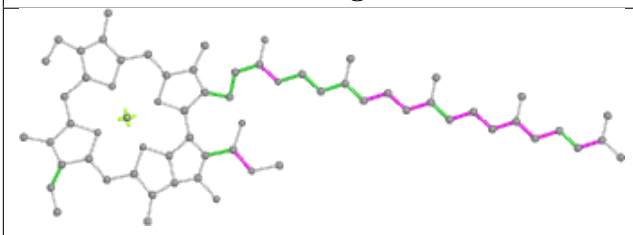
Ligand CLA b 619



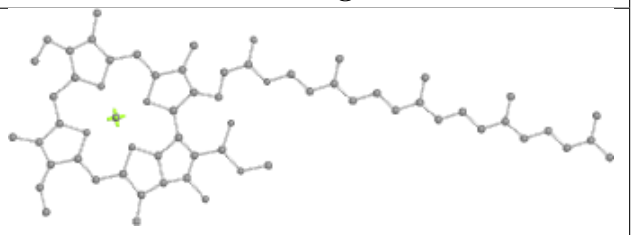
Bond lengths



Bond angles

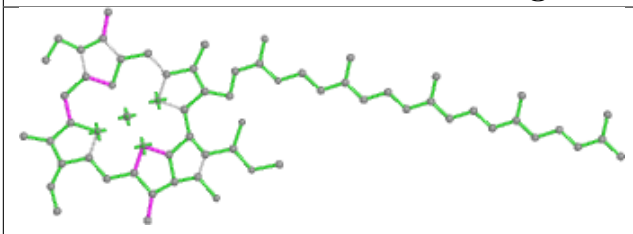


Torsions

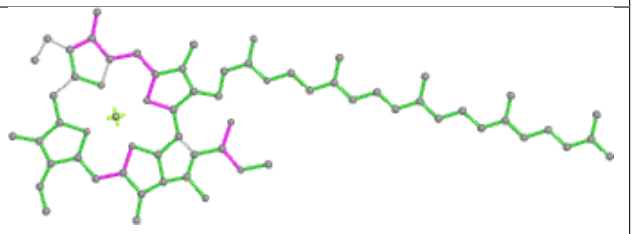


Rings

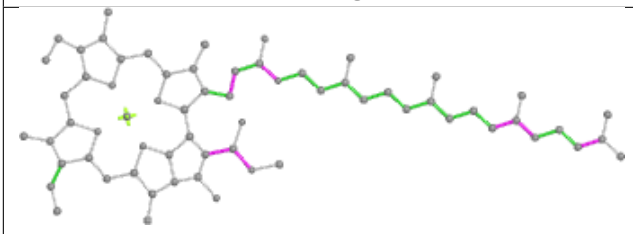
Ligand CLA c 507



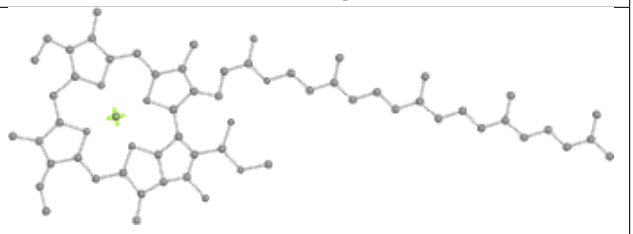
Bond lengths



Bond angles

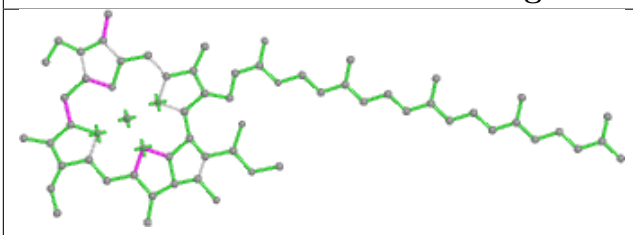


Torsions

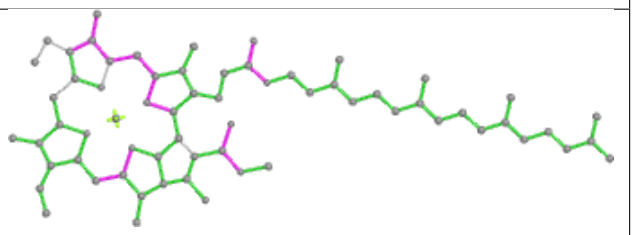


Rings

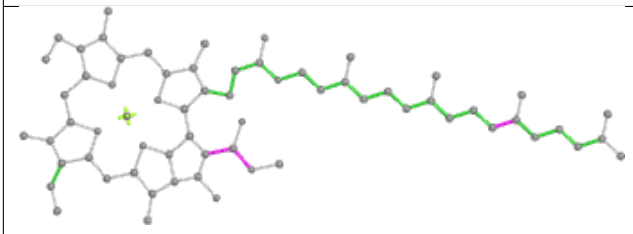
Ligand CLA C 502



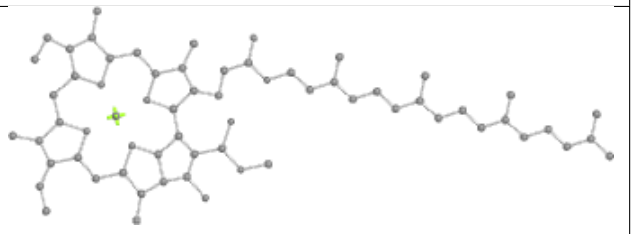
Bond lengths



Bond angles

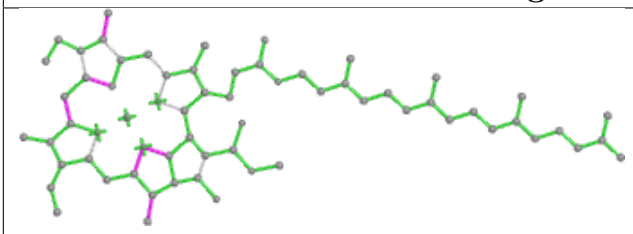


Torsions

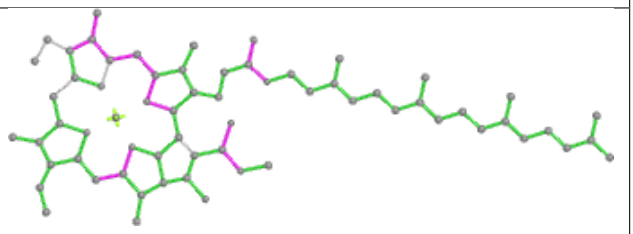


Rings

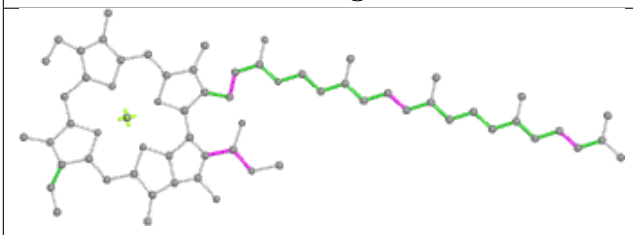
Ligand CLA b 606



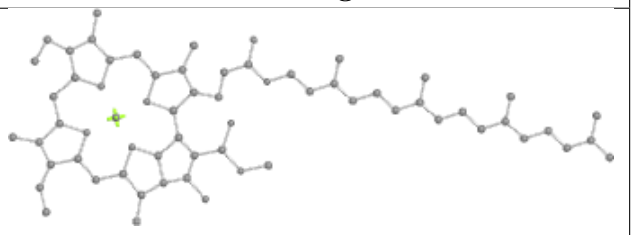
Bond lengths



Bond angles

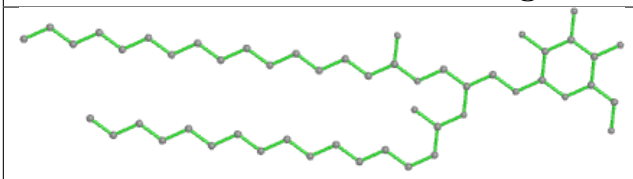


Torsions

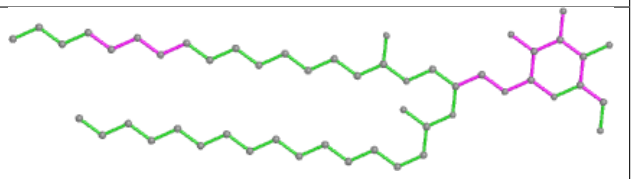


Rings

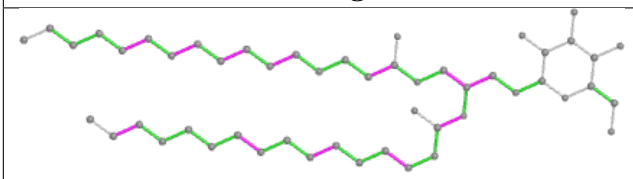
Ligand LMG A 613



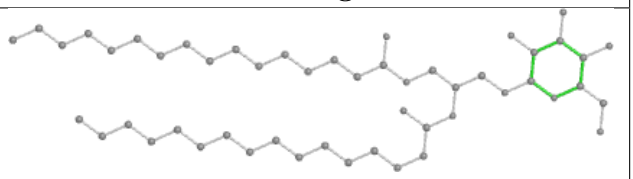
Bond lengths



Bond angles

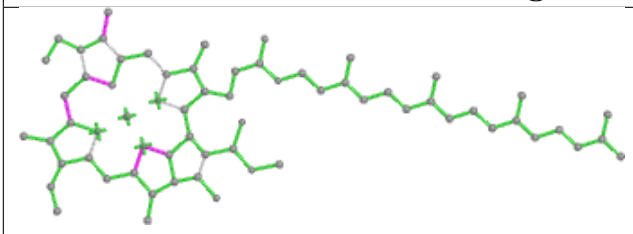


Torsions

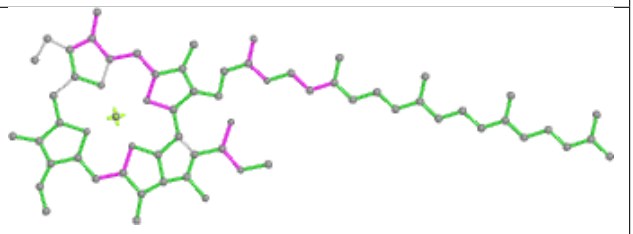


Rings

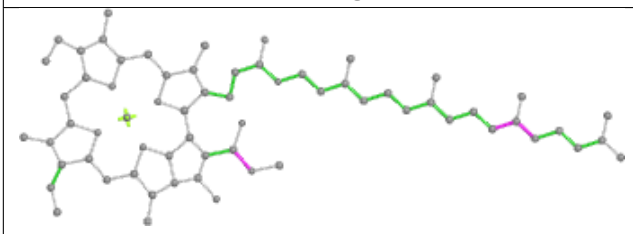
Ligand CLA b 614



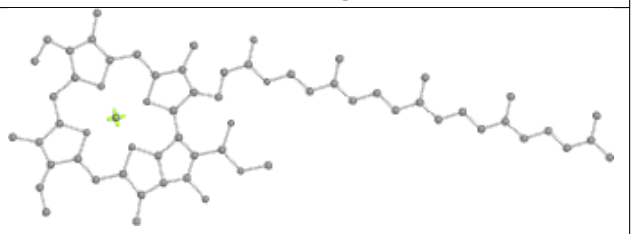
Bond lengths



Bond angles

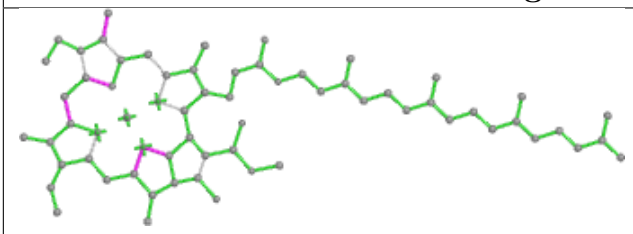


Torsions

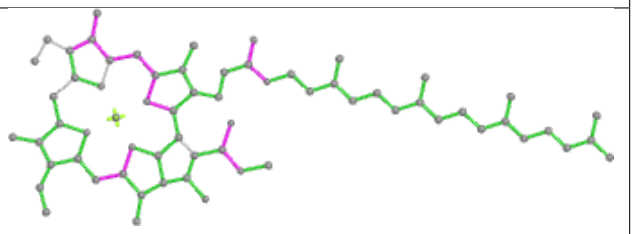


Rings

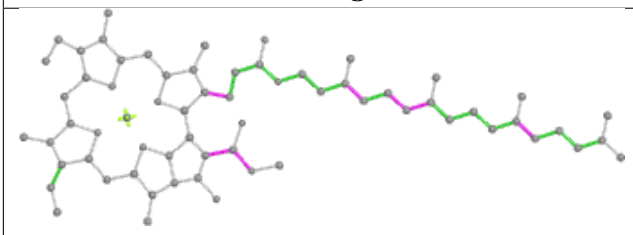
Ligand CLA B 609



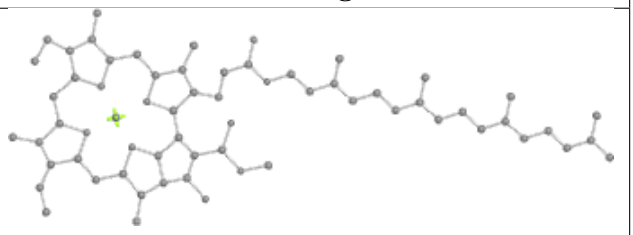
Bond lengths



Bond angles

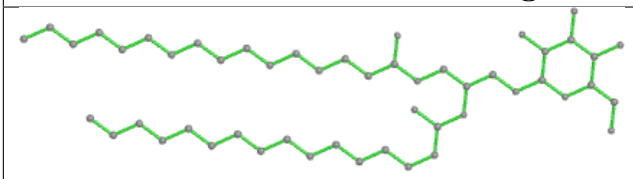


Torsions

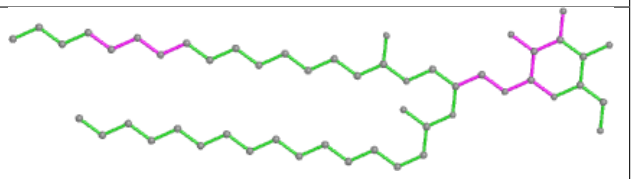


Rings

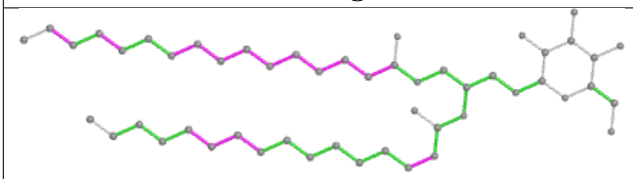
Ligand LMG B 620



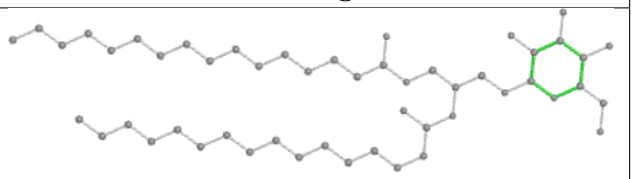
Bond lengths



Bond angles

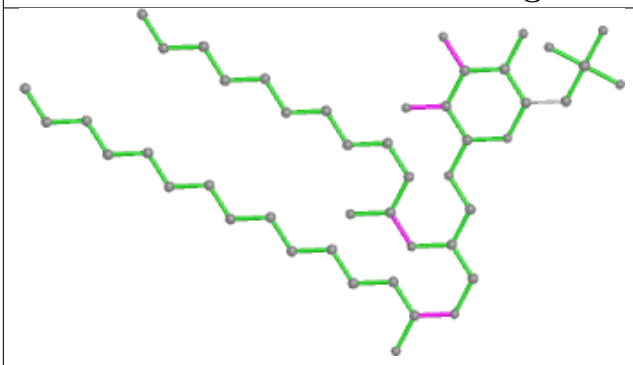


Torsions

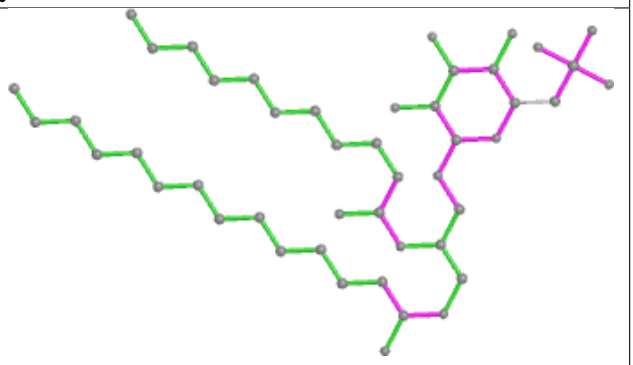


Rings

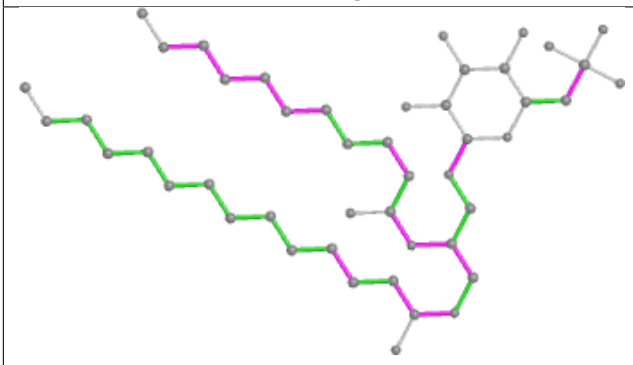
Ligand SQD D 408



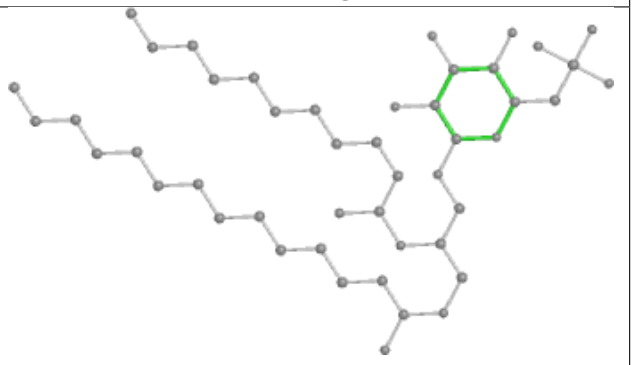
Bond lengths



Bond angles

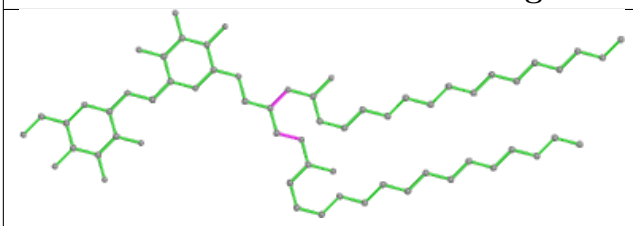


Torsions

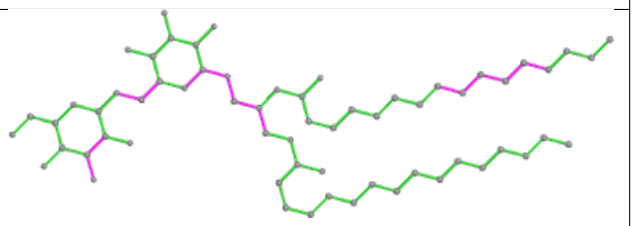


Rings

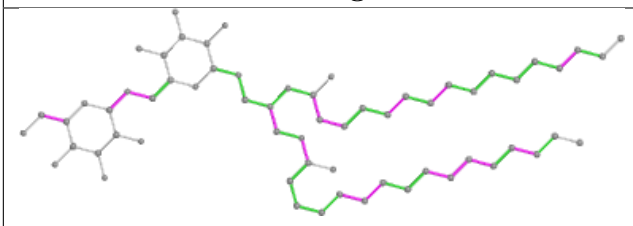
Ligand DGD c 519



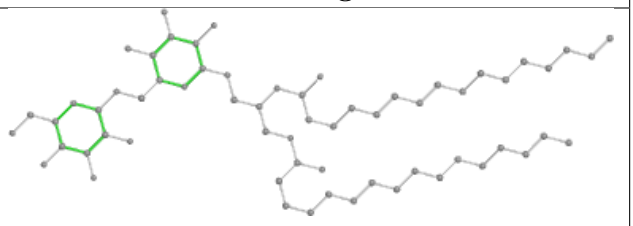
Bond lengths



Bond angles

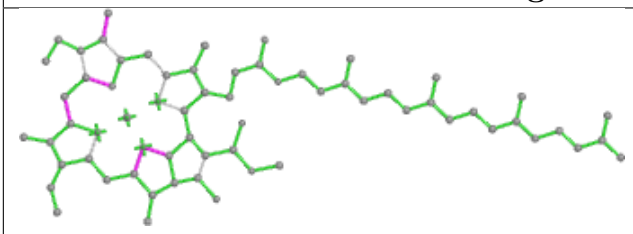


Torsions

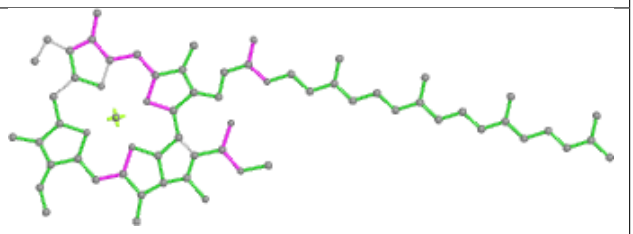


Rings

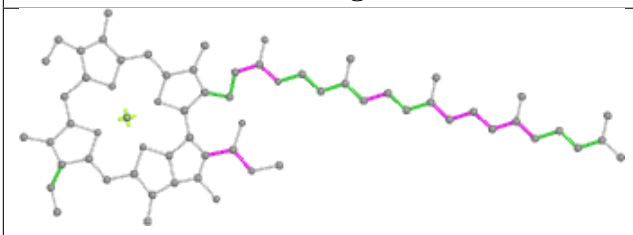
Ligand CLA b 604



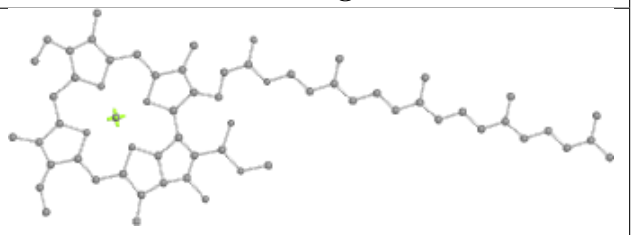
Bond lengths



Bond angles

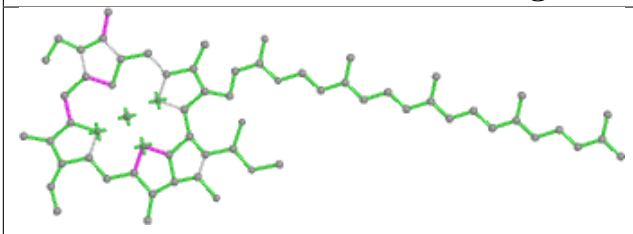


Torsions

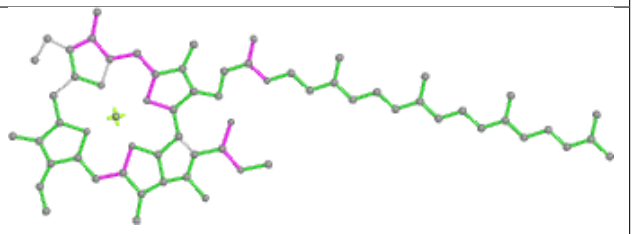


Rings

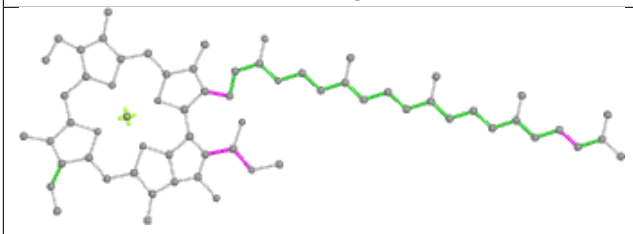
Ligand CLA c 505



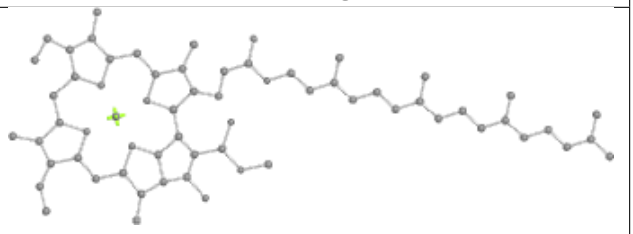
Bond lengths



Bond angles

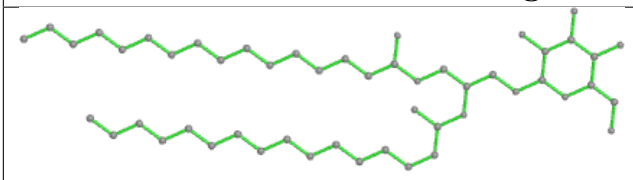


Torsions

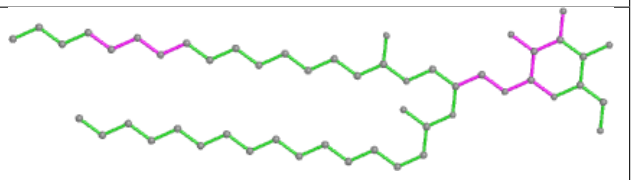


Rings

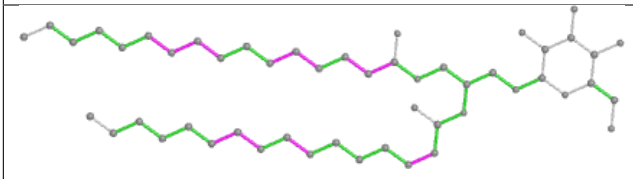
Ligand LMG b 623



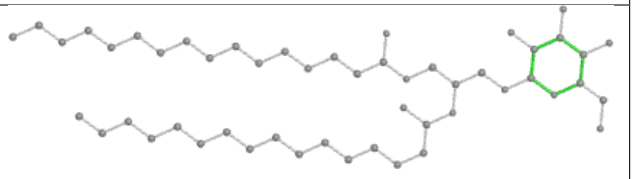
Bond lengths



Bond angles

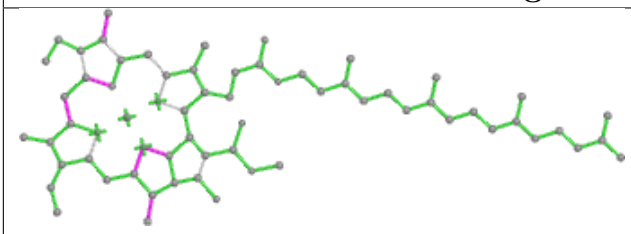


Torsions

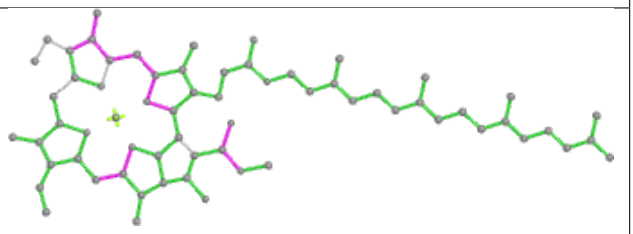


Rings

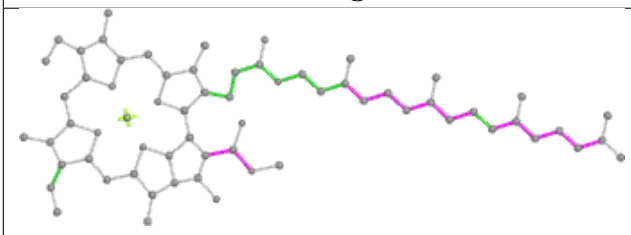
Ligand CLA B 614



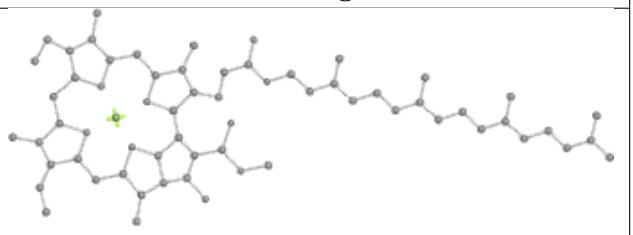
Bond lengths



Bond angles

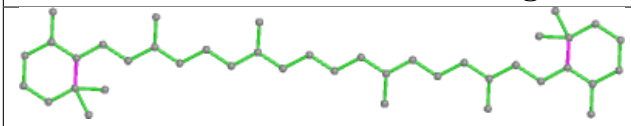


Torsions

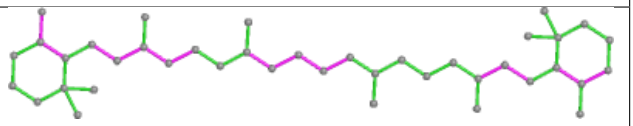


Rings

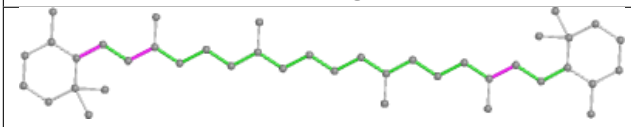
Ligand BCR D 404



Bond lengths



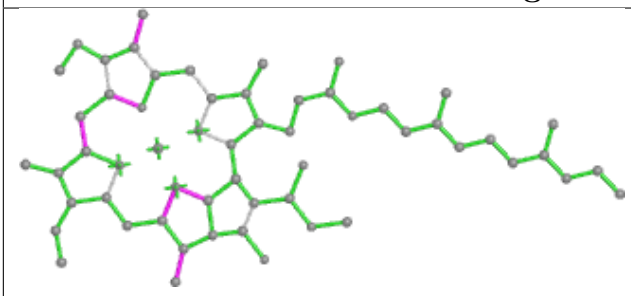
Bond angles



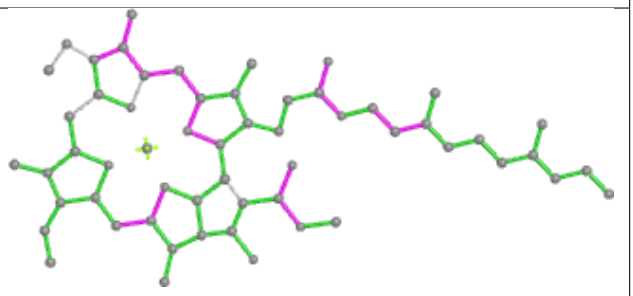
Torsions

Rings

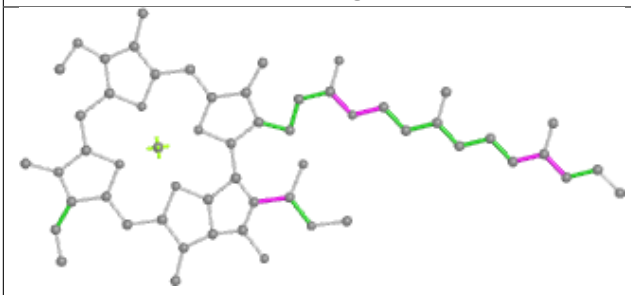
Ligand CLA A 607



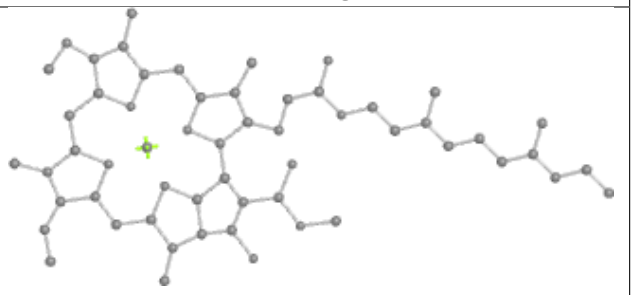
Bond lengths



Bond angles

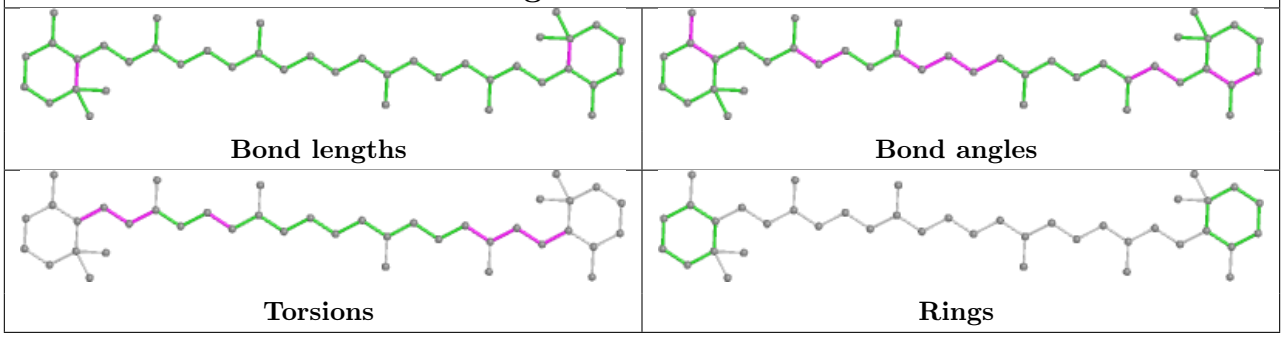


Torsions

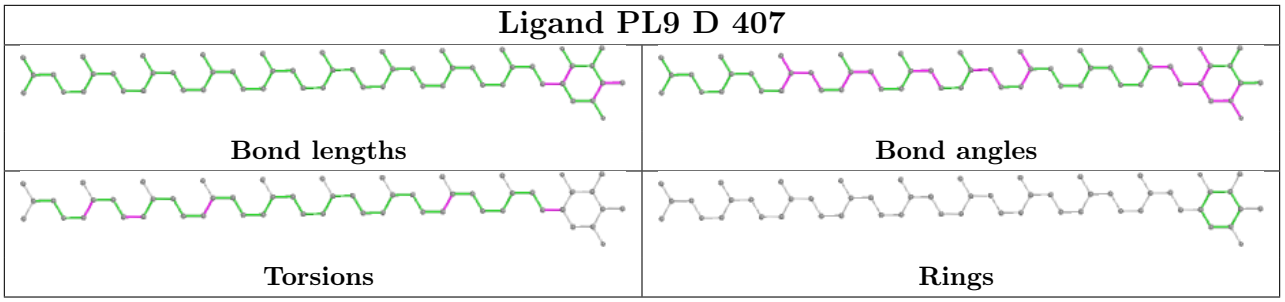


Rings

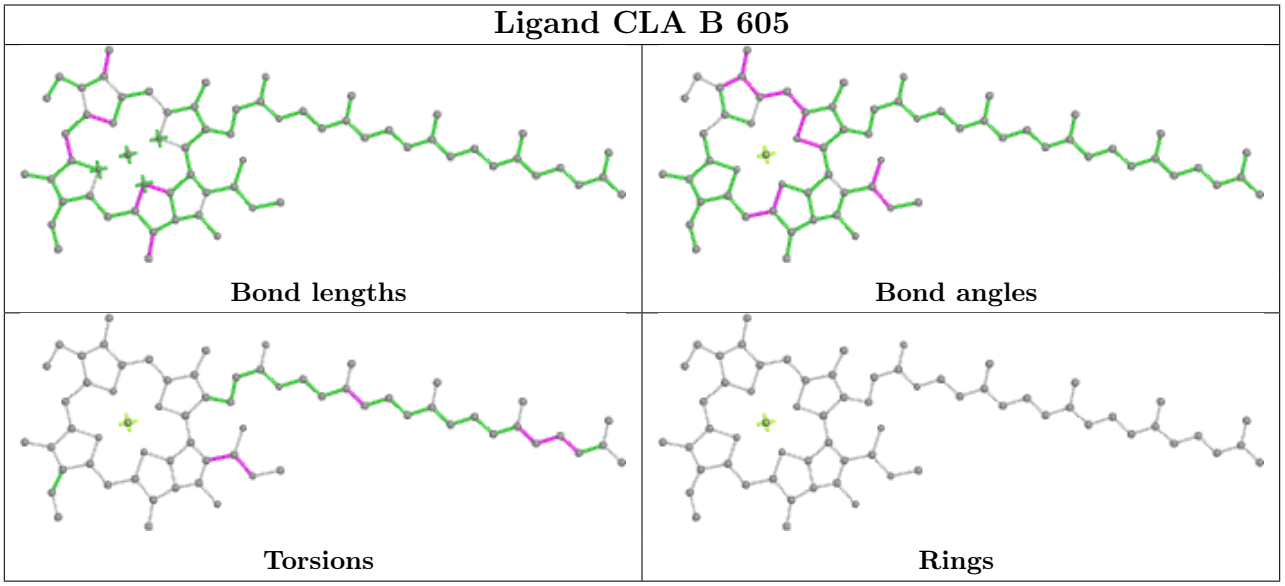
Ligand BCR T 101



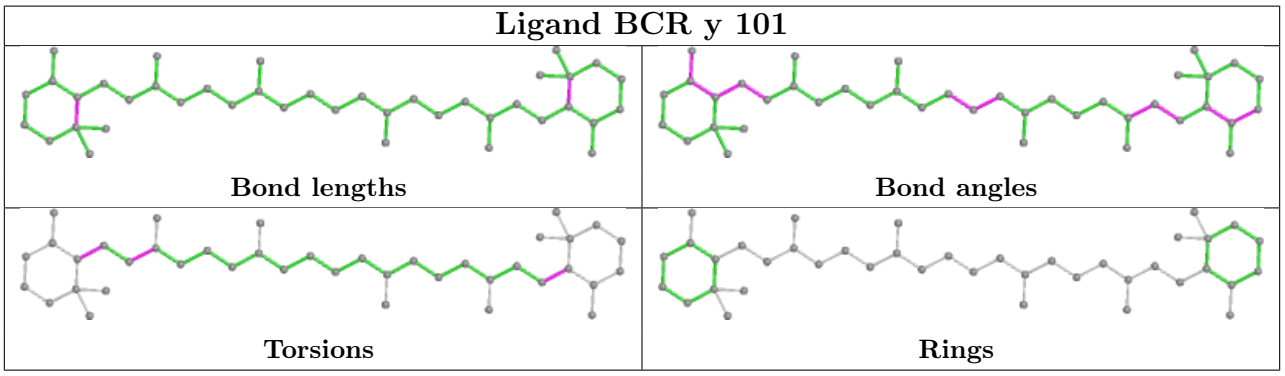
Ligand PL9 D 407



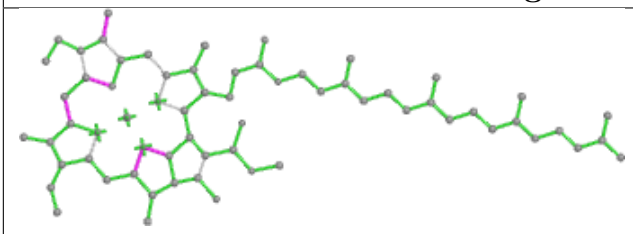
Ligand CLA B 605



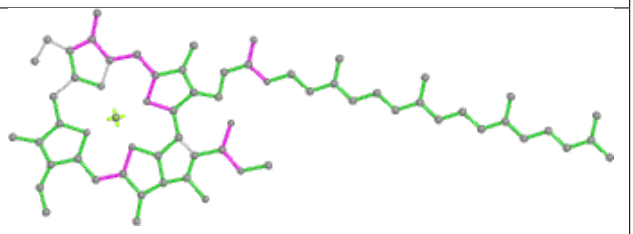
Ligand BCR y 101



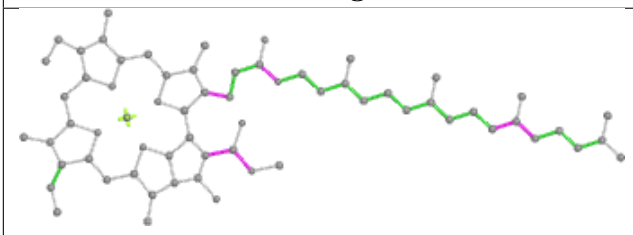
Ligand CLA B 607



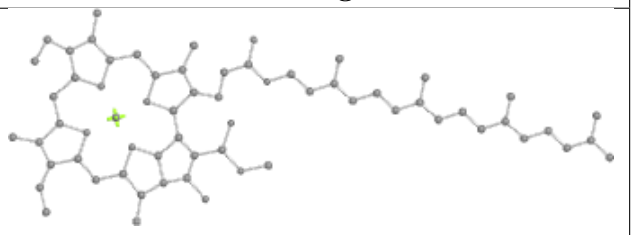
Bond lengths



Bond angles

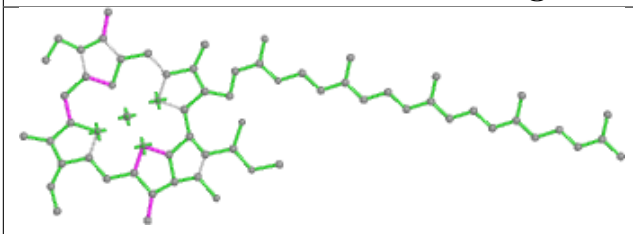


Torsions

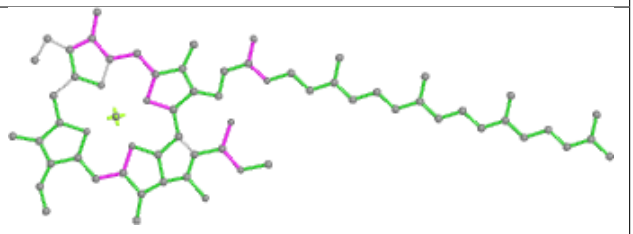


Rings

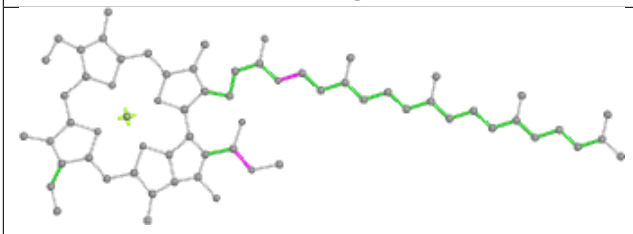
Ligand CLA a 606



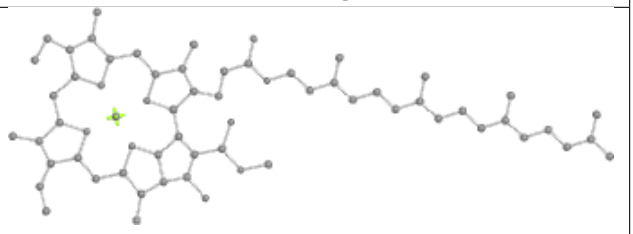
Bond lengths



Bond angles

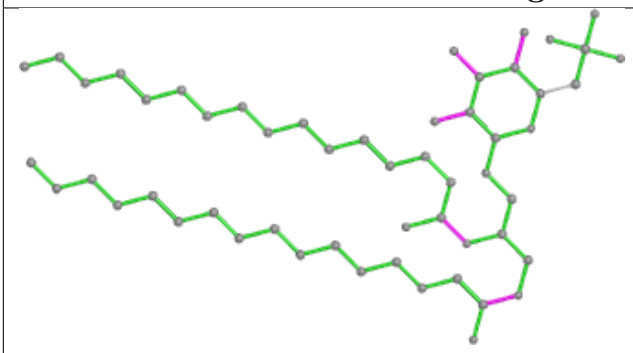


Torsions

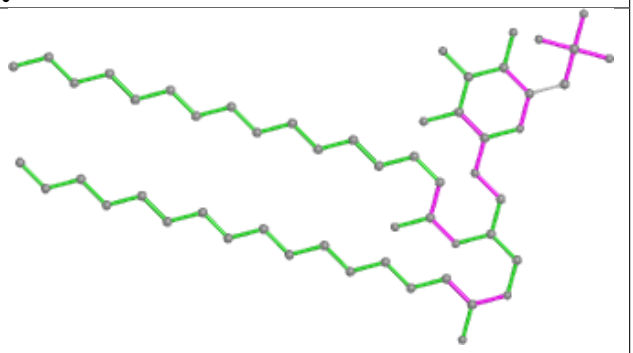


Rings

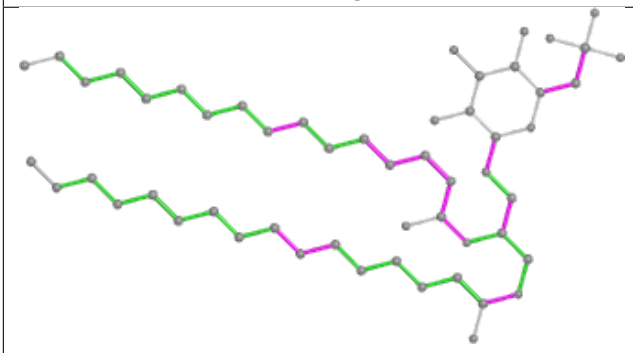
Ligand SQD b 601



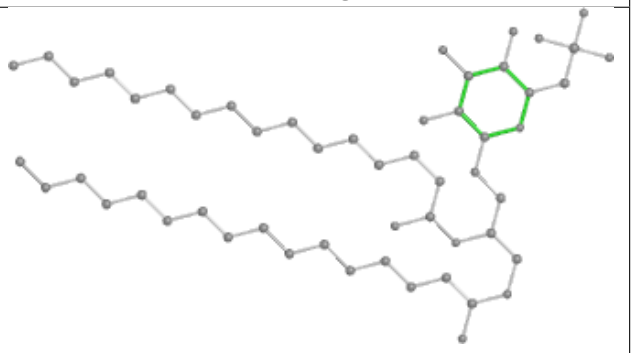
Bond lengths



Bond angles

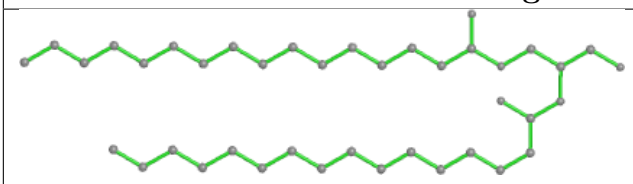


Torsions

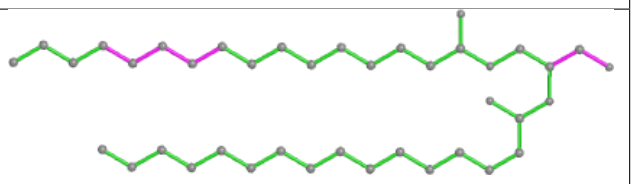


Rings

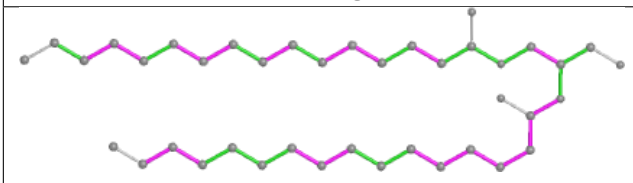
Ligand LMG d 409



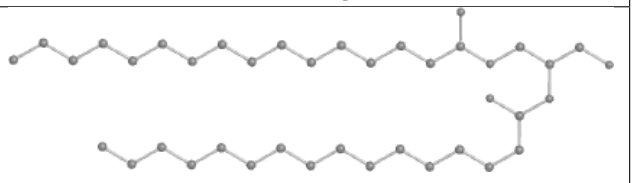
Bond lengths



Bond angles

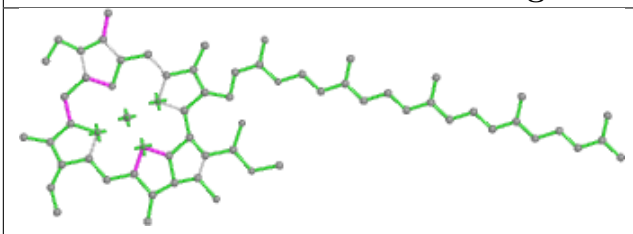


Torsions

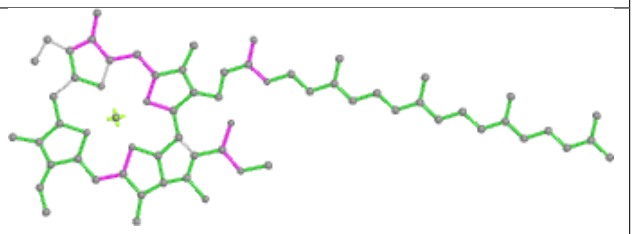


Rings

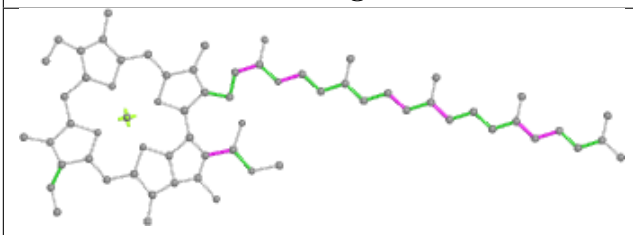
Ligand CLA b 616



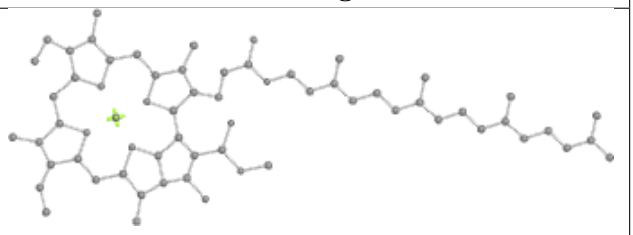
Bond lengths



Bond angles

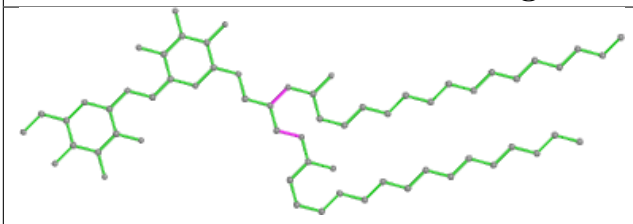


Torsions

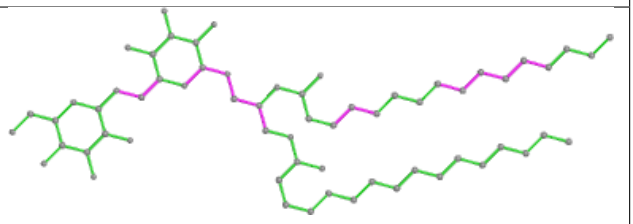


Rings

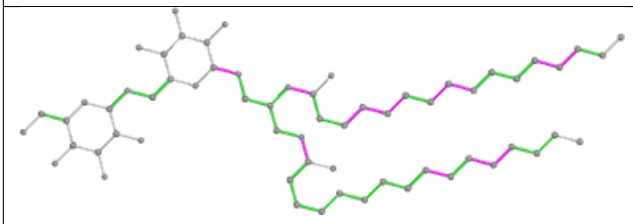
Ligand DGD C 518



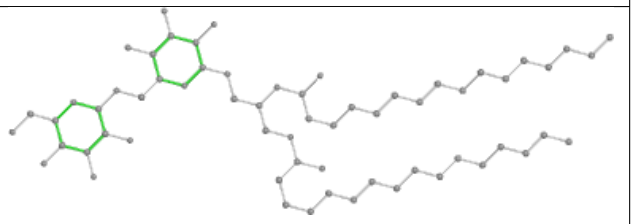
Bond lengths



Bond angles

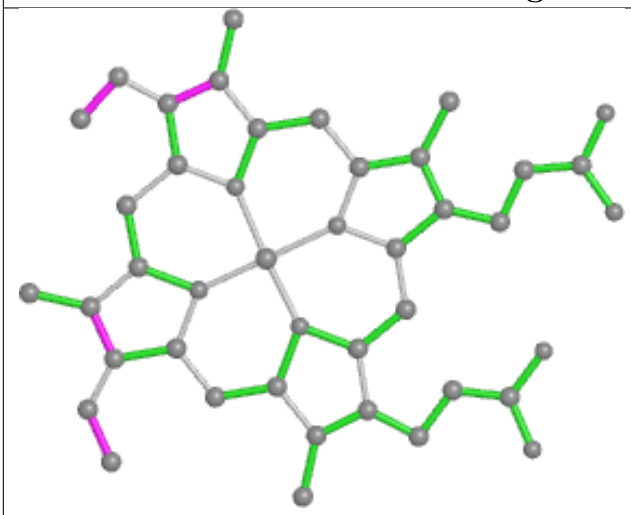


Torsions

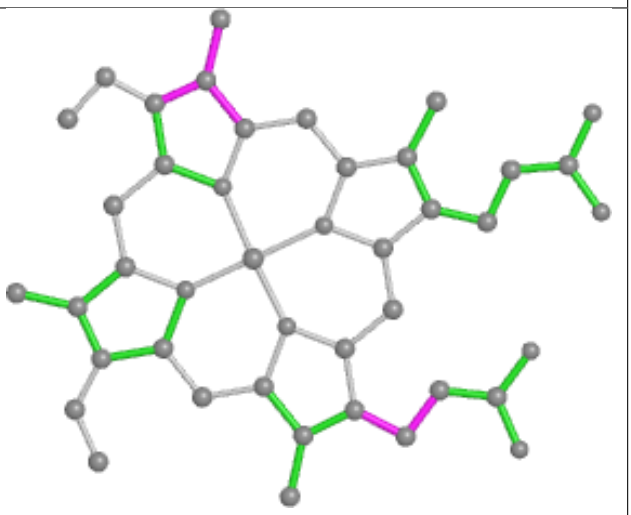


Rings

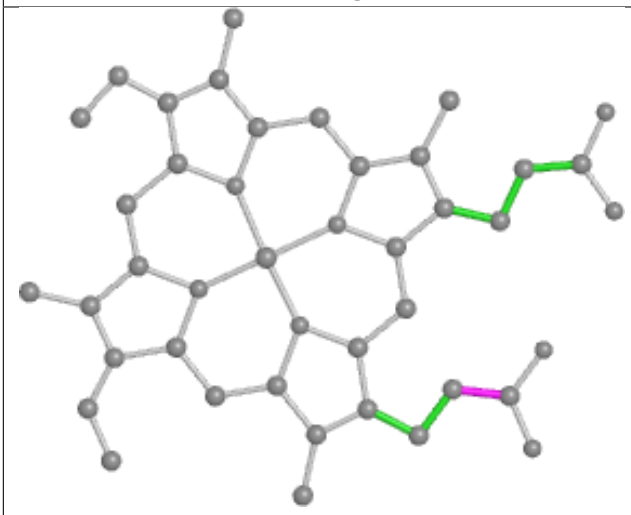
Ligand HEC v 201



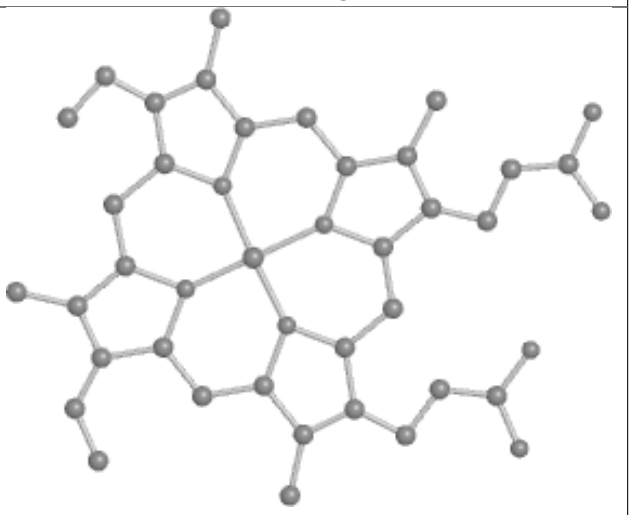
Bond lengths



Bond angles

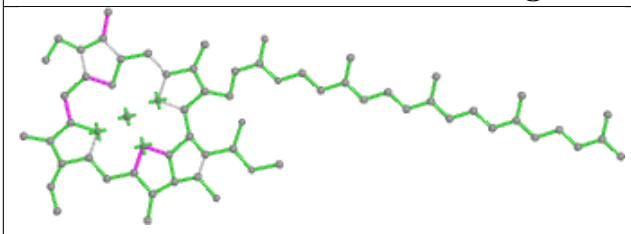


Torsions

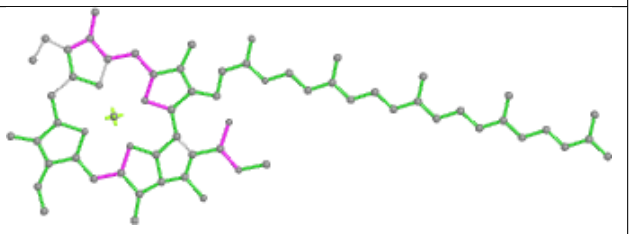


Rings

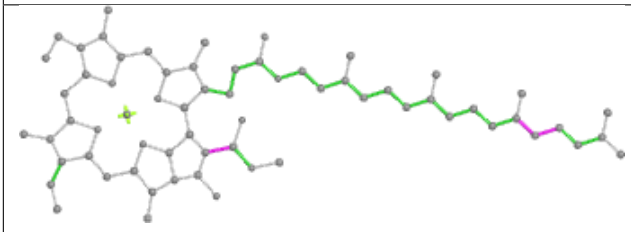
Ligand CLA C 504



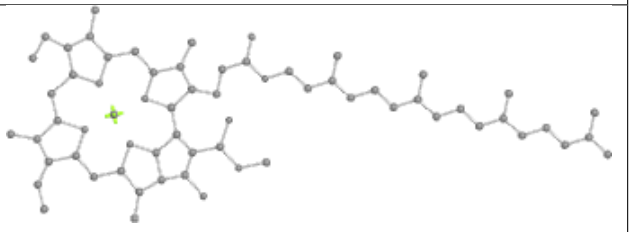
Bond lengths



Bond angles

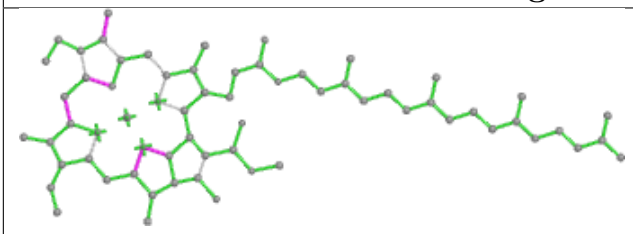


Torsions

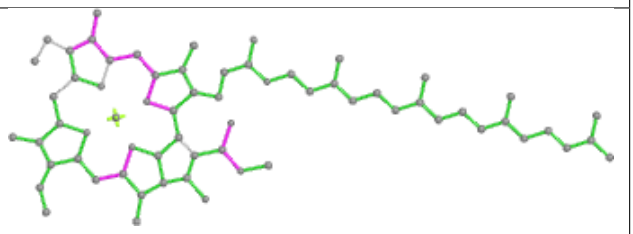


Rings

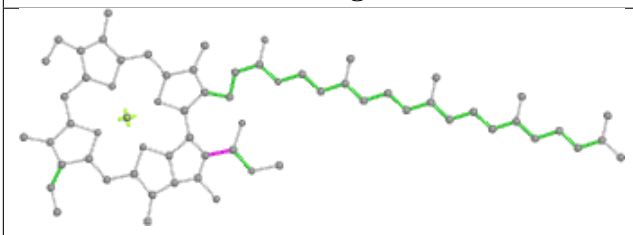
Ligand CLA a 612



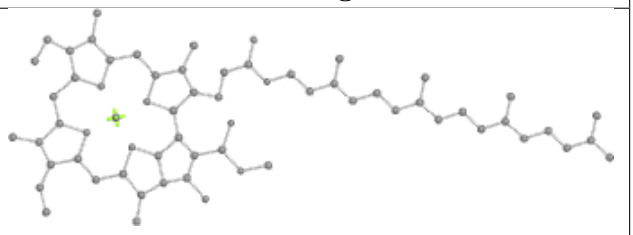
Bond lengths



Bond angles

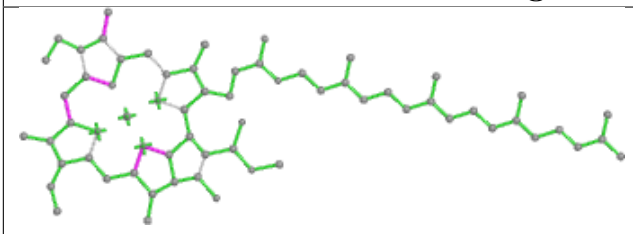


Torsions

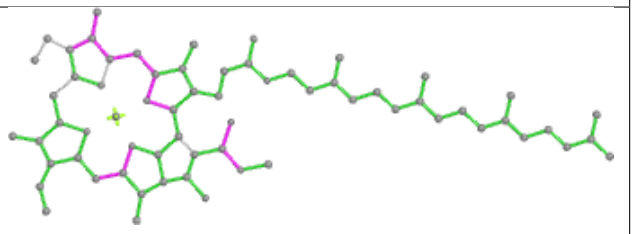


Rings

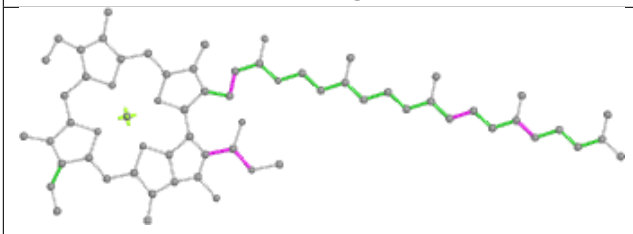
Ligand CLA b 609



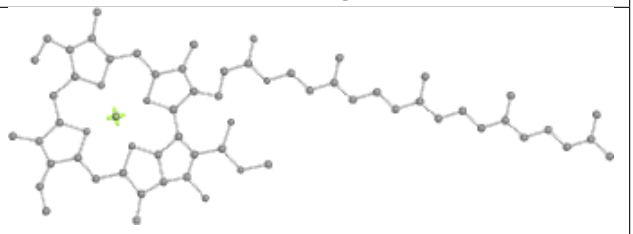
Bond lengths



Bond angles

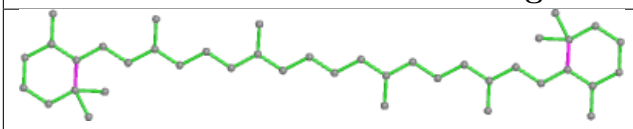


Torsions

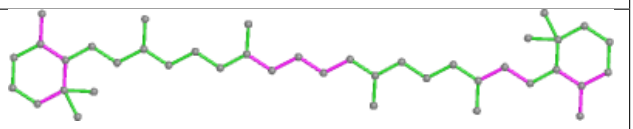


Rings

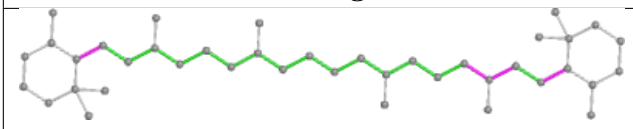
Ligand BCR b 622



Bond lengths



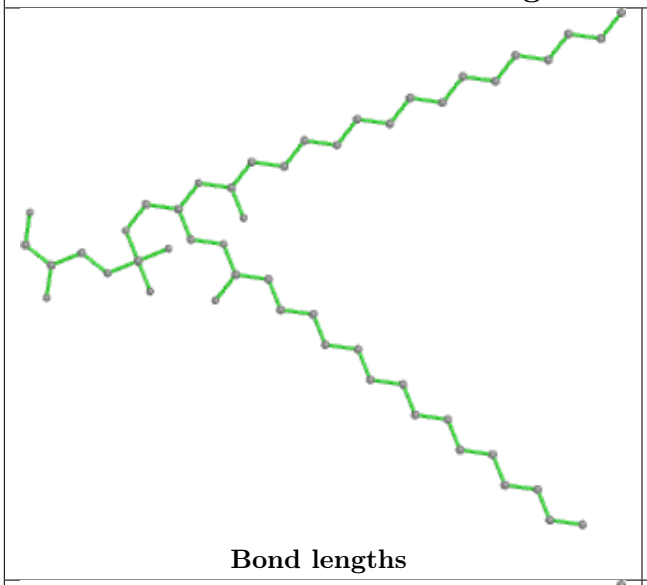
Bond angles



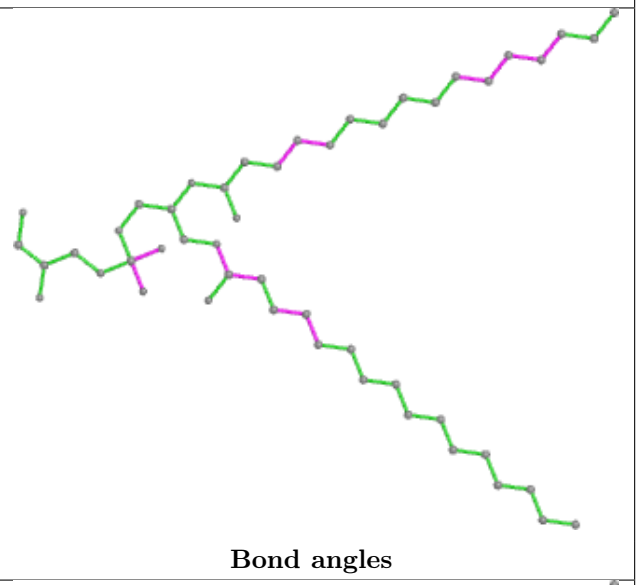
Torsions

Rings

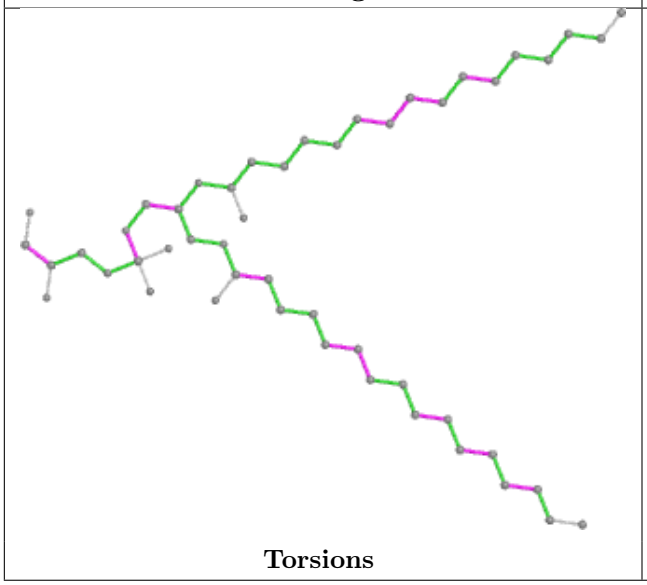
Ligand LHG A 617



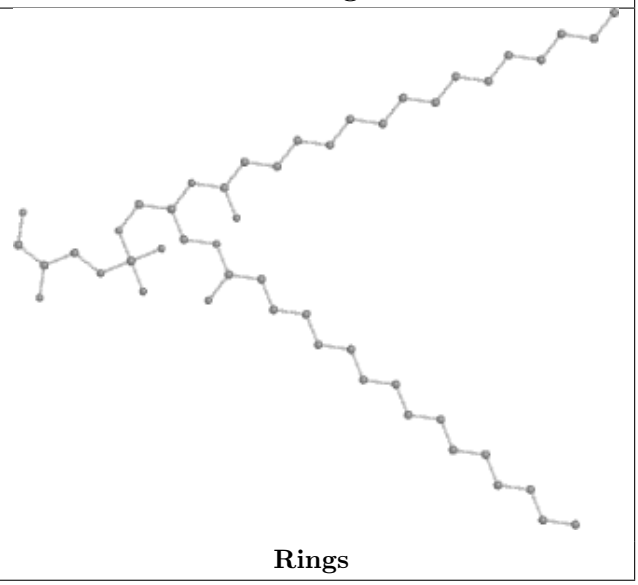
Bond lengths



Bond angles

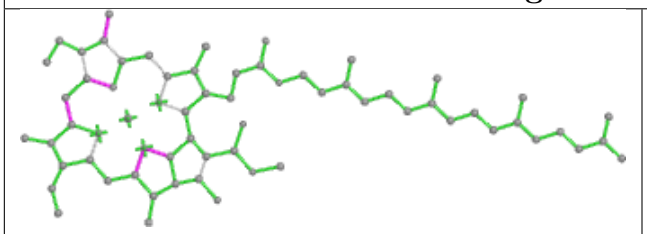


Torsions

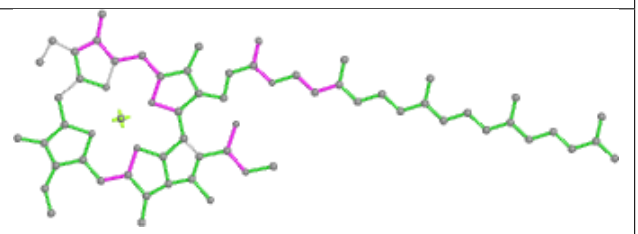


Rings

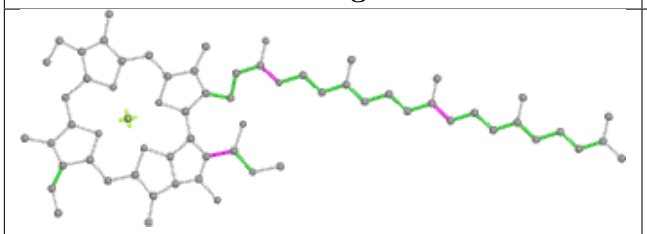
Ligand CLA C 508



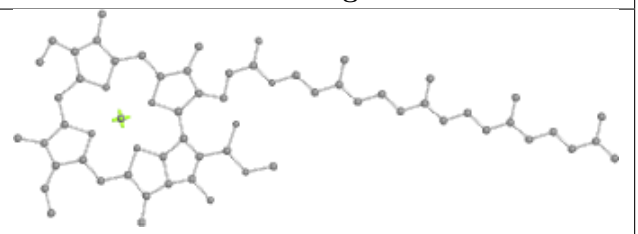
Bond lengths



Bond angles

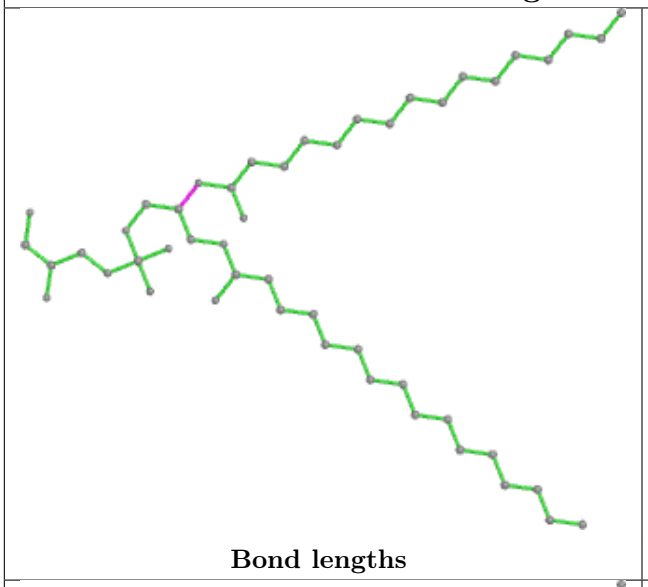


Torsions

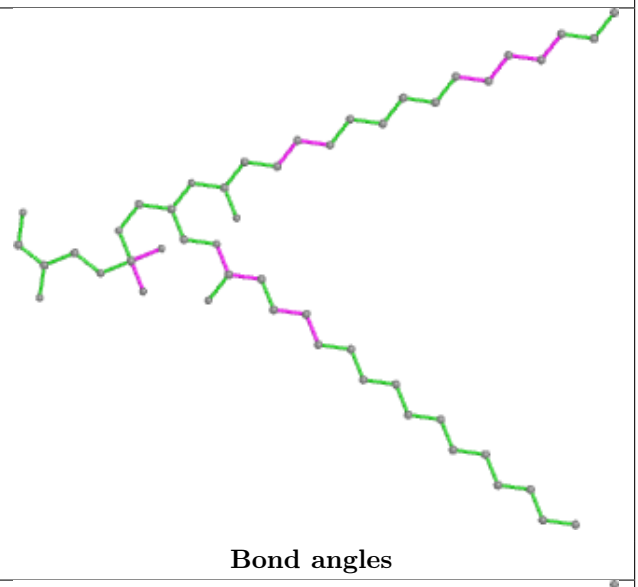


Rings

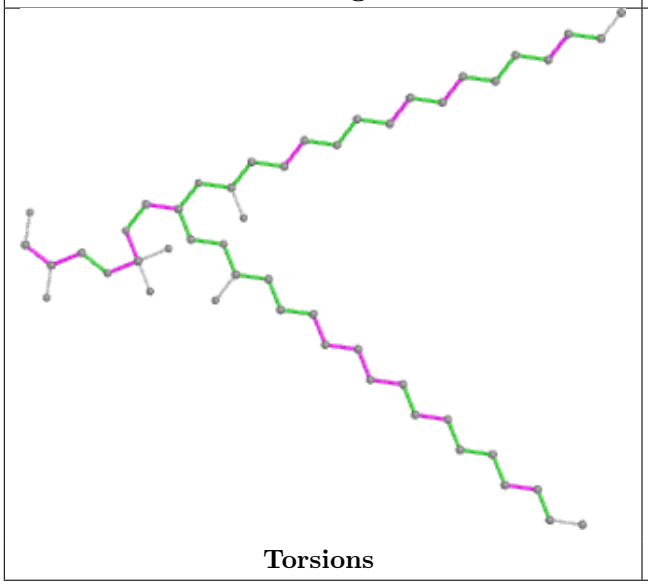
Ligand LHG D 406



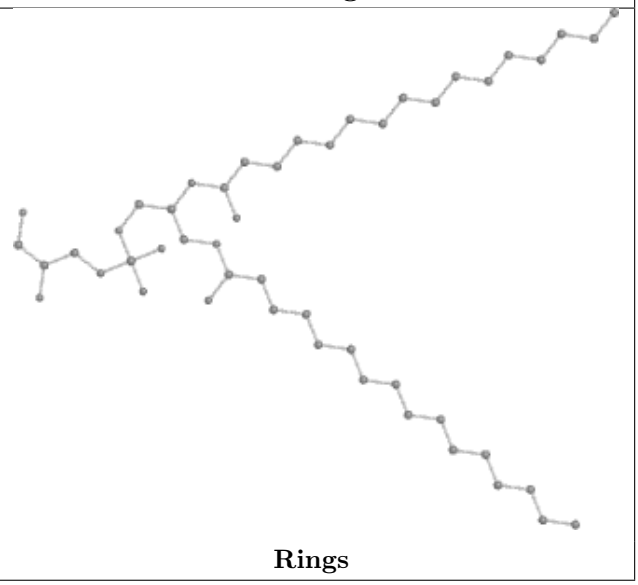
Bond lengths



Bond angles

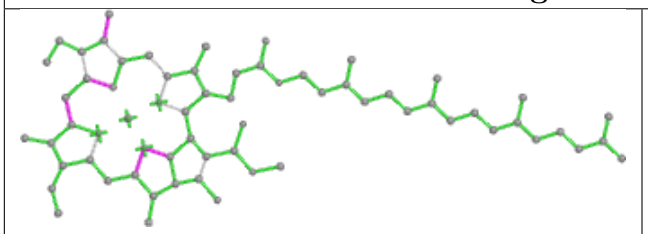


Torsions

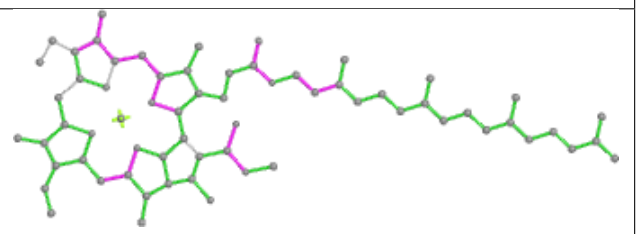


Rings

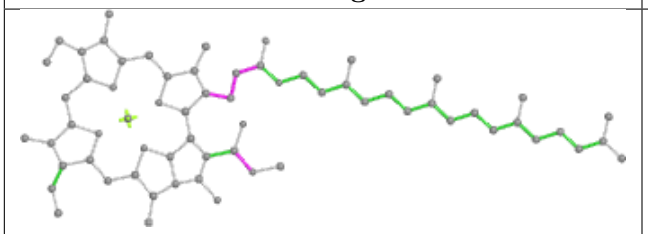
Ligand CLA c 503



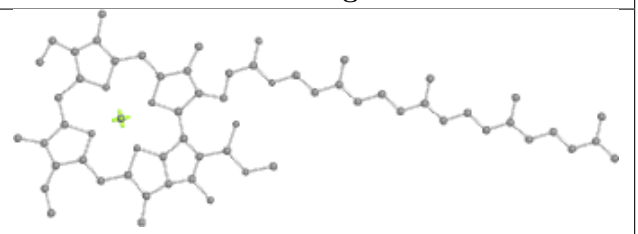
Bond lengths



Bond angles

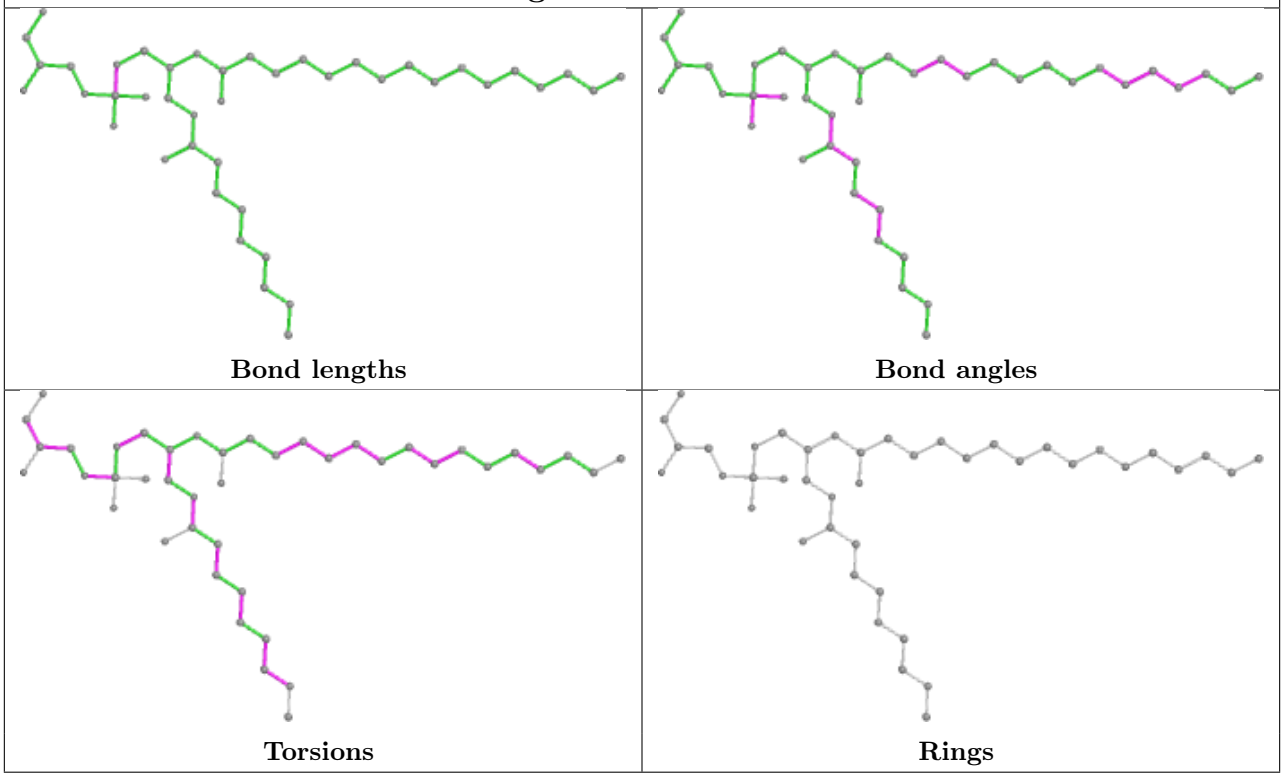


Torsions

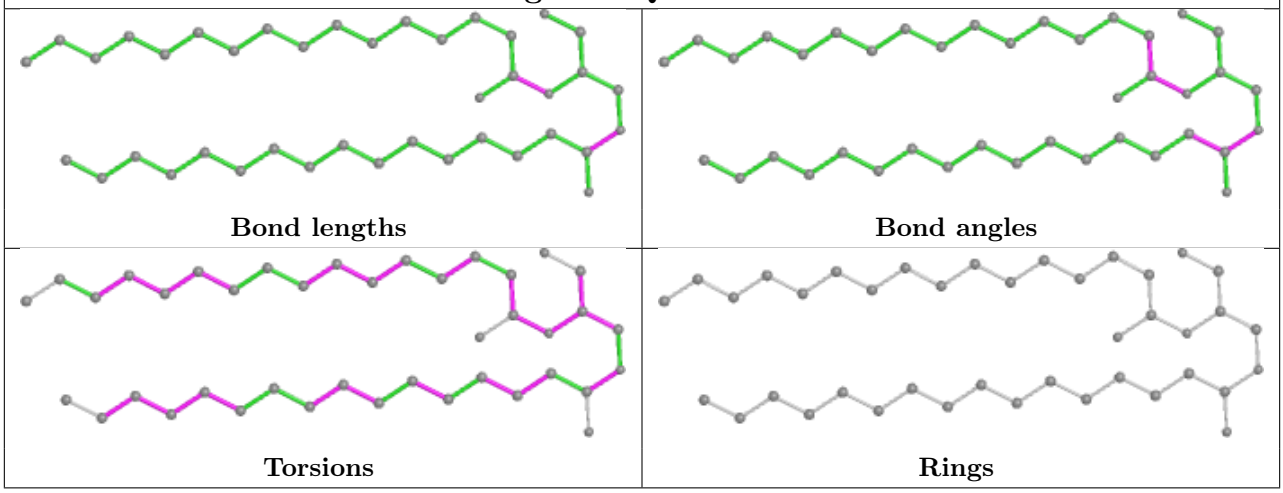


Rings

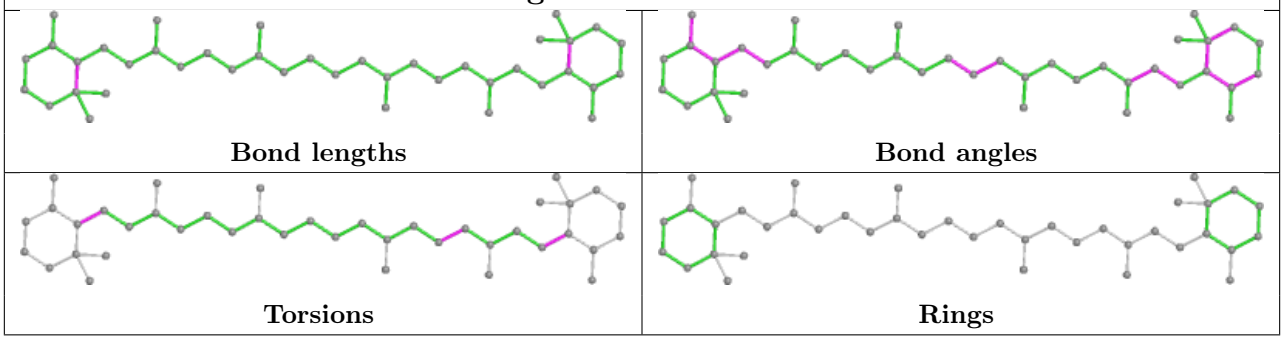
Ligand LHG a 615



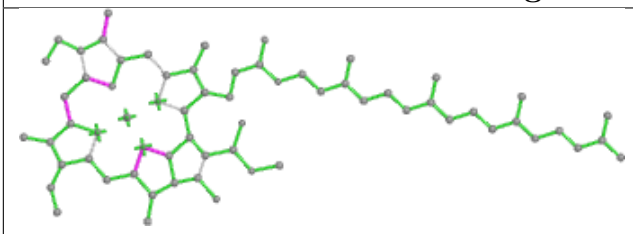
Ligand SQD A 619



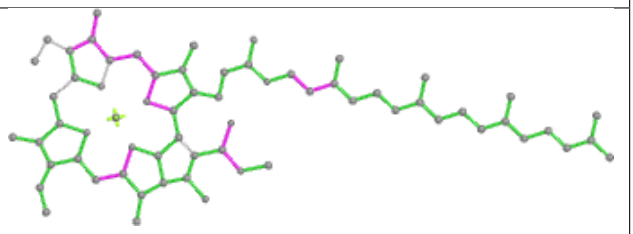
Ligand BCR k 101



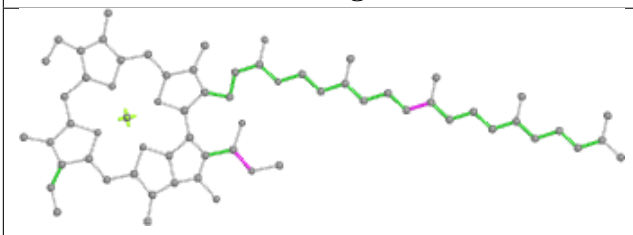
Ligand CLA C 511



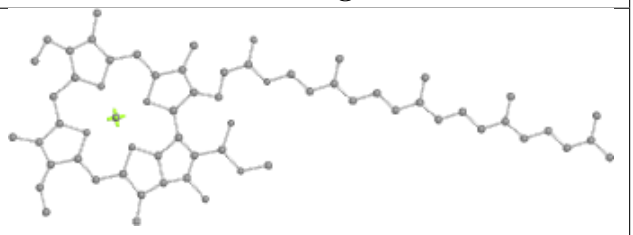
Bond lengths



Bond angles

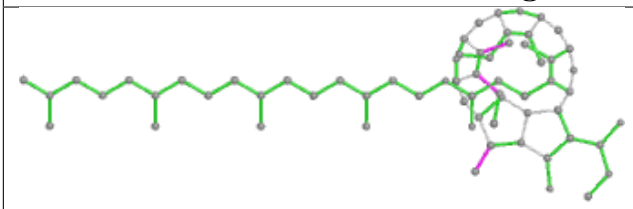


Torsions

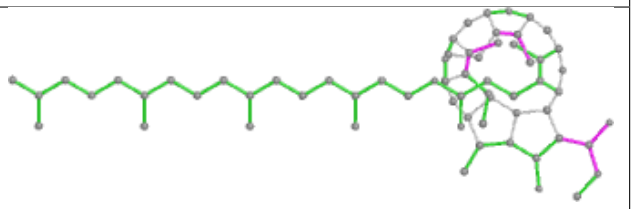


Rings

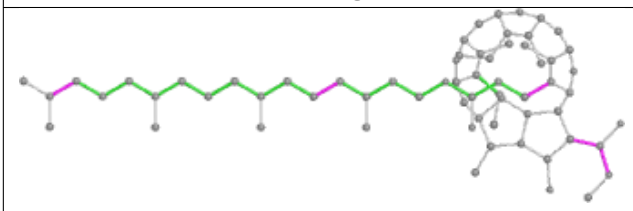
Ligand PHO D 401



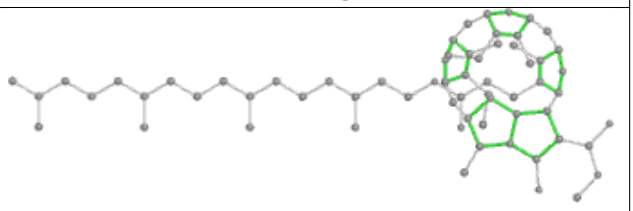
Bond lengths



Bond angles

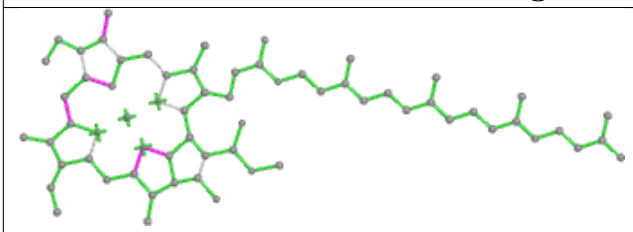


Torsions

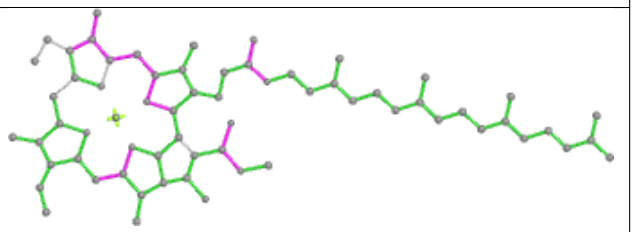


Rings

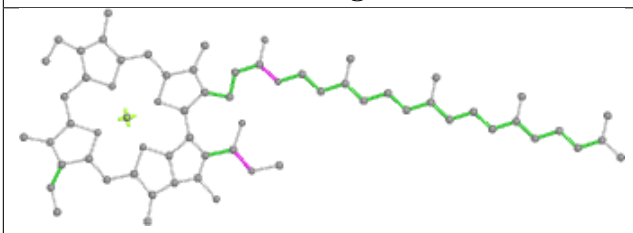
Ligand CLA c 513



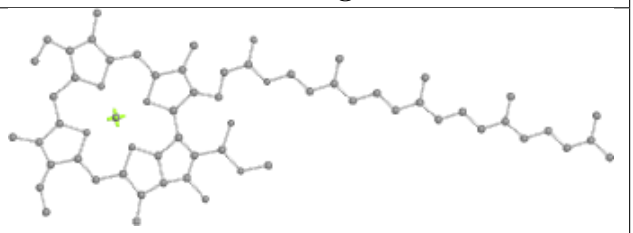
Bond lengths



Bond angles

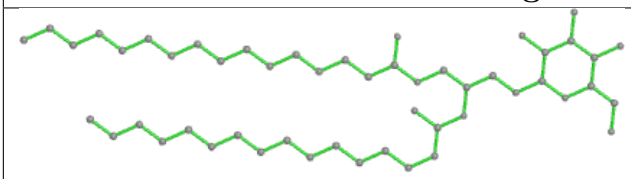


Torsions

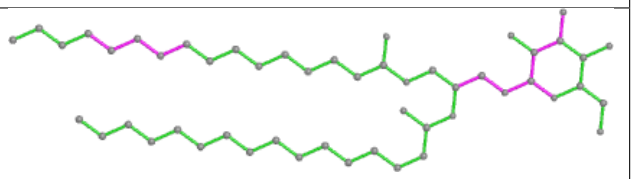


Rings

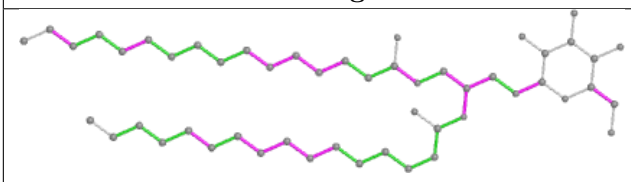
Ligand LMG b 624



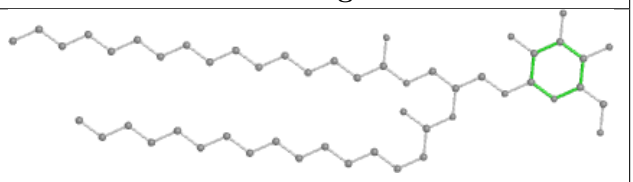
Bond lengths



Bond angles

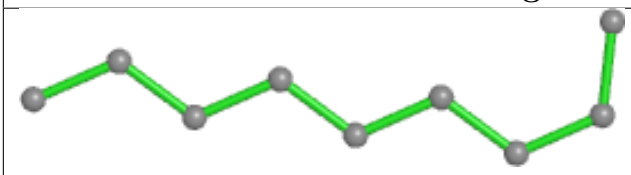


Torsions

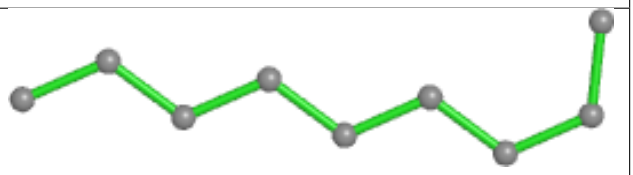


Rings

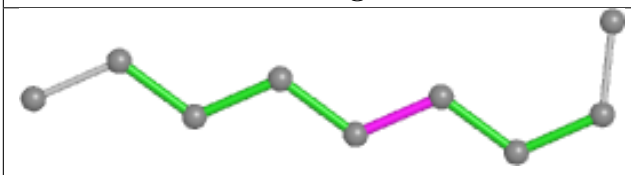
Ligand LMG b 625



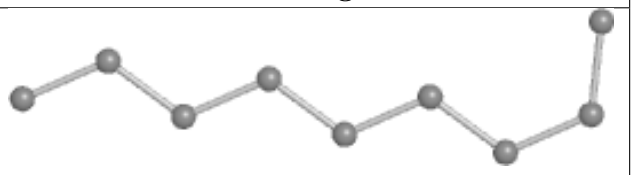
Bond lengths



Bond angles

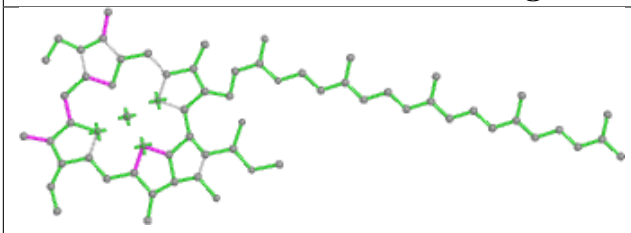


Torsions

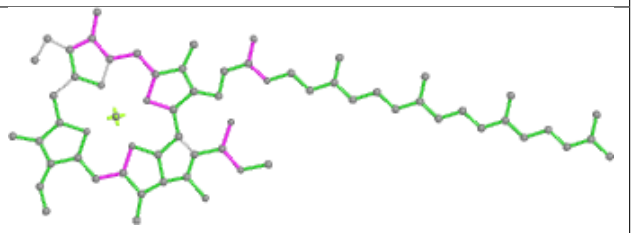


Rings

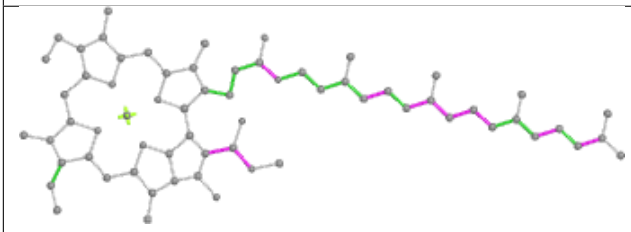
Ligand CLA B 616



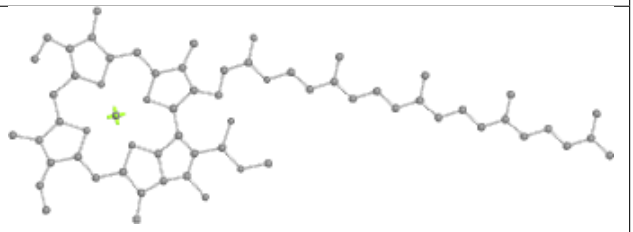
Bond lengths



Bond angles

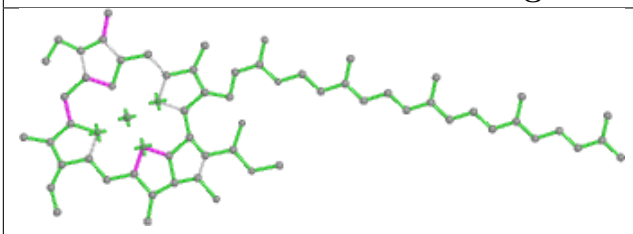


Torsions

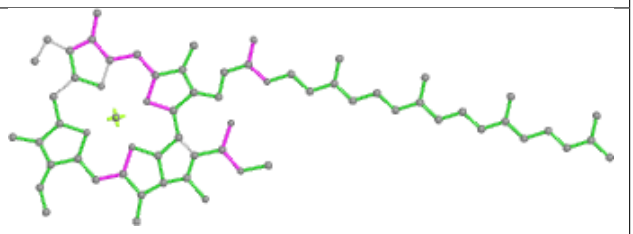


Rings

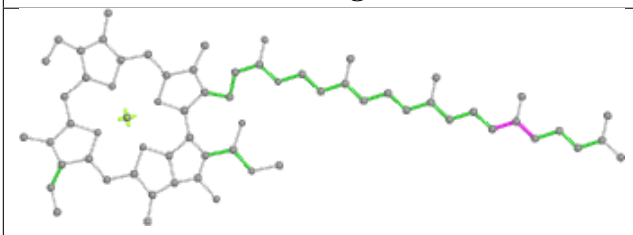
Ligand CLA B 615



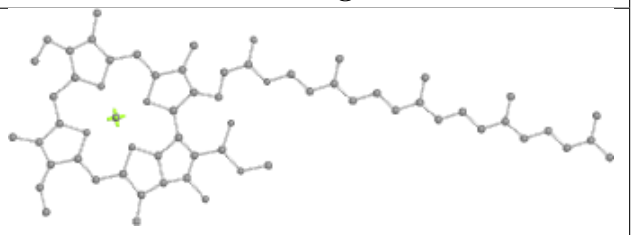
Bond lengths



Bond angles

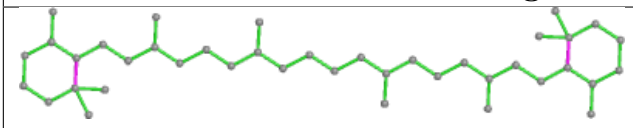


Torsions

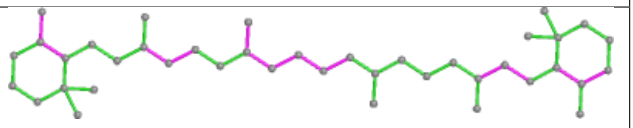


Rings

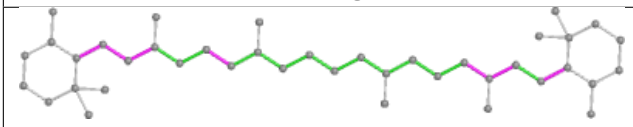
Ligand BCR B 627



Bond lengths



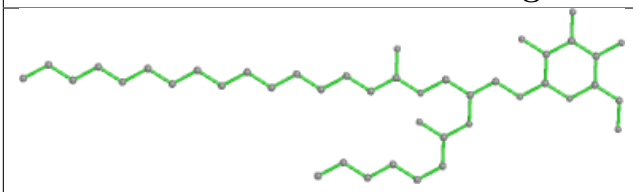
Bond angles



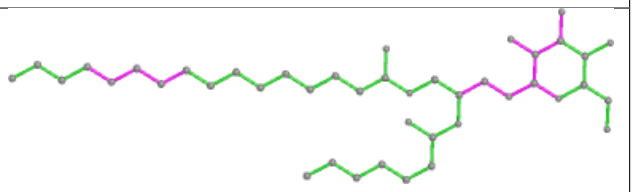
Torsions

Rings

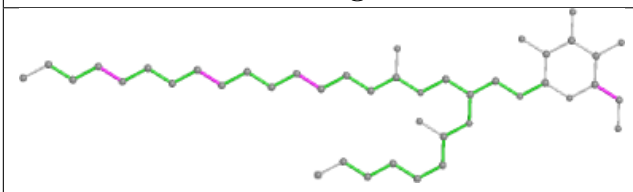
Ligand LMG d 406



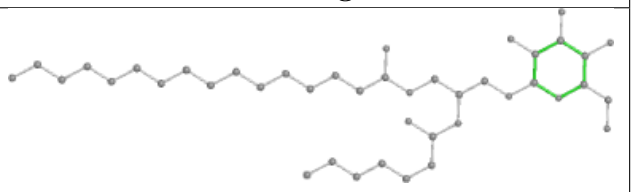
Bond lengths



Bond angles

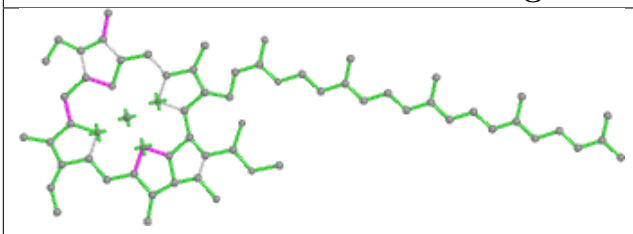


Torsions

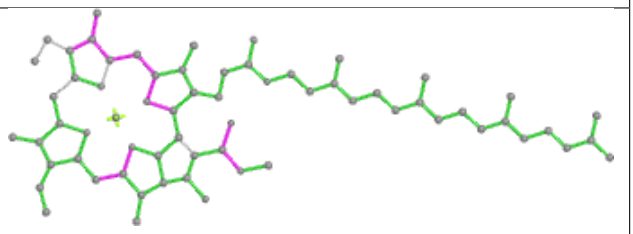


Rings

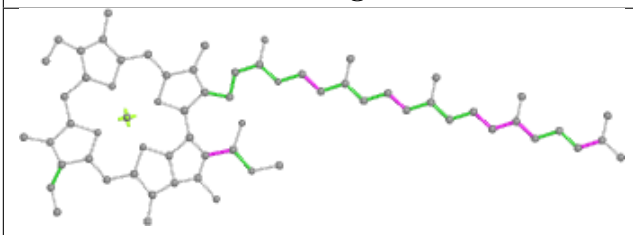
Ligand CLA C 509



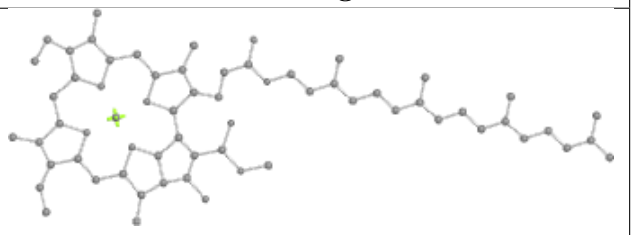
Bond lengths



Bond angles

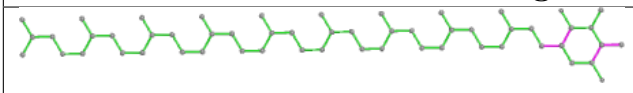


Torsions

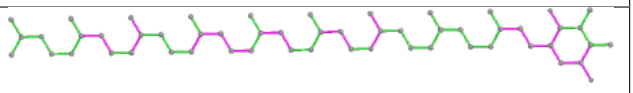


Rings

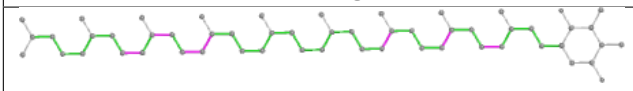
Ligand PL9 d 408



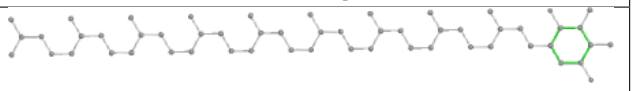
Bond lengths



Bond angles

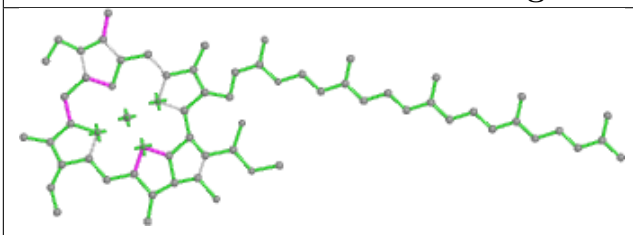


Torsions

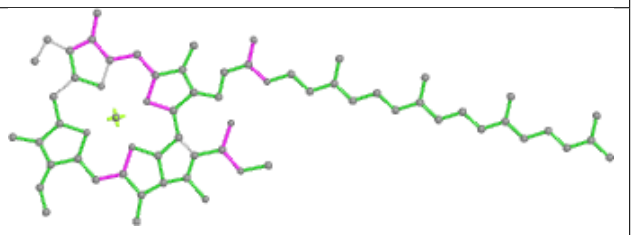


Rings

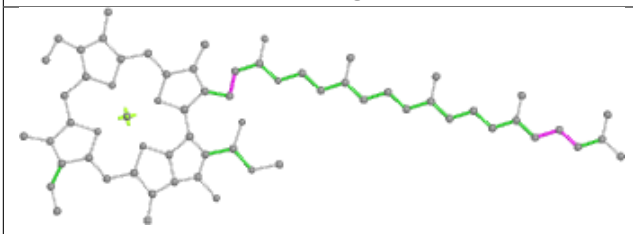
Ligand CLA b 611



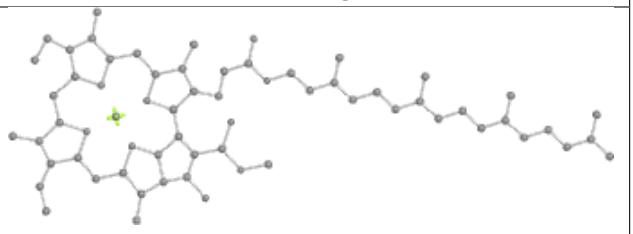
Bond lengths



Bond angles

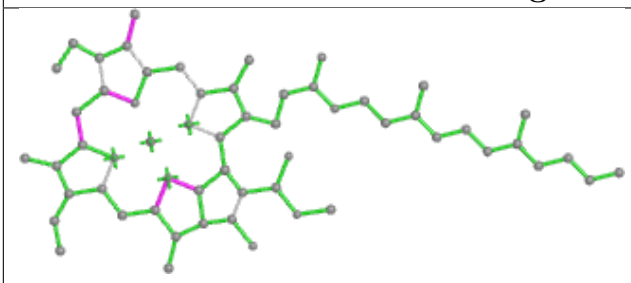


Torsions

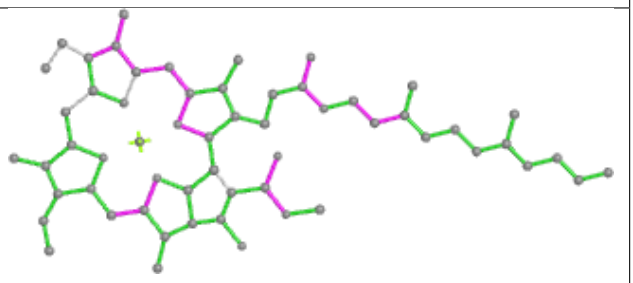


Rings

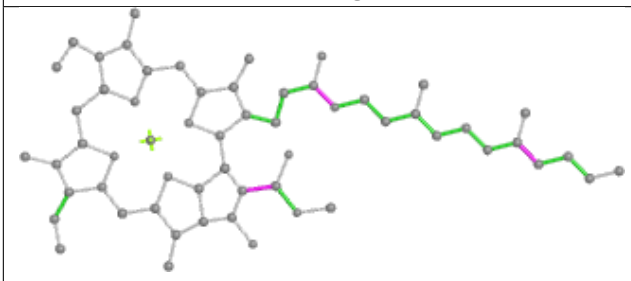
Ligand CLA c 510



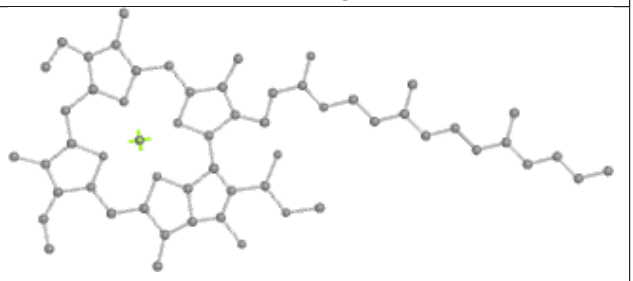
Bond lengths



Bond angles

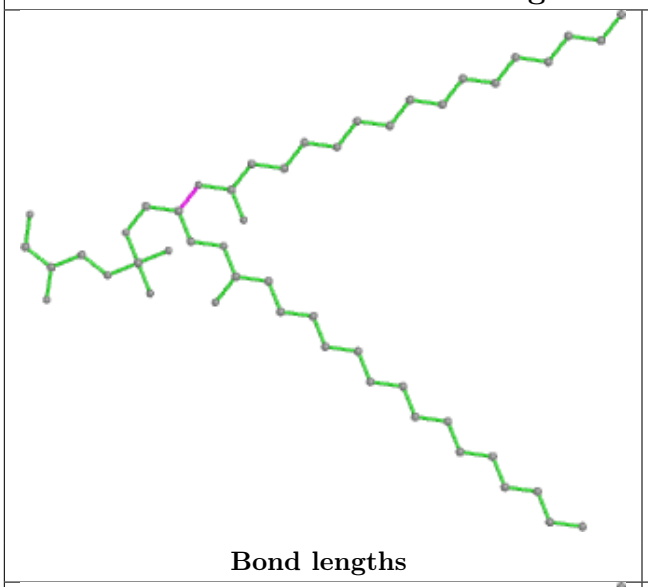


Torsions

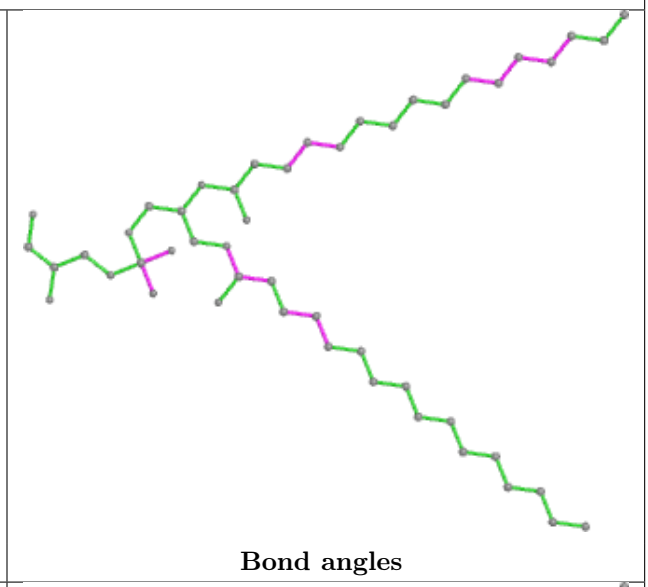


Rings

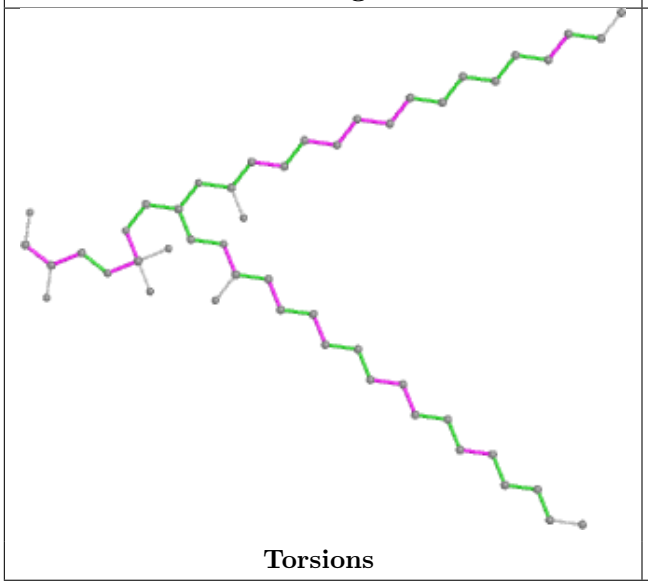
Ligand LHG a 613



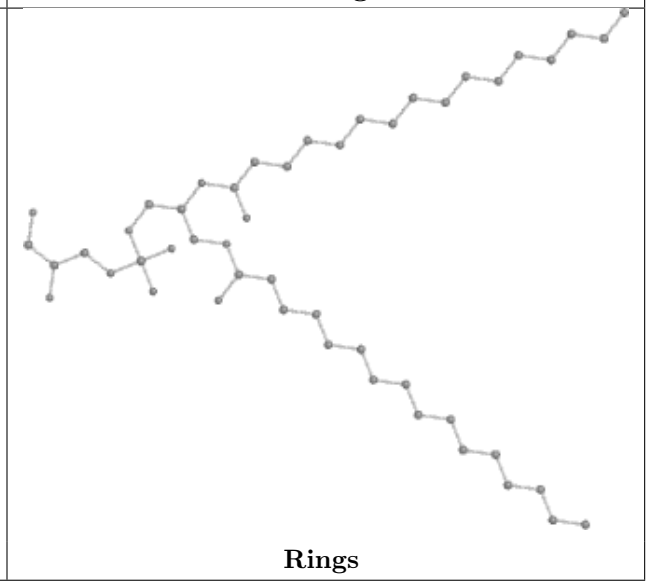
Bond lengths



Bond angles

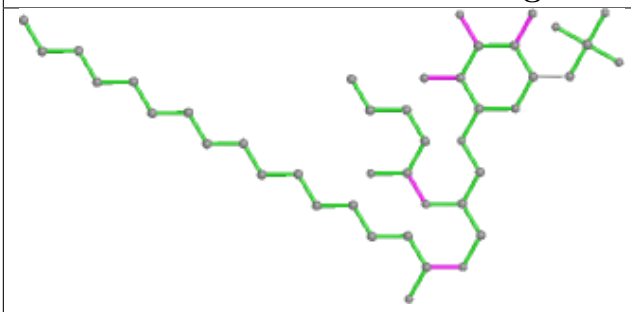


Torsions

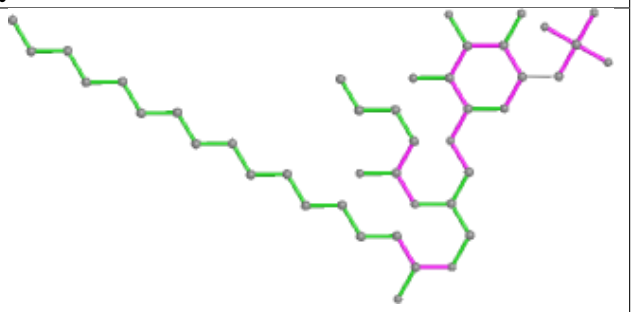


Rings

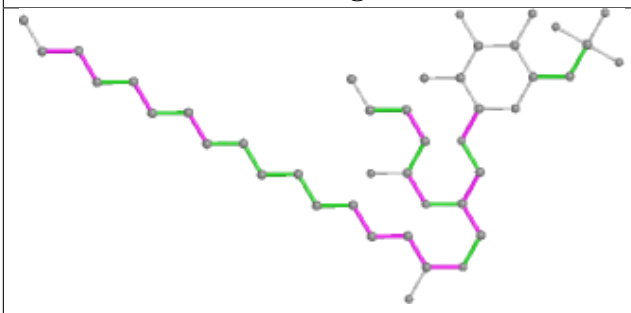
Ligand SQD D 409



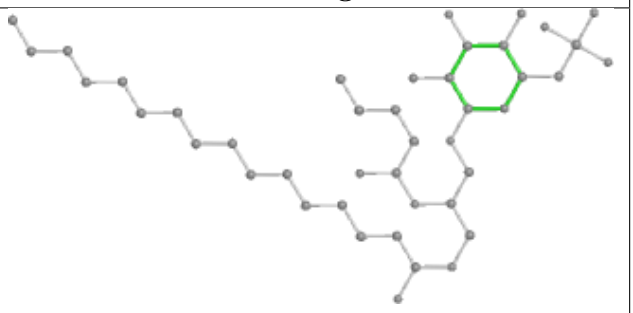
Bond lengths



Bond angles

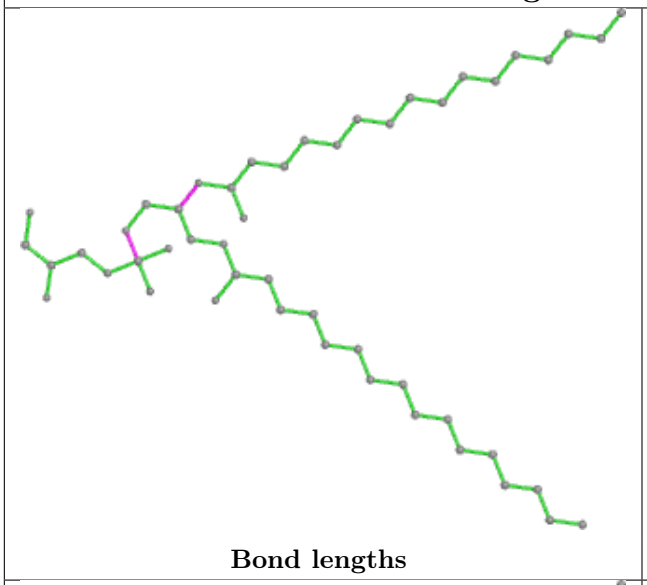


Torsions

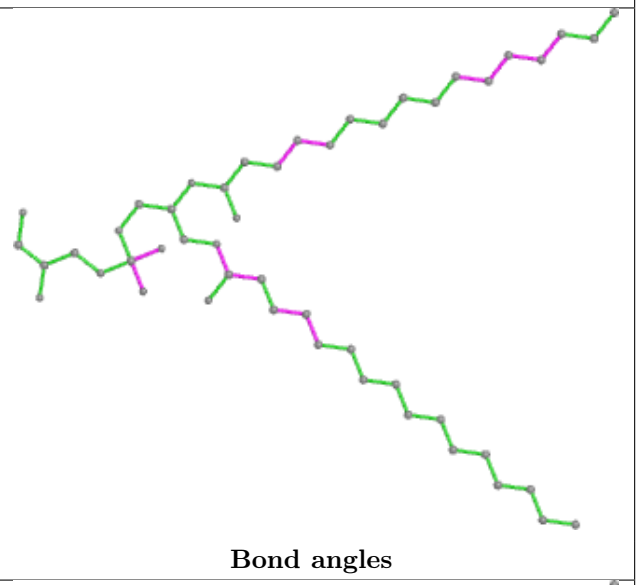


Rings

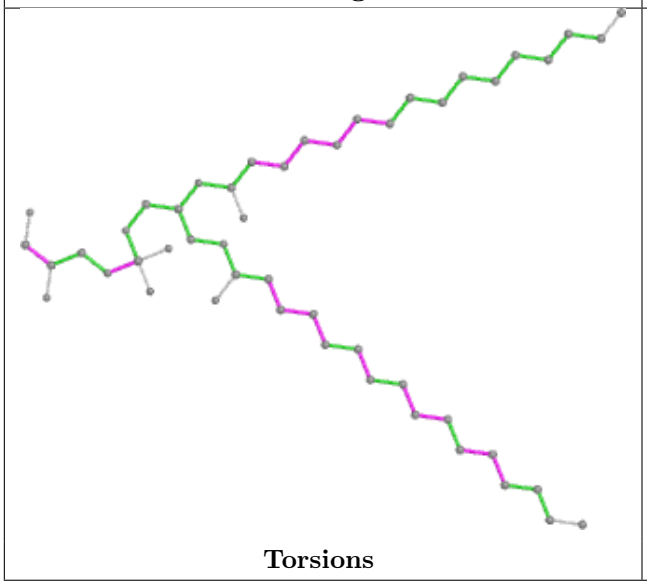
Ligand LHG A 616



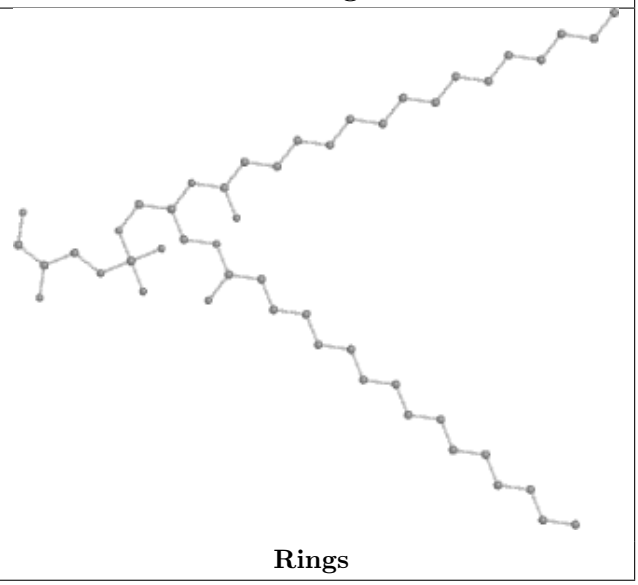
Bond lengths



Bond angles

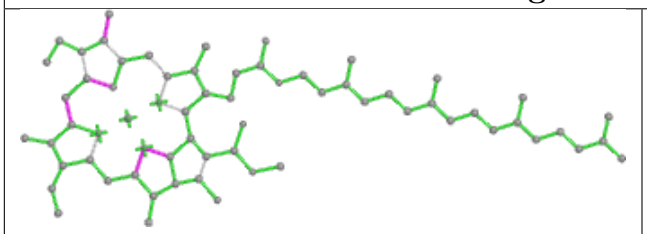


Torsions

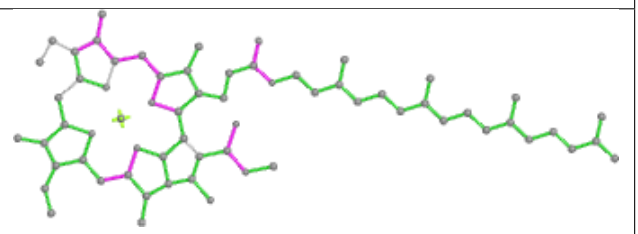


Rings

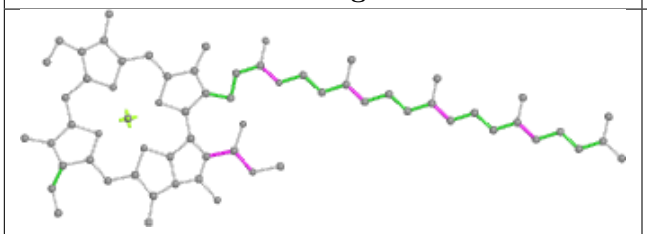
Ligand CLA b 612



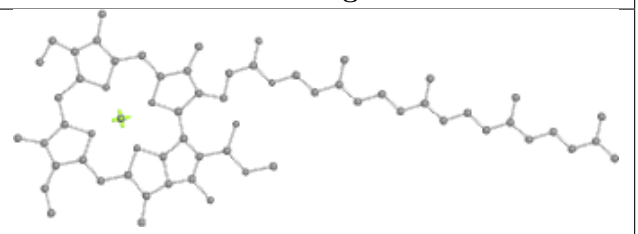
Bond lengths



Bond angles

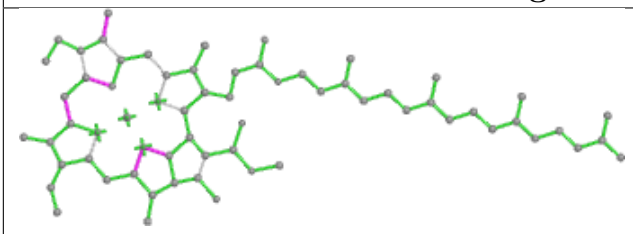


Torsions

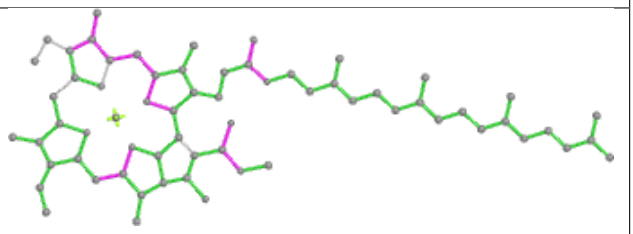


Rings

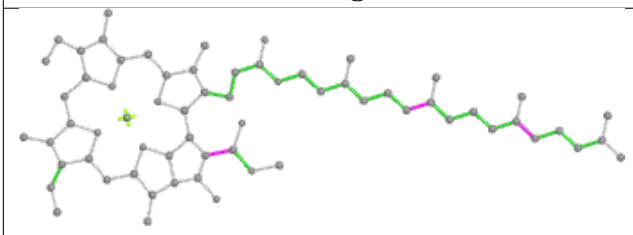
Ligand CLA c 504



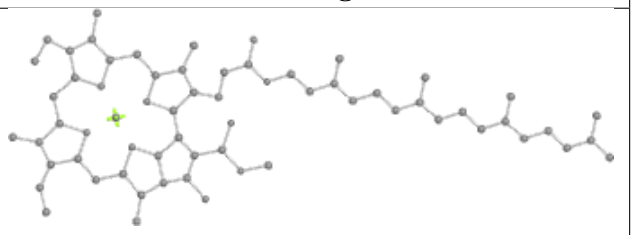
Bond lengths



Bond angles

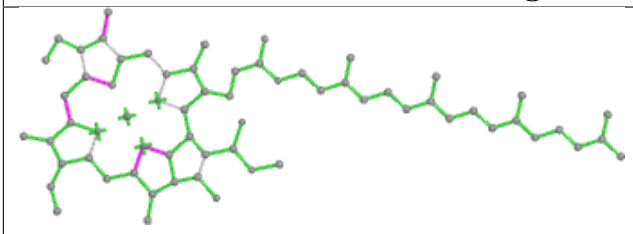


Torsions

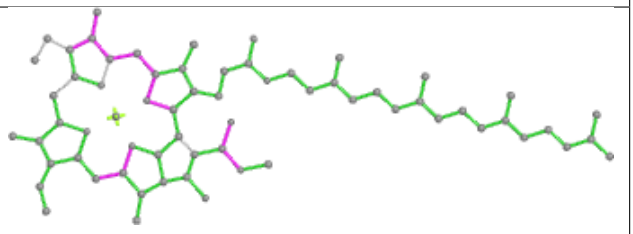


Rings

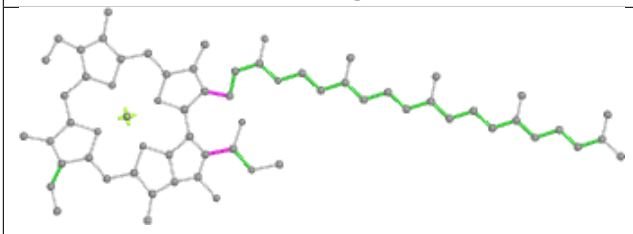
Ligand CLA A 615



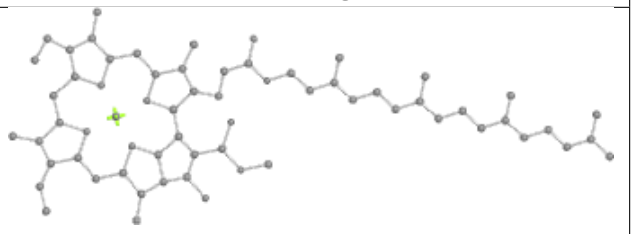
Bond lengths



Bond angles

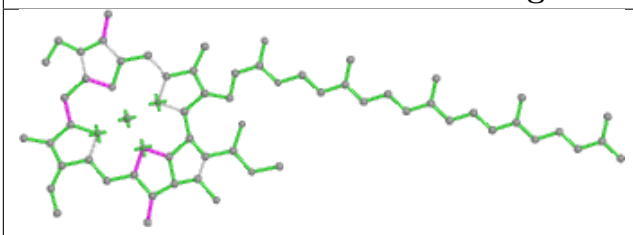


Torsions

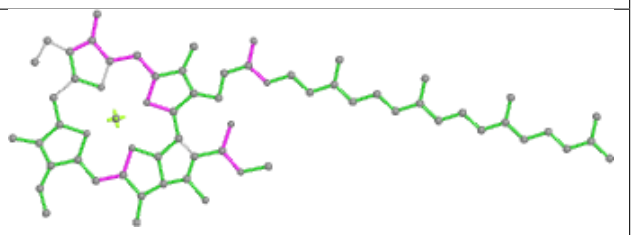


Rings

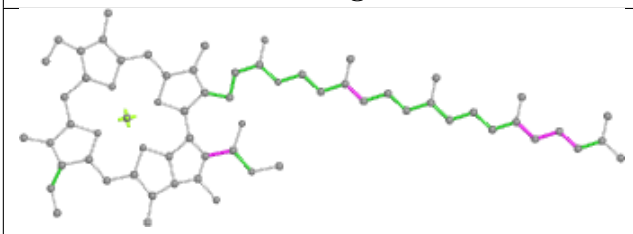
Ligand CLA b 608



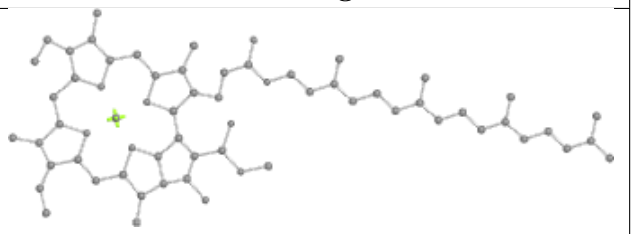
Bond lengths



Bond angles

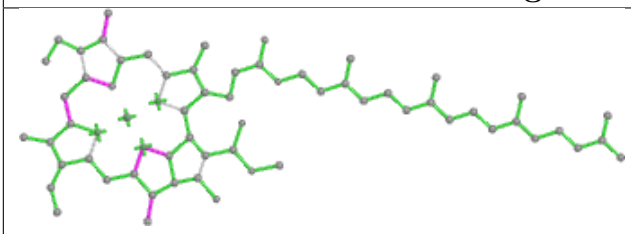


Torsions

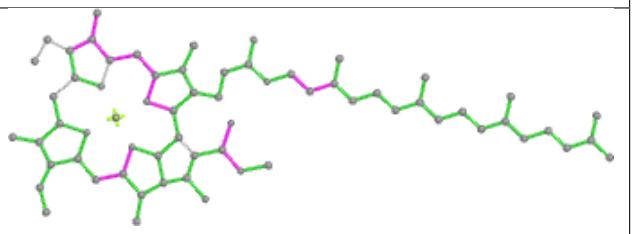


Rings

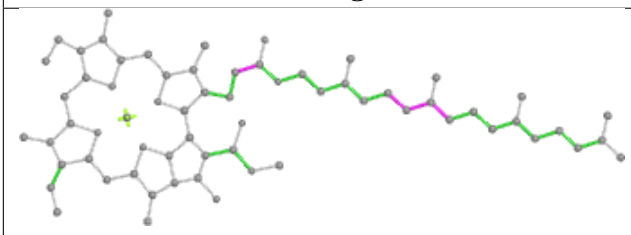
Ligand CLA C 510



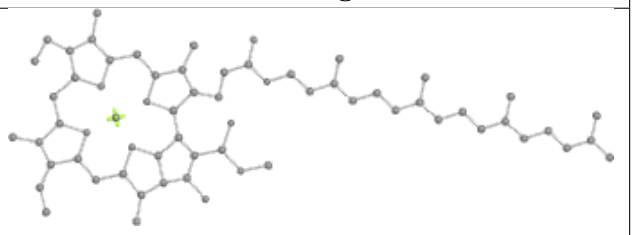
Bond lengths



Bond angles

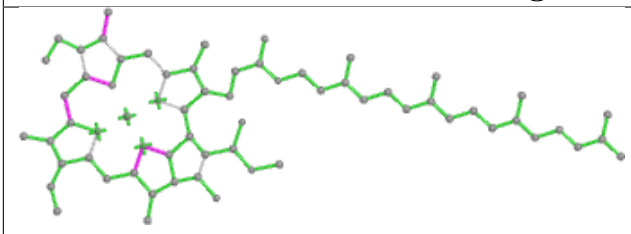


Torsions

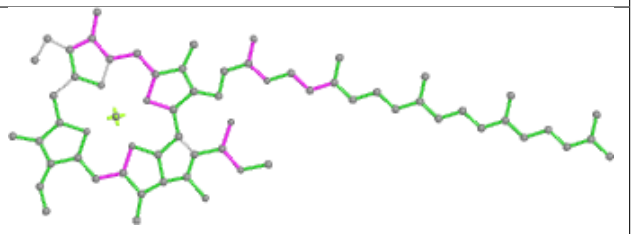


Rings

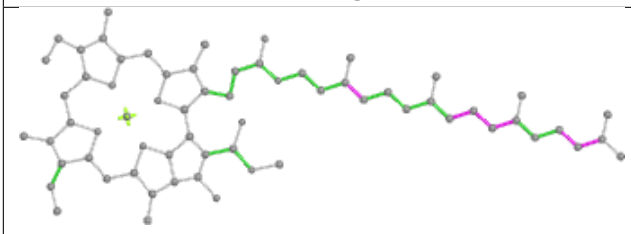
Ligand CLA a 609



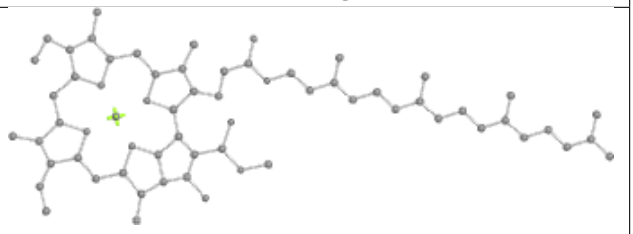
Bond lengths



Bond angles

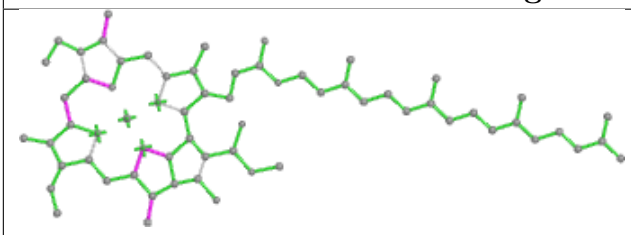


Torsions

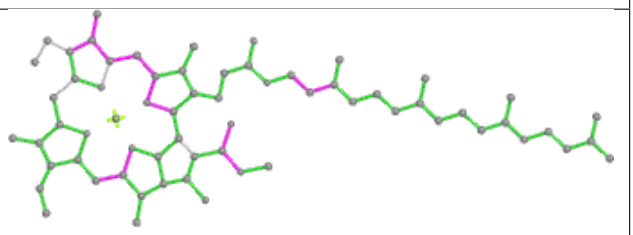


Rings

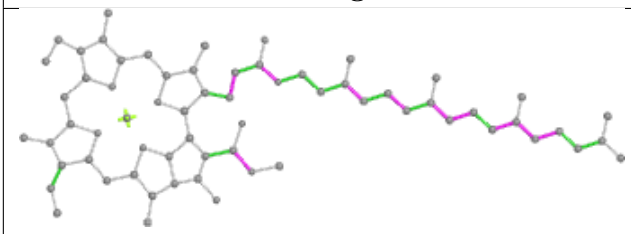
Ligand CLA C 505



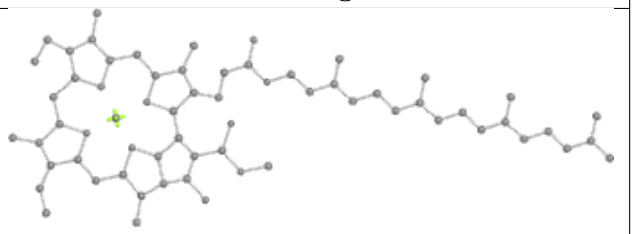
Bond lengths



Bond angles

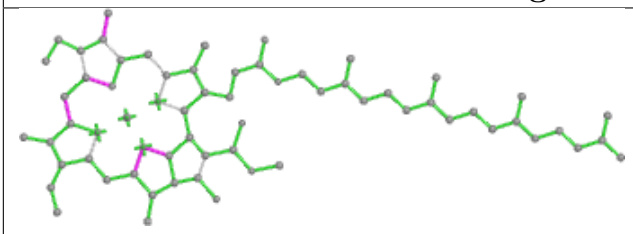


Torsions

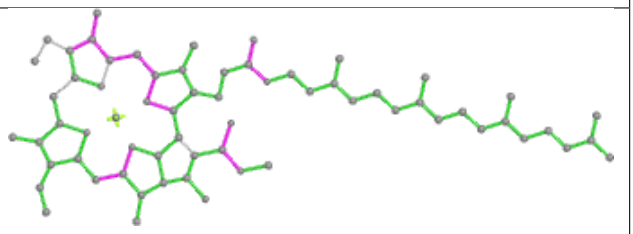


Rings

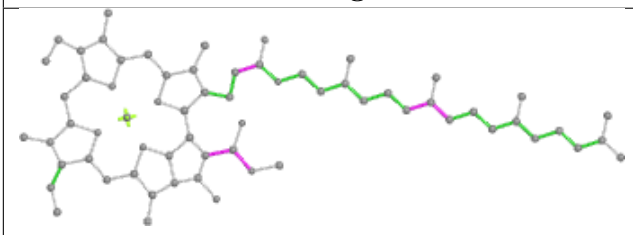
Ligand CLA c 512



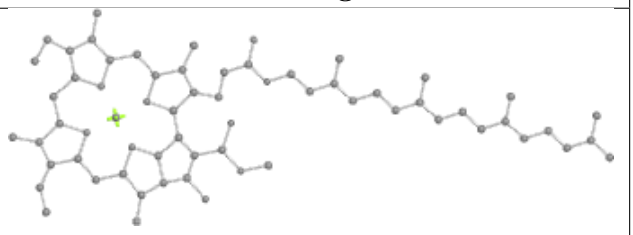
Bond lengths



Bond angles

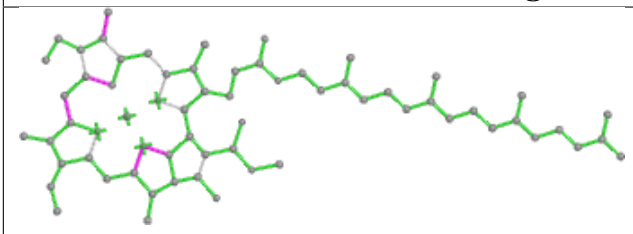


Torsions

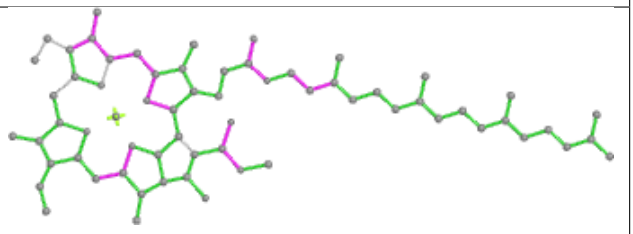


Rings

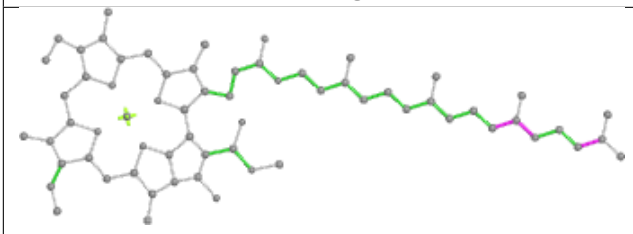
Ligand CLA B 611



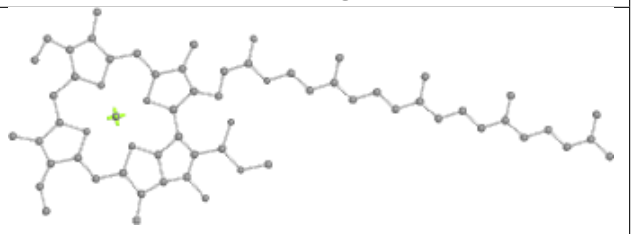
Bond lengths



Bond angles

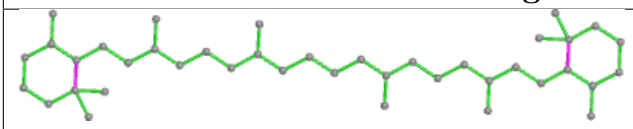


Torsions

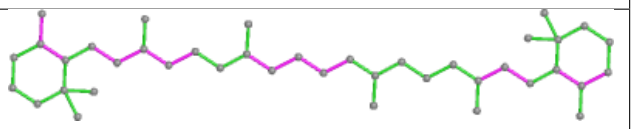


Rings

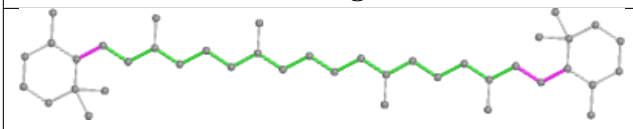
Ligand BCR B 617



Bond lengths



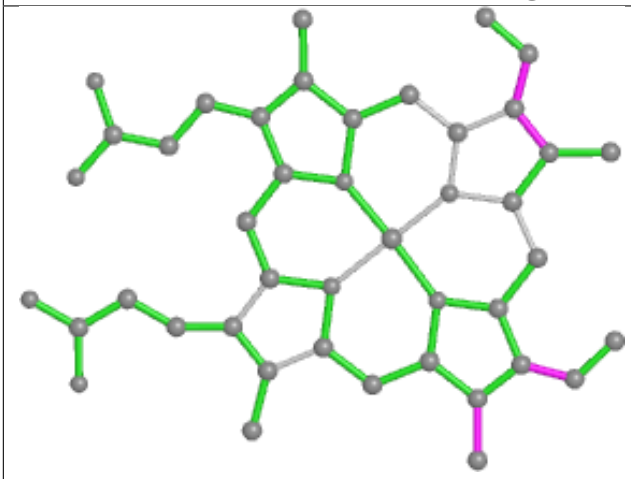
Bond angles



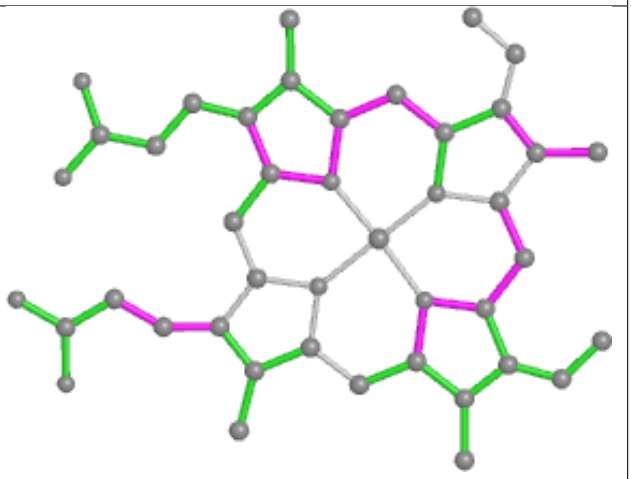
Torsions

Rings

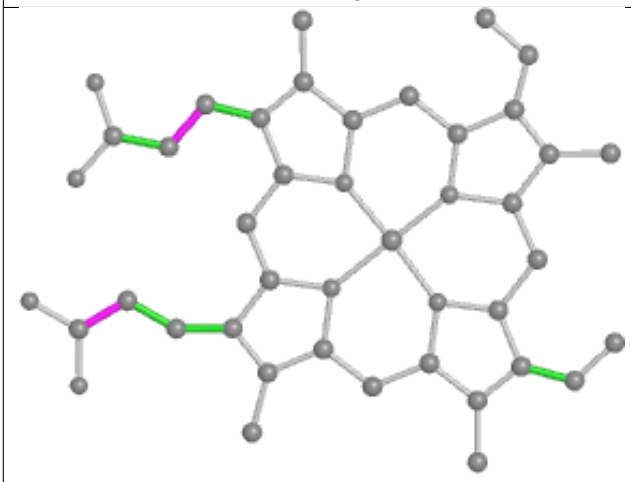
Ligand HEM e 101



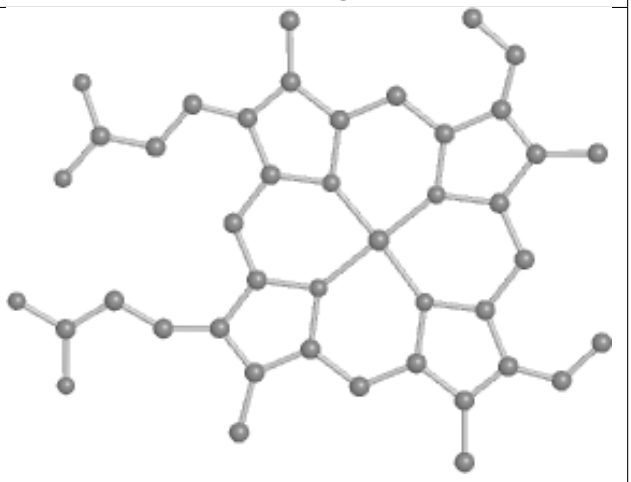
Bond lengths



Bond angles

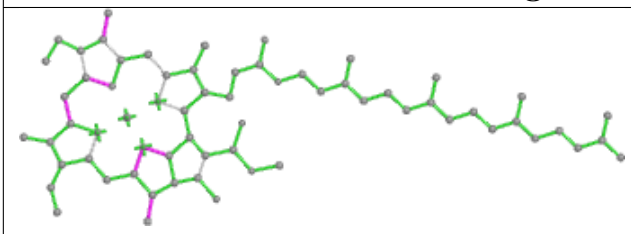


Torsions

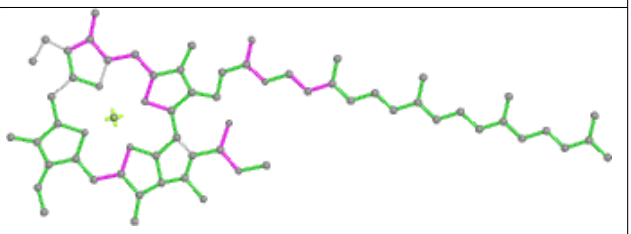


Rings

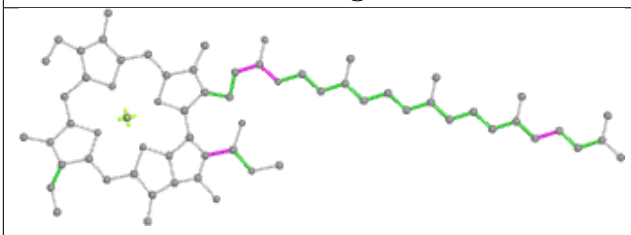
Ligand CLA B 612



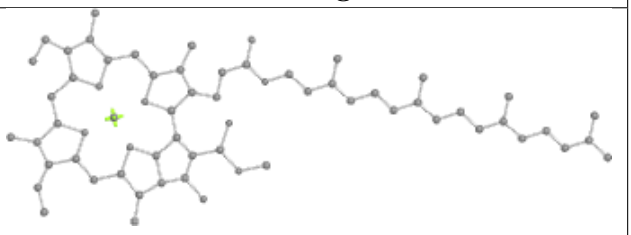
Bond lengths



Bond angles

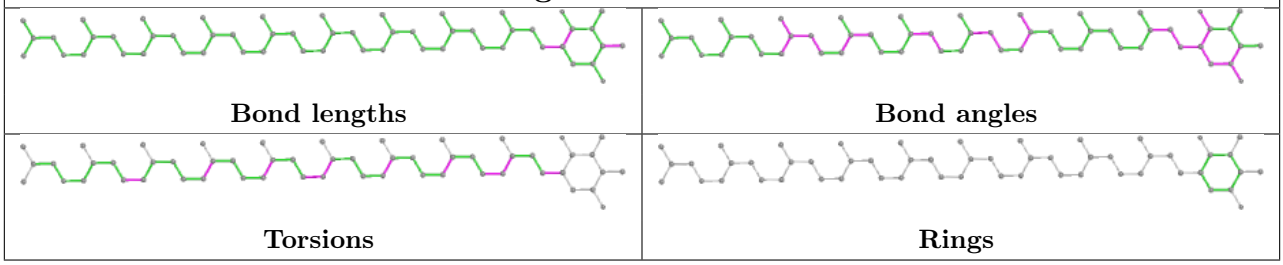


Torsions

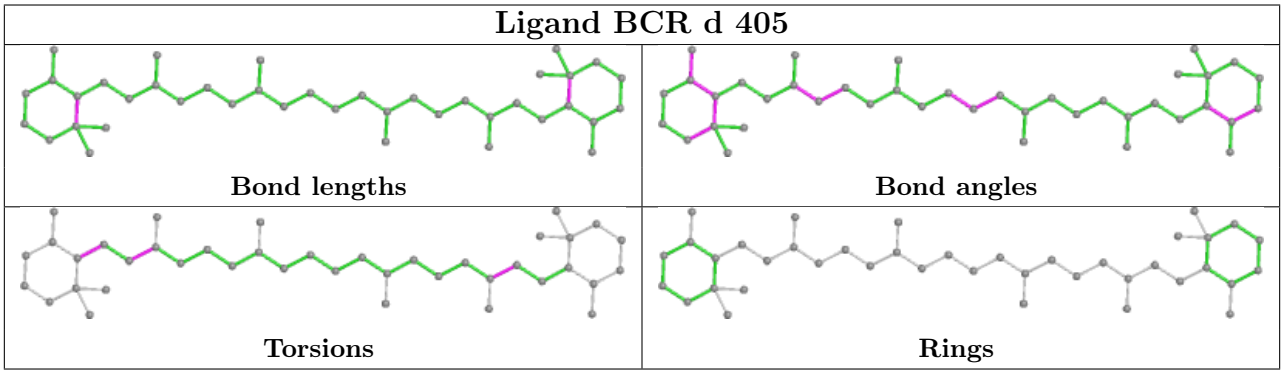


Rings

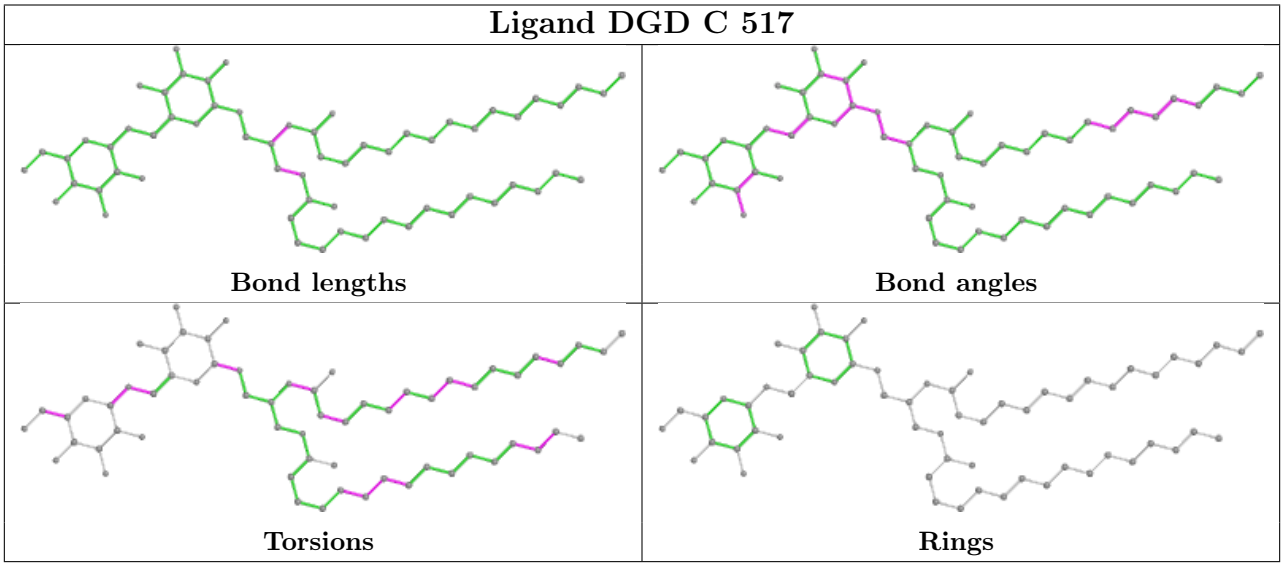
Ligand PL9 a 611



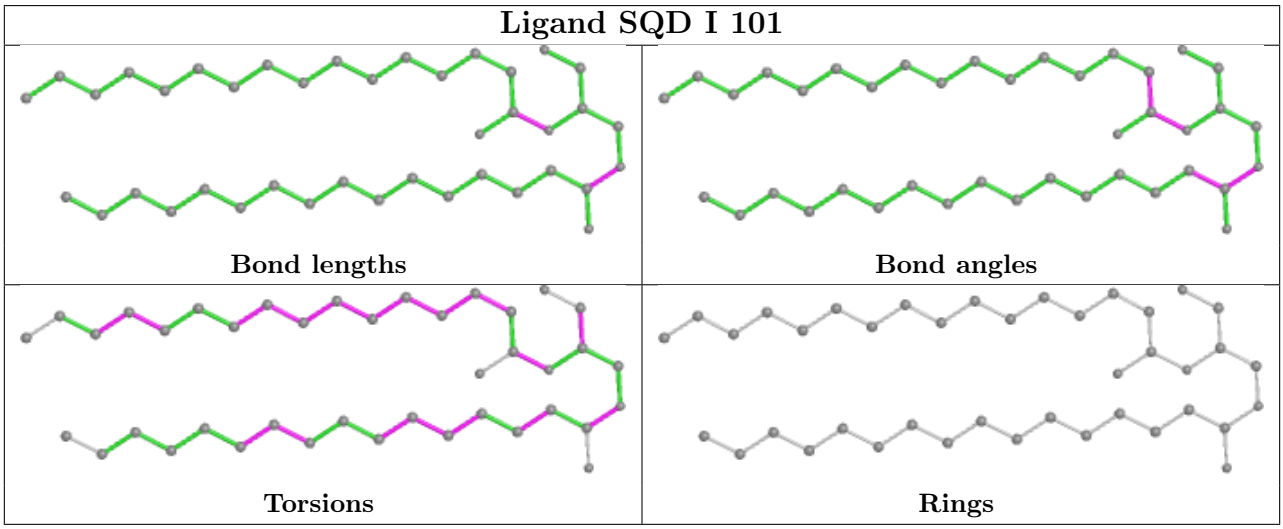
Ligand BCR d 405



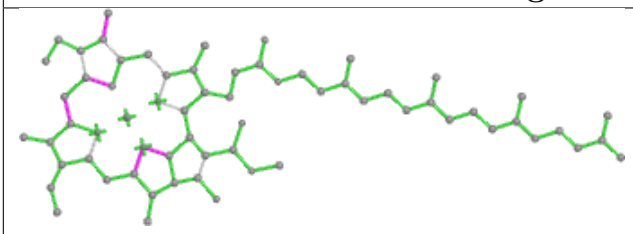
Ligand DGD C 517



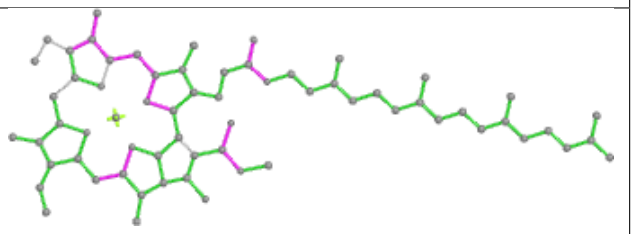
Ligand SQD I 101



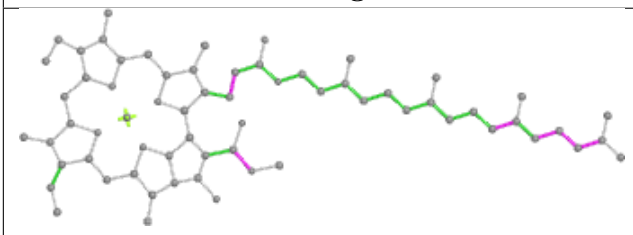
Ligand CLA b 613



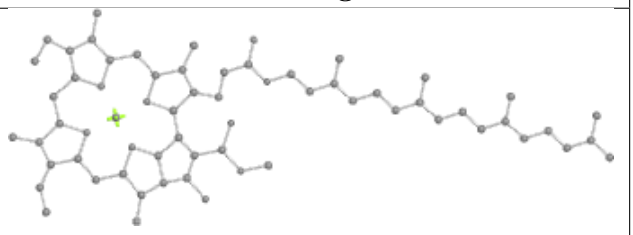
Bond lengths



Bond angles

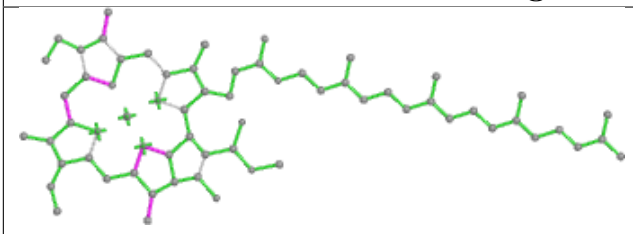


Torsions

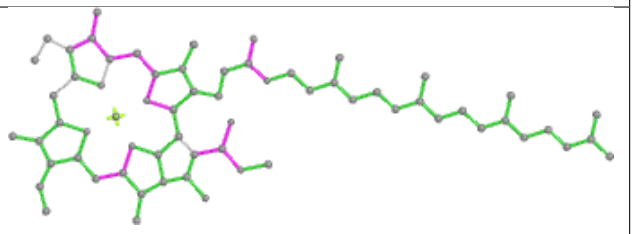


Rings

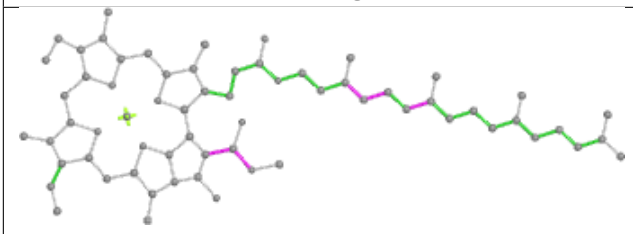
Ligand CLA b 607



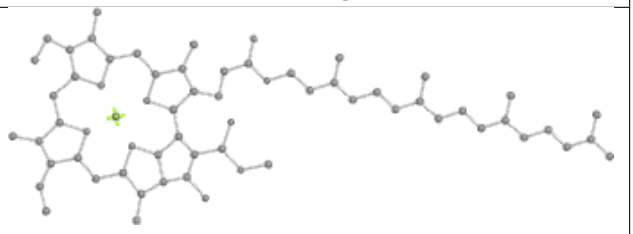
Bond lengths



Bond angles

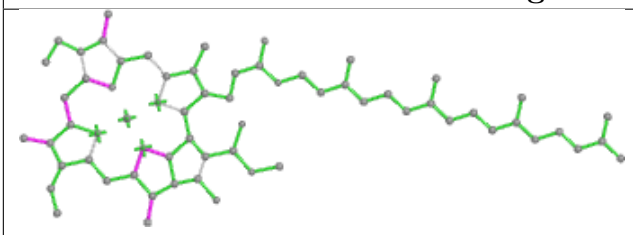


Torsions

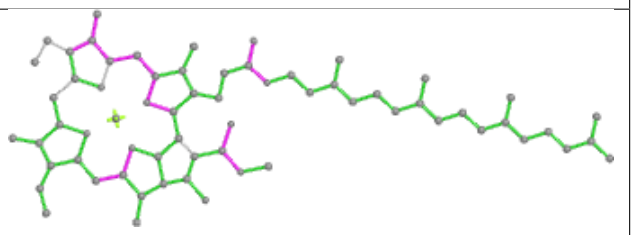


Rings

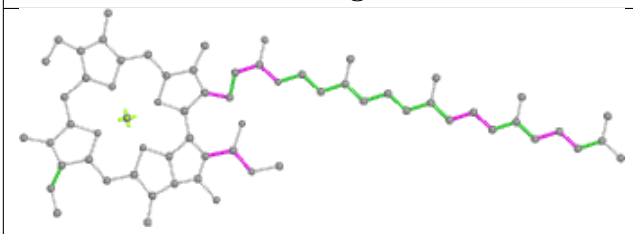
Ligand CLA b 615



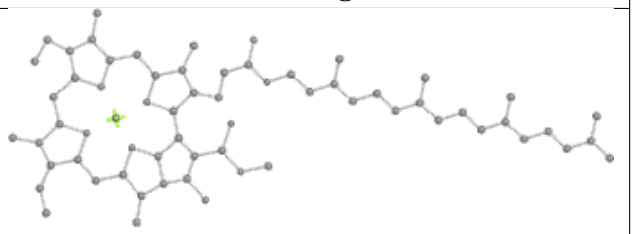
Bond lengths



Bond angles

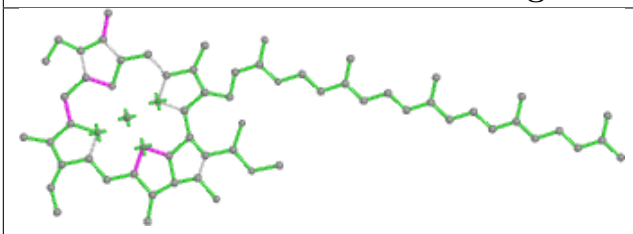


Torsions

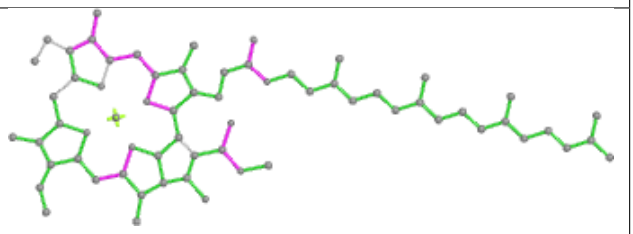


Rings

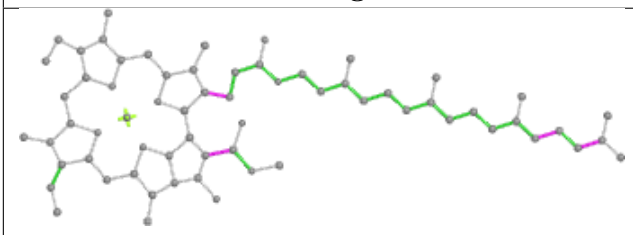
Ligand CLA d 404



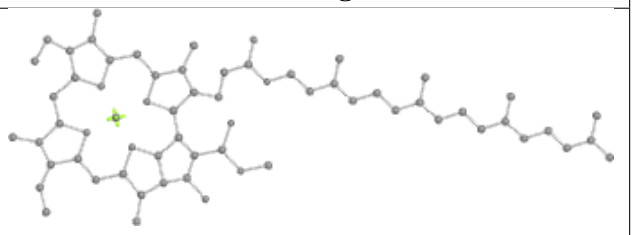
Bond lengths



Bond angles

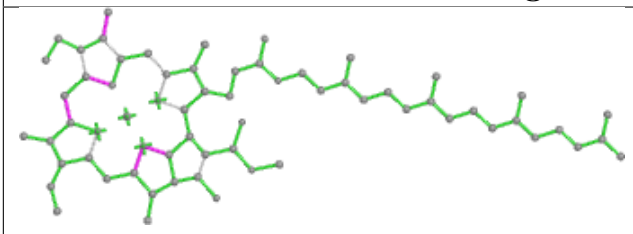


Torsions

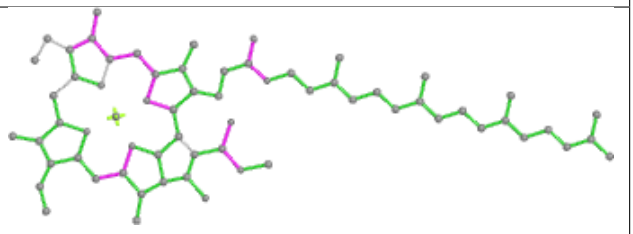


Rings

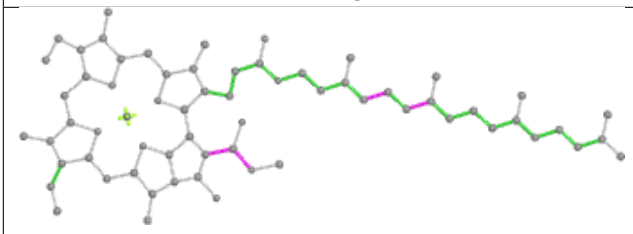
Ligand CLA B 604



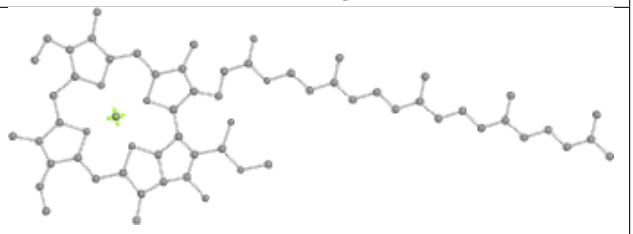
Bond lengths



Bond angles

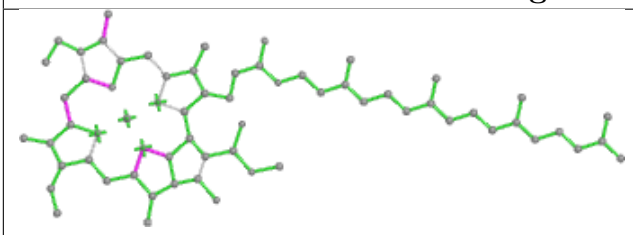


Torsions

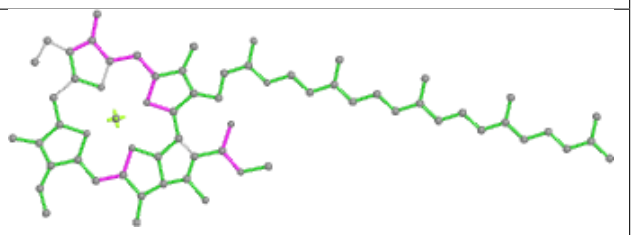


Rings

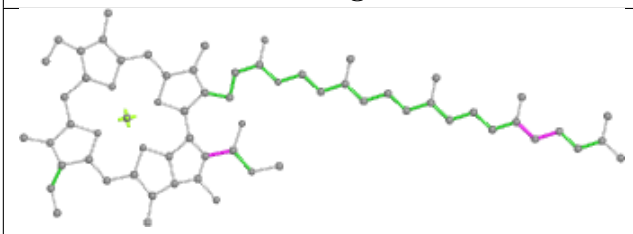
Ligand CLA c 506



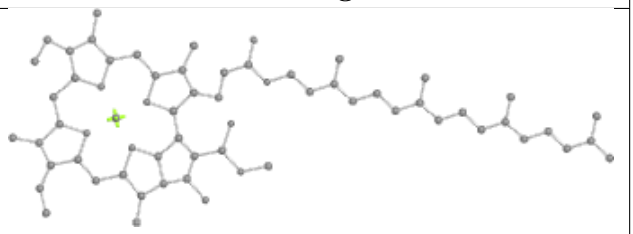
Bond lengths



Bond angles

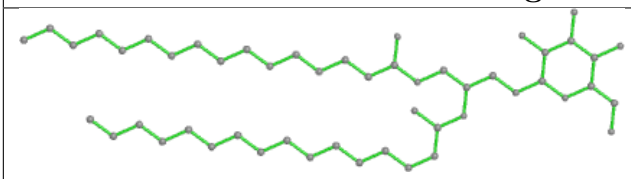


Torsions

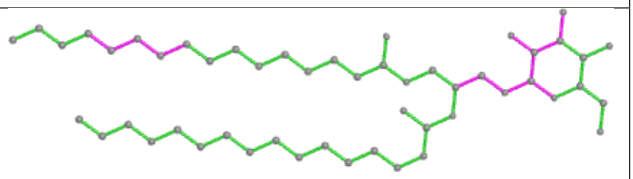


Rings

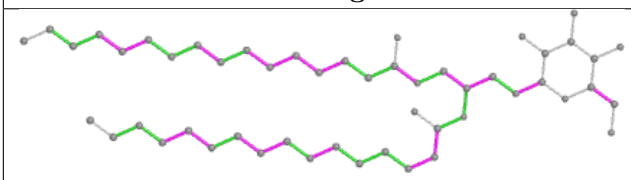
Ligand LMG c 521



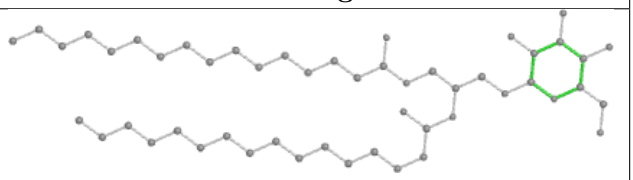
Bond lengths



Bond angles

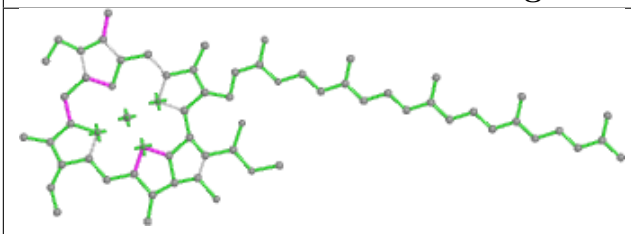


Torsions

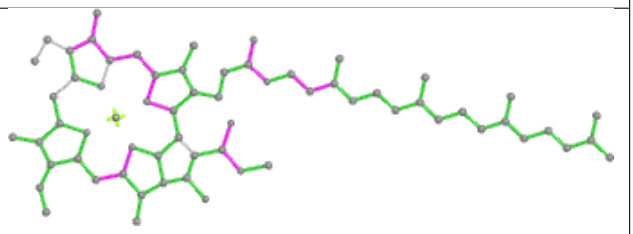


Rings

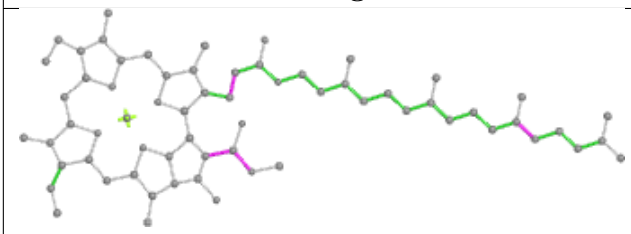
Ligand CLA B 606



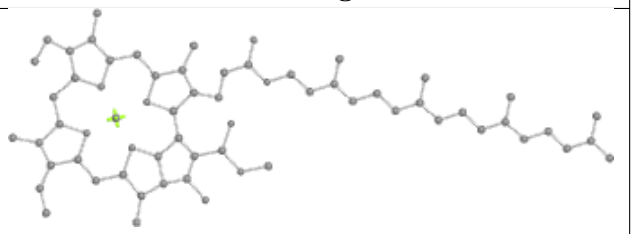
Bond lengths



Bond angles

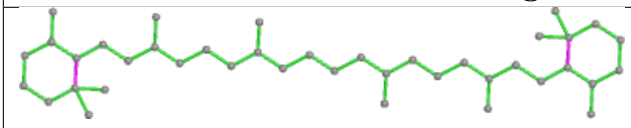


Torsions

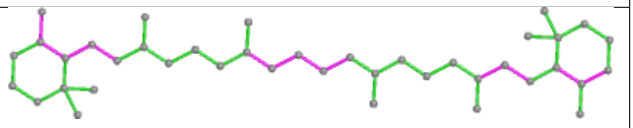


Rings

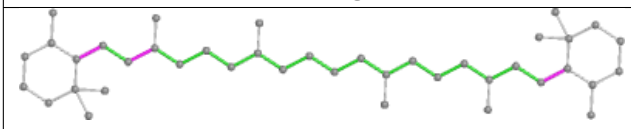
Ligand BCR A 610



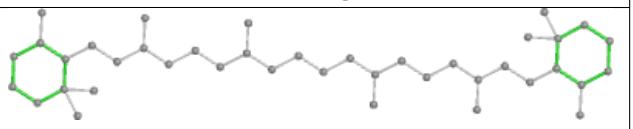
Bond lengths



Bond angles

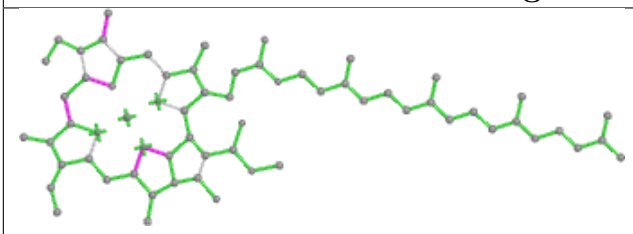


Torsions

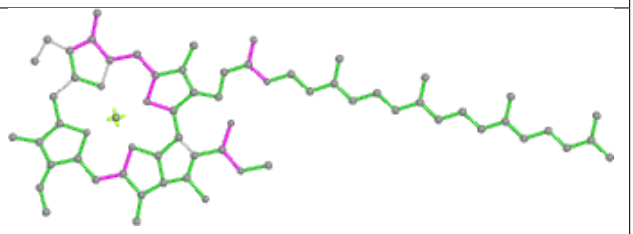


Rings

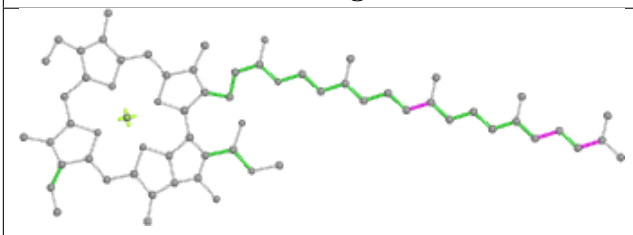
Ligand CLA D 403



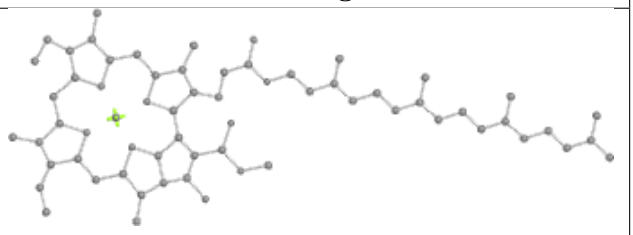
Bond lengths



Bond angles

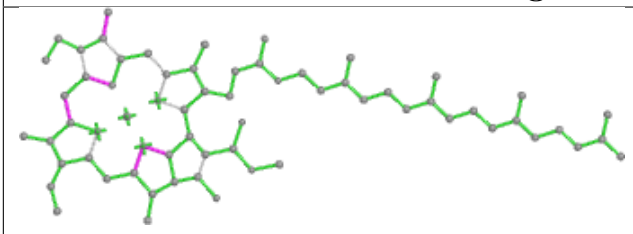


Torsions

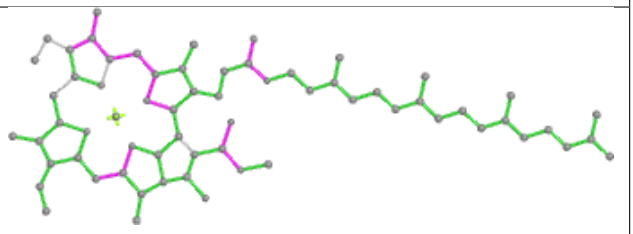


Rings

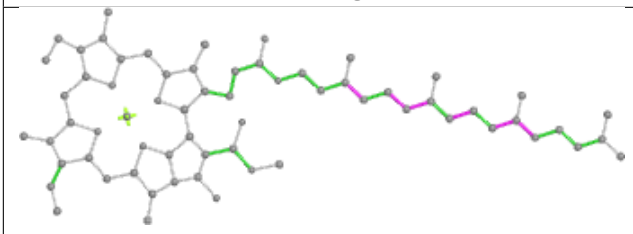
Ligand CLA b 605



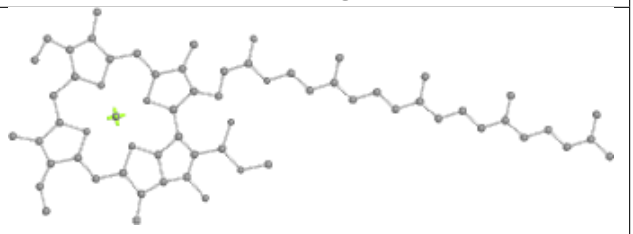
Bond lengths



Bond angles

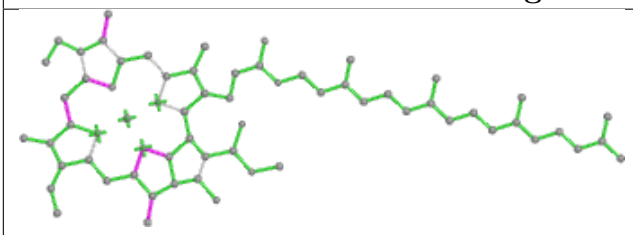


Torsions

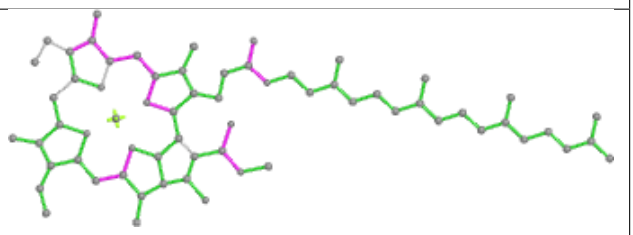


Rings

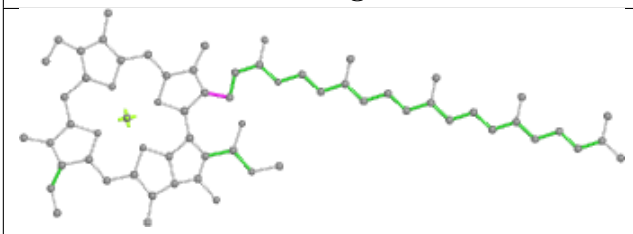
Ligand CLA C 503



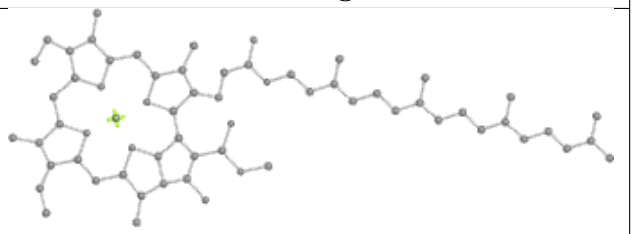
Bond lengths



Bond angles

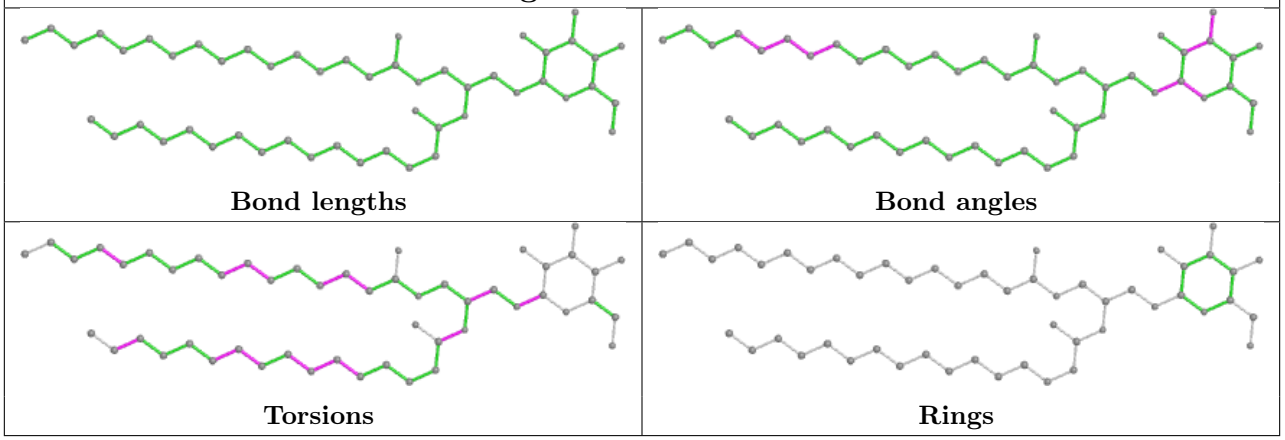


Torsions

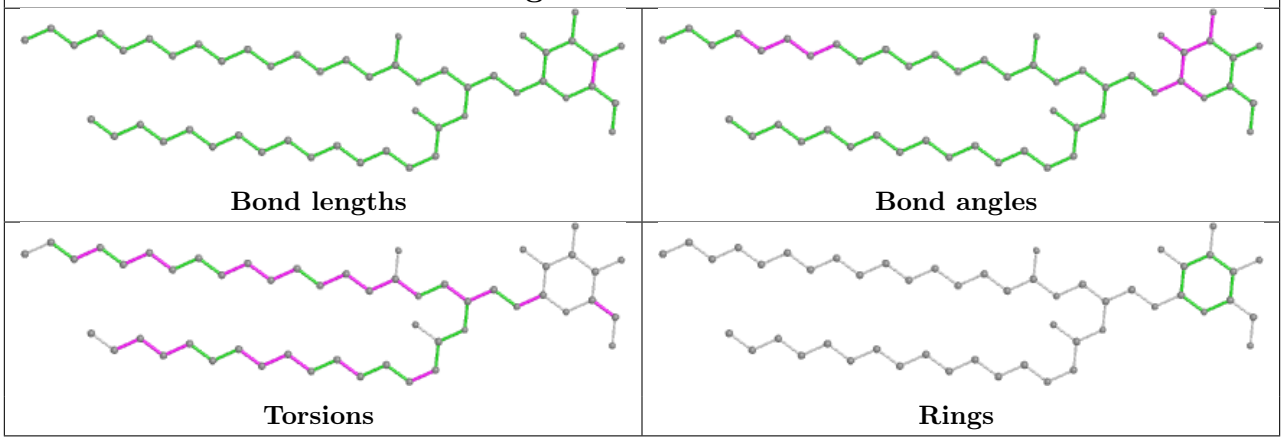


Rings

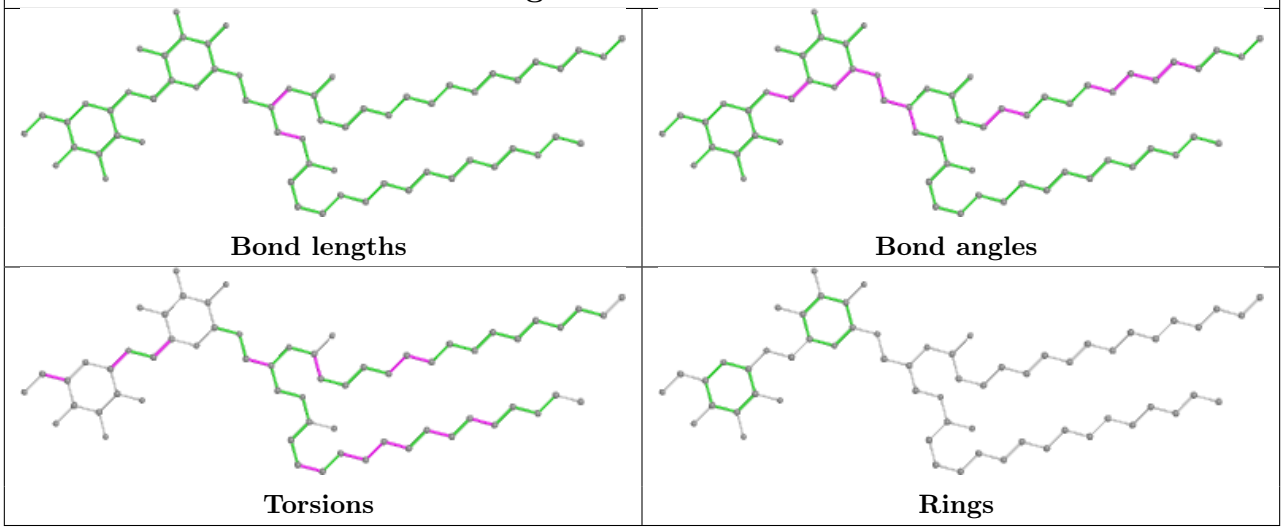
Ligand LMG A 612



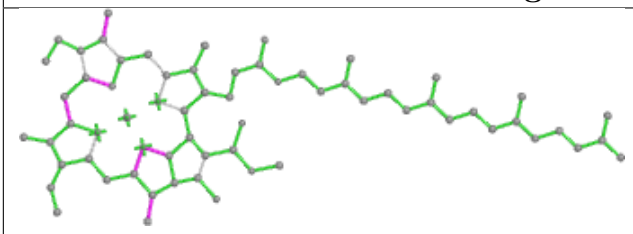
Ligand LMG c 502



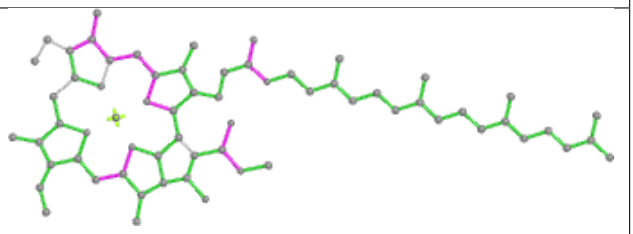
Ligand DGD c 518



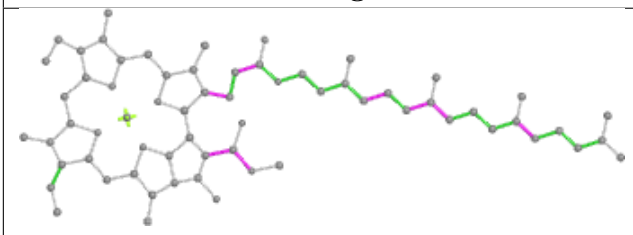
Ligand CLA C 512



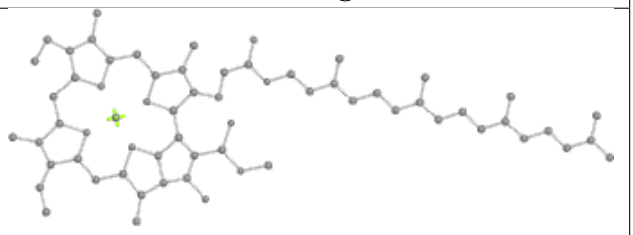
Bond lengths



Bond angles

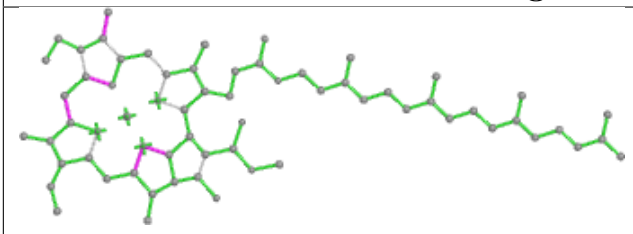


Torsions

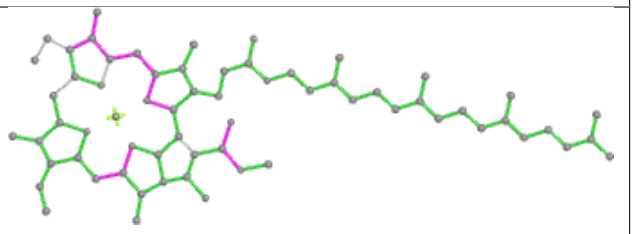


Rings

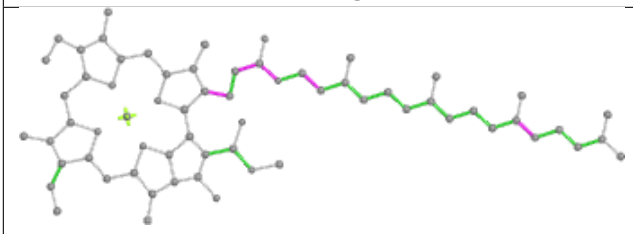
Ligand CLA d 403



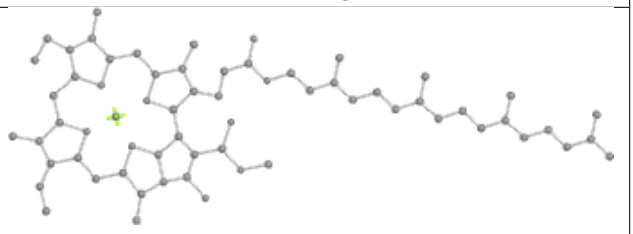
Bond lengths



Bond angles

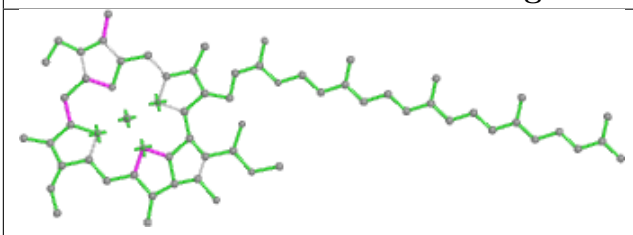


Torsions

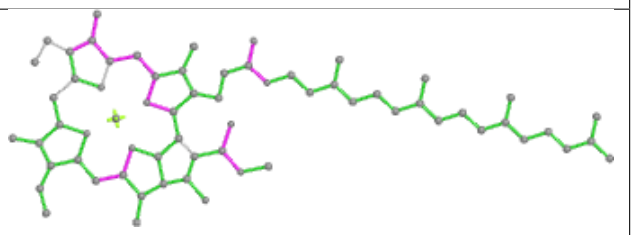


Rings

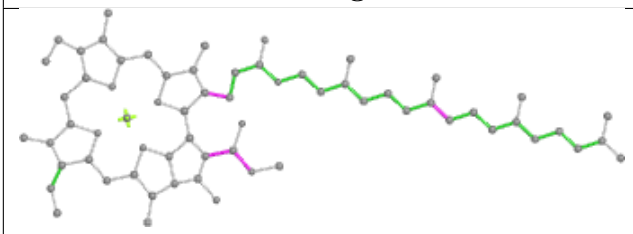
Ligand CLA C 513



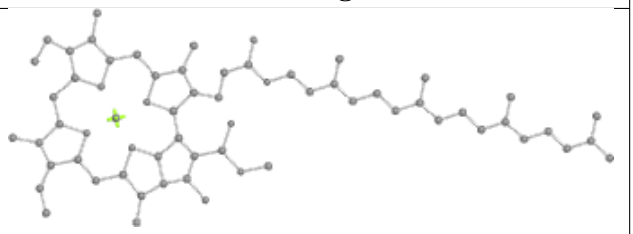
Bond lengths



Bond angles

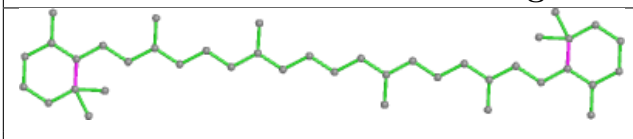


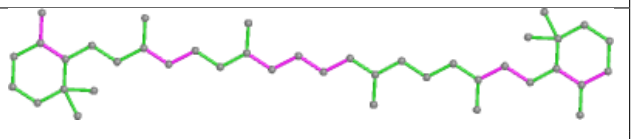
Torsions

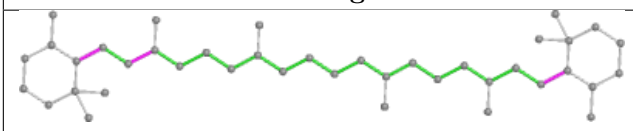


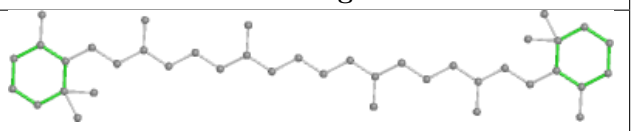
Rings

Ligand BCR c 517

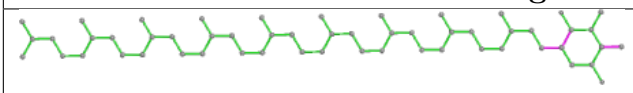

Bond lengths

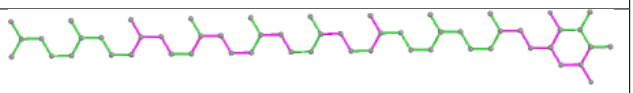

Bond angles

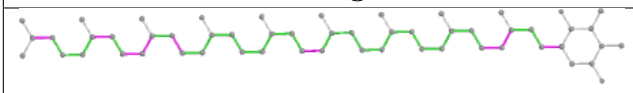

Torsions

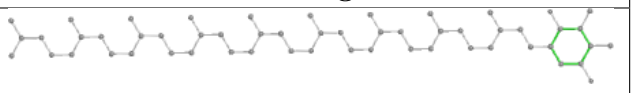

Rings

Ligand PL9 A 611

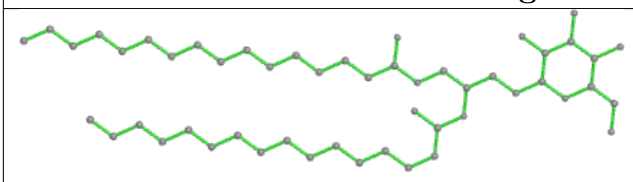

Bond lengths

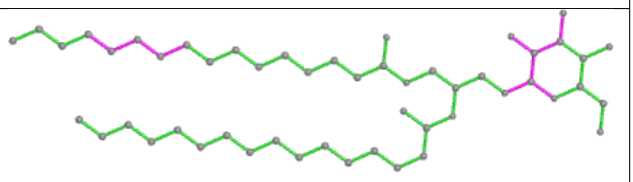

Bond angles

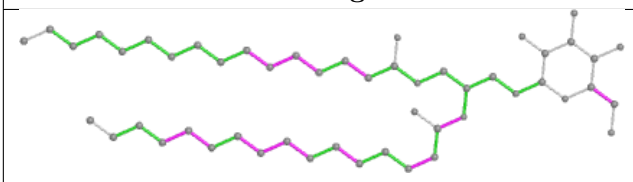

Torsions

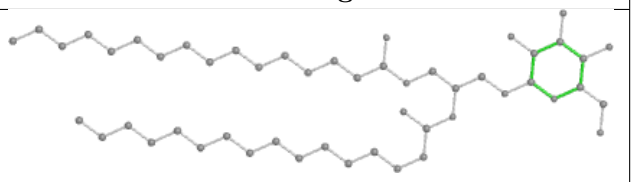

Rings

Ligand LMG D 405

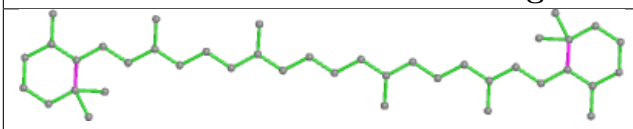

Bond lengths

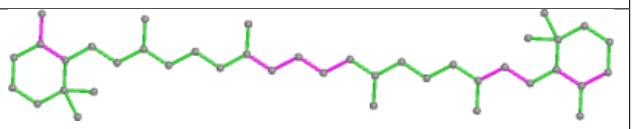

Bond angles

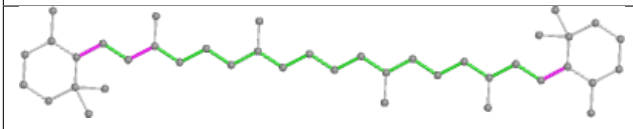

Torsions

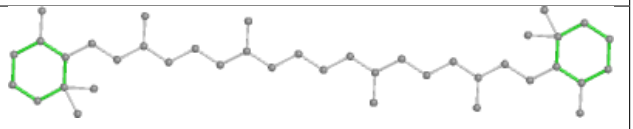

Rings

Ligand BCR a 610

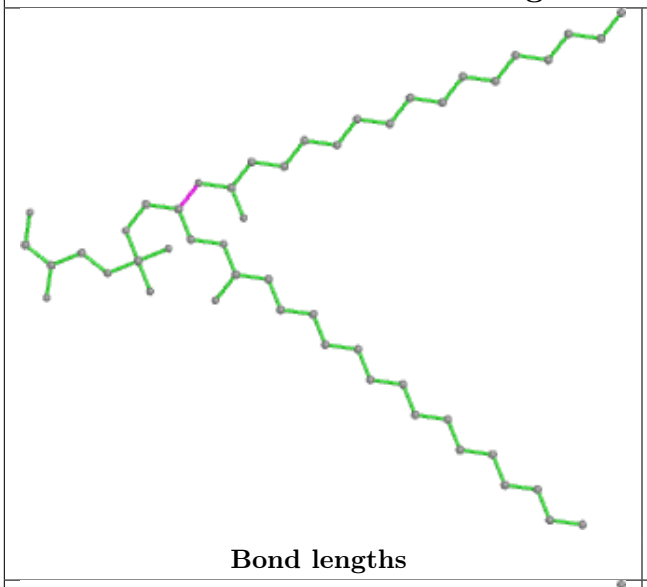

Bond lengths


Bond angles

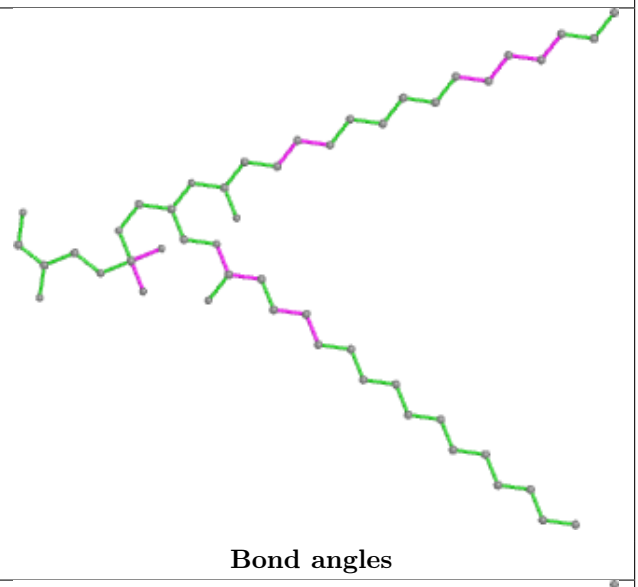

Torsions


Rings

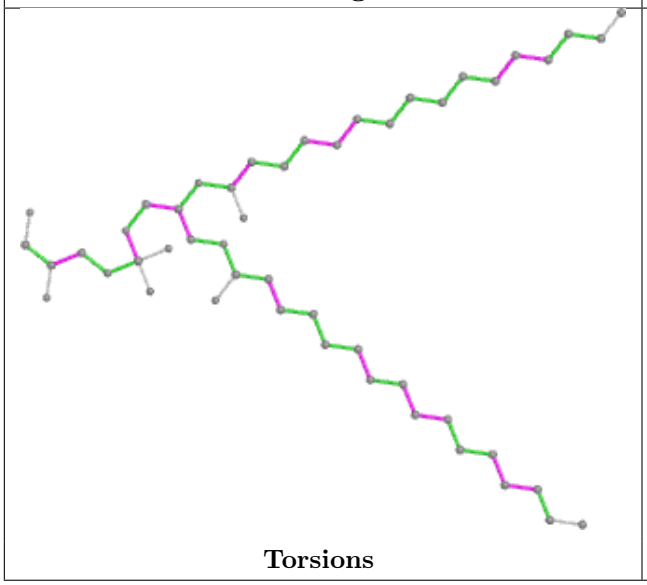
Ligand LHG L 101



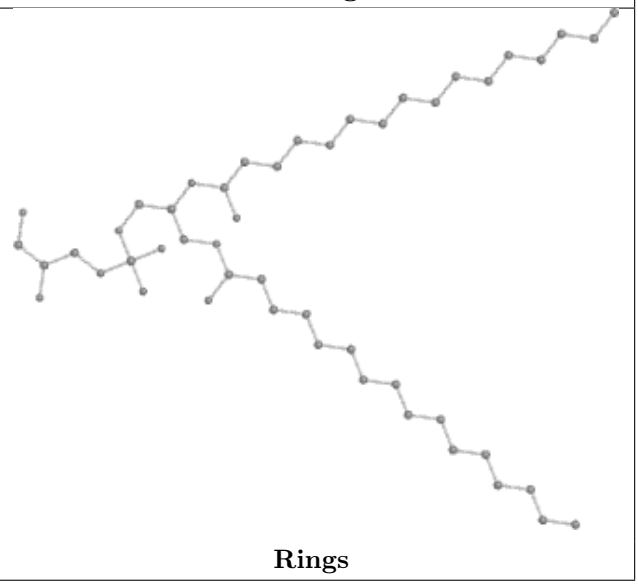
Bond lengths



Bond angles

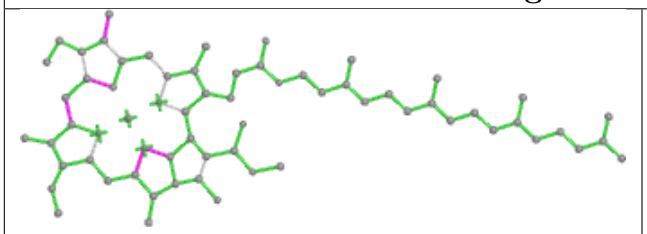


Torsions

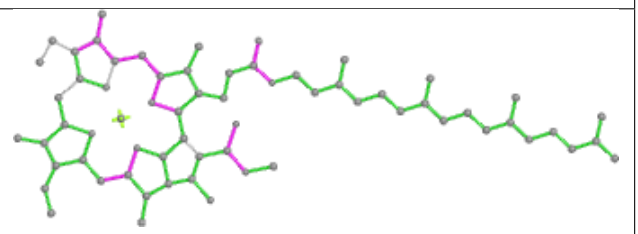


Rings

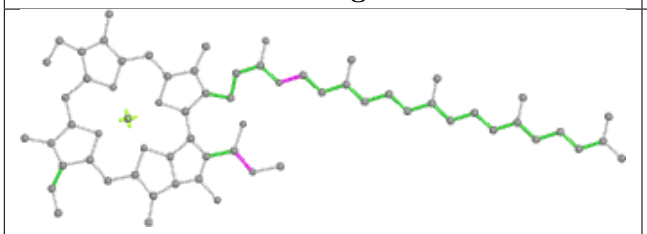
Ligand CLA A 606



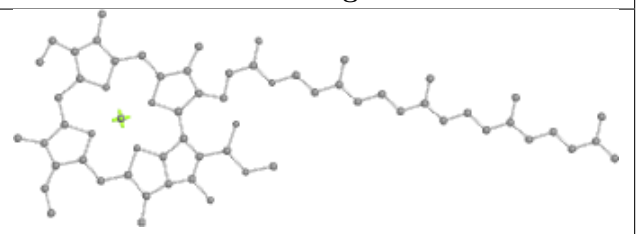
Bond lengths



Bond angles

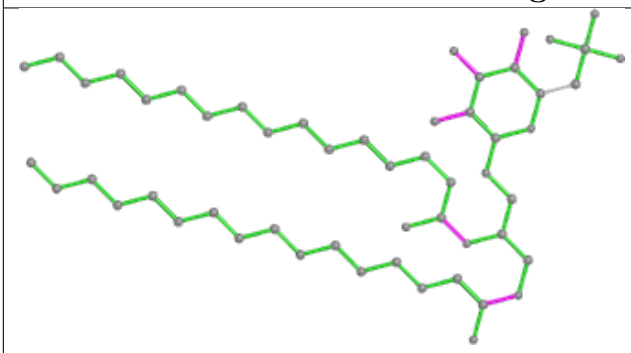


Torsions

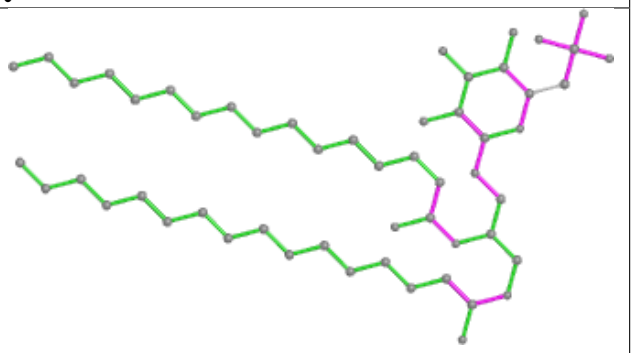


Rings

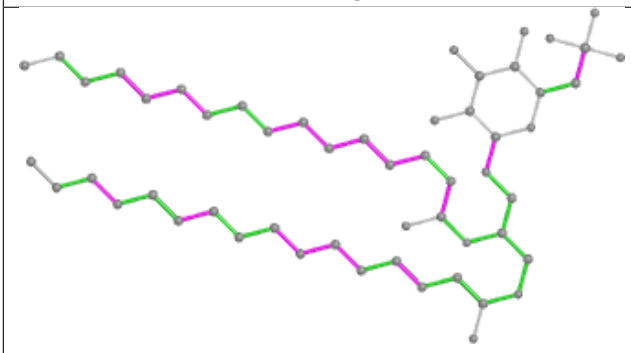
Ligand SQD c 501



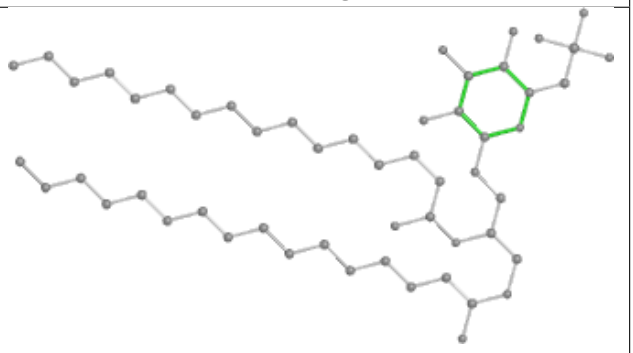
Bond lengths



Bond angles

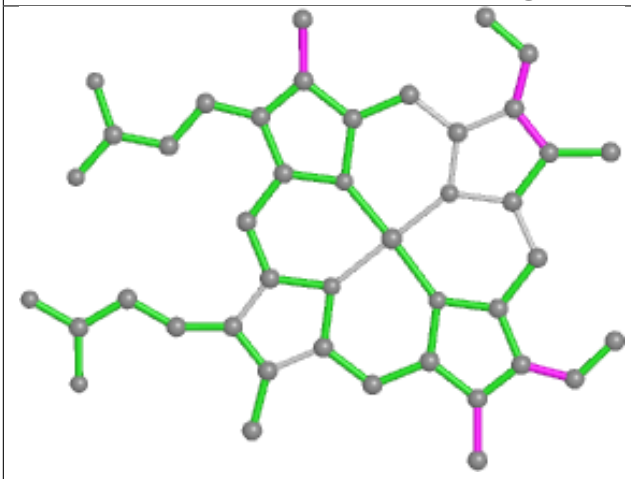


Torsions

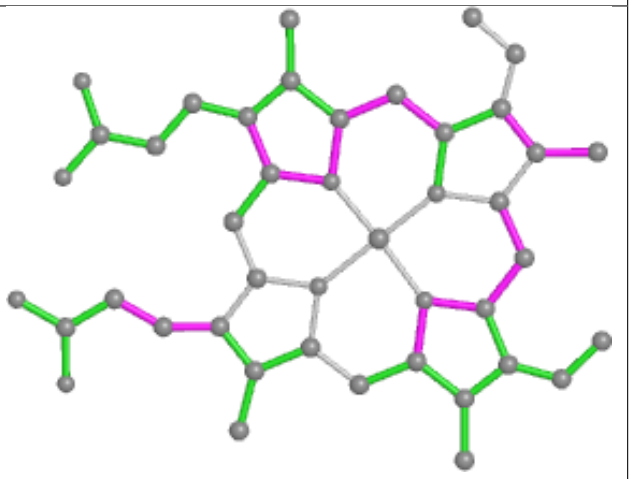


Rings

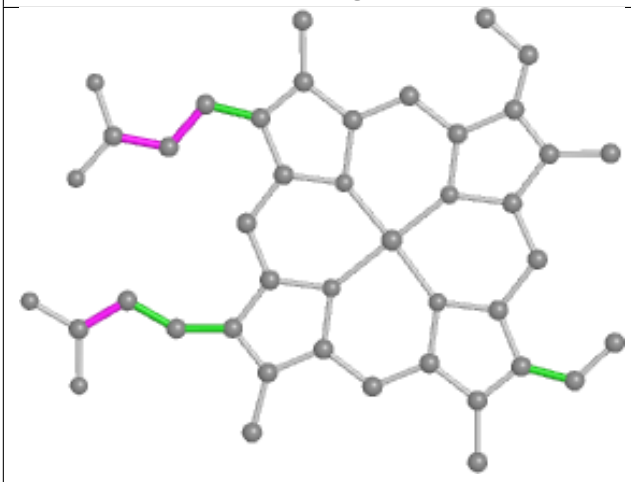
Ligand HEM E 101



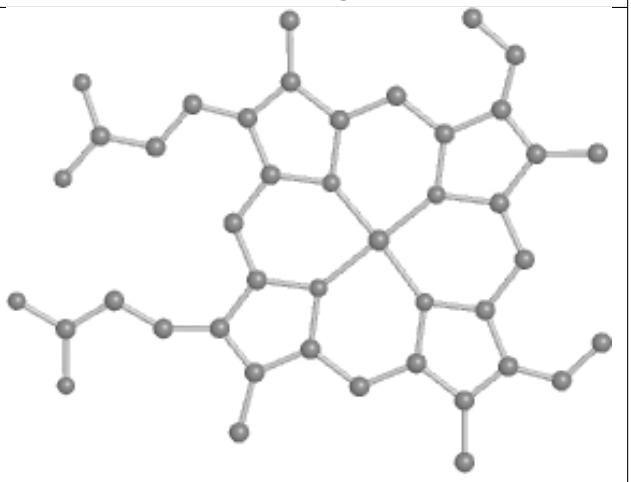
Bond lengths



Bond angles

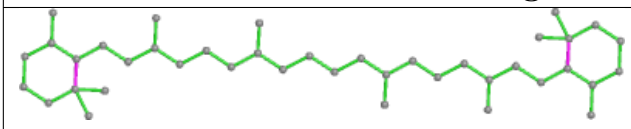


Torsions

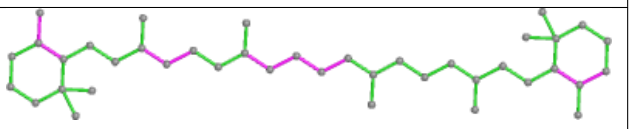


Rings

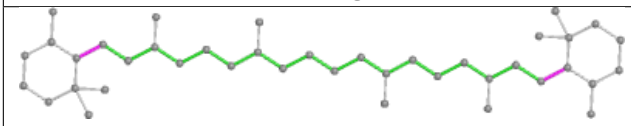
Ligand BCR B 618



Bond lengths



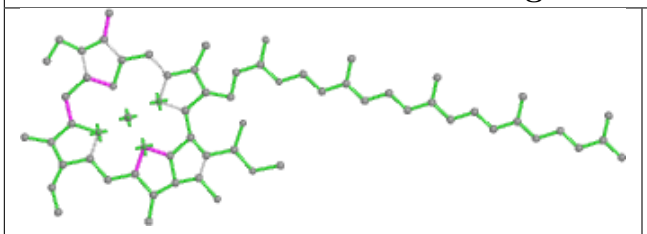
Bond angles



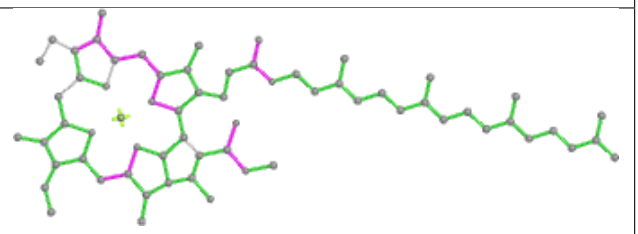
Torsions

Rings

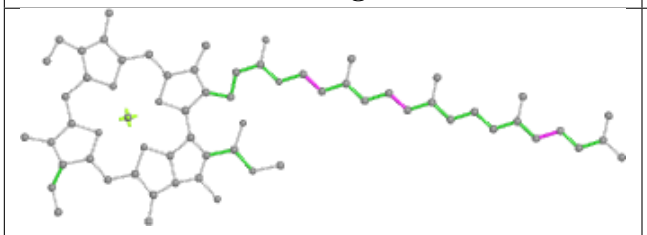
Ligand CLA B 613



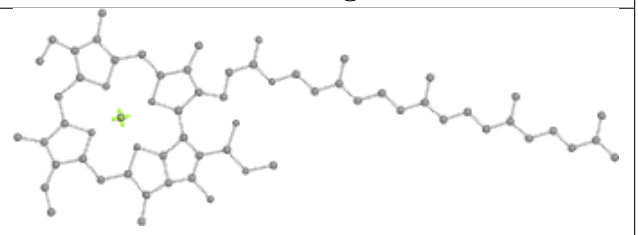
Bond lengths



Bond angles

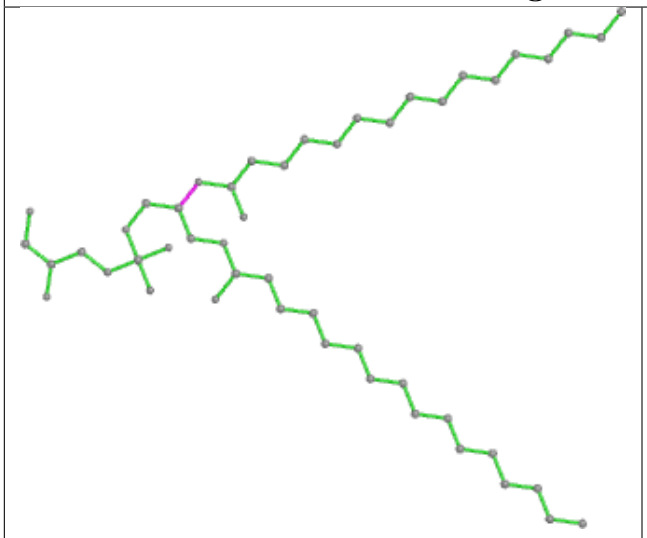


Torsions

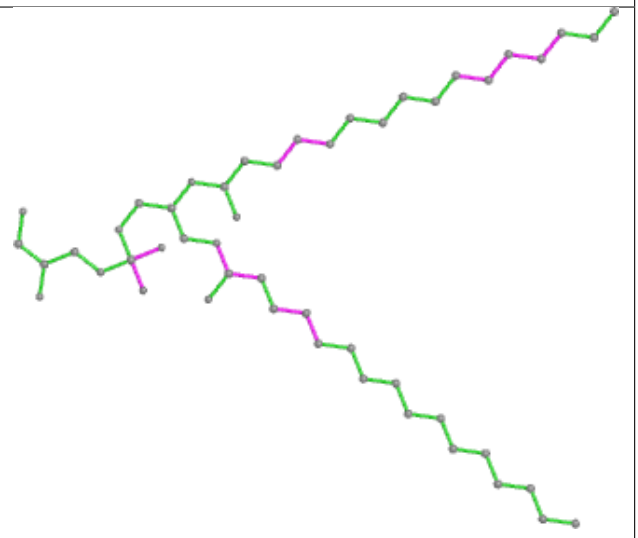


Rings

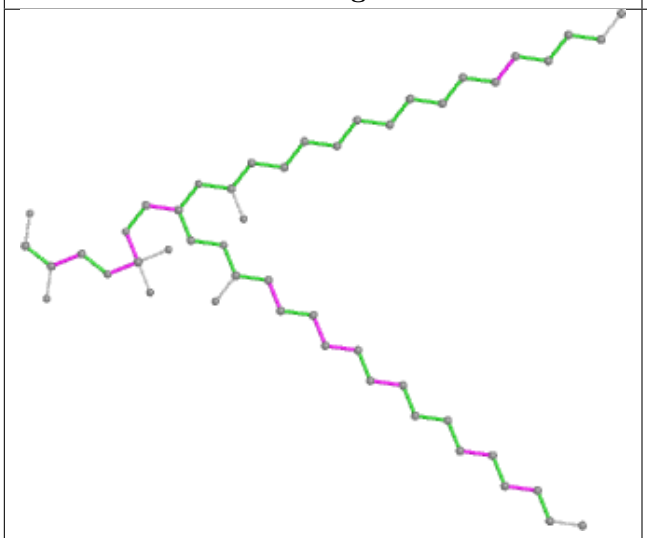
Ligand LHG d 407



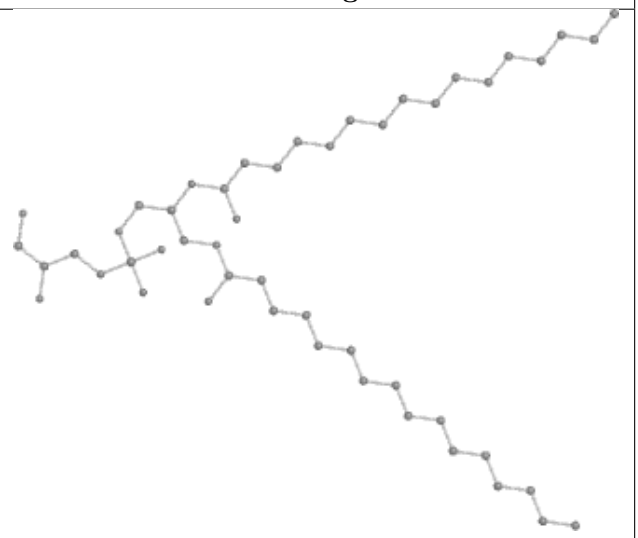
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.35	1 (0%) 94 84	28, 38, 60, 76	0
1	a	334/344 (97%)	-0.43	0 100 100	28, 38, 60, 76	0
2	B	504/510 (98%)	-0.17	12 (2%) 59 30	27, 41, 66, 86	0
2	b	504/510 (98%)	-0.22	4 (0%) 86 65	29, 42, 67, 85	0
3	C	451/461 (97%)	-0.26	5 (1%) 80 56	30, 45, 61, 75	0
3	c	451/461 (97%)	-0.23	4 (0%) 84 63	31, 46, 63, 93	0
4	D	341/352 (96%)	-0.39	2 (0%) 89 72	28, 39, 56, 67	0
4	d	341/352 (96%)	-0.37	0 100 100	29, 40, 55, 78	0
5	E	81/84 (96%)	-0.05	0 100 100	39, 54, 72, 89	0
5	e	82/84 (97%)	0.25	3 (3%) 41 17	43, 61, 75, 80	0
6	F	34/45 (75%)	-0.35	1 (2%) 51 23	40, 50, 63, 77	0
6	f	34/45 (75%)	-0.42	0 100 100	39, 51, 69, 72	0
7	H	63/66 (95%)	0.03	1 (1%) 72 44	39, 47, 57, 63	0
7	h	63/66 (95%)	-0.09	1 (1%) 72 44	35, 47, 58, 68	0
8	I	35/38 (92%)	0.10	1 (2%) 51 23	29, 44, 71, 73	0
8	i	35/38 (92%)	0.05	3 (8%) 10 3	33, 43, 74, 94	0
9	J	36/40 (90%)	-0.24	0 100 100	44, 58, 68, 75	0
9	j	36/40 (90%)	0.00	2 (5%) 24 8	49, 57, 72, 79	0
10	K	37/46 (80%)	-0.00	0 100 100	45, 59, 75, 89	0
10	k	37/46 (80%)	-0.07	0 100 100	47, 56, 72, 79	0
11	L	37/37 (100%)	-0.33	1 (2%) 54 26	32, 38, 62, 84	0
11	l	37/37 (100%)	-0.34	1 (2%) 54 26	29, 38, 69, 81	0
12	M	32/36 (88%)	-0.15	2 (6%) 20 6	33, 38, 56, 74	0
12	m	32/36 (88%)	0.03	3 (9%) 8 3	31, 41, 59, 64	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/272 (89%)	-0.06	8 (3%) 46 20	30, 47, 81, 111	0
13	o	244/272 (89%)	-0.06	6 (2%) 57 29	31, 46, 80, 127	0
14	T	29/32 (90%)	-0.39	0 100 100	30, 39, 60, 74	0
14	t	29/32 (90%)	-0.46	0 100 100	31, 36, 63, 66	0
15	U	97/134 (72%)	-0.03	0 100 100	36, 49, 69, 75	0
15	u	97/134 (72%)	-0.27	0 100 100	32, 44, 58, 76	0
16	V	137/163 (84%)	-0.18	0 100 100	34, 47, 59, 74	0
16	v	137/163 (84%)	-0.03	1 (0%) 87 69	34, 54, 67, 81	0
17	Y	30/46 (65%)	0.52	3 (10%) 7 2	60, 73, 84, 87	0
17	y	30/46 (65%)	0.15	2 (6%) 17 5	49, 65, 78, 83	0
18	X	38/41 (92%)	0.14	2 (5%) 26 10	41, 50, 65, 79	0
18	x	38/41 (92%)	0.19	2 (5%) 26 10	46, 55, 74, 76	0
19	Z	62/62 (100%)	0.48	5 (8%) 12 3	52, 69, 88, 98	0
19	z	62/62 (100%)	0.56	8 (12%) 3 1	51, 72, 97, 105	0
20	R	34/41 (82%)	0.89	3 (8%) 10 3	65, 73, 83, 86	0
20	r	34/41 (82%)	0.59	0 100 100	65, 78, 86, 90	0
All	All	5313/5700 (93%)	-0.18	87 (1%) 72 44	27, 44, 72, 127	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	35	SER	6.9
13	o	3	GLN	6.1
12	M	33	GLN	5.1
16	v	18	THR	5.0
12	m	31	SER	4.6
2	B	487	SER	4.2
18	x	2	THR	4.1
13	O	62	GLU	4.0
12	m	32	GLN	4.0
13	o	4	THR	3.9
12	m	33	GLN	3.7
11	l	1	MET	3.6
19	z	34	ASP	3.5
2	B	494	GLY	3.4
3	c	24	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	504	THR	3.3
11	L	1	MET	3.3
18	X	38	GLN	3.2
8	i	35	LYS	3.2
8	i	34	ARG	3.2
8	I	34	ARG	3.1
13	O	4	THR	3.1
19	z	62	VAL	3.1
3	C	27	ASP	3.1
8	i	36	ASP	3.0
6	F	12	SER	3.0
13	O	34	SER	2.9
2	B	351	GLY	2.9
13	O	63	ALA	2.9
3	c	192	GLY	2.8
20	R	6	LEU	2.8
19	z	3	ILE	2.8
19	z	1	MET	2.8
13	o	35	SER	2.8
2	B	497	GLN	2.7
2	b	482	ILE	2.7
2	B	294	SER	2.7
17	Y	20	ALA	2.7
3	C	29	GLU	2.6
13	o	6	THR	2.6
13	O	207	ARG	2.6
19	Z	32	ASP	2.6
2	B	127	ARG	2.5
9	j	7	ARG	2.5
12	M	31	SER	2.5
19	Z	33	TRP	2.4
18	x	38	GLN	2.4
2	B	503	THR	2.4
9	j	5	GLY	2.4
3	c	23	ALA	2.4
7	h	63	LYS	2.3
2	b	496	TYR	2.3
3	C	30	SER	2.3
13	O	55	GLU	2.3
13	O	23	ASP	2.3
18	X	2	THR	2.3
19	z	35	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	Y	41	VAL	2.2
1	A	11	ALA	2.2
19	z	31	GLN	2.2
7	H	5	THR	2.2
3	C	142	GLU	2.2
2	B	495	PHE	2.2
17	y	42	ARG	2.2
2	B	490	GLN	2.2
2	B	130	GLU	2.2
5	e	81	GLU	2.1
17	y	20	ALA	2.1
13	o	61	GLN	2.1
19	Z	29	SER	2.1
19	z	30	PRO	2.1
19	Z	3	ILE	2.1
19	Z	62	VAL	2.1
13	o	245	PRO	2.1
4	D	238	THR	2.1
4	D	240	ALA	2.1
5	e	62	SER	2.1
2	B	412	THR	2.1
3	C	23	ALA	2.1
5	e	12	ASP	2.1
2	b	294	SER	2.0
20	R	25	PRO	2.0
17	Y	43	ARG	2.0
19	z	41	PHE	2.0
2	B	292	LEU	2.0
3	c	32	GLY	2.0
20	R	10	LEU	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
8	FME	I	1	10/11	0.91	0.29	43,56,63,71	0
8	FME	i	1	10/11	0.91	0.22	35,50,56,61	0
12	FME	m	1	10/11	0.91	0.23	26,45,55,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.92	0.25	39,42,63,72	0
14	FME	T	1	10/11	0.93	0.13	44,47,53,54	0
12	FME	M	1	10/11	0.93	0.29	30,43,53,54	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMG	b	625	9/55	0.65	0.42	40,46,52,55	0
23	SQD	I	101	40/54	0.70	0.39	31,52,84,89	0
29	LMG	C	520	51/55	0.74	0.38	49,62,82,100	0
28	PL9	A	611	55/55	0.74	0.37	39,58,75,79	0
31	LHG	A	618	49/49	0.74	0.29	41,72,85,94	0
30	UNL	t	101	10/-	0.76	0.28	26,41,47,47	0
29	LMG	b	624	51/55	0.76	0.32	45,64,76,86	0
30	UNL	b	603	13/-	0.77	0.29	39,48,61,62	0
31	LHG	a	615	42/49	0.77	0.32	54,78,89,100	0
29	LMG	c	502	51/55	0.78	0.31	34,57,80,83	0
23	SQD	D	409	43/54	0.79	0.29	37,68,89,98	0
29	LMG	d	409	40/55	0.79	0.31	40,55,76,77	0
23	SQD	A	619	40/54	0.79	0.28	25,48,67,69	0
29	LMG	c	521	51/55	0.80	0.32	33,65,83,88	0
29	LMG	c	522	51/55	0.80	0.38	36,68,83,90	0
29	LMG	B	621	51/55	0.80	0.30	32,56,71,74	0
27	BCR	H	102	40/40	0.80	0.32	34,51,59,65	0
30	UNL	j	101	9/-	0.80	0.28	40,49,60,63	0
23	SQD	D	408	47/54	0.80	0.27	17,53,103,121	0
29	LMG	A	612	51/55	0.80	0.33	34,59,76,85	0
29	LMG	A	613	51/55	0.80	0.30	31,53,78,84	0
30	UNL	m	101	5/-	0.81	0.28	26,32,37,41	0
30	UNL	B	623	11/-	0.81	0.23	35,40,47,48	0
29	LMG	B	625	51/55	0.81	0.26	28,52,74,78	0
23	SQD	b	601	54/54	0.81	0.28	39,60,90,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	LMG	C	519	51/55	0.82	0.28	42,61,73,85	0
24	CL	a	603	1/1	0.82	0.23	59,59,59,59	0
30	UNL	z	101	11/-	0.82	0.29	31,53,58,60	0
30	UNL	d	402	22/-	0.82	0.31	26,43,60,78	0
29	LMG	b	623	51/55	0.82	0.30	29,48,71,74	0
33	DGD	h	102	62/66	0.82	0.29	35,47,63,73	0
30	UNL	m	102	16/-	0.83	0.27	37,45,51,54	0
30	UNL	M	101	6/-	0.83	0.31	41,46,52,65	0
27	BCR	y	101	40/40	0.83	0.29	50,63,70,74	0
25	CLA	c	515	65/65	0.83	0.30	45,60,78,81	0
25	CLA	C	512	65/65	0.83	0.30	42,58,68,79	0
27	BCR	k	101	40/40	0.83	0.26	37,53,59,61	0
28	PL9	a	611	55/55	0.84	0.29	40,59,72,73	0
27	BCR	Y	101	40/40	0.84	0.26	46,60,72,76	0
27	BCR	h	101	40/40	0.84	0.27	31,45,55,62	0
30	UNL	C	521	9/-	0.84	0.28	36,42,46,49	0
30	UNL	H	101	8/-	0.84	0.20	29,35,43,47	0
25	CLA	b	604	65/65	0.84	0.28	44,59,76,88	0
23	SQD	B	626	54/54	0.84	0.24	33,52,85,90	0
23	SQD	c	501	54/54	0.84	0.32	38,58,76,77	0
25	CLA	c	514	65/65	0.85	0.27	45,59,78,83	0
30	UNL	i	101	12/-	0.85	0.28	24,39,51,51	0
25	CLA	B	601	65/65	0.85	0.29	41,59,84,96	0
27	BCR	C	514	40/40	0.85	0.29	45,56,64,66	0
33	DGD	H	103	62/66	0.85	0.27	26,41,53,61	0
25	CLA	C	511	65/65	0.85	0.26	45,57,66,70	0
25	CLA	B	606	65/65	0.86	0.28	29,44,65,84	0
27	BCR	c	516	40/40	0.86	0.32	33,63,70,72	0
27	BCR	B	627	40/40	0.86	0.26	30,41,49,53	0
25	CLA	C	504	65/65	0.86	0.27	33,51,70,78	0
30	UNL	B	622	6/-	0.86	0.24	26,42,50,56	0
29	LMG	B	620	51/55	0.86	0.24	27,46,67,75	0
23	SQD	A	603	52/54	0.86	0.30	38,60,78,82	0
25	CLA	c	508	65/65	0.87	0.25	34,49,72,78	0
27	BCR	T	101	40/40	0.87	0.28	31,43,58,62	0
25	CLA	C	502	65/65	0.87	0.26	35,51,62,69	0
27	BCR	b	622	40/40	0.87	0.25	33,43,52,54	0
25	CLA	C	503	65/65	0.87	0.25	37,49,58,65	0
31	LHG	A	617	49/49	0.87	0.33	33,55,78,82	0
30	UNL	b	602	13/-	0.87	0.25	30,36,41,45	0
25	CLA	d	404	65/65	0.87	0.24	32,46,73,91	0
23	SQD	f	101	43/54	0.87	0.25	51,70,77,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	DGD	c	519	62/66	0.87	0.26	37,57,86,95	0
33	DGD	c	520	62/66	0.87	0.27	36,47,72,80	0
25	CLA	c	505	65/65	0.87	0.27	32,51,62,68	0
25	CLA	c	510	58/65	0.88	0.24	34,46,59,67	0
27	BCR	d	405	40/40	0.88	0.23	29,43,56,62	0
25	CLA	B	614	65/65	0.88	0.22	32,42,63,82	0
30	UNL	B	624	11/-	0.88	0.18	26,31,38,41	0
27	BCR	C	515	40/40	0.88	0.23	32,42,52,53	0
27	BCR	D	404	40/40	0.88	0.25	28,46,63,67	0
25	CLA	C	513	65/65	0.88	0.29	41,62,74,83	0
30	UNL	M	102	17/-	0.88	0.22	31,37,49,51	0
33	DGD	C	518	62/66	0.88	0.25	33,48,65,74	0
27	BCR	K	101	40/40	0.88	0.24	45,53,60,66	0
25	CLA	D	403	65/65	0.88	0.24	21,37,63,69	0
27	BCR	B	618	40/40	0.88	0.25	28,40,48,52	0
27	BCR	B	619	40/40	0.88	0.21	33,44,58,60	0
25	CLA	c	504	65/65	0.89	0.26	32,46,59,65	0
25	CLA	C	510	65/65	0.89	0.24	41,51,58,60	0
25	CLA	c	506	65/65	0.89	0.23	36,49,70,74	0
25	CLA	B	609	65/65	0.89	0.20	24,44,52,58	0
25	CLA	A	606	65/65	0.89	0.22	26,34,45,48	0
30	UNL	A	614	7/-	0.89	0.19	32,38,42,42	0
25	CLA	c	511	65/65	0.89	0.24	38,46,55,57	0
25	CLA	c	513	65/65	0.89	0.22	42,52,58,60	0
25	CLA	B	616	65/65	0.89	0.24	32,44,70,76	0
27	BCR	b	620	40/40	0.89	0.23	33,45,53,54	0
25	CLA	C	507	65/65	0.89	0.22	32,42,52,67	0
25	CLA	C	509	65/65	0.89	0.25	33,46,59,67	0
29	LMG	D	405	51/55	0.89	0.27	34,53,88,92	0
25	CLA	b	611	65/65	0.89	0.24	27,41,54,57	0
25	CLA	b	617	65/65	0.89	0.22	34,45,63,73	0
34	HEM	e	101	43/43	0.89	0.21	50,62,69,70	0
25	CLA	B	608	65/65	0.90	0.28	29,37,47,52	0
25	CLA	b	605	65/65	0.90	0.22	31,43,56,58	0
25	CLA	b	609	65/65	0.90	0.23	21,35,59,81	0
25	CLA	C	506	65/65	0.90	0.20	32,47,64,68	0
25	CLA	B	604	65/65	0.90	0.23	28,37,57,65	0
27	BCR	b	621	40/40	0.90	0.22	31,42,57,59	0
25	CLA	b	618	65/65	0.90	0.20	28,40,47,56	0
31	LHG	L	101	49/49	0.90	0.23	29,41,51,57	0
31	LHG	a	614	35/49	0.90	0.23	36,47,56,58	0
25	CLA	b	619	65/65	0.90	0.24	30,44,72,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LHG	l	101	49/49	0.90	0.21	30,45,54,56	0
25	CLA	C	508	65/65	0.90	0.22	38,49,82,90	0
25	CLA	D	402	65/65	0.90	0.22	24,36,48,59	0
33	DGD	c	518	62/66	0.90	0.21	28,46,63,79	0
25	CLA	B	603	65/65	0.90	0.25	28,37,45,47	0
25	CLA	c	507	65/65	0.90	0.21	32,44,61,64	0
25	CLA	a	609	65/65	0.90	0.25	19,34,71,81	0
28	PL9	D	407	55/55	0.90	0.23	26,35,45,50	0
29	LMG	d	406	42/55	0.91	0.21	38,48,63,73	0
33	DGD	C	516	62/66	0.91	0.21	21,39,63,71	0
25	CLA	C	505	65/65	0.91	0.21	33,41,55,62	0
25	CLA	b	612	65/65	0.91	0.19	28,41,55,61	0
25	CLA	c	512	65/65	0.91	0.23	31,47,56,64	0
25	CLA	B	607	65/65	0.91	0.20	26,36,44,54	0
25	CLA	b	607	65/65	0.91	0.20	24,34,48,53	0
22	FE2	a	602	1/1	0.91	0.08	62,62,62,62	0
25	CLA	c	509	65/65	0.91	0.20	30,39,51,55	0
25	CLA	b	616	65/65	0.92	0.20	25,33,51,62	0
25	CLA	A	615	65/65	0.92	0.22	22,34,43,47	0
25	CLA	B	610	65/65	0.92	0.21	25,33,39,45	0
31	LHG	A	616	49/49	0.92	0.20	24,41,54,58	0
28	PL9	d	408	55/55	0.92	0.21	21,33,43,45	0
25	CLA	B	613	65/65	0.92	0.23	19,33,48,69	0
31	LHG	D	406	49/49	0.92	0.24	25,40,50,59	0
25	CLA	A	609	65/65	0.92	0.23	17,29,79,89	0
25	CLA	b	608	65/65	0.92	0.19	30,40,46,51	0
25	CLA	d	403	65/65	0.92	0.19	24,36,45,50	0
25	CLA	B	615	65/65	0.92	0.19	27,41,51,57	0
26	PHO	D	401	64/64	0.92	0.21	27,37,47,54	0
33	DGD	C	517	62/66	0.92	0.22	39,51,74,83	0
26	PHO	d	401	64/64	0.92	0.21	24,39,45,49	0
27	BCR	A	610	40/40	0.92	0.20	22,34,44,47	0
27	BCR	c	517	40/40	0.92	0.20	19,39,50,52	0
27	BCR	B	617	40/40	0.92	0.20	32,41,49,50	0
25	CLA	B	605	65/65	0.92	0.19	24,34,40,42	0
25	CLA	C	501	65/65	0.92	0.21	34,42,49,54	0
34	HEM	E	101	43/43	0.92	0.20	42,54,67,69	0
25	CLA	b	613	65/65	0.92	0.20	24,35,43,45	0
31	LHG	a	613	49/49	0.93	0.20	26,43,56,60	0
27	BCR	a	610	40/40	0.93	0.19	19,32,45,47	0
24	CL	A	604	1/1	0.93	0.10	43,43,43,43	0
31	LHG	d	407	49/49	0.93	0.20	20,37,47,51	0

Continued on next page...

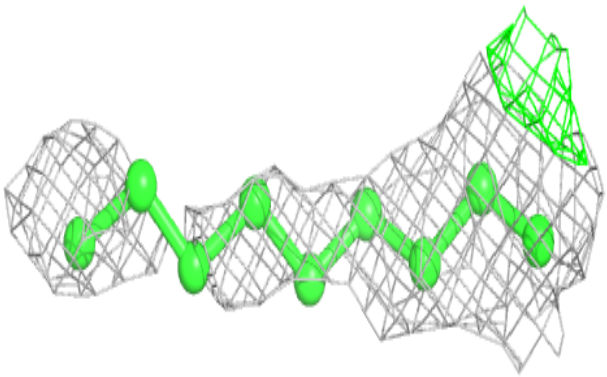
Continued from previous page...

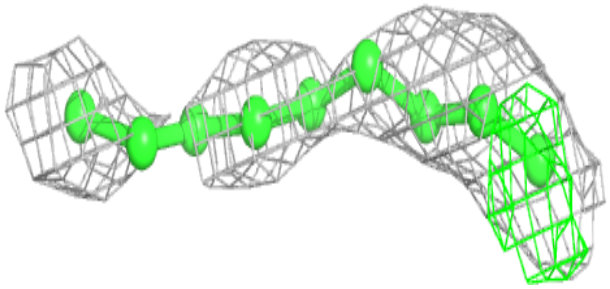
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	CLA	B	611	65/65	0.93	0.22	21,31,38,44	0
25	CLA	a	606	65/65	0.93	0.18	23,31,38,39	0
25	CLA	c	503	65/65	0.93	0.21	27,40,46,52	0
25	CLA	b	610	65/65	0.93	0.19	23,37,51,54	0
25	CLA	B	612	65/65	0.93	0.20	26,35,42,46	0
25	CLA	A	607	57/65	0.93	0.20	29,37,49,67	0
24	CL	a	604	1/1	0.93	0.14	42,42,42,42	0
26	PHO	A	608	64/64	0.93	0.21	23,32,37,43	0
25	CLA	b	614	65/65	0.93	0.18	25,35,41,50	0
26	PHO	a	608	64/64	0.93	0.20	19,28,38,42	0
25	CLA	b	606	65/65	0.93	0.20	24,36,50,58	0
35	HEC	V	201	43/43	0.93	0.17	31,44,52,56	0
25	CLA	b	615	65/65	0.94	0.18	22,32,41,50	0
25	CLA	a	612	65/65	0.94	0.17	17,29,37,39	0
25	CLA	a	607	59/65	0.94	0.17	27,37,55,72	0
25	CLA	B	602	65/65	0.94	0.22	29,39,47,52	0
35	HEC	v	201	43/43	0.94	0.17	32,41,48,52	0
24	CL	A	605	1/1	0.95	0.13	44,44,44,44	0
32	BCT	A	620	4/4	0.95	0.15	26,36,37,44	0
22	FE2	A	602	1/1	0.96	0.05	46,46,46,46	0
32	BCT	a	605	4/4	0.96	0.10	44,47,49,50	0
21	OEX	A	601	10/10	0.98	0.10	33,40,45,46	0
21	OEX	a	601	10/10	0.98	0.08	40,44,48,51	0

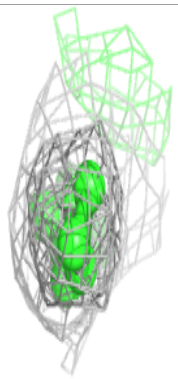
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG b 625:

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

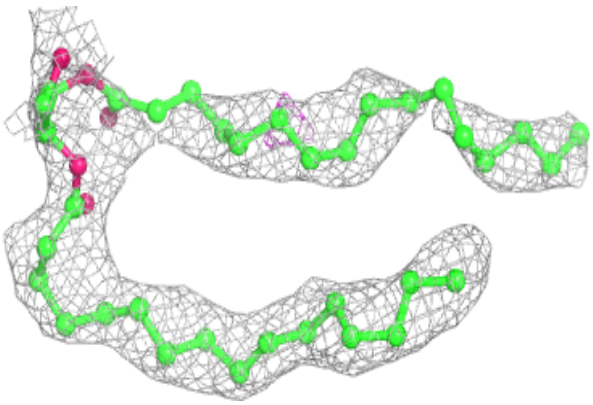


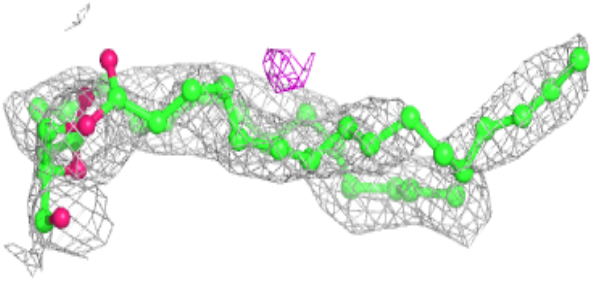


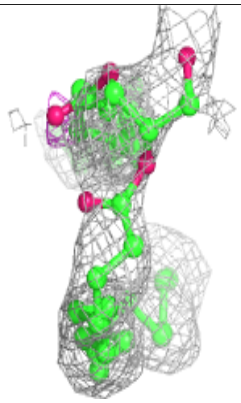


Electron density around SQD I 101:

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

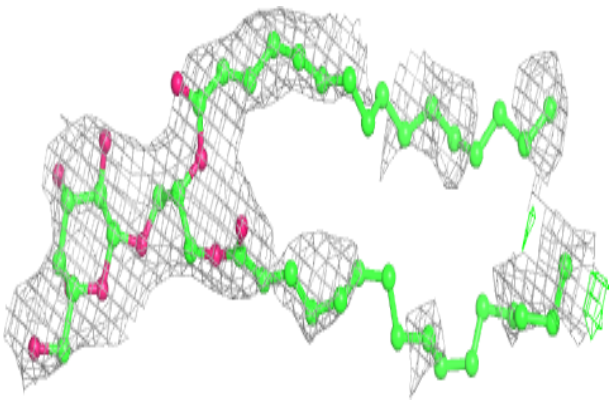


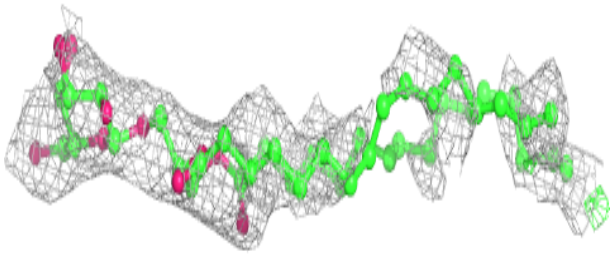


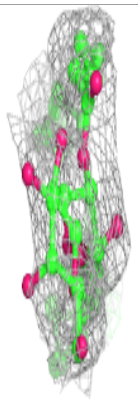


Electron density around LMG C 520:

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

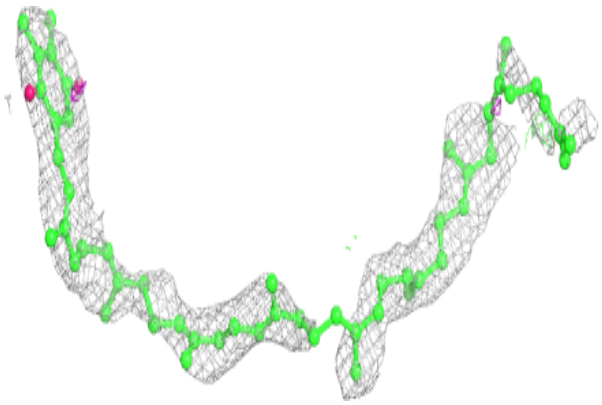


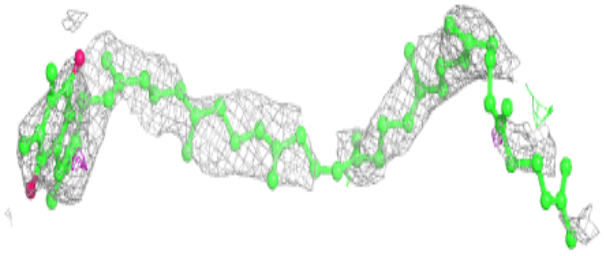


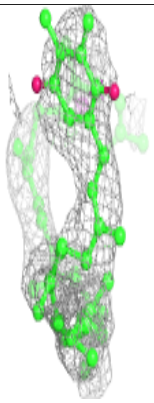


Electron density around PL9 A 611:

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

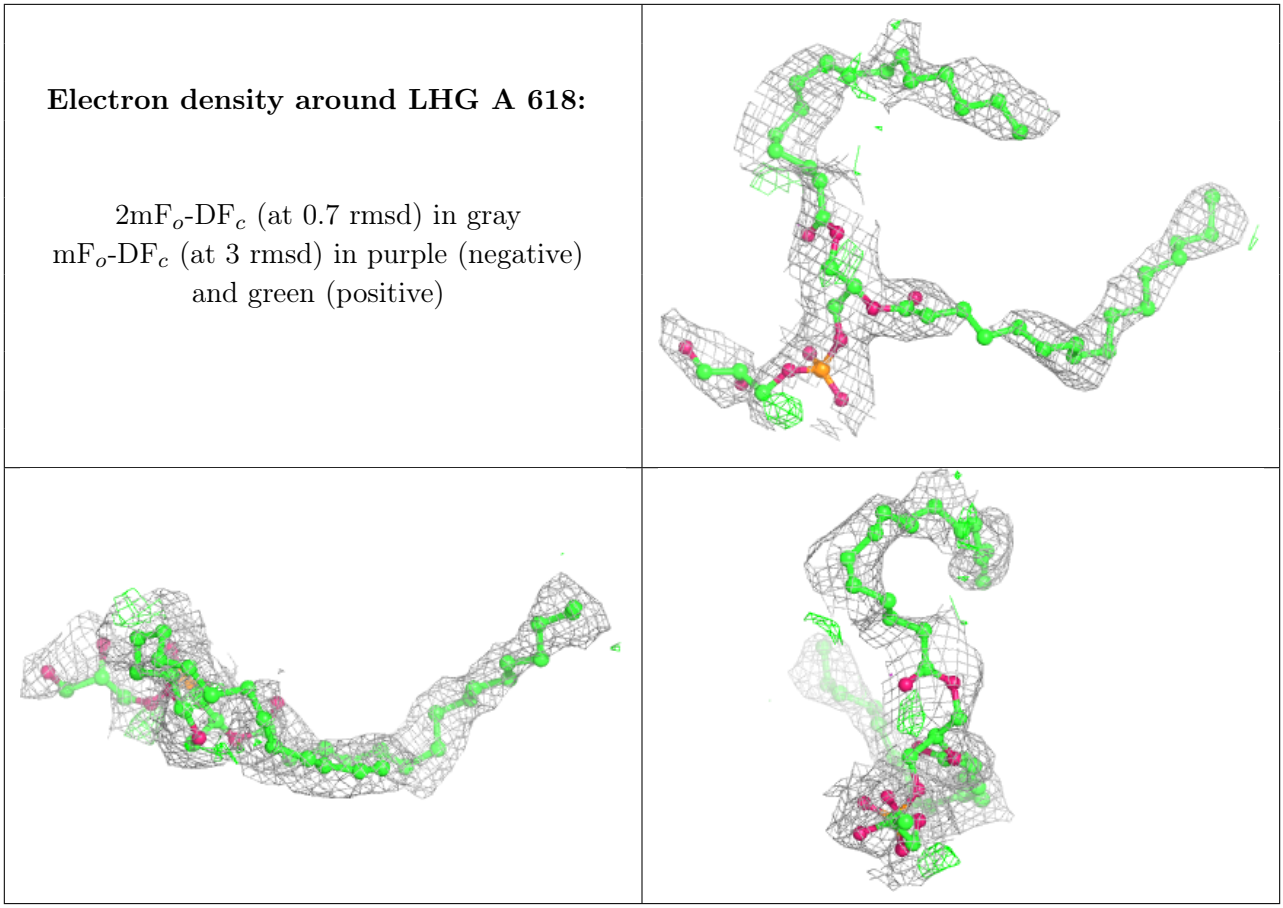






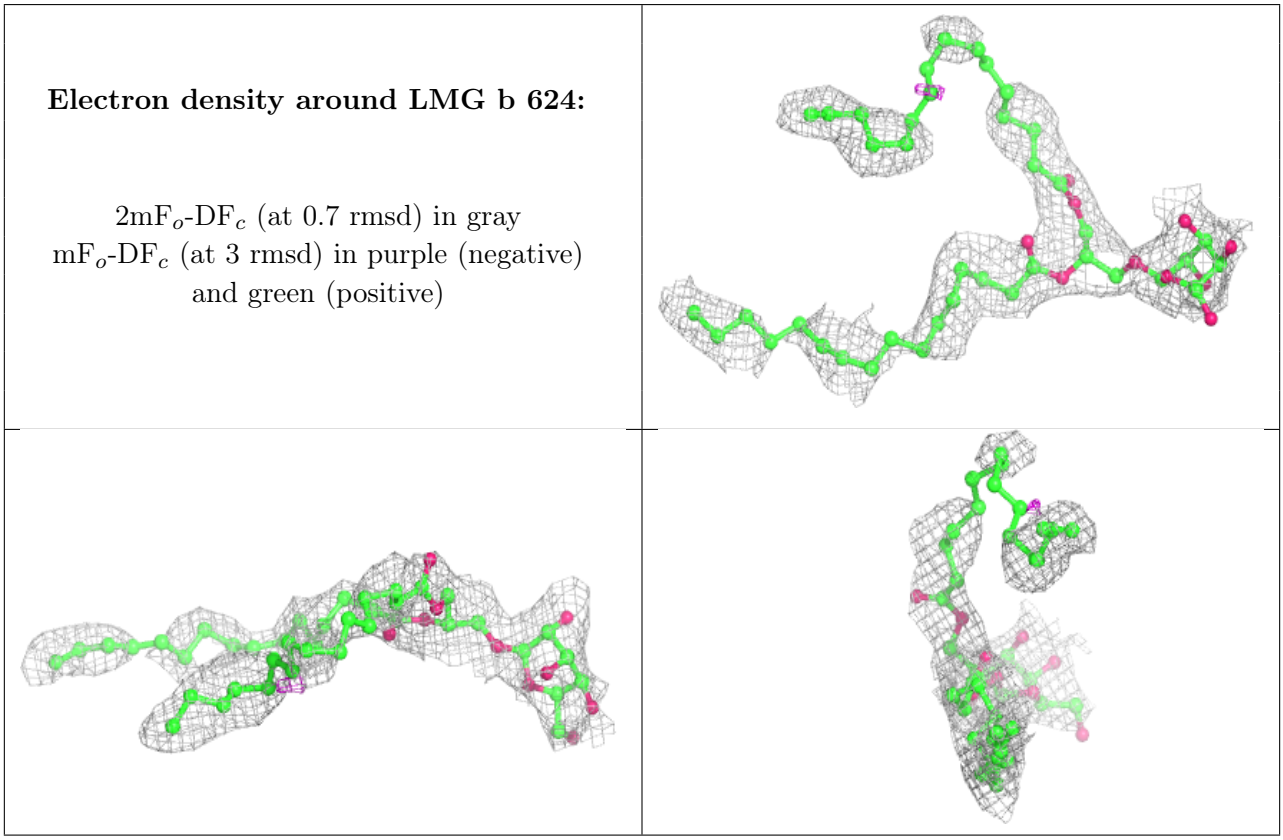
Electron density around LHG A 618:

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



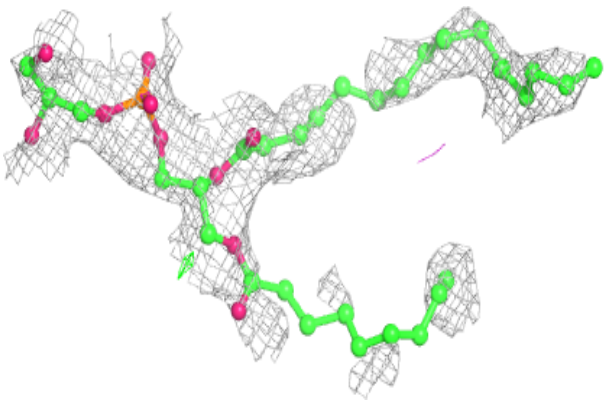
Electron density around LMG b 624:

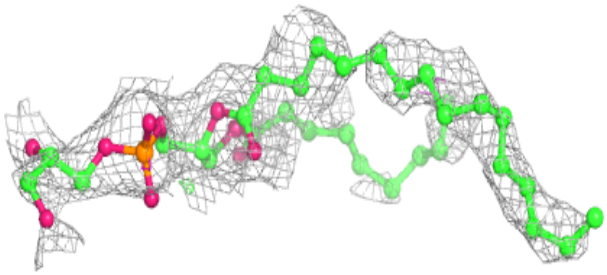
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

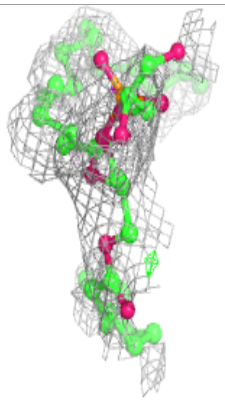


Electron density around LHG a 615:

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

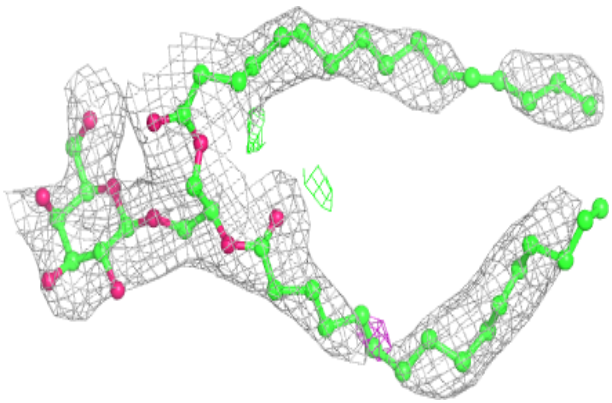


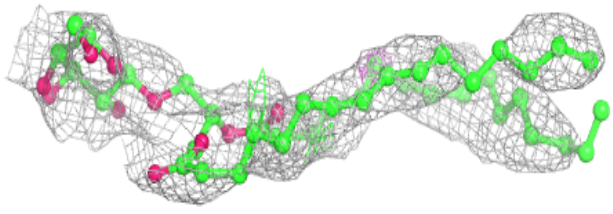


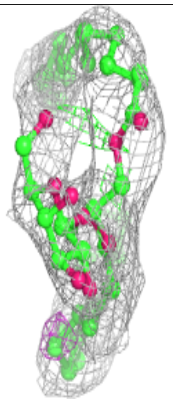


Electron density around LMG c 502:

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

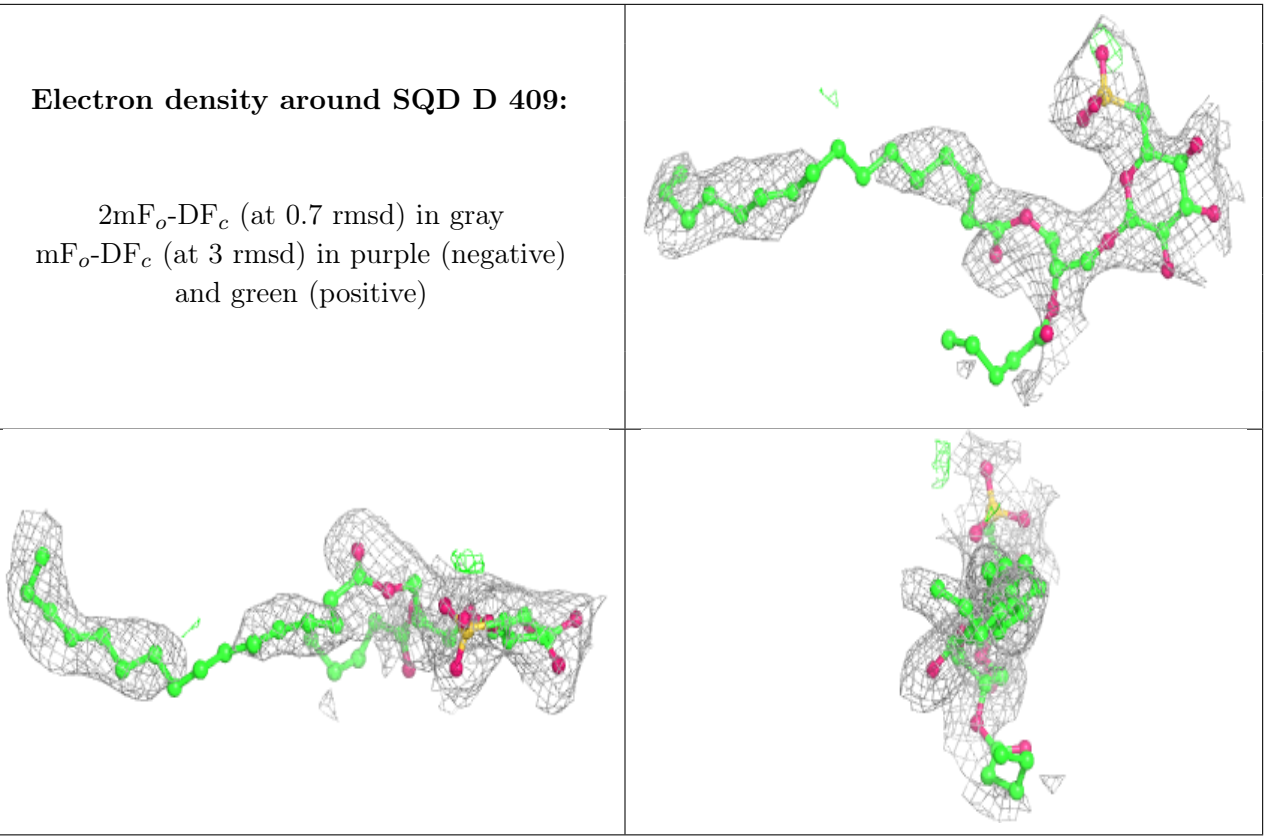






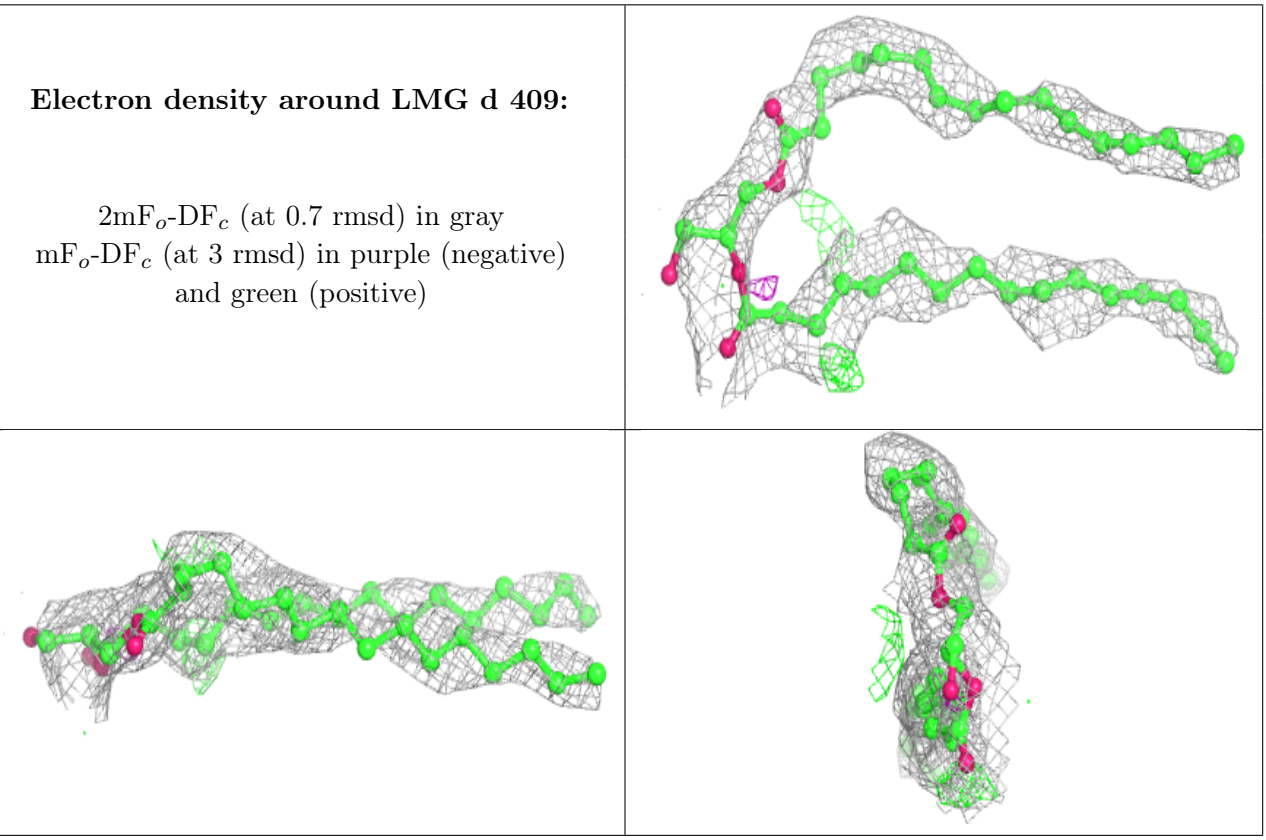
Electron density around SQD D 409:

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



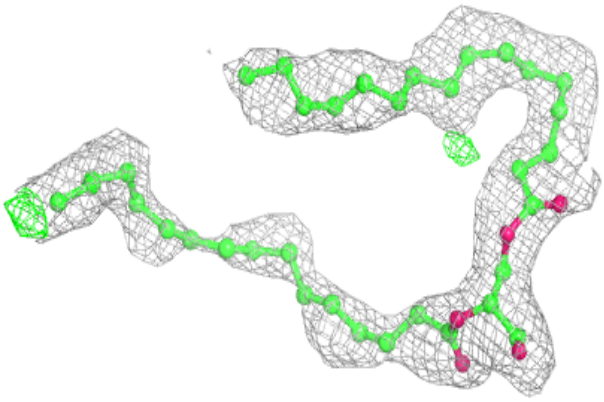
Electron density around LMG d 409:

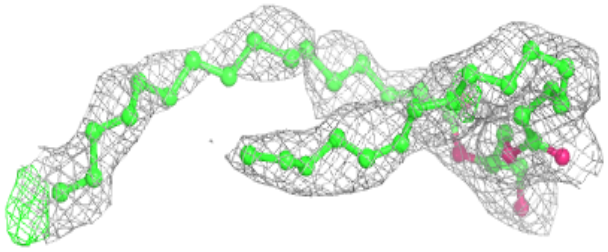
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

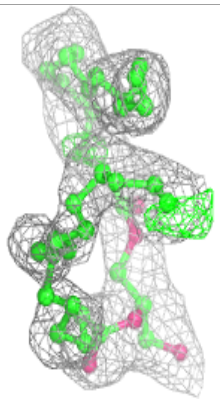


Electron density around SQD A 619:

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

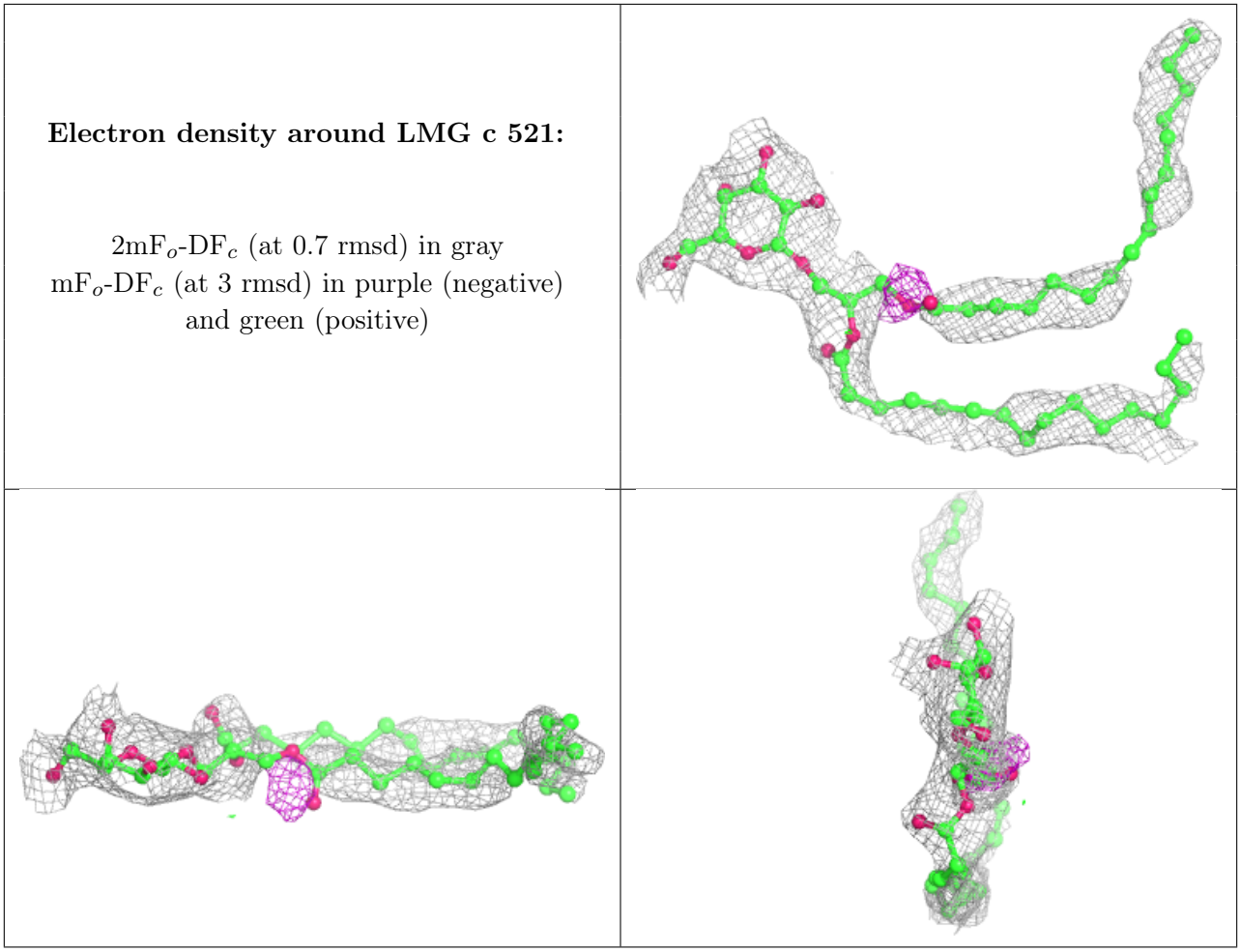






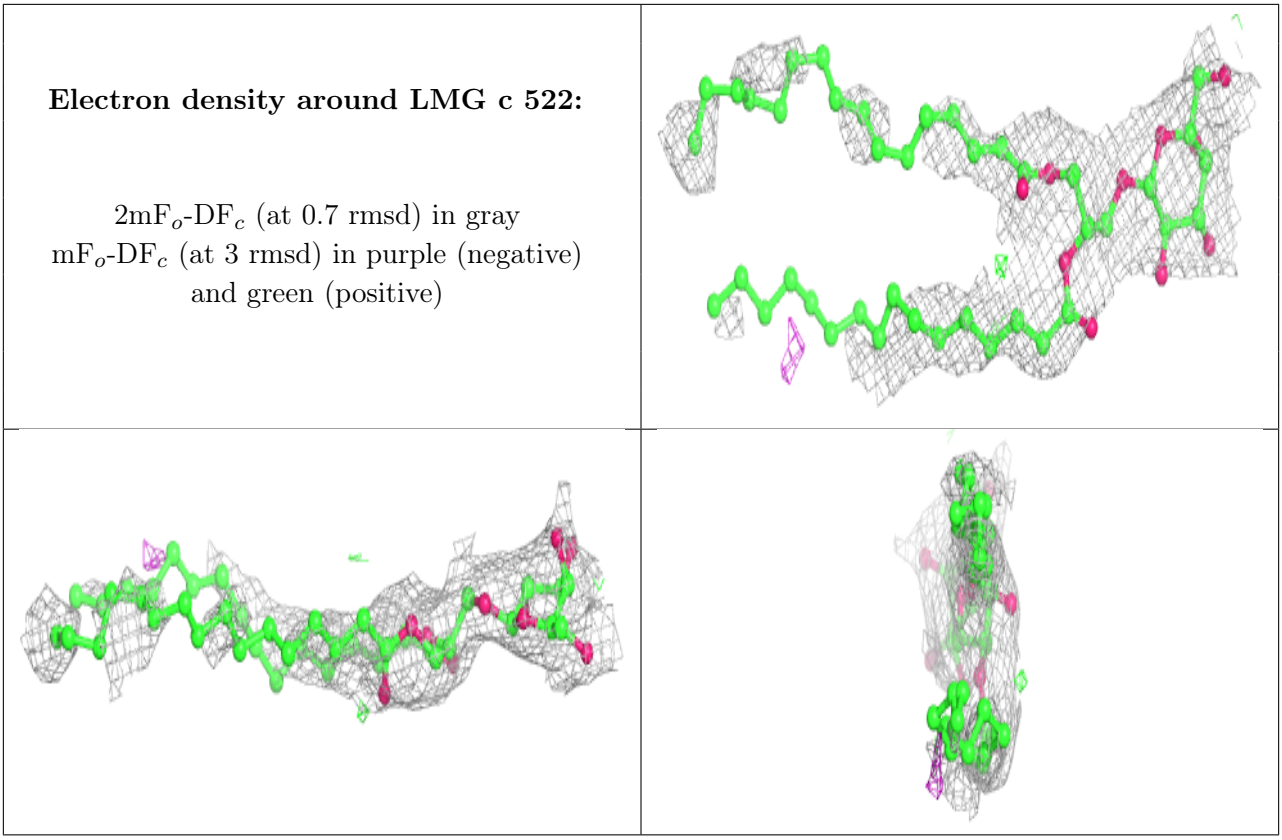
Electron density around LMG c 521:

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



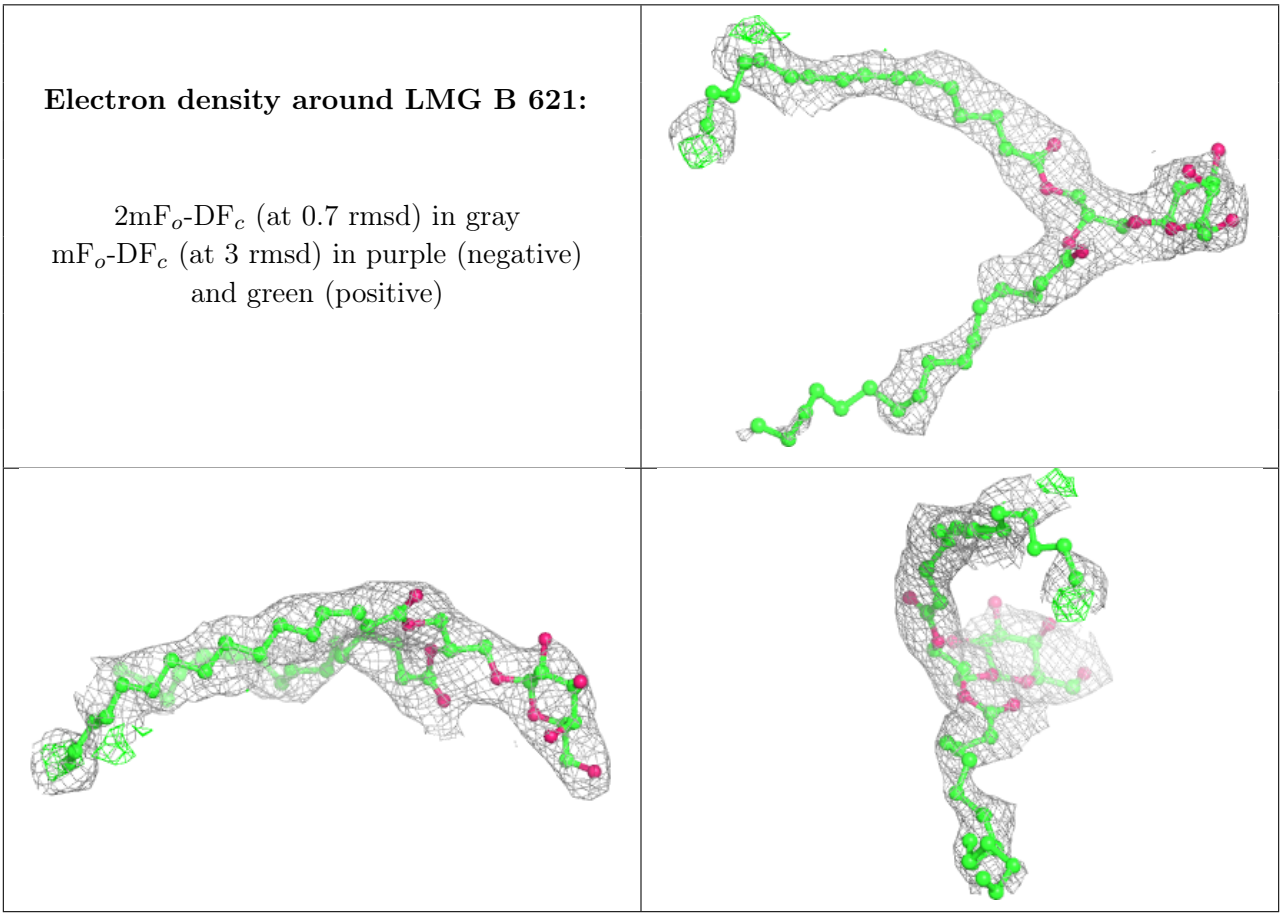
Electron density around LMG c 522:

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



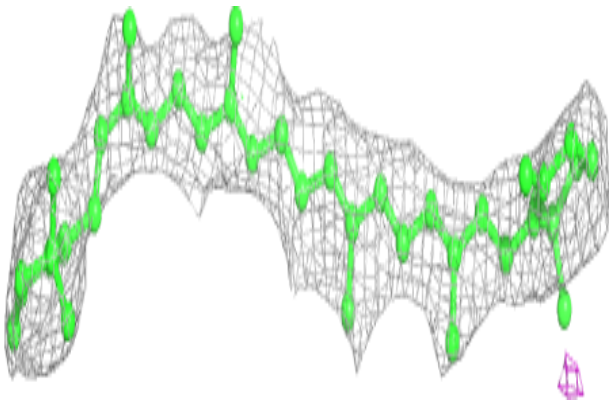
Electron density around LMG B 621:

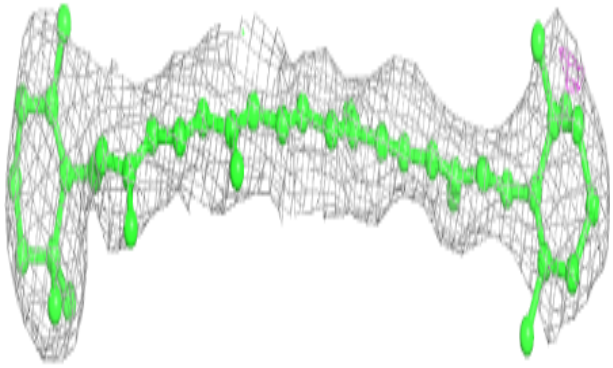
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

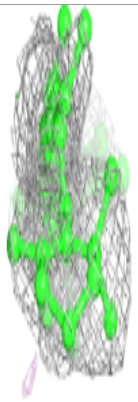


Electron density around BCR H 102:

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

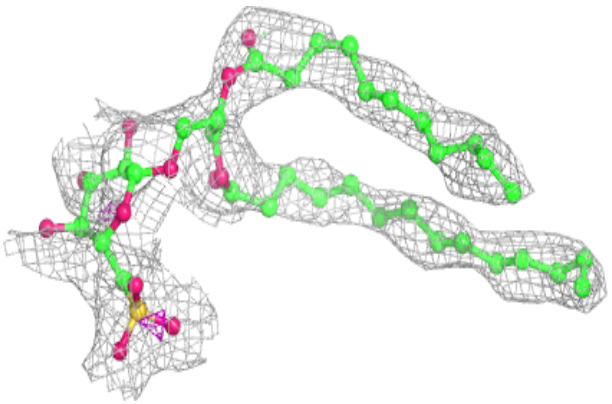


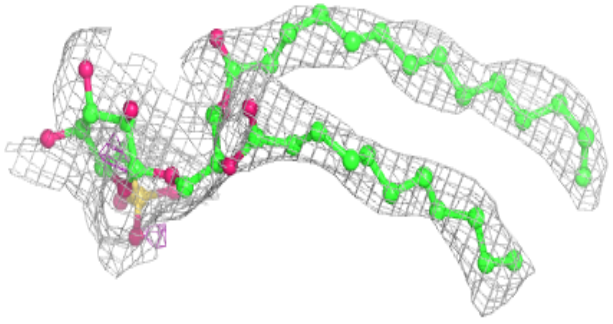


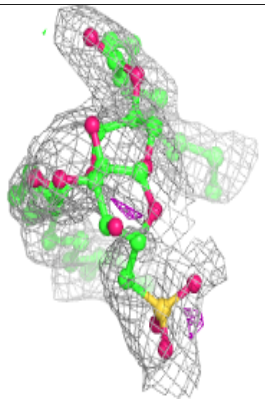


Electron density around SQD D 408:

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

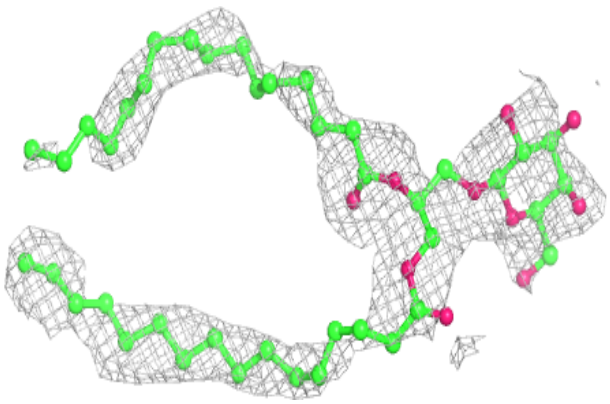


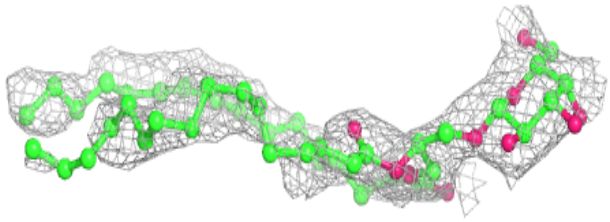


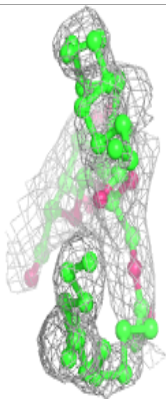


Electron density around LMG A 612:

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

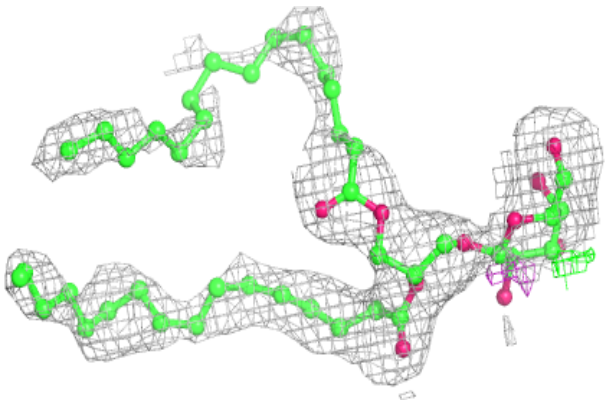


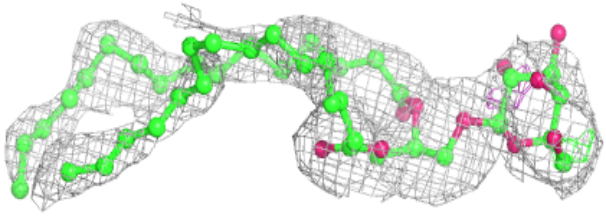


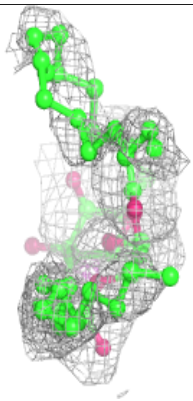


Electron density around LMG A 613:

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

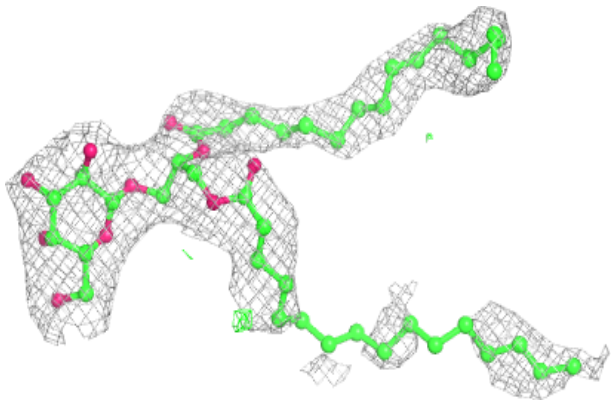


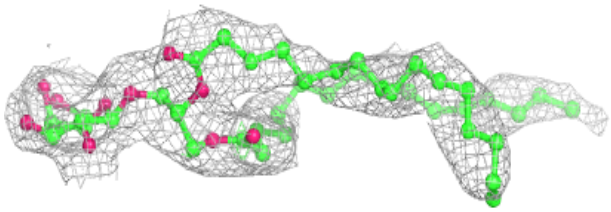


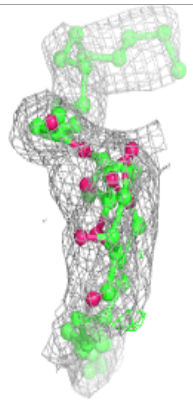


Electron density around LMG B 625:

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

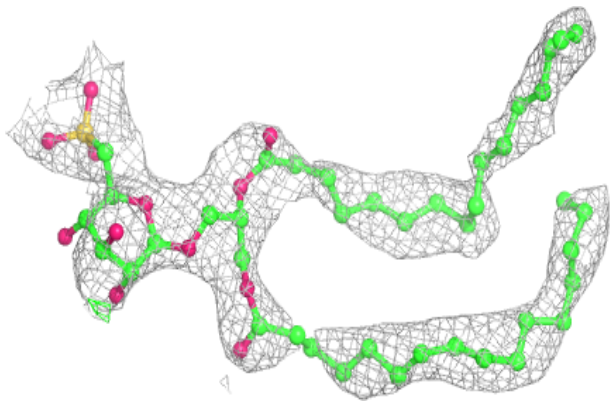


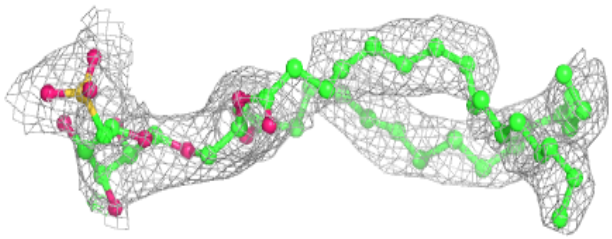


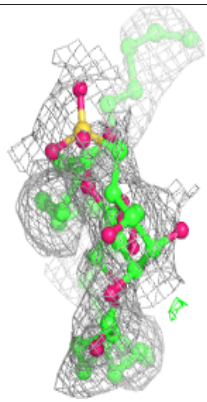


Electron density around SQD b 601:

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

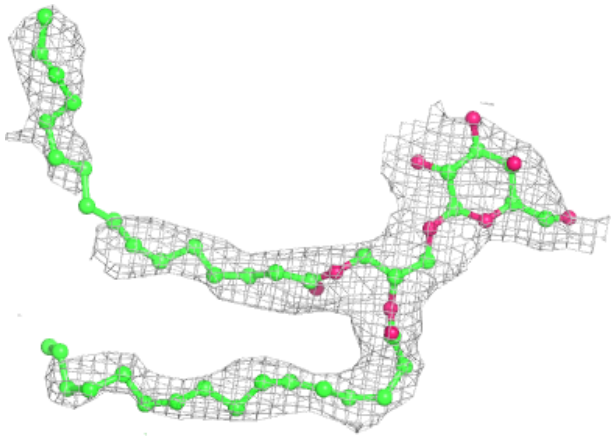


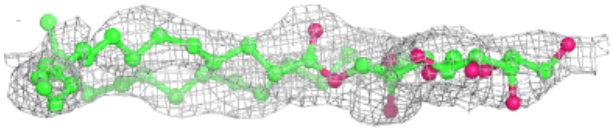


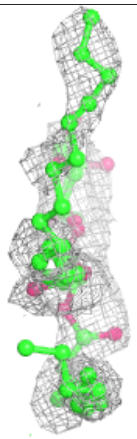


Electron density around LMG C 519:

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

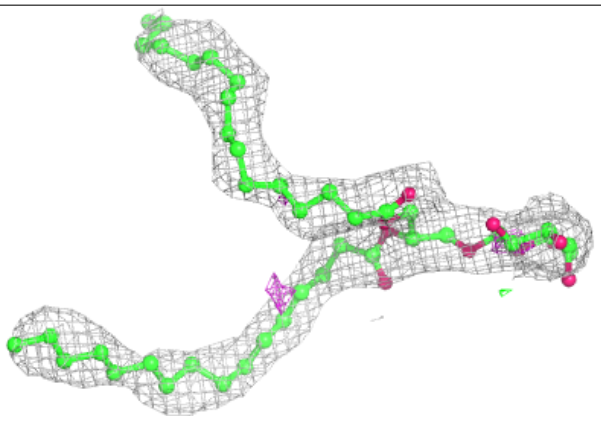


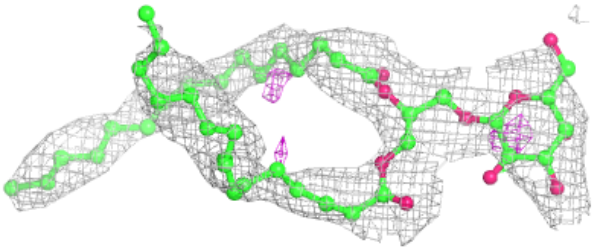


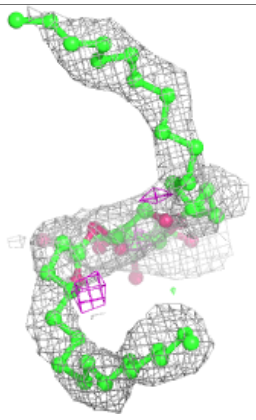


Electron density around LMG b 623:

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

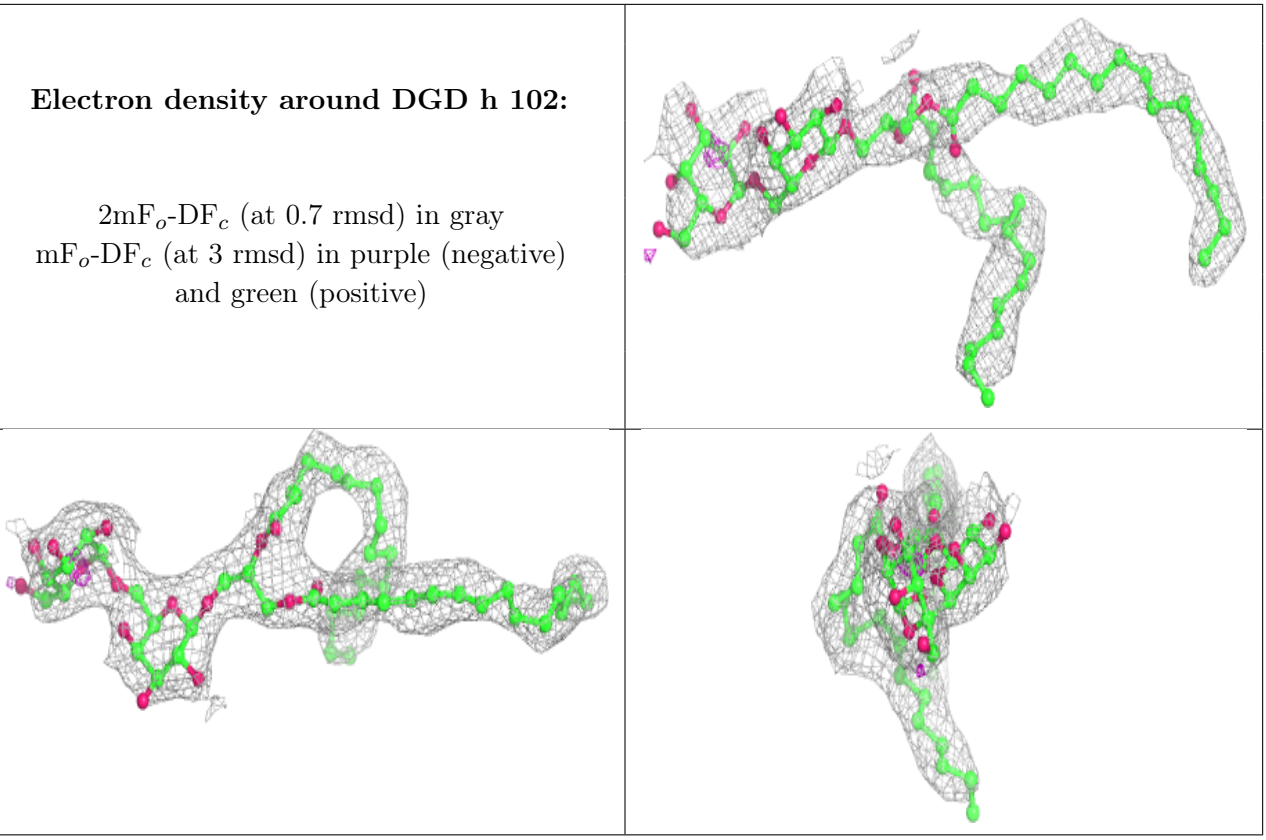






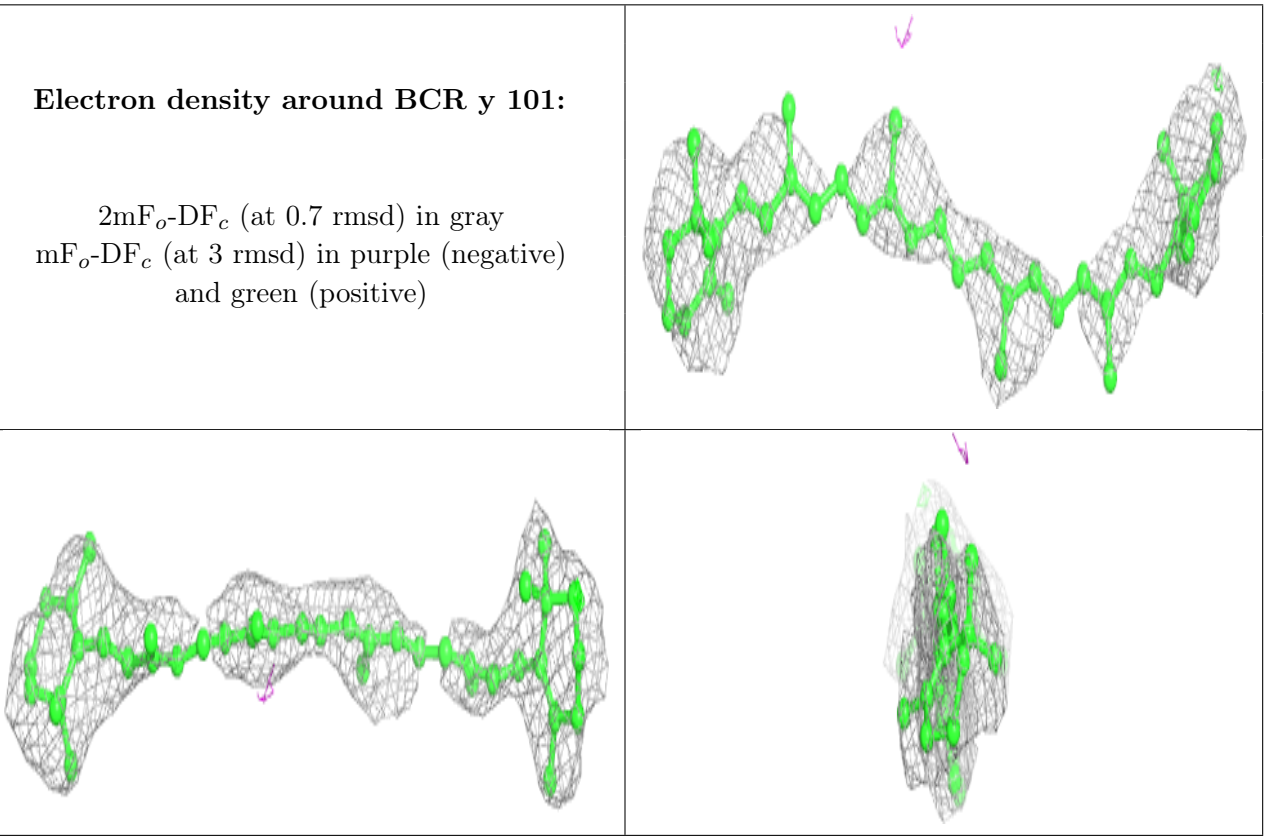
Electron density around DGD h 102:

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



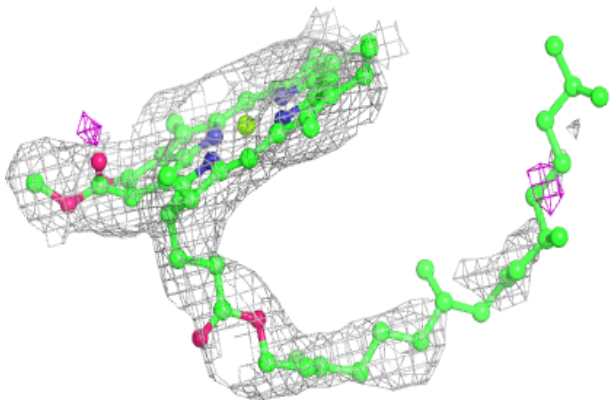
Electron density around BCR y 101:

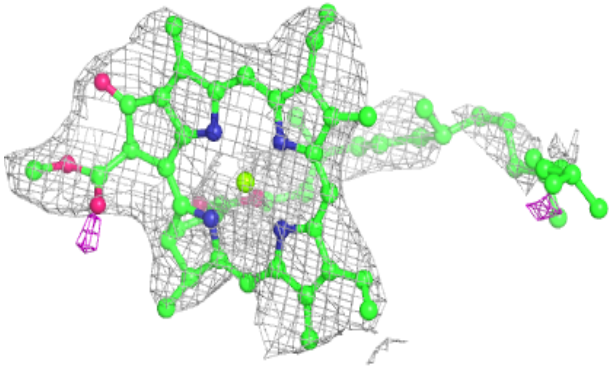
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

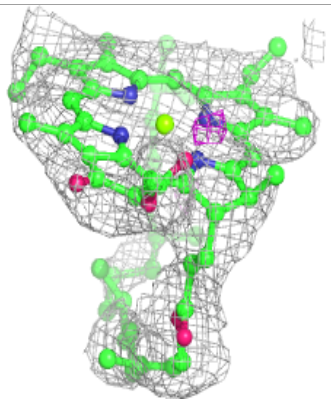


Electron density around CLA c 515:

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

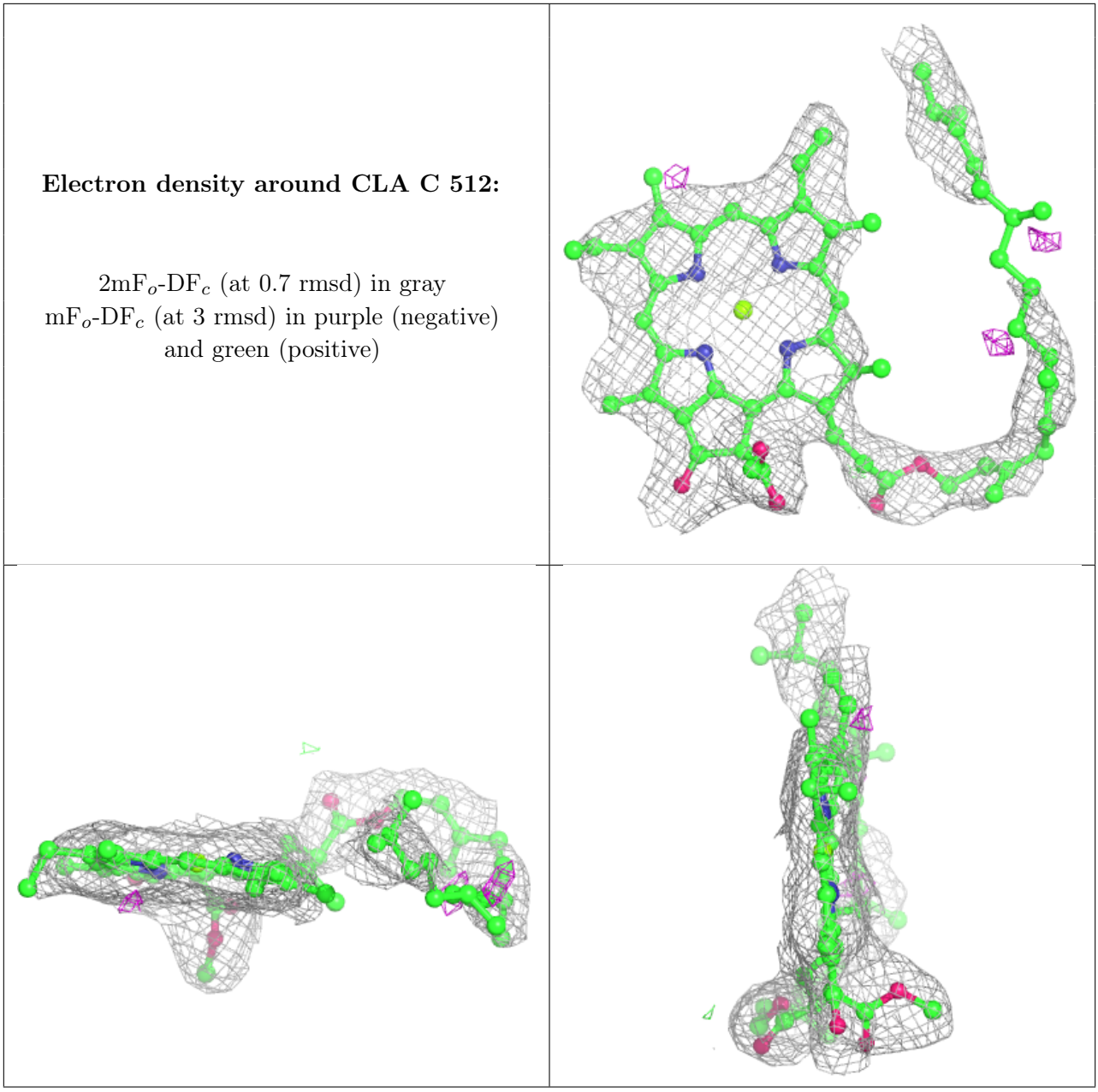






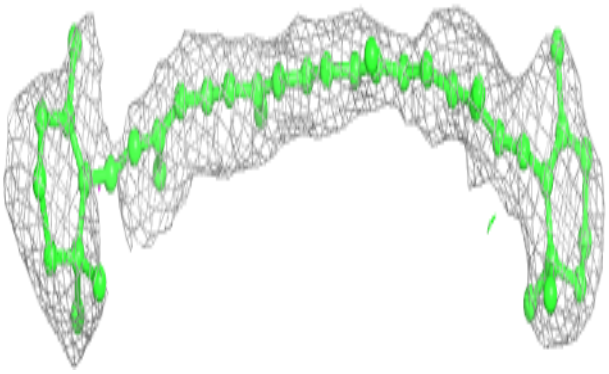
Electron density around CLA C 512:

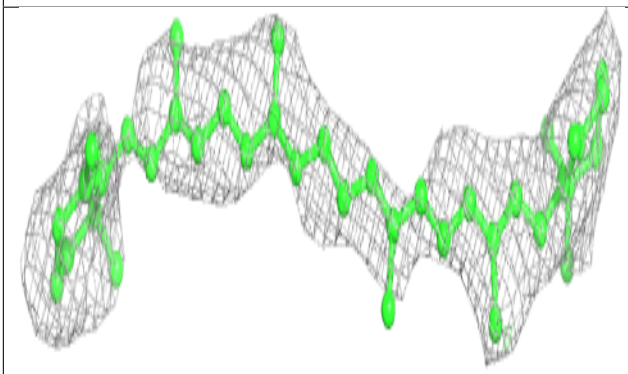
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

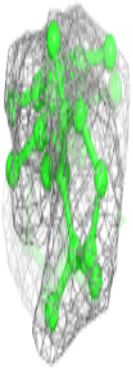


Electron density around BCR k 101:

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

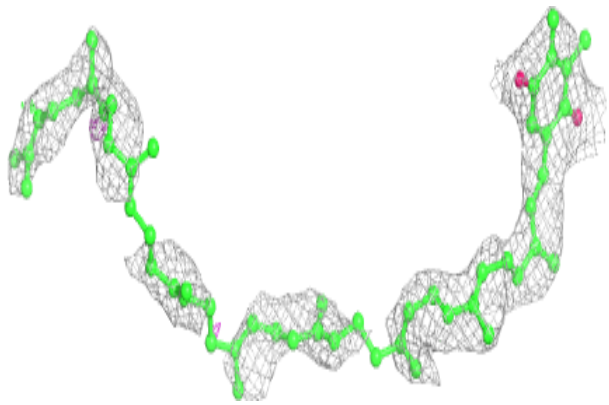


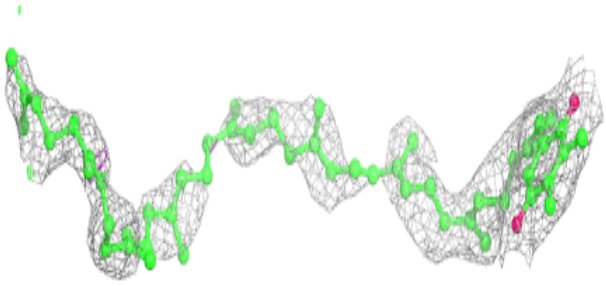


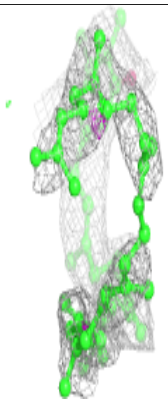


Electron density around PL9 a 611:

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

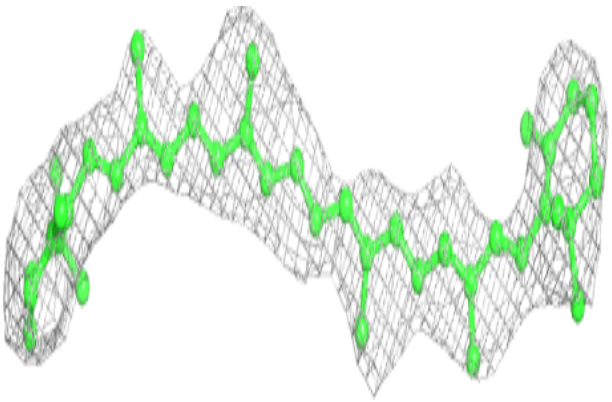


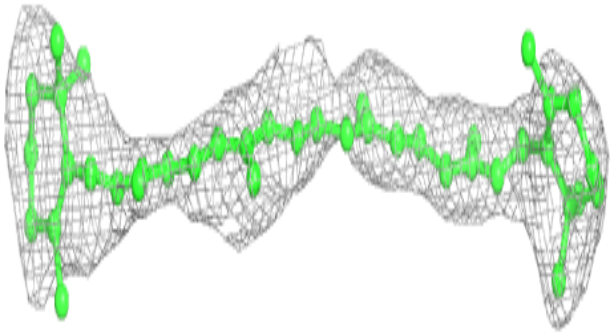


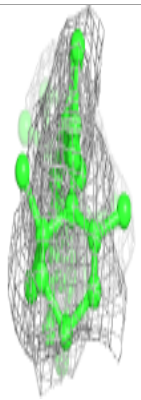


Electron density around BCR Y 101:

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

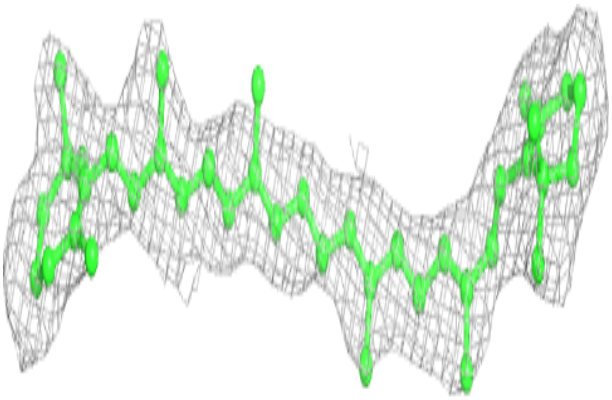


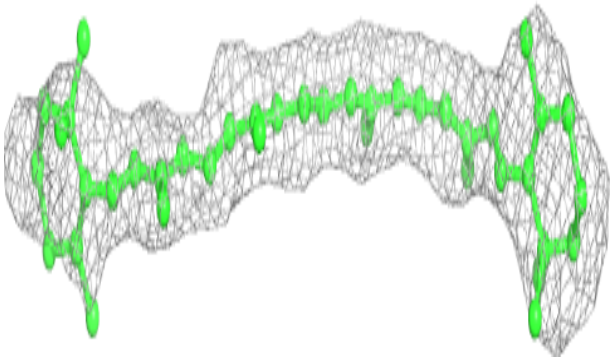


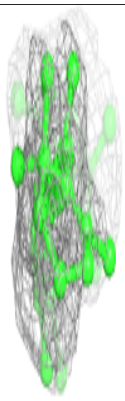


Electron density around BCR h 101:

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

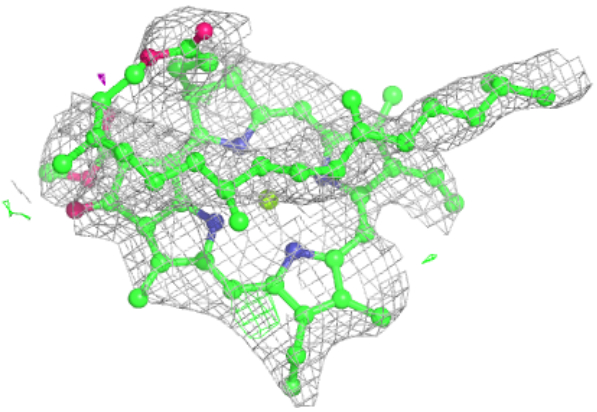


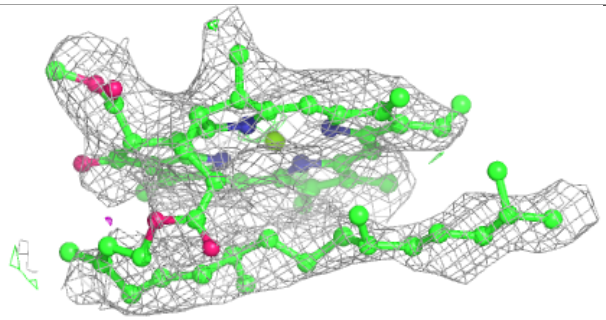


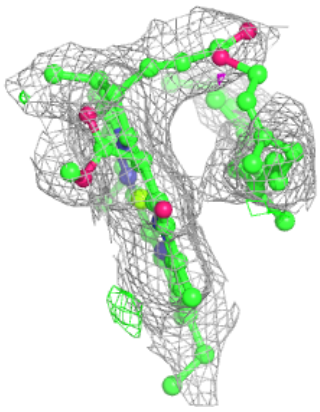


Electron density around CLA b 604:

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

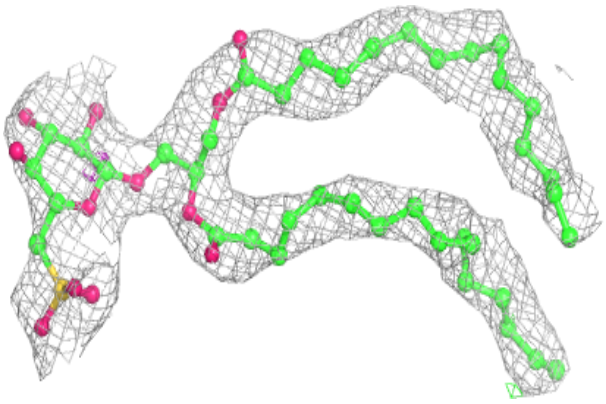


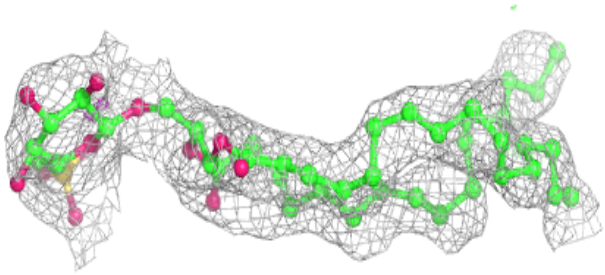


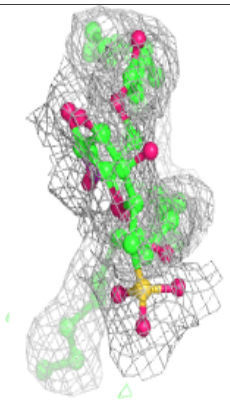


Electron density around SQD B 626:

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

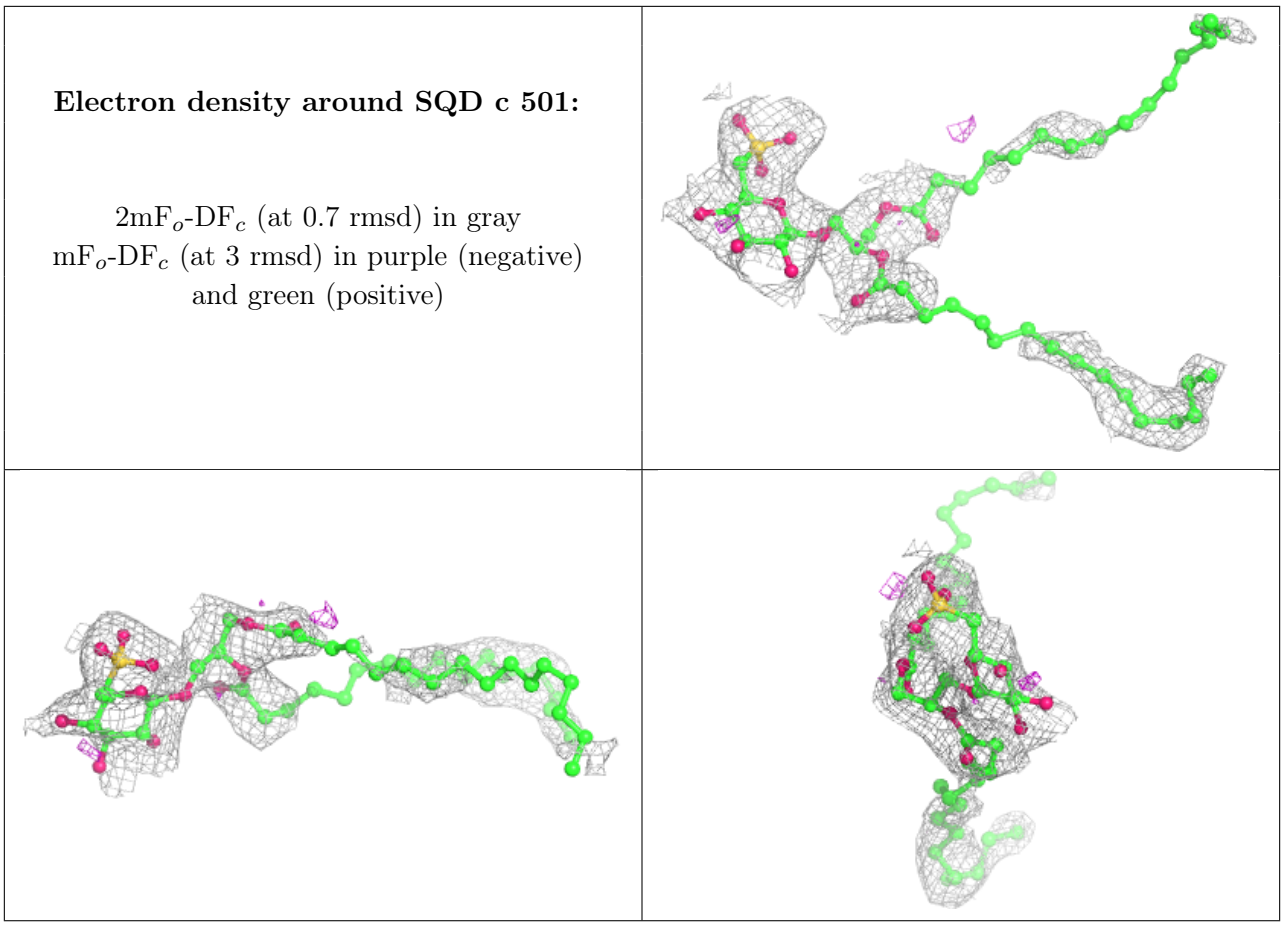






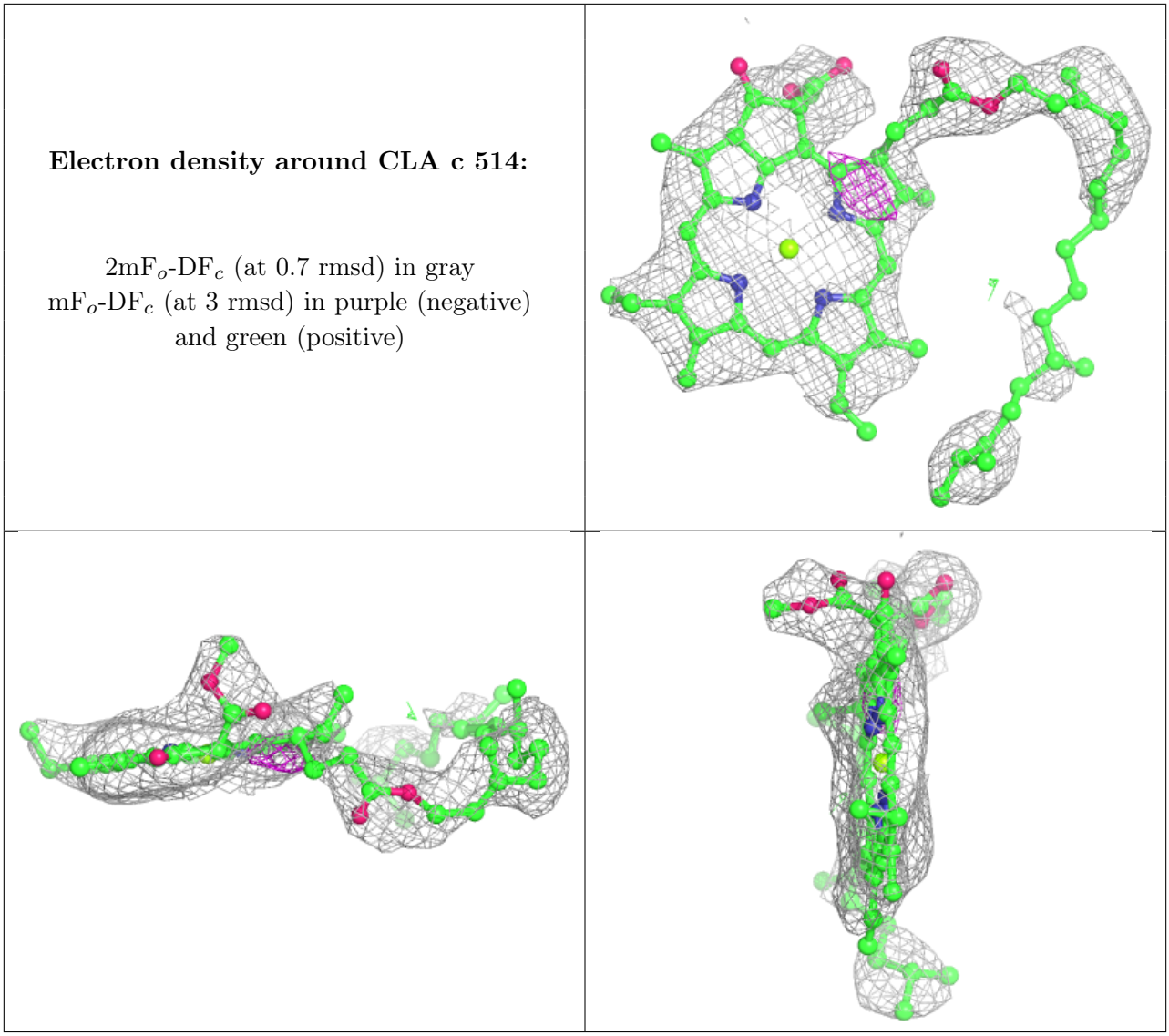
Electron density around SQD c 501:

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



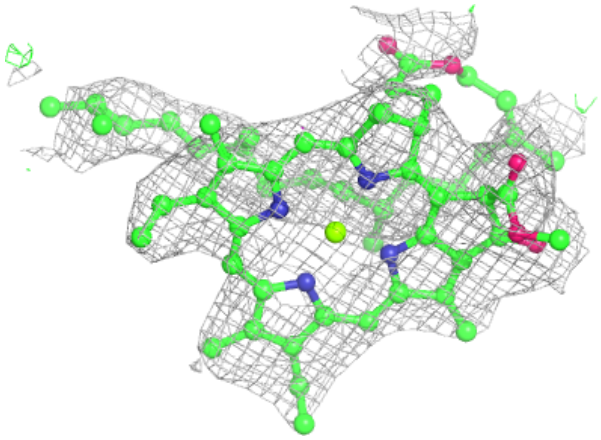
Electron density around CLA c 514:

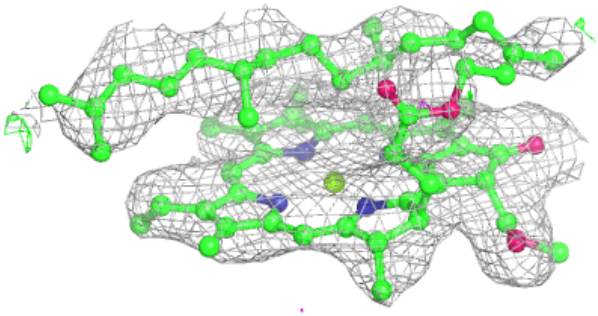
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

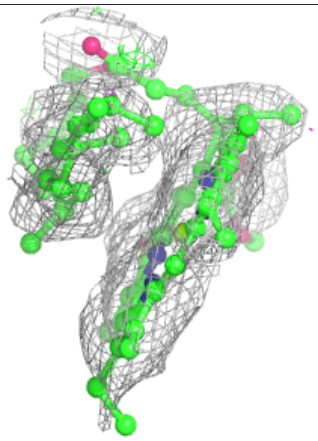


Electron density around CLA B 601:

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

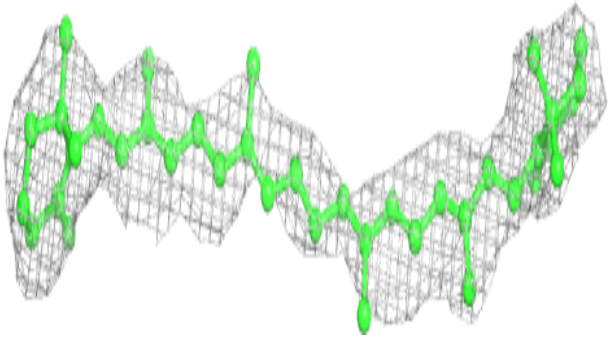


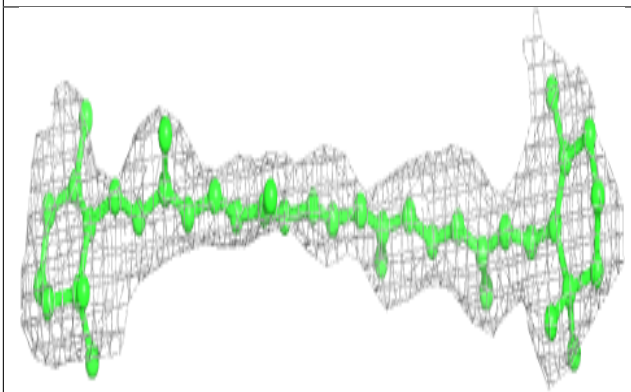


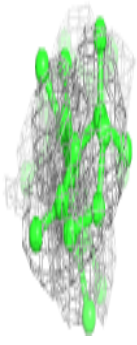


Electron density around BCR C 514:

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

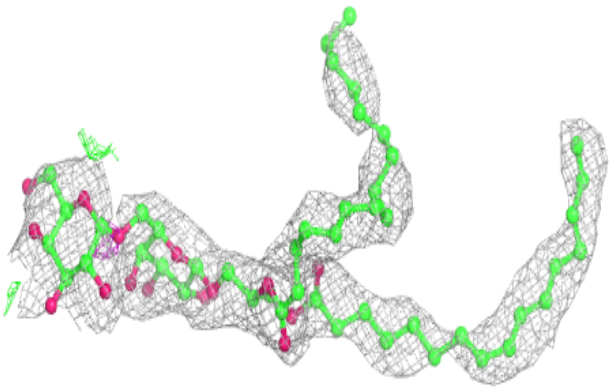


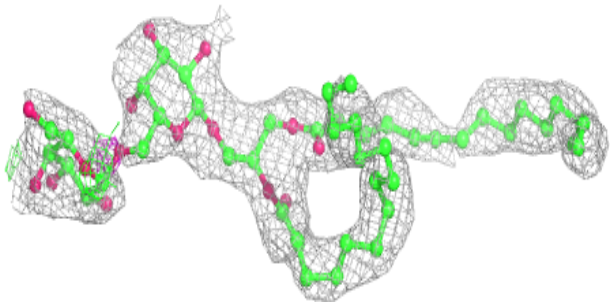


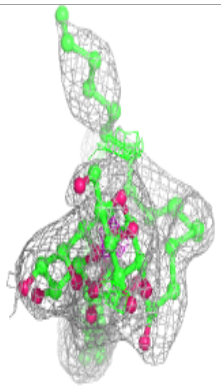


Electron density around DGD H 103:

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

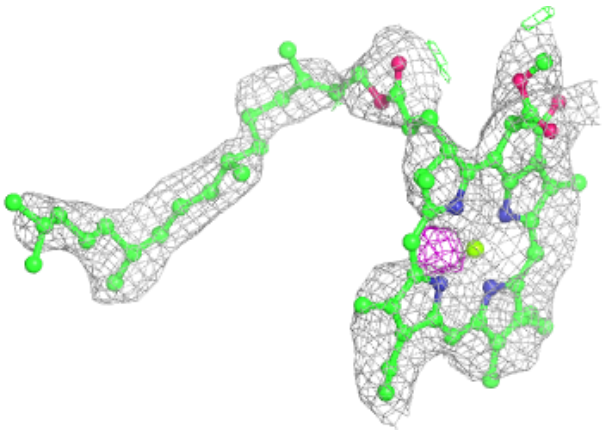


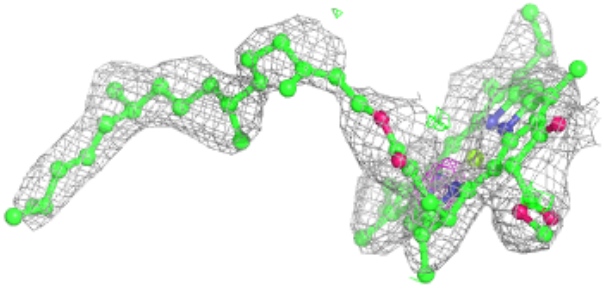


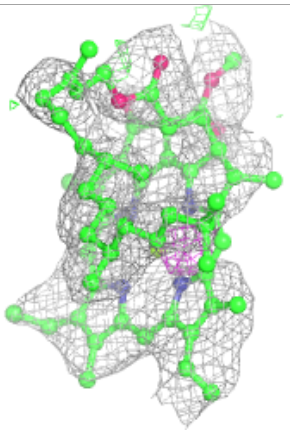


Electron density around CLA C 511:

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

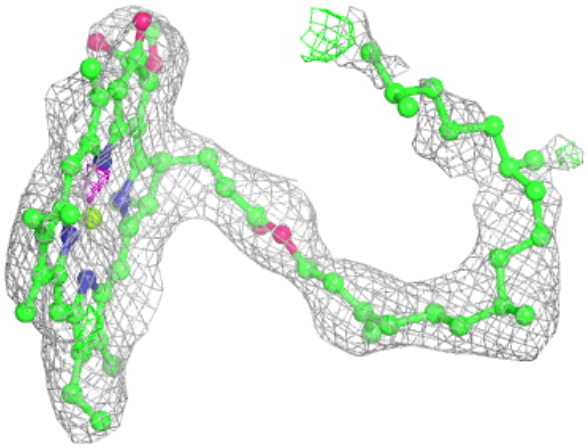


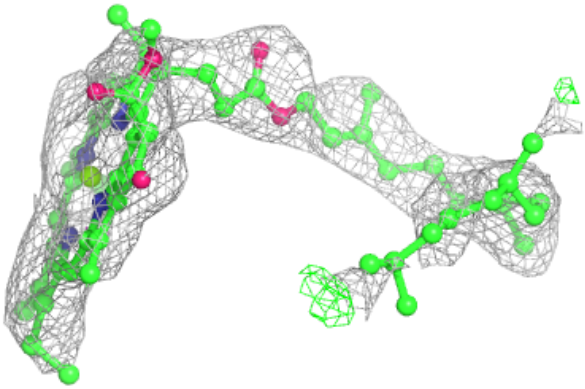


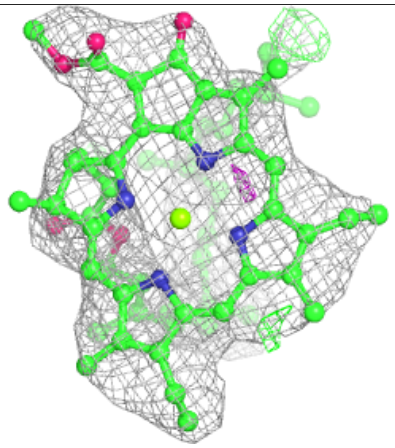


Electron density around CLA B 606:

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

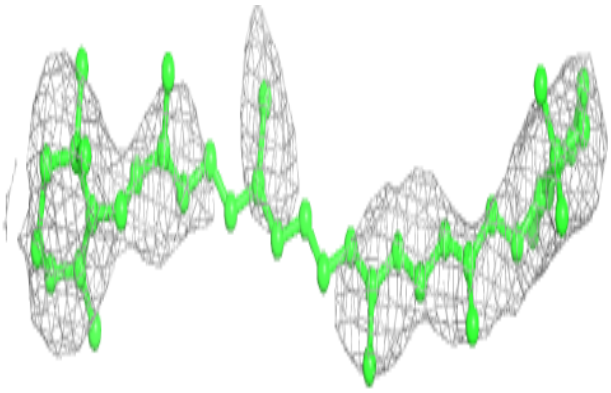


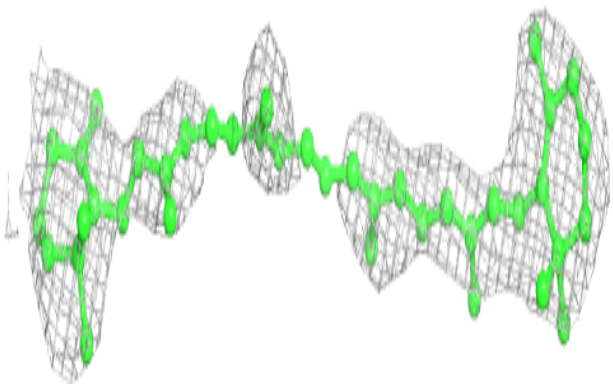


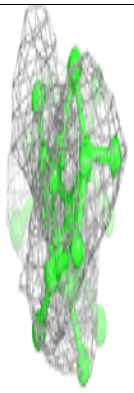


Electron density around BCR c 516:

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

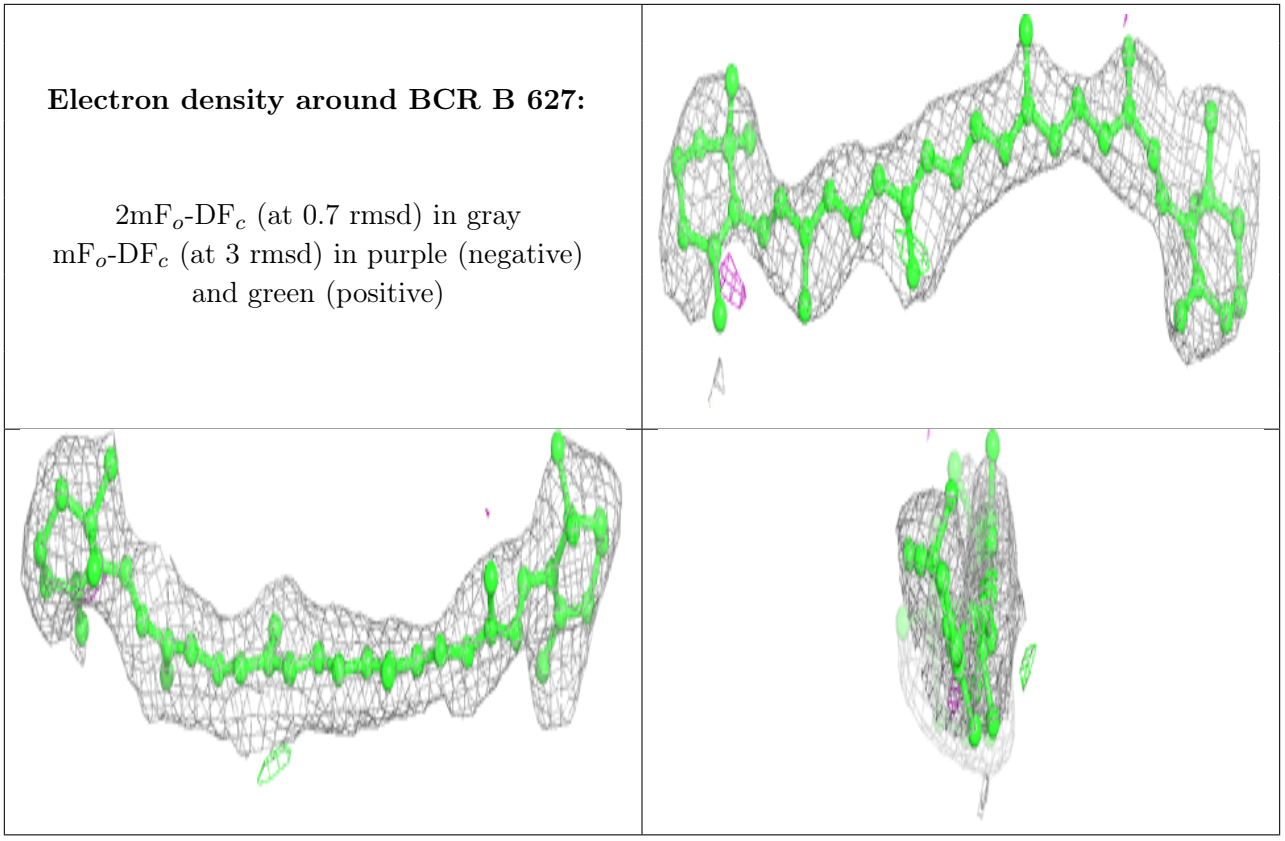






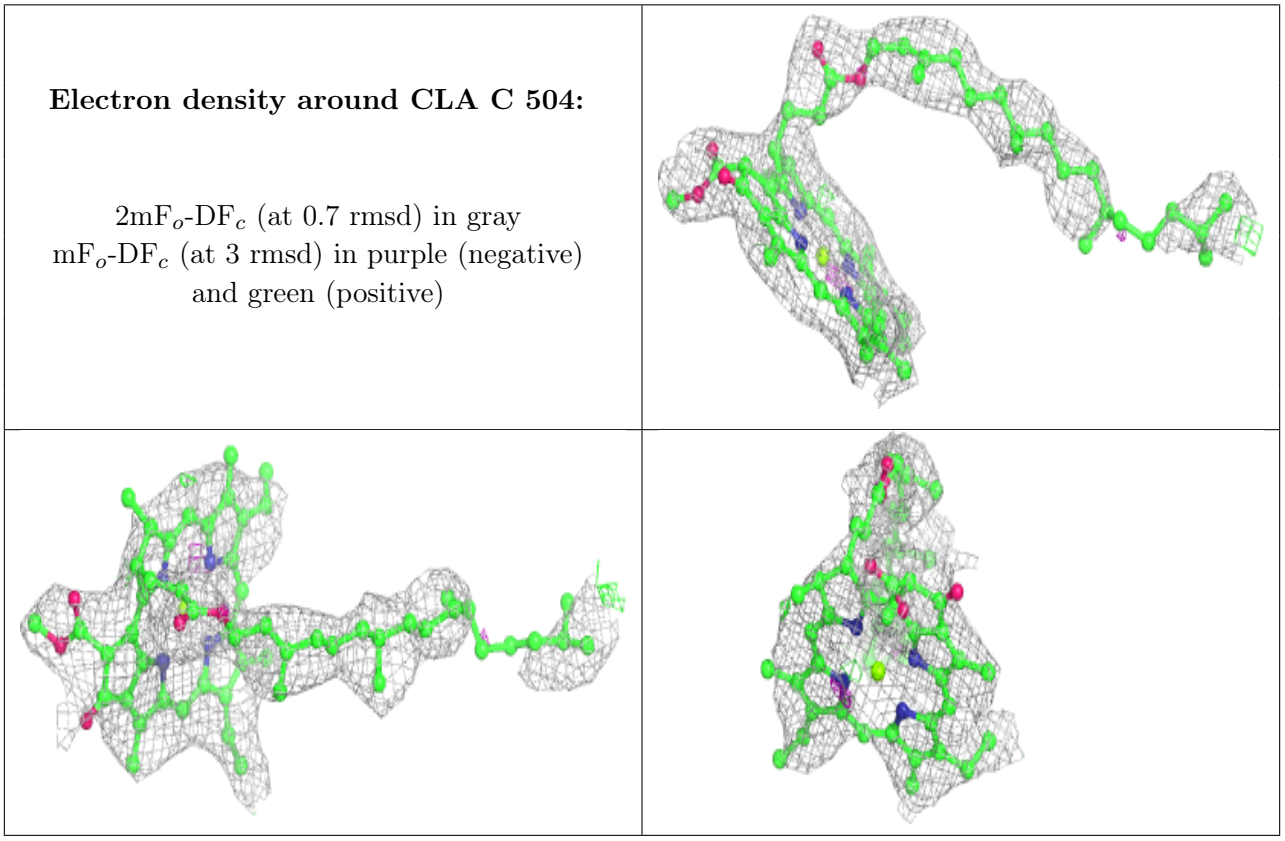
Electron density around BCR B 627:

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



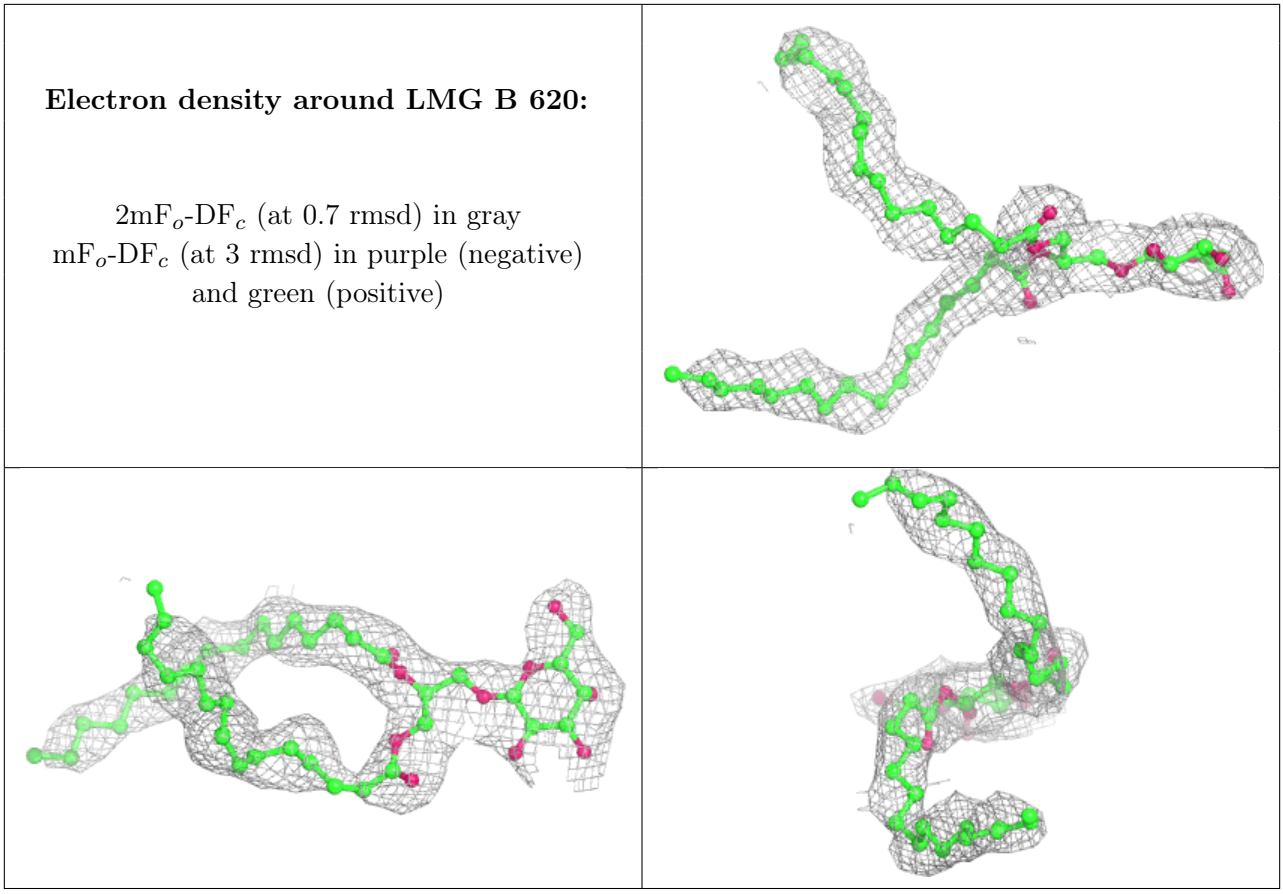
Electron density around CLA C 504:

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



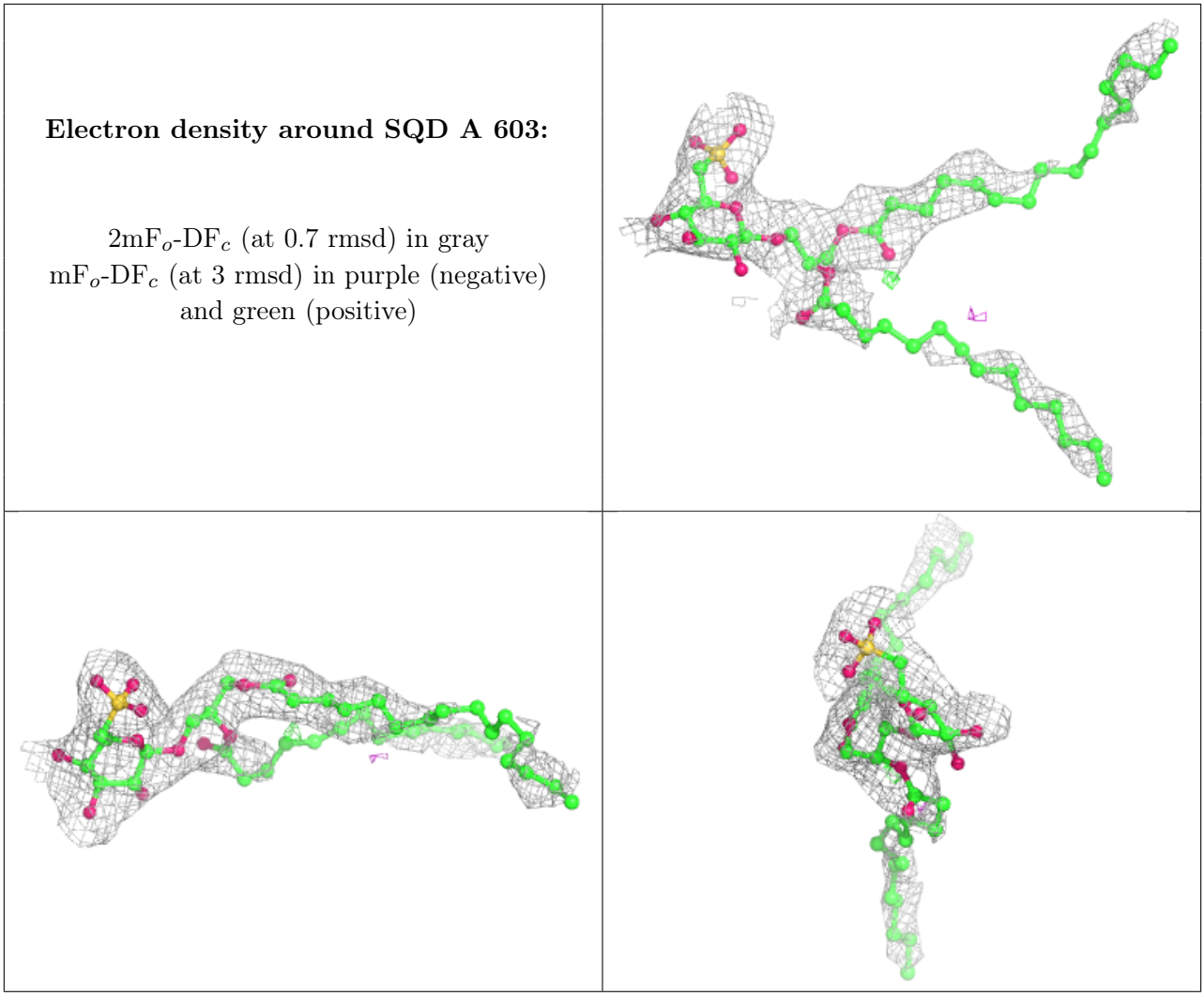
Electron density around LMG B 620:

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



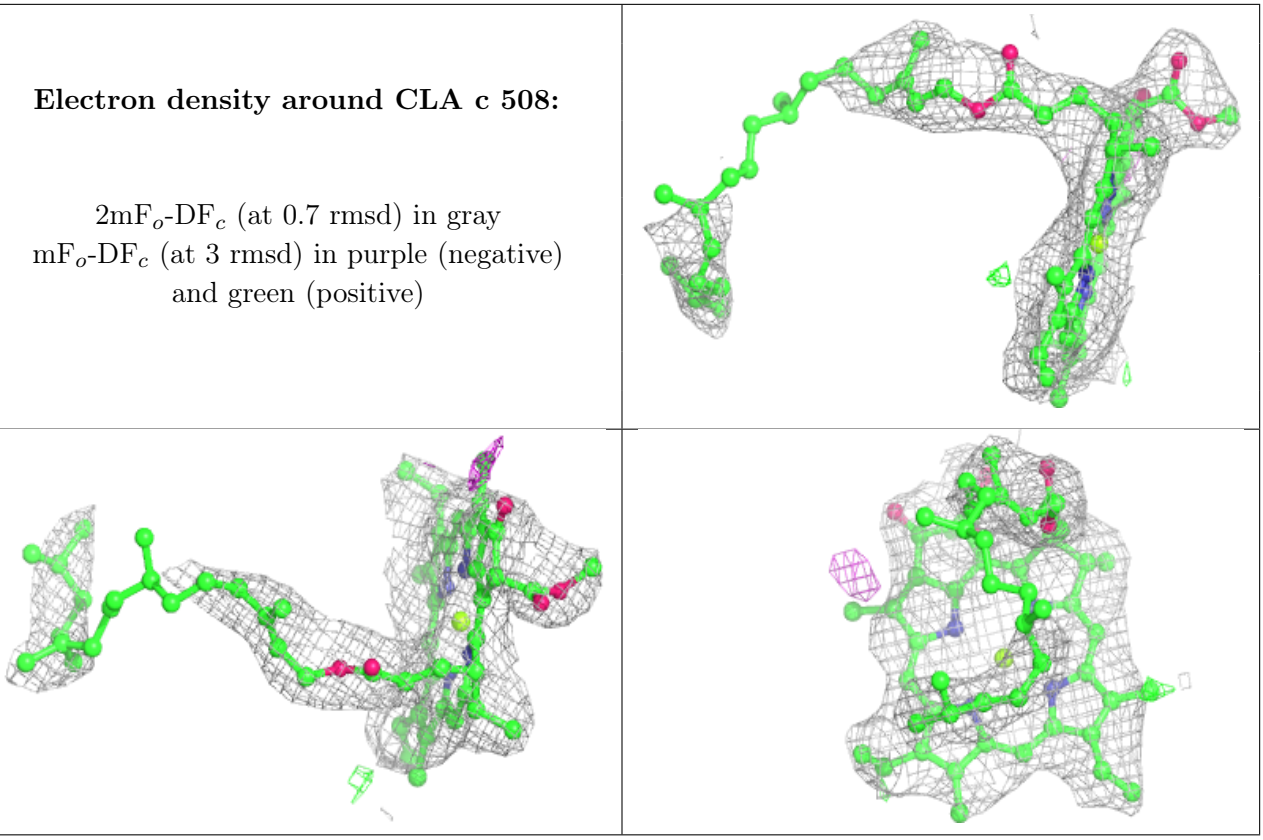
Electron density around SQD A 603:

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



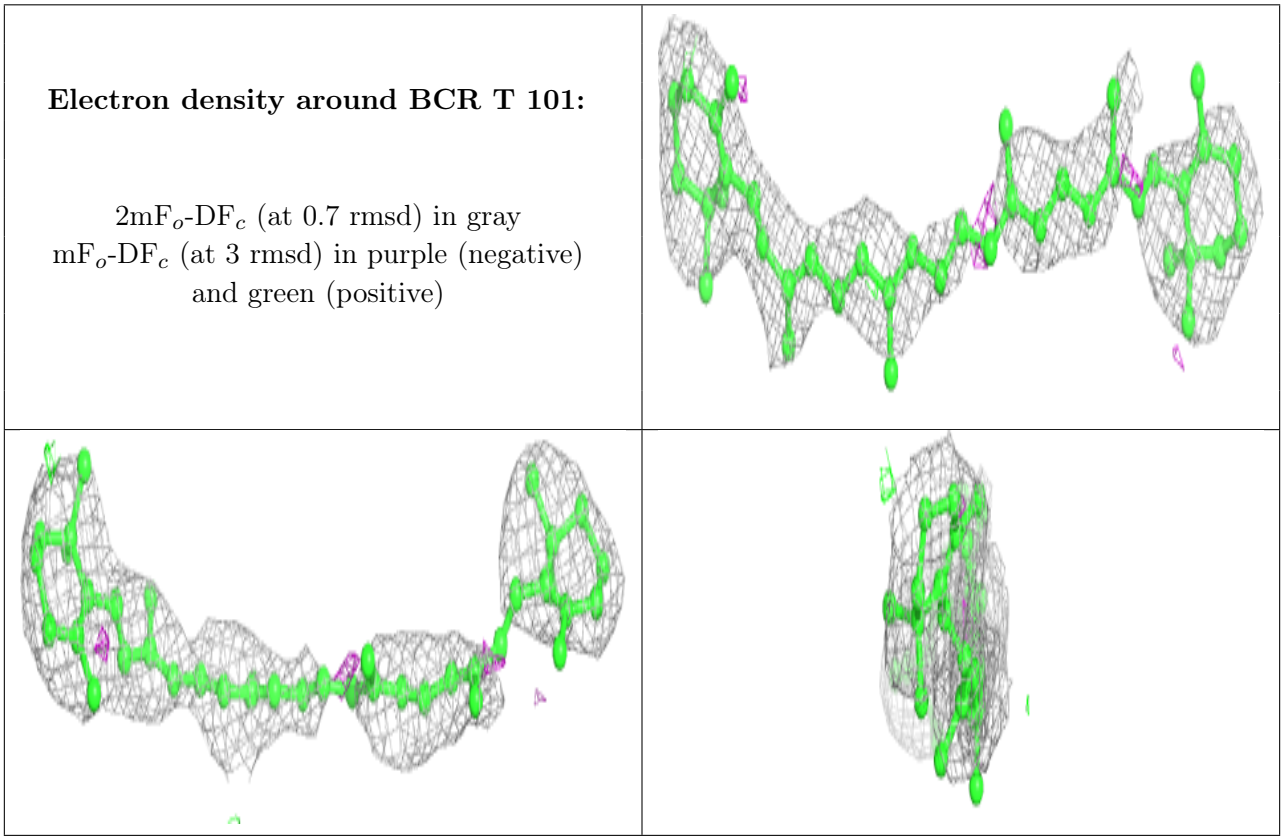
Electron density around CLA c 508:

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



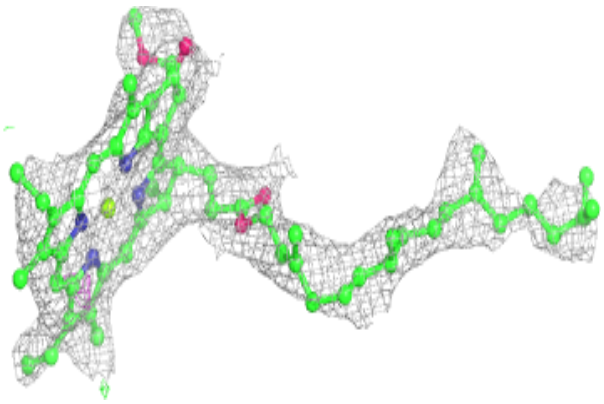
Electron density around BCR T 101:

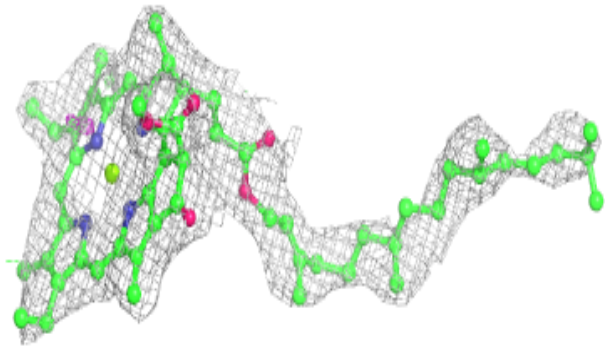
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

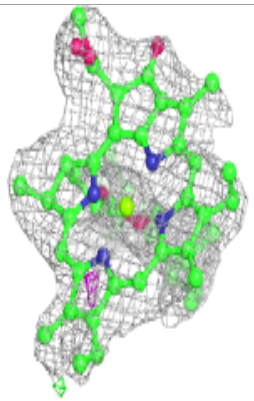


Electron density around CLA C 502:

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

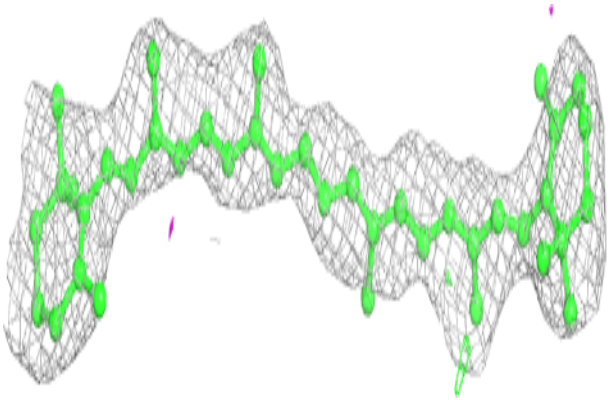


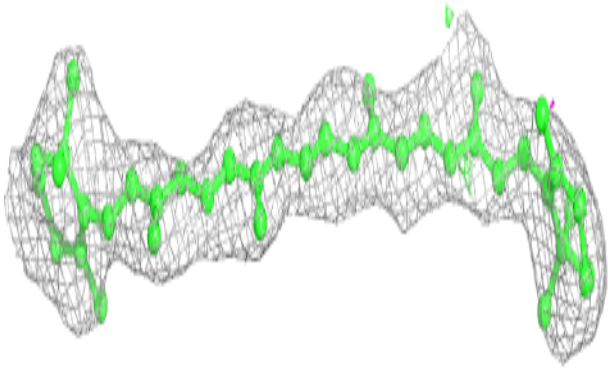


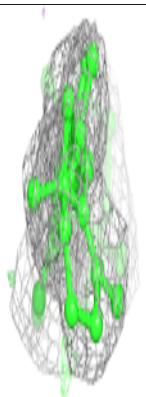


Electron density around BCR b 622:

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

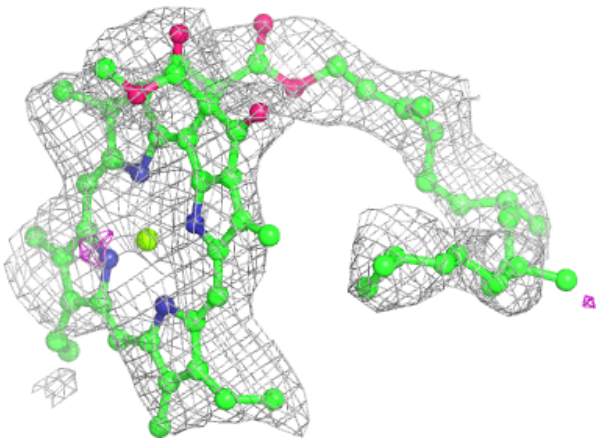


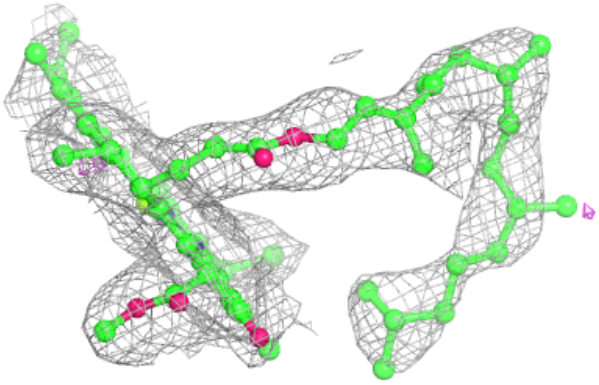


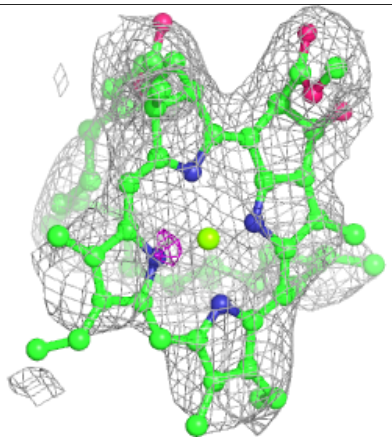


Electron density around CLA C 503:

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

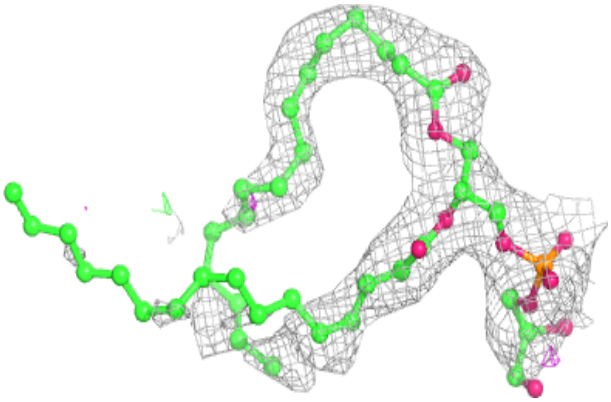


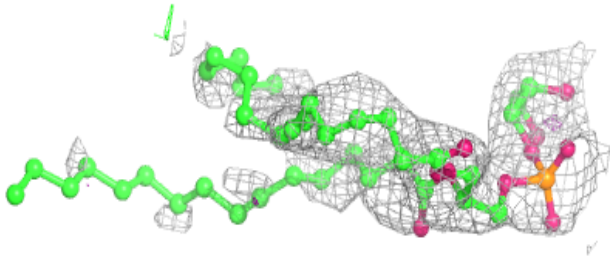


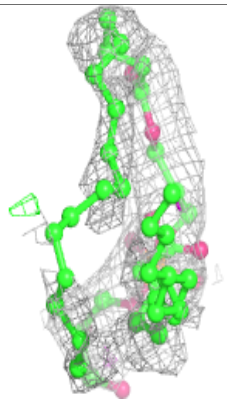


Electron density around LHG A 617:

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

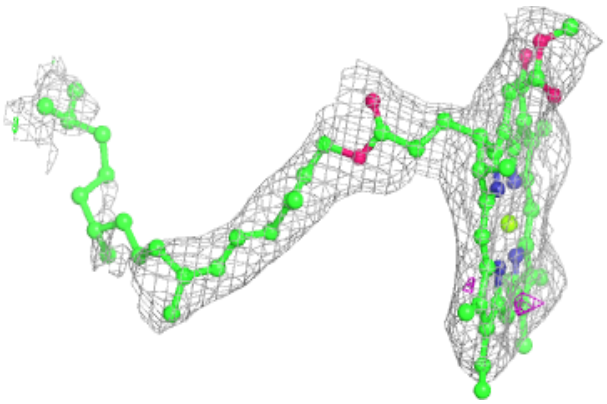


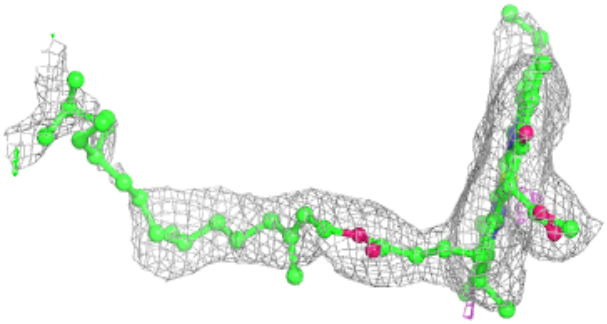


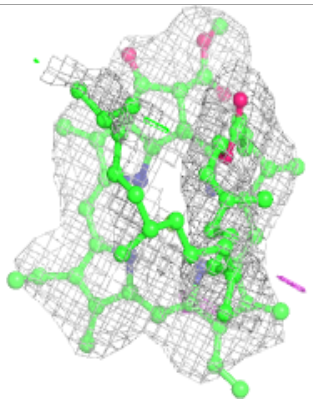


Electron density around CLA d 404:

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

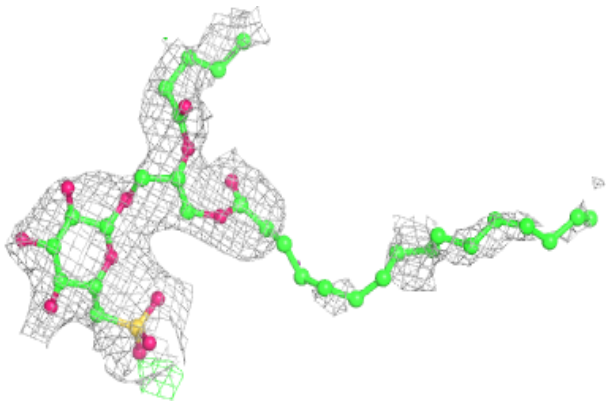


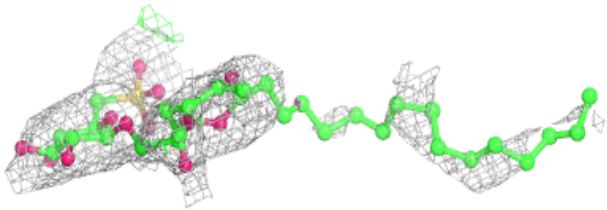


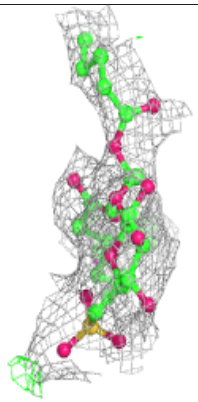


Electron density around SQD f 101:

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

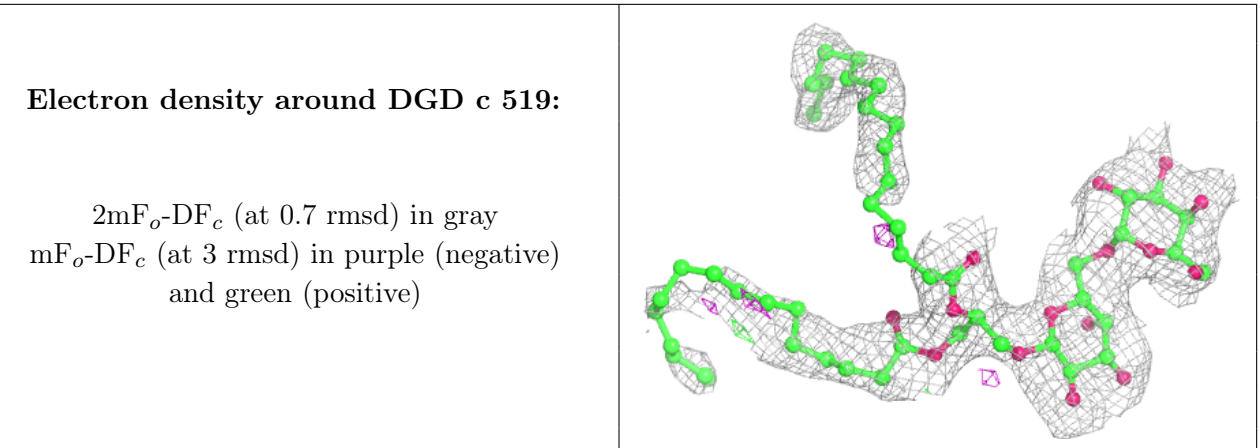


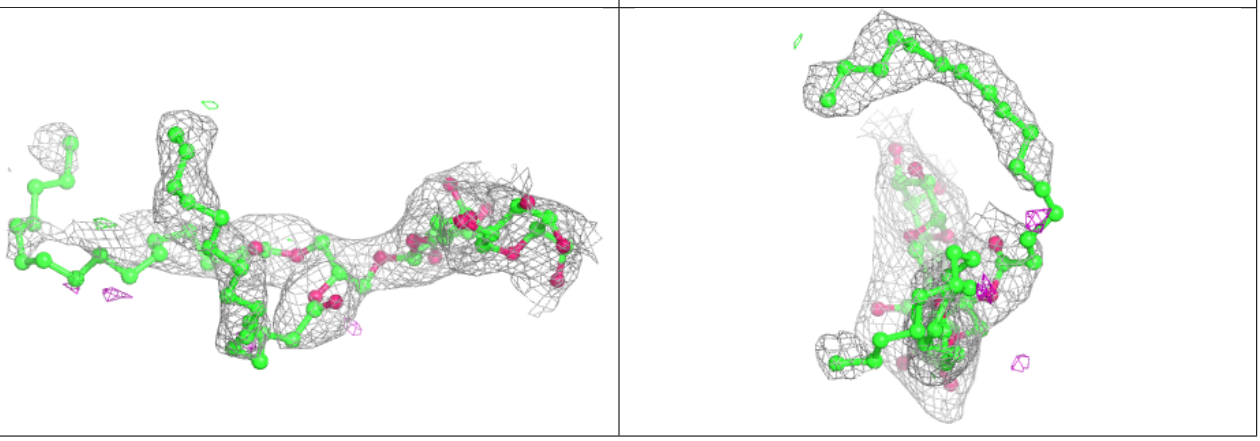




Electron density around DGD c 519:

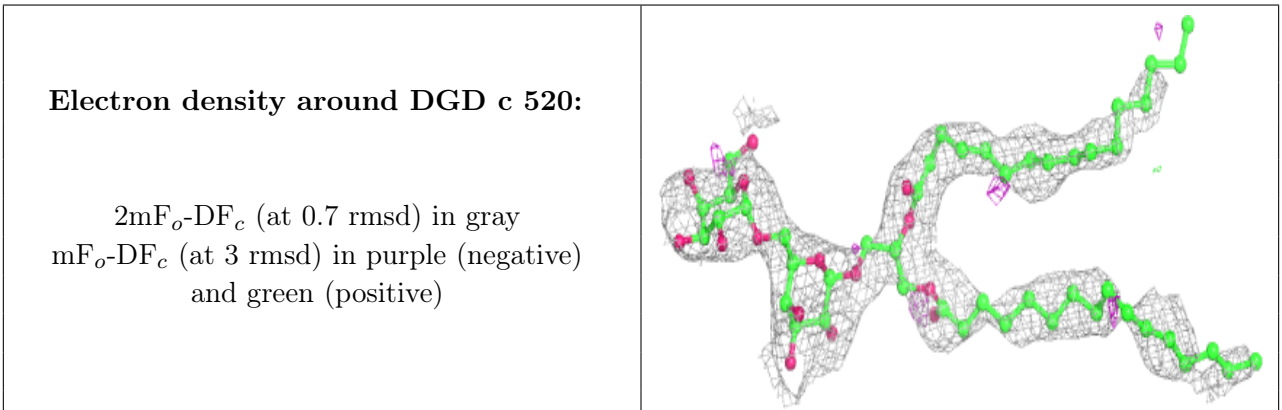
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

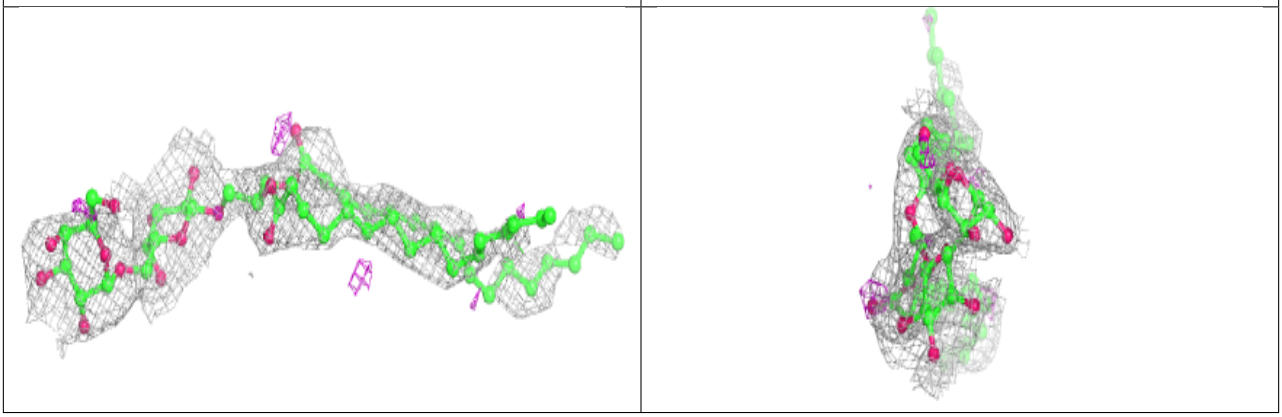




Electron density around DGD c 520:

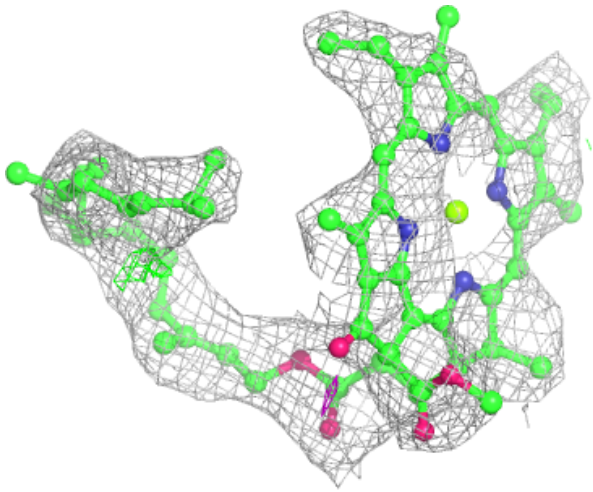
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

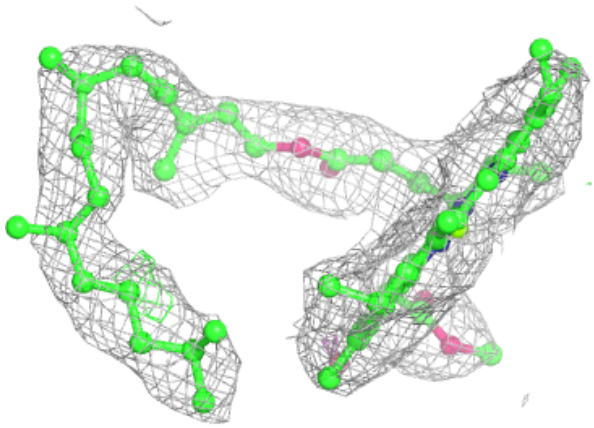


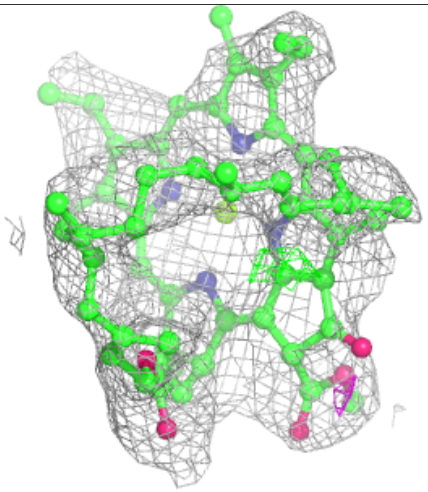


Electron density around CLA c 505:

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

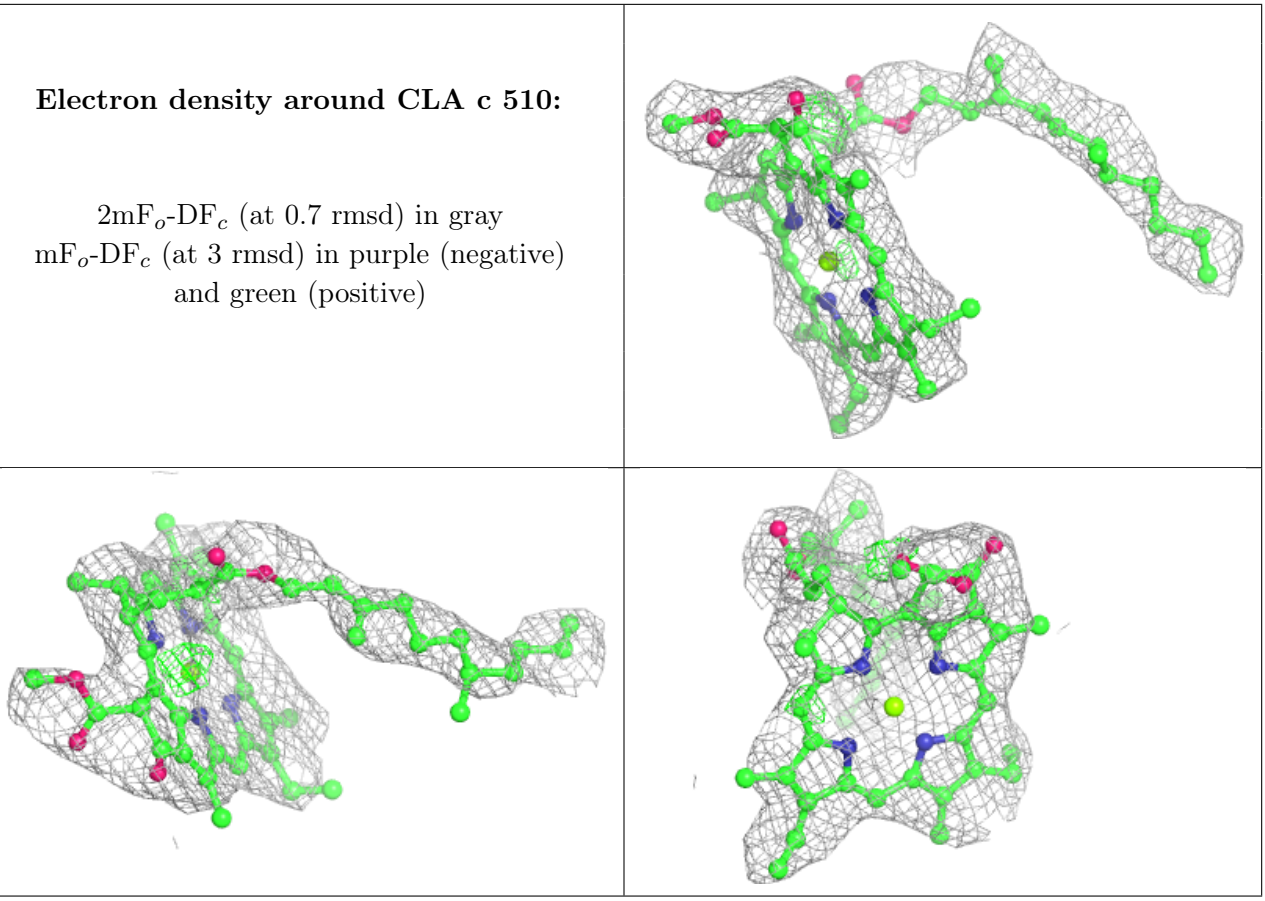






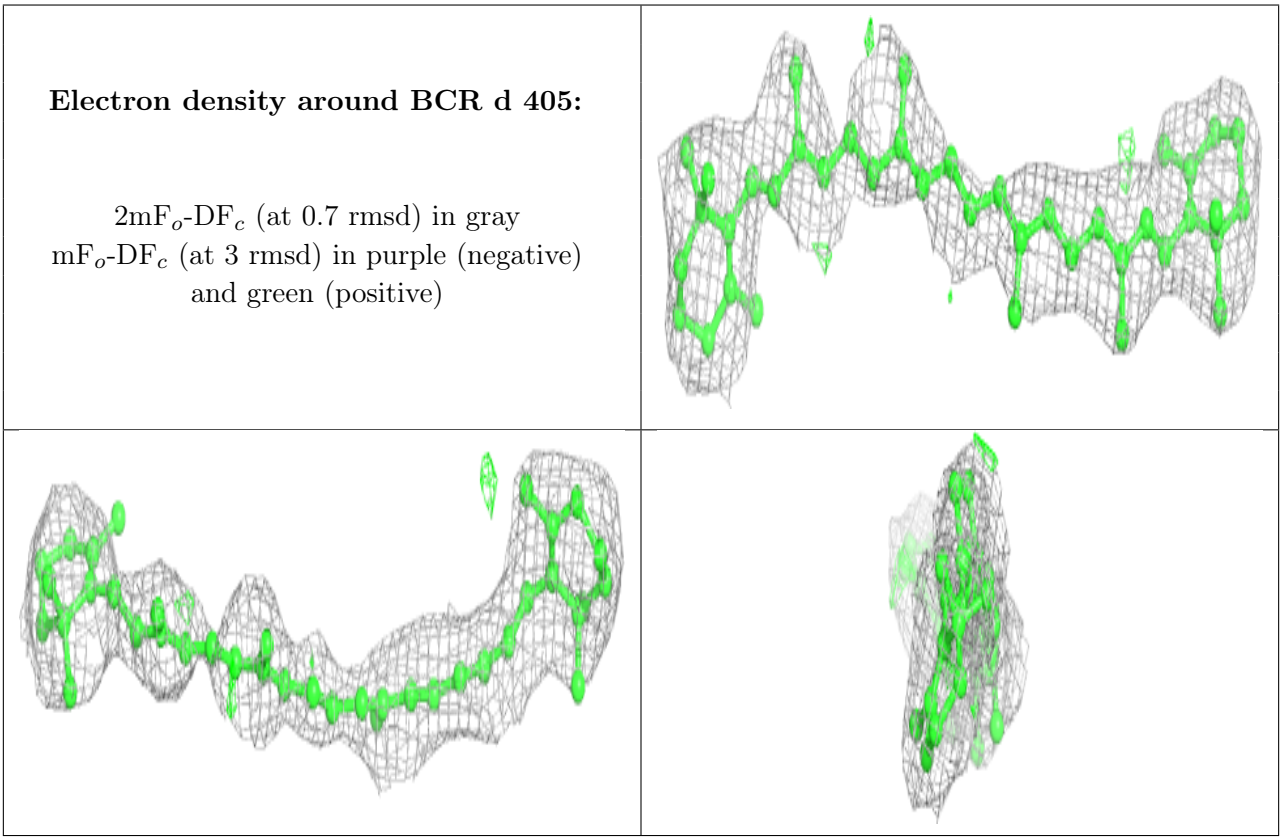
Electron density around CLA c 510:

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



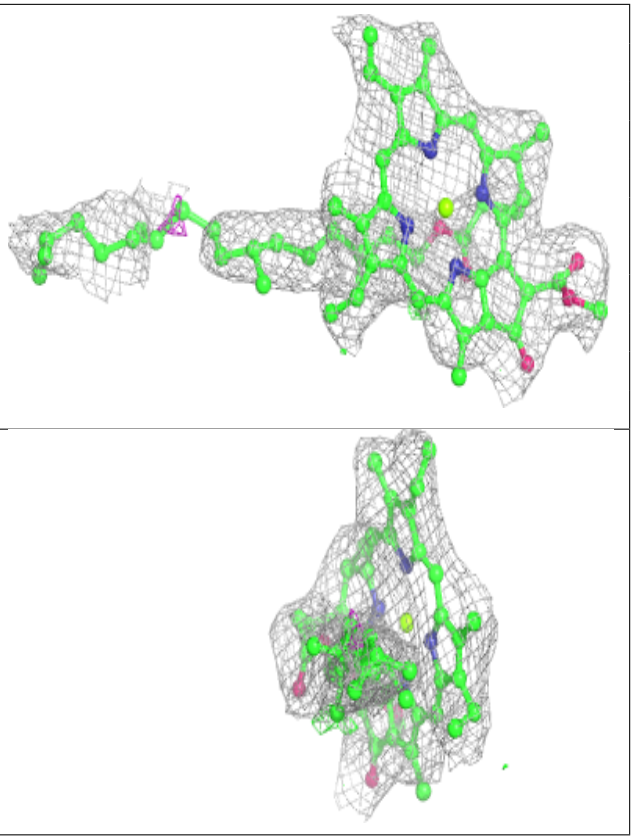
Electron density around BCR d 405:

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



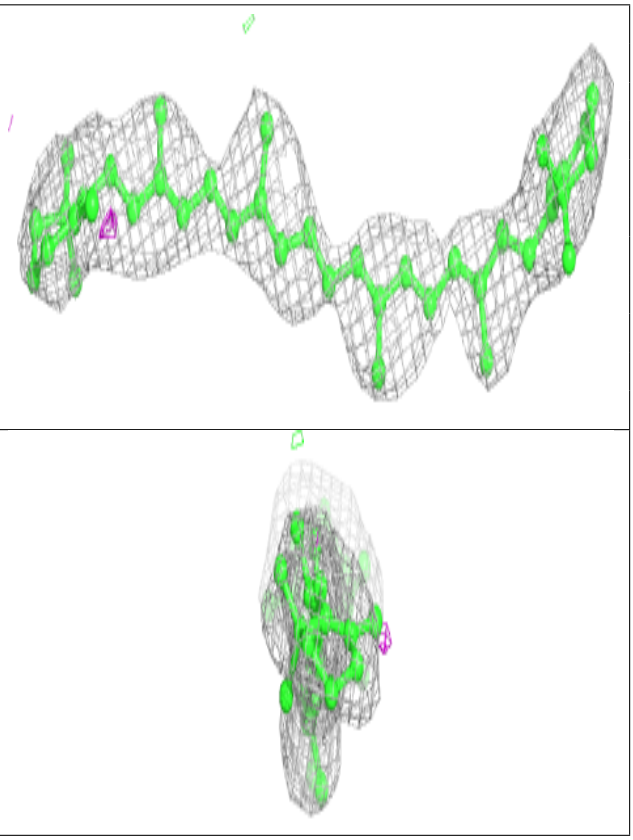
Electron density around CLA B 614:

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



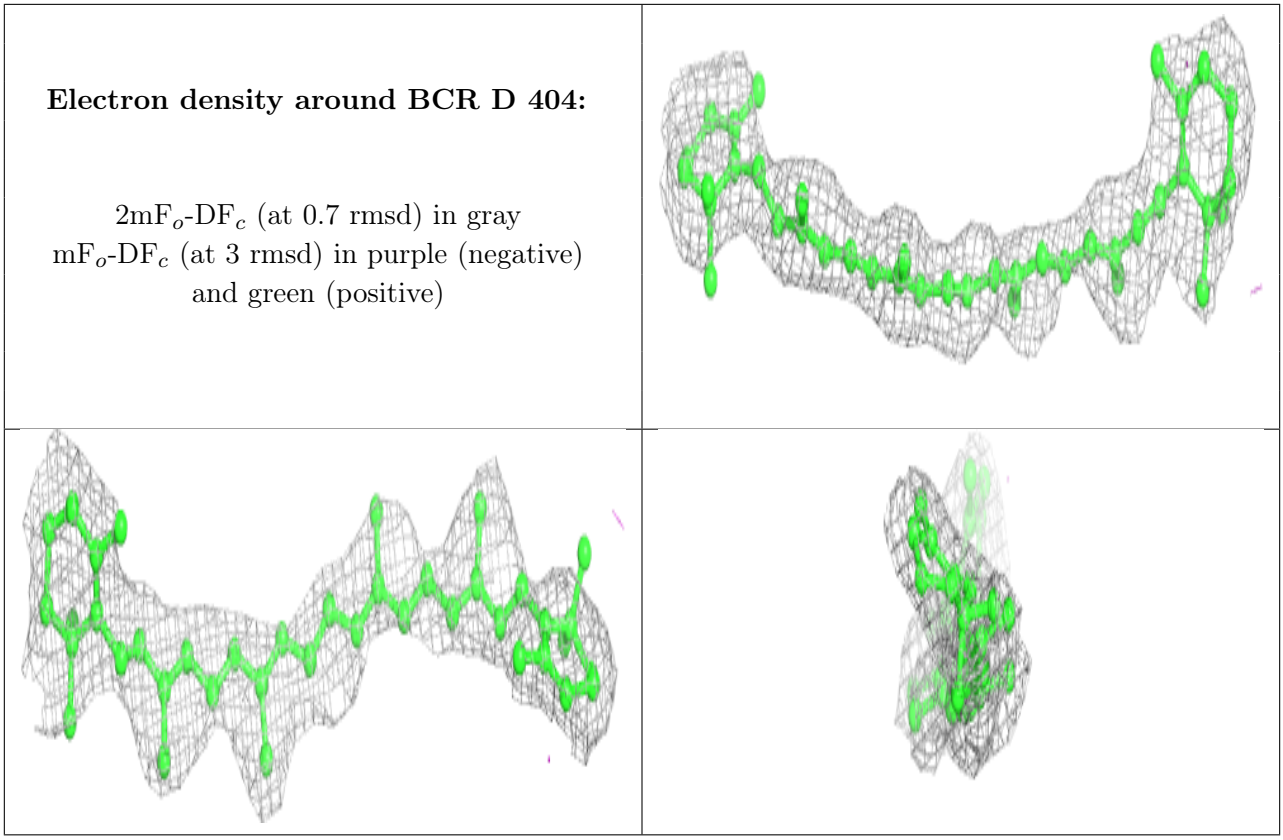
Electron density around BCR C 515:

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



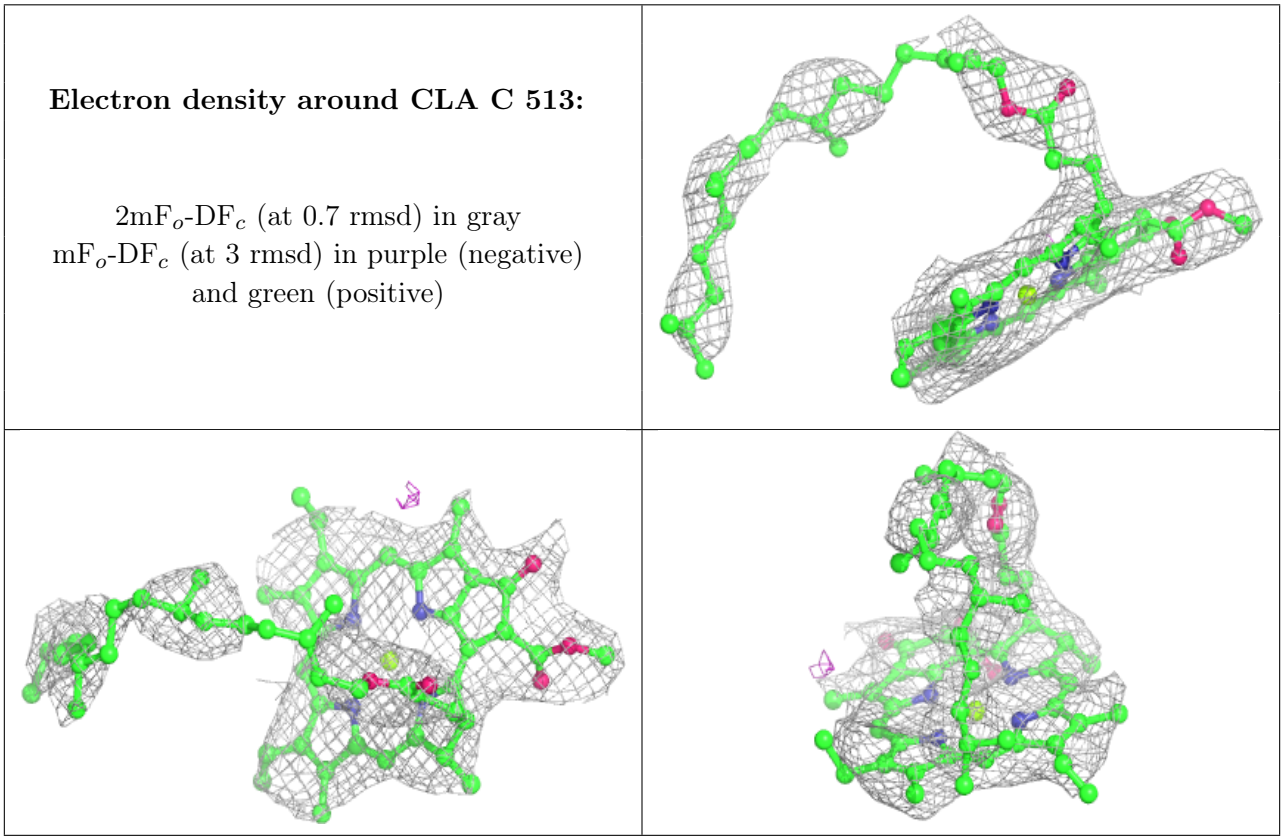
Electron density around BCR D 404:

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



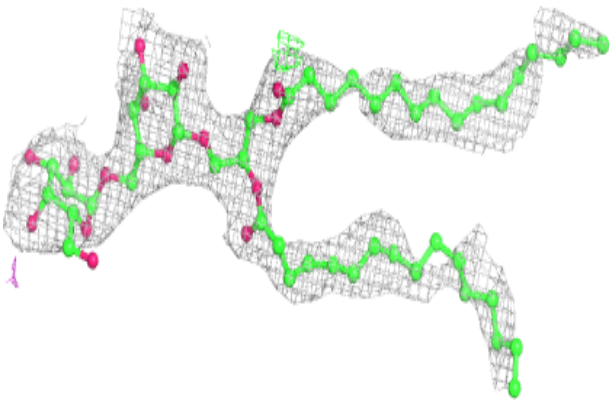
Electron density around CLA C 513:

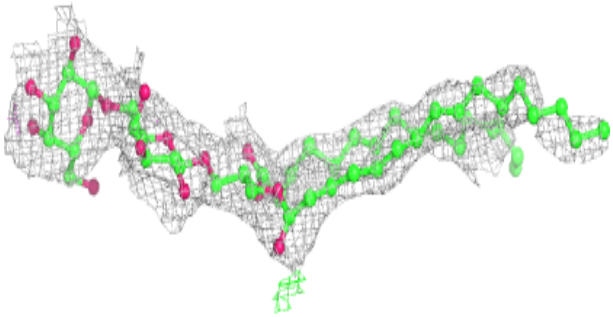
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

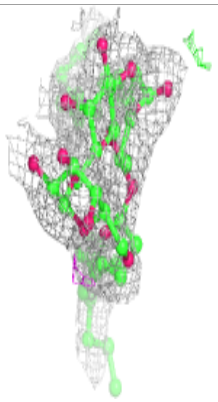


Electron density around DGD C 518:

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

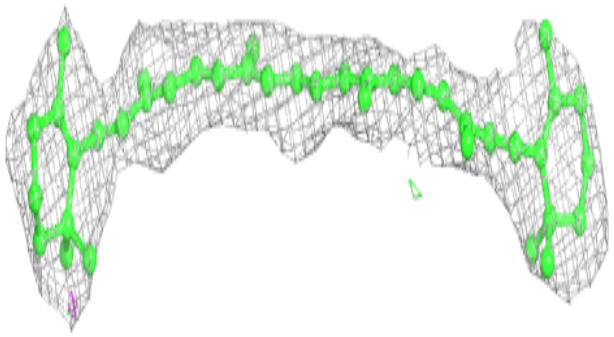


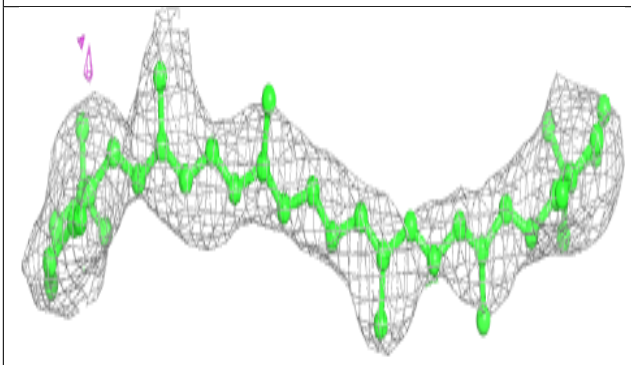


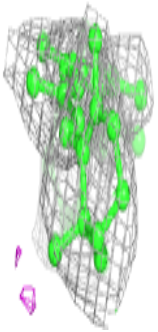


Electron density around BCR K 101:

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

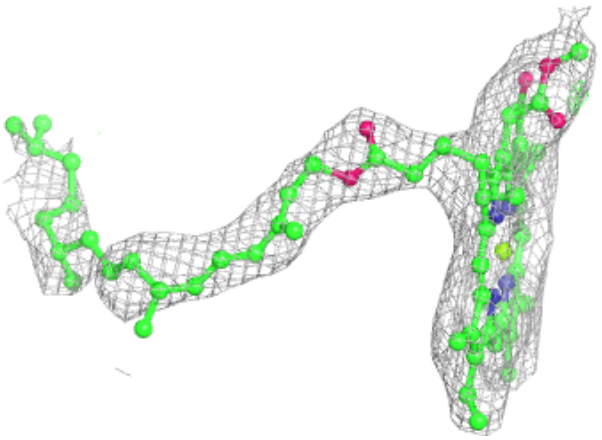


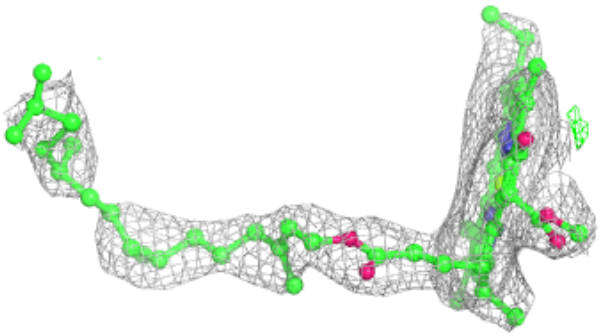


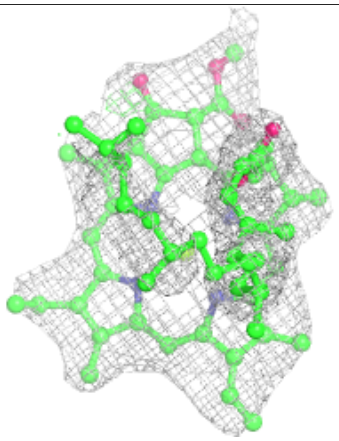


Electron density around CLA D 403:

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

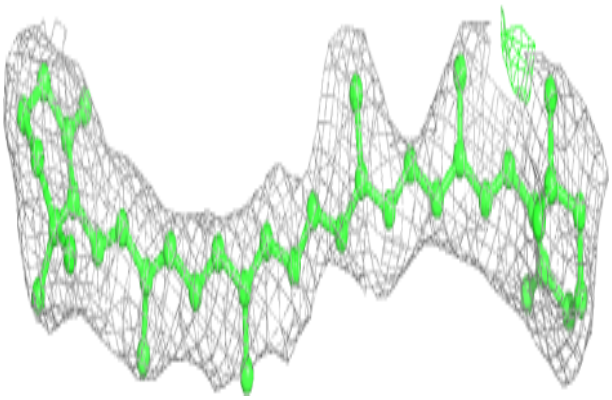


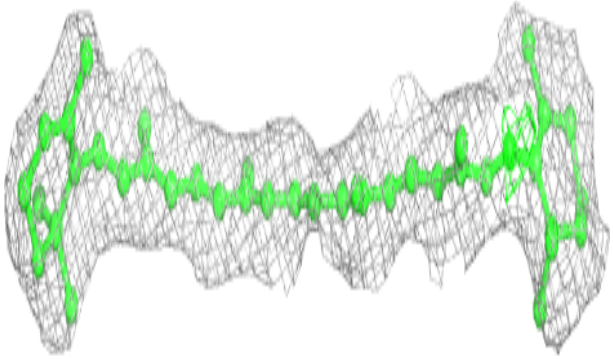


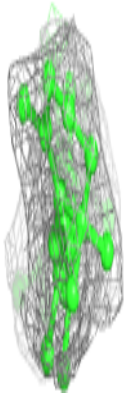


Electron density around BCR B 618:

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

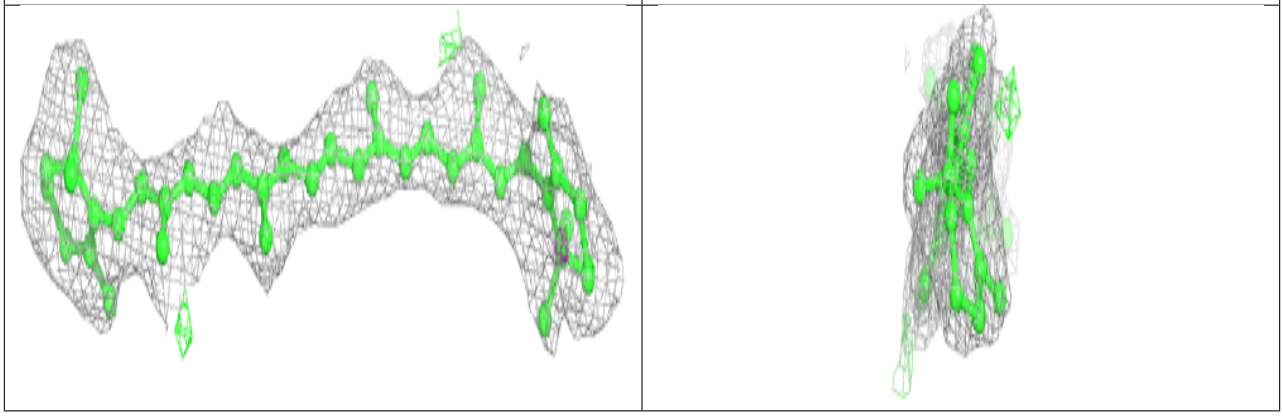






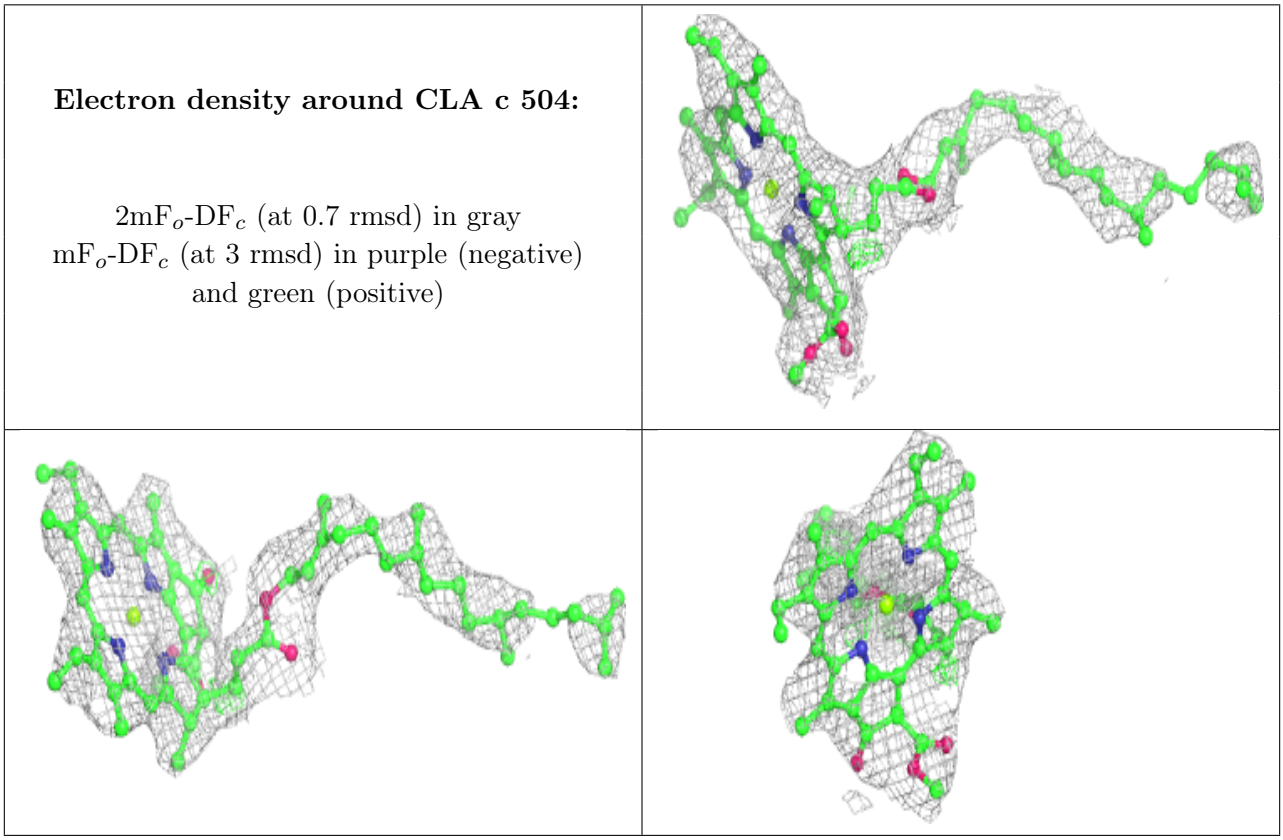
Electron density around BCR B 619:

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



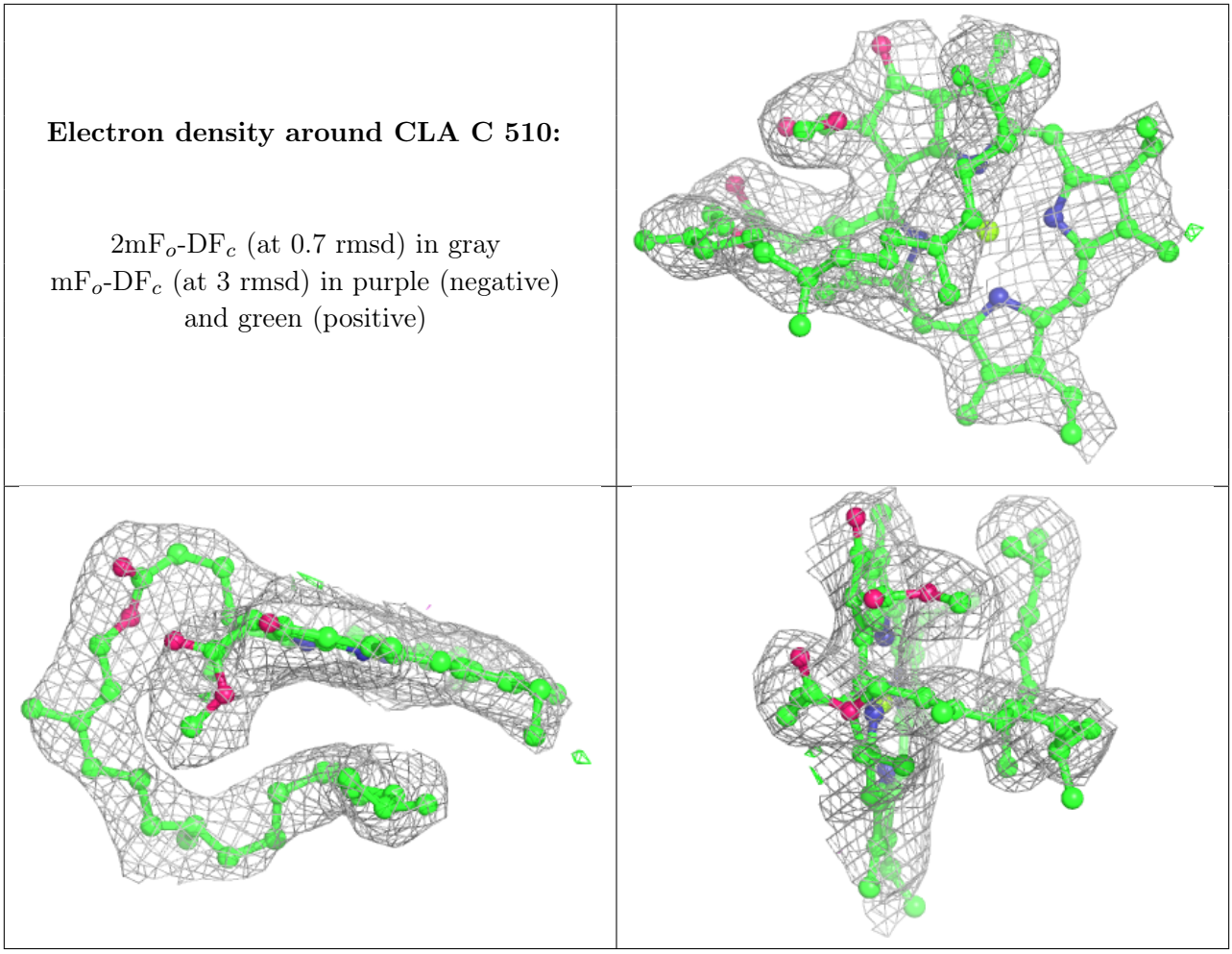
Electron density around CLA c 504:

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



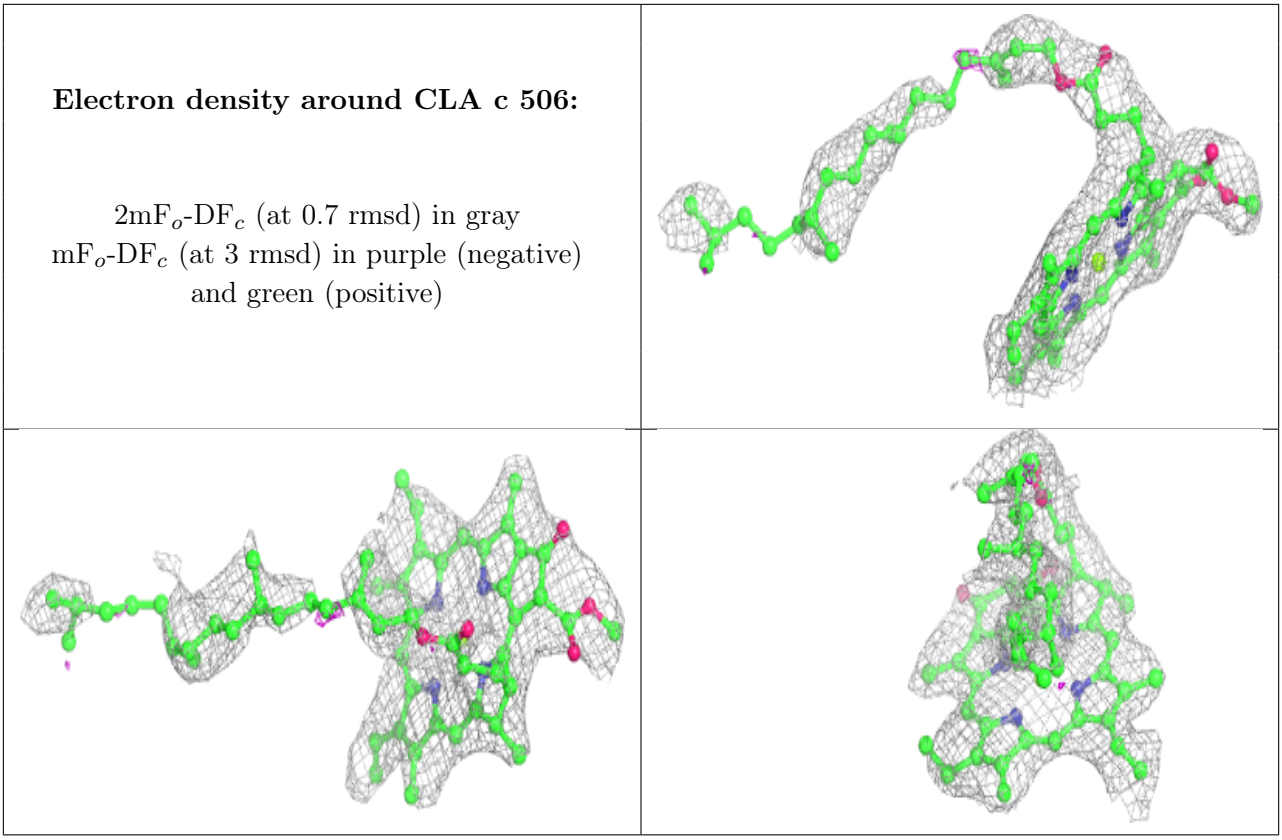
Electron density around CLA C 510:

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



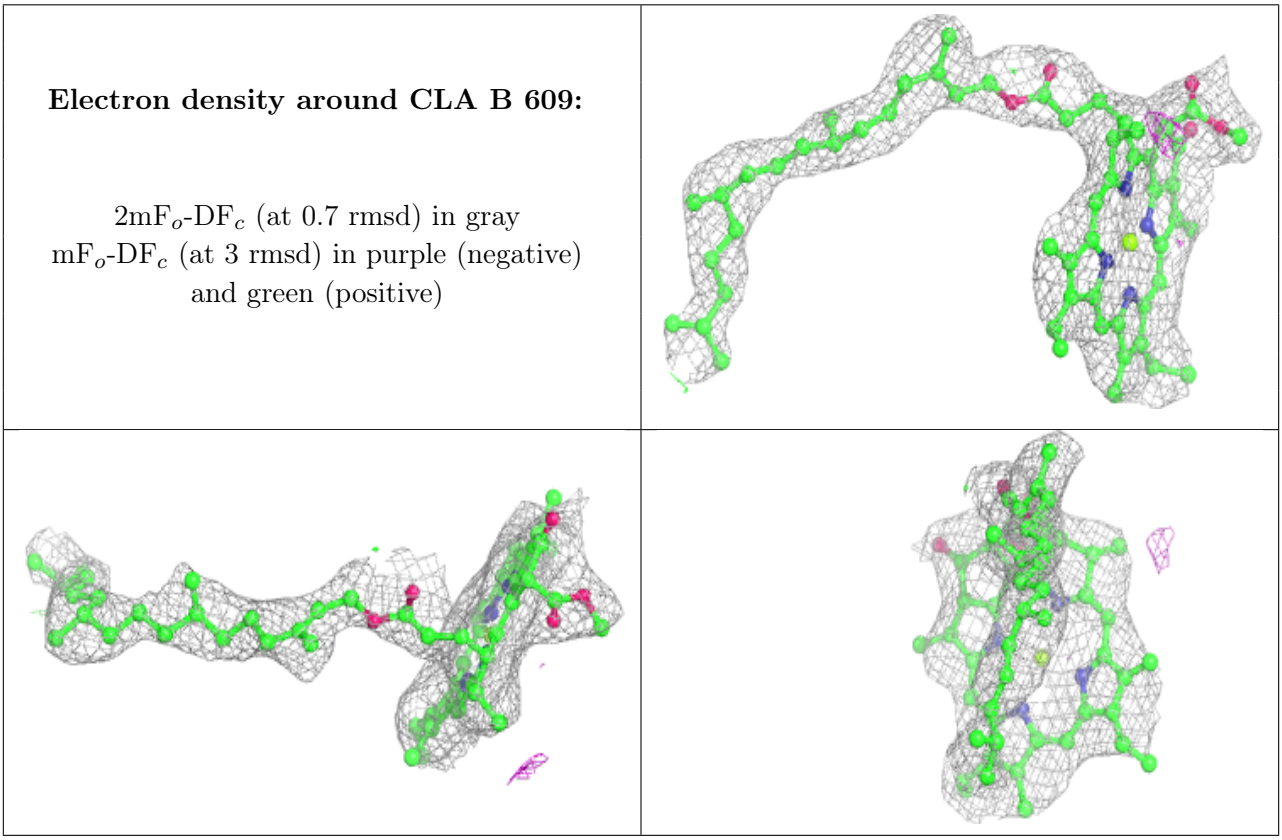
Electron density around CLA c 506:

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



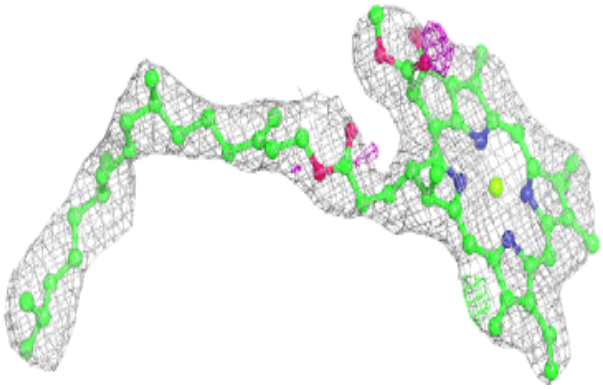
Electron density around CLA B 609:

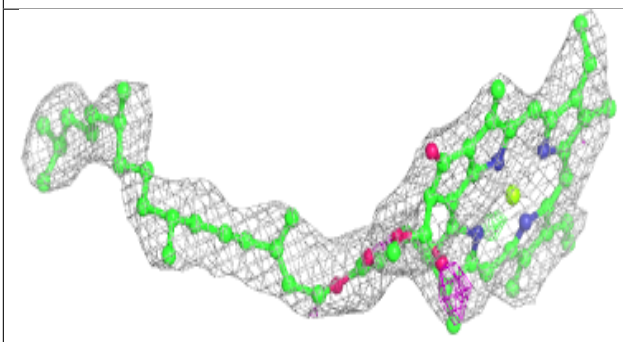
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

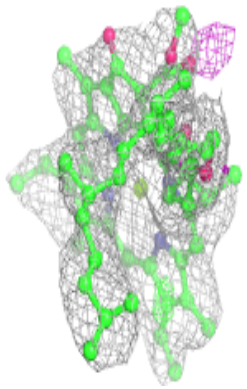


Electron density around CLA A 606:

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

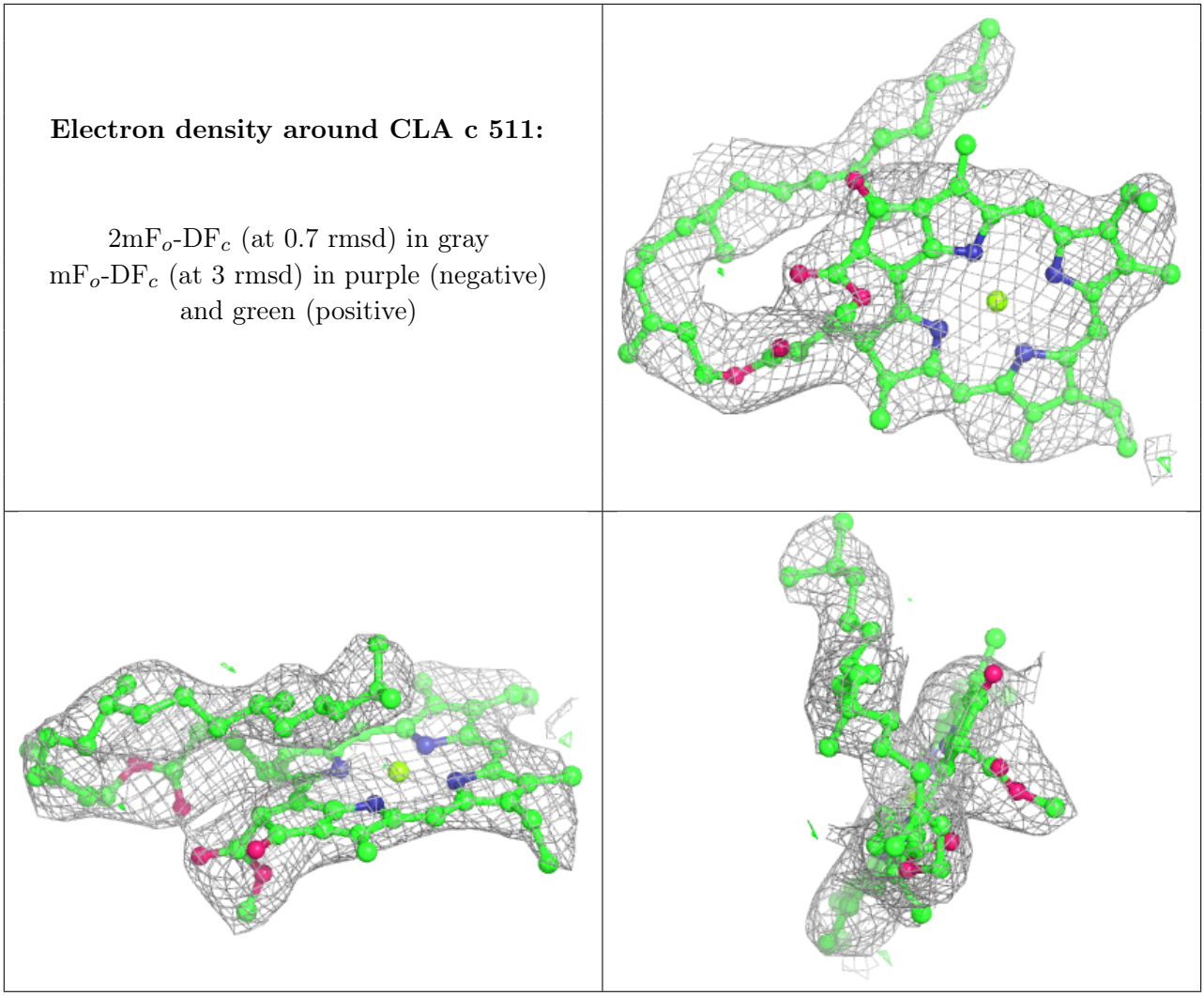






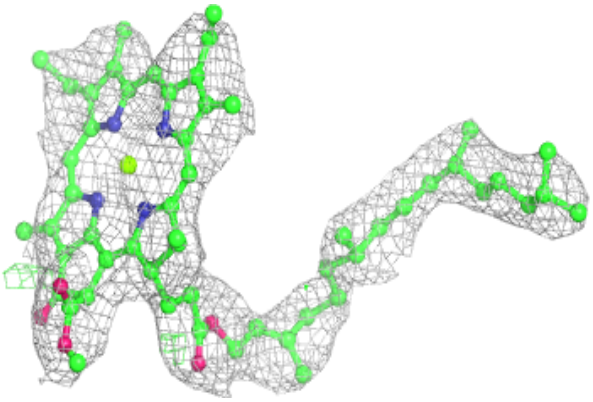
Electron density around CLA c 511:

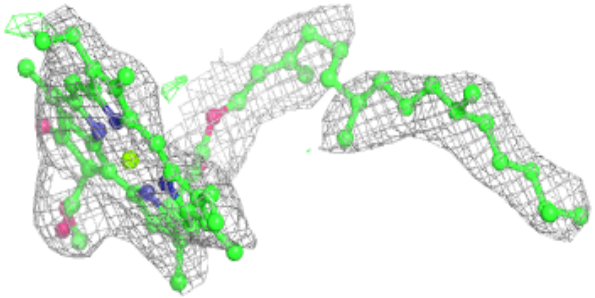
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

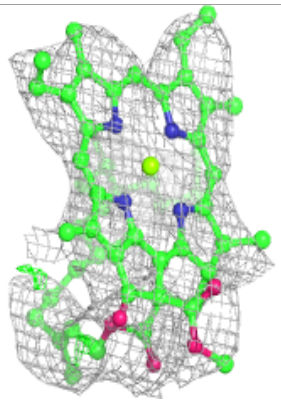


Electron density around CLA c 513:

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

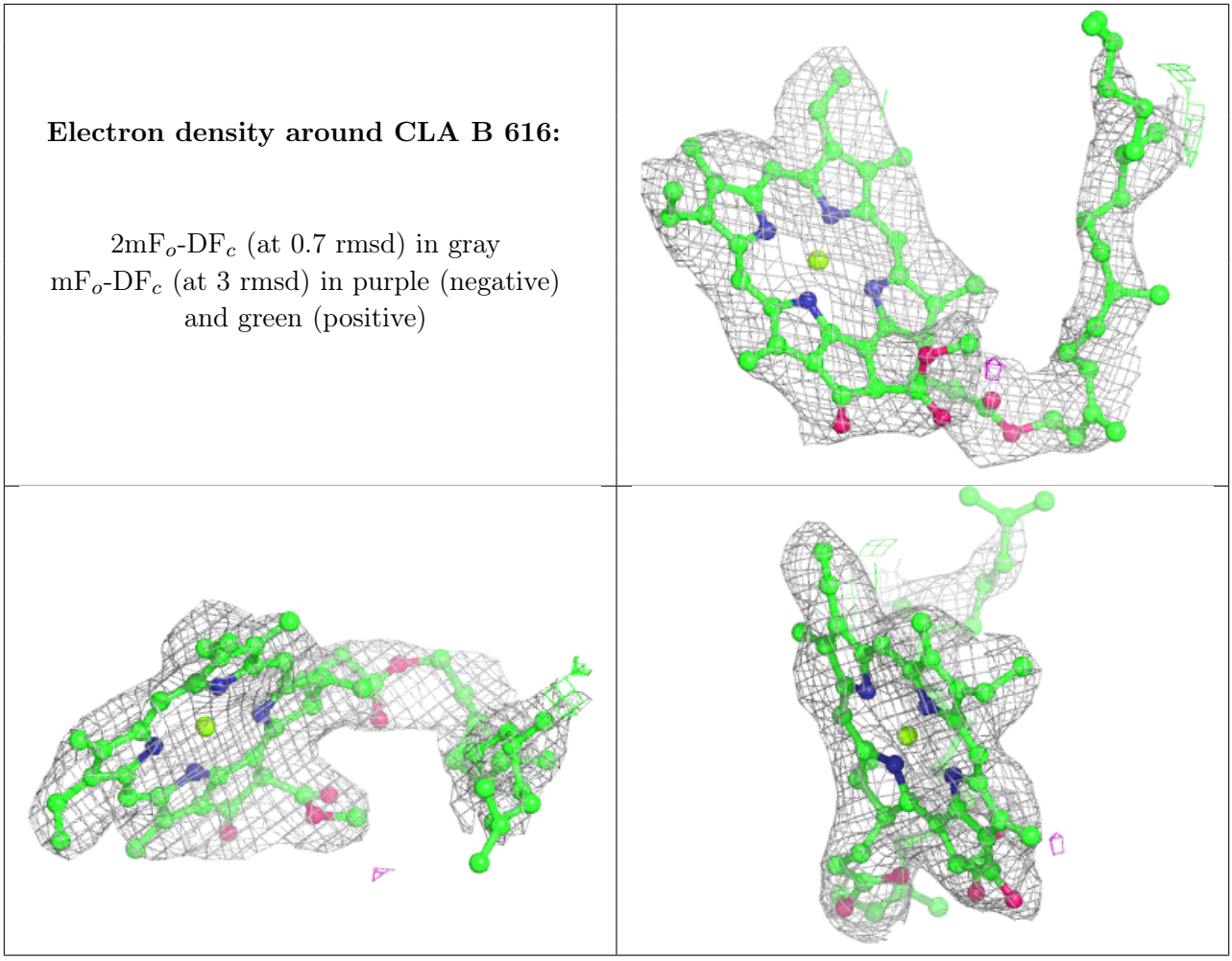






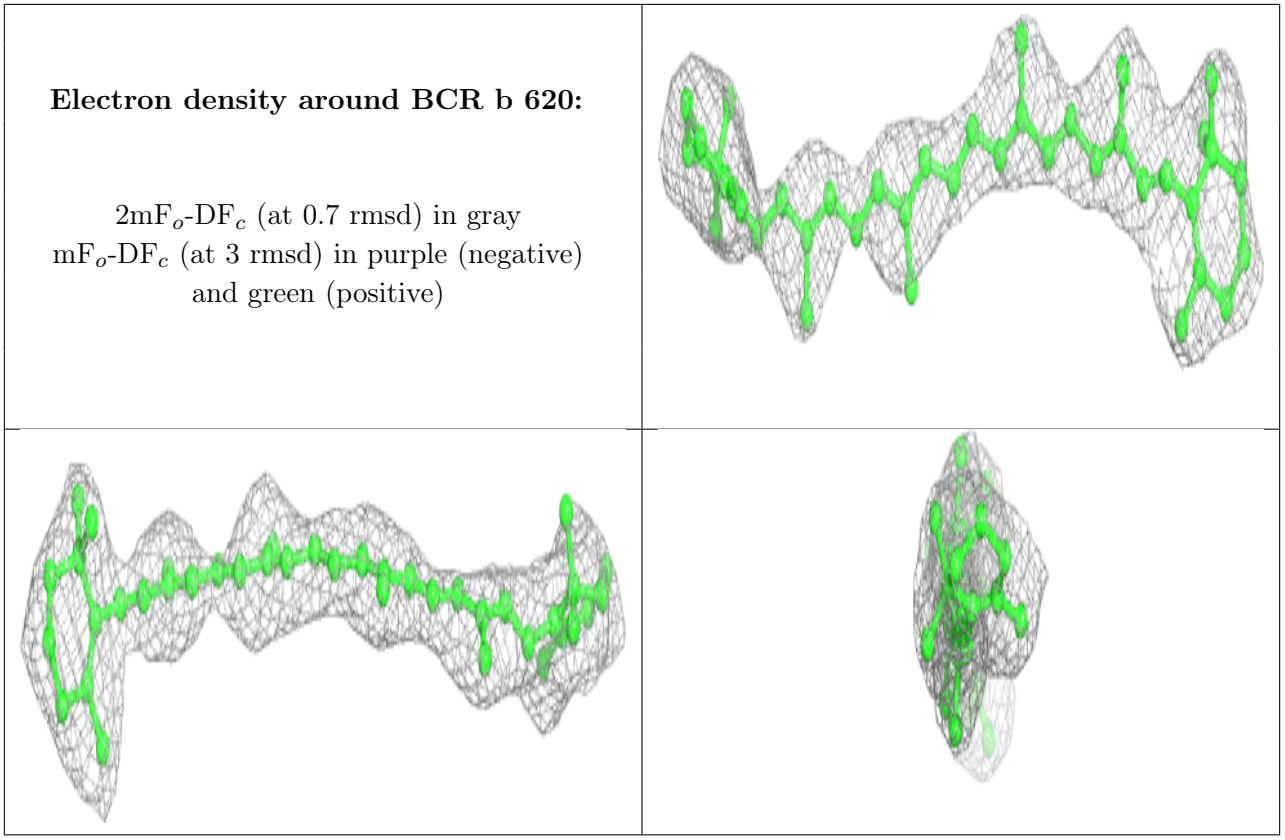
Electron density around CLA B 616:

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



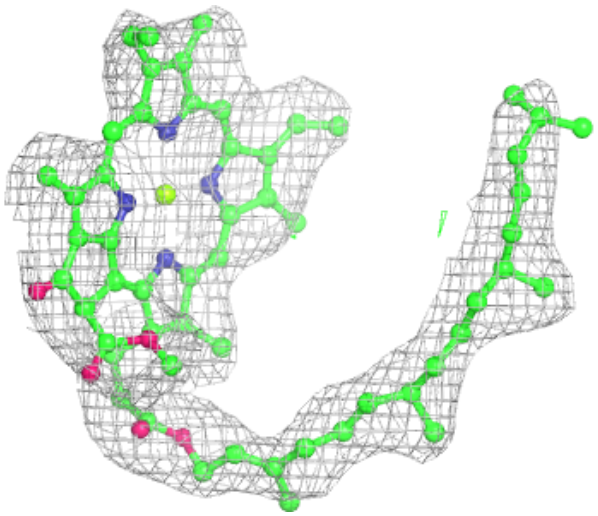
Electron density around BCR b 620:

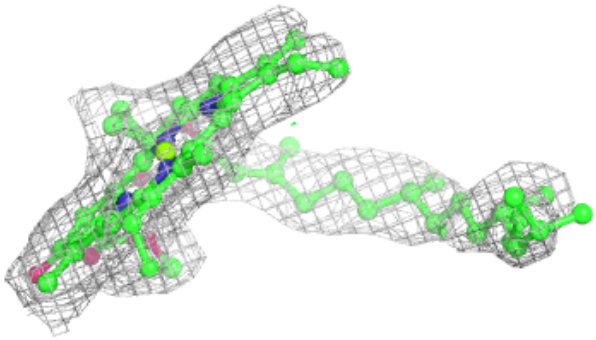
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

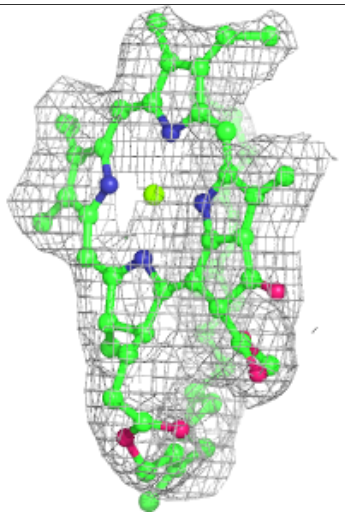


Electron density around CLA C 507:

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

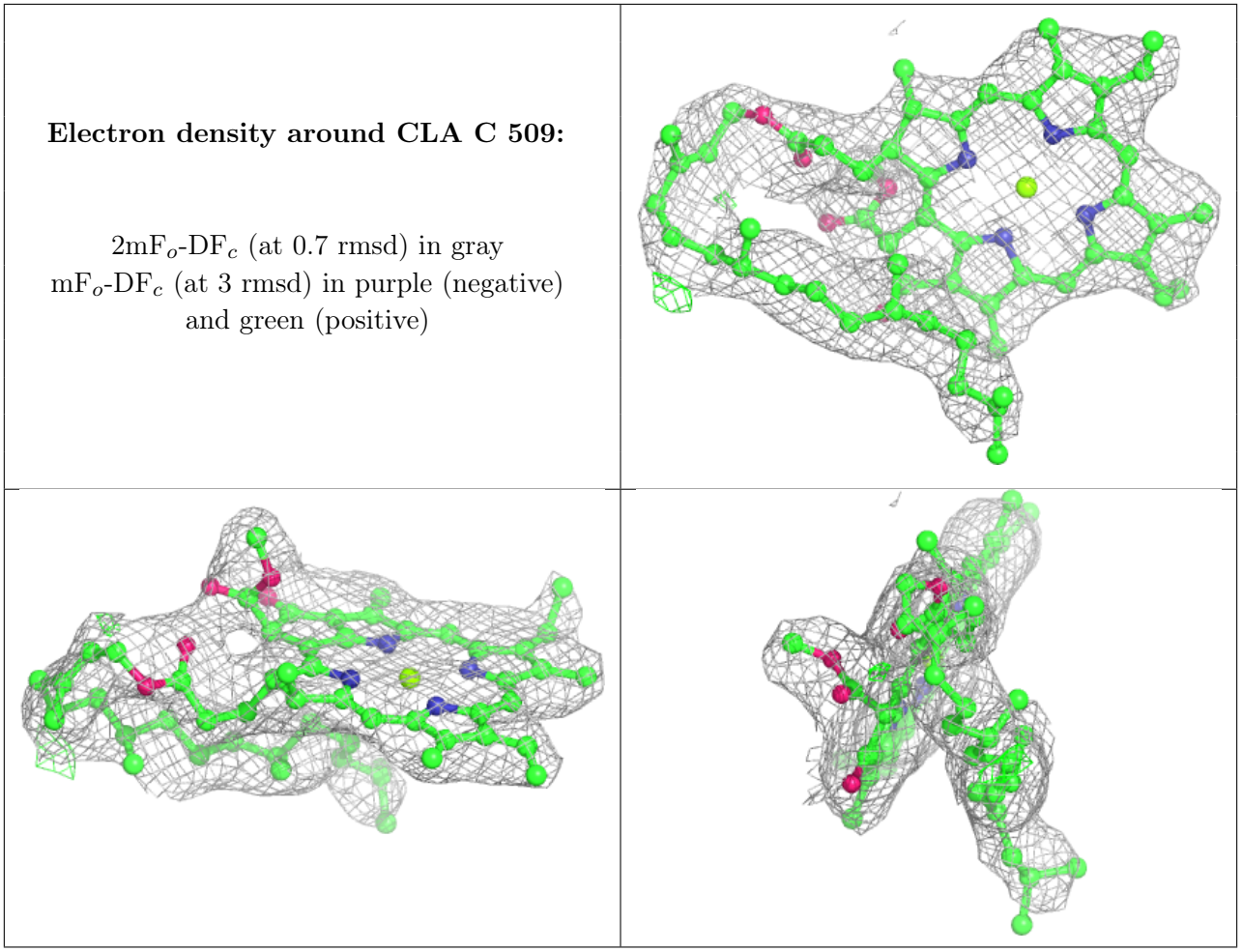






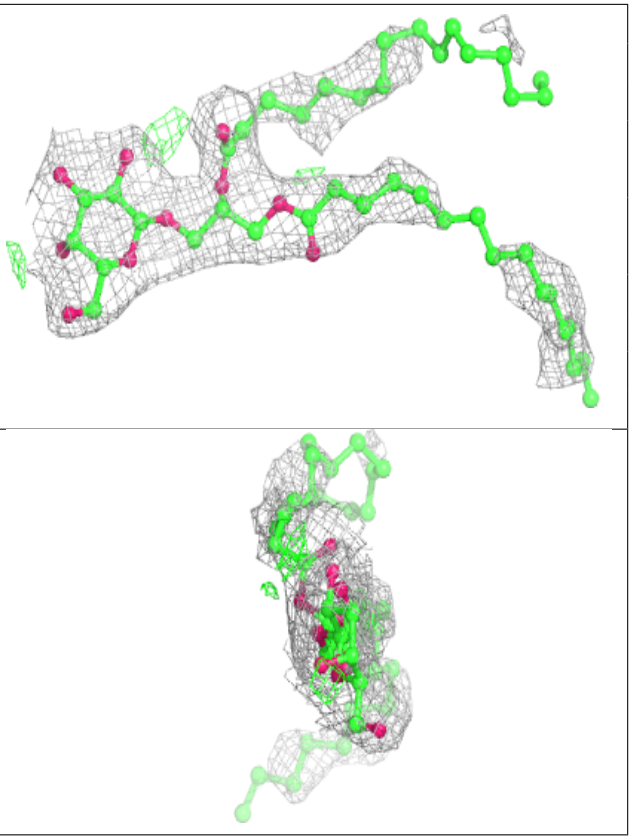
Electron density around CLA C 509:

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



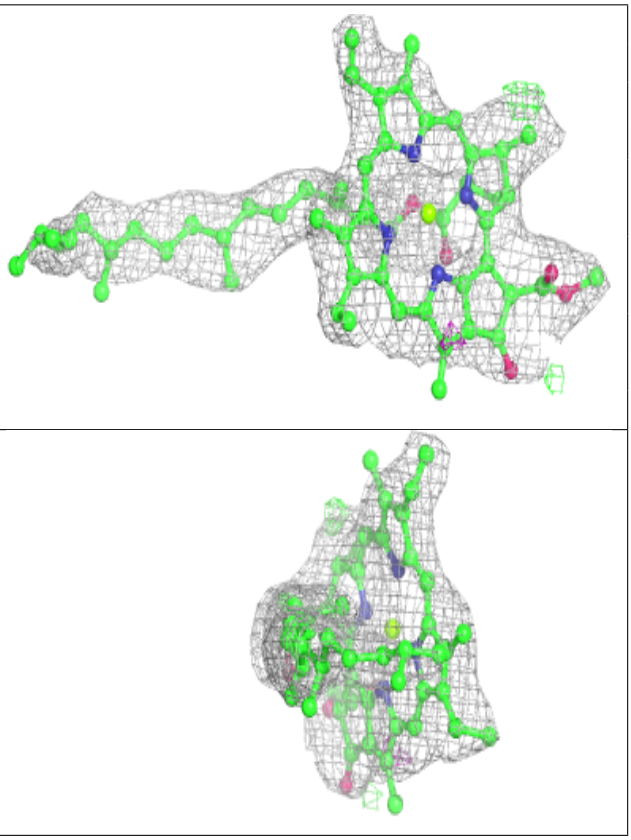
Electron density around LMG D 405:

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



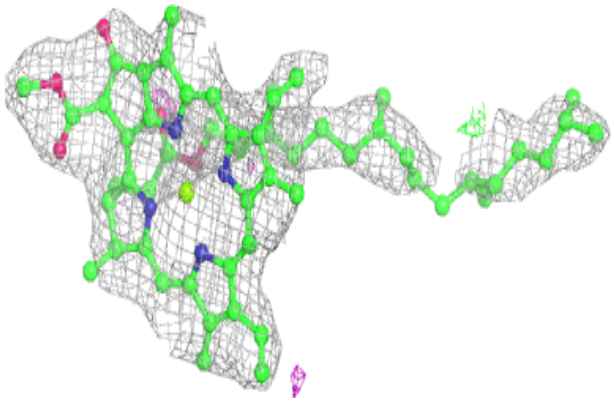
Electron density around CLA b 611:

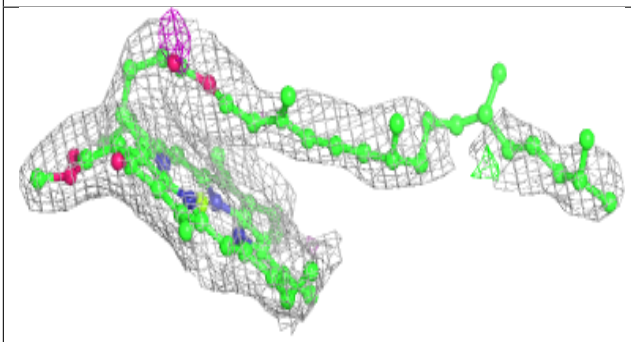
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

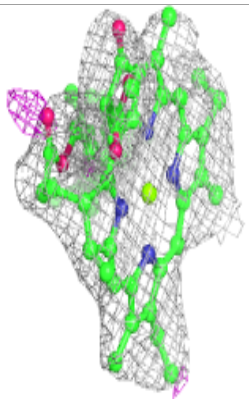


Electron density around CLA b 617:

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

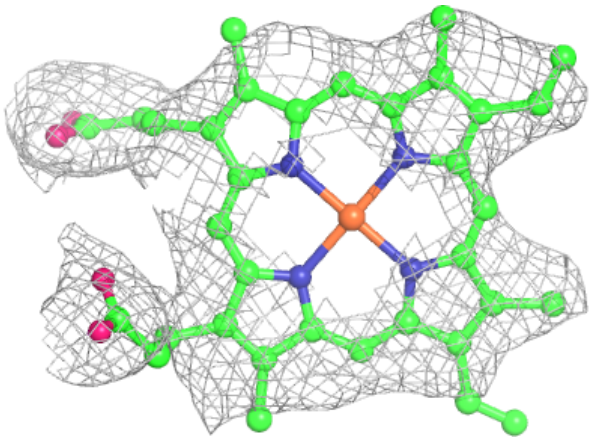


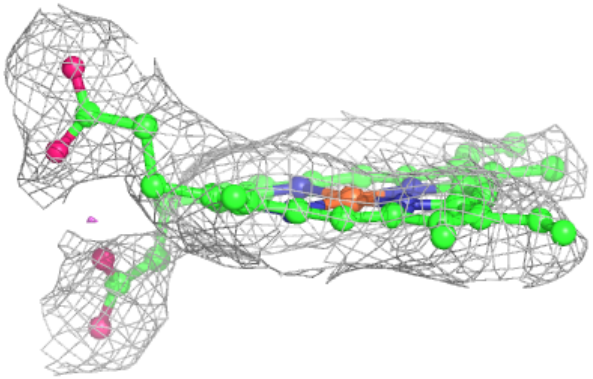


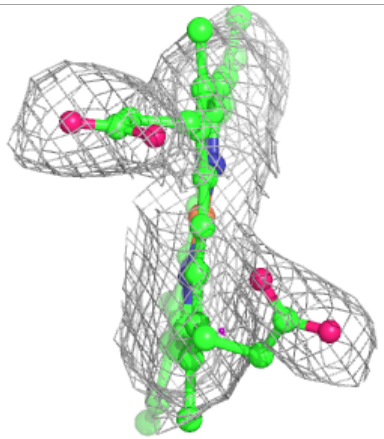


Electron density around HEM e 101:

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

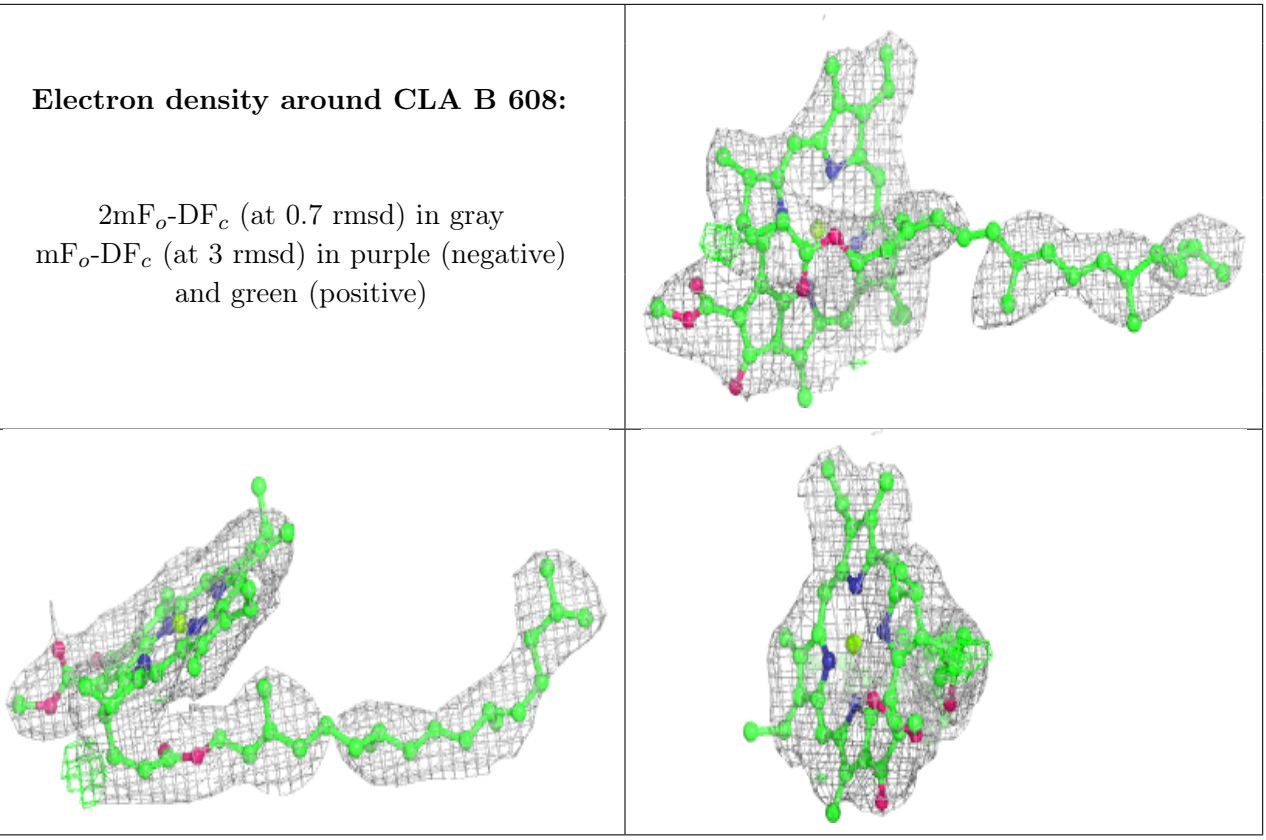






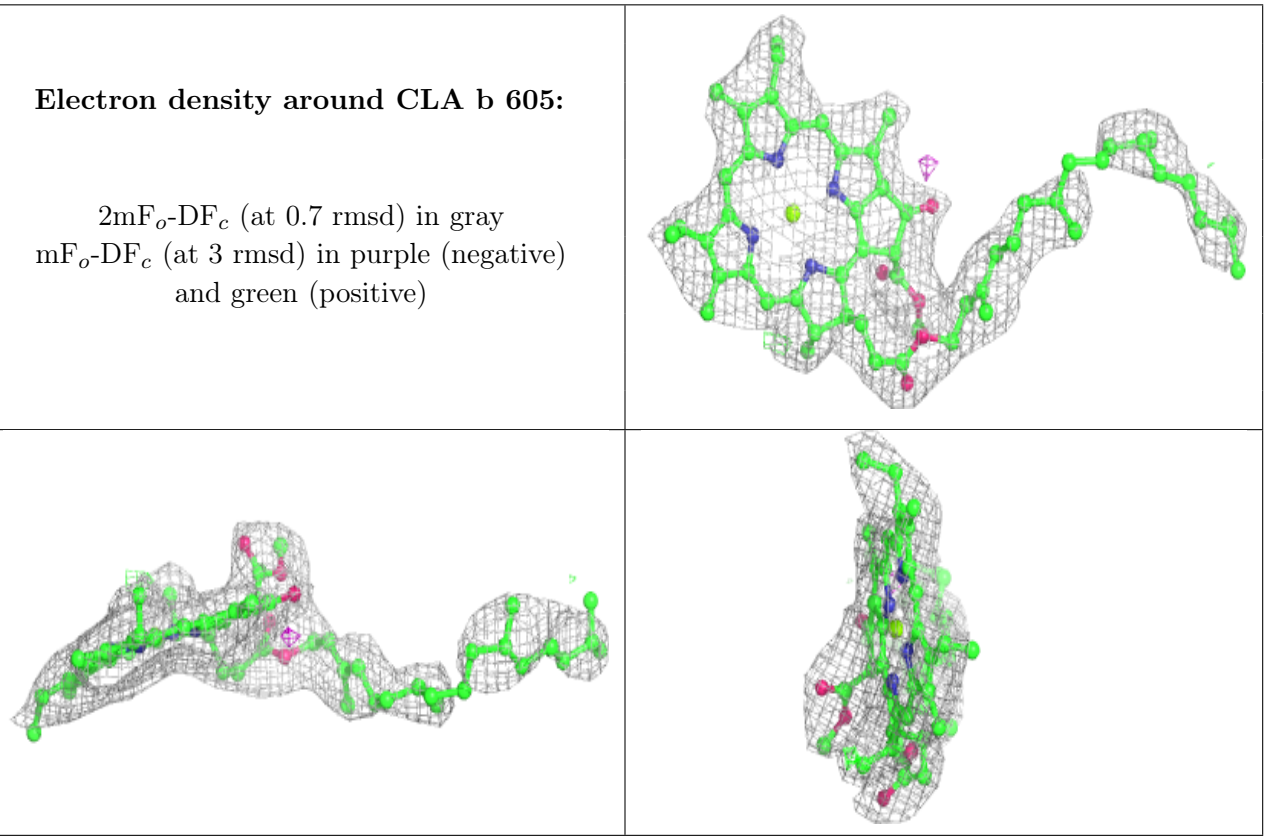
Electron density around CLA B 608:

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



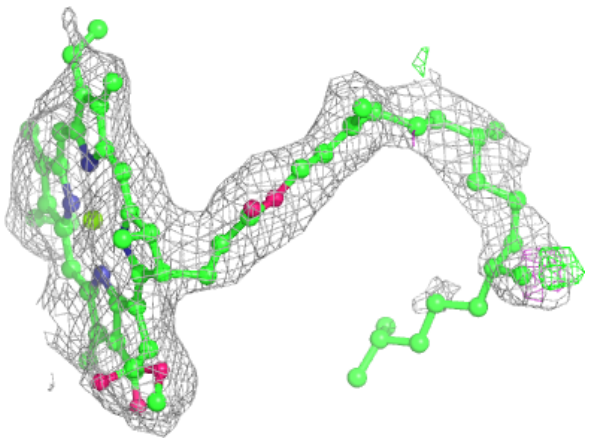
Electron density around CLA b 605:

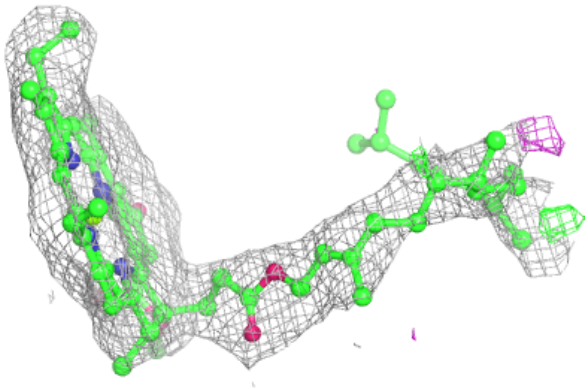
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

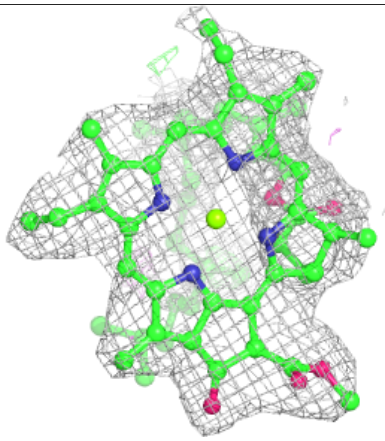


Electron density around CLA b 609:

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

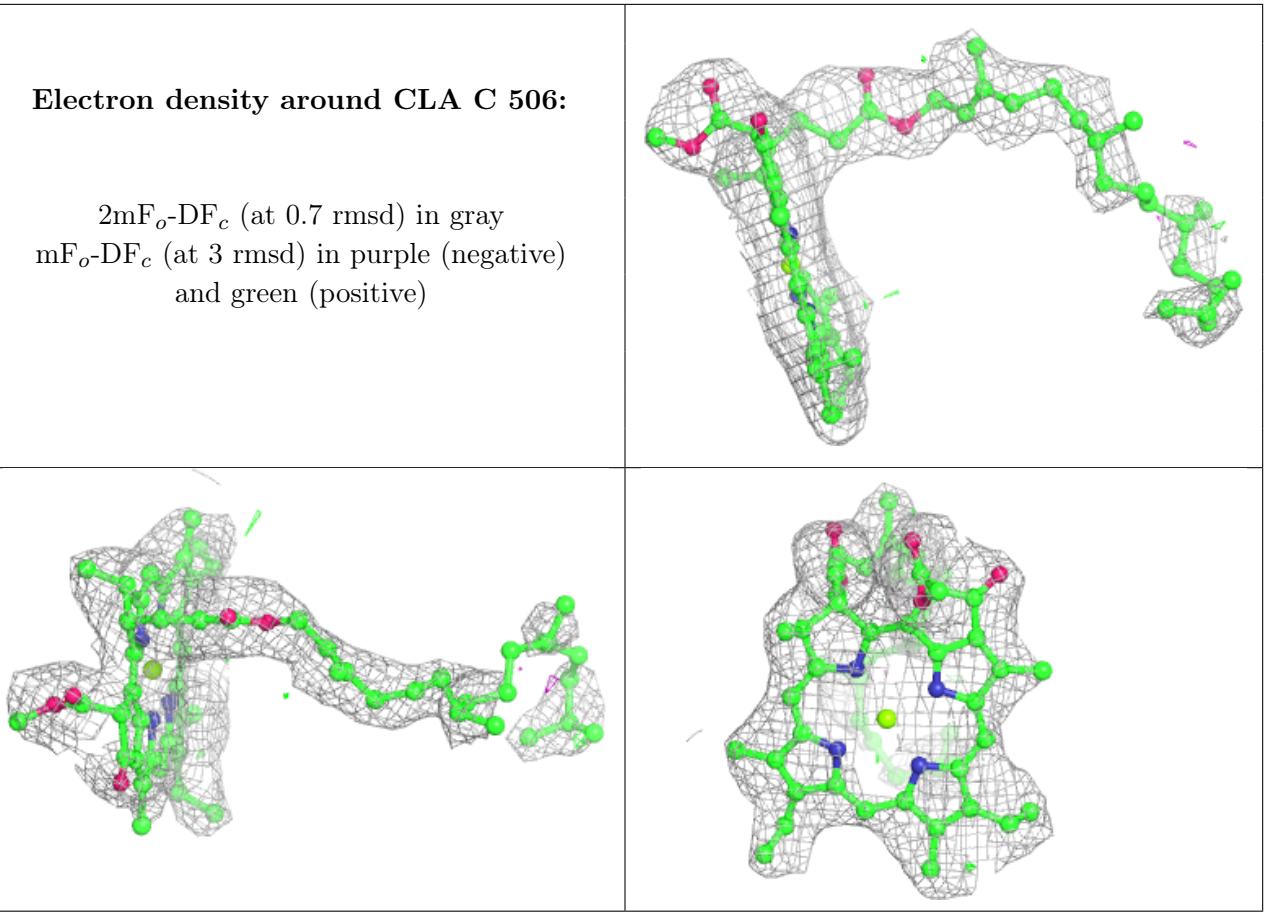






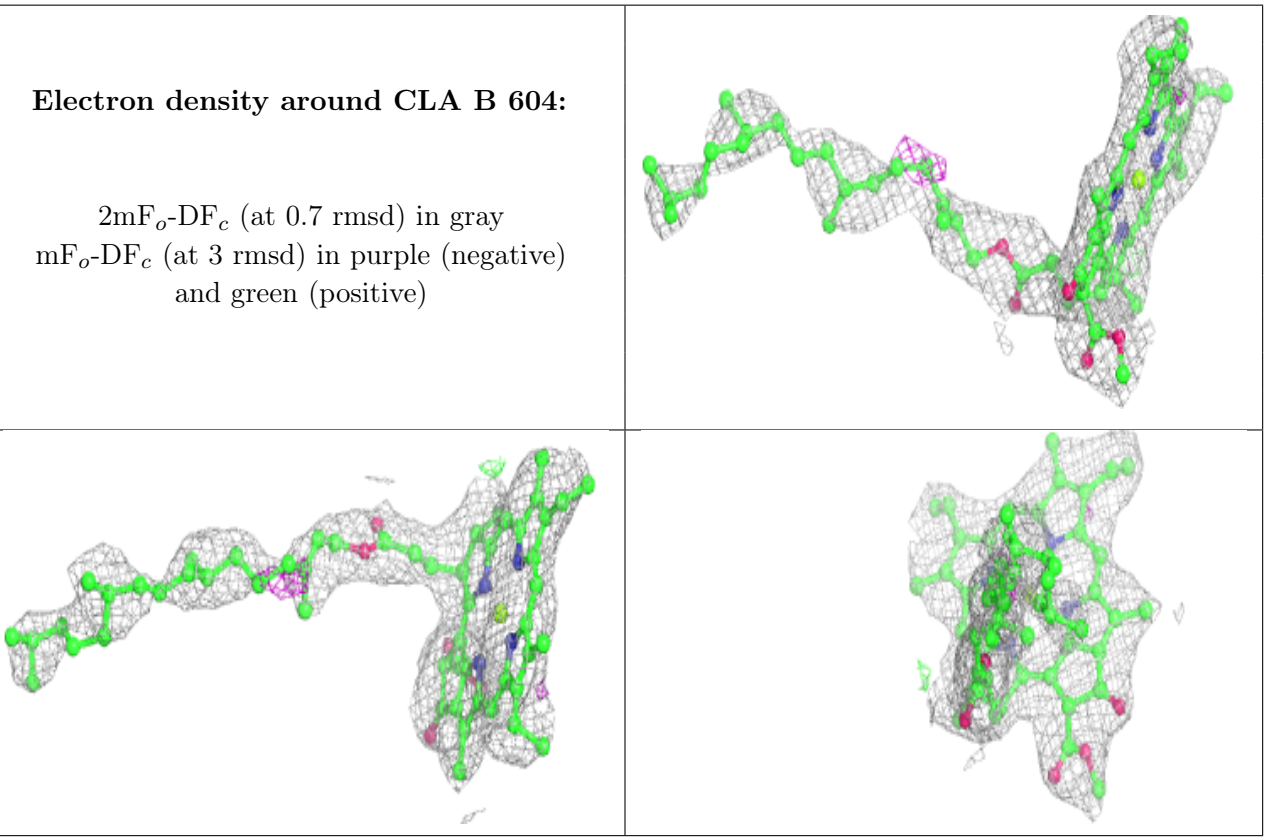
Electron density around CLA C 506:

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



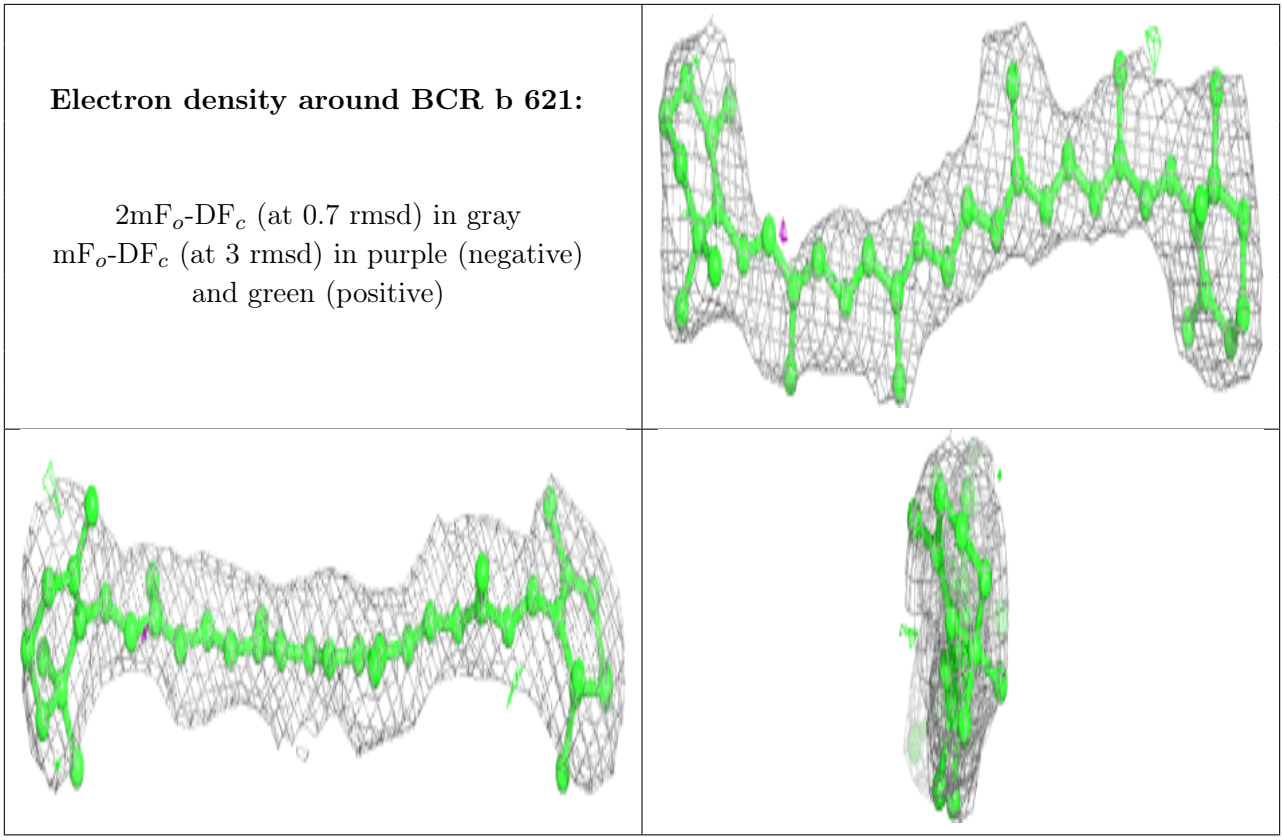
Electron density around CLA B 604:

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



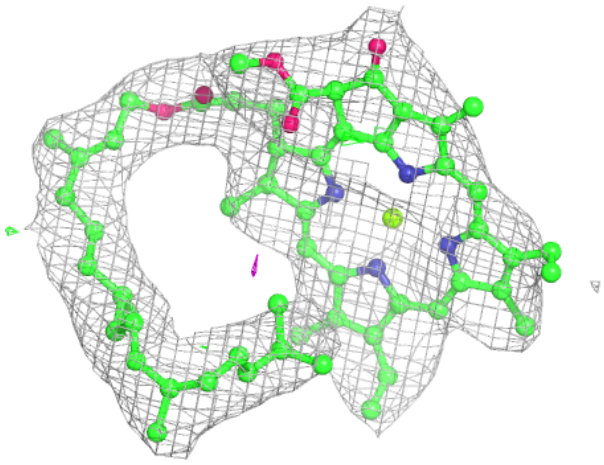
Electron density around BCR b 621:

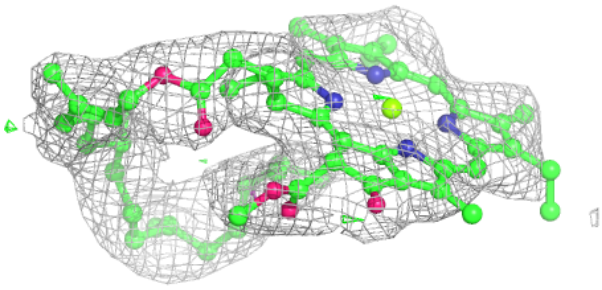
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

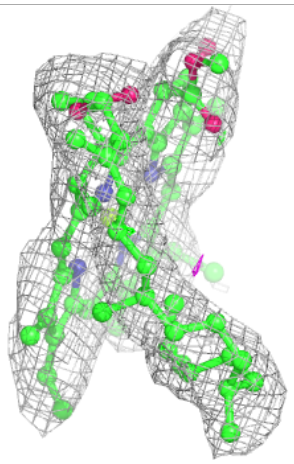


Electron density around CLA b 618:

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

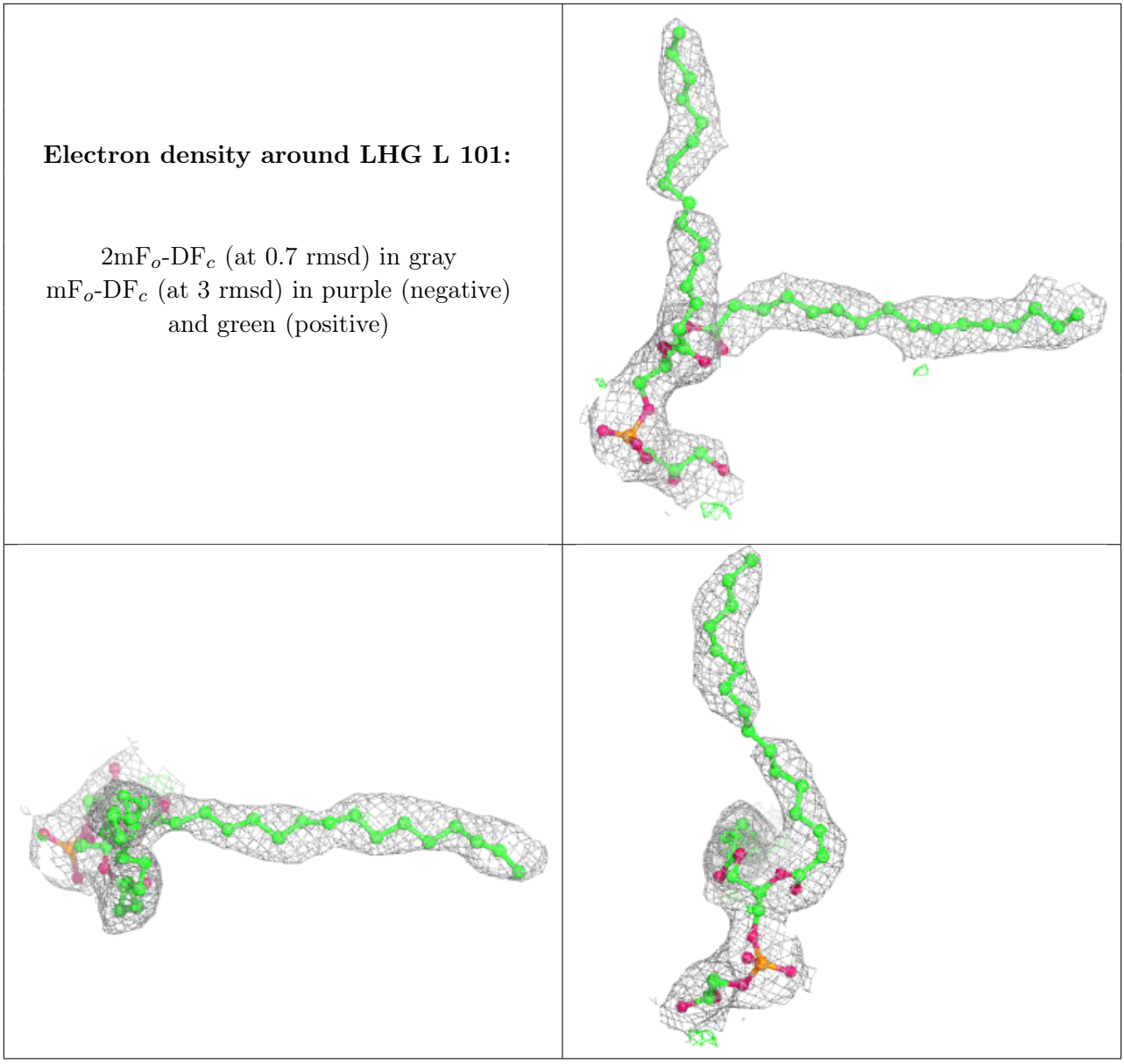






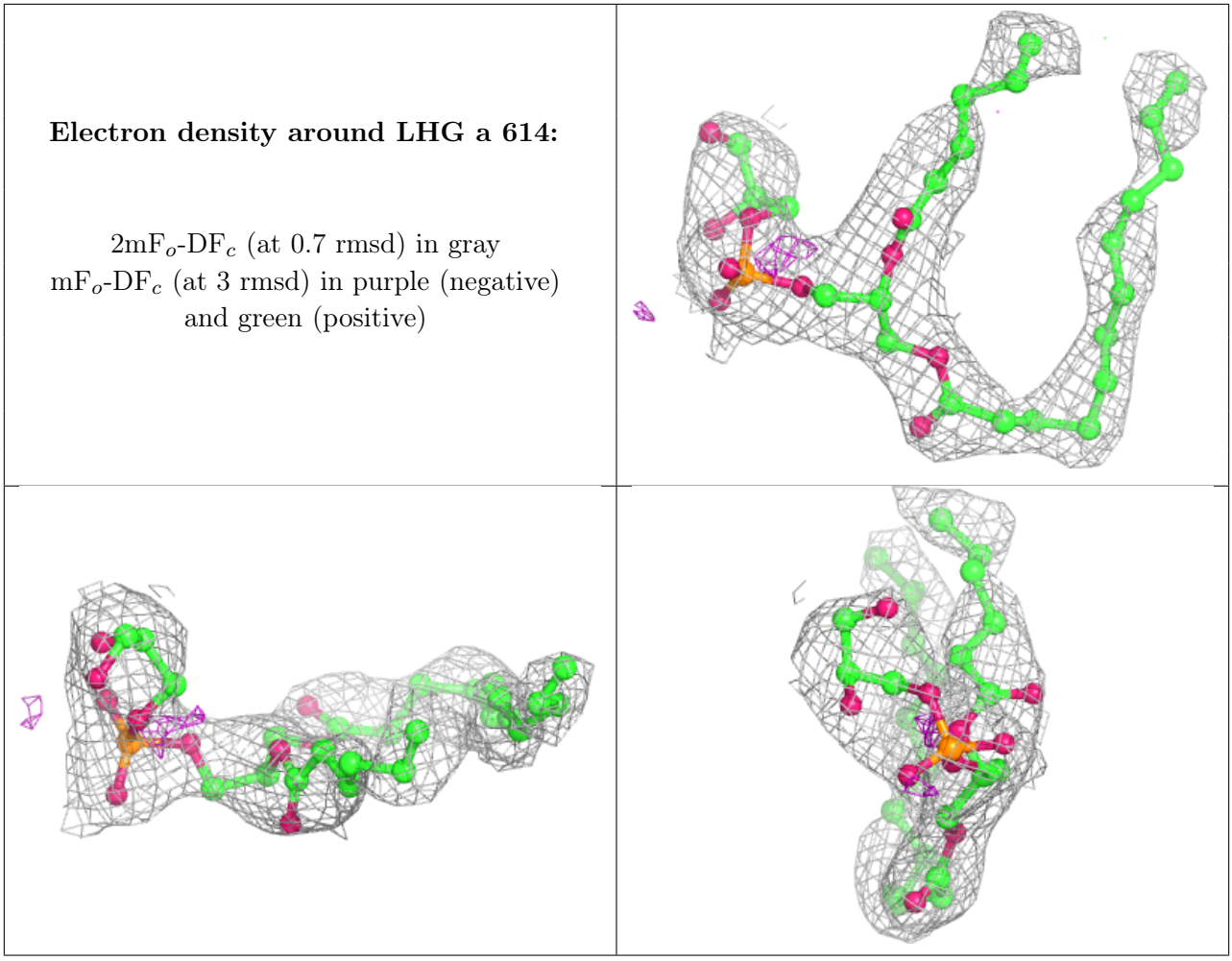
Electron density around LHG L 101:

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



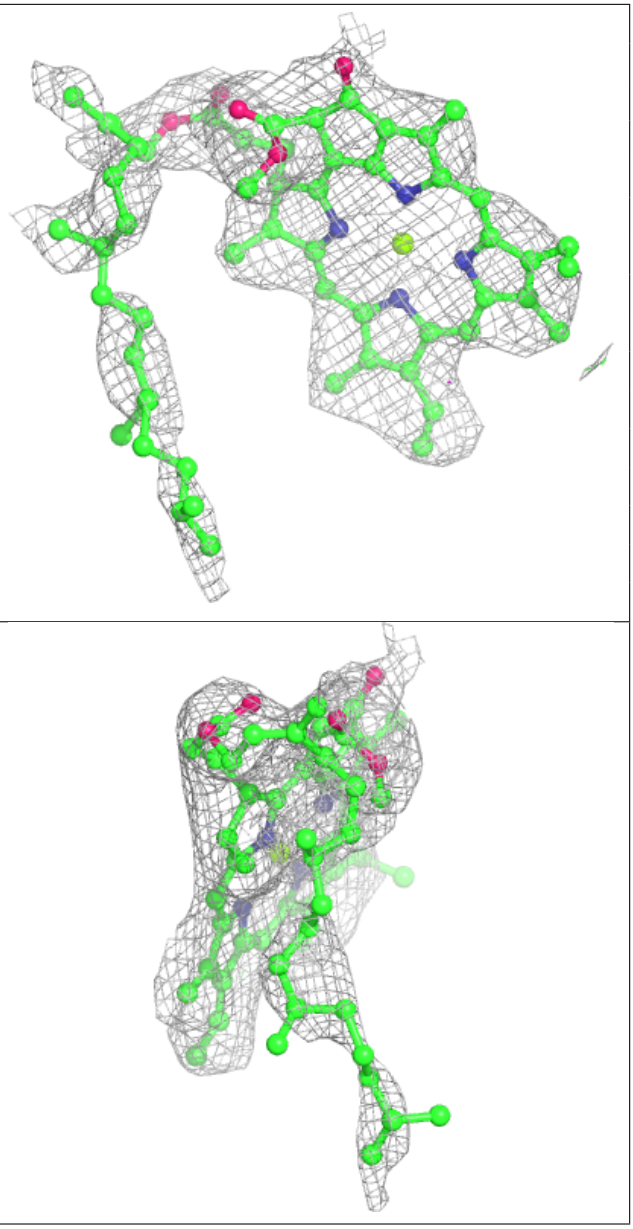
Electron density around LHG a 614:

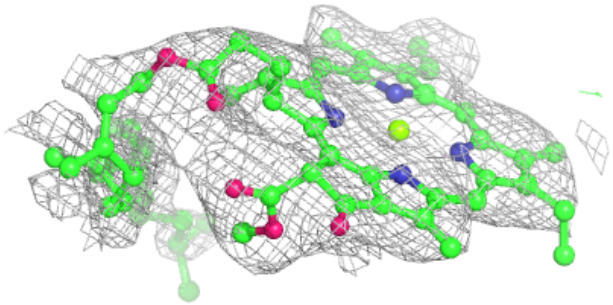
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 619:

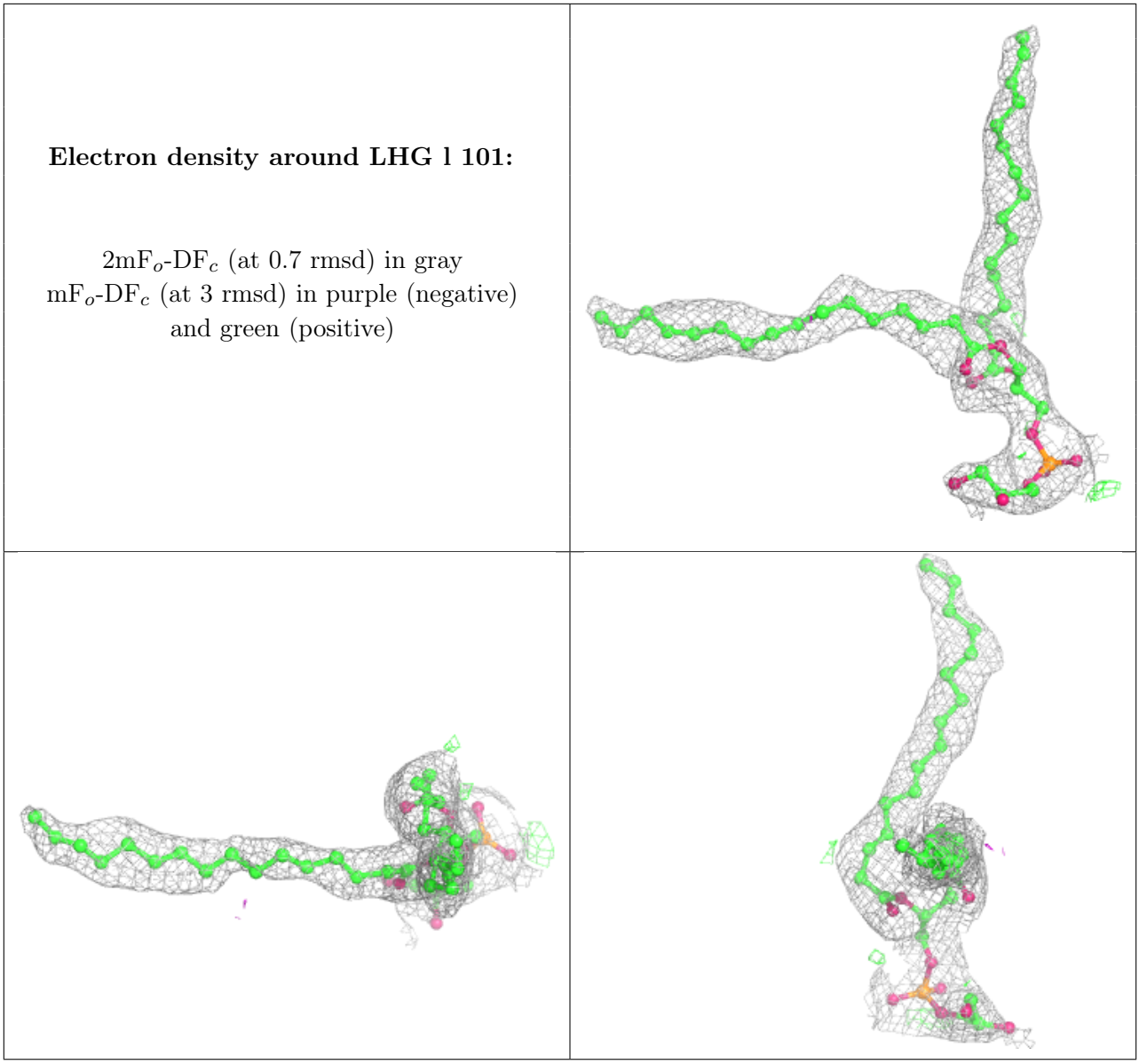
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





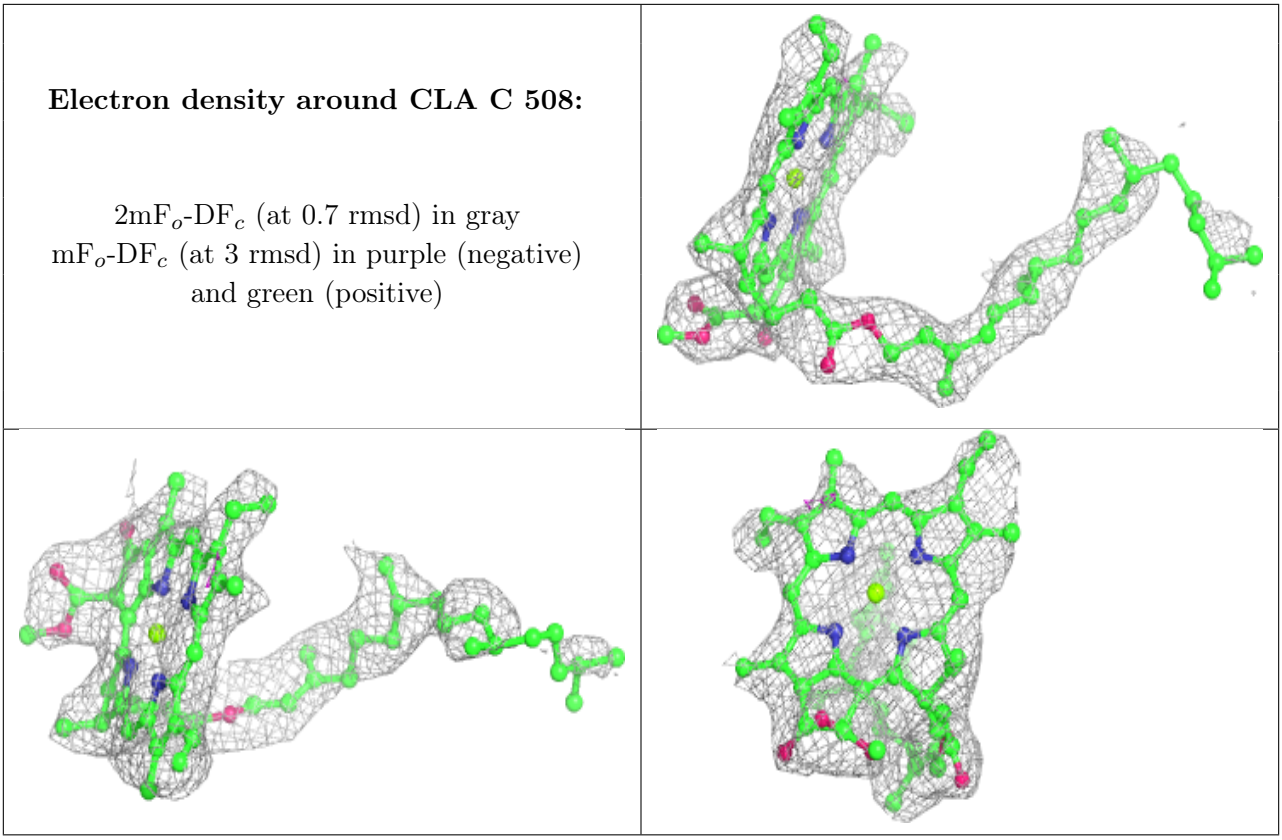
Electron density around LHG l 101:

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



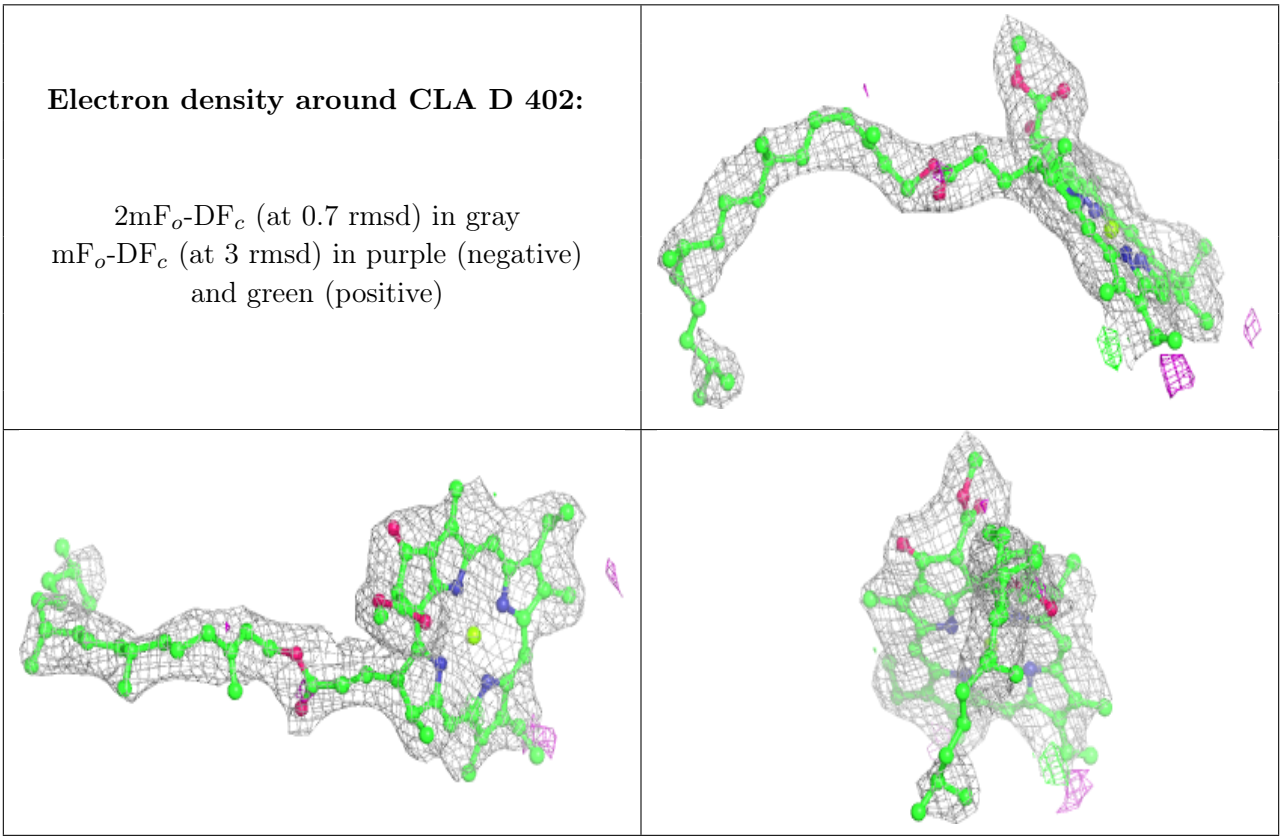
Electron density around CLA C 508:

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



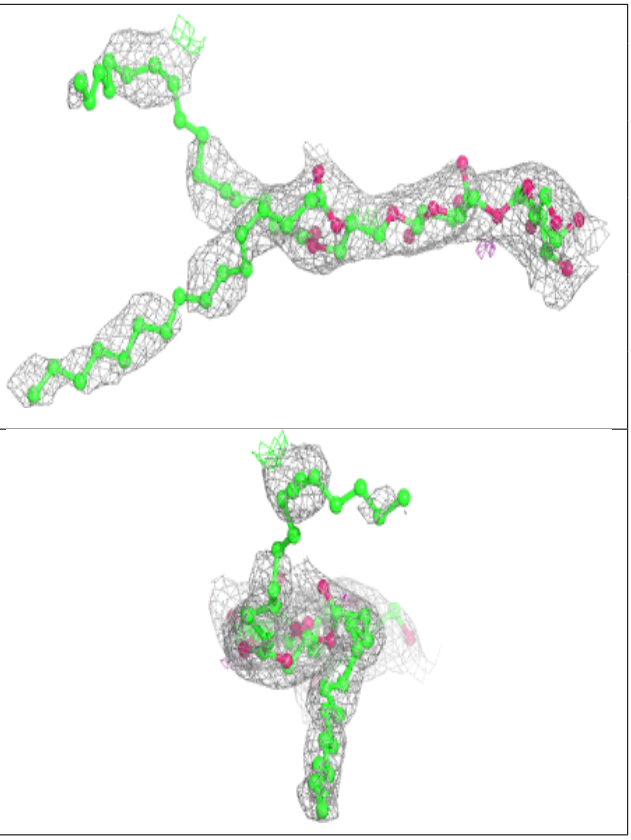
Electron density around CLA D 402:

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



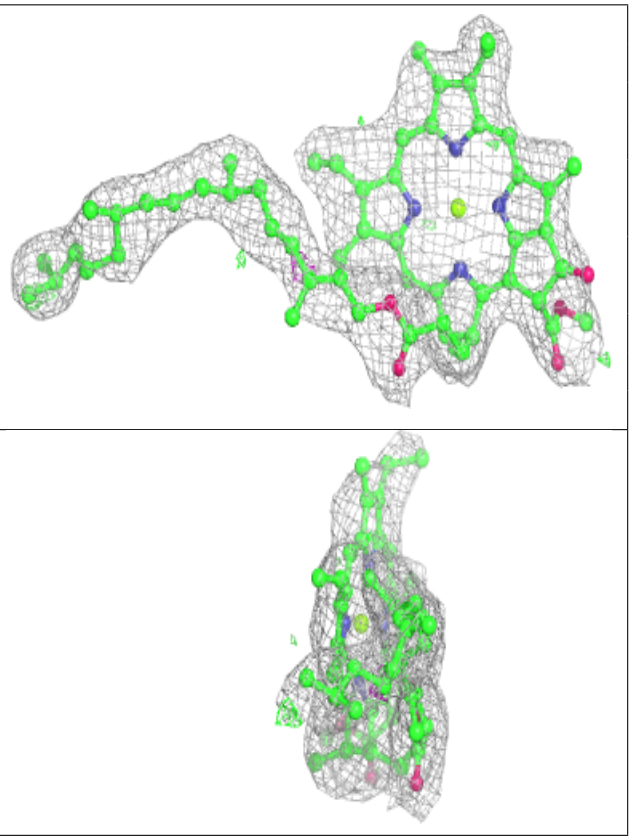
Electron density around DGD c 518:

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



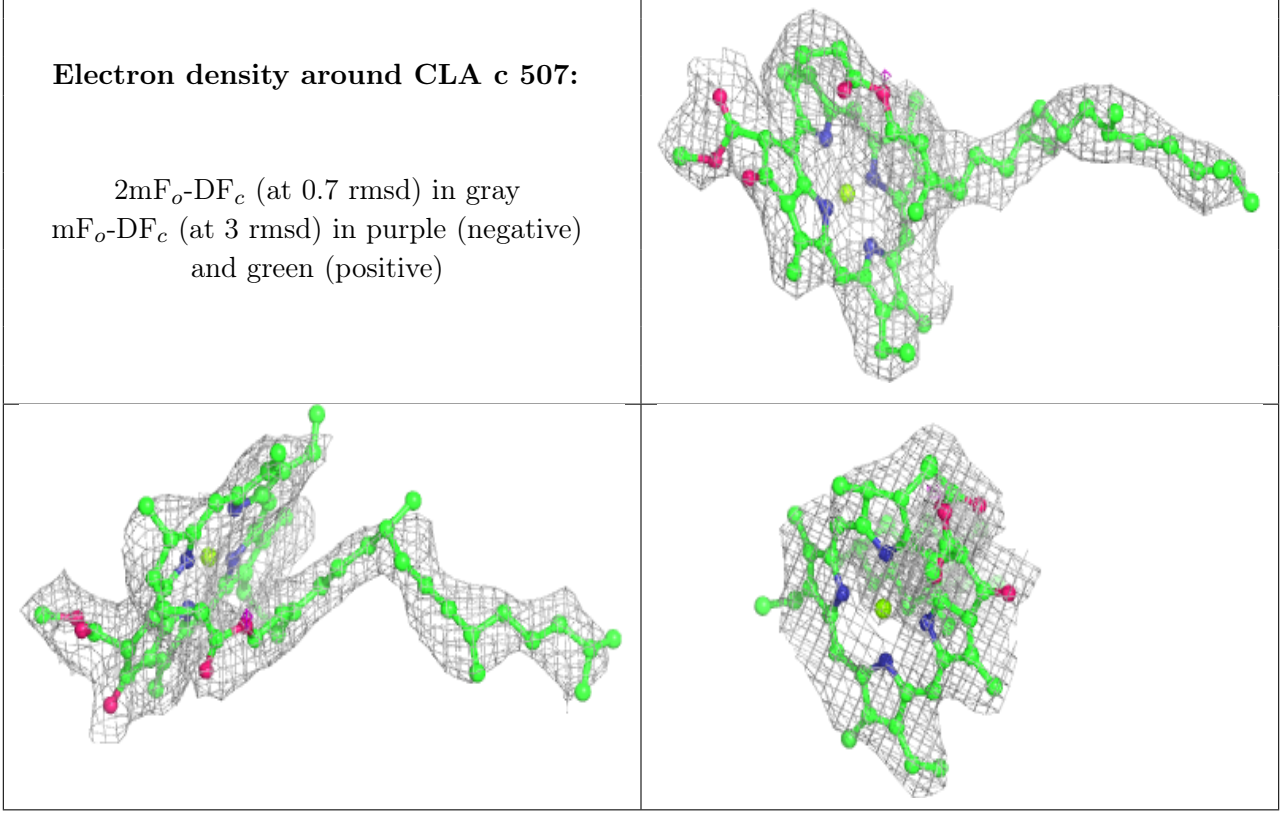
Electron density around CLA B 603:

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



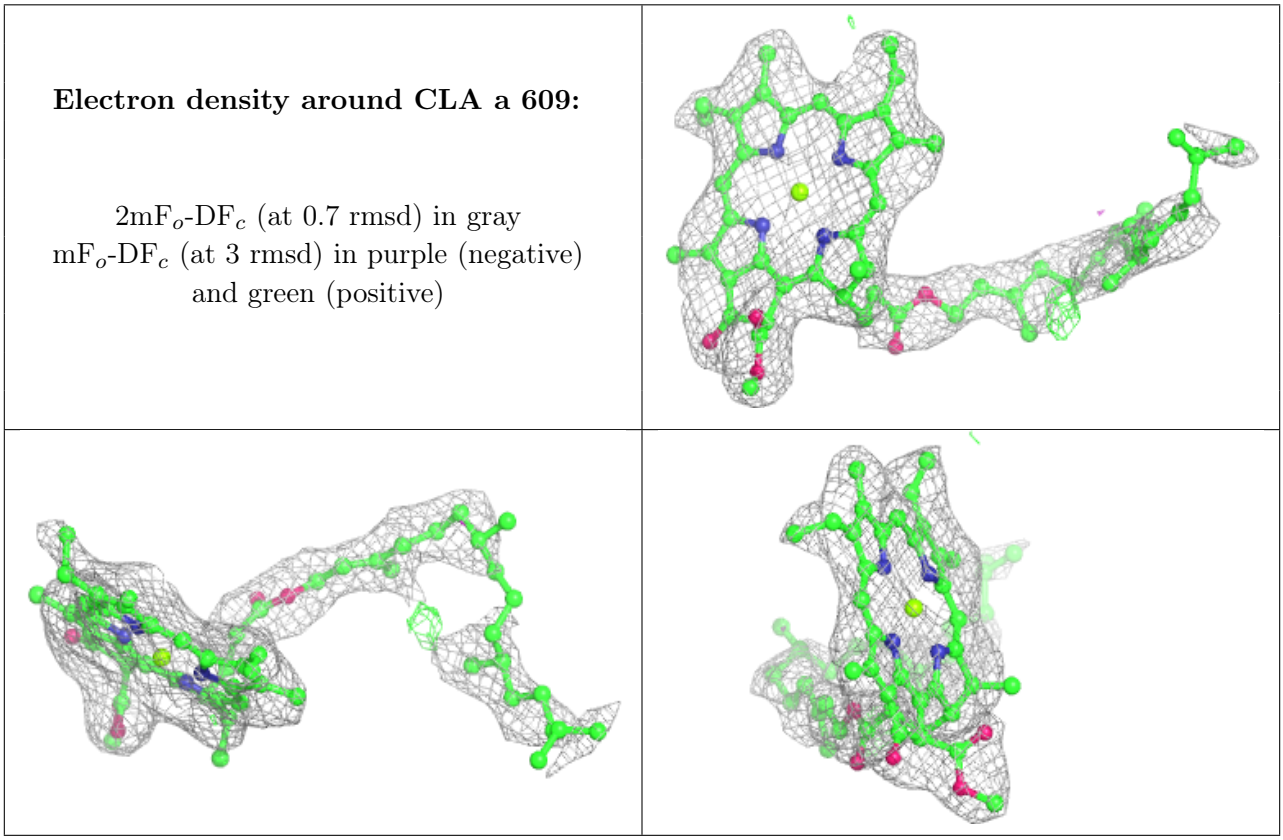
Electron density around CLA c 507:

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



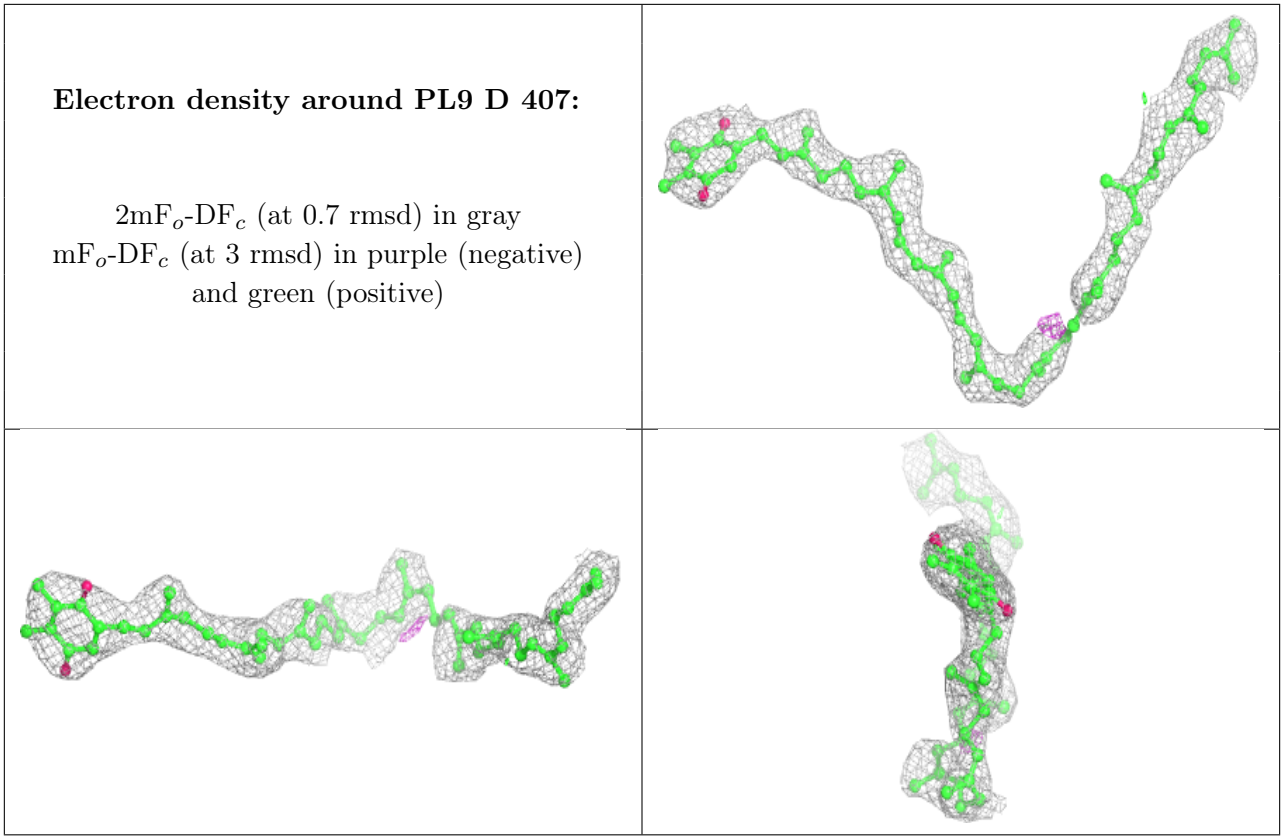
Electron density around CLA a 609:

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



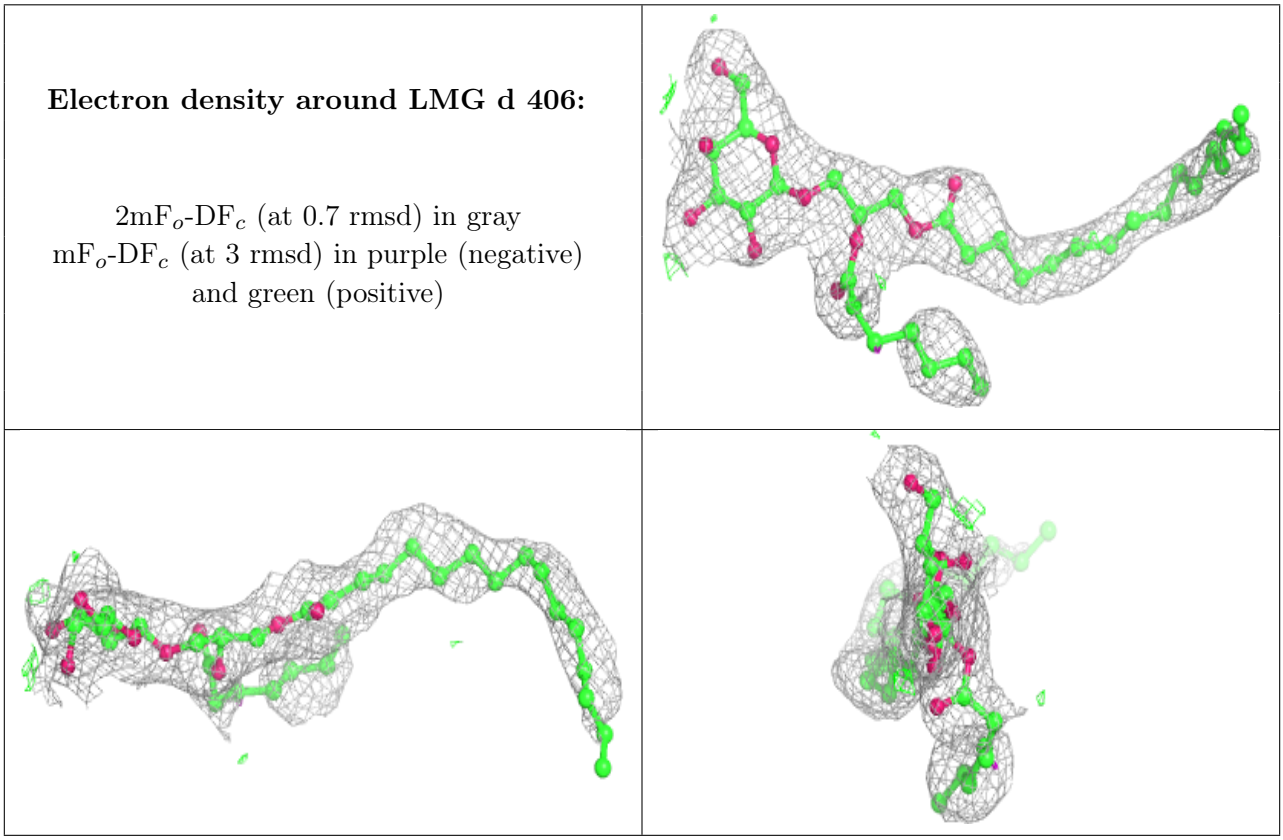
Electron density around PL9 D 407:

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



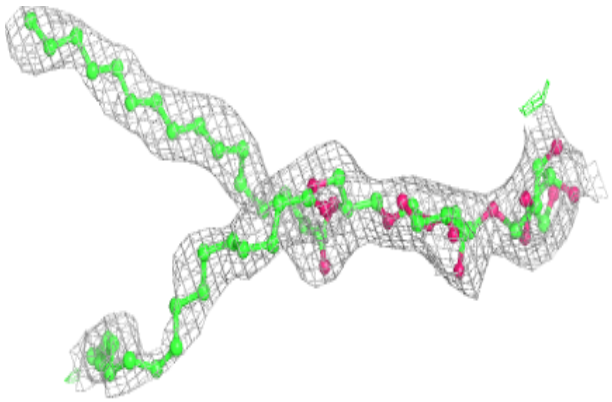
Electron density around LMG d 406:

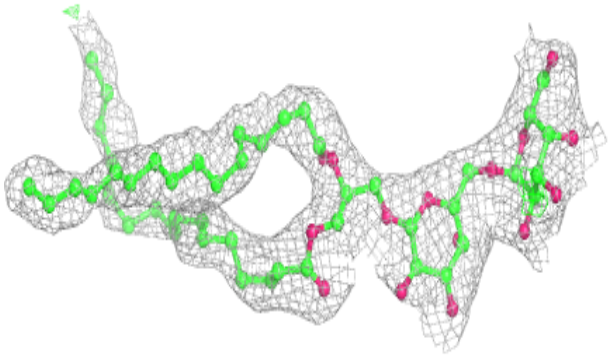
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

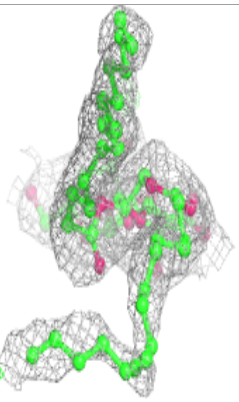


Electron density around DGD C 516:

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

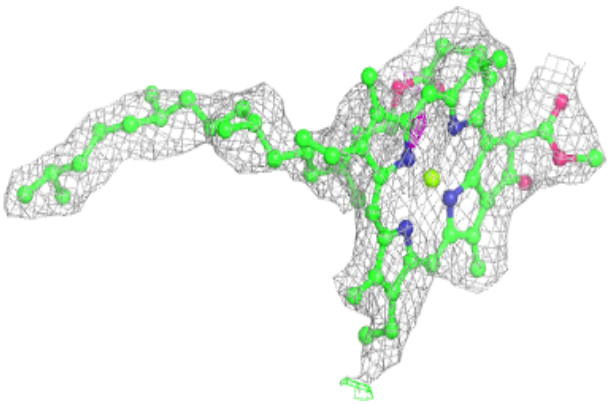


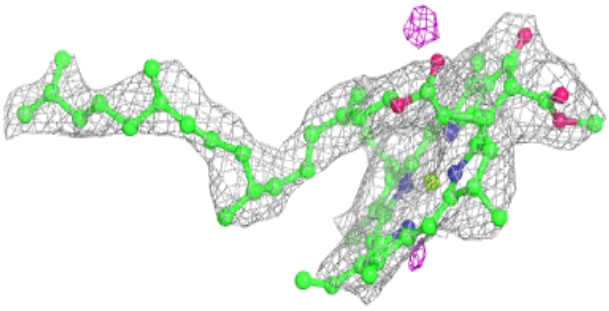


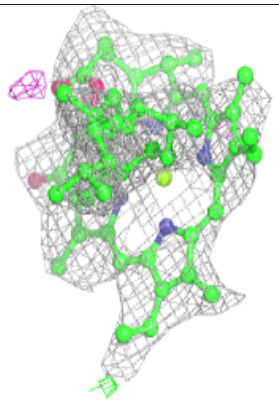


Electron density around CLA C 505:

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

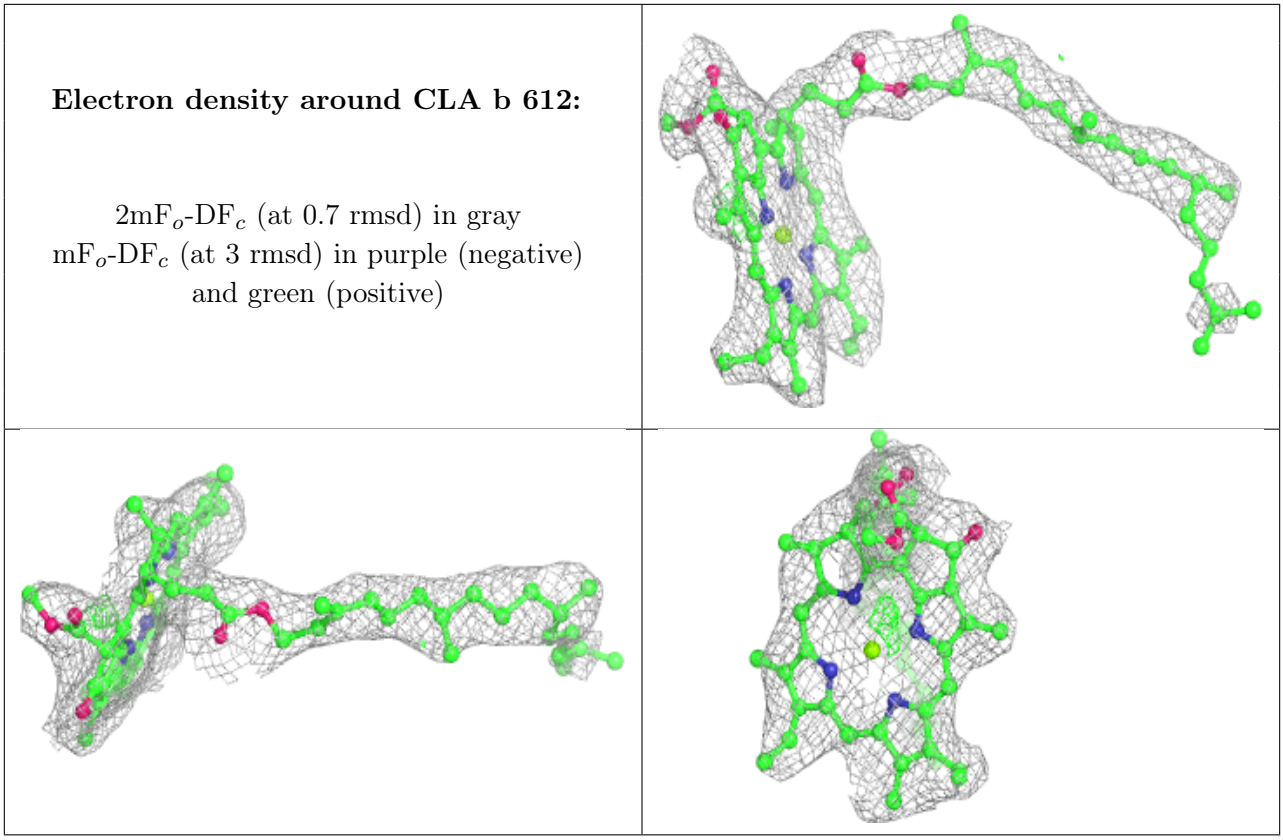






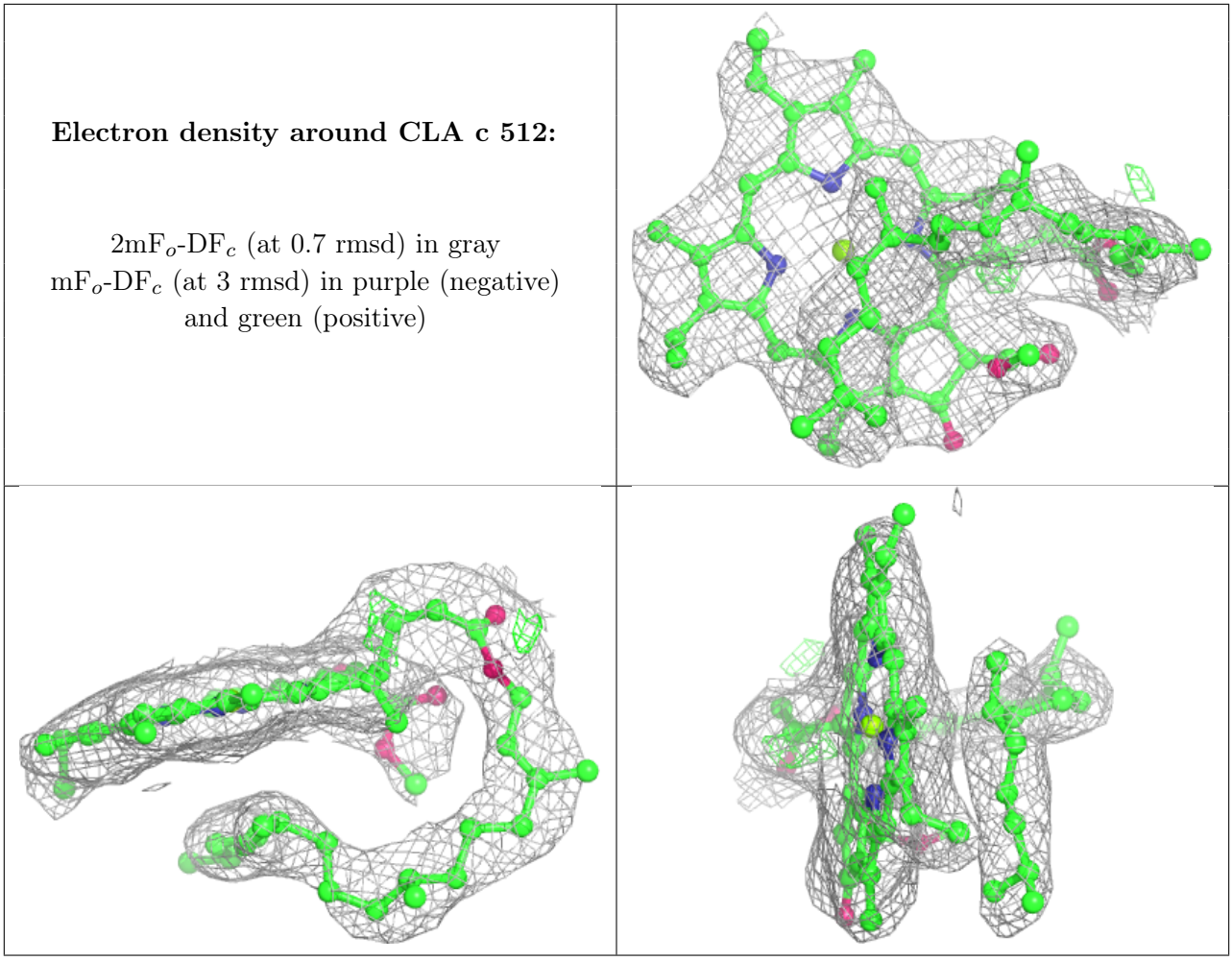
Electron density around CLA b 612:

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



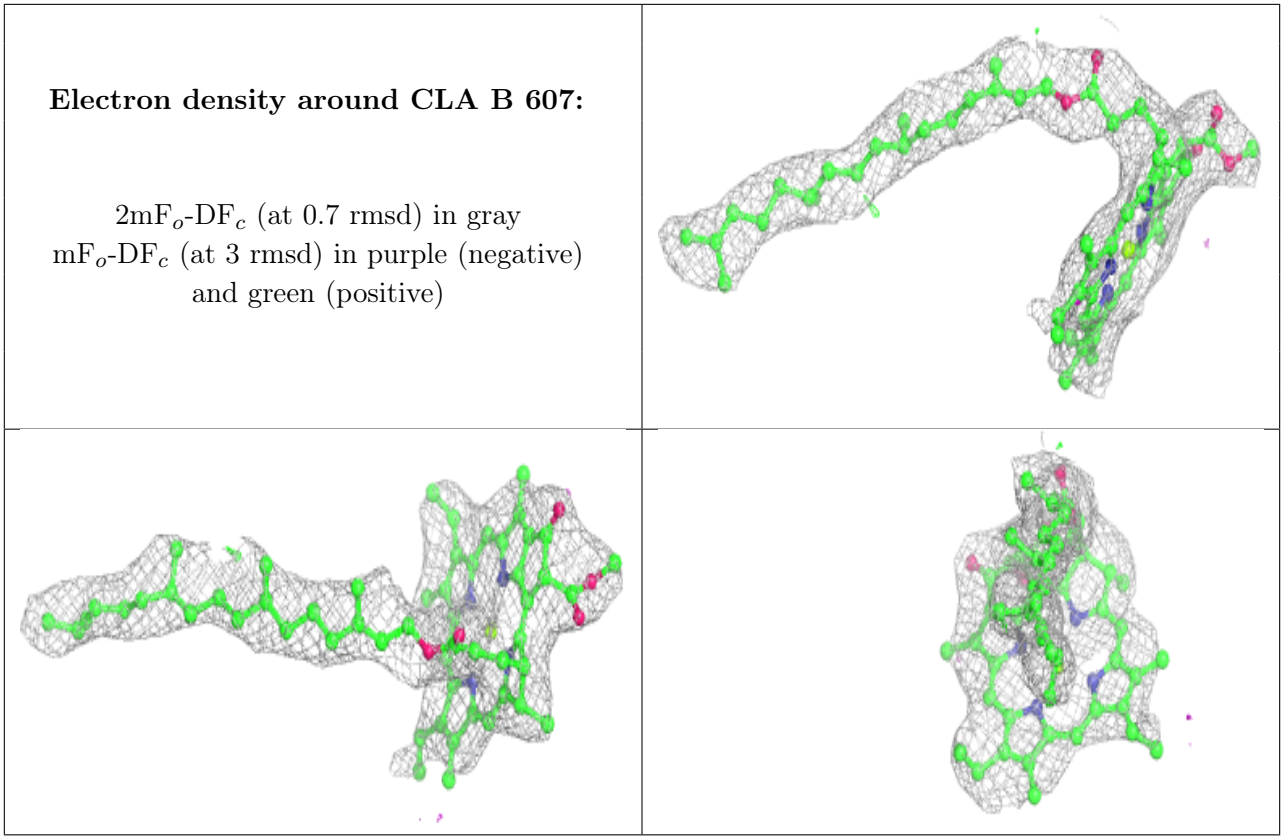
Electron density around CLA c 512:

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



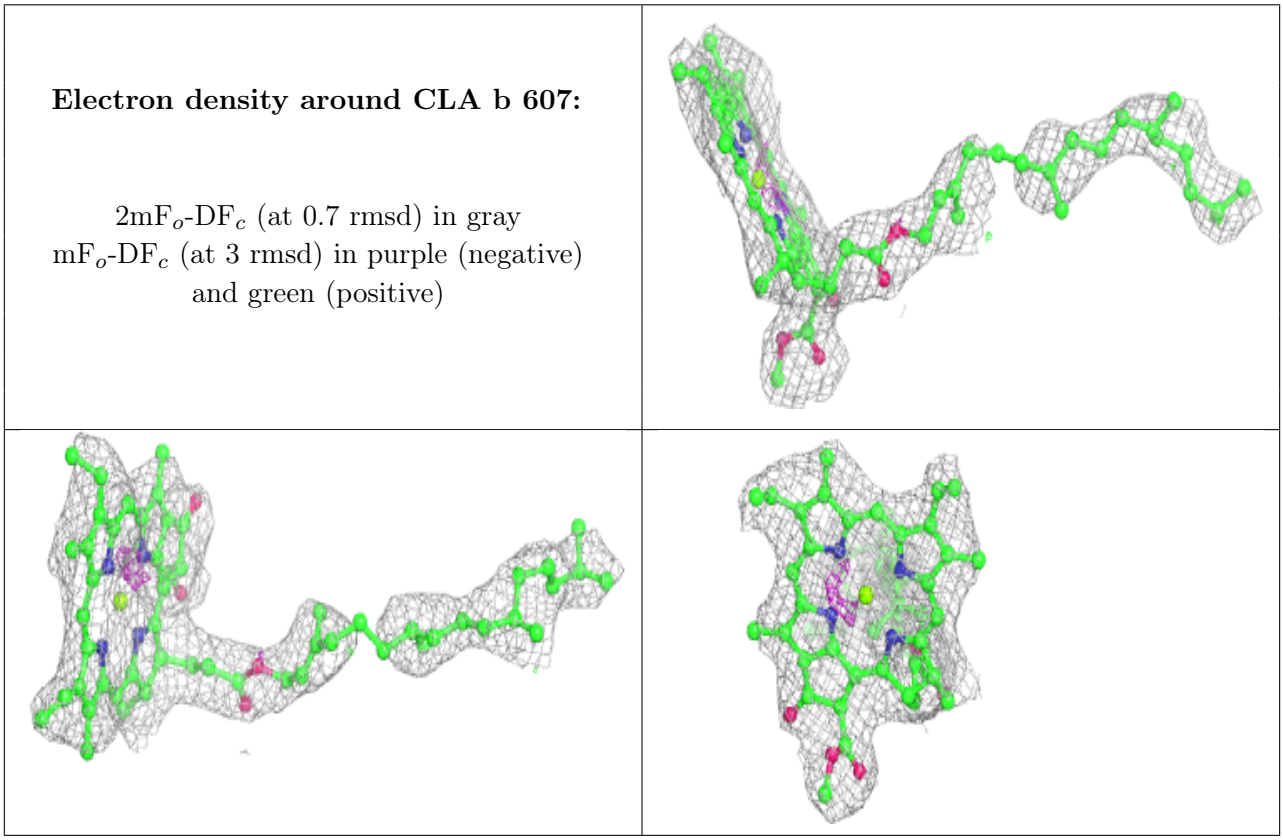
Electron density around CLA B 607:

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



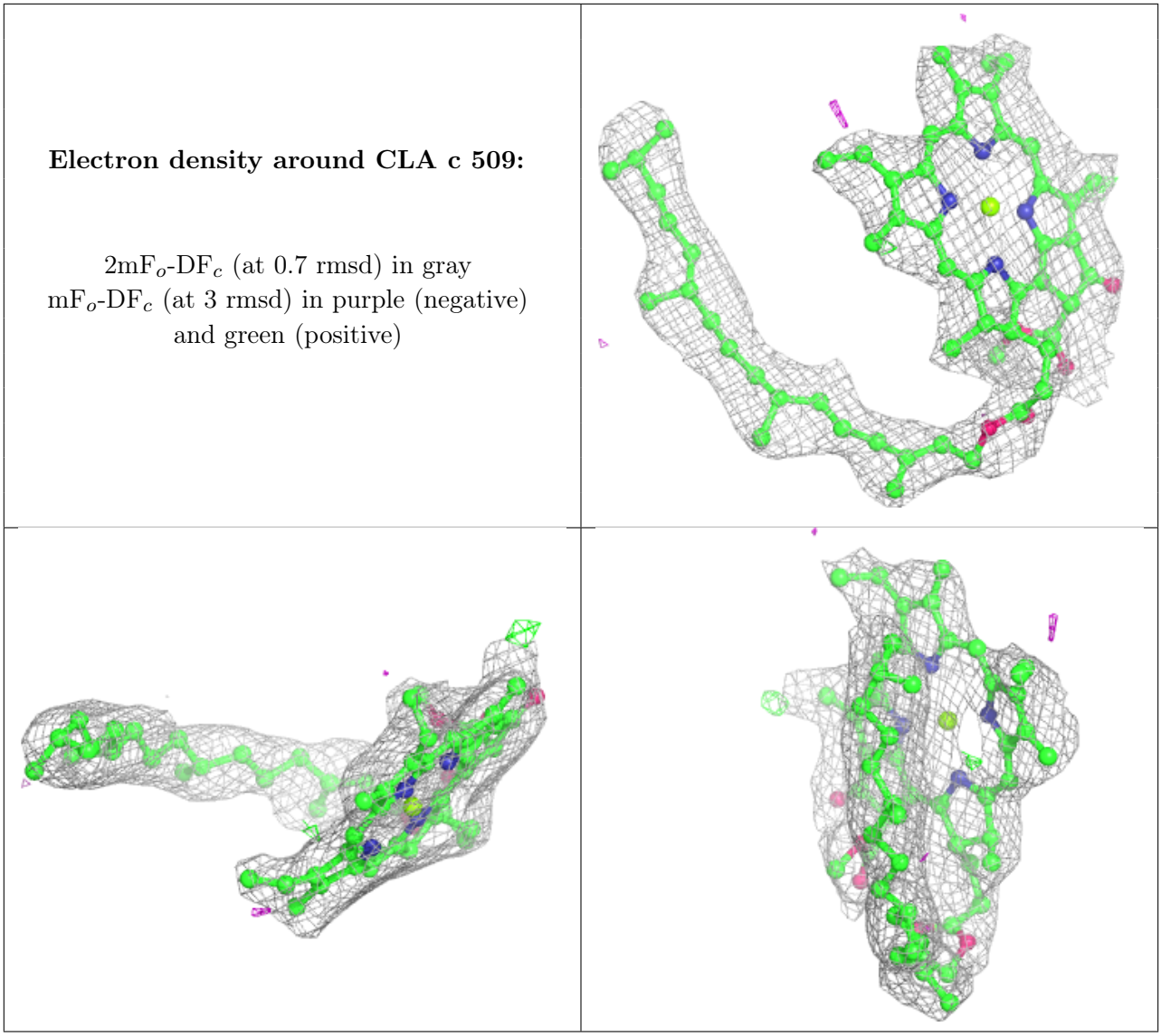
Electron density around CLA b 607:

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



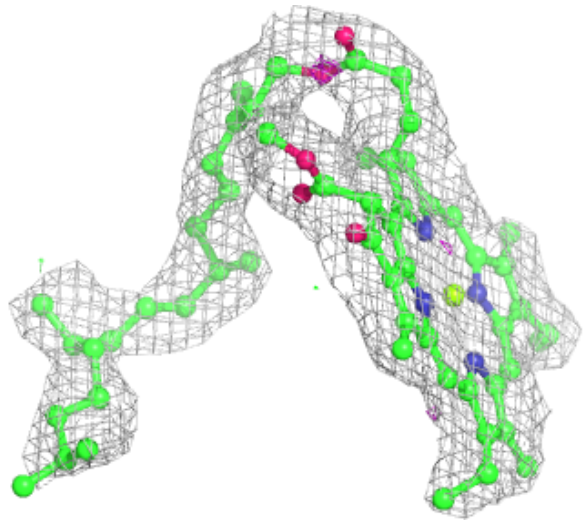
Electron density around CLA c 509:

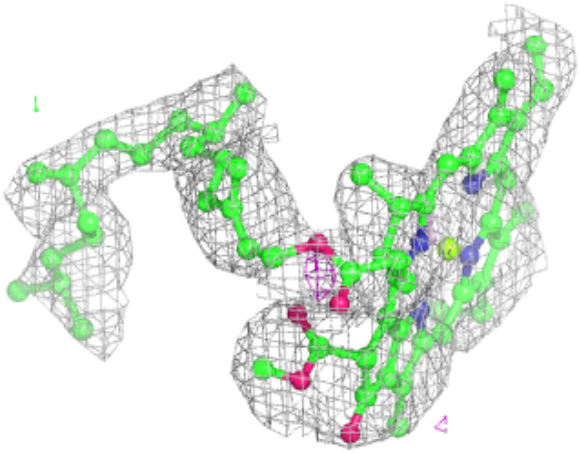
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

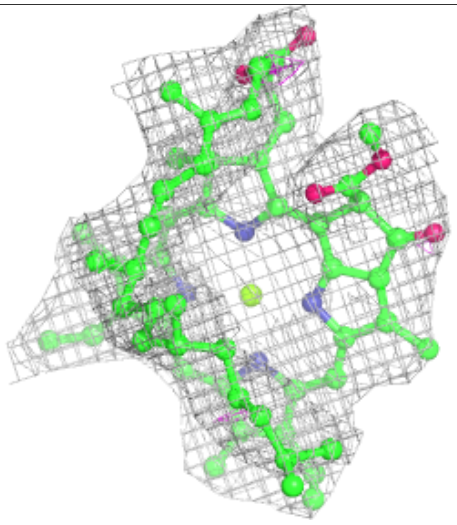


Electron density around CLA b 616:

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

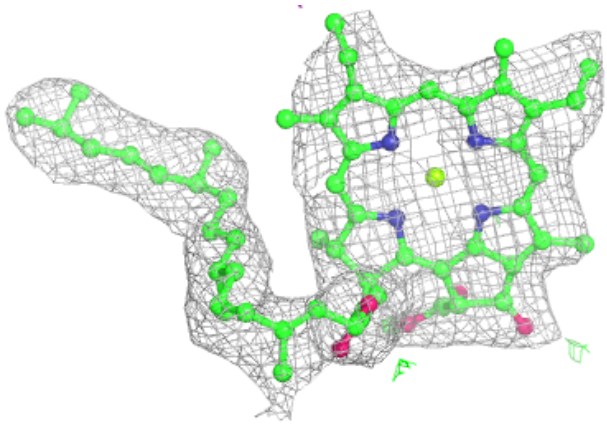


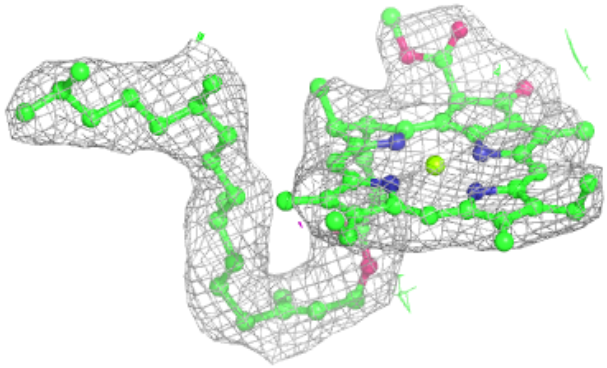




Electron density around CLA A 615:

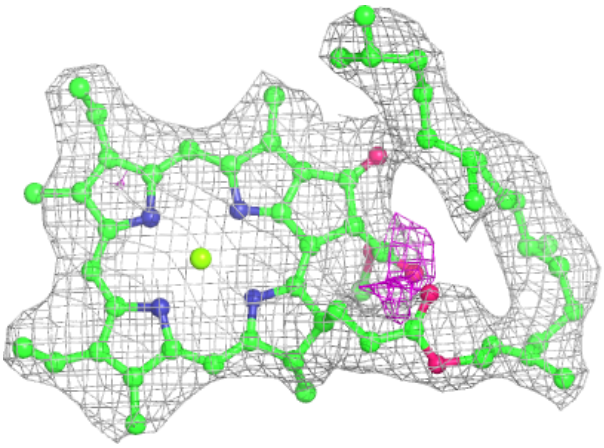
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

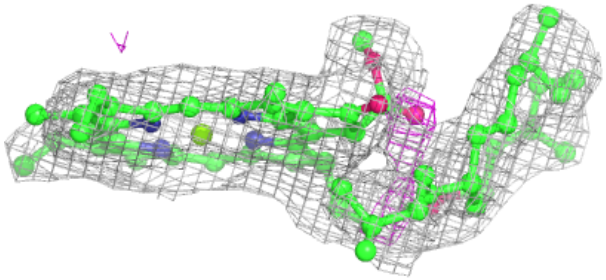


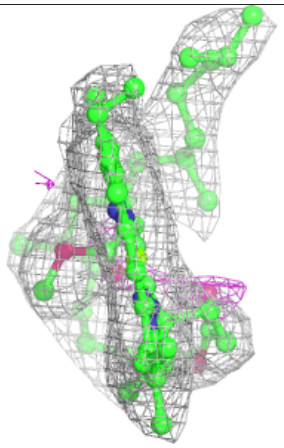


Electron density around CLA B 610:

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

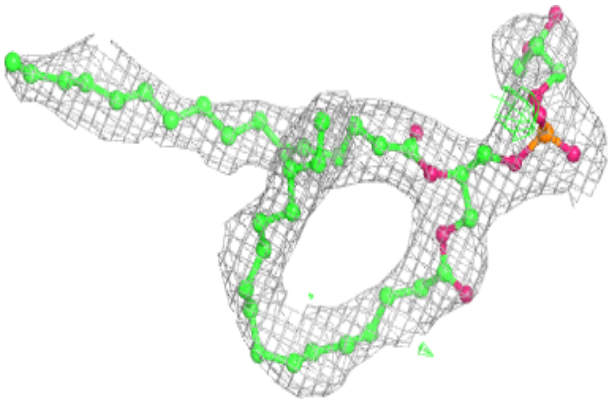


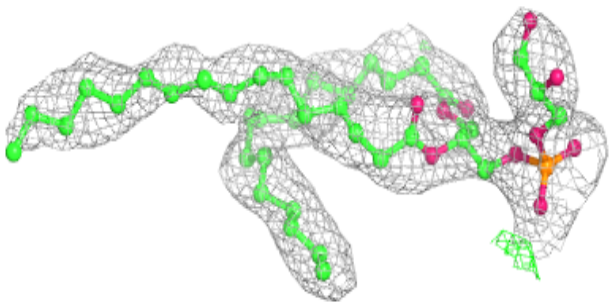


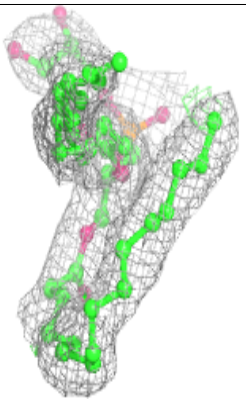


Electron density around LHG A 616:

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

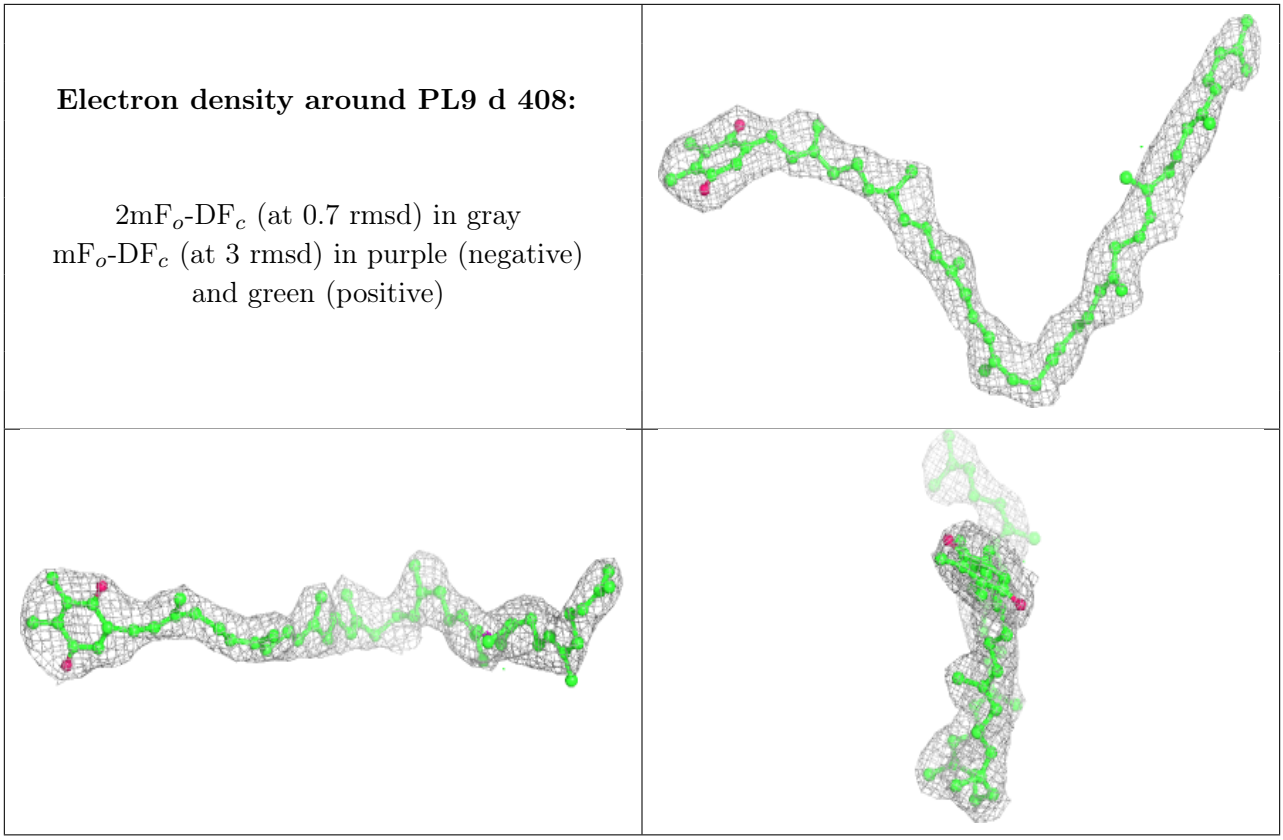






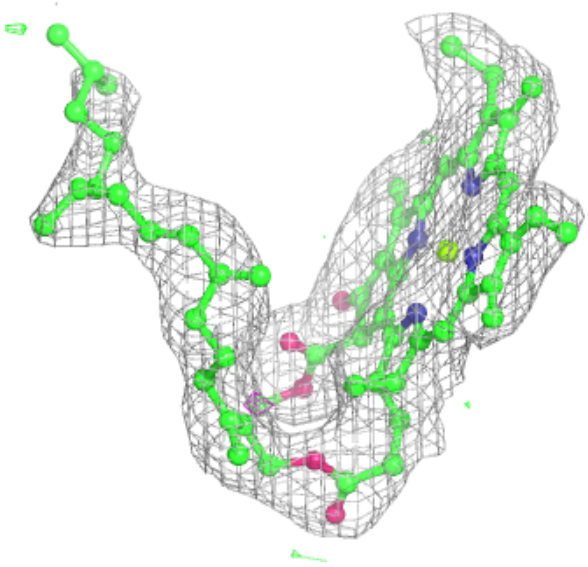
Electron density around PL9 d 408:

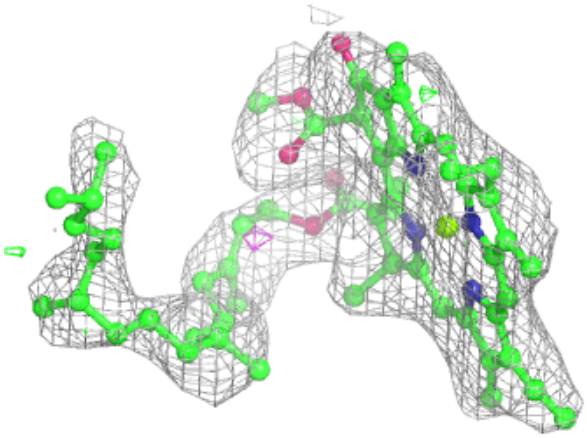
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

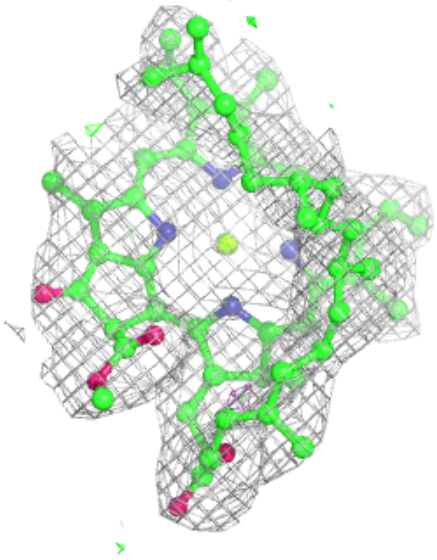


Electron density around CLA B 613:

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

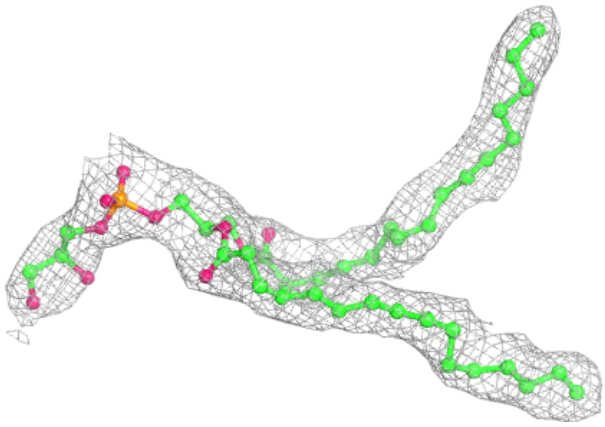


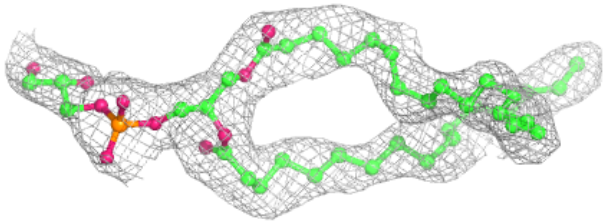


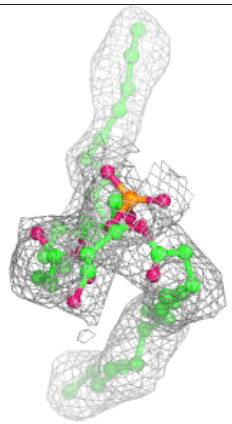


Electron density around LHG D 406:

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

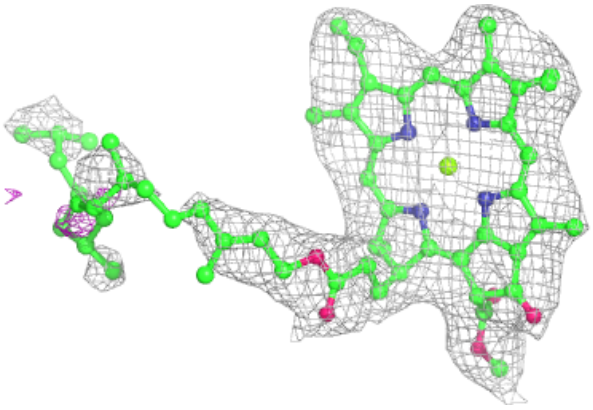


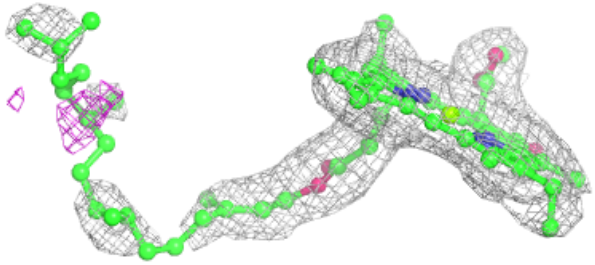


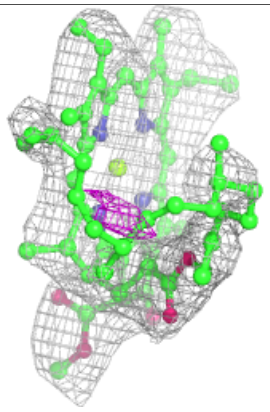


Electron density around CLA A 609:

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

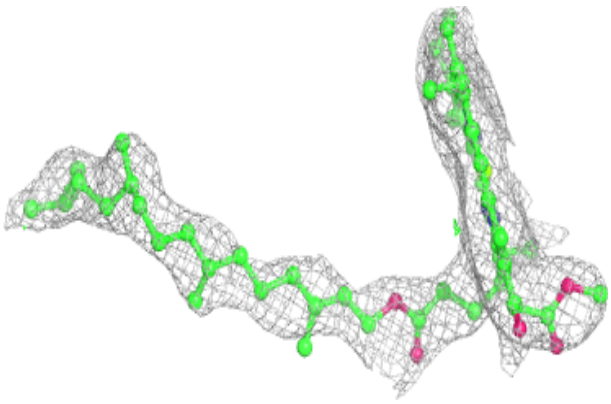


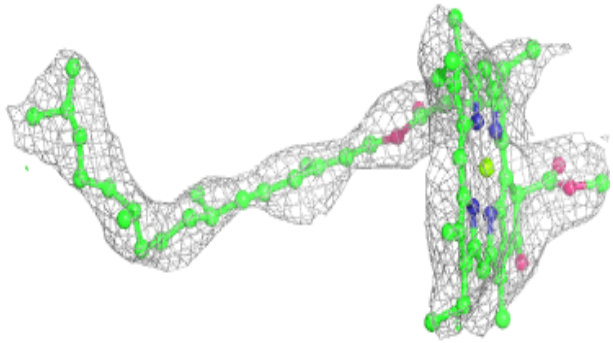


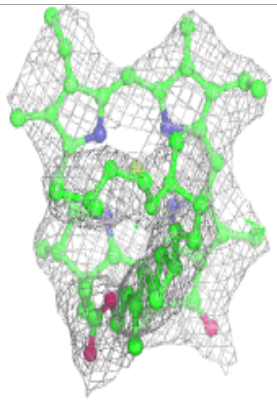


Electron density around CLA b 608:

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

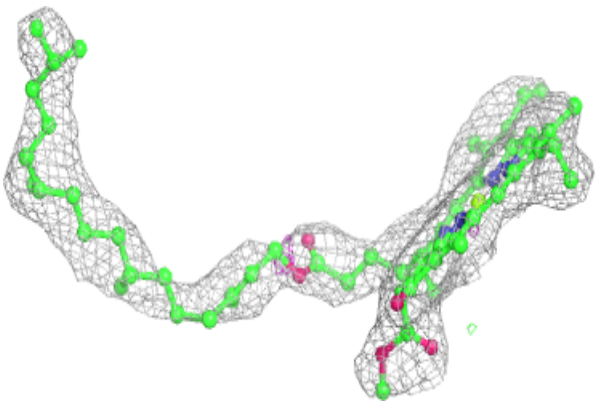


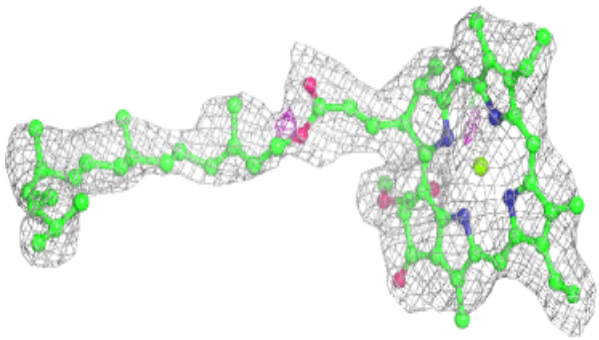


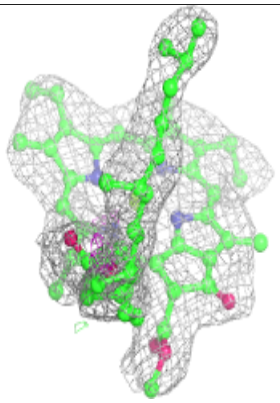


Electron density around CLA d 403:

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

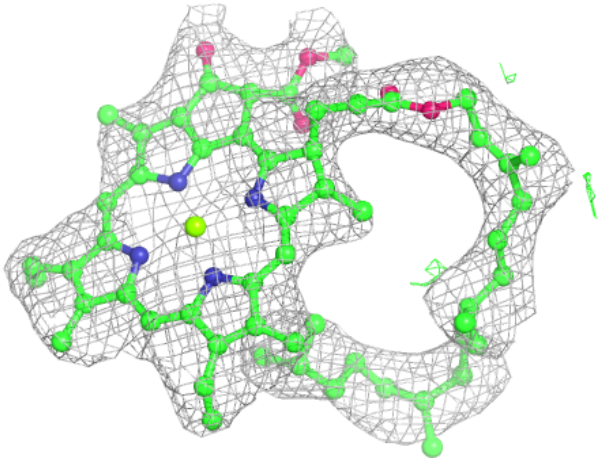


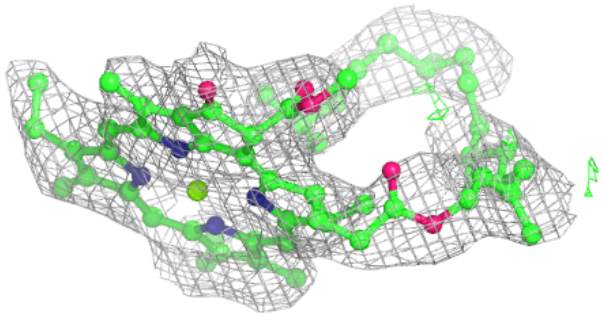


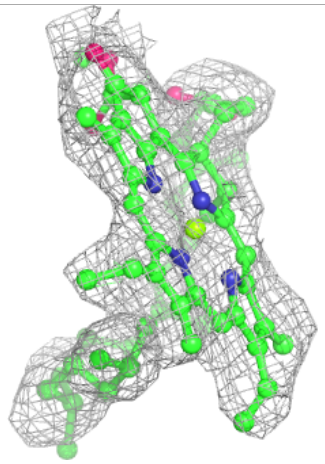


Electron density around CLA B 615:

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

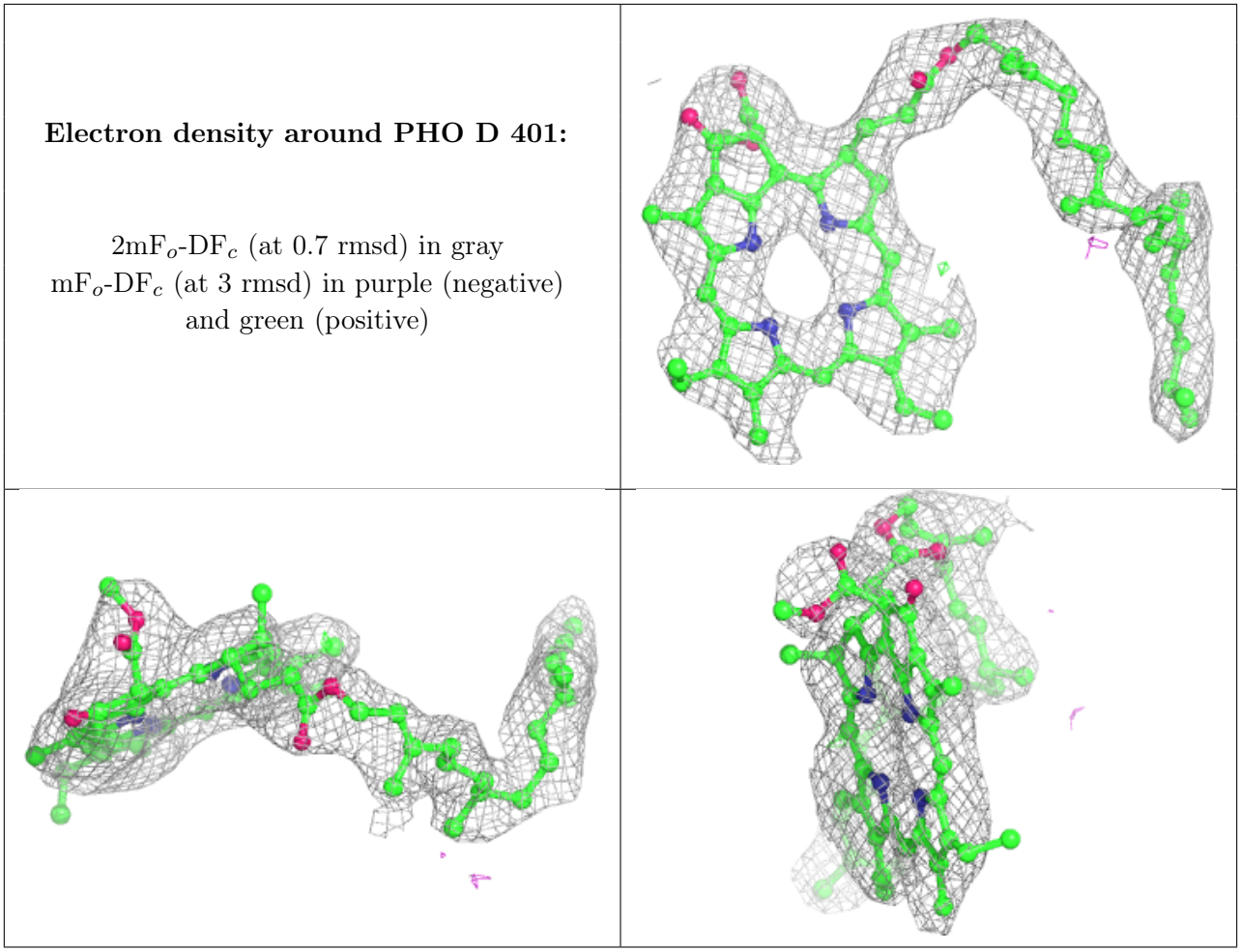






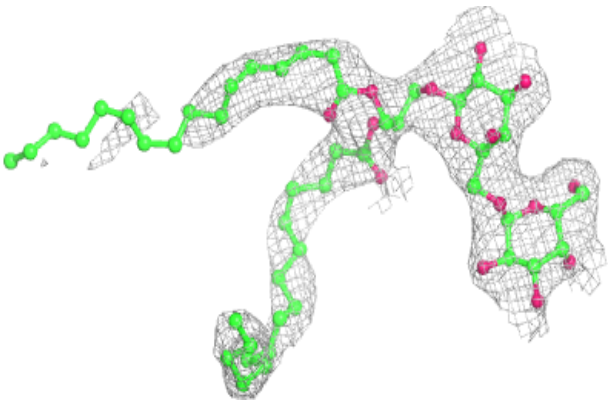
Electron density around PHO D 401:

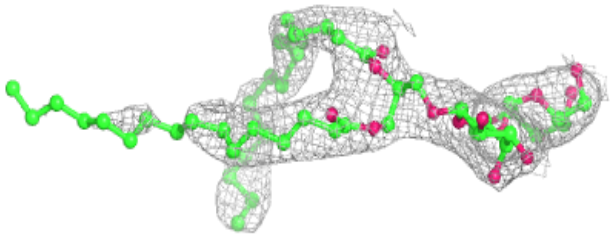
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

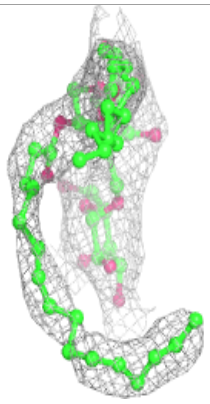


Electron density around DGD C 517:

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

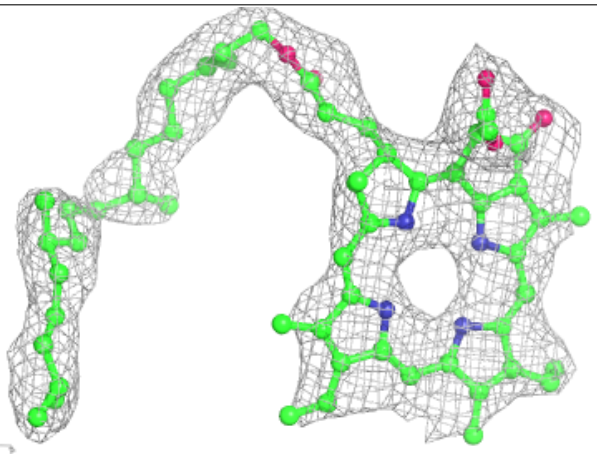


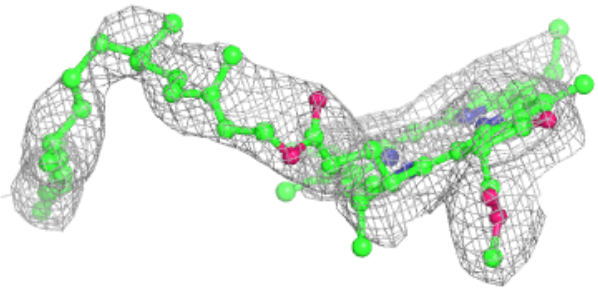


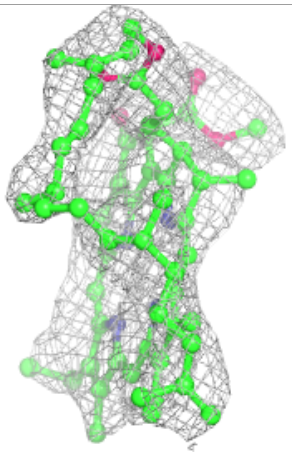


Electron density around PHO d 401:

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

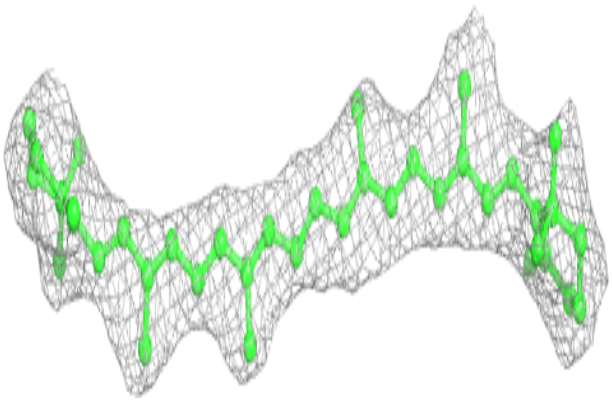


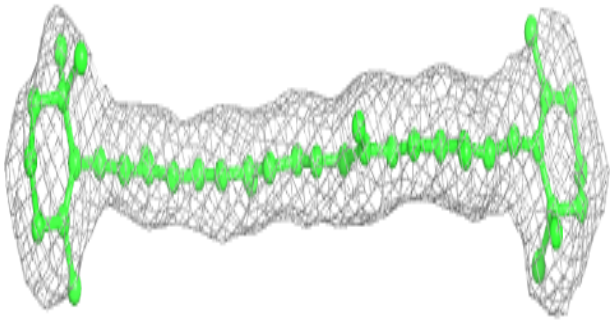


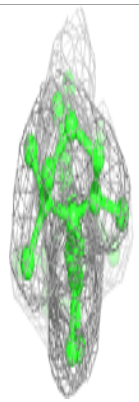


Electron density around BCR A 610:

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

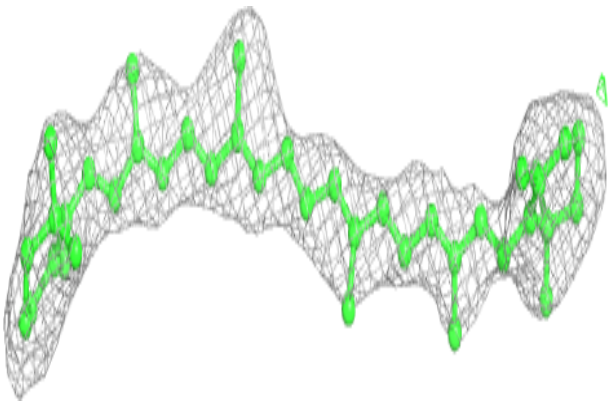


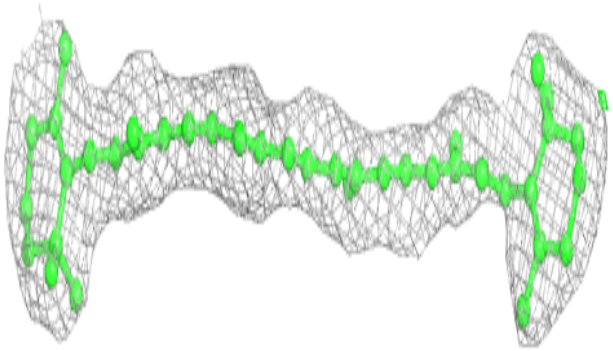


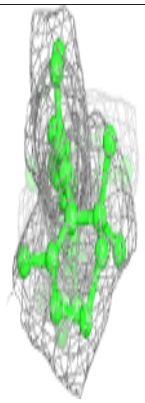


Electron density around BCR c 517:

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

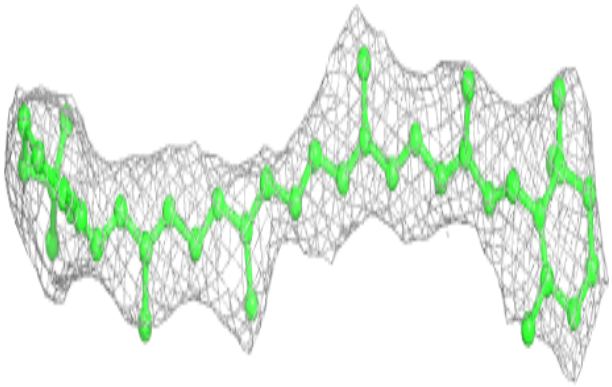


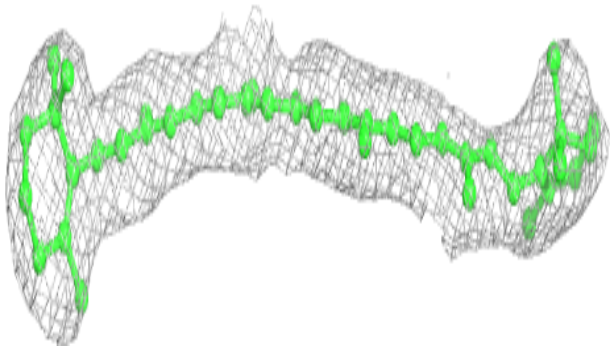


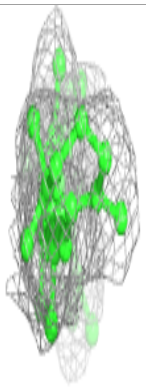


Electron density around BCR B 617:

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

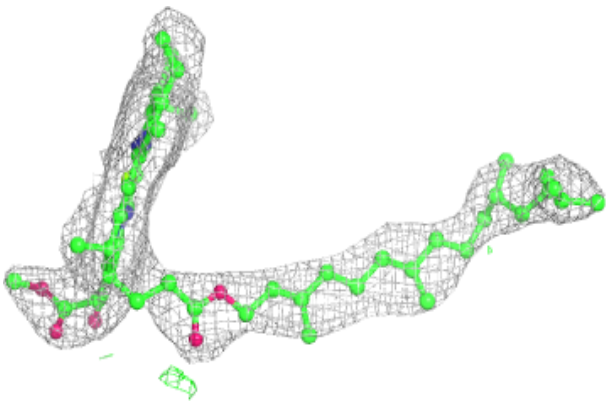


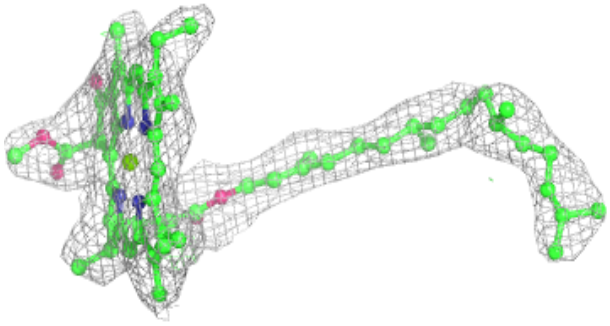


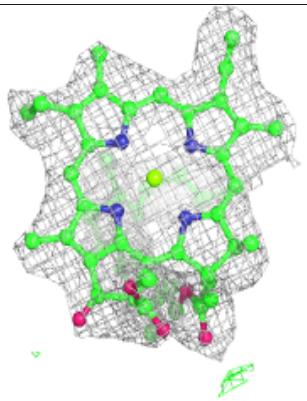


Electron density around CLA B 605:

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

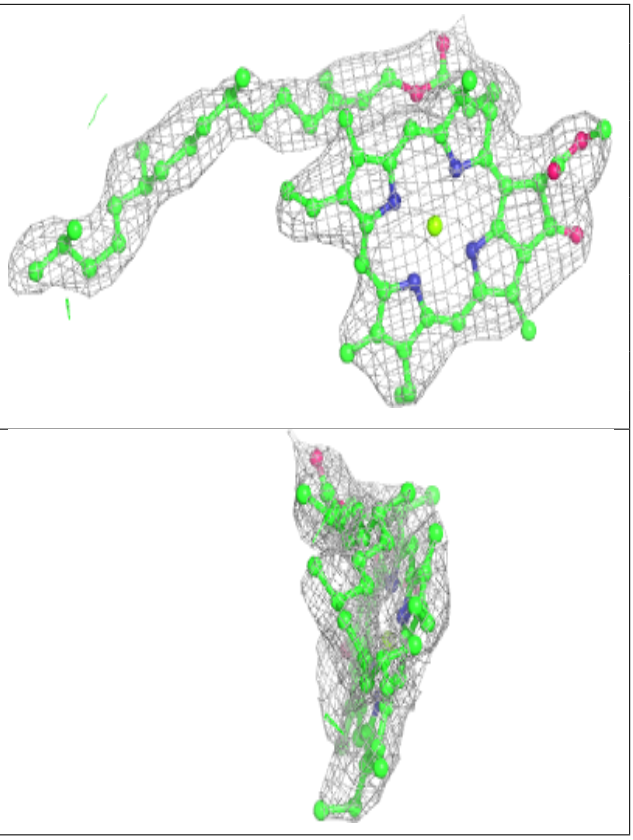


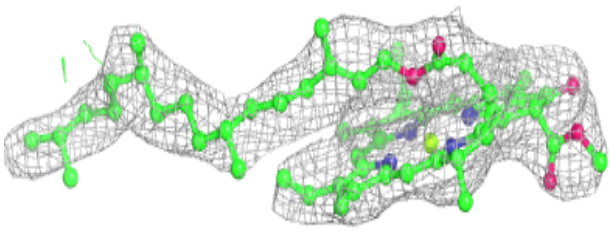




Electron density around CLA C 501:

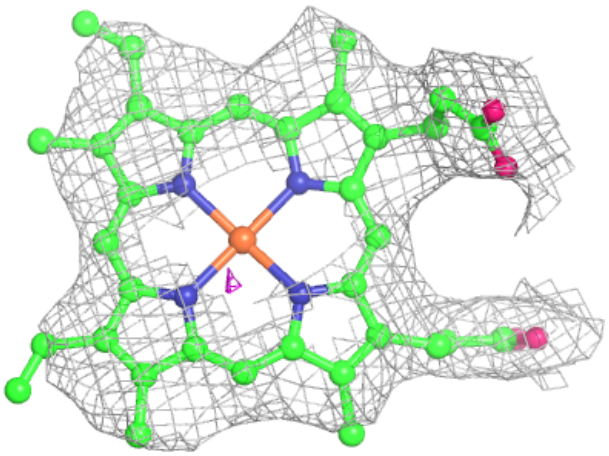
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

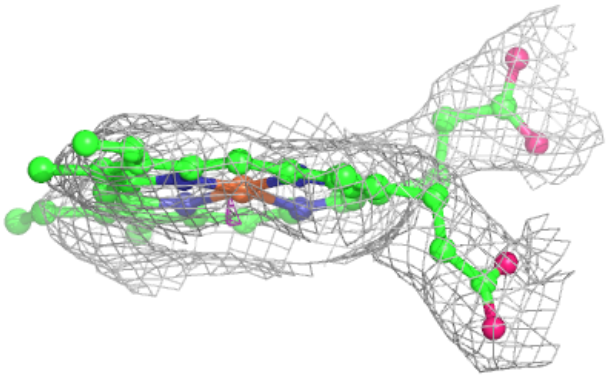


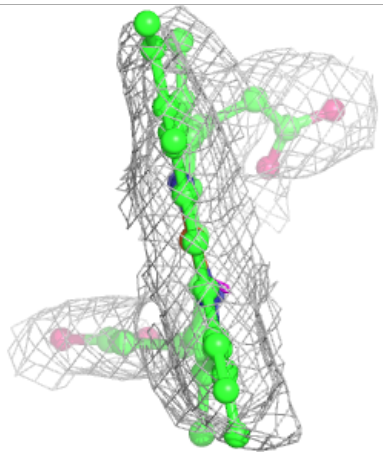


Electron density around HEM E 101:

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

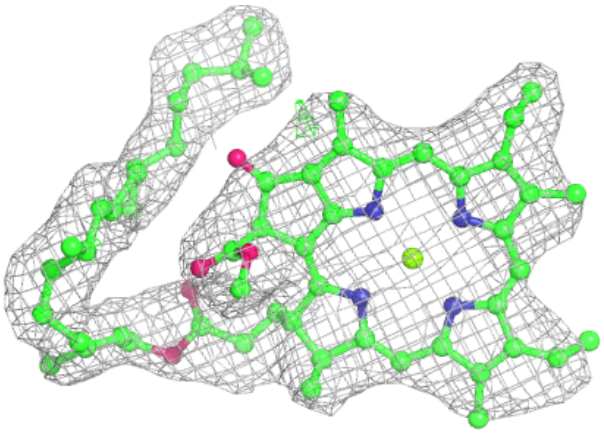


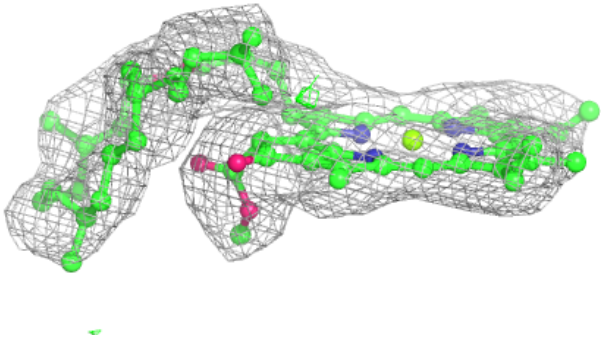


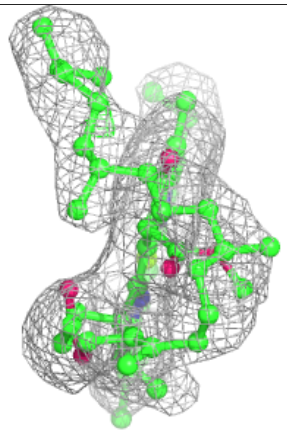


Electron density around CLA b 613:

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

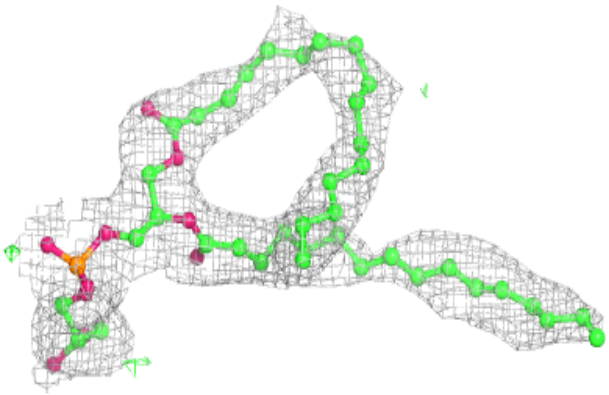


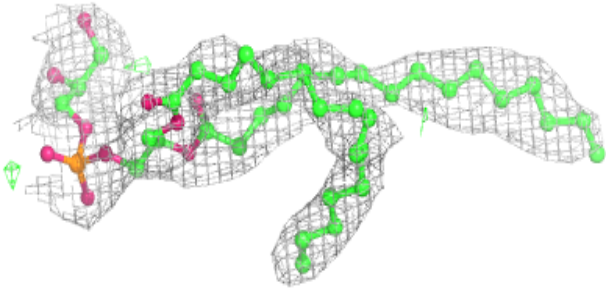


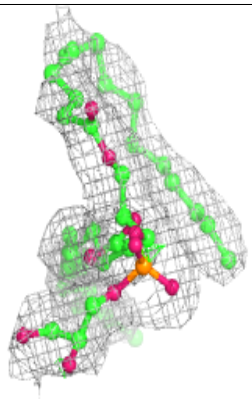


Electron density around LHG a 613:

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

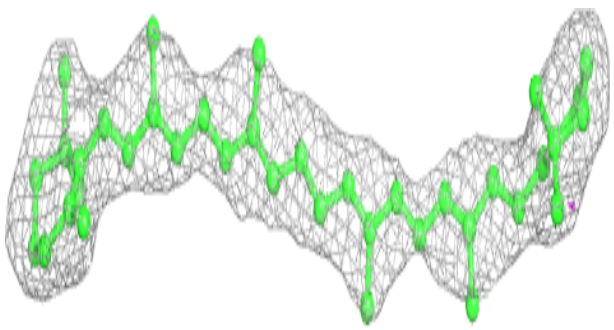


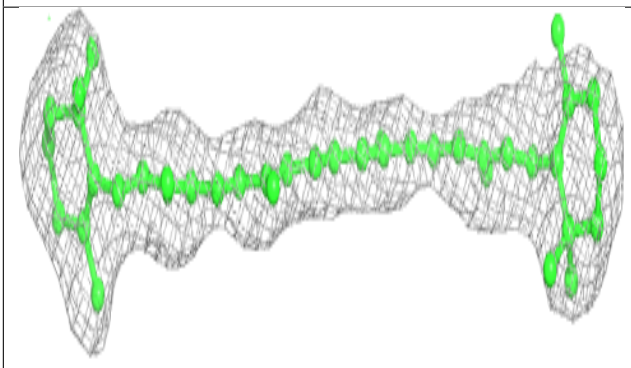


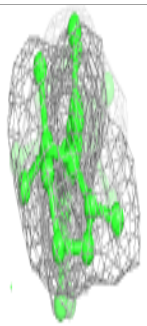


Electron density around BCR a 610:

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

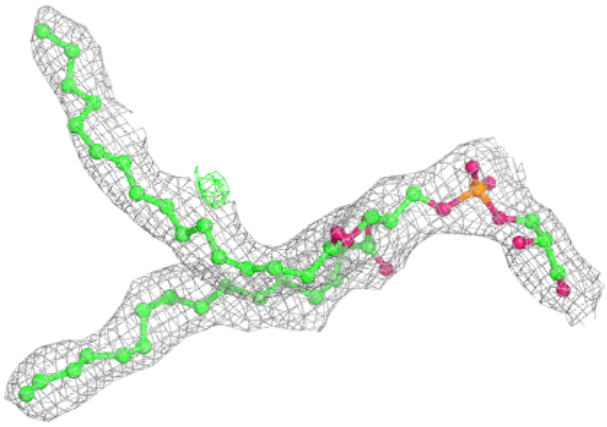


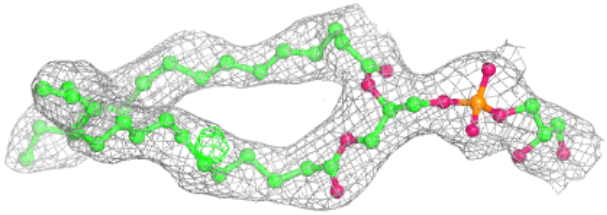


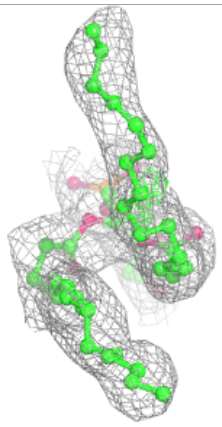


Electron density around LHG d 407:

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

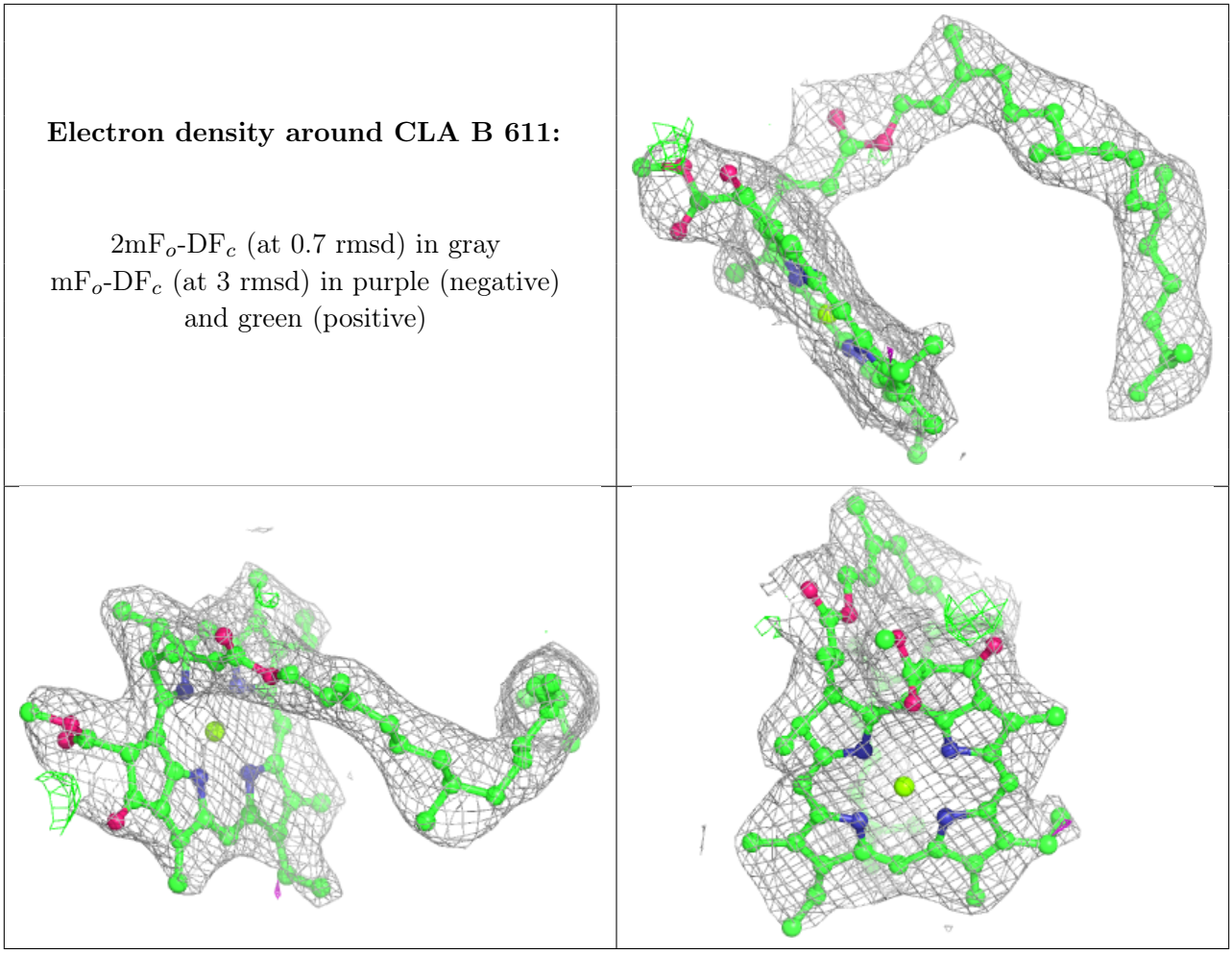






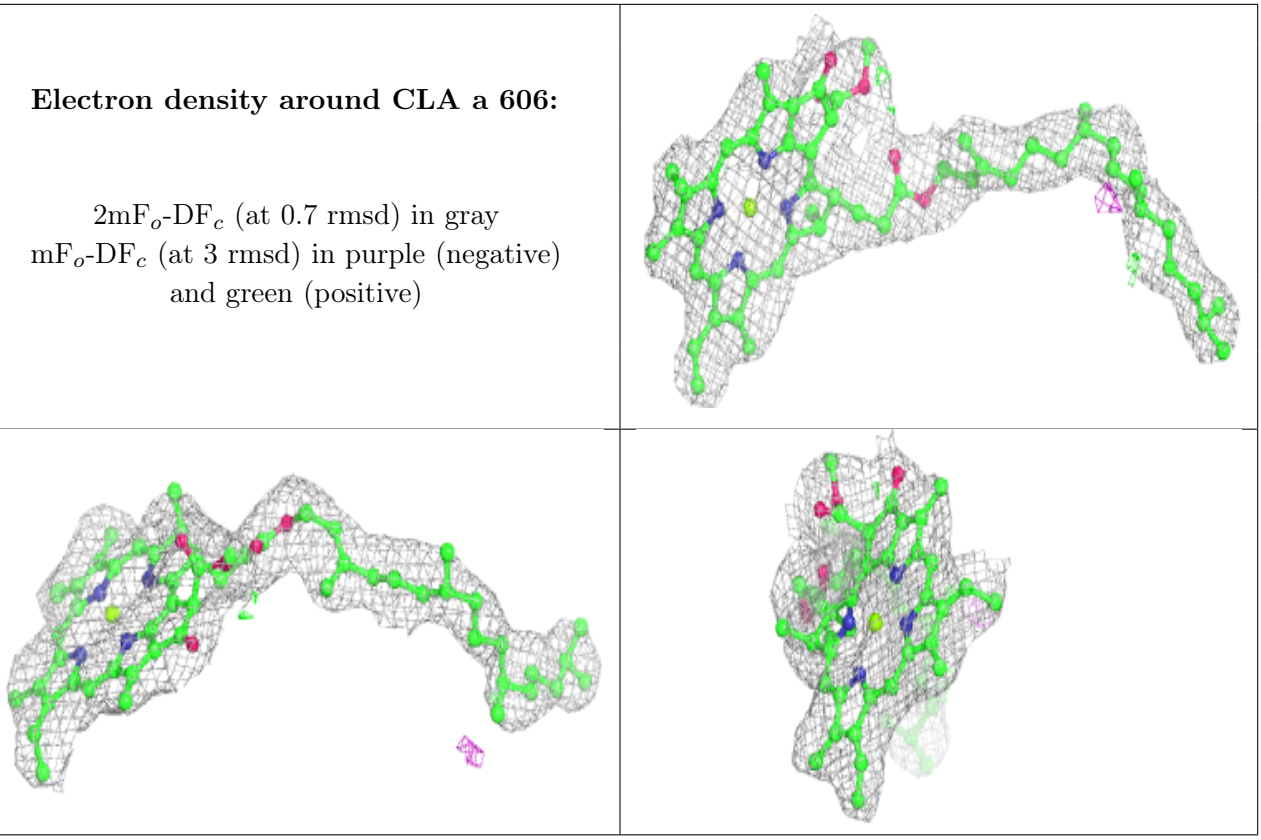
Electron density around CLA B 611:

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



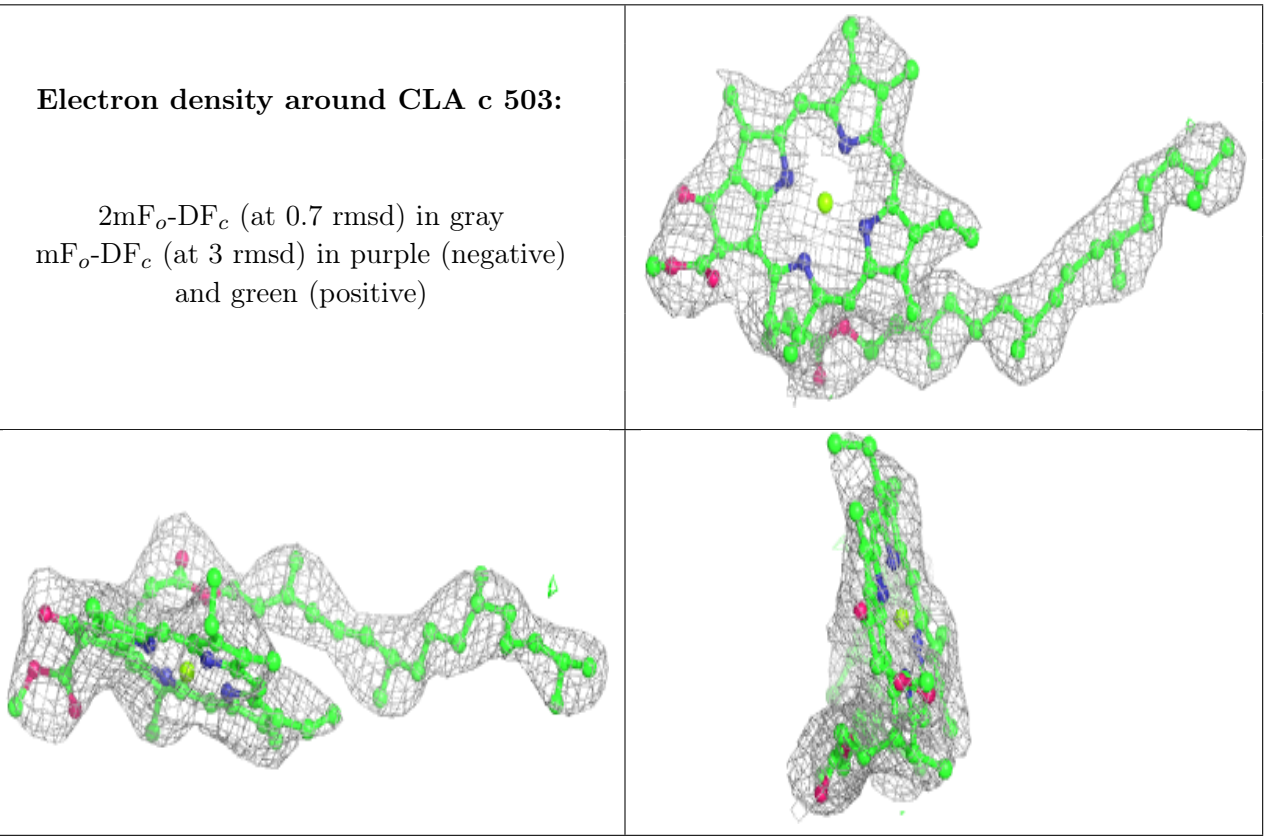
Electron density around CLA a 606:

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



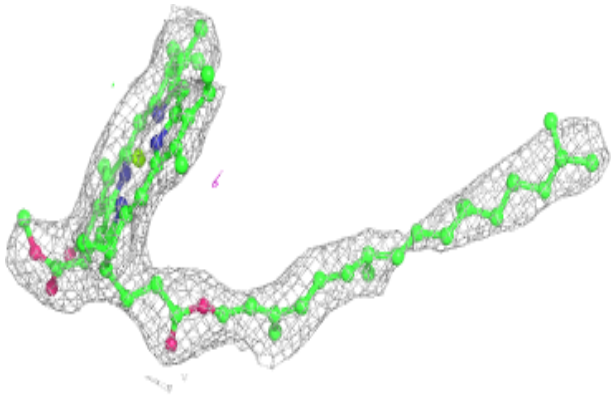
Electron density around CLA c 503:

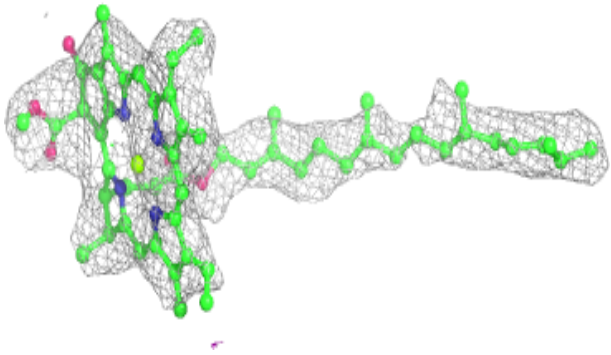
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

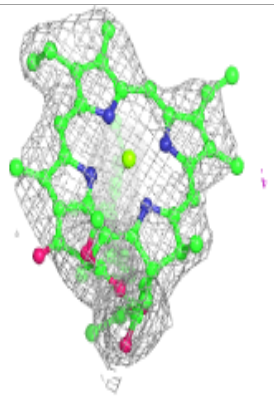


Electron density around CLA b 610:

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

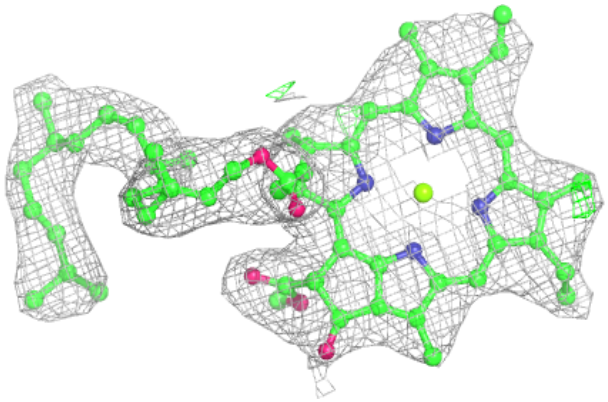


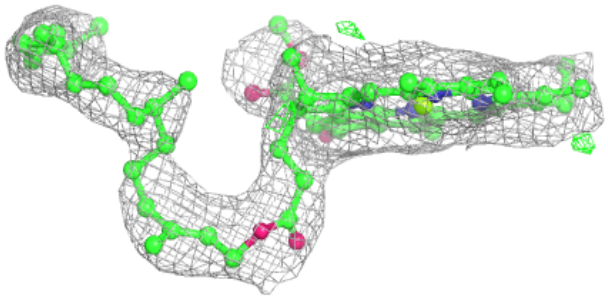


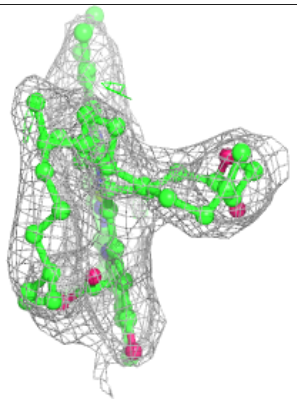


Electron density around CLA B 612:

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

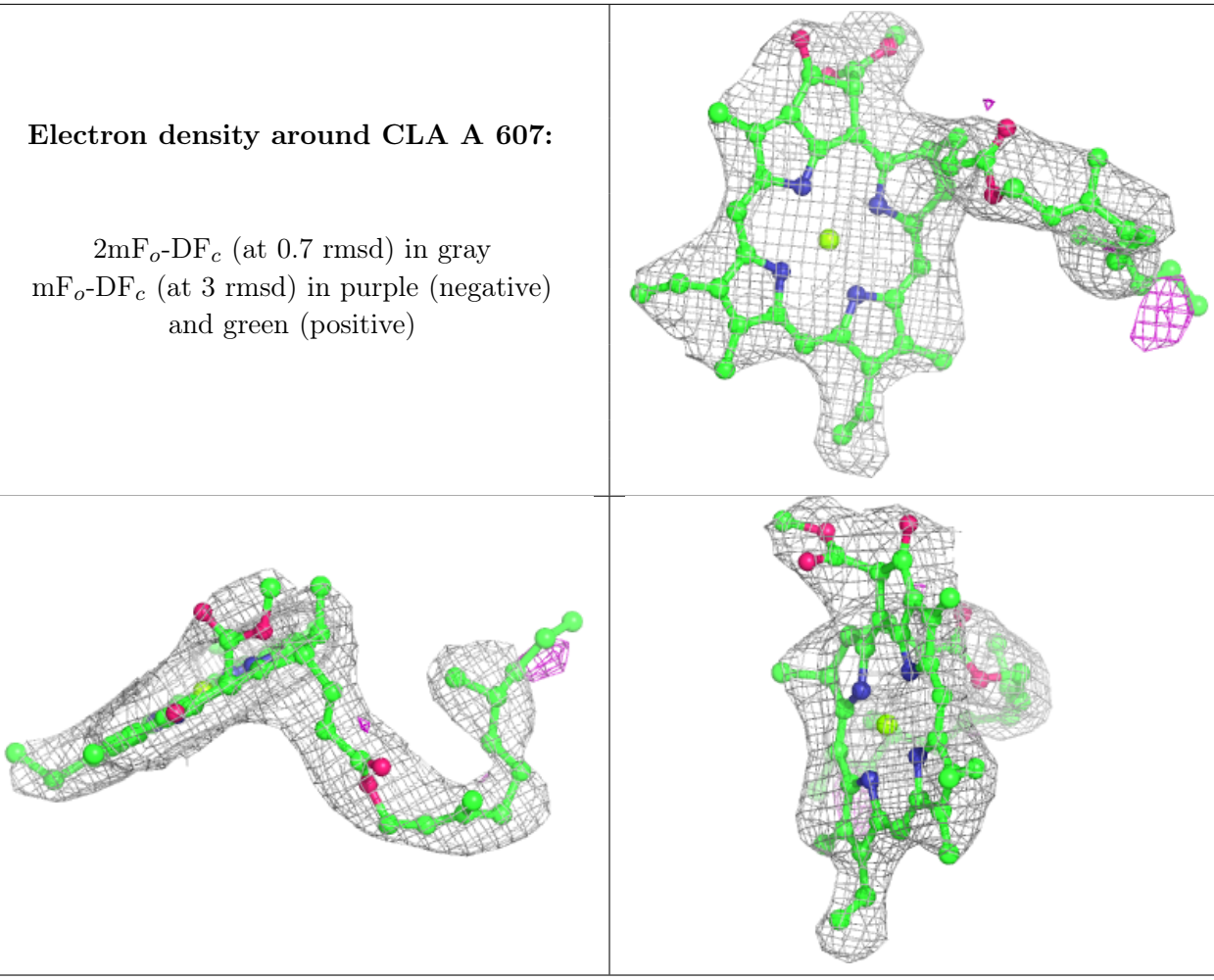






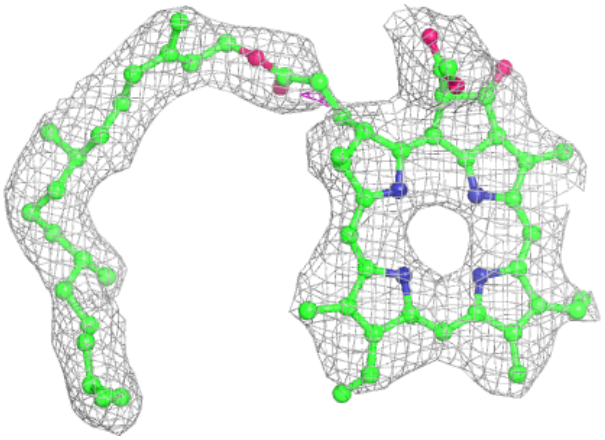
Electron density around CLA A 607:

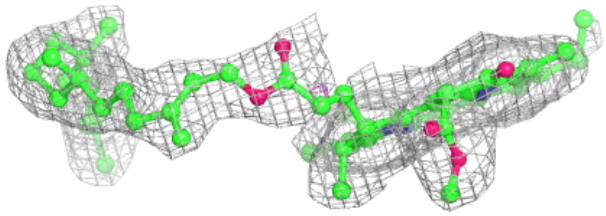
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

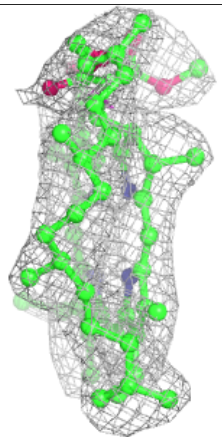


Electron density around PHO A 608:

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

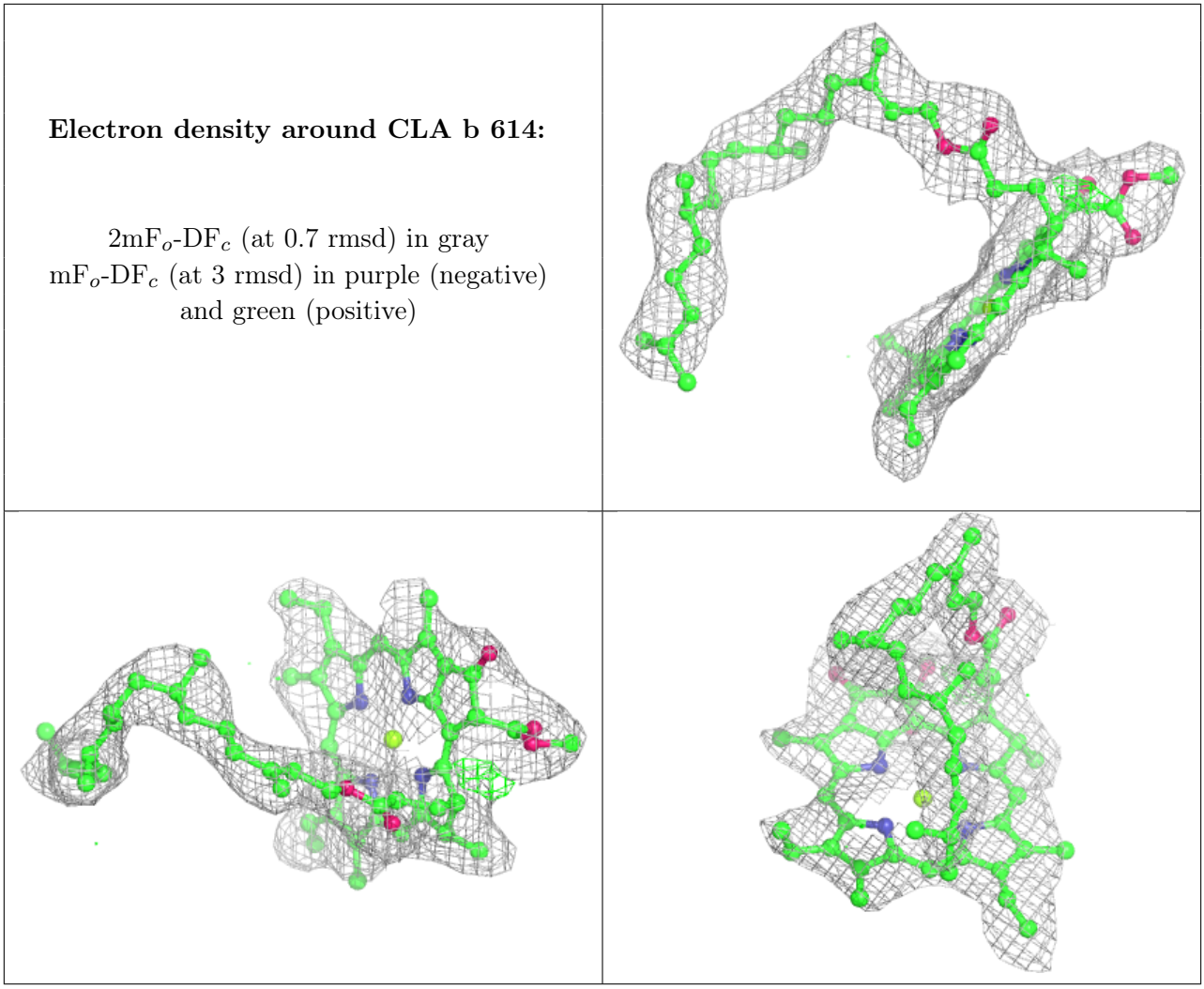






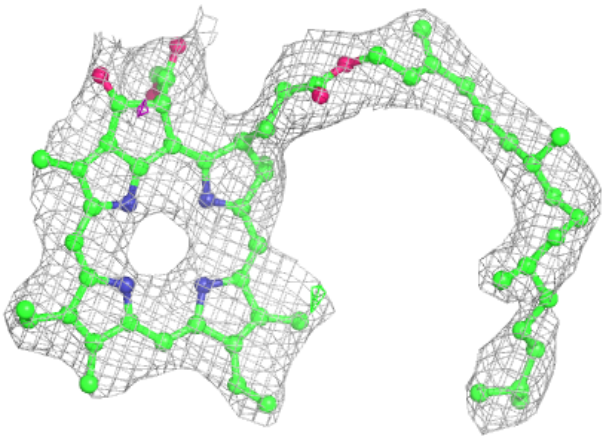
Electron density around CLA b 614:

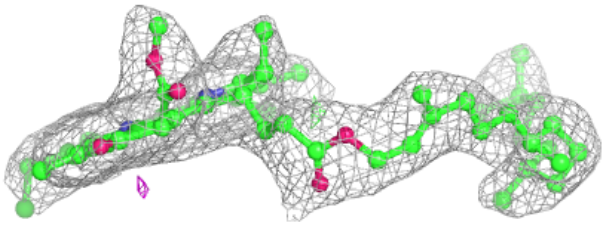
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

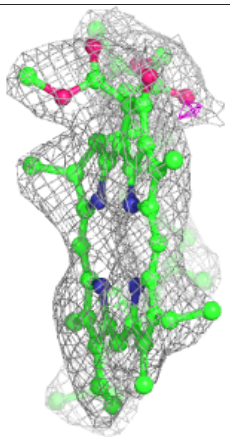


Electron density around PHO a 608:

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

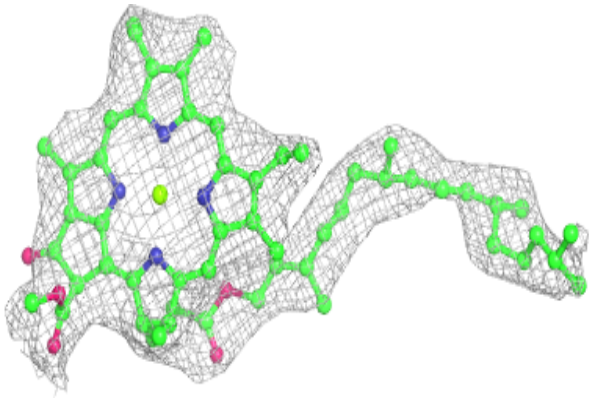


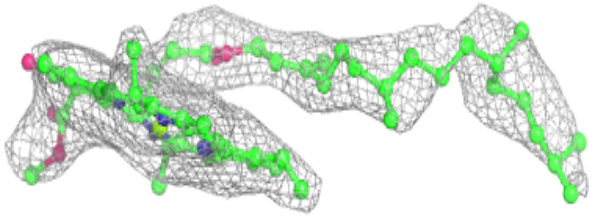


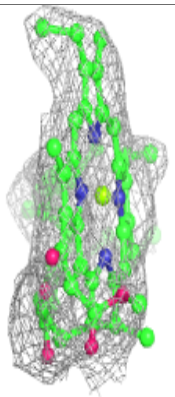


Electron density around CLA b 606:

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

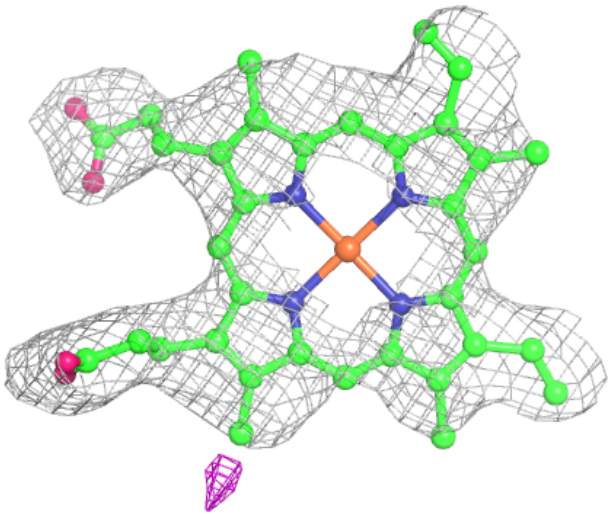


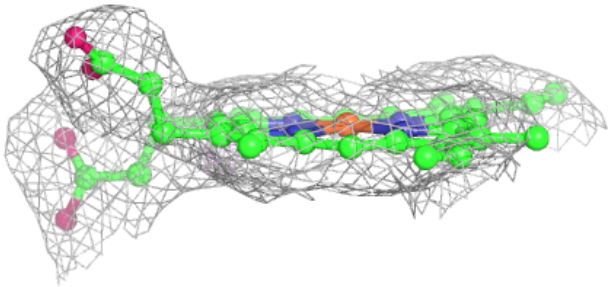


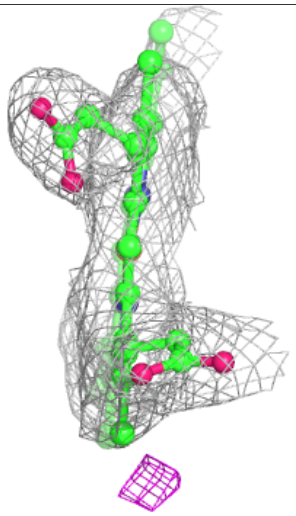


Electron density around HEC V 201:

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

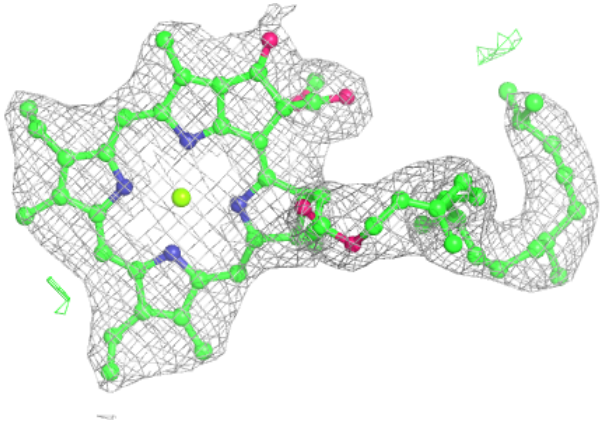


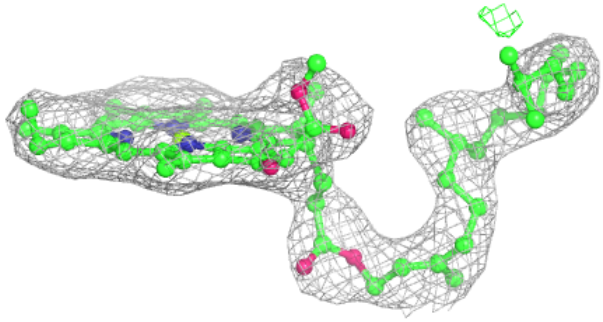


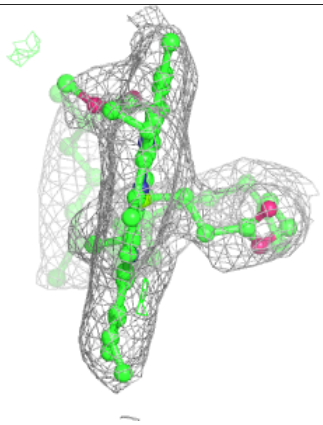


Electron density around CLA b 615:

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

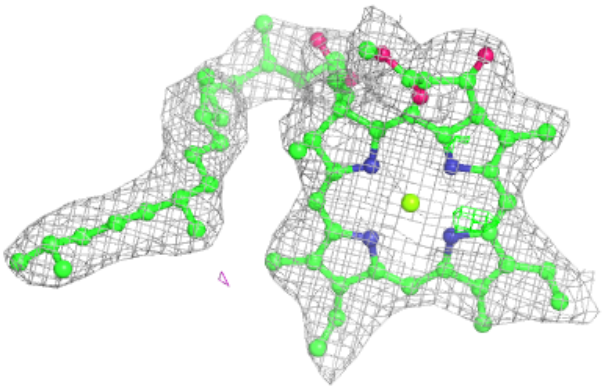


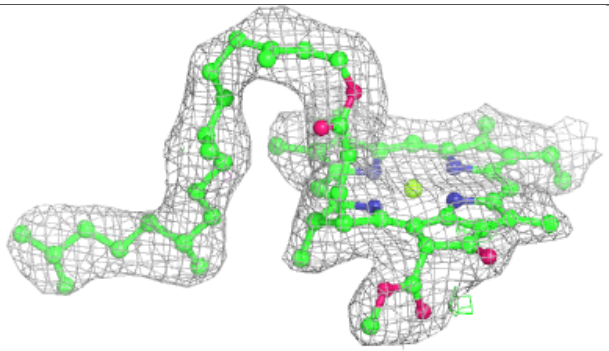


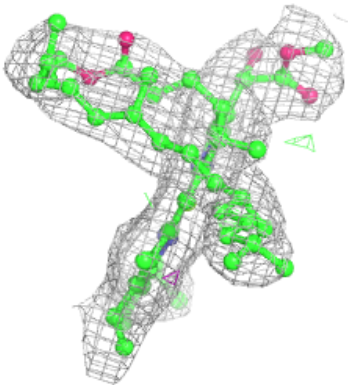


Electron density around CLA a 612:

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

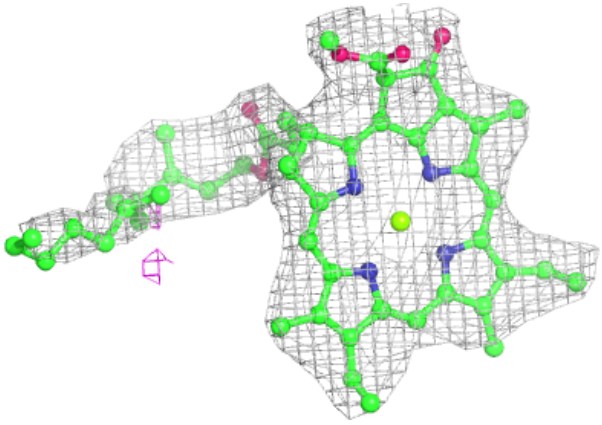


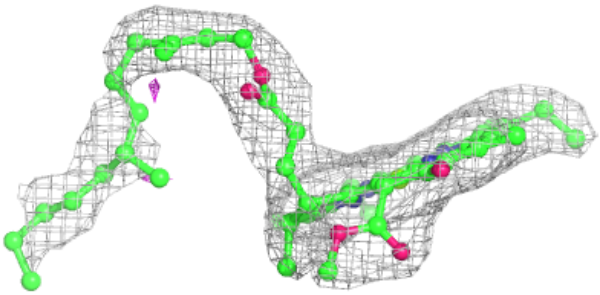


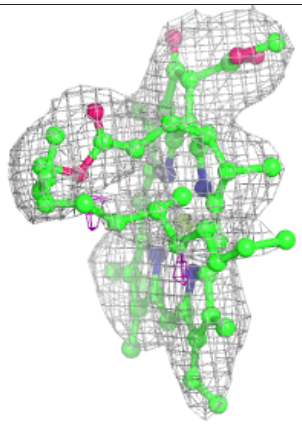


Electron density around CLA a 607:

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

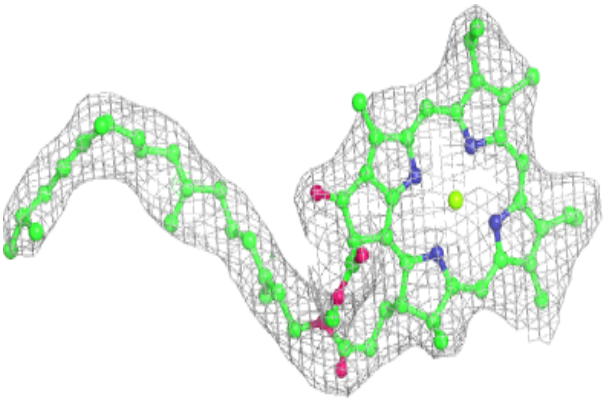


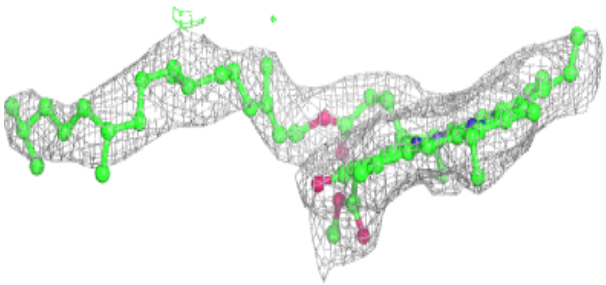


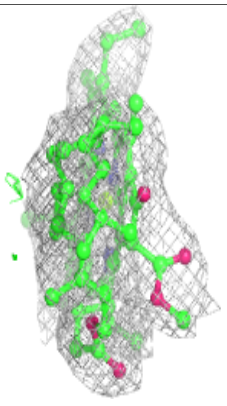


Electron density around CLA B 602:

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

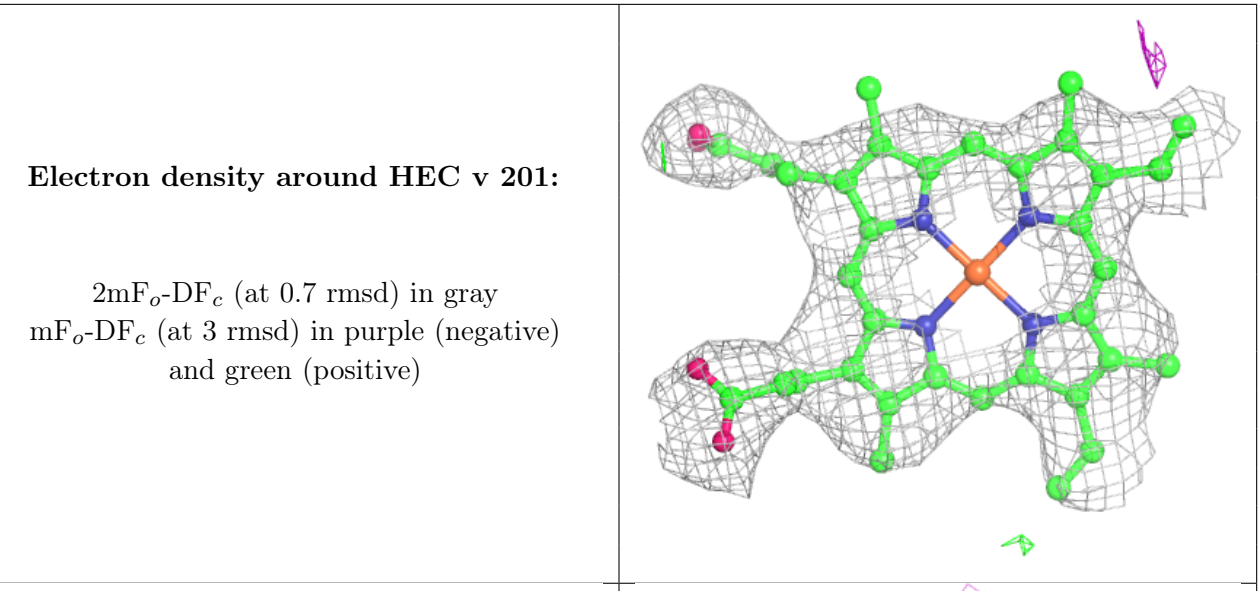






Electron density around HEC v 201:

$2mF_o$-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

There are no such residues in this entry.