Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 07:07 AM EDT

PDB ID	:	4IXQ
Title	:	RT fs X-ray diffraction of Photosystem II, dark state
Authors	:	Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on	:	2013-01-27
Resolution	:	5.70 Å(reported)

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

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

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

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

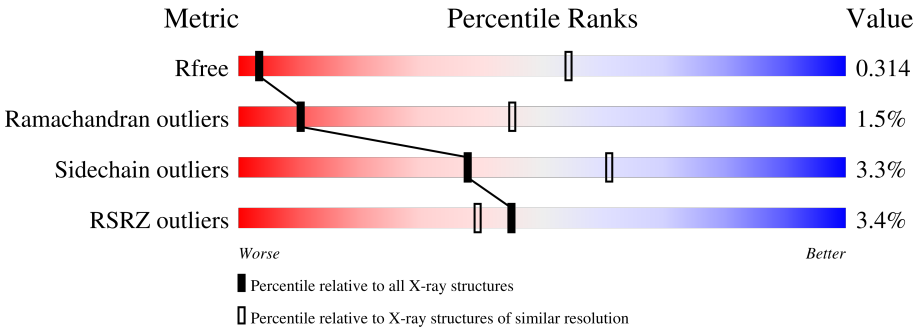
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

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 5.70 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	1003 (7.54-3.86)
Ramachandran outliers	138981	1011 (7.54-3.84)
Sidechain outliers	138945	1002 (7.58-3.82)
RSRZ outliers	127900	1002 (7.60-3.78)

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	360	2% 91% · 7%
1	a	360	% 91% · 7%
2	B	510	4% 93% · ·

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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

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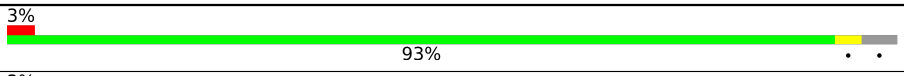
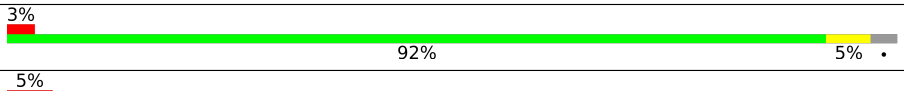
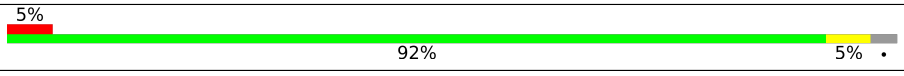
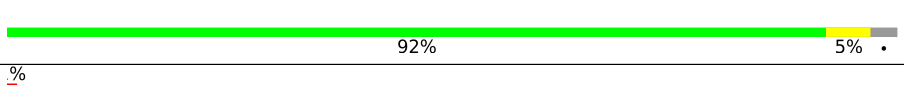
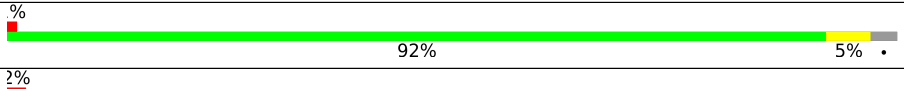
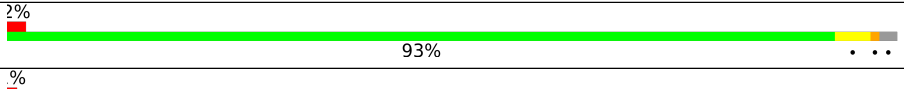
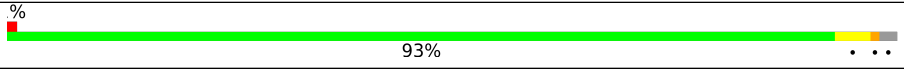
Mol	Chain	Length	Quality of chain
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
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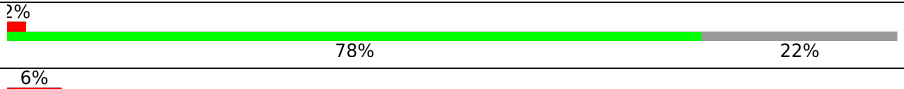
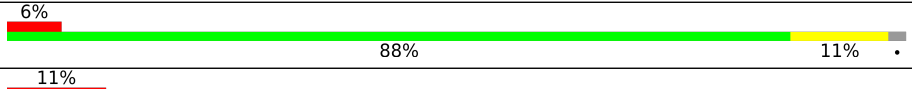
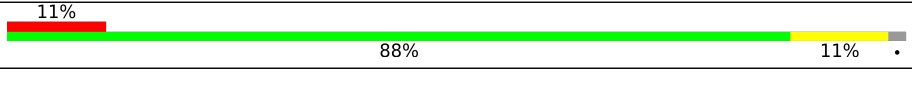
6	f	45	
7	H	66	
7	h	66	
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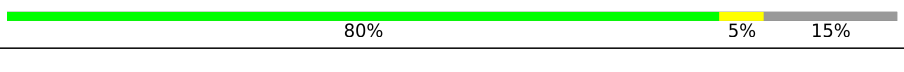
8	i	38	
9	J	40	
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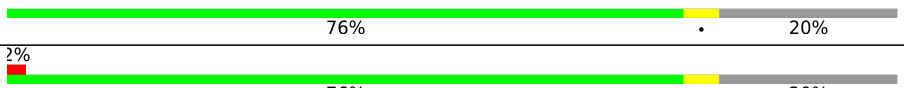
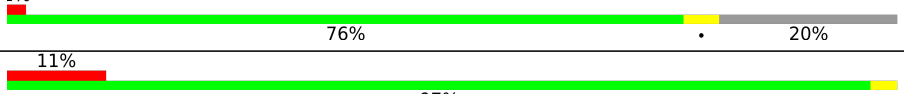
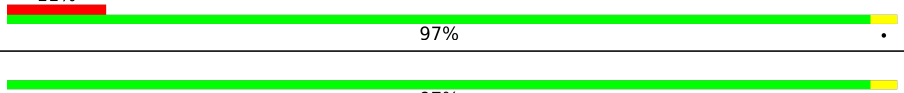
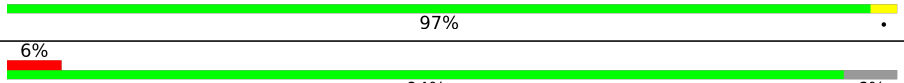
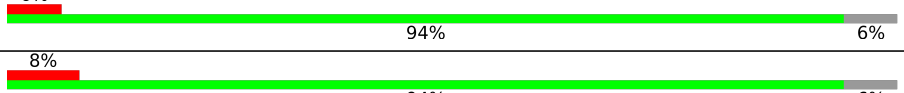
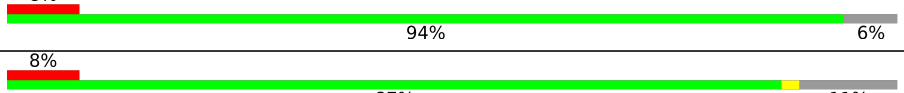
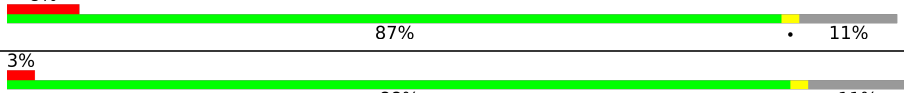
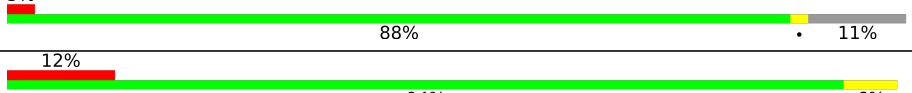
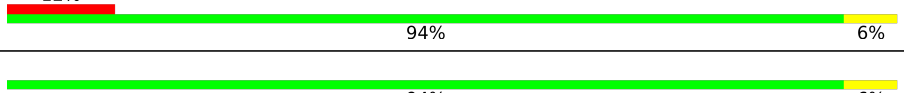
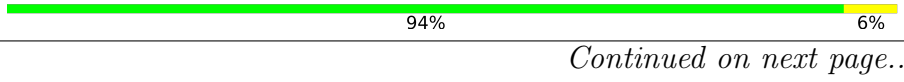
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	

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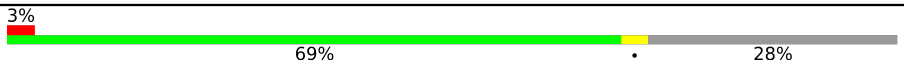
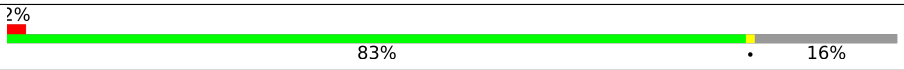
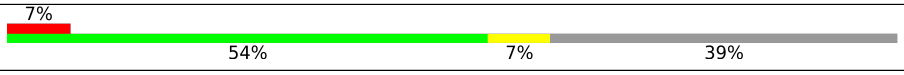
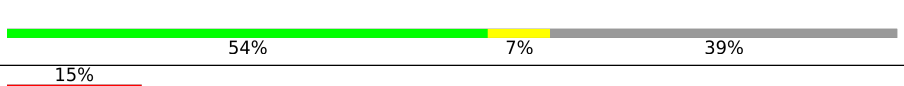
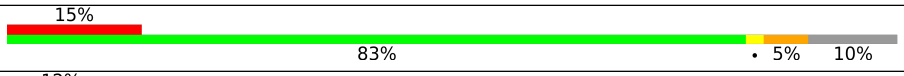
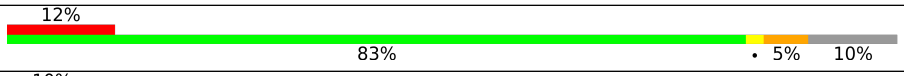
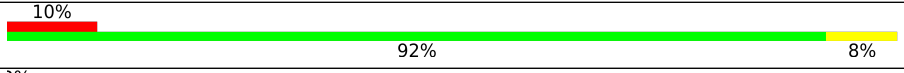
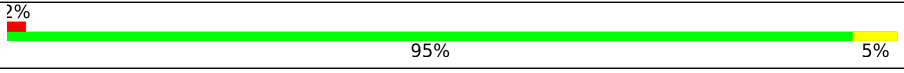
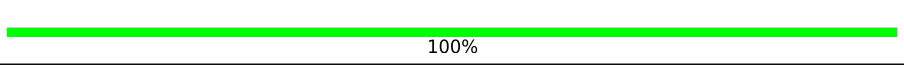
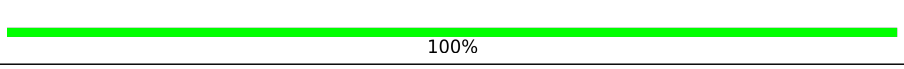
Mol	Chain	Length	Quality of chain
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	X
23	CLA	B	601	X	-	-	X
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	X
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	X
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	X
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	X
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	X
23	CLA	b	613	X	-	-	X
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	X
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	X
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	X
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	j	101	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	514	-	-	-	X
27	BCR	C	515	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	K	102	-	-	-	X
27	BCR	Z	101	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	621	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	c	516	-	-	-	X
27	BCR	f	102	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	x	101	-	-	-	X
28	DGD	B	621	-	-	-	X
28	DGD	B	626	-	-	-	X
28	DGD	D	410	-	-	-	X
28	DGD	b	602	-	-	-	X
28	DGD	d	408	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	417	-	-	-	X
30	SQD	D	409	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	d	407	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	f	103	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	520	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	M	101	-	-	-	X
31	LMG	M	102	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	520	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	101	-	-	-	X
31	LMG	k	103	-	-	-	X
33	LMT	B	623	-	-	-	X
33	LMT	B	624	-	-	-	X
33	LMT	B	627	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	D	411	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	T	101	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	625	-	-	-	X
33	LMT	b	626	-	-	-	X
33	LMT	i	102	-	-	-	X
33	LMT	m	101	-	-	-	X
33	LMT	x	102	-	-	-	X
35	CA	K	101	-	-	-	X
35	CA	o	301	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total 666	C 434	N 108	O 124	0	0	0
5	e	82	Total 666	C 434	N 108	O 124	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total 282	C 192	N 46	O 43	S 1	0	0	0
6	f	35	Total 282	C 192	N 46	O 43	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total 507	C 338	N 81	O 86	S 2	0	0	0
7	h	65	Total 507	C 338	N 81	O 86	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	35	Total 286	C 195	N 45	O 45	S 1	0	0	0
8	i	35	Total 286	C 195	N 45	O 45	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total 249	C 170	N 38	O 40	S 1	0	0	0
9	j	34	Total 249	C 170	N 38	O 40	S 1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total 293	C 204	N 43	O 46	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total 293	C 204	N 43	O 46	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total 304	C 202	N 48	O 53	S 1	0	0	0
11	l	37	Total 304	C 202	N 48	O 53	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total 267	C 178	N 40	O 48	S 1	0	0	0
12	m	34	Total 267	C 178	N 40	O 48	S 1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total 1845	C 1154	N 308	O 379	S 4	0	0	0
13	o	243	Total 1845	C 1154	N 308	O 379	S 4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total 275	C 192	N 40	O 41	S 2	0	0	0
14	t	32	Total 275	C 192	N 40	O 41	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	x	37	Total	C	N	O	0	0	0
			270	182	41	47			

- 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			

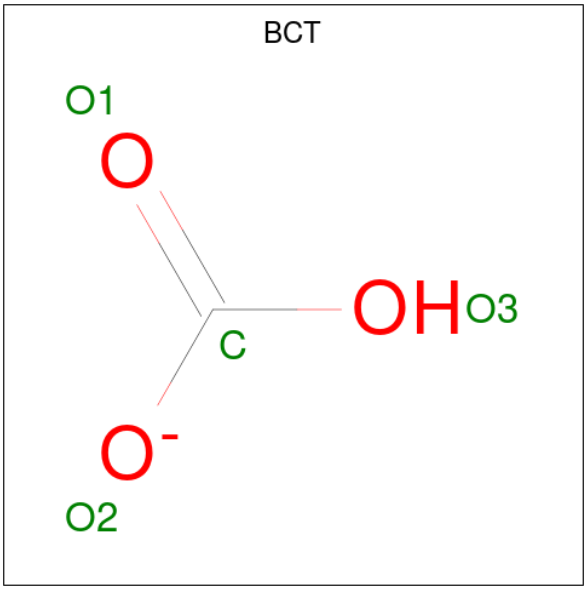
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			
20	G	28	Total	C	N	O	0	0	0
			140	84	28	28			

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

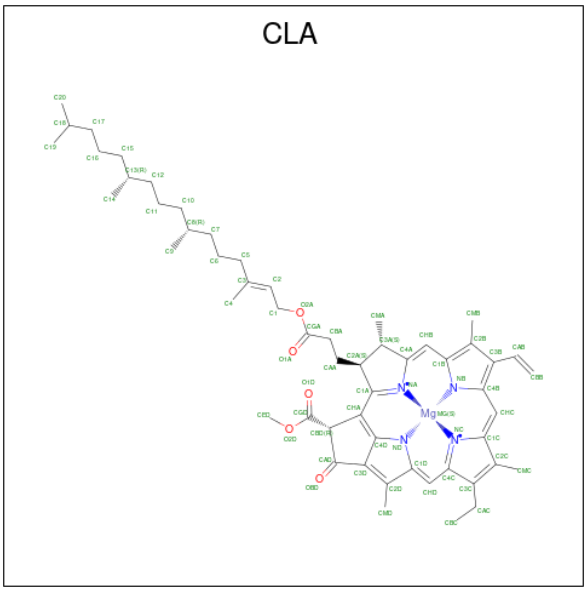
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe 1 1	0	0
21	a	1	Total Fe 1 1	0	0

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O 4 1 3	0	0
22	d	1	Total C O 4 1 3	0	0

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



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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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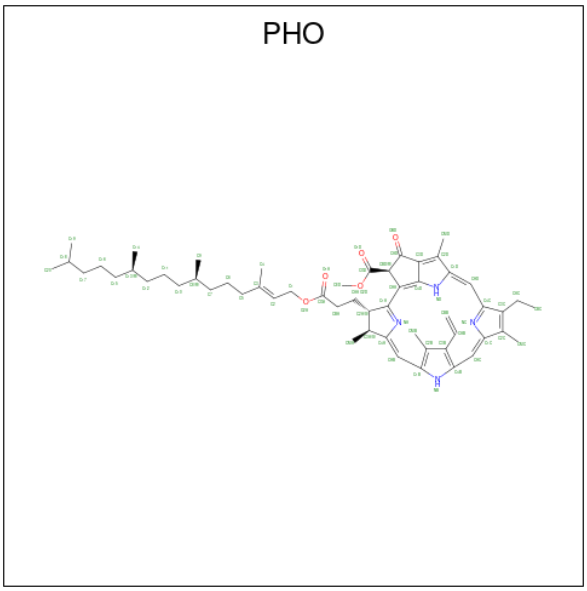
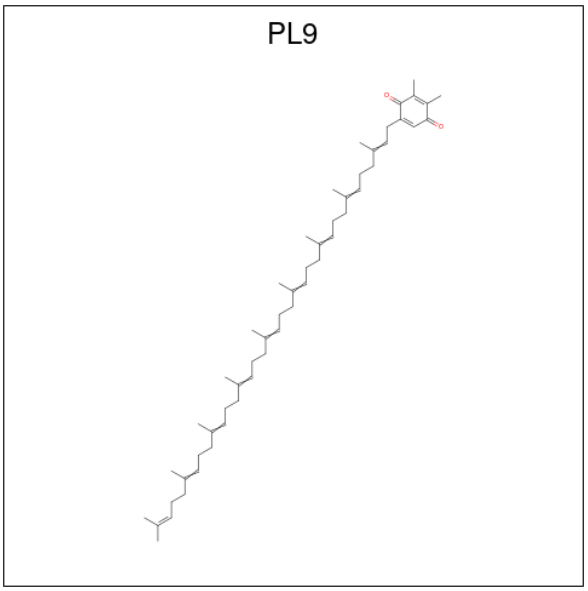
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



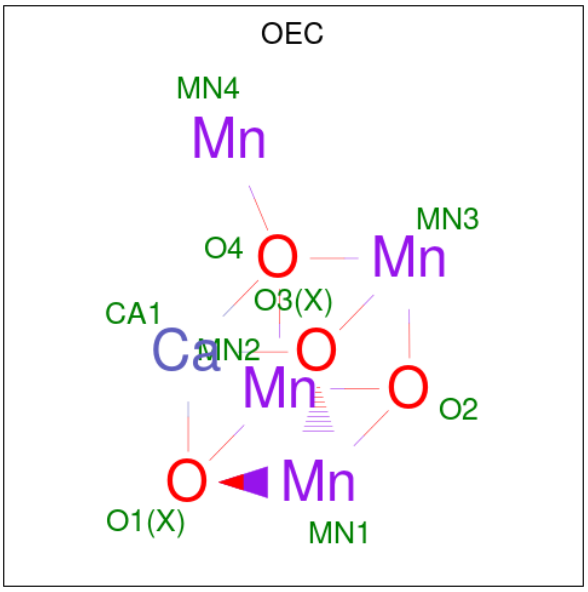
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 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: $C_{53}H_{80}O_2$).



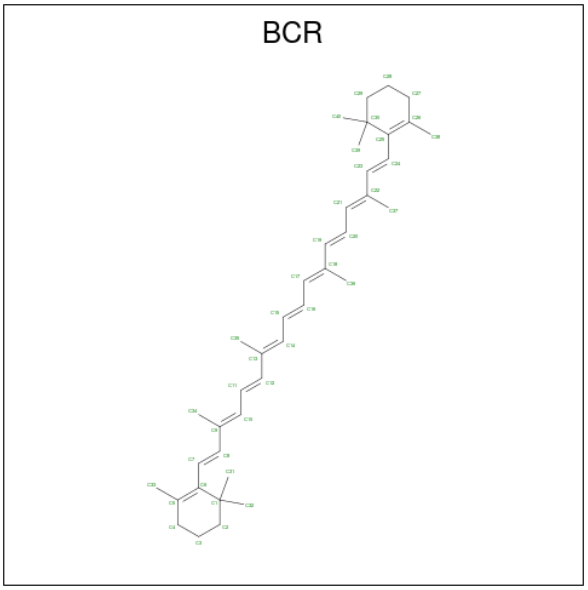
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 45 43 2	0	0
25	D	1	Total C O 55 53 2	0	0
25	J	1	Total C O 35 33 2	0	0
25	a	1	Total C O 45 43 2	0	0
25	d	1	Total C O 55 53 2	0	0
25	j	1	Total C O 35 33 2	0	0

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total Ca Mn 5 1 4	0	0
26	a	1	Total Ca Mn 5 1 4	0	0

- 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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	J	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	T	1	Total C 40 40	0	0
27	Z	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	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	f	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

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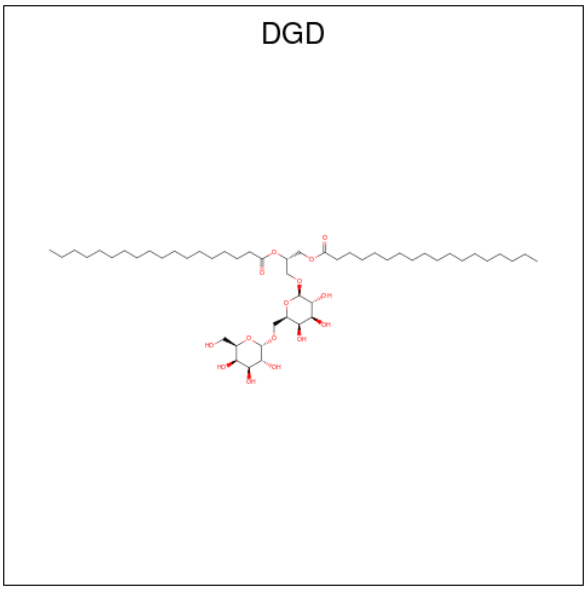
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	x	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52 37 15	0	0
28	b	1	Total C O 58 43 15	0	0

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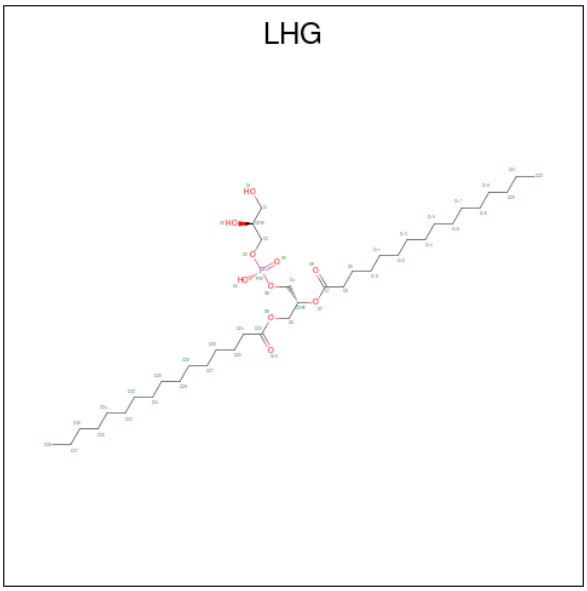
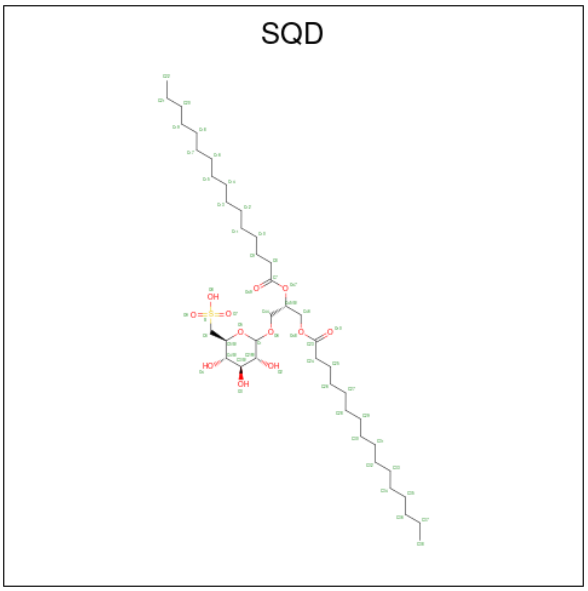
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C O 53 38 15	0	0
28	c	1	Total C O 62 47 15	0	0
28	c	1	Total C O 66 51 15	0	0
28	d	1	Total C O 63 48 15	0	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



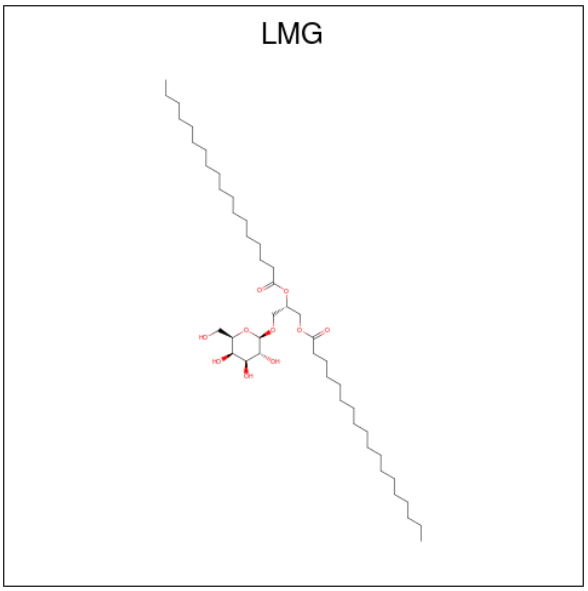
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O P 39 28 10 1	0	0
29	A	1	Total C O P 37 26 10 1	0	0
29	a	1	Total C O P 39 28 10 1	0	0
29	a	1	Total C O P 37 26 10 1	0	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 51 41 10	0	0
31	A	1	Total C O 42 32 10	0	0
31	B	1	Total C O 49 39 10	0	0
31	C	1	Total C O 48 38 10	0	0
31	C	1	Total C O 45 35 10	0	0
31	D	1	Total C O 46 36 10	0	0
31	D	1	Total C O 49 39 10	0	0
31	D	1	Total C O 48 38 10	0	0
31	E	1	Total C O 44 34 10	0	0
31	I	1	Total C O 43 33 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	a	1	Total C O 42 32 10	0	0
31	a	1	Total C O 51 41 10	0	0

Continued on next page...

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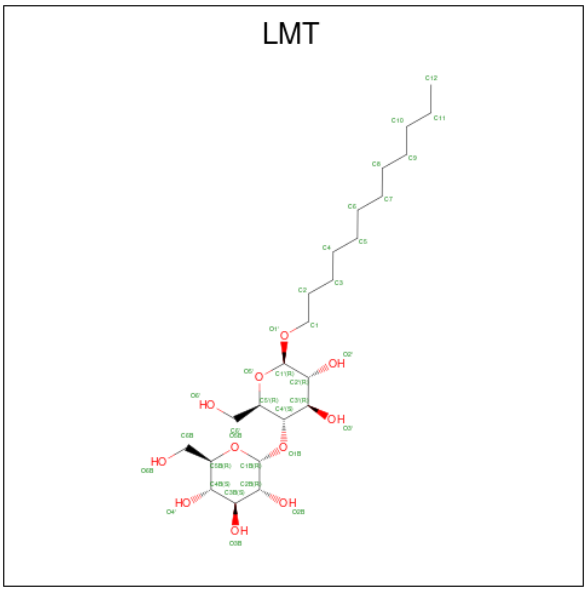
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C O 49 39 10	0	0
31	b	1	Total C O 49 39 10	0	0
31	c	1	Total C O 45 35 10	0	0
31	d	1	Total C O 46 36 10	0	0
31	d	1	Total C O 48 38 10	0	0
31	e	1	Total C O 44 34 10	0	0
31	i	1	Total C O 43 33 10	0	0
31	k	1	Total C O 48 38 10	0	0

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

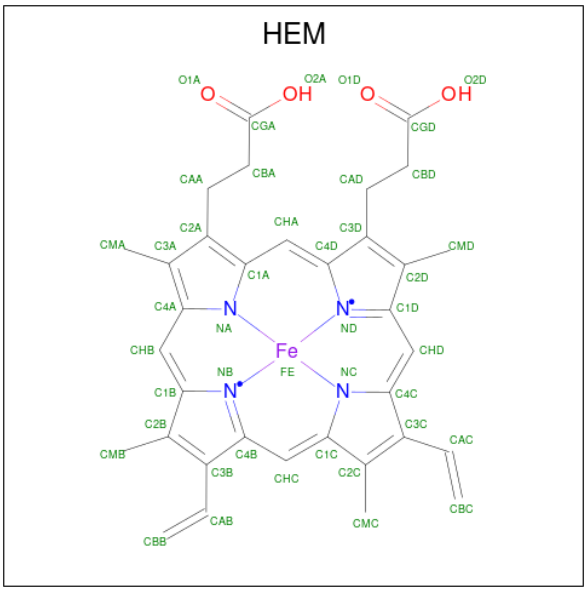
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Cl 1 1	0	0
32	d	1	Total Cl 1 1	0	0

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	D	1	Total	C	O	0	0
			31	20	11		
33	I	1	Total	C	O	0	0
			35	24	11		
33	M	1	Total	C	O	0	0
			35	24	11		
33	T	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			35	24	11		
33	i	1	Total	C	O	0	0
			35	24	11		
33	m	1	Total	C	O	0	0
			35	24	11		
33	x	1	Total	C	O	0	0
			31	20	11		

- 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	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
34	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

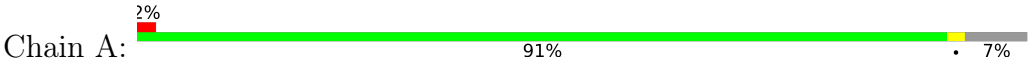
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

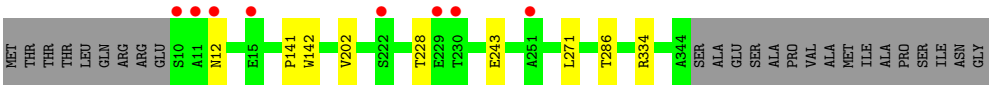
3 Residue-property plots (i)

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 Q(B) protein 1

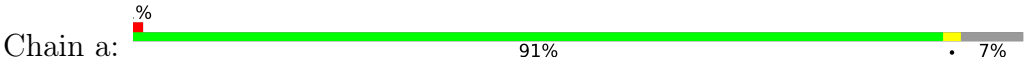
Chain A:





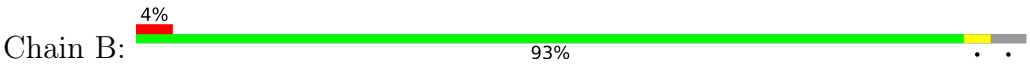
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



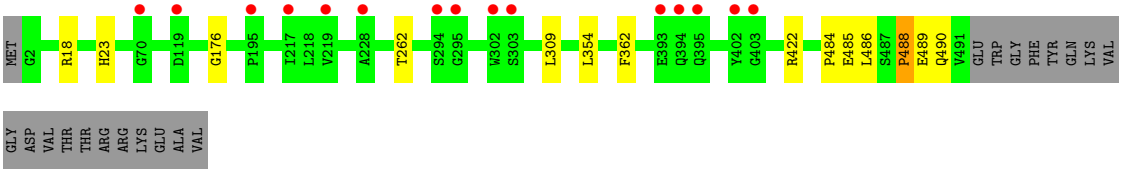
• Molecule 2: Photosystem II core light harvesting protein

Chain B:



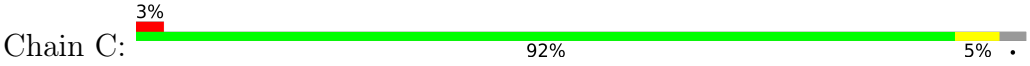
• Molecule 2: Photosystem II core light harvesting protein

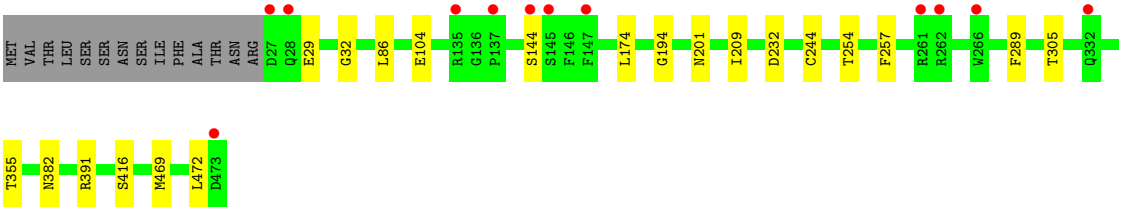
Chain b:



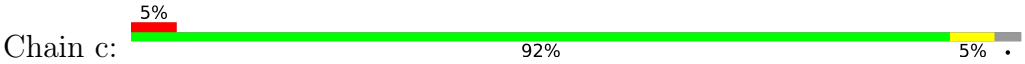
• Molecule 3: Photosystem II CP43 protein

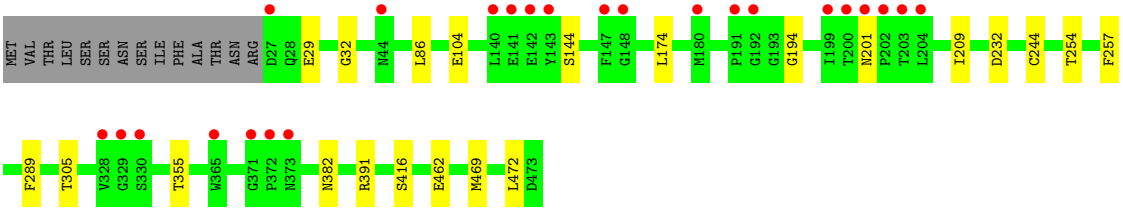
Chain C:



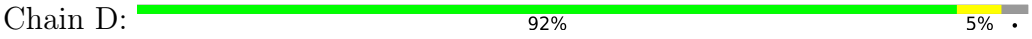


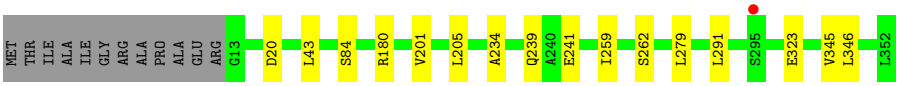
• Molecule 3: Photosystem II CP43 protein



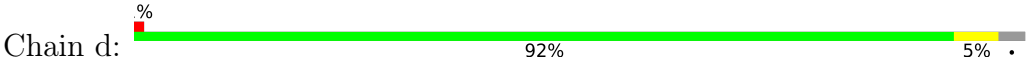


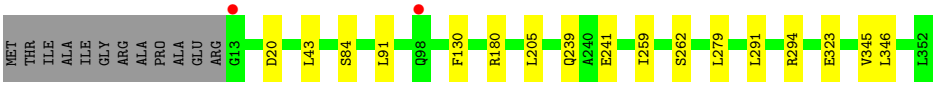
• Molecule 4: Photosystem II D2 protein



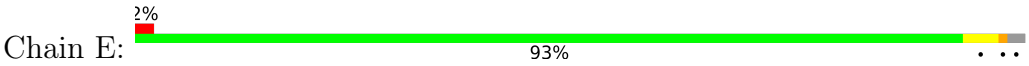


• Molecule 4: Photosystem II D2 protein





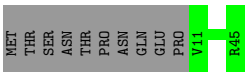
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

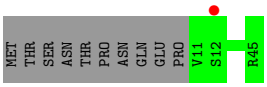
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



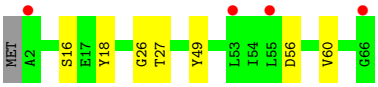
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



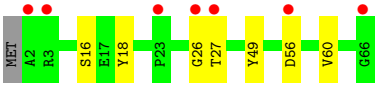
• Molecule 7: Photosystem II reaction center protein H

Chain H:



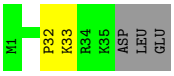
• Molecule 7: Photosystem II reaction center protein H

Chain h:



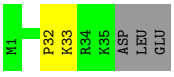
• Molecule 8: Photosystem II reaction center protein I

Chain I:



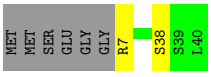
• Molecule 8: Photosystem II reaction center protein I

Chain i:



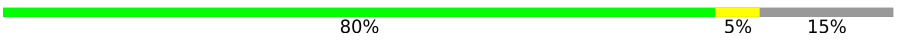
• Molecule 9: Photosystem II reaction center protein J

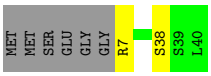
Chain J:



• Molecule 9: Photosystem II reaction center protein J

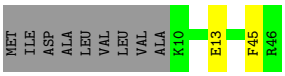
Chain j:





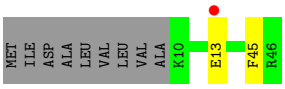
• Molecule 10: Photosystem II reaction center protein K

Chain K:



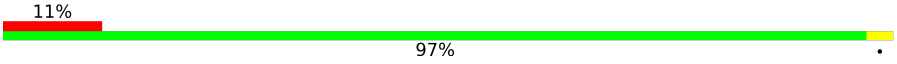
• Molecule 10: Photosystem II reaction center protein K

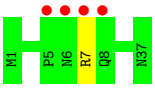
Chain k:



• Molecule 11: Photosystem II reaction center protein L

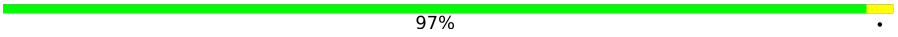
Chain L:





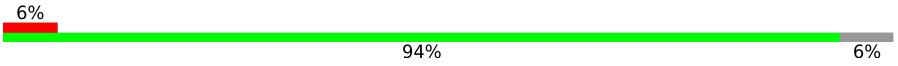
• Molecule 11: Photosystem II reaction center protein L

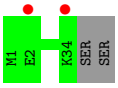
Chain l:



• Molecule 12: Photosystem II reaction center protein M

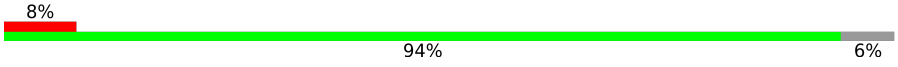
Chain M:

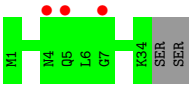




• Molecule 12: Photosystem II reaction center protein M

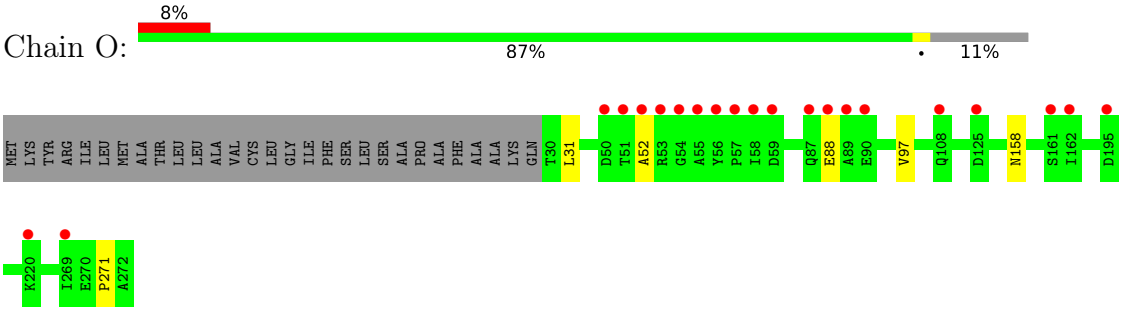
Chain m:





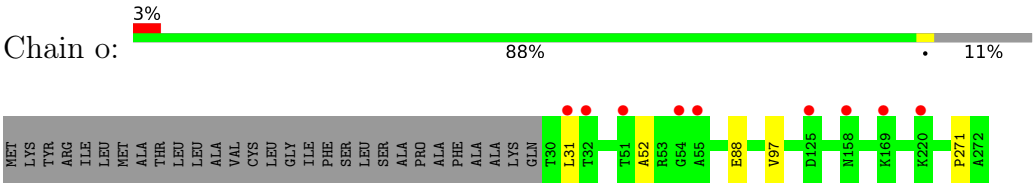
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



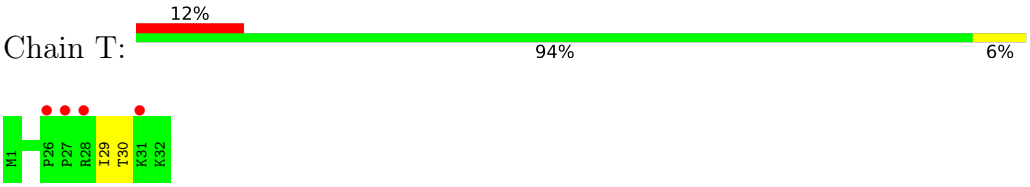
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



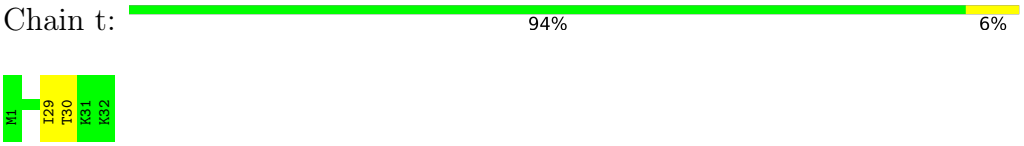
• Molecule 14: Photosystem II reaction center protein T

Chain T:



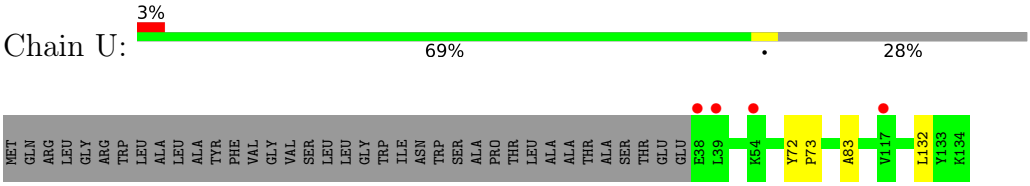
• Molecule 14: Photosystem II reaction center protein T

Chain t:



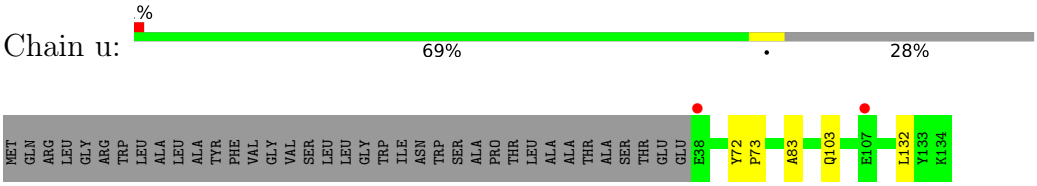
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



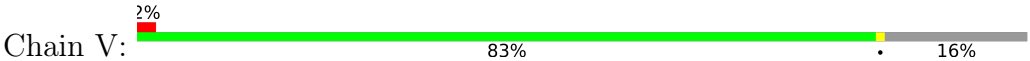
• Molecule 15: Photosystem II 12 kDa extrinsic protein

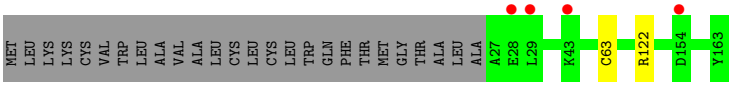
Chain u:



• Molecule 16: Cytochrome c-550

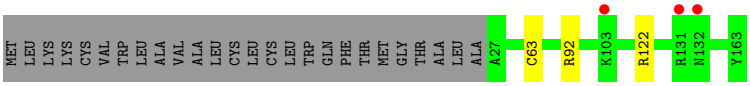
Chain V:





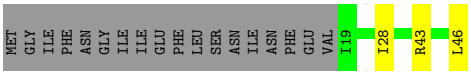
• Molecule 16: Cytochrome c-550

Chain v:



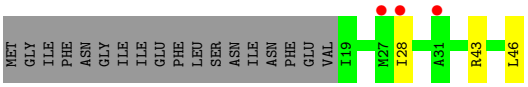
• Molecule 17: Photosystem II reaction center protein ycf12

Chain y:



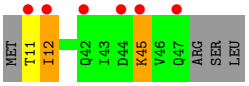
• Molecule 17: Photosystem II reaction center protein ycf12

Chain g:



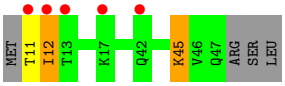
• Molecule 18: Photosystem II reaction center X protein

Chain X:



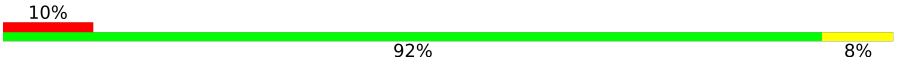
• Molecule 18: Photosystem II reaction center X protein

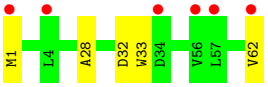
Chain x:



• Molecule 19: Photosystem II reaction center protein Z

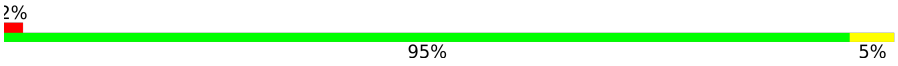
Chain Z:

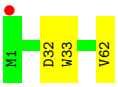




• Molecule 19: Photosystem II reaction center protein Z

Chain z:





• Molecule 20: Photosystem II reaction center protein Y

Chain Y:

There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Y

Chain G:

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.86Å 227.51Å 307.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.94 – 5.70 82.94 – 5.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (82.94-5.70) 98.3 (82.94-5.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.277 , 0.314 0.277 , 0.314	Depositor DCC
R_{free} test set	1325 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	3.698	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: BCR, SQD, FE2, BCT, CL, HEM, OEC, DGD, CA, LMG, PHO, PL9, LMT, LHG, CLA

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	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.29	0/3986	0.46	0/5433
3	C	0.29	0/3556	0.46	0/4842
3	c	0.28	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.28	0/685	0.48	0/933
5	e	0.27	0/685	0.46	0/933
6	F	0.26	0/291	0.44	0/397
6	f	0.26	0/291	0.42	0/397
7	H	0.27	0/520	0.50	0/709
7	h	0.28	0/520	0.51	0/709
8	I	0.28	0/293	0.47	0/395
8	i	0.31	0/293	0.49	0/395
9	J	0.25	0/255	0.44	0/346
9	j	0.27	0/255	0.45	0/346
10	K	0.28	0/303	0.53	0/416
10	k	0.29	0/303	0.53	0/416
11	L	0.27	0/311	0.47	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.66	0/367
12	m	0.41	0/270	0.66	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.35	0/284	0.47	0/381
14	t	0.36	0/284	0.48	0/381
15	U	0.28	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.31	0/1081	0.51	0/1468
16	v	0.26	0/1081	0.47	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	g	0.24	0/202	0.52	0/272
17	y	0.25	0/202	0.51	0/272
18	X	0.31	0/273	0.49	0/370
18	x	0.31	0/273	0.53	0/370
19	Z	0.29	0/490	0.50	0/669
19	z	0.27	0/490	0.47	0/669
All	All	0.29	0/41948	0.48	0/57100

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	333/360 (92%)	311 (93%)	18 (5%)	4 (1%)	13	49
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	13	49
2	B	488/510 (96%)	448 (92%)	35 (7%)	5 (1%)	15	54
2	b	488/510 (96%)	448 (92%)	36 (7%)	4 (1%)	19	60
3	C	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	12	48
3	c	445/461 (96%)	405 (91%)	33 (7%)	7 (2%)	9	43
4	D	338/352 (96%)	315 (93%)	20 (6%)	3 (1%)	17	56
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12 48
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12 48
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100 100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100 100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2 20
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2 20
8	I	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	4 28
8	i	33/38 (87%)	27 (82%)	5 (15%)	1 (3%)	4 28
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4 27
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4 27
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1 18
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1 18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
13	O	241/272 (89%)	207 (86%)	30 (12%)	4 (2%)	9 42
13	o	241/272 (89%)	209 (87%)	29 (12%)	3 (1%)	13 49
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4 26
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4 26
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4 26
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4 26
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100 100
16	v	135/163 (83%)	126 (93%)	9 (7%)	0	100 100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3 24
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3 24
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1 18
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1 18
19	Z	60/62 (97%)	54 (90%)	4 (7%)	2 (3%)	4 26
19	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9 42
All	All	5138/5650 (91%)	4681 (91%)	382 (7%)	75 (2%)	10 45

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA
14	T	30	THR
18	X	45	LYS
1	a	12	ASN
1	a	142	TRP
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
14	t	30	THR
18	x	45	LYS
1	A	141	PRO
1	A	142	TRP
2	B	489	GLU
3	C	32	GLY
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
7	H	26	GLY
17	y	43	ARG
19	Z	32	ASP
1	a	141	PRO
2	b	489	GLU
3	c	32	GLY
3	c	144	SER
3	c	257	PHE
3	c	416	SER
4	d	239	GLN
7	h	26	GLY
17	g	43	ARG
19	z	32	ASP
2	B	176	GLY
4	D	262	SER
5	E	82	GLN
9	J	38	SER
13	O	88	GLU
1	a	334	ARG

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Mol	Chain	Res	Type
2	b	176	GLY
3	c	194	GLY
5	e	82	GLN
9	j	38	SER
13	o	88	GLU
3	C	194	GLY
13	O	271	PRO
15	U	72	TYR
15	U	83	ALA
4	d	262	SER
7	h	16	SER
13	o	271	PRO
15	u	72	TYR
15	u	83	ALA
1	A	334	ARG
2	B	230	ARG
7	H	16	SER
10	K	13	GLU
13	O	158	ASN
18	X	12	ILE
10	k	13	GLU
10	k	45	PHE
18	x	12	ILE
4	D	234	ALA
10	K	45	PHE
19	Z	28	ALA
3	c	462	GLU
15	u	73	PRO
15	U	73	PRO
8	I	32	PRO
3	c	209	ILE
3	C	209	ILE
8	i	32	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/291 (93%)	266 (98%)	5 (2%)	59	77
1	a	271/291 (93%)	266 (98%)	5 (2%)	59	77
2	B	390/407 (96%)	379 (97%)	11 (3%)	43	64
2	b	390/407 (96%)	379 (97%)	11 (3%)	43	64
3	C	347/362 (96%)	332 (96%)	15 (4%)	29	53
3	c	347/362 (96%)	332 (96%)	15 (4%)	29	53
4	D	275/283 (97%)	262 (95%)	13 (5%)	26	51
4	d	275/283 (97%)	260 (94%)	15 (6%)	21	47
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	46
5	e	72/73 (99%)	68 (94%)	4 (6%)	21	46
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	13	38
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	38
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	62
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	54
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	54
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76	86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	83
15	u	84/112 (75%)	82 (98%)	2 (2%)	49	69
16	V	116/138 (84%)	114 (98%)	2 (2%)	60	78
16	v	116/138 (84%)	113 (97%)	3 (3%)	46	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	g	20/37 (54%)	18 (90%)	2 (10%)	7 26
17	y	20/37 (54%)	18 (90%)	2 (10%)	7 26
18	X	30/34 (88%)	27 (90%)	3 (10%)	7 26
18	x	30/34 (88%)	27 (90%)	3 (10%)	7 26
19	Z	52/52 (100%)	49 (94%)	3 (6%)	20 45
19	z	52/52 (100%)	50 (96%)	2 (4%)	33 57
All	All	4244/4616 (92%)	4103 (97%)	141 (3%)	38 61

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	VAL
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	354	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	488	PRO
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	232	ASP
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG

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Mol	Chain	Res	Type
3	C	469	MET
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	84	SER
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	323	GLU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU
16	V	63	CYS
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	45	LYS
19	Z	1	MET
19	Z	33	TRP
19	Z	62	VAL
1	a	202	VAL
1	a	228	THR

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Mol	Chain	Res	Type
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	354	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	488	PRO
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	232	ASP
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	305	THR
3	c	355	THR
3	c	382	ASN
3	c	391	ARG
3	c	469	MET
3	c	472	LEU
4	d	20	ASP
4	d	43	LEU
4	d	84	SER
4	d	91	LEU
4	d	130	PHE
4	d	180	ARG
4	d	205	LEU
4	d	241	GLU
4	d	259	ILE
4	d	279	LEU
4	d	291	LEU
4	d	294	ARG
4	d	323	GLU

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Mol	Chain	Res	Type
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	77	GLU
5	e	82	GLN
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	103	GLN
15	u	132	LEU
16	v	63	CYS
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	11	THR
18	x	12	ILE
18	x	45	LYS
19	z	33	TRP
19	z	62	VAL

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

Mol	Chain	Res	Type
1	A	241	GLN
1	A	261	GLN
2	B	201	HIS
2	B	409	GLN
4	D	117	HIS
4	D	332	GLN
1	a	241	GLN
2	b	201	HIS
4	d	142	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	$\#\|Z\| > 2$
31	LMG	k	103	-	48,48,55	1.15	6 (12%)	56,56,63	1.28	6 (10%)
24	PHO	D	402	-	51,69,69	1.03	5 (9%)	47,99,99	1.10	4 (8%)
23	CLA	C	506	-	65,73,73	1.53	5 (7%)	76,113,113	1.48	9 (11%)
33	LMT	B	627	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
34	HEM	f	101	6,5	41,50,50	1.93	5 (12%)	45,82,82	1.78	9 (20%)
23	CLA	B	610	-	65,73,73	1.51	5 (7%)	76,113,113	1.43	8 (10%)
23	CLA	b	613	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	8 (10%)
23	CLA	c	502	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	7 (9%)
23	CLA	c	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	6 (7%)
28	DGD	D	410	-	64,64,67	1.15	8 (12%)	78,78,81	1.39	8 (10%)
29	LHG	a	414	-	38,38,48	1.09	2 (5%)	41,44,54	0.96	2 (4%)
23	CLA	c	513	-	65,73,73	1.50	5 (7%)	76,113,113	1.44	9 (11%)
23	CLA	d	402	-	65,73,73	1.49	5 (7%)	76,113,113	1.43	8 (10%)
33	LMT	I	102	-	36,36,36	0.42	0	47,47,47	0.68	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DGD	c	518	-	63,63,67	1.23	9 (14%)	77,77,81	1.25	7 (9%)
23	CLA	a	404	-	65,73,73	1.54	6 (9%)	76,113,113	1.42	9 (11%)
30	SQD	a	401	-	53,54,54	0.98	5 (9%)	62,65,65	1.59	11 (17%)
23	CLA	c	512	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	7 (9%)
27	BCR	H	101	-	41,41,41	0.73	0	56,56,56	1.72	15 (26%)
24	PHO	a	407	-	51,69,69	1.02	4 (7%)	47,99,99	1.18	5 (10%)
27	BCR	b	621	-	41,41,41	0.75	0	56,56,56	2.18	18 (32%)
23	CLA	a	405	-	65,73,73	1.49	5 (7%)	76,113,113	1.46	9 (11%)
23	CLA	D	401	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
23	CLA	a	406	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	8 (10%)
23	CLA	B	608	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
30	SQD	D	409	-	42,43,54	1.11	4 (9%)	51,54,65	2.02	10 (19%)
23	CLA	C	513	-	65,73,73	1.51	5 (7%)	76,113,113	1.42	8 (10%)
25	PL9	D	404	-	55,55,55	1.22	8 (14%)	68,69,69	1.70	20 (29%)
27	BCR	Z	101	-	41,41,41	0.67	0	56,56,56	1.88	15 (26%)
23	CLA	A	407	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	6 (7%)
31	LMG	C	520	-	45,45,55	1.21	7 (15%)	53,53,63	1.44	8 (15%)
23	CLA	B	602	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	6 (7%)
31	LMG	d	406	-	48,48,55	1.16	8 (16%)	56,56,63	1.38	7 (12%)
27	BCR	j	102	-	41,41,41	0.73	0	56,56,56	3.35	24 (42%)
23	CLA	C	511	3	65,73,73	1.51	5 (7%)	76,113,113	1.47	8 (10%)
27	BCR	T	103	-	41,41,41	0.70	0	56,56,56	2.26	17 (30%)
33	LMT	D	411	-	32,32,36	0.48	0	43,43,47	0.71	1 (2%)
31	LMG	E	101	-	44,44,55	1.23	8 (18%)	52,52,63	1.36	8 (15%)
23	CLA	b	604	-	65,73,73	1.53	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	B	606	-	65,73,73	1.48	5 (7%)	76,113,113	1.35	6 (7%)
29	LHG	A	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.07	2 (5%)
27	BCR	K	102	-	41,41,41	0.73	0	56,56,56	1.85	12 (21%)
31	LMG	d	405	-	46,46,55	1.20	7 (15%)	54,54,63	1.38	6 (11%)
23	CLA	B	615	-	65,73,73	1.49	6 (9%)	76,113,113	1.41	8 (10%)
30	SQD	b	601	-	46,47,54	1.04	5 (10%)	55,58,65	1.61	9 (16%)
31	LMG	B	622	-	49,49,55	1.19	8 (16%)	57,57,63	1.38	9 (15%)
29	LHG	a	417	-	36,36,48	1.08	2 (5%)	39,42,54	1.07	2 (5%)
33	LMT	B	624	-	36,36,36	0.44	0	47,47,47	0.70	1 (2%)
33	LMT	m	101	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	601	-	65,73,73	1.56	6 (9%)	76,113,113	1.36	8 (10%)
28	DGD	C	516	-	54,54,67	1.26	6 (11%)	68,68,81	1.29	9 (13%)
23	CLA	c	509	-	65,73,73	1.52	5 (7%)	76,113,113	1.41	8 (10%)
27	BCR	f	102	-	41,41,41	0.69	0	56,56,56	2.17	19 (33%)
23	CLA	B	604	-	65,73,73	1.49	7 (10%)	76,113,113	1.35	8 (10%)
31	LMG	b	624	-	49,49,55	1.17	7 (14%)	57,57,63	1.39	9 (15%)
23	CLA	c	511	-	65,73,73	1.55	5 (7%)	76,113,113	1.42	7 (9%)
23	CLA	A	403	-	65,73,73	1.53	6 (9%)	76,113,113	1.41	7 (9%)
27	BCR	C	514	-	41,41,41	0.75	0	56,56,56	2.40	20 (35%)
28	DGD	C	518	-	67,67,67	1.16	7 (10%)	81,81,81	1.47	9 (11%)
28	DGD	d	408	-	64,64,67	1.13	7 (10%)	78,78,81	1.41	9 (11%)
31	LMG	D	406	-	46,46,55	1.17	6 (13%)	54,54,63	1.37	6 (11%)
23	CLA	c	506	-	65,73,73	1.53	6 (9%)	76,113,113	1.45	8 (10%)
31	LMG	D	407	-	49,49,55	1.19	7 (14%)	57,57,63	1.26	8 (14%)
33	LMT	M	103	-	36,36,36	0.41	0	47,47,47	0.68	1 (2%)
27	BCR	c	516	-	41,41,41	0.70	0	56,56,56	1.94	15 (26%)
23	CLA	b	616	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
28	DGD	b	622	-	59,59,67	1.25	9 (15%)	73,73,81	1.18	7 (9%)
33	LMT	T	101	-	36,36,36	0.41	0	47,47,47	0.85	1 (2%)
28	DGD	c	519	-	67,67,67	1.16	7 (10%)	81,81,81	1.46	10 (12%)
30	SQD	F	102	-	44,45,54	1.05	5 (11%)	53,56,65	1.69	10 (18%)
23	CLA	b	607	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	9 (11%)
31	LMG	e	101	-	44,44,55	1.23	8 (18%)	52,52,63	1.30	8 (15%)
23	CLA	D	403	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	10 (13%)
28	DGD	c	517	-	54,54,67	1.27	7 (12%)	68,68,81	1.27	8 (11%)
23	CLA	b	614	-	65,73,73	1.55	6 (9%)	76,113,113	1.36	8 (10%)
33	LMT	b	603	-	36,36,36	0.40	0	47,47,47	0.61	0
23	CLA	d	403	-	65,73,73	1.52	5 (7%)	76,113,113	1.35	6 (7%)
27	BCR	B	618	-	41,41,41	0.71	0	56,56,56	2.27	15 (26%)
27	BCR	A	410	-	41,41,41	0.76	0	56,56,56	1.98	15 (26%)
23	CLA	b	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	8 (10%)
23	CLA	B	605	-	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
23	CLA	c	508	-	65,73,73	1.49	5 (7%)	76,113,113	1.38	7 (9%)
23	CLA	a	409	-	65,73,73	1.51	5 (7%)	76,113,113	1.40	8 (10%)
33	LMT	B	623	-	36,36,36	0.41	0	47,47,47	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	503	-	65,73,73	1.53	6 (9%)	76,113,113	1.35	8 (10%)
23	CLA	B	612	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
23	CLA	C	509	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	9 (11%)
23	CLA	B	616	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	6 (7%)
30	SQD	d	407	-	42,43,54	1.14	4 (9%)	51,54,65	2.03	10 (19%)
27	BCR	T	102	-	41,41,41	0.75	0	56,56,56	1.93	13 (23%)
31	LMG	a	402	-	42,42,55	1.24	6 (14%)	50,50,63	1.49	8 (16%)
23	CLA	b	605	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	6 (7%)
23	CLA	C	510	-	65,73,73	1.53	6 (9%)	76,113,113	1.36	7 (9%)
25	PL9	A	408	-	45,45,55	1.28	7 (15%)	56,57,69	1.58	14 (25%)
30	SQD	B	625	-	46,47,54	1.04	5 (10%)	55,58,65	1.58	10 (18%)
31	LMG	a	416	-	51,51,55	1.15	6 (11%)	59,59,63	1.43	5 (8%)
23	CLA	A	404	-	65,73,73	1.51	6 (9%)	76,113,113	1.40	9 (11%)
23	CLA	c	503	-	65,73,73	1.52	5 (7%)	76,113,113	1.35	8 (10%)
27	BCR	B	617	-	41,41,41	0.74	0	56,56,56	1.94	14 (25%)
23	CLA	B	607	-	65,73,73	1.50	6 (9%)	76,113,113	1.47	9 (11%)
27	BCR	B	619	-	41,41,41	0.67	0	56,56,56	1.89	15 (26%)
31	LMG	M	102	-	42,42,55	1.29	7 (16%)	50,50,63	1.48	7 (14%)
23	CLA	C	501	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
27	BCR	D	405	-	41,41,41	0.69	0	56,56,56	2.23	20 (35%)
31	LMG	I	101	-	43,43,55	1.28	8 (18%)	51,51,63	1.35	7 (13%)
27	BCR	c	515	-	41,41,41	0.66	0	56,56,56	1.80	15 (26%)
33	LMT	x	102	-	32,32,36	0.49	1 (3%)	43,43,47	0.66	1 (2%)
27	BCR	k	102	-	41,41,41	0.72	0	56,56,56	1.90	16 (28%)
23	CLA	b	608	-	65,73,73	1.52	7 (10%)	76,113,113	1.39	6 (7%)
23	CLA	C	505	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
34	HEM	F	101	6,5	41,50,50	1.94	5 (12%)	45,82,82	1.76	9 (20%)
23	CLA	b	617	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	6 (7%)
31	LMG	M	101	-	42,42,55	1.32	7 (16%)	50,50,63	1.51	8 (16%)
23	CLA	C	508	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
23	CLA	b	619	-	65,73,73	1.50	5 (7%)	76,113,113	1.31	6 (7%)
25	PL9	d	404	-	55,55,55	1.25	9 (16%)	68,69,69	1.68	16 (23%)
27	BCR	C	515	-	41,41,41	0.70	0	56,56,56	1.98	16 (28%)
33	LMT	i	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.64	0
28	DGD	C	517	-	63,63,67	1.22	10 (15%)	77,77,81	1.23	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	505	-	65,73,73	1.54	6 (9%)	76,113,113	1.50	9 (11%)
23	CLA	B	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.41	8 (10%)
23	CLA	b	618	-	65,73,73	1.48	5 (7%)	76,113,113	1.44	9 (11%)
27	BCR	J	102	-	41,41,41	0.71	0	56,56,56	3.35	25 (44%)
30	SQD	A	417	-	53,54,54	1.02	5 (9%)	62,65,65	1.58	11 (17%)
23	CLA	C	512	-	65,73,73	1.51	6 (9%)	76,113,113	1.42	8 (10%)
23	CLA	c	504	-	65,73,73	1.54	6 (9%)	76,113,113	1.50	9 (11%)
23	CLA	c	507	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
28	DGD	B	621	-	59,59,67	1.28	9 (15%)	73,73,81	1.15	6 (8%)
34	HEM	v	201	16	41,50,50	2.06	8 (19%)	45,82,82	1.73	5 (11%)
27	BCR	c	514	-	41,41,41	0.72	0	56,56,56	2.44	18 (32%)
33	LMT	b	625	-	36,36,36	0.40	0	47,47,47	0.75	1 (2%)
23	CLA	B	613	-	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
25	PL9	a	410	-	45,45,55	1.23	7 (15%)	56,57,69	1.66	12 (21%)
30	SQD	f	103	-	44,45,54	1.04	5 (11%)	53,56,65	1.66	11 (20%)
24	PHO	A	406	-	51,69,69	1.02	4 (7%)	47,99,99	1.19	4 (8%)
33	LMT	B	628	-	36,36,36	0.46	0	47,47,47	0.63	0
28	DGD	b	602	-	53,53,67	1.26	7 (13%)	67,67,81	1.39	9 (13%)
31	LMG	D	408	-	48,48,55	1.21	8 (16%)	56,56,63	1.38	7 (12%)
23	CLA	B	611	-	65,73,73	1.49	6 (9%)	76,113,113	1.46	7 (9%)
30	SQD	a	415	-	50,51,54	1.01	5 (10%)	59,62,65	1.56	10 (16%)
31	LMG	A	414	-	51,51,55	1.17	6 (11%)	59,59,63	1.36	5 (8%)
34	HEM	V	201	16	41,50,50	2.00	7 (17%)	45,82,82	1.42	4 (8%)
23	CLA	b	610	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	9 (11%)
31	LMG	i	101	-	43,43,55	1.28	7 (16%)	51,51,63	1.32	8 (15%)
23	CLA	B	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	9 (11%)
25	PL9	J	101	-	35,35,55	1.19	5 (14%)	44,45,69	1.59	8 (18%)
23	CLA	b	611	-	65,73,73	1.52	6 (9%)	76,113,113	1.48	9 (11%)
27	BCR	B	620	-	41,41,41	0.73	0	56,56,56	2.13	16 (28%)
22	BCT	d	401	21	2,3,3	0.45	0	2,3,3	0.15	0
23	CLA	C	507	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
30	SQD	A	413	-	50,51,54	0.98	6 (12%)	59,62,65	1.55	9 (15%)
25	PL9	j	101	-	35,35,55	1.18	5 (14%)	44,45,69	1.60	9 (20%)
29	LHG	A	412	-	38,38,48	1.06	2 (5%)	41,44,54	0.98	2 (4%)
23	CLA	A	405	-	65,73,73	1.49	5 (7%)	76,113,113	1.29	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCT	A	402	21	2,3,3	0.45	0	2,3,3	0.09	0
28	DGD	a	413	-	57,57,67	1.23	8 (14%)	71,71,81	1.60	13 (18%)
23	CLA	b	615	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	6 (7%)
27	BCR	x	101	-	41,41,41	0.71	0	56,56,56	1.72	16 (28%)
27	BCR	b	620	-	41,41,41	0.67	0	56,56,56	1.94	15 (26%)
31	LMG	C	519	-	48,48,55	1.15	6 (12%)	56,56,63	1.36	7 (12%)
23	CLA	B	614	-	65,73,73	1.51	5 (7%)	76,113,113	1.31	6 (7%)
23	CLA	b	612	-	65,73,73	1.53	5 (7%)	76,113,113	1.31	7 (9%)
24	PHO	a	408	-	51,69,69	0.98	3 (5%)	47,99,99	1.11	3 (6%)
23	CLA	C	504	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
28	DGD	A	411	-	57,57,67	1.24	8 (14%)	71,71,81	1.64	13 (18%)
31	LMG	A	418	-	42,42,55	1.24	6 (14%)	50,50,63	1.54	11 (22%)
33	LMT	b	626	-	36,36,36	0.44	0	47,47,47	0.67	1 (2%)
23	CLA	b	606	-	65,73,73	1.47	5 (7%)	76,113,113	1.35	8 (10%)
27	BCR	a	412	-	41,41,41	0.72	0	56,56,56	1.90	15 (26%)
31	LMG	b	623	-	49,49,55	1.22	7 (14%)	57,57,63	1.35	7 (12%)
31	LMG	c	520	-	45,45,55	1.22	7 (15%)	53,53,63	1.41	8 (15%)
23	CLA	C	502	-	65,73,73	1.50	7 (10%)	76,113,113	1.42	7 (9%)
28	DGD	B	626	-	53,53,67	1.25	8 (15%)	67,67,81	1.40	9 (13%)
23	CLA	c	501	-	65,73,73	1.48	5 (7%)	76,113,113	1.42	9 (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
31	LMG	k	103	-	-	17/43/63/70	0/1/1/1
24	PHO	D	402	-	-	10/37/103/103	0/5/6/6
23	CLA	C	506	-	1/1/15/20	18/37/115/115	-
33	LMT	B	627	-	-	3/21/61/61	0/2/2/2
34	HEM	f	101	6,5	-	2/12/54/54	-
23	CLA	B	610	-	1/1/15/20	18/37/115/115	-
23	CLA	b	613	-	1/1/15/20	17/37/115/115	-
23	CLA	c	502	-	1/1/15/20	12/37/115/115	-
23	CLA	c	510	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	D	410	-	-	31/52/92/95	0/2/2/2
29	LHG	a	414	-	-	18/43/43/53	-
23	CLA	c	513	-	1/1/15/20	21/37/115/115	-
23	CLA	d	402	-	1/1/15/20	11/37/115/115	-
33	LMT	I	102	-	-	3/21/61/61	0/2/2/2
28	DGD	c	518	-	-	22/51/91/95	0/2/2/2
23	CLA	a	404	-	1/1/15/20	8/37/115/115	-
30	SQD	a	401	-	-	17/49/69/69	0/1/1/1
23	CLA	c	512	-	1/1/15/20	18/37/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	PHO	a	407	-	-	12/37/103/103	0/5/6/6
27	BCR	b	621	-	-	3/29/63/63	0/2/2/2
23	CLA	a	405	-	1/1/15/20	16/37/115/115	-
23	CLA	D	401	-	1/1/15/20	13/37/115/115	-
23	CLA	a	406	-	1/1/15/20	10/37/115/115	-
23	CLA	B	608	-	1/1/15/20	13/37/115/115	-
30	SQD	D	409	-	-	11/38/58/69	0/1/1/1
23	CLA	C	513	-	1/1/15/20	17/37/115/115	-
25	PL9	D	404	-	-	13/53/73/73	0/1/1/1
27	BCR	Z	101	-	-	2/29/63/63	0/2/2/2
23	CLA	A	407	-	1/1/15/20	8/37/115/115	-
31	LMG	C	520	-	-	19/40/60/70	0/1/1/1
23	CLA	B	602	-	1/1/15/20	17/37/115/115	-
31	LMG	d	406	-	-	20/43/63/70	0/1/1/1
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2
23	CLA	C	511	3	1/1/15/20	15/37/115/115	-
27	BCR	T	103	-	-	9/29/63/63	0/2/2/2
33	LMT	D	411	-	-	0/17/57/61	0/2/2/2
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
23	CLA	b	604	-	1/1/15/20	15/37/115/115	-
23	CLA	B	606	-	1/1/15/20	11/37/115/115	-
29	LHG	A	415	-	-	12/41/41/53	-
27	BCR	K	102	-	-	8/29/63/63	0/2/2/2
31	LMG	d	405	-	-	10/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	615	-	1/1/15/20	10/37/115/115	-
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1
31	LMG	B	622	-	-	15/44/64/70	0/1/1/1
29	LHG	a	417	-	-	13/41/41/53	-
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
23	CLA	B	601	-	1/1/15/20	16/37/115/115	-
28	DGD	C	516	-	-	19/42/82/95	0/2/2/2
23	CLA	c	509	-	1/1/15/20	16/37/115/115	-
27	BCR	f	102	-	-	6/29/63/63	0/2/2/2
23	CLA	B	604	-	1/1/15/20	8/37/115/115	-
31	LMG	b	624	-	-	15/44/64/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	15/37/115/115	-
23	CLA	A	403	-	1/1/15/20	8/37/115/115	-
27	BCR	C	514	-	-	7/29/63/63	0/2/2/2
28	DGD	C	518	-	-	23/55/95/95	0/2/2/2
28	DGD	d	408	-	-	29/52/92/95	0/2/2/2
31	LMG	D	406	-	-	11/41/61/70	0/1/1/1
23	CLA	c	506	-	1/1/15/20	16/37/115/115	-
31	LMG	D	407	-	-	23/44/64/70	0/1/1/1
33	LMT	M	103	-	-	0/21/61/61	0/2/2/2
27	BCR	c	516	-	-	8/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	16/37/115/115	-
28	DGD	b	622	-	-	19/47/87/95	0/2/2/2
33	LMT	T	101	-	-	3/21/61/61	0/2/2/2
28	DGD	c	519	-	-	21/55/95/95	0/2/2/2
30	SQD	F	102	-	-	16/40/60/69	0/1/1/1
23	CLA	b	607	-	1/1/15/20	7/37/115/115	-
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	D	403	-	1/1/15/20	7/37/115/115	-
28	DGD	c	517	-	-	20/42/82/95	0/2/2/2
23	CLA	b	614	-	1/1/15/20	9/37/115/115	-
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
23	CLA	b	609	-	1/1/15/20	12/37/115/115	-
23	CLA	B	605	-	1/1/15/20	15/37/115/115	-
23	CLA	c	508	-	1/1/15/20	14/37/115/115	-
23	CLA	a	409	-	1/1/15/20	7/37/115/115	-
33	LMT	B	623	-	-	2/21/61/61	0/2/2/2
23	CLA	C	503	-	1/1/15/20	15/37/115/115	-
23	CLA	B	612	-	1/1/15/20	11/37/115/115	-
23	CLA	C	509	-	1/1/15/20	16/37/115/115	-
23	CLA	B	616	-	1/1/15/20	19/37/115/115	-
30	SQD	d	407	-	-	12/38/58/69	0/1/1/1
27	BCR	T	102	-	-	2/29/63/63	0/2/2/2
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1
23	CLA	b	605	-	1/1/15/20	20/37/115/115	-
23	CLA	C	510	-	1/1/15/20	16/37/115/115	-
25	PL9	A	408	-	-	22/41/61/73	0/1/1/1
30	SQD	B	625	-	-	14/42/62/69	0/1/1/1
31	LMG	a	416	-	-	21/46/66/70	0/1/1/1
23	CLA	A	404	-	1/1/15/20	15/37/115/115	-
23	CLA	c	503	-	1/1/15/20	14/37/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	607	-	1/1/15/20	9/37/115/115	-
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	LMG	M	102	-	-	17/37/57/70	0/1/1/1
23	CLA	C	501	-	1/1/15/20	13/37/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
31	LMG	I	101	-	-	20/38/58/70	0/1/1/1
27	BCR	c	515	-	-	4/29/63/63	0/2/2/2
33	LMT	x	102	-	-	0/17/57/61	0/2/2/2
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
23	CLA	b	608	-	1/1/15/20	15/37/115/115	-
23	CLA	C	505	-	1/1/15/20	18/37/115/115	-
34	HEM	F	101	6,5	-	2/12/54/54	-
23	CLA	b	617	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
23	CLA	C	508	-	1/1/15/20	14/37/115/115	-
23	CLA	b	619	-	1/1/15/20	19/37/115/115	-
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1
27	BCR	C	515	-	-	7/29/63/63	0/2/2/2
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2
28	DGD	C	517	-	-	21/51/91/95	0/2/2/2
23	CLA	c	505	-	1/1/15/20	18/37/115/115	-
23	CLA	B	609	-	1/1/15/20	11/37/115/115	-
23	CLA	b	618	-	1/1/15/20	8/37/115/115	-
27	BCR	J	102	-	-	3/29/63/63	0/2/2/2
30	SQD	A	417	-	-	17/49/69/69	0/1/1/1
23	CLA	C	512	-	1/1/15/20	18/37/115/115	-
23	CLA	c	504	-	1/1/15/20	12/37/115/115	-
23	CLA	c	507	-	1/1/15/20	14/37/115/115	-
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
34	HEM	v	201	16	-	3/12/54/54	-
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
33	LMT	b	625	-	-	2/21/61/61	0/2/2/2
23	CLA	B	613	-	1/1/15/20	15/37/115/115	-
25	PL9	a	410	-	-	22/41/61/73	0/1/1/1
30	SQD	f	103	-	-	15/40/60/69	0/1/1/1
24	PHO	A	406	-	-	12/37/103/103	0/5/6/6
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
28	DGD	b	602	-	-	18/41/81/95	0/2/2/2
31	LMG	D	408	-	-	21/43/63/70	0/1/1/1
23	CLA	B	611	-	1/1/15/20	10/37/115/115	-
30	SQD	a	415	-	-	19/46/66/69	0/1/1/1
31	LMG	A	414	-	-	21/46/66/70	0/1/1/1
34	HEM	V	201	16	-	3/12/54/54	-
23	CLA	b	610	-	1/1/15/20	9/37/115/115	-
31	LMG	i	101	-	-	18/38/58/70	0/1/1/1
23	CLA	B	603	-	1/1/15/20	15/37/115/115	-
25	PL9	J	101	-	-	12/29/49/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	611	-	1/1/15/20	16/37/115/115	-
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
23	CLA	C	507	-	1/1/15/20	12/37/115/115	-
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
29	LHG	A	412	-	-	18/43/43/53	-
23	CLA	A	405	-	1/1/15/20	11/37/115/115	-
28	DGD	a	413	-	-	11/45/85/95	0/2/2/2
23	CLA	b	615	-	1/1/15/20	12/37/115/115	-
27	BCR	x	101	-	-	3/29/63/63	0/2/2/2
27	BCR	b	620	-	-	0/29/63/63	0/2/2/2
31	LMG	C	519	-	-	16/43/63/70	0/1/1/1
23	CLA	B	614	-	1/1/15/20	17/37/115/115	-
23	CLA	b	612	-	-	11/37/115/115	-
24	PHO	a	408	-	-	12/37/103/103	0/5/6/6
23	CLA	C	504	-	1/1/15/20	10/37/115/115	-
28	DGD	A	411	-	-	11/45/85/95	0/2/2/2
31	LMG	A	418	-	-	15/37/57/70	0/1/1/1
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
23	CLA	b	606	-	1/1/15/20	15/37/115/115	-
27	BCR	a	412	-	-	3/29/63/63	0/2/2/2
31	LMG	b	623	-	-	23/44/64/70	0/1/1/1
31	LMG	c	520	-	-	21/40/60/70	0/1/1/1
23	CLA	C	502	-	1/1/15/20	9/37/115/115	-
28	DGD	B	626	-	-	17/41/81/95	0/2/2/2
23	CLA	c	501	-	1/1/15/20	13/37/115/115	-

All (792) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3D-C2D	8.45	1.54	1.36
23	c	504	CLA	C4B-NB	8.24	1.42	1.35
34	F	101	HEM	C3D-C2D	8.14	1.54	1.36
34	V	201	HEM	C3D-C2D	8.06	1.53	1.36
23	a	404	CLA	C4B-NB	7.99	1.42	1.35
23	c	505	CLA	C4B-NB	7.91	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	403	CLA	C4B-NB	7.90	1.42	1.35
23	c	511	CLA	C4B-NB	7.89	1.42	1.35
34	f	101	HEM	C3D-C2D	7.87	1.53	1.36
23	C	503	CLA	C4B-NB	7.84	1.42	1.35
23	B	601	CLA	C4B-NB	7.80	1.42	1.35
23	B	614	CLA	C4B-NB	7.80	1.42	1.35
23	b	614	CLA	C4B-NB	7.78	1.42	1.35
23	b	612	CLA	C4B-NB	7.72	1.42	1.35
23	C	512	CLA	C4B-NB	7.69	1.42	1.35
23	c	506	CLA	C4B-NB	7.67	1.42	1.35
23	B	602	CLA	C4B-NB	7.67	1.42	1.35
23	B	607	CLA	C4B-NB	7.65	1.42	1.35
23	d	403	CLA	C4B-NB	7.64	1.42	1.35
23	A	407	CLA	C4B-NB	7.63	1.42	1.35
23	D	401	CLA	C4B-NB	7.62	1.42	1.35
23	C	505	CLA	C4B-NB	7.62	1.42	1.35
23	b	610	CLA	C4B-NB	7.61	1.42	1.35
23	B	603	CLA	C4B-NB	7.60	1.42	1.35
23	c	503	CLA	C4B-NB	7.59	1.42	1.35
23	C	506	CLA	C4B-NB	7.59	1.42	1.35
23	b	611	CLA	C4B-NB	7.59	1.42	1.35
23	C	508	CLA	C4B-NB	7.58	1.42	1.35
23	c	509	CLA	C4B-NB	7.57	1.42	1.35
23	b	619	CLA	C4B-NB	7.56	1.42	1.35
23	d	402	CLA	C4B-NB	7.54	1.41	1.35
23	C	501	CLA	C4B-NB	7.53	1.41	1.35
23	C	511	CLA	C4B-NB	7.53	1.41	1.35
23	C	510	CLA	C4B-NB	7.52	1.41	1.35
23	b	608	CLA	C4B-NB	7.50	1.41	1.35
23	a	409	CLA	C4B-NB	7.50	1.41	1.35
23	B	610	CLA	C4B-NB	7.49	1.41	1.35
23	C	502	CLA	C4B-NB	7.48	1.41	1.35
23	b	604	CLA	C4B-NB	7.48	1.41	1.35
23	B	611	CLA	C4B-NB	7.46	1.41	1.35
23	B	615	CLA	C4B-NB	7.46	1.41	1.35
23	c	513	CLA	C4B-NB	7.44	1.41	1.35
23	b	607	CLA	C4B-NB	7.44	1.41	1.35
23	C	509	CLA	C4B-NB	7.44	1.41	1.35
23	b	616	CLA	C4B-NB	7.42	1.41	1.35
23	c	512	CLA	C4B-NB	7.42	1.41	1.35
23	B	609	CLA	C4B-NB	7.41	1.41	1.35
23	a	406	CLA	C4B-NB	7.41	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	C4B-NB	7.39	1.41	1.35
23	b	605	CLA	C4B-NB	7.39	1.41	1.35
23	C	513	CLA	C4B-NB	7.39	1.41	1.35
23	b	609	CLA	C4B-NB	7.38	1.41	1.35
23	c	501	CLA	C4B-NB	7.37	1.41	1.35
23	b	613	CLA	C4B-NB	7.36	1.41	1.35
23	c	508	CLA	C4B-NB	7.36	1.41	1.35
23	b	617	CLA	C4B-NB	7.36	1.41	1.35
23	B	605	CLA	C4B-NB	7.36	1.41	1.35
23	A	405	CLA	C4B-NB	7.34	1.41	1.35
23	c	510	CLA	C4B-NB	7.32	1.41	1.35
23	b	615	CLA	C4B-NB	7.32	1.41	1.35
23	B	616	CLA	C4B-NB	7.30	1.41	1.35
23	b	618	CLA	C4B-NB	7.30	1.41	1.35
23	B	612	CLA	C4B-NB	7.28	1.41	1.35
23	b	606	CLA	C4B-NB	7.28	1.41	1.35
23	B	608	CLA	C4B-NB	7.27	1.41	1.35
23	B	613	CLA	C4B-NB	7.26	1.41	1.35
23	D	403	CLA	C4B-NB	7.26	1.41	1.35
23	A	404	CLA	C4B-NB	7.23	1.41	1.35
23	c	507	CLA	C4B-NB	7.21	1.41	1.35
23	c	502	CLA	C4B-NB	7.20	1.41	1.35
23	B	604	CLA	C4B-NB	7.19	1.41	1.35
23	C	504	CLA	C4B-NB	7.18	1.41	1.35
23	B	606	CLA	C4B-NB	7.13	1.41	1.35
23	C	507	CLA	C4B-NB	7.09	1.41	1.35
34	V	201	HEM	C3C-C2C	-4.90	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.76	1.33	1.40
29	a	414	LHG	O7-C7	4.38	1.46	1.34
29	a	414	LHG	O8-C23	4.37	1.46	1.33
29	A	412	LHG	O7-C7	4.32	1.46	1.34
23	B	601	CLA	C1D-ND	4.31	1.43	1.37
23	c	506	CLA	C1D-ND	4.25	1.43	1.37
29	A	415	LHG	O8-C23	4.24	1.45	1.33
23	b	611	CLA	C1D-ND	4.23	1.43	1.37
23	b	604	CLA	C1D-ND	4.19	1.42	1.37
29	A	415	LHG	O7-C7	4.19	1.46	1.34
29	a	417	LHG	O8-C23	4.17	1.45	1.33
29	A	412	LHG	O8-C23	4.16	1.45	1.33
23	c	509	CLA	C1D-ND	4.15	1.42	1.37
23	b	609	CLA	C1D-ND	4.14	1.42	1.37
23	C	506	CLA	C1D-ND	4.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1D-ND	4.13	1.42	1.37
29	a	417	LHG	O7-C7	4.12	1.45	1.34
23	c	503	CLA	C1D-ND	4.12	1.42	1.37
23	b	605	CLA	C1D-ND	4.11	1.42	1.37
23	b	618	CLA	C1D-ND	4.11	1.42	1.37
23	b	613	CLA	C1D-ND	4.11	1.42	1.37
23	A	404	CLA	C1D-ND	4.09	1.42	1.37
23	C	511	CLA	C1D-ND	4.05	1.42	1.37
23	b	608	CLA	C1D-ND	4.04	1.42	1.37
23	c	502	CLA	C1D-ND	4.04	1.42	1.37
23	B	608	CLA	C1D-ND	4.04	1.42	1.37
23	c	513	CLA	C1D-ND	4.04	1.42	1.37
23	d	403	CLA	C1D-ND	4.03	1.42	1.37
23	C	510	CLA	C1D-ND	4.02	1.42	1.37
23	B	609	CLA	C1D-ND	4.01	1.42	1.37
23	C	507	CLA	C1D-ND	4.01	1.42	1.37
23	C	501	CLA	C1D-ND	4.01	1.42	1.37
23	B	610	CLA	C1D-ND	4.00	1.42	1.37
23	a	404	CLA	C1D-ND	3.97	1.42	1.37
23	C	513	CLA	C1D-ND	3.97	1.42	1.37
23	c	504	CLA	C1D-ND	3.95	1.42	1.37
23	b	612	CLA	C1D-ND	3.95	1.42	1.37
23	C	503	CLA	C1D-ND	3.95	1.42	1.37
23	a	409	CLA	C1D-ND	3.94	1.42	1.37
23	C	512	CLA	C1D-ND	3.94	1.42	1.37
23	B	606	CLA	C1D-ND	3.93	1.42	1.37
23	A	407	CLA	C1D-ND	3.93	1.42	1.37
23	B	616	CLA	C1D-ND	3.92	1.42	1.37
34	f	101	HEM	C3C-CAC	3.91	1.55	1.47
23	B	602	CLA	C1D-ND	3.88	1.42	1.37
23	A	403	CLA	C1D-ND	3.88	1.42	1.37
23	c	512	CLA	C1D-ND	3.88	1.42	1.37
23	c	505	CLA	C1D-ND	3.88	1.42	1.37
23	b	616	CLA	C1D-ND	3.87	1.42	1.37
23	A	405	CLA	C1D-ND	3.85	1.42	1.37
23	c	510	CLA	C1D-ND	3.85	1.42	1.37
23	b	610	CLA	C1D-ND	3.85	1.42	1.37
23	c	501	CLA	C1D-ND	3.84	1.42	1.37
23	B	604	CLA	C1D-ND	3.84	1.42	1.37
23	C	502	CLA	C1D-ND	3.84	1.42	1.37
23	C	504	CLA	C1D-ND	3.84	1.42	1.37
23	c	508	CLA	C1D-ND	3.83	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C1D-ND	3.82	1.42	1.37
23	d	402	CLA	C1D-ND	3.82	1.42	1.37
23	C	508	CLA	C1D-ND	3.82	1.42	1.37
23	D	403	CLA	C1D-ND	3.81	1.42	1.37
23	B	607	CLA	C1D-ND	3.81	1.42	1.37
23	c	507	CLA	C1D-ND	3.81	1.42	1.37
23	a	405	CLA	C1D-ND	3.80	1.42	1.37
34	F	101	HEM	C3C-C2C	-3.77	1.35	1.40
34	v	201	HEM	C3C-CAC	3.76	1.55	1.47
23	b	607	CLA	C1D-ND	3.75	1.42	1.37
23	B	611	CLA	C1D-ND	3.75	1.42	1.37
23	B	613	CLA	C1D-ND	3.74	1.42	1.37
23	D	401	CLA	C1D-ND	3.74	1.42	1.37
23	b	619	CLA	C1D-ND	3.72	1.42	1.37
23	C	505	CLA	C1D-ND	3.71	1.42	1.37
34	V	201	HEM	C3C-CAC	3.71	1.55	1.47
34	f	101	HEM	C3C-C2C	-3.71	1.35	1.40
23	B	615	CLA	C1D-ND	3.70	1.42	1.37
23	b	614	CLA	C1D-ND	3.64	1.42	1.37
23	b	606	CLA	C1D-ND	3.63	1.42	1.37
34	F	101	HEM	C3C-CAC	3.62	1.55	1.47
23	b	615	CLA	C1D-ND	3.61	1.42	1.37
23	C	509	CLA	C1D-ND	3.61	1.42	1.37
23	B	612	CLA	C1D-ND	3.60	1.42	1.37
23	a	406	CLA	C1D-ND	3.59	1.42	1.37
23	B	614	CLA	C1D-ND	3.47	1.42	1.37
23	a	409	CLA	CHC-C1C	3.46	1.43	1.35
31	D	406	LMG	O7-C8	-3.45	1.38	1.46
23	b	617	CLA	C1D-ND	3.41	1.42	1.37
25	A	408	PL9	C33-C34	3.38	1.41	1.33
23	B	605	CLA	C1D-ND	3.38	1.41	1.37
23	b	605	CLA	CHC-C1C	3.38	1.43	1.35
28	C	516	DGD	O2G-C2G	-3.38	1.38	1.46
23	A	404	CLA	CHC-C1C	3.38	1.43	1.35
23	B	602	CLA	CHC-C1C	3.37	1.43	1.35
31	D	407	LMG	O7-C8	-3.37	1.38	1.46
23	b	611	CLA	CHC-C1C	3.36	1.43	1.35
23	b	617	CLA	C4D-ND	-3.33	1.33	1.37
28	B	621	DGD	O2G-C2G	-3.31	1.38	1.46
30	d	407	SQD	O48-C23	3.30	1.43	1.33
23	b	608	CLA	CHC-C1C	3.29	1.43	1.35
25	D	404	PL9	C38-C39	3.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C4D-ND	-3.28	1.33	1.37
25	d	404	PL9	C38-C39	3.28	1.40	1.33
23	C	506	CLA	CHC-C1C	3.28	1.43	1.35
23	c	508	CLA	CHC-C1C	3.27	1.43	1.35
23	b	618	CLA	CHC-C1C	3.26	1.43	1.35
23	b	613	CLA	CHC-C1C	3.26	1.43	1.35
25	a	410	PL9	C33-C34	3.25	1.40	1.33
28	b	622	DGD	O2G-C2G	-3.24	1.38	1.46
25	D	404	PL9	C33-C34	3.24	1.40	1.33
23	b	617	CLA	CHC-C1C	3.24	1.43	1.35
31	d	405	LMG	O7-C8	-3.23	1.38	1.46
23	c	506	CLA	CHC-C1C	3.23	1.43	1.35
23	C	504	CLA	CHC-C1C	3.23	1.43	1.35
23	B	610	CLA	CHC-C1C	3.22	1.43	1.35
23	d	403	CLA	CHC-C1C	3.21	1.43	1.35
28	b	602	DGD	O1G-C1A	3.21	1.42	1.33
23	C	503	CLA	CHC-C1C	3.21	1.43	1.35
23	B	615	CLA	CHC-C1C	3.21	1.43	1.35
25	d	404	PL9	C43-C44	3.20	1.40	1.33
31	a	416	LMG	O7-C10	3.20	1.43	1.34
30	B	625	SQD	O48-C23	3.20	1.42	1.33
23	a	409	CLA	C4D-ND	-3.20	1.33	1.37
23	c	502	CLA	CHC-C1C	3.20	1.43	1.35
23	a	405	CLA	C4D-ND	-3.20	1.33	1.37
30	b	601	SQD	O48-C23	3.19	1.42	1.33
23	B	606	CLA	CHC-C1C	3.19	1.43	1.35
25	d	404	PL9	C33-C34	3.19	1.40	1.33
23	C	502	CLA	CHC-C1C	3.19	1.43	1.35
23	b	614	CLA	CHC-C1C	3.19	1.43	1.35
23	c	504	CLA	CHC-C1C	3.18	1.43	1.35
23	b	606	CLA	CHC-C1C	3.18	1.43	1.35
30	A	413	SQD	O48-C23	3.18	1.42	1.33
23	B	607	CLA	CHC-C1C	3.18	1.43	1.35
23	b	612	CLA	CHC-C1C	3.18	1.43	1.35
23	B	613	CLA	C4D-ND	-3.17	1.33	1.37
23	c	509	CLA	CHC-C1C	3.17	1.43	1.35
23	C	513	CLA	CHC-C1C	3.16	1.43	1.35
23	a	404	CLA	CHC-C1C	3.16	1.43	1.35
23	b	615	CLA	CHC-C1C	3.16	1.43	1.35
28	c	517	DGD	O2G-C2G	-3.15	1.38	1.46
23	B	603	CLA	CHC-C1C	3.15	1.43	1.35
23	C	512	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	102	SQD	O48-C23	3.15	1.42	1.33
30	a	415	SQD	O48-C23	3.14	1.42	1.33
23	b	609	CLA	CHC-C1C	3.14	1.43	1.35
30	a	401	SQD	O48-C23	3.14	1.42	1.33
31	b	624	LMG	O7-C8	-3.14	1.38	1.46
31	M	102	LMG	O1-C7	-3.14	1.38	1.43
31	b	623	LMG	O7-C8	-3.14	1.38	1.46
23	b	614	CLA	C4D-ND	-3.13	1.33	1.37
31	C	520	LMG	O7-C10	3.13	1.43	1.34
23	b	616	CLA	CHC-C1C	3.13	1.43	1.35
23	c	510	CLA	CHC-C1C	3.13	1.43	1.35
23	B	608	CLA	CHC-C1C	3.13	1.43	1.35
23	B	601	CLA	CHC-C1C	3.13	1.43	1.35
23	C	511	CLA	CHC-C1C	3.13	1.43	1.35
31	k	103	LMG	O7-C8	-3.13	1.38	1.46
23	c	510	CLA	C4D-ND	-3.12	1.33	1.37
23	c	505	CLA	CHC-C1C	3.12	1.43	1.35
23	a	406	CLA	CHC-C1C	3.12	1.43	1.35
28	c	519	DGD	O2G-C1B	3.11	1.43	1.34
23	b	608	CLA	C4D-ND	-3.11	1.33	1.37
31	C	519	LMG	O7-C8	-3.11	1.38	1.46
31	I	101	LMG	O7-C8	-3.11	1.38	1.46
30	A	417	SQD	O48-C23	3.10	1.42	1.33
30	f	103	SQD	O48-C23	3.10	1.42	1.33
31	M	101	LMG	O1-C7	-3.10	1.38	1.43
23	C	507	CLA	CHC-C1C	3.09	1.42	1.35
23	c	511	CLA	CHC-C1C	3.09	1.42	1.35
23	D	401	CLA	CHC-C1C	3.09	1.42	1.35
31	A	418	LMG	O7-C8	-3.09	1.38	1.46
23	B	605	CLA	CHC-C1C	3.09	1.42	1.35
23	B	609	CLA	CHC-C1C	3.09	1.42	1.35
28	c	517	DGD	O1G-C1A	3.09	1.42	1.33
23	c	513	CLA	CHC-C1C	3.08	1.42	1.35
23	C	505	CLA	CHC-C1C	3.08	1.42	1.35
23	C	510	CLA	CHC-C1C	3.08	1.42	1.35
31	D	408	LMG	O7-C8	-3.08	1.38	1.46
28	C	518	DGD	O2G-C1B	3.07	1.43	1.34
23	A	403	CLA	CHC-C1C	3.07	1.42	1.35
30	D	409	SQD	O48-C23	3.07	1.42	1.33
23	B	612	CLA	CHC-C1C	3.07	1.42	1.35
23	B	614	CLA	CHC-C1C	3.07	1.42	1.35
23	B	613	CLA	CHC-C1C	3.07	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	407	SQD	O47-C7	3.06	1.42	1.34
23	D	401	CLA	C4D-ND	-3.06	1.33	1.37
23	D	403	CLA	CHC-C1C	3.06	1.42	1.35
23	B	611	CLA	CHC-C1C	3.05	1.42	1.35
23	c	512	CLA	CHC-C1C	3.05	1.42	1.35
23	B	616	CLA	CHC-C1C	3.04	1.42	1.35
31	M	102	LMG	O7-C8	-3.04	1.39	1.46
23	A	405	CLA	CHC-C1C	3.04	1.42	1.35
31	c	520	LMG	O7-C10	3.04	1.42	1.34
23	B	611	CLA	C4D-ND	-3.04	1.33	1.37
23	C	511	CLA	C4D-ND	-3.04	1.33	1.37
28	B	626	DGD	O2G-C1B	3.04	1.42	1.34
23	C	508	CLA	CHC-C1C	3.04	1.42	1.35
23	C	501	CLA	CHC-C1C	3.03	1.42	1.35
23	A	407	CLA	CHC-C1C	3.03	1.42	1.35
31	a	402	LMG	O7-C8	-3.03	1.39	1.46
23	A	403	CLA	C4D-ND	-3.03	1.33	1.37
23	C	509	CLA	CHC-C1C	3.03	1.42	1.35
23	b	610	CLA	CHC-C1C	3.02	1.42	1.35
23	c	503	CLA	CHC-C1C	3.02	1.42	1.35
23	b	607	CLA	C4D-ND	-3.02	1.33	1.37
28	C	517	DGD	O2G-C2G	-3.01	1.39	1.46
23	B	605	CLA	C4D-ND	-3.01	1.33	1.37
31	A	414	LMG	O7-C10	3.01	1.42	1.34
23	b	607	CLA	CHC-C1C	3.01	1.42	1.35
30	b	601	SQD	O47-C7	3.01	1.42	1.34
31	i	101	LMG	O7-C8	-3.00	1.39	1.46
25	a	410	PL9	C38-C39	3.00	1.41	1.32
23	c	501	CLA	CHC-C1C	3.00	1.42	1.35
24	a	407	PHO	CAC-C3C	-3.00	1.46	1.52
25	A	408	PL9	C38-C39	3.00	1.41	1.32
23	d	402	CLA	CHC-C1C	2.99	1.42	1.35
23	B	608	CLA	C4D-ND	-2.99	1.33	1.37
31	E	101	LMG	O7-C10	2.99	1.42	1.34
31	M	101	LMG	O7-C10	2.98	1.42	1.34
31	M	101	LMG	O7-C8	-2.98	1.39	1.46
25	D	404	PL9	C43-C44	2.97	1.40	1.33
23	C	505	CLA	C4D-ND	-2.97	1.33	1.37
31	B	622	LMG	O7-C10	2.96	1.42	1.34
23	c	507	CLA	C4D-ND	-2.96	1.33	1.37
28	D	410	DGD	O1G-C1A	2.96	1.42	1.33
30	A	417	SQD	O47-C7	2.96	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	102	SQD	O47-C7	2.96	1.42	1.34
23	b	619	CLA	CHC-C1C	2.96	1.42	1.35
23	B	614	CLA	C4D-ND	-2.95	1.33	1.37
23	B	612	CLA	C4D-ND	-2.94	1.33	1.37
28	D	410	DGD	O2G-C2G	-2.93	1.39	1.46
23	b	614	CLA	CMB-C2B	-2.93	1.45	1.51
23	a	405	CLA	CHC-C1C	2.93	1.42	1.35
23	B	604	CLA	C4D-ND	-2.92	1.33	1.37
23	C	507	CLA	C4D-ND	-2.92	1.33	1.37
23	b	606	CLA	C4D-ND	-2.92	1.33	1.37
34	F	101	HEM	CAB-C3B	2.92	1.55	1.47
28	B	626	DGD	O1G-C1A	2.91	1.41	1.33
23	B	616	CLA	C4D-ND	-2.91	1.33	1.37
31	M	102	LMG	O7-C10	2.91	1.42	1.34
31	D	408	LMG	O3-C3	-2.91	1.36	1.43
23	b	604	CLA	CHC-C1C	2.91	1.42	1.35
23	A	405	CLA	C4D-ND	-2.91	1.33	1.37
23	c	505	CLA	C4D-ND	-2.91	1.33	1.37
30	D	409	SQD	O47-C7	2.90	1.42	1.34
23	C	510	CLA	C4D-ND	-2.90	1.33	1.37
28	A	411	DGD	O2G-C1B	2.90	1.42	1.34
31	d	406	LMG	O3-C3	-2.90	1.36	1.43
23	b	615	CLA	C4D-ND	-2.90	1.33	1.37
23	C	509	CLA	C4D-ND	-2.90	1.33	1.37
31	d	406	LMG	O7-C8	-2.89	1.39	1.46
23	c	507	CLA	CHC-C1C	2.89	1.42	1.35
23	a	406	CLA	C4D-ND	-2.89	1.33	1.37
23	B	604	CLA	CHC-C1C	2.89	1.42	1.35
23	b	618	CLA	C4D-ND	-2.89	1.33	1.37
23	C	503	CLA	C4D-ND	-2.88	1.33	1.37
34	f	101	HEM	CAB-C3B	2.88	1.55	1.47
28	d	408	DGD	O2G-C2G	-2.88	1.39	1.46
23	B	609	CLA	C4D-ND	-2.87	1.33	1.37
31	a	416	LMG	O3-C3	-2.87	1.36	1.43
34	v	201	HEM	CAB-C3B	2.87	1.55	1.47
28	b	602	DGD	O2G-C2G	-2.86	1.39	1.46
28	c	518	DGD	O2G-C2G	-2.86	1.39	1.46
28	d	408	DGD	O1G-C1A	2.86	1.41	1.33
28	C	516	DGD	O1G-C1A	2.85	1.41	1.33
28	C	517	DGD	O1G-C1A	2.85	1.41	1.33
31	E	101	LMG	O8-C28	2.85	1.41	1.33
23	C	508	CLA	C4D-ND	-2.85	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	413	DGD	O2G-C2G	-2.85	1.39	1.46
28	c	518	DGD	O2G-C1B	2.85	1.42	1.34
28	c	519	DGD	O1G-C1A	2.84	1.41	1.33
23	A	407	CLA	C4D-ND	-2.84	1.33	1.37
23	d	402	CLA	C4D-ND	-2.84	1.33	1.37
31	A	414	LMG	O7-C8	-2.84	1.39	1.46
31	i	101	LMG	O7-C10	2.84	1.42	1.34
23	C	502	CLA	C4D-ND	-2.84	1.33	1.37
23	c	508	CLA	C4D-ND	-2.84	1.33	1.37
25	J	101	PL9	C23-C24	2.83	1.39	1.33
28	C	518	DGD	O2G-C2G	-2.83	1.39	1.46
31	c	520	LMG	O8-C28	2.83	1.41	1.33
23	C	504	CLA	C4D-ND	-2.83	1.33	1.37
23	c	509	CLA	C4D-ND	-2.83	1.33	1.37
31	B	622	LMG	O7-C8	-2.82	1.39	1.46
28	b	622	DGD	O1G-C1A	2.82	1.41	1.33
25	A	408	PL9	C13-C14	2.82	1.39	1.33
30	a	401	SQD	O47-C7	2.82	1.42	1.34
30	a	415	SQD	O47-C7	2.82	1.42	1.34
30	B	625	SQD	O47-C7	2.82	1.42	1.34
28	b	602	DGD	O2G-C1B	2.82	1.42	1.34
28	c	517	DGD	O2G-C1B	2.81	1.42	1.34
23	b	619	CLA	C4D-ND	-2.81	1.33	1.37
28	C	518	DGD	O1G-C1A	2.81	1.41	1.33
23	B	606	CLA	C4D-ND	-2.81	1.33	1.37
23	B	607	CLA	C4D-ND	-2.80	1.33	1.37
30	f	103	SQD	O47-C7	2.80	1.42	1.34
31	A	414	LMG	O3-C3	-2.80	1.36	1.43
31	i	101	LMG	O1-C7	-2.80	1.38	1.43
31	e	101	LMG	O7-C10	2.79	1.42	1.34
25	j	101	PL9	C23-C24	2.79	1.39	1.33
31	a	402	LMG	O7-C10	2.79	1.42	1.34
31	d	406	LMG	O7-C10	2.79	1.42	1.34
31	C	520	LMG	O8-C28	2.79	1.41	1.33
31	d	406	LMG	O8-C28	2.78	1.41	1.33
28	a	413	DGD	O2G-C1B	2.78	1.42	1.34
23	b	612	CLA	C4D-ND	-2.78	1.33	1.37
28	B	621	DGD	O1G-C1A	2.78	1.41	1.33
25	J	101	PL9	C8-C9	2.78	1.39	1.33
25	d	404	PL9	C18-C19	2.78	1.39	1.33
31	B	622	LMG	O3-C3	-2.77	1.36	1.43
28	c	518	DGD	O1G-C1A	2.77	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	j	101	PL9	C13-C14	2.77	1.39	1.33
31	C	519	LMG	O8-C28	2.77	1.41	1.33
23	B	602	CLA	C4D-ND	-2.76	1.33	1.37
23	A	404	CLA	C4D-ND	-2.76	1.33	1.37
31	i	101	LMG	O3-C3	-2.76	1.36	1.43
31	a	416	LMG	O8-C28	2.75	1.41	1.33
31	I	101	LMG	O3-C3	-2.75	1.36	1.43
23	D	403	CLA	C4D-ND	-2.75	1.33	1.37
31	a	416	LMG	O7-C8	-2.74	1.39	1.46
24	A	406	PHO	CAC-C3C	-2.74	1.47	1.52
31	b	623	LMG	O6-C5	-2.74	1.37	1.44
31	M	101	LMG	O8-C9	-2.74	1.38	1.45
25	d	404	PL9	C23-C24	2.74	1.39	1.33
23	B	611	CLA	CMB-C2B	-2.74	1.45	1.51
31	D	406	LMG	O3-C3	-2.74	1.36	1.43
31	b	623	LMG	O3-C3	-2.74	1.36	1.43
23	B	603	CLA	C4D-ND	-2.74	1.33	1.37
25	a	410	PL9	C23-C24	2.73	1.39	1.33
28	a	413	DGD	O1G-C1A	2.73	1.41	1.33
25	J	101	PL9	C18-C19	2.73	1.39	1.33
24	D	402	PHO	CAC-C3C	-2.73	1.47	1.52
23	c	506	CLA	C4D-ND	-2.73	1.33	1.37
23	c	511	CLA	C4D-ND	-2.73	1.33	1.37
31	b	624	LMG	O3-C3	-2.72	1.36	1.43
23	a	404	CLA	C4D-ND	-2.72	1.33	1.37
31	d	405	LMG	O3-C3	-2.72	1.36	1.43
28	c	519	DGD	O2G-C2G	-2.72	1.39	1.46
31	k	103	LMG	O8-C28	2.72	1.41	1.33
31	A	418	LMG	O7-C10	2.72	1.42	1.34
25	j	101	PL9	C18-C19	2.72	1.39	1.33
25	D	404	PL9	C18-C19	2.71	1.39	1.33
25	j	101	PL9	C8-C9	2.71	1.39	1.33
31	M	102	LMG	O8-C28	2.71	1.41	1.33
23	b	616	CLA	C4D-ND	-2.71	1.34	1.37
23	c	502	CLA	C4D-ND	-2.71	1.34	1.37
25	A	408	PL9	C23-C24	2.71	1.39	1.33
31	D	407	LMG	O8-C9	-2.70	1.39	1.45
31	b	624	LMG	O7-C10	2.70	1.41	1.34
24	a	408	PHO	CAC-C3C	-2.70	1.47	1.52
31	e	101	LMG	O7-C8	-2.70	1.39	1.46
31	A	414	LMG	O8-C28	2.69	1.41	1.33
31	a	402	LMG	O8-C28	2.69	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	411	DGD	O2G-C2G	-2.69	1.39	1.46
31	d	405	LMG	O7-C10	2.69	1.41	1.34
28	b	602	DGD	O6E-C5E	-2.68	1.37	1.44
31	D	408	LMG	O7-C10	2.68	1.41	1.34
25	J	101	PL9	C13-C14	2.68	1.39	1.33
31	M	101	LMG	O3-C3	-2.68	1.36	1.43
23	B	601	CLA	C4D-ND	-2.68	1.34	1.37
31	E	101	LMG	O3-C3	-2.67	1.36	1.43
25	A	408	PL9	C18-C19	2.67	1.39	1.33
31	b	623	LMG	O7-C10	2.67	1.41	1.34
23	b	605	CLA	C4D-ND	-2.67	1.34	1.37
28	B	621	DGD	O3G-C3G	-2.67	1.38	1.43
30	A	413	SQD	O47-C7	2.67	1.41	1.34
31	b	624	LMG	O8-C9	-2.67	1.39	1.45
25	A	408	PL9	C8-C9	2.66	1.39	1.33
28	B	626	DGD	O2G-C2G	-2.66	1.39	1.46
31	a	402	LMG	O3-C3	-2.66	1.36	1.43
23	d	403	CLA	C4D-ND	-2.66	1.34	1.37
23	c	513	CLA	C4D-ND	-2.66	1.34	1.37
28	d	408	DGD	O2G-C1B	2.65	1.41	1.34
31	A	414	LMG	O1-C7	-2.65	1.38	1.43
31	c	520	LMG	O3-C3	-2.65	1.36	1.43
28	b	622	DGD	O3G-C3G	-2.65	1.38	1.43
31	e	101	LMG	O8-C28	2.65	1.41	1.33
31	I	101	LMG	O7-C10	2.65	1.41	1.34
23	b	611	CLA	C4D-ND	-2.65	1.34	1.37
31	k	103	LMG	O7-C10	2.65	1.41	1.34
23	C	506	CLA	C4D-ND	-2.65	1.34	1.37
23	C	513	CLA	C4D-ND	-2.65	1.34	1.37
23	c	503	CLA	C4D-ND	-2.65	1.34	1.37
28	B	626	DGD	O6E-C5E	-2.64	1.37	1.44
23	b	610	CLA	C4D-ND	-2.64	1.34	1.37
31	I	101	LMG	O8-C28	2.64	1.41	1.33
31	C	519	LMG	O7-C10	2.64	1.41	1.34
34	V	201	HEM	CAB-C3B	2.63	1.54	1.47
31	C	519	LMG	O3-C3	-2.63	1.36	1.43
31	A	418	LMG	O3-C3	-2.63	1.36	1.43
28	A	411	DGD	O1G-C1A	2.63	1.41	1.33
31	M	101	LMG	O8-C28	2.63	1.41	1.33
31	C	520	LMG	O3-C3	-2.63	1.36	1.43
31	B	622	LMG	O8-C28	2.63	1.41	1.33
34	v	201	HEM	FE-ND	2.62	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	517	DGD	O2G-C1B	2.62	1.41	1.34
25	D	404	PL9	C13-C14	2.62	1.39	1.33
25	D	404	PL9	C23-C24	2.62	1.39	1.33
23	c	512	CLA	C4D-ND	-2.62	1.34	1.37
25	d	404	PL9	C13-C14	2.62	1.39	1.33
31	D	408	LMG	O8-C28	2.62	1.41	1.33
23	C	510	CLA	CMB-C2B	-2.61	1.46	1.51
31	B	622	LMG	O1-C7	-2.61	1.39	1.43
28	c	518	DGD	O4D-C4D	-2.61	1.36	1.43
25	a	410	PL9	C18-C19	2.61	1.39	1.33
31	b	623	LMG	O8-C28	2.60	1.40	1.33
31	e	101	LMG	O8-C9	-2.60	1.39	1.45
31	A	418	LMG	O8-C9	-2.60	1.39	1.45
23	C	512	CLA	C4D-ND	-2.60	1.34	1.37
31	D	407	LMG	O1-C7	-2.60	1.39	1.43
31	e	101	LMG	O3-C3	-2.60	1.36	1.43
31	D	407	LMG	O3-C3	-2.60	1.36	1.43
31	M	102	LMG	O8-C9	-2.59	1.39	1.45
23	b	604	CLA	CMB-C2B	-2.59	1.46	1.51
25	d	404	PL9	C8-C9	2.59	1.39	1.33
31	c	520	LMG	O7-C8	-2.59	1.40	1.46
31	d	405	LMG	O8-C28	2.59	1.40	1.33
28	C	516	DGD	O6E-C5E	-2.58	1.38	1.44
31	D	407	LMG	O8-C28	2.58	1.40	1.33
31	k	103	LMG	O3-C3	-2.58	1.36	1.43
31	i	101	LMG	O8-C9	-2.58	1.39	1.45
23	B	604	CLA	CMB-C2B	-2.58	1.46	1.51
23	c	508	CLA	CMB-C2B	-2.58	1.46	1.51
31	b	624	LMG	O8-C28	2.58	1.40	1.33
31	M	102	LMG	O3-C3	-2.57	1.36	1.43
23	c	501	CLA	C4D-ND	-2.57	1.34	1.37
31	i	101	LMG	O8-C28	2.57	1.40	1.33
31	D	407	LMG	O7-C10	2.55	1.41	1.34
31	A	418	LMG	O8-C28	2.55	1.40	1.33
23	B	608	CLA	CMB-C2B	-2.55	1.46	1.51
34	f	101	HEM	FE-ND	2.55	2.09	1.96
25	a	410	PL9	C13-C14	2.54	1.39	1.33
31	b	623	LMG	O8-C9	-2.54	1.39	1.45
23	A	404	CLA	CMB-C2B	-2.54	1.46	1.51
31	D	408	LMG	O8-C9	-2.54	1.39	1.45
31	A	414	LMG	O8-C9	-2.54	1.39	1.45
31	C	520	LMG	O7-C8	-2.54	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	406	LMG	O8-C9	-2.54	1.39	1.45
28	C	516	DGD	O2G-C1B	2.53	1.41	1.34
30	A	417	SQD	C4-C5	-2.53	1.47	1.53
25	a	410	PL9	C28-C29	2.52	1.39	1.33
34	V	201	HEM	FE-ND	2.52	2.09	1.96
23	b	611	CLA	CMB-C2B	-2.52	1.46	1.51
31	I	101	LMG	O8-C9	-2.52	1.39	1.45
31	E	101	LMG	O7-C8	-2.52	1.40	1.46
23	C	508	CLA	CMB-C2B	-2.52	1.46	1.51
23	b	616	CLA	CMB-C2B	-2.52	1.46	1.51
23	B	601	CLA	CMB-C2B	-2.52	1.46	1.51
23	B	610	CLA	CMB-C2B	-2.51	1.46	1.51
28	B	626	DGD	O5D-C6D	-2.51	1.39	1.43
31	k	103	LMG	O1-C7	-2.51	1.39	1.43
25	a	410	PL9	C8-C9	2.51	1.39	1.33
28	c	517	DGD	O6E-C5E	-2.51	1.38	1.44
23	C	501	CLA	C4D-ND	-2.51	1.34	1.37
31	a	416	LMG	O8-C9	-2.51	1.39	1.45
23	b	605	CLA	CMB-C2B	-2.51	1.46	1.51
28	B	621	DGD	O6D-C5D	-2.51	1.38	1.44
23	b	613	CLA	C4D-ND	-2.50	1.34	1.37
28	C	517	DGD	O4D-C4D	-2.50	1.37	1.43
31	E	101	LMG	O8-C9	-2.50	1.39	1.45
23	B	606	CLA	CMB-C2B	-2.50	1.46	1.51
23	b	604	CLA	C4D-ND	-2.49	1.34	1.37
31	b	624	LMG	O1-C7	-2.49	1.39	1.43
30	A	417	SQD	O2-C2	-2.49	1.37	1.43
31	d	405	LMG	O1-C7	-2.49	1.39	1.43
31	k	103	LMG	O8-C9	-2.49	1.39	1.45
23	A	405	CLA	CMB-C2B	-2.49	1.46	1.51
23	b	609	CLA	CMB-C2B	-2.49	1.46	1.51
23	c	501	CLA	CMB-C2B	-2.49	1.46	1.51
28	A	411	DGD	O1G-C1G	-2.49	1.39	1.45
28	c	518	DGD	O6E-C5E	-2.48	1.38	1.44
23	c	510	CLA	CMB-C2B	-2.48	1.46	1.51
31	D	406	LMG	O8-C28	2.47	1.40	1.33
31	a	402	LMG	O1-C7	-2.47	1.39	1.43
23	a	406	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	513	CLA	CMB-C2B	-2.47	1.46	1.51
28	b	622	DGD	O2G-C1B	2.47	1.41	1.34
31	B	622	LMG	O8-C9	-2.47	1.39	1.45
23	a	404	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CMB-C2B	-2.46	1.46	1.51
31	a	402	LMG	O8-C9	-2.46	1.39	1.45
23	B	616	CLA	CMB-C2B	-2.46	1.46	1.51
31	b	623	LMG	O1-C7	-2.46	1.39	1.43
31	c	520	LMG	O8-C9	-2.46	1.39	1.45
23	c	502	CLA	CMB-C2B	-2.46	1.46	1.51
23	b	607	CLA	CMB-C2B	-2.45	1.46	1.51
23	b	609	CLA	C4D-ND	-2.45	1.34	1.37
23	B	610	CLA	C4D-ND	-2.45	1.34	1.37
23	B	613	CLA	CMB-C2B	-2.45	1.46	1.51
28	D	410	DGD	O2G-C1B	2.44	1.41	1.34
25	A	408	PL9	C28-C29	2.43	1.38	1.33
28	b	622	DGD	O6D-C5D	-2.43	1.38	1.44
31	I	101	LMG	O1-C7	-2.43	1.39	1.43
28	C	517	DGD	O6E-C5E	-2.43	1.38	1.44
31	C	520	LMG	O8-C9	-2.43	1.39	1.45
23	C	511	CLA	CMB-C2B	-2.43	1.46	1.51
28	C	517	DGD	C4D-C5D	-2.42	1.47	1.53
23	C	501	CLA	CMB-C2B	-2.42	1.46	1.51
31	d	405	LMG	O8-C9	-2.42	1.39	1.45
23	a	409	CLA	CMB-C2B	-2.42	1.46	1.51
23	a	405	CLA	CMB-C2B	-2.42	1.46	1.51
25	d	404	PL9	C28-C29	2.42	1.38	1.33
23	b	619	CLA	CMB-C2B	-2.42	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.42	1.46	1.51
23	b	613	CLA	CMB-C2B	-2.42	1.46	1.51
23	B	602	CLA	CMB-C2B	-2.41	1.46	1.51
23	C	502	CLA	CMB-C2B	-2.41	1.46	1.51
25	D	404	PL9	C8-C9	2.41	1.38	1.33
23	A	403	CLA	CMB-C2B	-2.41	1.46	1.51
28	c	518	DGD	O6D-C5D	-2.41	1.38	1.44
23	C	512	CLA	CMB-C2B	-2.41	1.46	1.51
23	C	504	CLA	CMB-C2B	-2.41	1.46	1.51
23	b	606	CLA	CMB-C2B	-2.40	1.46	1.51
23	c	513	CLA	CMB-C2B	-2.40	1.46	1.51
23	C	509	CLA	CMB-C2B	-2.40	1.46	1.51
31	D	406	LMG	O7-C10	2.40	1.41	1.34
23	B	603	CLA	CMB-C2B	-2.40	1.46	1.51
23	c	506	CLA	CMB-C2B	-2.40	1.46	1.51
31	C	519	LMG	O8-C9	-2.40	1.39	1.45
28	C	518	DGD	O3G-C3G	-2.40	1.39	1.43
23	c	504	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	418	LMG	O1-C7	-2.39	1.39	1.43
23	C	503	CLA	CMB-C2B	-2.39	1.46	1.51
23	B	609	CLA	CMB-C2B	-2.39	1.46	1.51
23	D	401	CLA	CMB-C2B	-2.39	1.46	1.51
23	B	614	CLA	CMB-C2B	-2.39	1.46	1.51
28	c	518	DGD	O5D-C6D	-2.38	1.39	1.43
23	c	503	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	610	CLA	CMB-C2B	-2.38	1.46	1.51
23	B	612	CLA	CMB-C2B	-2.38	1.46	1.51
23	D	403	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	618	CLA	CMB-C2B	-2.38	1.46	1.51
28	B	621	DGD	O5D-C6D	-2.38	1.39	1.43
23	B	605	CLA	CMB-C2B	-2.37	1.46	1.51
28	c	519	DGD	O3G-C3G	-2.37	1.39	1.43
23	d	403	CLA	CMB-C2B	-2.37	1.46	1.51
31	D	408	LMG	O1-C7	-2.37	1.39	1.43
23	b	617	CLA	CMB-C2B	-2.37	1.46	1.51
23	c	512	CLA	CMB-C2B	-2.37	1.46	1.51
23	B	615	CLA	CMB-C2B	-2.36	1.46	1.51
23	c	511	CLA	CMB-C2B	-2.36	1.46	1.51
23	C	506	CLA	CMB-C2B	-2.36	1.46	1.51
23	C	507	CLA	CMB-C2B	-2.36	1.46	1.51
23	b	615	CLA	CMB-C2B	-2.36	1.46	1.51
31	D	407	LMG	O6-C5	-2.35	1.38	1.44
28	c	517	DGD	O4D-C4D	-2.35	1.37	1.43
23	b	608	CLA	CMB-C2B	-2.35	1.46	1.51
25	D	404	PL9	C28-C29	2.35	1.38	1.33
23	b	612	CLA	CMB-C2B	-2.34	1.46	1.51
28	C	516	DGD	C4E-C5E	-2.34	1.48	1.53
28	a	413	DGD	O1G-C1G	-2.33	1.39	1.45
25	J	101	PL9	C28-C29	2.33	1.39	1.32
23	c	509	CLA	CMB-C2B	-2.33	1.46	1.51
23	c	504	CLA	C4D-ND	-2.33	1.34	1.37
23	B	607	CLA	CMB-C2B	-2.33	1.46	1.51
23	A	407	CLA	CMB-C2B	-2.32	1.46	1.51
28	D	410	DGD	O5D-C6D	-2.32	1.39	1.43
31	a	416	LMG	O1-C7	-2.32	1.39	1.43
28	B	621	DGD	O2G-C1B	2.32	1.40	1.34
31	D	408	LMG	O6-C5	-2.31	1.38	1.44
28	a	413	DGD	O4D-C4D	-2.30	1.37	1.43
28	c	518	DGD	C4D-C5D	-2.30	1.48	1.53
23	A	404	CLA	C3B-C2B	-2.30	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	406	LMG	O1-C7	-2.29	1.39	1.43
30	a	401	SQD	O2-C2	-2.29	1.37	1.43
28	b	602	DGD	O5D-C6D	-2.29	1.39	1.43
25	j	101	PL9	C28-C29	2.28	1.38	1.32
23	d	402	CLA	CMB-C2B	-2.28	1.46	1.51
28	c	519	DGD	O4D-C4D	-2.28	1.37	1.43
31	B	622	LMG	O6-C5	-2.28	1.38	1.44
31	I	101	LMG	O6-C5	-2.28	1.38	1.44
31	C	519	LMG	O1-C7	-2.27	1.39	1.43
34	F	101	HEM	FE-ND	2.27	2.08	1.96
28	C	517	DGD	O6D-C5D	-2.27	1.38	1.44
34	V	201	HEM	CAA-C2A	2.26	1.55	1.52
30	B	625	SQD	O2-C2	-2.26	1.37	1.43
31	e	101	LMG	O6-C5	-2.26	1.38	1.44
23	c	505	CLA	CMB-C2B	-2.26	1.46	1.51
28	C	518	DGD	O6E-C5E	-2.26	1.38	1.44
28	B	621	DGD	O6E-C5E	-2.25	1.38	1.44
28	b	622	DGD	O6E-C5E	-2.25	1.38	1.44
31	d	406	LMG	O8-C9	-2.24	1.40	1.45
28	C	518	DGD	O4D-C4D	-2.24	1.37	1.43
28	A	411	DGD	O4D-C4D	-2.24	1.37	1.43
30	b	601	SQD	O2-C2	-2.23	1.37	1.43
31	c	520	LMG	O1-C7	-2.22	1.39	1.43
28	c	519	DGD	O6E-C5E	-2.22	1.39	1.44
28	C	517	DGD	O5D-C6D	-2.22	1.39	1.43
28	a	413	DGD	O6E-C5E	-2.22	1.39	1.44
34	v	201	HEM	CAA-C2A	2.21	1.55	1.52
28	A	411	DGD	O3G-C3G	-2.20	1.39	1.43
28	b	602	DGD	O4D-C4D	-2.20	1.37	1.43
33	i	102	LMT	O1'-C1'	2.19	1.43	1.40
28	a	413	DGD	O3G-C3G	-2.18	1.39	1.43
28	A	411	DGD	O6E-C5E	-2.18	1.39	1.44
31	c	520	LMG	O6-C5	-2.18	1.39	1.44
28	B	621	DGD	O4D-C4D	-2.18	1.37	1.43
28	D	410	DGD	O6E-C5E	-2.18	1.39	1.44
28	c	518	DGD	O1G-C1G	-2.18	1.40	1.45
23	B	612	CLA	CMD-C2D	-2.18	1.46	1.50
23	c	505	CLA	CMD-C2D	-2.18	1.46	1.50
24	a	407	PHO	CMD-C2D	-2.18	1.46	1.51
31	C	520	LMG	O6-C5	-2.17	1.39	1.44
31	I	101	LMG	C4-C5	-2.16	1.48	1.53
31	e	101	LMG	O1-C7	-2.15	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	622	DGD	O5D-C6D	-2.15	1.39	1.43
23	c	510	CLA	CMD-C2D	-2.15	1.46	1.50
28	C	516	DGD	O4D-C4D	-2.15	1.37	1.43
28	C	518	DGD	O1G-C1G	-2.15	1.40	1.45
28	A	411	DGD	C4D-C5D	-2.15	1.48	1.53
30	D	409	SQD	O3-C3	-2.14	1.37	1.43
34	v	201	HEM	FE-NB	2.14	2.07	1.96
31	i	101	LMG	O6-C5	-2.14	1.39	1.44
23	a	404	CLA	CMD-C2D	-2.14	1.46	1.50
23	b	617	CLA	CMD-C2D	-2.14	1.46	1.50
30	A	413	SQD	O2-C2	-2.14	1.37	1.43
23	C	505	CLA	CMD-C2D	-2.14	1.46	1.50
30	B	625	SQD	O4-C4	-2.12	1.38	1.43
34	v	201	HEM	CMB-C2B	2.12	1.55	1.50
31	E	101	LMG	O6-C5	-2.12	1.39	1.44
31	D	406	LMG	O1-C7	-2.12	1.39	1.43
24	a	407	PHO	CMC-C2C	-2.12	1.46	1.51
31	M	101	LMG	O6-C5	-2.12	1.39	1.44
24	D	402	PHO	CMC-C2C	-2.11	1.46	1.51
30	a	415	SQD	O3-C3	-2.11	1.38	1.43
28	b	622	DGD	O4D-C4D	-2.11	1.38	1.43
30	d	407	SQD	O4-C4	-2.11	1.38	1.43
30	b	601	SQD	O3-C3	-2.11	1.38	1.43
23	B	604	CLA	CMD-C2D	-2.11	1.46	1.50
24	D	402	PHO	CMD-C2D	-2.11	1.46	1.51
31	D	408	LMG	O2-C2	-2.11	1.38	1.43
23	b	615	CLA	CMD-C2D	-2.11	1.46	1.50
30	f	103	SQD	O2-C2	-2.10	1.38	1.43
23	b	614	CLA	CMD-C2D	-2.10	1.46	1.50
28	d	408	DGD	O6E-C5E	-2.10	1.39	1.44
30	d	407	SQD	O3-C3	-2.09	1.38	1.43
28	D	410	DGD	O4D-C4D	-2.09	1.38	1.43
30	a	401	SQD	C4-C5	-2.09	1.48	1.53
23	C	501	CLA	C1D-C2D	2.09	1.49	1.45
24	A	406	PHO	CMB-C2B	-2.09	1.46	1.51
28	d	408	DGD	O4D-C4D	-2.09	1.38	1.43
24	a	407	PHO	CMB-C2B	-2.09	1.46	1.51
30	A	417	SQD	O4-C4	-2.08	1.38	1.43
31	b	624	LMG	O6-C5	-2.08	1.39	1.44
23	B	616	CLA	CMC-C2C	-2.08	1.46	1.50
23	a	406	CLA	CMD-C2D	-2.08	1.46	1.50
28	d	408	DGD	O5D-C6D	-2.08	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CMD-C2D	-2.08	1.46	1.50
23	B	608	CLA	CMD-C2D	-2.08	1.46	1.50
28	B	626	DGD	C4E-C5E	-2.08	1.48	1.53
30	b	601	SQD	O4-C4	-2.08	1.38	1.43
30	F	102	SQD	O3-C3	-2.07	1.38	1.43
24	a	408	PHO	CMD-C2D	-2.07	1.46	1.51
23	A	403	CLA	CMD-C2D	-2.07	1.46	1.50
23	B	605	CLA	CMD-C2D	-2.07	1.46	1.50
25	d	404	PL9	C48-C49	2.07	1.38	1.32
30	F	102	SQD	O2-C2	-2.06	1.38	1.43
23	c	506	CLA	C3D-C4D	2.06	1.48	1.44
23	C	510	CLA	CMD-C2D	-2.06	1.46	1.50
28	B	621	DGD	O1G-C1G	-2.06	1.40	1.45
30	B	625	SQD	O3-C3	-2.06	1.38	1.43
24	A	406	PHO	CMD-C2D	-2.06	1.46	1.51
23	B	601	CLA	C3D-C4D	2.06	1.48	1.44
30	f	103	SQD	O3-C3	-2.06	1.38	1.43
28	c	519	DGD	O1G-C1G	-2.06	1.40	1.45
30	D	409	SQD	O4-C4	-2.06	1.38	1.43
23	b	608	CLA	CMC-C2C	-2.06	1.46	1.50
30	a	415	SQD	O4-C4	-2.06	1.38	1.43
30	a	415	SQD	O2-C2	-2.06	1.38	1.43
28	c	517	DGD	C4D-C5D	-2.05	1.48	1.53
28	B	626	DGD	O1G-C1G	-2.05	1.40	1.45
34	V	201	HEM	CMB-C2B	2.05	1.55	1.50
23	C	502	CLA	CMD-C2D	-2.05	1.46	1.50
30	f	103	SQD	O4-C4	-2.05	1.38	1.43
24	a	408	PHO	CMC-C2C	-2.05	1.46	1.51
28	b	622	DGD	O1G-C1G	-2.05	1.40	1.45
28	c	517	DGD	C4E-C5E	-2.05	1.48	1.53
31	E	101	LMG	O1-C7	-2.05	1.40	1.43
31	E	101	LMG	O4-C4	-2.04	1.38	1.43
28	d	408	DGD	O6D-C5D	-2.04	1.39	1.44
23	C	512	CLA	C3D-C4D	2.04	1.48	1.44
28	C	517	DGD	O1G-C1G	-2.04	1.40	1.45
30	F	102	SQD	O4-C4	-2.04	1.38	1.43
31	d	406	LMG	O6-C5	-2.04	1.39	1.44
23	B	604	CLA	C3B-CAB	-2.04	1.43	1.47
28	D	410	DGD	C4D-C5D	-2.03	1.48	1.53
28	a	413	DGD	C4D-C5D	-2.03	1.48	1.53
24	D	402	PHO	CMB-C2B	-2.03	1.46	1.51
28	C	517	DGD	C4E-C5E	-2.03	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	CMD-C2D	-2.03	1.46	1.50
24	D	402	PHO	C3B-C2B	-2.03	1.37	1.40
31	e	101	LMG	O4-C4	-2.03	1.38	1.43
30	A	413	SQD	O4-C4	-2.03	1.38	1.43
31	d	406	LMG	O2-C2	-2.03	1.38	1.43
24	A	406	PHO	CMC-C2C	-2.02	1.46	1.51
23	C	503	CLA	CMD-C2D	-2.02	1.46	1.50
23	b	607	CLA	CMD-C2D	-2.02	1.46	1.50
30	A	413	SQD	O3-C3	-2.02	1.38	1.43
30	a	401	SQD	O4-C4	-2.02	1.38	1.43
23	C	508	CLA	CMD-C2D	-2.02	1.46	1.50
23	C	502	CLA	CMC-C2C	-2.02	1.46	1.50
28	b	602	DGD	C4E-C5E	-2.02	1.48	1.53
30	A	413	SQD	O47-C45	-2.02	1.41	1.46
31	d	405	LMG	O6-C5	-2.02	1.39	1.44
23	B	603	CLA	CMD-C2D	-2.02	1.46	1.50
23	c	502	CLA	CMD-C2D	-2.02	1.46	1.50
28	D	410	DGD	O6D-C5D	-2.01	1.39	1.44
23	B	615	CLA	CMD-C2D	-2.01	1.46	1.50
23	b	604	CLA	CMC-C2C	-2.01	1.46	1.50
23	B	611	CLA	CMD-C2D	-2.01	1.46	1.50
31	M	102	LMG	O6-C5	-2.01	1.39	1.44
31	C	520	LMG	O1-C7	-2.01	1.40	1.43
23	b	608	CLA	CMD-C2D	-2.01	1.46	1.50
23	D	401	CLA	CMD-C2D	-2.01	1.46	1.50
31	B	622	LMG	O2-C2	-2.01	1.38	1.43
23	B	602	CLA	CMD-C2D	-2.00	1.46	1.50
33	x	102	LMT	O1'-C1'	2.00	1.43	1.40
28	B	626	DGD	O4D-C4D	-2.00	1.38	1.43
23	b	611	CLA	CMD-C2D	-2.00	1.46	1.50

All (1465) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J	102	BCR	C32-C1-C6	-13.60	88.24	110.30
27	j	102	BCR	C32-C1-C6	-13.52	88.37	110.30
27	j	102	BCR	C32-C1-C31	-8.60	82.13	108.53
27	B	618	BCR	C7-C8-C9	-8.58	113.28	126.23
27	J	102	BCR	C32-C1-C31	-8.52	82.39	108.53
27	C	514	BCR	C7-C8-C9	8.41	138.94	126.23
23	c	505	CLA	C4A-NA-C1A	8.28	110.43	106.71
27	T	103	BCR	C7-C8-C9	-8.24	113.79	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	514	BCR	C7-C8-C9	8.10	138.47	126.23
23	c	504	CLA	C4A-NA-C1A	7.86	110.24	106.71
23	C	511	CLA	C4A-NA-C1A	7.77	110.20	106.71
23	B	607	CLA	C4A-NA-C1A	7.64	110.14	106.71
23	d	402	CLA	C4A-NA-C1A	7.61	110.13	106.71
23	c	502	CLA	C4A-NA-C1A	7.58	110.12	106.71
23	C	512	CLA	C4A-NA-C1A	7.35	110.01	106.71
23	c	513	CLA	C4A-NA-C1A	7.31	109.99	106.71
23	A	403	CLA	C4A-NA-C1A	7.30	109.99	106.71
23	C	505	CLA	C4A-NA-C1A	7.20	109.94	106.71
23	c	509	CLA	C4A-NA-C1A	7.19	109.94	106.71
23	b	615	CLA	C4A-NA-C1A	7.18	109.93	106.71
23	C	502	CLA	C4A-NA-C1A	7.05	109.88	106.71
23	C	513	CLA	C4A-NA-C1A	7.05	109.87	106.71
23	b	616	CLA	C4A-NA-C1A	7.04	109.87	106.71
23	c	511	CLA	C4A-NA-C1A	7.02	109.86	106.71
23	c	506	CLA	C4A-NA-C1A	6.97	109.84	106.71
23	b	605	CLA	C4A-NA-C1A	6.95	109.83	106.71
23	c	501	CLA	C4A-NA-C1A	6.95	109.83	106.71
23	b	607	CLA	C4A-NA-C1A	6.86	109.79	106.71
23	B	610	CLA	C4A-NA-C1A	6.82	109.77	106.71
23	B	615	CLA	C4A-NA-C1A	6.81	109.77	106.71
23	B	602	CLA	C4A-NA-C1A	6.81	109.77	106.71
23	B	611	CLA	C4A-NA-C1A	6.80	109.77	106.71
23	C	503	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	b	618	CLA	C4A-NA-C1A	6.79	109.76	106.71
30	D	409	SQD	O6-C1-C2	6.78	118.89	108.30
23	b	608	CLA	C4A-NA-C1A	6.78	109.75	106.71
34	v	201	HEM	C4D-ND-C1D	6.77	112.07	105.07
23	C	504	CLA	C4A-NA-C1A	6.76	109.74	106.71
23	b	617	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	a	409	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	C	501	CLA	C4A-NA-C1A	6.65	109.69	106.71
23	a	404	CLA	C4A-NA-C1A	6.62	109.68	106.71
28	A	411	DGD	C3G-O3G-C1D	6.61	126.66	113.74
23	B	605	CLA	C4A-NA-C1A	6.58	109.67	106.71
27	j	102	BCR	C31-C1-C6	6.57	120.96	110.30
23	C	507	CLA	C4A-NA-C1A	6.57	109.66	106.71
23	B	601	CLA	C4A-NA-C1A	6.53	109.64	106.71
23	b	610	CLA	C4A-NA-C1A	6.52	109.64	106.71
23	c	512	CLA	C4A-NA-C1A	6.51	109.64	106.71
23	C	508	CLA	C4A-NA-C1A	6.50	109.63	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	b	611	CLA	C4A-NA-C1A	6.50	109.63	106.71
23	C	506	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	C	509	CLA	C4A-NA-C1A	6.47	109.61	106.71
23	d	403	CLA	C4A-NA-C1A	6.46	109.61	106.71
27	J	102	BCR	C31-C1-C6	6.44	120.75	110.30
30	d	407	SQD	O6-C1-C2	6.43	118.35	108.30
23	D	401	CLA	C4A-NA-C1A	6.41	109.59	106.71
28	a	413	DGD	C3G-O3G-C1D	6.41	126.26	113.74
23	B	603	CLA	C4A-NA-C1A	6.39	109.58	106.71
28	c	519	DGD	C3G-O3G-C1D	6.31	126.08	113.74
23	b	604	CLA	C4A-NA-C1A	6.31	109.55	106.71
27	D	405	BCR	C7-C8-C9	-6.31	116.70	126.23
23	A	407	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	b	609	CLA	C4A-NA-C1A	6.30	109.54	106.71
23	B	604	CLA	C4A-NA-C1A	6.29	109.53	106.71
23	c	508	CLA	C4A-NA-C1A	6.25	109.52	106.71
23	B	606	CLA	C4A-NA-C1A	6.25	109.51	106.71
23	c	503	CLA	C4A-NA-C1A	6.23	109.50	106.71
23	B	613	CLA	C4A-NA-C1A	6.20	109.49	106.71
23	c	507	CLA	C4A-NA-C1A	6.19	109.49	106.71
27	c	514	BCR	C15-C14-C13	-6.19	118.48	127.31
23	B	614	CLA	C4A-NA-C1A	6.17	109.48	106.71
27	f	102	BCR	C7-C8-C9	-6.16	116.92	126.23
23	A	404	CLA	C4A-NA-C1A	6.12	109.46	106.71
23	a	406	CLA	C4A-NA-C1A	6.10	109.45	106.71
23	b	619	CLA	C4A-NA-C1A	6.07	109.44	106.71
23	a	405	CLA	C4A-NA-C1A	6.05	109.42	106.71
23	C	510	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	b	606	CLA	C4A-NA-C1A	6.03	109.42	106.71
23	D	403	CLA	C4A-NA-C1A	6.00	109.40	106.71
23	B	608	CLA	C4A-NA-C1A	5.93	109.37	106.71
30	D	409	SQD	C44-O6-C1	5.93	125.33	113.74
23	b	614	CLA	C4A-NA-C1A	5.91	109.36	106.71
28	C	518	DGD	C3G-O3G-C1D	5.89	125.25	113.74
23	b	613	CLA	C4A-NA-C1A	5.89	109.35	106.71
34	F	101	HEM	C4D-ND-C1D	5.87	111.14	105.07
23	B	612	CLA	C4A-NA-C1A	5.84	109.33	106.71
23	c	510	CLA	C4A-NA-C1A	5.80	109.31	106.71
27	J	102	BCR	C15-C14-C13	-5.77	119.08	127.31
23	b	612	CLA	C4A-NA-C1A	5.74	109.29	106.71
27	B	618	BCR	C11-C10-C9	-5.73	119.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	d	407	SQD	C44-O6-C1	5.62	124.72	113.74
23	B	616	CLA	C4A-NA-C1A	5.62	109.23	106.71
34	f	101	HEM	C4D-ND-C1D	5.60	110.86	105.07
27	j	102	BCR	C15-C14-C13	-5.51	119.44	127.31
27	B	620	BCR	C3-C4-C5	-5.44	104.36	114.08
23	A	405	CLA	C4A-NA-C1A	5.43	109.15	106.71
34	V	201	HEM	C4D-ND-C1D	5.35	110.59	105.07
27	J	102	BCR	C32-C1-C2	-5.34	87.56	108.91
27	j	102	BCR	C20-C21-C22	-5.31	119.73	127.31
27	f	102	BCR	C15-C14-C13	-5.29	119.77	127.31
30	b	601	SQD	O7-S-C6	5.26	113.19	106.94
27	T	103	BCR	C11-C10-C9	-5.25	119.81	127.31
27	j	102	BCR	C32-C1-C2	-5.25	87.91	108.91
27	c	515	BCR	C15-C14-C13	-5.21	119.88	127.31
27	D	405	BCR	C28-C27-C26	-5.15	104.87	114.08
27	J	102	BCR	C28-C27-C26	-5.13	104.91	114.08
27	D	405	BCR	C11-C10-C9	-5.13	119.99	127.31
27	A	410	BCR	C33-C5-C6	-5.09	118.81	124.53
27	j	102	BCR	C28-C27-C26	-5.07	105.03	114.08
27	C	514	BCR	C15-C14-C13	-5.05	120.11	127.31
27	B	618	BCR	C3-C4-C5	-5.02	105.11	114.08
28	d	408	DGD	O3G-C1D-C2D	4.98	116.08	108.30
27	b	621	BCR	C24-C23-C22	-4.98	118.71	126.23
25	j	101	PL9	C7-C3-C4	4.94	120.89	116.88
25	J	101	PL9	C7-C3-C4	4.93	120.89	116.88
27	A	410	BCR	C16-C17-C18	-4.93	120.27	127.31
27	j	102	BCR	C24-C23-C22	-4.93	118.78	126.23
27	c	514	BCR	C33-C5-C6	-4.93	118.99	124.53
27	J	102	BCR	C11-C10-C9	-4.92	120.29	127.31
30	B	625	SQD	O7-S-C6	4.85	112.70	106.94
27	J	102	BCR	C20-C21-C22	-4.84	120.40	127.31
27	b	621	BCR	C3-C4-C5	-4.84	105.43	114.08
27	k	102	BCR	C15-C14-C13	-4.79	120.47	127.31
27	f	102	BCR	C28-C27-C26	-4.79	105.52	114.08
30	d	407	SQD	O9-S-C6	4.78	112.61	106.94
27	Z	101	BCR	C15-C14-C13	-4.71	120.59	127.31
27	C	514	BCR	C33-C5-C6	-4.64	119.32	124.53
27	B	620	BCR	C24-C23-C22	-4.62	119.25	126.23
27	T	103	BCR	C3-C4-C5	-4.62	105.82	114.08
27	T	102	BCR	C15-C14-C13	-4.61	120.73	127.31
27	B	617	BCR	C15-C14-C13	-4.60	120.75	127.31
27	A	410	BCR	C15-C14-C13	-4.60	120.75	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	514	BCR	C8-C7-C6	4.57	140.04	127.20
30	D	409	SQD	O9-S-C6	4.57	112.37	106.94
27	J	102	BCR	C24-C23-C22	-4.57	119.33	126.23
27	j	102	BCR	C11-C10-C9	-4.54	120.83	127.31
27	T	102	BCR	C16-C17-C18	-4.53	120.84	127.31
27	b	620	BCR	C7-C8-C9	-4.52	119.40	126.23
30	f	103	SQD	O7-S-C6	4.50	112.29	106.94
27	B	618	BCR	C28-C27-C26	-4.50	106.05	114.08
27	B	619	BCR	C28-C27-C26	-4.50	106.05	114.08
27	f	102	BCR	C16-C17-C18	-4.48	120.91	127.31
28	C	518	DGD	C1D-O6D-C5D	-4.47	104.91	113.69
28	c	519	DGD	C1D-O6D-C5D	-4.47	104.91	113.69
28	D	410	DGD	O3G-C1D-C2D	4.47	115.28	108.30
28	A	411	DGD	O2G-C1B-C2B	4.45	121.08	111.50
31	a	416	LMG	O7-C10-C11	4.42	121.02	111.50
25	d	404	PL9	C7-C3-C4	4.42	120.47	116.88
27	J	102	BCR	C16-C17-C18	-4.39	121.04	127.31
27	c	514	BCR	C8-C7-C6	4.36	139.45	127.20
27	B	620	BCR	C7-C8-C9	-4.36	119.65	126.23
27	j	102	BCR	C7-C8-C9	-4.35	119.66	126.23
27	C	515	BCR	C15-C14-C13	-4.35	121.11	127.31
27	C	515	BCR	C7-C8-C9	-4.34	119.67	126.23
27	k	102	BCR	C16-C17-C18	-4.32	121.14	127.31
27	b	621	BCR	C11-C10-C9	-4.31	121.16	127.31
27	a	412	BCR	C33-C5-C6	-4.31	119.69	124.53
27	B	617	BCR	C16-C17-C18	-4.29	121.18	127.31
27	f	102	BCR	C33-C5-C6	-4.27	119.73	124.53
31	a	416	LMG	C7-O1-C1	4.27	122.08	113.74
27	T	103	BCR	C28-C27-C26	-4.27	106.46	114.08
27	b	621	BCR	C7-C8-C9	-4.26	119.80	126.23
27	C	515	BCR	C28-C27-C26	-4.24	106.51	114.08
25	a	410	PL9	C7-C3-C4	4.23	120.32	116.88
30	d	407	SQD	O47-C7-C8	4.23	120.61	111.50
27	b	620	BCR	C15-C14-C13	-4.23	121.28	127.31
27	C	514	BCR	C3-C4-C5	-4.20	106.57	114.08
27	a	412	BCR	C16-C17-C18	-4.20	121.31	127.31
27	D	405	BCR	C24-C23-C22	-4.19	119.91	126.23
27	c	514	BCR	C16-C17-C18	-4.18	121.34	127.31
27	H	101	BCR	C33-C5-C6	-4.18	119.83	124.53
31	A	414	LMG	O7-C10-C11	4.18	120.51	111.50
30	A	413	SQD	O7-S-C6	4.18	111.91	106.94
27	k	102	BCR	C38-C26-C25	-4.17	119.85	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	102	BCR	C24-C23-C22	-4.17	119.94	126.23
27	c	514	BCR	C11-C10-C9	-4.16	121.38	127.31
27	a	412	BCR	C15-C14-C13	-4.15	121.39	127.31
27	c	516	BCR	C15-C14-C13	-4.14	121.40	127.31
27	c	516	BCR	C7-C8-C9	-4.14	119.98	126.23
28	a	413	DGD	O2G-C1B-C2B	4.13	120.41	111.50
27	B	617	BCR	C7-C8-C9	-4.13	119.99	126.23
27	K	102	BCR	C3-C4-C5	-4.13	106.71	114.08
27	c	516	BCR	C16-C17-C18	-4.13	121.42	127.31
27	c	516	BCR	C28-C27-C26	-4.13	106.71	114.08
27	b	620	BCR	C28-C27-C26	-4.12	106.73	114.08
27	B	619	BCR	C15-C14-C13	-4.10	121.46	127.31
27	Z	101	BCR	C16-C17-C18	-4.09	121.48	127.31
31	b	624	LMG	O7-C10-C11	4.09	120.31	111.50
27	Z	101	BCR	C24-C23-C22	-4.08	120.07	126.23
27	b	621	BCR	C16-C17-C18	-4.07	121.50	127.31
23	A	407	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
27	B	620	BCR	C16-C17-C18	-4.06	121.51	127.31
27	b	621	BCR	C15-C14-C13	-4.06	121.52	127.31
30	F	102	SQD	O7-S-C6	4.05	111.75	106.94
27	D	405	BCR	C15-C14-C13	-4.04	121.54	127.31
27	B	617	BCR	C24-C23-C22	-4.03	120.14	126.23
23	B	613	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
27	K	102	BCR	C7-C8-C9	-4.02	120.16	126.23
27	A	410	BCR	C3-C4-C5	-4.02	106.91	114.08
31	M	101	LMG	O7-C10-C11	4.01	120.15	111.50
27	b	620	BCR	C24-C23-C22	-4.01	120.17	126.23
31	d	405	LMG	O7-C10-C11	4.01	120.14	111.50
30	D	409	SQD	O47-C7-C8	4.01	120.14	111.50
30	F	102	SQD	O9-S-C6	4.00	111.70	106.94
27	B	617	BCR	C33-C5-C6	-4.00	120.04	124.53
31	B	622	LMG	O7-C10-C11	3.99	120.10	111.50
31	M	102	LMG	O7-C10-C11	3.98	120.08	111.50
27	x	101	BCR	C24-C23-C22	-3.98	120.22	126.23
27	a	412	BCR	C38-C26-C25	-3.98	120.06	124.53
27	x	101	BCR	C33-C5-C6	-3.98	120.06	124.53
23	b	611	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
30	a	401	SQD	O47-C7-C8	3.97	120.06	111.50
34	v	201	HEM	C4C-CHD-C1D	3.97	127.80	122.56
27	B	620	BCR	C38-C26-C25	-3.96	120.08	124.53
27	T	103	BCR	C38-C26-C25	-3.96	120.08	124.53
30	F	102	SQD	O47-C7-C8	3.96	120.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	K	102	BCR	C38-C26-C25	-3.95	120.09	124.53
28	d	408	DGD	C3G-O3G-C1D	3.94	121.44	113.74
23	c	508	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
30	A	413	SQD	O9-S-C6	3.92	111.60	106.94
23	B	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
27	b	621	BCR	C20-C21-C22	-3.92	121.72	127.31
31	C	520	LMG	O7-C10-C11	3.91	119.94	111.50
30	A	417	SQD	O47-C7-C8	3.91	119.93	111.50
27	b	621	BCR	C38-C26-C25	-3.90	120.15	124.53
31	c	520	LMG	O7-C10-C11	3.90	119.90	111.50
23	B	612	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
23	B	608	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
31	b	623	LMG	O7-C10-C11	3.87	119.83	111.50
27	J	102	BCR	C7-C8-C9	-3.86	120.40	126.23
31	D	408	LMG	O1-C1-C2	3.86	114.34	108.30
23	C	508	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
30	F	102	SQD	C1-O5-C5	3.85	121.24	113.69
27	T	102	BCR	C33-C5-C6	-3.85	120.21	124.53
28	d	408	DGD	O2D-C2D-C1D	3.84	119.37	110.05
29	a	417	LHG	O7-C7-C8	3.84	119.77	111.50
30	f	103	SQD	O47-C7-C8	3.84	119.77	111.50
31	d	405	LMG	C7-O1-C1	3.83	121.22	113.74
27	k	102	BCR	C3-C4-C5	-3.82	107.26	114.08
27	D	405	BCR	C16-C17-C18	-3.81	121.87	127.31
29	A	415	LHG	O7-C7-C8	3.81	119.72	111.50
27	c	516	BCR	C11-C10-C9	-3.81	121.87	127.31
27	D	405	BCR	C33-C5-C6	-3.80	120.26	124.53
23	b	618	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
30	A	413	SQD	O9-S-O7	-3.79	100.83	113.95
23	b	606	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
27	k	102	BCR	C20-C21-C22	-3.77	121.92	127.31
27	B	620	BCR	C15-C14-C13	-3.76	121.94	127.31
28	D	410	DGD	O2D-C2D-C1D	3.76	119.18	110.05
30	f	103	SQD	O9-S-O7	-3.76	100.94	113.95
23	a	405	CLA	C1-C2-C3	-3.76	119.55	126.04
30	F	102	SQD	O9-S-O7	-3.75	100.97	113.95
28	c	518	DGD	O2G-C1B-C2B	3.75	119.58	111.50
28	D	410	DGD	C3G-O3G-C1D	3.74	121.05	113.74
23	B	603	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
30	d	407	SQD	C1-O5-C5	3.74	121.02	113.69
30	d	407	SQD	O9-S-O7	-3.73	101.03	113.95
31	C	519	LMG	O7-C10-C11	3.73	119.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	618	BCR	C38-C26-C25	-3.73	120.34	124.53
23	b	616	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
28	A	411	DGD	C1D-O6D-C5D	-3.72	106.38	113.69
27	B	620	BCR	C11-C10-C9	-3.71	122.01	127.31
27	K	102	BCR	C16-C17-C18	-3.71	122.02	127.31
23	a	405	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
30	D	409	SQD	O9-S-O7	-3.70	101.13	113.95
28	b	622	DGD	C1D-O6D-C5D	-3.70	106.42	113.69
27	C	515	BCR	C38-C26-C25	-3.70	120.38	124.53
23	b	609	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
28	A	411	DGD	O6D-C5D-C6D	3.69	114.11	106.67
30	a	415	SQD	O7-S-C6	3.69	111.32	106.94
28	B	621	DGD	C1D-O6D-C5D	-3.68	106.46	113.69
34	v	201	HEM	C4B-CHC-C1C	3.68	127.42	122.56
27	A	410	BCR	C38-C26-C25	-3.67	120.40	124.53
27	b	621	BCR	C4-C5-C6	-3.67	117.41	122.73
27	Z	101	BCR	C3-C4-C5	-3.66	107.53	114.08
23	C	507	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
27	B	620	BCR	C4-C5-C6	-3.66	117.42	122.73
25	d	404	PL9	C25-C24-C26	3.66	121.43	115.27
25	A	408	PL9	C25-C24-C26	3.66	121.43	115.27
27	B	620	BCR	C20-C21-C22	-3.65	122.10	127.31
30	a	415	SQD	O9-S-O7	-3.65	101.31	113.95
23	b	611	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
30	B	625	SQD	C44-O6-C1	3.64	120.86	113.74
30	a	401	SQD	C1-O5-C5	3.64	120.84	113.69
31	A	418	LMG	O7-C10-C11	3.64	119.35	111.50
31	D	406	LMG	O7-C10-C11	3.64	119.35	111.50
30	b	601	SQD	C44-O6-C1	3.64	120.85	113.74
27	c	515	BCR	C20-C21-C22	-3.64	122.12	127.31
28	B	626	DGD	C3G-O3G-C1D	3.63	120.84	113.74
27	c	515	BCR	C3-C4-C5	-3.63	107.59	114.08
30	A	417	SQD	C44-O6-C1	3.63	120.83	113.74
23	b	613	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
27	j	102	BCR	C16-C17-C18	-3.62	122.15	127.31
25	a	410	PL9	C35-C34-C36	3.62	121.36	115.27
31	D	407	LMG	O7-C10-C11	3.61	119.29	111.50
27	B	619	BCR	C20-C21-C22	-3.61	122.16	127.31
28	d	408	DGD	O5D-C1E-C2E	3.61	113.93	108.30
27	C	515	BCR	C20-C21-C22	-3.61	122.16	127.31
27	B	617	BCR	C38-C26-C25	-3.61	120.48	124.53
30	f	103	SQD	C1-O5-C5	3.61	120.77	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	412	BCR	C3-C4-C5	-3.60	107.65	114.08
30	a	415	SQD	O47-C7-C8	3.60	119.25	111.50
23	b	615	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
23	B	606	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
31	a	402	LMG	O7-C10-C11	3.59	119.24	111.50
30	A	413	SQD	O47-C7-C8	3.59	119.23	111.50
23	c	507	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	c	506	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
25	A	408	PL9	C7-C3-C4	3.58	119.79	116.88
25	D	404	PL9	C7-C3-C4	3.58	119.78	116.88
28	b	602	DGD	O5D-C1E-C2E	3.58	113.89	108.30
30	a	401	SQD	O5-C1-C2	3.57	117.92	110.35
28	b	602	DGD	C3G-O3G-C1D	3.57	120.71	113.74
23	B	610	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	D	404	PL9	C7-C8-C9	-3.57	120.86	126.79
23	b	617	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
28	C	517	DGD	O2G-C1B-C2B	3.56	119.17	111.50
29	A	412	LHG	O7-C7-C8	3.56	119.17	111.50
31	k	103	LMG	O7-C10-C11	3.56	119.17	111.50
30	B	625	SQD	O9-S-O7	-3.56	101.64	113.95
23	B	614	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
30	b	601	SQD	O9-S-O7	-3.55	101.66	113.95
28	C	518	DGD	O6D-C5D-C6D	3.54	113.81	106.67
27	c	514	BCR	C3-C4-C5	-3.54	107.76	114.08
27	T	102	BCR	C38-C26-C25	-3.53	120.56	124.53
30	A	413	SQD	C1-O5-C5	3.53	120.61	113.69
27	f	102	BCR	C24-C23-C22	-3.52	120.91	126.23
27	a	412	BCR	C24-C23-C22	-3.52	120.91	126.23
27	T	102	BCR	C20-C21-C22	-3.52	122.28	127.31
23	B	616	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
34	F	101	HEM	C4C-CHD-C1D	3.52	127.20	122.56
23	B	606	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
30	A	417	SQD	C1-O5-C5	3.51	120.58	113.69
27	J	102	BCR	C2-C1-C6	3.50	115.87	110.48
23	c	503	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
30	a	401	SQD	O5-C5-C4	3.50	116.04	109.69
27	C	515	BCR	C11-C10-C9	-3.49	122.32	127.31
23	C	506	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
27	c	515	BCR	C33-C5-C6	-3.49	120.61	124.53
23	c	504	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
30	b	601	SQD	O9-S-C6	3.48	111.08	106.94
23	C	504	CLA	CMB-C2B-C1B	-3.48	123.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	409	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
34	F	101	HEM	C3B-C2B-C1B	3.48	109.06	106.49
27	c	514	BCR	C35-C13-C14	-3.47	118.06	122.92
23	A	407	CLA	CMB-C2B-C3B	3.47	131.17	124.68
27	B	617	BCR	C20-C21-C22	-3.47	122.36	127.31
23	c	512	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
28	c	519	DGD	C2G-O2G-C1B	3.46	126.32	117.79
31	M	101	LMG	C6-C5-C4	-3.46	104.89	113.00
27	K	102	BCR	C15-C14-C13	-3.46	122.37	127.31
28	C	518	DGD	O5D-C1E-C2E	3.46	113.70	108.30
27	T	102	BCR	C11-C10-C9	-3.46	122.38	127.31
28	B	626	DGD	O2G-C1B-C2B	3.45	118.94	111.50
27	C	515	BCR	C16-C17-C18	-3.45	122.39	127.31
28	b	602	DGD	C3D-C4D-C5D	3.45	116.39	110.24
31	A	418	LMG	C7-O1-C1	3.44	120.47	113.74
27	b	620	BCR	C11-C10-C9	-3.44	122.39	127.31
29	a	414	LHG	O7-C7-C8	3.44	118.92	111.50
27	b	620	BCR	C20-C21-C22	-3.44	122.40	127.31
24	A	406	PHO	O2D-CGD-O1D	-3.44	117.11	123.84
25	D	404	PL9	C22-C23-C24	-3.43	119.39	127.66
27	B	617	BCR	C11-C10-C9	-3.43	122.41	127.31
27	H	101	BCR	C16-C17-C18	-3.43	122.42	127.31
27	c	516	BCR	C33-C5-C6	-3.43	120.68	124.53
27	B	619	BCR	C16-C17-C18	-3.42	122.42	127.31
31	d	406	LMG	O1-C1-C2	3.42	113.64	108.30
23	b	614	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
30	a	401	SQD	O9-S-O7	-3.42	102.13	113.95
23	c	504	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
23	c	510	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
27	C	514	BCR	C11-C10-C9	-3.41	122.45	127.31
27	j	102	BCR	C29-C30-C25	3.40	115.72	110.48
23	B	615	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
27	c	515	BCR	C16-C17-C18	-3.40	122.46	127.31
30	B	625	SQD	O9-S-C6	3.40	110.98	106.94
27	k	102	BCR	C7-C8-C9	-3.40	121.10	126.23
31	D	406	LMG	C7-O1-C1	3.39	120.37	113.74
23	D	403	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	b	611	CLA	CMB-C2B-C3B	3.39	131.02	124.68
23	b	610	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
27	Z	101	BCR	C33-C5-C6	-3.38	120.73	124.53
25	a	410	PL9	C25-C24-C26	3.38	120.95	115.27
28	C	516	DGD	O2G-C1B-C2B	3.38	118.78	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
27	c	514	BCR	C7-C6-C5	-3.37	113.30	121.46
25	A	408	PL9	C35-C34-C36	3.37	120.94	115.27
23	B	602	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
31	C	520	LMG	C7-O1-C1	3.37	120.32	113.74
23	b	619	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
23	b	609	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
23	C	502	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
27	B	619	BCR	C24-C23-C22	-3.36	121.16	126.23
34	f	101	HEM	C4C-CHD-C1D	3.36	126.99	122.56
31	i	101	LMG	O7-C10-C11	3.36	118.73	111.50
23	B	609	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
23	B	613	CLA	CMB-C2B-C3B	3.35	130.95	124.68
27	b	621	BCR	C33-C5-C4	3.35	120.05	113.62
34	f	101	HEM	C4B-CHC-C1C	3.35	126.97	122.56
30	D	409	SQD	C1-O5-C5	3.35	120.26	113.69
28	a	413	DGD	O6D-C5D-C6D	3.35	113.42	106.67
23	b	606	CLA	CMB-C2B-C3B	3.34	130.92	124.68
27	f	102	BCR	C11-C10-C9	-3.34	122.55	127.31
30	A	417	SQD	O9-S-O7	-3.33	102.41	113.95
23	a	404	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
27	B	620	BCR	C33-C5-C4	3.33	120.01	113.62
27	B	619	BCR	C3-C4-C5	-3.33	108.14	114.08
30	d	407	SQD	O5-C5-C4	3.32	115.73	109.69
31	M	101	LMG	C1-O6-C5	-3.31	107.18	113.69
27	x	101	BCR	C20-C21-C22	-3.31	122.58	127.31
23	B	605	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
27	c	514	BCR	C1-C6-C7	3.31	125.14	115.78
27	j	102	BCR	C31-C1-C2	3.31	122.13	108.91
31	A	414	LMG	C1-O6-C5	-3.30	107.20	113.69
30	a	401	SQD	O7-S-C6	3.30	110.87	106.94
28	C	517	DGD	O5D-C6D-C5D	-3.30	102.95	109.05
30	a	415	SQD	C1-O5-C5	3.30	120.16	113.69
23	d	402	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
27	b	620	BCR	C3-C4-C5	-3.29	108.19	114.08
27	a	412	BCR	C11-C10-C9	-3.29	122.61	127.31
30	f	103	SQD	C44-O6-C1	3.29	120.17	113.74
27	C	515	BCR	C33-C5-C6	-3.29	120.83	124.53
25	J	101	PL9	C25-C24-C26	3.29	120.80	115.27
27	A	410	BCR	C24-C23-C22	-3.29	121.27	126.23
23	A	403	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
23	D	401	CLA	CMB-C2B-C1B	-3.28	123.42	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	414	LMG	C7-O1-C1	3.28	120.14	113.74
23	b	605	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
25	j	101	PL9	C25-C24-C26	3.27	120.78	115.27
31	D	408	LMG	C7-O1-C1	3.27	120.14	113.74
27	C	515	BCR	C3-C4-C5	-3.27	108.23	114.08
23	B	607	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
27	x	101	BCR	C15-C14-C13	-3.27	122.64	127.31
27	J	102	BCR	C29-C30-C25	3.27	115.52	110.48
23	C	512	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
23	c	508	CLA	CMB-C2B-C3B	3.27	130.79	124.68
30	A	413	SQD	O8-S-C6	3.27	110.95	105.74
23	B	612	CLA	CMB-C2B-C3B	3.27	130.79	124.68
23	b	618	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	b	610	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
31	k	103	LMG	O8-C28-C29	3.26	122.13	111.91
27	j	102	BCR	C2-C1-C6	3.26	115.49	110.48
27	J	102	BCR	C31-C1-C2	3.26	121.93	108.91
27	C	514	BCR	C28-C27-C26	-3.25	108.27	114.08
23	b	614	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
30	f	103	SQD	O9-S-C6	3.25	110.80	106.94
23	C	509	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
27	H	101	BCR	C24-C23-C22	-3.25	121.32	126.23
28	C	518	DGD	C2G-O2G-C1B	3.25	125.79	117.79
23	d	403	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
27	T	102	BCR	C7-C8-C9	-3.25	121.33	126.23
30	a	401	SQD	C44-O6-C1	3.25	120.08	113.74
23	B	607	CLA	O2D-CGD-O1D	-3.24	117.49	123.84
28	a	413	DGD	C1D-O6D-C5D	-3.24	107.33	113.69
30	A	417	SQD	O5-C5-C4	3.24	115.58	109.69
27	C	514	BCR	C20-C21-C22	-3.24	122.69	127.31
31	M	102	LMG	C3-C4-C5	3.24	116.01	110.24
30	F	102	SQD	C44-O6-C1	3.23	120.05	113.74
25	D	404	PL9	C35-C34-C36	3.22	120.69	115.27
31	C	519	LMG	C1-O6-C5	-3.22	107.36	113.69
28	c	518	DGD	O3G-C1D-C2D	3.22	113.33	108.30
30	a	415	SQD	O9-S-C6	3.22	110.76	106.94
23	C	506	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
31	A	418	LMG	C6-C5-C4	-3.21	105.48	113.00
25	d	404	PL9	C7-C8-C9	-3.21	121.44	126.79
27	x	101	BCR	C10-C11-C12	-3.21	113.20	123.22
25	d	404	PL9	C7-C3-C2	-3.21	119.08	123.30
27	Z	101	BCR	C20-C21-C22	-3.21	122.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b	620	BCR	C16-C17-C18	-3.21	122.73	127.31
27	c	516	BCR	C38-C26-C25	-3.20	120.93	124.53
31	D	406	LMG	O8-C28-C29	3.20	121.94	111.91
23	b	604	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
23	C	513	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
31	D	408	LMG	C1-O6-C5	-3.19	107.42	113.69
27	B	619	BCR	C11-C10-C9	-3.19	122.76	127.31
27	T	103	BCR	C2-C1-C6	3.18	115.38	110.48
27	b	620	BCR	C33-C5-C6	-3.18	120.95	124.53
23	C	510	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	c	503	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	A	404	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
34	f	101	HEM	C3B-C2B-C1B	3.17	108.84	106.49
23	b	608	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
31	M	102	LMG	C6-C5-C4	-3.17	105.58	113.00
27	B	618	BCR	C4-C5-C6	-3.17	118.13	122.73
23	C	506	CLA	CMB-C2B-C3B	3.17	130.60	124.68
23	C	507	CLA	CMB-C2B-C3B	3.16	130.58	124.68
27	C	514	BCR	C34-C9-C10	-3.16	118.50	122.92
30	F	102	SQD	O5-C5-C4	3.16	115.42	109.69
31	M	102	LMG	C1-O6-C5	-3.16	107.50	113.69
34	V	201	HEM	C4C-CHD-C1D	3.15	126.72	122.56
23	a	406	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
23	B	603	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	d	404	PL9	C35-C34-C36	3.15	120.57	115.27
23	a	406	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	C	508	CLA	CMB-C2B-C3B	3.15	130.56	124.68
31	C	519	LMG	O8-C28-C29	3.15	121.78	111.91
23	C	503	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
25	d	404	PL9	C37-C38-C39	-3.14	120.09	127.66
27	C	514	BCR	C35-C13-C14	-3.14	118.52	122.92
27	j	102	BCR	C27-C26-C25	-3.14	118.17	122.73
23	b	615	CLA	CMB-C2B-C3B	3.14	130.55	124.68
30	A	417	SQD	O7-S-C6	3.14	110.67	106.94
28	c	517	DGD	O5D-C1E-C2E	3.13	113.19	108.30
27	a	412	BCR	C20-C21-C22	-3.13	122.84	127.31
28	a	413	DGD	C4D-C3D-C2D	-3.13	105.36	110.82
27	c	514	BCR	C34-C9-C10	-3.13	118.54	122.92
31	c	520	LMG	C1-O6-C5	-3.13	107.55	113.69
27	c	516	BCR	C3-C4-C5	-3.12	108.50	114.08
23	C	506	CLA	CHB-C4A-NA	3.12	128.83	124.51
23	c	511	CLA	CMB-C2B-C1B	-3.12	123.67	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	520	LMG	O8-C28-C29	3.11	121.68	111.91
23	b	607	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
30	a	415	SQD	C44-O6-C1	3.11	119.82	113.74
31	C	520	LMG	O1-C1-C2	3.11	113.16	108.30
28	c	518	DGD	O5D-C6D-C5D	-3.11	103.29	109.05
23	c	509	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
23	b	612	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
24	a	408	PHO	O1D-CGD-CBD	3.10	129.90	124.74
23	B	608	CLA	CMB-C2B-C3B	3.10	130.47	124.68
27	C	514	BCR	C1-C6-C7	3.09	124.53	115.78
23	c	513	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
23	B	614	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	c	507	CLA	CMB-C2B-C3B	3.09	130.46	124.68
23	c	506	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
28	c	517	DGD	O2G-C1B-C2B	3.09	118.15	111.50
30	a	415	SQD	O5-C5-C4	3.08	115.30	109.69
31	M	101	LMG	C3-C4-C5	3.08	115.74	110.24
23	b	609	CLA	CMB-C2B-C3B	3.08	130.44	124.68
23	b	616	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
23	c	501	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
31	e	101	LMG	C7-O1-C1	3.08	119.75	113.74
31	d	406	LMG	C7-O1-C1	3.07	119.75	113.74
23	A	405	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
31	d	406	LMG	O7-C10-C11	3.07	118.12	111.50
23	C	511	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
27	T	103	BCR	C4-C5-C6	-3.07	118.27	122.73
23	b	613	CLA	CMB-C2B-C3B	3.07	130.42	124.68
30	D	409	SQD	O5-C5-C4	3.06	115.26	109.69
27	T	103	BCR	C38-C26-C27	3.06	119.50	113.62
23	B	607	CLA	CHB-C4A-NA	3.06	128.75	124.51
23	b	617	CLA	CMB-C2B-C3B	3.06	130.41	124.68
24	a	408	PHO	CMB-C2B-C3B	3.06	130.40	124.68
23	C	510	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
34	f	101	HEM	C1B-NB-C4B	3.06	108.23	105.07
27	K	102	BCR	C24-C23-C22	-3.06	121.62	126.23
23	C	503	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
31	a	402	LMG	C6-C5-C4	-3.05	105.85	113.00
23	c	501	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
28	A	411	DGD	C3G-C2G-C1G	-3.05	104.58	111.79
27	Z	101	BCR	C11-C10-C9	-3.05	122.96	127.31
23	B	611	CLA	CMB-C2B-C3B	3.05	130.38	124.68
31	c	520	LMG	O8-C28-C29	3.04	121.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405	CLA	CMB-C2B-C3B	3.04	130.36	124.68
28	B	626	DGD	C3D-C4D-C5D	3.04	115.66	110.24
23	b	619	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
30	f	103	SQD	O8-S-C6	3.03	110.57	105.74
25	j	101	PL9	C7-C3-C2	-3.03	119.32	123.30
23	C	511	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
27	C	514	BCR	C16-C17-C18	-3.02	122.99	127.31
31	c	520	LMG	C7-O1-C1	3.02	119.64	113.74
23	b	616	CLA	CMB-C2B-C3B	3.02	130.33	124.68
30	A	417	SQD	O5-C1-C2	3.02	116.74	110.35
27	D	405	BCR	C16-C15-C14	-3.02	117.29	123.47
23	B	601	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
27	b	621	BCR	C2-C1-C6	3.02	115.12	110.48
23	b	608	CLA	CMB-C2B-C3B	3.01	130.32	124.68
31	b	623	LMG	O1-C1-C2	3.01	113.00	108.30
23	C	504	CLA	CMB-C2B-C3B	3.01	130.31	124.68
27	B	619	BCR	C7-C8-C9	-3.01	121.69	126.23
23	c	505	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
27	c	514	BCR	C28-C27-C26	-3.00	108.71	114.08
27	T	103	BCR	C33-C5-C4	3.00	119.39	113.62
23	B	610	CLA	CMB-C2B-C3B	3.00	130.29	124.68
27	C	514	BCR	C24-C23-C22	-3.00	121.70	126.23
31	B	622	LMG	O8-C28-C29	3.00	121.31	111.91
28	d	408	DGD	O5D-C6D-C5D	3.00	114.59	109.05
27	C	514	BCR	C7-C6-C5	-2.99	114.21	121.46
24	a	408	PHO	O2D-CGD-O1D	-2.99	118.00	123.84
23	B	604	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
28	B	626	DGD	C6D-C5D-C4D	-2.99	105.86	112.09
23	c	502	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
23	b	608	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
23	A	407	CLA	CHB-C4A-NA	2.98	128.63	124.51
23	a	409	CLA	CMB-C2B-C3B	2.98	130.25	124.68
34	F	101	HEM	C1B-NB-C4B	2.98	108.15	105.07
31	A	414	LMG	O8-C28-C29	2.98	121.25	111.91
28	c	519	DGD	O1G-C1A-C2A	2.97	121.24	111.91
23	b	608	CLA	CHB-C4A-NA	2.97	128.62	124.51
23	c	513	CLA	CHB-C4A-NA	2.97	128.62	124.51
31	d	406	LMG	C1-O6-C5	-2.97	107.86	113.69
23	B	606	CLA	CMB-C2B-C3B	2.97	130.24	124.68
27	D	405	BCR	C3-C4-C5	-2.97	108.78	114.08
23	b	613	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
23	b	606	CLA	O2D-CGD-O1D	-2.97	118.04	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	407	PHO	O2D-CGD-O1D	-2.97	118.04	123.84
23	b	604	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
23	B	616	CLA	CMB-C2B-C3B	2.96	130.22	124.68
23	C	502	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
25	J	101	PL9	C7-C3-C2	-2.96	119.41	123.30
23	c	506	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	D	403	CLA	CMB-C2B-C3B	2.96	130.21	124.68
23	C	505	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
27	j	102	BCR	C38-C26-C27	2.95	119.29	113.62
31	b	623	LMG	O4-C4-C3	-2.95	103.53	110.35
27	K	102	BCR	C33-C5-C6	-2.95	121.22	124.53
23	B	609	CLA	CMB-C2B-C3B	2.94	130.19	124.68
24	D	402	PHO	O2D-CGD-O1D	-2.94	118.08	123.84
31	D	408	LMG	O7-C10-C11	2.94	117.83	111.50
23	B	605	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	b	624	LMG	O8-C28-C29	2.94	121.13	111.91
23	c	503	CLA	CMB-C2B-C3B	2.94	130.17	124.68
25	a	410	PL9	C22-C23-C24	-2.93	120.60	127.66
27	J	102	BCR	C27-C26-C25	-2.93	118.47	122.73
27	f	102	BCR	C29-C30-C25	2.93	114.98	110.48
27	B	619	BCR	C33-C5-C6	-2.92	121.24	124.53
23	c	512	CLA	CMB-C2B-C3B	2.92	130.15	124.68
31	a	402	LMG	C3-C4-C5	2.92	115.45	110.24
27	c	514	BCR	C20-C21-C22	-2.92	123.14	127.31
28	a	413	DGD	C3G-C2G-C1G	-2.92	104.89	111.79
30	f	103	SQD	O5-C5-C4	2.92	114.99	109.69
23	D	401	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
31	E	101	LMG	O8-C28-C29	2.91	121.05	111.91
31	I	101	LMG	O7-C10-C11	2.91	117.78	111.50
31	D	407	LMG	O8-C28-C29	2.91	121.05	111.91
23	B	611	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	D	403	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
31	b	624	LMG	O1-C1-C2	2.91	112.85	108.30
31	a	416	LMG	O8-C28-C29	2.91	121.04	111.91
27	f	102	BCR	C38-C26-C27	2.90	119.20	113.62
27	C	514	BCR	C38-C26-C25	-2.90	121.27	124.53
23	B	604	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
31	k	103	LMG	C1-O6-C5	-2.90	108.00	113.69
25	a	410	PL9	C7-C3-C2	-2.90	119.49	123.30
30	a	415	SQD	O8-S-C6	2.90	110.36	105.74
27	c	516	BCR	C20-C21-C22	-2.90	123.18	127.31
28	A	411	DGD	O4D-C4D-C5D	-2.89	102.11	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	CMB-C2B-C3B	2.89	130.09	124.68
23	B	601	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	D	405	BCR	C38-C26-C27	2.89	119.17	113.62
25	D	404	PL9	C7-C3-C2	-2.88	119.51	123.30
34	v	201	HEM	C1B-NB-C4B	2.88	108.05	105.07
23	c	502	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	c	509	CLA	CHB-C4A-NA	2.88	128.50	124.51
27	j	102	BCR	C33-C5-C6	-2.88	121.29	124.53
23	B	605	CLA	CMB-C2B-C3B	2.88	130.07	124.68
31	D	406	LMG	O8-C28-O10	-2.88	116.33	123.59
25	D	404	PL9	C25-C24-C26	2.88	120.11	115.27
28	b	602	DGD	O2G-C1B-C2B	2.87	117.70	111.50
23	c	511	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	C	505	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
28	B	621	DGD	O3D-C3D-C4D	2.87	116.99	110.35
28	C	516	DGD	O5D-C1E-C2E	2.87	112.78	108.30
31	E	101	LMG	C7-O1-C1	2.87	119.34	113.74
23	B	609	CLA	C1-C2-C3	-2.87	121.08	126.04
31	a	402	LMG	C7-O1-C1	2.87	119.34	113.74
23	B	614	CLA	CMB-C2B-C3B	2.87	130.04	124.68
31	d	405	LMG	O8-C28-C29	2.87	120.91	111.91
27	K	102	BCR	C11-C10-C9	-2.87	123.22	127.31
23	c	504	CLA	CHB-C4A-NA	2.86	128.47	124.51
31	a	416	LMG	C1-O6-C5	-2.86	108.07	113.69
30	a	401	SQD	C1-C2-C3	2.86	115.95	110.00
28	B	626	DGD	O5D-C1E-C2E	2.86	112.77	108.30
28	D	410	DGD	O5D-C1E-C2E	2.86	112.77	108.30
24	A	406	PHO	CMB-C2B-C3B	2.86	130.02	124.68
28	C	518	DGD	O1G-C1A-C2A	2.86	120.87	111.91
27	H	101	BCR	C15-C14-C13	-2.86	123.23	127.31
24	a	407	PHO	O1D-CGD-CBD	2.85	129.48	124.74
23	b	605	CLA	CMB-C2B-C3B	2.84	130.00	124.68
31	C	519	LMG	C7-O1-C1	2.84	119.29	113.74
23	d	402	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
23	b	612	CLA	CMB-C2B-C3B	2.84	129.99	124.68
31	A	418	LMG	C3-C4-C5	2.84	115.30	110.24
25	d	404	PL9	C22-C23-C24	-2.84	120.83	127.66
23	B	615	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
27	b	620	BCR	C29-C30-C25	2.83	114.84	110.48
23	c	509	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	B	618	BCR	C33-C5-C4	2.83	119.06	113.62
23	C	502	CLA	CMB-C2B-C3B	2.83	129.97	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	E	101	LMG	C8-O7-C10	2.83	124.75	117.79
30	d	407	SQD	O7-S-C6	2.83	110.30	106.94
27	B	618	BCR	C2-C1-C6	2.82	114.82	110.48
27	B	617	BCR	C3-C4-C5	-2.82	109.05	114.08
31	A	418	LMG	O8-C28-C29	2.82	120.75	111.91
23	b	611	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
28	c	519	DGD	C4D-C3D-C2D	-2.81	105.91	110.82
23	A	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	B	602	CLA	CMB-C2B-C3B	2.81	129.94	124.68
28	c	517	DGD	C1D-O6D-C5D	-2.81	108.17	113.69
28	b	622	DGD	O3D-C3D-C4D	2.81	116.84	110.35
23	a	409	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
28	C	517	DGD	O1G-C1A-C2A	2.81	120.72	111.91
31	b	623	LMG	C1-O6-C5	-2.81	108.18	113.69
27	T	103	BCR	C23-C24-C25	-2.81	119.32	127.20
23	b	611	CLA	CHB-C4A-NA	2.81	128.39	124.51
30	a	415	SQD	O6-C1-C2	2.80	112.68	108.30
23	C	513	CLA	CHB-C4A-NA	2.80	128.39	124.51
23	d	402	CLA	CMB-C2B-C3B	2.80	129.92	124.68
24	A	406	PHO	O1D-CGD-CBD	2.80	129.40	124.74
27	J	102	BCR	C33-C5-C6	-2.80	121.38	124.53
23	C	507	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
28	c	519	DGD	O6D-C5D-C6D	2.80	112.32	106.67
27	K	102	BCR	C20-C21-C22	-2.80	123.31	127.31
23	b	610	CLA	CMB-C2B-C3B	2.80	129.91	124.68
27	A	410	BCR	C11-C10-C9	-2.80	123.32	127.31
23	C	501	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
27	c	515	BCR	C24-C23-C22	-2.79	122.02	126.23
23	C	509	CLA	CHB-C4A-NA	2.79	128.37	124.51
23	c	508	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
28	C	518	DGD	C4D-C3D-C2D	-2.79	105.96	110.82
27	f	102	BCR	C38-C26-C25	-2.79	121.40	124.53
23	b	617	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	b	605	CLA	CHB-C4A-NA	2.78	128.35	124.51
23	D	401	CLA	CMB-C2B-C3B	2.78	129.88	124.68
31	b	624	LMG	C1-O6-C5	-2.78	108.24	113.69
23	C	506	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
23	c	502	CLA	CHB-C4A-NA	2.77	128.35	124.51
23	C	509	CLA	CMB-C2B-C3B	2.77	129.86	124.68
25	A	408	PL9	C22-C23-C24	-2.77	120.99	127.66
27	H	101	BCR	C38-C26-C25	-2.77	121.42	124.53
23	B	615	CLA	CMB-C2B-C3B	2.77	129.86	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	c	513	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
25	d	404	PL9	C40-C39-C41	2.77	119.92	115.27
23	c	507	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
31	a	402	LMG	O8-C28-C29	2.76	120.57	111.91
31	B	622	LMG	O1-C1-C2	2.76	112.61	108.30
23	a	405	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
27	H	101	BCR	C20-C21-C22	-2.76	123.38	127.31
23	c	510	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
30	A	417	SQD	C1-C2-C3	2.75	115.73	110.00
23	c	510	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	b	615	CLA	CHB-C4A-NA	2.75	128.32	124.51
31	I	101	LMG	O8-C28-C29	2.75	120.53	111.91
27	x	101	BCR	C16-C17-C18	-2.75	123.39	127.31
27	J	102	BCR	C35-C13-C14	-2.75	119.08	122.92
30	b	601	SQD	O47-C7-C8	2.75	117.42	111.50
27	B	618	BCR	C38-C26-C27	2.74	118.88	113.62
27	A	410	BCR	C20-C21-C22	-2.74	123.40	127.31
23	B	610	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
27	k	102	BCR	C33-C5-C6	-2.74	121.46	124.53
27	D	405	BCR	C23-C24-C25	-2.74	119.52	127.20
30	B	625	SQD	O5-C5-C4	2.73	114.66	109.69
23	b	612	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
28	a	413	DGD	O4D-C4D-C5D	-2.73	102.52	109.30
28	c	518	DGD	C4D-C3D-C2D	-2.73	106.06	110.82
31	I	101	LMG	C7-O1-C1	2.73	119.06	113.74
23	C	512	CLA	CHB-C4A-NA	2.72	128.28	124.51
30	b	601	SQD	O5-C5-C4	2.72	114.64	109.69
23	c	505	CLA	CHB-C4A-NA	2.72	128.28	124.51
28	D	410	DGD	O5D-C6D-C5D	2.72	114.08	109.05
31	C	520	LMG	C1-O6-C5	-2.72	108.34	113.69
23	b	610	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	C	513	CLA	CMB-C2B-C3B	2.72	129.76	124.68
23	c	513	CLA	CMB-C2B-C3B	2.72	129.76	124.68
31	C	520	LMG	C6-C5-C4	-2.72	106.64	113.00
31	A	418	LMG	C1-O6-C5	-2.72	108.36	113.69
27	B	618	BCR	C29-C30-C25	2.72	114.66	110.48
23	a	409	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
31	d	405	LMG	O8-C28-O10	-2.71	116.75	123.59
23	A	404	CLA	CMB-C2B-C3B	2.71	129.74	124.68
23	a	404	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
30	D	409	SQD	O7-S-C6	2.70	110.15	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Z	101	BCR	C28-C27-C26	-2.70	109.26	114.08
31	b	623	LMG	O8-C28-C29	2.70	120.37	111.91
27	f	102	BCR	C16-C15-C14	-2.70	117.95	123.47
23	b	618	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
23	a	409	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	B	608	CLA	C1-C2-C3	-2.69	121.39	126.04
23	d	403	CLA	CMB-C2B-C3B	2.69	129.71	124.68
28	d	408	DGD	O1G-C1A-C2A	2.69	120.34	111.91
31	i	101	LMG	C7-O1-C1	2.69	118.99	113.74
27	H	101	BCR	C8-C7-C6	-2.69	119.66	127.20
23	b	618	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	B	616	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	B	609	CLA	CHB-C4A-NA	2.68	128.22	124.51
27	H	101	BCR	C10-C11-C12	-2.68	114.85	123.22
23	C	502	CLA	CHB-C4A-NA	2.68	128.22	124.51
27	T	103	BCR	C29-C30-C25	2.68	114.61	110.48
33	D	411	LMT	C1B-O1B-C4'	-2.68	111.33	117.96
31	D	407	LMG	C7-O1-C1	2.68	118.97	113.74
23	B	609	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	C	504	CLA	CHB-C4A-NA	2.68	128.21	124.51
27	B	618	BCR	C21-C20-C19	-2.67	114.87	123.22
31	i	101	LMG	O8-C28-C29	2.67	120.30	111.91
25	J	101	PL9	C15-C14-C16	2.67	119.77	115.27
23	d	403	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
23	c	506	CLA	CHB-C4A-NA	2.67	128.20	124.51
31	a	402	LMG	C1-O6-C5	-2.67	108.45	113.69
25	a	410	PL9	C12-C13-C14	-2.67	121.24	127.66
23	a	405	CLA	CHB-C4A-NA	2.67	128.20	124.51
33	B	627	LMT	O1B-C4'-C3'	2.66	114.37	107.28
23	b	606	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
27	J	102	BCR	C38-C26-C27	2.66	118.73	113.62
31	D	408	LMG	O8-C28-C29	2.66	120.26	111.91
23	A	407	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
23	C	512	CLA	CMB-C2B-C3B	2.66	129.65	124.68
23	A	404	CLA	CHD-C1D-ND	-2.66	122.01	124.45
23	a	404	CLA	C1-C2-C3	-2.65	121.45	126.04
31	d	406	LMG	C1-C2-C3	-2.65	104.48	110.00
23	b	619	CLA	CMB-C2B-C3B	2.65	129.63	124.68
31	e	101	LMG	O8-C28-C29	2.64	120.21	111.91
23	c	508	CLA	CHB-C4A-NA	2.64	128.17	124.51
25	D	404	PL9	C37-C38-C39	-2.64	121.30	127.66
23	B	611	CLA	CHB-C4A-NA	2.64	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	C	513	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
27	T	102	BCR	C36-C18-C17	-2.64	119.23	122.92
31	E	101	LMG	O7-C10-C11	2.64	117.18	111.50
25	D	404	PL9	C12-C13-C14	-2.64	121.31	127.66
23	c	509	CLA	CMB-C2B-C3B	2.63	129.61	124.68
23	B	607	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
27	c	516	BCR	C29-C30-C25	2.63	114.53	110.48
27	B	620	BCR	C2-C1-C6	2.63	114.53	110.48
23	c	504	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	c	506	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
30	A	413	SQD	O5-C5-C4	2.63	114.46	109.69
24	D	402	PHO	O1D-CGD-CBD	2.63	129.11	124.74
27	J	102	BCR	C1-C6-C5	-2.62	118.92	122.61
27	j	102	BCR	C39-C30-C25	-2.62	106.05	110.30
28	A	411	DGD	C4D-C3D-C2D	-2.62	106.25	110.82
30	A	413	SQD	C44-O6-C1	2.61	118.84	113.74
23	c	508	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
28	a	413	DGD	C6E-C5E-C4E	-2.61	106.89	113.00
31	A	418	LMG	O3-C3-C4	-2.61	104.31	110.35
30	B	625	SQD	O47-C7-C8	2.61	117.12	111.50
28	b	602	DGD	O1G-C1A-C2A	2.61	120.09	111.91
28	D	410	DGD	O1G-C1A-C2A	2.61	120.09	111.91
23	C	513	CLA	CHD-C1D-ND	-2.61	122.06	124.45
28	b	622	DGD	O2G-C1B-C2B	2.61	117.12	111.50
27	B	617	BCR	C23-C24-C25	-2.61	119.88	127.20
23	b	607	CLA	C1-C2-C3	-2.60	121.54	126.04
27	Z	101	BCR	C8-C7-C6	-2.60	119.89	127.20
28	b	622	DGD	C3G-O3G-C1D	2.60	118.82	113.74
23	c	511	CLA	CMB-C2B-C3B	2.60	129.54	124.68
28	A	411	DGD	C6D-C5D-C4D	-2.60	106.67	112.09
23	b	605	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
33	T	101	LMT	O1B-C4'-C3'	2.59	114.16	107.28
23	A	405	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	d	406	LMG	O8-C28-C29	2.59	120.02	111.91
23	c	512	CLA	CHB-C4A-NA	2.58	128.08	124.51
27	x	101	BCR	C3-C4-C5	-2.58	109.47	114.08
27	T	103	BCR	C21-C20-C19	-2.58	115.16	123.22
23	C	501	CLA	CHB-C4A-NA	2.58	128.08	124.51
27	T	102	BCR	C3-C4-C5	-2.58	109.47	114.08
23	B	606	CLA	CHB-C4A-NA	2.58	128.07	124.51
23	B	605	CLA	CHB-C4A-NA	2.58	128.07	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	612	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
23	a	404	CLA	CHB-C4A-NA	2.57	128.07	124.51
27	H	101	BCR	C33-C5-C4	2.57	118.56	113.62
30	D	409	SQD	O8-S-C6	2.57	109.83	105.74
23	b	616	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	D	405	BCR	C29-C30-C25	2.57	114.44	110.48
31	D	408	LMG	C1-C2-C3	-2.57	104.65	110.00
23	C	512	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	b	608	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	c	502	CLA	CMB-C2B-C3B	2.57	129.48	124.68
23	c	501	CLA	CMB-C2B-C3B	2.56	129.48	124.68
27	H	101	BCR	C35-C13-C12	2.56	122.11	118.08
27	c	515	BCR	C8-C7-C6	-2.56	120.01	127.20
28	C	516	DGD	C3G-O3G-C1D	2.56	118.74	113.74
23	C	511	CLA	CMB-C2B-C3B	2.56	129.46	124.68
31	D	406	LMG	C3-C4-C5	2.56	114.80	110.24
27	c	515	BCR	C7-C8-C9	-2.55	122.38	126.23
23	b	606	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	a	410	PL9	C20-C19-C21	2.55	119.57	115.27
23	d	403	CLA	CHB-C4A-NA	2.55	128.04	124.51
30	B	625	SQD	O48-C23-C24	2.55	119.92	111.91
23	A	403	CLA	CHB-C4A-NA	2.55	128.04	124.51
34	F	101	HEM	CBA-CAA-C2A	-2.55	108.27	112.62
28	A	411	DGD	O1G-C1A-C2A	2.55	119.90	111.91
27	D	405	BCR	C27-C26-C25	-2.54	119.04	122.73
23	C	501	CLA	CHD-C1D-ND	-2.54	122.12	124.45
23	B	609	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
23	C	511	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	J	101	PL9	C12-C13-C14	-2.54	121.54	127.66
23	b	612	CLA	CHB-C4A-NA	2.54	128.02	124.51
28	B	621	DGD	C3G-O3G-C1D	2.54	118.70	113.74
30	A	417	SQD	O8-S-C6	2.54	109.78	105.74
31	M	102	LMG	O8-C28-C29	2.54	119.87	111.91
23	b	618	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
25	D	404	PL9	C42-C43-C44	-2.53	121.56	127.66
31	M	101	LMG	O8-C28-C29	2.53	119.86	111.91
25	d	404	PL9	C15-C14-C16	2.53	119.53	115.27
23	A	404	CLA	C1-C2-C3	-2.53	121.67	126.04
27	j	102	BCR	C11-C12-C13	-2.53	119.31	126.42
27	B	618	BCR	C23-C24-C25	-2.53	120.10	127.20
23	C	508	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
27	K	102	BCR	C33-C5-C4	2.53	118.47	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
29	A	415	LHG	O8-C23-C24	2.52	119.82	111.91
27	c	514	BCR	C24-C23-C22	-2.52	122.43	126.23
31	I	101	LMG	C1-O6-C5	-2.52	108.75	113.69
23	C	509	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
23	b	607	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	b	607	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
23	a	404	CLA	O2A-CGA-O1A	-2.51	117.25	123.59
23	B	611	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
27	j	102	BCR	C37-C22-C21	-2.51	119.40	122.92
27	B	619	BCR	C29-C30-C25	2.51	114.35	110.48
27	T	102	BCR	C36-C18-C19	2.51	122.03	118.08
23	C	504	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	B	613	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	D	405	BCR	C21-C20-C19	-2.51	115.39	123.22
23	A	404	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	A	405	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	C	507	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
23	c	513	CLA	CHD-C1D-ND	-2.50	122.15	124.45
31	C	519	LMG	C6-C5-C4	-2.50	107.14	113.00
31	e	101	LMG	O1-C1-C2	2.50	112.21	108.30
23	B	615	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	c	503	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	b	610	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	b	617	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	C	504	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
23	b	605	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
31	c	520	LMG	O1-C1-C2	2.49	112.20	108.30
23	A	403	CLA	CMB-C2B-C3B	2.49	129.34	124.68
23	a	405	CLA	CHD-C1D-ND	-2.49	122.16	124.45
23	C	512	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
23	B	602	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	c	513	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
28	a	413	DGD	O1G-C1A-C2A	2.49	119.72	111.91
23	b	609	CLA	CHB-C4A-NA	2.49	127.95	124.51
31	D	407	LMG	C4-C3-C2	2.49	115.17	110.82
23	A	404	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
31	k	103	LMG	O8-C28-O10	-2.49	117.31	123.59
28	C	516	DGD	C6E-C5E-C4E	-2.48	107.19	113.00
27	C	515	BCR	C29-C30-C25	2.48	114.30	110.48
23	B	602	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
28	b	622	DGD	O1G-C1A-C2A	2.48	119.68	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	501	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	a	406	CLA	CMB-C2B-C3B	2.48	129.31	124.68
27	C	515	BCR	C38-C26-C27	2.47	118.36	113.62
23	a	404	CLA	CMB-C2B-C3B	2.47	129.30	124.68
23	c	511	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	B	619	BCR	C27-C26-C25	-2.47	119.15	122.73
31	b	623	LMG	C7-O1-C1	2.47	118.56	113.74
31	B	622	LMG	C1-O6-C5	-2.46	108.85	113.69
27	H	101	BCR	C3-C4-C5	-2.46	109.68	114.08
23	a	406	CLA	C1-C2-C3	-2.46	121.78	126.04
23	B	603	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	d	404	PL9	C32-C33-C34	-2.46	121.73	127.66
23	D	403	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	B	604	CLA	CMB-C2B-C3B	2.46	129.28	124.68
23	B	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
31	e	101	LMG	C8-O7-C10	2.46	123.84	117.79
31	I	101	LMG	O1-C1-C2	2.46	112.14	108.30
27	J	102	BCR	C36-C18-C17	-2.46	119.48	122.92
23	b	618	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
23	C	506	CLA	CAA-CBA-CGA	-2.46	106.08	113.25
23	C	501	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
27	D	405	BCR	C38-C26-C25	-2.45	121.77	124.53
23	B	616	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
23	B	604	CLA	C1-C2-C3	-2.45	121.80	126.04
23	B	612	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
23	D	403	CLA	CHB-C4A-NA	2.45	127.90	124.51
28	a	413	DGD	C3D-C4D-C5D	2.45	114.61	110.24
23	B	613	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
34	f	101	HEM	CBA-CAA-C2A	-2.45	108.44	112.62
25	j	101	PL9	C12-C13-C14	-2.45	121.76	127.66
23	B	605	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	C	503	CLA	CMB-C2B-C3B	2.44	129.25	124.68
28	B	621	DGD	O2G-C1B-C2B	2.44	116.77	111.50
23	A	403	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
23	C	508	CLA	CHB-C4A-NA	2.44	127.89	124.51
29	a	417	LHG	O8-C23-C24	2.44	119.57	111.91
27	T	103	BCR	C24-C23-C22	-2.44	122.55	126.23
23	c	505	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
23	c	512	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
27	J	102	BCR	C11-C12-C13	-2.44	119.57	126.42
27	j	102	BCR	C1-C6-C5	-2.44	119.18	122.61
23	b	614	CLA	CMB-C2B-C3B	2.44	129.23	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	517	DGD	O1G-C1A-C2A	2.43	119.55	111.91
28	B	626	DGD	O6D-C1D-O3G	2.43	115.73	109.97
30	a	401	SQD	O8-S-C6	2.43	109.61	105.74
28	c	519	DGD	O5D-C1E-C2E	2.43	112.09	108.30
33	b	625	LMT	C1B-O1B-C4'	-2.43	111.96	117.96
28	c	518	DGD	O1G-C1A-C2A	2.43	119.52	111.91
27	Z	101	BCR	C15-C16-C17	-2.42	118.51	123.47
30	b	601	SQD	O48-C23-C24	2.42	119.51	111.91
31	c	520	LMG	C6-C5-C4	-2.42	107.33	113.00
23	a	409	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
23	a	404	CLA	CHD-C1D-ND	-2.42	122.23	124.45
23	c	509	CLA	C1-C2-C3	-2.42	121.86	126.04
25	A	408	PL9	C20-C19-C21	2.42	119.34	115.27
31	i	101	LMG	C1-O6-C5	-2.42	108.94	113.69
28	A	411	DGD	O3D-C3D-C4D	2.42	115.94	110.35
23	c	507	CLA	C1-C2-C3	-2.42	121.86	126.04
33	B	624	LMT	C1B-O1B-C4'	-2.41	111.99	117.96
27	f	102	BCR	C3-C4-C5	-2.41	109.77	114.08
30	A	413	SQD	O48-C23-C24	2.41	119.47	111.91
25	D	404	PL9	C32-C33-C34	-2.41	121.85	127.66
31	D	408	LMG	O8-C28-O10	-2.41	117.51	123.59
23	c	505	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	b	611	CLA	CHD-C1D-ND	-2.41	122.24	124.45
30	F	102	SQD	O8-S-C6	2.41	109.58	105.74
30	d	407	SQD	O8-S-C6	2.41	109.58	105.74
23	B	613	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
23	b	609	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
27	C	515	BCR	C23-C24-C25	-2.41	120.44	127.20
25	D	404	PL9	C40-C39-C41	2.40	119.31	115.27
27	H	101	BCR	C16-C15-C14	-2.40	118.56	123.47
23	B	611	CLA	C1-C2-C3	-2.40	121.89	126.04
23	b	614	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	B	605	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
28	C	517	DGD	O6E-C1E-C2E	2.39	115.42	110.35
27	b	620	BCR	C27-C26-C25	-2.39	119.26	122.73
34	F	101	HEM	C4B-CHC-C1C	2.39	125.72	122.56
23	C	510	CLA	CHD-C1D-ND	-2.39	122.25	124.45
25	D	404	PL9	C15-C14-C16	2.39	119.30	115.27
27	C	514	BCR	C23-C24-C25	-2.39	120.49	127.20
25	j	101	PL9	C22-C23-C24	-2.39	121.91	127.66
27	k	102	BCR	C24-C23-C22	-2.39	122.63	126.23
27	c	516	BCR	C23-C24-C25	-2.39	120.50	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
27	x	101	BCR	C34-C9-C8	2.39	121.84	118.08
27	B	617	BCR	C36-C18-C17	-2.39	119.58	122.92
27	J	102	BCR	C37-C22-C21	-2.39	119.58	122.92
23	b	613	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
24	a	407	PHO	CMC-C2C-C3C	2.38	129.43	124.94
23	b	617	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
27	T	103	BCR	C15-C16-C17	-2.38	118.60	123.47
31	E	101	LMG	O9-C10-C11	-2.38	114.45	123.73
27	c	514	BCR	C38-C26-C25	-2.38	121.86	124.53
23	B	603	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
27	c	516	BCR	C15-C16-C17	-2.38	118.61	123.47
34	F	101	HEM	CMC-C2C-C3C	2.38	129.12	124.68
28	b	602	DGD	O6D-C1D-O3G	2.38	115.60	109.97
28	C	517	DGD	O3G-C1D-C2D	2.38	112.01	108.30
23	B	603	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
31	C	519	LMG	O8-C28-O10	-2.37	117.60	123.59
23	c	502	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
30	B	625	SQD	C1-O5-C5	2.37	118.35	113.69
23	c	510	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
27	C	515	BCR	C15-C16-C17	-2.37	118.61	123.47
30	F	102	SQD	O5-C1-C2	2.37	115.37	110.35
34	F	101	HEM	CHB-C1B-NB	2.37	127.31	124.38
23	d	402	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
27	c	515	BCR	C38-C26-C25	-2.37	121.87	124.53
25	a	410	PL9	C32-C33-C34	-2.37	121.96	127.66
23	b	613	CLA	CHB-C4A-NA	2.37	127.79	124.51
30	D	409	SQD	O48-C23-C24	2.37	119.34	111.91
23	B	608	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
31	b	624	LMG	C3-C4-C5	2.37	114.46	110.24
23	b	607	CLA	CHB-C4A-NA	2.37	127.78	124.51
28	c	517	DGD	C6E-C5E-C4E	-2.37	107.46	113.00
27	k	102	BCR	C37-C22-C21	-2.37	119.61	122.92
28	d	408	DGD	O2G-C1B-C2B	2.37	116.60	111.50
31	e	101	LMG	O7-C10-O9	-2.37	117.99	123.70
27	j	102	BCR	C35-C13-C14	-2.37	119.61	122.92
23	B	615	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
25	j	101	PL9	C15-C14-C16	2.36	119.24	115.27
31	D	407	LMG	C1-O6-C5	-2.36	109.06	113.69
27	f	102	BCR	C23-C24-C25	-2.36	120.58	127.20
23	b	604	CLA	CMB-C2B-C3B	2.36	129.09	124.68
27	C	514	BCR	C39-C30-C25	-2.36	106.47	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
27	x	101	BCR	C35-C13-C12	2.36	121.79	118.08
27	a	412	BCR	C28-C27-C26	-2.35	109.88	114.08
23	c	507	CLA	CHB-C4A-NA	2.35	127.77	124.51
28	D	410	DGD	O2G-C1B-C2B	2.35	116.57	111.50
25	A	408	PL9	C10-C9-C11	2.35	119.22	115.27
31	i	101	LMG	O8-C28-O10	-2.34	117.67	123.59
28	B	621	DGD	O1G-C1A-C2A	2.34	119.27	111.91
31	b	624	LMG	C7-O1-C1	2.34	118.32	113.74
23	B	603	CLA	CHD-C1D-ND	-2.34	122.30	124.45
31	I	101	LMG	C6-C5-C4	-2.34	107.52	113.00
27	b	620	BCR	C38-C26-C27	2.34	118.12	113.62
23	d	403	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	B	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
27	J	102	BCR	C39-C30-C25	-2.34	106.50	110.30
23	c	507	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	c	513	CLA	C1-C2-C3	-2.34	122.00	126.04
30	F	102	SQD	O48-C23-C24	2.34	119.24	111.91
27	x	101	BCR	C38-C26-C25	-2.34	121.91	124.53
27	c	516	BCR	C38-C26-C27	2.34	118.10	113.62
27	k	102	BCR	C15-C16-C17	-2.33	118.69	123.47
31	d	405	LMG	C3-C4-C5	2.33	114.40	110.24
23	b	615	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
24	a	407	PHO	CMB-C2B-C3B	2.33	129.04	124.68
23	a	405	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
23	C	511	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
28	a	413	DGD	O3D-C3D-C4D	2.33	115.73	110.35
27	T	102	BCR	C28-C27-C26	-2.33	109.92	114.08
27	Z	101	BCR	C23-C24-C25	-2.33	120.67	127.20
25	d	404	PL9	C36-C34-C33	-2.32	116.41	121.12
27	f	102	BCR	C33-C5-C4	2.32	118.08	113.62
23	B	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	C	507	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
25	j	101	PL9	C20-C19-C21	2.32	119.18	115.27
28	B	626	DGD	O1G-C1A-C2A	2.32	119.19	111.91
27	B	620	BCR	C32-C1-C6	-2.32	106.53	110.30
27	b	621	BCR	C28-C27-C26	-2.32	109.93	114.08
27	D	405	BCR	C36-C18-C19	2.32	121.73	118.08
31	k	103	LMG	C6-C5-C4	-2.32	107.57	113.00
25	D	404	PL9	C10-C9-C11	2.32	119.17	115.27
31	e	101	LMG	O7-C10-C11	2.32	116.50	111.50
27	A	410	BCR	C34-C9-C10	-2.31	119.68	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	403	CLA	CHD-C1D-ND	-2.31	122.33	124.45
23	d	402	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
27	T	102	BCR	C23-C24-C25	-2.31	120.71	127.20
25	J	101	PL9	C20-C19-C21	2.31	119.16	115.27
23	B	604	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
28	C	517	DGD	C1D-O6D-C5D	-2.31	109.15	113.69
23	C	513	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
27	Z	101	BCR	C7-C8-C9	-2.31	122.75	126.23
25	d	404	PL9	C12-C13-C14	-2.31	122.10	127.66
28	b	602	DGD	C6D-C5D-C4D	-2.31	107.27	112.09
23	B	610	CLA	CHD-C1D-ND	-2.31	122.33	124.45
23	B	616	CLA	CHB-C4A-NA	2.31	127.70	124.51
27	c	515	BCR	C28-C27-C26	-2.31	109.96	114.08
23	B	607	CLA	O2D-CGD-CBD	2.31	115.36	111.27
27	f	102	BCR	C27-C26-C25	-2.31	119.38	122.73
23	B	601	CLA	CMB-C2B-C3B	2.30	128.99	124.68
34	V	201	HEM	C4B-CHC-C1C	2.30	125.60	122.56
27	c	514	BCR	C33-C5-C4	2.30	118.04	113.62
23	C	505	CLA	CBA-CAA-C2A	2.30	120.66	113.86
30	a	401	SQD	O48-C23-C24	2.30	119.13	111.91
23	b	611	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
28	C	516	DGD	O1G-C1A-C2A	2.30	119.12	111.91
25	a	410	PL9	C15-C14-C16	2.30	119.13	115.27
23	B	612	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	C	506	CLA	CHD-C1D-ND	-2.29	122.34	124.45
23	c	511	CLA	CHD-C1D-ND	-2.29	122.35	124.45
27	f	102	BCR	C21-C20-C19	-2.29	116.06	123.22
23	B	606	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	C	502	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
27	f	102	BCR	C36-C18-C19	2.29	121.68	118.08
27	x	101	BCR	C8-C7-C6	-2.29	120.77	127.20
23	C	505	CLA	CMB-C2B-C3B	2.29	128.96	124.68
30	a	415	SQD	O48-C23-C24	2.29	119.08	111.91
31	D	407	LMG	O1-C1-C2	2.29	111.87	108.30
28	d	408	DGD	O2G-C1B-O1B	-2.29	118.18	123.70
27	b	621	BCR	C34-C9-C10	-2.29	119.72	122.92
25	D	404	PL9	C51-C49-C50	2.28	119.64	114.60
23	C	510	CLA	CMB-C2B-C3B	2.28	128.94	124.68
23	b	607	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
23	A	403	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
23	c	509	CLA	CHD-C1D-ND	-2.27	122.36	124.45
28	c	519	DGD	O1G-C1A-O1A	-2.27	117.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	103	BCR	C16-C17-C18	-2.27	124.07	127.31
23	D	401	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
27	a	412	BCR	C23-C24-C25	-2.26	120.85	127.20
31	A	418	LMG	O8-C28-O10	-2.26	117.88	123.59
23	C	509	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
33	M	103	LMT	C1B-O1B-C4'	-2.26	112.37	117.96
23	b	613	CLA	O2D-CGD-CBD	2.26	115.28	111.27
23	B	604	CLA	CHB-C4A-NA	2.26	127.64	124.51
27	A	410	BCR	C32-C1-C6	-2.26	106.64	110.30
23	A	405	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	B	609	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
30	f	103	SQD	O48-C23-C24	2.26	118.99	111.91
23	D	401	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
23	c	503	CLA	CHD-C1D-ND	-2.26	122.38	124.45
23	B	607	CLA	CHD-C1D-ND	-2.25	122.38	124.45
23	B	601	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
27	f	102	BCR	C36-C18-C17	-2.25	119.77	122.92
25	a	410	PL9	C7-C8-C9	-2.25	123.04	126.79
31	a	416	LMG	O1-C7-C8	2.25	116.33	110.90
23	B	601	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
31	k	103	LMG	C7-O1-C1	2.24	118.12	113.74
23	C	507	CLA	C1-C2-C3	-2.24	122.17	126.04
28	D	410	DGD	O2G-C1B-O1B	-2.24	118.28	123.70
23	C	512	CLA	CHD-C1D-ND	-2.24	122.39	124.45
23	c	501	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	C	508	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
25	j	101	PL9	C10-C9-C11	2.24	119.04	115.27
23	b	607	CLA	CAA-CBA-CGA	-2.24	106.71	113.25
28	C	516	DGD	O3G-C3G-C2G	2.24	116.30	110.90
27	a	412	BCR	C8-C7-C6	-2.24	120.92	127.20
27	B	619	BCR	C15-C16-C17	-2.24	118.89	123.47
27	x	101	BCR	C33-C5-C4	2.24	117.91	113.62
23	b	604	CLA	CHB-C4A-NA	2.24	127.60	124.51
28	d	408	DGD	C2G-O2G-C1B	2.24	123.30	117.79
23	C	503	CLA	CHB-C4A-NA	2.23	127.60	124.51
25	d	404	PL9	C20-C19-C21	2.23	119.02	115.27
23	c	501	CLA	CHD-C1D-ND	-2.23	122.41	124.45
23	a	404	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
23	b	611	CLA	C1-C2-C3	-2.23	122.19	126.04
25	a	410	PL9	C53-C6-C1	2.23	119.54	114.99
30	A	417	SQD	O48-C23-C24	2.23	118.89	111.91
25	D	404	PL9	C36-C34-C33	-2.22	116.62	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	403	CLA	CHD-C1D-ND	-2.22	122.41	124.45
27	B	620	BCR	C8-C7-C6	-2.22	120.97	127.20
25	A	408	PL9	C30-C29-C31	2.22	119.01	115.27
31	b	623	LMG	C4-C3-C2	2.22	114.70	110.82
28	A	411	DGD	C3D-C4D-C5D	2.22	114.20	110.24
25	A	408	PL9	C11-C9-C8	-2.22	116.62	121.12
25	A	408	PL9	C12-C13-C14	-2.22	122.32	127.66
28	A	411	DGD	C6E-C5E-C4E	-2.22	107.81	113.00
23	B	610	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
31	a	402	LMG	O1-C1-C2	2.22	111.77	108.30
27	Z	101	BCR	C38-C26-C25	-2.22	122.04	124.53
27	B	619	BCR	C38-C26-C27	2.22	117.87	113.62
23	C	506	CLA	C1-C2-C3	-2.22	122.21	126.04
31	M	102	LMG	O6-C5-C4	2.21	113.72	109.69
23	C	502	CLA	C1-C2-C3	-2.21	122.21	126.04
23	C	513	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
25	A	408	PL9	C53-C6-C1	2.21	119.51	114.99
27	B	619	BCR	C2-C1-C6	2.21	113.89	110.48
31	a	402	LMG	O3-C3-C4	-2.21	105.24	110.35
23	c	504	CLA	CHD-C1D-ND	-2.21	122.42	124.45
33	m	101	LMT	C1B-O1B-C4'	-2.21	112.50	117.96
27	A	410	BCR	C33-C5-C4	2.21	117.86	113.62
30	A	417	SQD	O2-C2-C3	-2.21	105.25	110.35
29	A	412	LHG	O8-C23-C24	2.21	118.83	111.91
23	c	502	CLA	C1-C2-C3	-2.21	122.23	126.04
27	C	515	BCR	C21-C20-C19	-2.21	116.33	123.22
23	b	604	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
25	A	408	PL9	C32-C33-C34	-2.21	122.35	127.66
23	d	402	CLA	CHB-C4A-NA	2.20	127.56	124.51
27	a	412	BCR	C16-C15-C14	-2.20	118.96	123.47
23	A	407	CLA	CHD-C1D-ND	-2.20	122.43	124.45
27	D	405	BCR	C33-C5-C4	2.20	117.84	113.62
28	B	621	DGD	C4D-C3D-C2D	-2.20	106.98	110.82
23	b	607	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
28	C	518	DGD	O1G-C1A-O1A	-2.20	118.04	123.59
23	b	618	CLA	C1-C2-C3	-2.20	122.24	126.04
28	a	413	DGD	C6D-C5D-C4D	-2.20	107.51	112.09
31	e	101	LMG	C1-O6-C5	-2.20	109.38	113.69
25	D	404	PL9	C45-C44-C43	-2.20	118.04	123.68
27	B	617	BCR	C28-C27-C26	-2.20	110.16	114.08
28	C	516	DGD	C1D-O6D-C5D	-2.19	109.38	113.69
25	J	101	PL9	C22-C23-C24	-2.19	122.38	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	CHD-C1D-ND	-2.19	122.44	124.45
27	b	621	BCR	C40-C30-C25	-2.19	106.75	110.30
27	A	410	BCR	C23-C24-C25	-2.19	121.06	127.20
23	A	405	CLA	C1-C2-C3	-2.19	122.26	126.04
23	b	606	CLA	C1-C2-C3	-2.19	122.26	126.04
23	C	505	CLA	CHB-C4A-NA	2.19	127.53	124.51
28	c	517	DGD	C1G-O1G-C1A	2.19	125.21	117.12
27	c	515	BCR	C15-C16-C17	-2.19	119.00	123.47
28	c	519	DGD	O3D-C3D-C4D	2.18	115.40	110.35
31	I	101	LMG	O3-C3-C4	-2.18	105.30	110.35
23	C	510	CLA	C1-C2-C3	-2.18	122.27	126.04
23	B	614	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
28	B	626	DGD	O4D-C4D-C5D	-2.18	103.88	109.30
31	A	414	LMG	O8-C28-O10	-2.18	118.09	123.59
27	k	102	BCR	C35-C13-C14	-2.18	119.87	122.92
24	D	402	PHO	O2A-CGA-O1A	-2.18	118.10	123.59
27	K	102	BCR	C32-C1-C6	-2.18	106.77	110.30
23	B	610	CLA	C1-C2-C3	-2.18	122.28	126.04
23	c	503	CLA	O2D-CGD-CBD	2.18	115.14	111.27
27	C	514	BCR	C33-C5-C4	2.18	117.80	113.62
23	A	405	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
28	C	516	DGD	O3D-C3D-C4D	2.17	115.38	110.35
23	b	615	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
23	C	501	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
31	E	101	LMG	O1-C1-C2	2.17	111.69	108.30
23	B	604	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
28	C	517	DGD	O4D-C4D-C5D	-2.17	103.91	109.30
31	b	624	LMG	O8-C28-O10	-2.17	118.11	123.59
25	d	404	PL9	C51-C49-C50	2.17	119.39	114.60
27	C	515	BCR	C2-C1-C6	2.17	113.82	110.48
27	D	405	BCR	C34-C9-C10	-2.17	119.89	122.92
23	C	512	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
27	B	617	BCR	C8-C7-C6	-2.17	121.12	127.20
23	B	615	CLA	C1-C2-C3	-2.16	122.30	126.04
33	x	102	LMT	C1B-O1B-C4'	-2.16	112.61	117.96
28	c	518	DGD	C1D-O6D-C5D	-2.16	109.45	113.69
23	c	503	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
28	c	518	DGD	O6E-C1E-C2E	2.16	114.92	110.35
27	k	102	BCR	C33-C5-C4	2.16	117.76	113.62
23	D	403	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	a	406	CLA	CHB-C4A-NA	2.15	127.49	124.51
34	f	101	HEM	CAD-CBD-CGD	-2.15	108.97	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Z	101	BCR	C10-C11-C12	-2.15	116.50	123.22
23	C	505	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
27	x	101	BCR	C15-C16-C17	-2.15	119.07	123.47
31	i	101	LMG	C3-C4-C5	2.15	114.08	110.24
23	b	610	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	c	513	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
31	A	418	LMG	O1-C1-C2	2.15	111.66	108.30
27	C	514	BCR	C29-C30-C25	2.15	113.79	110.48
25	D	404	PL9	C20-C19-C21	2.15	118.88	115.27
30	f	103	SQD	O6-C1-C2	2.15	111.65	108.30
23	c	504	CLA	O2D-CGD-CBD	2.14	115.08	111.27
23	B	601	CLA	C1-C2-C3	-2.14	122.34	126.04
23	c	506	CLA	C1-C2-C3	-2.14	122.34	126.04
25	A	408	PL9	C41-C39-C40	2.14	119.33	114.60
27	b	620	BCR	C33-C5-C4	2.14	117.73	113.62
31	B	622	LMG	C6-C5-C4	-2.14	107.99	113.00
34	f	101	HEM	CHC-C4B-C3B	2.14	127.84	124.57
27	B	619	BCR	C23-C24-C25	-2.14	121.19	127.20
23	b	614	CLA	CHB-C4A-NA	2.14	127.47	124.51
33	b	626	LMT	C1B-O1B-C4'	-2.14	112.67	117.96
27	H	101	BCR	C36-C18-C19	2.14	121.45	118.08
27	a	412	BCR	C34-C9-C10	-2.14	119.93	122.92
31	e	101	LMG	O9-C10-C11	-2.14	115.39	123.73
24	a	407	PHO	O2A-CGA-O1A	-2.14	118.20	123.59
23	b	614	CLA	O2D-CGD-CBD	2.14	115.06	111.27
25	D	404	PL9	C27-C28-C29	-2.14	122.52	127.66
23	a	409	CLA	C1-C2-C3	-2.13	122.35	126.04
31	E	101	LMG	C1-O6-C5	-2.13	109.50	113.69
31	C	520	LMG	O3-C3-C4	-2.13	105.42	110.35
23	B	613	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
31	M	101	LMG	O4-C4-C3	-2.13	105.42	110.35
25	a	410	PL9	C41-C39-C40	2.13	119.31	114.60
31	c	520	LMG	O3-C3-C4	-2.13	105.43	110.35
28	c	519	DGD	O2G-C1B-C2B	2.13	116.09	111.50
30	B	625	SQD	O8-S-C6	2.13	109.13	105.74
28	a	413	DGD	C6D-O5D-C1E	2.13	117.90	113.74
25	A	408	PL9	C26-C24-C23	-2.13	116.81	121.12
27	B	620	BCR	C40-C30-C25	-2.13	106.85	110.30
23	C	501	CLA	CMB-C2B-C3B	2.13	128.66	124.68
23	c	507	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
31	D	406	LMG	C6-C5-C4	-2.12	108.03	113.00
31	d	406	LMG	O8-C28-O10	-2.12	118.23	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	404	PL9	C53-C6-C1	2.12	119.33	114.99
27	B	620	BCR	C38-C26-C27	2.12	117.69	113.62
30	d	407	SQD	O48-C23-C24	2.12	118.56	111.91
28	b	622	DGD	O5D-C6D-C5D	2.12	112.97	109.05
23	c	511	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
27	H	101	BCR	C15-C16-C17	-2.12	119.13	123.47
30	f	103	SQD	O5-C1-C2	2.12	114.83	110.35
27	B	617	BCR	C33-C5-C4	2.12	117.68	113.62
28	b	602	DGD	C1E-C2E-C3E	2.12	114.40	110.00
23	B	614	CLA	CHB-C4A-NA	2.11	127.44	124.51
31	B	622	LMG	O8-C28-O10	-2.11	118.26	123.59
23	c	512	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
27	j	102	BCR	C20-C19-C18	-2.11	120.48	126.42
28	b	622	DGD	C4D-C3D-C2D	-2.11	107.14	110.82
23	C	511	CLA	C1-C2-C3	-2.11	122.40	126.04
31	M	101	LMG	O8-C9-C8	-2.11	102.30	108.43
23	c	510	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	C	511	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
30	a	401	SQD	O6-C1-C2	2.11	111.59	108.30
23	C	508	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	c	504	CLA	C1-C2-C3	-2.10	122.40	126.04
23	b	604	CLA	C1-C2-C3	-2.10	122.40	126.04
31	B	622	LMG	C3-C4-C5	2.10	113.99	110.24
33	I	102	LMT	O1B-C4'-C3'	2.10	112.87	107.28
25	A	408	PL9	C7-C3-C2	-2.10	120.54	123.30
23	B	607	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	A	406	PHO	C1B-NB-C4B	2.10	111.40	107.09
27	J	102	BCR	C34-C9-C10	-2.10	119.99	122.92
23	B	612	CLA	CAA-CBA-CGA	-2.09	107.13	113.25
31	D	407	LMG	O8-C28-O10	-2.09	118.31	123.59
23	b	610	CLA	O2D-CGD-CBD	2.09	114.99	111.27
27	A	410	BCR	C8-C7-C6	-2.09	121.33	127.20
23	b	609	CLA	CHD-C1D-ND	-2.09	122.53	124.45
31	C	519	LMG	O1-C1-C2	2.09	111.57	108.30
23	b	616	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
28	A	411	DGD	C6D-O5D-C1E	2.09	117.82	113.74
27	B	618	BCR	C34-C9-C10	-2.09	120.00	122.92
23	a	406	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	c	505	CLA	CMB-C2B-C3B	2.09	128.58	124.68
23	a	406	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
23	C	509	CLA	C1-C2-C3	-2.08	122.44	126.04
27	Z	101	BCR	C33-C5-C4	2.08	117.61	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c	517	DGD	C4D-C3D-C2D	-2.08	107.19	110.82
31	E	101	LMG	O7-C10-O9	-2.08	118.68	123.70
27	c	516	BCR	C21-C20-C19	-2.08	116.73	123.22
23	C	503	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
23	C	510	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
23	b	606	CLA	O2D-CGD-CBD	2.08	114.96	111.27
27	H	101	BCR	C21-C20-C19	-2.08	116.73	123.22
27	J	102	BCR	C15-C16-C17	-2.08	119.22	123.47
27	b	621	BCR	C38-C26-C27	2.07	117.60	113.62
23	A	405	CLA	CHD-C1D-ND	-2.07	122.55	124.45
27	C	514	BCR	C2-C3-C4	-2.07	106.75	111.38
27	k	102	BCR	C38-C26-C27	2.07	117.60	113.62
23	B	615	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	B	612	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
31	i	101	LMG	C6-C5-C4	-2.07	108.16	113.00
23	B	608	CLA	CHD-C1D-ND	-2.07	122.55	124.45
27	D	405	BCR	C35-C13-C12	2.07	121.33	118.08
31	C	520	LMG	O8-C28-O10	-2.07	118.38	123.59
27	a	412	BCR	C21-C20-C19	-2.07	116.77	123.22
23	d	402	CLA	O1D-CGD-CBD	2.06	128.71	124.48
23	B	603	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	b	613	CLA	CHD-C1D-ND	-2.06	122.56	124.45
28	C	518	DGD	O2G-C1B-C2B	2.06	115.94	111.50
27	c	515	BCR	C35-C13-C14	-2.06	120.04	122.92
23	b	609	CLA	C2D-C1D-ND	-2.06	108.59	110.10
28	B	626	DGD	C1E-C2E-C3E	2.06	114.28	110.00
27	T	103	BCR	C34-C9-C10	-2.06	120.04	122.92
31	b	624	LMG	O6-C5-C4	2.06	113.43	109.69
31	d	405	LMG	O6-C5-C4	2.06	113.43	109.69
28	C	516	DGD	O2G-C1B-O1B	-2.05	118.74	123.70
23	b	619	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
27	A	410	BCR	C34-C9-C8	2.05	121.31	118.08
23	b	610	CLA	CHD-C1D-ND	-2.05	122.57	124.45
27	k	102	BCR	C36-C18-C19	2.05	121.30	118.08
25	j	101	PL9	C53-C6-C1	2.05	119.18	114.99
31	D	407	LMG	O4-C4-C3	-2.05	105.62	110.35
27	k	102	BCR	C11-C10-C9	-2.05	124.39	127.31
23	b	616	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
27	k	102	BCR	C23-C24-C25	-2.04	121.46	127.20
25	D	404	PL9	C45-C44-C46	2.04	118.71	115.27
27	c	514	BCR	C29-C30-C25	2.04	113.63	110.48
34	V	201	HEM	C1B-NB-C4B	2.04	107.18	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	K	102	BCR	C38-C26-C27	2.04	117.54	113.62
23	c	501	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	b	619	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	b	616	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	i	101	LMG	C8-O7-C10	2.04	122.81	117.79
27	b	621	BCR	C16-C15-C14	-2.04	119.30	123.47
23	C	503	CLA	O2D-CGD-CBD	2.04	114.89	111.27
23	C	504	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
23	D	403	CLA	O2D-CGD-CBD	2.04	114.89	111.27
27	b	620	BCR	C2-C1-C6	2.04	113.61	110.48
28	b	602	DGD	O4D-C4D-C5D	-2.04	104.24	109.30
27	j	102	BCR	C15-C16-C17	-2.03	119.31	123.47
27	T	103	BCR	C32-C1-C6	-2.03	107.00	110.30
27	x	101	BCR	C16-C15-C14	-2.03	119.31	123.47
27	c	514	BCR	C34-C9-C8	2.03	121.28	118.08
27	D	405	BCR	C20-C21-C22	-2.03	124.41	127.31
31	M	101	LMG	O1-C1-C2	2.03	111.47	108.30
27	C	515	BCR	C33-C5-C4	2.03	117.52	113.62
31	M	102	LMG	O4-C4-C3	-2.03	105.65	110.35
27	x	101	BCR	C11-C10-C9	-2.03	124.41	127.31
23	C	509	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	c	505	CLA	C6-C7-C8	-2.03	109.36	115.92
23	D	401	CLA	CHB-C4A-NA	2.03	127.32	124.51
27	B	618	BCR	C35-C13-C12	2.03	121.27	118.08
27	B	620	BCR	C16-C15-C14	-2.03	119.32	123.47
30	b	601	SQD	C1-O5-C5	2.03	117.67	113.69
23	D	403	CLA	C1-C2-C3	-2.03	122.54	126.04
31	B	622	LMG	O6-C5-C4	2.03	113.38	109.69
30	b	601	SQD	O6-C1-C2	2.03	111.47	108.30
23	c	501	CLA	C1-C2-C3	-2.02	122.54	126.04
23	C	503	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
27	c	515	BCR	C33-C5-C4	2.02	117.50	113.62
23	C	501	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
23	c	505	CLA	CBA-CAA-C2A	2.02	119.84	113.86
27	x	101	BCR	C36-C18-C19	2.02	121.26	118.08
34	F	101	HEM	C2B-C1B-NB	-2.02	107.44	109.84
23	c	508	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
27	A	410	BCR	C21-C20-C19	-2.02	116.91	123.22
34	v	201	HEM	CHC-C4B-NB	2.02	126.63	124.43
23	b	612	CLA	C1-C2-C3	-2.02	122.55	126.04
23	a	405	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	b	618	CLA	CHD-C1D-ND	-2.02	122.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	516	BCR	C2-C1-C6	2.02	113.59	110.48
25	J	101	PL9	C10-C9-C11	2.02	118.66	115.27
31	c	520	LMG	O8-C28-O10	-2.02	118.50	123.59
27	c	515	BCR	C11-C10-C9	-2.02	124.43	127.31
31	A	418	LMG	O6-C5-C4	2.01	113.35	109.69
31	B	622	LMG	C7-O1-C1	2.01	117.67	113.74
31	b	624	LMG	C6-C5-C4	-2.01	108.29	113.00
23	B	603	CLA	C1-C2-C3	-2.01	122.56	126.04
25	d	404	PL9	C53-C6-C1	2.01	119.10	114.99
28	c	517	DGD	O6D-C1D-O3G	2.01	114.73	109.97
23	c	505	CLA	C3A-C2A-C1A	2.01	104.35	101.34
25	d	404	PL9	C30-C29-C31	2.01	118.65	115.27
27	B	618	BCR	C15-C14-C13	-2.01	124.44	127.31
23	c	504	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
27	c	515	BCR	C23-C24-C25	-2.01	121.57	127.20
34	f	101	HEM	CAB-C3B-C2B	-2.01	122.00	128.60
24	D	402	PHO	CMC-C2C-C3C	2.01	128.72	124.94
27	b	620	BCR	C39-C30-C25	-2.00	107.05	110.30
23	B	613	CLA	C1-C2-C3	-2.00	122.58	126.04
23	b	614	CLA	C1-C2-C3	-2.00	122.58	126.04
27	b	621	BCR	C35-C13-C12	2.00	121.23	118.08
30	B	625	SQD	C10-C9-C8	-2.00	105.99	113.19
27	f	102	BCR	C35-C13-C14	-2.00	120.12	122.92
29	a	414	LHG	C6-O8-C23	2.00	124.53	117.12
27	a	412	BCR	C36-C18-C19	2.00	121.23	118.08
27	b	621	BCR	C32-C1-C6	-2.00	107.05	110.30
23	c	506	CLA	C3A-C2A-C1A	2.00	104.33	101.34
31	A	418	LMG	O7-C10-O9	-2.00	118.87	123.70
23	b	604	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	608	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	401	CLA	ND
23	D	403	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	406	CLA	ND
23	a	409	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (2114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-C2A-CAA-CBA
23	A	404	CLA	C3A-C2A-CAA-CBA
23	A	404	CLA	CHA-CBD-CGD-O1D
23	A	404	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C2-C3-C5-C6
23	B	602	CLA	C4-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	604	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C1A-C2A-CAA-CBA
23	B	606	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C1A-C2A-CAA-CBA
23	B	607	CLA	C2A-CAA-CBA-CGA
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	505	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C3A-C2A-CAA-CBA
23	C	505	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	C2A-CAA-CBA-CGA
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C3A-C2A-CAA-CBA
23	D	401	CLA	C2-C3-C5-C6
23	D	401	CLA	C4-C3-C5-C6
23	a	405	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	CHA-CBD-CGD-O1D
23	a	405	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	CBD-CGD-O2D-CED
23	b	605	CLA	C1A-C2A-CAA-CBA
23	b	605	CLA	C3A-C2A-CAA-CBA
23	b	605	CLA	C2-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	605	CLA	C6-C7-C8-C9
23	b	606	CLA	CBD-CGD-O2D-CED
23	b	606	CLA	C2-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	C1A-C2A-CAA-CBA
23	b	609	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	C1A-C2A-CAA-CBA
23	b	611	CLA	C3A-C2A-CAA-CBA
23	b	613	CLA	C2A-CAA-CBA-CGA
23	b	613	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CHA-CBD-CGD-O1D
23	b	617	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	617	CLA	CAD-CBD-CGD-O2D
23	b	619	CLA	C3A-C2A-CAA-CBA
23	b	619	CLA	CBD-CGD-O2D-CED
23	c	504	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	C1A-C2A-CAA-CBA
23	c	505	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O2D
23	d	402	CLA	C2-C3-C5-C6
23	d	402	CLA	C4-C3-C5-C6
25	A	408	PL9	C7-C8-C9-C11
25	A	408	PL9	C12-C13-C14-C16
25	A	408	PL9	C17-C18-C19-C20
25	A	408	PL9	C17-C18-C19-C21
25	A	408	PL9	C22-C23-C24-C25
25	A	408	PL9	C24-C26-C27-C28
25	A	408	PL9	C27-C28-C29-C30
25	A	408	PL9	C27-C28-C29-C31
25	A	408	PL9	C28-C29-C31-C32
25	A	408	PL9	C30-C29-C31-C32
25	A	408	PL9	C33-C34-C36-C37
25	A	408	PL9	C35-C34-C36-C37
25	A	408	PL9	C37-C38-C39-C41
25	D	404	PL9	C27-C28-C29-C30
25	D	404	PL9	C27-C28-C29-C31
25	D	404	PL9	C34-C36-C37-C38
25	J	101	PL9	C7-C8-C9-C10
25	J	101	PL9	C7-C8-C9-C11
25	J	101	PL9	C22-C23-C24-C25
25	J	101	PL9	C22-C23-C24-C26
25	a	410	PL9	C7-C8-C9-C11
25	a	410	PL9	C12-C13-C14-C16
25	a	410	PL9	C17-C18-C19-C20
25	a	410	PL9	C17-C18-C19-C21
25	a	410	PL9	C22-C23-C24-C25
25	a	410	PL9	C24-C26-C27-C28
25	a	410	PL9	C27-C28-C29-C30
25	a	410	PL9	C27-C28-C29-C31
25	a	410	PL9	C28-C29-C31-C32
25	a	410	PL9	C30-C29-C31-C32
25	a	410	PL9	C33-C34-C36-C37
25	d	404	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	d	404	PL9	C27-C28-C29-C30
25	d	404	PL9	C27-C28-C29-C31
25	j	101	PL9	C7-C8-C9-C10
25	j	101	PL9	C7-C8-C9-C11
25	j	101	PL9	C22-C23-C24-C25
25	j	101	PL9	C22-C23-C24-C26
27	B	617	BCR	C1-C6-C7-C8
27	B	618	BCR	C21-C22-C23-C24
27	B	618	BCR	C37-C22-C23-C24
27	B	618	BCR	C23-C24-C25-C26
27	C	514	BCR	C11-C12-C13-C14
27	C	514	BCR	C11-C12-C13-C35
27	C	515	BCR	C1-C6-C7-C8
27	C	515	BCR	C7-C8-C9-C10
27	C	515	BCR	C7-C8-C9-C34
27	D	405	BCR	C7-C8-C9-C10
27	D	405	BCR	C7-C8-C9-C34
27	K	102	BCR	C1-C6-C7-C8
27	K	102	BCR	C7-C8-C9-C10
27	K	102	BCR	C21-C22-C23-C24
27	K	102	BCR	C37-C22-C23-C24
27	K	102	BCR	C23-C24-C25-C30
27	T	103	BCR	C21-C22-C23-C24
27	T	103	BCR	C37-C22-C23-C24
27	T	103	BCR	C23-C24-C25-C26
27	Z	101	BCR	C1-C6-C7-C8
27	c	514	BCR	C11-C12-C13-C14
27	c	514	BCR	C11-C12-C13-C35
27	c	515	BCR	C1-C6-C7-C8
27	c	516	BCR	C1-C6-C7-C8
27	c	516	BCR	C7-C8-C9-C34
27	c	516	BCR	C23-C24-C25-C30
27	f	102	BCR	C7-C8-C9-C10
27	f	102	BCR	C7-C8-C9-C34
27	f	102	BCR	C37-C22-C23-C24
27	k	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C7-C8-C9-C10
27	k	102	BCR	C7-C8-C9-C34
27	k	102	BCR	C21-C22-C23-C24
27	k	102	BCR	C37-C22-C23-C24
27	x	101	BCR	C1-C6-C7-C8
27	x	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	A	411	DGD	C2D-C1D-O3G-C3G
28	A	411	DGD	O6D-C1D-O3G-C3G
28	B	621	DGD	C2E-C1E-O5D-C6D
28	B	621	DGD	O6E-C1E-O5D-C6D
28	B	626	DGD	C2B-C1B-O2G-C2G
28	B	626	DGD	O1B-C1B-O2G-C2G
28	B	626	DGD	O2G-C2G-C3G-O3G
28	B	626	DGD	C2E-C1E-O5D-C6D
28	B	626	DGD	O6E-C1E-O5D-C6D
28	C	516	DGD	C2D-C1D-O3G-C3G
28	C	516	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C2B-C1B-O2G-C2G
28	C	517	DGD	O1B-C1B-O2G-C2G
28	C	517	DGD	O2G-C2G-C3G-O3G
28	C	518	DGD	C2D-C1D-O3G-C3G
28	C	518	DGD	O6D-C1D-O3G-C3G
28	D	410	DGD	C2B-C1B-O2G-C2G
28	D	410	DGD	O6D-C1D-O3G-C3G
28	a	413	DGD	C2D-C1D-O3G-C3G
28	a	413	DGD	O6D-C1D-O3G-C3G
28	b	602	DGD	C2B-C1B-O2G-C2G
28	b	602	DGD	O1B-C1B-O2G-C2G
28	b	602	DGD	C2E-C1E-O5D-C6D
28	b	622	DGD	C2E-C1E-O5D-C6D
28	b	622	DGD	O6E-C1E-O5D-C6D
28	c	517	DGD	C2D-C1D-O3G-C3G
28	c	517	DGD	C2E-C1E-O5D-C6D
28	c	518	DGD	C2B-C1B-O2G-C2G
28	c	518	DGD	O1B-C1B-O2G-C2G
28	c	518	DGD	O2G-C2G-C3G-O3G
28	c	519	DGD	C2D-C1D-O3G-C3G
28	c	519	DGD	O6D-C1D-O3G-C3G
28	d	408	DGD	C2B-C1B-O2G-C2G
28	d	408	DGD	O6D-C1D-O3G-C3G
29	A	412	LHG	C3-O3-P-O5
29	A	412	LHG	C4-O6-P-O4
29	A	415	LHG	C4-O6-P-O4
29	A	415	LHG	C4-O6-P-O5
29	a	414	LHG	C3-O3-P-O5
29	a	414	LHG	C4-O6-P-O4
29	a	414	LHG	C4-O6-P-O5
29	a	417	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
29	a	417	LHG	C4-O6-P-O5
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	O5-C1-O6-C44
30	A	417	SQD	O6-C44-C45-O47
30	A	417	SQD	C24-C23-O48-C46
30	B	625	SQD	O5-C5-C6-S
30	D	409	SQD	C2-C1-O6-C44
30	D	409	SQD	O6-C44-C45-O47
30	D	409	SQD	O49-C7-O47-C45
30	D	409	SQD	C8-C7-O47-C45
30	F	102	SQD	O5-C1-O6-C44
30	F	102	SQD	C8-C7-O47-C45
30	a	401	SQD	O6-C44-C45-O47
30	a	401	SQD	C24-C23-O48-C46
30	a	415	SQD	C2-C1-O6-C44
30	a	415	SQD	O5-C1-O6-C44
30	b	601	SQD	O5-C5-C6-S
30	d	407	SQD	C2-C1-O6-C44
30	d	407	SQD	O6-C44-C45-O47
30	d	407	SQD	O49-C7-O47-C45
30	d	407	SQD	C8-C7-O47-C45
30	f	103	SQD	O5-C1-O6-C44
30	f	103	SQD	C8-C7-O47-C45
30	f	103	SQD	O10-C23-O48-C46
31	B	622	LMG	O9-C10-O7-C8
31	B	622	LMG	C11-C10-O7-C8
31	C	519	LMG	C2-C1-O1-C7
31	C	519	LMG	O6-C1-O1-C7
31	C	520	LMG	C2-C1-O1-C7
31	C	520	LMG	O6-C1-O1-C7
31	C	520	LMG	C8-C9-O8-C28
31	C	520	LMG	O9-C10-O7-C8
31	C	520	LMG	C11-C10-O7-C8
31	D	406	LMG	C11-C10-O7-C8
31	D	407	LMG	O1-C7-C8-O7
31	D	407	LMG	O9-C10-O7-C8
31	D	407	LMG	C11-C10-O7-C8
31	D	408	LMG	C2-C1-O1-C7
31	D	408	LMG	O6-C1-O1-C7
31	E	101	LMG	C2-C1-O1-C7
31	E	101	LMG	O6-C1-O1-C7
31	M	101	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
31	M	101	LMG	O6-C1-O1-C7
31	M	101	LMG	O9-C10-O7-C8
31	M	102	LMG	C2-C1-O1-C7
31	M	102	LMG	O9-C10-O7-C8
31	b	623	LMG	O1-C7-C8-O7
31	b	623	LMG	O9-C10-O7-C8
31	b	623	LMG	C11-C10-O7-C8
31	b	624	LMG	O9-C10-O7-C8
31	b	624	LMG	C11-C10-O7-C8
31	c	520	LMG	C2-C1-O1-C7
31	c	520	LMG	O6-C1-O1-C7
31	c	520	LMG	C8-C9-O8-C28
31	c	520	LMG	O9-C10-O7-C8
31	c	520	LMG	C11-C10-O7-C8
31	d	405	LMG	C11-C10-O7-C8
31	d	406	LMG	C2-C1-O1-C7
31	d	406	LMG	O6-C1-O1-C7
31	d	406	LMG	O10-C28-O8-C9
31	e	101	LMG	C2-C1-O1-C7
31	e	101	LMG	O6-C1-O1-C7
31	k	103	LMG	C2-C1-O1-C7
31	k	103	LMG	O6-C1-O1-C7
31	k	103	LMG	C11-C10-O7-C8
34	v	201	HEM	C3D-CAD-CBD-CGD
23	A	403	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	O1D-CGD-O2D-CED
23	C	505	CLA	O1D-CGD-O2D-CED
23	a	404	CLA	O1D-CGD-O2D-CED
23	c	505	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	CBD-CGD-O2D-CED
23	B	611	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED
23	C	501	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	506	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	a	404	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBD-CGD-O2D-CED
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
30	A	417	SQD	O10-C23-O48-C46
30	a	401	SQD	O10-C23-O48-C46
31	D	407	LMG	O10-C28-O8-C9
31	D	408	LMG	O10-C28-O8-C9
31	b	623	LMG	O10-C28-O8-C9
33	B	627	LMT	C3'-C4'-O1B-C1B
33	T	101	LMT	C3'-C4'-O1B-C1B
23	B	601	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	O1D-CGD-O2D-CED
23	b	619	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	O1D-CGD-O2D-CED
28	b	622	DGD	C4D-C5D-C6D-O5D
23	C	504	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	O1D-CGD-O2D-CED
31	A	414	LMG	C29-C28-O8-C9
31	D	408	LMG	C29-C28-O8-C9
31	d	406	LMG	C29-C28-O8-C9
25	A	408	PL9	C37-C38-C39-C40
25	a	410	PL9	C37-C38-C39-C40
25	a	410	PL9	C37-C38-C39-C41
23	B	606	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	CBD-CGD-O2D-CED
23	C	512	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	CBD-CGD-O2D-CED
23	b	614	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
24	A	406	PHO	CBD-CGD-O2D-CED
28	D	410	DGD	O1A-C1A-O1G-C1G
28	d	408	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
30	F	102	SQD	O10-C23-O48-C46
31	A	414	LMG	O10-C28-O8-C9
31	C	520	LMG	O10-C28-O8-C9
31	E	101	LMG	O10-C28-O8-C9
31	a	416	LMG	O10-C28-O8-C9
31	c	520	LMG	O10-C28-O8-C9
31	e	101	LMG	O10-C28-O8-C9
23	B	605	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	O1D-CGD-O2D-CED
23	b	604	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
28	a	413	DGD	O6E-C5E-C6E-O5E
28	C	517	DGD	C4E-C5E-C6E-O5E
28	c	518	DGD	C4E-C5E-C6E-O5E
23	c	504	CLA	O1D-CGD-O2D-CED
28	D	410	DGD	O6D-C5D-C6D-O5D
28	d	408	DGD	O6D-C5D-C6D-O5D
23	B	612	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	O1D-CGD-O2D-CED
23	b	613	CLA	O1D-CGD-O2D-CED
28	C	516	DGD	O1B-C1B-O2G-C2G
28	C	518	DGD	O1B-C1B-O2G-C2G
28	D	410	DGD	O1B-C1B-O2G-C2G
28	c	517	DGD	O1B-C1B-O2G-C2G
28	d	408	DGD	O1B-C1B-O2G-C2G
31	A	418	LMG	O9-C10-O7-C8
31	D	406	LMG	O9-C10-O7-C8
31	E	101	LMG	O9-C10-O7-C8
31	I	101	LMG	O9-C10-O7-C8
31	d	405	LMG	O9-C10-O7-C8
31	e	101	LMG	O9-C10-O7-C8
31	i	101	LMG	O9-C10-O7-C8
23	A	405	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
23	a	406	CLA	C3-C5-C6-C7
24	D	402	PHO	C3-C5-C6-C7
24	a	407	PHO	C3-C5-C6-C7
28	D	410	DGD	C2A-C1A-O1G-C1G
30	F	102	SQD	C24-C23-O48-C46
30	f	103	SQD	C24-C23-O48-C46
31	C	519	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
31	C	520	LMG	C29-C28-O8-C9
31	D	407	LMG	C29-C28-O8-C9
31	E	101	LMG	C29-C28-O8-C9
31	b	623	LMG	C29-C28-O8-C9
31	c	520	LMG	C29-C28-O8-C9
31	e	101	LMG	C29-C28-O8-C9
28	C	516	DGD	C2B-C1B-O2G-C2G
28	c	517	DGD	C2B-C1B-O2G-C2G
31	C	519	LMG	C11-C10-O7-C8
31	M	101	LMG	C11-C10-O7-C8
31	M	102	LMG	C11-C10-O7-C8
23	B	613	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	O1D-CGD-O2D-CED
23	b	615	CLA	CBD-CGD-O2D-CED
28	A	411	DGD	O6E-C5E-C6E-O5E
33	b	603	LMT	C3'-C4'-O1B-C1B
23	A	404	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
25	D	404	PL9	C35-C34-C36-C37
25	a	410	PL9	C35-C34-C36-C37
25	d	404	PL9	C35-C34-C36-C37
23	B	601	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C2A-CAA-CBA-CGA
33	B	628	LMT	C3'-C4'-O1B-C1B
23	B	608	CLA	C3-C5-C6-C7
23	b	611	CLA	C3-C5-C6-C7
23	b	617	CLA	C3-C5-C6-C7
28	d	408	DGD	C2A-C1A-O1G-C1G
31	a	416	LMG	C29-C28-O8-C9
31	i	101	LMG	C29-C28-O8-C9
31	k	103	LMG	C29-C28-O8-C9
31	k	103	LMG	O6-C5-C6-O5
23	c	508	CLA	O1D-CGD-O2D-CED
28	B	621	DGD	C4D-C5D-C6D-O5D
25	A	408	PL9	C12-C13-C14-C15
25	a	410	PL9	C12-C13-C14-C15
23	B	609	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	C	517	DGD	O6E-C5E-C6E-O5E
30	F	102	SQD	O49-C7-O47-C45
31	a	402	LMG	O9-C10-O7-C8
25	A	408	PL9	C22-C23-C24-C26
25	a	410	PL9	C22-C23-C24-C26
23	C	506	CLA	O1D-CGD-O2D-CED
31	C	519	LMG	O6-C5-C6-O5
23	b	611	CLA	CBD-CGD-O2D-CED
24	a	408	PHO	CBD-CGD-O2D-CED
23	b	610	CLA	O1D-CGD-O2D-CED
29	A	412	LHG	O2-C2-C3-O3
29	a	414	LHG	O2-C2-C3-O3
23	C	509	CLA	C3-C5-C6-C7
28	D	410	DGD	C4D-C5D-C6D-O5D
28	d	408	DGD	C4D-C5D-C6D-O5D
31	I	101	LMG	C29-C28-O8-C9
33	I	102	LMT	C3'-C4'-O1B-C1B
28	c	518	DGD	O6E-C5E-C6E-O5E
23	C	501	CLA	O1D-CGD-O2D-CED
31	A	418	LMG	C11-C10-O7-C8
31	I	101	LMG	C11-C10-O7-C8
31	a	402	LMG	C11-C10-O7-C8
31	d	406	LMG	C11-C10-O7-C8
31	i	101	LMG	C11-C10-O7-C8
33	i	102	LMT	C3'-C4'-O1B-C1B
23	B	608	CLA	CBD-CGD-O2D-CED
28	C	516	DGD	O6E-C5E-C6E-O5E
31	A	418	LMG	O6-C5-C6-O5
31	D	407	LMG	O6-C5-C6-O5
31	M	101	LMG	O6-C5-C6-O5
31	a	402	LMG	O6-C5-C6-O5
28	A	411	DGD	C4E-C5E-C6E-O5E
28	B	621	DGD	C4E-C5E-C6E-O5E
31	C	519	LMG	O10-C28-O8-C9
31	M	102	LMG	O6-C5-C6-O5
28	a	413	DGD	C4E-C5E-C6E-O5E
23	B	611	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	C3-C5-C6-C7
28	B	621	DGD	O6E-C5E-C6E-O5E
31	c	520	LMG	O6-C5-C6-O5
28	b	622	DGD	C4E-C5E-C6E-O5E
31	k	103	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	V	201	HEM	C3D-CAD-CBD-CGD
31	C	520	LMG	O6-C5-C6-O5
31	b	623	LMG	O6-C5-C6-O5
24	D	402	PHO	C4-C3-C5-C6
24	a	407	PHO	C4-C3-C5-C6
31	b	623	LMG	C4-C5-C6-O5
23	B	605	CLA	C2-C3-C5-C6
24	D	402	PHO	C2-C3-C5-C6
24	a	407	PHO	C2-C3-C5-C6
23	B	610	CLA	C2A-CAA-CBA-CGA
23	C	509	CLA	O1D-CGD-O2D-CED
28	b	622	DGD	O6E-C5E-C6E-O5E
28	c	517	DGD	O6E-C5E-C6E-O5E
28	B	621	DGD	O6D-C1D-O3G-C3G
28	b	602	DGD	O6E-C1E-O5D-C6D
28	b	622	DGD	O6D-C1D-O3G-C3G
28	c	517	DGD	O6D-C1D-O3G-C3G
28	c	517	DGD	O6E-C1E-O5D-C6D
31	A	418	LMG	O6-C1-O1-C7
31	M	102	LMG	O6-C1-O1-C7
25	a	410	PL9	C29-C31-C32-C33
31	a	416	LMG	O6-C5-C6-O5
23	B	614	CLA	O1D-CGD-O2D-CED
23	C	513	CLA	O1D-CGD-O2D-CED
23	b	616	CLA	O1D-CGD-O2D-CED
30	b	601	SQD	C8-C7-O47-C45
28	C	516	DGD	C4E-C5E-C6E-O5E
31	D	407	LMG	C4-C5-C6-O5
23	B	606	CLA	O1D-CGD-O2D-CED
23	b	614	CLA	O1D-CGD-O2D-CED
29	A	412	LHG	C1-C2-C3-O3
29	a	414	LHG	C1-C2-C3-O3
31	A	414	LMG	O6-C5-C6-O5
28	c	517	DGD	C4E-C5E-C6E-O5E
31	k	103	LMG	C4-C5-C6-O5
23	B	602	CLA	C3-C5-C6-C7
23	b	612	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
23	b	619	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
24	D	402	PHO	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	a	407	PHO	CBA-CGA-O2A-C1
30	b	601	SQD	C24-C23-O48-C46
31	C	520	LMG	C4-C5-C6-O5
31	a	416	LMG	C4-C5-C6-O5
31	D	406	LMG	C10-C11-C12-C13
23	B	607	CLA	C15-C16-C17-C18
31	C	519	LMG	C4-C5-C6-O5
23	b	610	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
31	E	101	LMG	C28-C29-C30-C31
31	e	101	LMG	C28-C29-C30-C31
28	b	602	DGD	O2G-C2G-C3G-O3G
24	a	407	PHO	O1A-CGA-O2A-C1
31	I	101	LMG	O10-C28-O8-C9
31	A	414	LMG	C4-C5-C6-O5
23	A	404	CLA	C2-C3-C5-C6
23	B	608	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	C	509	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	b	611	CLA	C6-C7-C8-C9
23	b	613	CLA	C14-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	b	617	CLA	O1D-CGD-O2D-CED
23	c	501	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	C13-C15-C16-C17
23	B	612	CLA	C5-C6-C7-C8
23	B	616	CLA	C10-C11-C12-C13
23	c	509	CLA	C5-C6-C7-C8
27	B	618	BCR	C7-C8-C9-C34
27	B	618	BCR	C11-C12-C13-C35
27	D	405	BCR	C37-C22-C23-C24
27	K	102	BCR	C7-C8-C9-C34
27	T	103	BCR	C7-C8-C9-C34
27	c	516	BCR	C37-C22-C23-C24
27	j	102	BCR	C7-C8-C9-C34
27	B	618	BCR	C7-C8-C9-C10
27	C	514	BCR	C7-C8-C9-C10
27	T	103	BCR	C7-C8-C9-C10
27	c	514	BCR	C7-C8-C9-C10
30	B	625	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
31	c	520	LMG	C4-C5-C6-O5
23	B	616	CLA	O1A-CGA-O2A-C1
23	b	619	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
24	D	402	PHO	O1A-CGA-O2A-C1
23	B	601	CLA	C13-C15-C16-C17
23	D	401	CLA	C15-C16-C17-C18
23	a	406	CLA	C10-C11-C12-C13
23	b	619	CLA	C10-C11-C12-C13
23	d	402	CLA	C15-C16-C17-C18
23	C	512	CLA	O1D-CGD-O2D-CED
23	b	605	CLA	C3-C5-C6-C7
23	B	604	CLA	C13-C15-C16-C17
23	B	610	CLA	C8-C10-C11-C12
23	B	616	CLA	C5-C6-C7-C8
23	C	501	CLA	C15-C16-C17-C18
23	C	503	CLA	C10-C11-C12-C13
23	b	615	CLA	C13-C15-C16-C17
23	c	504	CLA	C13-C15-C16-C17
23	c	506	CLA	C5-C6-C7-C8
23	c	506	CLA	C15-C16-C17-C18
23	c	508	CLA	C15-C16-C17-C18
24	A	406	PHO	C15-C16-C17-C18
28	c	517	DGD	C1B-C2B-C3B-C4B
31	c	520	LMG	C28-C29-C30-C31
31	d	405	LMG	C10-C11-C12-C13
23	B	607	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	C10-C11-C12-C13
23	B	607	CLA	C13-C15-C16-C17
23	B	608	CLA	C15-C16-C17-C18
23	B	611	CLA	C15-C16-C17-C18
23	B	612	CLA	C13-C15-C16-C17
23	C	504	CLA	C13-C15-C16-C17
23	C	506	CLA	C15-C16-C17-C18
23	C	508	CLA	C10-C11-C12-C13
23	C	509	CLA	C5-C6-C7-C8
23	a	405	CLA	C15-C16-C17-C18
23	b	607	CLA	C13-C15-C16-C17
23	b	610	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	b	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	C8-C10-C11-C12
23	b	614	CLA	C15-C16-C17-C18
23	b	619	CLA	C5-C6-C7-C8
23	c	503	CLA	C10-C11-C12-C13
24	a	408	PHO	C15-C16-C17-C18
25	D	404	PL9	C22-C23-C24-C25
25	J	101	PL9	C12-C13-C14-C15
28	A	411	DGD	C1B-C2B-C3B-C4B
28	B	626	DGD	C1A-C2A-C3A-C4A
28	C	516	DGD	C1B-C2B-C3B-C4B
28	D	410	DGD	C1B-C2B-C3B-C4B
28	a	413	DGD	C1B-C2B-C3B-C4B
28	b	602	DGD	C1A-C2A-C3A-C4A
28	d	408	DGD	C1B-C2B-C3B-C4B
30	a	415	SQD	C7-C8-C9-C10
31	B	622	LMG	C10-C11-C12-C13
31	C	520	LMG	C10-C11-C12-C13
31	C	520	LMG	C28-C29-C30-C31
31	b	624	LMG	C10-C11-C12-C13
23	A	404	CLA	C15-C16-C17-C18
23	C	504	CLA	C15-C16-C17-C18
23	b	604	CLA	C13-C15-C16-C17
23	B	605	CLA	CBA-CGA-O2A-C1
23	b	609	CLA	O1D-CGD-O2D-CED
31	I	101	LMG	O6-C5-C6-O5
28	c	519	DGD	O1B-C1B-O2G-C2G
30	f	103	SQD	O49-C7-O47-C45
31	k	103	LMG	O9-C10-O7-C8
23	C	508	CLA	C15-C16-C17-C18
23	c	501	CLA	C15-C16-C17-C18
23	c	504	CLA	C15-C16-C17-C18
23	c	505	CLA	C10-C11-C12-C13
23	c	507	CLA	C5-C6-C7-C8
23	c	508	CLA	C10-C11-C12-C13
31	C	519	LMG	C10-C11-C12-C13
31	c	520	LMG	C10-C11-C12-C13
23	C	501	CLA	C8-C10-C11-C12
23	C	506	CLA	C13-C15-C16-C17
23	c	501	CLA	C8-C10-C11-C12
23	d	402	CLA	C13-C15-C16-C17
23	A	405	CLA	C6-C7-C8-C10
23	C	507	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C11-C10-C8-C7
23	a	406	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C10-C8-C7
23	c	513	CLA	C11-C10-C8-C7
23	A	404	CLA	C3-C5-C6-C7
23	C	513	CLA	O1A-CGA-O2A-C1
28	C	516	DGD	C1A-C2A-C3A-C4A
23	c	512	CLA	CBA-CGA-O2A-C1
23	b	609	CLA	C2A-CAA-CBA-CGA
23	B	612	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
24	A	406	PHO	O1D-CGD-O2D-CED
23	B	613	CLA	C5-C6-C7-C8
23	C	504	CLA	C10-C11-C12-C13
23	C	507	CLA	C5-C6-C7-C8
23	c	506	CLA	C13-C15-C16-C17
31	i	101	LMG	O10-C28-O8-C9
28	C	516	DGD	O6D-C1D-O3G-C3G
28	C	516	DGD	O6E-C1E-O5D-C6D
31	a	402	LMG	O6-C1-O1-C7
23	C	510	CLA	C15-C16-C17-C18
23	C	513	CLA	C15-C16-C17-C18
25	D	404	PL9	C29-C31-C32-C33
25	d	404	PL9	C29-C31-C32-C33
25	d	404	PL9	C34-C36-C37-C38
28	c	517	DGD	C1A-C2A-C3A-C4A
31	i	101	LMG	O6-C5-C6-O5
31	C	519	LMG	O9-C10-O7-C8
23	A	405	CLA	C15-C16-C17-C18
23	C	505	CLA	C10-C11-C12-C13
23	b	616	CLA	C5-C6-C7-C8
23	c	501	CLA	C10-C11-C12-C13
23	c	504	CLA	C10-C11-C12-C13
23	c	513	CLA	C15-C16-C17-C18
28	b	622	DGD	C1B-C2B-C3B-C4B
23	B	615	CLA	C13-C15-C16-C17
23	b	619	CLA	C13-C15-C16-C17
23	c	511	CLA	C5-C6-C7-C8
23	b	615	CLA	O1D-CGD-O2D-CED
30	b	601	SQD	O10-C23-O48-C46
31	D	408	LMG	C11-C10-O7-C8
23	B	616	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C5-C6-C7-C8
23	C	511	CLA	C5-C6-C7-C8
23	D	401	CLA	C13-C15-C16-C17
23	c	510	CLA	C15-C16-C17-C18
29	A	415	LHG	C3-O3-P-O6
29	A	415	LHG	C4-O6-P-O3
29	a	414	LHG	C4-O6-P-O3
29	a	417	LHG	C3-O3-P-O6
29	a	417	LHG	C4-O6-P-O3
30	A	413	SQD	C7-C8-C9-C10
23	A	403	CLA	C3-C5-C6-C7
23	b	619	CLA	C3-C5-C6-C7
31	M	101	LMG	C29-C28-O8-C9
31	M	102	LMG	C29-C28-O8-C9
23	B	608	CLA	C5-C6-C7-C8
23	C	501	CLA	C10-C11-C12-C13
23	b	618	CLA	C13-C15-C16-C17
30	B	625	SQD	O10-C23-O48-C46
23	B	606	CLA	C2A-CAA-CBA-CGA
30	B	625	SQD	C24-C23-O48-C46
23	a	406	CLA	C15-C16-C17-C18
28	B	621	DGD	C1B-C2B-C3B-C4B
28	c	518	DGD	O6D-C5D-C6D-O5D
28	c	518	DGD	C4D-C5D-C6D-O5D
31	M	101	LMG	C4-C5-C6-O5
28	d	408	DGD	C3A-C4A-C5A-C6A
28	d	408	DGD	C7B-C8B-C9B-CAB
29	a	417	LHG	C11-C10-C9-C8
30	B	625	SQD	C11-C10-C9-C8
31	A	414	LMG	C34-C35-C36-C37
31	D	408	LMG	C36-C37-C38-C39
28	C	517	DGD	O6D-C5D-C6D-O5D
28	b	622	DGD	O6D-C5D-C6D-O5D
23	B	616	CLA	C3-C5-C6-C7
28	C	518	DGD	C9B-CAB-CBB-CCB
28	D	410	DGD	C3A-C4A-C5A-C6A
30	b	601	SQD	C11-C10-C9-C8
31	A	414	LMG	C29-C30-C31-C32
31	A	418	LMG	C11-C12-C13-C14
31	B	622	LMG	C31-C32-C33-C34
31	a	416	LMG	C14-C15-C16-C17
31	b	623	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
31	b	623	LMG	C31-C32-C33-C34
31	d	406	LMG	C36-C37-C38-C39
28	B	621	DGD	C6B-C7B-C8B-C9B
28	C	516	DGD	C3A-C4A-C5A-C6A
28	D	410	DGD	C7B-C8B-C9B-CAB
28	c	517	DGD	C3A-C4A-C5A-C6A
30	A	413	SQD	C14-C15-C16-C17
31	A	414	LMG	C14-C15-C16-C17
31	D	407	LMG	C31-C32-C33-C34
31	a	416	LMG	C29-C30-C31-C32
31	a	416	LMG	C34-C35-C36-C37
28	D	410	DGD	C1G-C2G-O2G-C1B
28	d	408	DGD	C1G-C2G-O2G-C1B
31	E	101	LMG	C7-C8-O7-C10
31	e	101	LMG	C7-C8-O7-C10
23	B	609	CLA	O1D-CGD-O2D-CED
28	B	626	DGD	C2A-C3A-C4A-C5A
28	b	602	DGD	C2A-C3A-C4A-C5A
28	b	622	DGD	C6B-C7B-C8B-C9B
28	c	519	DGD	C9B-CAB-CBB-CCB
30	f	103	SQD	C12-C13-C14-C15
31	M	101	LMG	C29-C30-C31-C32
31	M	102	LMG	C29-C30-C31-C32
31	b	624	LMG	C31-C32-C33-C34
28	A	411	DGD	C5B-C6B-C7B-C8B
31	a	402	LMG	C11-C12-C13-C14
23	a	409	CLA	C10-C11-C12-C13
34	f	101	HEM	C3D-CAD-CBD-CGD
29	A	415	LHG	C24-C25-C26-C27
30	F	102	SQD	C12-C13-C14-C15
30	a	415	SQD	C14-C15-C16-C17
23	C	502	CLA	C3-C5-C6-C7
31	k	103	LMG	C10-C11-C12-C13
28	C	517	DGD	C2D-C1D-O3G-C3G
28	C	517	DGD	C2E-C1E-O5D-C6D
28	c	518	DGD	C2E-C1E-O5D-C6D
31	B	622	LMG	C2-C1-O1-C7
31	I	101	LMG	C2-C1-O1-C7
31	a	402	LMG	C4-C5-C6-O5
29	A	412	LHG	C25-C26-C27-C28
29	A	415	LHG	C11-C10-C9-C8
29	a	417	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
31	B	622	LMG	C34-C35-C36-C37
31	d	406	LMG	C15-C16-C17-C18
23	C	503	CLA	C5-C6-C7-C8
23	B	605	CLA	O1A-CGA-O2A-C1
25	A	408	PL9	C7-C8-C9-C10
28	C	518	DGD	C3B-C4B-C5B-C6B
28	c	519	DGD	C3B-C4B-C5B-C6B
28	d	408	DGD	CCB-CDB-CEB-CFB
29	a	414	LHG	C25-C26-C27-C28
31	c	520	LMG	C12-C13-C14-C15
23	B	601	CLA	C11-C12-C13-C14
23	B	612	CLA	C6-C7-C8-C9
23	C	505	CLA	C11-C10-C8-C9
23	C	506	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	a	405	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C12-C13-C14
23	c	505	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C10-C8-C9
24	A	406	PHO	C11-C10-C8-C9
24	a	408	PHO	C11-C10-C8-C9
28	a	413	DGD	C5B-C6B-C7B-C8B
28	d	408	DGD	C2A-C3A-C4A-C5A
28	d	408	DGD	CAB-CBB-CCB-CDB
28	d	408	DGD	CDB-CEB-CFB-CGB
30	A	413	SQD	C27-C28-C29-C30
30	f	103	SQD	C11-C12-C13-C14
31	C	520	LMG	C12-C13-C14-C15
31	D	407	LMG	C30-C31-C32-C33
31	D	408	LMG	C15-C16-C17-C18
31	I	101	LMG	C16-C17-C18-C19
31	a	402	LMG	C18-C19-C20-C21
31	i	101	LMG	C16-C17-C18-C19
23	b	611	CLA	C5-C6-C7-C8
23	c	512	CLA	O1A-CGA-O2A-C1
28	C	517	DGD	C4D-C5D-C6D-O5D
27	C	514	BCR	C7-C8-C9-C34
27	c	514	BCR	C7-C8-C9-C34
27	c	515	BCR	C7-C8-C9-C34
30	F	102	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	D	408	LMG	C19-C20-C21-C22
33	B	627	LMT	C2-C3-C4-C5
27	c	516	BCR	C7-C8-C9-C10
27	f	102	BCR	C21-C22-C23-C24
23	a	404	CLA	C3-C5-C6-C7
23	a	405	CLA	C3-C5-C6-C7
28	C	518	DGD	C2B-C1B-O2G-C2G
31	D	408	LMG	C14-C15-C16-C17
31	I	101	LMG	C14-C15-C16-C17
31	b	624	LMG	C34-C35-C36-C37
31	A	418	LMG	C4-C5-C6-O5
28	C	517	DGD	C1A-C2A-C3A-C4A
31	b	623	LMG	C28-C29-C30-C31
28	C	517	DGD	C2A-C3A-C4A-C5A
28	D	410	DGD	C2A-C3A-C4A-C5A
28	D	410	DGD	C4B-C5B-C6B-C7B
28	D	410	DGD	CAB-CBB-CCB-CDB
28	D	410	DGD	CDB-CEB-CFB-CGB
28	D	410	DGD	CEB-CFB-CGB-CHB
28	c	517	DGD	C3B-C4B-C5B-C6B
28	d	408	DGD	C4B-C5B-C6B-C7B
30	a	415	SQD	C27-C28-C29-C30
31	A	418	LMG	C18-C19-C20-C21
31	d	406	LMG	C14-C15-C16-C17
33	B	627	LMT	C7-C8-C9-C10
30	D	409	SQD	O5-C1-O6-C44
25	A	408	PL9	C29-C31-C32-C33
28	C	516	DGD	C3B-C4B-C5B-C6B
28	D	410	DGD	CCB-CDB-CEB-CFB
31	d	406	LMG	C19-C20-C21-C22
31	i	101	LMG	C14-C15-C16-C17
33	I	102	LMT	C6-C7-C8-C9
31	b	624	LMG	C13-C14-C15-C16
31	i	101	LMG	C13-C14-C15-C16
33	T	101	LMT	C7-C8-C9-C10
31	D	407	LMG	C28-C29-C30-C31
23	A	407	CLA	C10-C11-C12-C13
23	C	506	CLA	C10-C11-C12-C13
30	B	625	SQD	C9-C10-C11-C12
31	c	520	LMG	C29-C30-C31-C32
33	T	101	LMT	C2-C3-C4-C5
23	b	611	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	CBA-CGA-O2A-C1
31	E	101	LMG	C15-C16-C17-C18
31	I	101	LMG	C13-C14-C15-C16
31	e	101	LMG	C15-C16-C17-C18
23	B	602	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C3A-C2A-CAA-CBA
23	B	608	CLA	C3A-C2A-CAA-CBA
23	B	616	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
23	a	405	CLA	C3A-C2A-CAA-CBA
23	c	505	CLA	C3A-C2A-CAA-CBA
23	c	507	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
23	c	503	CLA	C5-C6-C7-C8
25	J	101	PL9	C27-C28-C29-C31
28	B	626	DGD	C5B-C6B-C7B-C8B
28	C	516	DGD	C4A-C5A-C6A-C7A
28	c	517	DGD	C4A-C5A-C6A-C7A
31	C	520	LMG	C29-C30-C31-C32
33	i	102	LMT	C6-C7-C8-C9
23	B	613	CLA	C16-C17-C18-C19
28	C	516	DGD	C4B-C5B-C6B-C7B
28	d	408	DGD	CEB-CFB-CGB-CHB
31	B	622	LMG	C13-C14-C15-C16
31	D	408	LMG	C13-C14-C15-C16
31	b	623	LMG	C18-C19-C20-C21
31	d	406	LMG	C13-C14-C15-C16
28	C	518	DGD	O1G-C1G-C2G-C3G
28	c	519	DGD	O1G-C1G-C2G-C3G
28	c	518	DGD	CCB-CDB-CEB-CFB
28	c	518	DGD	C1A-C2A-C3A-C4A
28	d	408	DGD	C3B-C4B-C5B-C6B
23	C	510	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
23	C	510	CLA	C2-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
28	c	517	DGD	C4B-C5B-C6B-C7B
31	i	101	LMG	C12-C13-C14-C15
28	b	602	DGD	C9B-CAB-CBB-CCB
28	b	622	DGD	C5B-C6B-C7B-C8B
30	f	103	SQD	C10-C11-C12-C13
31	I	101	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	a	402	LMG	C31-C32-C33-C34
31	b	623	LMG	C19-C20-C21-C22
28	C	518	DGD	CAB-CBB-CCB-CDB
28	c	518	DGD	C2A-C3A-C4A-C5A
31	A	418	LMG	C31-C32-C33-C34
30	B	625	SQD	C11-C12-C13-C14
31	b	623	LMG	C36-C37-C38-C39
31	d	406	LMG	O9-C10-O7-C8
33	b	625	LMT	C1-C2-C3-C4
23	C	509	CLA	C2-C1-O2A-CGA
28	C	517	DGD	CCB-CDB-CEB-CFB
28	D	410	DGD	C5A-C6A-C7A-C8A
33	B	623	LMT	C1-C2-C3-C4
28	d	408	DGD	C6B-C7B-C8B-C9B
31	D	407	LMG	C18-C19-C20-C21
31	a	416	LMG	C30-C31-C32-C33
27	B	617	BCR	C5-C6-C7-C8
27	B	618	BCR	C23-C24-C25-C30
27	C	514	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	405	BCR	C1-C6-C7-C8
27	D	405	BCR	C5-C6-C7-C8
27	H	101	BCR	C1-C6-C7-C8
27	H	101	BCR	C5-C6-C7-C8
27	K	102	BCR	C23-C24-C25-C26
27	T	103	BCR	C23-C24-C25-C30
27	Z	101	BCR	C5-C6-C7-C8
27	c	515	BCR	C5-C6-C7-C8
27	c	516	BCR	C5-C6-C7-C8
27	c	516	BCR	C23-C24-C25-C26
27	f	102	BCR	C1-C6-C7-C8
27	f	102	BCR	C5-C6-C7-C8
27	j	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C26
27	k	102	BCR	C23-C24-C25-C30
28	b	602	DGD	C5B-C6B-C7B-C8B
31	b	623	LMG	C13-C14-C15-C16
24	a	408	PHO	O1D-CGD-O2D-CED
23	C	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C15-C16-C17-C18
23	b	604	CLA	C10-C11-C12-C13
23	c	506	CLA	C10-C11-C12-C13
34	F	101	HEM	C3D-CAD-CBD-CGD
28	c	519	DGD	C2B-C1B-O2G-C2G
30	A	417	SQD	C18-C19-C20-C21
31	A	414	LMG	C30-C31-C32-C33
28	D	410	DGD	C3B-C4B-C5B-C6B
28	b	602	DGD	C3A-C4A-C5A-C6A
30	a	415	SQD	C17-C18-C19-C20
25	j	101	PL9	C27-C28-C29-C31
23	C	513	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
28	B	621	DGD	C5B-C6B-C7B-C8B
28	D	410	DGD	C6B-C7B-C8B-C9B
30	b	601	SQD	C9-C10-C11-C12
30	b	601	SQD	C11-C12-C13-C14
23	b	608	CLA	C4-C3-C5-C6
23	B	601	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C12-C13-C15
23	B	612	CLA	C6-C7-C8-C10
23	C	505	CLA	C11-C10-C8-C7
23	C	506	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C10-C8-C7
23	C	511	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C10-C8-C7
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
24	A	406	PHO	C11-C10-C8-C7
24	a	408	PHO	C11-C10-C8-C7
23	C	512	CLA	O1A-CGA-O2A-C1
31	D	407	LMG	C36-C37-C38-C39
23	c	512	CLA	C13-C15-C16-C17
23	d	403	CLA	C15-C16-C17-C18
23	b	616	CLA	C16-C17-C18-C19
28	B	621	DGD	O6D-C5D-C6D-O5D
23	B	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	b	608	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
31	b	624	LMG	C29-C28-O8-C9
30	A	413	SQD	C17-C18-C19-C20
30	F	102	SQD	C10-C11-C12-C13
23	C	501	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
23	B	604	CLA	C8-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
23	c	513	CLA	C13-C15-C16-C17
28	B	626	DGD	C9B-CAB-CBB-CCB
29	a	414	LHG	C30-C31-C32-C33
31	A	418	LMG	C32-C33-C34-C35
23	B	602	CLA	C13-C15-C16-C17
28	C	516	DGD	C5A-C6A-C7A-C8A
28	c	519	DGD	CAB-CBB-CCB-CDB
28	D	410	DGD	C5B-C6B-C7B-C8B
30	A	417	SQD	C32-C33-C34-C35
31	D	408	LMG	C32-C33-C34-C35
31	M	102	LMG	O10-C28-O8-C9
23	b	614	CLA	CBA-CGA-O2A-C1
28	c	518	DGD	O6E-C1E-O5D-C6D
31	B	622	LMG	O6-C1-O1-C7
31	I	101	LMG	O6-C1-O1-C7
23	C	503	CLA	C8-C10-C11-C12
25	A	408	PL9	C14-C16-C17-C18
31	a	402	LMG	C32-C33-C34-C35
31	A	414	LMG	C11-C10-O7-C8
31	E	101	LMG	C11-C10-O7-C8
31	e	101	LMG	C11-C10-O7-C8
31	D	406	LMG	O6-C5-C6-O5
28	d	408	DGD	C5B-C6B-C7B-C8B
29	A	412	LHG	C30-C31-C32-C33
25	d	404	PL9	C47-C48-C49-C51
30	D	409	SQD	C9-C10-C11-C12
31	D	408	LMG	O9-C10-O7-C8
28	d	408	DGD	C5A-C6A-C7A-C8A
28	c	518	DGD	C2D-C1D-O3G-C3G
31	b	624	LMG	C2-C1-O1-C7
28	C	518	DGD	O1G-C1G-C2G-O2G
28	c	519	DGD	O1G-C1G-C2G-O2G
30	A	413	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
28	b	602	DGD	C2B-C3B-C4B-C5B
23	b	613	CLA	C16-C17-C18-C20
30	A	413	SQD	C11-C10-C9-C8
31	D	407	LMG	C20-C21-C22-C23
31	E	101	LMG	C17-C18-C19-C20
23	A	405	CLA	C6-C7-C8-C9
23	B	601	CLA	C6-C7-C8-C9
23	B	603	CLA	C11-C12-C13-C14
23	B	613	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	a	406	CLA	C6-C7-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	612	CLA	C6-C7-C8-C9
23	c	503	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C10-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	c	513	CLA	C11-C10-C8-C9
23	c	513	CLA	C14-C13-C15-C16
23	c	510	CLA	CBD-CGD-O2D-CED
28	B	621	DGD	C3B-C4B-C5B-C6B
28	c	517	DGD	C5A-C6A-C7A-C8A
23	C	513	CLA	C2A-CAA-CBA-CGA
23	c	513	CLA	C2A-CAA-CBA-CGA
31	E	101	LMG	O6-C5-C6-O5
23	B	614	CLA	C15-C16-C17-C18
23	C	512	CLA	C5-C6-C7-C8
23	c	503	CLA	C8-C10-C11-C12
30	d	407	SQD	C9-C10-C11-C12
23	b	608	CLA	O1A-CGA-O2A-C1
23	B	616	CLA	C1A-C2A-CAA-CBA
23	C	501	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	b	619	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
23	b	613	CLA	C16-C17-C18-C19
23	A	407	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	a	409	CLA	C5-C6-C7-C8
29	A	412	LHG	C4-O6-P-O3
28	B	626	DGD	C3A-C4A-C5A-C6A
31	d	406	LMG	C32-C33-C34-C35
33	B	624	LMT	C2B-C1B-O1B-C4'
23	c	502	CLA	C3-C5-C6-C7
31	I	101	LMG	C4-C5-C6-O5
28	C	517	DGD	CAB-CBB-CCB-CDB
31	D	407	LMG	C19-C20-C21-C22
23	b	607	CLA	C8-C10-C11-C12
23	D	403	CLA	CBA-CGA-O2A-C1
23	c	504	CLA	CBA-CGA-O2A-C1
31	a	416	LMG	C15-C16-C17-C18
31	D	408	LMG	C28-C29-C30-C31
31	d	406	LMG	C10-C11-C12-C13
31	d	406	LMG	C28-C29-C30-C31
23	B	613	CLA	C16-C17-C18-C20
28	b	622	DGD	C3B-C4B-C5B-C6B
31	e	101	LMG	O6-C5-C6-O5
31	A	414	LMG	C15-C16-C17-C18
30	a	415	SQD	C11-C10-C9-C8
23	d	403	CLA	CBA-CGA-O2A-C1
31	A	414	LMG	C20-C21-C22-C23
23	c	509	CLA	O1A-CGA-O2A-C1
23	b	604	CLA	C16-C17-C18-C20
23	c	512	CLA	C16-C17-C18-C20
28	B	621	DGD	O1G-C1G-C2G-C3G
28	B	626	DGD	C2B-C3B-C4B-C5B
28	D	410	DGD	C1G-C2G-C3G-O3G
28	b	602	DGD	C1G-C2G-C3G-O3G
28	b	622	DGD	O1G-C1G-C2G-C3G
28	d	408	DGD	C1G-C2G-C3G-O3G
30	A	417	SQD	O6-C44-C45-C46
30	B	625	SQD	C44-C45-C46-O48
30	a	401	SQD	O6-C44-C45-C46
30	b	601	SQD	C44-C45-C46-O48
31	A	414	LMG	O1-C7-C8-C9
31	C	519	LMG	C7-C8-C9-O8
31	D	407	LMG	O1-C7-C8-C9
31	D	408	LMG	O1-C7-C8-C9
31	I	101	LMG	O1-C7-C8-C9
31	d	406	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	k	103	LMG	C7-C8-C9-O8
23	B	602	CLA	C5-C6-C7-C8
23	c	505	CLA	C15-C16-C17-C18
28	d	408	DGD	C8B-C9B-CAB-CBB
31	a	416	LMG	C20-C21-C22-C23
31	D	408	LMG	C8-C7-O1-C1
31	a	416	LMG	C8-C7-O1-C1
31	e	101	LMG	C19-C20-C21-C22
23	C	505	CLA	C15-C16-C17-C18
33	b	626	LMT	C2B-C1B-O1B-C4'
31	E	101	LMG	C19-C20-C21-C22
31	e	101	LMG	C17-C18-C19-C20
28	c	519	DGD	C1A-C2A-C3A-C4A
23	b	614	CLA	O1A-CGA-O2A-C1
31	B	622	LMG	O10-C28-O8-C9
31	a	402	LMG	C28-C29-C30-C31
31	M	102	LMG	C4-C5-C6-O5
23	C	505	CLA	C4-C3-C5-C6
25	j	101	PL9	C15-C14-C16-C17
31	d	405	LMG	C31-C32-C33-C34
31	d	405	LMG	C38-C39-C40-C41
28	C	518	DGD	C1A-C2A-C3A-C4A
29	a	414	LHG	C23-C24-C25-C26
31	D	408	LMG	C10-C11-C12-C13
23	B	610	CLA	C16-C17-C18-C20
23	b	616	CLA	C16-C17-C18-C20
23	B	611	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
23	C	507	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
23	B	604	CLA	C15-C16-C17-C18
31	d	405	LMG	O6-C5-C6-O5
23	A	403	CLA	C2A-CAA-CBA-CGA
23	a	404	CLA	C2A-CAA-CBA-CGA
23	A	403	CLA	C2-C1-O2A-CGA
23	B	610	CLA	C2-C1-O2A-CGA
23	c	509	CLA	C2-C1-O2A-CGA
30	A	417	SQD	C12-C13-C14-C15
31	D	406	LMG	C38-C39-C40-C41
31	D	407	LMG	C17-C18-C19-C20
30	A	417	SQD	C10-C11-C12-C13
31	d	406	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	a	409	CLA	C13-C15-C16-C17
31	D	406	LMG	C31-C32-C33-C34
23	C	505	CLA	CBA-CGA-O2A-C1
31	B	622	LMG	C29-C28-O8-C9
29	a	417	LHG	O6-C4-C5-O7
28	B	621	DGD	CAB-CBB-CCB-CDB
23	c	502	CLA	C13-C15-C16-C17
28	C	516	DGD	C2A-C3A-C4A-C5A
31	k	103	LMG	C16-C17-C18-C19
31	D	407	LMG	C15-C16-C17-C18
23	B	605	CLA	C15-C16-C17-C18
23	b	617	CLA	C15-C16-C17-C18
28	D	410	DGD	C2D-C1D-O3G-C3G
28	d	408	DGD	C2D-C1D-O3G-C3G
33	B	624	LMT	O5B-C1B-O1B-C4'
28	B	626	DGD	CAB-CBB-CCB-CDB
30	a	401	SQD	C32-C33-C34-C35
30	a	415	SQD	O6-C44-C45-O47
31	I	101	LMG	O1-C7-C8-O7
30	A	413	SQD	C10-C11-C12-C13
31	b	623	LMG	C20-C21-C22-C23
25	D	404	PL9	C47-C48-C49-C51
23	D	403	CLA	O1A-CGA-O2A-C1
23	c	504	CLA	O1A-CGA-O2A-C1
28	b	622	DGD	CAB-CBB-CCB-CDB
31	D	408	LMG	C11-C12-C13-C14
31	e	101	LMG	C18-C19-C20-C21
23	c	505	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6
25	j	101	PL9	C12-C13-C14-C15
28	D	410	DGD	C8B-C9B-CAB-CBB
23	B	601	CLA	C6-C7-C8-C10
23	B	610	CLA	C11-C12-C13-C15
23	B	611	CLA	C11-C10-C8-C7
23	B	613	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C10-C8-C7
23	B	615	CLA	C12-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C15
23	C	503	CLA	C11-C10-C8-C7
23	C	503	CLA	C11-C12-C13-C15
23	C	505	CLA	C6-C7-C8-C10
23	C	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C7
23	b	604	CLA	C11-C12-C13-C15
23	b	605	CLA	C6-C7-C8-C10
23	b	606	CLA	C6-C7-C8-C10
23	b	613	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C10-C8-C7
23	b	616	CLA	C11-C10-C8-C7
23	b	618	CLA	C12-C13-C15-C16
23	b	619	CLA	C11-C10-C8-C7
23	b	619	CLA	C12-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C12-C13-C15
23	c	505	CLA	C2-C3-C5-C6
23	c	508	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
23	d	402	CLA	C12-C13-C15-C16
24	a	408	PHO	C12-C13-C15-C16
23	C	510	CLA	C3-C5-C6-C7
23	C	512	CLA	C3-C5-C6-C7
23	A	403	CLA	C11-C12-C13-C14
23	B	603	CLA	C6-C7-C8-C9
23	B	606	CLA	C14-C13-C15-C16
23	B	609	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C14
23	C	502	CLA	C14-C13-C15-C16
23	C	503	CLA	C11-C10-C8-C9
23	C	503	CLA	C11-C12-C13-C14
23	C	505	CLA	C6-C7-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	D	401	CLA	C14-C13-C15-C16
23	b	609	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C9
23	b	618	CLA	C11-C10-C8-C9
23	b	618	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	502	CLA	C11-C12-C13-C14
23	c	502	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	505	CLA	C14-C13-C15-C16
23	c	506	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C9
23	c	511	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C14
23	d	402	CLA	C14-C13-C15-C16
24	A	406	PHO	C14-C13-C15-C16
24	a	407	PHO	C6-C7-C8-C9
24	a	408	PHO	C14-C13-C15-C16
30	A	417	SQD	C30-C31-C32-C33
23	C	504	CLA	CBA-CGA-O2A-C1
28	c	518	DGD	CAB-CBB-CCB-CDB
27	B	620	BCR	C37-C22-C23-C24
23	B	610	CLA	C16-C17-C18-C19
23	C	512	CLA	C16-C17-C18-C20
27	D	405	BCR	C21-C22-C23-C24
31	a	402	LMG	C15-C16-C17-C18
23	b	607	CLA	C15-C16-C17-C18
23	b	608	CLA	C15-C16-C17-C18
23	c	509	CLA	C15-C16-C17-C18
31	a	416	LMG	C11-C10-O7-C8
23	d	403	CLA	O1A-CGA-O2A-C1
29	A	415	LHG	C24-C23-O8-C6
28	c	517	DGD	C2A-C3A-C4A-C5A
23	C	502	CLA	C13-C15-C16-C17
23	b	619	CLA	C8-C10-C11-C12
28	D	410	DGD	CBA-CCA-CDA-CEA
31	A	418	LMG	C12-C13-C14-C15
34	V	201	HEM	C4D-C3D-CAD-CBD
23	b	604	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C19
29	A	412	LHG	O6-C4-C5-C6
29	a	417	LHG	O6-C4-C5-C6
23	c	510	CLA	C3-C5-C6-C7
31	D	407	LMG	C13-C14-C15-C16
28	D	410	DGD	C1A-C2A-C3A-C4A
33	b	626	LMT	O5B-C1B-O1B-C4'
30	a	401	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	i	101	LMG	C18-C19-C20-C21
23	A	407	CLA	C13-C15-C16-C17
23	C	513	CLA	C4-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	C	513	CLA	C2-C3-C5-C6
23	c	513	CLA	C2-C3-C5-C6
30	D	409	SQD	C7-C8-C9-C10
31	A	414	LMG	C31-C32-C33-C34
31	C	519	LMG	C12-C13-C14-C15
23	B	601	CLA	C16-C17-C18-C20
31	C	519	LMG	C16-C17-C18-C19
23	c	504	CLA	C2A-CAA-CBA-CGA
23	B	610	CLA	CBA-CGA-O2A-C1
23	C	509	CLA	CBA-CGA-O2A-C1
23	b	613	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
23	B	616	CLA	C8-C10-C11-C12
31	E	101	LMG	C18-C19-C20-C21
23	a	405	CLA	C5-C6-C7-C8
23	b	619	CLA	C15-C16-C17-C18
28	B	626	DGD	C1G-C2G-C3G-O3G
28	C	517	DGD	C1G-C2G-C3G-O3G
28	c	518	DGD	C1G-C2G-C3G-O3G
30	A	413	SQD	O6-C44-C45-C46
30	a	415	SQD	O6-C44-C45-C46
31	B	622	LMG	C7-C8-C9-O8
31	M	101	LMG	C7-C8-C9-O8
31	M	102	LMG	C7-C8-C9-O8
31	b	624	LMG	C7-C8-C9-O8
31	i	101	LMG	O1-C7-C8-C9
28	c	519	DGD	CFA-CGA-CHA-CIA
31	k	103	LMG	C30-C31-C32-C33
28	d	408	DGD	C1A-C2A-C3A-C4A
33	i	102	LMT	C5'-C4'-O1B-C1B
23	b	608	CLA	C5-C6-C7-C8
30	A	413	SQD	C15-C16-C17-C18
31	I	101	LMG	C18-C19-C20-C21
34	V	201	HEM	C2D-C3D-CAD-CBD
30	A	413	SQD	C31-C32-C33-C34
23	b	608	CLA	C2-C3-C5-C6
31	A	418	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	a	415	SQD	C10-C11-C12-C13
23	c	505	CLA	C8-C10-C11-C12
31	A	418	LMG	C28-C29-C30-C31
31	b	624	LMG	O10-C28-O8-C9
31	C	520	LMG	C13-C14-C15-C16
31	M	101	LMG	C11-C12-C13-C14
23	c	507	CLA	C3-C5-C6-C7
28	d	408	DGD	CBA-CCA-CDA-CEA
31	b	623	LMG	C17-C18-C19-C20
29	a	414	LHG	O6-C4-C5-O7
23	B	611	CLA	O1A-CGA-O2A-C1
23	C	511	CLA	O1A-CGA-O2A-C1
31	M	101	LMG	O10-C28-O8-C9
23	B	610	CLA	C10-C11-C12-C13
24	a	407	PHO	C5-C6-C7-C8
23	C	505	CLA	O1A-CGA-O2A-C1
31	a	416	LMG	C31-C32-C33-C34
30	A	413	SQD	O47-C45-C46-O48
30	B	625	SQD	O47-C45-C46-O48
30	a	415	SQD	O47-C45-C46-O48
30	b	601	SQD	O47-C45-C46-O48
30	f	103	SQD	O47-C45-C46-O48
31	A	414	LMG	O1-C7-C8-O7
31	B	622	LMG	O7-C8-C9-O8
31	b	624	LMG	O7-C8-C9-O8
31	e	101	LMG	O1-C7-C8-O7
31	i	101	LMG	O1-C7-C8-O7
31	k	103	LMG	O7-C8-C9-O8
29	A	412	LHG	C8-C7-O7-C5
30	d	407	SQD	O5-C1-O6-C44
31	b	624	LMG	O6-C1-O1-C7
25	a	410	PL9	C14-C16-C17-C18
31	a	402	LMG	C12-C13-C14-C15
30	b	601	SQD	O49-C7-O47-C45
23	B	613	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
23	b	616	CLA	C2-C1-O2A-CGA
28	c	519	DGD	C8B-C9B-CAB-CBB
23	B	616	CLA	C15-C16-C17-C18
23	C	508	CLA	C5-C6-C7-C8
23	A	404	CLA	C6-C7-C8-C9
23	B	615	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C11-C12-C13-C14
23	D	401	CLA	C6-C7-C8-C9
23	a	404	CLA	C11-C12-C13-C14
23	b	606	CLA	C6-C7-C8-C9
23	b	618	CLA	C6-C7-C8-C9
23	d	402	CLA	C6-C7-C8-C9
28	C	518	DGD	CDB-CEB-CFB-CGB
30	a	415	SQD	C31-C32-C33-C34
31	a	402	LMG	C30-C31-C32-C33
28	b	602	DGD	CAB-CBB-CCB-CDB
30	a	415	SQD	C15-C16-C17-C18
31	b	624	LMG	C15-C16-C17-C18
31	c	520	LMG	C13-C14-C15-C16
23	C	504	CLA	O1A-CGA-O2A-C1
30	A	417	SQD	C33-C34-C35-C36
30	B	625	SQD	C12-C13-C14-C15
23	C	512	CLA	C16-C17-C18-C19
23	c	512	CLA	C3-C5-C6-C7
27	C	514	BCR	C5-C6-C7-C8
27	J	102	BCR	C5-C6-C7-C8
27	K	102	BCR	C5-C6-C7-C8
27	T	102	BCR	C1-C6-C7-C8
27	T	102	BCR	C5-C6-C7-C8
27	a	412	BCR	C23-C24-C25-C26
27	a	412	BCR	C23-C24-C25-C30
27	j	102	BCR	C1-C6-C7-C8
23	c	508	CLA	C5-C6-C7-C8
33	I	102	LMT	C5'-C4'-O1B-C1B
27	B	618	BCR	C11-C12-C13-C14
27	c	516	BCR	C21-C22-C23-C24
27	j	102	BCR	C7-C8-C9-C10
31	i	101	LMG	C4-C5-C6-O5
29	A	412	LHG	O9-C7-O7-C5
28	B	621	DGD	C7A-C8A-C9A-CAA
34	v	201	HEM	C2D-C3D-CAD-CBD
30	d	407	SQD	C7-C8-C9-C10
23	c	501	CLA	C13-C15-C16-C17
31	b	623	LMG	C15-C16-C17-C18
29	a	414	LHG	O6-C4-C5-C6
28	C	516	DGD	C2B-C3B-C4B-C5B
30	b	601	SQD	C12-C13-C14-C15
31	A	418	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	B	622	LMG	C15-C16-C17-C18
23	A	404	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	B	603	CLA	C6-C7-C8-C10
23	B	605	CLA	C11-C10-C8-C7
23	B	606	CLA	C12-C13-C15-C16
23	B	608	CLA	C6-C7-C8-C10
23	B	613	CLA	C11-C12-C13-C15
23	B	616	CLA	C11-C10-C8-C7
23	C	501	CLA	C11-C12-C13-C15
23	C	502	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	508	CLA	C12-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C7
23	C	511	CLA	C6-C7-C8-C10
23	C	512	CLA	C11-C12-C13-C15
23	C	512	CLA	C12-C13-C15-C16
23	D	401	CLA	C12-C13-C15-C16
23	a	405	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C10-C8-C7
23	b	609	CLA	C12-C13-C15-C16
23	b	611	CLA	C6-C7-C8-C10
23	b	612	CLA	C12-C13-C15-C16
23	b	616	CLA	C11-C12-C13-C15
23	b	618	CLA	C11-C10-C8-C7
23	c	501	CLA	C11-C12-C13-C15
23	c	502	CLA	C12-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C10
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
23	c	508	CLA	C12-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C7
23	c	511	CLA	C6-C7-C8-C10
23	c	511	CLA	C12-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
24	A	406	PHO	C12-C13-C15-C16
28	A	411	DGD	C3B-C4B-C5B-C6B
23	b	608	CLA	C10-C11-C12-C13
30	a	401	SQD	C23-C24-C25-C26
31	D	407	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	a	401	SQD	C10-C11-C12-C13
31	D	406	LMG	C11-C12-C13-C14
23	B	601	CLA	C16-C17-C18-C19
24	a	408	PHO	C10-C11-C12-C13
23	c	507	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	CAD-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
28	C	518	DGD	C3G-C2G-O2G-C1B
31	C	520	LMG	C9-C8-O7-C10
23	C	507	CLA	C3-C5-C6-C7
28	C	517	DGD	C4B-C5B-C6B-C7B
23	C	509	CLA	C15-C16-C17-C18
23	c	509	CLA	C10-C11-C12-C13
28	C	517	DGD	C7B-C8B-C9B-CAB
28	c	519	DGD	CDB-CEB-CFB-CGB
23	b	605	CLA	CBA-CGA-O2A-C1
29	a	417	LHG	C24-C23-O8-C6
23	b	615	CLA	C4-C3-C5-C6
29	a	417	LHG	C25-C26-C27-C28
28	C	517	DGD	O6E-C1E-O5D-C6D
31	i	101	LMG	O6-C1-O1-C7
25	J	101	PL9	C19-C21-C22-C23
25	j	101	PL9	C19-C21-C22-C23
29	A	412	LHG	C2-C3-O3-P
30	D	409	SQD	O6-C44-C45-C46
30	d	407	SQD	O6-C44-C45-C46
31	b	623	LMG	O1-C7-C8-C9
23	C	509	CLA	O1A-CGA-O2A-C1
31	M	102	LMG	C30-C31-C32-C33
23	B	605	CLA	C5-C6-C7-C8
34	F	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4B-C3B-CAB-CBB
23	B	614	CLA	C16-C17-C18-C19
31	A	418	LMG	C13-C14-C15-C16
31	M	102	LMG	C11-C12-C13-C14
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O1D
23	b	617	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1A-CGA-O2A-C1
23	c	505	CLA	O1A-CGA-O2A-C1
28	a	413	DGD	C8B-C9B-CAB-CBB
23	C	507	CLA	O1D-CGD-O2D-CED
30	F	102	SQD	C2-C1-O6-C44
31	i	101	LMG	C2-C1-O1-C7
28	b	622	DGD	C4B-C5B-C6B-C7B
28	D	410	DGD	O2G-C2G-C3G-O3G
28	b	602	DGD	O1G-C1G-C2G-O2G
30	F	102	SQD	O47-C45-C46-O48
31	E	101	LMG	O1-C7-C8-O7
31	M	102	LMG	O7-C8-C9-O8
29	A	415	LHG	O10-C23-O8-C6
31	C	519	LMG	C30-C31-C32-C33
23	b	617	CLA	C16-C17-C18-C20
23	A	405	CLA	C5-C6-C7-C8
23	B	608	CLA	C13-C15-C16-C17
23	b	613	CLA	C5-C6-C7-C8
25	D	404	PL9	C15-C14-C16-C17
25	J	101	PL9	C15-C14-C16-C17
23	c	511	CLA	O1A-CGA-O2A-C1
30	B	625	SQD	O49-C7-O47-C45
23	B	609	CLA	C14-C13-C15-C16
23	a	405	CLA	C14-C13-C15-C16
23	b	612	CLA	C14-C13-C15-C16
23	b	605	CLA	O1D-CGD-O2D-CED
31	B	622	LMG	C35-C36-C37-C38
27	j	102	BCR	C37-C22-C23-C24
28	C	518	DGD	C8B-C9B-CAB-CBB
23	B	612	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	c	518	DGD	C7B-C8B-C9B-CAB
31	b	624	LMG	C35-C36-C37-C38
23	B	603	CLA	C16-C17-C18-C19
23	A	404	CLA	C5-C6-C7-C8
23	c	507	CLA	O1D-CGD-O2D-CED
29	A	412	LHG	C3-O3-P-O6
31	k	103	LMG	C12-C13-C14-C15
30	f	103	SQD	C29-C30-C31-C32
31	A	418	LMG	C30-C31-C32-C33
29	a	414	LHG	C2-C3-O3-P
23	b	605	CLA	O1A-CGA-O2A-C1
29	A	412	LHG	C4-O6-P-O5
29	A	415	LHG	C3-O3-P-O5
29	a	417	LHG	C3-O3-P-O5
23	B	614	CLA	C16-C17-C18-C20
23	B	605	CLA	C10-C11-C12-C13
23	b	607	CLA	CBA-CGA-O2A-C1
25	A	408	PL9	C19-C21-C22-C23
25	j	101	PL9	C24-C26-C27-C28
30	a	401	SQD	C26-C27-C28-C29
31	i	101	LMG	C29-C30-C31-C32
31	b	623	LMG	C10-C11-C12-C13
28	B	626	DGD	C8B-C9B-CAB-CBB
30	a	415	SQD	C16-C17-C18-C19
31	a	402	LMG	C17-C18-C19-C20
23	A	407	CLA	C16-C17-C18-C19
28	C	518	DGD	CDA-CEA-CFA-CGA
33	B	623	LMT	C4-C5-C6-C7
33	b	625	LMT	C4-C5-C6-C7
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
30	D	409	SQD	O5-C5-C6-S
34	v	201	HEM	C4D-C3D-CAD-CBD
23	b	615	CLA	C10-C11-C12-C13
28	C	518	DGD	CEA-CFA-CGA-CHA
23	B	604	CLA	CBA-CGA-O2A-C1
23	b	611	CLA	CBA-CGA-O2A-C1
28	B	621	DGD	C7B-C8B-C9B-CAB
30	b	601	SQD	C15-C16-C17-C18
31	I	101	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
31	b	623	LMG	C29-C30-C31-C32
23	b	606	CLA	C16-C17-C18-C19
23	A	407	CLA	C11-C10-C8-C7
23	B	608	CLA	C11-C12-C13-C15
23	B	609	CLA	C12-C13-C15-C16
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	a	409	CLA	C11-C10-C8-C7
23	b	611	CLA	C11-C12-C13-C15
23	b	613	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
23	d	403	CLA	C11-C10-C8-C7
29	A	412	LHG	O6-C4-C5-O7
29	A	415	LHG	O6-C4-C5-O7
23	B	606	CLA	C13-C15-C16-C17
23	b	606	CLA	C8-C10-C11-C12
30	A	413	SQD	C8-C7-O47-C45
28	a	413	DGD	C3B-C4B-C5B-C6B
29	A	415	LHG	C25-C26-C27-C28
23	b	611	CLA	O1A-CGA-O2A-C1
28	A	411	DGD	C8B-C9B-CAB-CBB
28	c	517	DGD	C2B-C3B-C4B-C5B
33	B	628	LMT	C5'-C4'-O1B-C1B
23	C	504	CLA	C2A-CAA-CBA-CGA
25	a	410	PL9	C7-C8-C9-C10
23	c	510	CLA	C16-C17-C18-C19
30	A	417	SQD	C23-C24-C25-C26
28	C	518	DGD	CBA-CCA-CDA-CEA
28	b	602	DGD	C8B-C9B-CAB-CBB
28	b	622	DGD	C7A-C8A-C9A-CAA
28	c	519	DGD	CEA-CFA-CGA-CHA
30	F	102	SQD	C44-C45-C46-O48
30	f	103	SQD	C44-C45-C46-O48
31	e	101	LMG	O1-C7-C8-C9
28	B	621	DGD	O1G-C1G-C2G-O2G
28	b	622	DGD	O1G-C1G-C2G-O2G
28	d	408	DGD	O2G-C2G-C3G-O3G
31	D	408	LMG	O1-C7-C8-O7
31	M	101	LMG	O7-C8-C9-O8
31	a	416	LMG	O1-C7-C8-O7
31	c	520	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
31	c	520	LMG	O7-C8-C9-O8
28	a	413	DGD	C2A-C3A-C4A-C5A
28	B	621	DGD	C4B-C5B-C6B-C7B
28	c	518	DGD	C3A-C4A-C5A-C6A
31	D	406	LMG	C17-C18-C19-C20
23	c	510	CLA	O1D-CGD-O2D-CED
30	A	417	SQD	C45-C44-O6-C1
31	A	414	LMG	C8-C7-O1-C1
31	d	406	LMG	C8-C7-O1-C1
23	b	617	CLA	C16-C17-C18-C19
29	a	417	LHG	O10-C23-O8-C6
23	c	512	CLA	C5-C6-C7-C8
25	d	404	PL9	C15-C14-C16-C17
30	f	103	SQD	C24-C25-C26-C27
30	F	102	SQD	C29-C30-C31-C32
23	b	609	CLA	C13-C15-C16-C17
23	A	404	CLA	C14-C13-C15-C16
23	B	605	CLA	C11-C10-C8-C9
23	B	609	CLA	C11-C12-C13-C14
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C10-C8-C9
23	B	613	CLA	C11-C12-C13-C14
23	B	616	CLA	C11-C10-C8-C9
23	C	501	CLA	C11-C12-C13-C14
23	C	503	CLA	C6-C7-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	b	608	CLA	C11-C10-C8-C9
23	b	616	CLA	C11-C12-C13-C14
23	b	619	CLA	C11-C10-C8-C9
23	c	501	CLA	C11-C12-C13-C14
23	c	508	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C9
23	c	512	CLA	C14-C13-C15-C16
28	c	518	DGD	C4B-C5B-C6B-C7B
25	J	101	PL9	C12-C13-C14-C16
25	d	404	PL9	C32-C33-C34-C36
31	D	406	LMG	O10-C28-O8-C9
23	c	512	CLA	CAA-CBA-CGA-O2A
28	c	519	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
27	T	103	BCR	C11-C12-C13-C35
27	a	412	BCR	C7-C8-C9-C34
30	a	401	SQD	C17-C18-C19-C20
27	B	620	BCR	C21-C22-C23-C24
23	B	614	CLA	C5-C6-C7-C8
23	C	510	CLA	O1D-CGD-O2D-CED
29	a	414	LHG	O9-C7-O7-C5
23	B	604	CLA	O1A-CGA-O2A-C1
23	b	607	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	C10-C11-C12-C13
24	D	402	PHO	C5-C6-C7-C8
23	b	617	CLA	C5-C6-C7-C8
30	B	625	SQD	C15-C16-C17-C18
28	c	519	DGD	C3G-C2G-O2G-C1B
31	c	520	LMG	C9-C8-O7-C10
29	A	415	LHG	O6-C4-C5-C6
23	B	614	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	b	617	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
24	a	407	PHO	C2-C1-O2A-CGA
23	b	616	CLA	C13-C15-C16-C17
30	A	413	SQD	C16-C17-C18-C19
23	C	510	CLA	C16-C17-C18-C19
29	A	412	LHG	C23-C24-C25-C26
23	B	611	CLA	C4-C3-C5-C6
23	a	405	CLA	C4-C3-C5-C6
33	b	603	LMT	C5'-C4'-O1B-C1B
27	J	102	BCR	C1-C6-C7-C8
27	c	514	BCR	C5-C6-C7-C8
23	b	615	CLA	C2-C3-C5-C6
31	a	416	LMG	C38-C39-C40-C41
23	b	617	CLA	C4C-C3C-CAC-CBC
31	i	101	LMG	C17-C18-C19-C20
28	A	411	DGD	C2A-C3A-C4A-C5A
28	C	518	DGD	CFA-CGA-CHA-CIA
23	a	409	CLA	C16-C17-C18-C19
23	b	613	CLA	C10-C11-C12-C13
23	b	606	CLA	C2A-CAA-CBA-CGA
31	D	407	LMG	C2-C1-O1-C7
31	C	519	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
31	C	520	LMG	O1-C7-C8-O7
31	d	406	LMG	O1-C7-C8-O7
23	C	509	CLA	C10-C11-C12-C13
24	A	406	PHO	C13-C15-C16-C17
30	D	409	SQD	C10-C11-C12-C13
29	a	414	LHG	C3-O3-P-O6
23	B	610	CLA	C5-C6-C7-C8
24	A	406	PHO	C10-C11-C12-C13
28	D	410	DGD	O1G-C1G-C2G-C3G
30	A	413	SQD	C44-C45-C46-O48
30	a	415	SQD	C44-C45-C46-O48
28	c	518	DGD	C7A-C8A-C9A-CAA
23	B	602	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C10-C8-C7
23	C	503	CLA	C6-C7-C8-C10
23	C	506	CLA	C6-C7-C8-C10
23	C	509	CLA	C6-C7-C8-C10
23	C	512	CLA	CAA-CBA-CGA-O2A
23	B	602	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C12-C13-C14
23	D	403	CLA	C11-C10-C8-C9
23	a	409	CLA	C11-C10-C8-C9
23	b	613	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C10-C8-C9
23	b	619	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C10-C8-C9
24	D	402	PHO	C6-C7-C8-C9
29	a	414	LHG	C8-C7-O7-C5
23	B	603	CLA	C16-C17-C18-C20
29	A	412	LHG	C24-C25-C26-C27
31	d	406	LMG	C34-C35-C36-C37
23	A	405	CLA	C2C-C3C-CAC-CBC
27	C	515	BCR	C37-C22-C23-C24
23	A	407	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
30	a	401	SQD	C33-C34-C35-C36
30	F	102	SQD	C26-C27-C28-C29
23	b	606	CLA	C15-C16-C17-C18
31	a	416	LMG	C35-C36-C37-C38
23	C	501	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	a	406	CLA	C2C-C3C-CAC-CBC
31	d	405	LMG	C17-C18-C19-C20
25	j	101	PL9	C17-C18-C19-C21
28	C	518	DGD	O6E-C5E-C6E-O5E
25	D	404	PL9	C47-C48-C49-C50
25	d	404	PL9	C47-C48-C49-C50
23	B	606	CLA	C16-C17-C18-C20
31	b	623	LMG	O6-C1-O1-C7
27	B	618	BCR	C13-C14-C15-C16
33	B	628	LMT	C1-C2-C3-C4
25	D	404	PL9	C9-C11-C12-C13
25	J	101	PL9	C24-C26-C27-C28
25	a	410	PL9	C19-C21-C22-C23
31	D	408	LMG	C34-C35-C36-C37
31	d	405	LMG	C11-C12-C13-C14
31	d	405	LMG	O10-C28-O8-C9
23	b	609	CLA	C16-C17-C18-C20
28	D	410	DGD	CAA-CBA-CCA-CDA
23	B	612	CLA	C4-C3-C5-C6
31	D	407	LMG	C16-C17-C18-C19
23	B	603	CLA	C15-C16-C17-C18
28	D	410	DGD	CBB-CCB-CDB-CEB
23	A	404	CLA	C2-C1-O2A-CGA
23	B	614	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA
30	a	401	SQD	C18-C19-C20-C21
23	a	406	CLA	C5-C6-C7-C8
23	b	611	CLA	C13-C15-C16-C17
23	b	617	CLA	C2C-C3C-CAC-CBC
28	a	413	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C7A-C8A-C9A-CAA
23	A	404	CLA	C2A-CAA-CBA-CGA
28	b	602	DGD	C5A-C6A-C7A-C8A
23	A	403	CLA	C3A-C2A-CAA-CBA
23	C	513	CLA	C3A-C2A-CAA-CBA
23	a	404	CLA	C3A-C2A-CAA-CBA
23	c	513	CLA	C3A-C2A-CAA-CBA
31	A	414	LMG	C38-C39-C40-C41
31	D	407	LMG	C29-C30-C31-C32
23	b	611	CLA	C4-C3-C5-C6
31	b	624	LMG	C28-C29-C30-C31
28	c	519	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
25	A	408	PL9	C4-C3-C7-C8
25	a	410	PL9	C4-C3-C7-C8
23	B	616	CLA	C11-C12-C13-C14
23	b	619	CLA	C11-C12-C13-C14
23	c	503	CLA	C6-C7-C8-C9
23	C	510	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
31	I	101	LMG	C17-C18-C19-C20
28	A	411	DGD	C4B-C5B-C6B-C7B
31	a	402	LMG	C13-C14-C15-C16
31	i	101	LMG	C19-C20-C21-C22
28	C	518	DGD	C1G-C2G-C3G-O3G
28	b	602	DGD	O1G-C1G-C2G-C3G
31	c	520	LMG	C34-C35-C36-C37
23	c	511	CLA	C2A-CAA-CBA-CGA
30	A	417	SQD	C26-C27-C28-C29
28	C	517	DGD	O6D-C1D-O3G-C3G
31	D	407	LMG	O6-C1-O1-C7
24	a	408	PHO	C13-C15-C16-C17
29	a	414	LHG	C4-C5-O7-C7
23	A	403	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
23	B	605	CLA	C11-C12-C13-C15
23	D	401	CLA	C11-C10-C8-C7
23	b	605	CLA	C11-C10-C8-C7
23	b	608	CLA	C11-C12-C13-C15
23	c	507	CLA	C11-C12-C13-C15
23	c	508	CLA	C11-C12-C13-C15
23	c	509	CLA	C6-C7-C8-C10
23	B	613	CLA	C8-C10-C11-C12
23	b	616	CLA	C8-C10-C11-C12
23	B	613	CLA	C10-C11-C12-C13
23	C	509	CLA	C2A-CAA-CBA-CGA
23	d	403	CLA	C2A-CAA-CBA-CGA
23	D	403	CLA	C8-C10-C11-C12
28	C	517	DGD	C3A-C4A-C5A-C6A
28	c	518	DGD	C4A-C5A-C6A-C7A
23	B	613	CLA	C13-C15-C16-C17
23	b	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	C	518	DGD	C7A-C8A-C9A-CAA
30	a	401	SQD	C25-C26-C27-C28
28	C	518	DGD	O1A-C1A-O1G-C1G
31	C	520	LMG	O7-C8-C9-O8
33	b	603	LMT	C1-C2-C3-C4
31	M	101	LMG	C30-C31-C32-C33
27	T	103	BCR	C13-C14-C15-C16
23	C	505	CLA	C8-C10-C11-C12
23	d	403	CLA	C8-C10-C11-C12
24	D	402	PHO	C2-C1-O2A-CGA
23	B	611	CLA	C2-C3-C5-C6
23	B	612	CLA	C2-C3-C5-C6
25	D	404	PL9	C13-C14-C16-C17
30	a	415	SQD	C29-C30-C31-C32
31	A	414	LMG	C35-C36-C37-C38
31	e	101	LMG	C31-C32-C33-C34
23	B	615	CLA	C11-C12-C13-C14
23	b	612	CLA	C11-C12-C13-C14
23	b	615	CLA	C6-C7-C8-C9
30	d	407	SQD	C10-C11-C12-C13
23	a	405	CLA	C2A-CAA-CBA-CGA
28	d	408	DGD	CAA-CBA-CCA-CDA
31	a	402	LMG	O10-C28-O8-C9
27	C	514	BCR	C23-C24-C25-C30
27	b	621	BCR	C23-C24-C25-C30
27	c	514	BCR	C1-C6-C7-C8
31	a	416	LMG	O1-C7-C8-C9
28	c	519	DGD	CBB-CCB-CDB-CEB
23	B	614	CLA	C4C-C3C-CAC-CBC
30	f	103	SQD	C26-C27-C28-C29
25	A	408	PL9	C15-C14-C16-C17
27	T	103	BCR	C11-C12-C13-C14
27	c	515	BCR	C7-C8-C9-C10
23	B	606	CLA	C16-C17-C18-C19
23	B	610	CLA	C13-C15-C16-C17
31	B	622	LMG	C12-C13-C14-C15
25	d	404	PL9	C13-C14-C16-C17
23	a	406	CLA	C4C-C3C-CAC-CBC
31	I	101	LMG	C19-C20-C21-C22
28	C	517	DGD	C5D-C6D-O5D-C1E
30	a	401	SQD	C45-C44-O6-C1
23	b	609	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C2A-CAA-CBA-CGA
23	D	403	CLA	C2A-CAA-CBA-CGA
23	b	617	CLA	C2A-CAA-CBA-CGA
23	B	609	CLA	C11-C12-C13-C15
23	B	615	CLA	C11-C12-C13-C15
23	b	615	CLA	C6-C7-C8-C10
23	c	503	CLA	C6-C7-C8-C10
23	d	402	CLA	C11-C10-C8-C7
28	c	517	DGD	C2A-C1A-O1G-C1G
28	C	518	DGD	CBB-CCB-CDB-CEB
30	F	102	SQD	C9-C10-C11-C12
31	C	519	LMG	C29-C30-C31-C32
31	b	623	LMG	C14-C15-C16-C17
30	f	103	SQD	C2-C1-O6-C44
31	b	623	LMG	C2-C1-O1-C7
30	F	102	SQD	C24-C25-C26-C27
28	a	413	DGD	C4B-C5B-C6B-C7B
28	B	626	DGD	O1G-C1G-C2G-O2G
23	B	614	CLA	C2C-C3C-CAC-CBC
31	d	406	LMG	C29-C30-C31-C32
31	E	101	LMG	O9-C10-C11-C12
30	A	413	SQD	C29-C30-C31-C32
23	B	603	CLA	C8-C10-C11-C12
23	B	605	CLA	C8-C10-C11-C12
23	C	511	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
25	J	101	PL9	C13-C14-C16-C17
25	j	101	PL9	C13-C14-C16-C17
23	c	513	CLA	C16-C17-C18-C20
23	C	507	CLA	CAA-CBA-CGA-O2A
23	b	616	CLA	CAA-CBA-CGA-O2A
30	A	417	SQD	C17-C18-C19-C20
23	A	407	CLA	C11-C10-C8-C9
23	B	603	CLA	C11-C10-C8-C9
23	B	608	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C14
23	b	611	CLA	C11-C12-C13-C14
23	c	507	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C10-C8-C9
30	B	625	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	c	504	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	501	CLA	CAA-CBA-CGA-O2A
31	a	416	LMG	C12-C13-C14-C15
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	b	613	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	b	619	CLA	CAD-CBD-CGD-O2D
24	D	402	PHO	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
29	a	414	LHG	C6-C5-O7-C7
31	M	102	LMG	C9-C8-O7-C10
23	b	608	CLA	C8-C10-C11-C12
24	a	407	PHO	C15-C16-C17-C18
23	A	405	CLA	C4C-C3C-CAC-CBC
30	a	401	SQD	C30-C31-C32-C33
23	B	601	CLA	C2-C1-O2A-CGA
23	C	512	CLA	C2-C1-O2A-CGA
25	j	101	PL9	C12-C13-C14-C16
23	B	604	CLA	C4C-C3C-CAC-CBC
29	a	417	LHG	C7-C8-C9-C10
23	D	401	CLA	CAA-CBA-CGA-O2A
23	c	501	CLA	CAA-CBA-CGA-O2A
31	k	103	LMG	O8-C28-C29-C30
28	d	408	DGD	CBB-CCB-CDB-CEB
30	f	103	SQD	C15-C16-C17-C18
23	c	511	CLA	C4-C3-C5-C6
23	b	615	CLA	C3-C5-C6-C7
23	b	614	CLA	C2-C3-C5-C6
23	d	402	CLA	CAA-CBA-CGA-O2A
31	A	414	LMG	O7-C10-C11-C12
31	a	416	LMG	O7-C10-C11-C12
30	B	625	SQD	C19-C20-C21-C22
31	k	103	LMG	C34-C35-C36-C37
27	j	102	BCR	C21-C22-C23-C24
31	C	520	LMG	O1-C7-C8-C9
31	C	520	LMG	C7-C8-C9-O8
31	E	101	LMG	O1-C7-C8-C9
31	c	520	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
28	b	622	DGD	C7B-C8B-C9B-CAB
23	b	609	CLA	C16-C17-C18-C19
28	C	518	DGD	C4B-C5B-C6B-C7B
23	B	616	CLA	O2A-C1-C2-C3
23	b	619	CLA	O2A-C1-C2-C3
23	c	512	CLA	O2A-C1-C2-C3
24	A	406	PHO	O2A-C1-C2-C3
24	a	408	PHO	O2A-C1-C2-C3
28	c	519	DGD	C4B-C5B-C6B-C7B
23	B	603	CLA	C2A-CAA-CBA-CGA
31	e	101	LMG	O9-C10-C11-C12
23	c	502	CLA	C16-C17-C18-C20
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	CHA-CBD-CGD-O1D
23	b	605	CLA	CHA-CBD-CGD-O2D
23	b	610	CLA	CHA-CBD-CGD-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	513	CLA	CHA-CBD-CGD-O2D
31	D	408	LMG	C29-C30-C31-C32
23	c	510	CLA	CAA-CBA-CGA-O2A
28	B	621	DGD	O2G-C1B-C2B-C3B
28	b	622	DGD	O2G-C1B-C2B-C3B
23	a	405	CLA	C2C-C3C-CAC-CBC
31	M	102	LMG	O1-C7-C8-O7
31	d	405	LMG	O1-C7-C8-O7
29	A	412	LHG	C28-C29-C30-C31
30	a	401	SQD	O47-C7-C8-C9
23	B	602	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C2A-CAA-CBA-CGA
24	D	402	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	a	408	PHO	CHA-CBD-CGD-O1D
23	C	503	CLA	C15-C16-C17-C18
30	a	415	SQD	C8-C7-O47-C45
23	C	510	CLA	CAA-CBA-CGA-O2A
23	b	617	CLA	CAA-CBA-CGA-O2A
23	B	601	CLA	C12-C13-C15-C16
23	C	507	CLA	C11-C12-C13-C15
23	C	508	CLA	C11-C12-C13-C15
23	b	605	CLA	C11-C12-C13-C15
23	b	612	CLA	C11-C12-C13-C15
23	c	504	CLA	C6-C7-C8-C10
23	c	506	CLA	C6-C7-C8-C10
23	A	404	CLA	C2C-C3C-CAC-CBC
31	E	101	LMG	C31-C32-C33-C34
30	D	409	SQD	O47-C7-C8-C9
30	d	407	SQD	O47-C7-C8-C9
23	C	506	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C12-C13-C14
23	D	401	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	605	CLA	C11-C12-C13-C14
23	b	606	CLA	C11-C10-C8-C9
23	b	618	CLA	C11-C12-C13-C14
23	c	504	CLA	C6-C7-C8-C9
23	c	508	CLA	C11-C12-C13-C14
23	c	513	CLA	C11-C12-C13-C14
31	D	406	LMG	C19-C20-C21-C22
23	c	502	CLA	CBA-CGA-O2A-C1
23	c	507	CLA	CAA-CBA-CGA-O2A
28	c	517	DGD	O1G-C1A-C2A-C3A
31	M	101	LMG	O8-C28-C29-C30
25	d	404	PL9	C21-C22-C23-C24
31	I	101	LMG	C15-C16-C17-C18
31	I	101	LMG	C20-C21-C22-C23
31	C	519	LMG	O8-C28-C29-C30
31	M	102	LMG	O8-C28-C29-C30
23	a	405	CLA	C4C-C3C-CAC-CBC
28	B	626	DGD	C5A-C6A-C7A-C8A
23	b	616	CLA	CAA-CBA-CGA-O1A
28	B	621	DGD	O1B-C1B-C2B-C3B
23	c	513	CLA	C16-C17-C18-C19
23	a	405	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B	612	CLA	CAA-CBA-CGA-O2A
23	D	401	CLA	C5-C6-C7-C8
28	b	622	DGD	O1B-C1B-C2B-C3B
23	B	615	CLA	CBA-CGA-O2A-C1
24	A	406	PHO	CBA-CGA-O2A-C1
23	B	601	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C1A-C2A-CAA-CBA
23	b	604	CLA	C1A-C2A-CAA-CBA
23	c	504	CLA	C1A-C2A-CAA-CBA
23	d	402	CLA	CAA-CBA-CGA-O1A
25	D	404	PL9	C46-C47-C48-C49
25	a	410	PL9	C16-C17-C18-C19
23	c	502	CLA	O1A-CGA-O2A-C1
31	c	520	LMG	C36-C37-C38-C39
31	M	102	LMG	O1-C7-C8-C9
31	c	520	LMG	O1-C7-C8-C9
29	a	414	LHG	C24-C25-C26-C27
23	C	510	CLA	C13-C15-C16-C17
23	c	507	CLA	CAA-CBA-CGA-O1A
30	A	413	SQD	O49-C7-O47-C45
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	507	CLA	CAA-CBA-CGA-O1A
23	D	401	CLA	CAA-CBA-CGA-O1A
28	c	517	DGD	O1A-C1A-C2A-C3A
28	B	626	DGD	C2D-C1D-O3G-C3G
28	b	602	DGD	C2D-C1D-O3G-C3G
30	F	102	SQD	C15-C16-C17-C18
30	b	601	SQD	C19-C20-C21-C22
28	c	519	DGD	CBA-CCA-CDA-CEA
31	k	103	LMG	O10-C28-C29-C30
23	C	505	CLA	CAA-CBA-CGA-O2A
27	b	621	BCR	C23-C24-C25-C26
25	d	404	PL9	C9-C11-C12-C13
23	c	501	CLA	CAA-CBA-CGA-O1A
28	C	516	DGD	O1A-C1A-C2A-C3A
24	a	407	PHO	C13-C15-C16-C17
28	c	518	DGD	CBB-CCB-CDB-CEB
23	C	501	CLA	CAA-CBA-CGA-O1A
27	x	101	BCR	C9-C10-C11-C12
23	A	405	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	501	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	502	CLA	CAD-CBD-CGD-O1D
23	b	608	CLA	CAD-CBD-CGD-O1D
23	b	612	CLA	CAD-CBD-CGD-O1D
23	c	501	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	510	CLA	CAD-CBD-CGD-O1D
23	c	513	CLA	CAD-CBD-CGD-O1D
29	A	412	LHG	C4-C5-O7-C7
30	d	407	SQD	O5-C5-C6-S
31	M	101	LMG	C9-C8-O7-C10
24	A	406	PHO	O1A-CGA-O2A-C1
31	a	416	LMG	O9-C10-C11-C12
23	B	614	CLA	CAA-CBA-CGA-O2A
23	A	407	CLA	C6-C7-C8-C9
23	B	601	CLA	C14-C13-C15-C16
23	B	605	CLA	C11-C12-C13-C14
23	C	504	CLA	C6-C7-C8-C9
23	c	507	CLA	C6-C7-C8-C9
28	D	410	DGD	C8A-C9A-CAA-CBA
23	C	502	CLA	CBA-CGA-O2A-C1
30	A	417	SQD	O47-C7-C8-C9
28	A	411	DGD	C7A-C8A-C9A-CAA
31	A	414	LMG	C19-C20-C21-C22
23	c	502	CLA	C5-C6-C7-C8
23	B	615	CLA	O1A-CGA-O2A-C1
23	C	502	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	CAA-CBA-CGA-O1A
30	A	413	SQD	O49-C7-C8-C9
28	c	519	DGD	CCB-CDB-CEB-CFB
23	c	505	CLA	CAA-CBA-CGA-O2A
25	j	101	PL9	C21-C22-C23-C24
30	A	417	SQD	C25-C26-C27-C28
23	B	606	CLA	C4-C3-C5-C6
31	D	408	LMG	C31-C32-C33-C34
23	B	602	CLA	C11-C10-C8-C7
23	B	611	CLA	C6-C7-C8-C10
23	C	504	CLA	C6-C7-C8-C10
23	C	513	CLA	C11-C12-C13-C15
23	b	604	CLA	C12-C13-C15-C16
23	b	605	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C7
23	b	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	618	CLA	C11-C12-C13-C15
23	c	513	CLA	C11-C12-C13-C15
24	a	407	PHO	C12-C13-C15-C16
31	a	416	LMG	C16-C17-C18-C19
23	b	604	CLA	CAA-CBA-CGA-O2A
23	b	613	CLA	CAA-CBA-CGA-O2A
30	A	413	SQD	O47-C7-C8-C9
30	a	415	SQD	O47-C7-C8-C9
31	E	101	LMG	O7-C10-C11-C12
23	B	602	CLA	CBA-CGA-O2A-C1
31	A	414	LMG	C12-C13-C14-C15
27	J	102	BCR	C7-C8-C9-C10
27	b	621	BCR	C21-C22-C23-C24
23	b	604	CLA	CAA-CBA-CGA-O1A
23	b	617	CLA	CAA-CBA-CGA-O1A
30	a	415	SQD	O49-C7-C8-C9
23	B	610	CLA	CAA-CBA-CGA-O2A
23	b	615	CLA	CAA-CBA-CGA-O2A
31	e	101	LMG	O7-C10-C11-C12
28	c	518	DGD	O6D-C1D-O3G-C3G
23	c	510	CLA	C13-C15-C16-C17
23	B	612	CLA	CAA-CBA-CGA-O1A
23	B	614	CLA	CAA-CBA-CGA-O1A
23	C	510	CLA	CAA-CBA-CGA-O1A
31	D	406	LMG	O9-C10-C11-C12
25	D	404	PL9	C39-C41-C42-C43
25	J	101	PL9	C9-C11-C12-C13
23	B	601	CLA	CAA-CBA-CGA-O2A
23	B	602	CLA	CAA-CBA-CGA-O2A
30	A	417	SQD	O49-C7-C8-C9
31	A	414	LMG	C11-C12-C13-C14
23	C	506	CLA	C8-C10-C11-C12
30	a	401	SQD	O49-C7-C8-C9
30	d	407	SQD	O49-C7-C8-C9
23	B	608	CLA	C4-C3-C5-C6
28	C	516	DGD	O1G-C1A-C2A-C3A

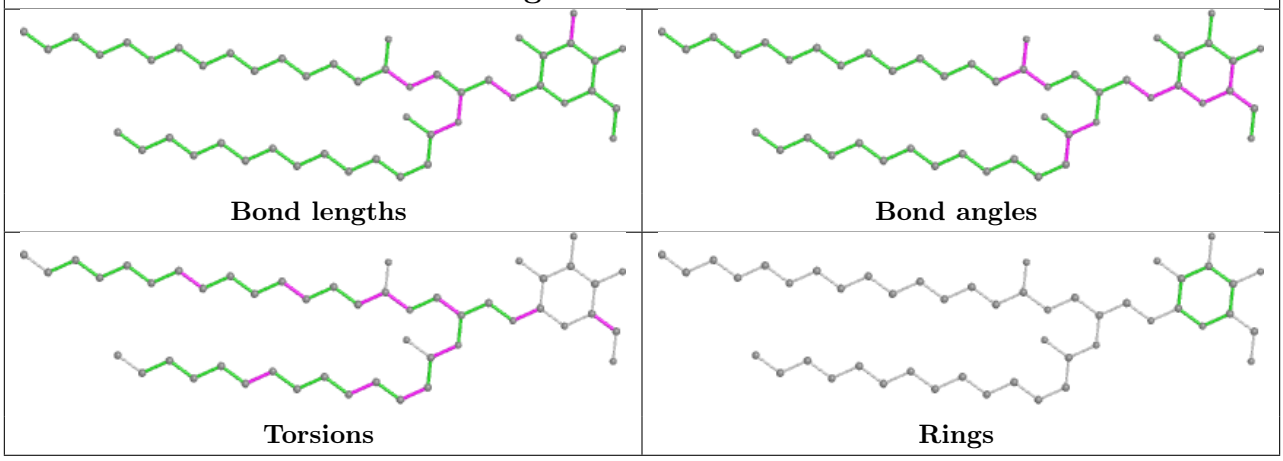
There are no ring outliers.

No monomer is involved in short contacts.

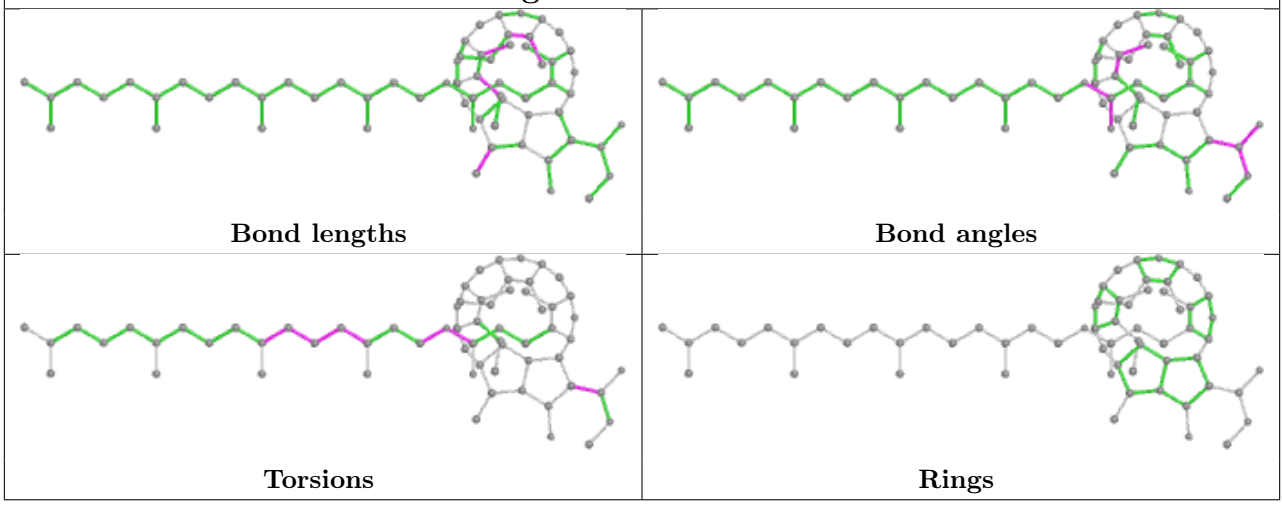
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

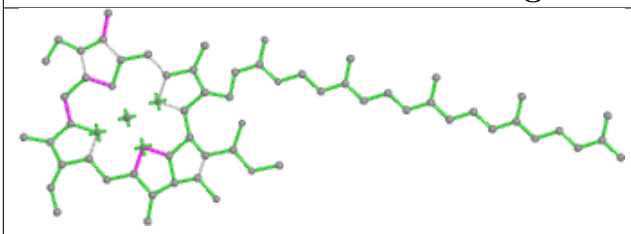
Ligand LMG k 103



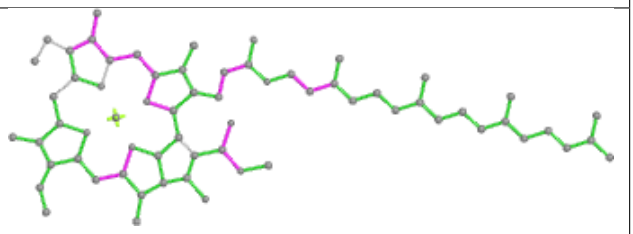
Ligand PHO D 402



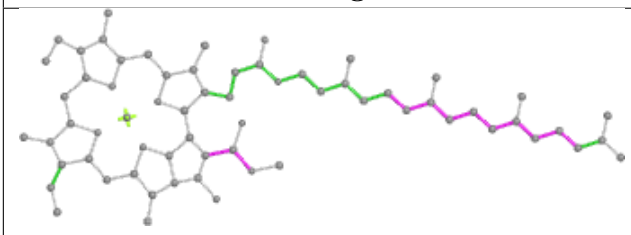
Ligand CLA C 506



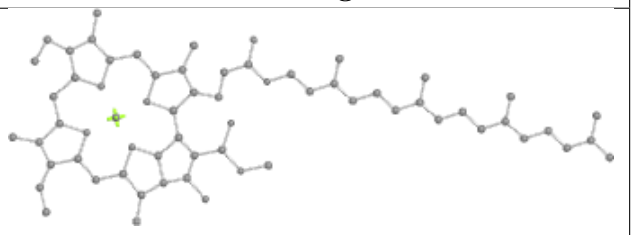
Bond lengths



Bond angles

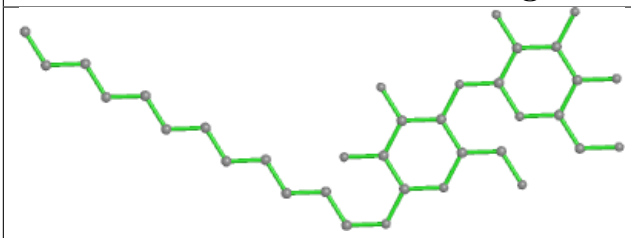


Torsions

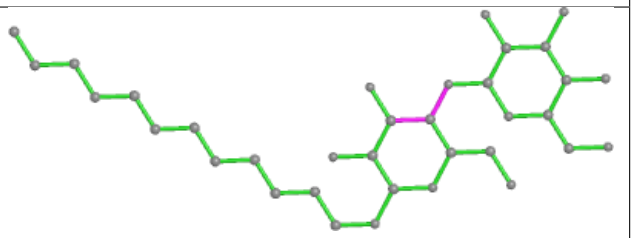


Rings

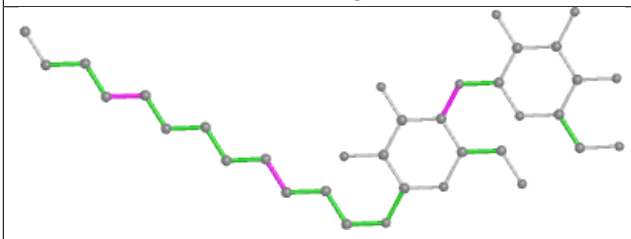
Ligand LMT B 627



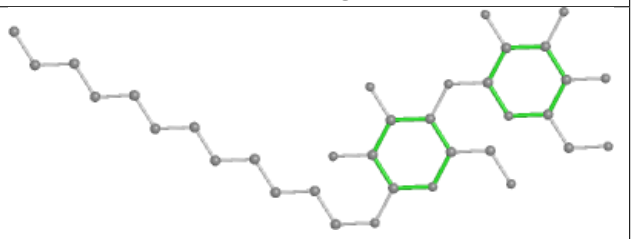
Bond lengths



Bond angles

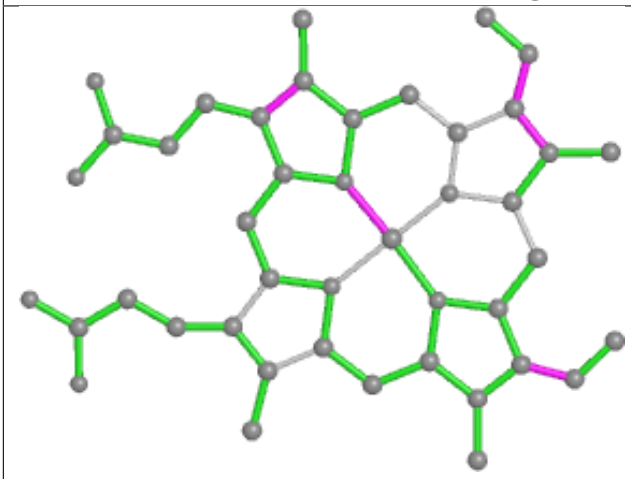


Torsions

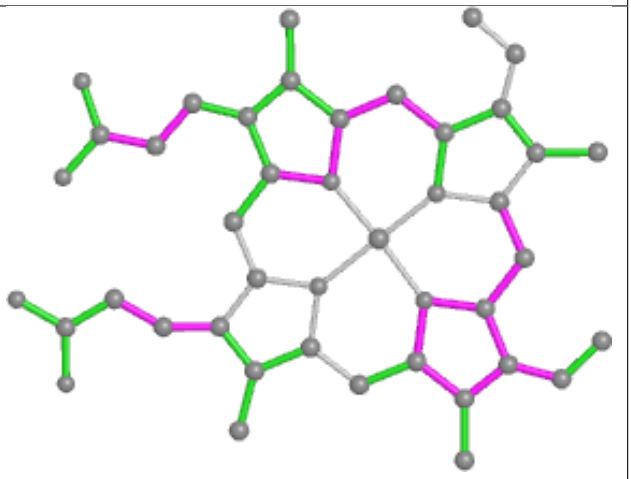


Rings

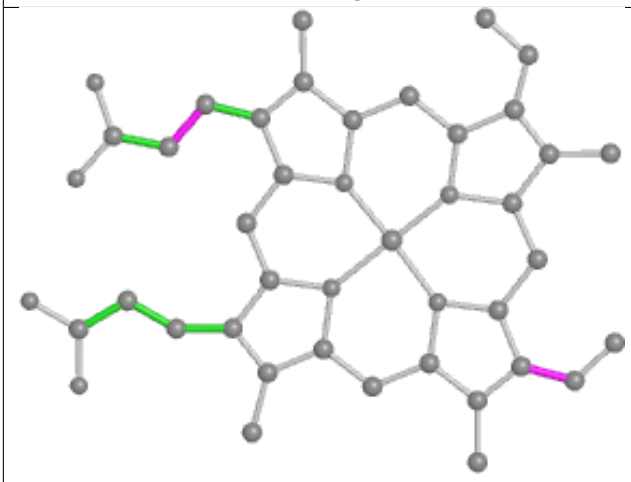
Ligand HEM f 101



Bond lengths



Bond angles



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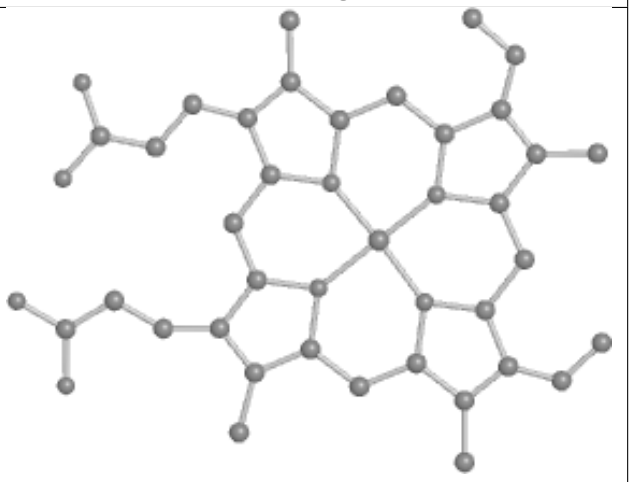
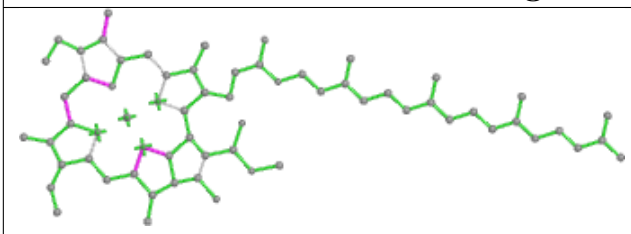
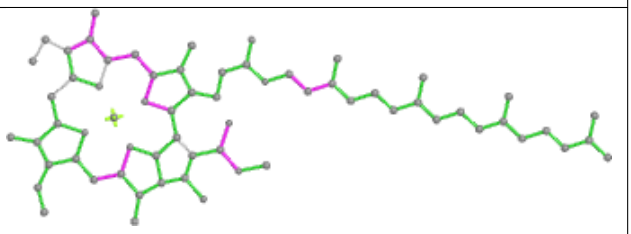


Rings

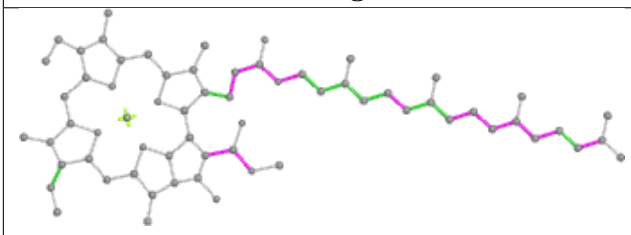
Ligand CLA B 610



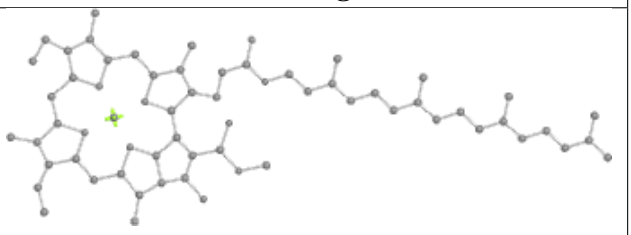
Bond lengths



Bond angles

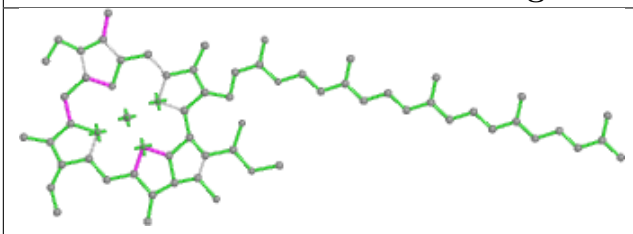


Torsions

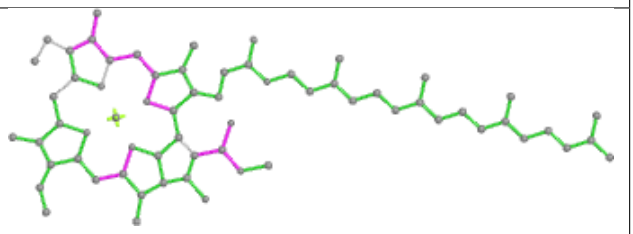


Rings

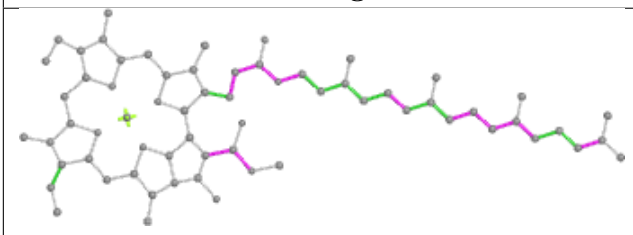
Ligand CLA b 613



Bond lengths



Bond angles



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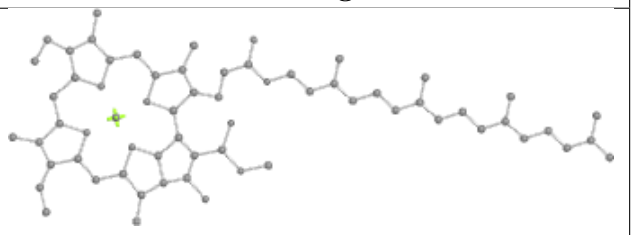
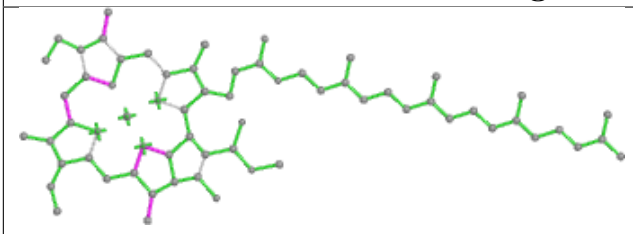
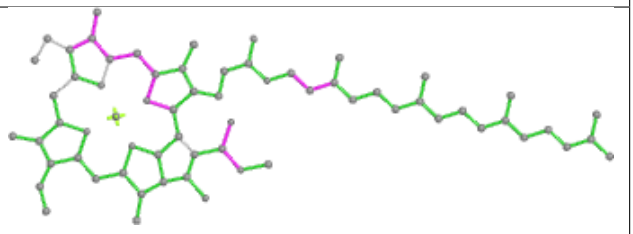


Rings

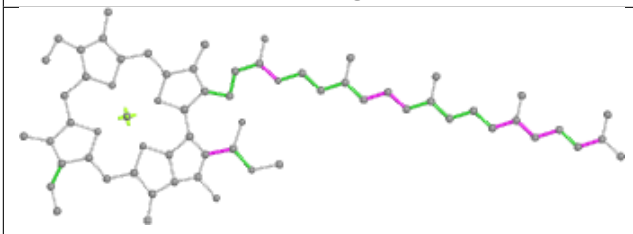
Ligand CLA c 502



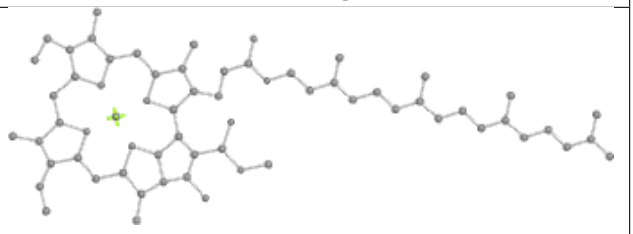
Bond lengths



Bond angles

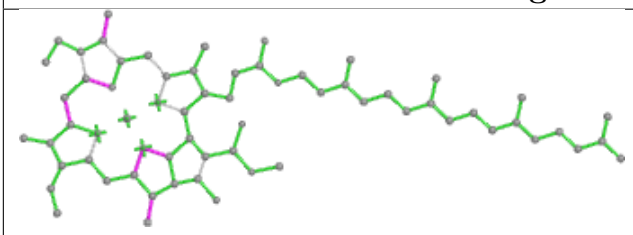


Torsions

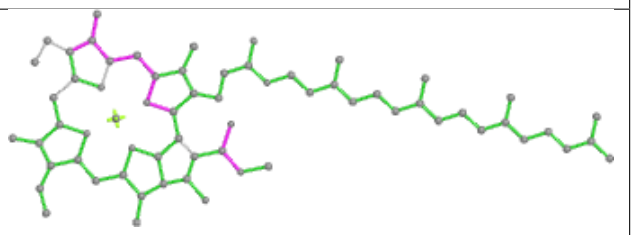


Rings

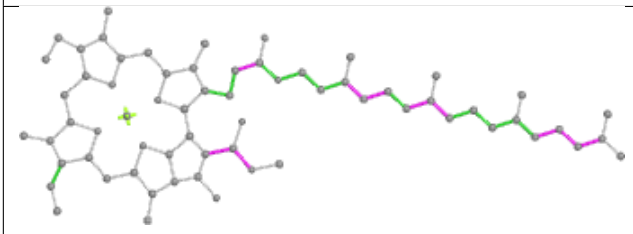
Ligand CLA c 510



Bond lengths



Bond angles



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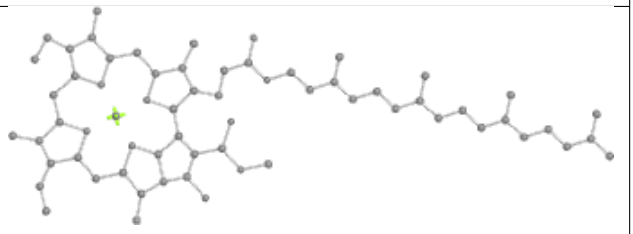
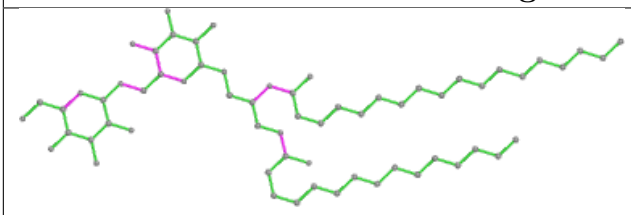


Rings

Ligand DGD D 410



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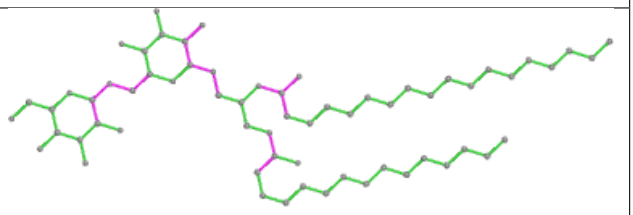
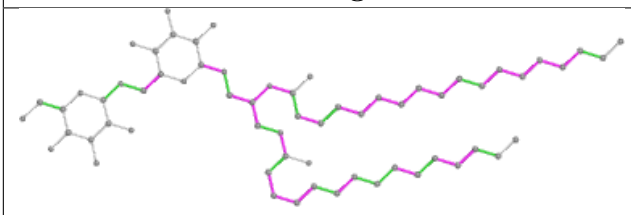
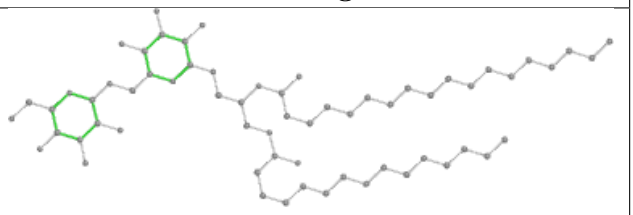


Bond angles

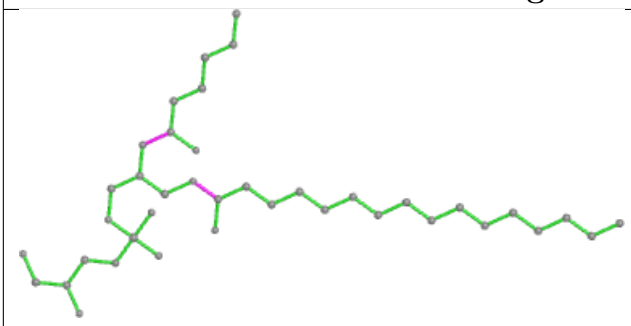


Torsions



Rings

Ligand LHG a 414



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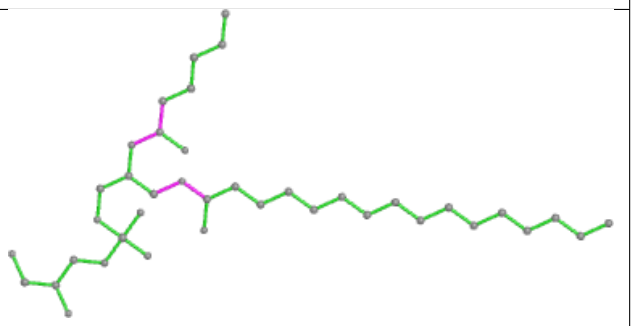
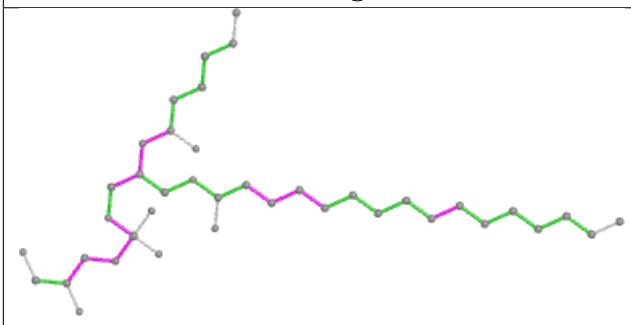
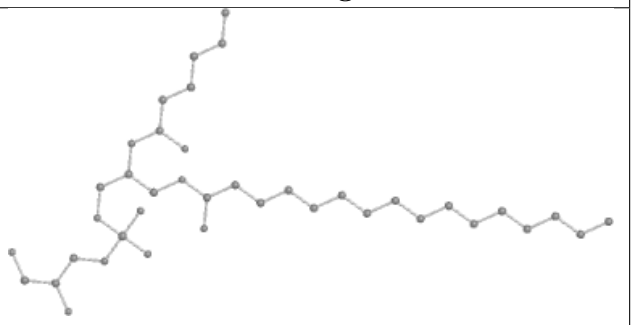


Bond angles

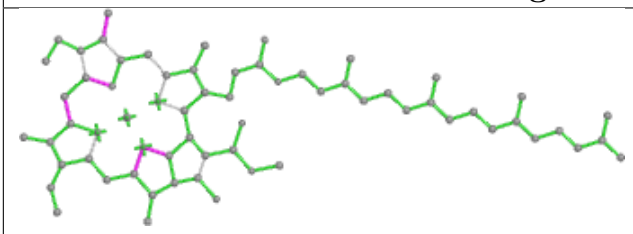


Torsions

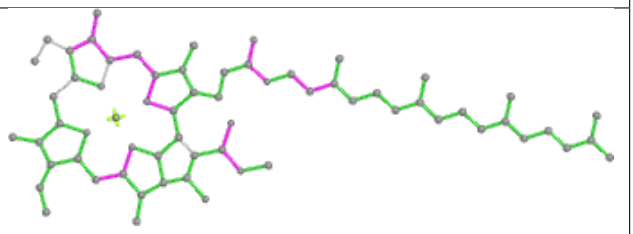


Rings

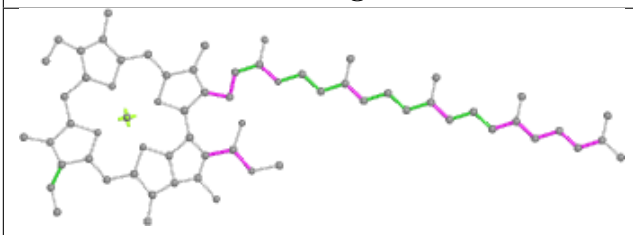
Ligand CLA c 513



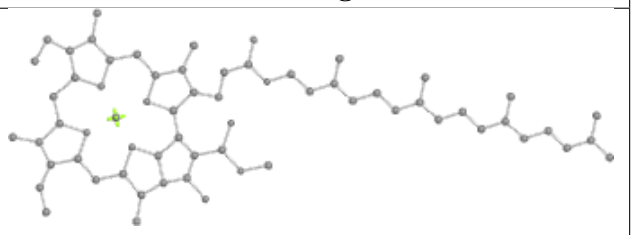
Bond lengths



Bond angles

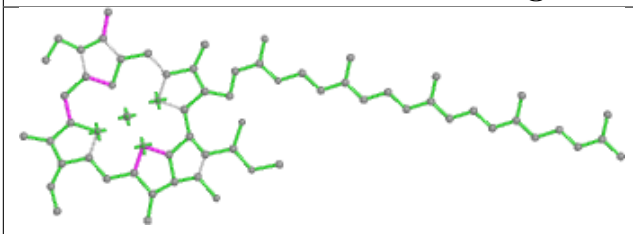


Torsions

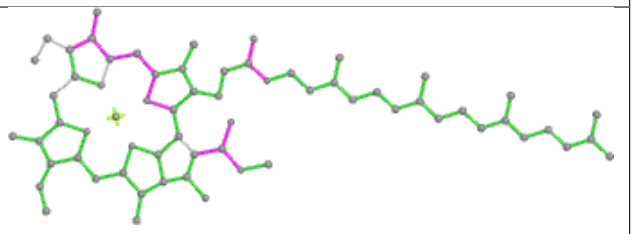


Rings

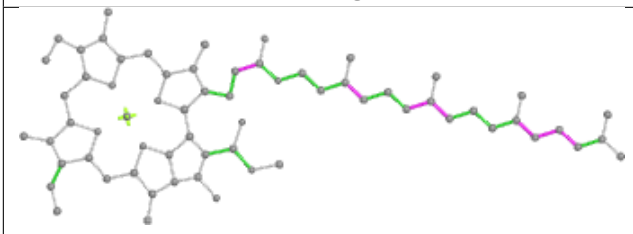
Ligand CLA d 402



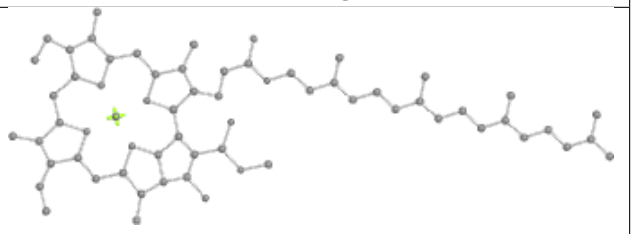
Bond lengths



Bond angles

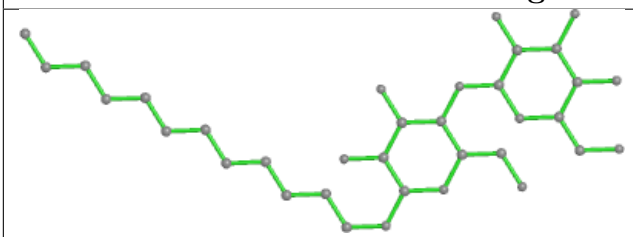


Torsions

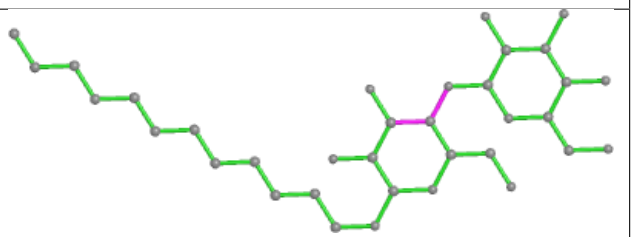


Rings

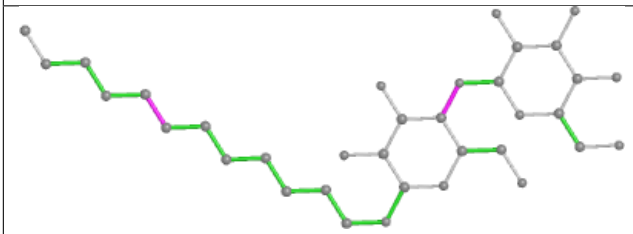
Ligand LMT I 102



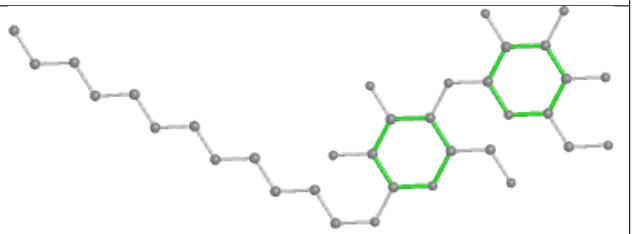
Bond lengths



Bond angles

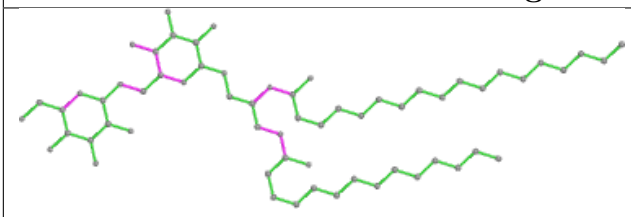


Torsions



Rings

Ligand DGD c 518



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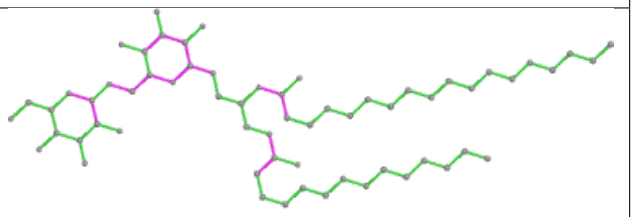
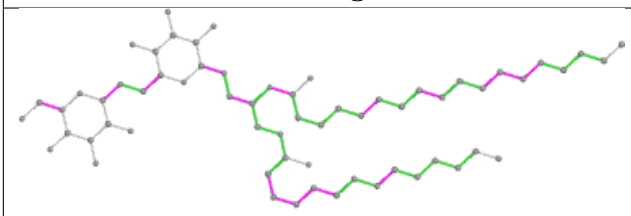
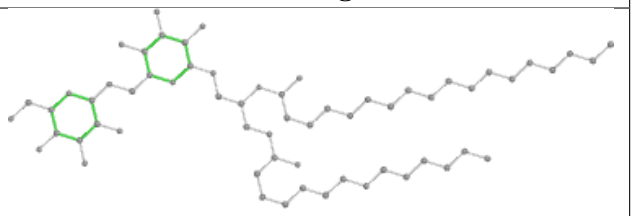


Bond angles

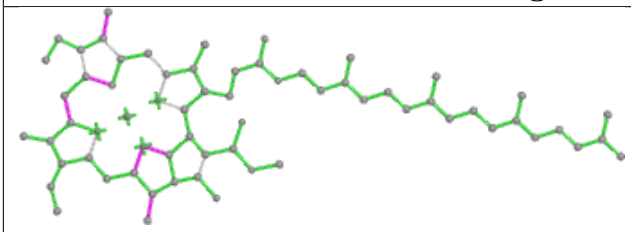


Torsions

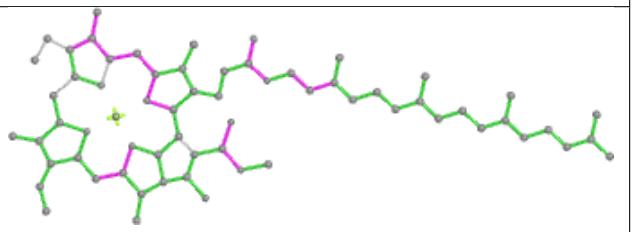


Rings

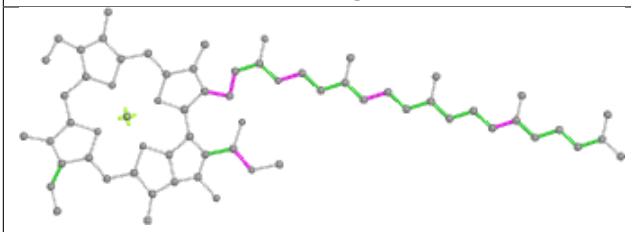
Ligand CLA a 404



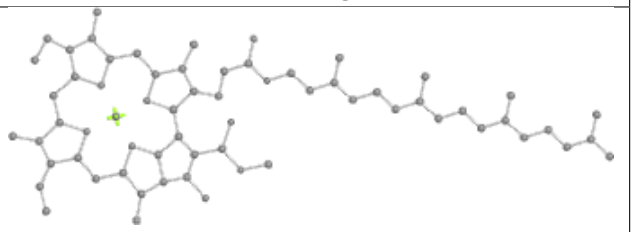
Bond lengths



Bond angles

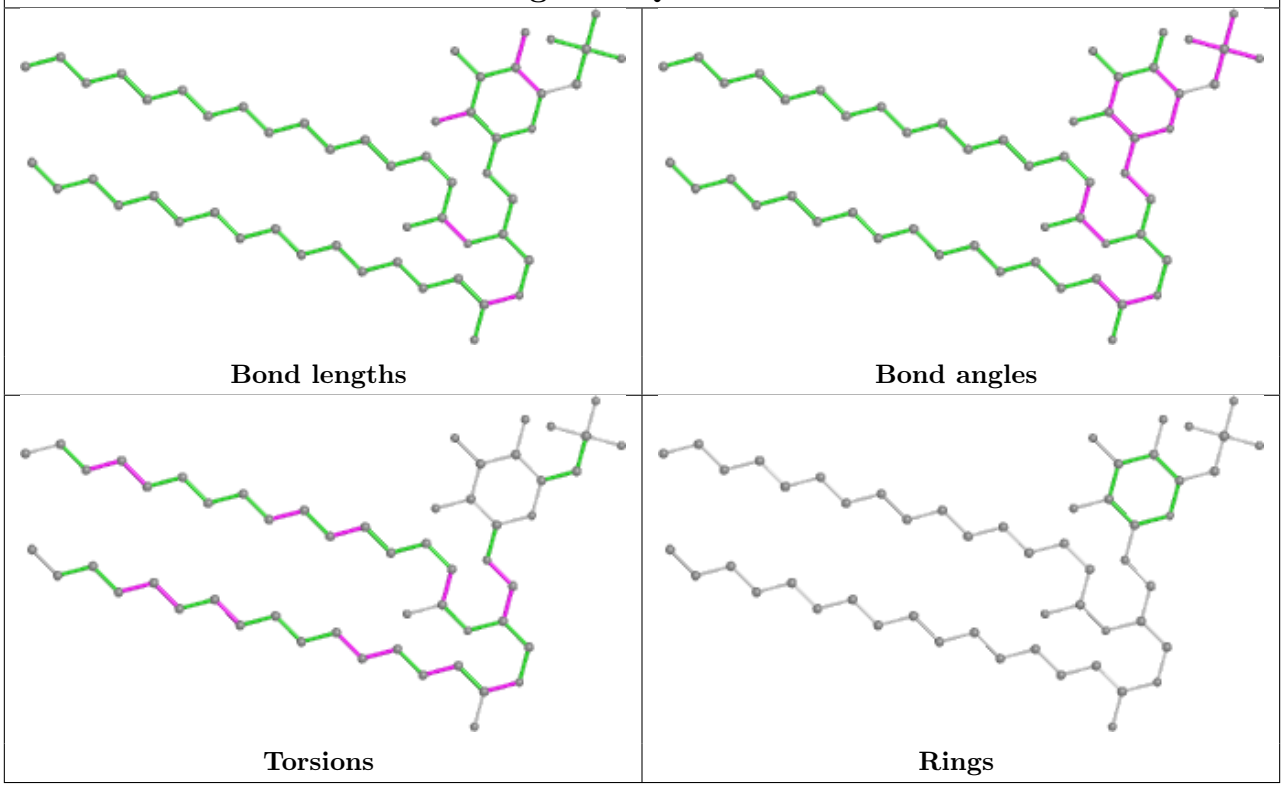


Torsions

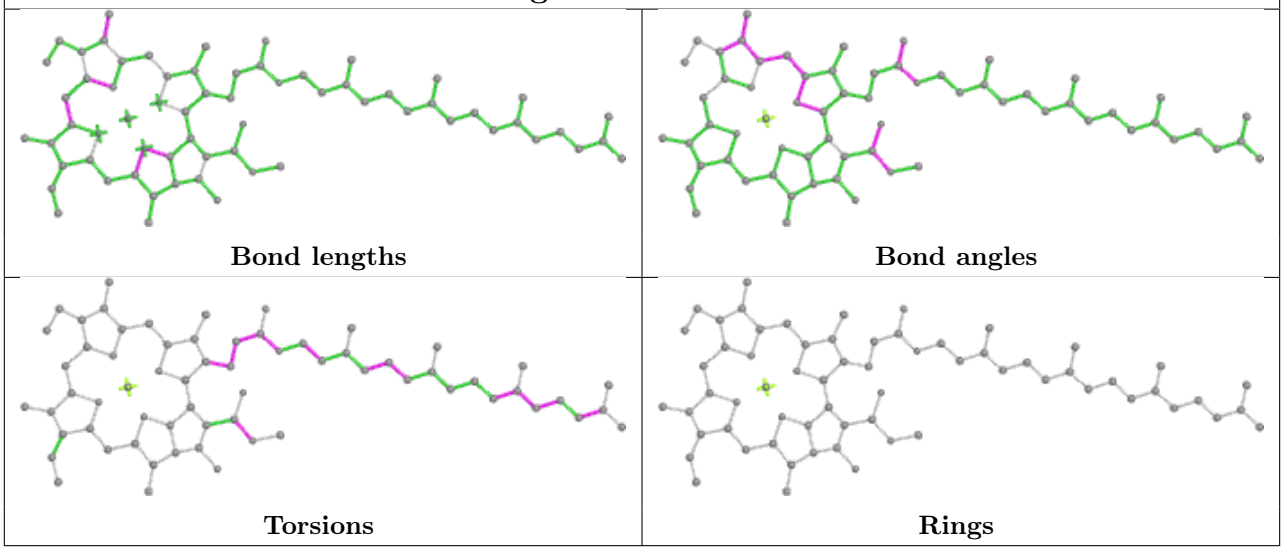


Rings

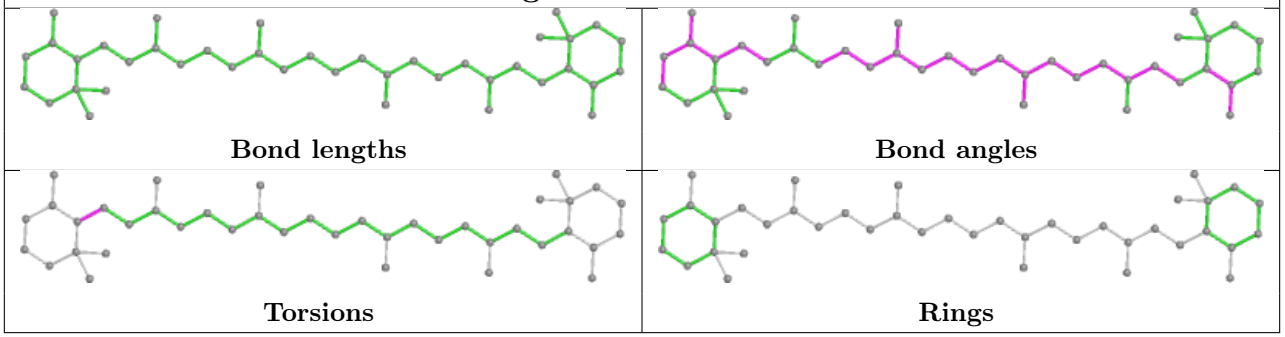
Ligand SQD a 401



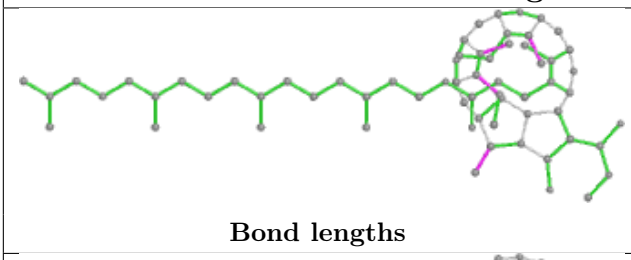
Ligand CLA c 512



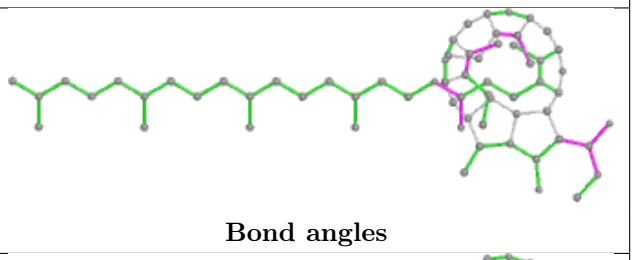
Ligand BCR H 101



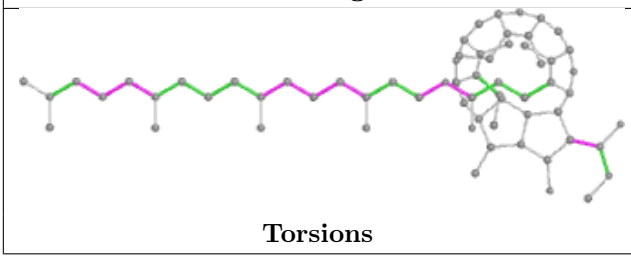
Ligand PHO a 407



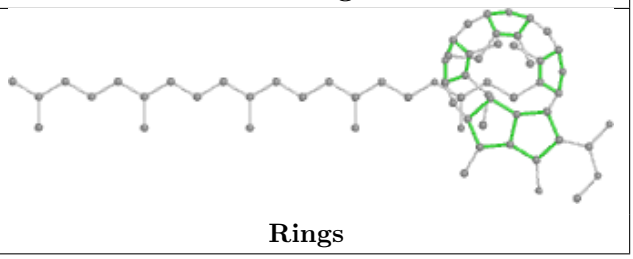
Bond lengths



Bond angles

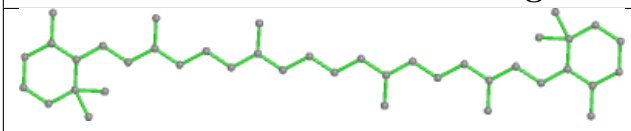


Torsions

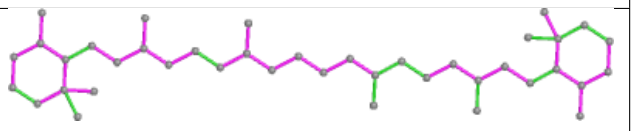


Rings

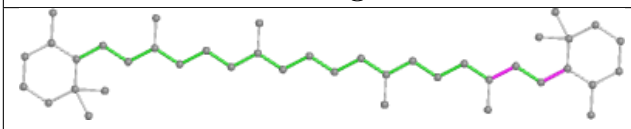
Ligand BCR b 621



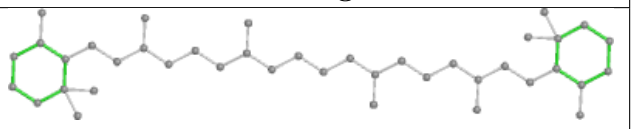
Bond lengths



Bond angles

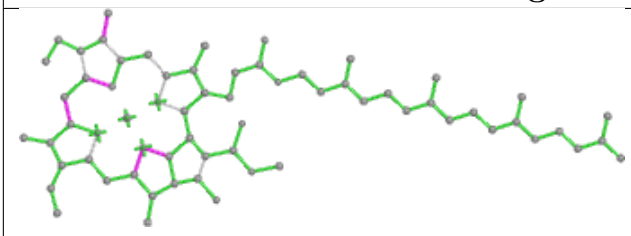


Torsions

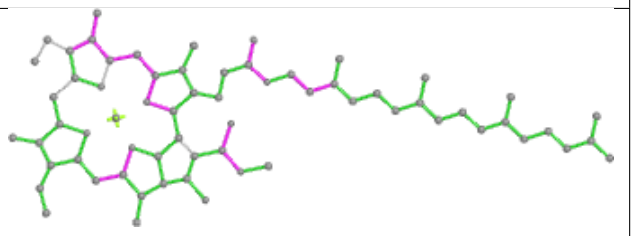


Rings

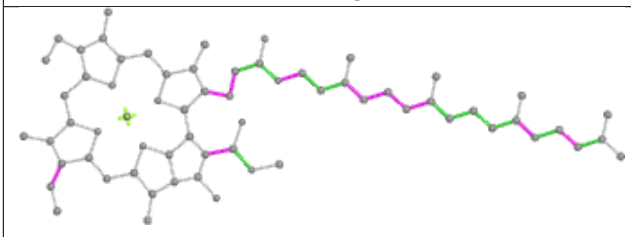
Ligand CLA a 405



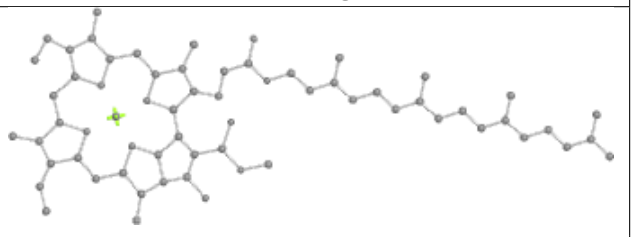
Bond lengths



Bond angles

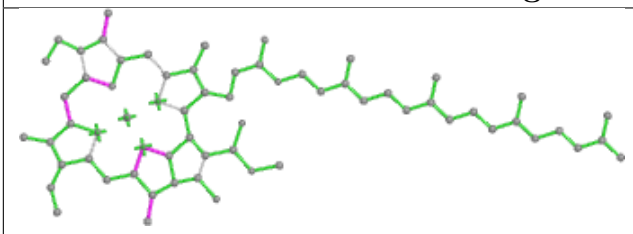


Torsions

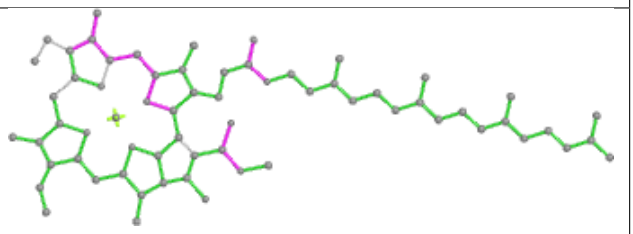


Rings

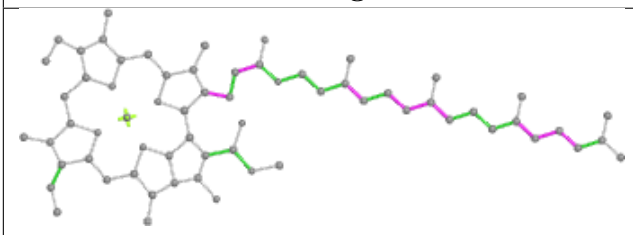
Ligand CLA D 401



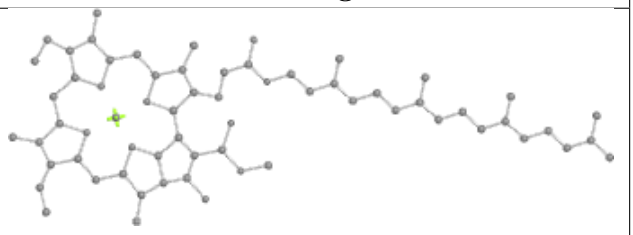
Bond lengths



Bond angles

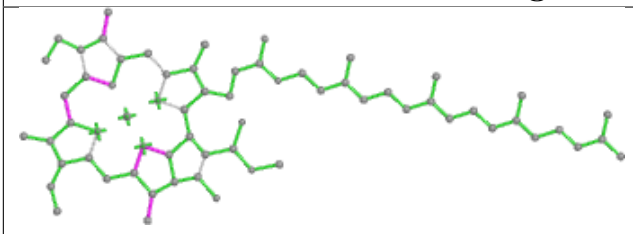


Torsions

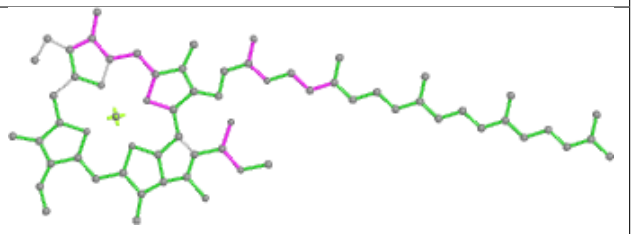


Rings

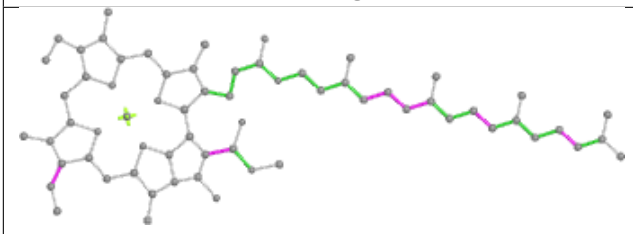
Ligand CLA a 406



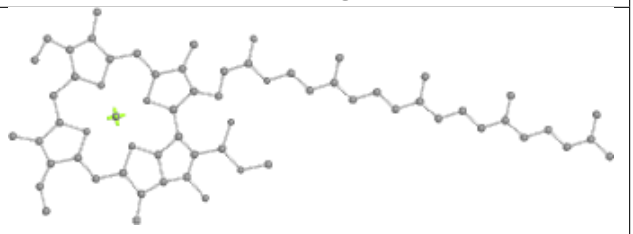
Bond lengths



Bond angles

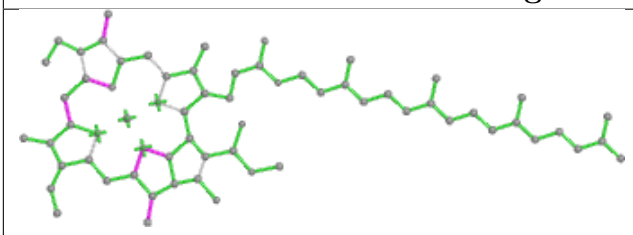


Torsions



Rings

Ligand CLA B 608



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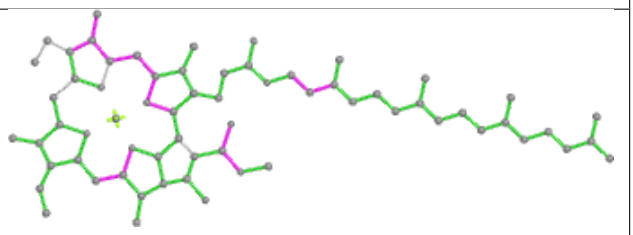
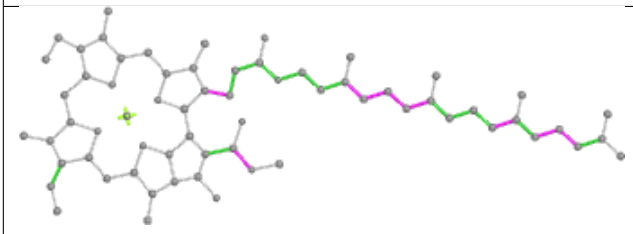
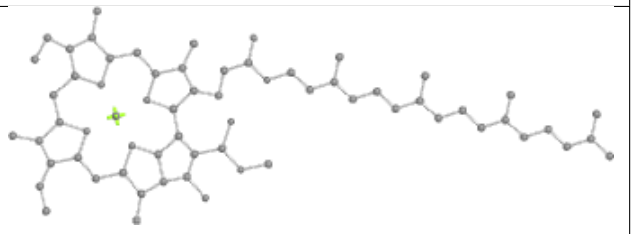


Bond angles

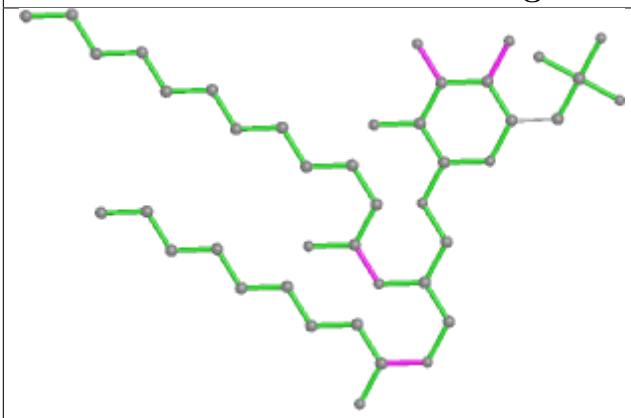


Torsions



Rings

Ligand SQD D 409



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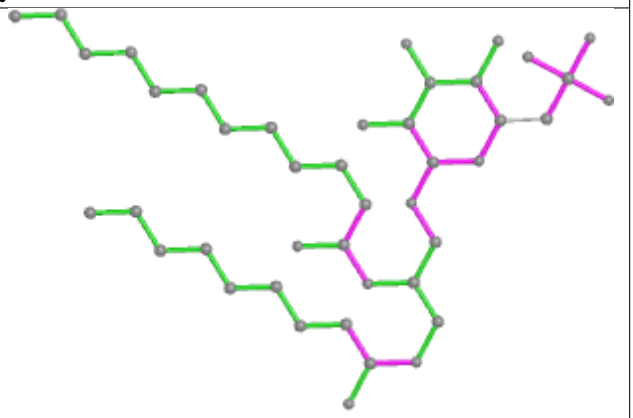
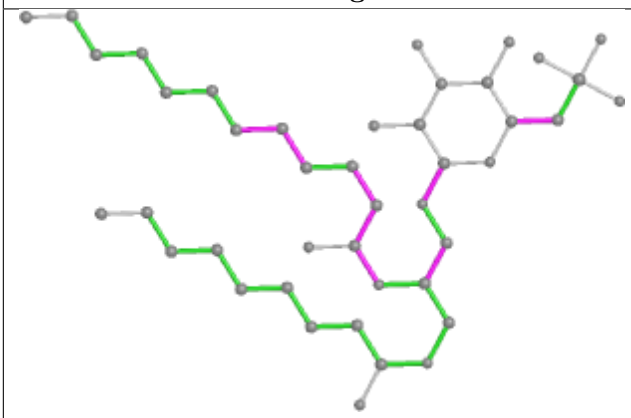
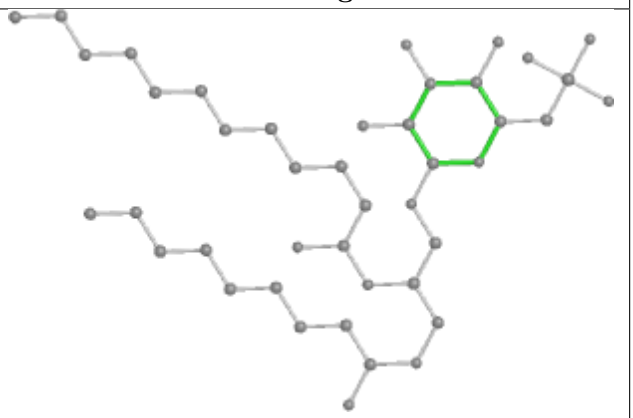


Bond angles

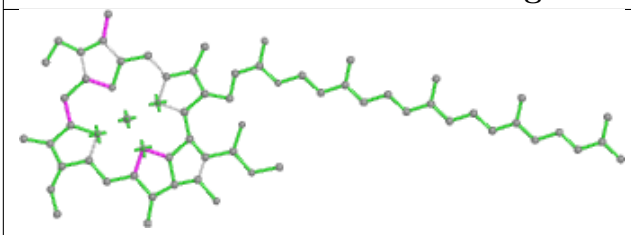


Torsions

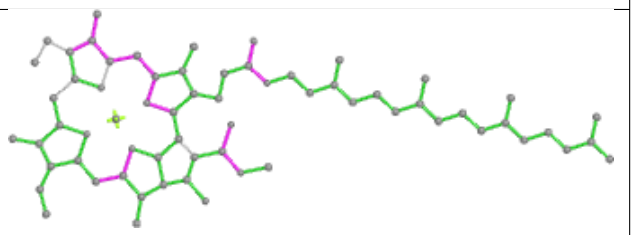


Rings

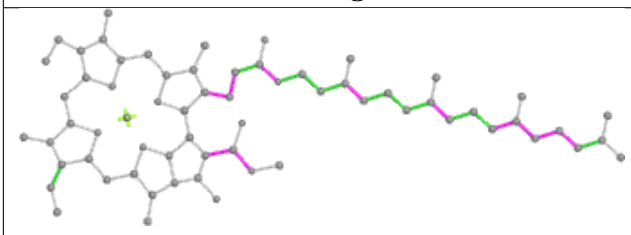
Ligand CLA C 513



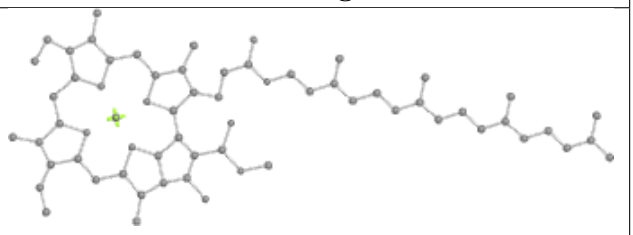
Bond lengths



Bond angles

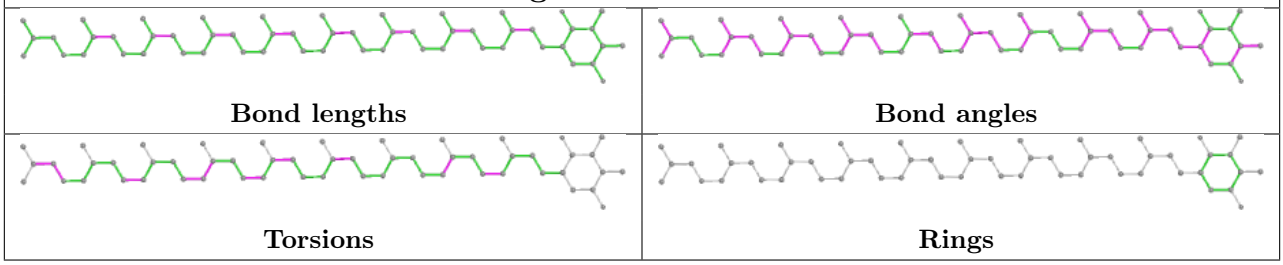


Torsions

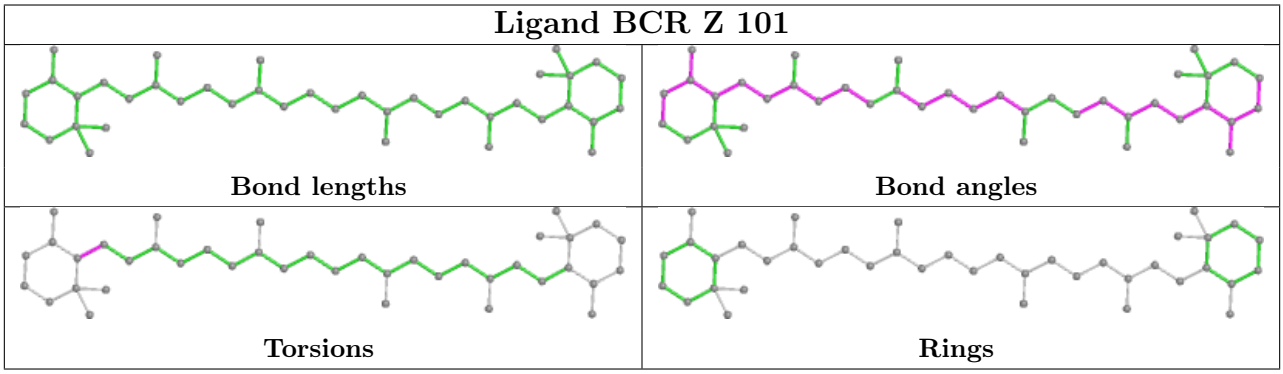


Rings

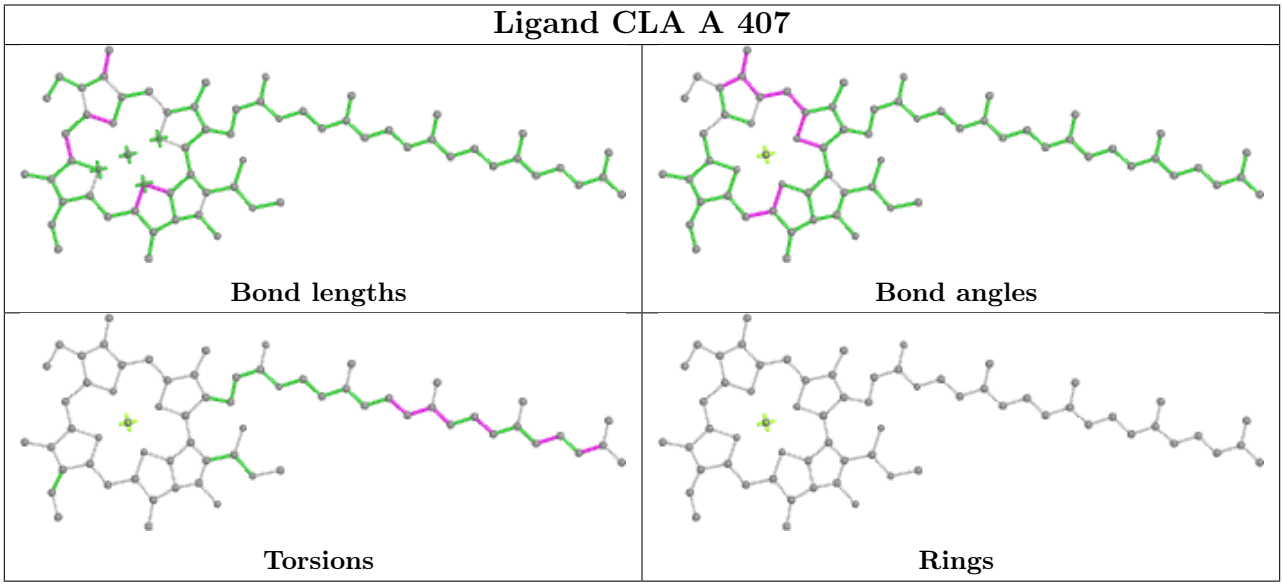
Ligand PL9 D 404



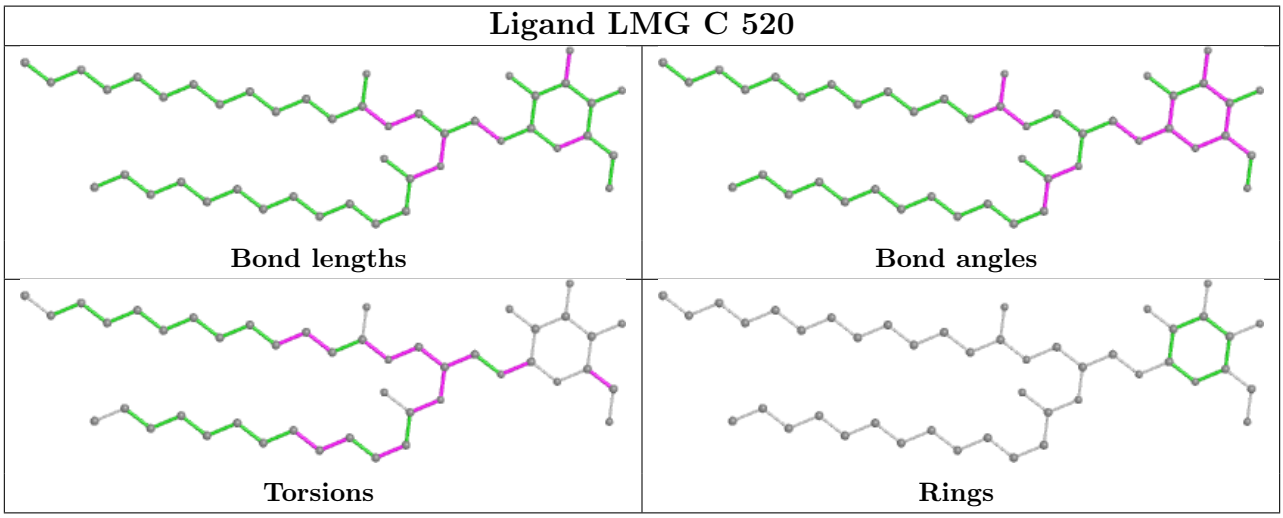
Ligand BCR Z 101



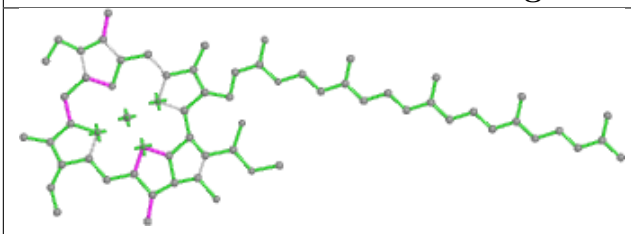
Ligand CLA A 407



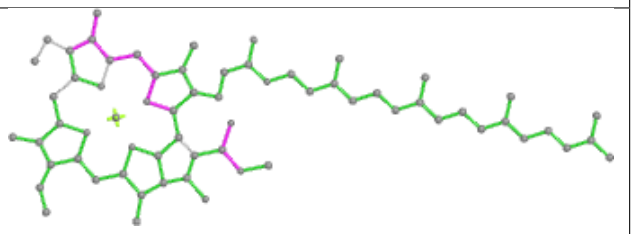
Ligand LMG C 520



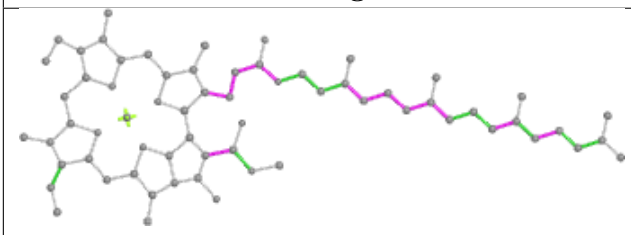
Ligand CLA B 602



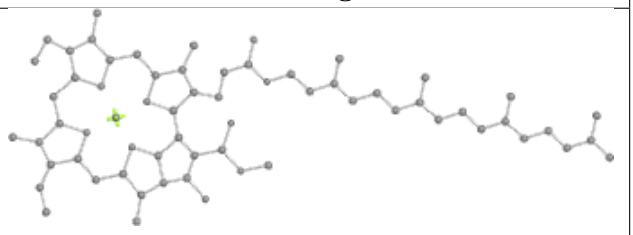
Bond lengths



Bond angles

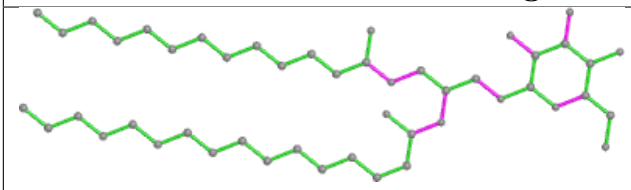


Torsions



Rings

Ligand LMG d 406



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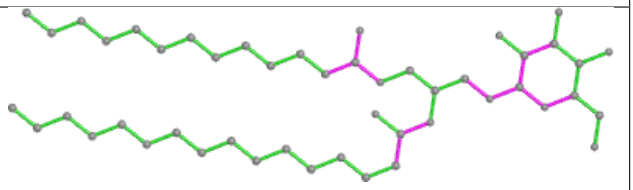
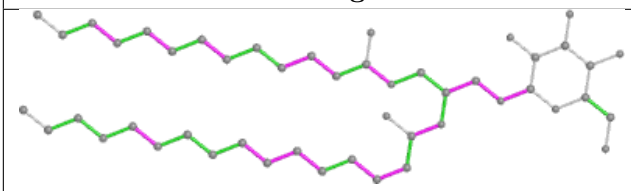
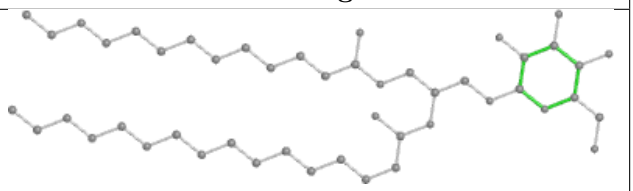


Bond angles

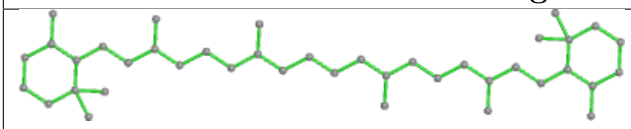


Torsions



Rings

Ligand BCR j 102



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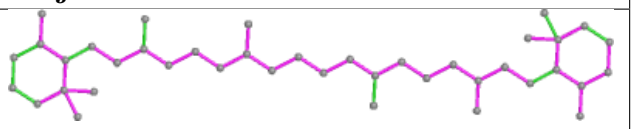
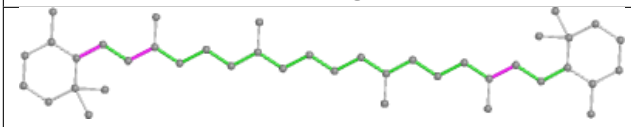


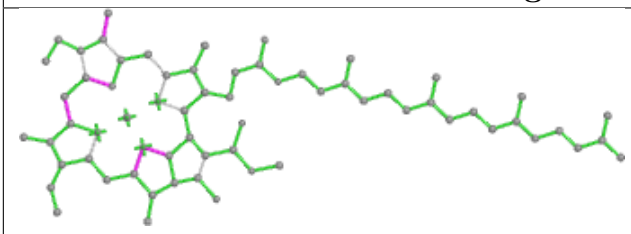
Bond angles



Torsions

Rings

Ligand CLA C 511



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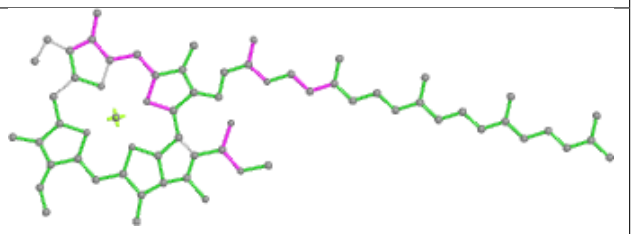
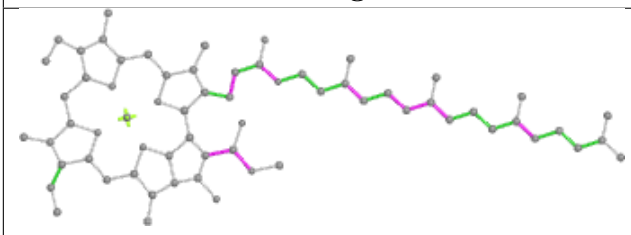
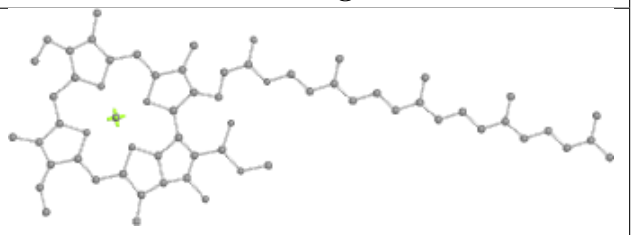


Bond angles

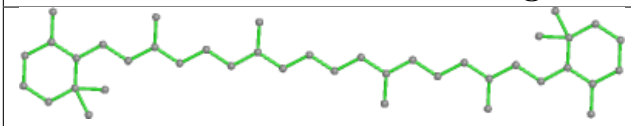


Torsions



Rings

Ligand BCR T 103



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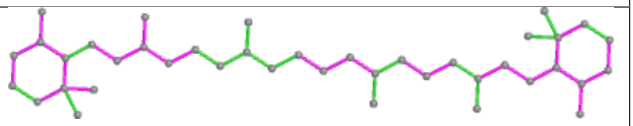
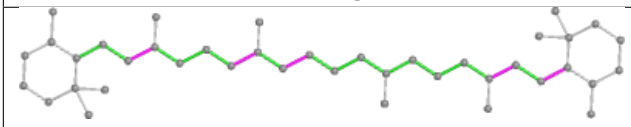


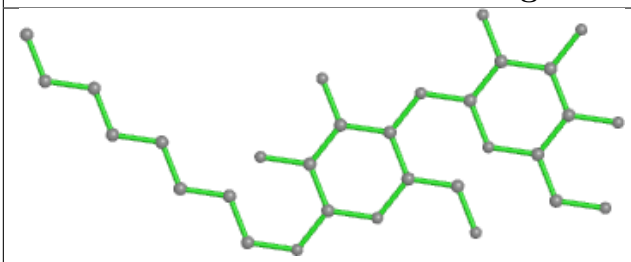
Bond angles



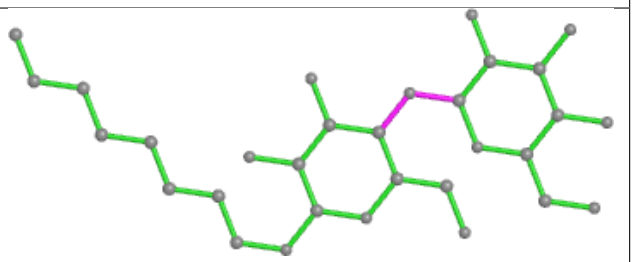
Torsions

Rings

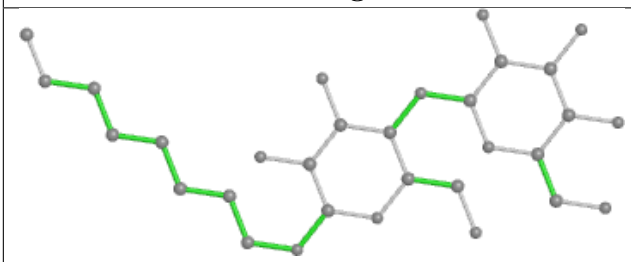
Ligand LMT D 411



Bond lengths



Bond angles



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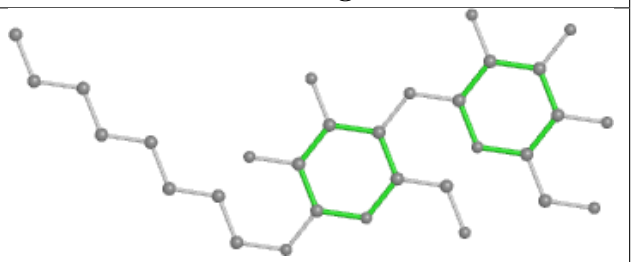
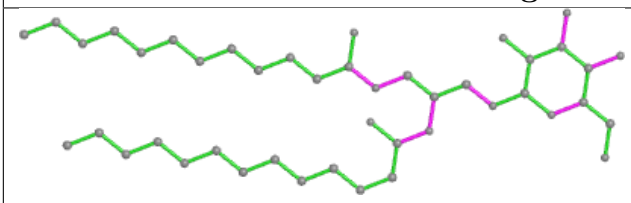


Rings

Ligand LMG E 101



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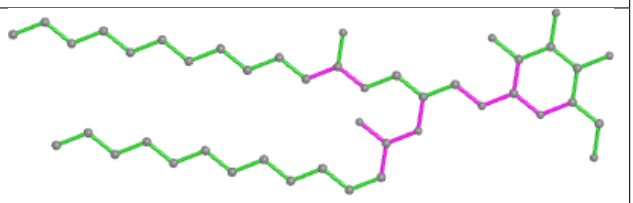
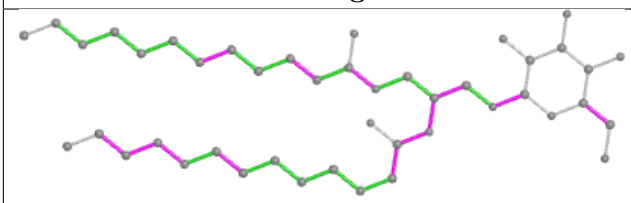


Bond angles



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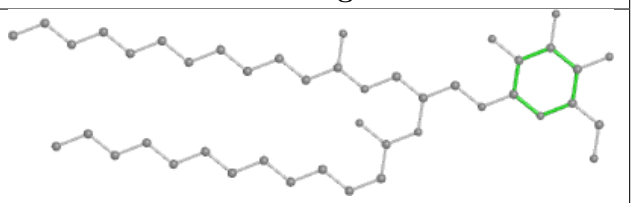
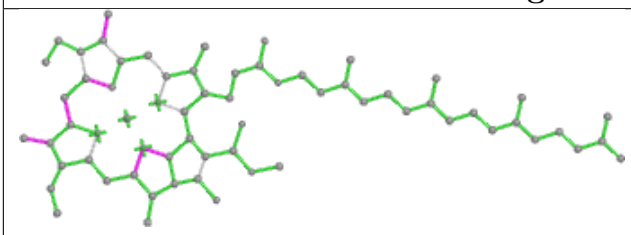


Rings

Ligand CLA b 604



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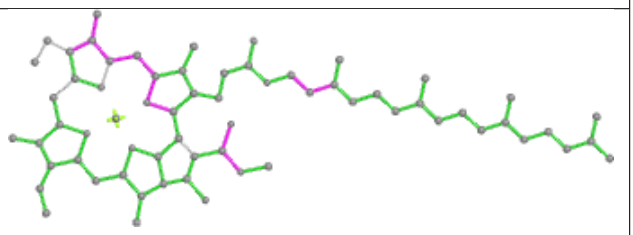
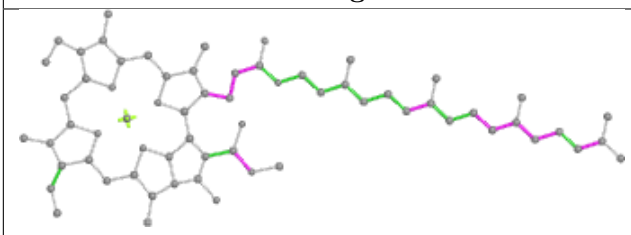


Bond angles



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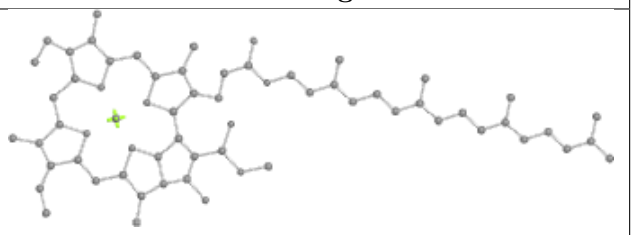
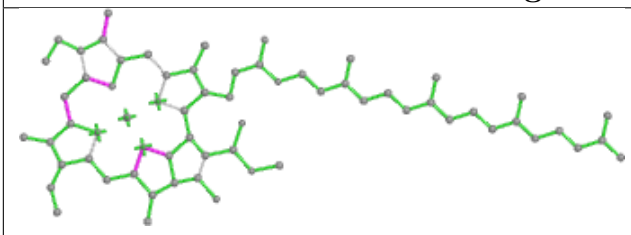
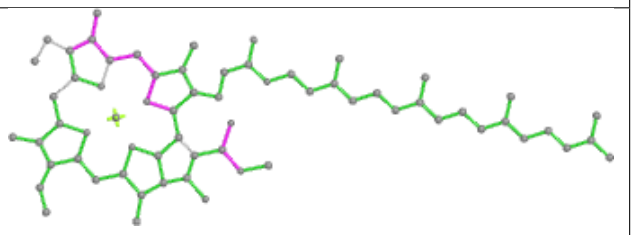


Rings

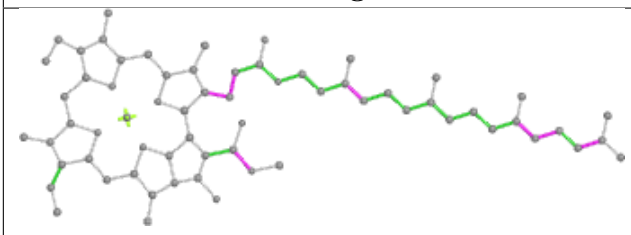
Ligand CLA B 606



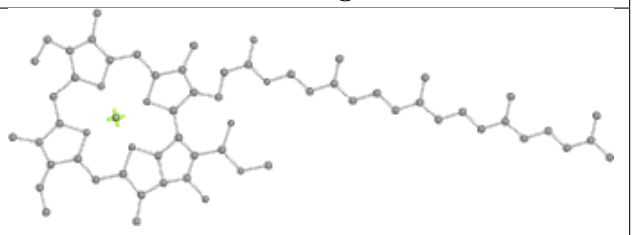
Bond lengths



Bond angles

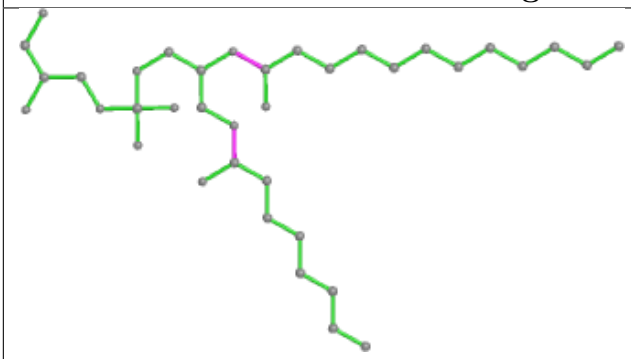


Torsions

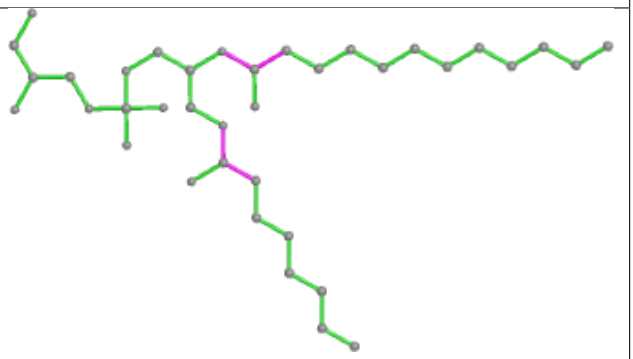


Rings

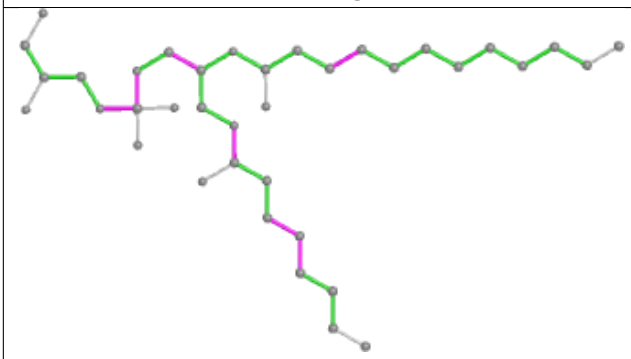
Ligand LHG A 415



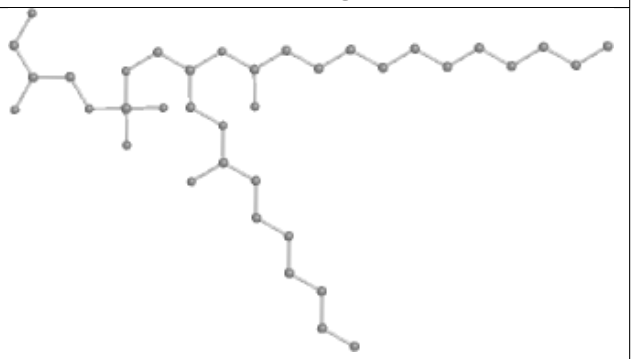
Bond lengths



Bond angles

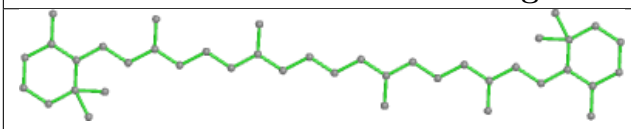


Torsions

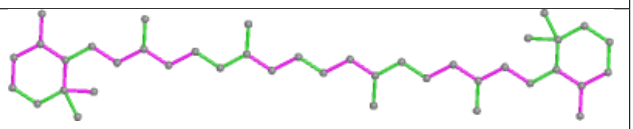


Rings

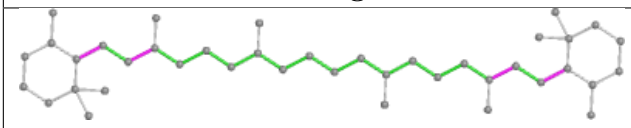
Ligand BCR K 102



Bond lengths



Bond angles



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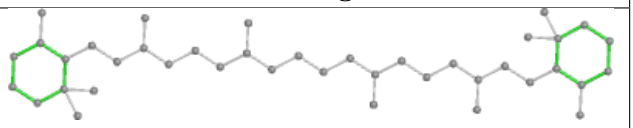
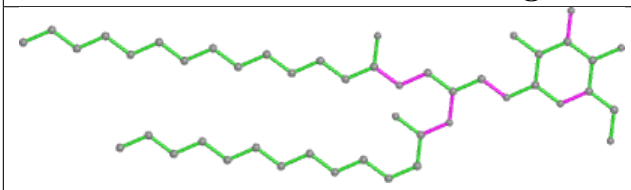
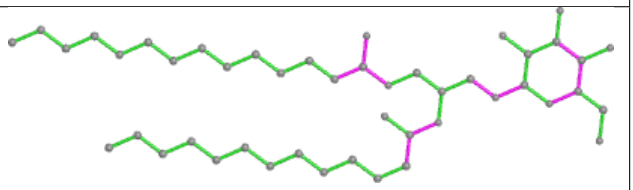


Rings

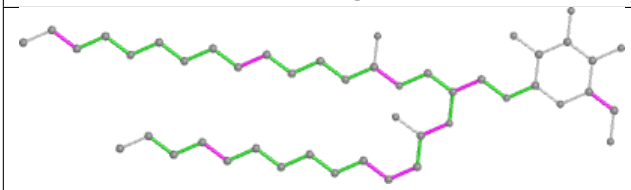
Ligand LMG d 405



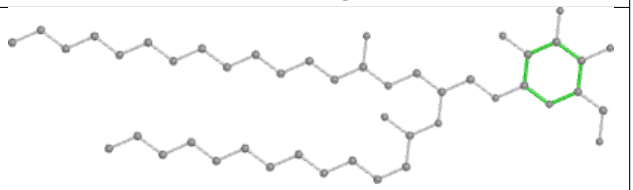
Bond lengths



Bond angles

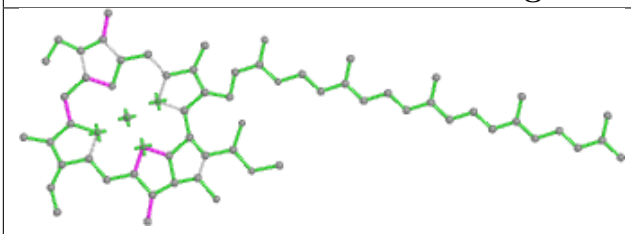


Torsions



Rings

Ligand CLA B 615



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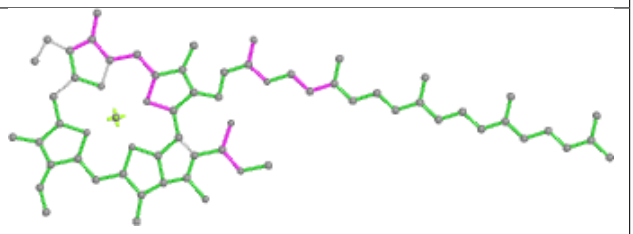
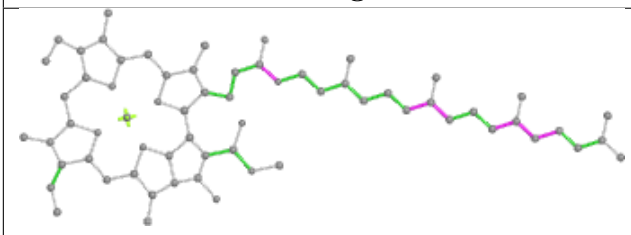
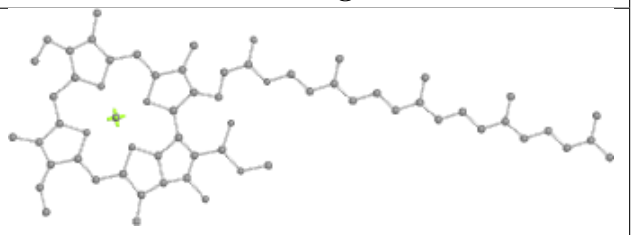


Bond angles

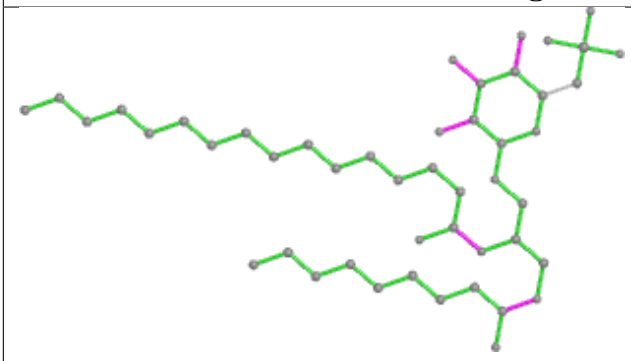


Torsions

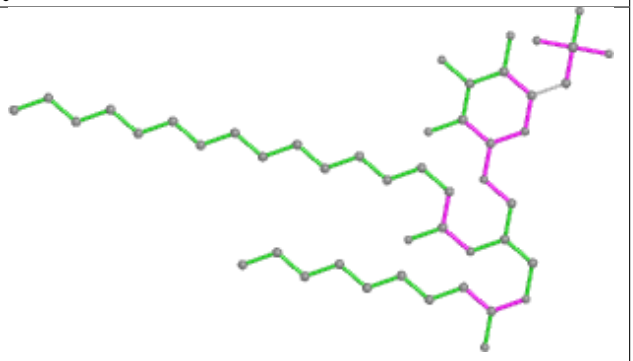


Rings

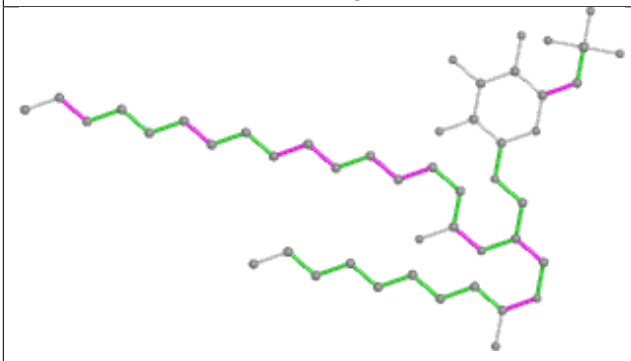
Ligand SQD b 601



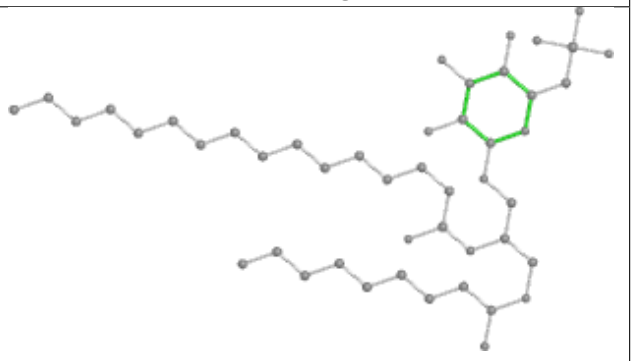
Bond lengths



Bond angles

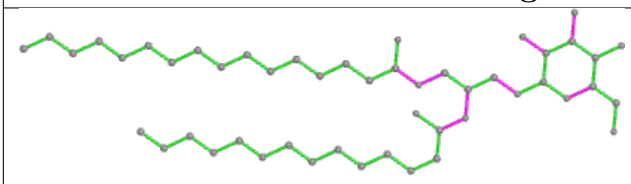


Torsions



Rings

Ligand LMG B 622



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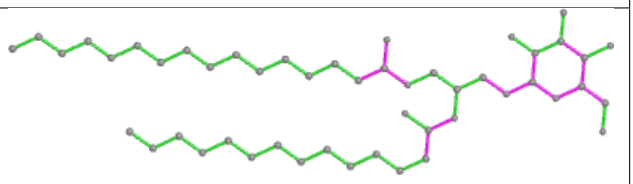
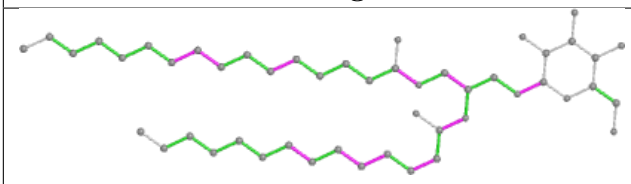


Bond angles



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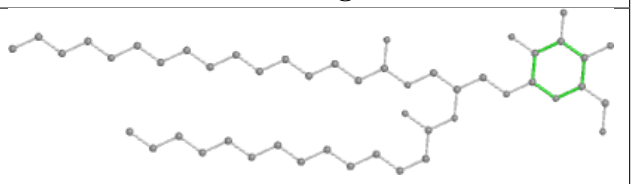
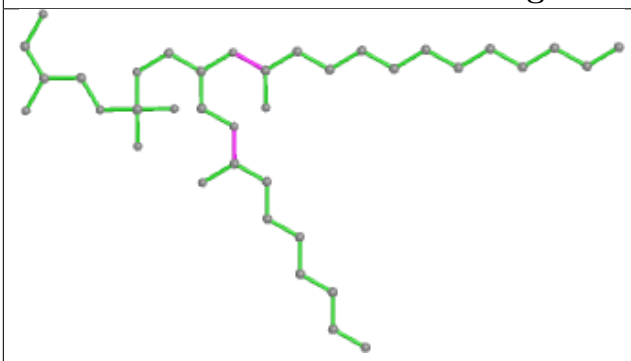


Rings

Ligand LHG a 417



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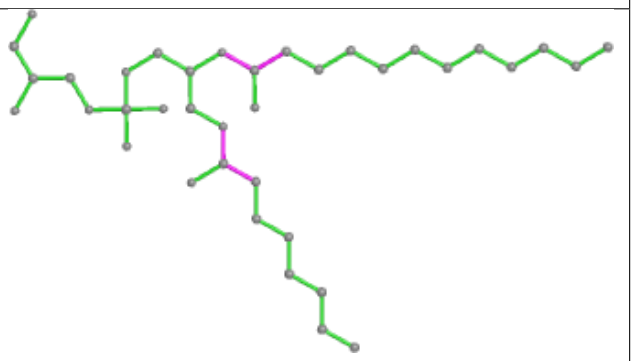
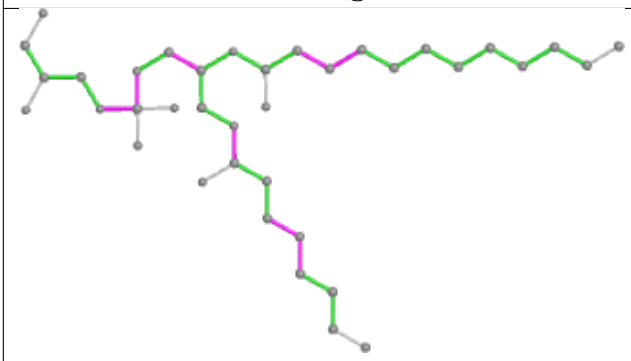


Bond angles



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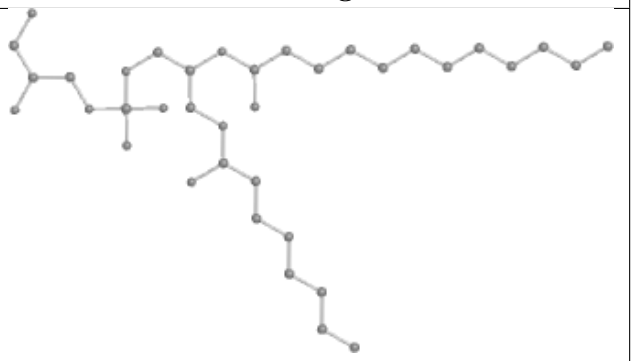
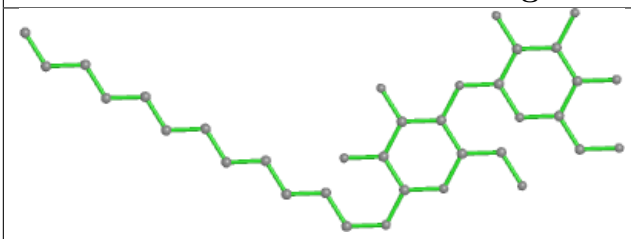


Rings

Ligand LMT B 624



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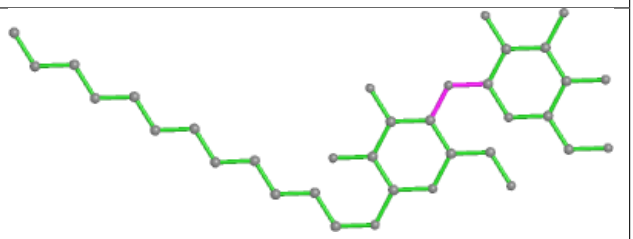
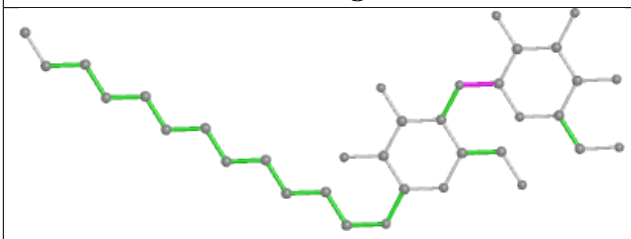


Bond angles



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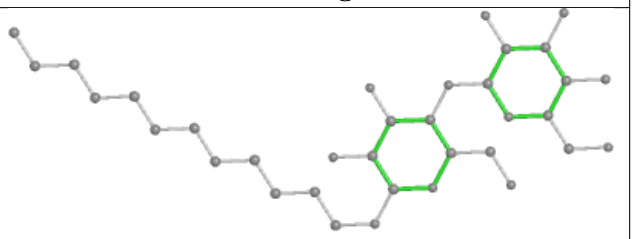
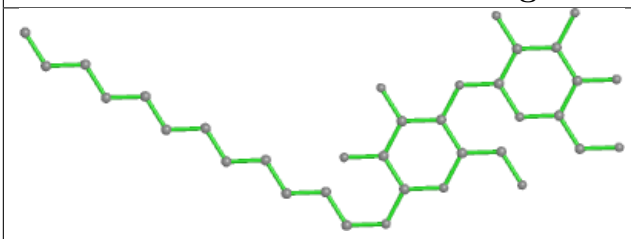


Rings

Ligand LMT m 101



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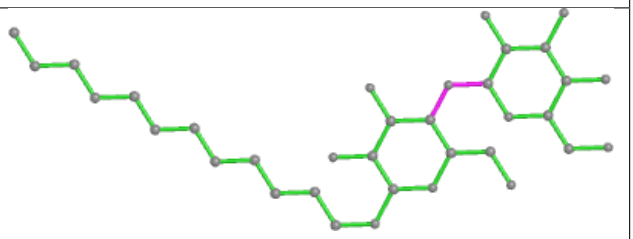
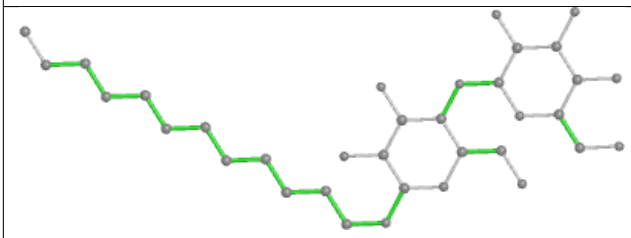
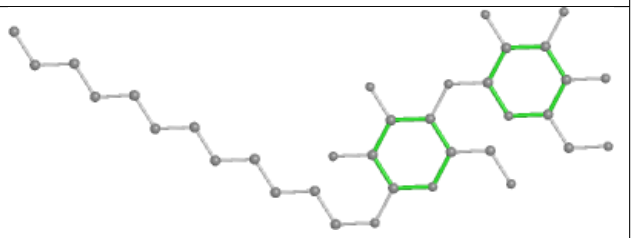


Bond angles

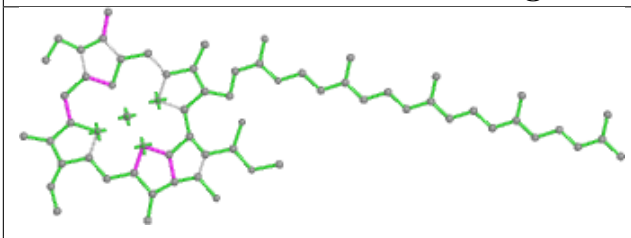


Torsions



Rings

Ligand CLA B 601



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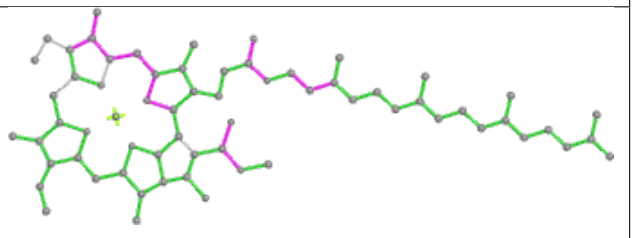
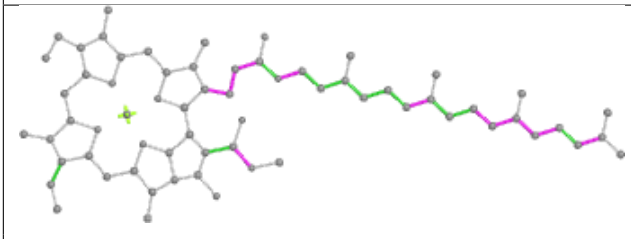


Bond angles



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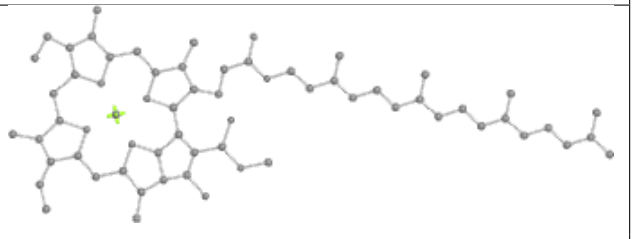
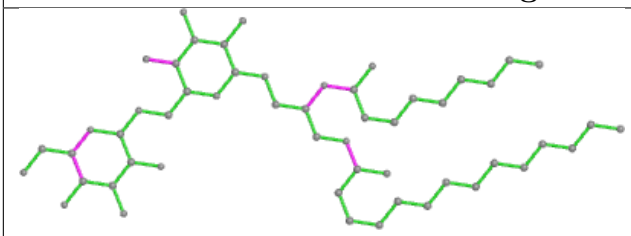


Rings

Ligand DGD C 516



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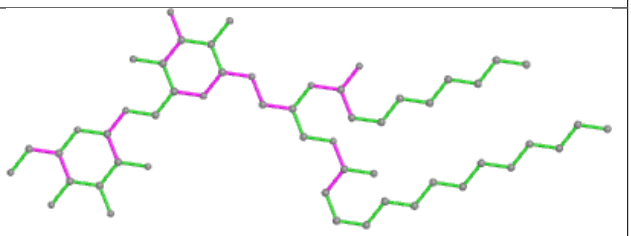

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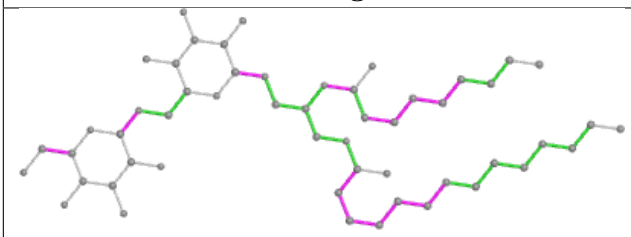

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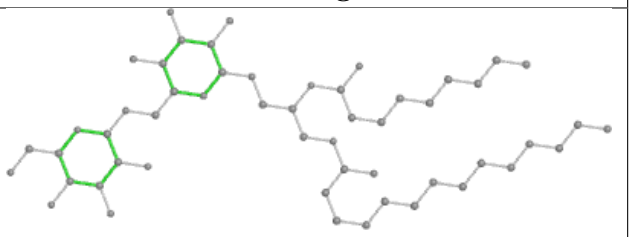
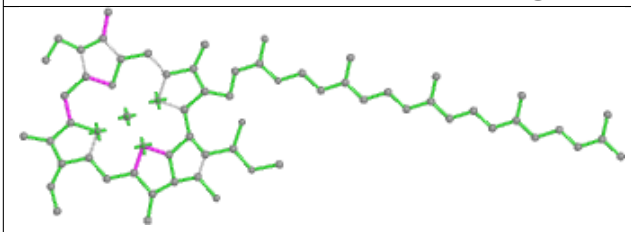


Rings

Ligand CLA c 509



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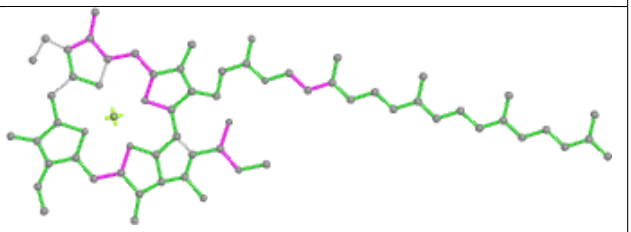
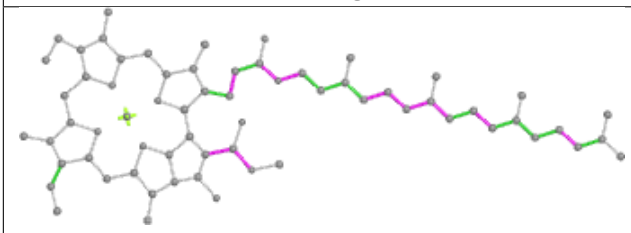


Bond angles



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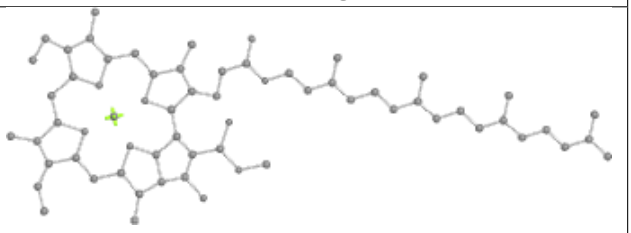
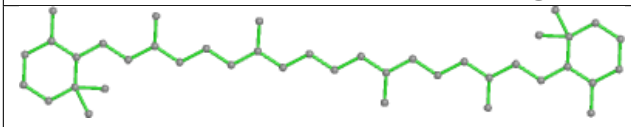
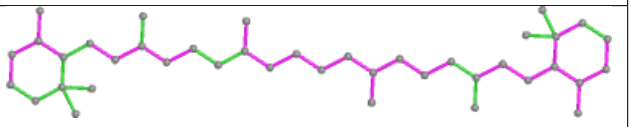


Rings

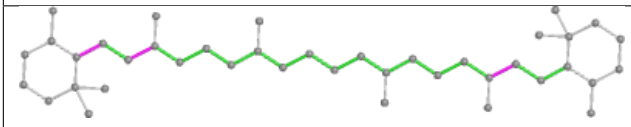
Ligand BCR f 102



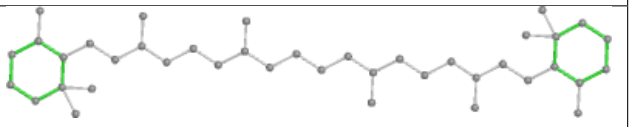
Bond lengths



Bond angles

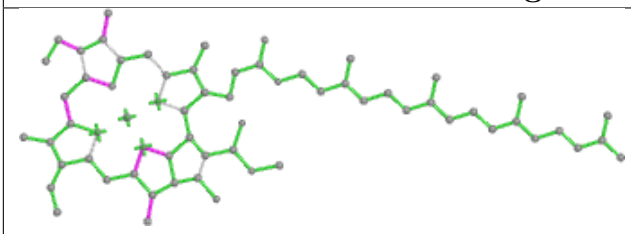


Torsions

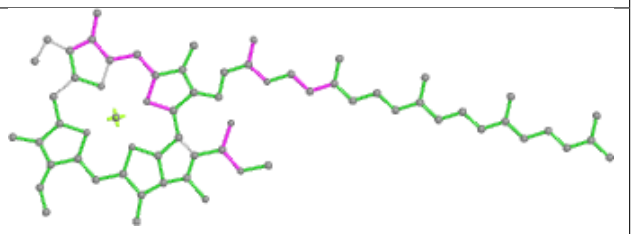


Rings

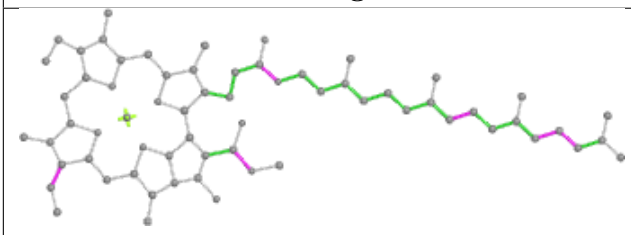
Ligand CLA B 604



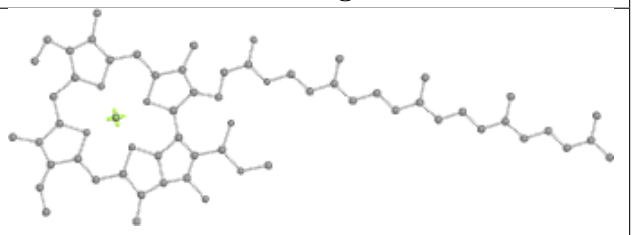
Bond lengths



Bond angles

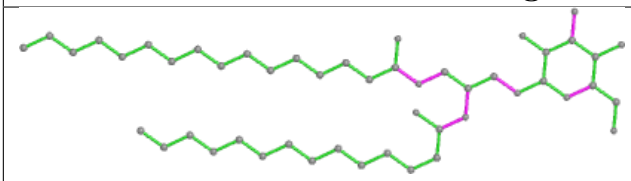


Torsions

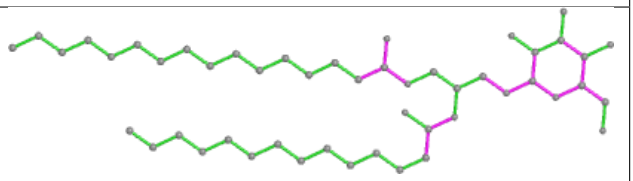


Rings

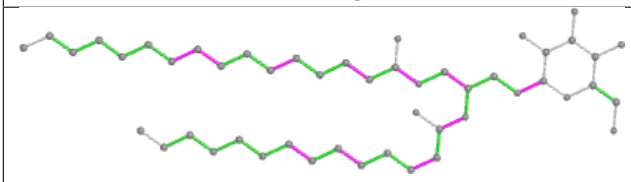
Ligand LMG b 624



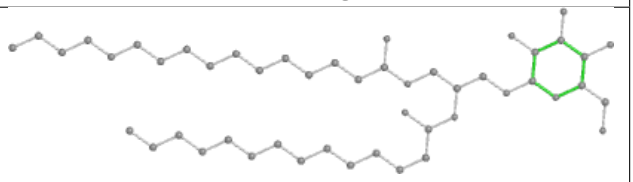
Bond lengths



Bond angles

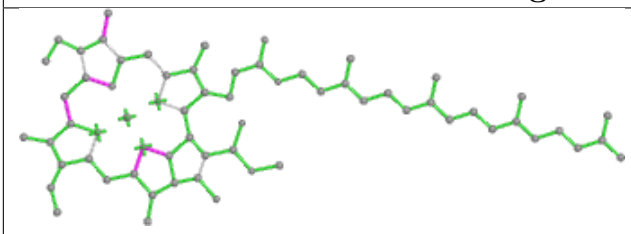


Torsions

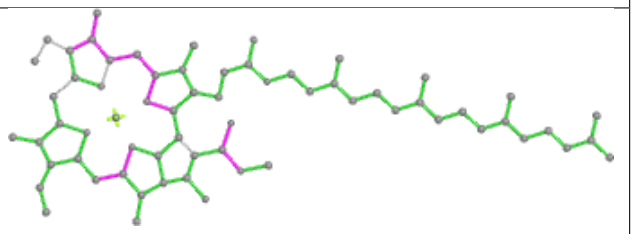


Rings

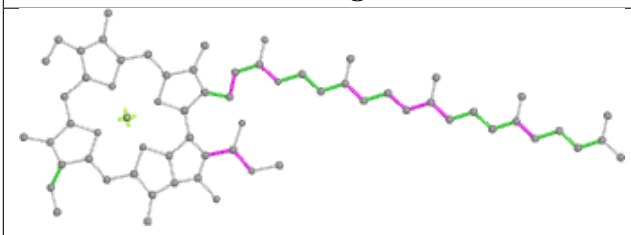
Ligand CLA c 511



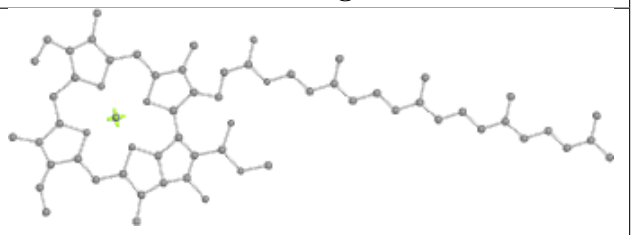
Bond lengths



Bond angles

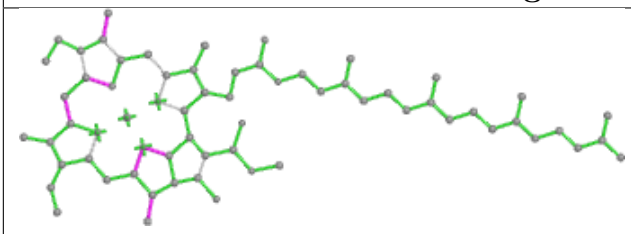


Torsions

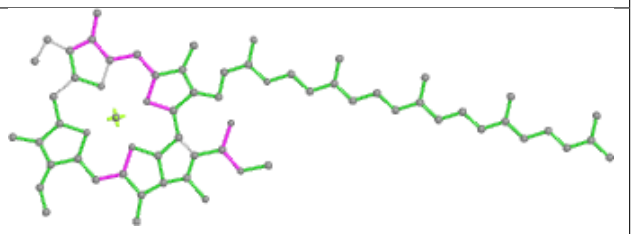


Rings

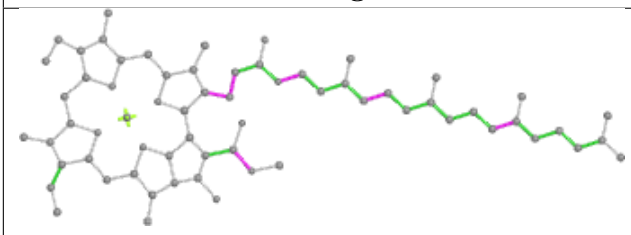
Ligand CLA A 403



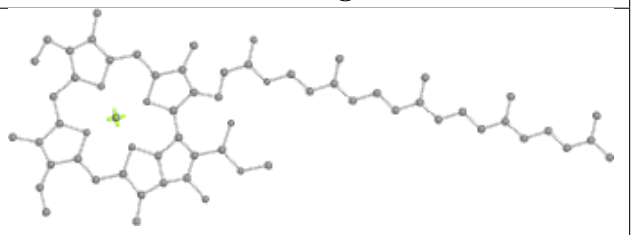
Bond lengths



Bond angles

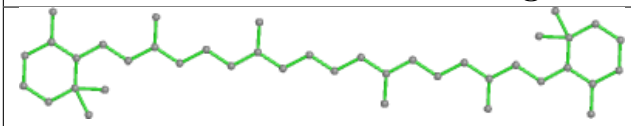


Torsions

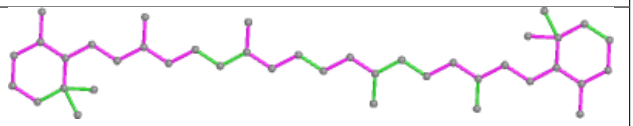


Rings

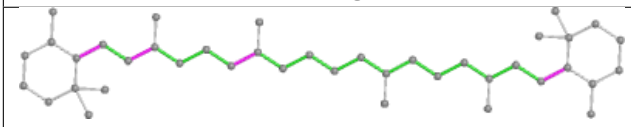
Ligand BCR C 514



Bond lengths



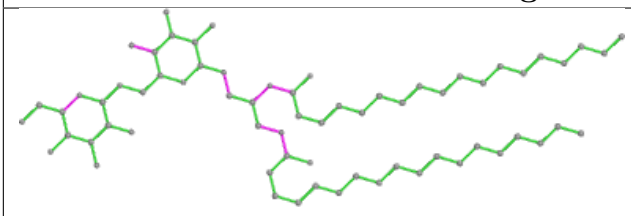
Bond angles



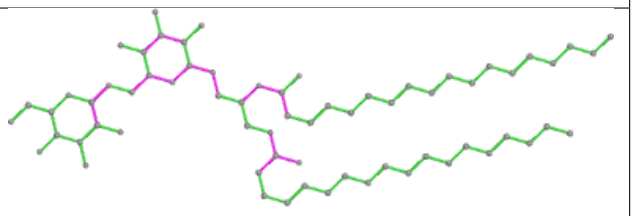
Torsions

Rings

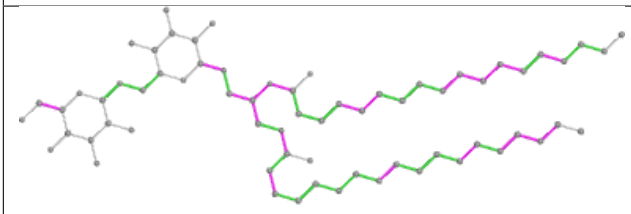
Ligand DGD C 518



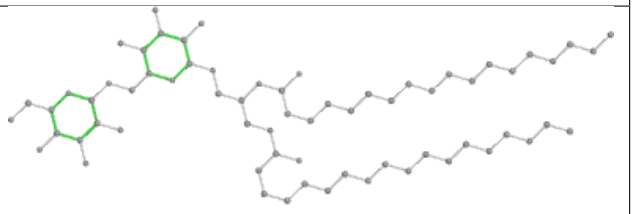
Bond lengths



Bond angles

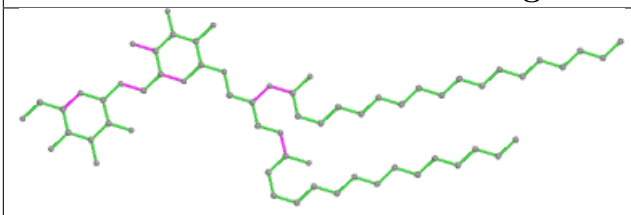


Torsions

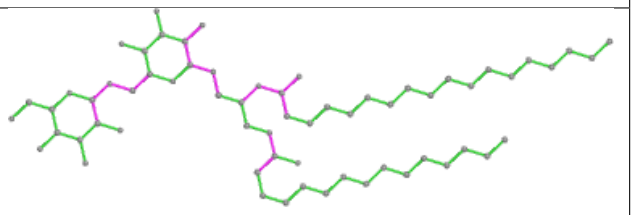


Rings

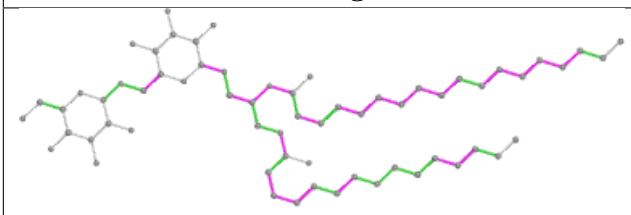
Ligand DGD d 408



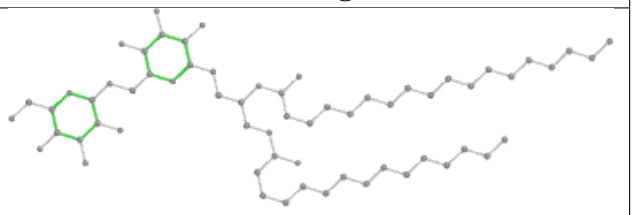
Bond lengths



Bond angles

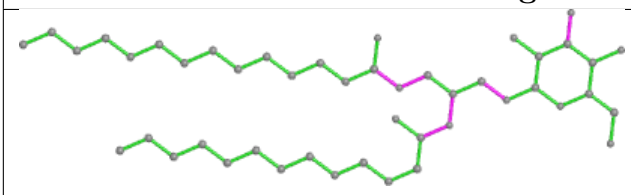


Torsions

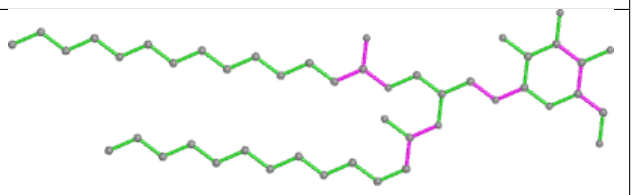


Rings

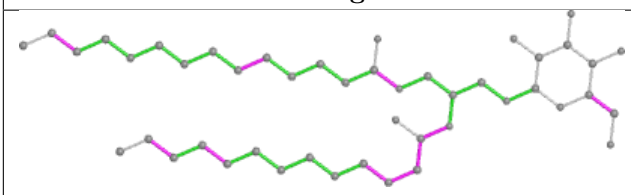
Ligand LMG D 406



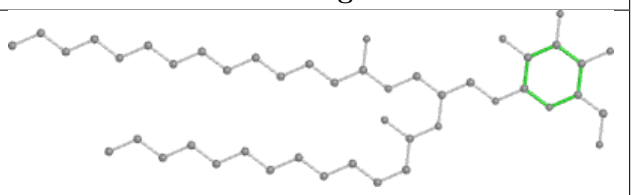
Bond lengths



Bond angles

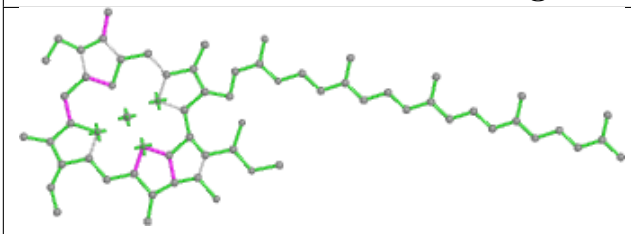


Torsions

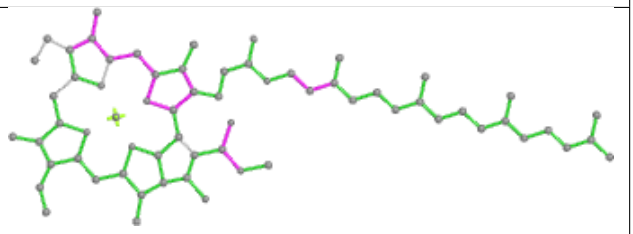


Rings

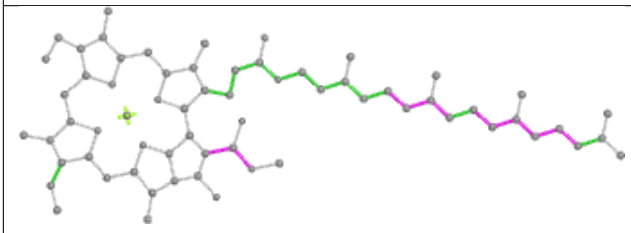
Ligand CLA c 506



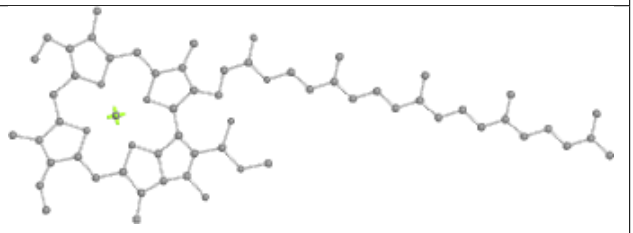
Bond lengths



Bond angles

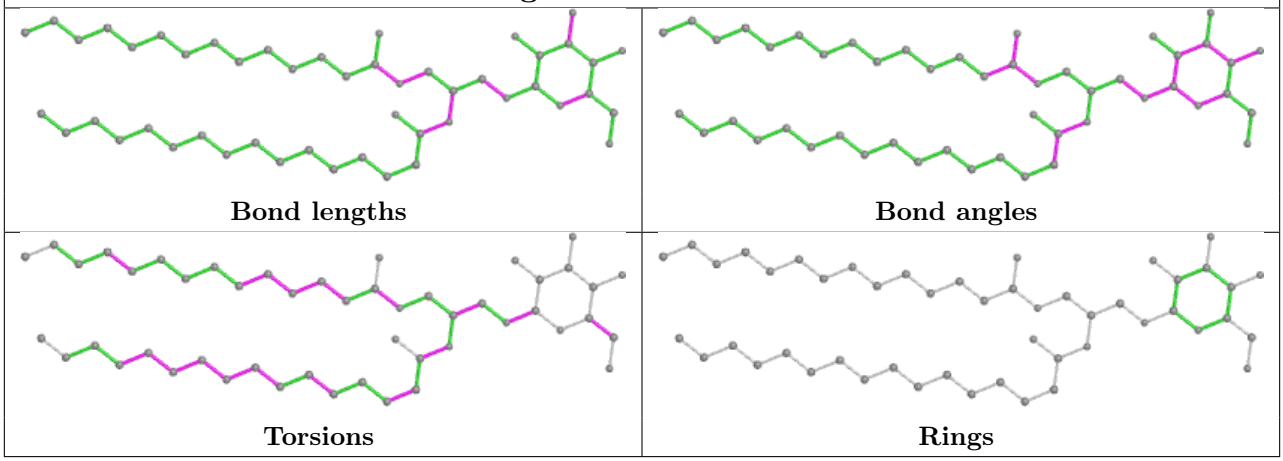


Torsions

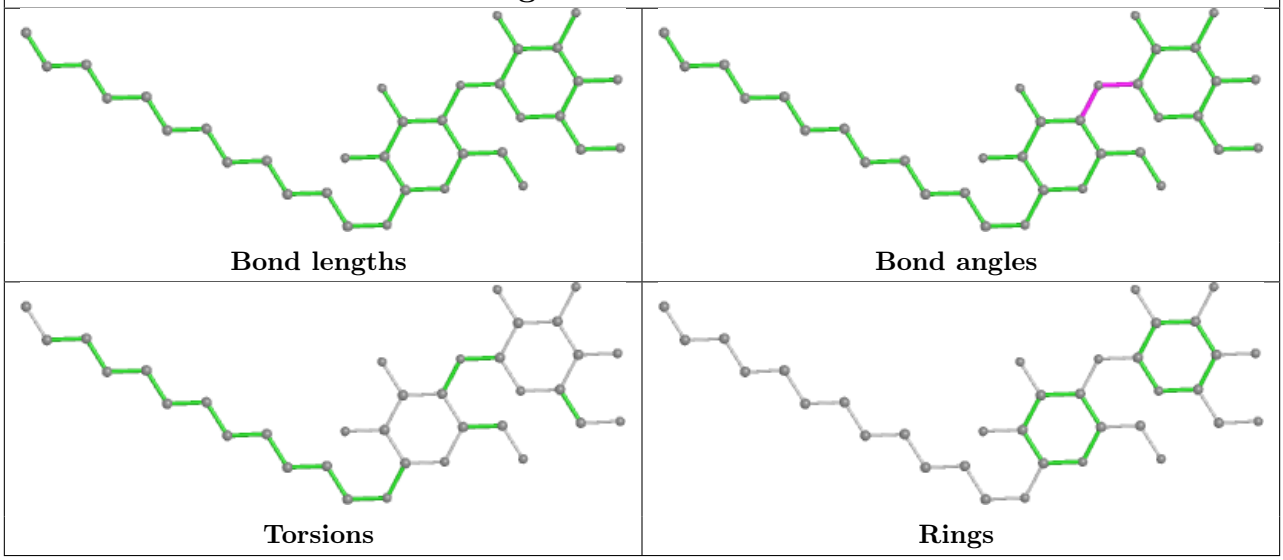


Rings

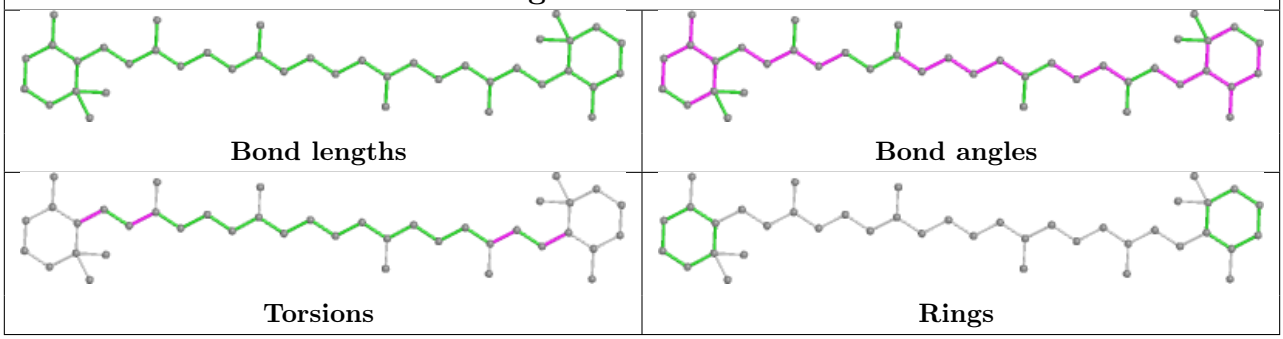
Ligand LMG D 407



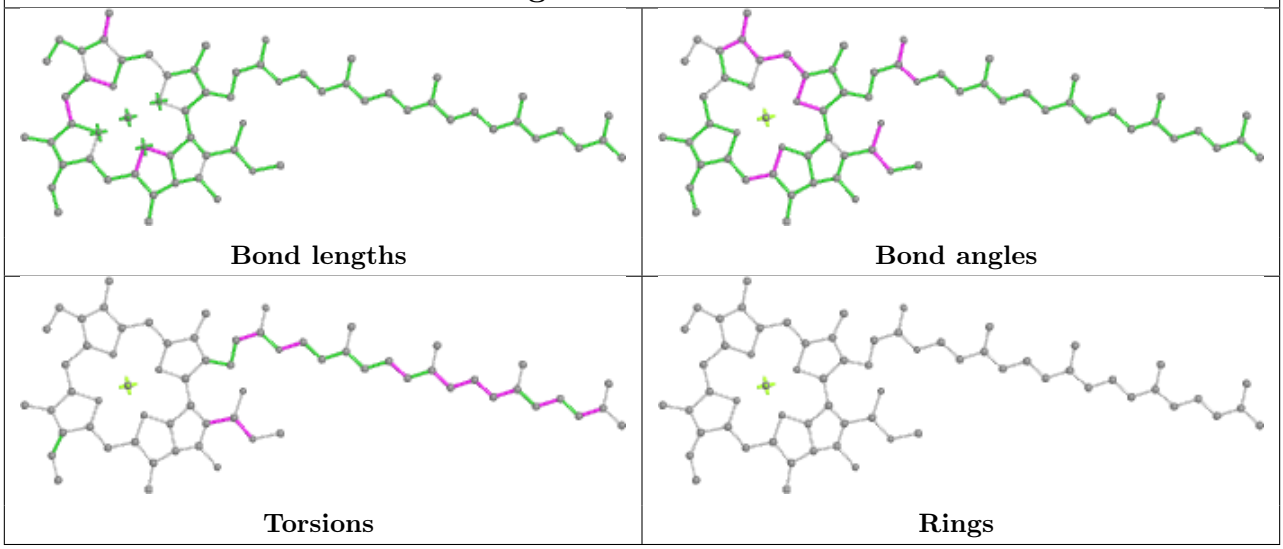
Ligand LMT M 103



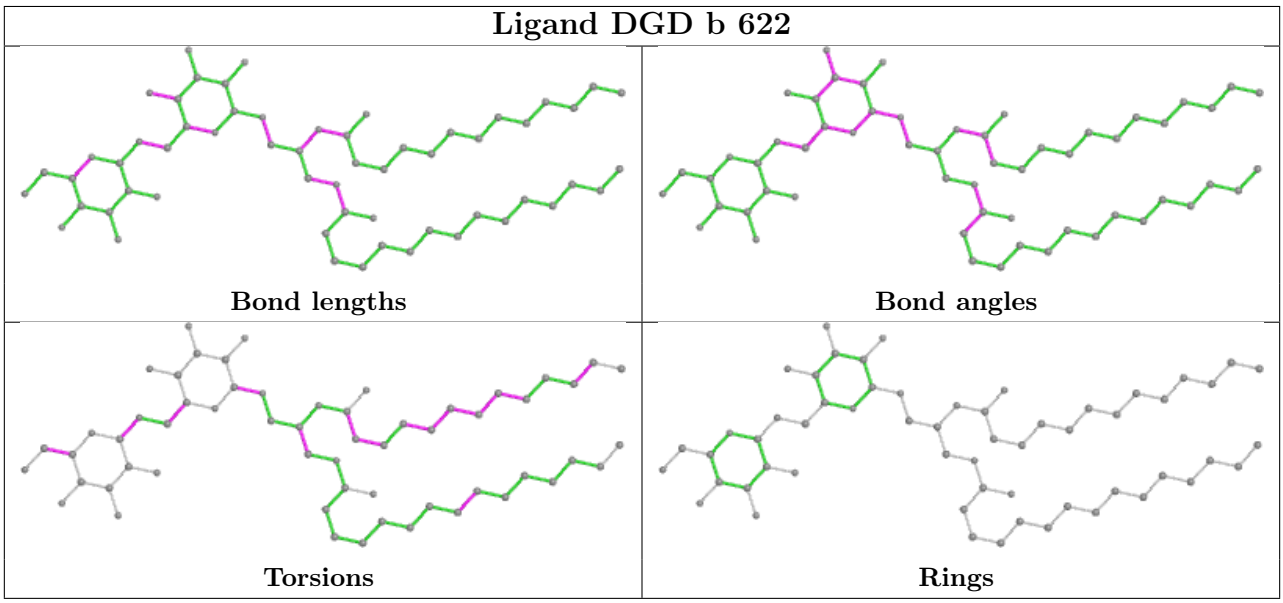
Ligand BCR c 516



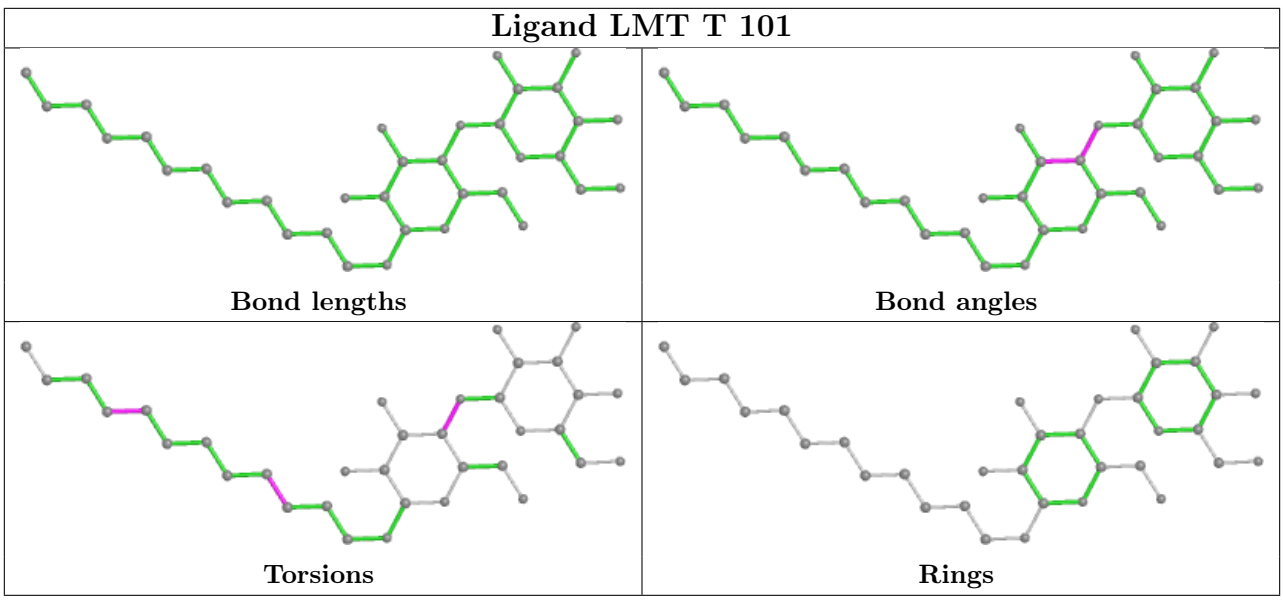
Ligand CLA b 616



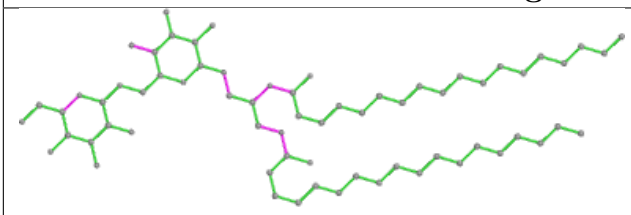
Ligand DGD b 622



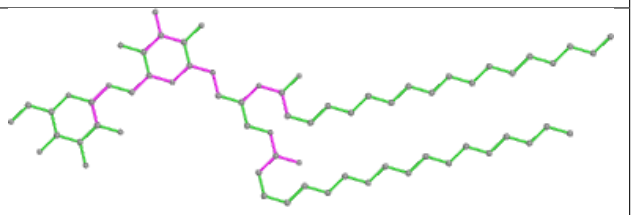
Ligand LMT T 101



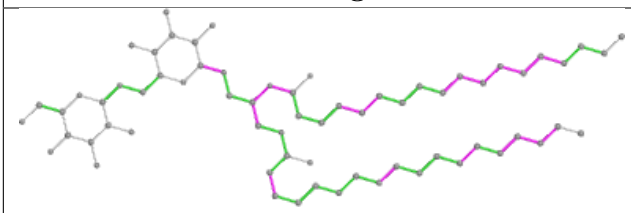
Ligand DGD c 519



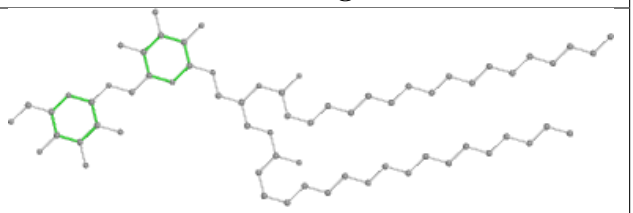
Bond lengths



Bond angles

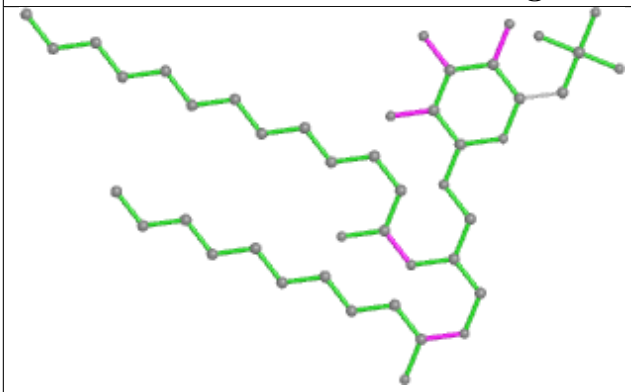


Torsions

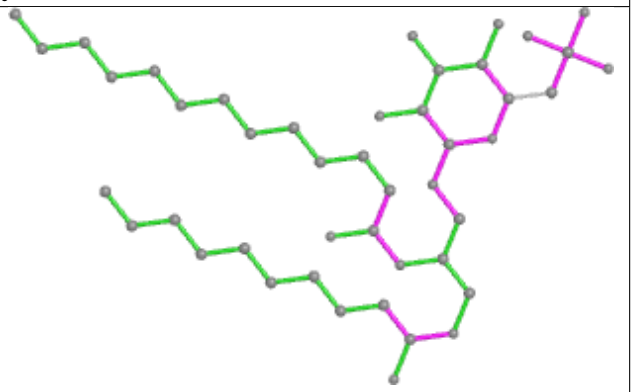


Rings

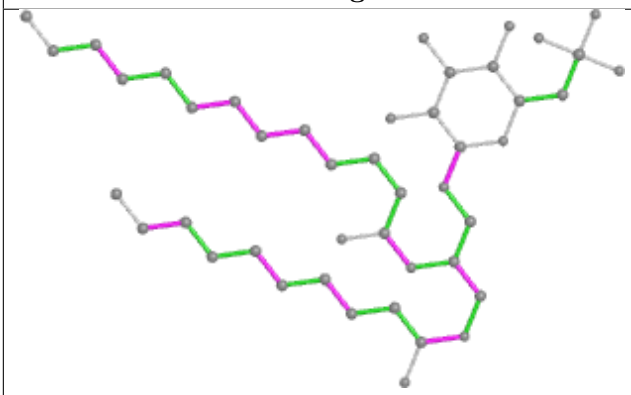
Ligand SQD F 102



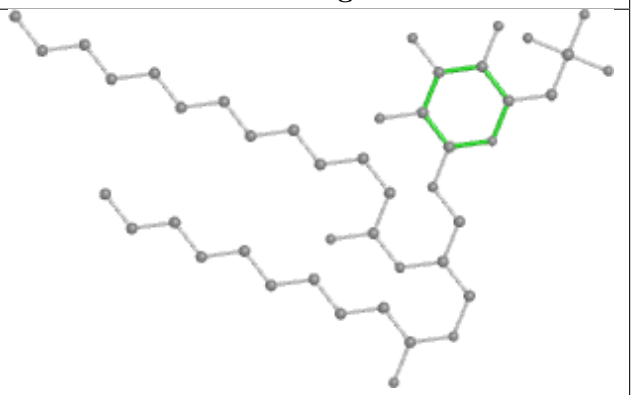
Bond lengths



Bond angles

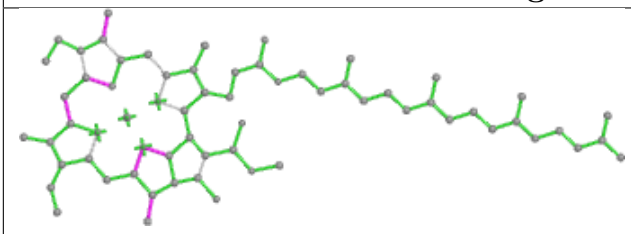


Torsions

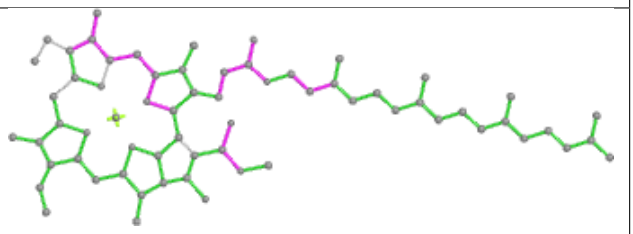


Rings

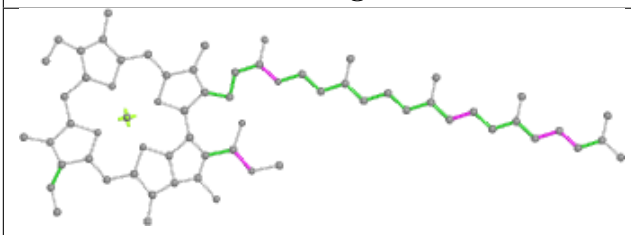
Ligand CLA b 607



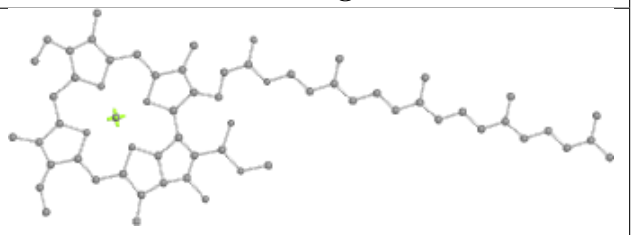
Bond lengths



Bond angles

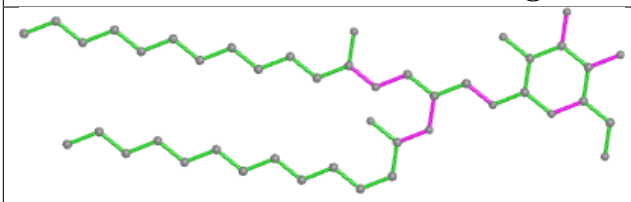


Torsions



Rings

Ligand LMG e 101



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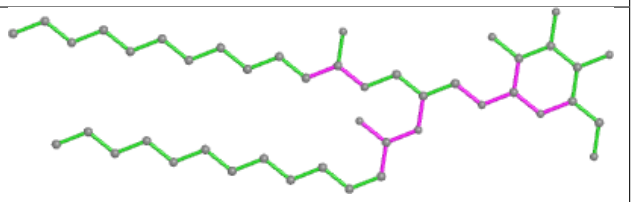
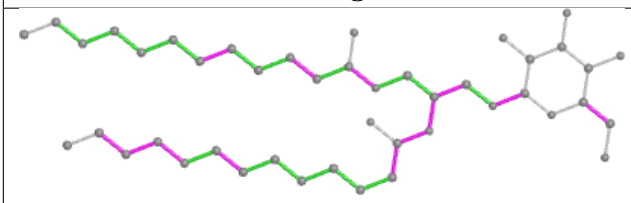
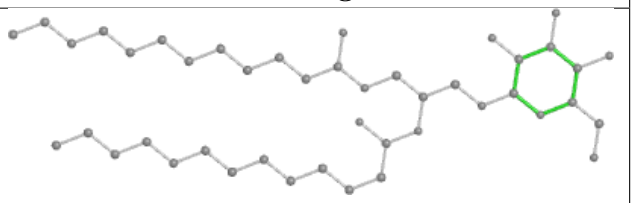


Bond angles

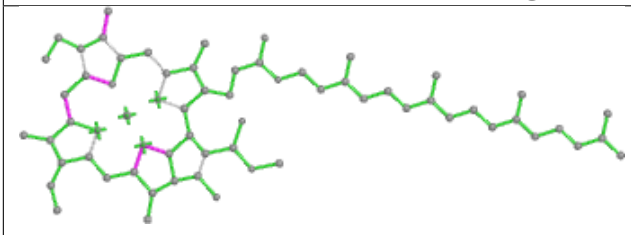


Torsions

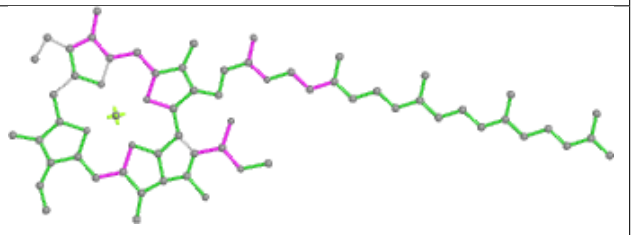


Rings

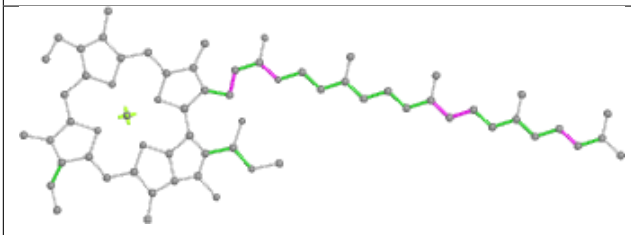
Ligand CLA D 403



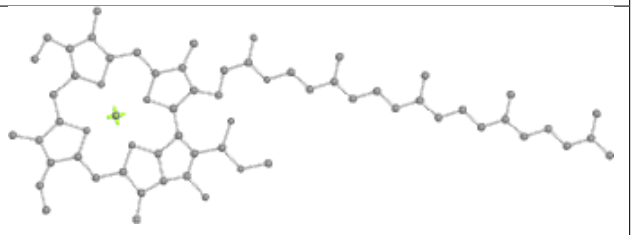
Bond lengths



Bond angles

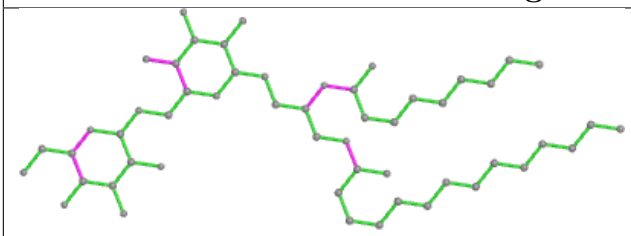


Torsions

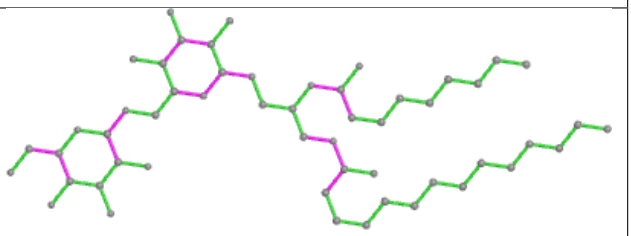


Rings

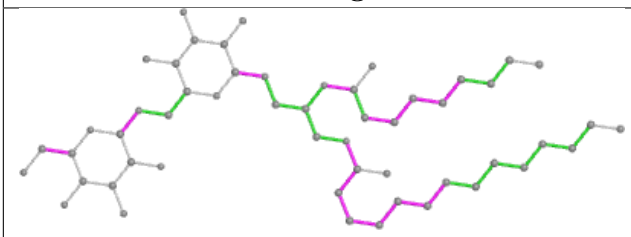
Ligand DGD c 517



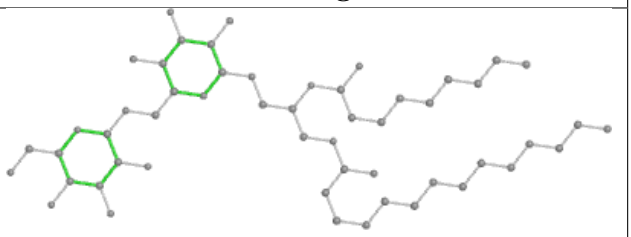
Bond lengths



Bond angles

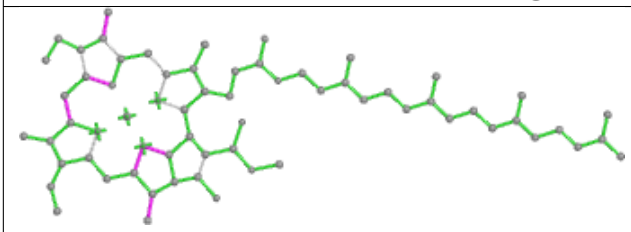


Torsions



Rings

Ligand CLA b 614



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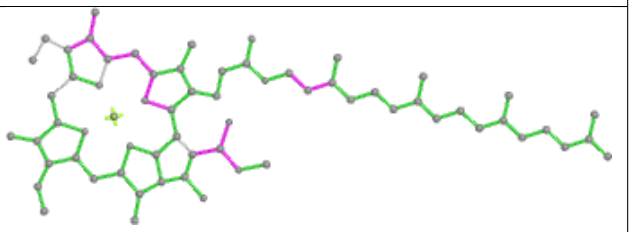
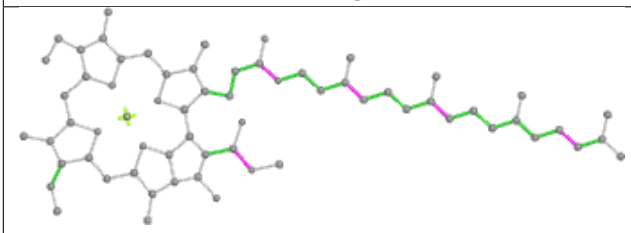
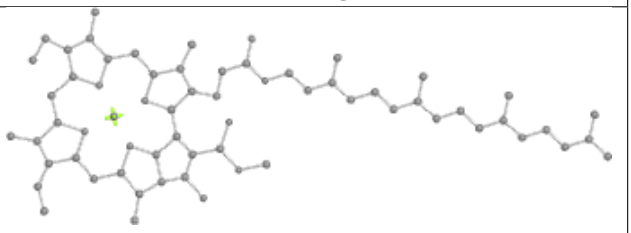


Bond angles

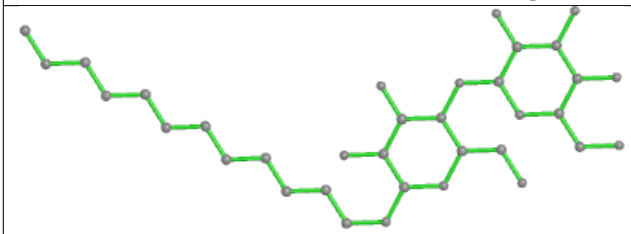


Torsions



Rings

Ligand LMT b 603



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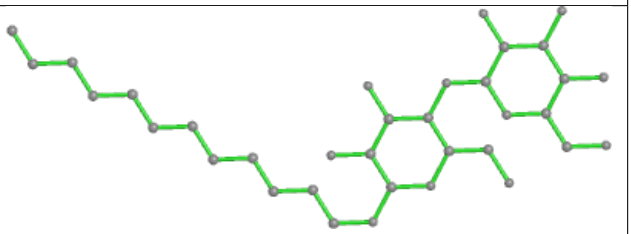
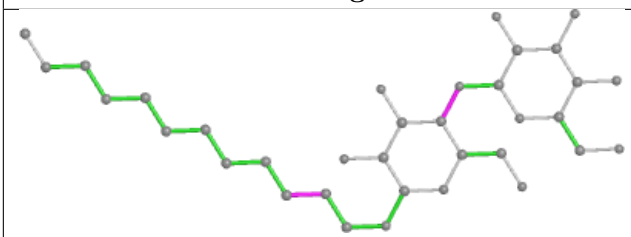
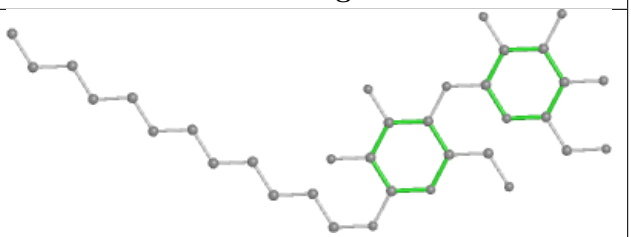


Bond angles

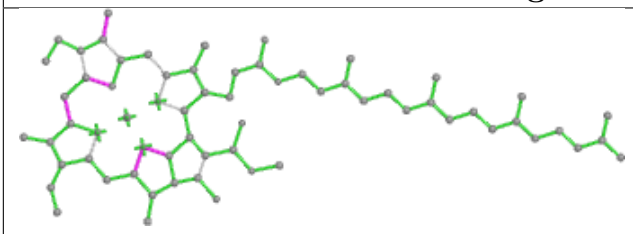


Torsions

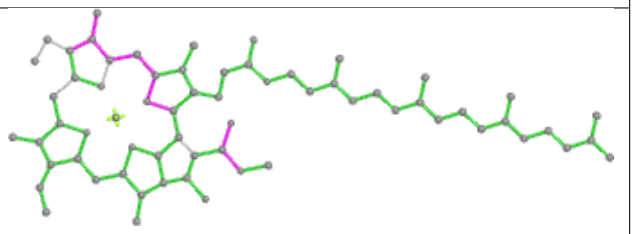


Rings

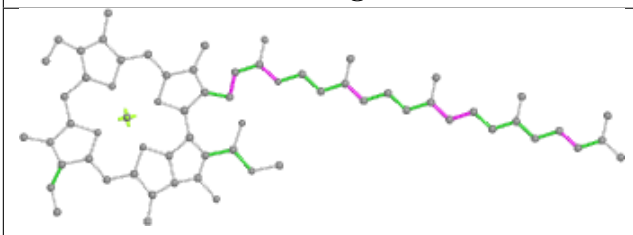
Ligand CLA d 403



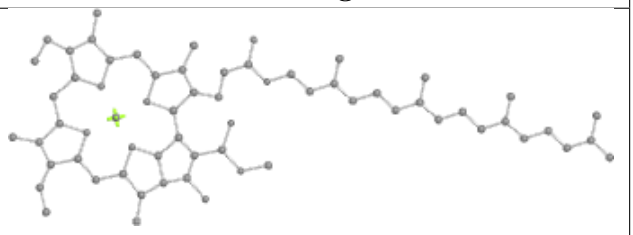
Bond lengths



Bond angles

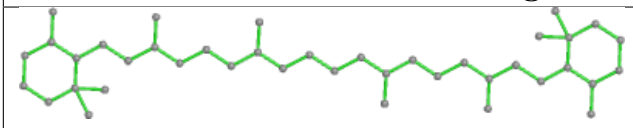


Torsions



Rings

Ligand BCR B 618



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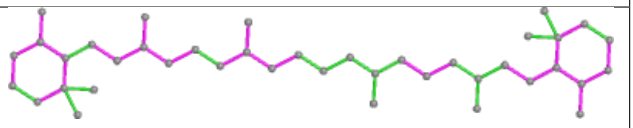
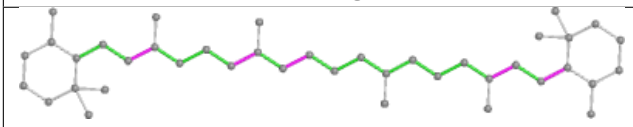


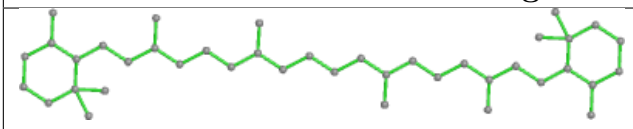
Bond angles



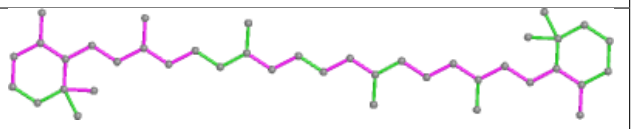
Torsions

Rings

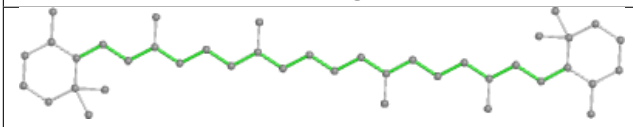
Ligand BCR A 410



Bond lengths



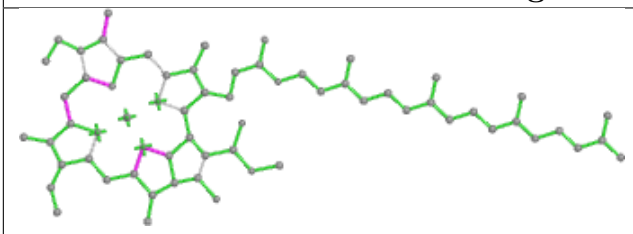
Bond angles



Torsions

Rings

Ligand CLA b 609



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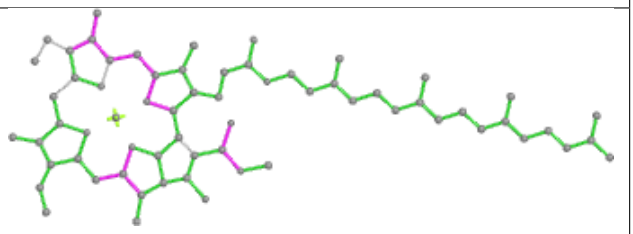
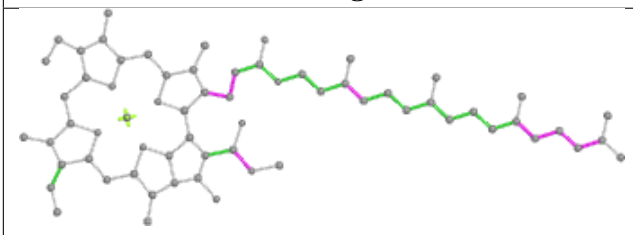


Bond angles



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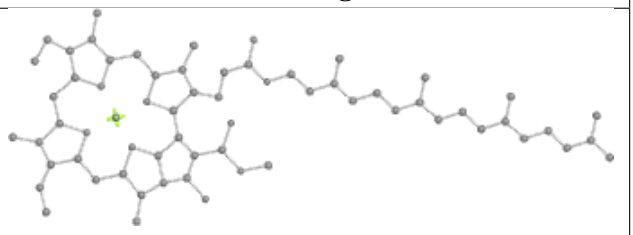
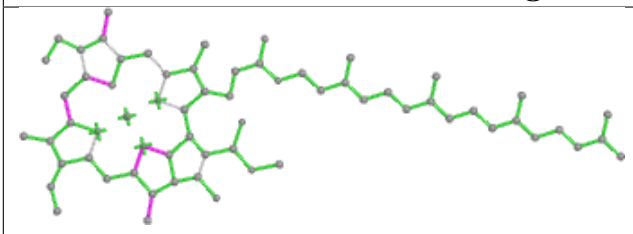


Rings

Ligand CLA B 605



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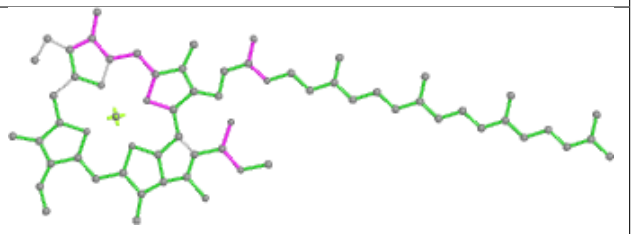
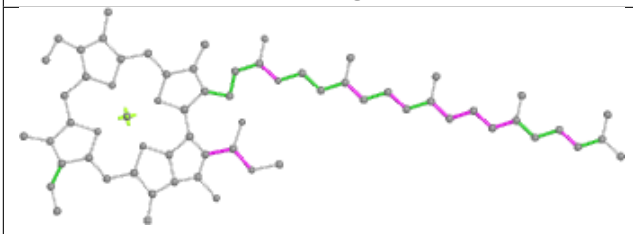
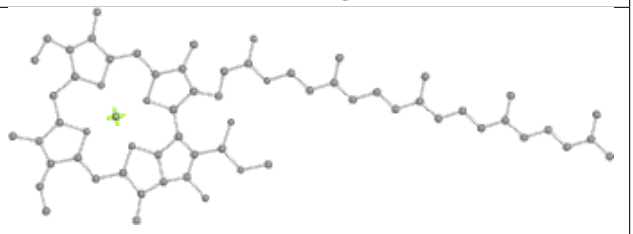


Bond angles

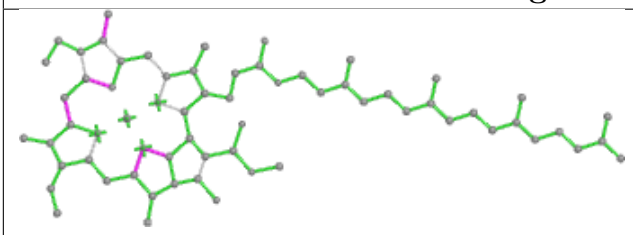


Torsions



Rings

Ligand CLA c 508



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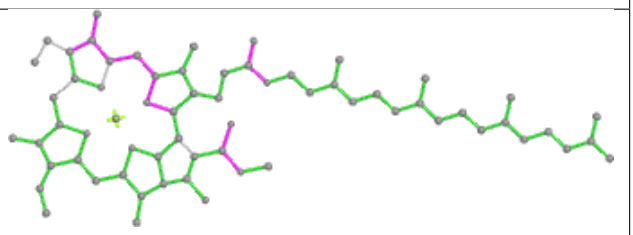
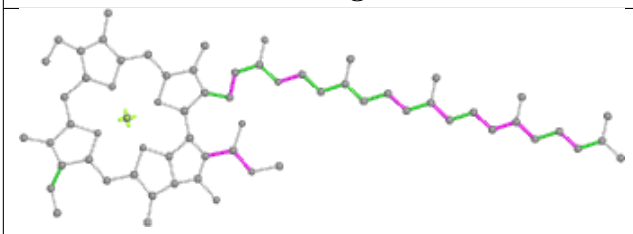


Bond angles



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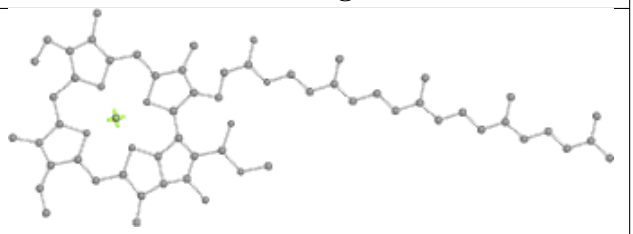
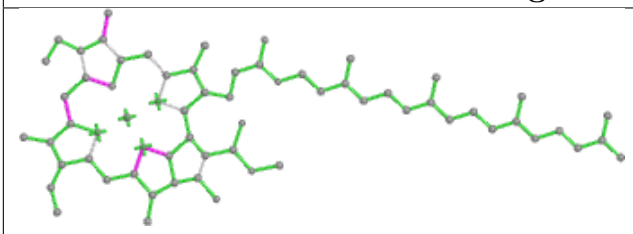


Rings

Ligand CLA a 409



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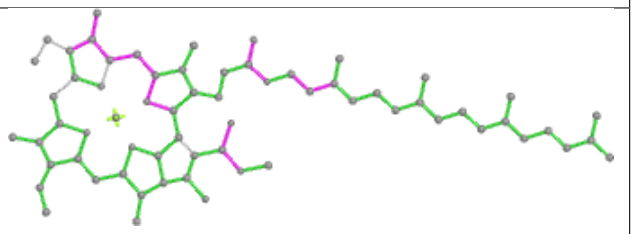
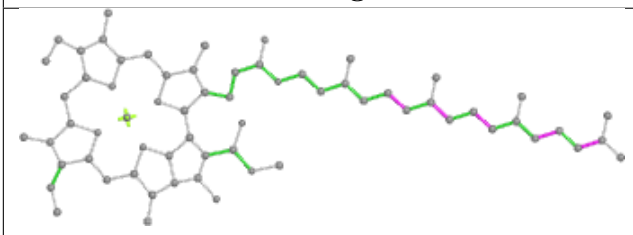
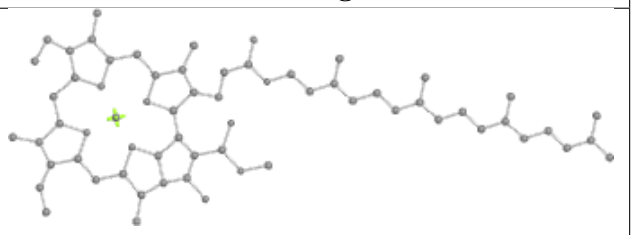


Bond angles

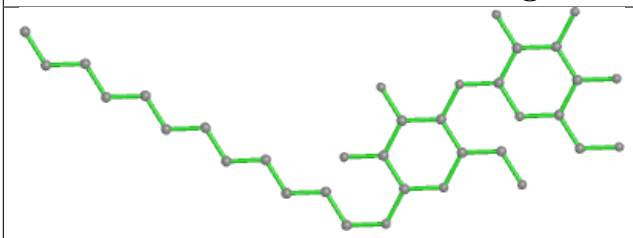


Torsions



Rings

Ligand LMT B 623



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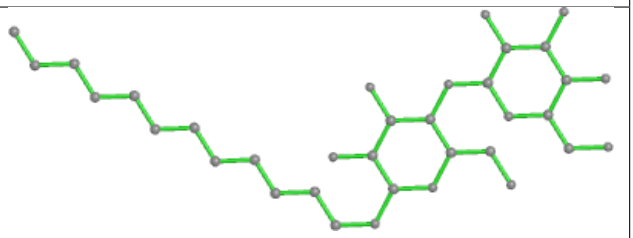
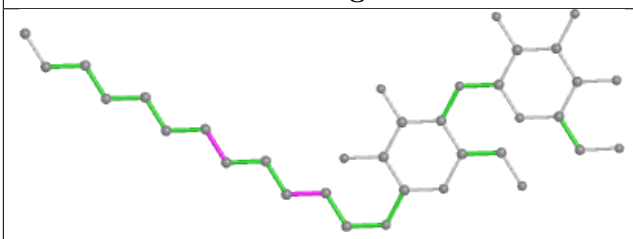
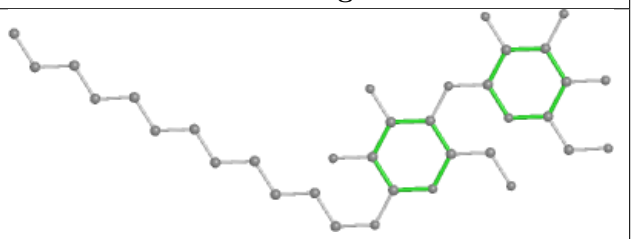


Bond angles

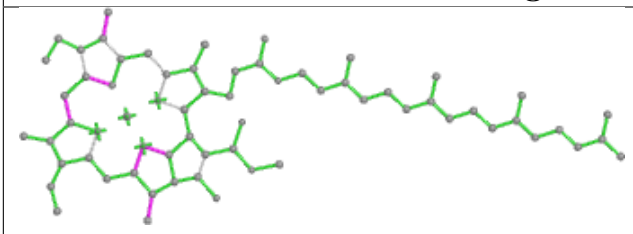


Torsions



Rings

Ligand CLA C 503



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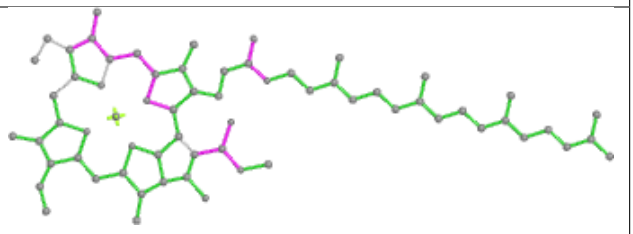
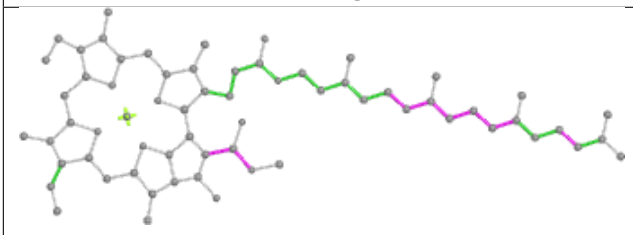
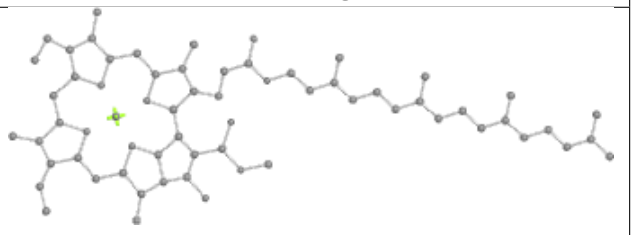


Bond angles

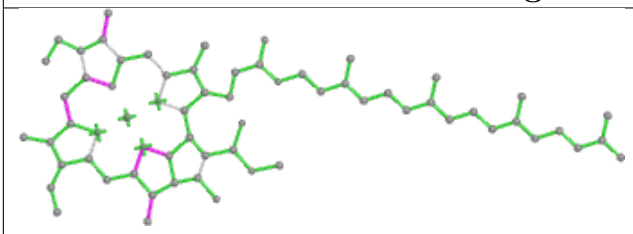


Torsions



Rings

Ligand CLA B 612



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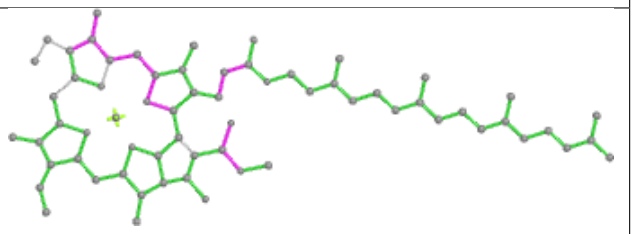
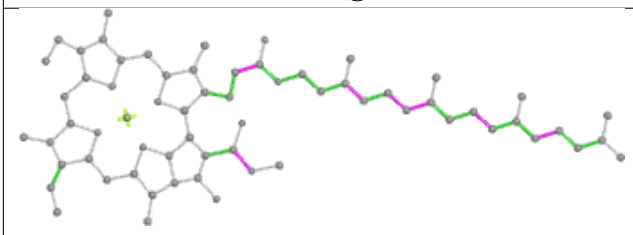
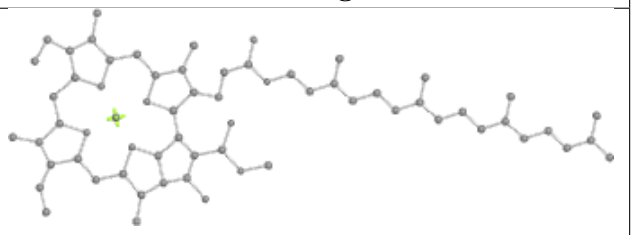


Bond angles

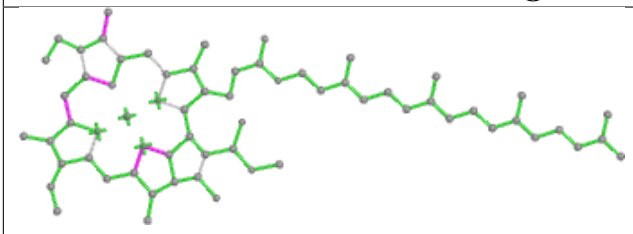


Torsions

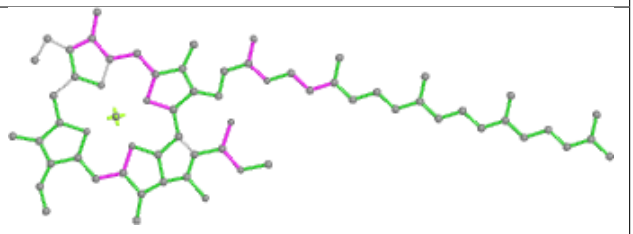


Rings

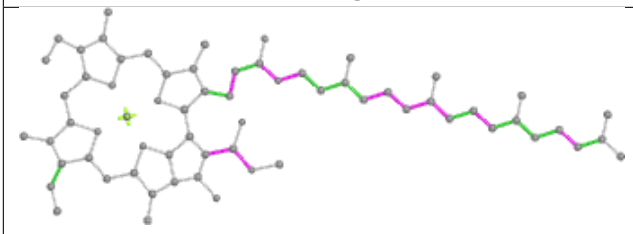
Ligand CLA C 509



Bond lengths



Bond angles



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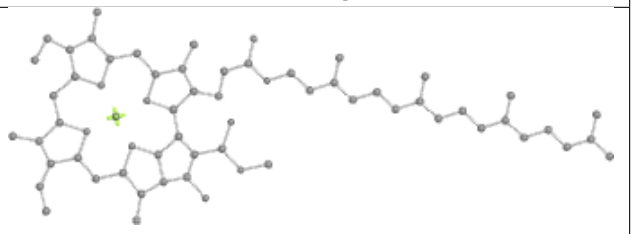
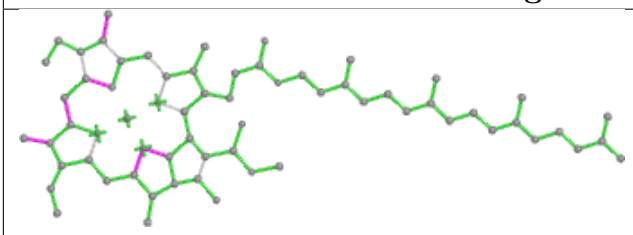
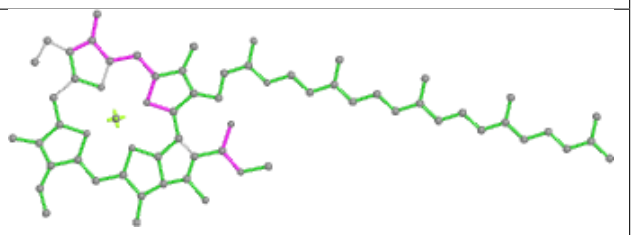


Rings

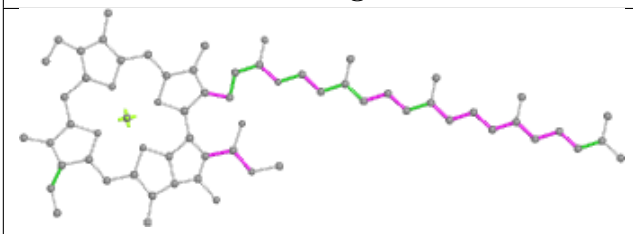
Ligand CLA B 616



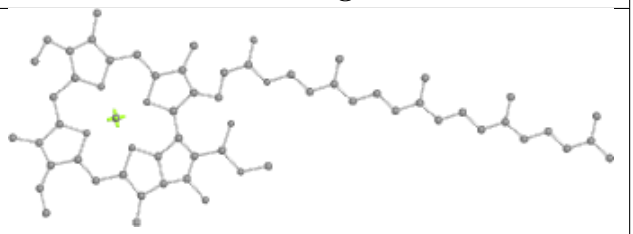
Bond lengths



Bond angles

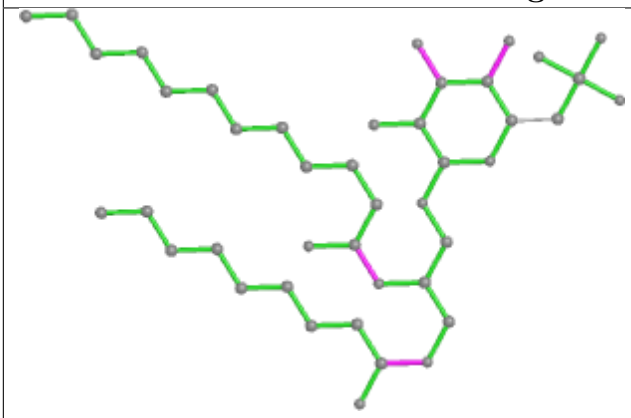


Torsions

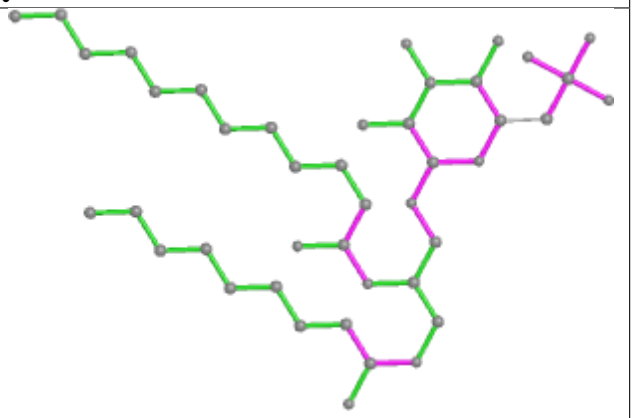


Rings

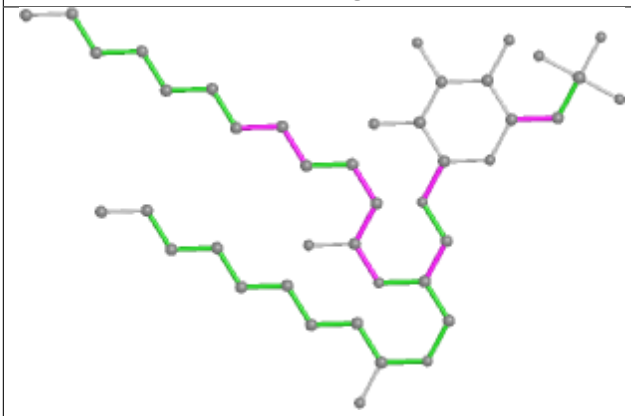
Ligand SQD d 407



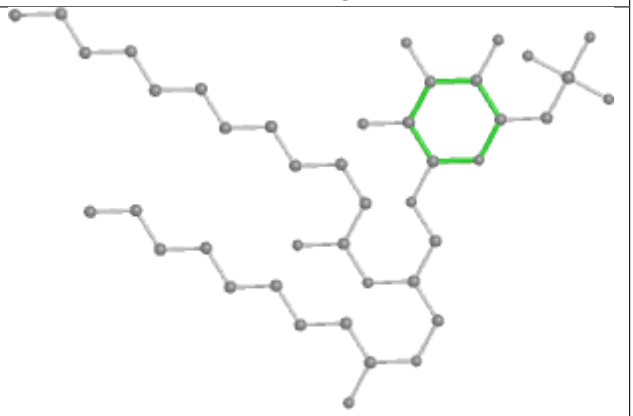
Bond lengths



Bond angles



Torsions

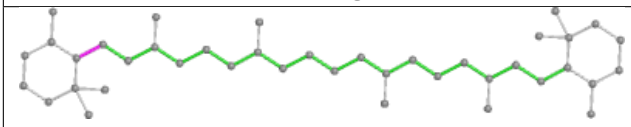


Rings

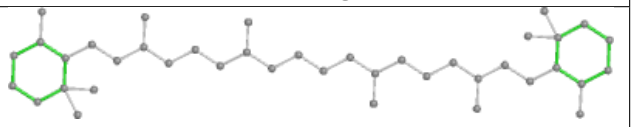
Ligand BCR T 102

Bond lengths

Bond angles

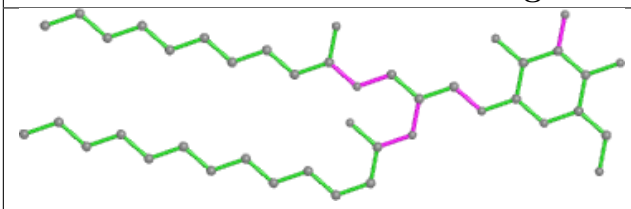


Torsions

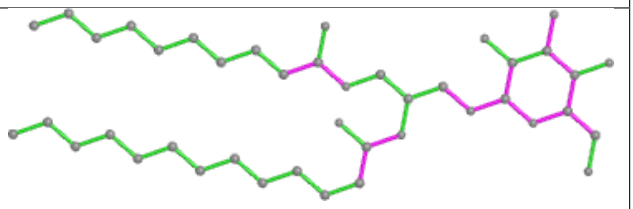


Rings

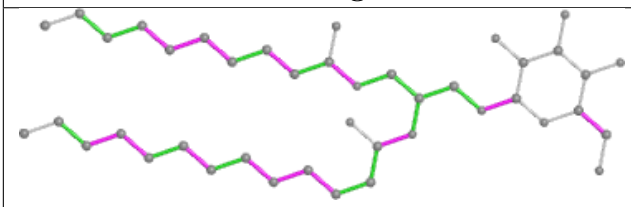
Ligand LMG a 402



Bond lengths



Bond angles



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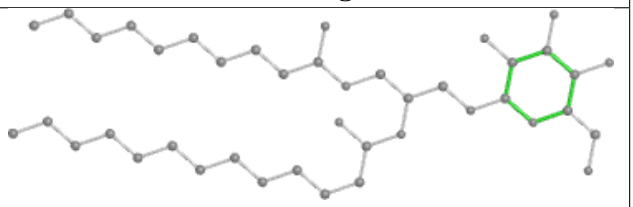
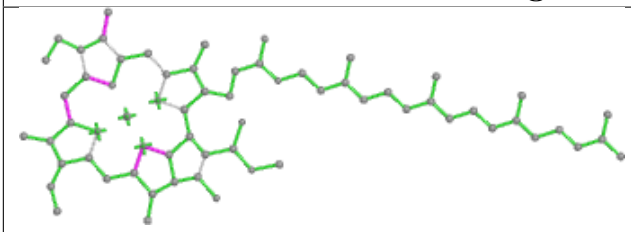
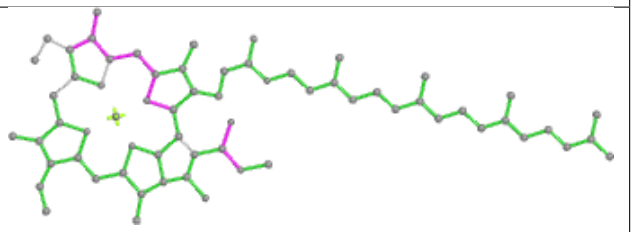


Rings

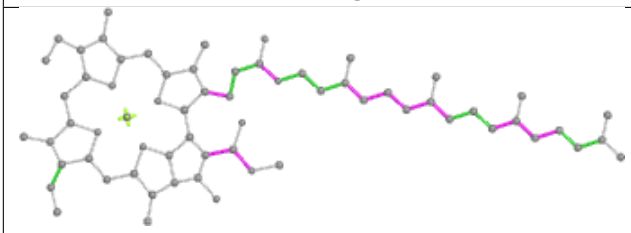
Ligand CLA b 605



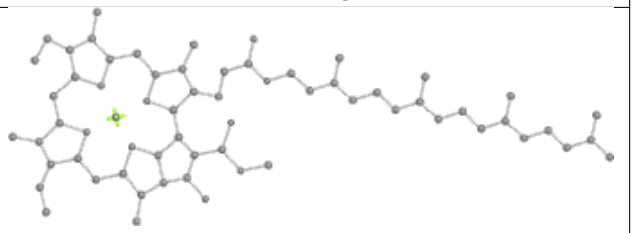
Bond lengths



Bond angles

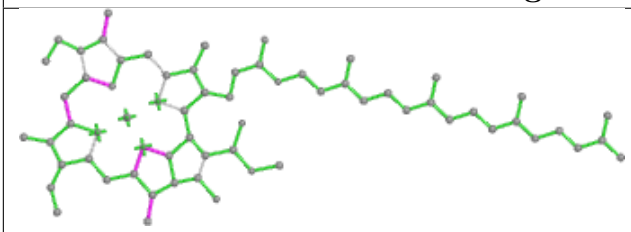


Torsions

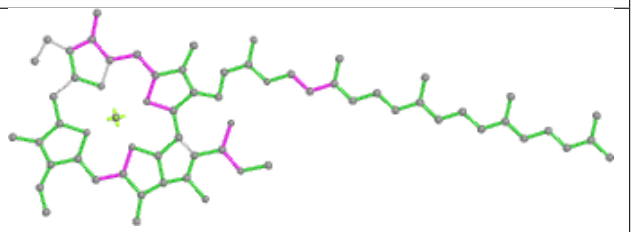


Rings

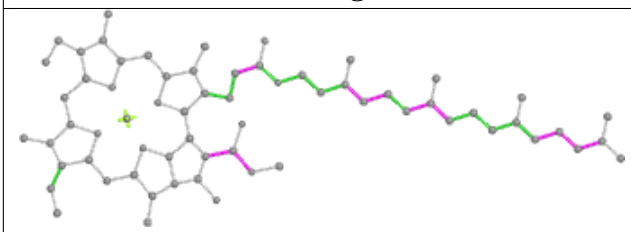
Ligand CLA C 510



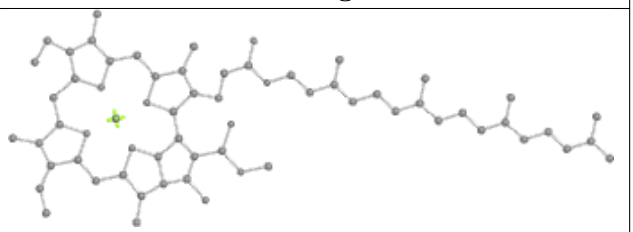
Bond lengths



Bond angles

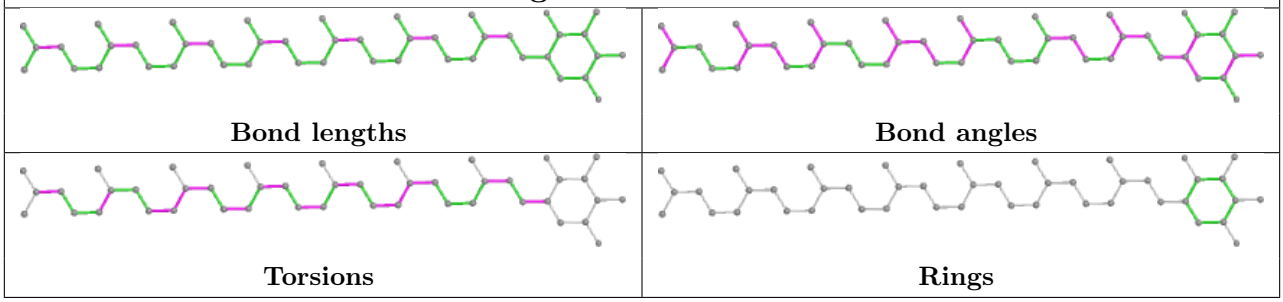


Torsions

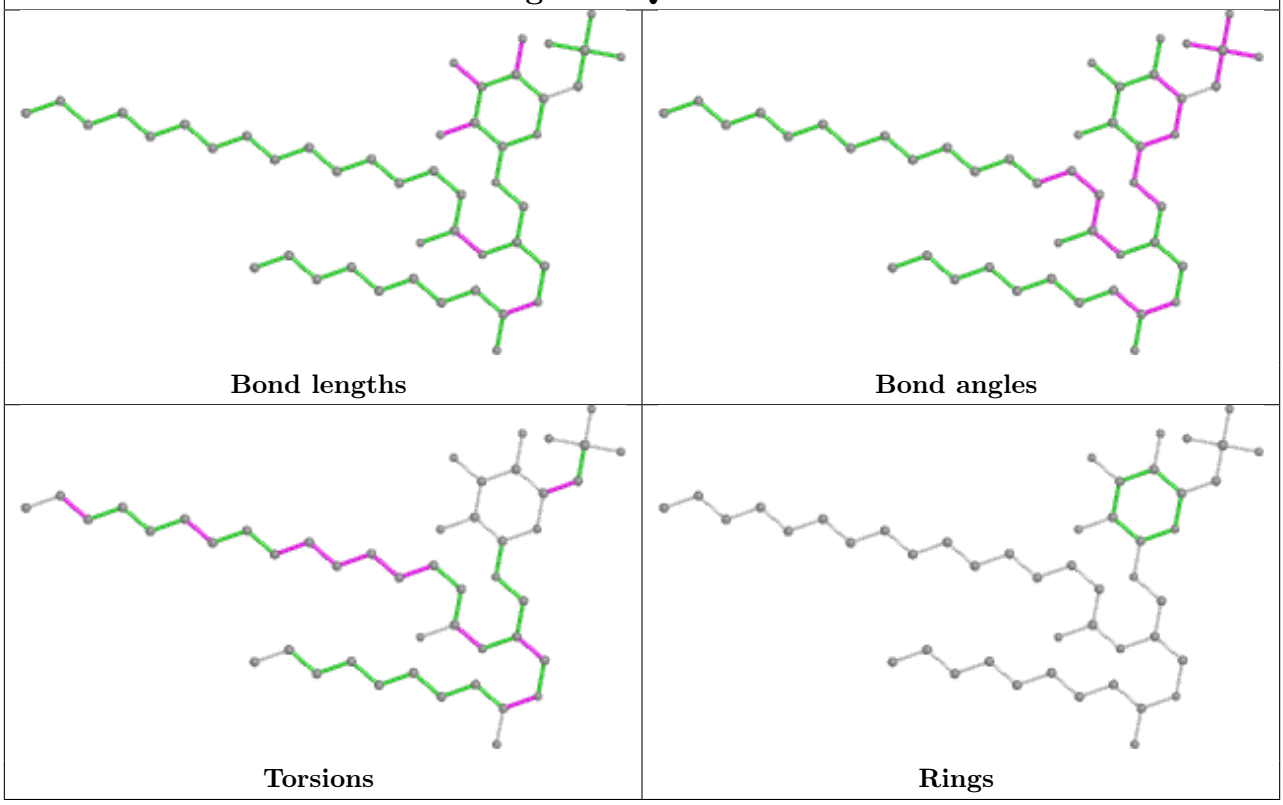


Rings

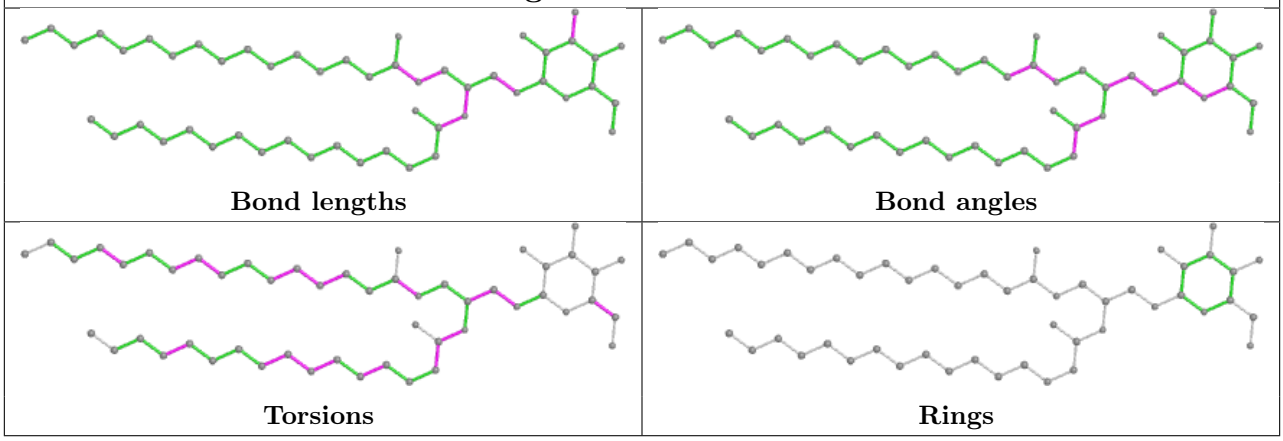
Ligand PL9 A 408



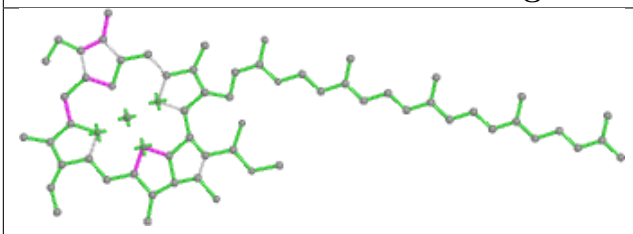
Ligand SQD B 625



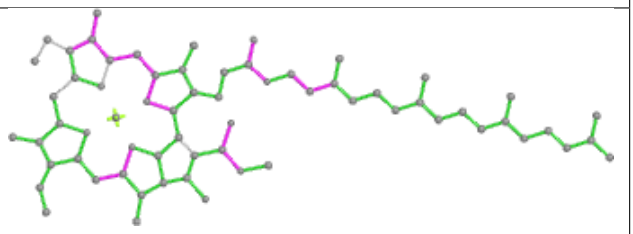
Ligand LMG a 416



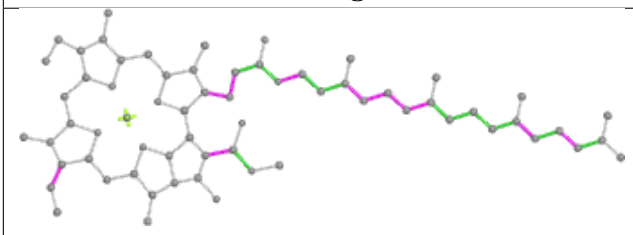
Ligand CLA A 404



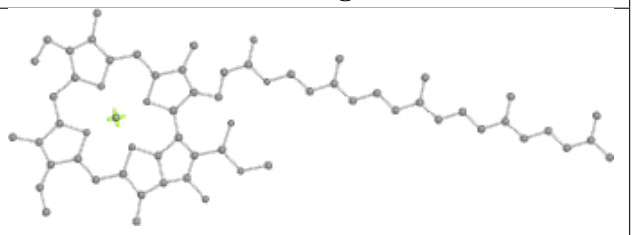
Bond lengths



Bond angles

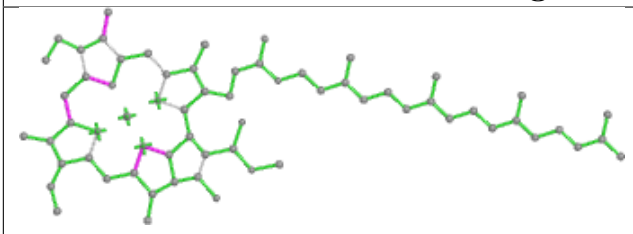


Torsions

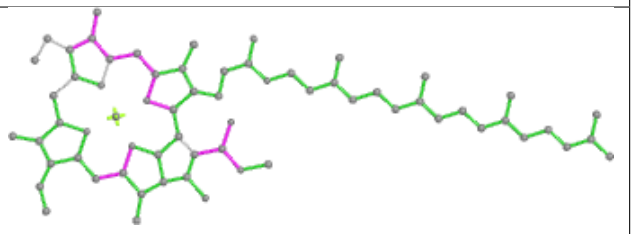


Rings

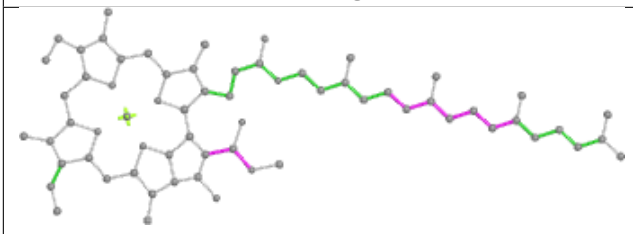
Ligand CLA c 503



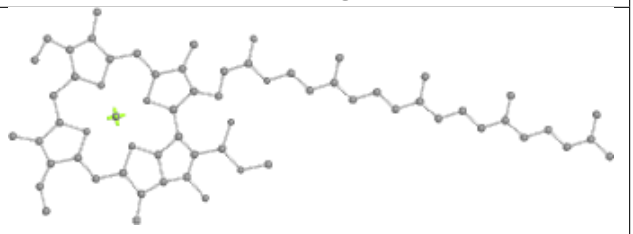
Bond lengths



Bond angles

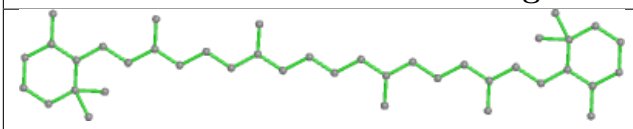


Torsions

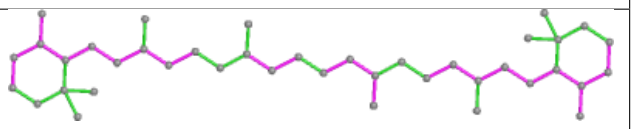


Rings

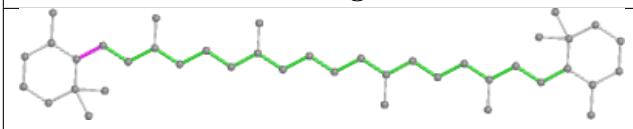
Ligand BCR B 617



Bond lengths



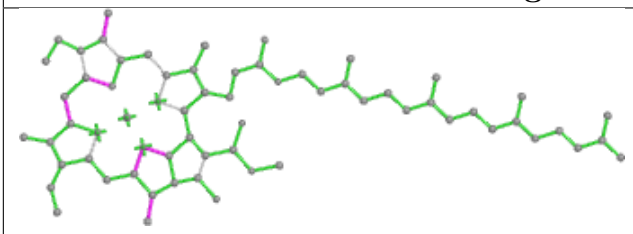
Bond angles



Torsions

Rings

Ligand CLA B 607



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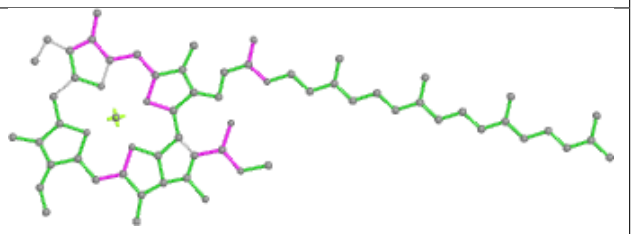
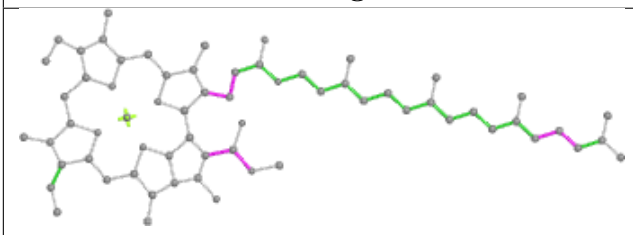
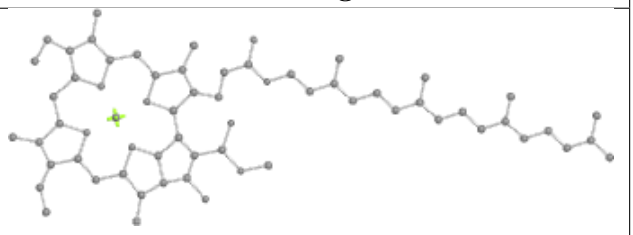


Bond angles

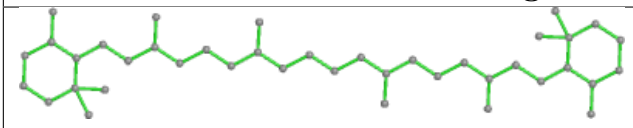


Torsions



Rings

Ligand BCR B 619



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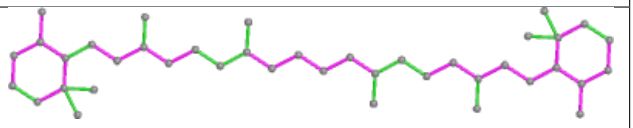
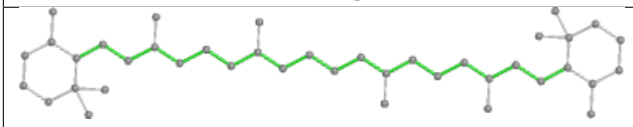


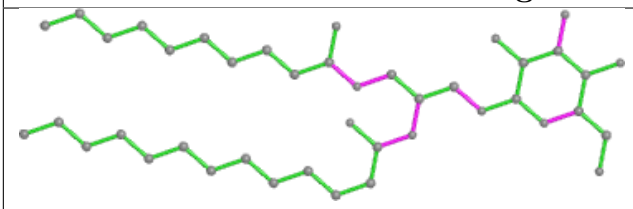
Bond angles



Torsions

Rings

Ligand LMG M 102



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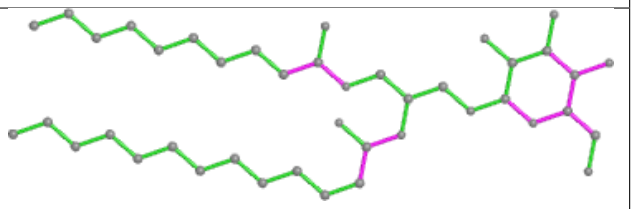
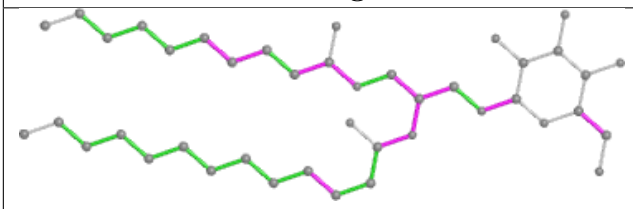
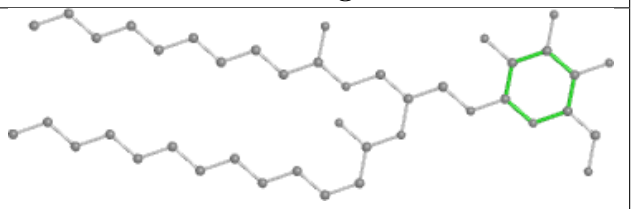


Bond angles

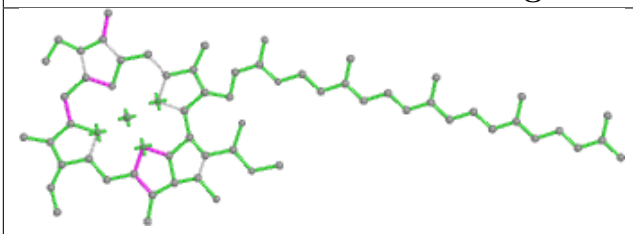


Torsions

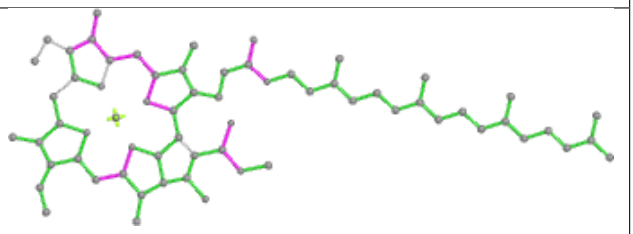


Rings

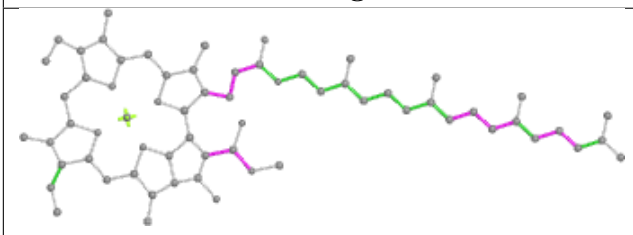
Ligand CLA C 501



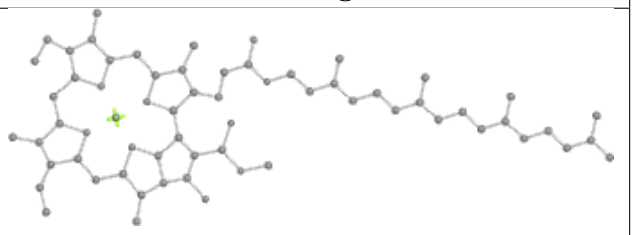
Bond lengths



Bond angles

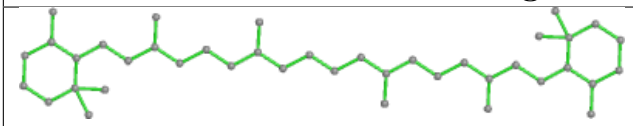


Torsions



Rings

Ligand BCR D 405



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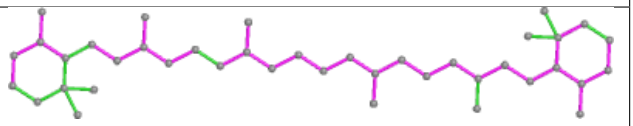
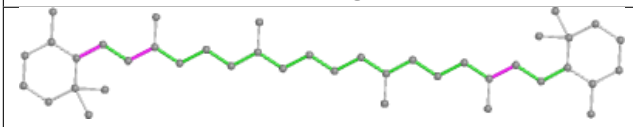


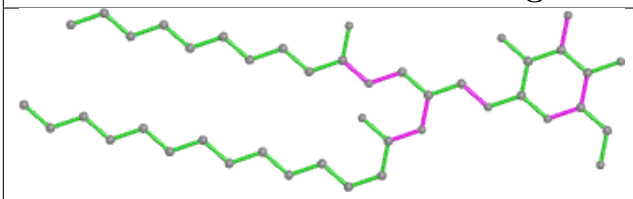
Bond angles



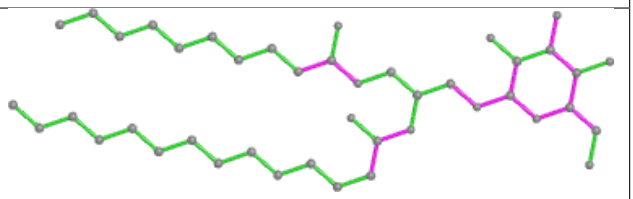
Torsions

Rings

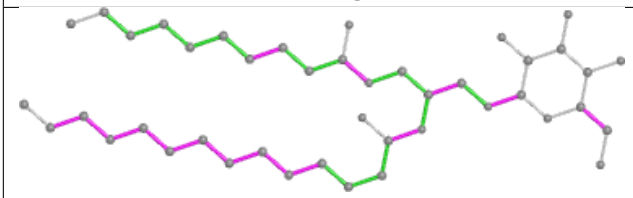
Ligand LMG I 101



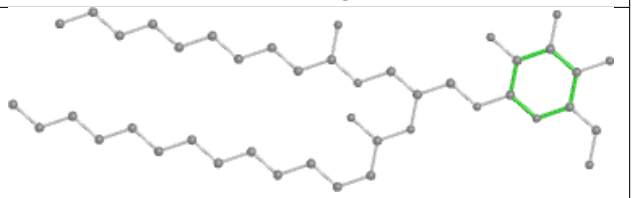
Bond lengths



Bond angles

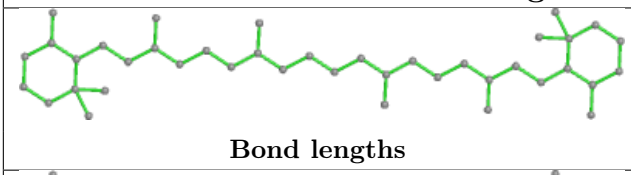


Torsions



Rings

Ligand BCR c 515



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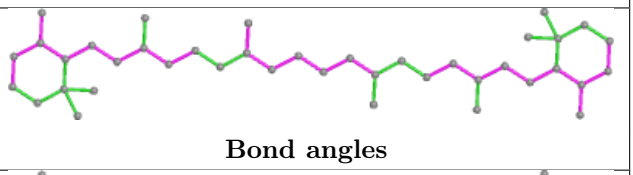
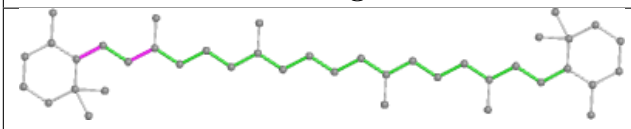
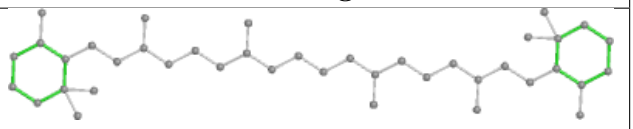


Bond angles

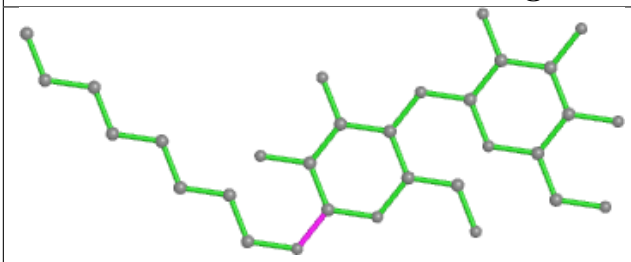


Torsions

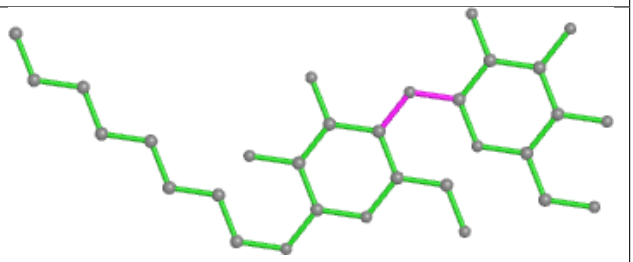


Rings

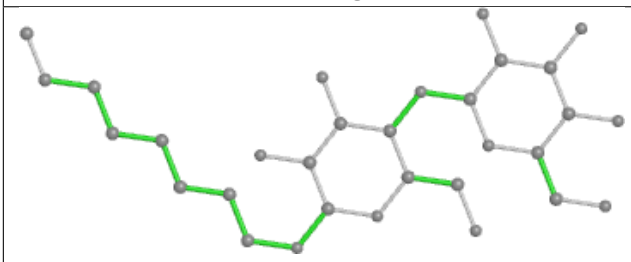
Ligand LMT x 102



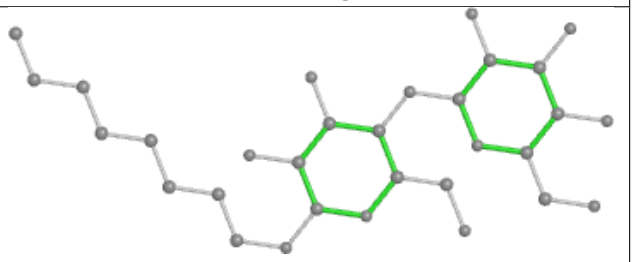
Bond lengths



Bond angles

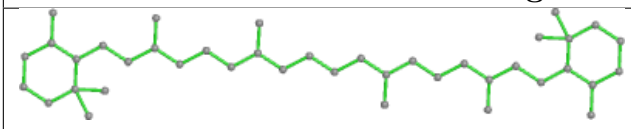


Torsions



Rings

Ligand BCR k 102



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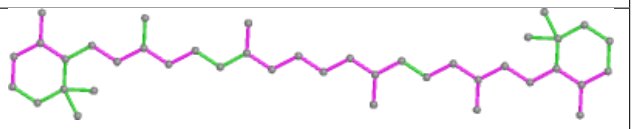
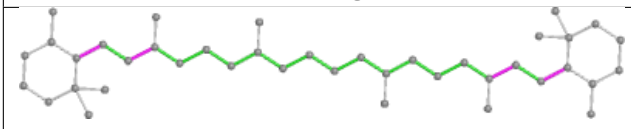


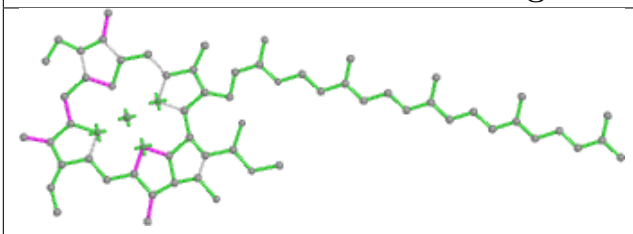
Bond angles



Torsions

Rings

Ligand CLA b 608



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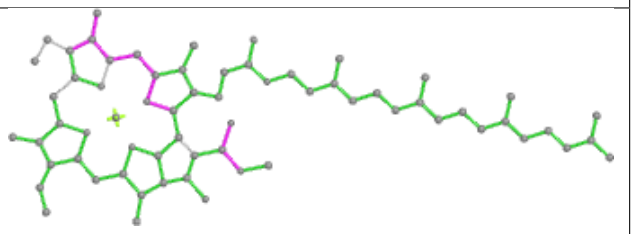
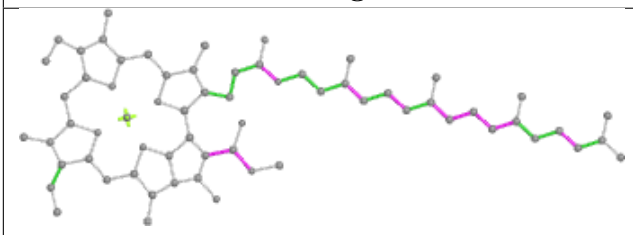


Bond angles



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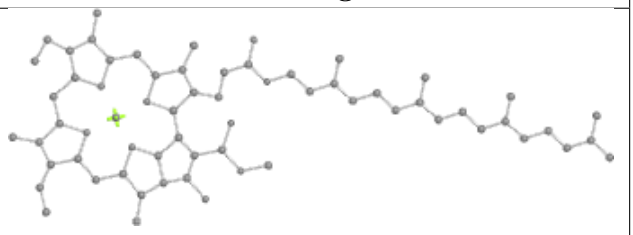
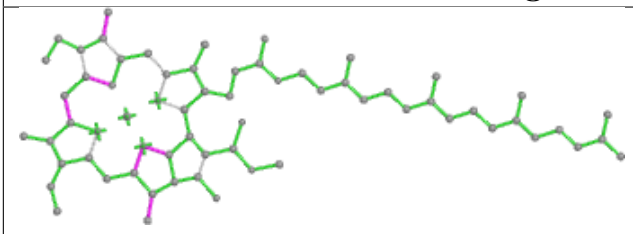


Rings

Ligand CLA C 505



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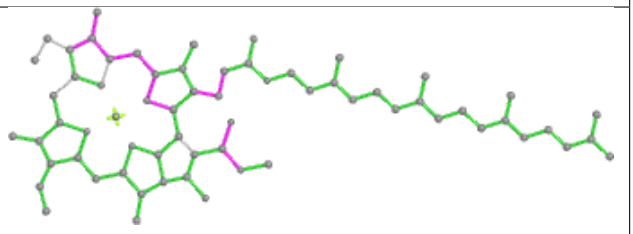
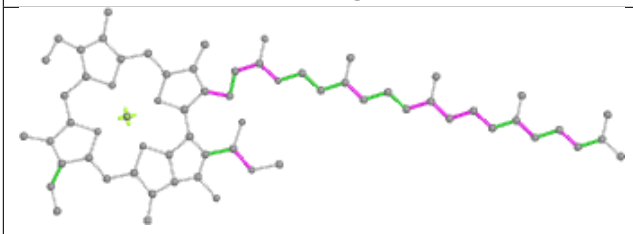


Bond angles



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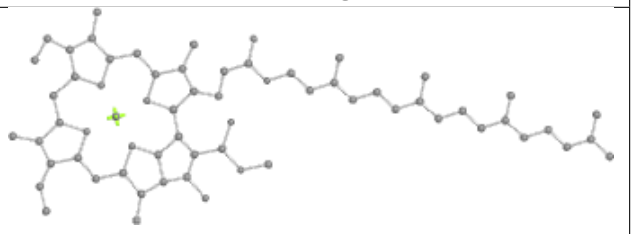
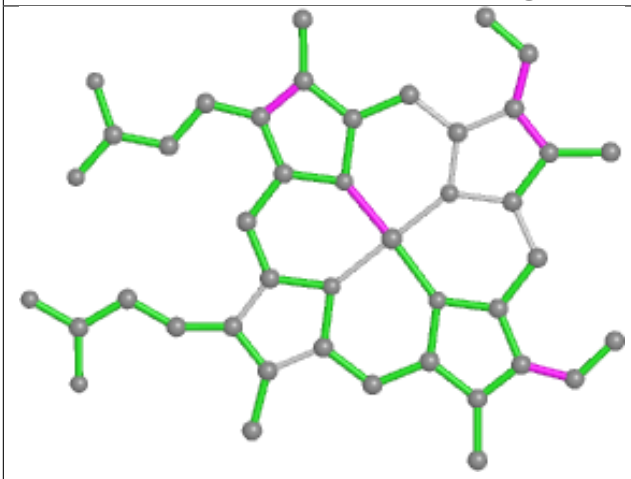


Rings

Ligand HEM F 101



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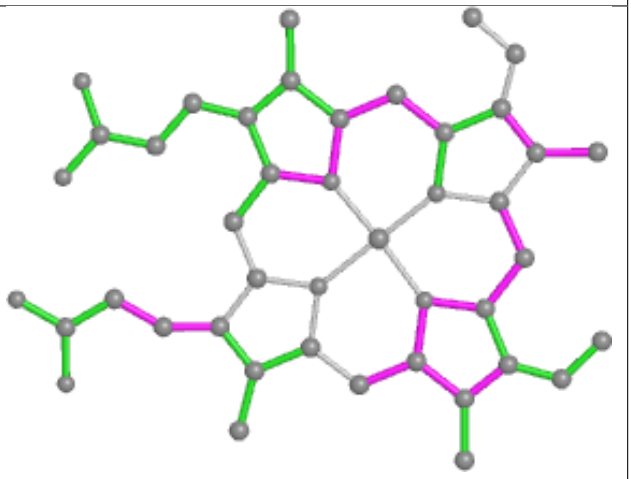
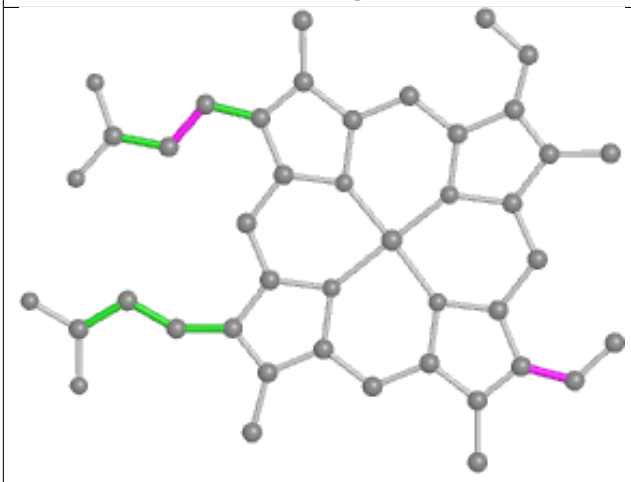


Bond angles



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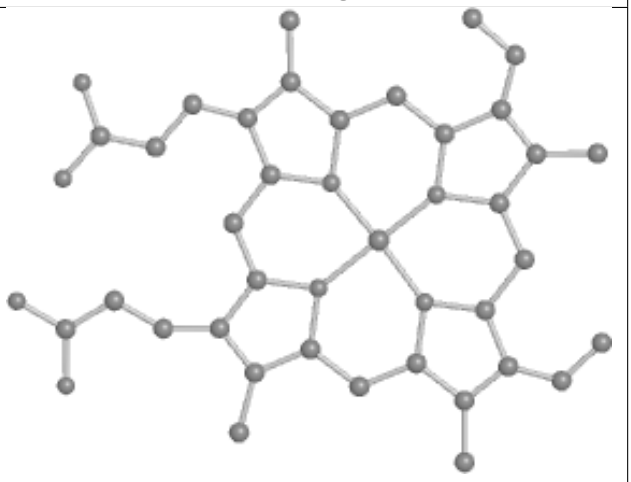
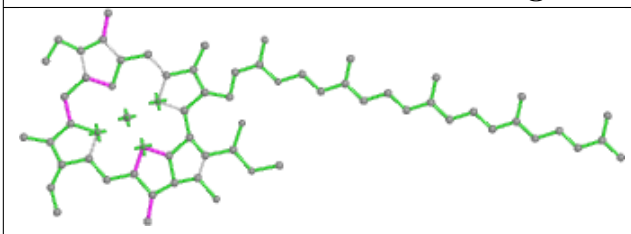


Rings

Ligand CLA b 617



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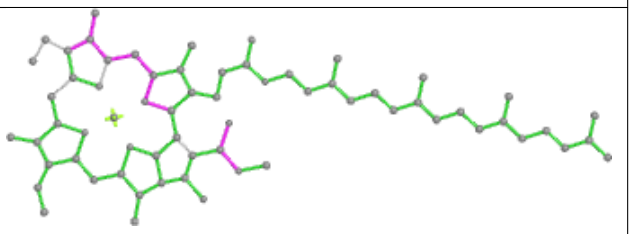
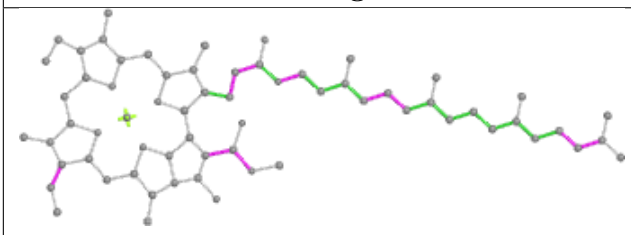


Bond angles



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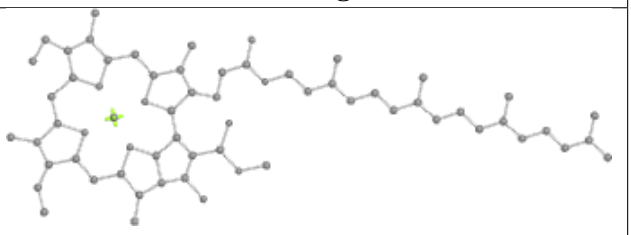
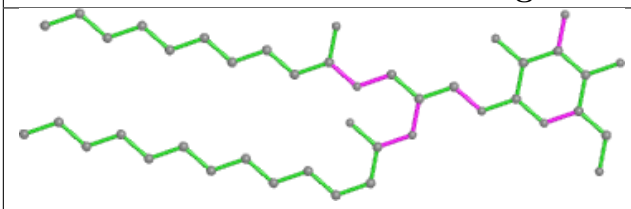


Rings

Ligand LMG M 101



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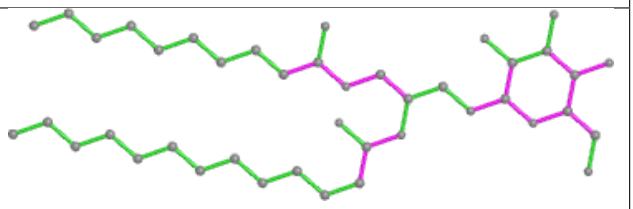
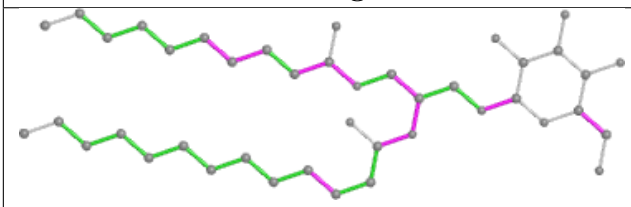


Bond angles



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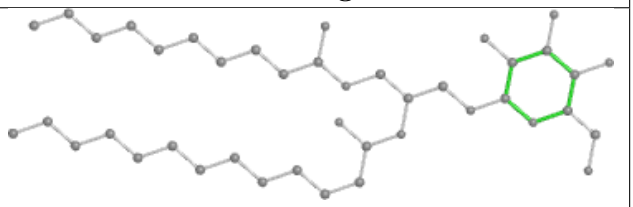
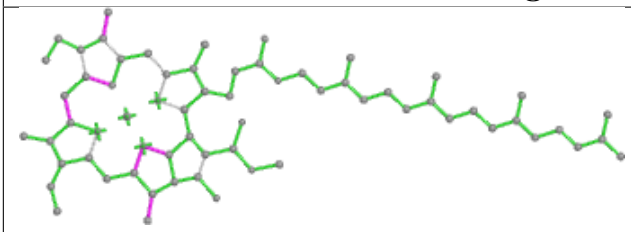


Rings

Ligand CLA C 508



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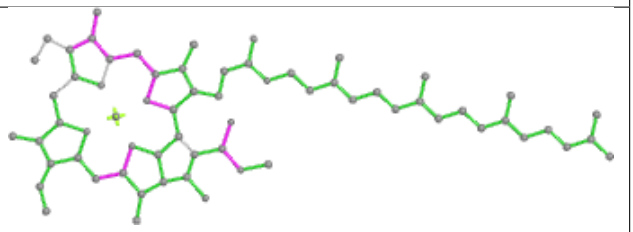
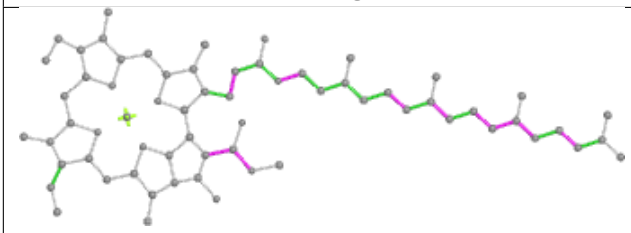
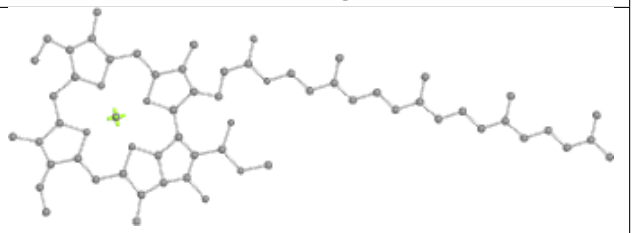


Bond angles

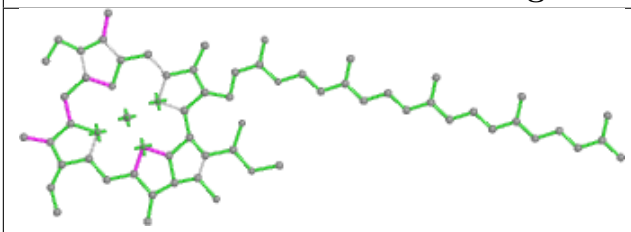


Torsions



Rings

Ligand CLA b 619



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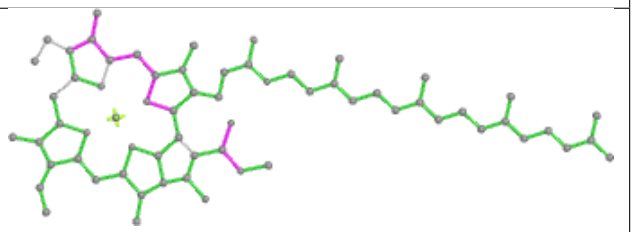
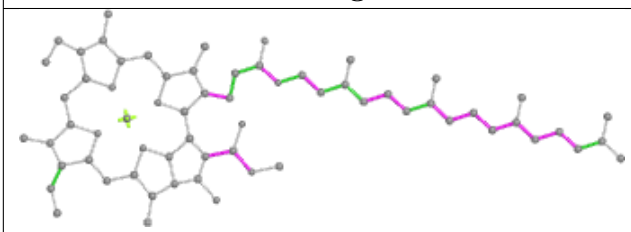


Bond angles



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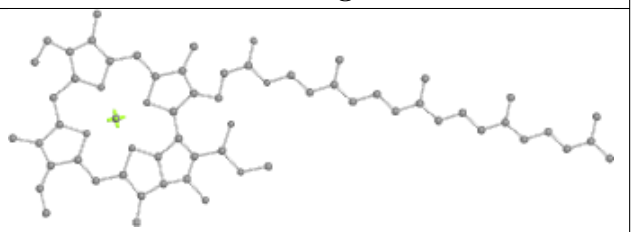
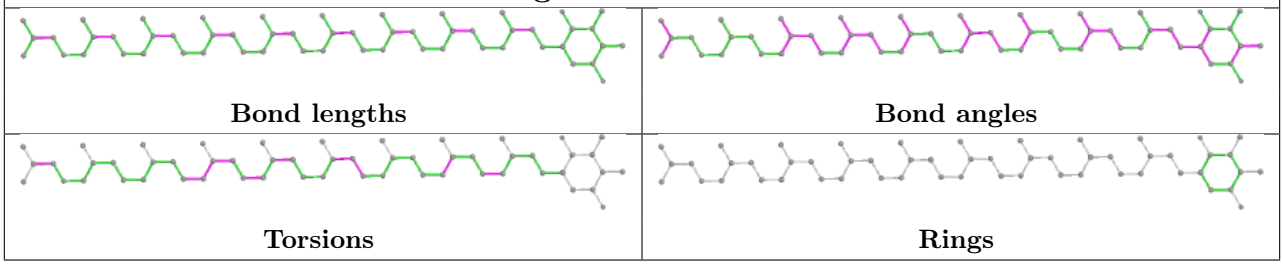
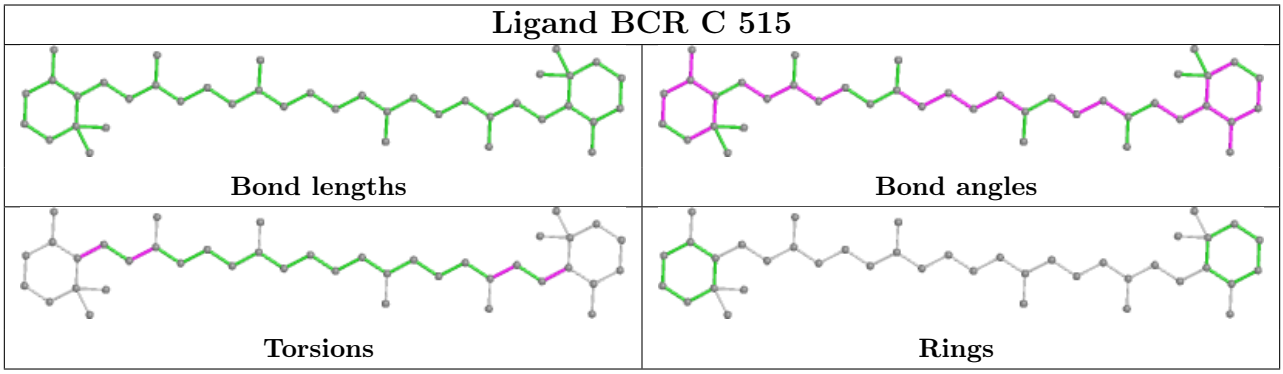


Rings

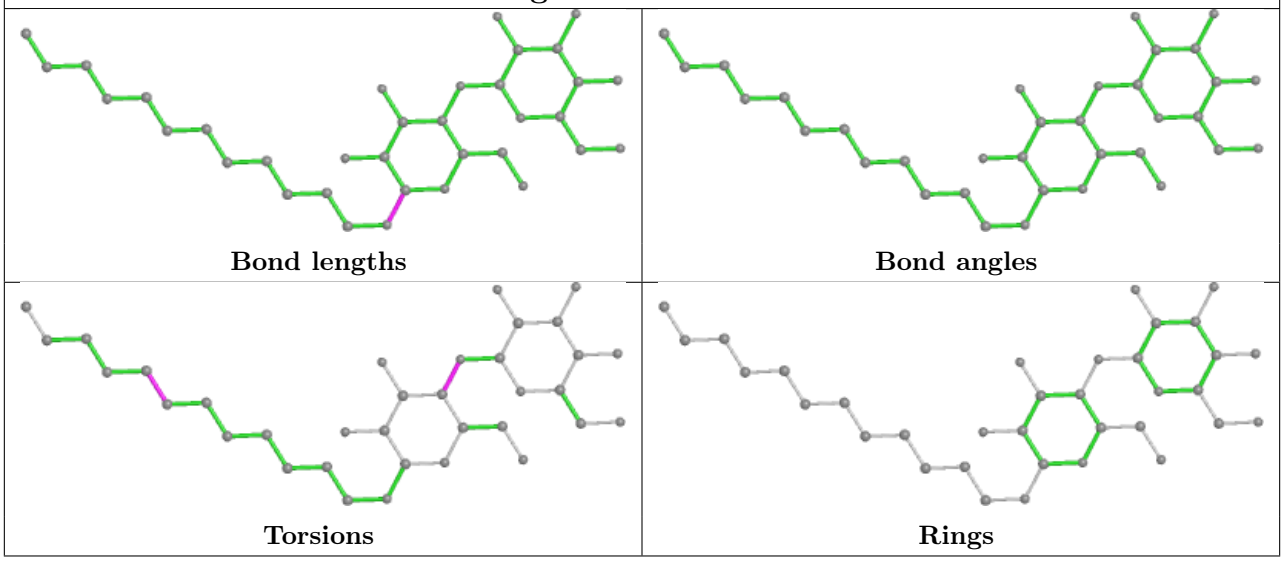
Ligand PL9 d 404



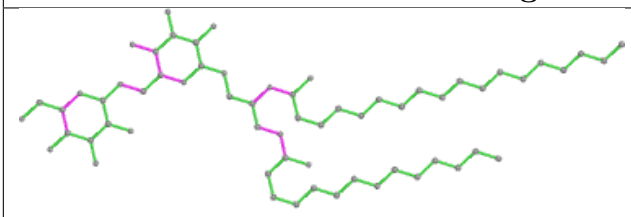
Ligand BCR C 515



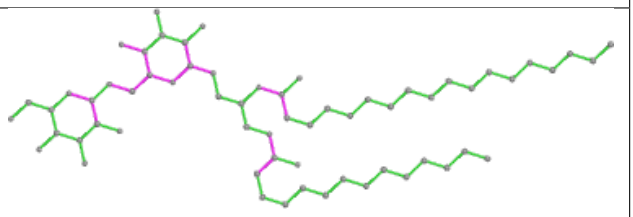
Ligand LMT i 102



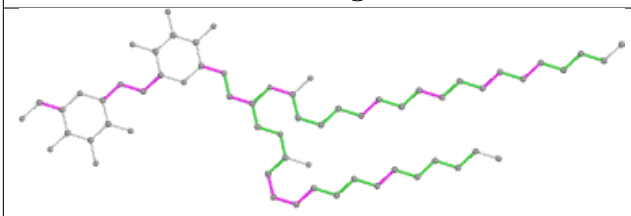
Ligand DGD C 517



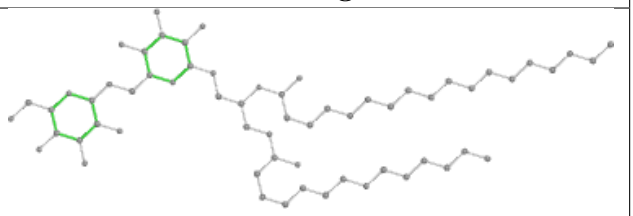
Bond lengths



Bond angles

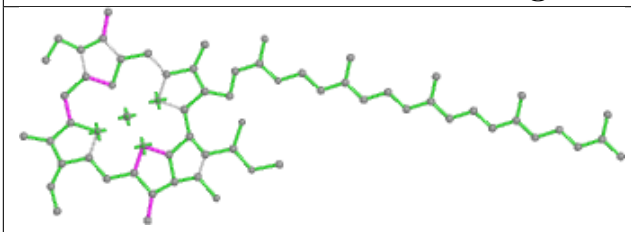


Torsions



Rings

Ligand CLA c 505



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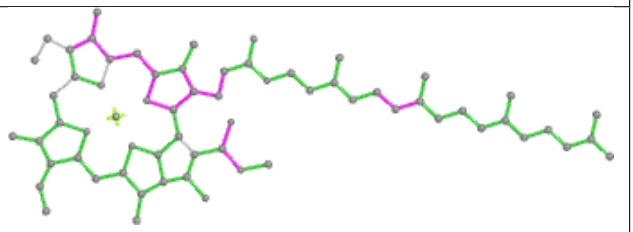
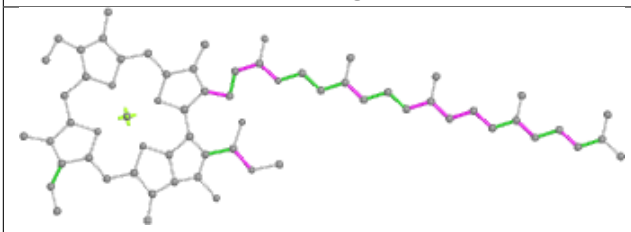


Bond angles



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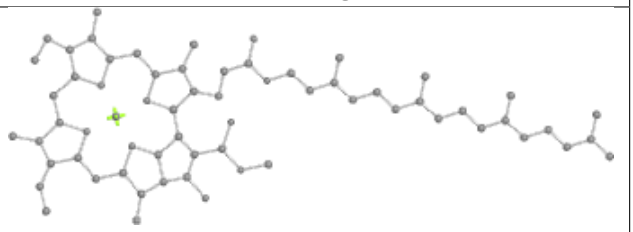
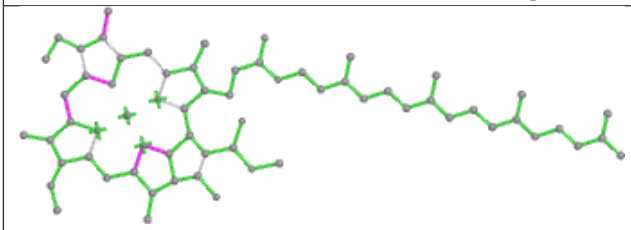
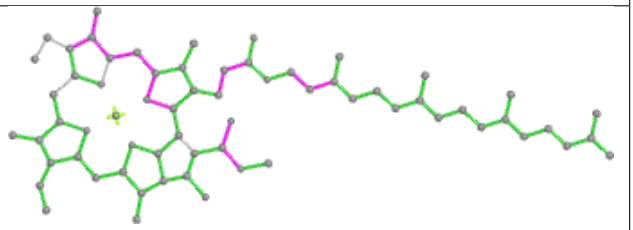


Rings

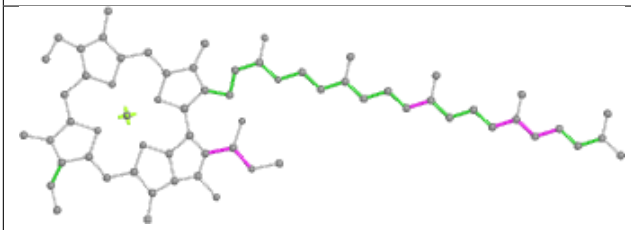
Ligand CLA B 609



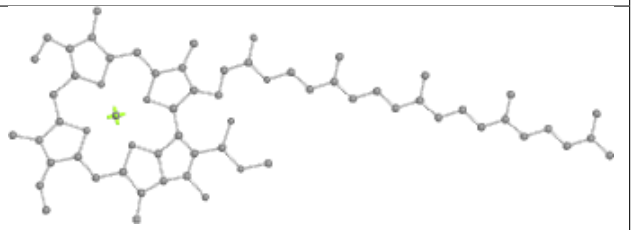
Bond lengths



Bond angles

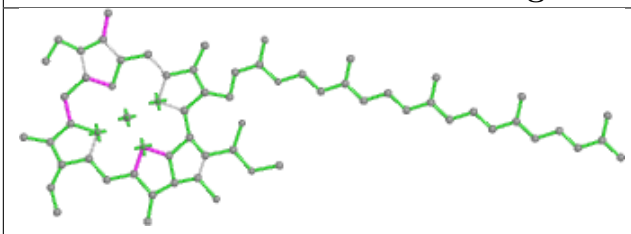


Torsions

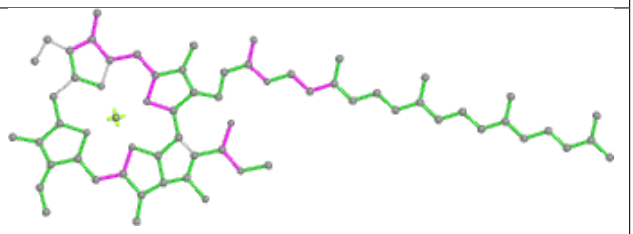


Rings

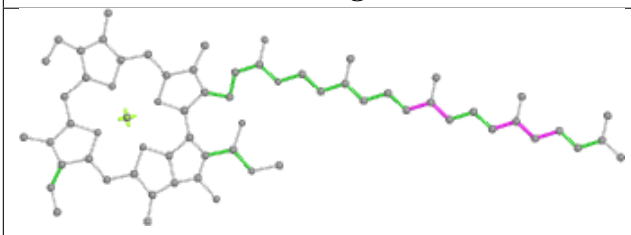
Ligand CLA b 618



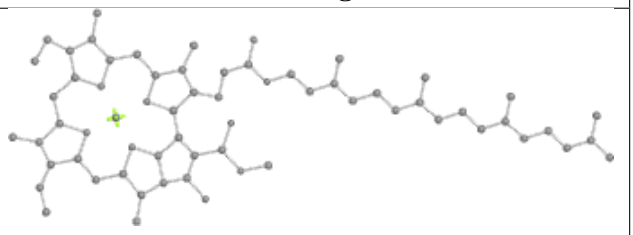
Bond lengths



Bond angles

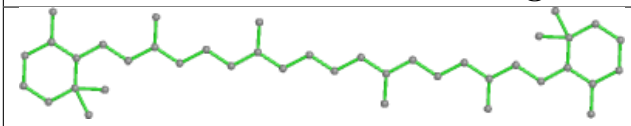


Torsions



Rings

Ligand BCR J 102



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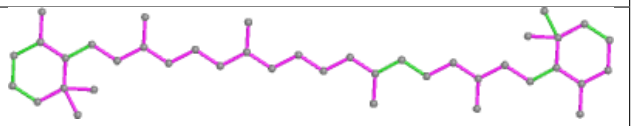
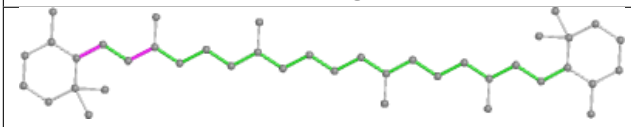


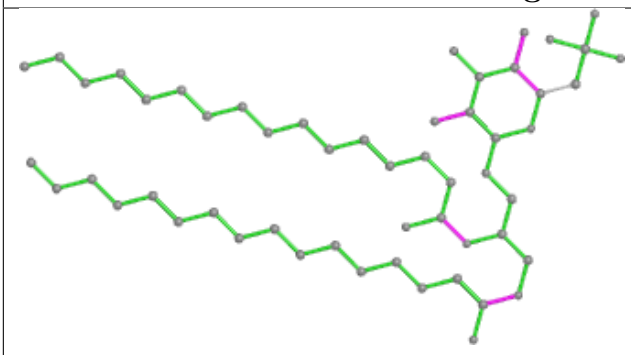
Bond angles



Torsions

Rings

Ligand SQD A 417



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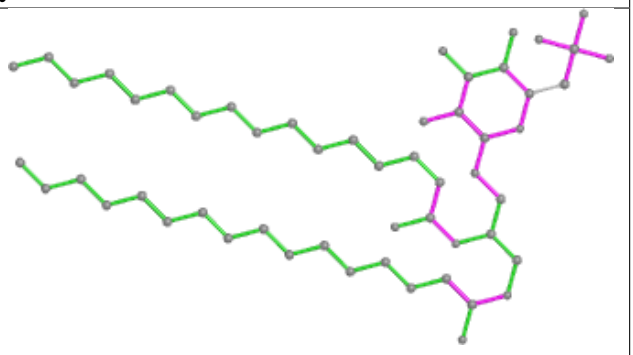
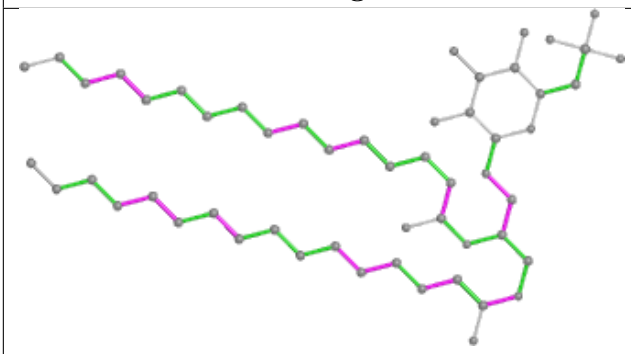
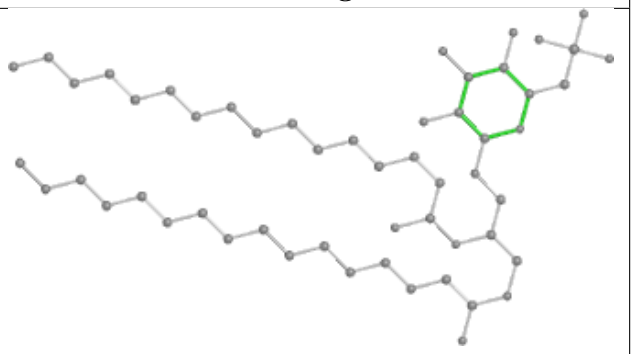


Bond angles

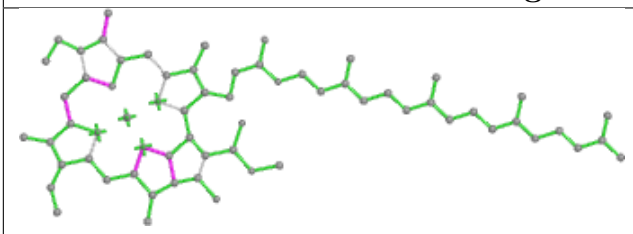


Torsions



Rings

Ligand CLA C 512



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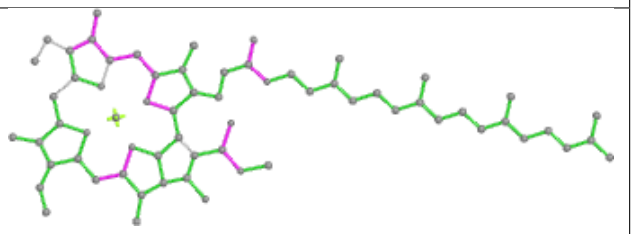
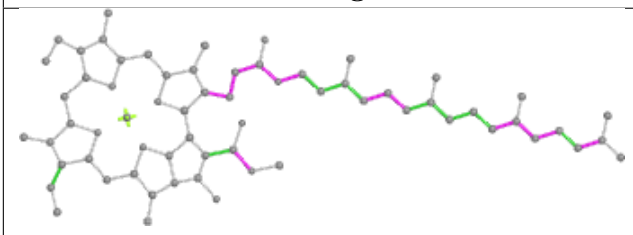
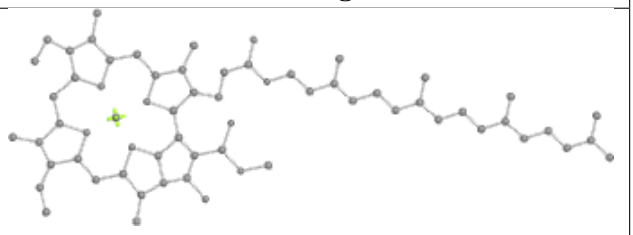


Bond angles

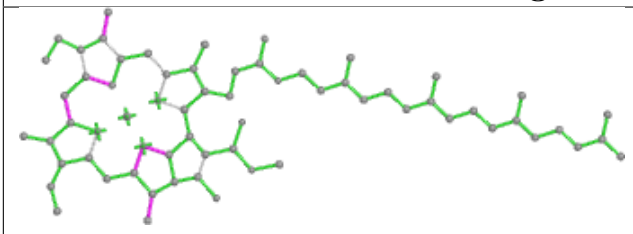


Torsions

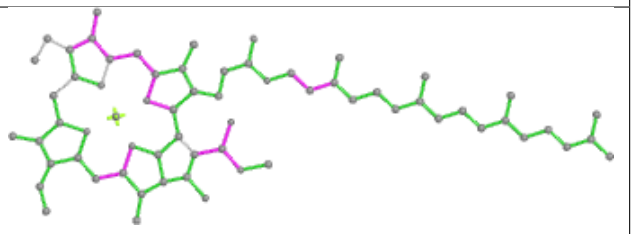


Rings

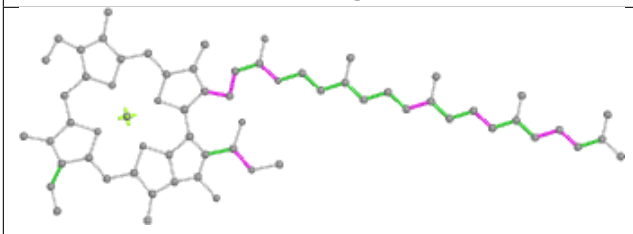
Ligand CLA c 504



Bond lengths



Bond angles



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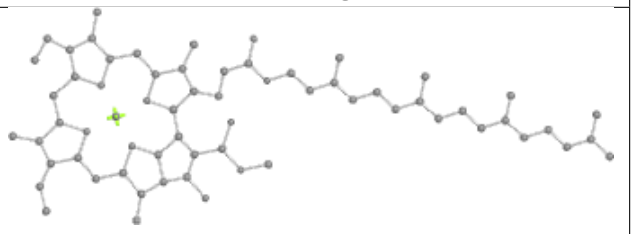
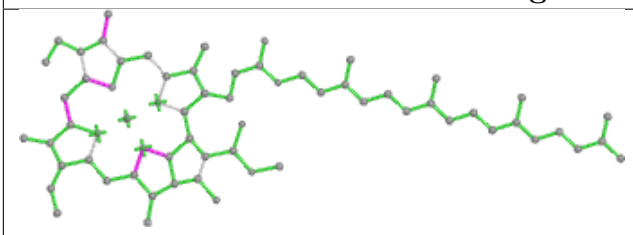


Rings

Ligand CLA c 507



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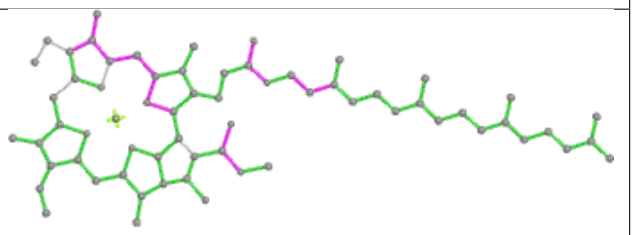
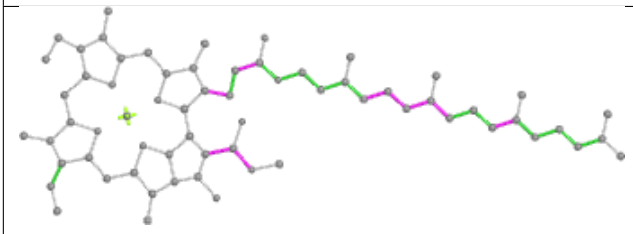


Bond angles



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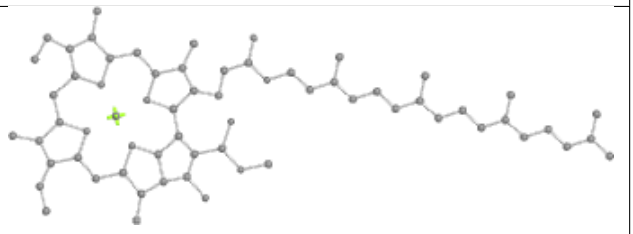
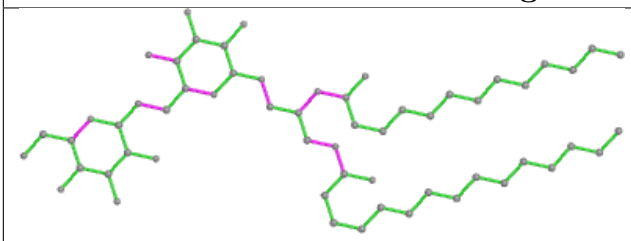


Rings

Ligand DGD B 621



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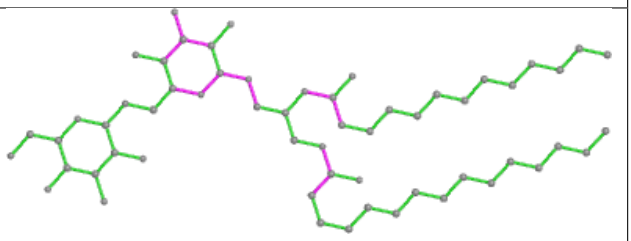
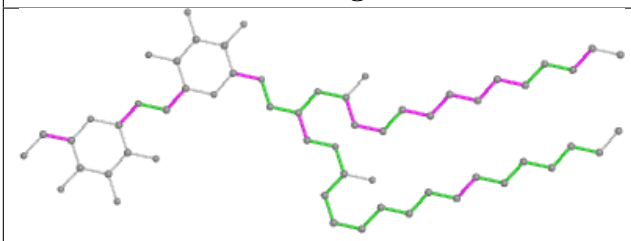


Bond angles



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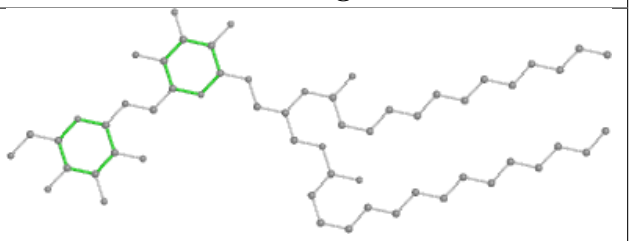
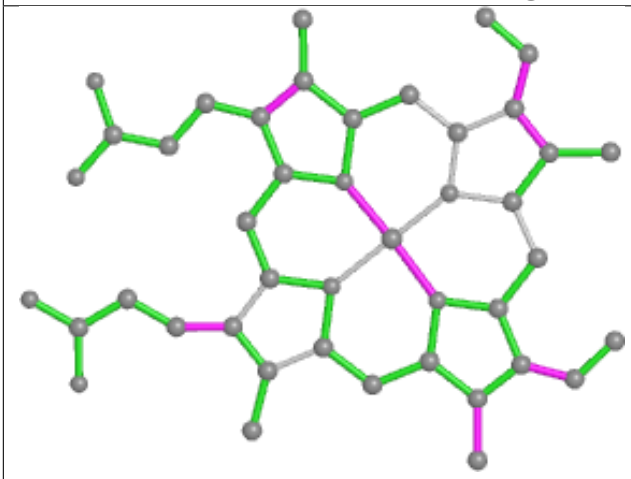


Rings

Ligand HEM v 201



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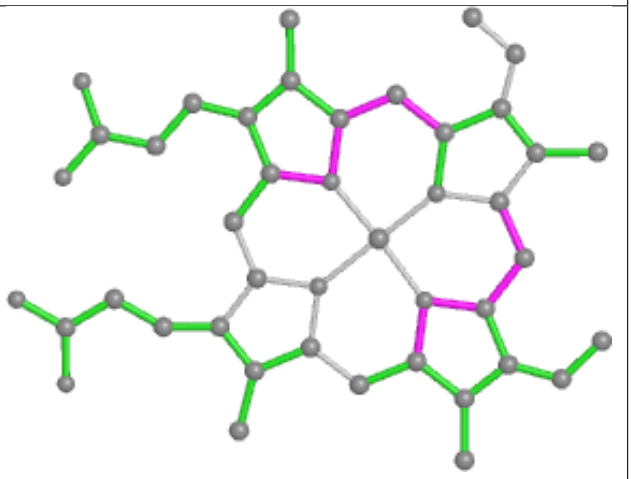
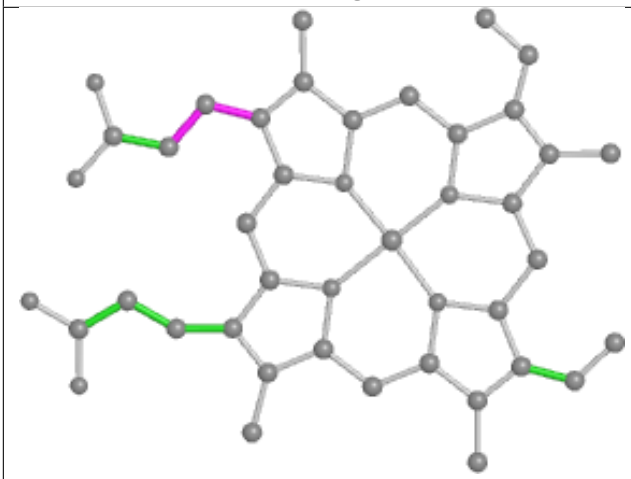


Bond angles



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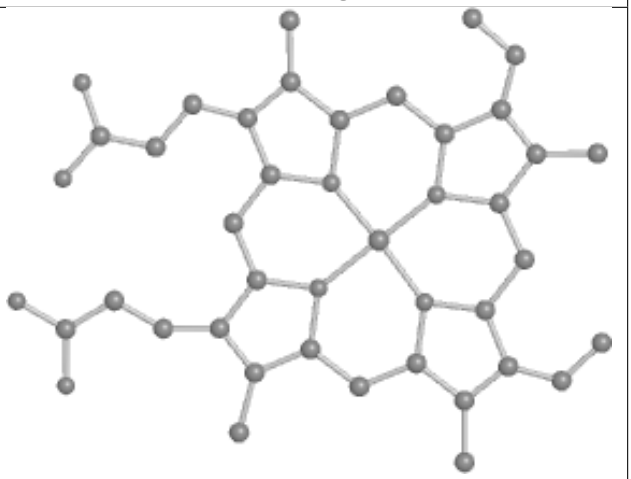
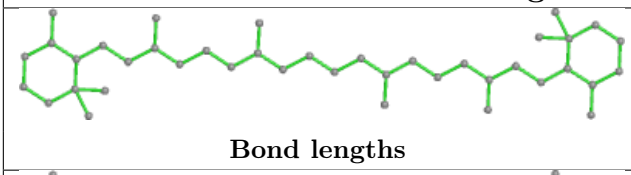


Rings

Ligand BCR c 514



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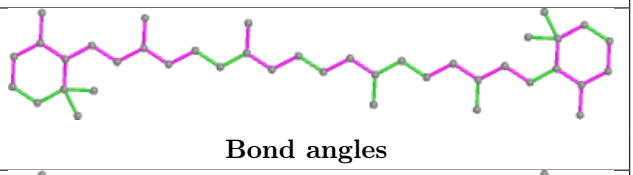
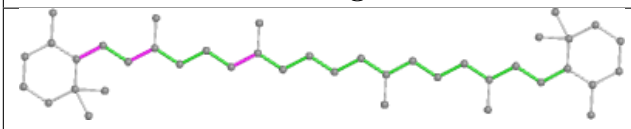


Bond angles



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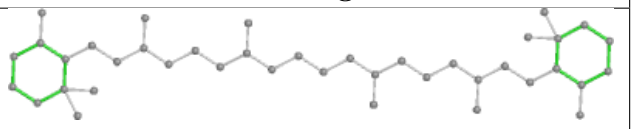
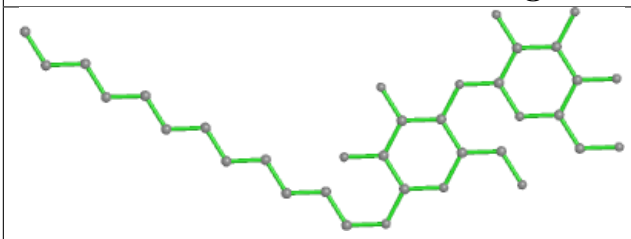


Rings

Ligand LMT b 625



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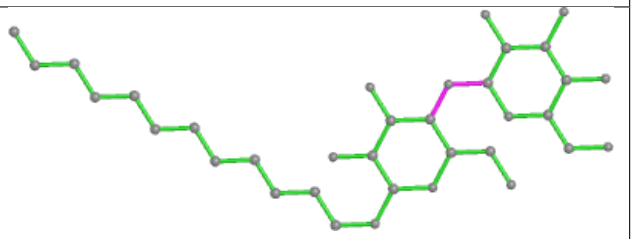
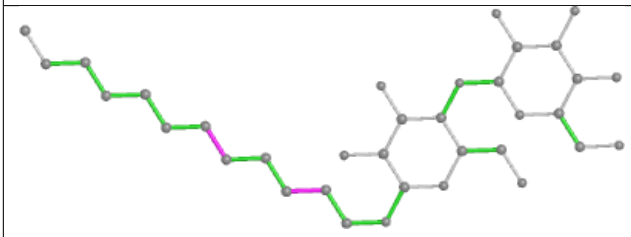


Bond angles



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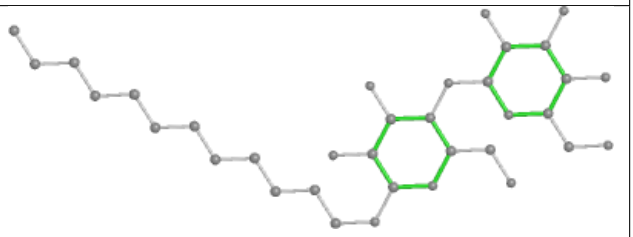
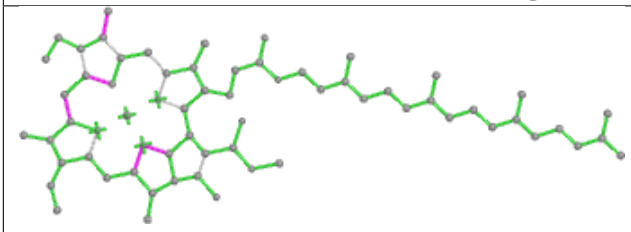


Rings

Ligand CLA B 613



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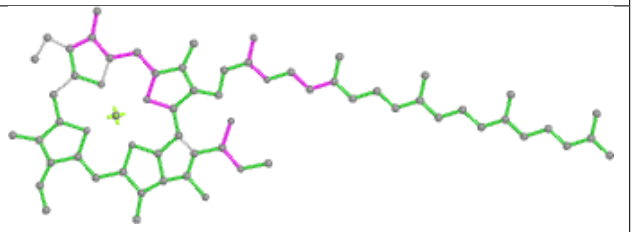
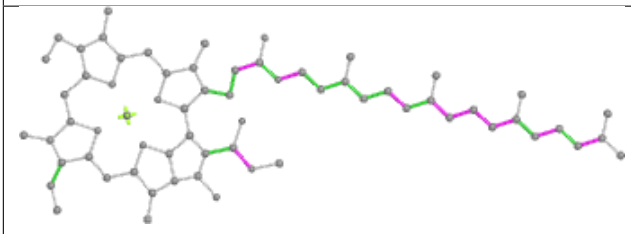
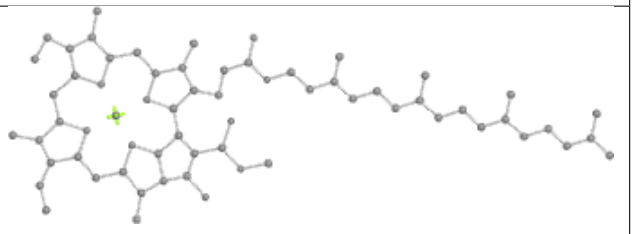


Bond angles

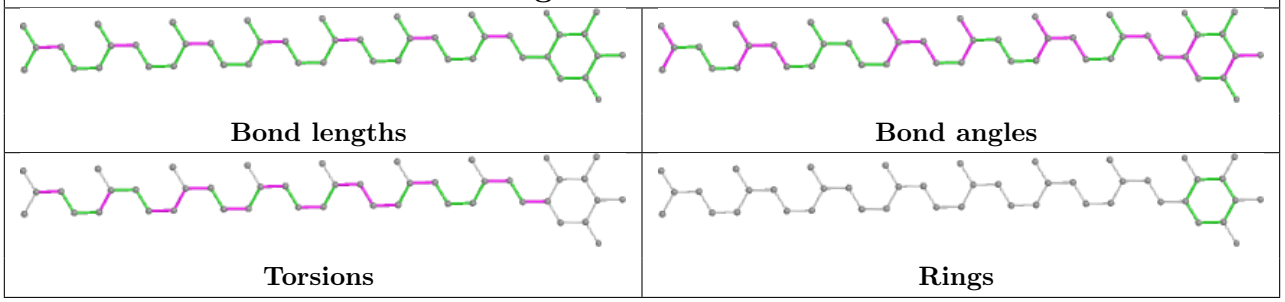


Torsions

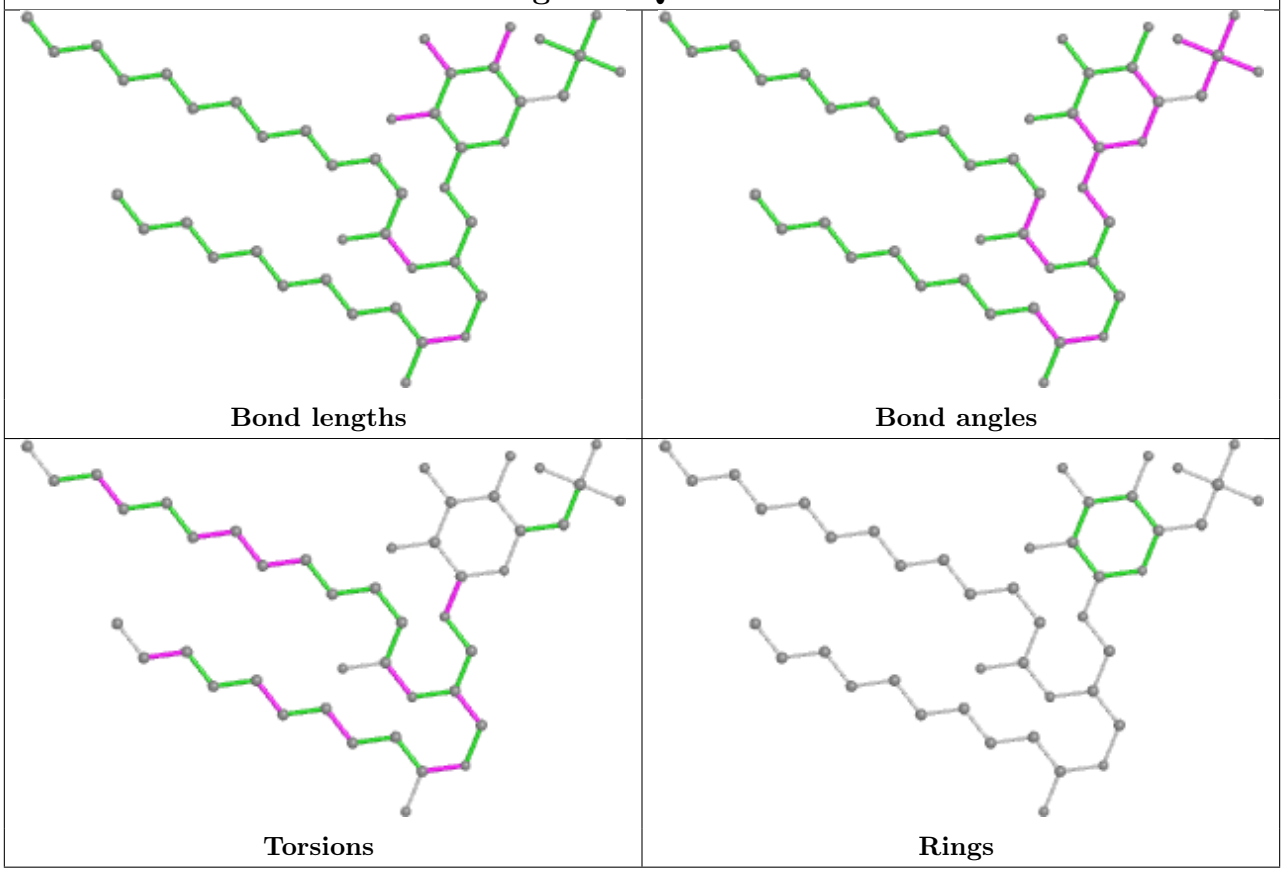


Rings

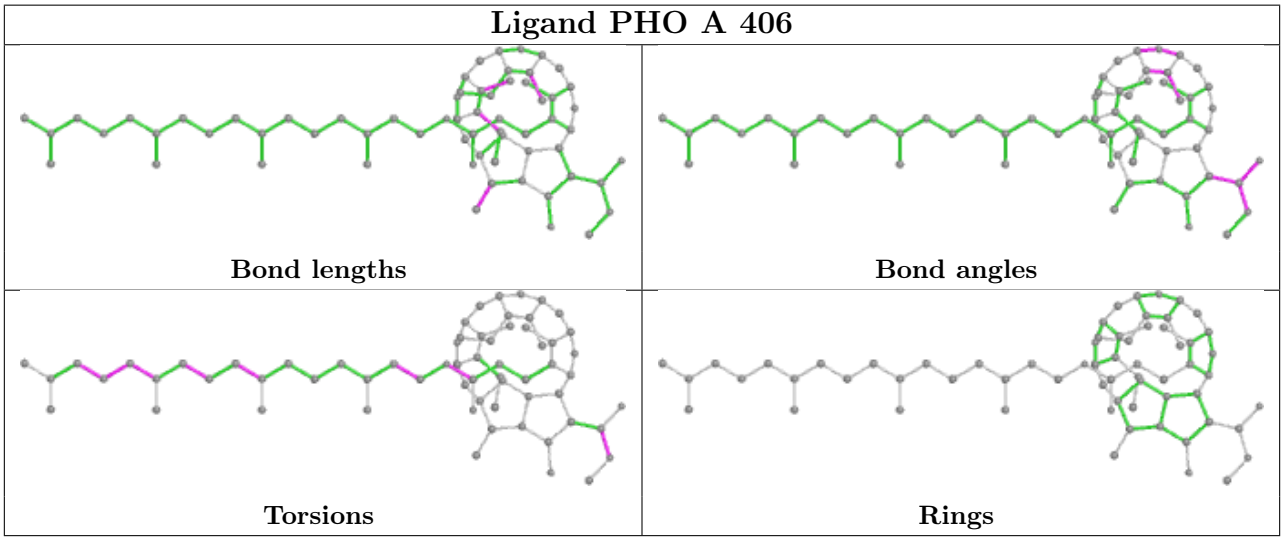
Ligand PL9 a 410



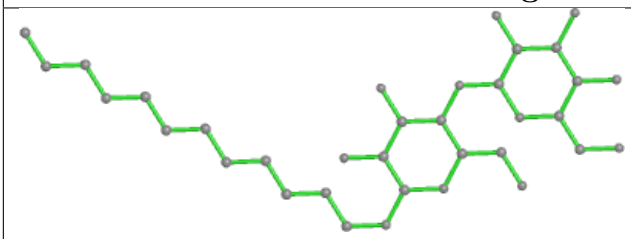
Ligand SQD f 103

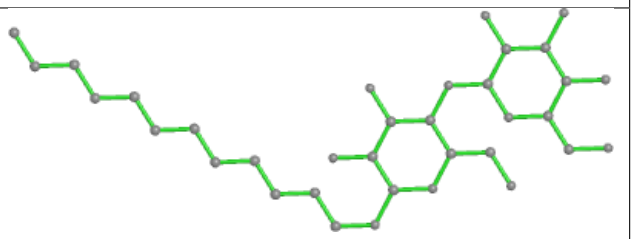


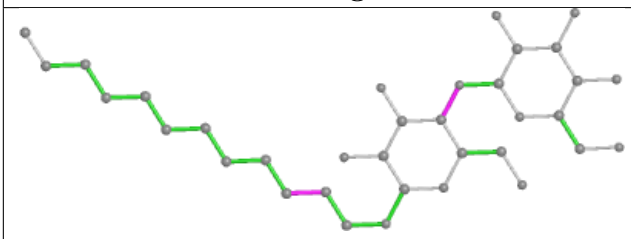
Ligand PHO A 406

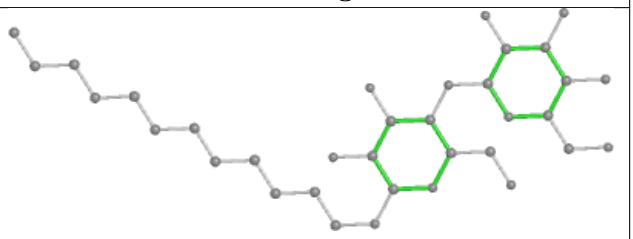


Ligand LMT B 628

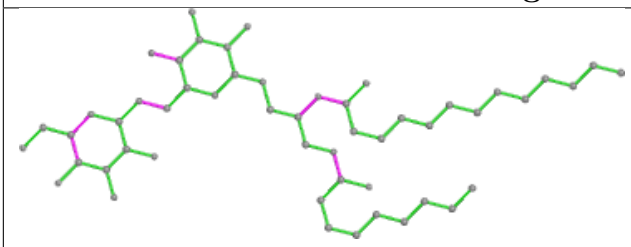

Bond lengths

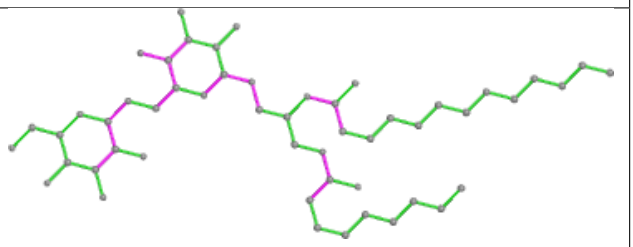

Bond angles

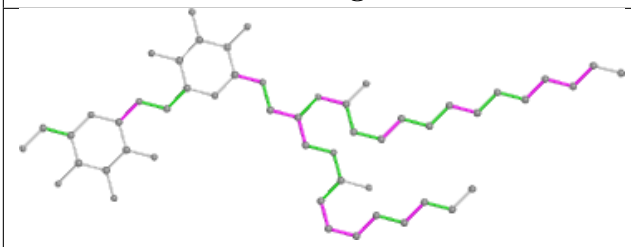

Torsions

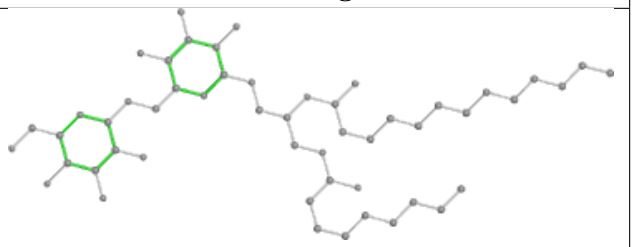

Rings

Ligand DGD b 602

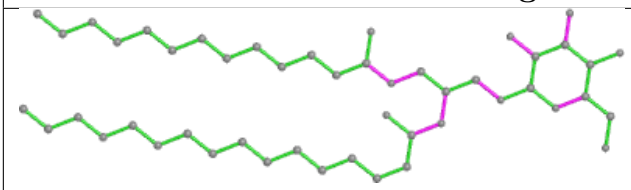

Bond lengths

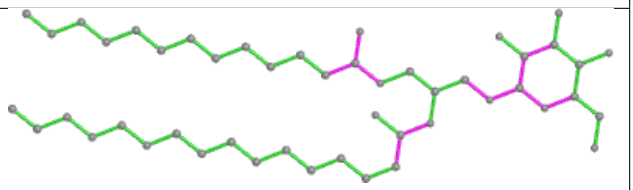

Bond angles

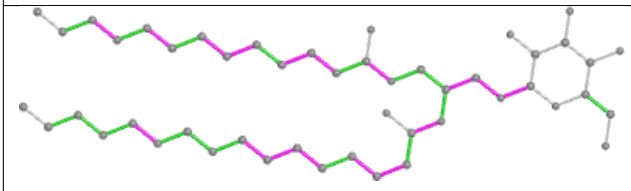

Torsions

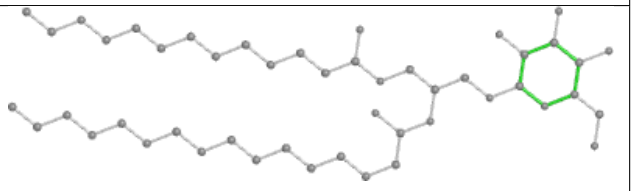

Rings

Ligand LMG D 408

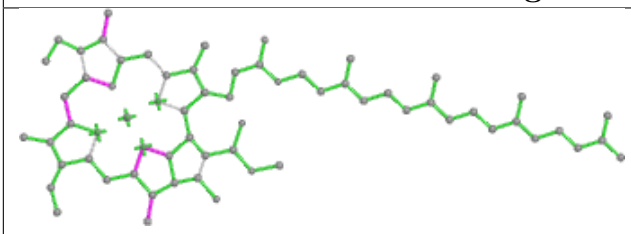

Bond lengths


Bond angles

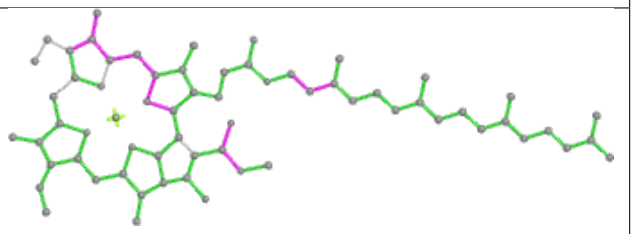

Torsions


Rings

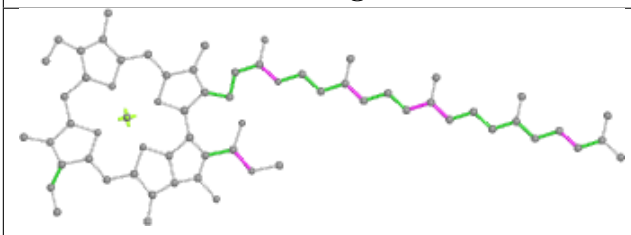
Ligand CLA B 611



Bond lengths



Bond angles



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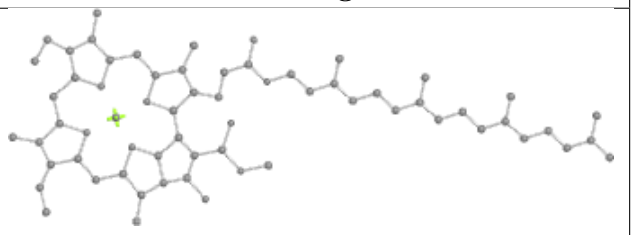
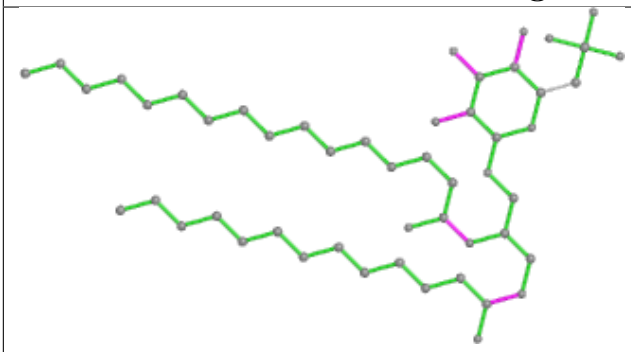


Rings

Ligand SQD a 415



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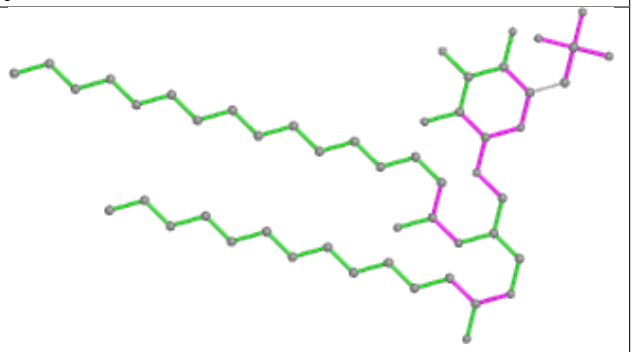

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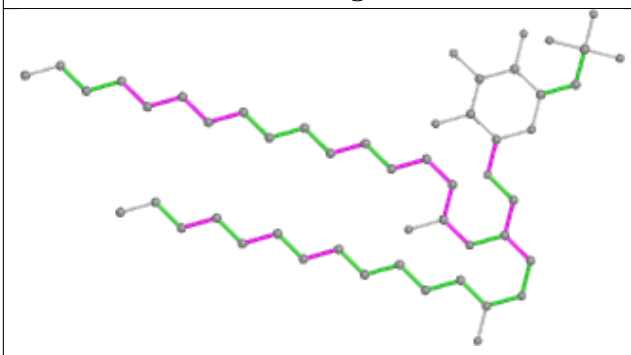

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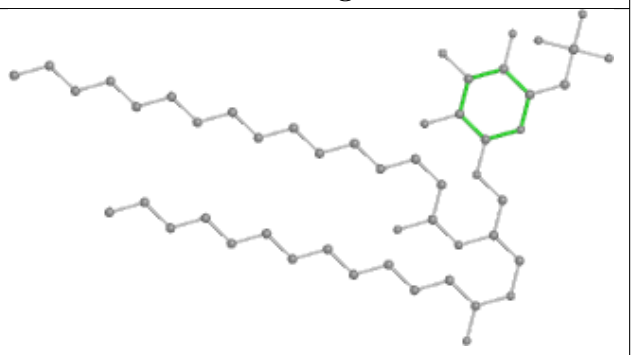
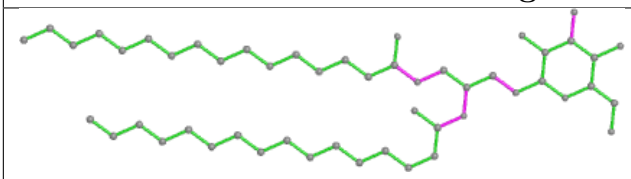


Rings

Ligand LMG A 414



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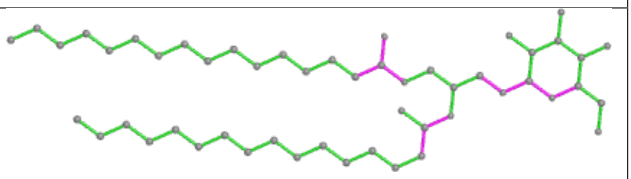
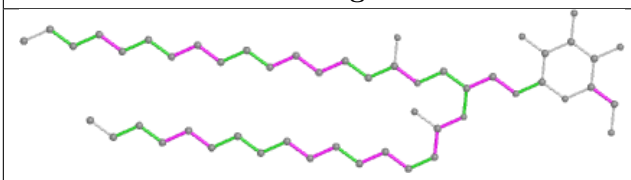


Bond angles



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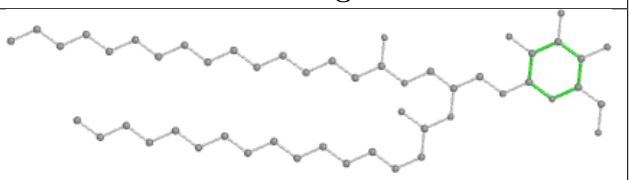
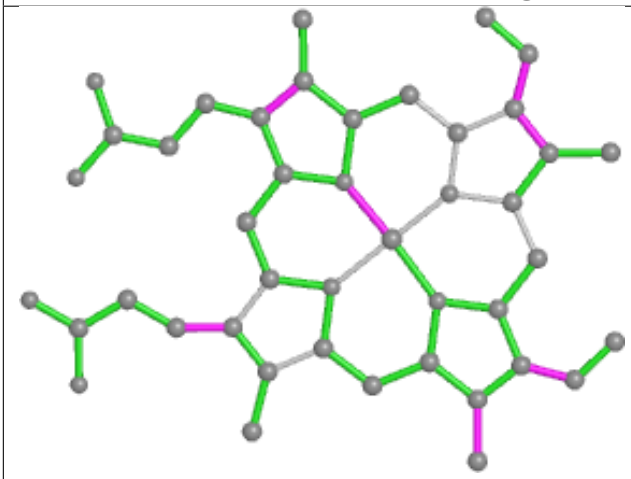


Rings

Ligand HEM V 201



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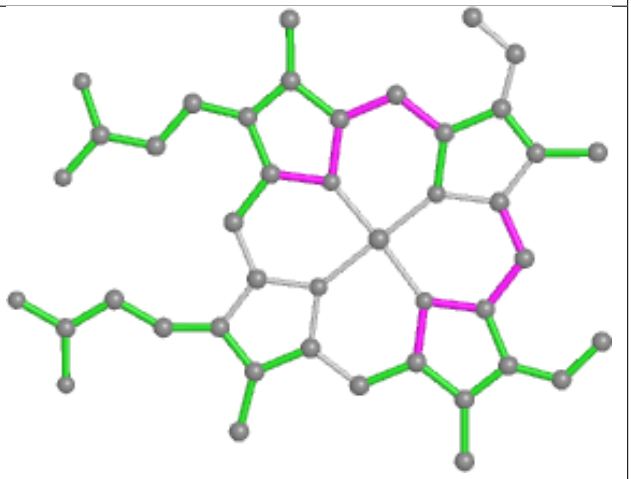

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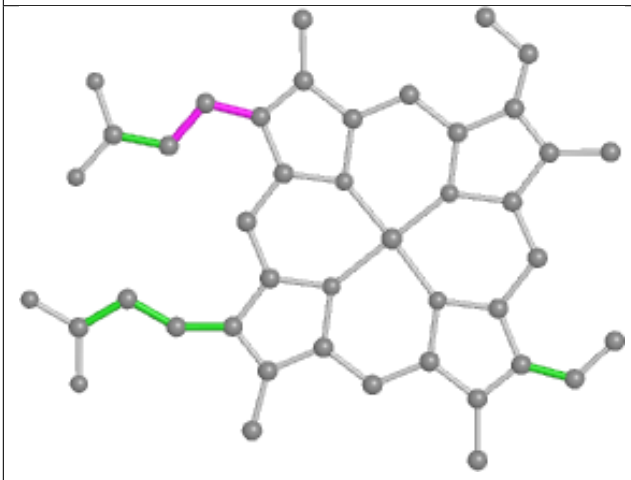

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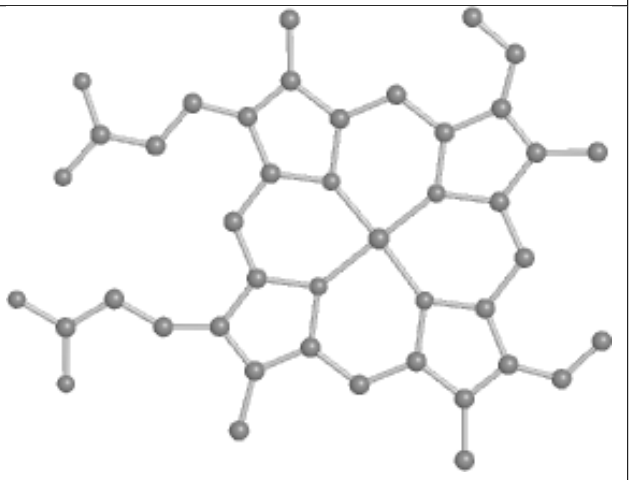
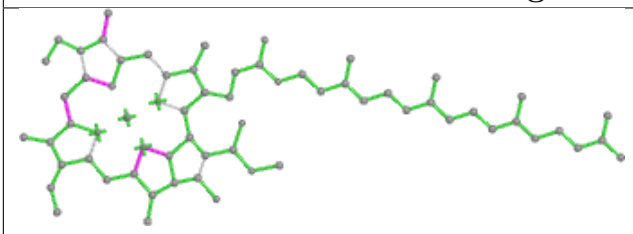


Rings

Ligand CLA b 610



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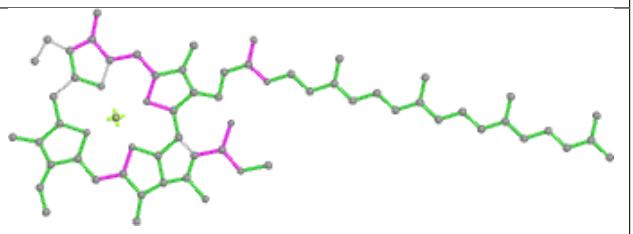
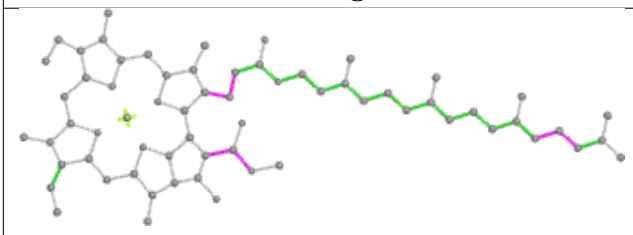


Bond angles



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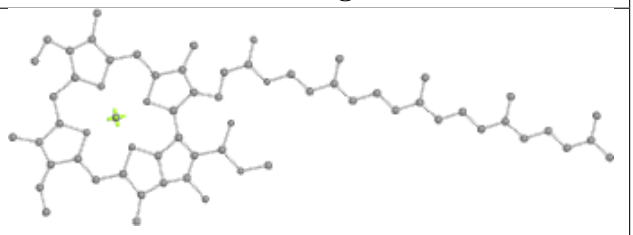
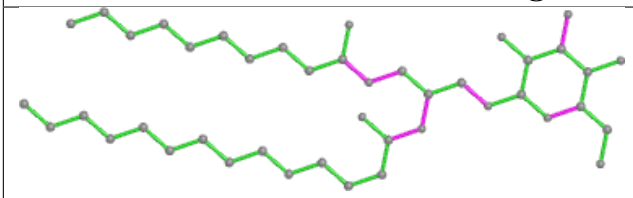


Rings

Ligand LMG i 101



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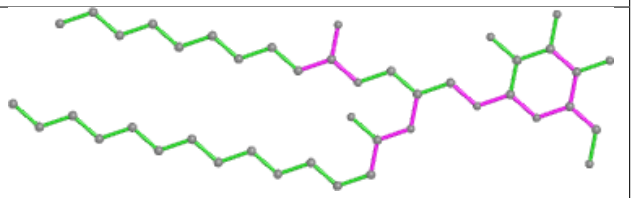
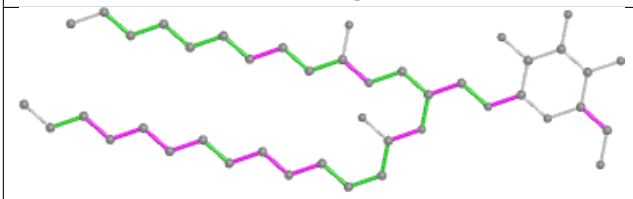
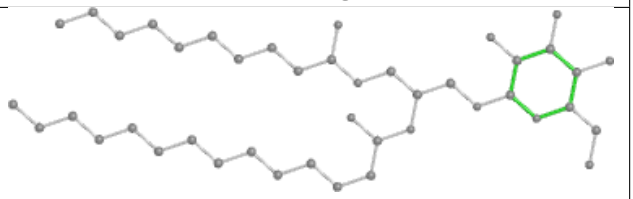


Bond angles

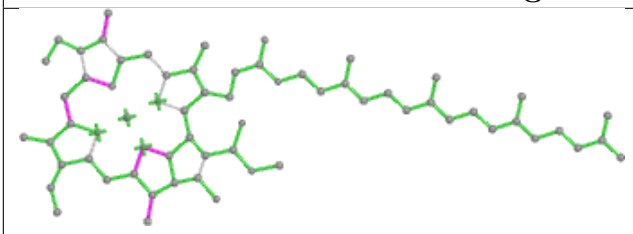


Torsions

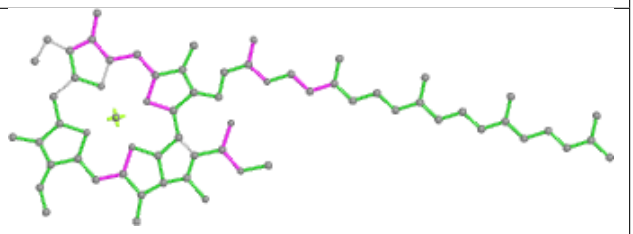


Rings

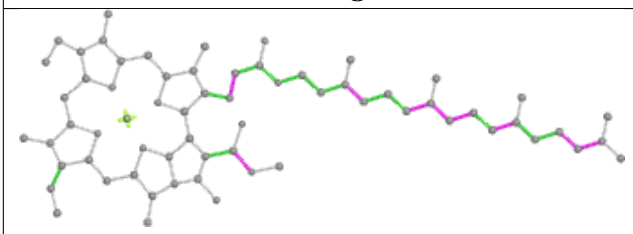
Ligand CLA B 603



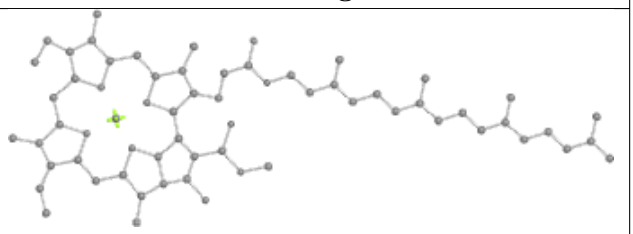
Bond lengths



Bond angles

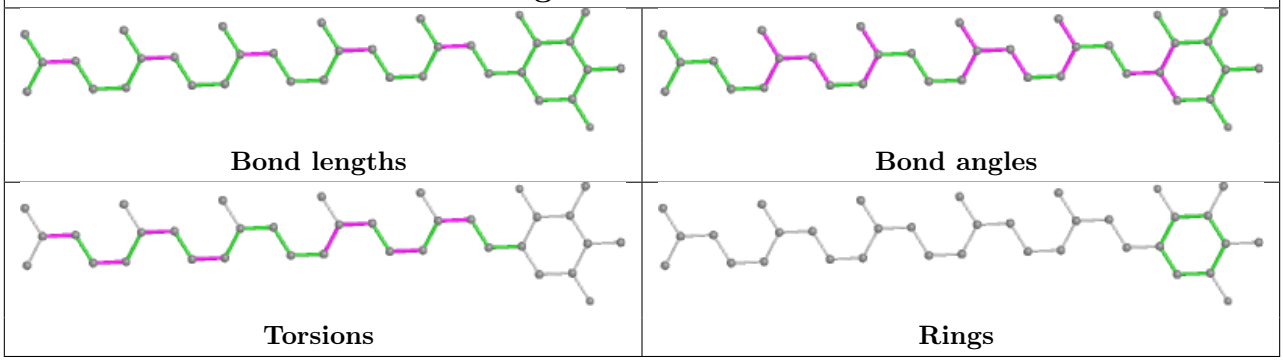


Torsions

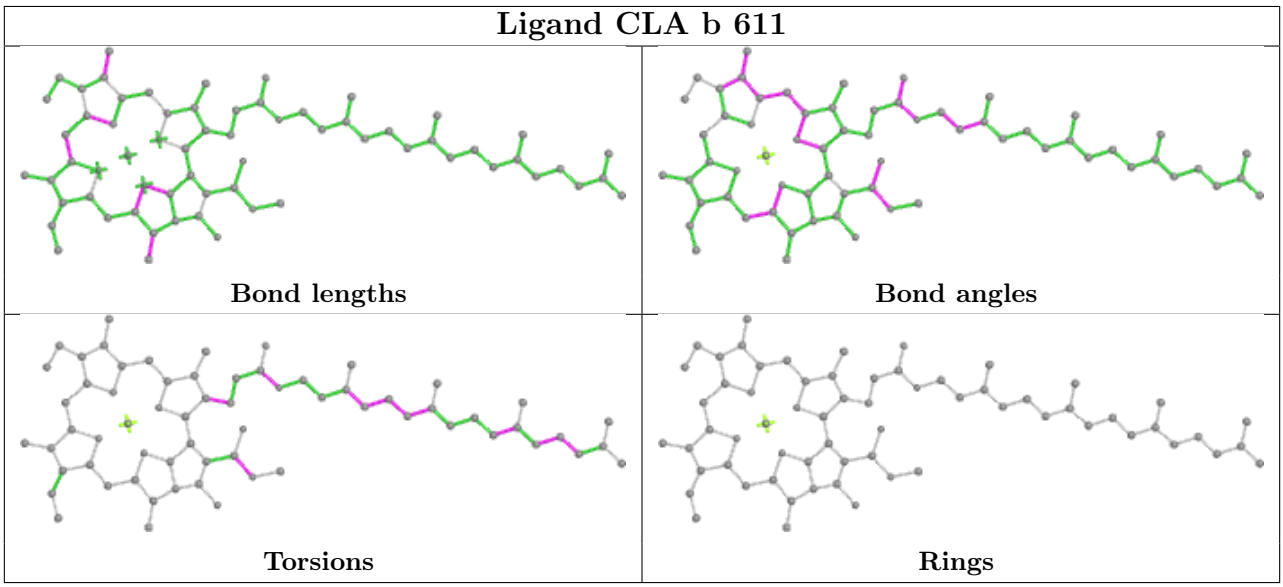


Rings

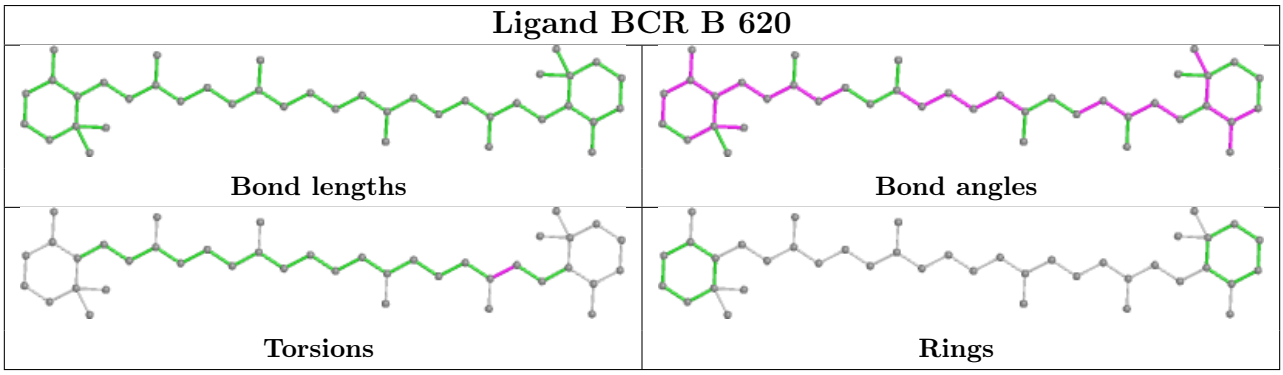
Ligand PL9 J 101



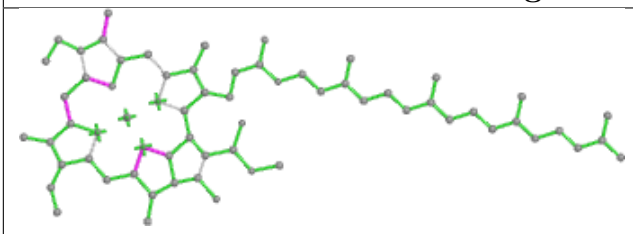
Ligand CLA b 611



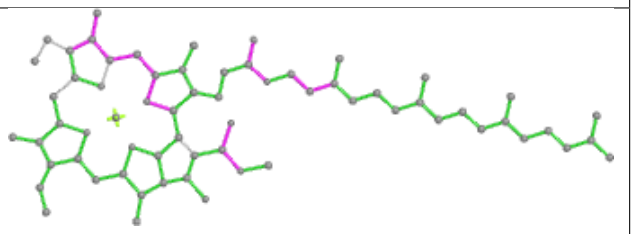
Ligand BCR B 620



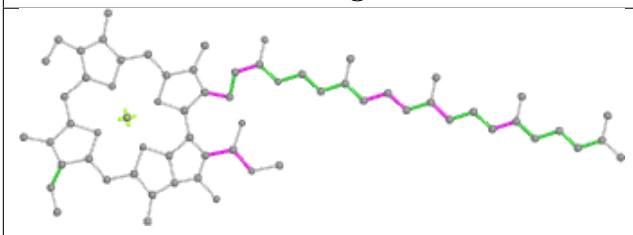
Ligand CLA C 507



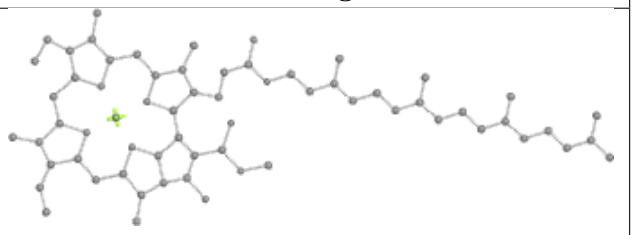
Bond lengths



Bond angles

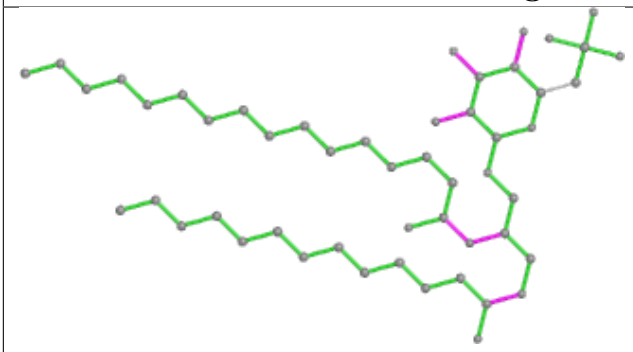


Torsions



Rings

Ligand SQD A 413



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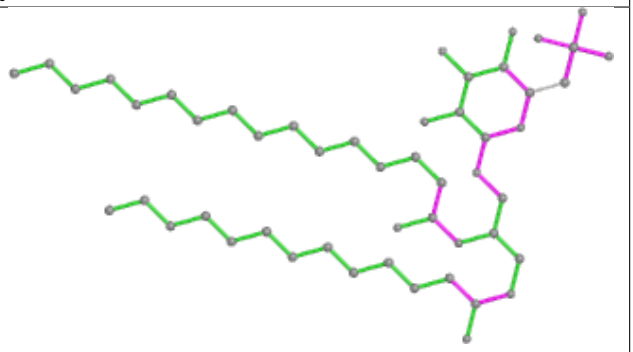
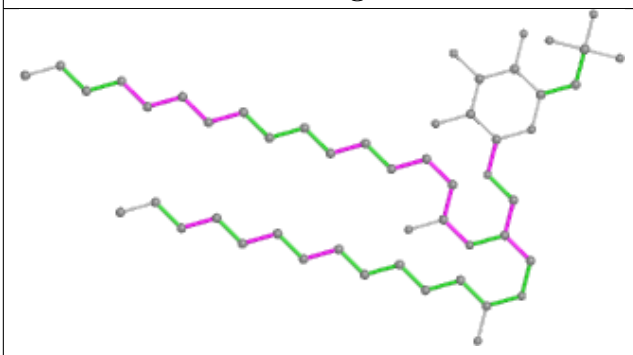


Bond angles



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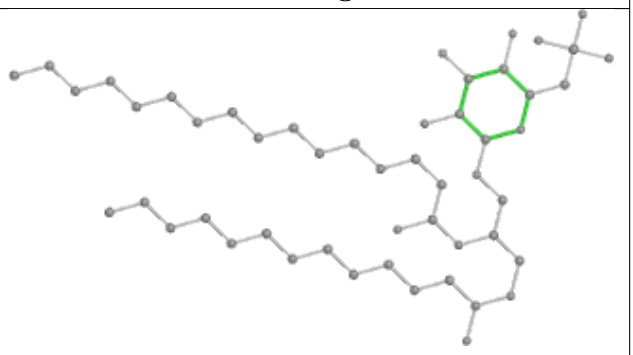
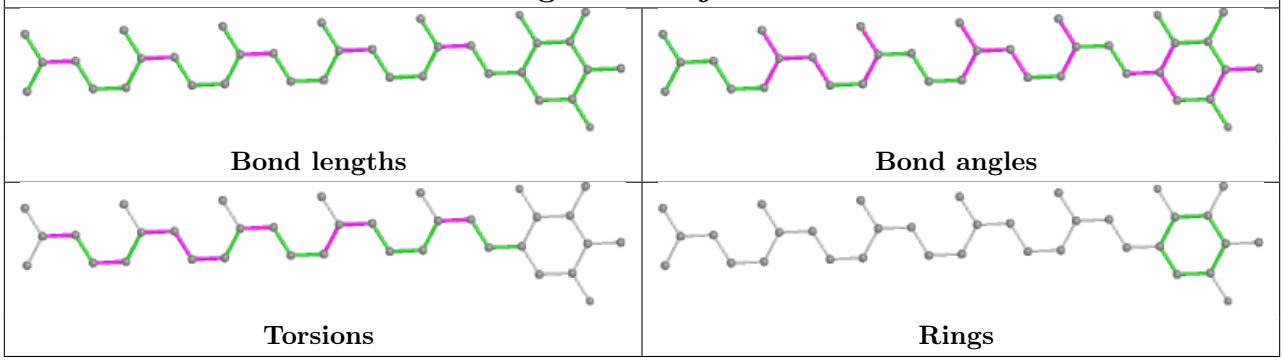
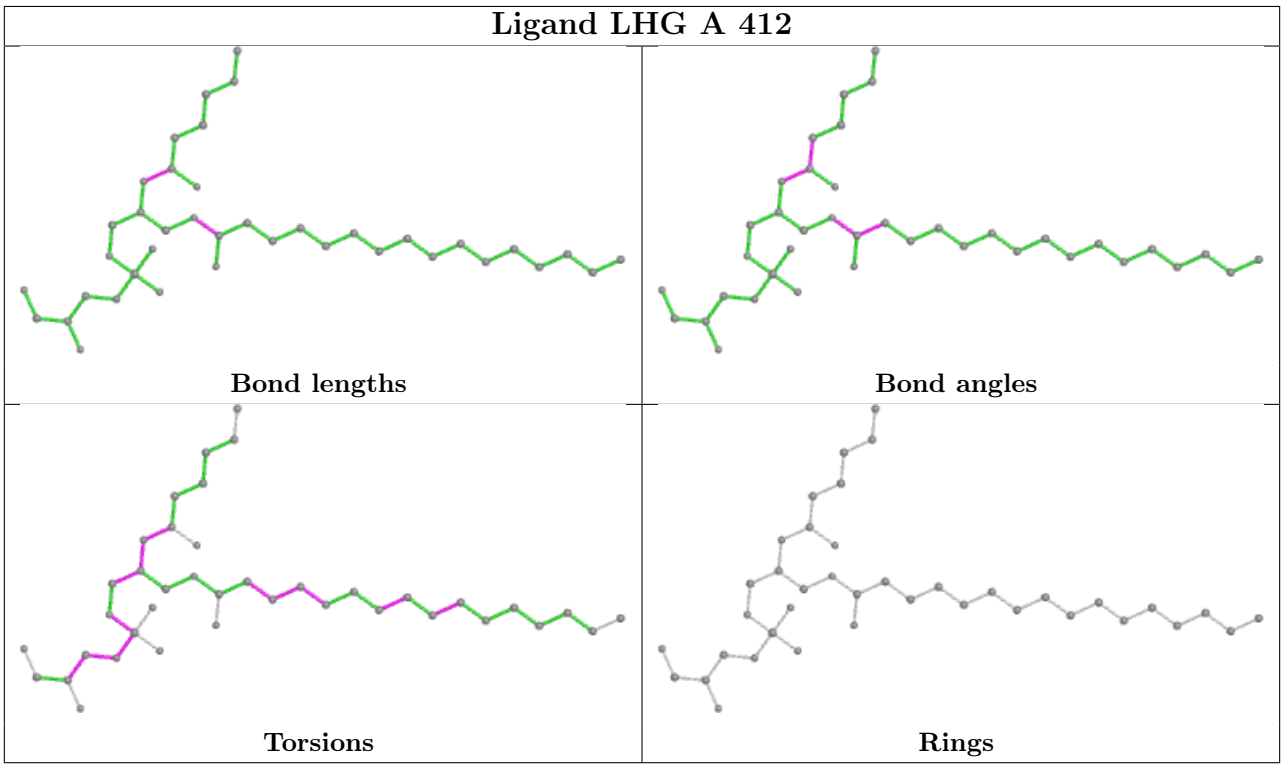


Rings

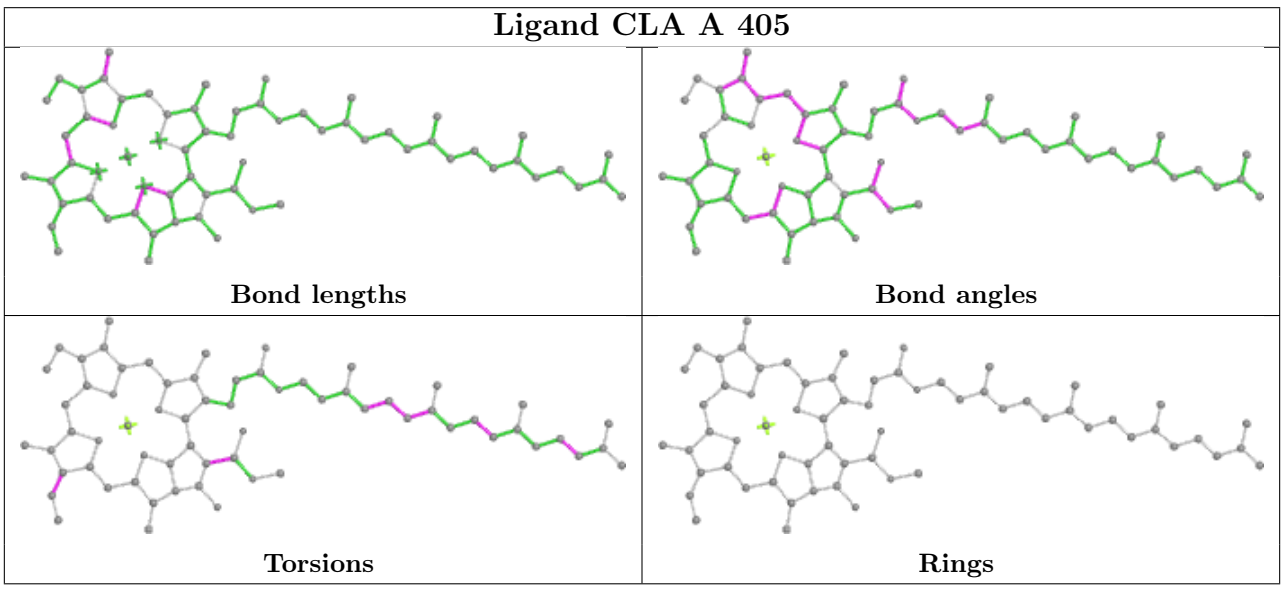
Ligand PL9 j 101



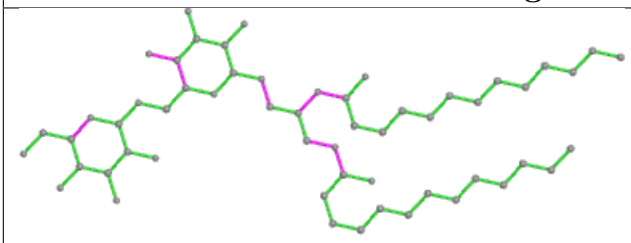
Ligand LHG A 412



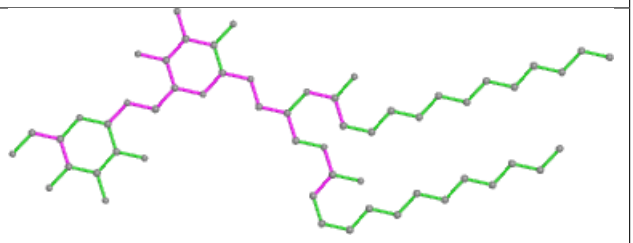
Ligand CLA A 405



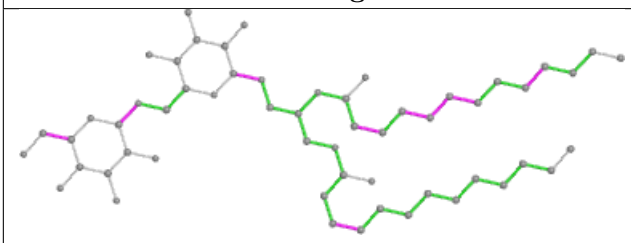
Ligand DGD a 413



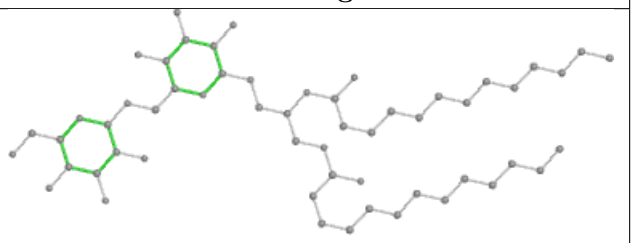
Bond lengths



Bond angles

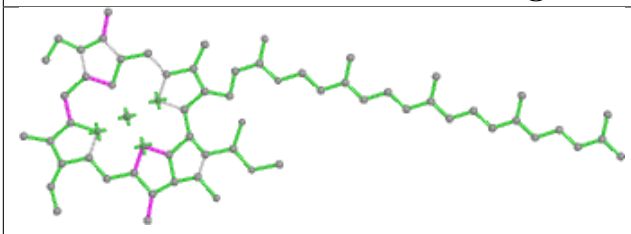


Torsions

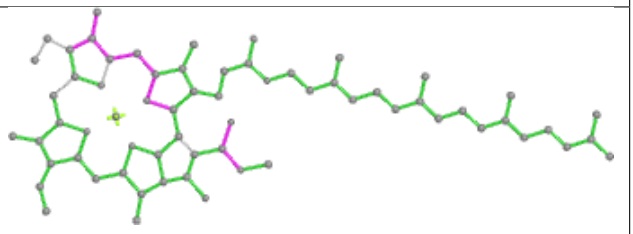


Rings

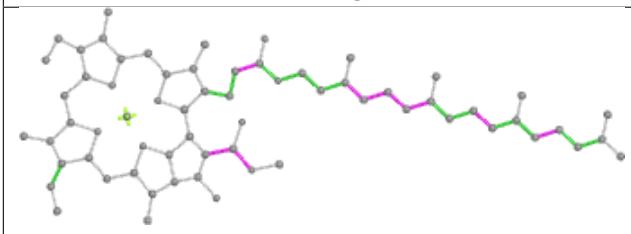
Ligand CLA b 615



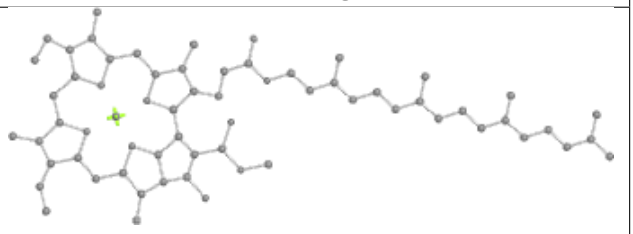
Bond lengths



Bond angles

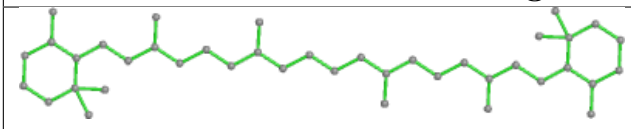


Torsions

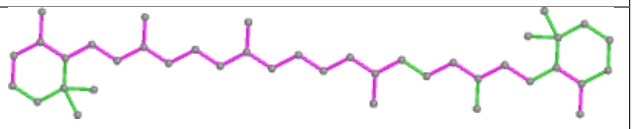


Rings

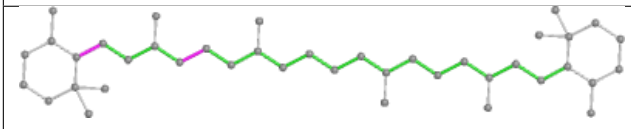
Ligand BCR x 101



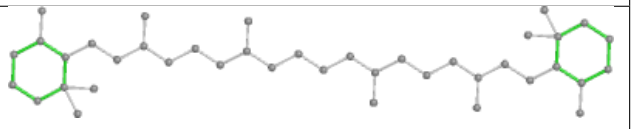
Bond lengths



Bond angles

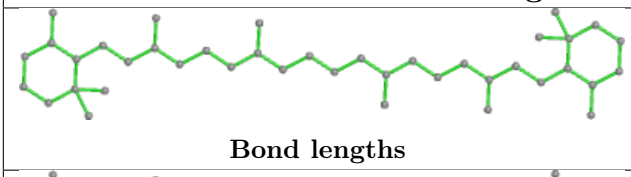


Torsions

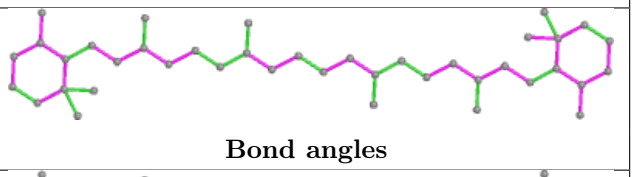


Rings

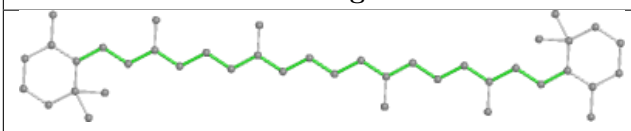
Ligand BCR b 620



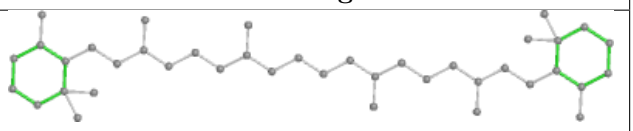
Bond lengths



Bond angles

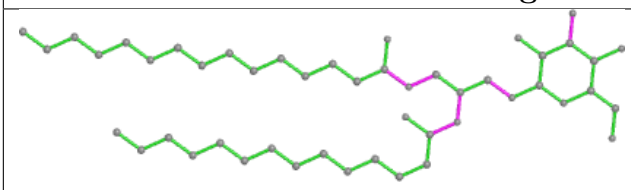


Torsions

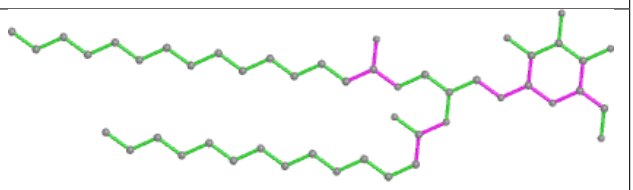


Rings

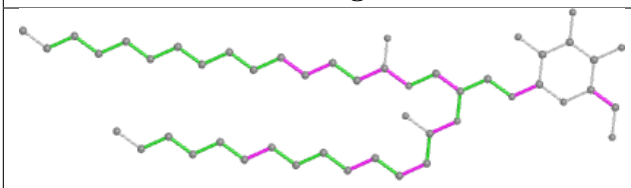
Ligand LMG C 519



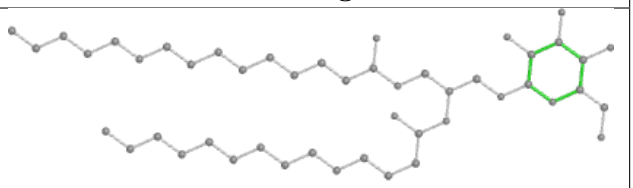
Bond lengths



Bond angles

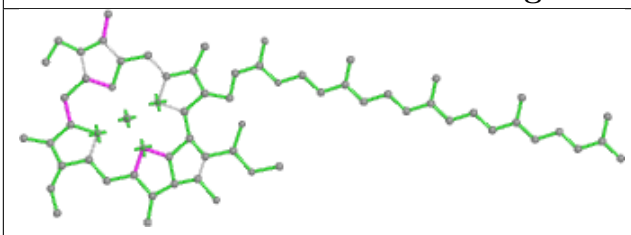


Torsions



Rings

Ligand CLA B 614



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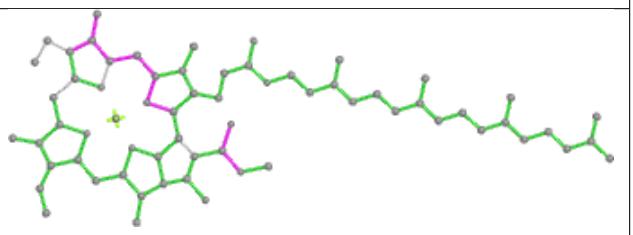
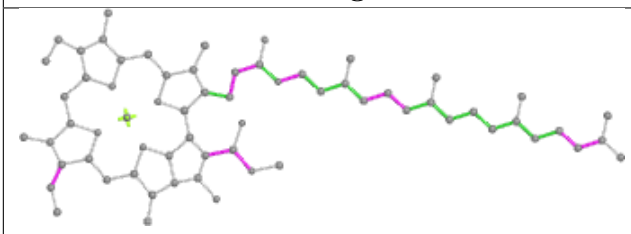
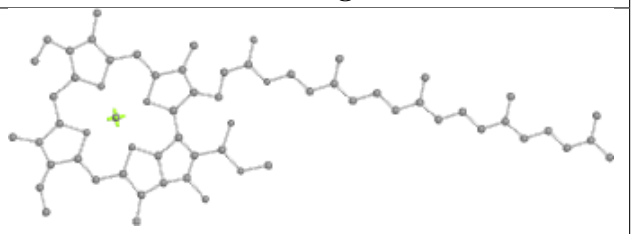


Bond angles

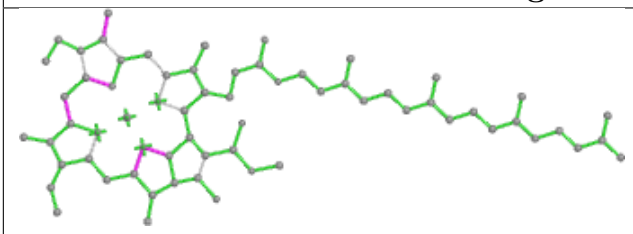


Torsions

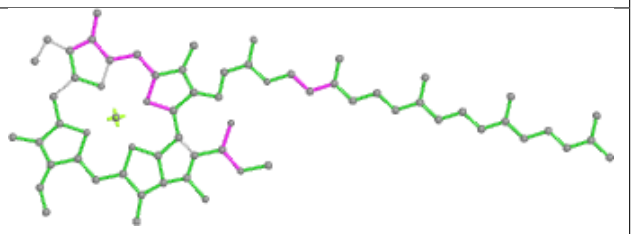


Rings

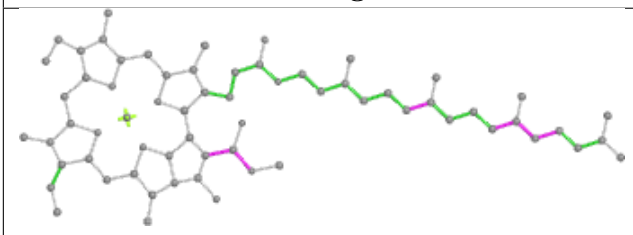
Ligand CLA b 612



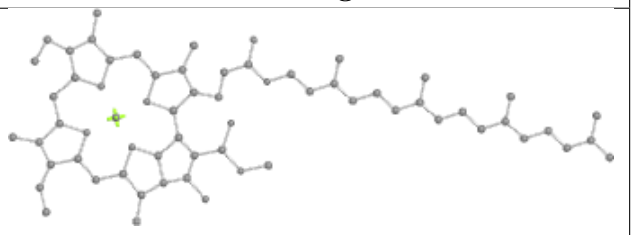
Bond lengths



Bond angles

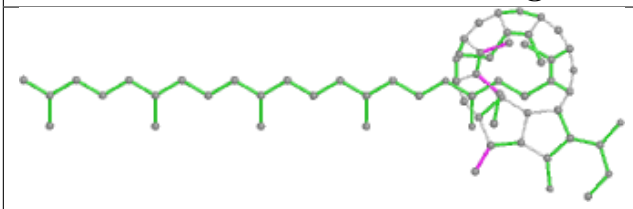


Torsions



Rings

Ligand PHO a 408



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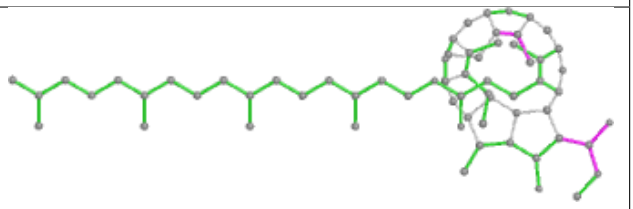
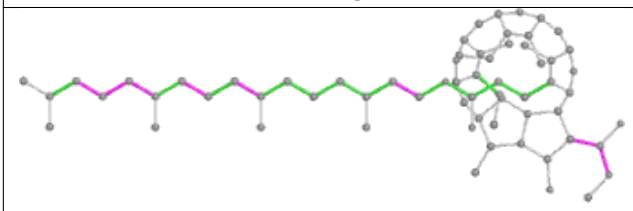
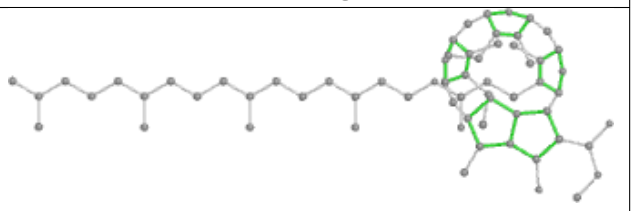


Bond angles

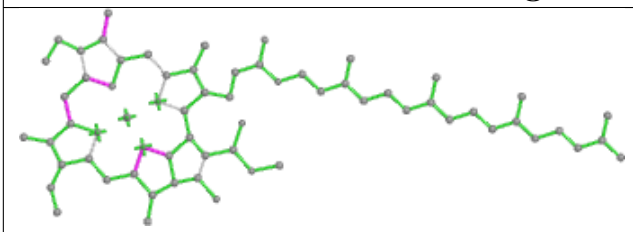


Torsions

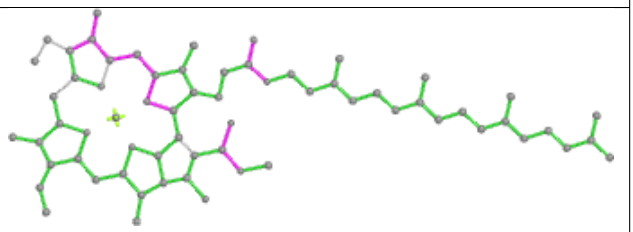


Rings

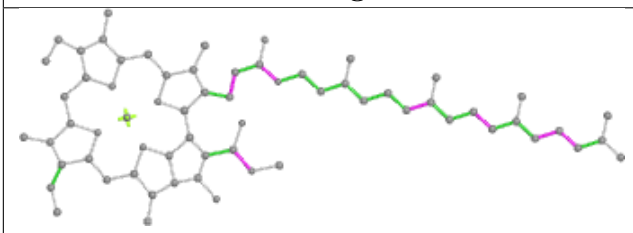
Ligand CLA C 504



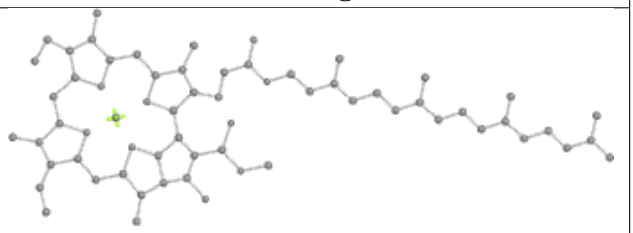
Bond lengths



Bond angles

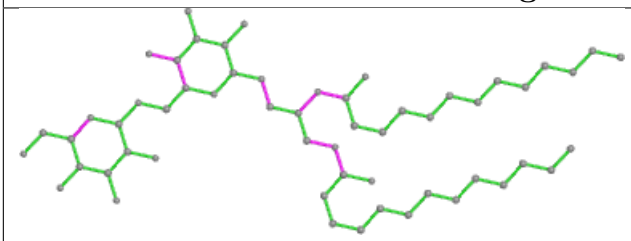


Torsions

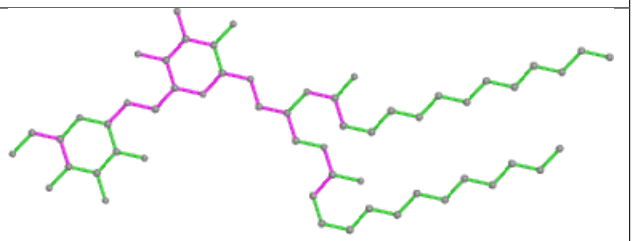


Rings

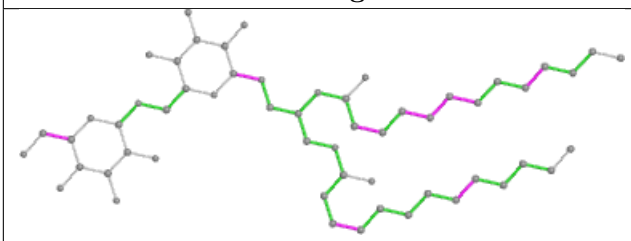
Ligand DGD A 411



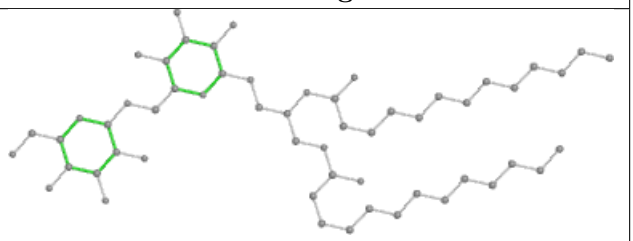
Bond lengths



Bond angles

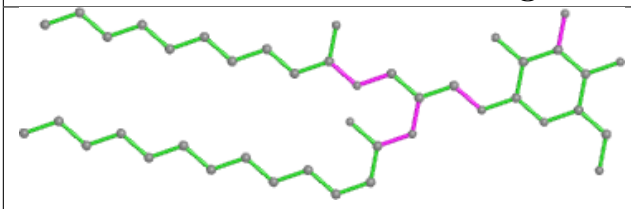


Torsions

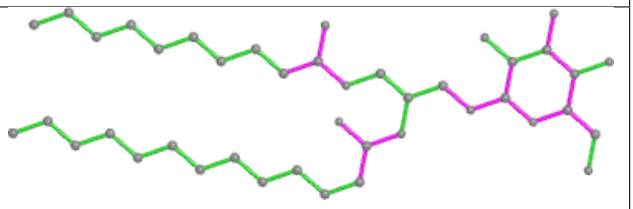


Rings

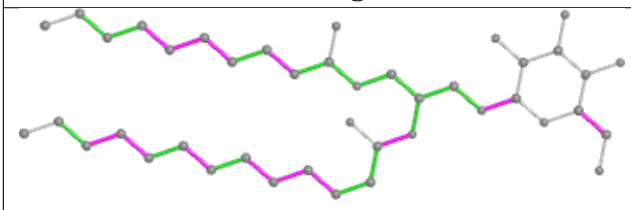
Ligand LMG A 418



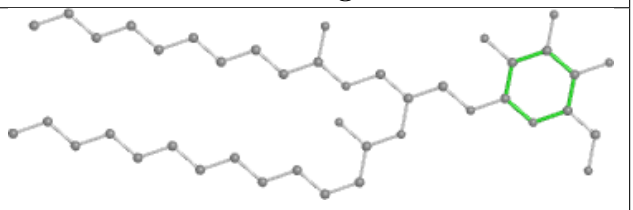
Bond lengths



Bond angles

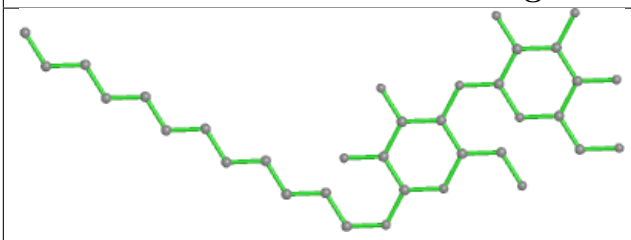


Torsions



Rings

Ligand LMT b 626



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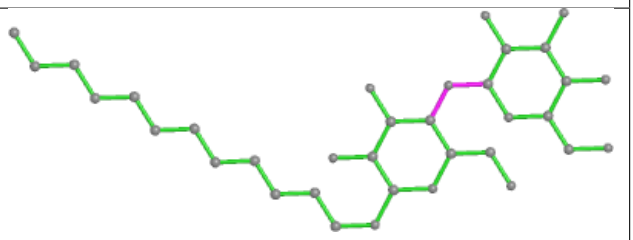
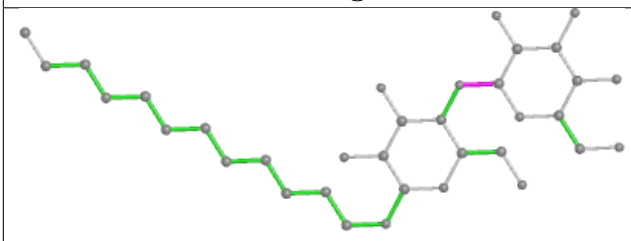
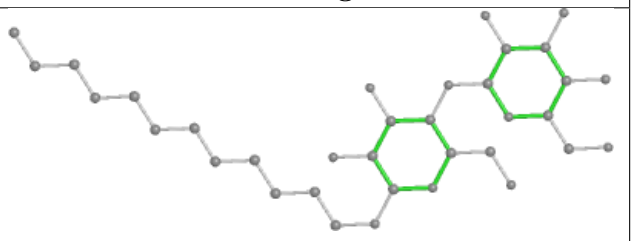


Bond angles

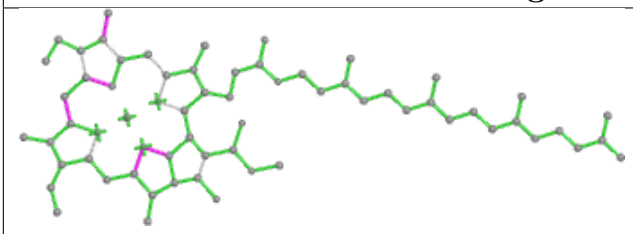


Torsions



Rings

Ligand CLA b 606



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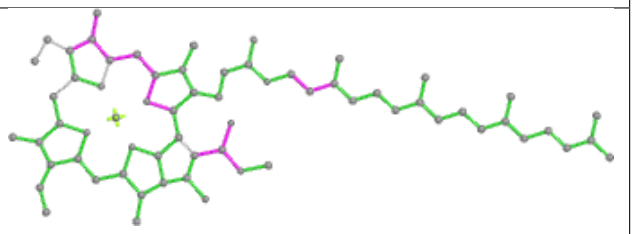
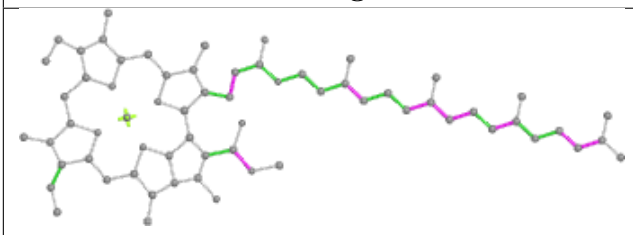
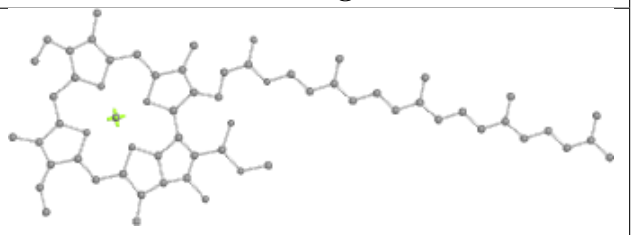


Bond angles

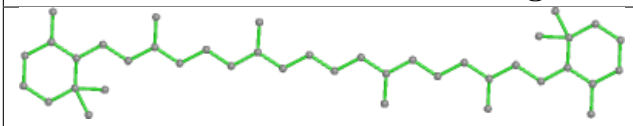


Torsions



Rings

Ligand BCR a 412



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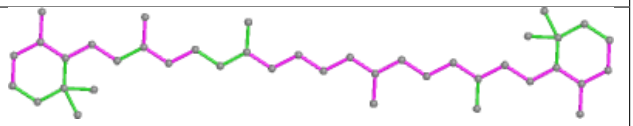
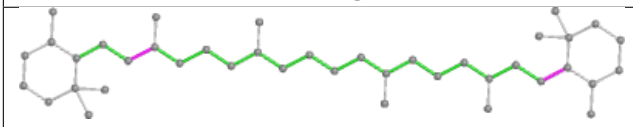


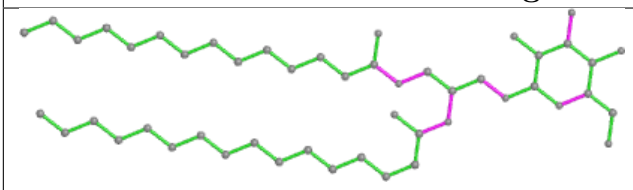
Bond angles



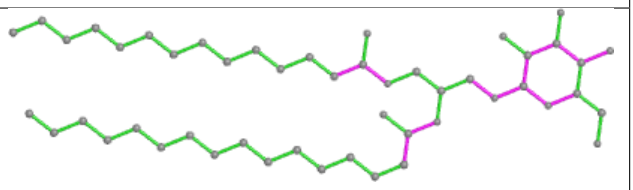
Torsions

Rings

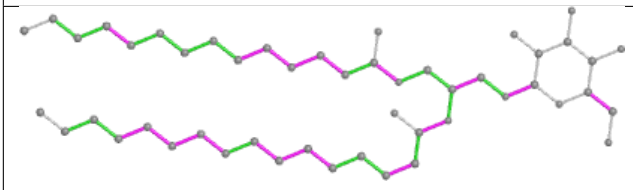
Ligand LMG b 623



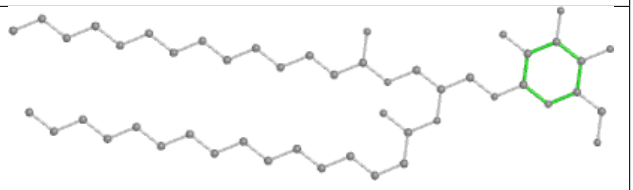
Bond lengths



Bond angles

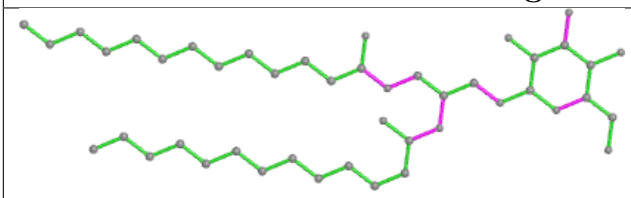


Torsions

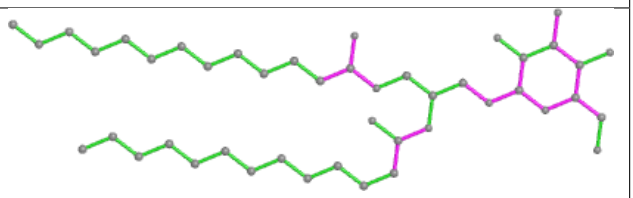


Rings

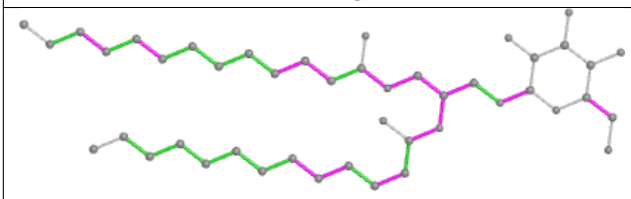
Ligand LMG c 520



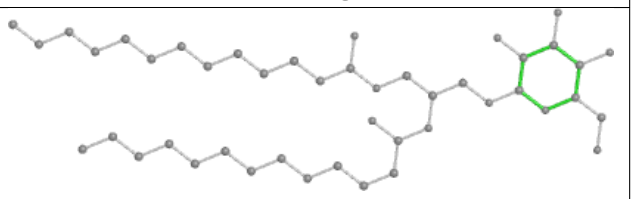
Bond lengths



Bond angles

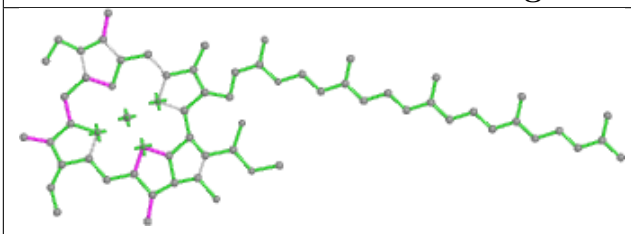


Torsions

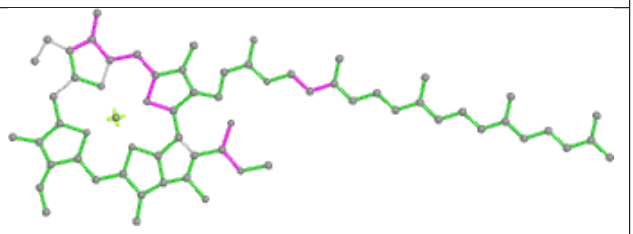


Rings

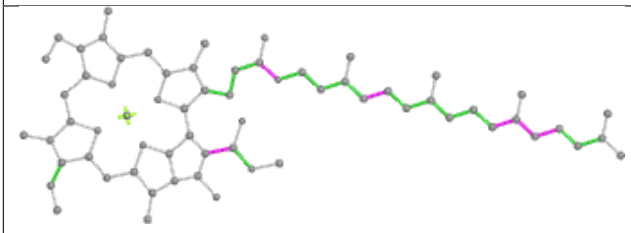
Ligand CLA C 502



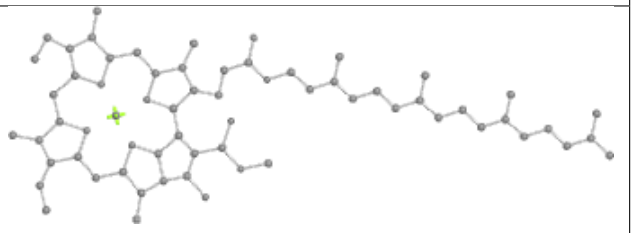
Bond lengths



Bond angles

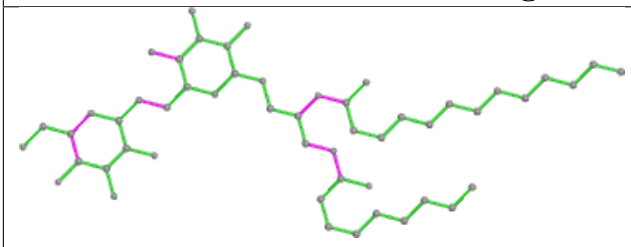


Torsions

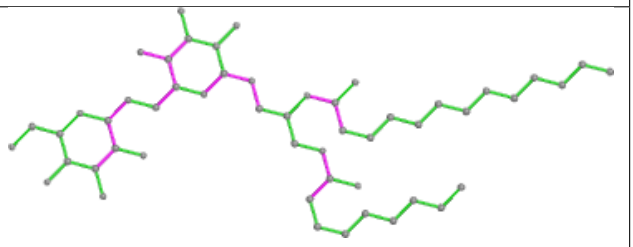


Rings

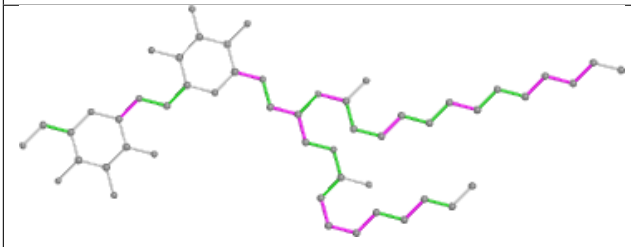
Ligand DGD B 626



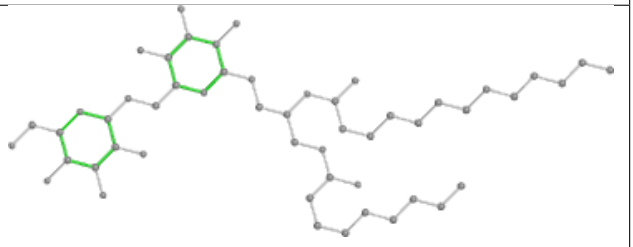
Bond lengths



Bond angles

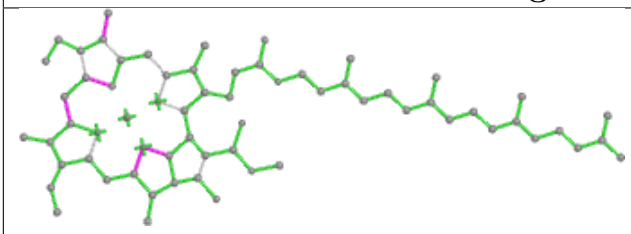


Torsions

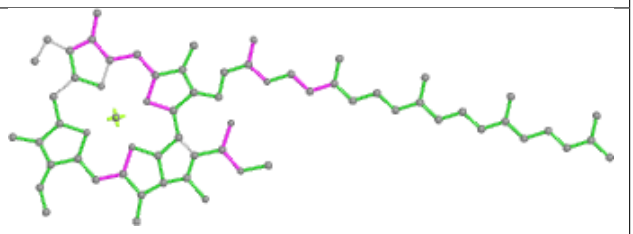


Rings

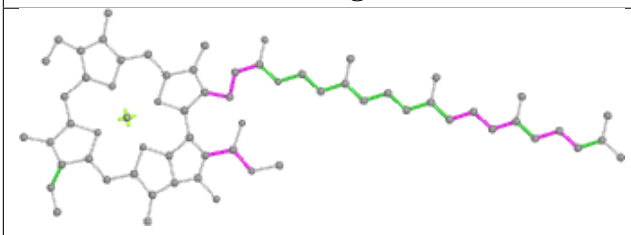
Ligand CLA c 501



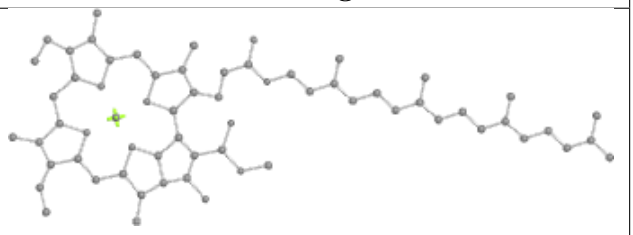
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/360 (93%)	0.03	8 (2%) 59 51	44, 65, 104, 152	0
1	a	335/360 (93%)	-0.18	2 (0%) 89 83	46, 65, 104, 153	0
2	B	490/510 (96%)	0.22	21 (4%) 35 32	46, 70, 103, 156	0
2	b	490/510 (96%)	0.21	15 (3%) 49 41	43, 70, 103, 160	0
3	C	447/461 (96%)	0.01	12 (2%) 54 47	52, 79, 105, 133	0
3	c	447/461 (96%)	0.14	24 (5%) 25 25	56, 81, 106, 135	0
4	D	340/352 (96%)	-0.13	1 (0%) 94 90	44, 66, 102, 139	0
4	d	340/352 (96%)	-0.10	2 (0%) 89 83	43, 66, 102, 135	0
5	E	82/84 (97%)	0.08	2 (2%) 59 51	68, 92, 123, 132	0
5	e	82/84 (97%)	-0.14	1 (1%) 79 70	70, 92, 123, 127	0
6	F	35/45 (77%)	-0.30	0 100 100	67, 84, 119, 143	0
6	f	35/45 (77%)	-0.21	1 (2%) 51 44	72, 83, 121, 141	0
7	H	65/66 (98%)	0.39	4 (6%) 20 19	74, 93, 119, 145	0
7	h	65/66 (98%)	0.63	7 (10%) 5 8	73, 94, 119, 148	0
8	I	35/38 (92%)	0.18	0 100 100	65, 80, 106, 120	0
8	i	35/38 (92%)	-0.08	0 100 100	68, 80, 105, 120	0
9	J	34/40 (85%)	-0.24	0 100 100	72, 85, 95, 112	0
9	j	34/40 (85%)	-0.06	0 100 100	77, 87, 96, 115	0
10	K	37/46 (80%)	-0.15	0 100 100	76, 88, 99, 125	0
10	k	37/46 (80%)	0.41	1 (2%) 54 47	73, 89, 104, 126	0
11	L	37/37 (100%)	0.35	4 (10%) 5 8	50, 63, 126, 156	0
11	l	37/37 (100%)	0.05	0 100 100	51, 63, 127, 155	0
12	M	34/36 (94%)	0.14	2 (5%) 22 21	53, 69, 107, 165	0
12	m	34/36 (94%)	0.21	3 (8%) 10 11	55, 69, 109, 163	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.54	21 (8%) 10 11	49, 79, 122, 167	0
13	o	243/272 (89%)	0.44	9 (3%) 41 36	49, 79, 121, 167	0
14	T	32/32 (100%)	0.22	4 (12%) 3 7	57, 69, 159, 169	0
14	t	32/32 (100%)	-0.08	0 100 100	56, 67, 158, 170	0
15	U	97/134 (72%)	0.57	4 (4%) 37 33	56, 70, 90, 112	0
15	u	97/134 (72%)	0.52	2 (2%) 63 55	56, 70, 89, 111	0
16	V	137/163 (84%)	0.02	4 (2%) 51 44	55, 71, 85, 100	0
16	v	137/163 (84%)	0.43	3 (2%) 62 54	58, 71, 86, 96	0
17	g	28/46 (60%)	0.85	3 (10%) 6 8	96, 108, 125, 129	0
17	y	28/46 (60%)	0.03	0 100 100	92, 108, 128, 129	0
18	X	37/41 (90%)	0.84	6 (16%) 1 4	77, 92, 120, 140	0
18	x	37/41 (90%)	0.76	5 (13%) 3 5	75, 90, 124, 145	0
19	Z	62/62 (100%)	0.83	6 (9%) 7 9	87, 103, 170, 186	0
19	z	62/62 (100%)	0.36	1 (1%) 72 63	88, 104, 169, 184	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.15	178 (3%) 45 39	43, 75, 115, 186	0

All (178) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.2
16	v	132	ASN	5.2
1	A	10	SER	4.6
1	A	11	ALA	4.6
7	h	66	GLY	4.2
5	E	84	LYS	4.0
3	c	180	MET	3.8
1	A	230	THR	3.7
1	A	12	ASN	3.7
13	o	55	ALA	3.7
1	a	10	SER	3.7
3	c	200	THR	3.7
2	B	129	GLY	3.7
3	c	201	ASN	3.6
2	B	379	ALA	3.6
2	B	128	THR	3.5

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Mol	Chain	Res	Type	RSRZ
13	O	51	THR	3.5
15	U	38	GLU	3.5
2	B	127	ARG	3.5
2	B	477	ASP	3.5
4	d	13	GLY	3.4
3	c	372	PRO	3.4
7	h	23	PRO	3.4
2	B	126	PRO	3.3
7	h	27	THR	3.3
13	o	220	LYS	3.3
2	b	393	GLU	3.2
7	h	2	ALA	3.2
3	c	202	PRO	3.2
3	c	373	ASN	3.2
18	X	42	GLN	3.1
18	x	12	ILE	3.1
13	O	269	ILE	3.1
12	m	7	GLY	3.1
13	O	57	PRO	3.1
16	v	131	ARG	3.1
3	C	27	ASP	3.1
3	C	332	GLN	3.0
2	B	132	ALA	3.0
18	X	47	GLN	3.0
2	b	119	ASP	3.0
7	H	2	ALA	2.9
2	b	303	SER	2.9
13	O	195	ASP	2.9
16	V	28	GLU	2.9
18	X	11	THR	2.9
3	c	329	GLY	2.9
2	b	394	GLN	2.9
3	c	330	SER	2.9
3	c	140	LEU	2.8
3	c	142	GLU	2.8
19	z	1	MET	2.8
3	c	147	PHE	2.7
3	c	365	TRP	2.7
13	O	54	GLY	2.7
3	c	199	ILE	2.7
19	Z	57	LEU	2.7
13	O	58	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	c	27	ASP	2.7
3	C	473	ASP	2.7
3	c	203	THR	2.7
2	b	195	PRO	2.7
1	A	229	GLU	2.7
2	b	302	TRP	2.7
2	B	476	ARG	2.6
14	T	27	PRO	2.6
5	e	84	LYS	2.6
2	B	2	GLY	2.6
12	M	2	GLU	2.6
14	T	28	ARG	2.6
2	B	3	LEU	2.5
13	O	88	GLU	2.5
2	B	397	VAL	2.5
7	h	3	ARG	2.5
12	m	5	GLN	2.5
2	b	402	TYR	2.5
2	B	162	PHE	2.5
3	c	191	PRO	2.5
13	O	87	GLN	2.5
15	U	54	LYS	2.5
1	A	15	GLU	2.4
3	c	148	GLY	2.4
3	C	262	ARG	2.4
13	O	55	ALA	2.4
13	O	90	GLU	2.4
1	a	224	ILE	2.4
13	O	89	ALA	2.4
2	B	347	ARG	2.4
18	X	12	ILE	2.4
3	c	204	LEU	2.4
3	C	261	ARG	2.4
2	b	219	VAL	2.4
3	c	192	GLY	2.4
12	m	4	ASN	2.4
3	C	137	PRO	2.4
1	A	222	SER	2.4
3	C	28	GLN	2.4
18	x	42	GLN	2.4
6	f	12	SER	2.4
11	L	7	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
13	O	56	TYR	2.3
18	X	45	LYS	2.3
13	o	169	LYS	2.3
13	o	158	ASN	2.3
13	o	54	GLY	2.3
7	H	66	GLY	2.3
2	B	295	GLY	2.3
2	B	84	THR	2.3
3	C	266	TRP	2.3
19	Z	56	VAL	2.3
2	B	4	PRO	2.3
13	O	59	ASP	2.3
19	Z	34	ASP	2.3
19	Z	62	VAL	2.3
13	O	52	ALA	2.3
5	E	83	LEU	2.3
2	b	295	GLY	2.3
13	O	125	ASP	2.3
1	A	251	ALA	2.3
2	b	228	ALA	2.3
13	O	53	ARG	2.3
3	C	135	ARG	2.3
12	M	34	LYS	2.3
11	L	5	PRO	2.3
10	k	13	GLU	2.3
13	o	125	ASP	2.2
4	d	98	GLN	2.2
18	x	13	THR	2.2
7	h	26	GLY	2.2
17	g	28	ILE	2.2
13	o	31	LEU	2.2
2	b	217	ILE	2.2
17	g	31	ALA	2.2
3	c	371	GLY	2.2
14	T	26	PRO	2.2
2	b	403	GLY	2.2
11	L	8	GLN	2.2
19	Z	1	MET	2.2
2	B	294	SER	2.2
3	C	144	SER	2.2
2	b	70	GLY	2.2
13	o	51	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	259	GLY	2.2
3	C	147	PHE	2.2
16	V	154	ASP	2.2
4	D	295	SER	2.2
3	c	141	GLU	2.2
3	C	145	SER	2.2
15	u	107	GLU	2.1
13	o	32	THR	2.1
2	B	214	LEU	2.1
7	h	56	ASP	2.1
16	V	43	LYS	2.1
3	c	143	TYR	2.1
11	L	6	ASN	2.1
2	B	370	LEU	2.1
2	b	395	GLN	2.1
15	u	38	GLU	2.1
15	U	117	VAL	2.1
13	O	108	GLN	2.1
7	H	55	LEU	2.1
2	B	474	LEU	2.1
2	b	294	SER	2.1
3	c	44	ASN	2.1
13	O	220	LYS	2.1
14	T	31	LYS	2.1
13	O	50	ASP	2.1
18	x	17	LYS	2.1
7	H	53	LEU	2.0
16	V	29	LEU	2.0
13	O	161	SER	2.0
19	Z	4	LEU	2.0
16	v	103	LYS	2.0
17	g	27	MET	2.0
3	c	328	VAL	2.0
13	O	162	ILE	2.0
18	X	44	ASP	2.0
15	U	39	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
31	LMG	C	520	45/55	0.27	1.27	80,119,142,171	0
25	PL9	J	101	35/55	0.30	0.52	119,157,183,185	0
25	PL9	j	101	35/55	0.34	0.46	120,159,178,180	0
33	LMT	i	102	35/35	0.35	1.16	99,136,146,150	0
33	LMT	I	102	35/35	0.39	0.94	94,136,147,149	0
35	CA	K	101	1/1	0.42	0.51	72,72,72,72	0
33	LMT	B	623	35/35	0.45	0.86	76,136,170,172	0
31	LMG	E	101	44/55	0.49	0.62	85,123,134,138	0
27	BCR	j	102	40/40	0.50	0.51	107,125,176,178	0
27	BCR	J	102	40/40	0.51	0.41	109,129,176,177	0
31	LMG	c	520	45/55	0.54	1.18	82,119,140,168	0
33	LMT	b	626	35/35	0.54	1.07	99,143,152,153	0
33	LMT	x	102	31/35	0.55	0.68	79,130,156,157	0
28	DGD	d	408	63/66	0.56	0.65	104,127,184,187	0
28	DGD	D	410	63/66	0.56	0.74	104,127,181,188	0
33	LMT	B	627	35/35	0.57	0.57	71,122,138,140	0
23	CLA	b	604	65/65	0.58	0.88	93,108,130,134	0
27	BCR	D	405	40/40	0.58	0.57	65,80,101,108	0
33	LMT	D	411	31/35	0.59	1.00	82,132,156,156	0
23	CLA	B	601	65/65	0.59	0.90	94,108,129,134	0
27	BCR	B	620	40/40	0.60	0.80	77,87,92,92	0
33	LMT	T	101	35/35	0.60	0.57	63,115,136,143	0
28	DGD	b	602	52/66	0.61	0.57	81,104,177,178	0
29	LHG	A	415	37/49	0.63	0.41	108,137,192,202	0
29	LHG	a	417	37/49	0.63	0.43	111,134,197,206	0
33	LMT	B	624	35/35	0.64	0.64	91,142,154,155	0
31	LMG	A	418	42/55	0.64	0.43	76,107,120,142	0
31	LMG	a	402	42/55	0.64	0.52	76,105,121,142	0
27	BCR	A	410	40/40	0.65	0.46	53,68,81,91	0
33	LMT	b	603	35/35	0.65	0.52	76,131,155,156	0
27	BCR	H	101	40/40	0.66	1.12	82,95,131,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	SQD	d	407	43/54	0.66	0.86	73,107,144,149	0
31	LMG	I	101	43/55	0.67	0.70	87,115,159,171	0
31	LMG	M	102	42/55	0.67	0.44	70,109,133,139	0
31	LMG	i	101	43/55	0.67	0.69	85,120,158,176	0
33	LMT	B	628	35/35	0.67	0.49	72,137,162,163	0
27	BCR	B	618	40/40	0.68	0.35	68,80,90,92	0
31	LMG	C	519	48/55	0.68	0.38	86,99,110,116	0
23	CLA	c	513	65/65	0.68	0.93	94,107,138,149	0
28	DGD	C	518	66/66	0.69	0.36	58,72,106,121	0
27	BCR	b	621	40/40	0.69	0.67	72,83,92,94	0
30	SQD	F	102	45/54	0.69	0.69	86,129,153,154	0
27	BCR	c	516	40/40	0.69	0.80	76,86,93,103	0
23	CLA	C	506	65/65	0.69	0.46	75,91,123,134	0
27	BCR	x	101	40/40	0.70	0.72	81,97,129,130	0
23	CLA	B	614	65/65	0.70	0.42	64,83,124,132	0
31	LMG	e	101	44/55	0.70	0.42	85,122,133,140	0
27	BCR	C	515	40/40	0.70	0.57	76,87,95,98	0
35	CA	o	301	1/1	0.70	0.41	106,106,106,106	0
27	BCR	a	412	40/40	0.71	0.44	51,71,82,84	0
28	DGD	B	626	52/66	0.71	0.46	77,104,179,183	0
27	BCR	k	102	40/40	0.71	0.80	69,85,106,109	0
28	DGD	A	411	56/66	0.72	0.40	79,100,145,149	0
23	CLA	b	619	65/65	0.72	0.62	78,99,142,147	0
23	CLA	C	502	65/65	0.72	0.49	62,72,104,112	0
25	PL9	A	408	45/55	0.72	0.46	84,103,119,127	0
30	SQD	D	409	43/54	0.72	0.58	72,103,147,151	0
30	SQD	b	601	47/54	0.73	0.38	86,99,139,146	0
31	LMG	M	101	42/55	0.73	0.40	78,110,135,144	0
25	PL9	d	404	55/55	0.73	0.31	48,65,76,86	0
30	SQD	f	103	45/54	0.73	0.67	88,129,148,155	0
27	BCR	K	102	40/40	0.73	0.76	74,85,102,103	0
27	BCR	f	102	40/40	0.73	0.45	64,83,107,110	0
23	CLA	C	507	65/65	0.73	0.59	77,92,101,105	0
31	LMG	k	103	48/55	0.73	0.43	80,100,118,120	0
32	CL	A	416	1/1	0.73	0.38	49,49,49,49	0
31	LMG	D	407	49/55	0.73	0.36	59,80,109,117	0
30	SQD	a	401	54/54	0.73	0.45	75,116,152,156	0
28	DGD	a	413	56/66	0.74	0.39	74,101,145,149	0
23	CLA	a	409	65/65	0.74	0.58	55,69,129,134	0
30	SQD	a	415	51/54	0.74	0.38	81,102,128,134	0
33	LMT	b	625	35/35	0.75	0.58	78,139,172,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	BCR	Z	101	40/40	0.75	0.90	81,93,117,118	0
23	CLA	C	503	65/65	0.76	0.51	76,88,99,101	0
28	DGD	c	519	66/66	0.76	0.34	61,72,104,113	0
25	PL9	a	410	45/55	0.76	0.35	82,98,119,127	0
23	CLA	c	502	65/65	0.76	0.52	67,75,101,107	0
23	CLA	C	513	65/65	0.76	0.84	93,108,142,149	0
30	SQD	A	413	51/54	0.76	0.34	81,95,126,130	0
33	LMT	m	101	35/35	0.76	0.51	71,95,109,109	0
30	SQD	B	625	47/54	0.76	0.38	73,102,139,146	0
31	LMG	a	416	51/55	0.76	0.33	61,80,92,99	0
23	CLA	b	613	65/65	0.76	0.66	71,81,88,91	0
27	BCR	c	515	40/40	0.77	1.10	83,95,112,115	0
28	DGD	B	621	58/66	0.77	0.45	51,69,99,106	0
27	BCR	T	103	40/40	0.77	0.32	69,79,87,95	0
31	LMG	b	624	49/55	0.77	0.29	56,76,88,91	0
27	BCR	c	514	40/40	0.77	0.85	66,80,89,91	0
30	SQD	A	417	54/54	0.77	0.37	81,116,146,153	0
33	LMT	M	103	35/35	0.78	0.35	68,98,108,115	0
27	BCR	C	514	40/40	0.78	0.83	70,80,86,90	0
23	CLA	A	407	65/65	0.78	0.49	57,69,128,131	0
23	CLA	c	509	65/65	0.78	0.60	73,82,91,98	0
35	CA	O	301	1/1	0.78	0.30	123,123,123,123	0
23	CLA	c	511	65/65	0.78	0.61	72,91,102,106	0
23	CLA	C	501	65/65	0.79	0.49	66,80,90,95	0
27	BCR	B	617	40/40	0.79	0.28	64,73,79,80	0
23	CLA	c	506	65/65	0.79	0.45	79,94,122,126	0
27	BCR	b	620	40/40	0.79	0.30	59,72,79,80	0
24	PHO	A	406	64/64	0.79	0.39	57,69,74,76	0
23	CLA	b	611	65/65	0.79	0.47	63,76,96,100	0
29	LHG	A	412	39/49	0.80	0.33	61,80,92,94	0
25	PL9	D	404	55/55	0.80	0.30	47,59,70,74	0
23	CLA	B	606	65/65	0.80	0.59	68,84,111,123	0
23	CLA	B	610	65/65	0.80	0.73	68,82,87,91	0
24	PHO	a	408	64/64	0.80	0.36	58,71,81,87	0
23	CLA	C	504	65/65	0.80	0.36	67,83,133,136	0
28	DGD	C	517	62/66	0.80	0.33	61,84,132,147	0
31	LMG	B	622	49/55	0.80	0.31	50,74,85,91	0
23	CLA	B	616	65/65	0.81	0.61	75,93,144,150	0
23	CLA	C	509	65/65	0.81	0.73	65,81,95,98	0
23	CLA	b	618	65/65	0.81	0.56	78,97,109,116	0
27	BCR	B	619	40/40	0.81	0.27	62,76,82,84	0
23	CLA	c	512	65/65	0.81	0.96	90,102,148,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	511	65/65	0.81	0.49	73,90,100,109	0
23	CLA	d	403	65/65	0.81	0.57	72,88,124,128	0
23	CLA	b	609	65/65	0.81	0.58	71,86,111,121	0
23	CLA	D	403	65/65	0.82	0.85	73,85,121,124	0
23	CLA	B	609	65/65	0.82	0.81	73,89,105,112	0
28	DGD	b	622	58/66	0.82	0.34	57,71,97,102	0
28	DGD	c	518	62/66	0.82	0.33	65,86,138,143	0
29	LHG	a	414	39/49	0.82	0.36	62,79,91,94	0
23	CLA	C	512	65/65	0.83	0.93	83,101,147,151	0
24	PHO	D	402	64/64	0.83	0.30	48,61,71,77	0
24	PHO	a	407	64/64	0.83	0.32	52,62,71,76	0
23	CLA	b	607	65/65	0.83	0.39	62,67,112,117	0
23	CLA	c	507	65/65	0.83	0.65	84,94,102,109	0
23	CLA	b	612	65/65	0.83	0.66	69,89,104,106	0
31	LMG	d	405	46/55	0.83	0.33	65,71,116,128	0
23	CLA	b	605	65/65	0.84	0.44	73,87,96,98	0
23	CLA	b	606	65/65	0.84	0.61	69,79,93,100	0
31	LMG	d	406	48/55	0.84	0.26	56,71,86,120	0
23	CLA	b	617	65/65	0.84	0.31	67,82,130,135	0
23	CLA	a	406	65/65	0.84	0.29	53,70,143,149	0
23	CLA	b	608	65/65	0.84	0.45	58,76,85,89	0
23	CLA	C	505	65/65	0.84	0.34	69,77,84,88	0
23	CLA	B	604	65/65	0.84	0.44	55,66,109,121	0
31	LMG	D	408	48/55	0.85	0.27	52,73,83,120	0
23	CLA	c	505	65/65	0.85	0.30	66,78,83,86	0
23	CLA	B	605	65/65	0.85	0.60	58,77,87,92	0
23	CLA	C	508	65/65	0.85	0.31	70,84,123,140	0
23	CLA	B	608	65/65	0.85	0.61	62,74,94,97	0
23	CLA	C	510	65/65	0.85	0.32	63,73,85,93	0
27	BCR	T	102	40/40	0.85	0.27	66,73,83,85	0
23	CLA	a	405	65/65	0.85	0.33	40,54,65,72	0
23	CLA	A	405	65/65	0.86	0.27	48,69,139,145	0
31	LMG	A	414	51/55	0.86	0.27	61,74,88,96	0
28	DGD	c	517	53/66	0.86	0.28	58,75,98,102	0
23	CLA	d	402	65/65	0.86	0.30	49,59,79,91	0
23	CLA	c	504	65/65	0.86	0.28	69,82,132,136	0
23	CLA	b	610	65/65	0.86	0.31	52,64,82,88	0
31	LMG	D	406	46/55	0.86	0.29	55,74,116,125	0
23	CLA	c	501	65/65	0.86	0.63	68,81,89,95	0
34	HEM	F	101	43/43	0.87	0.44	92,104,127,128	0
23	CLA	b	614	65/65	0.87	0.34	57,71,79,93	0
23	CLA	b	615	65/65	0.87	0.33	62,72,83,94	0

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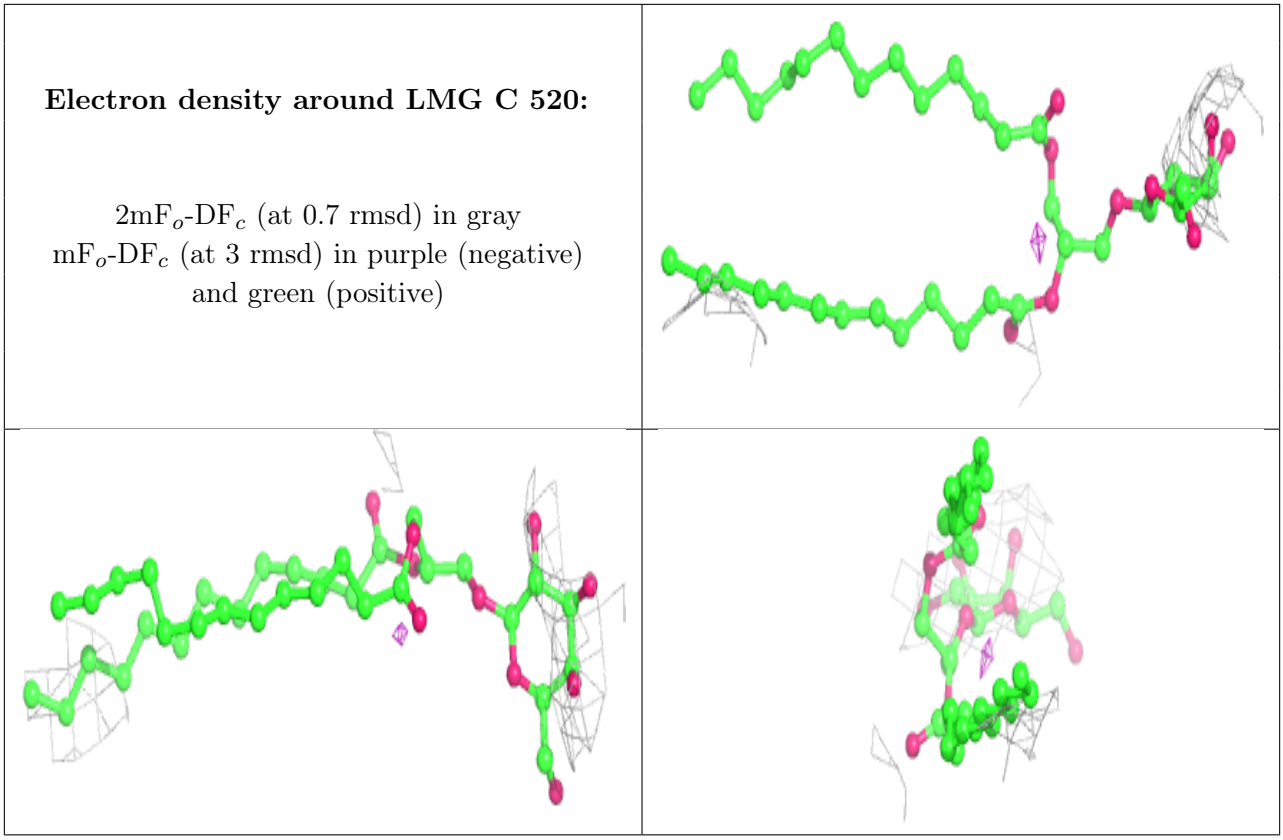
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	615	65/65	0.87	0.63	82,94,108,116	0
22	BCT	d	401	4/4	0.88	0.26	77,80,82,85	0
23	CLA	B	602	65/65	0.88	0.53	68,87,96,99	0
23	CLA	c	503	65/65	0.88	0.80	73,89,97,103	0
23	CLA	B	603	65/65	0.88	0.69	65,80,91,105	0
23	CLA	B	611	65/65	0.88	0.32	65,73,80,81	0
35	CA	k	101	1/1	0.88	0.21	94,94,94,94	0
23	CLA	B	612	65/65	0.88	0.40	56,69,84,87	0
23	CLA	c	508	65/65	0.89	0.30	73,84,120,134	0
23	CLA	A	403	65/65	0.89	0.27	47,58,67,68	0
32	CL	d	409	1/1	0.89	0.25	49,49,49,49	0
34	HEM	v	201	43/43	0.89	0.46	61,68,75,78	0
23	CLA	c	510	65/65	0.90	0.33	66,74,85,87	0
23	CLA	B	607	65/65	0.90	0.25	56,64,84,91	0
23	CLA	B	613	65/65	0.90	0.27	44,63,88,92	0
34	HEM	V	201	43/43	0.90	0.35	46,65,74,79	0
34	HEM	f	101	43/43	0.90	0.38	77,103,125,130	0
23	CLA	a	404	65/65	0.91	0.35	44,58,65,73	0
31	LMG	b	623	49/55	0.91	0.25	57,80,96,113	0
23	CLA	D	401	65/65	0.91	0.26	47,58,85,99	0
23	CLA	A	404	65/65	0.92	0.33	39,54,66,70	0
28	DGD	C	516	53/66	0.92	0.25	58,75,97,102	0
22	BCT	A	402	4/4	0.92	0.43	84,88,89,93	0
23	CLA	b	616	65/65	0.93	0.32	54,68,90,92	0
21	FE2	A	401	1/1	0.94	0.15	60,60,60,60	0
26	OEC	a	411	5/9	0.94	0.39	35,44,62,62	0
26	OEC	A	409	5/9	0.96	0.43	35,44,46,62	0
21	FE2	a	403	1/1	0.97	0.13	70,70,70,70	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.

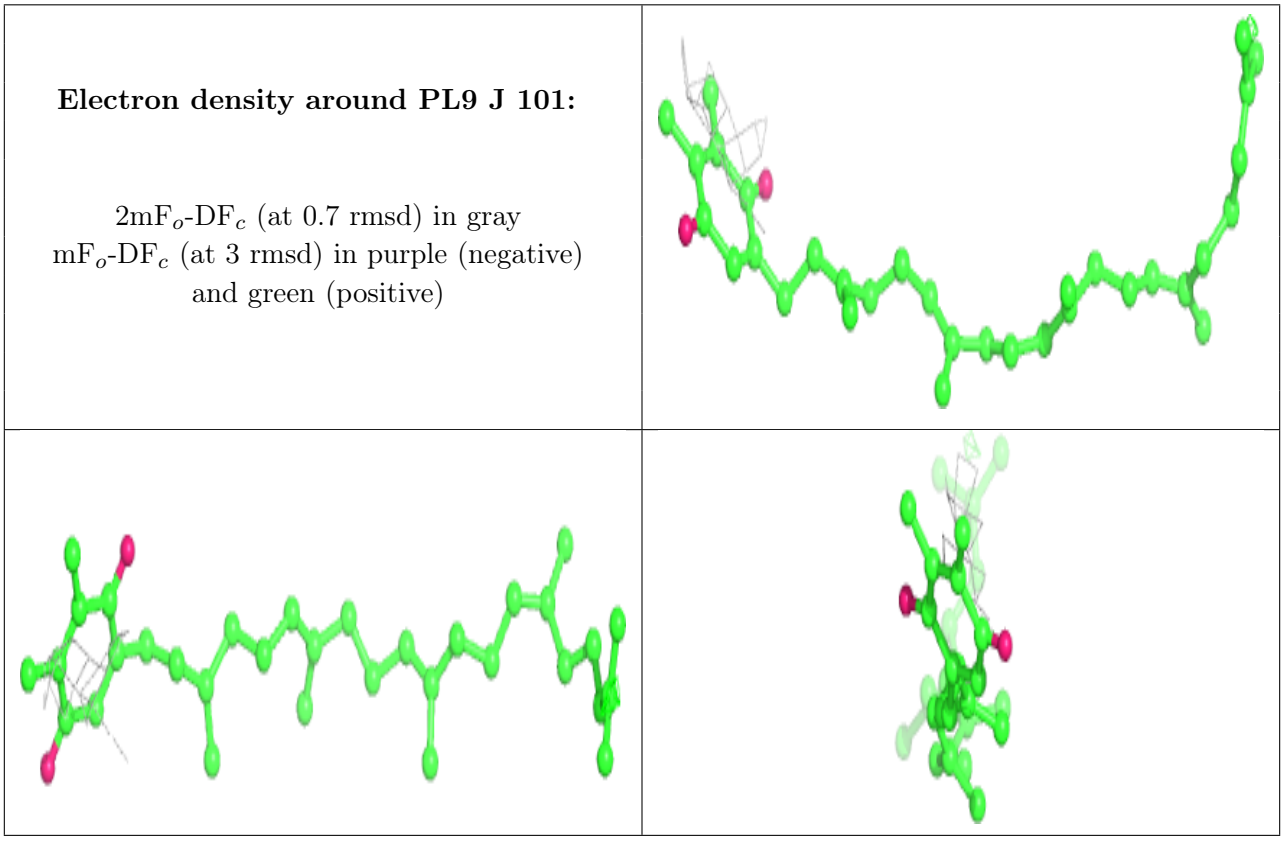
Electron density around LMG C 520:

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



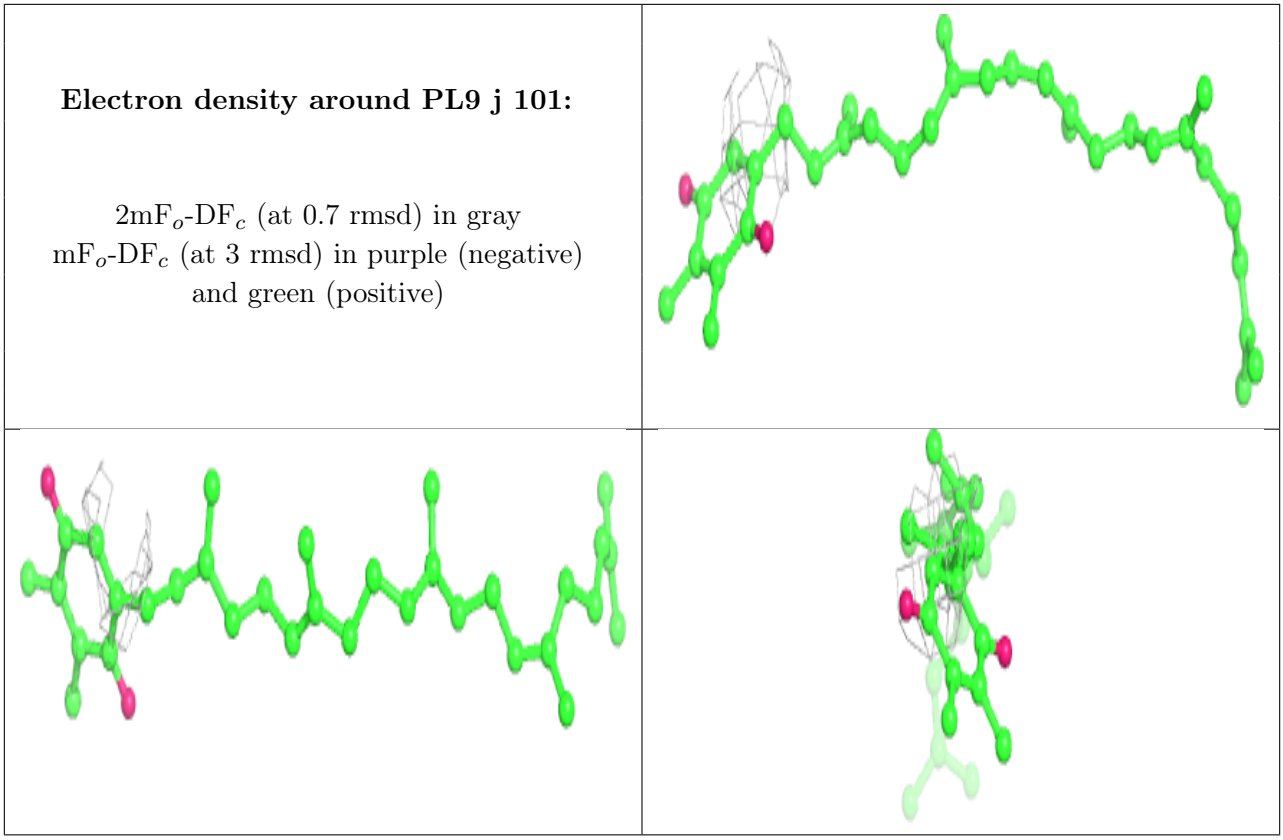
Electron density around PL9 J 101:

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



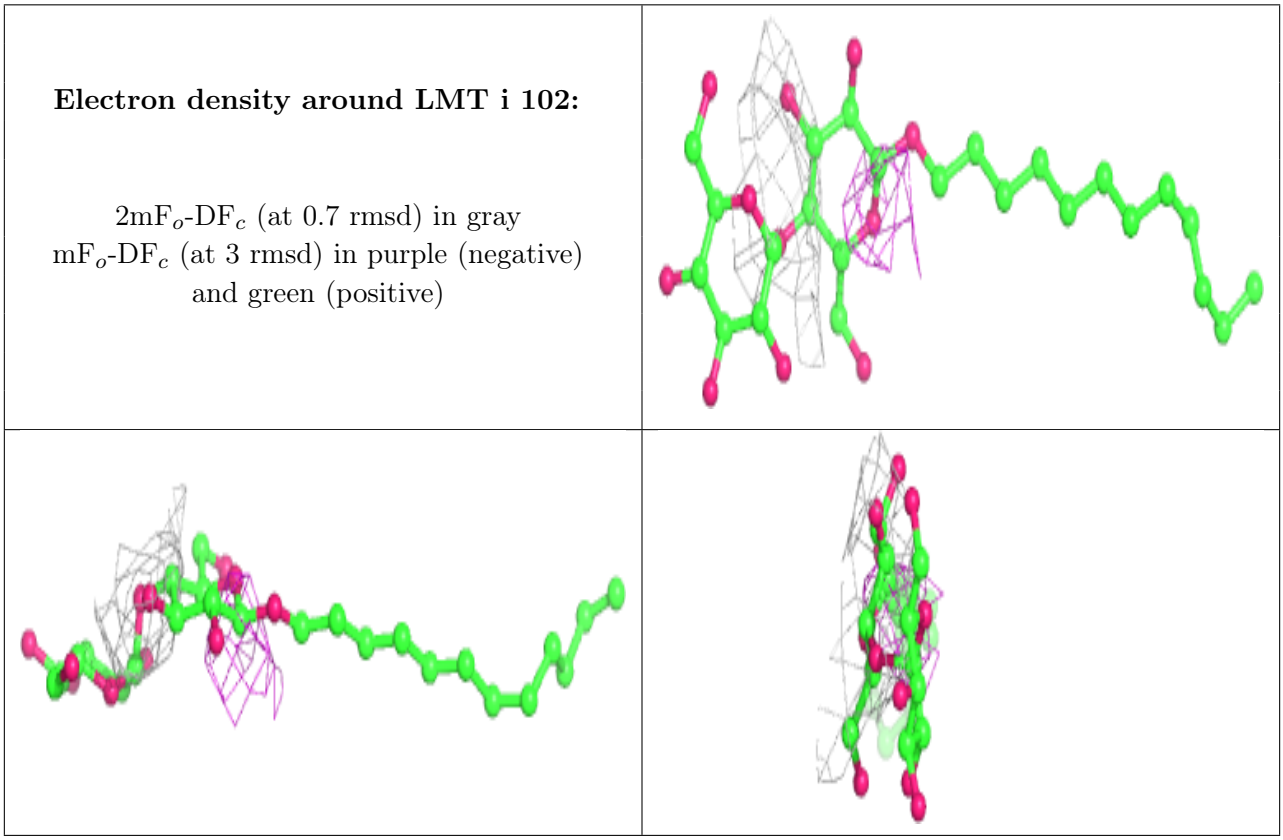
Electron density around PL9 j 101:

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



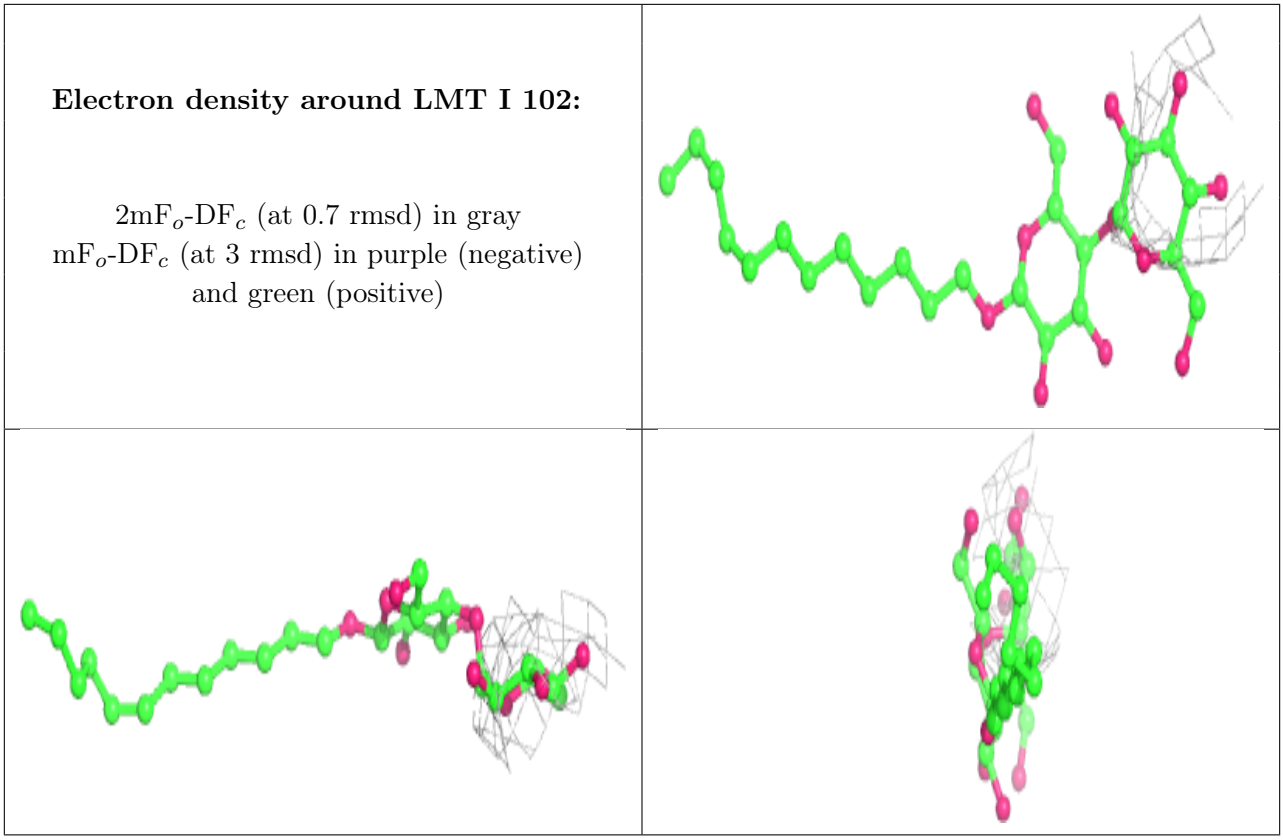
Electron density around LMT i 102:

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



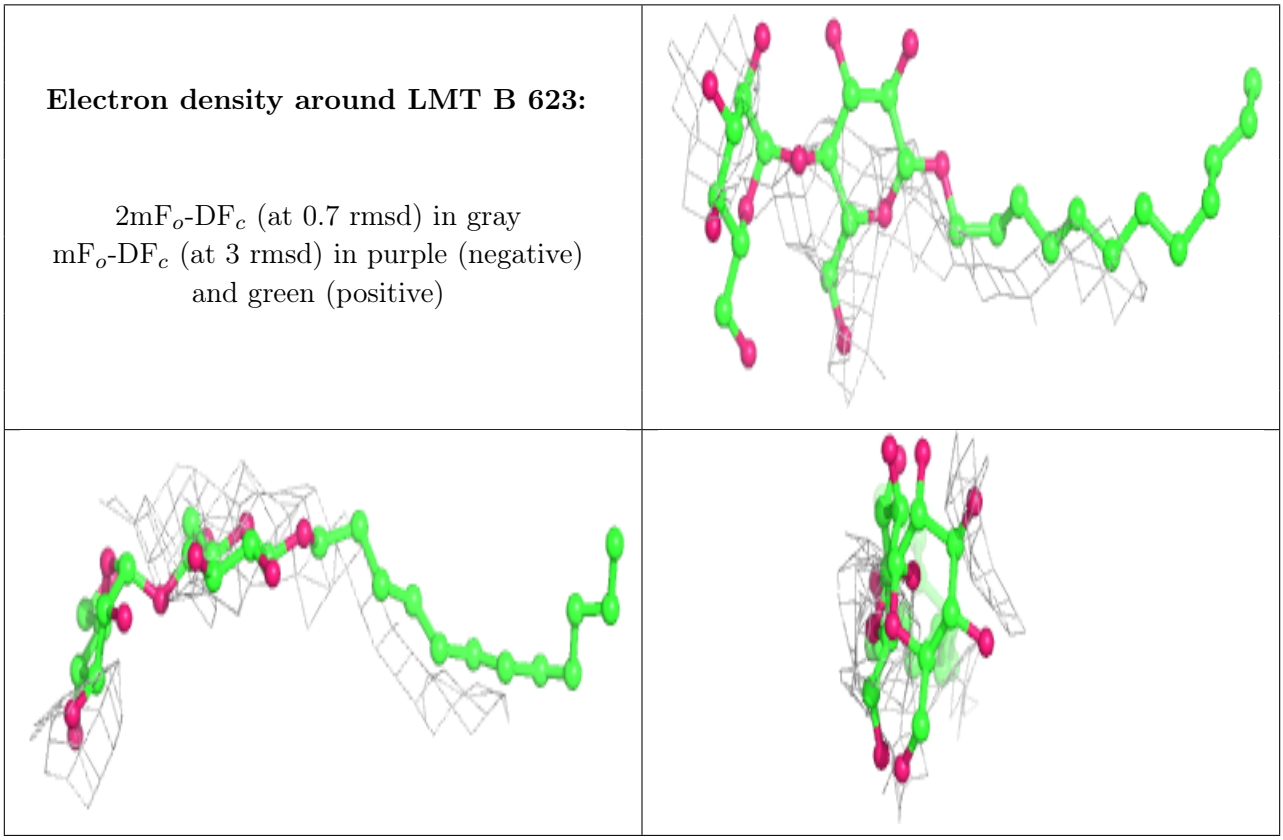
Electron density around LMT I 102:

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



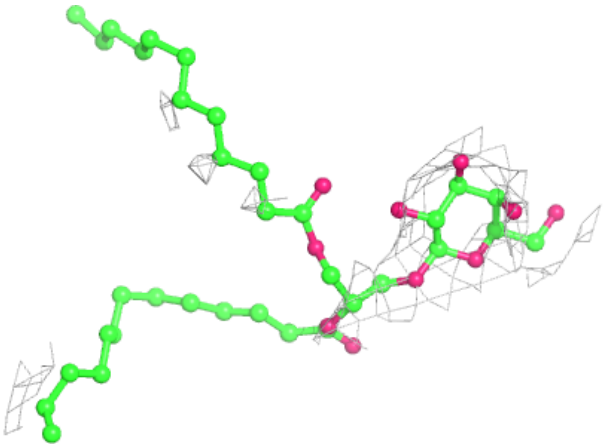
Electron density around LMT B 623:

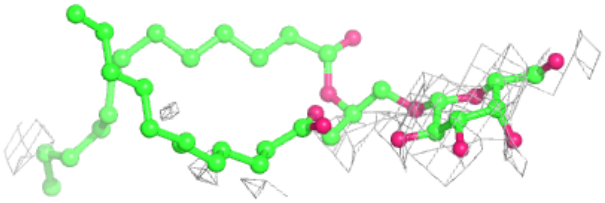
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

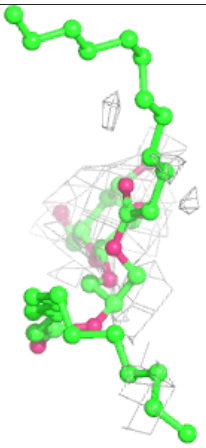


Electron density around LMG E 101:

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

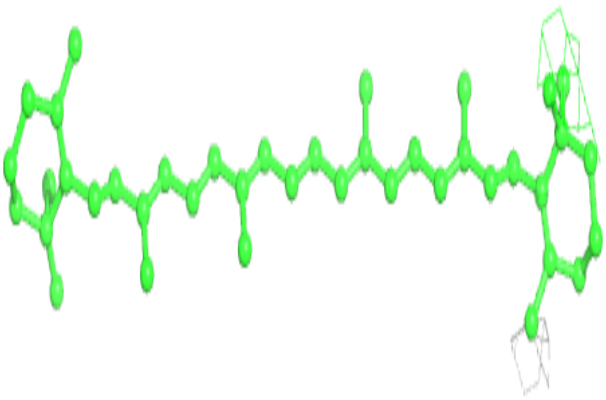


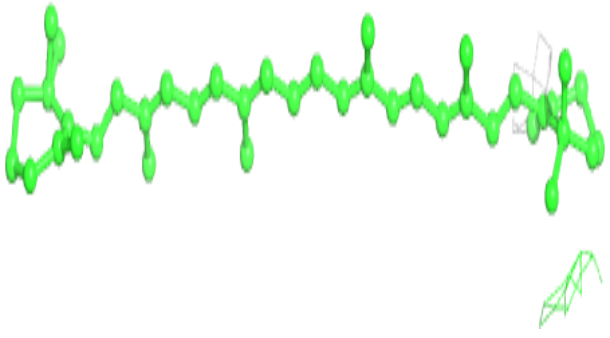




Electron density around BCR j 102:

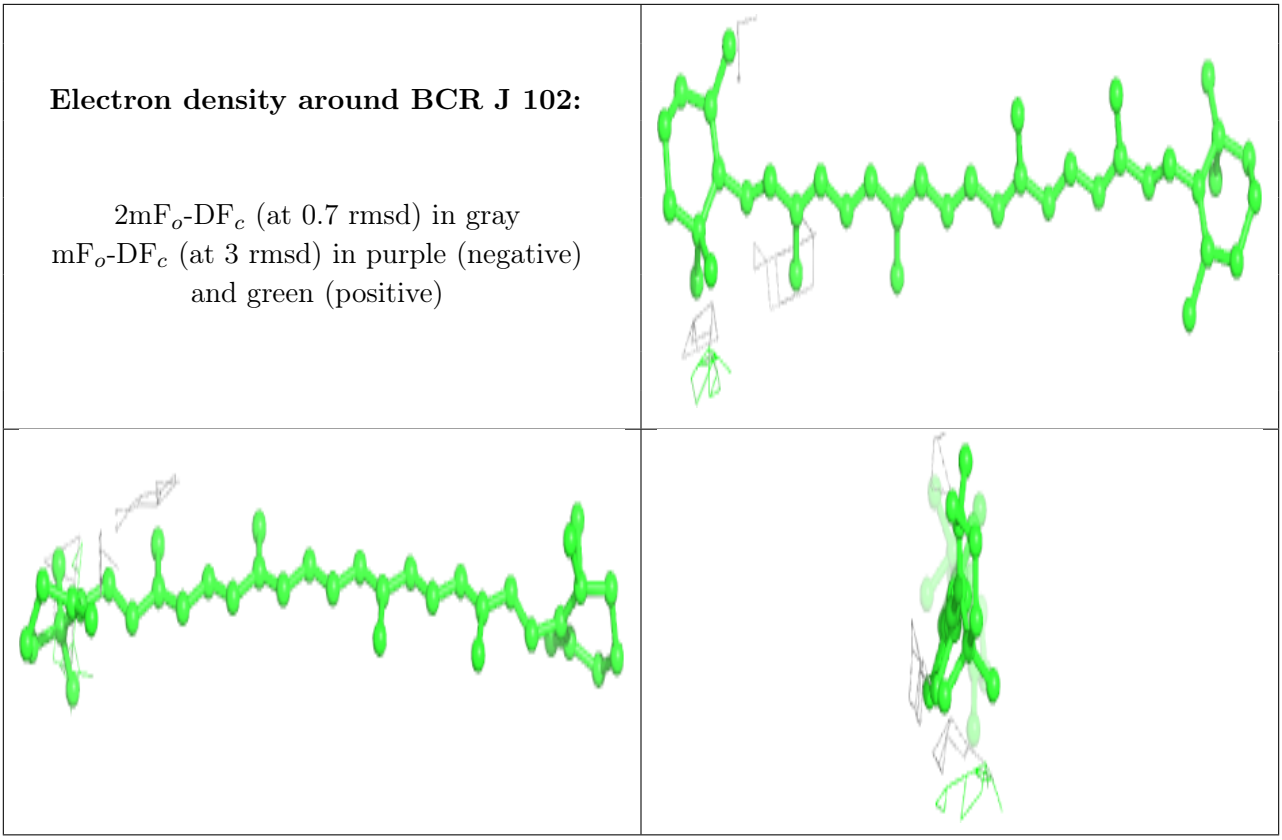
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





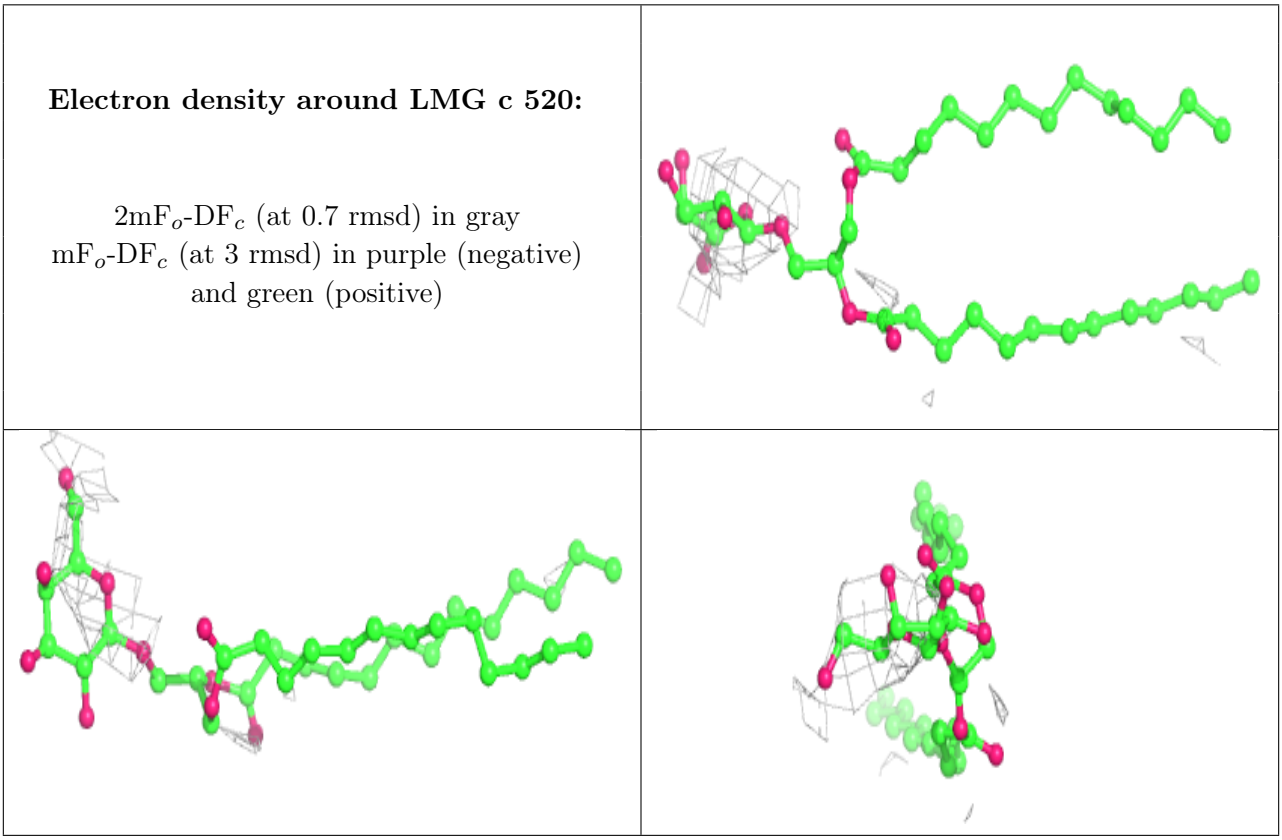
Electron density around BCR J 102:

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



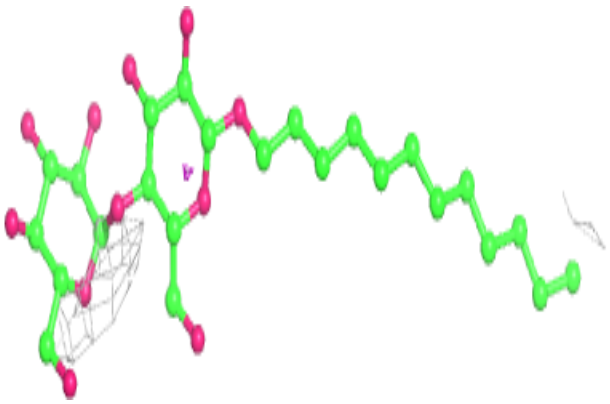
Electron density around LMG c 520:

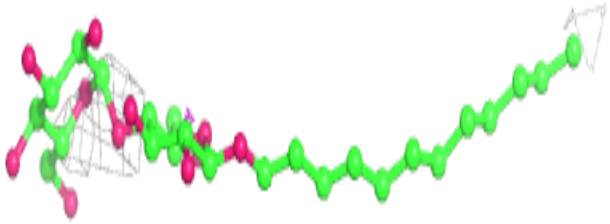
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

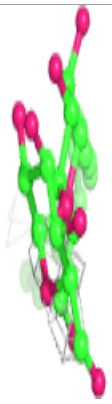


Electron density around LMT b 626:

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

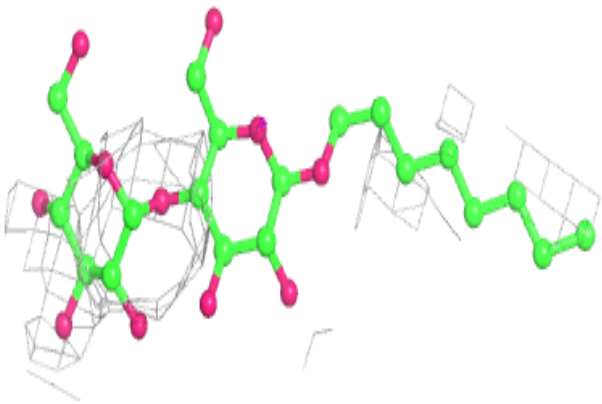


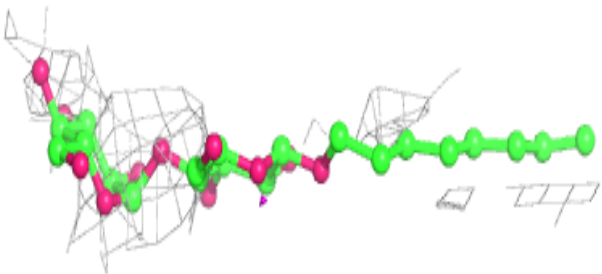




Electron density around LMT x 102:

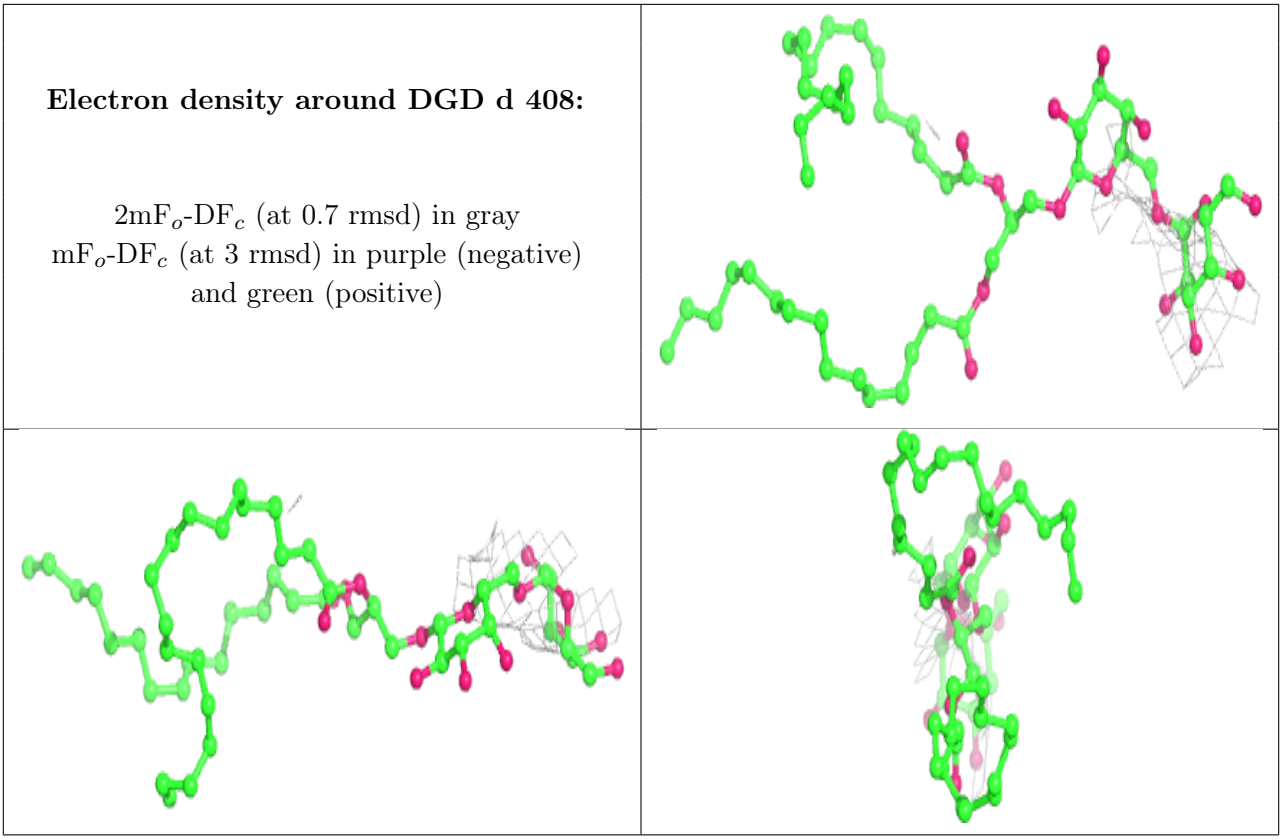
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





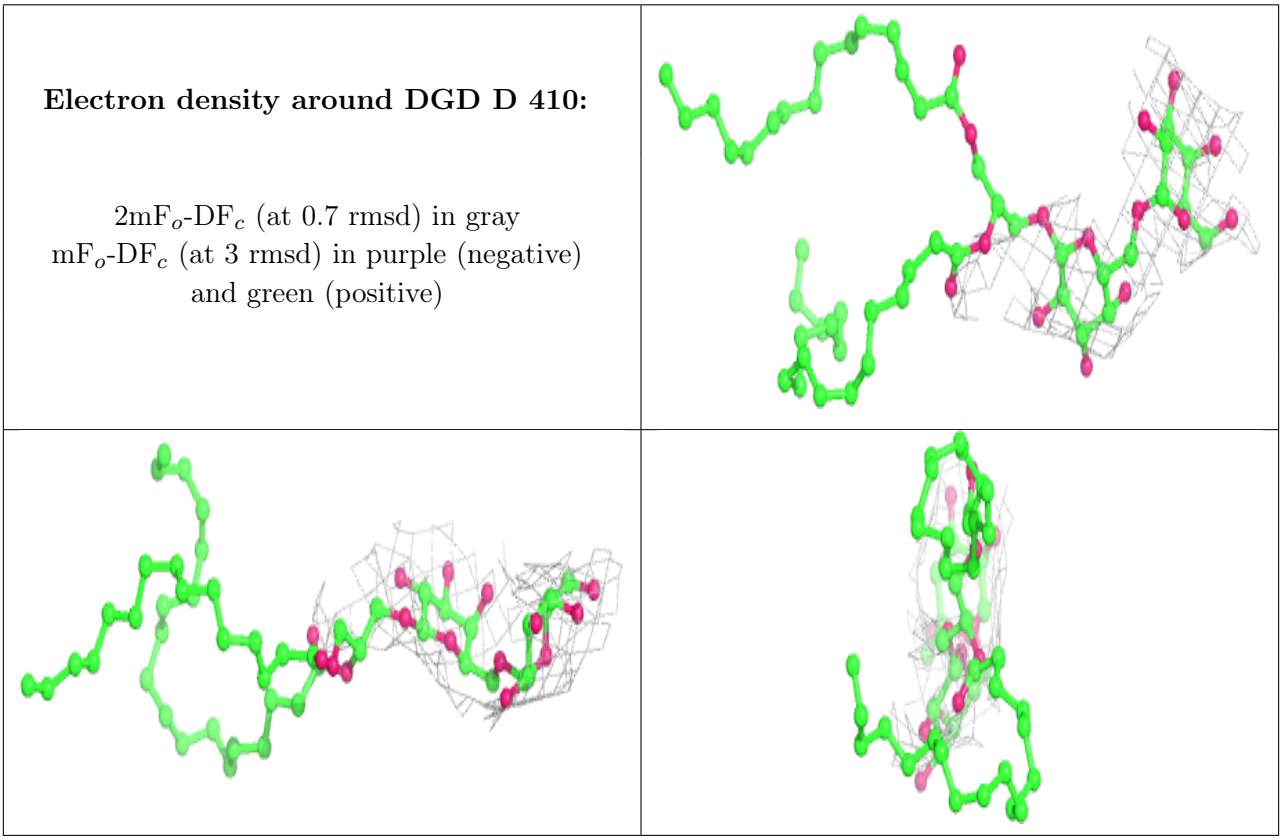
Electron density around DGD d 408:

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



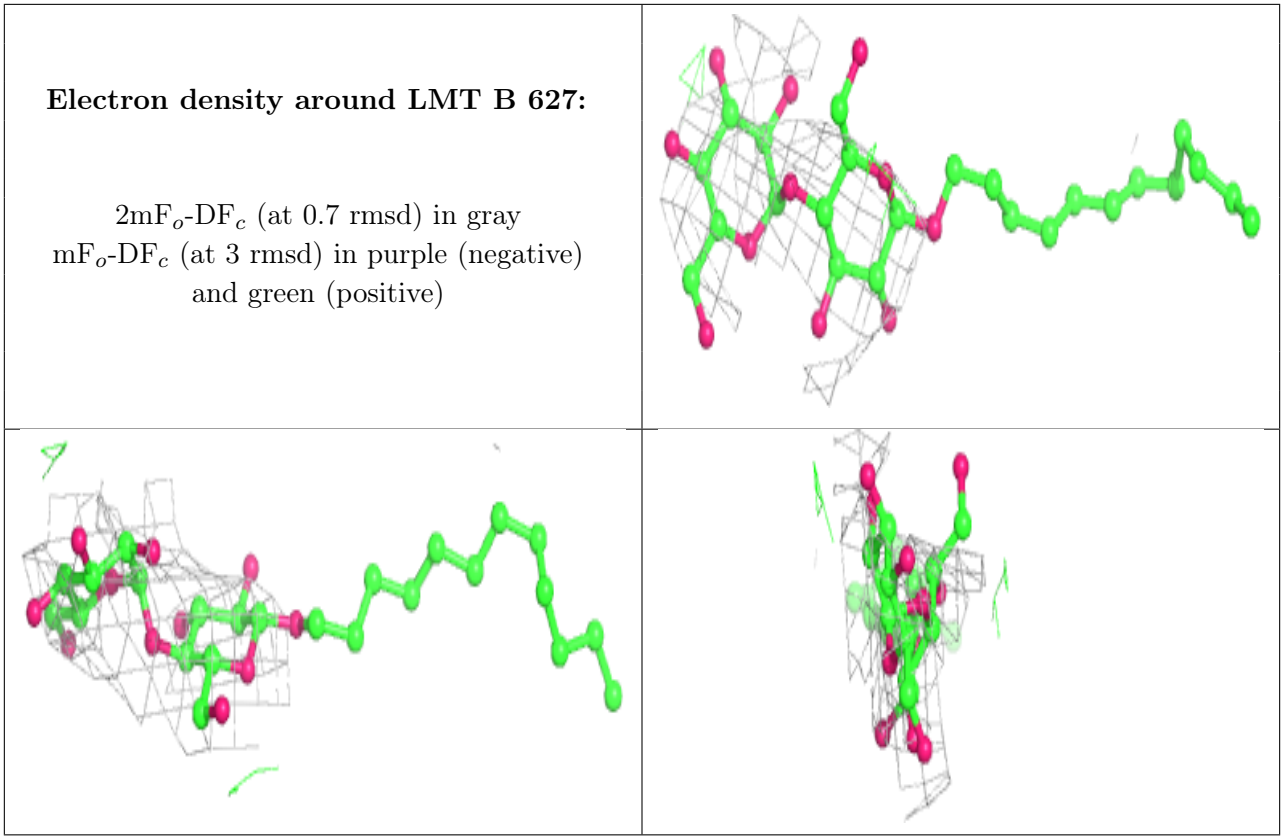
Electron density around DGD D 410:

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



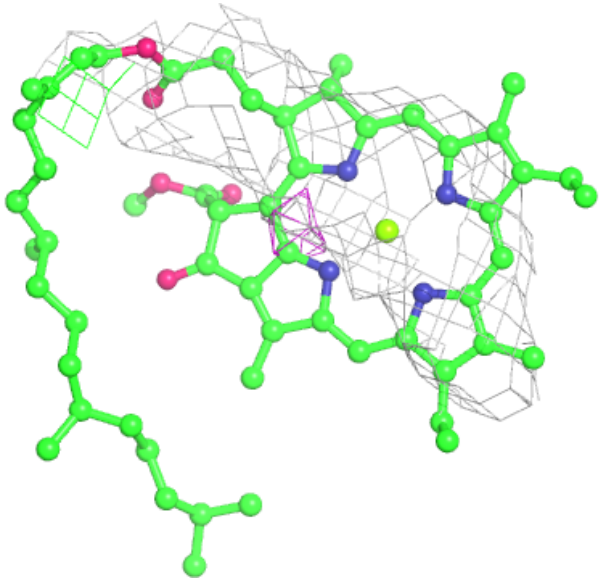
Electron density around LMT B 627:

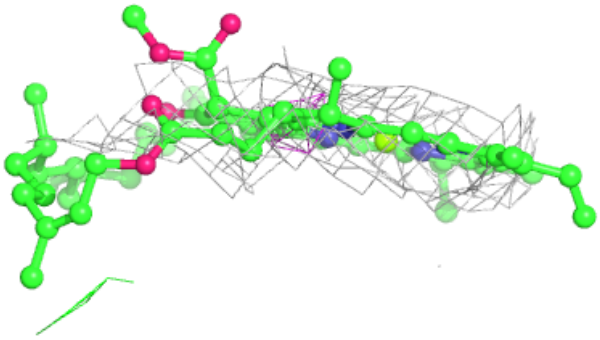
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

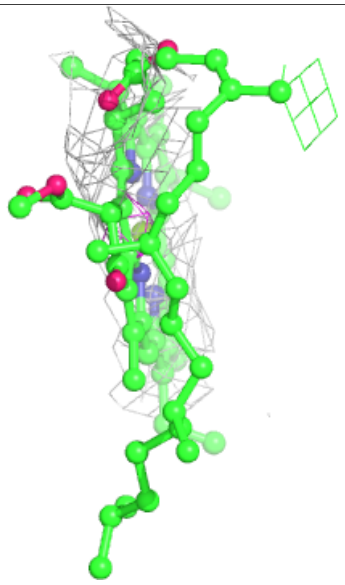


Electron density around CLA b 604:

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

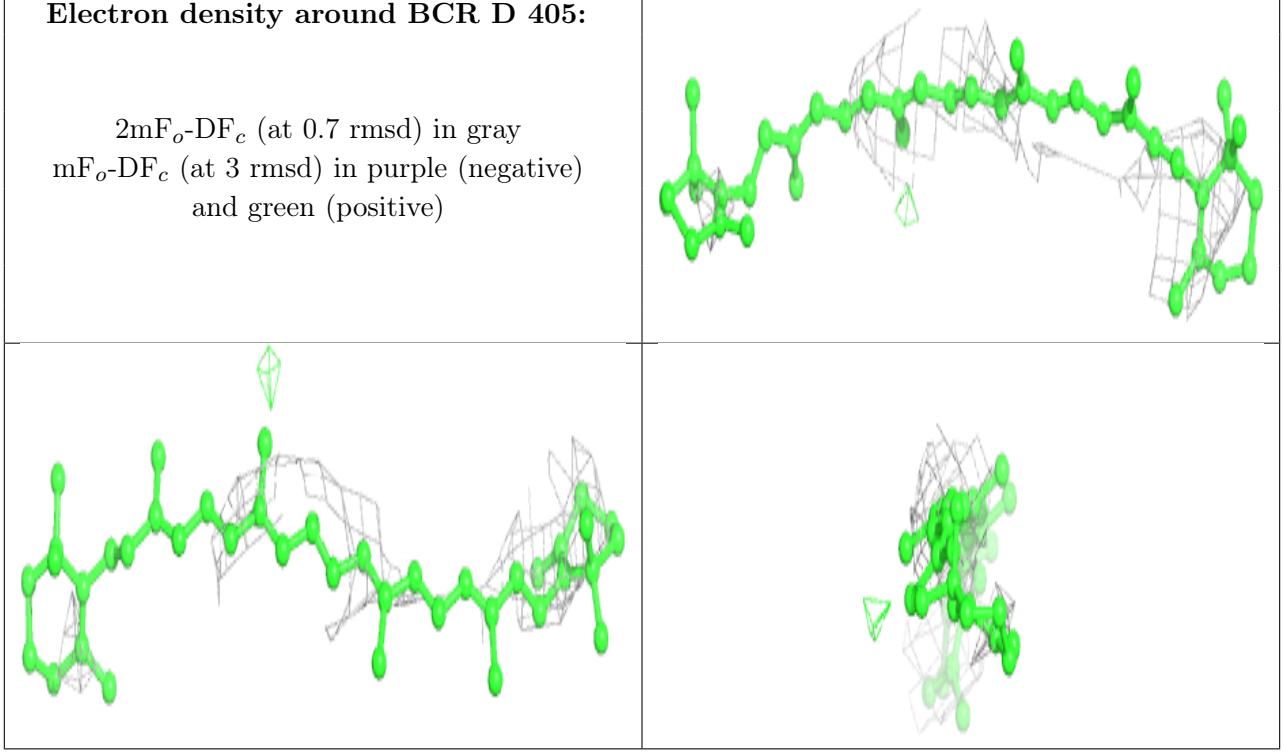






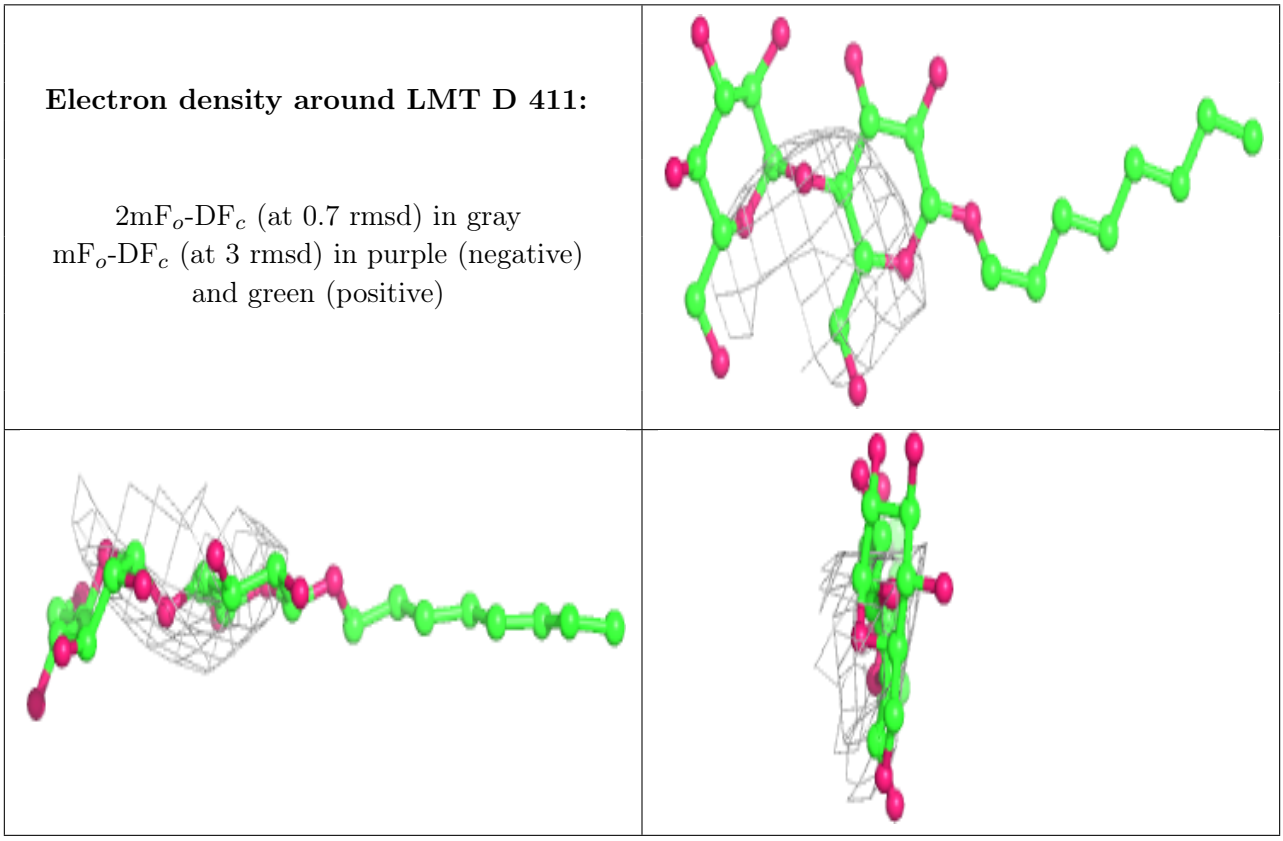
Electron density around BCR D 405:

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



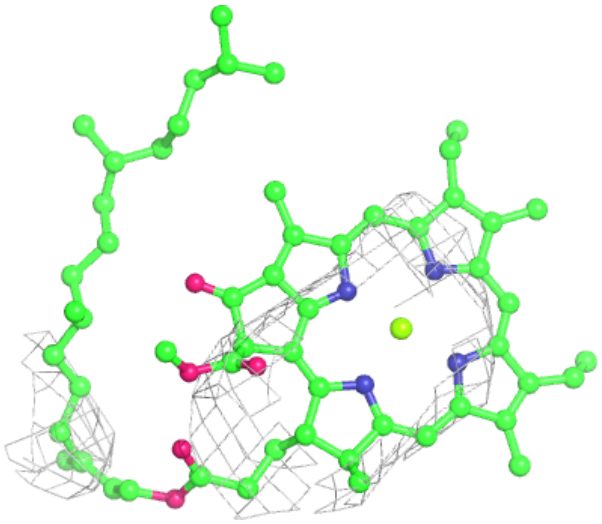
Electron density around LMT D 411:

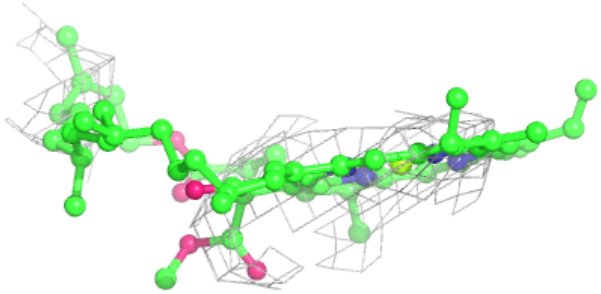
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

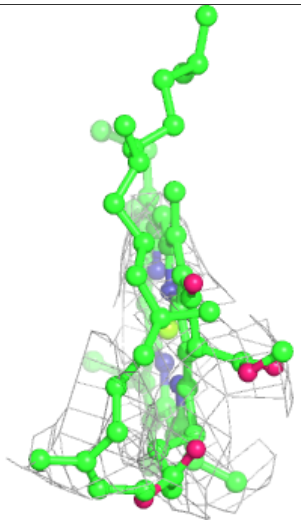


Electron density around CLA B 601:

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

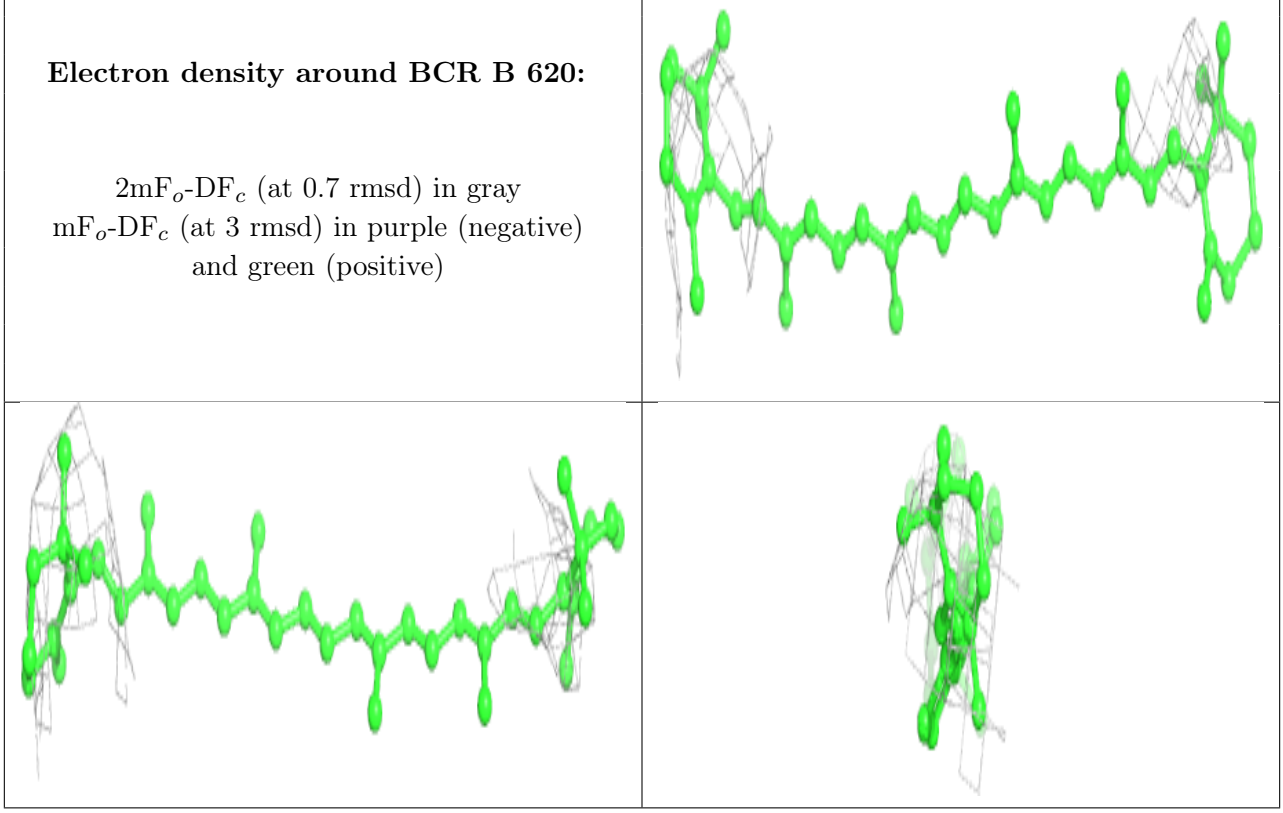






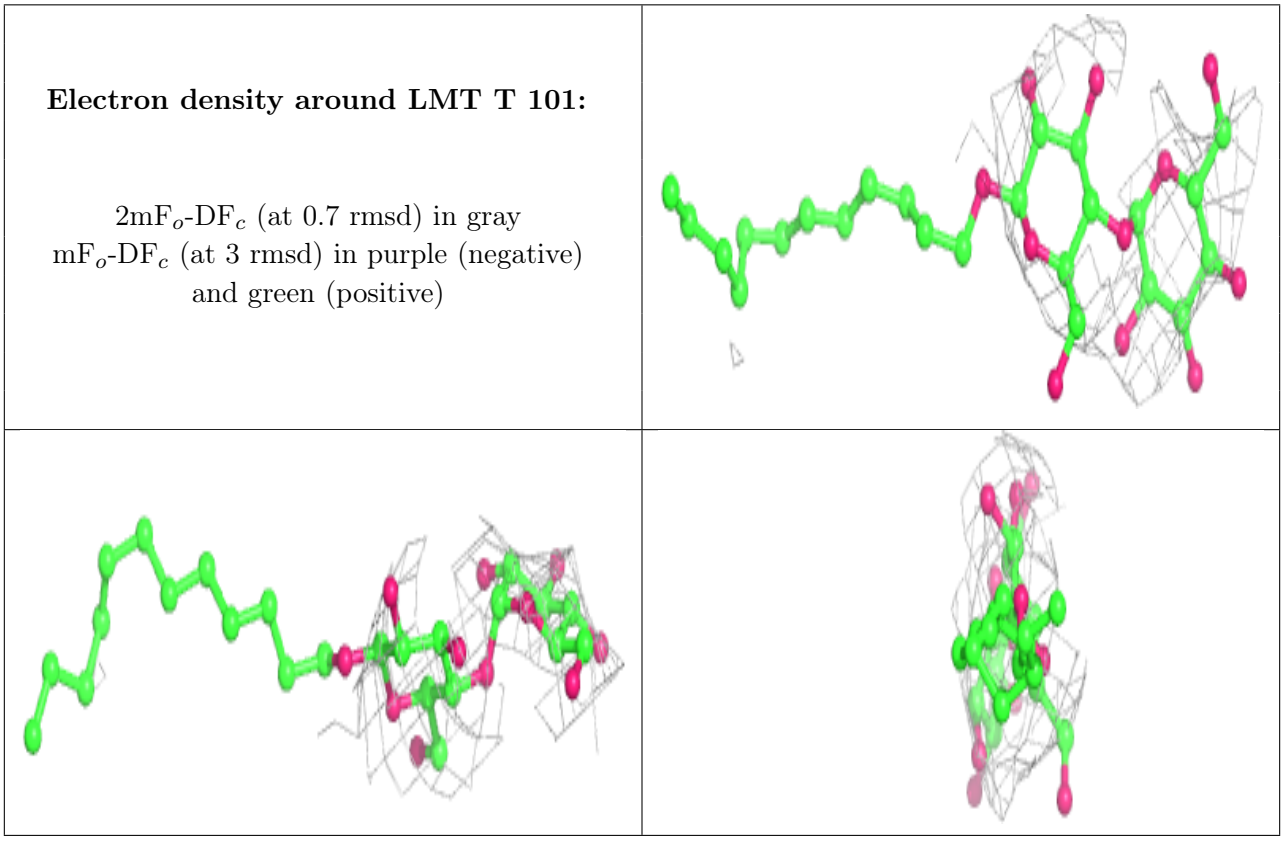
Electron density around BCR B 620:

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



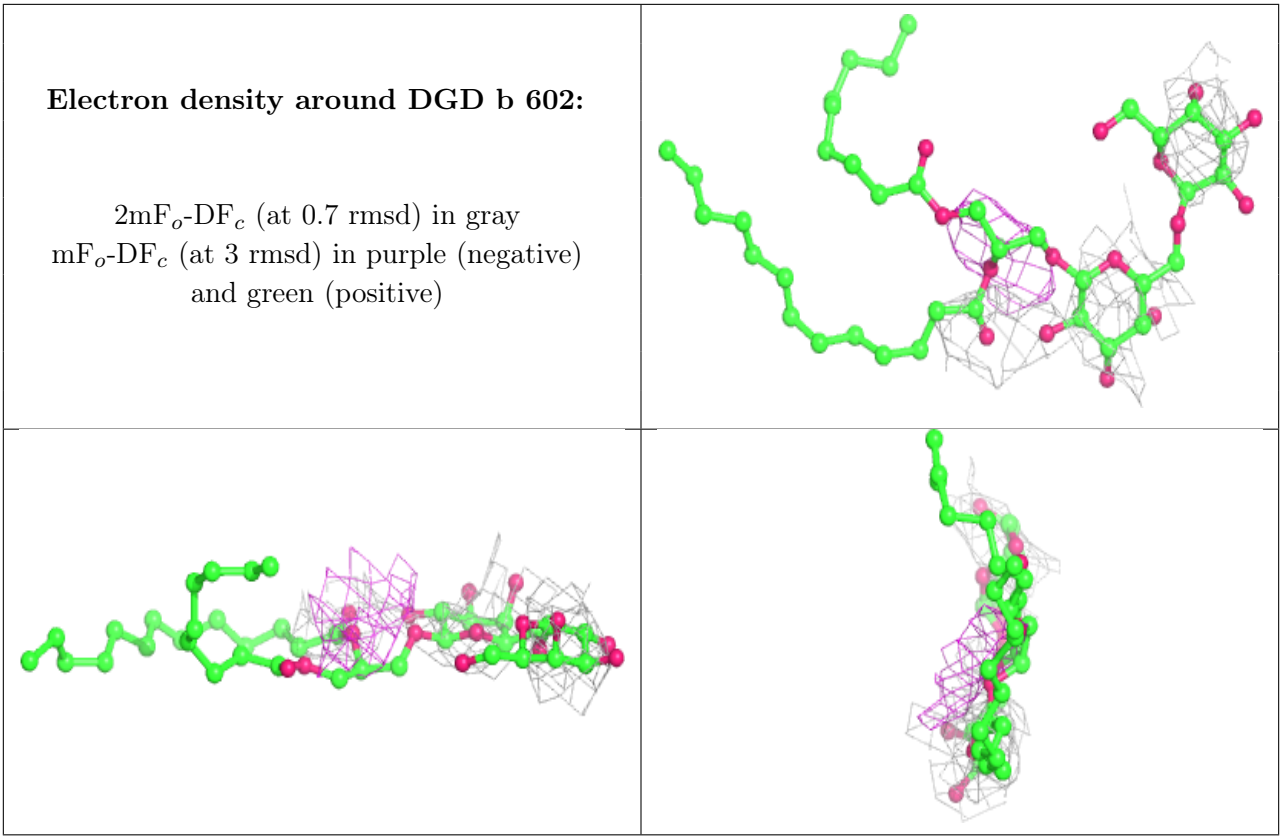
Electron density around LMT T 101:

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



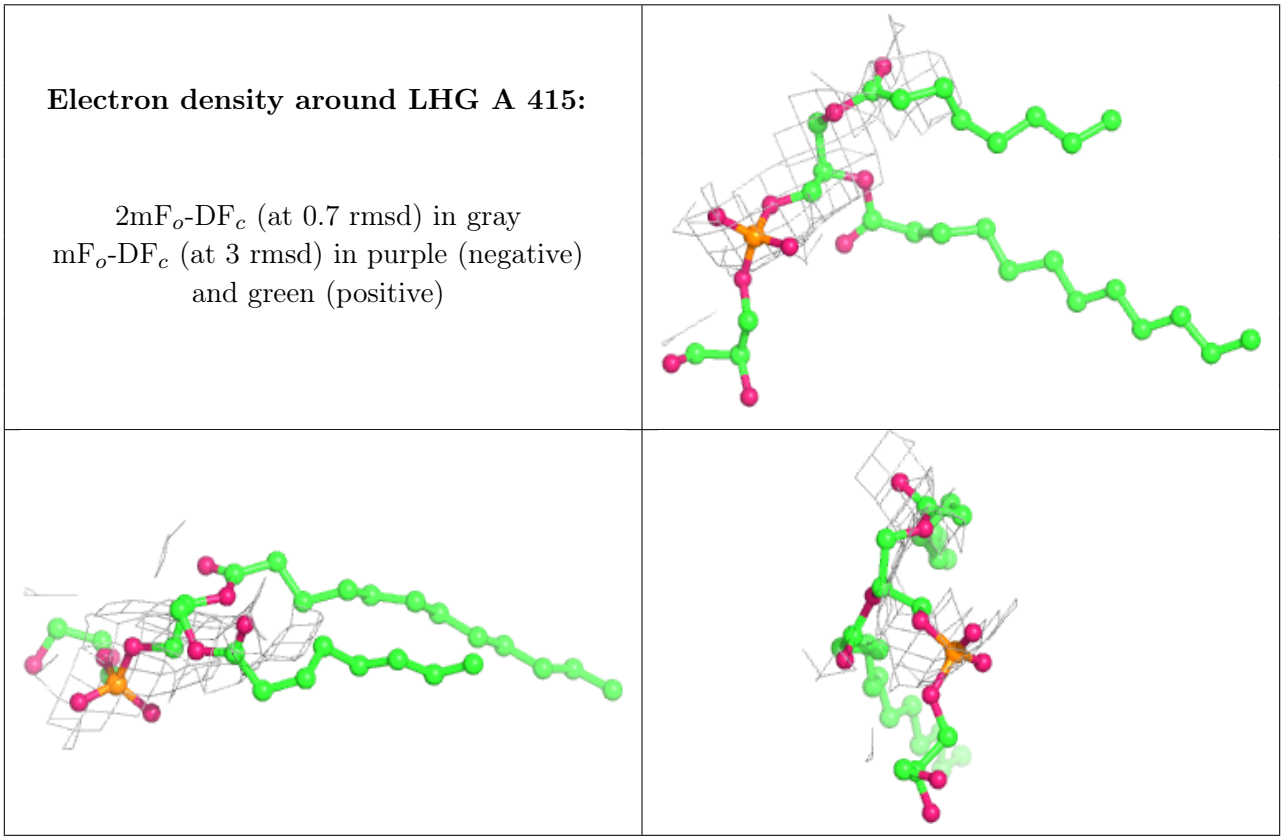
Electron density around DGD b 602:

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



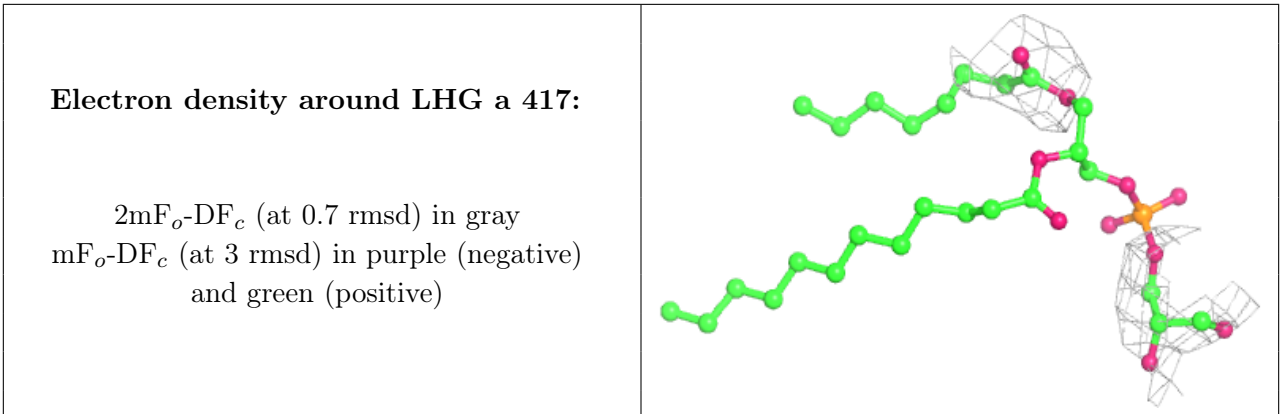
Electron density around LHG A 415:

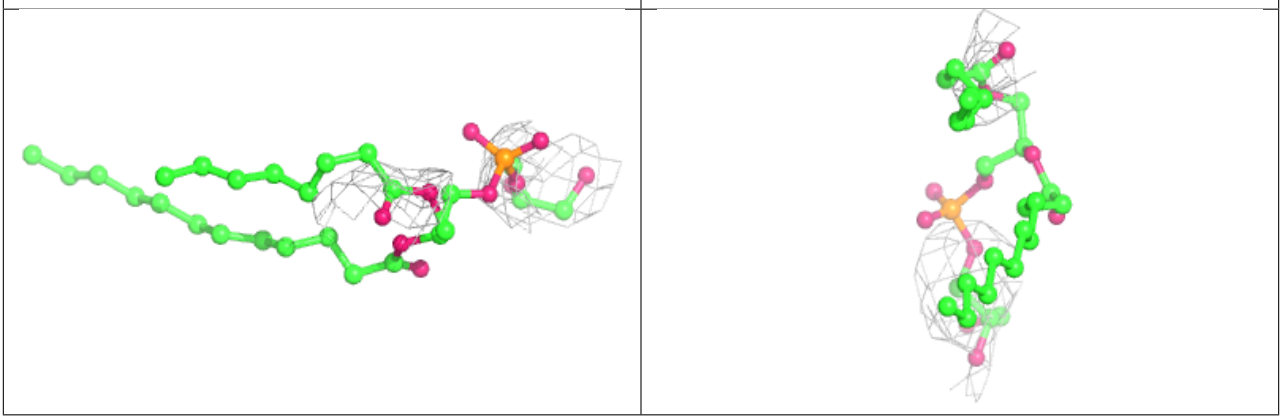
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG a 417:

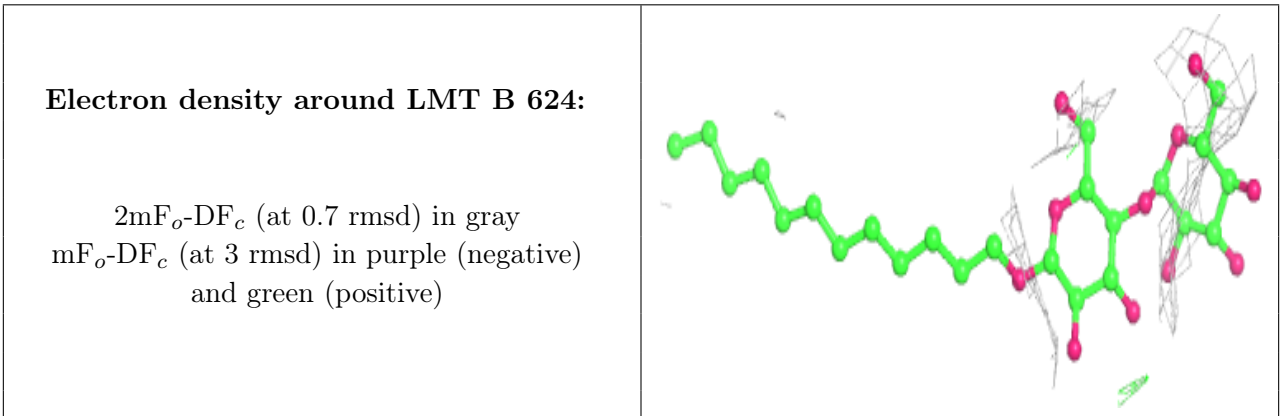
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

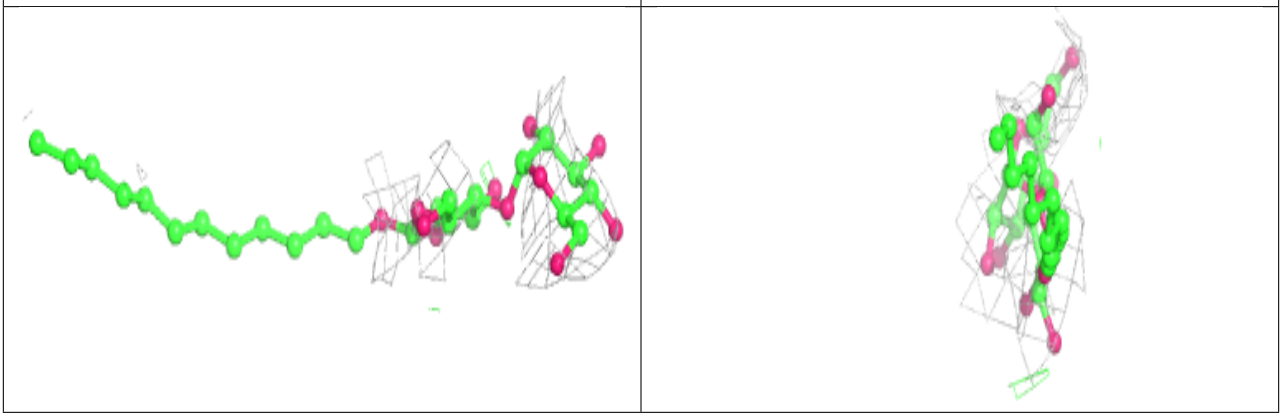




Electron density around LMT B 624:

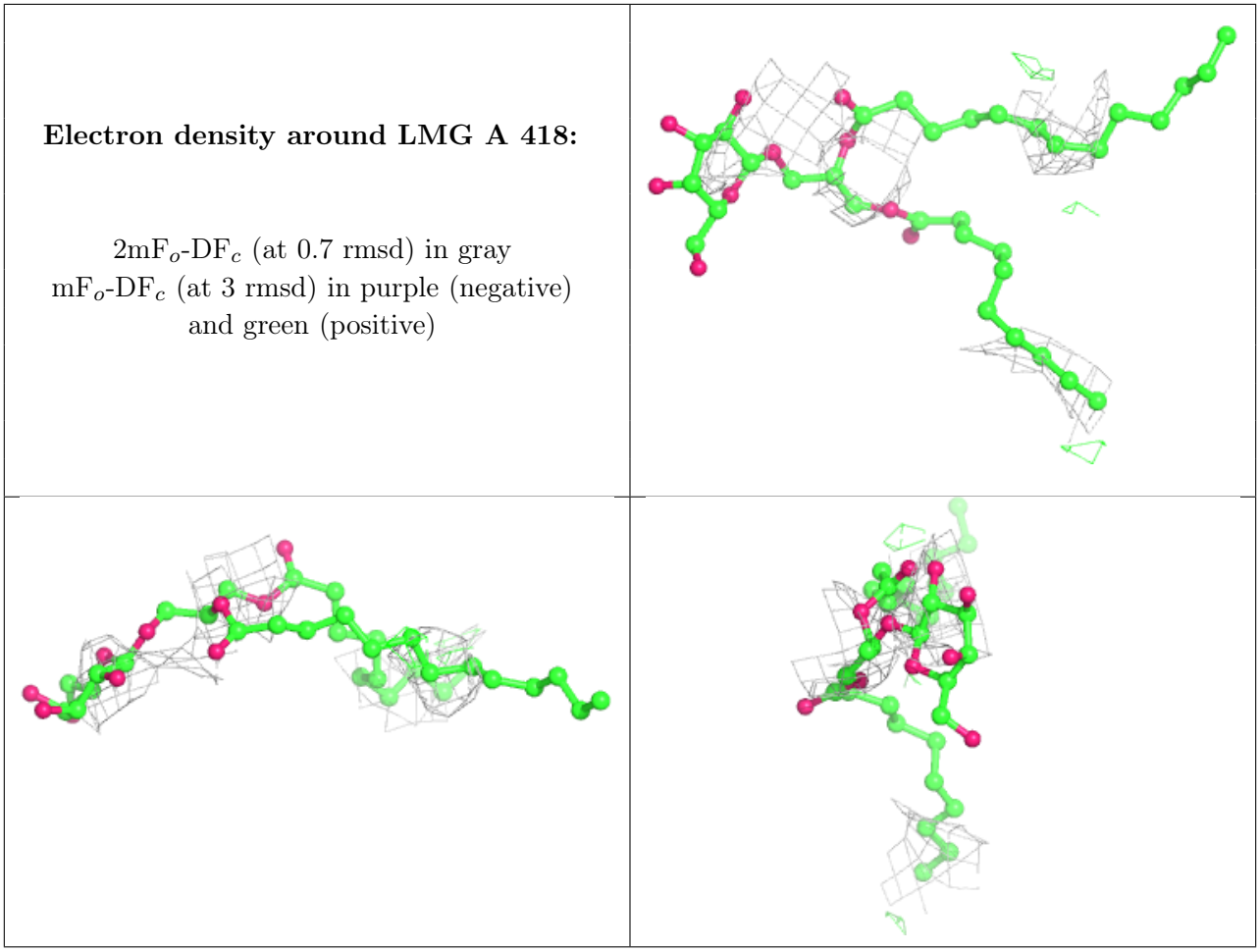
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





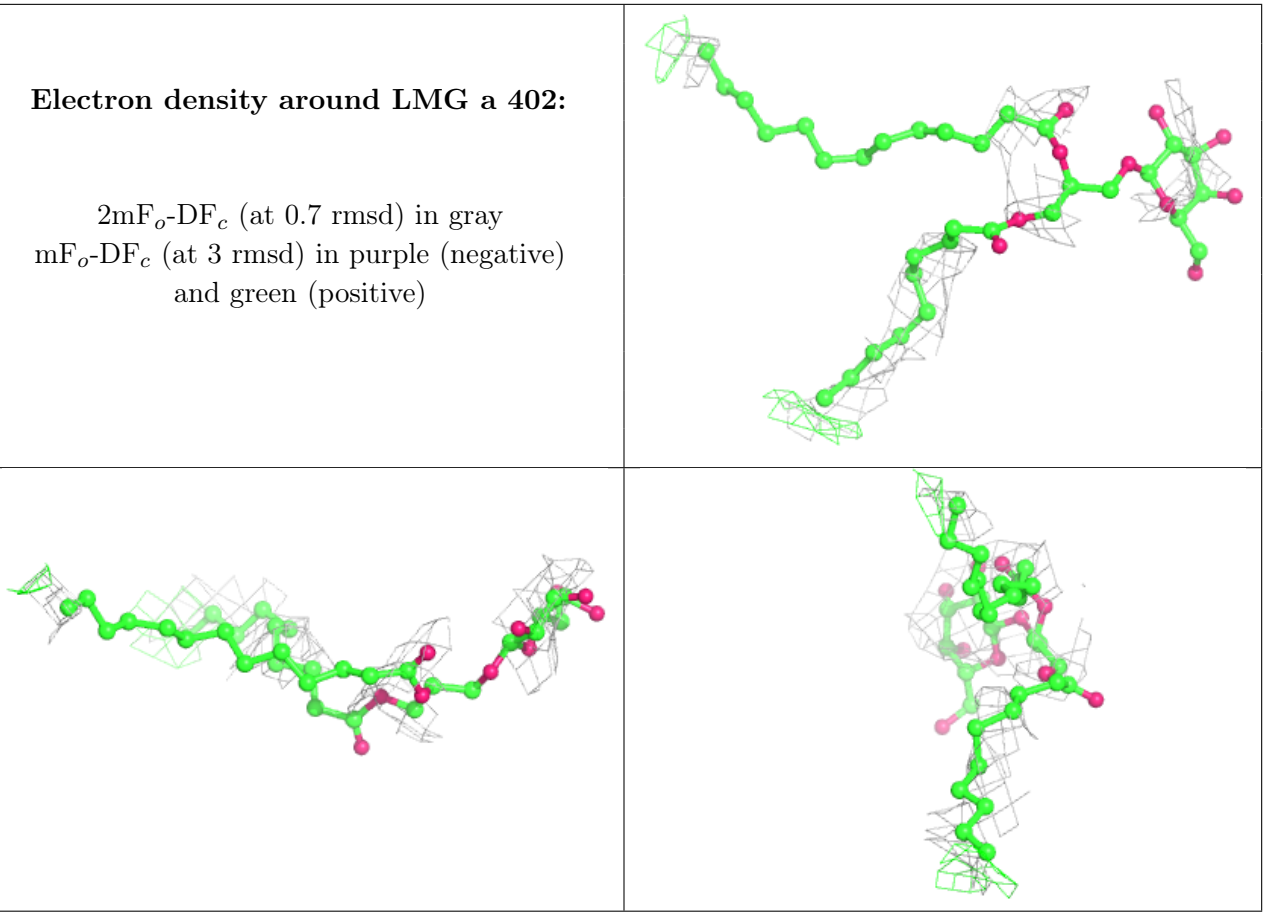
Electron density around LMG A 418:

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



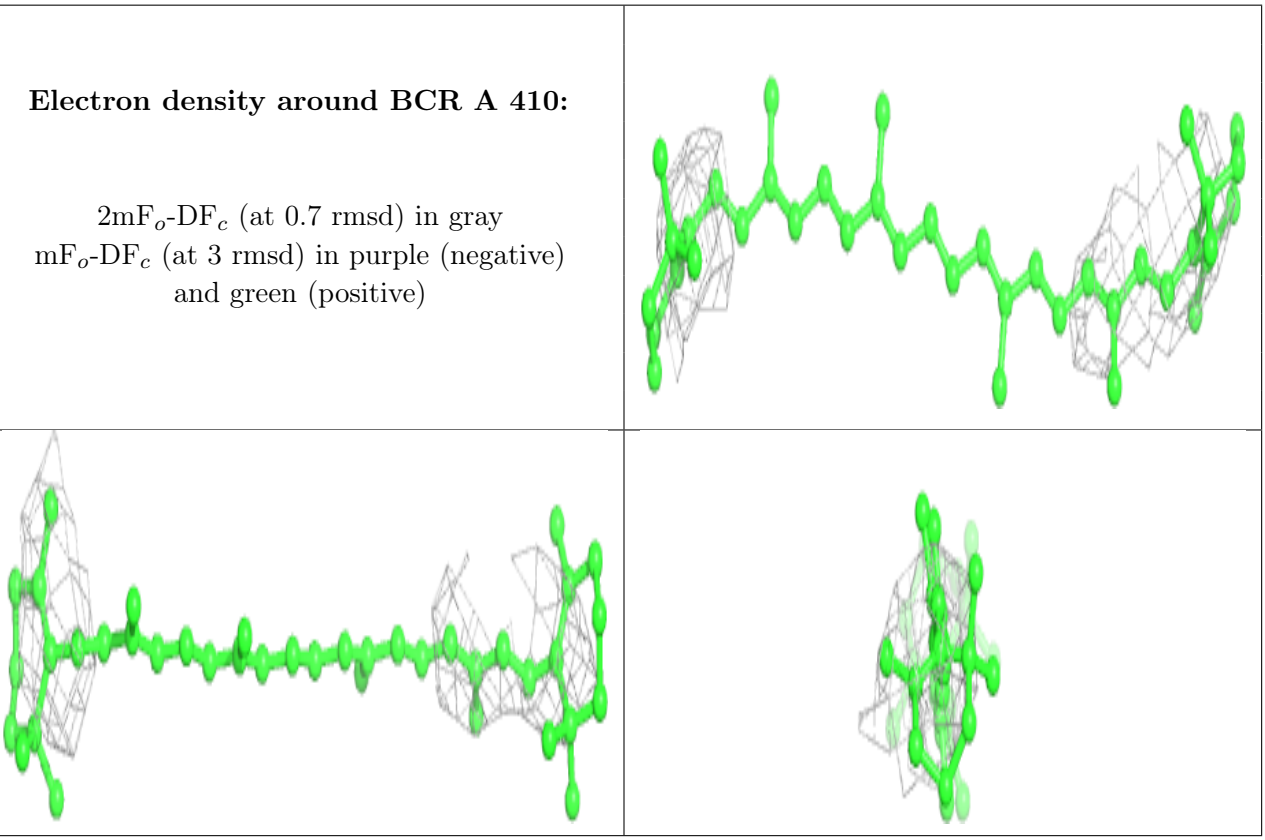
Electron density around LMG a 402:

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



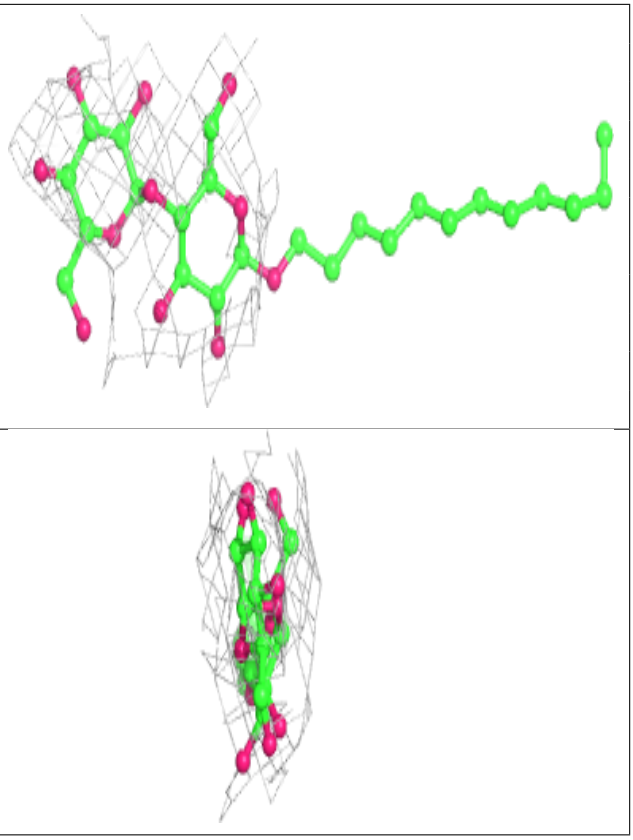
Electron density around BCR A 410:

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



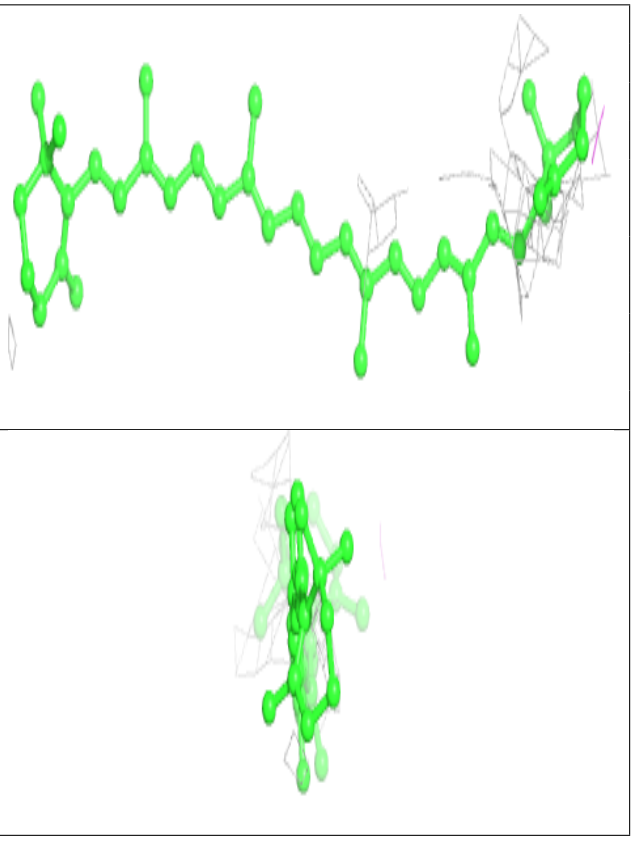
Electron density around LMT b 603:

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



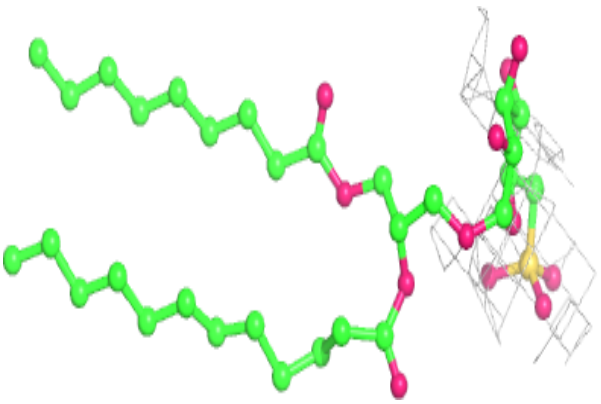
Electron density around BCR H 101:

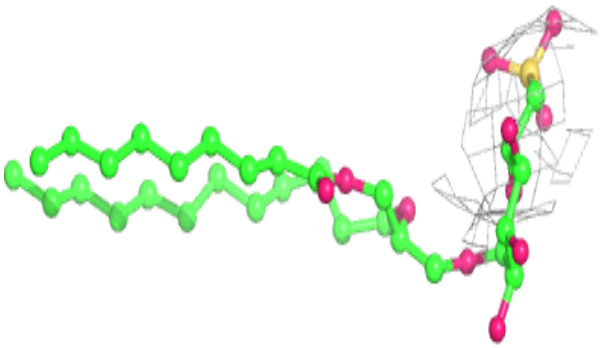
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

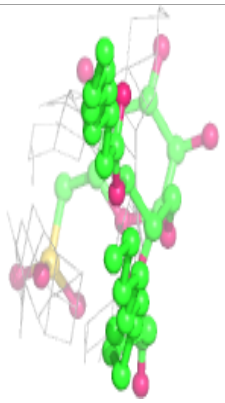


Electron density around SQD d 407:

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

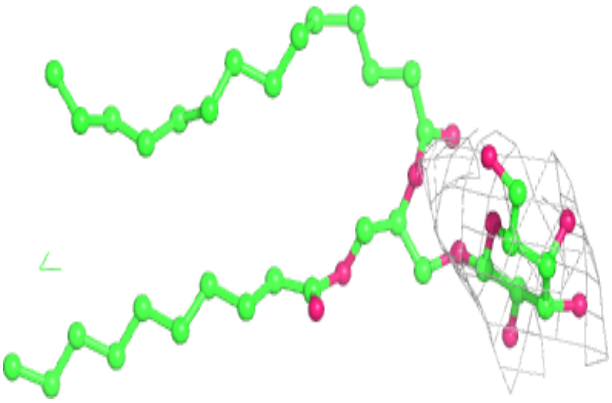


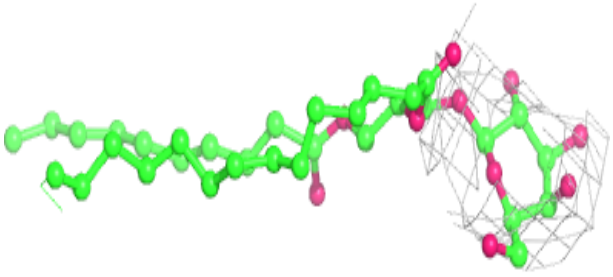


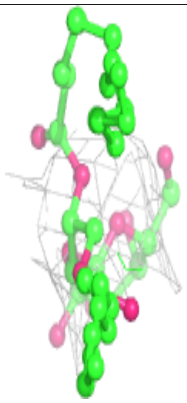


Electron density around LMG I 101:

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

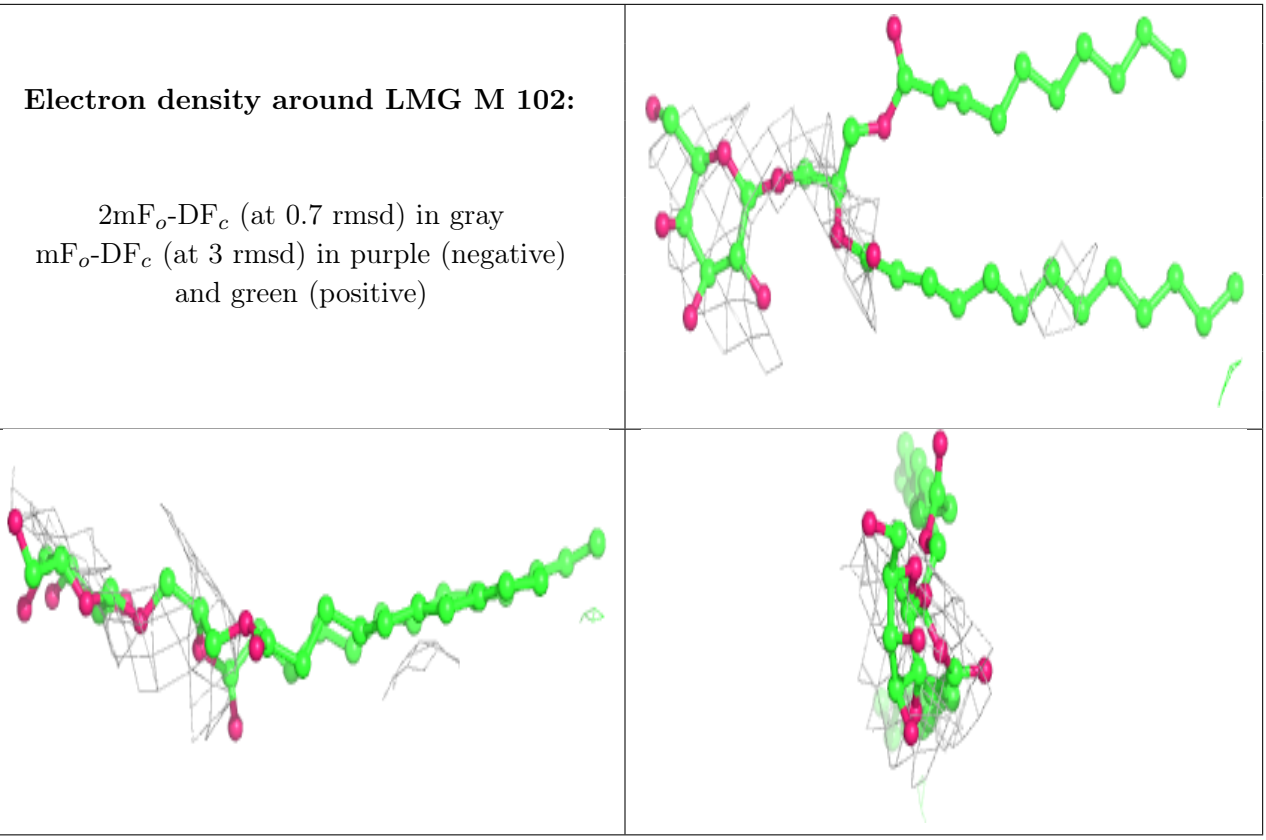






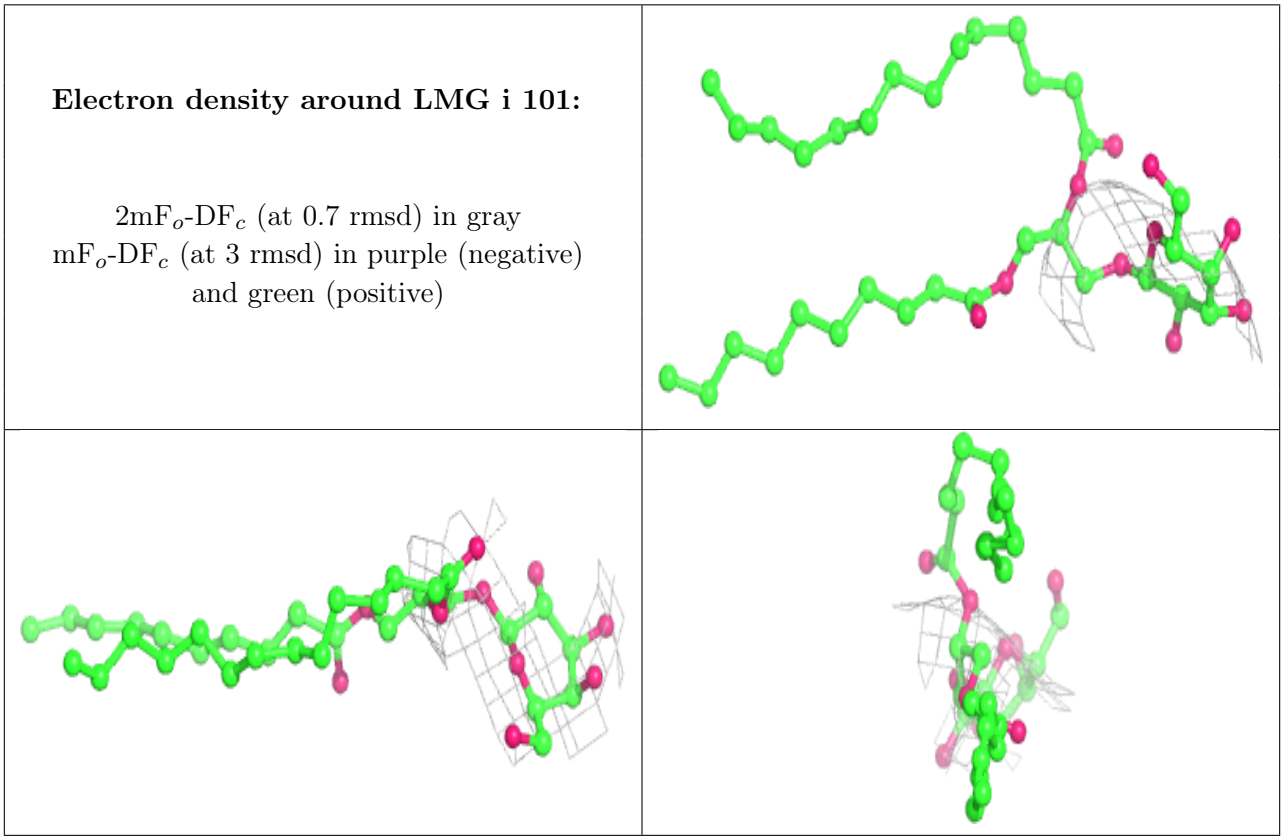
Electron density around LMG M 102:

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



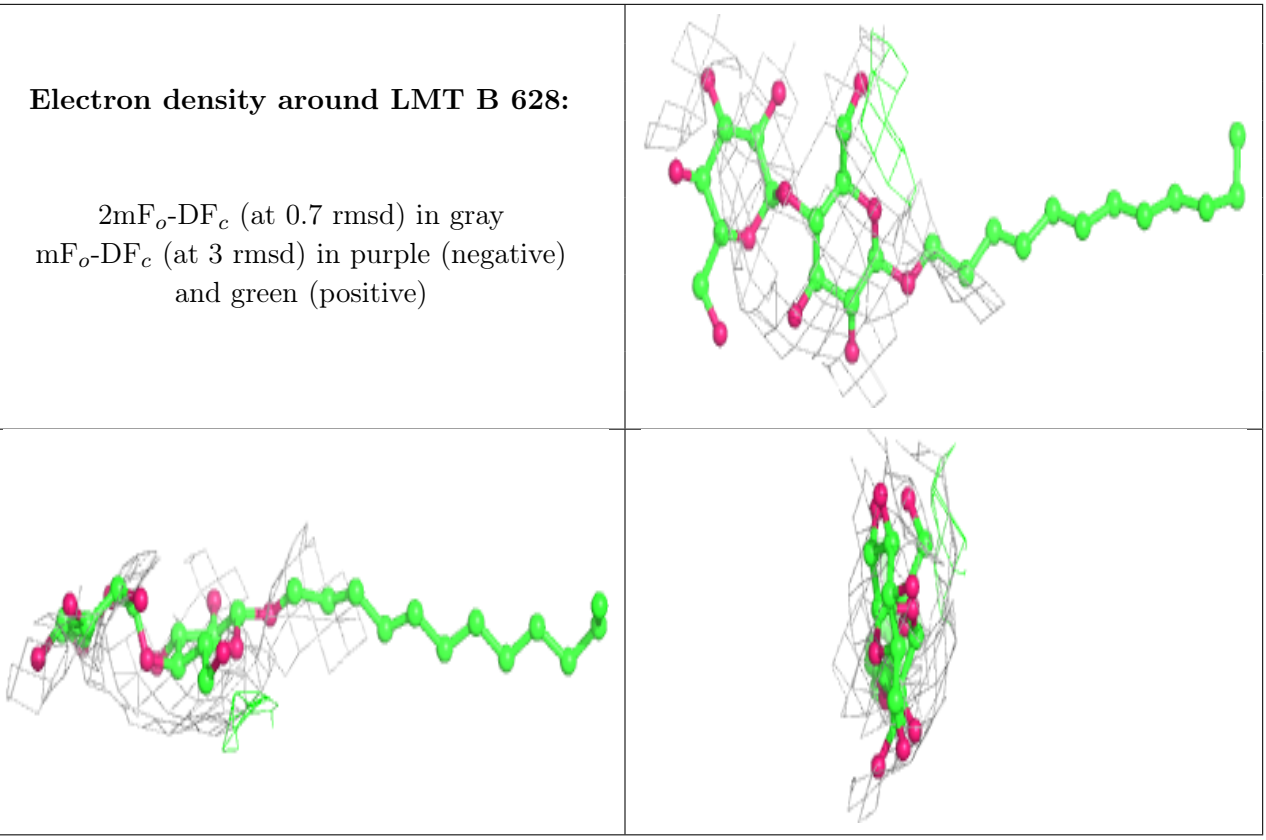
Electron density around LMG i 101:

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



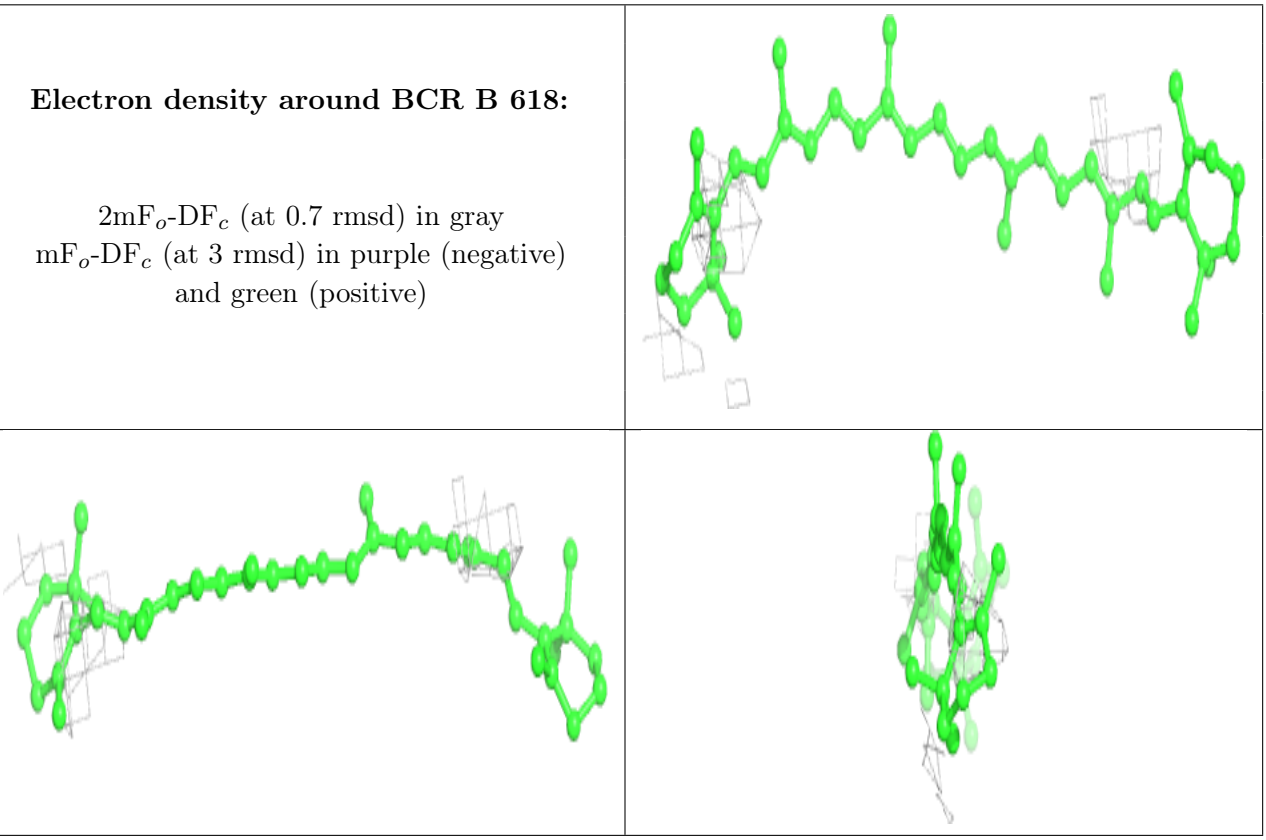
Electron density around LMT B 628:

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



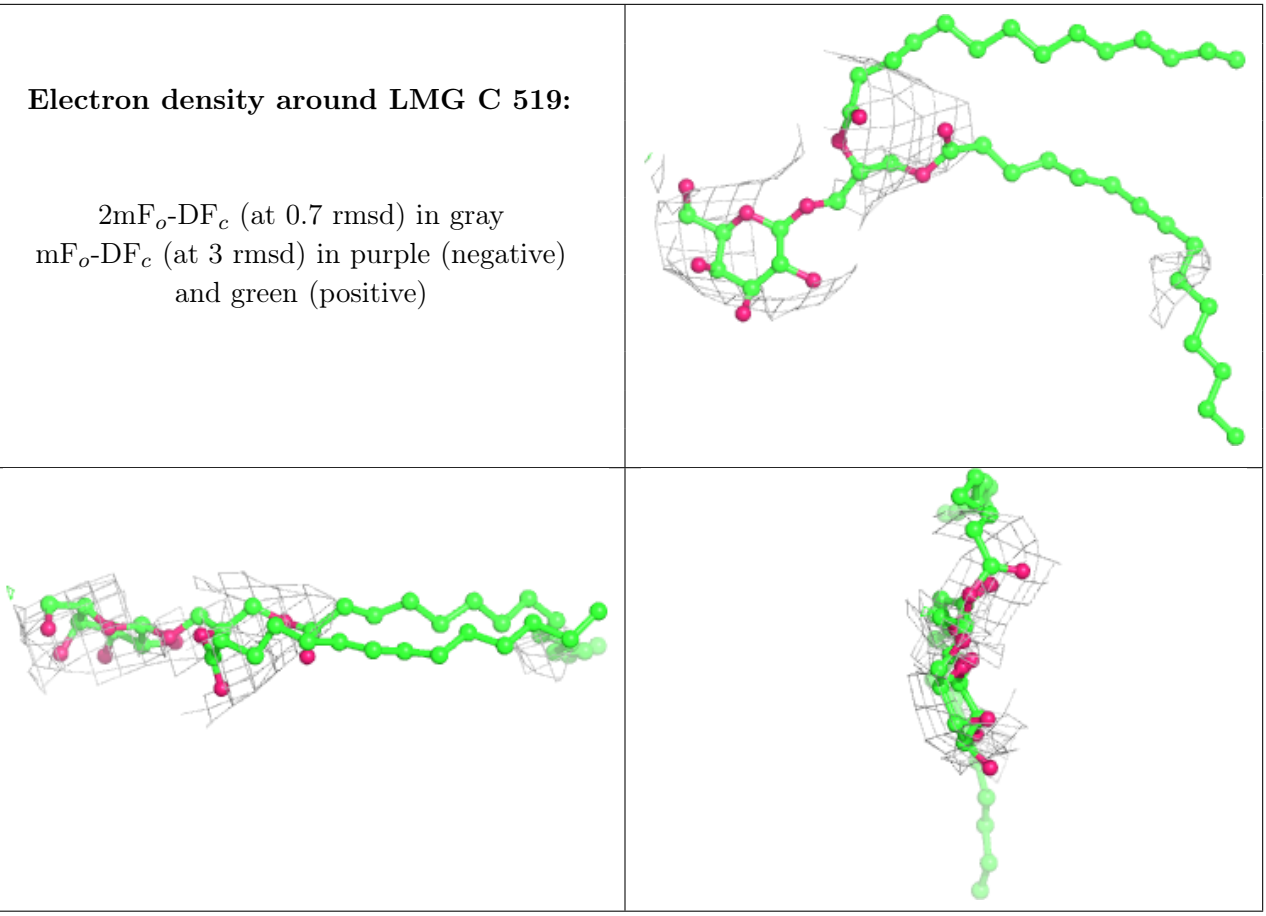
Electron density around BCR B 618:

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



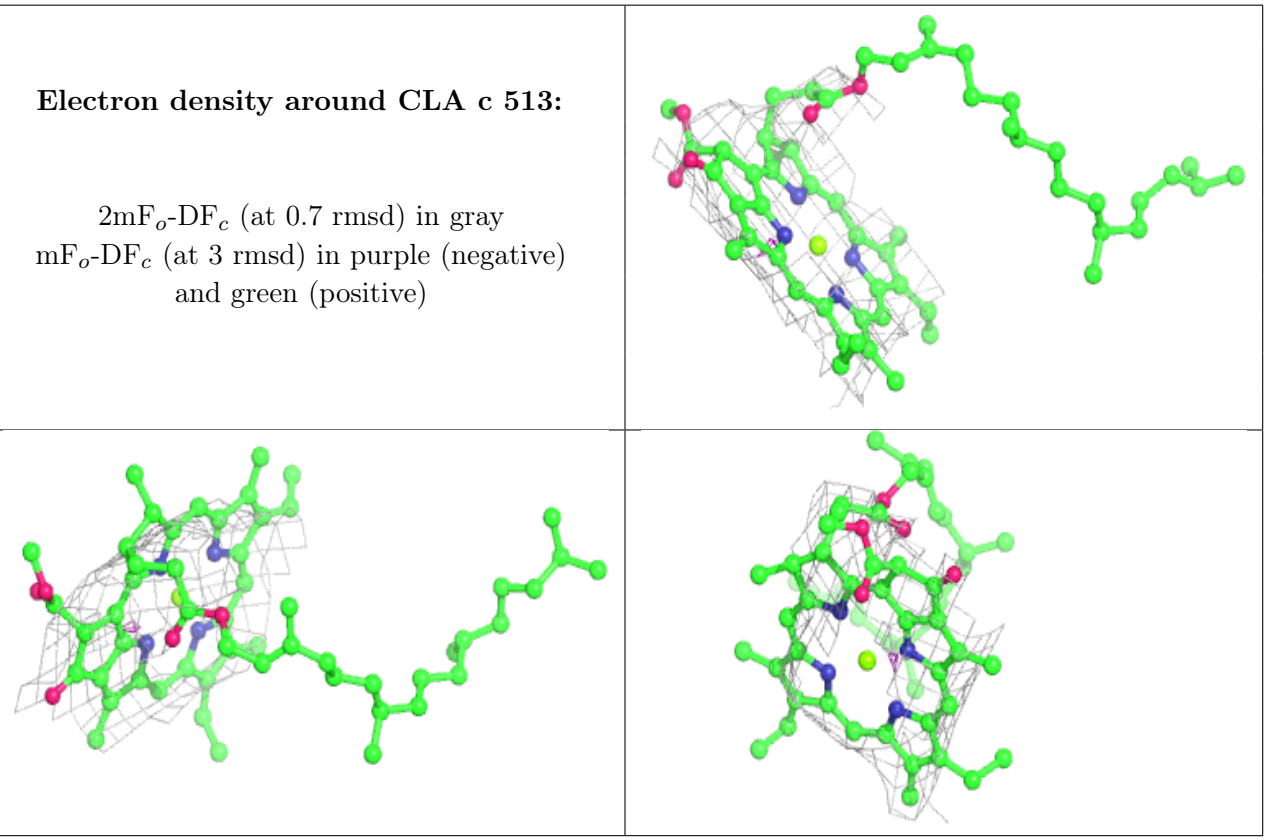
Electron density around LMG C 519:

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



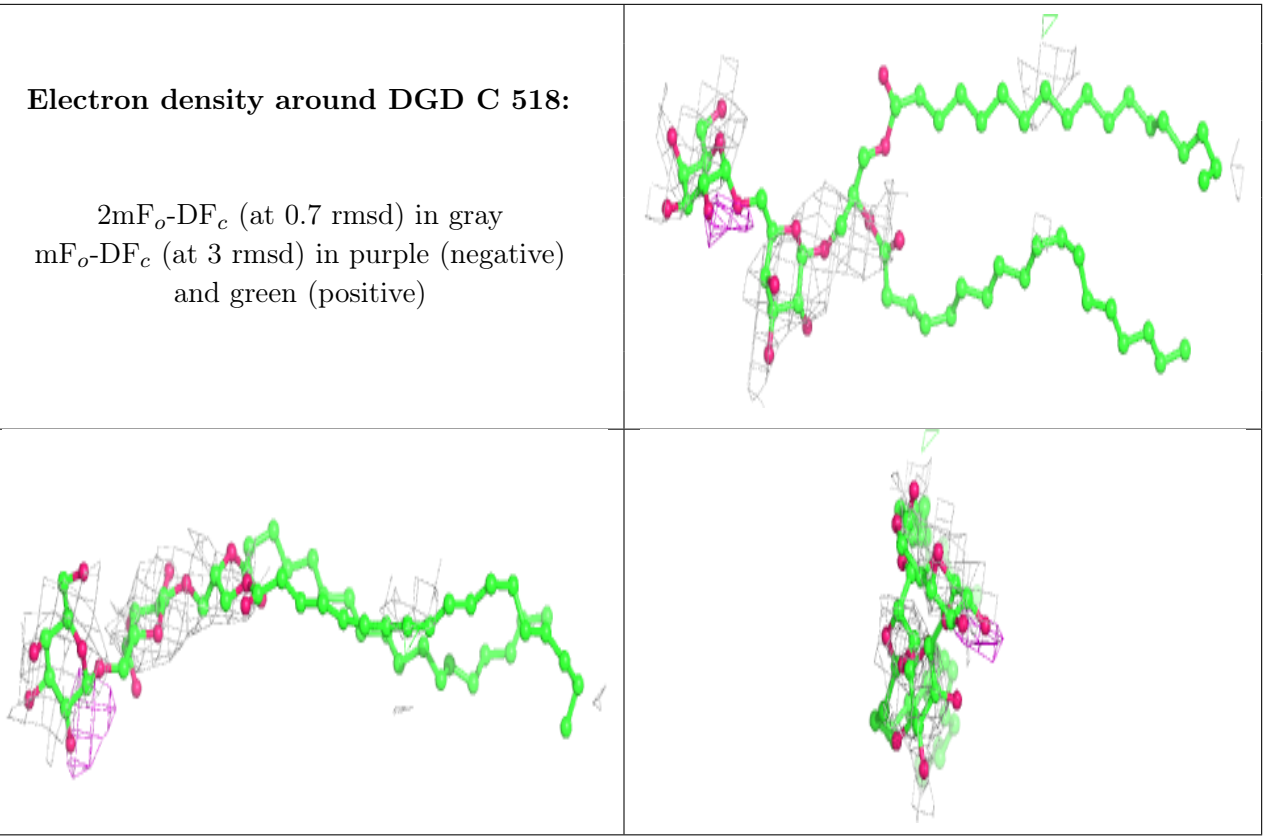
Electron density around CLA c 513:

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



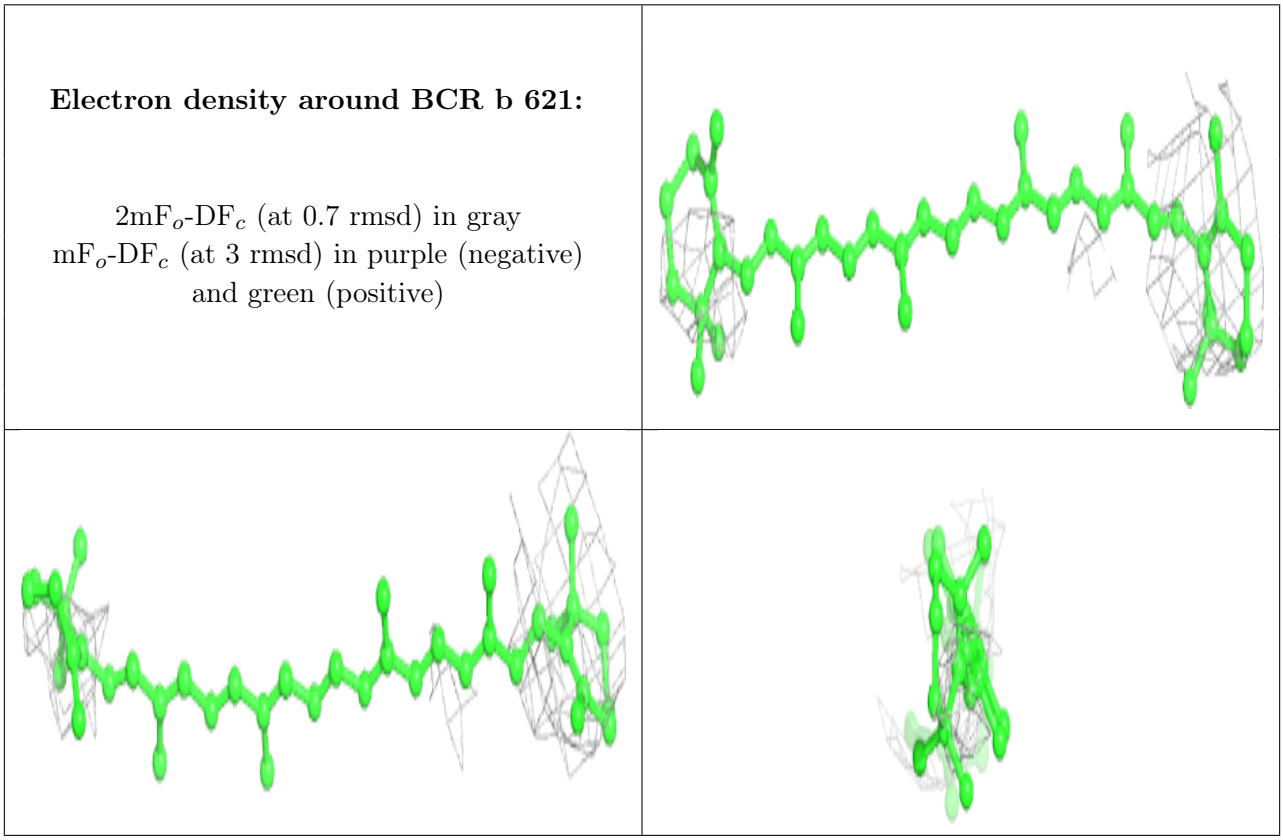
Electron density around DGD C 518:

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



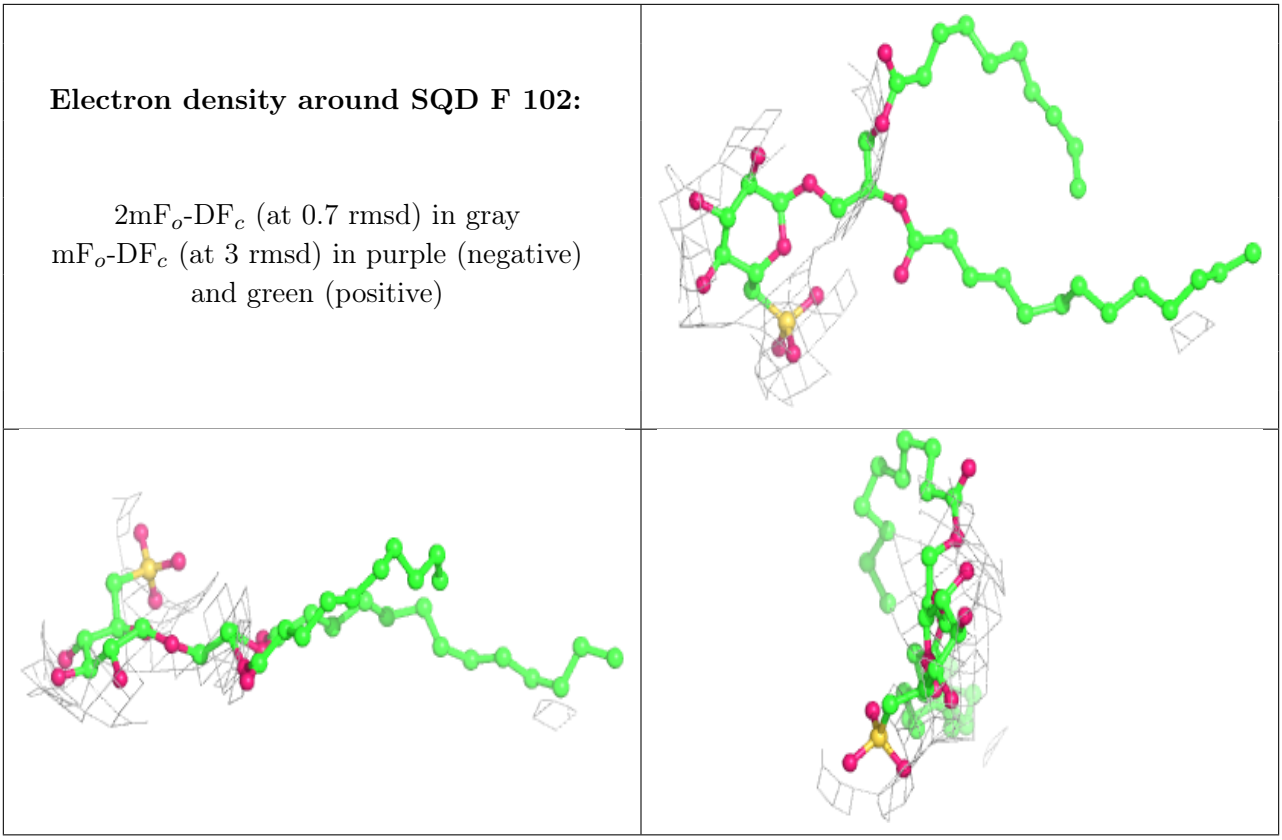
Electron density around BCR b 621:

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



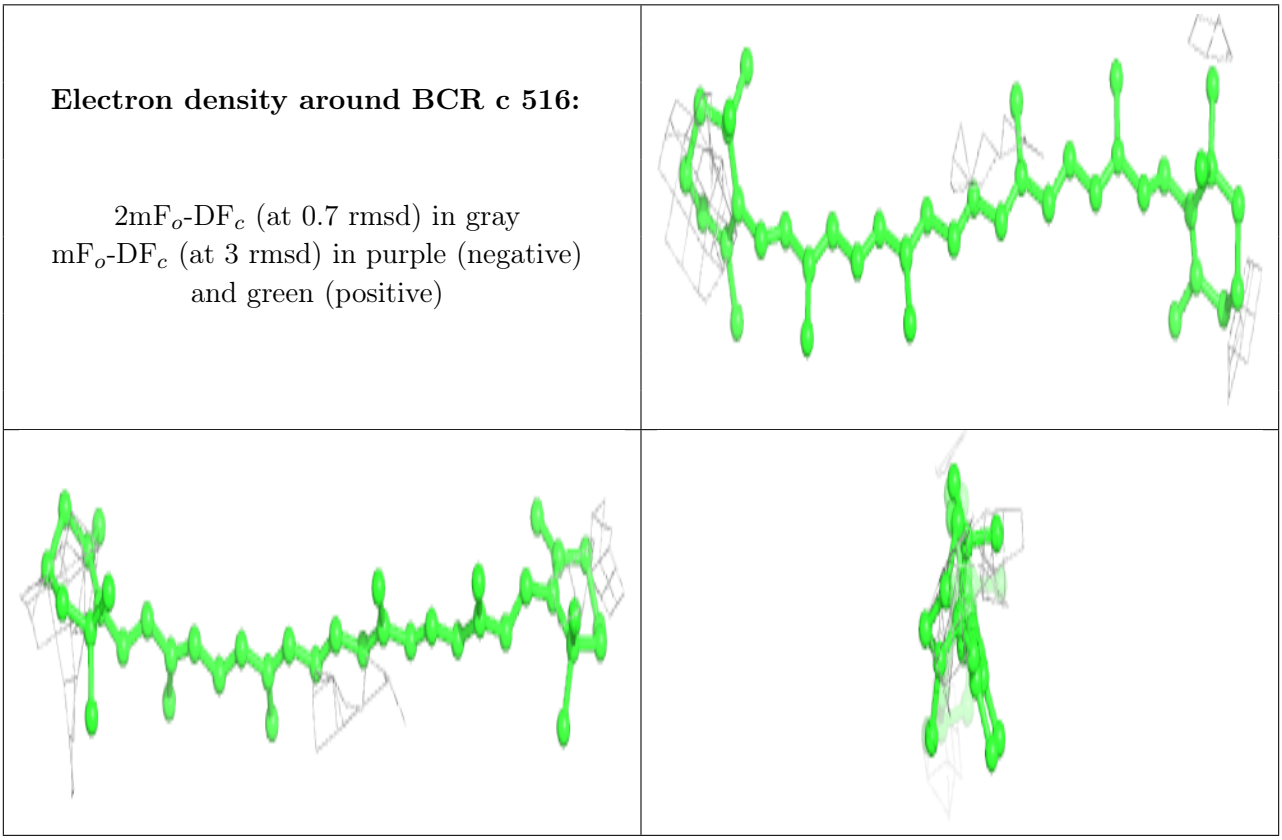
Electron density around SQD F 102:

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



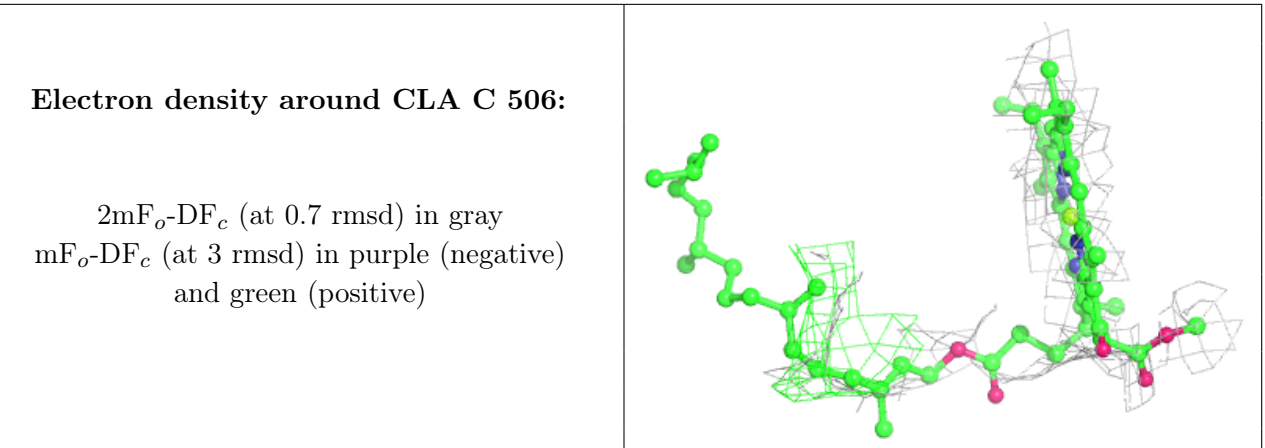
Electron density around BCR c 516:

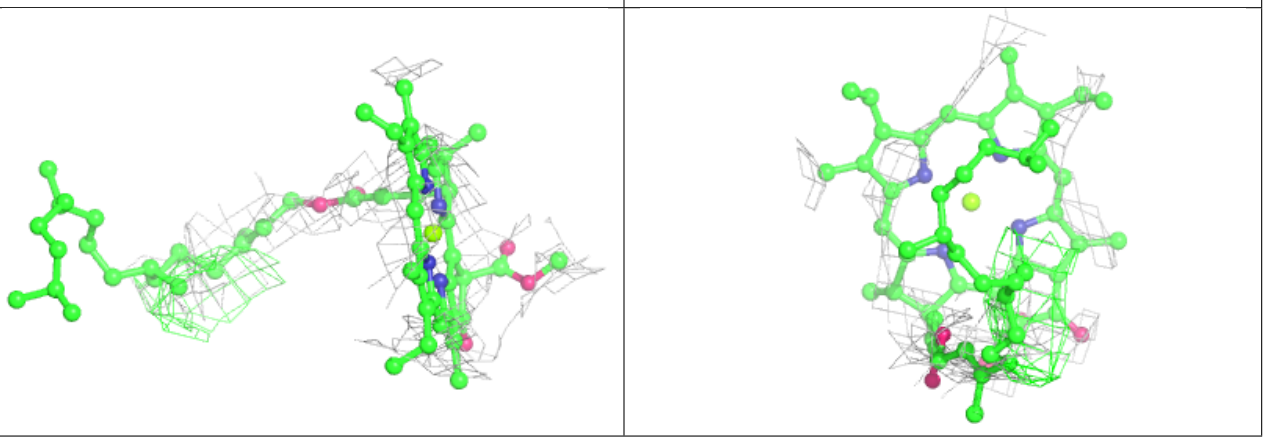
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA C 506:

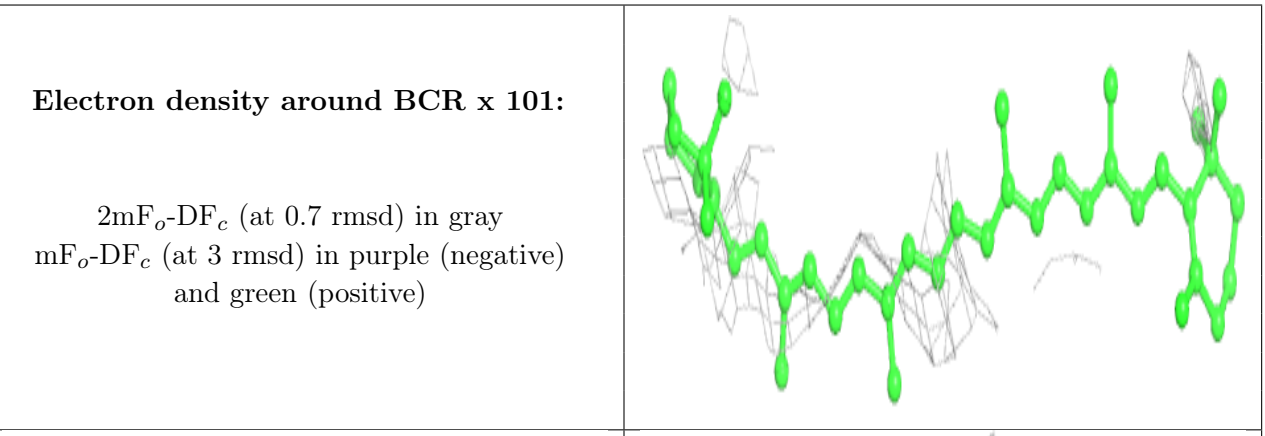
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

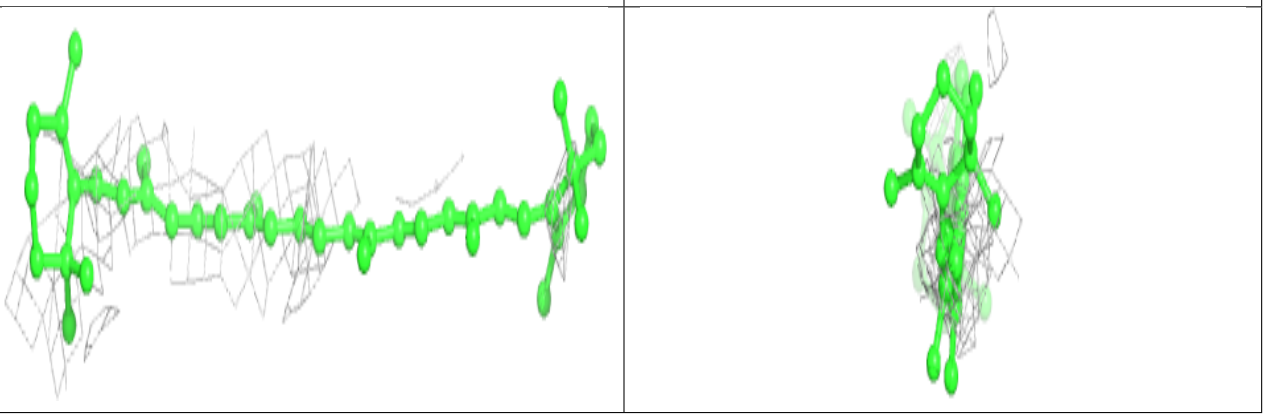




Electron density around BCR x 101:

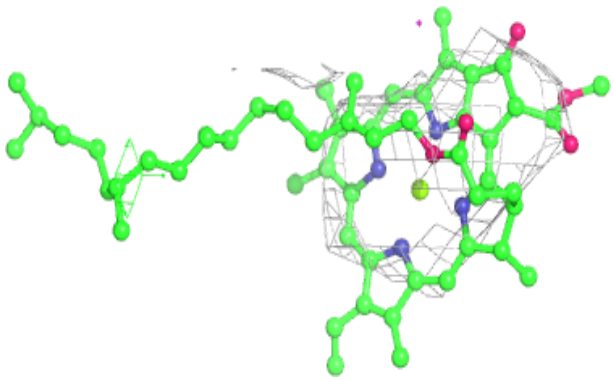
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

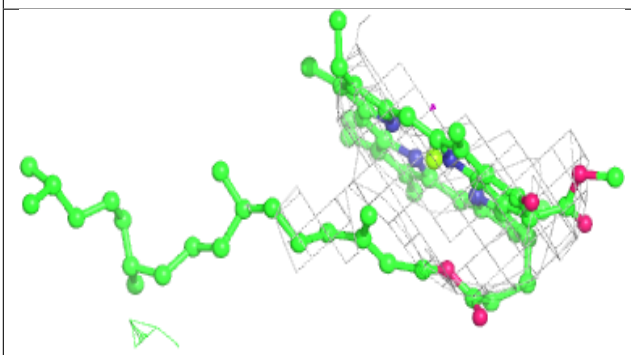


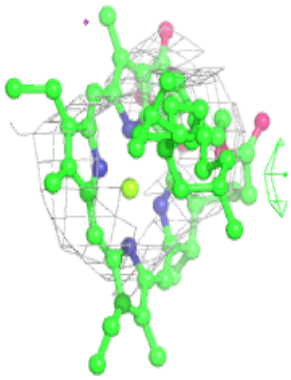


Electron density around CLA B 614:

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

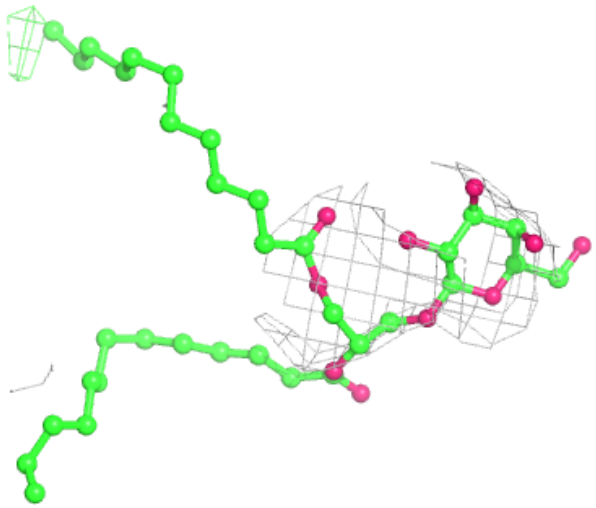


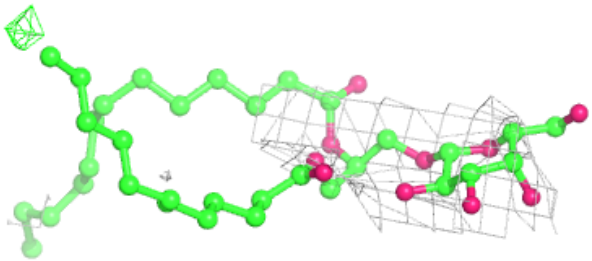


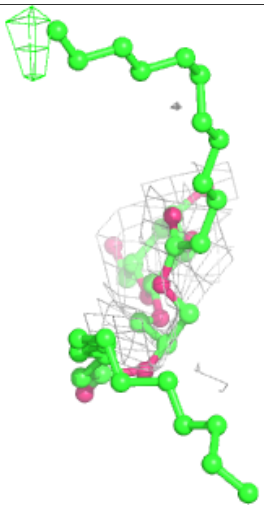


Electron density around LMG e 101:

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

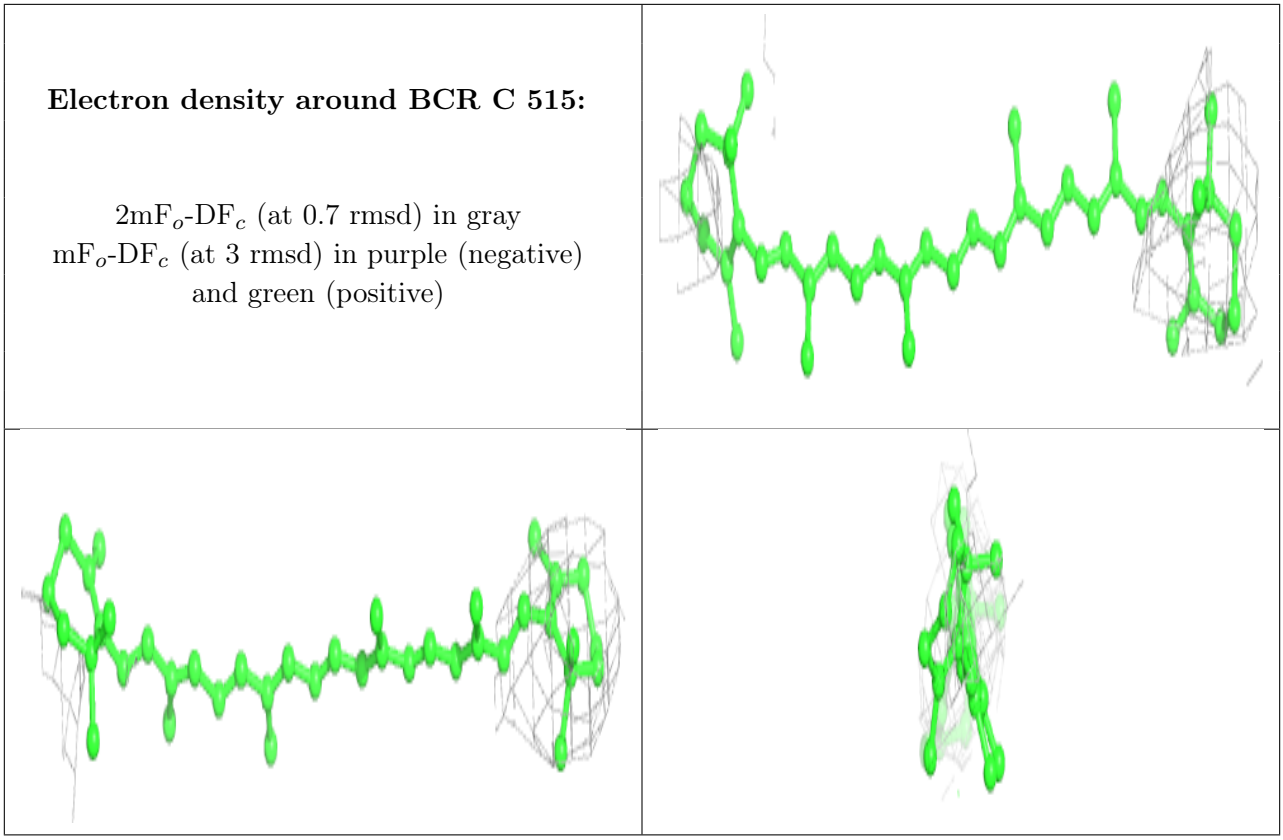






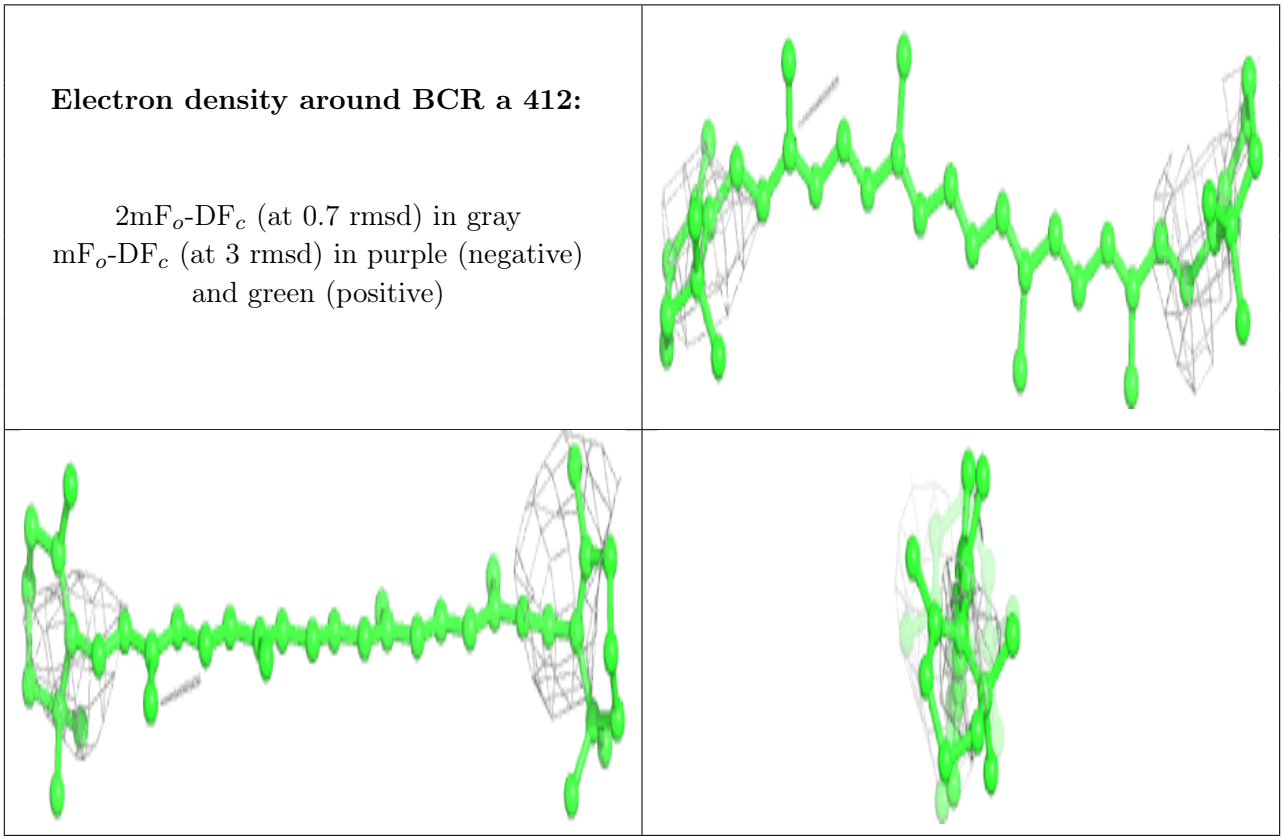
Electron density around BCR C 515:

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



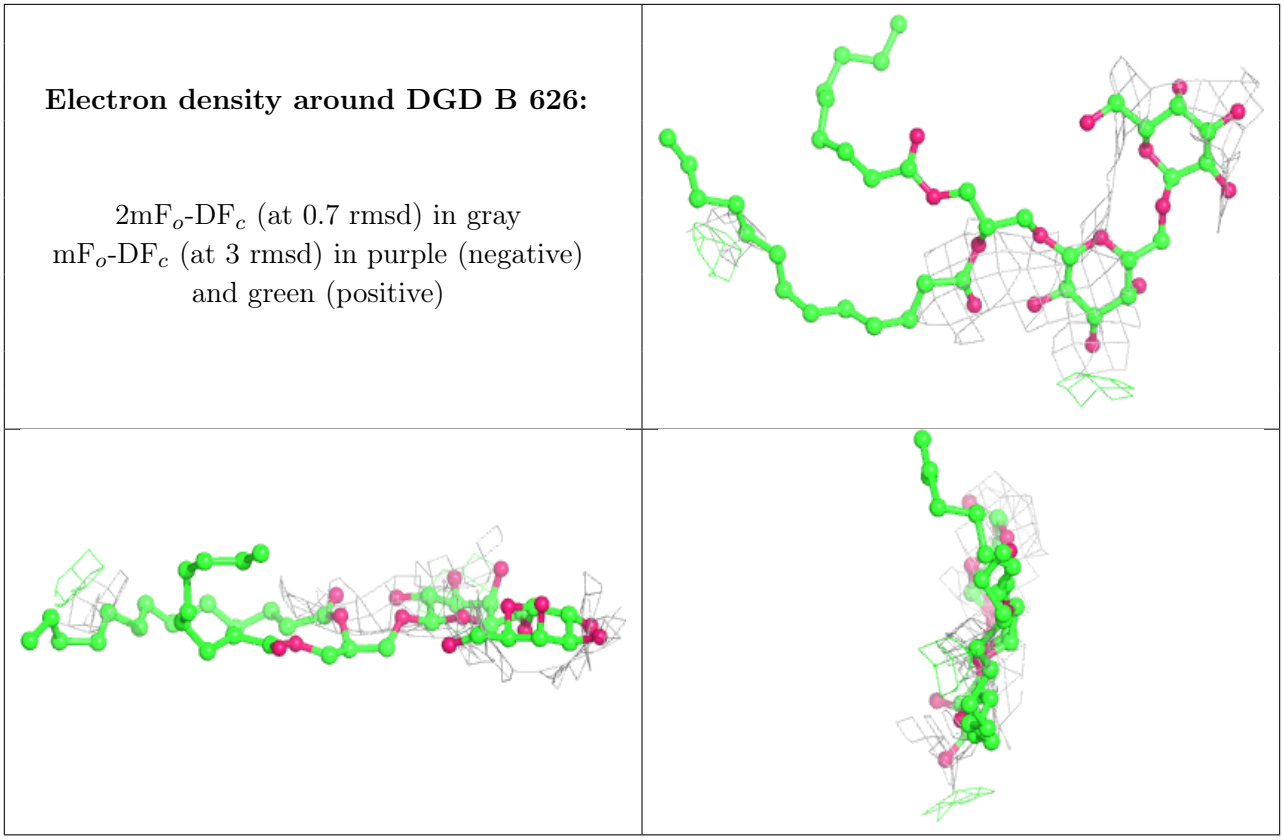
Electron density around BCR a 412:

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



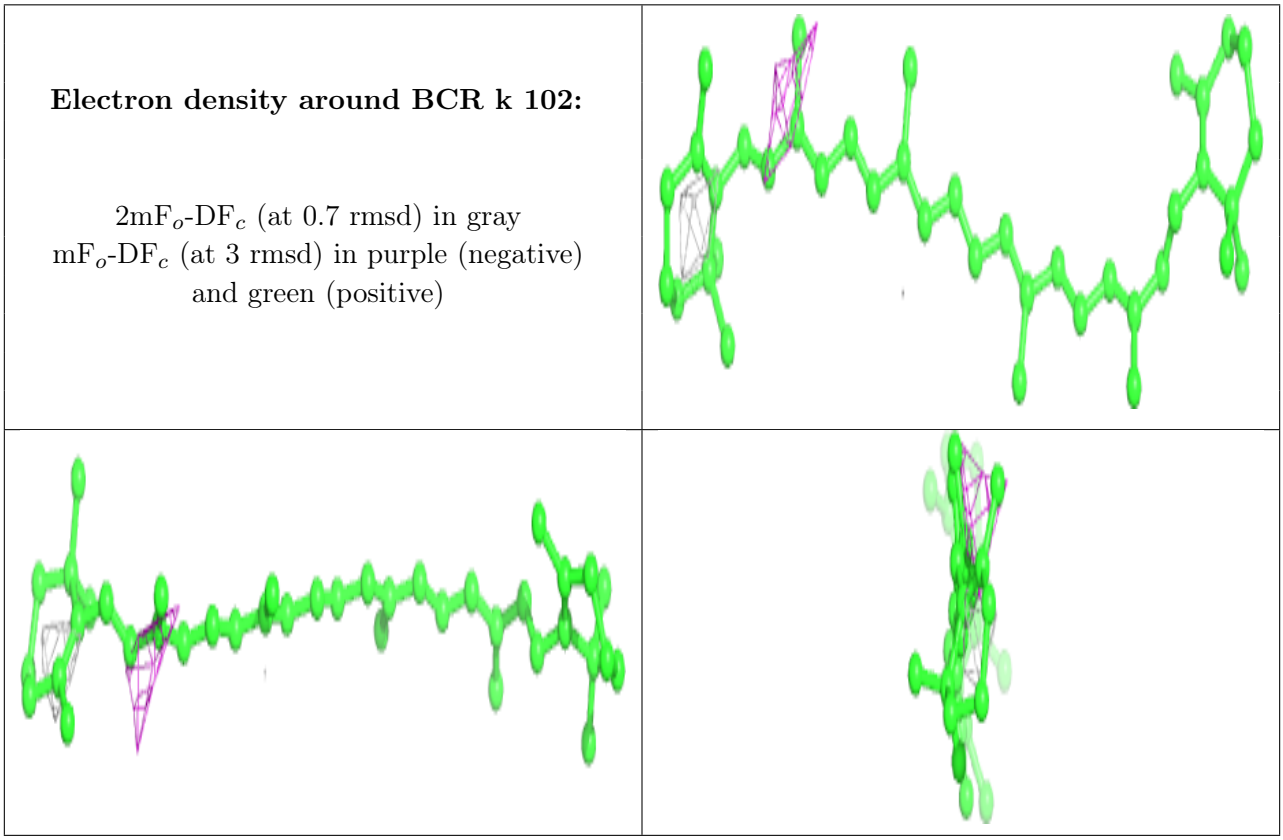
Electron density around DGD B 626:

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



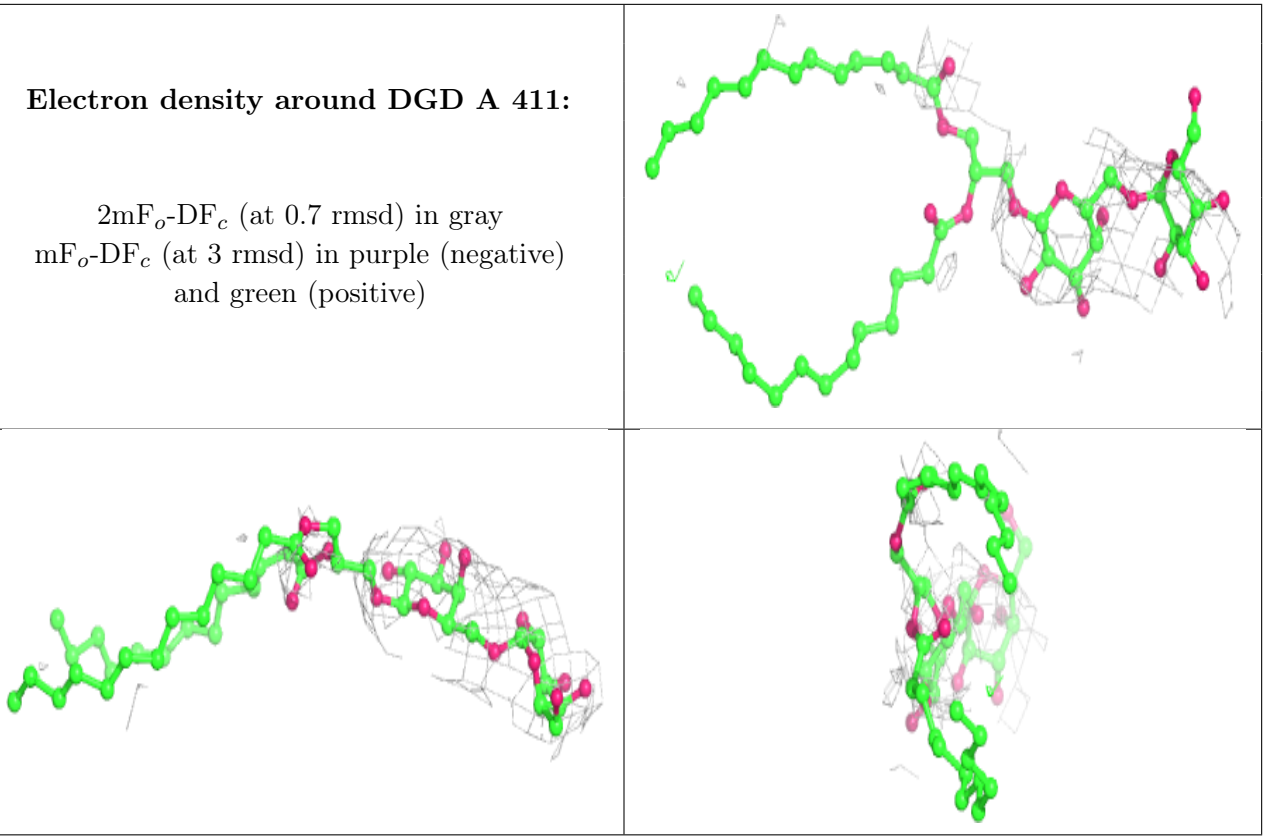
Electron density around BCR k 102:

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



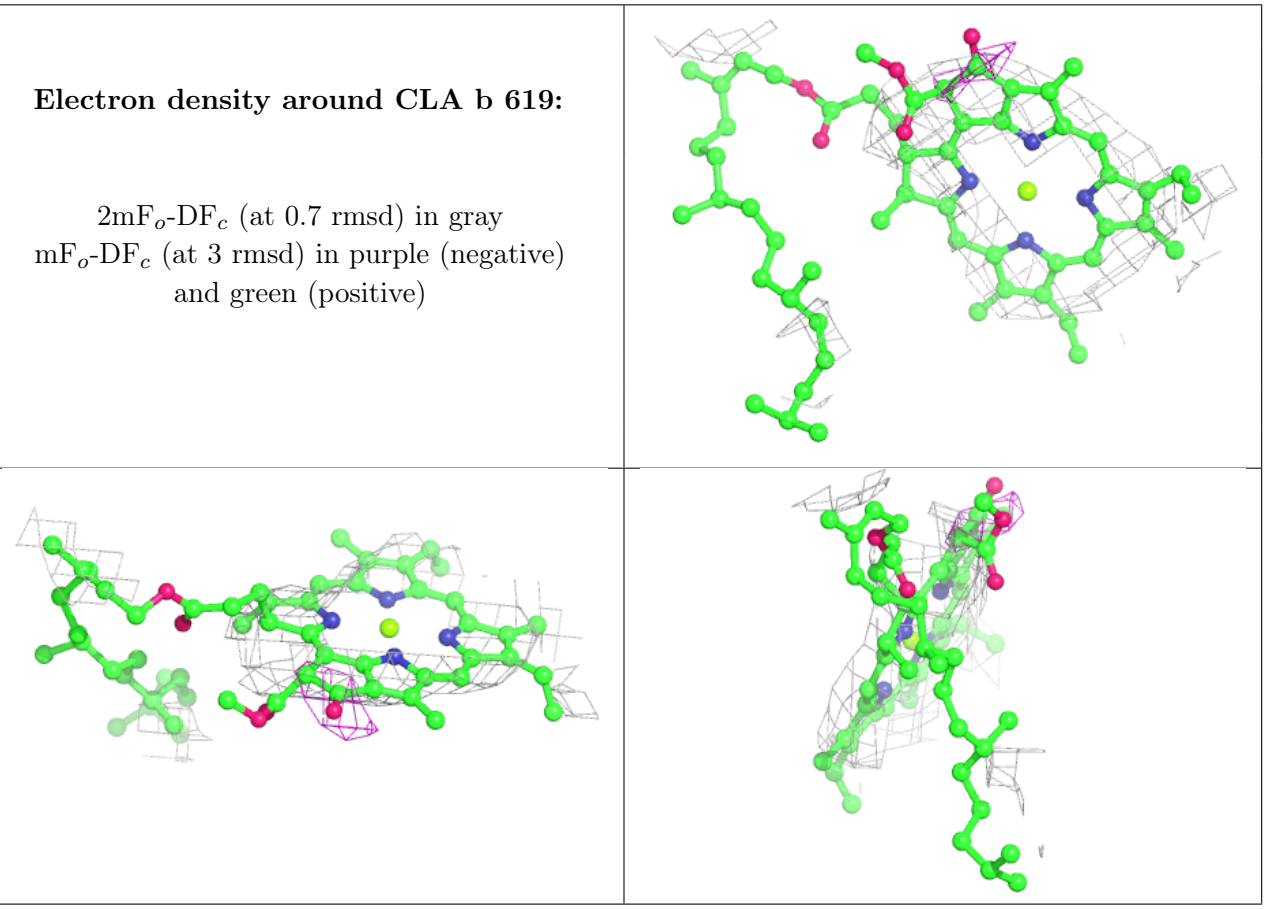
Electron density around DGD A 411:

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



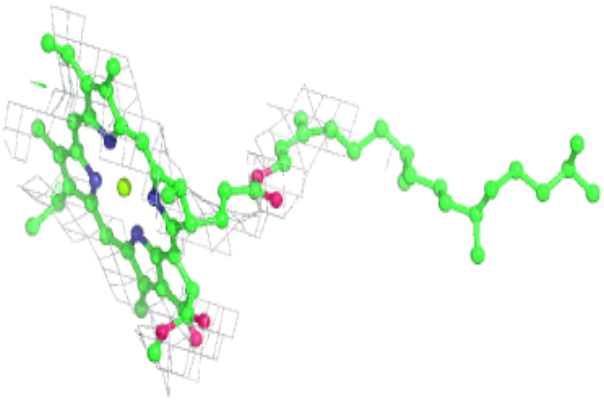
Electron density around CLA b 619:

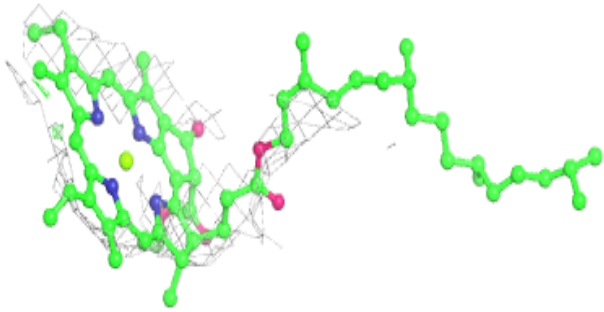
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

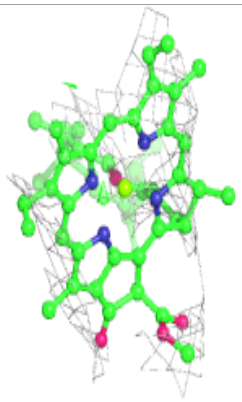


Electron density around CLA C 502:

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

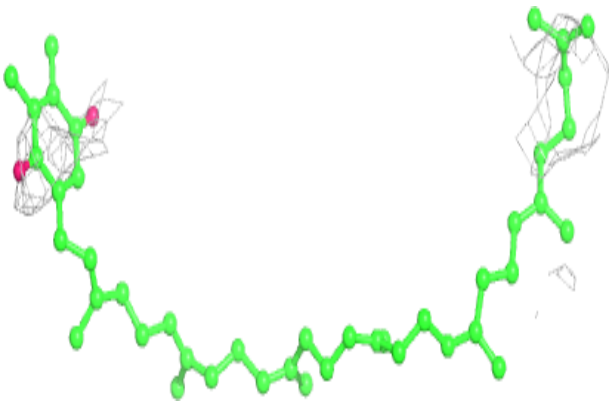


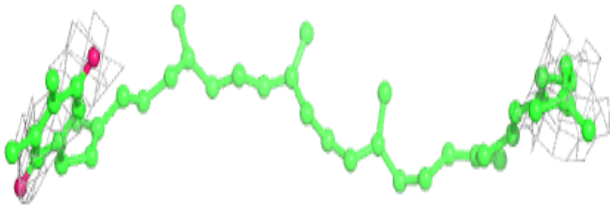


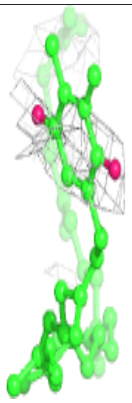


Electron density around PL9 A 408:

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

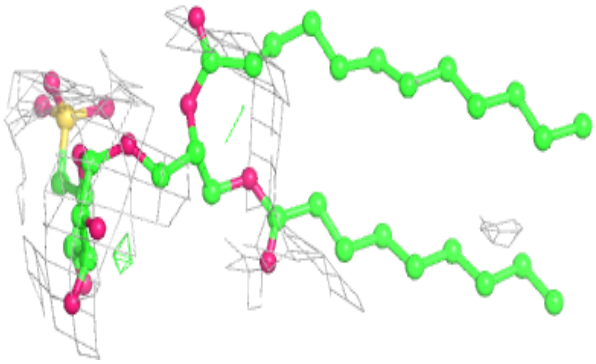


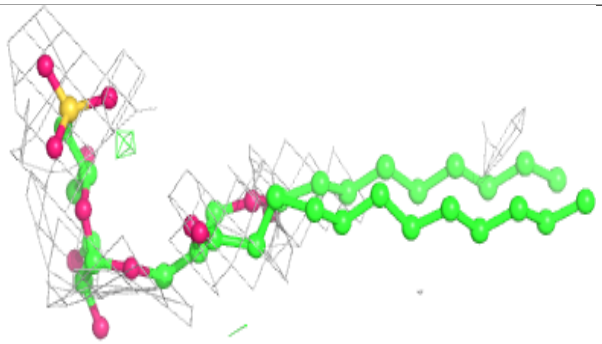


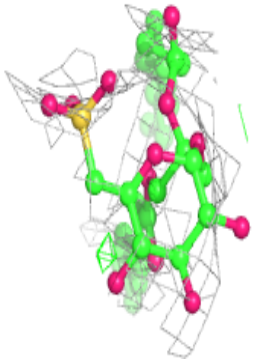


Electron density around SQD D 409:

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

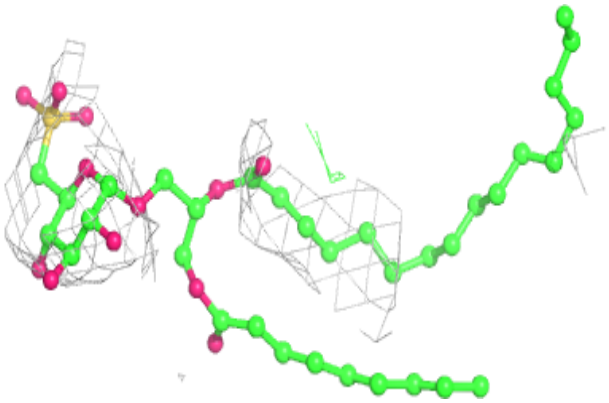


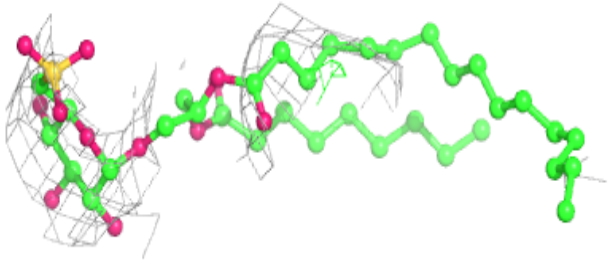


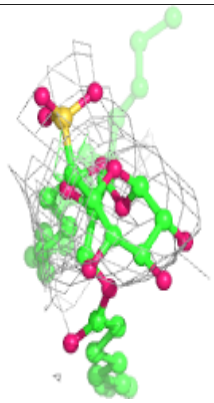


Electron density around SQD b 601:

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

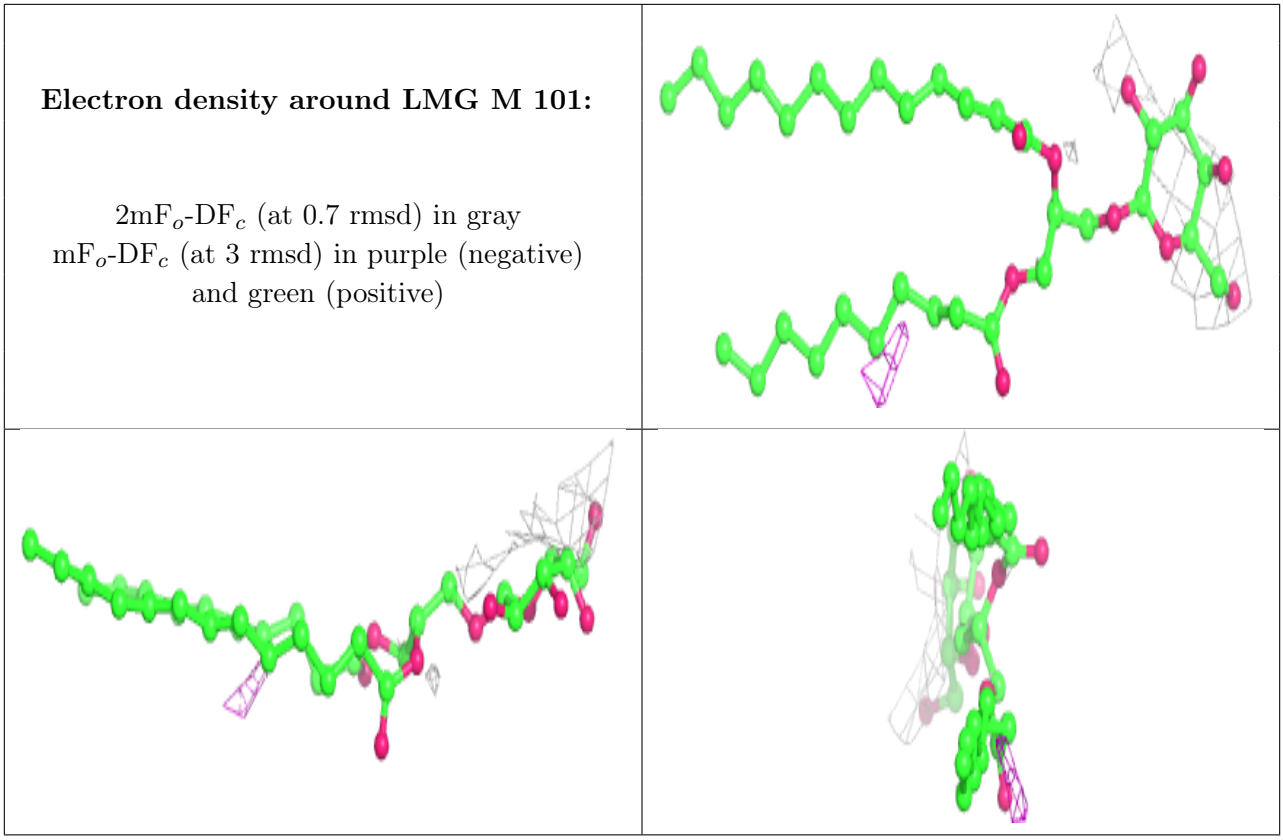






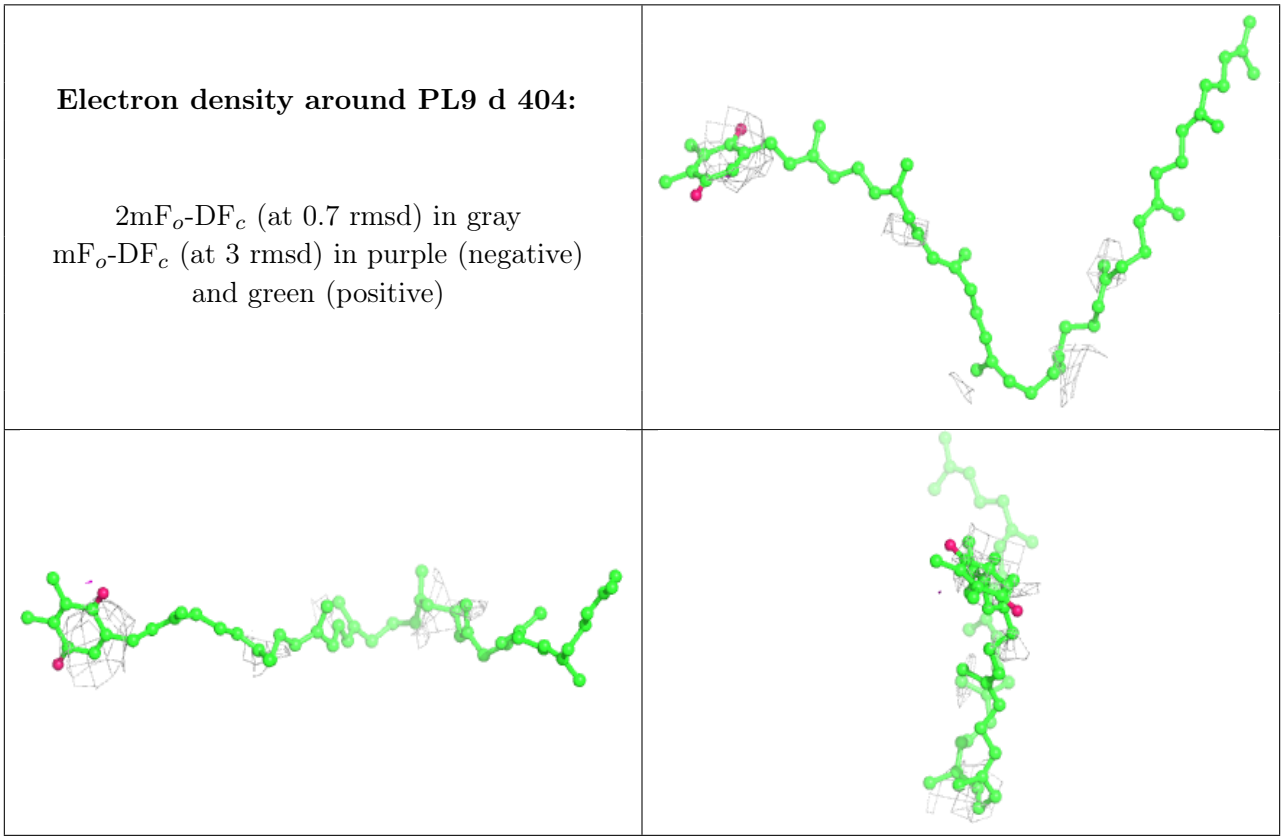
Electron density around LMG M 101:

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



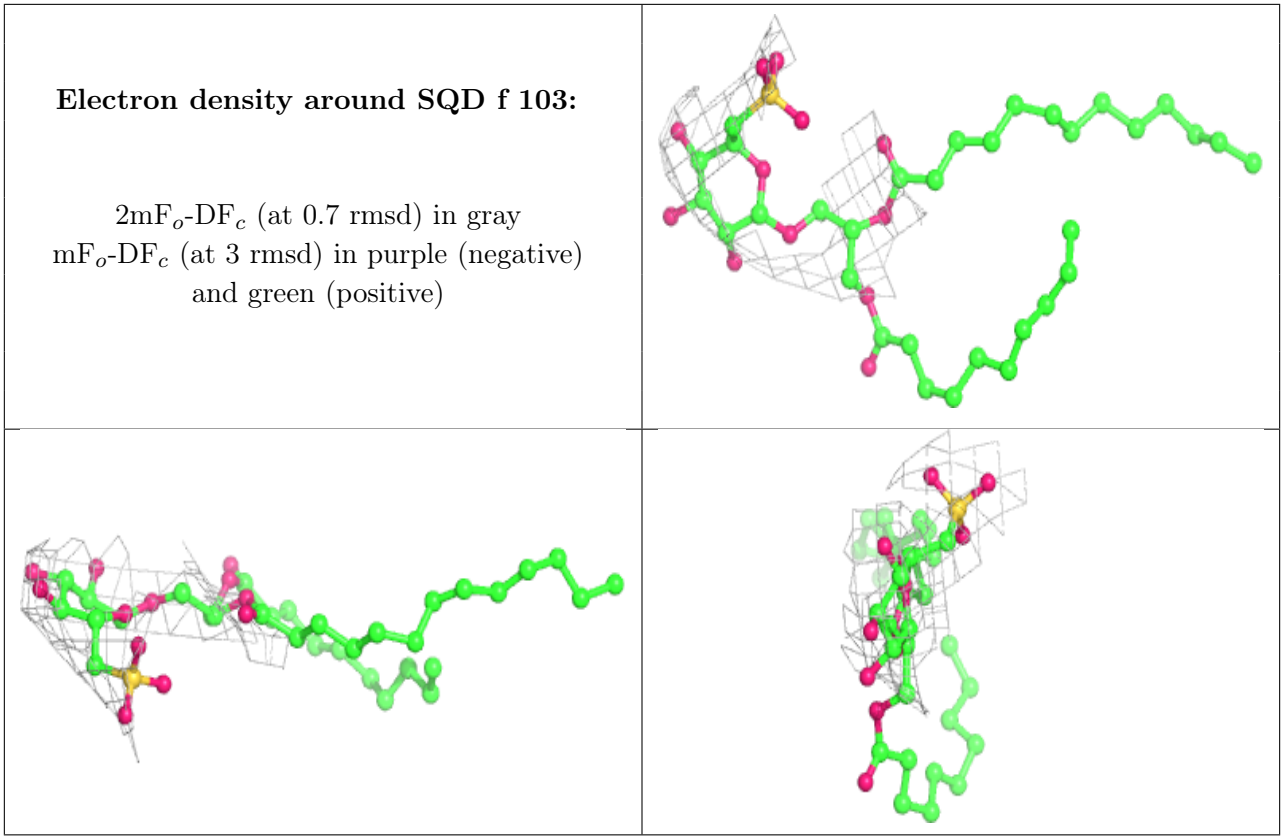
Electron density around PL9 d 404:

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



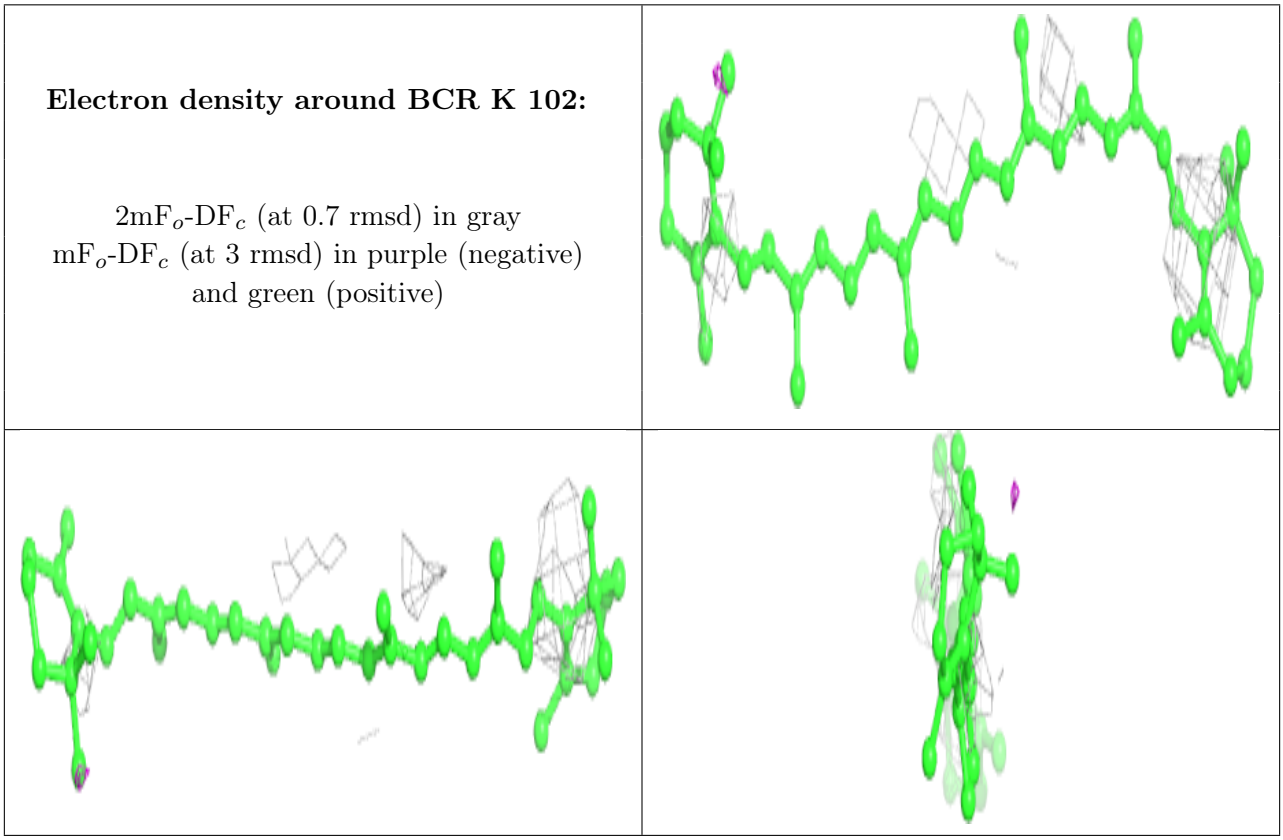
Electron density around SQD f 103:

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



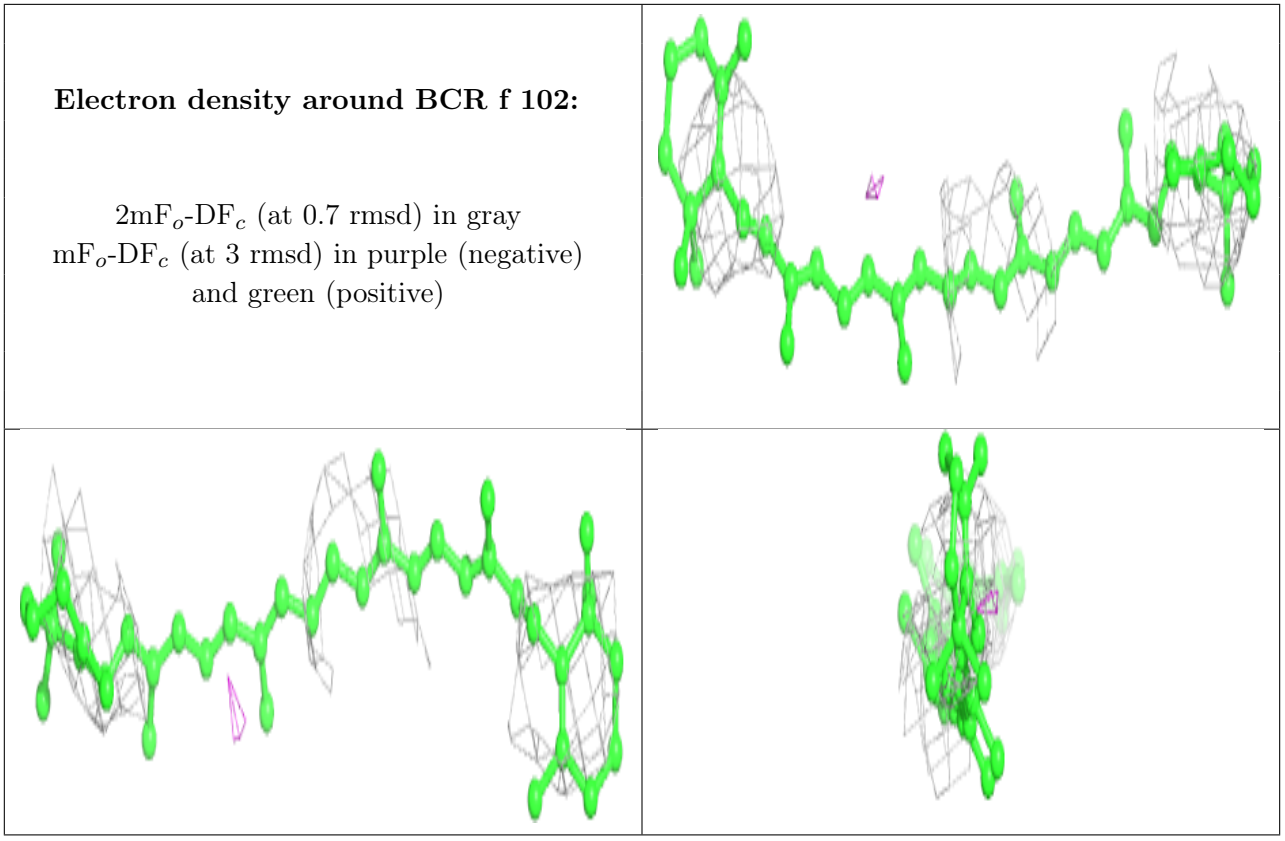
Electron density around BCR K 102:

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



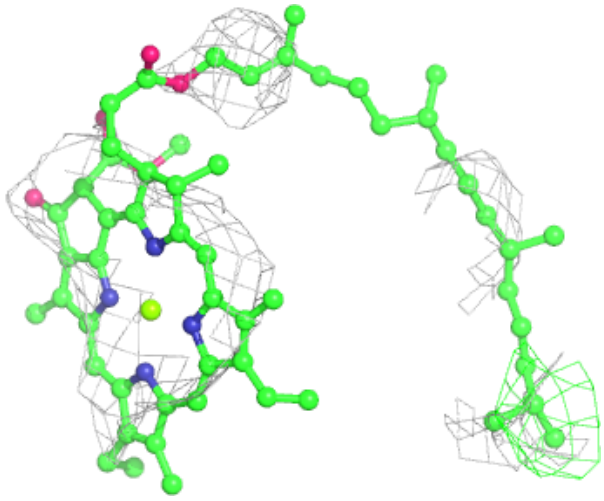
Electron density around BCR f 102:

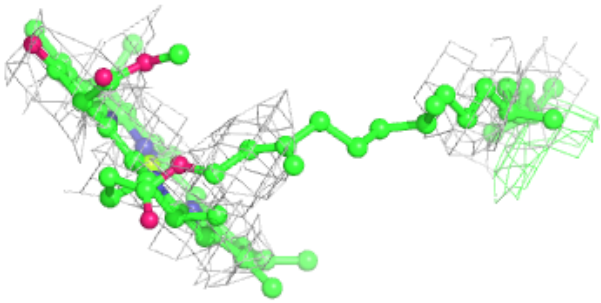
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

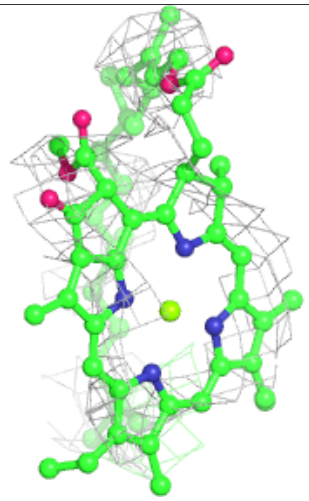


Electron density around CLA C 507:

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

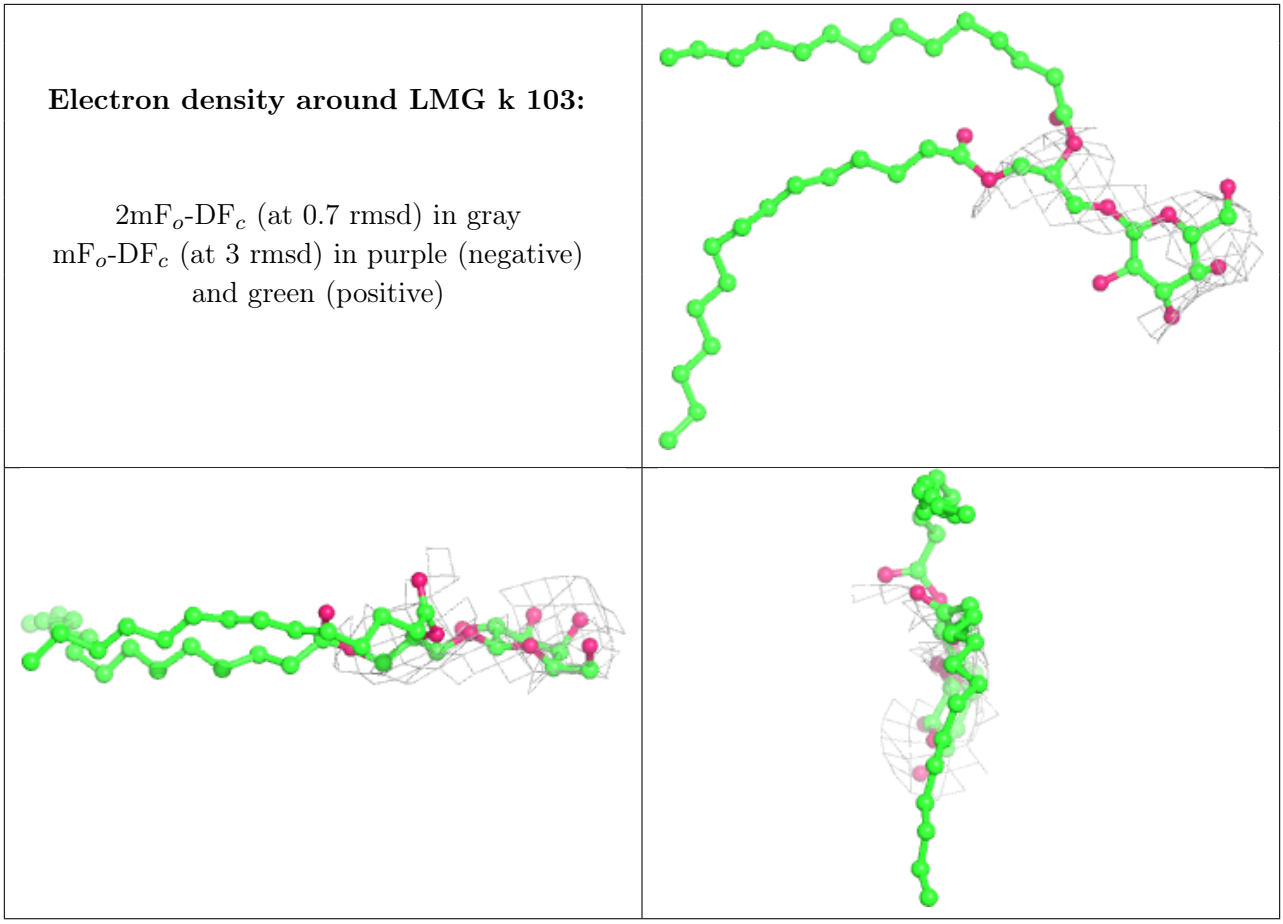






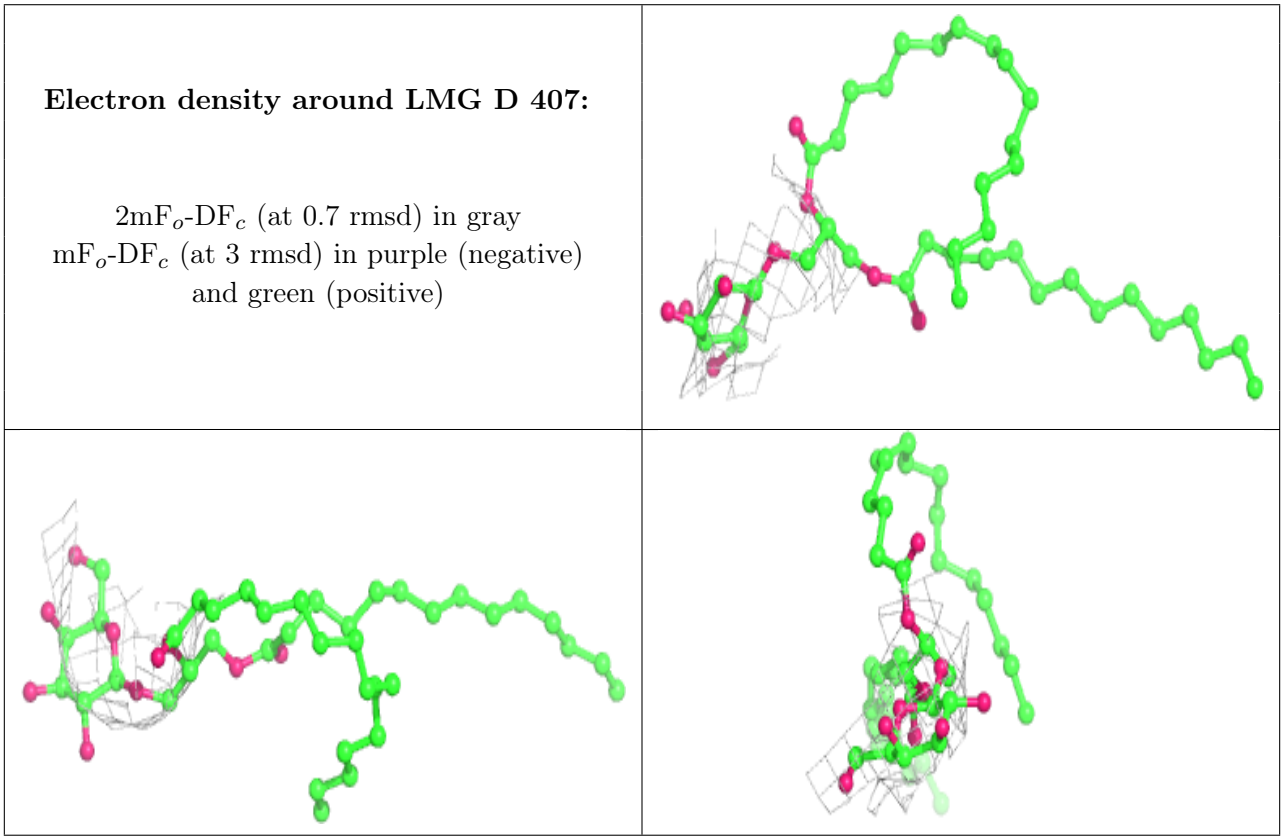
Electron density around LMG k 103:

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



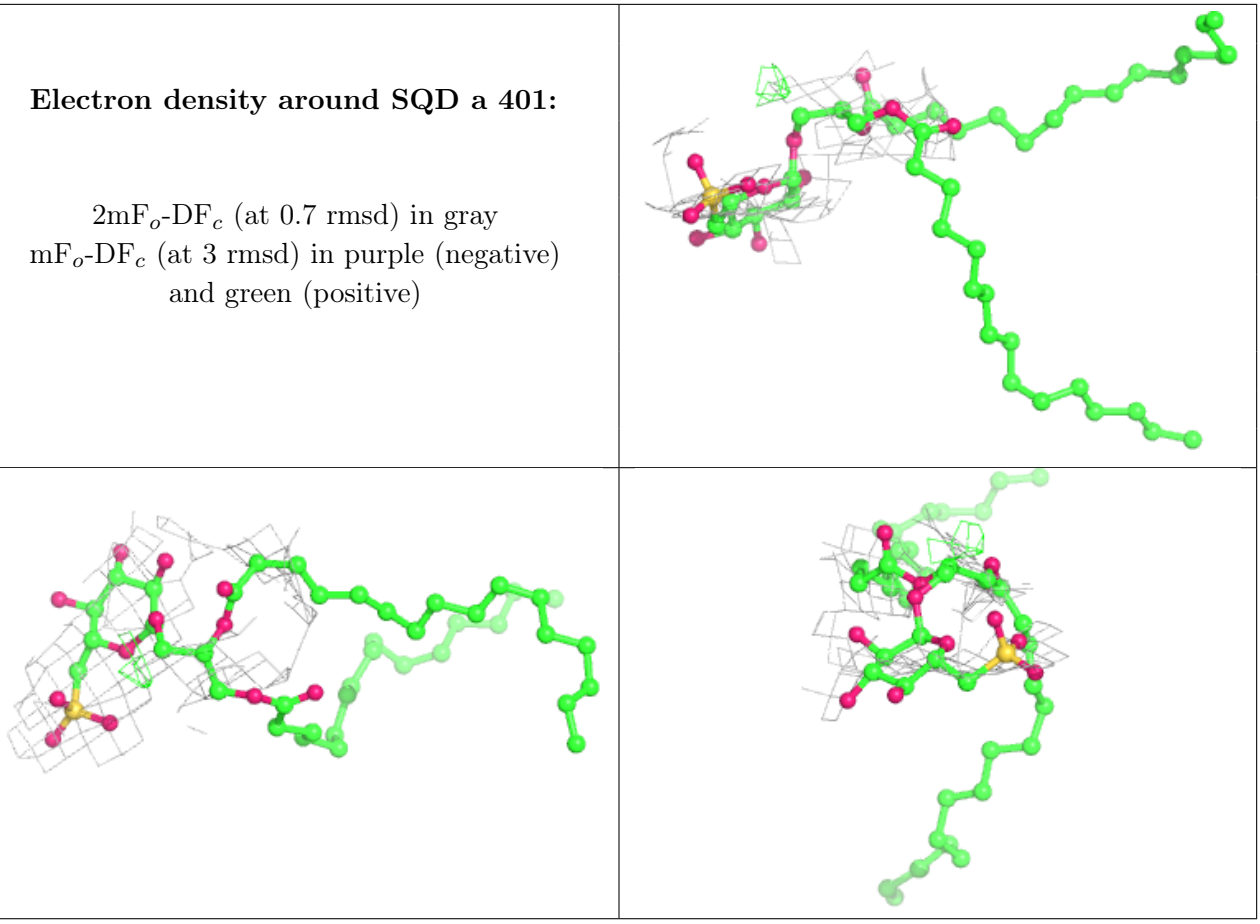
Electron density around LMG D 407:

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



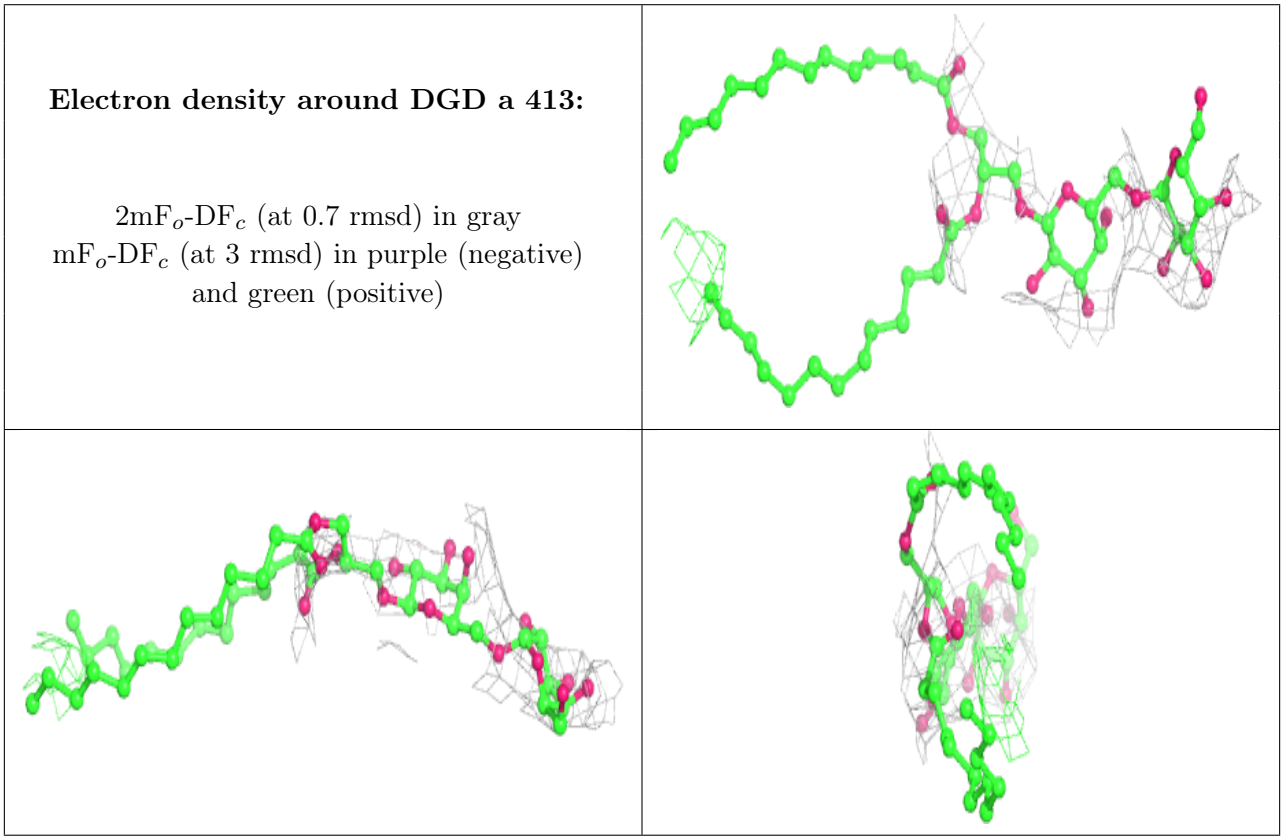
Electron density around SQD a 401:

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



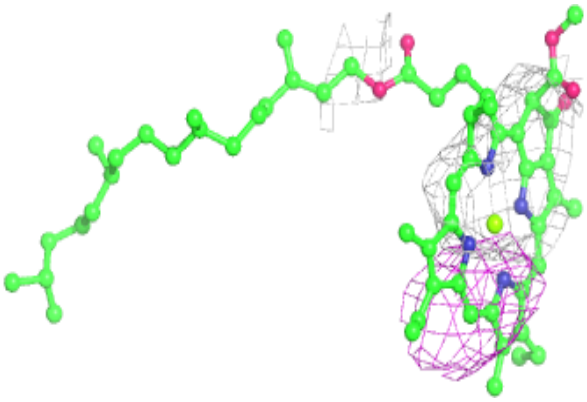
Electron density around DGD a 413:

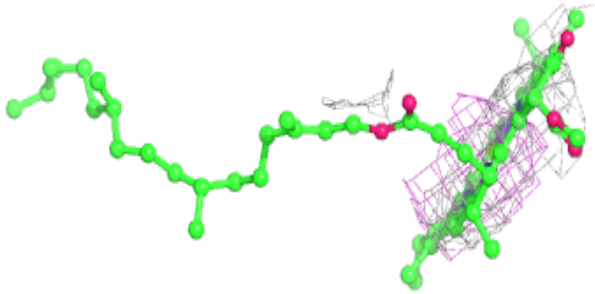
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

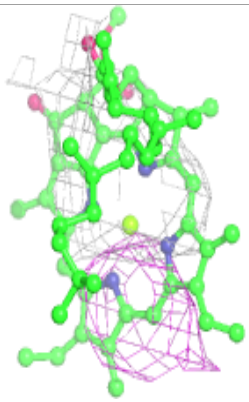


Electron density around CLA a 409:

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

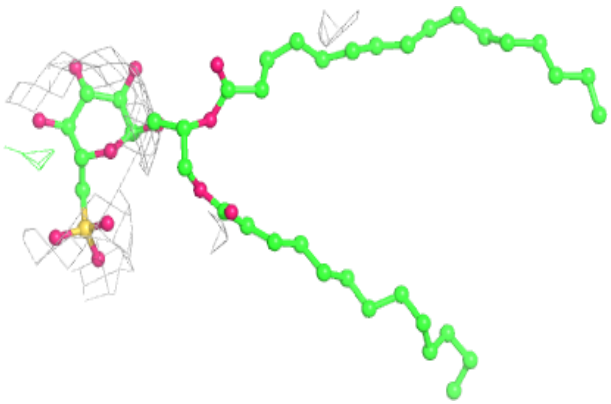


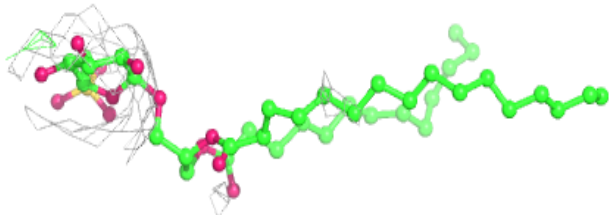


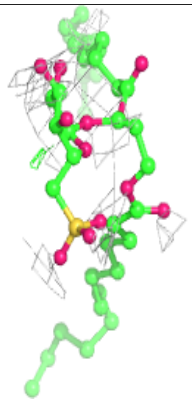


Electron density around SQD a 415:

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

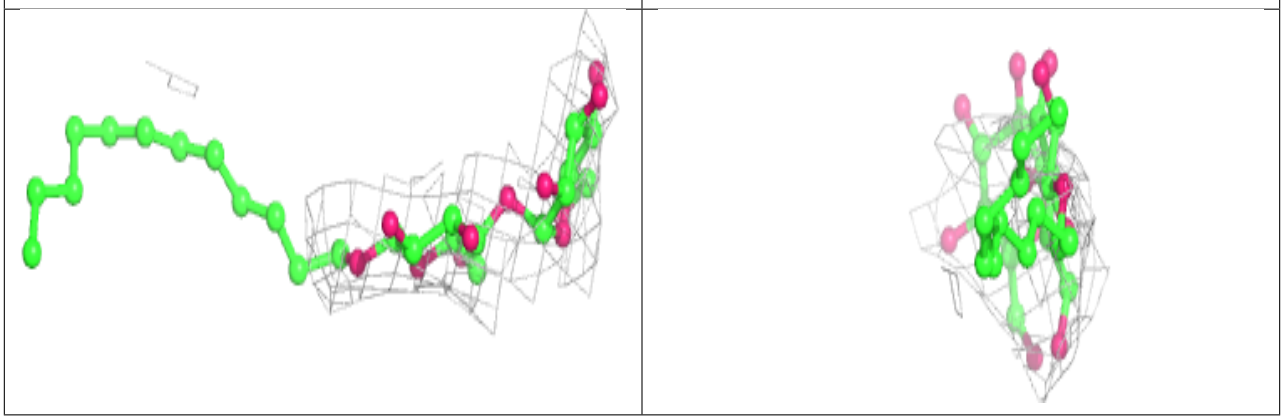






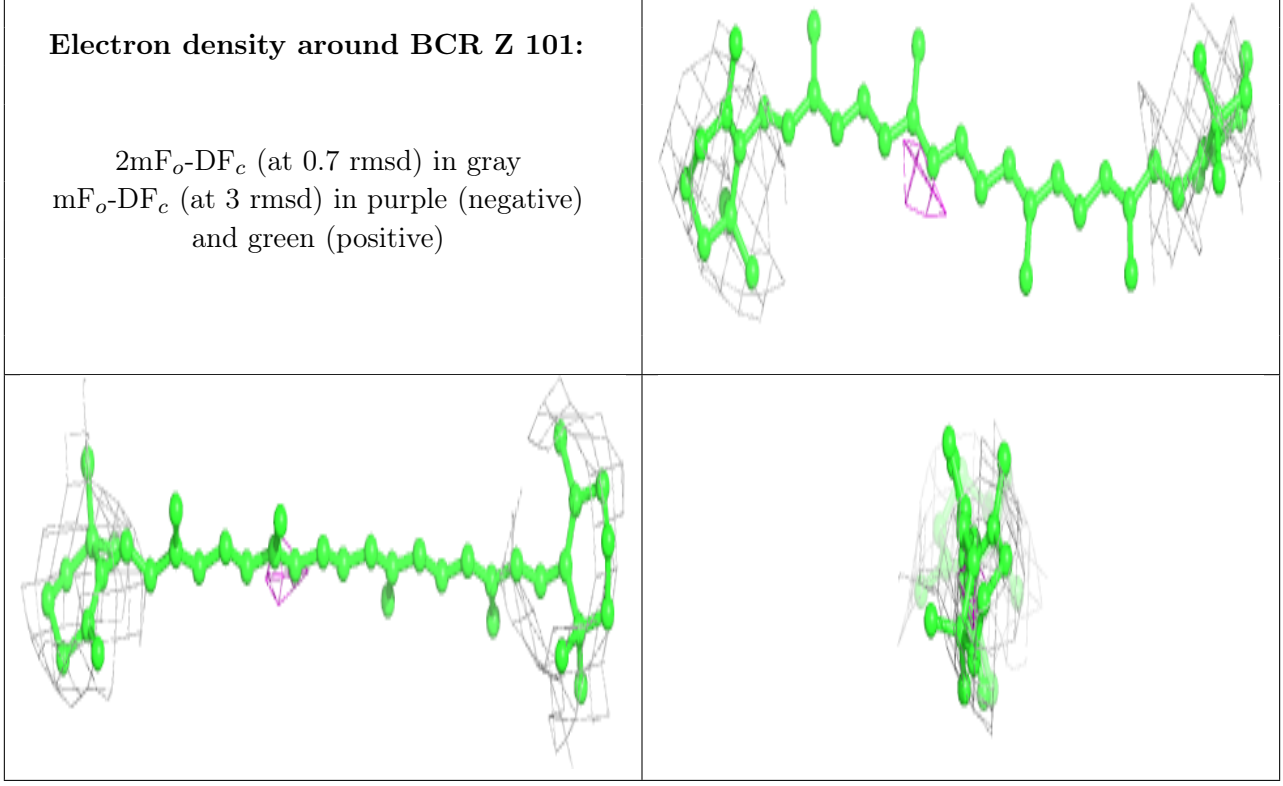
Electron density around LMT b 625:

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



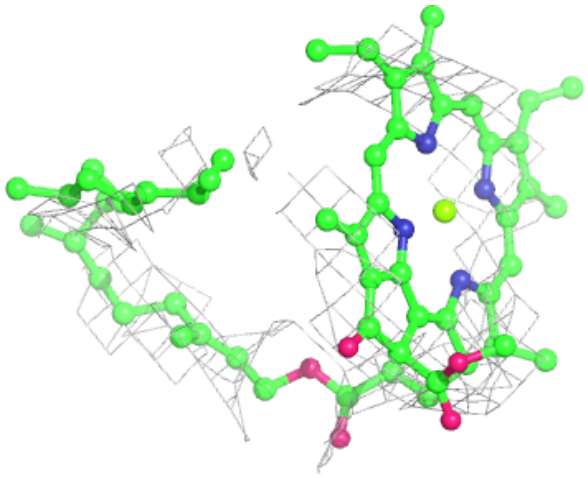
Electron density around BCR Z 101:

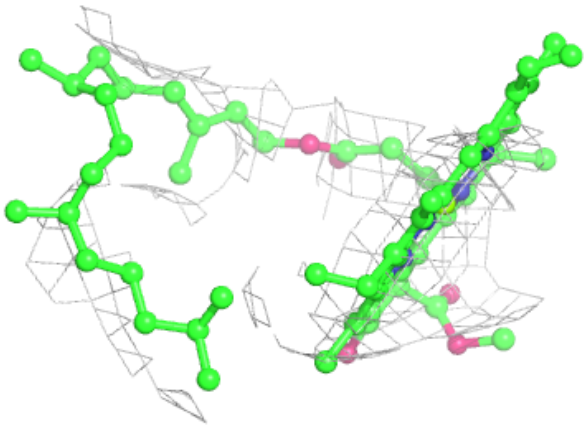
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

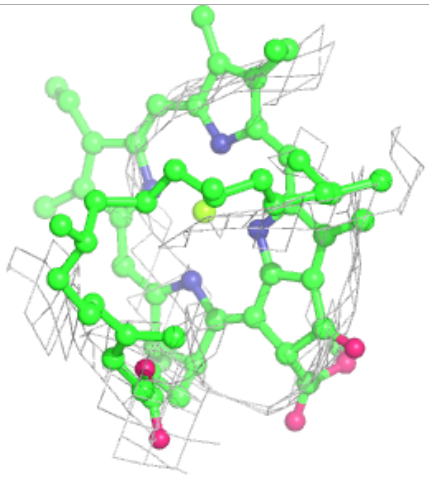


Electron density around CLA C 503:

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

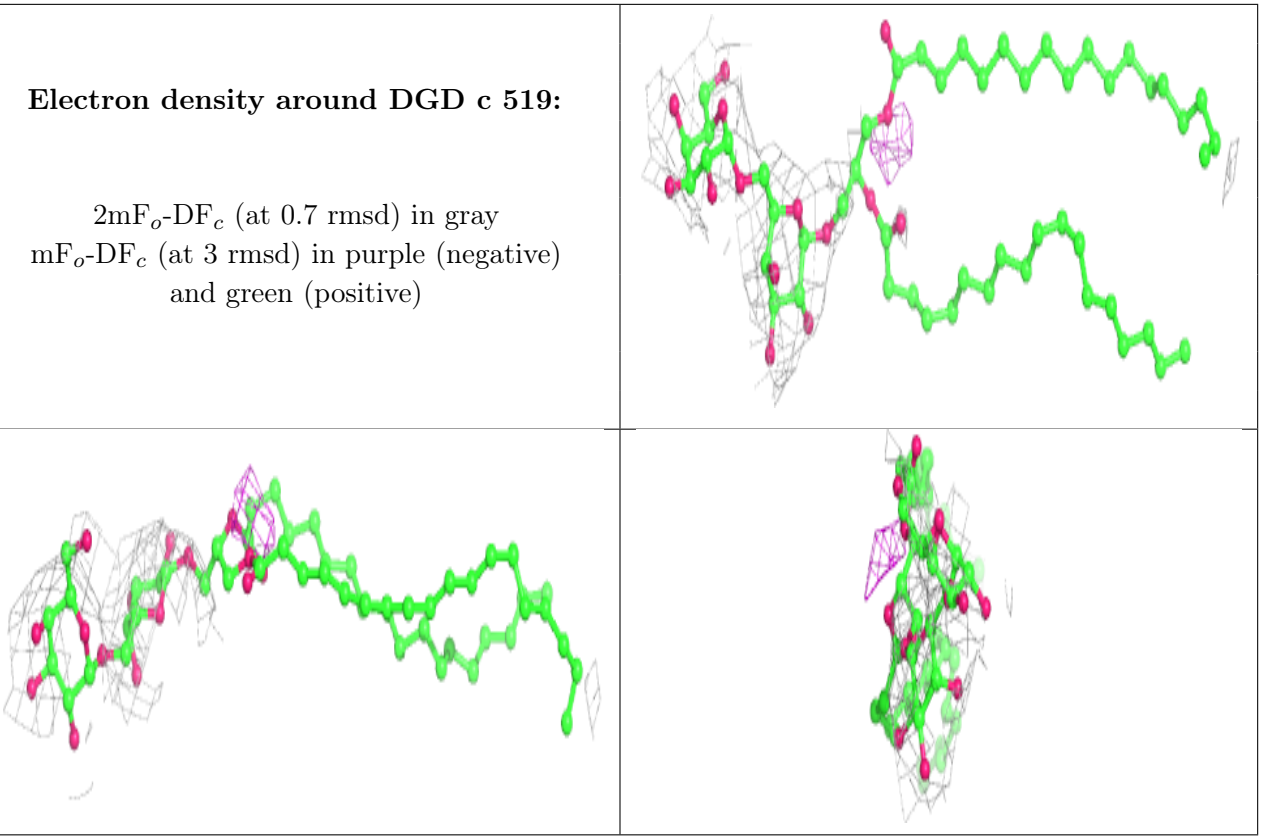






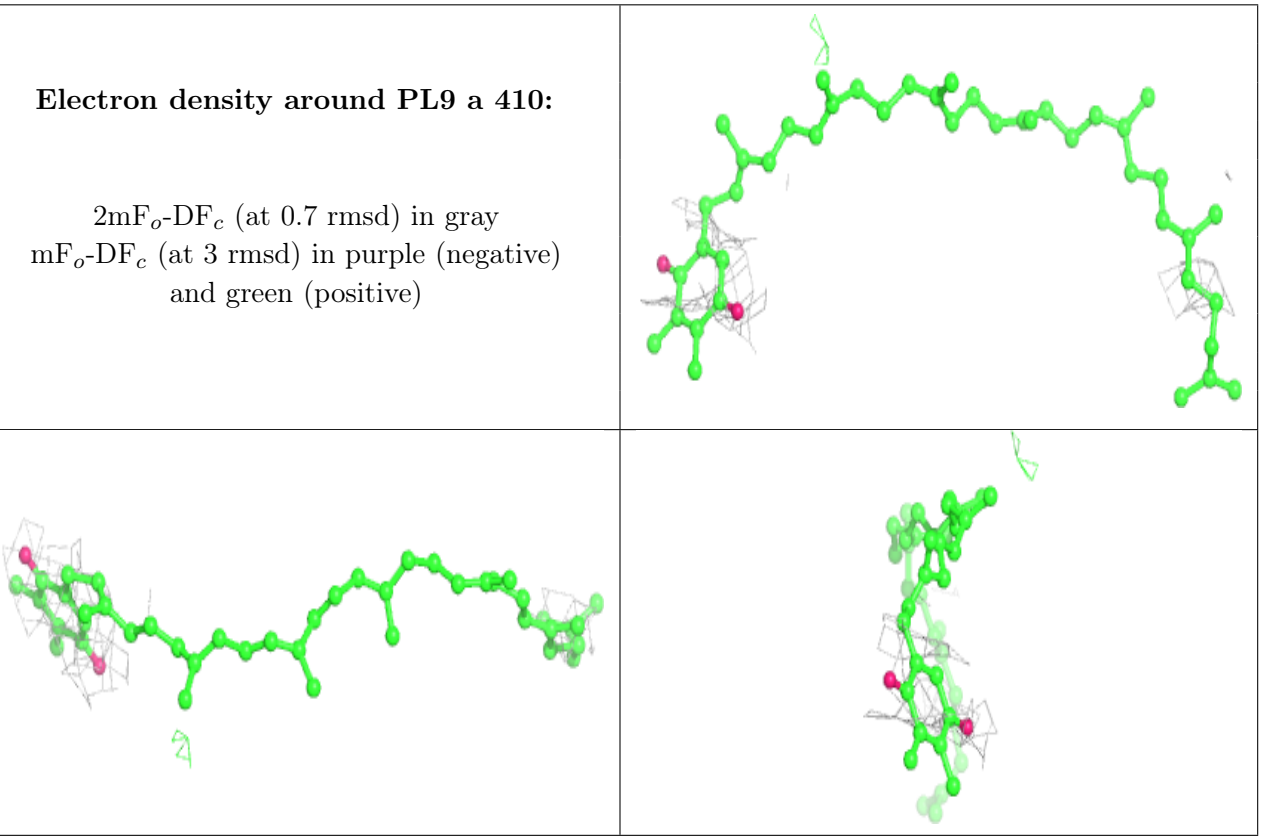
Electron density around DGD c 519:

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



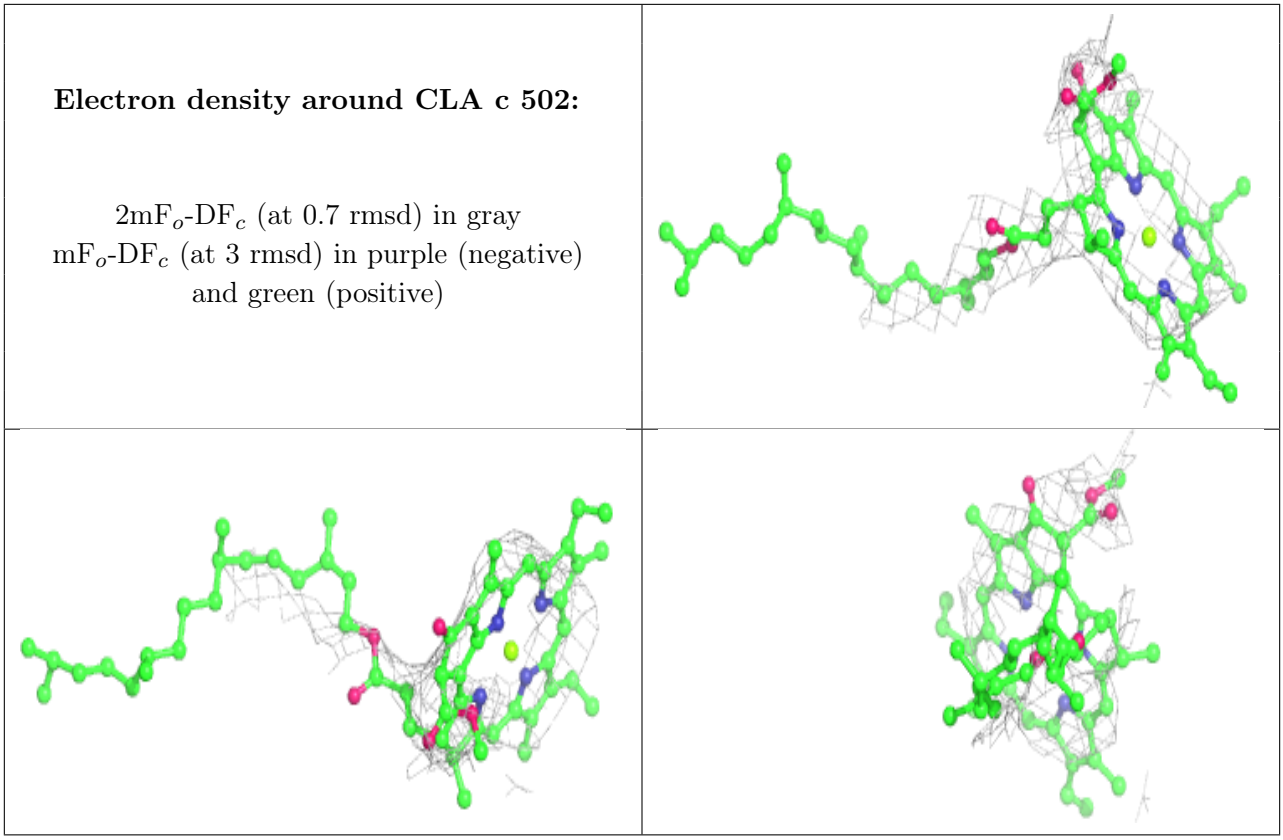
Electron density around PL9 a 410:

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



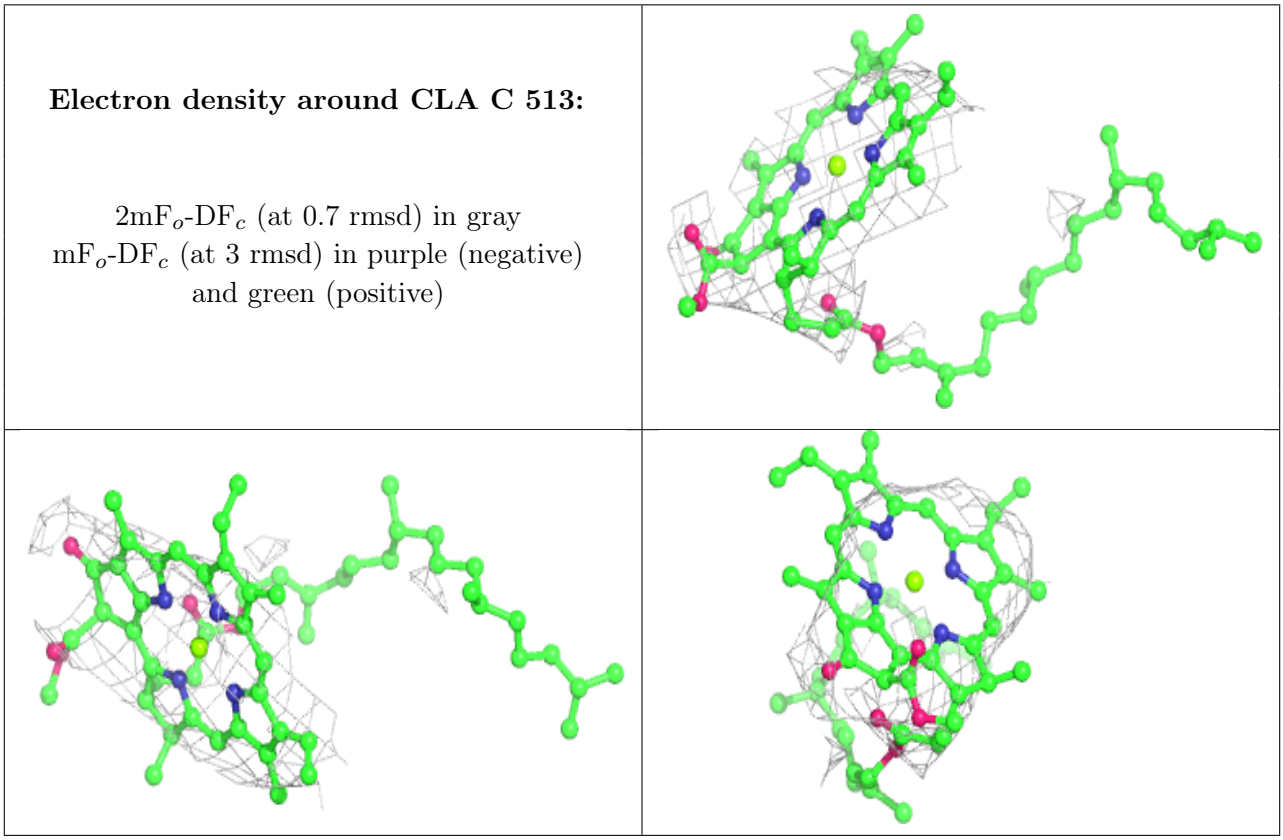
Electron density around CLA c 502:

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



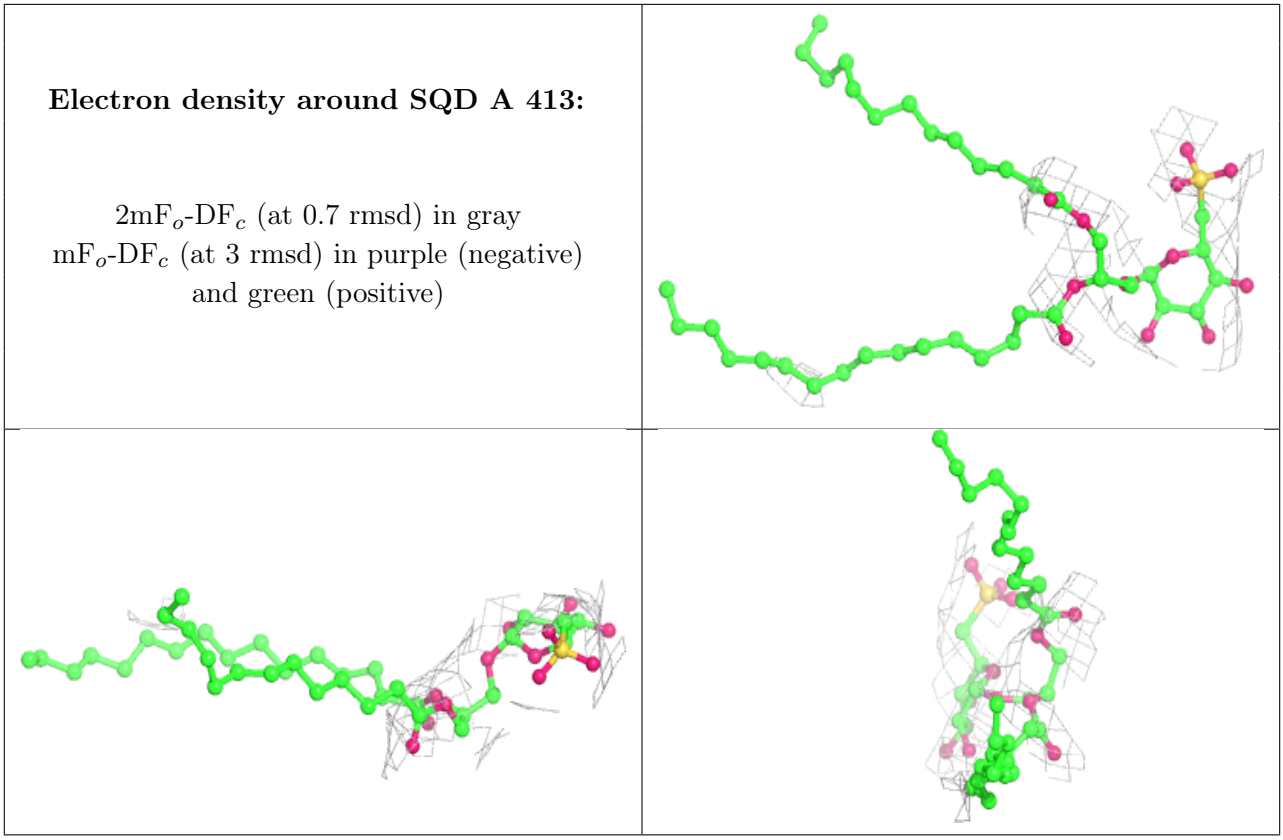
Electron density around CLA C 513:

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



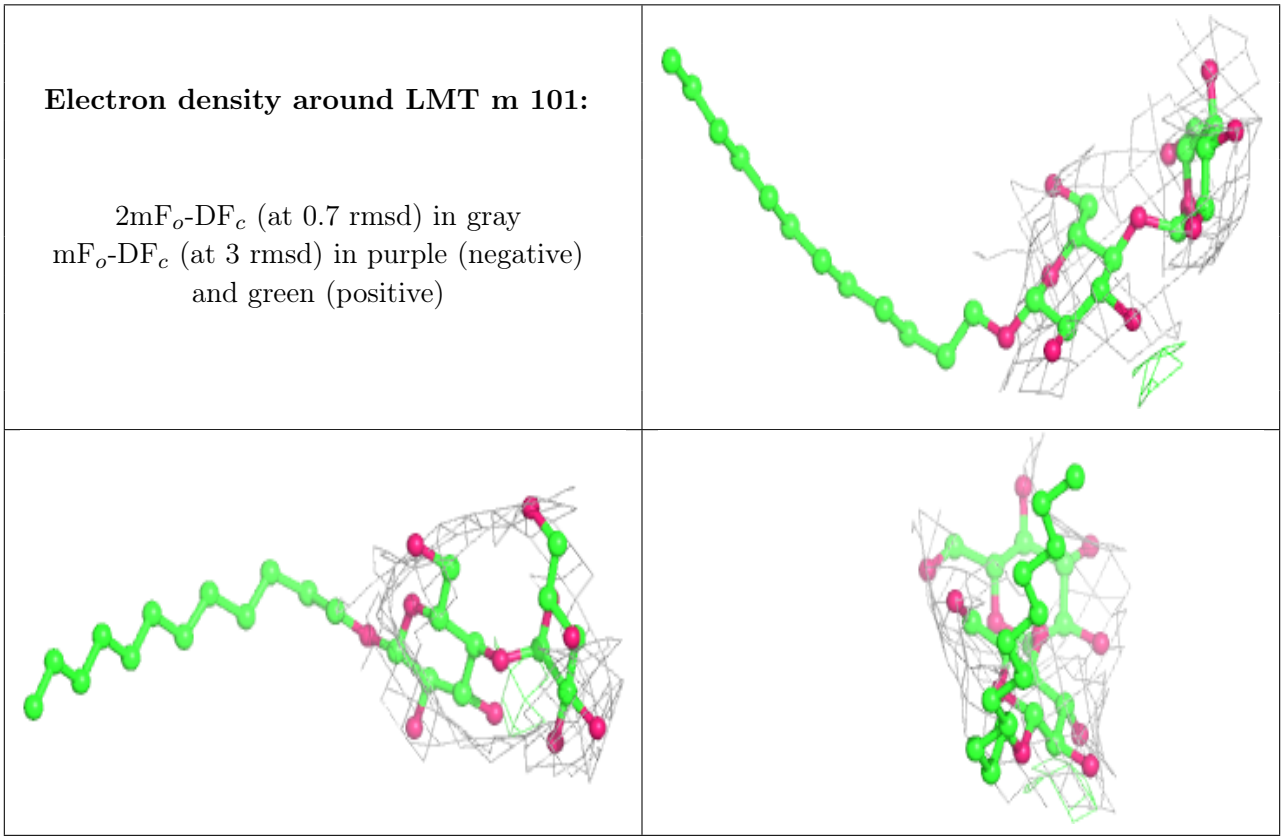
Electron density around SQD A 413:

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



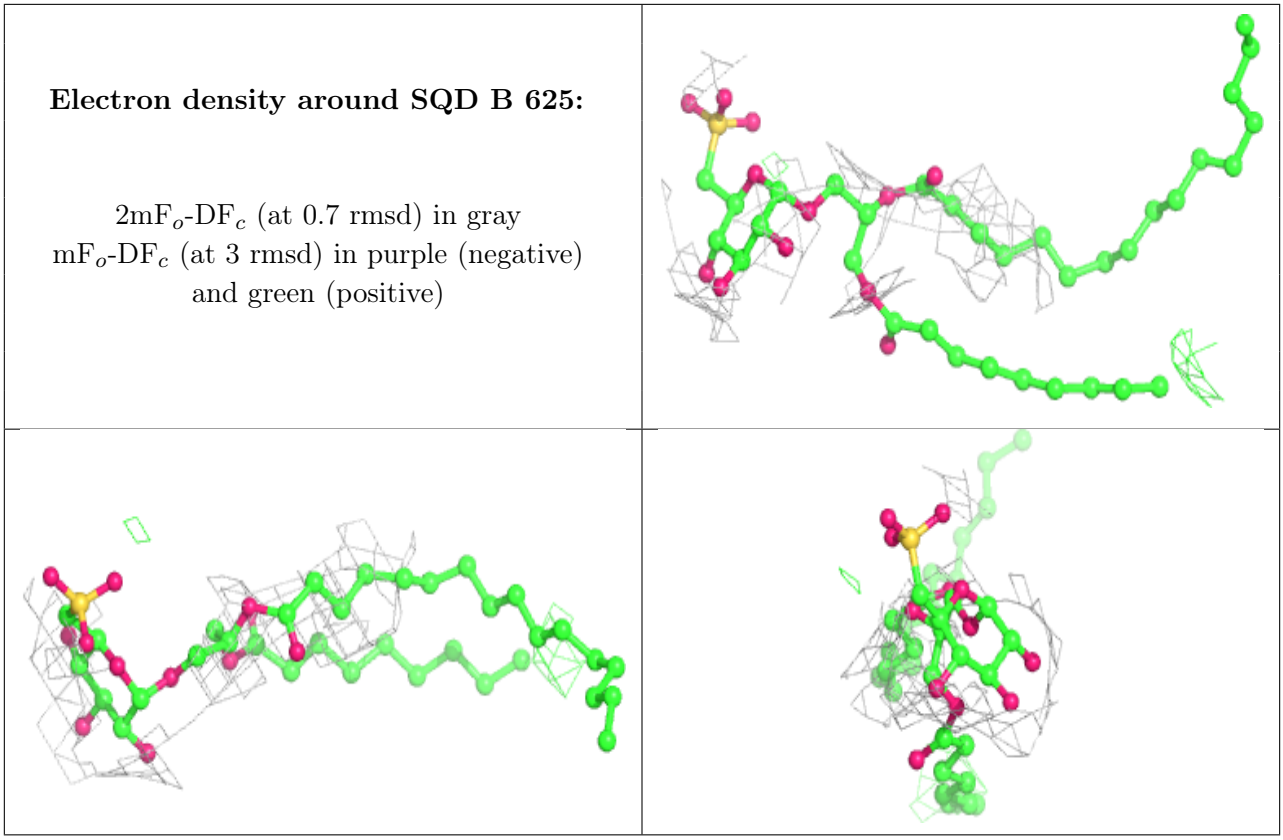
Electron density around LMT m 101:

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



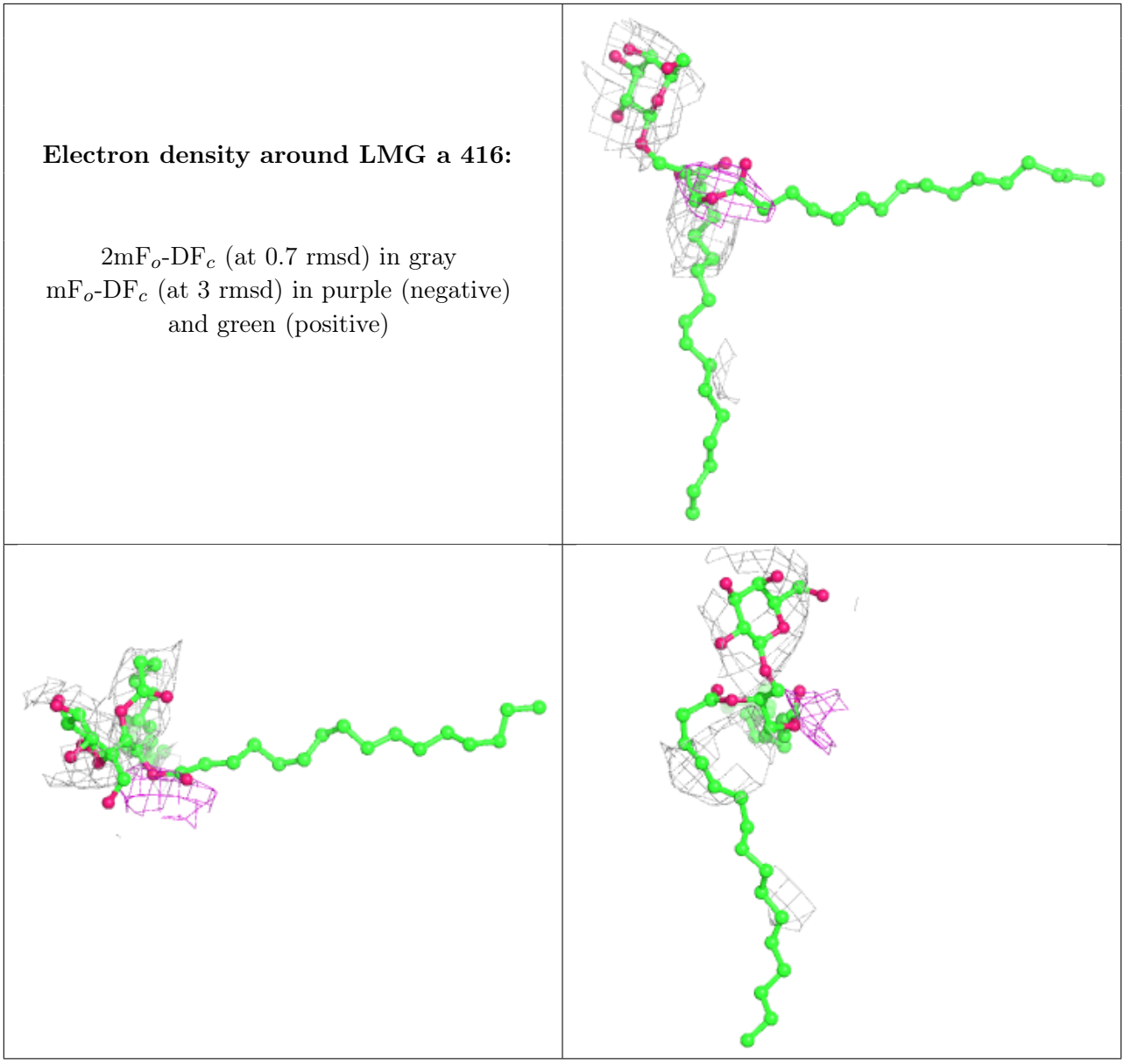
Electron density around SQD B 625:

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



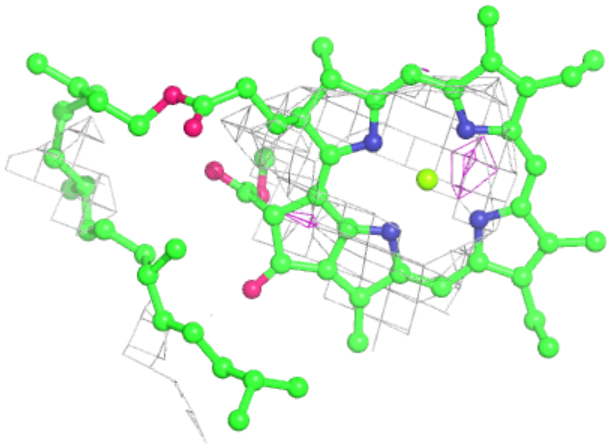
Electron density around LMG a 416:

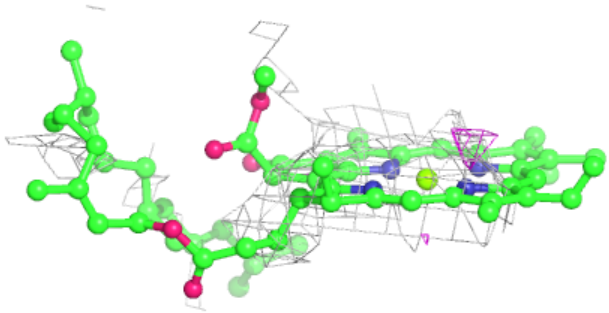
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

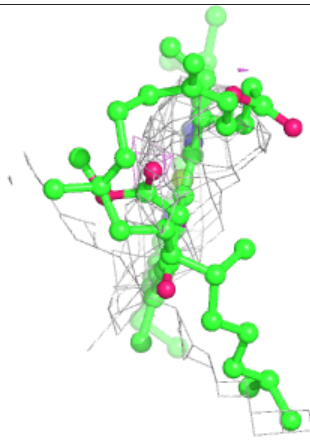


Electron density around CLA b 613:

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

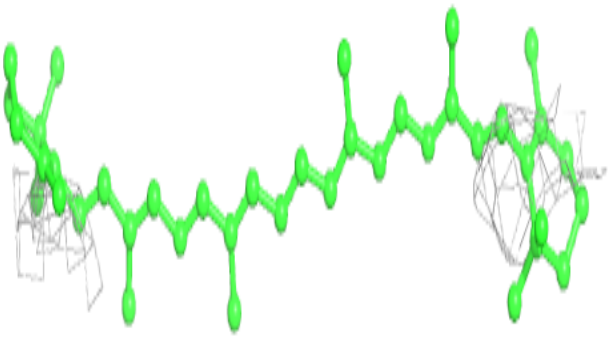


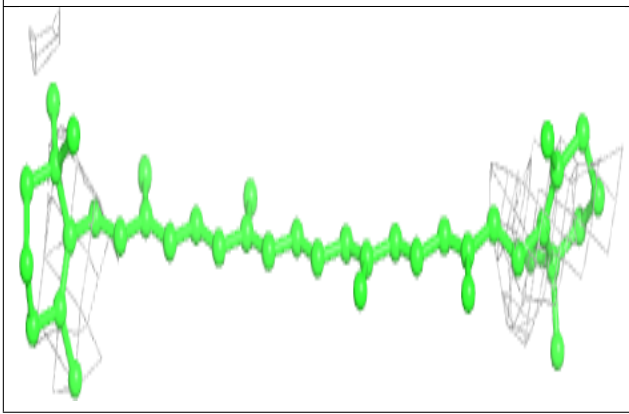


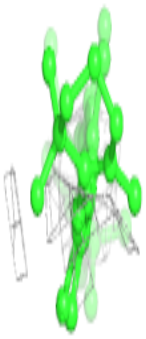


Electron density around BCR c 515:

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

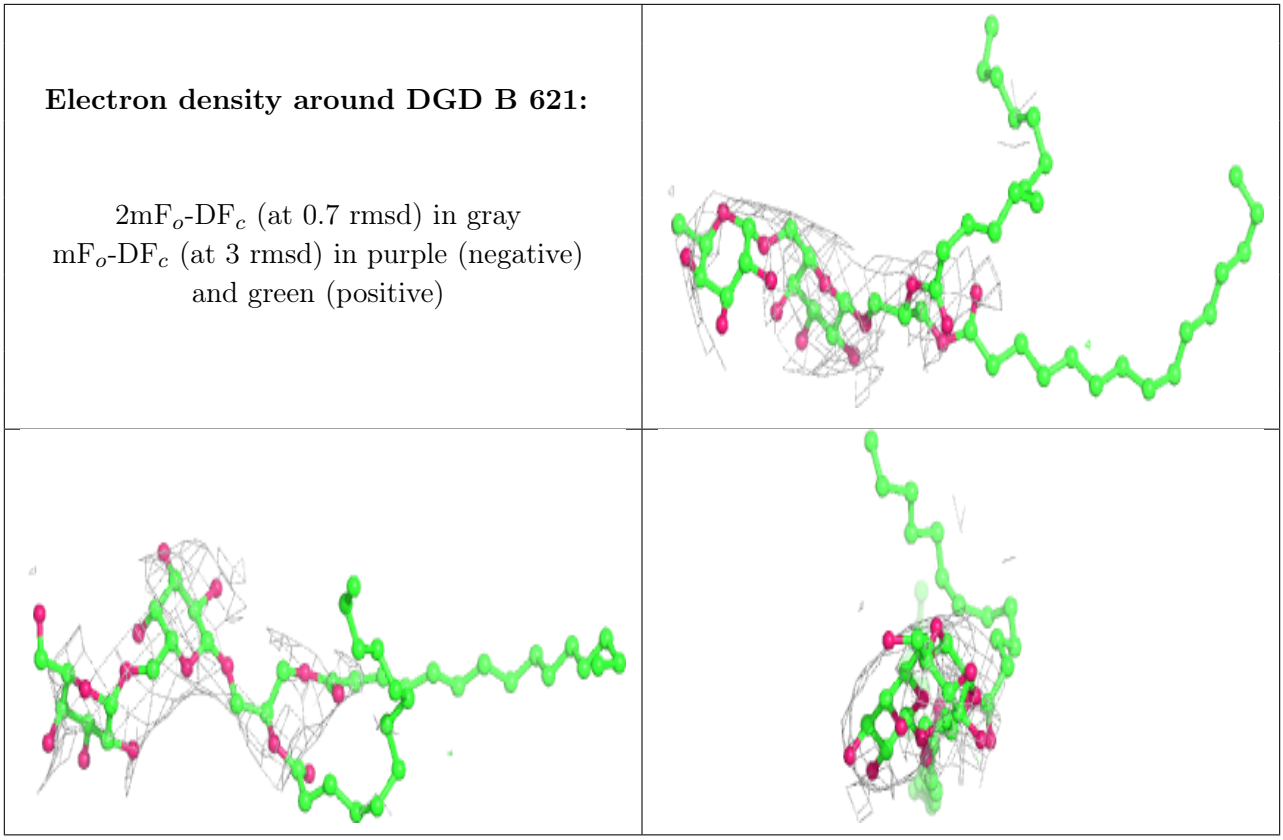






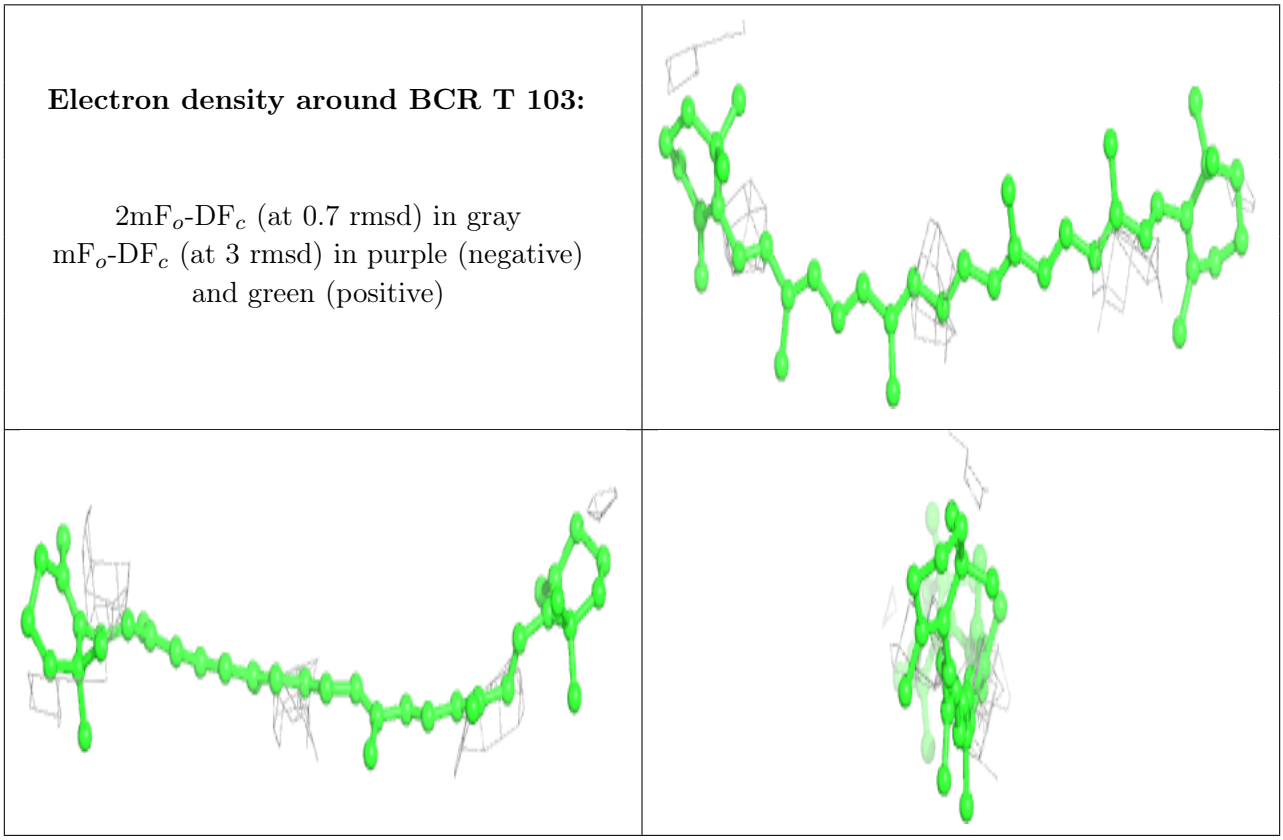
Electron density around DGD B 621:

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



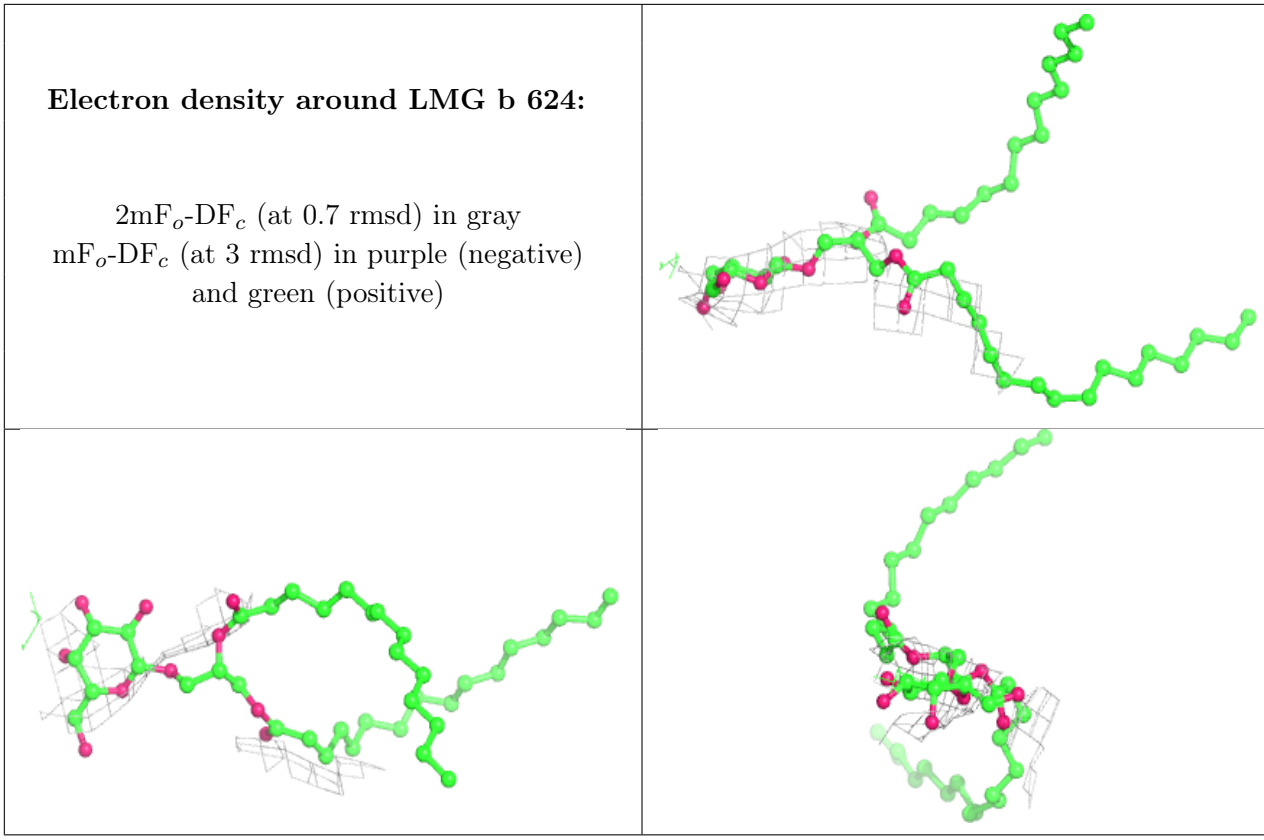
Electron density around BCR T 103:

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



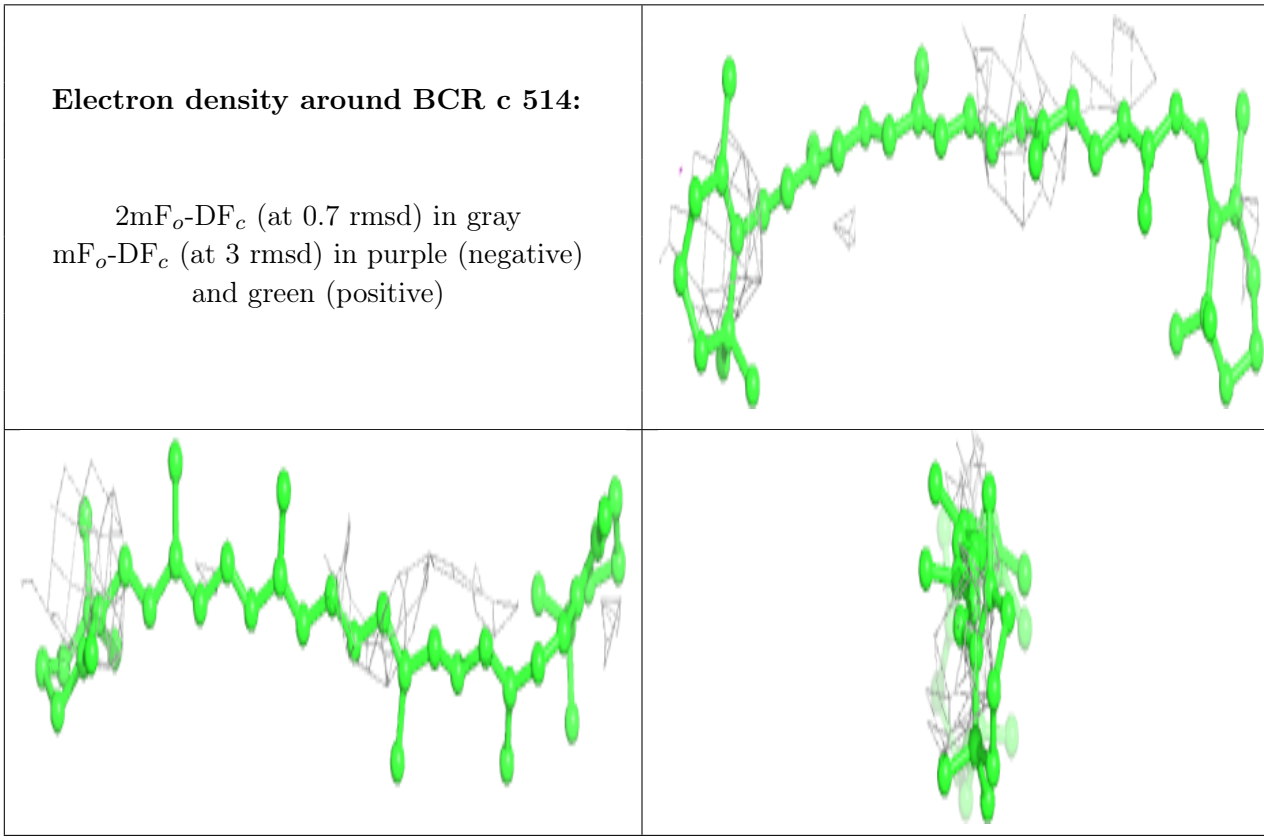
Electron density around LMG b 624:

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



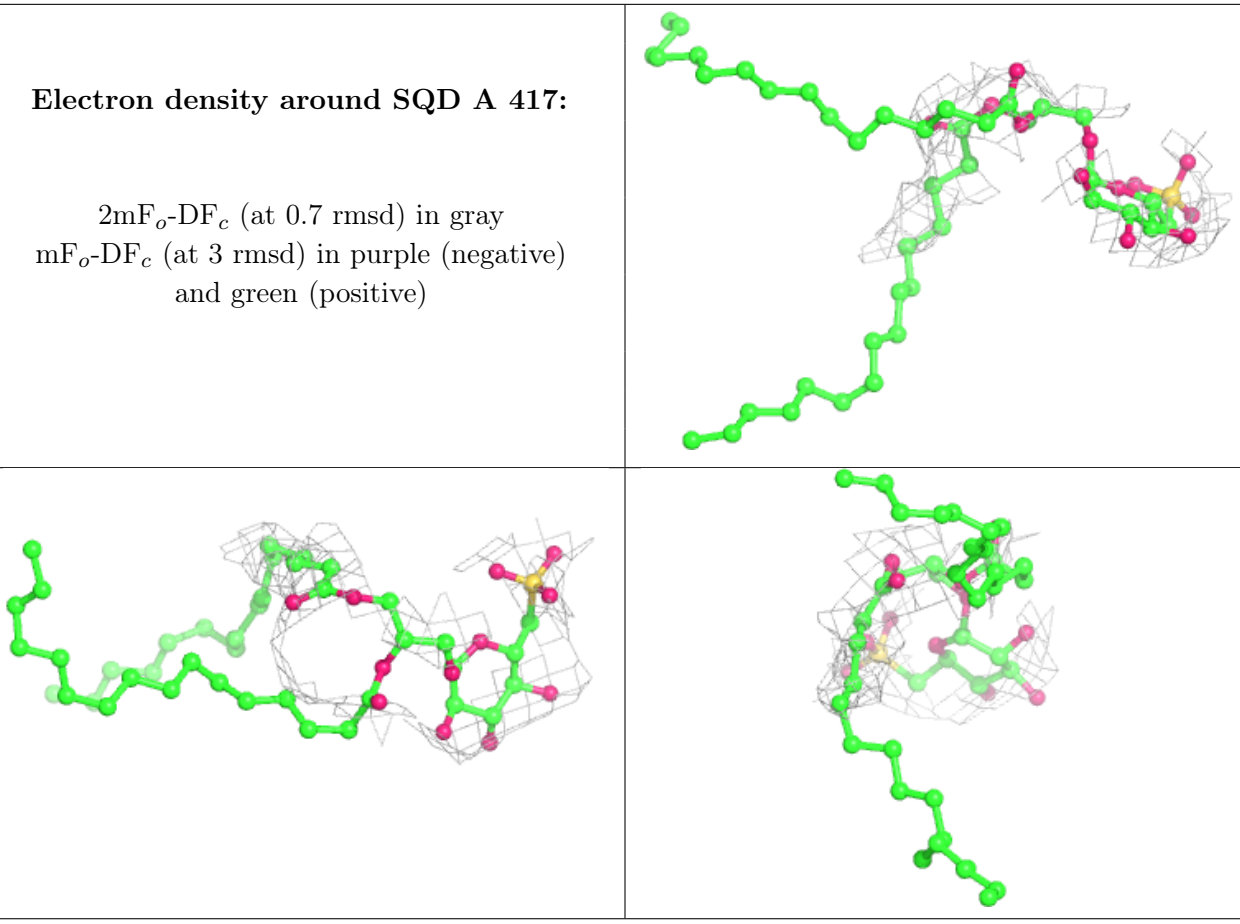
Electron density around BCR c 514:

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



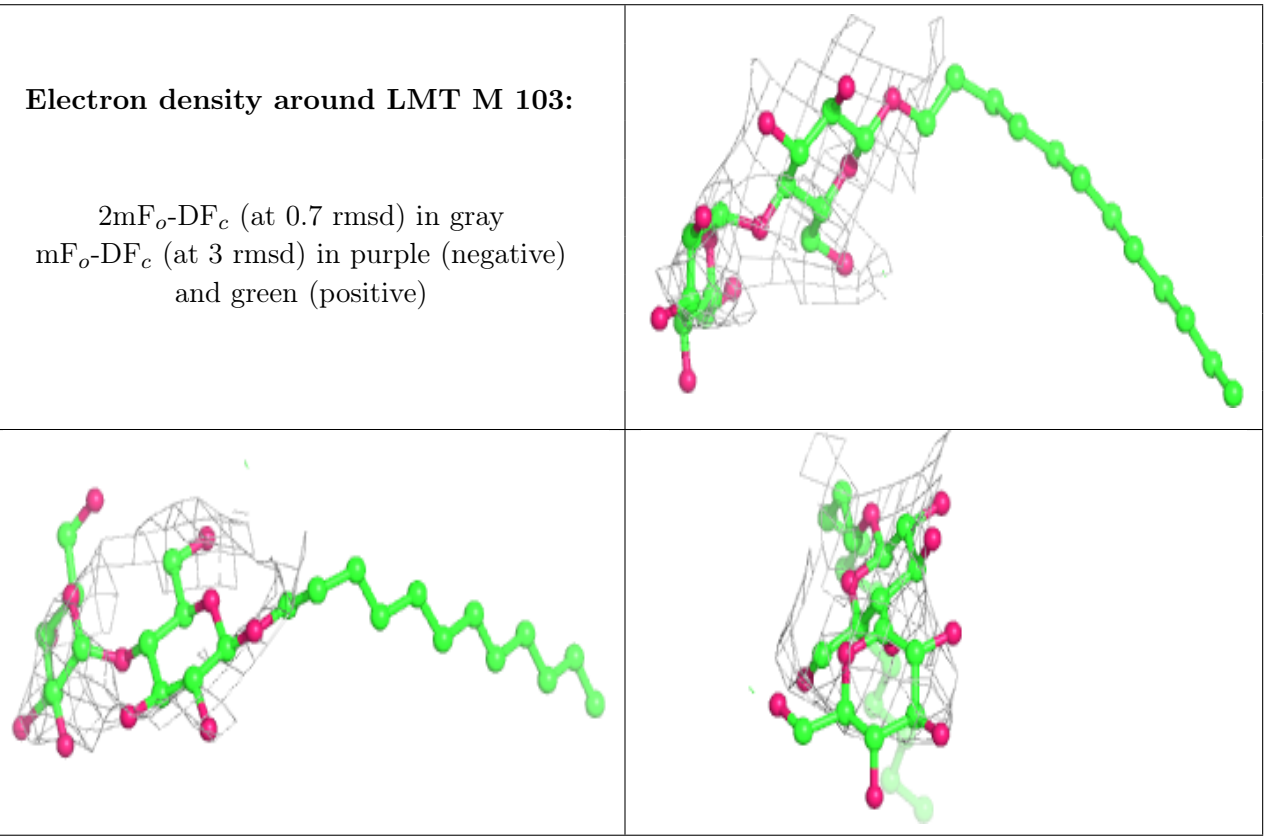
Electron density around SQD A 417:

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



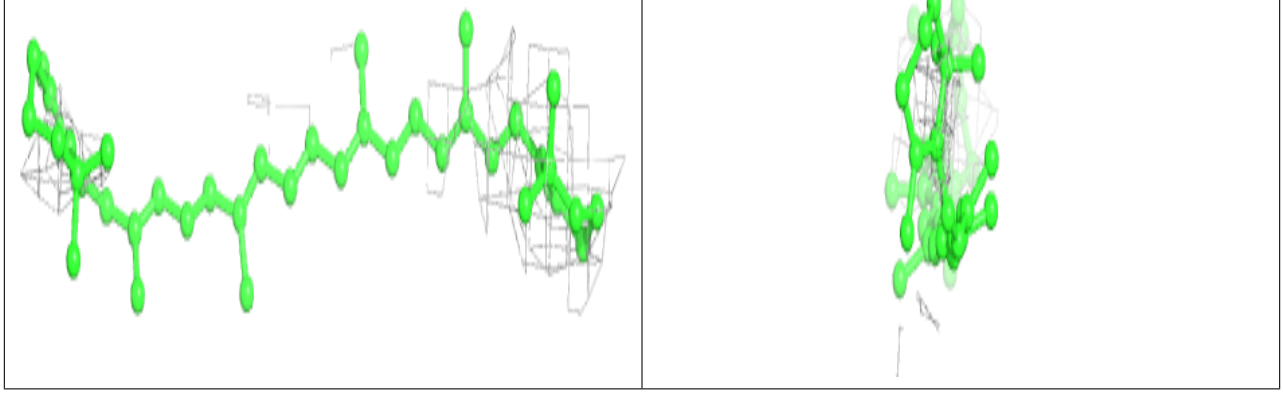
Electron density around LMT M 103:

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



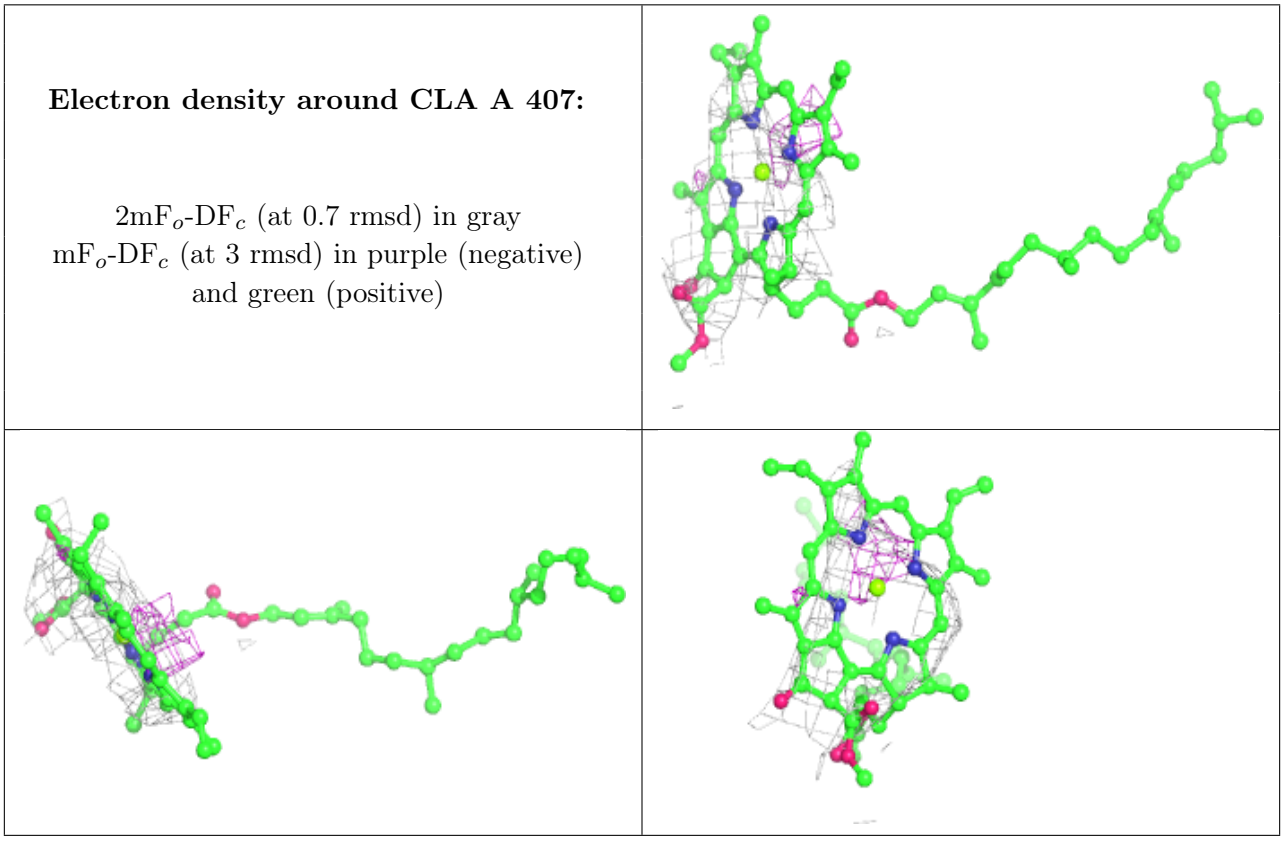
Electron density around BCR C 514:

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



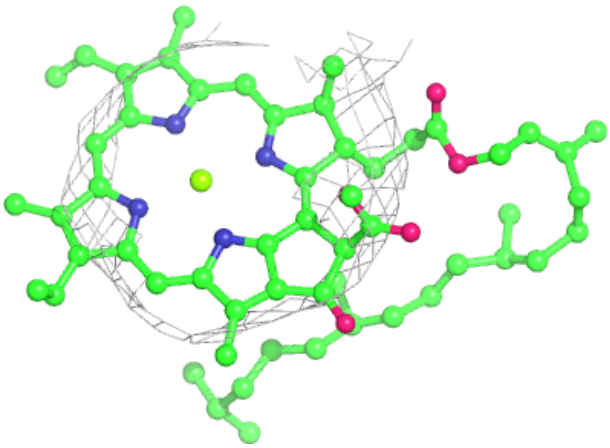
Electron density around CLA A 407:

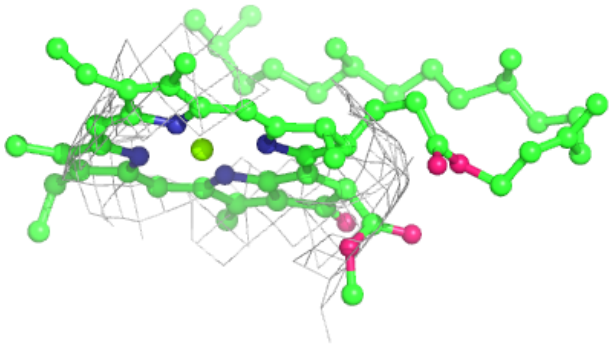
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

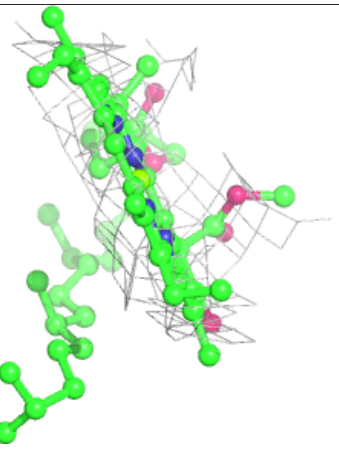


Electron density around CLA c 509:

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

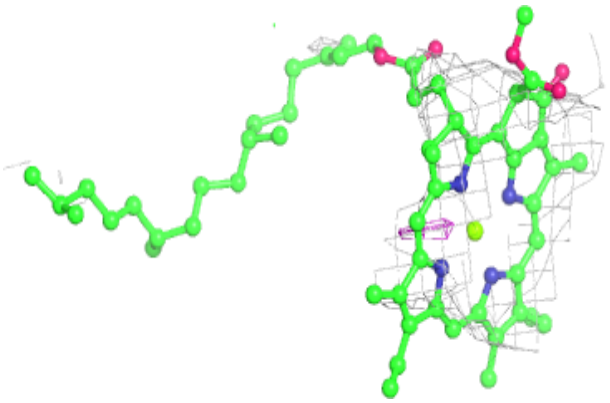


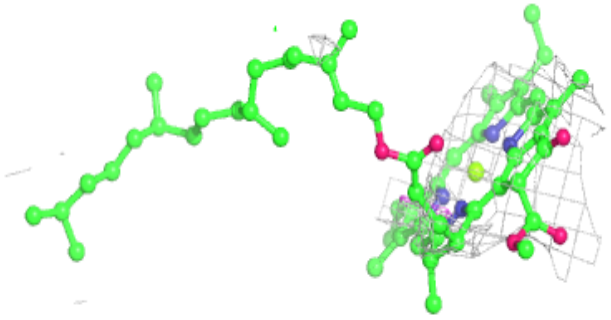


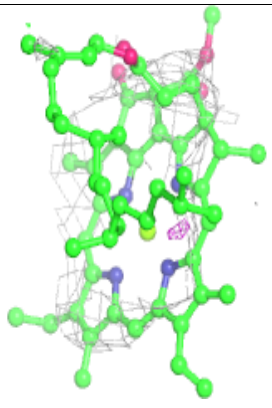


Electron density around CLA c 511:

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

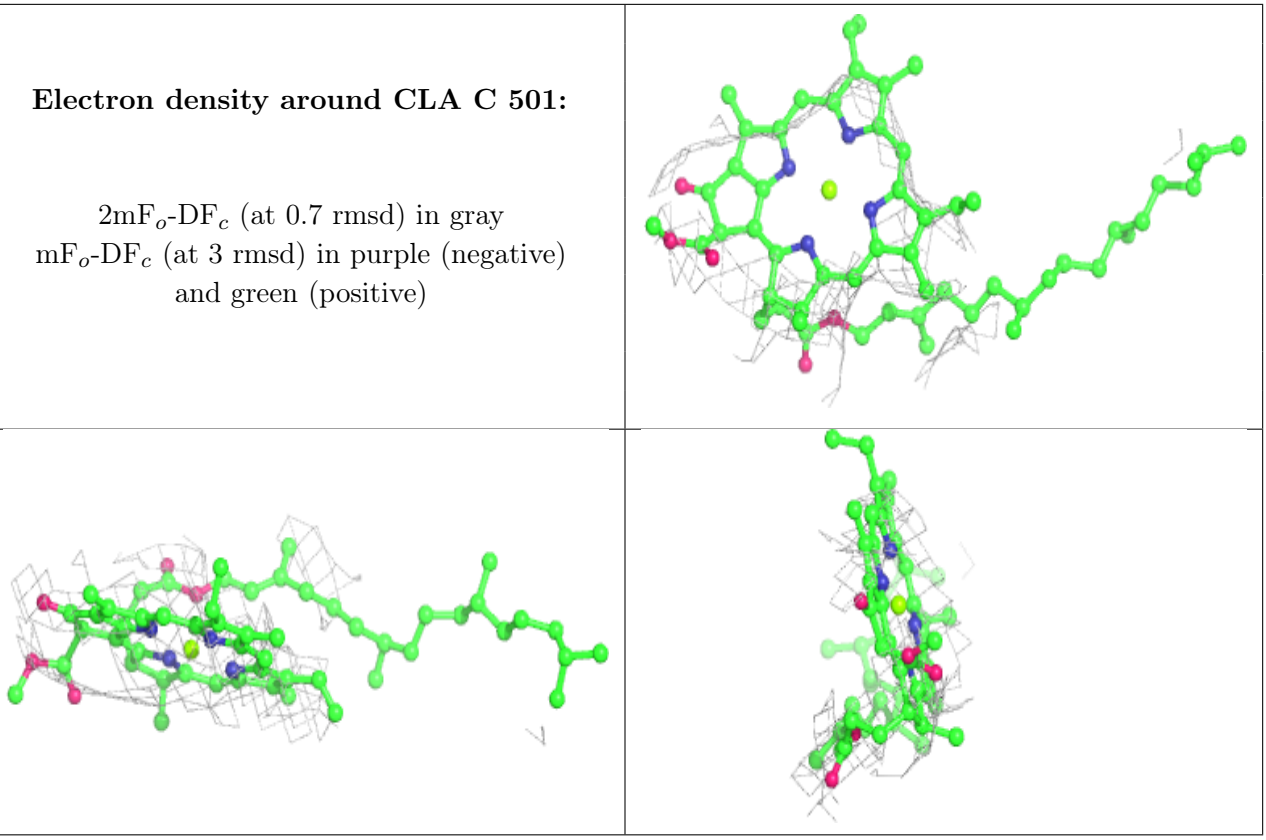






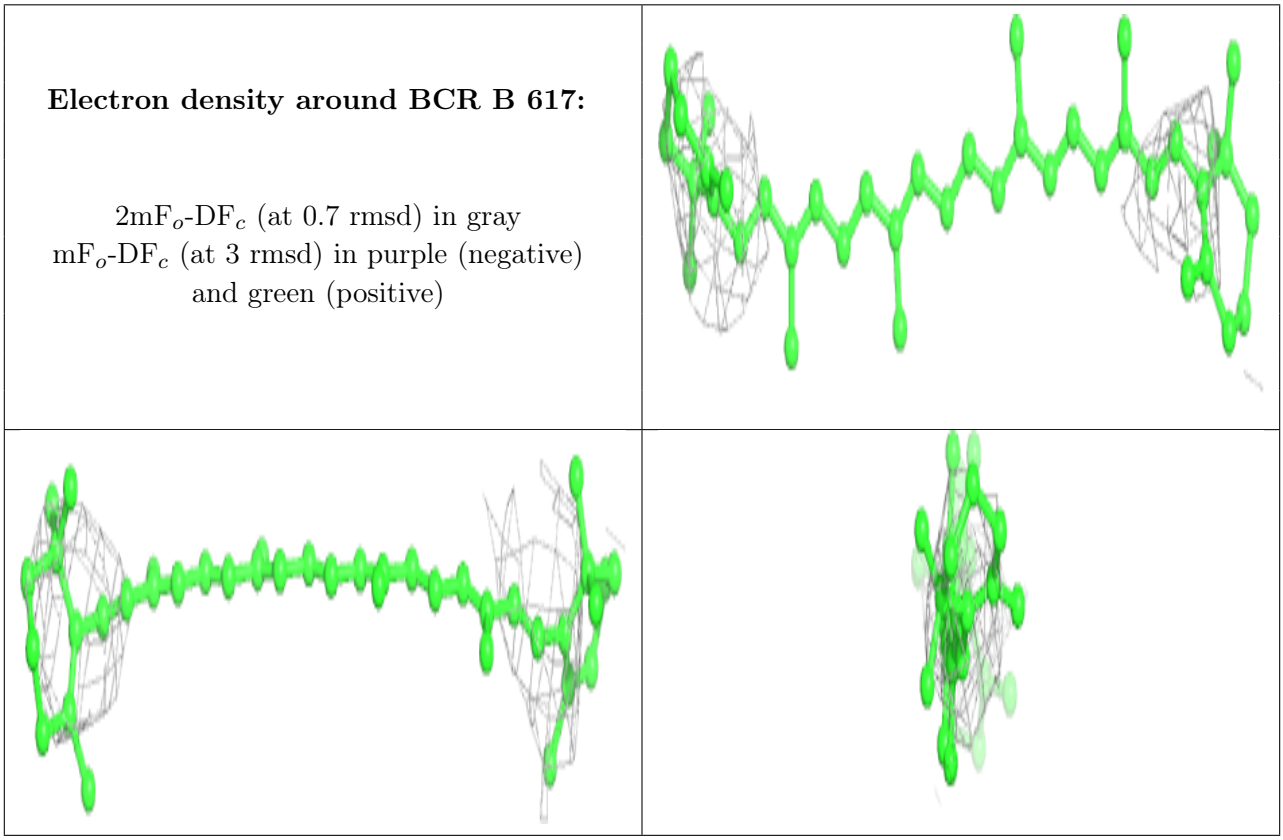
Electron density around CLA C 501:

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



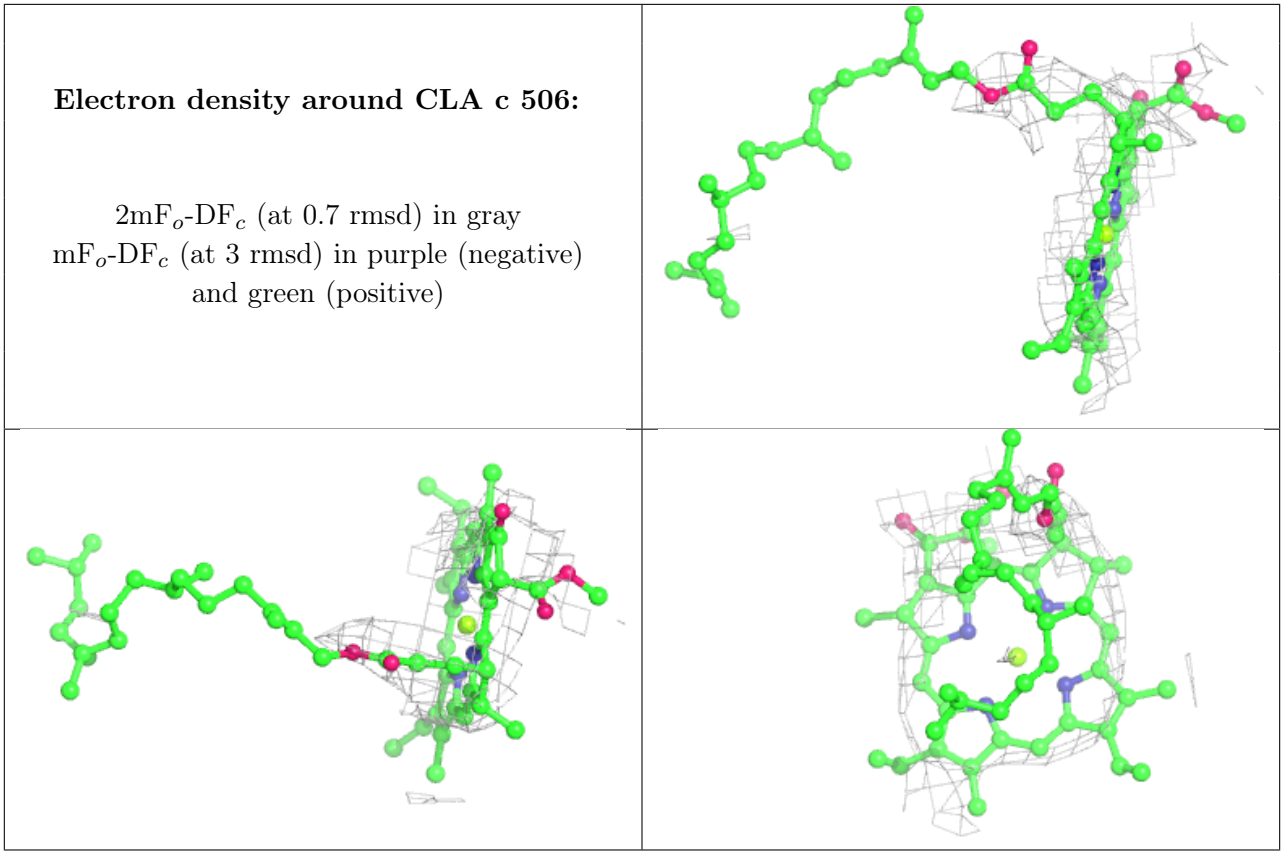
Electron density around BCR B 617:

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



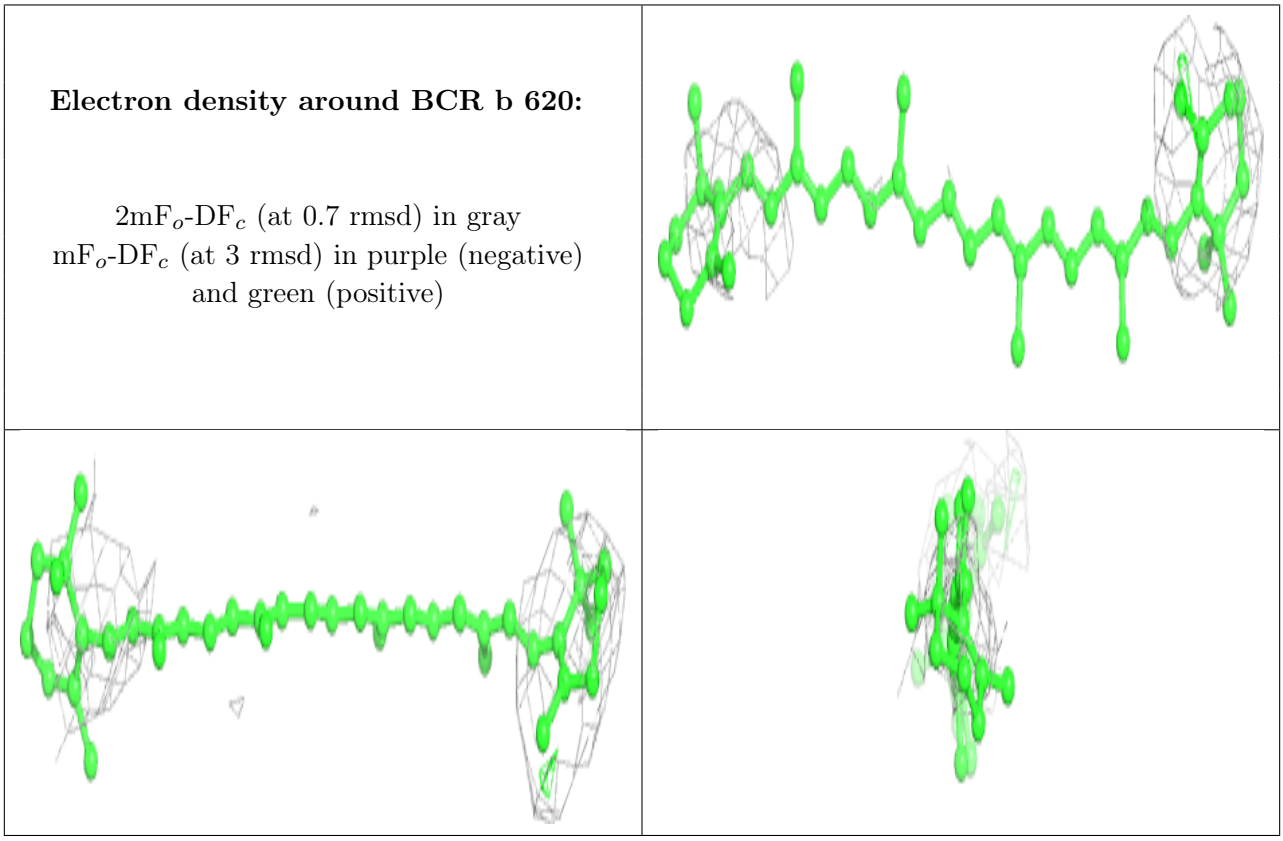
Electron density around CLA c 506:

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



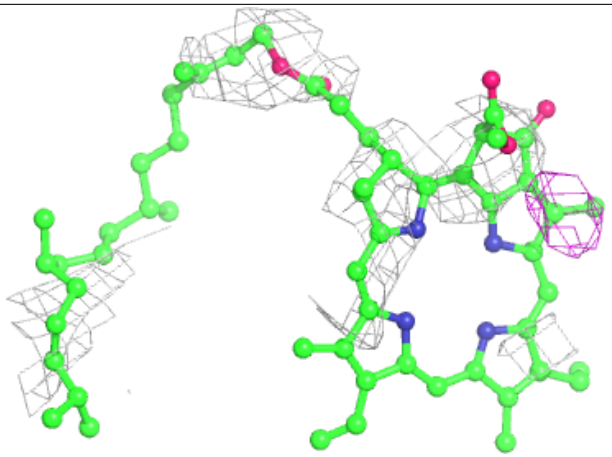
Electron density around BCR b 620:

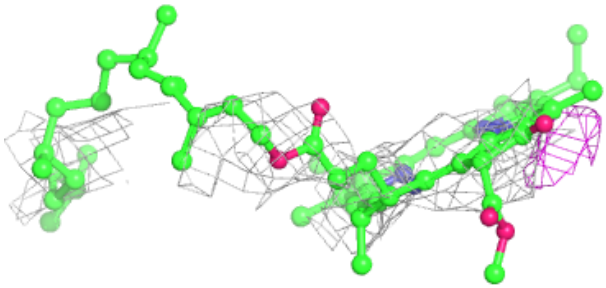
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

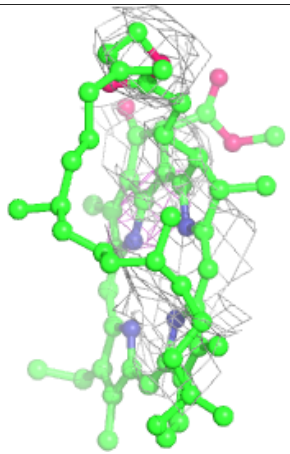


Electron density around PHO A 406:

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

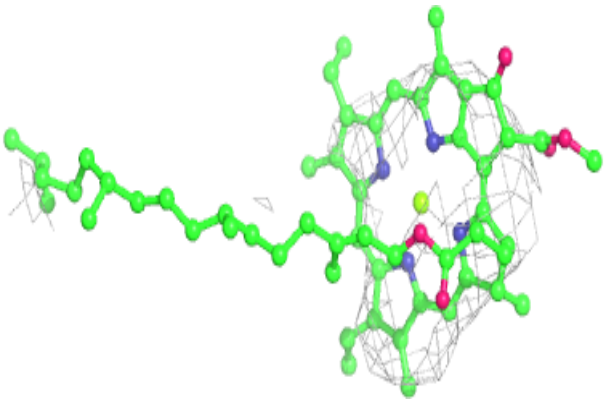


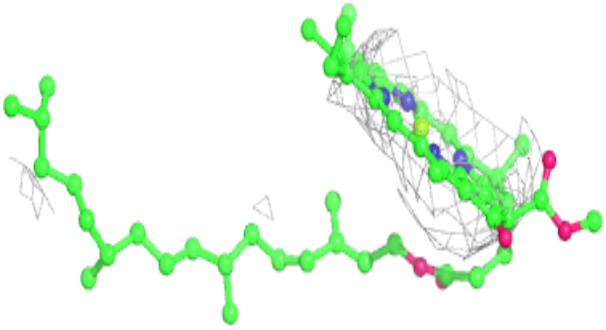


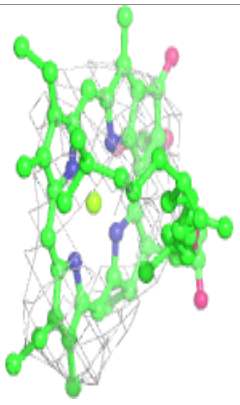


Electron density around CLA b 611:

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

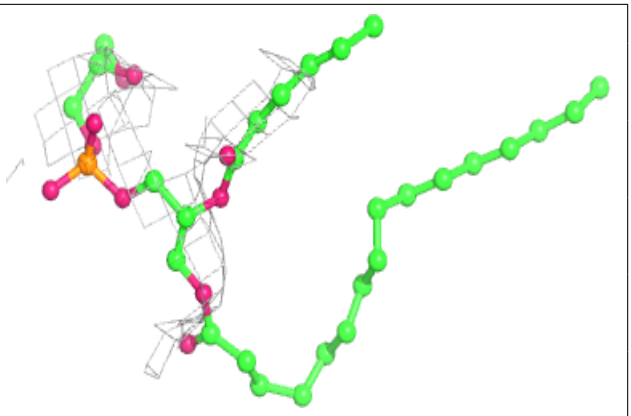


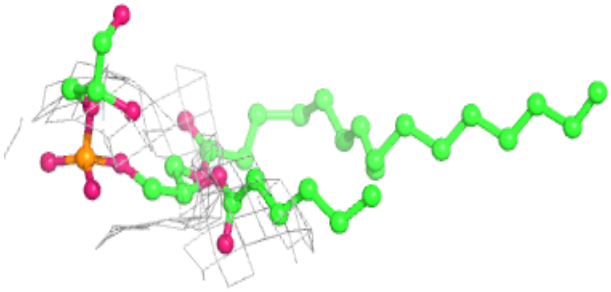


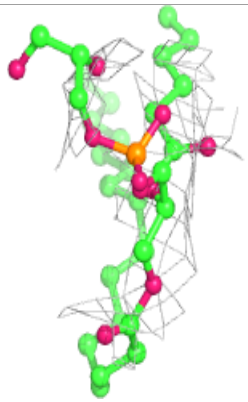


Electron density around LHG A 412:

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

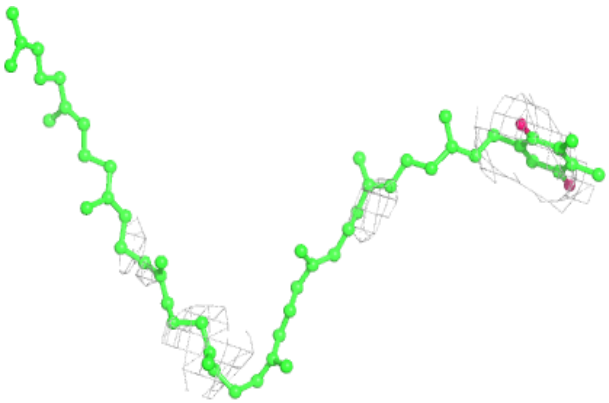


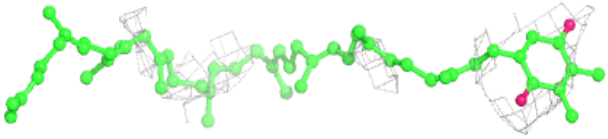




Electron density around PL9 D 404:

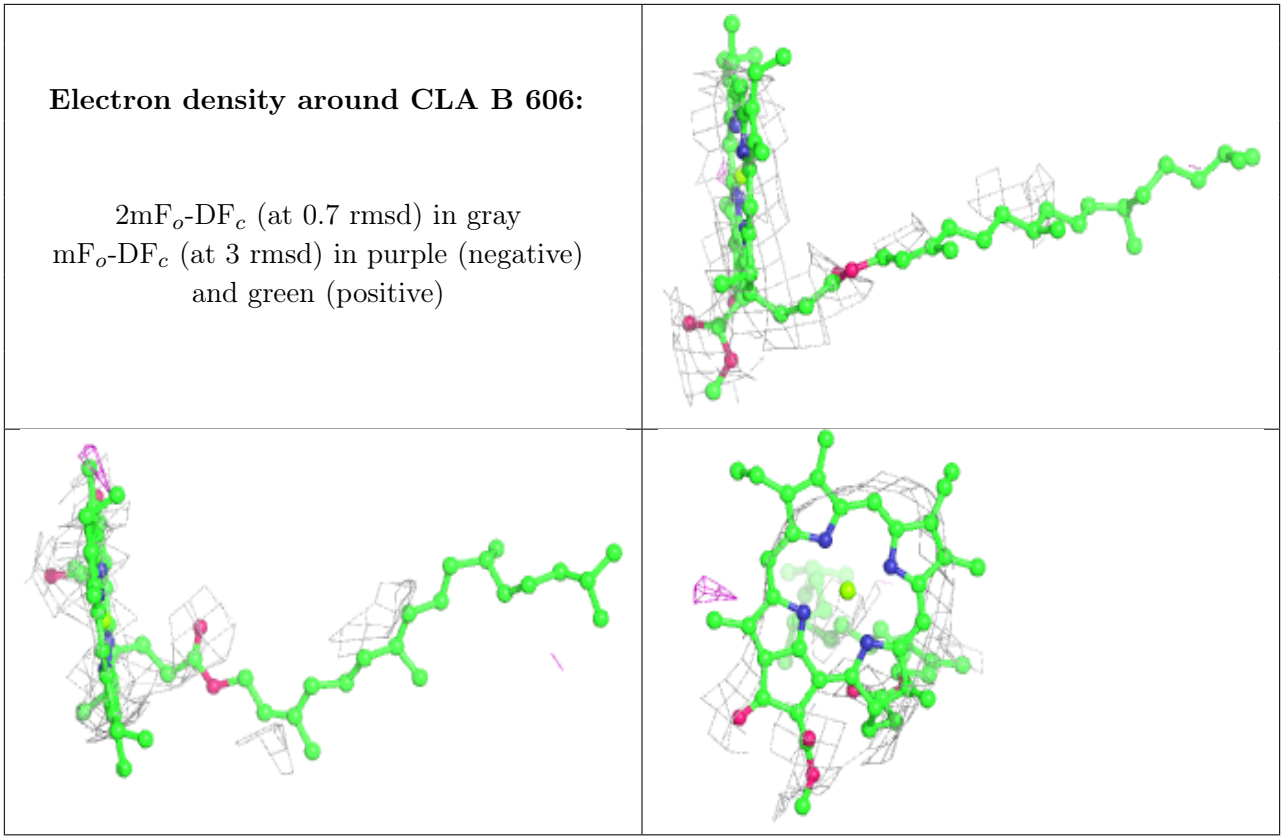
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





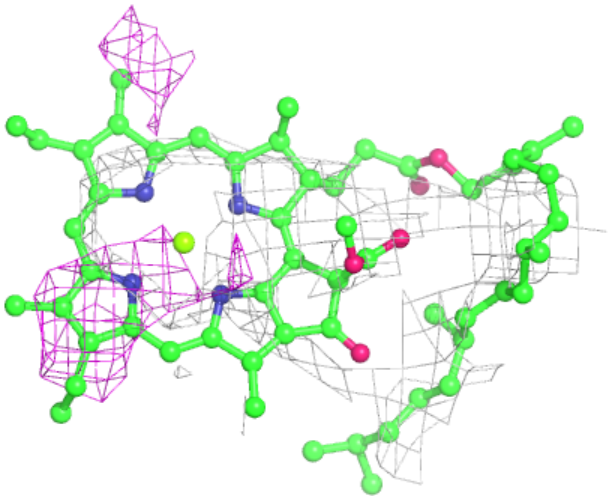
Electron density around CLA B 606:

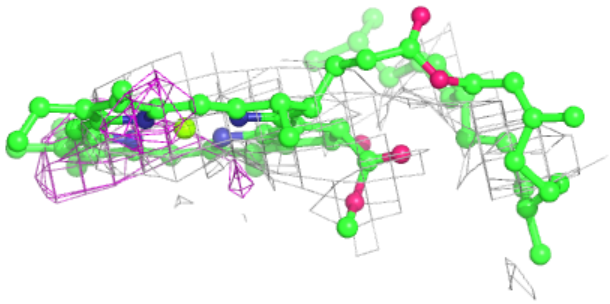
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

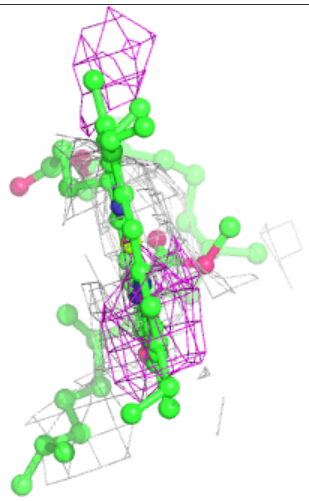


Electron density around CLA B 610:

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

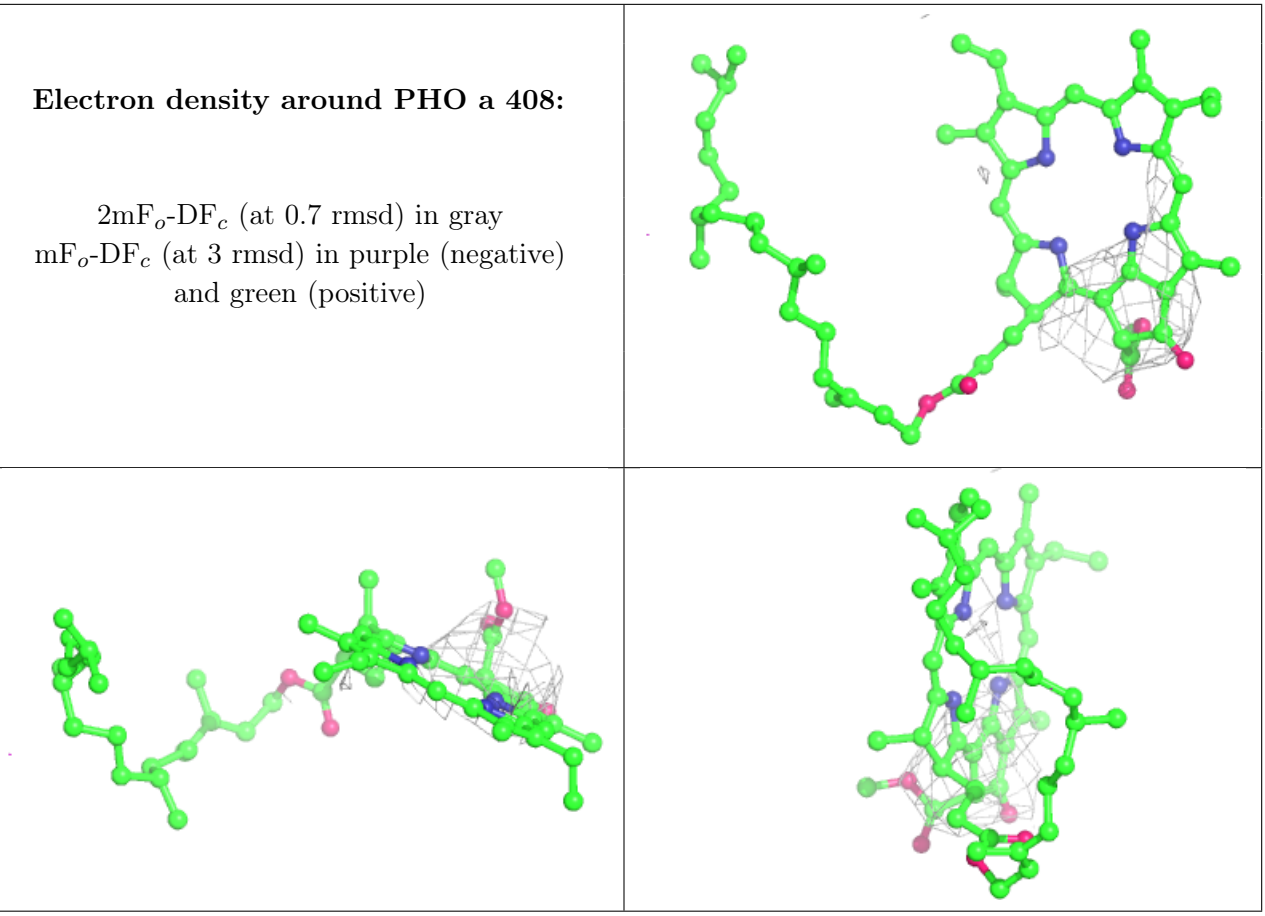






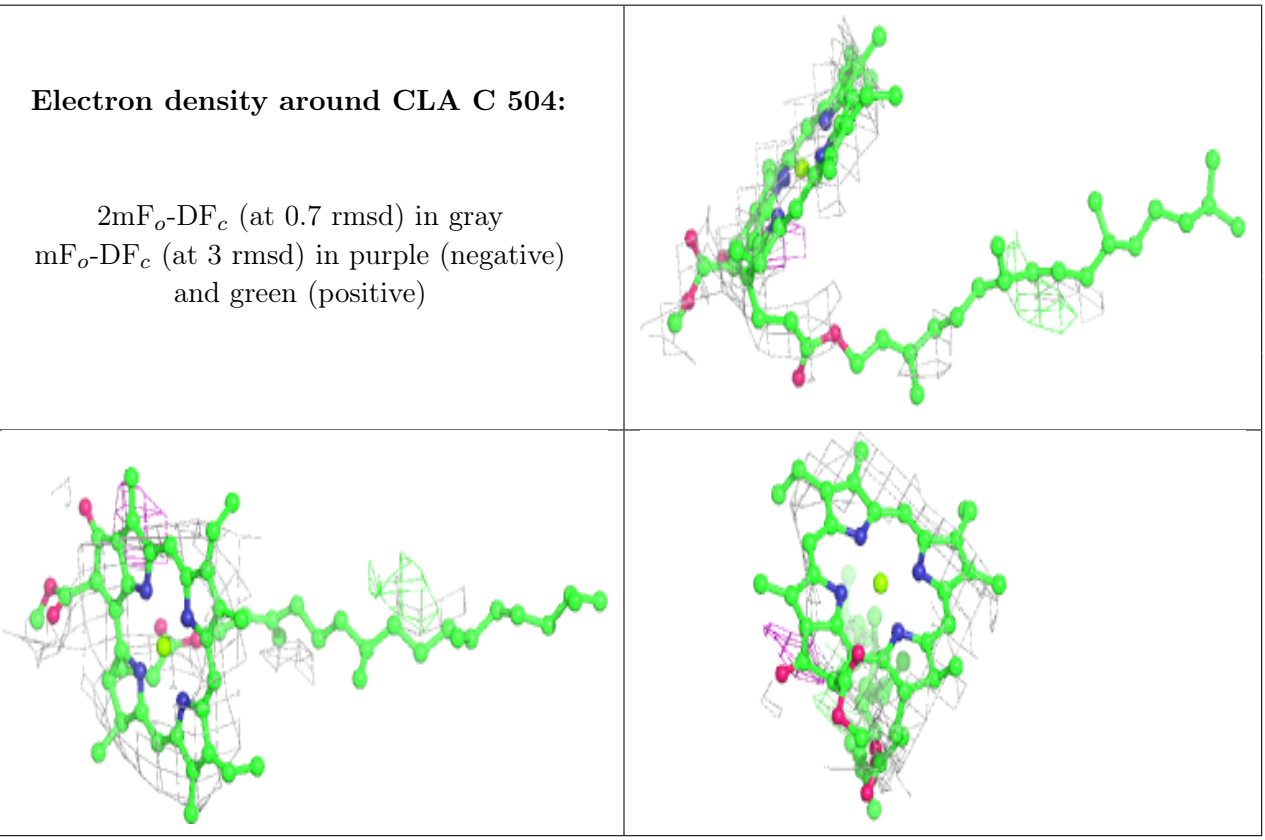
Electron density around PHO a 408:

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



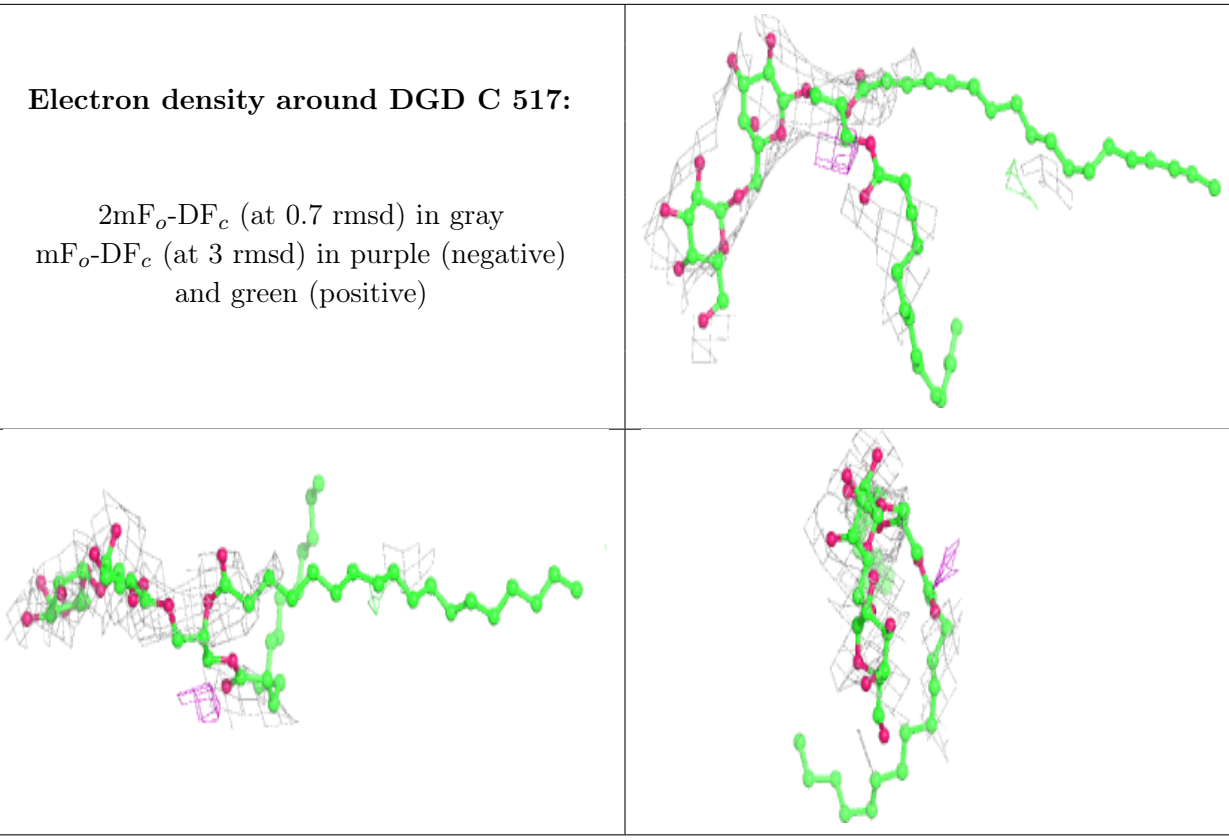
Electron density around CLA C 504:

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



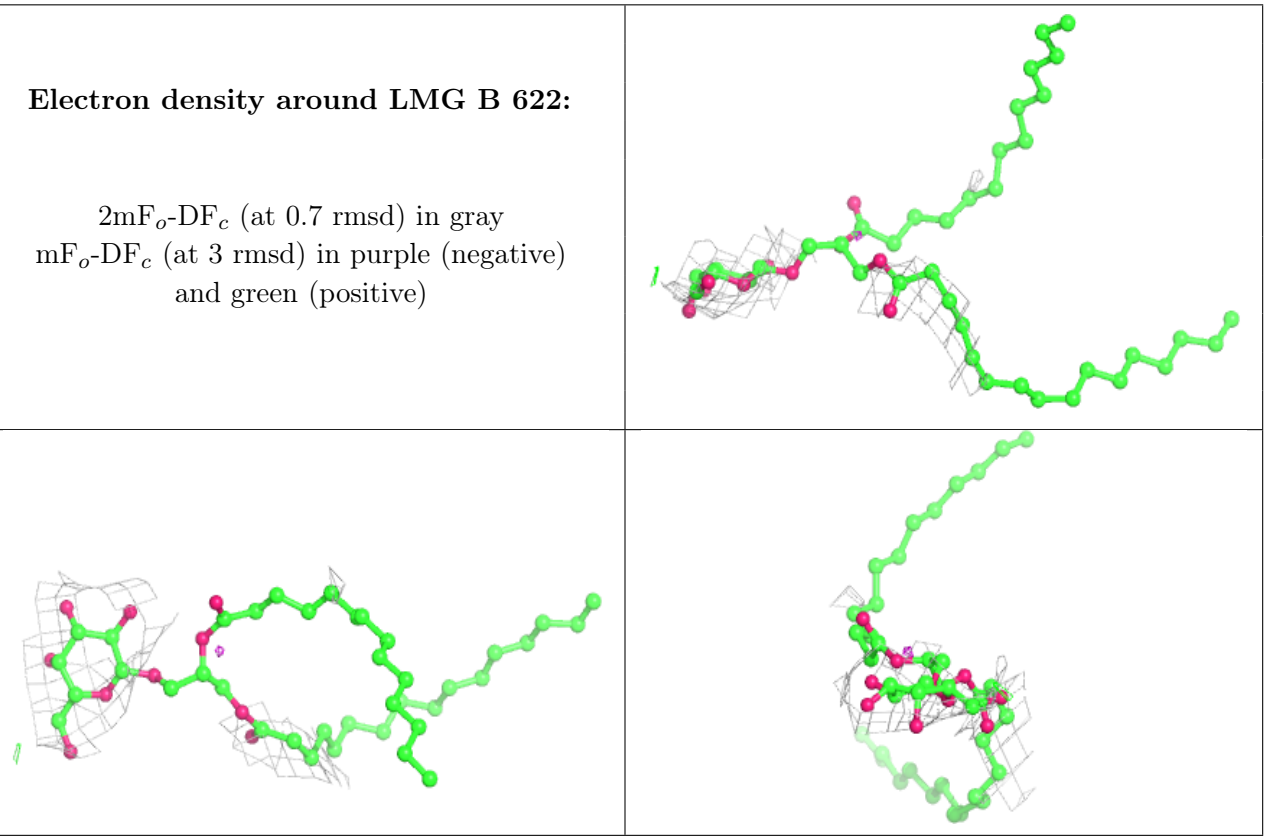
Electron density around DGD C 517:

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



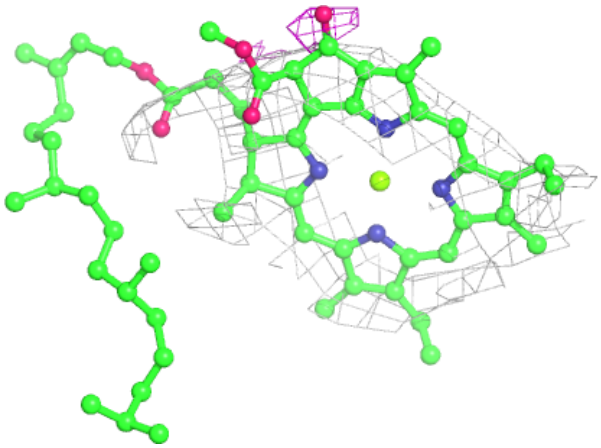
Electron density around LMG B 622:

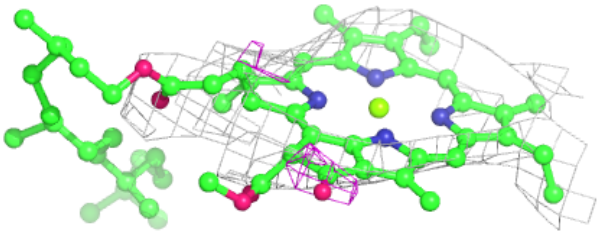
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

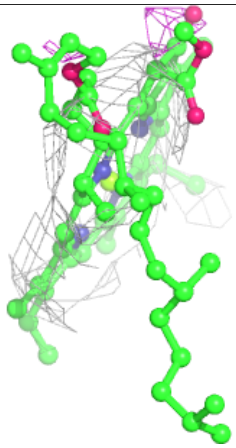


Electron density around CLA B 616:

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

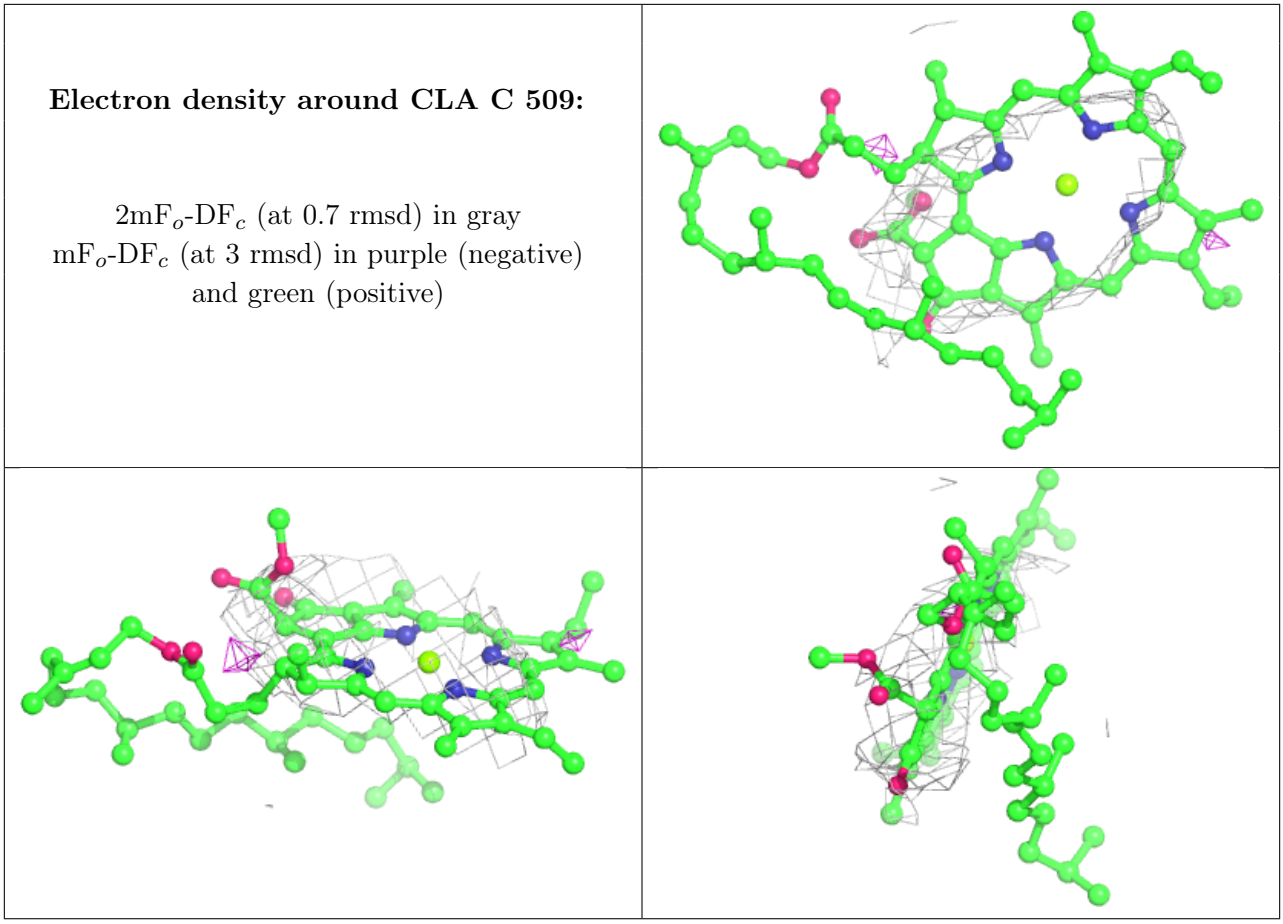






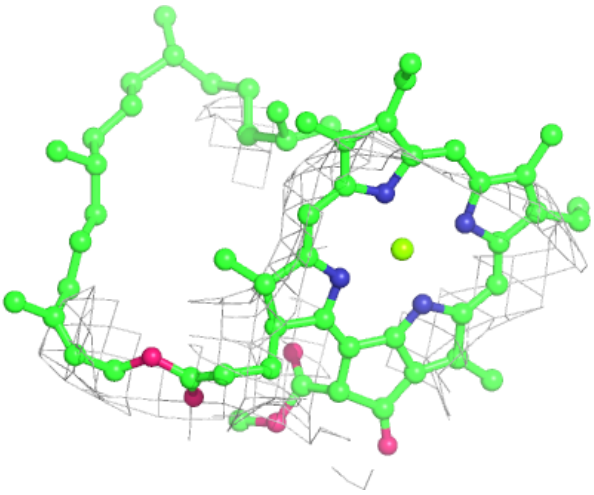
Electron density around CLA C 509:

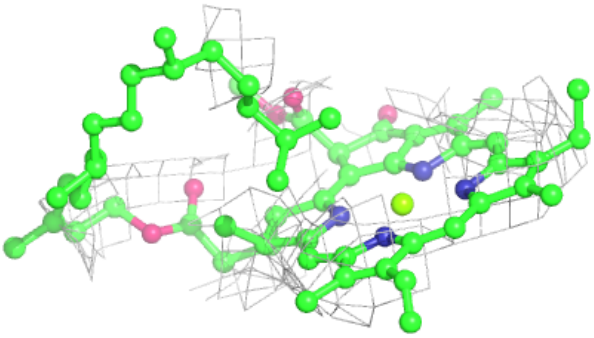
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

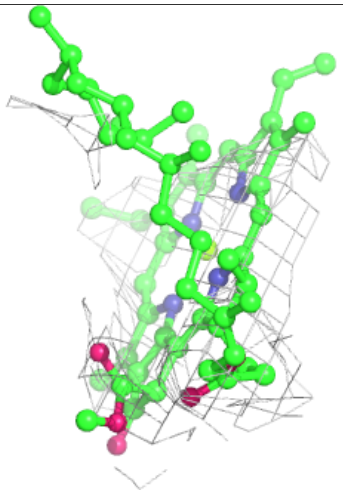


Electron density around CLA b 618:

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

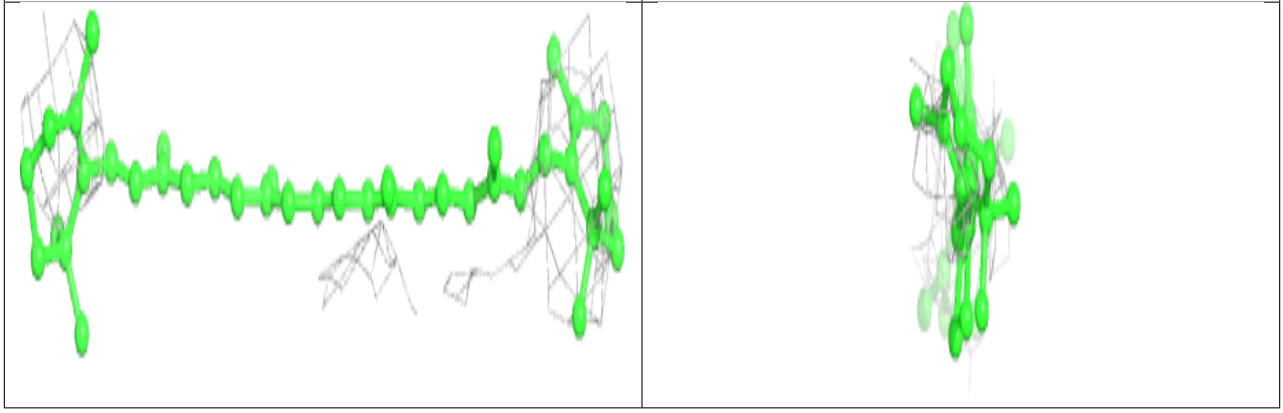






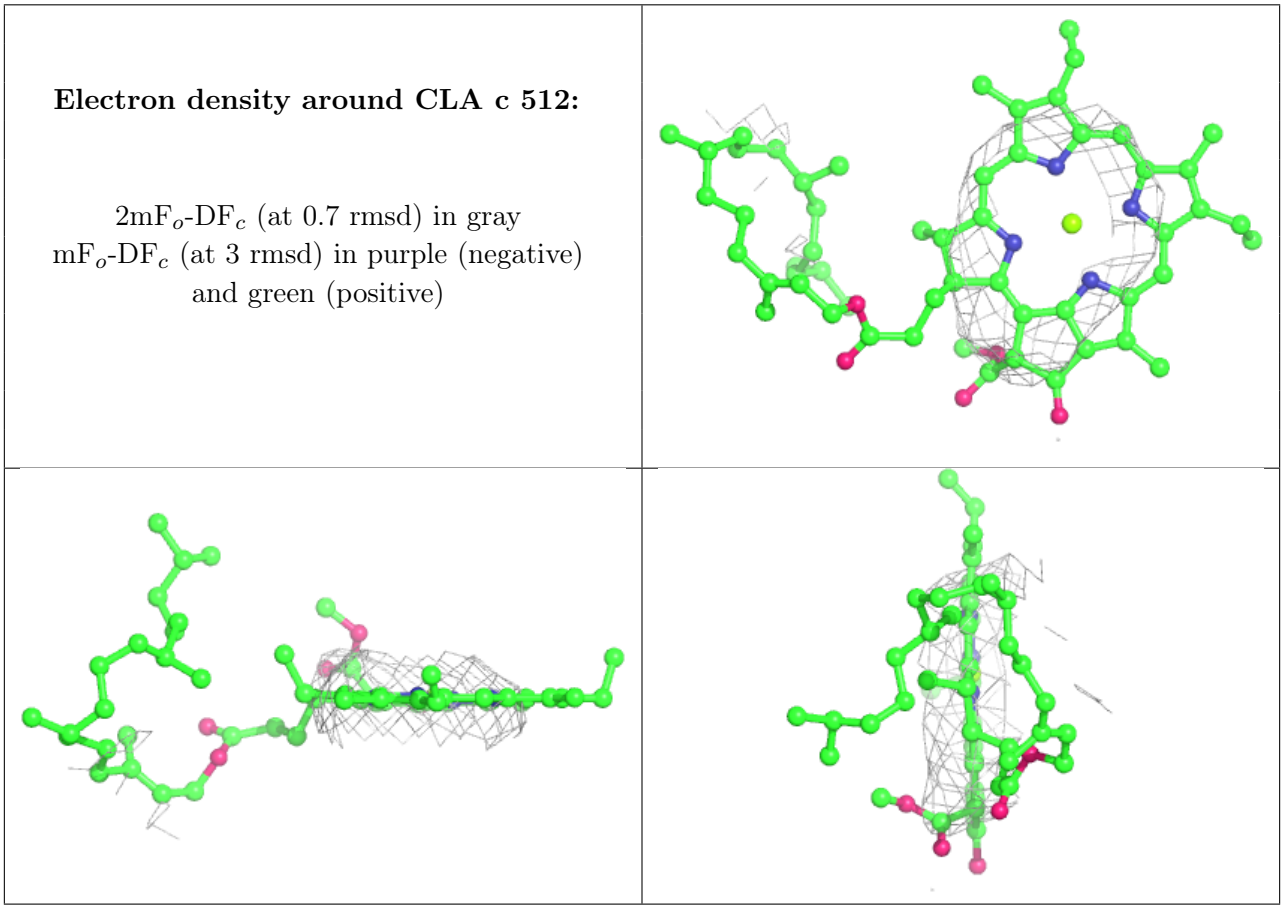
Electron density around BCR B 619:

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



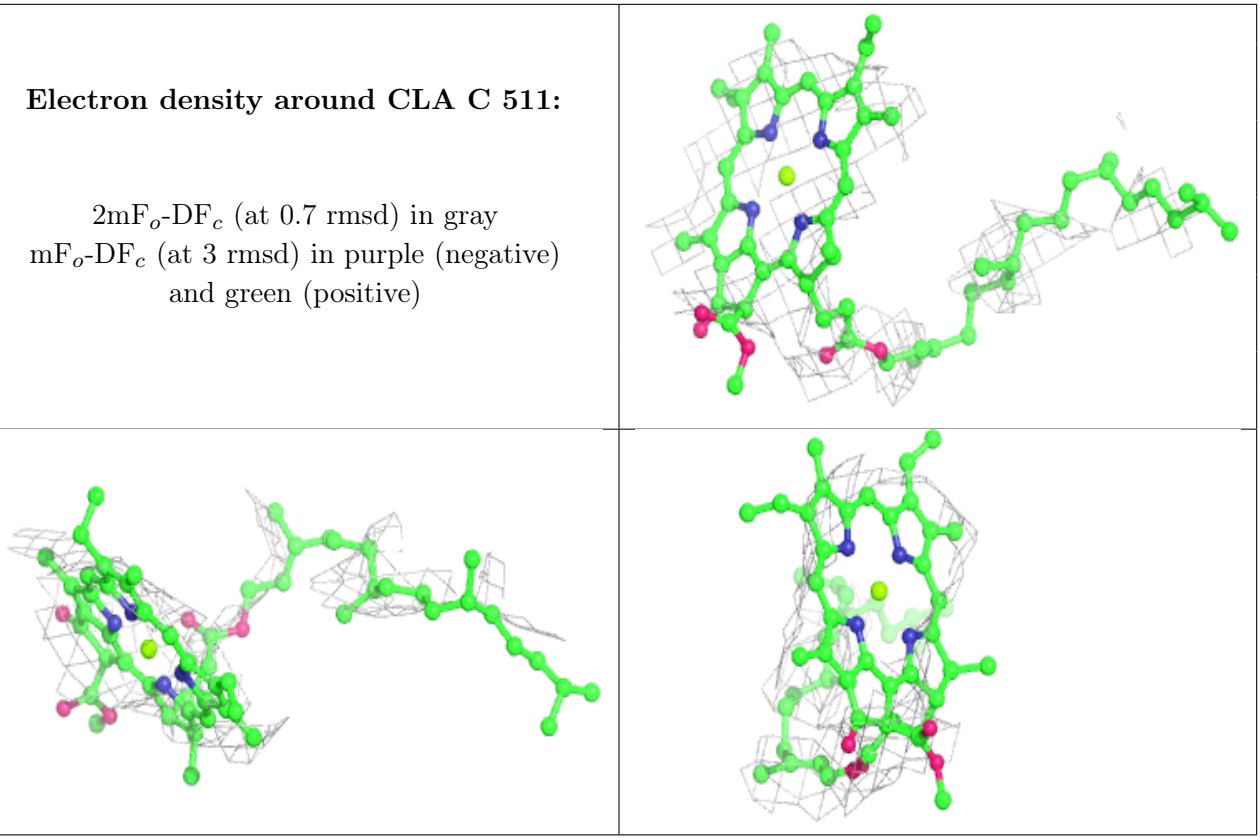
Electron density around CLA c 512:

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



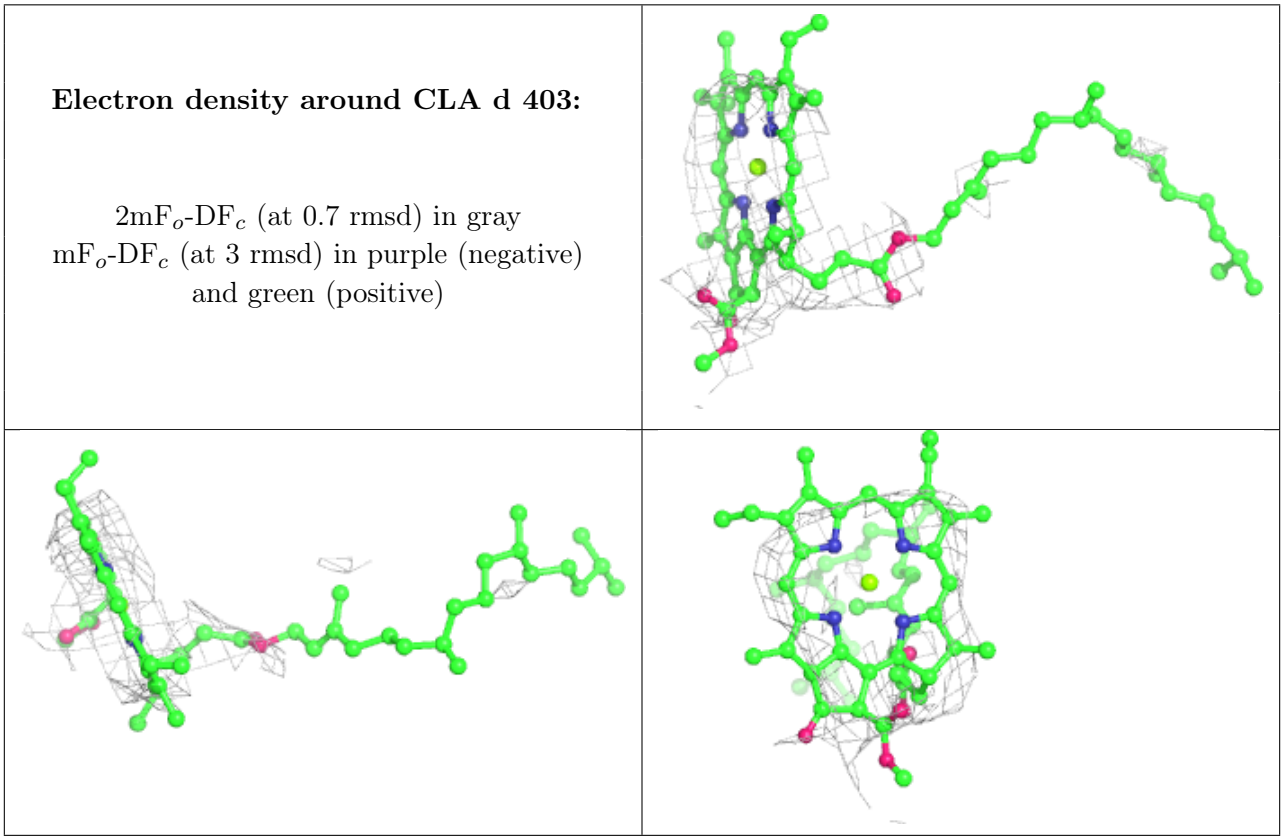
Electron density around CLA C 511:

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



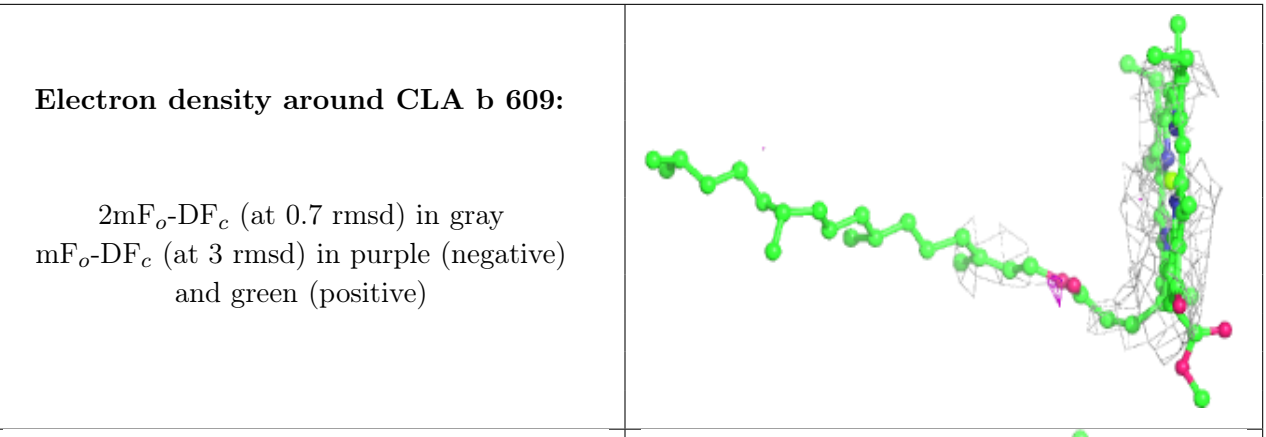
Electron density around CLA d 403:

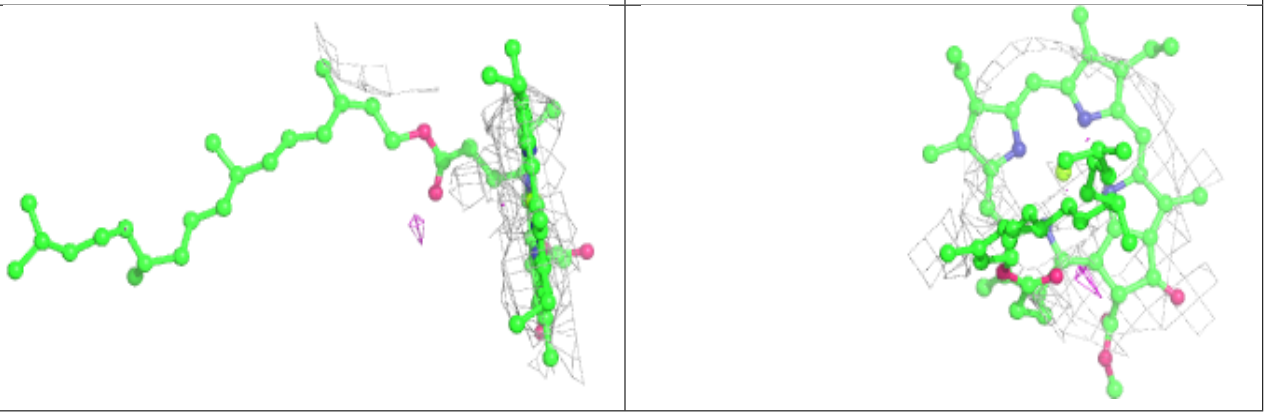
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA b 609:

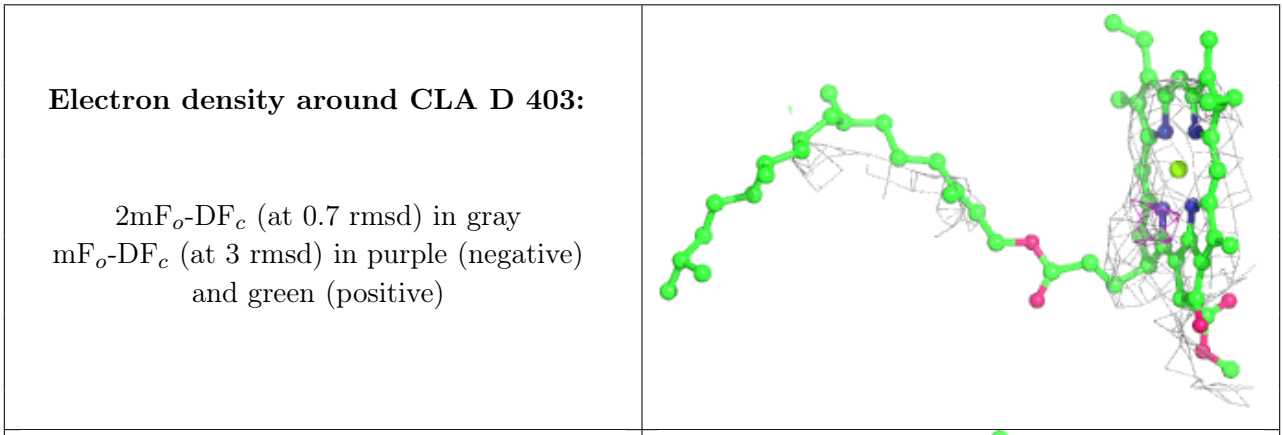
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

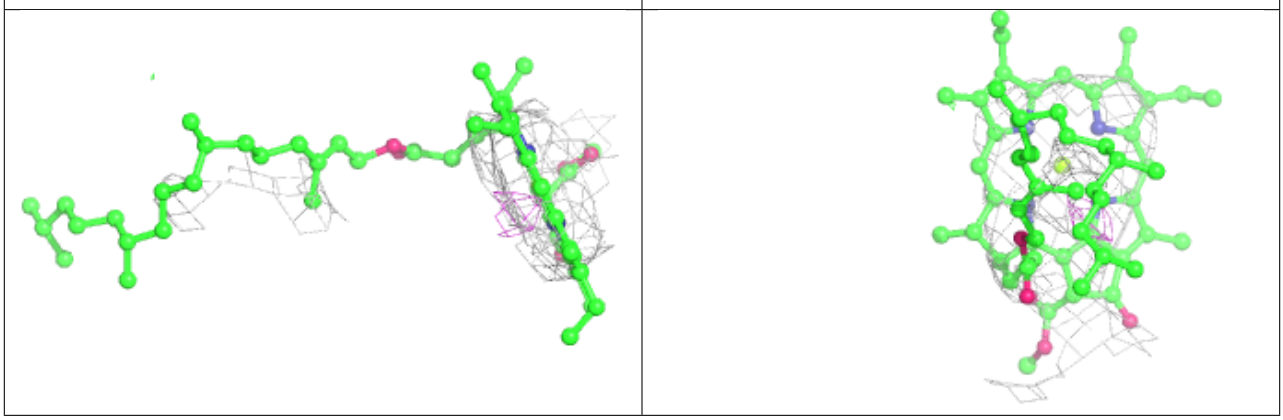




Electron density around CLA D 403:

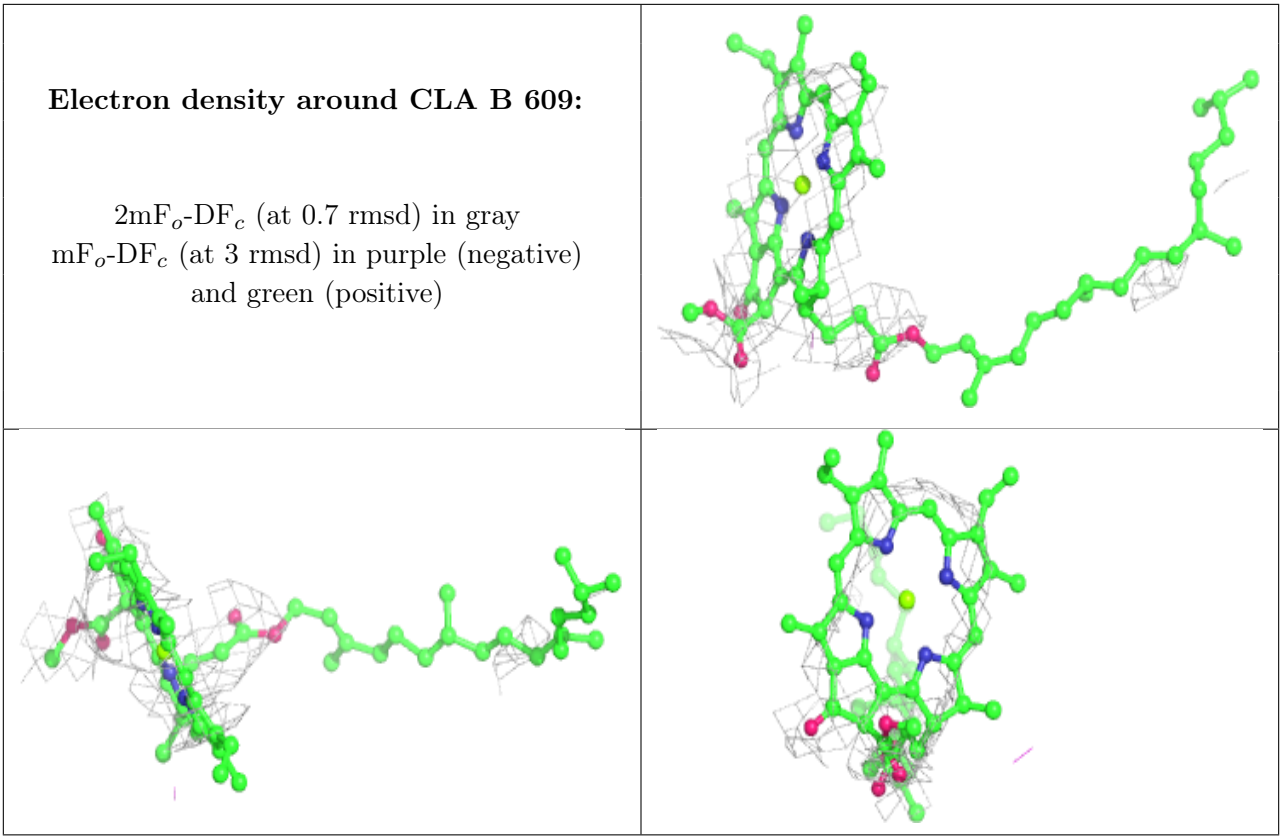
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





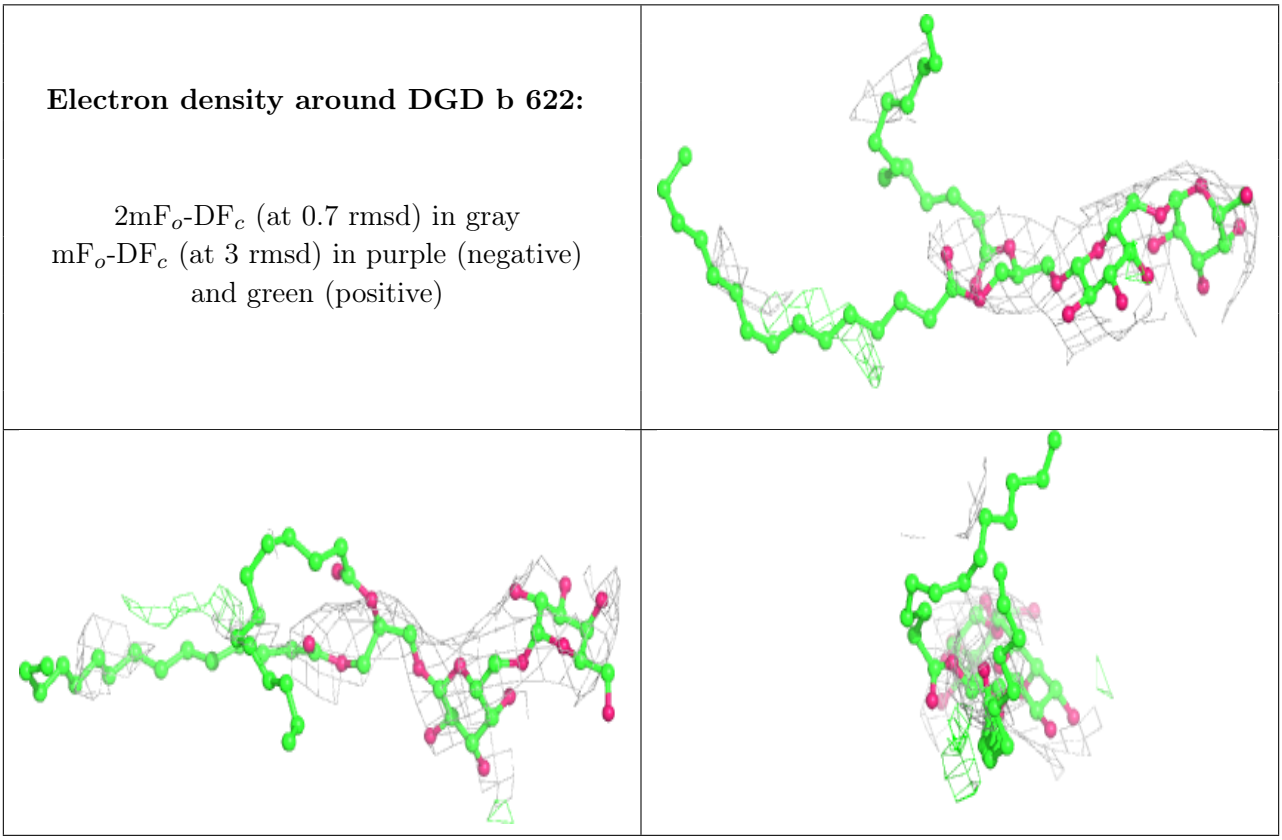
Electron density around CLA B 609:

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



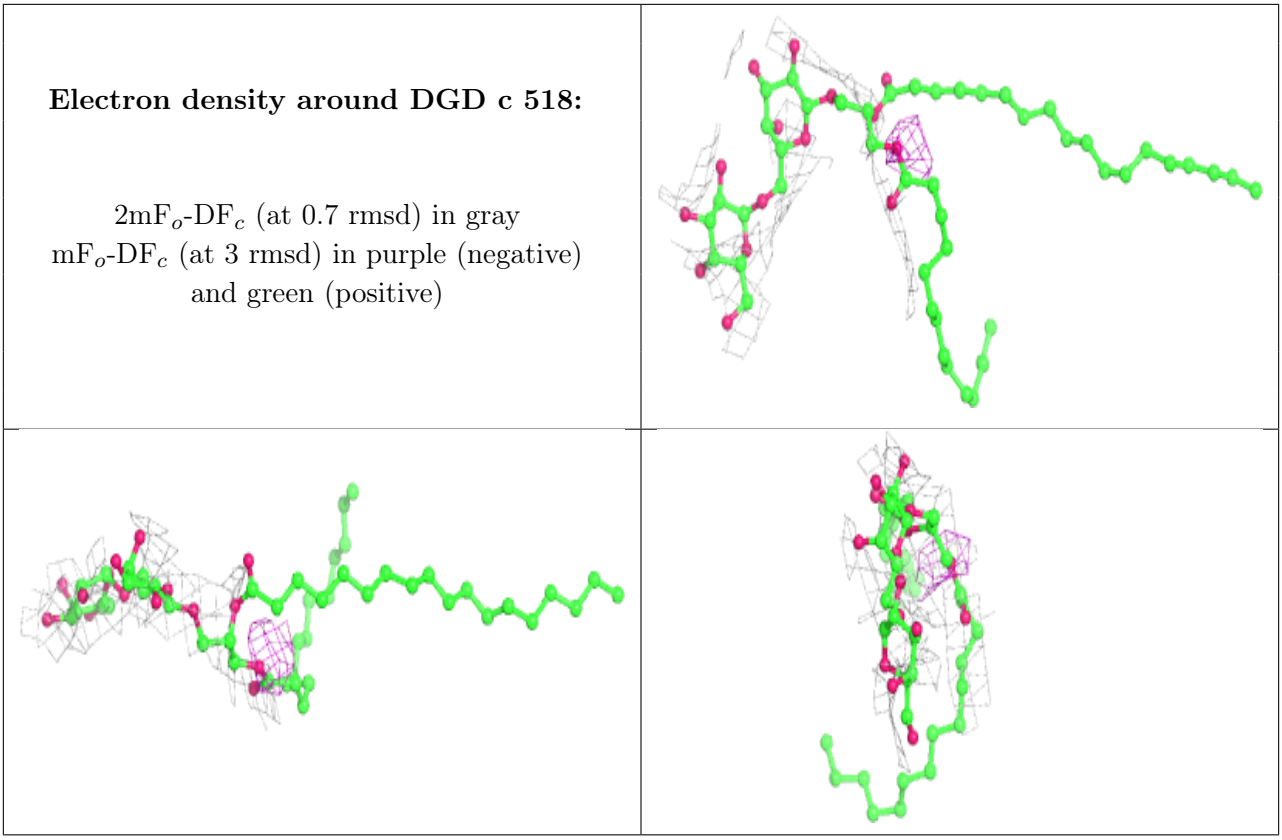
Electron density around DGD b 622:

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



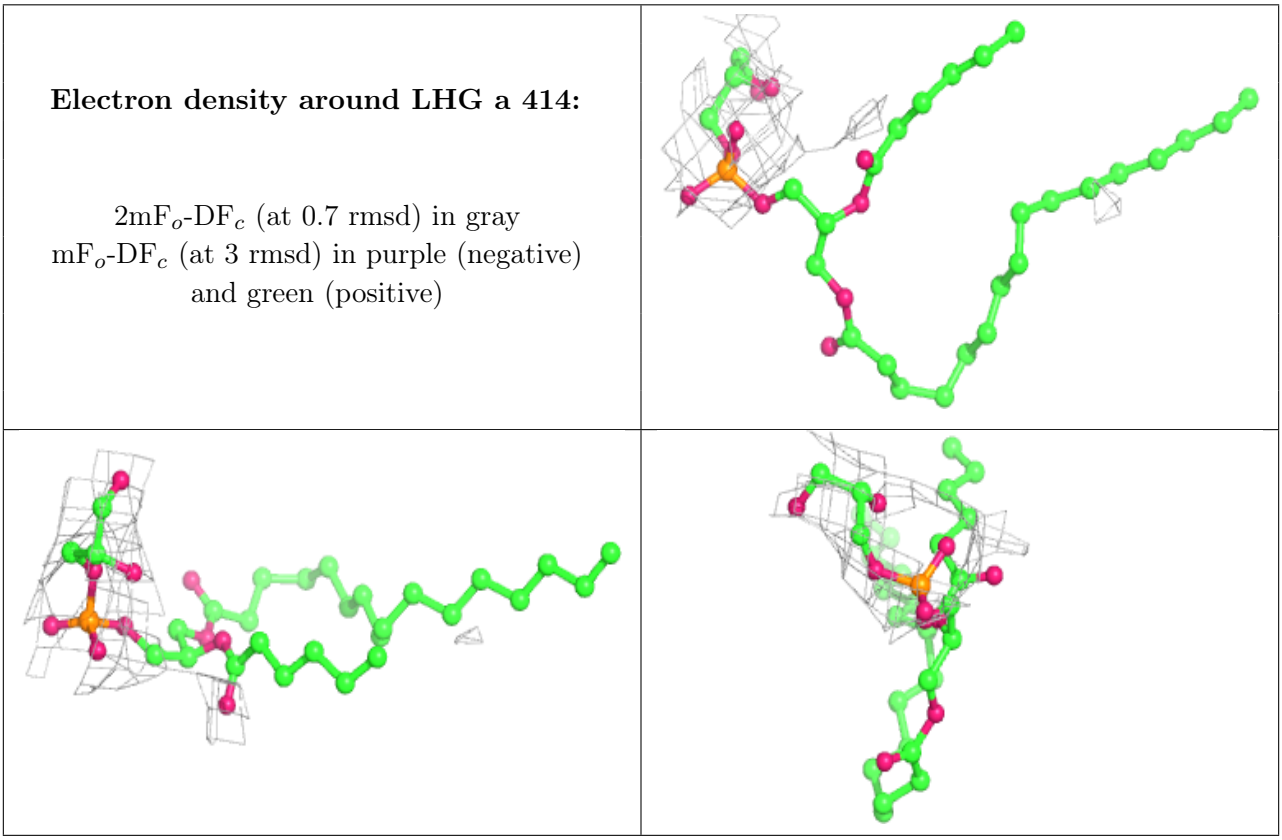
Electron density around DGD c 518:

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



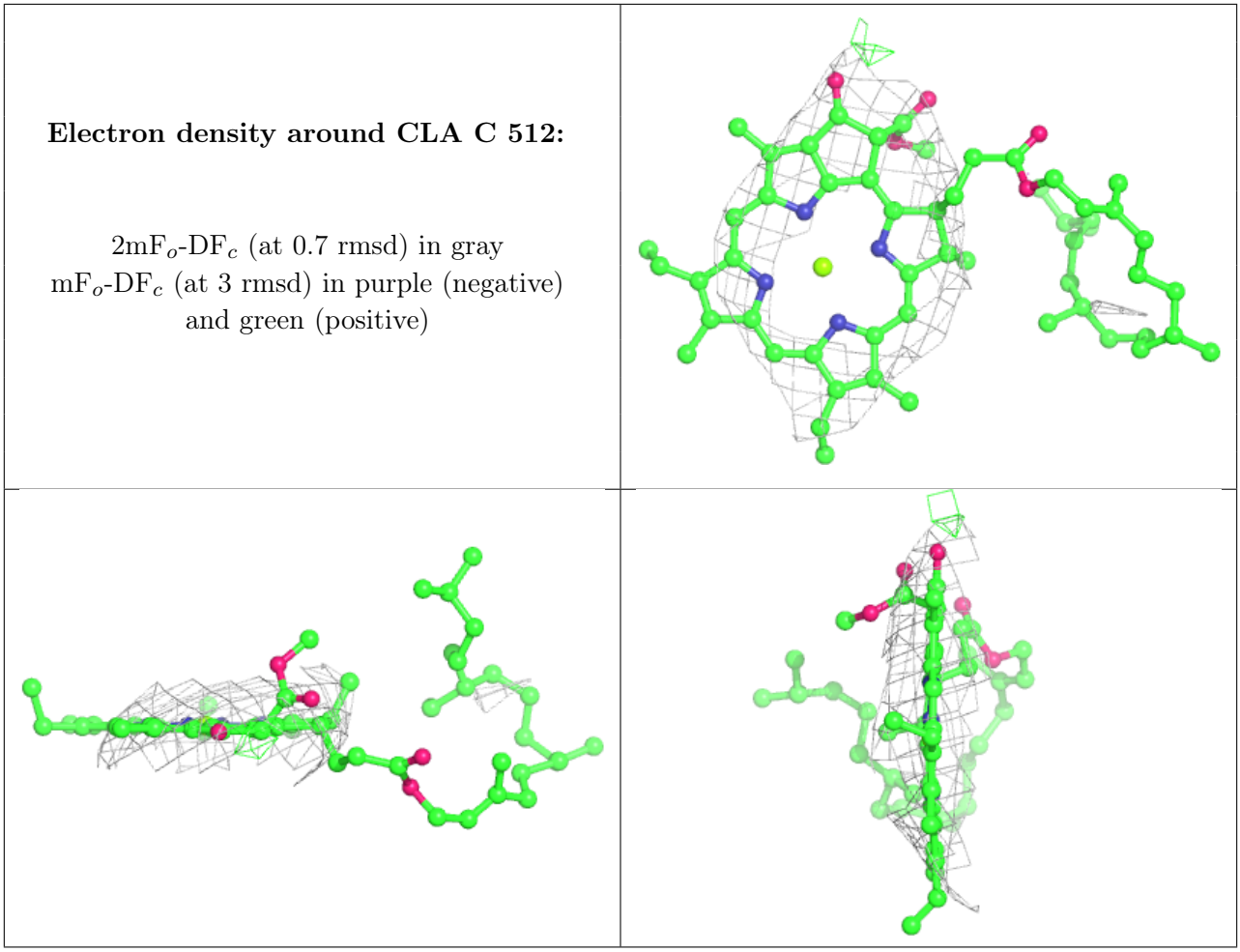
Electron density around LHG a 414:

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



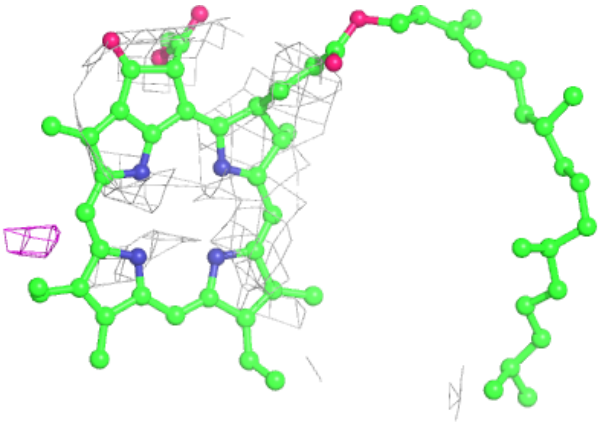
Electron density around CLA C 512:

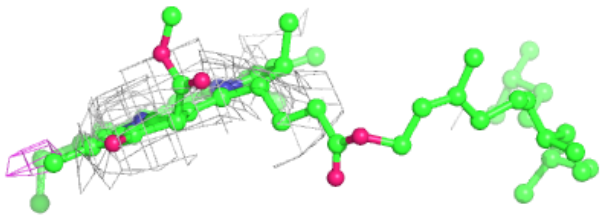
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

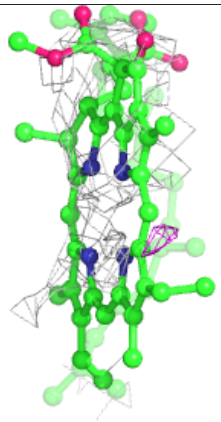


Electron density around PHO D 402:

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

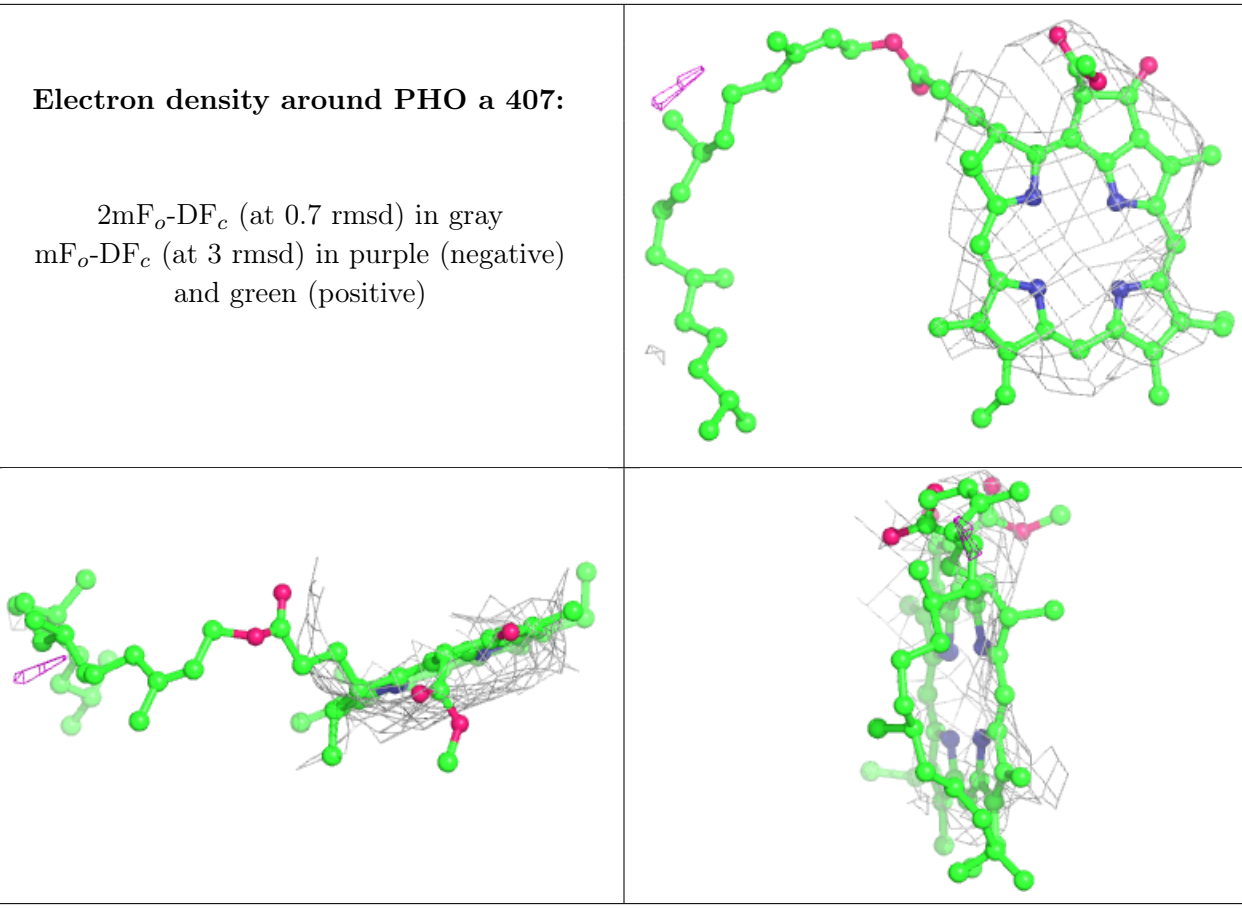






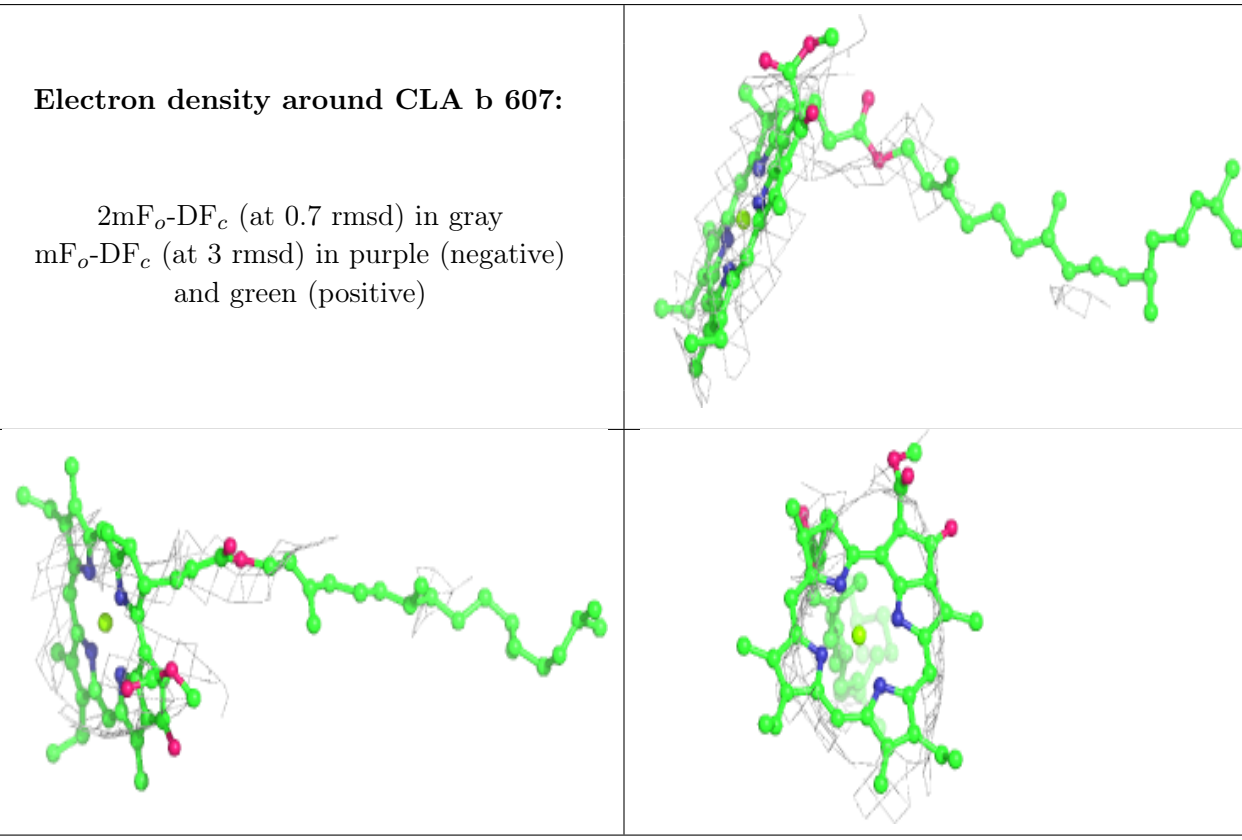
Electron density around PHO a 407:

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



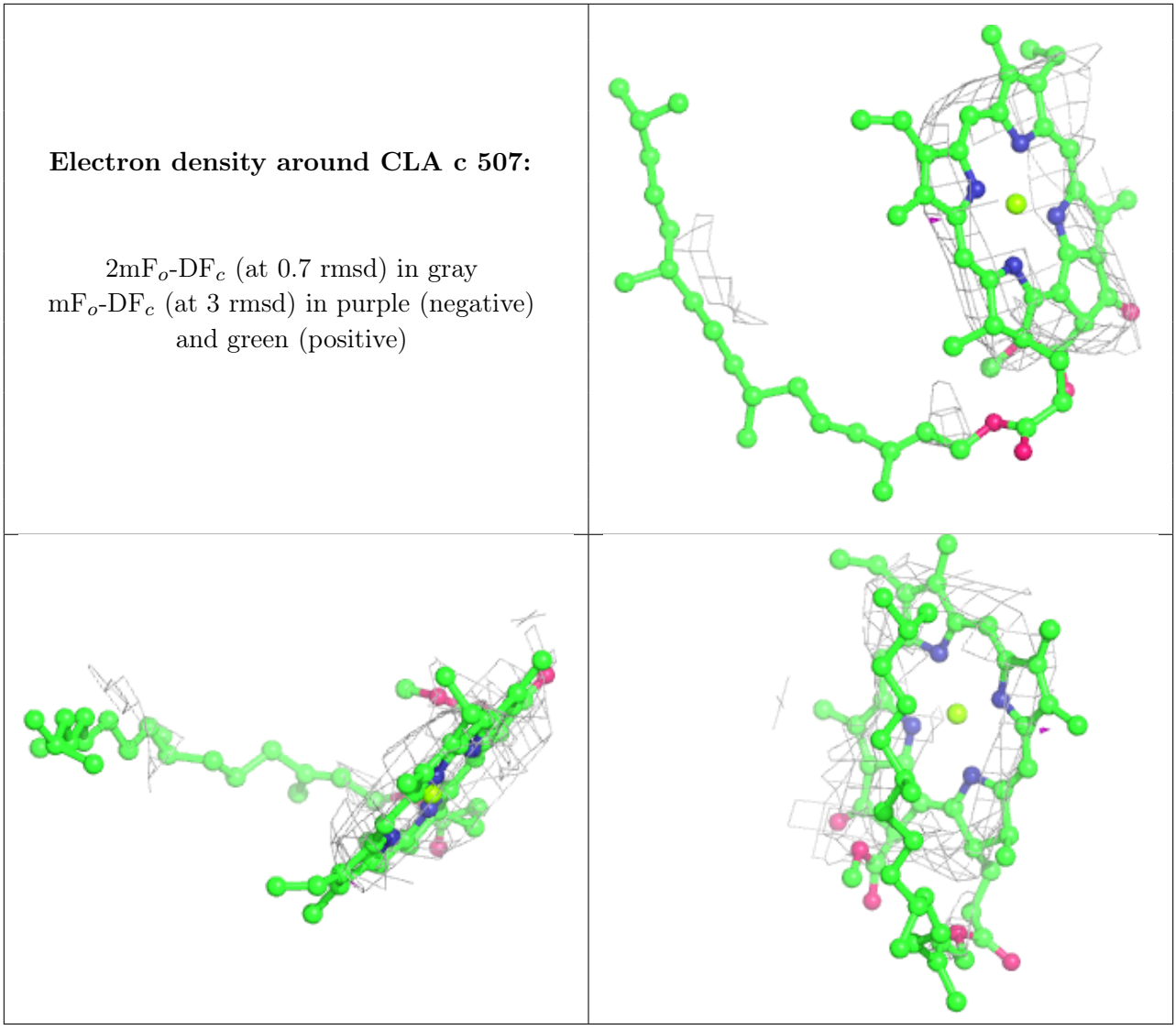
Electron density around CLA b 607:

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



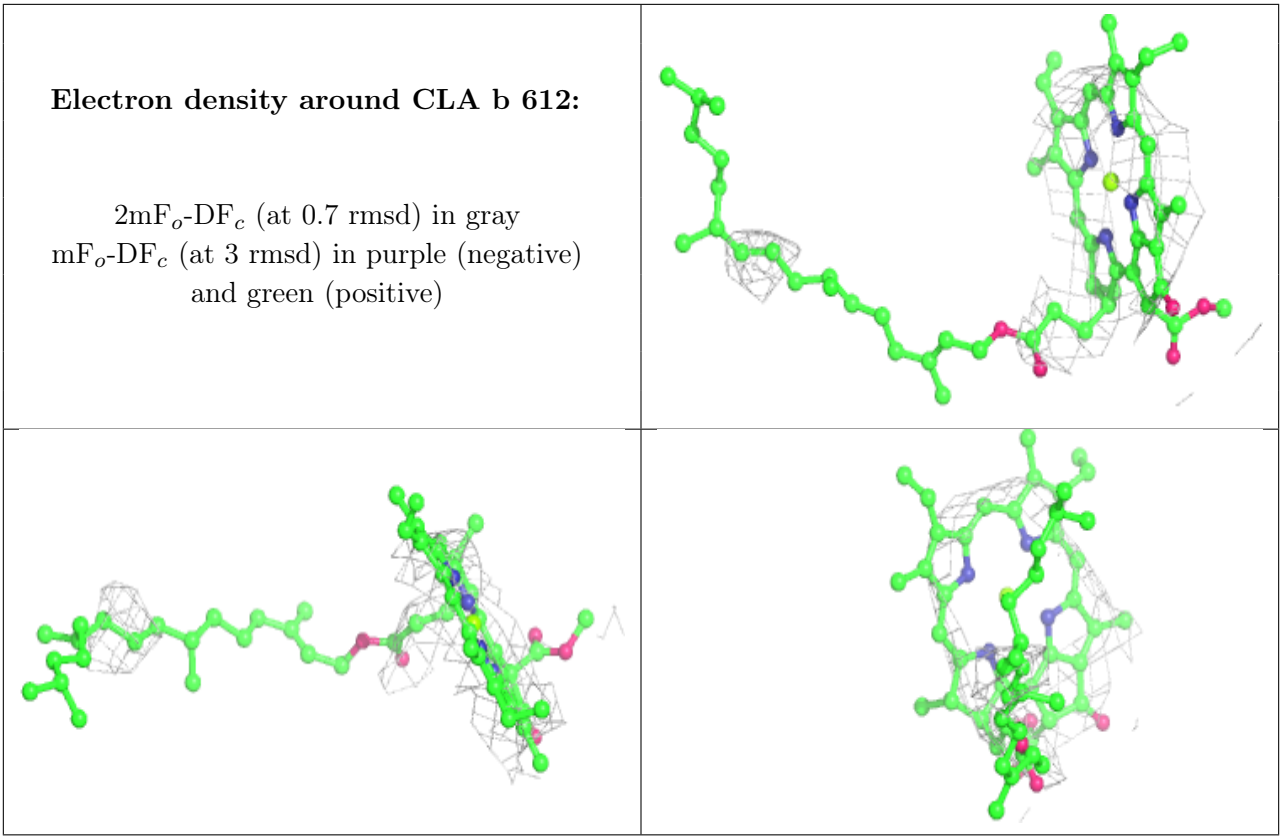
Electron density around CLA c 507:

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



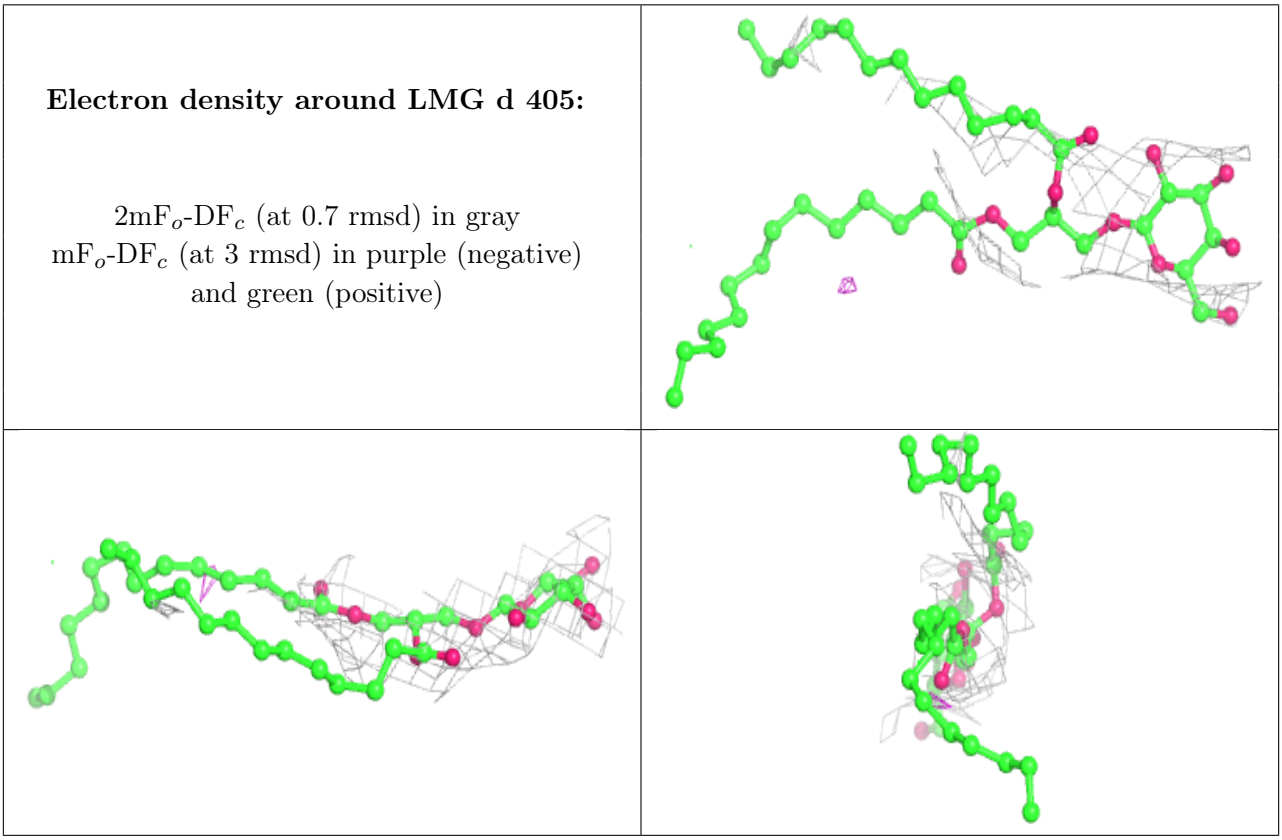
Electron density around CLA b 612:

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



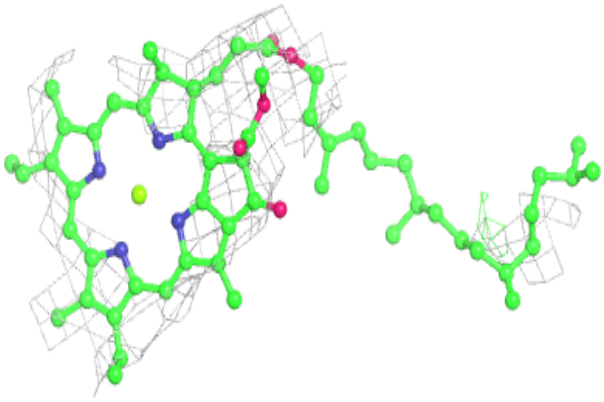
Electron density around LMG d 405:

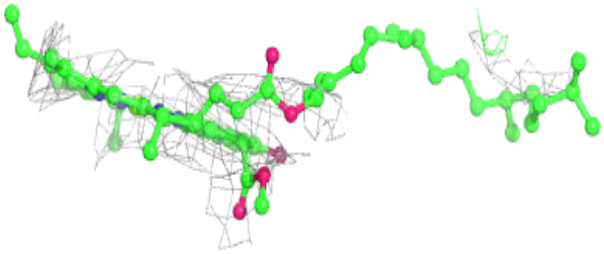
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

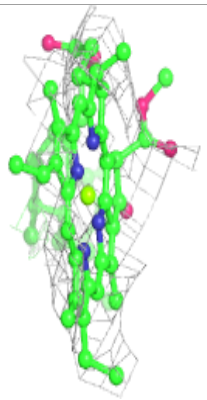


Electron density around CLA b 605:

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

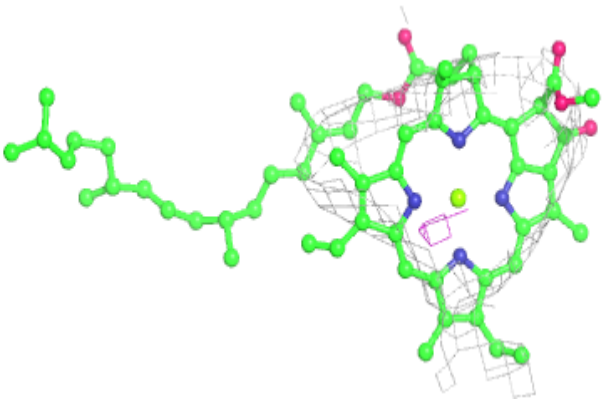


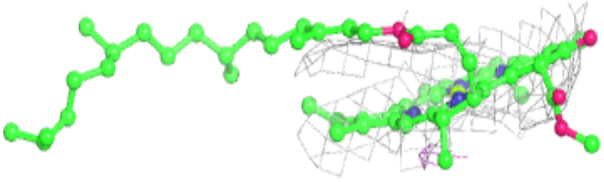


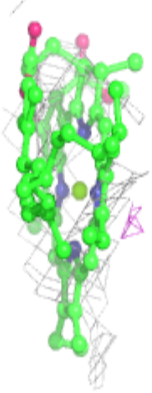


Electron density around CLA b 606:

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

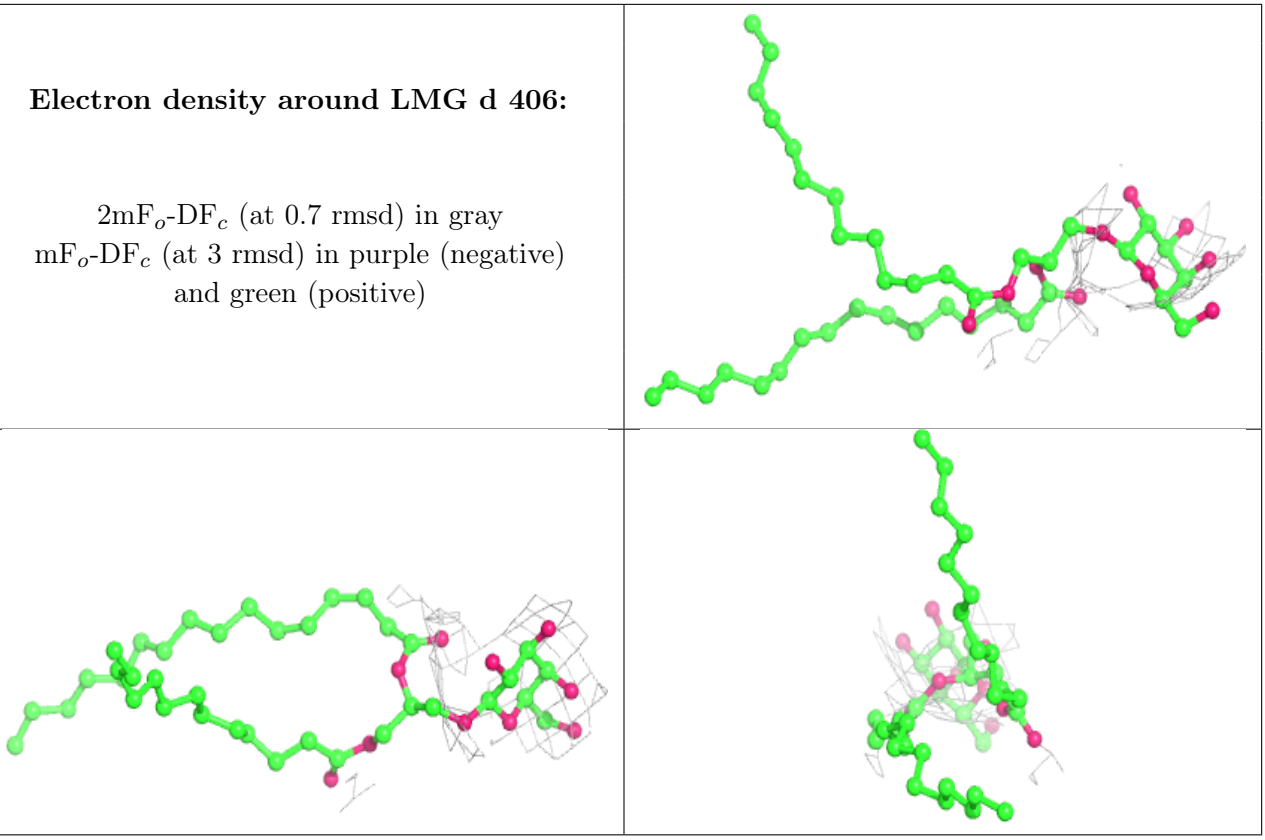






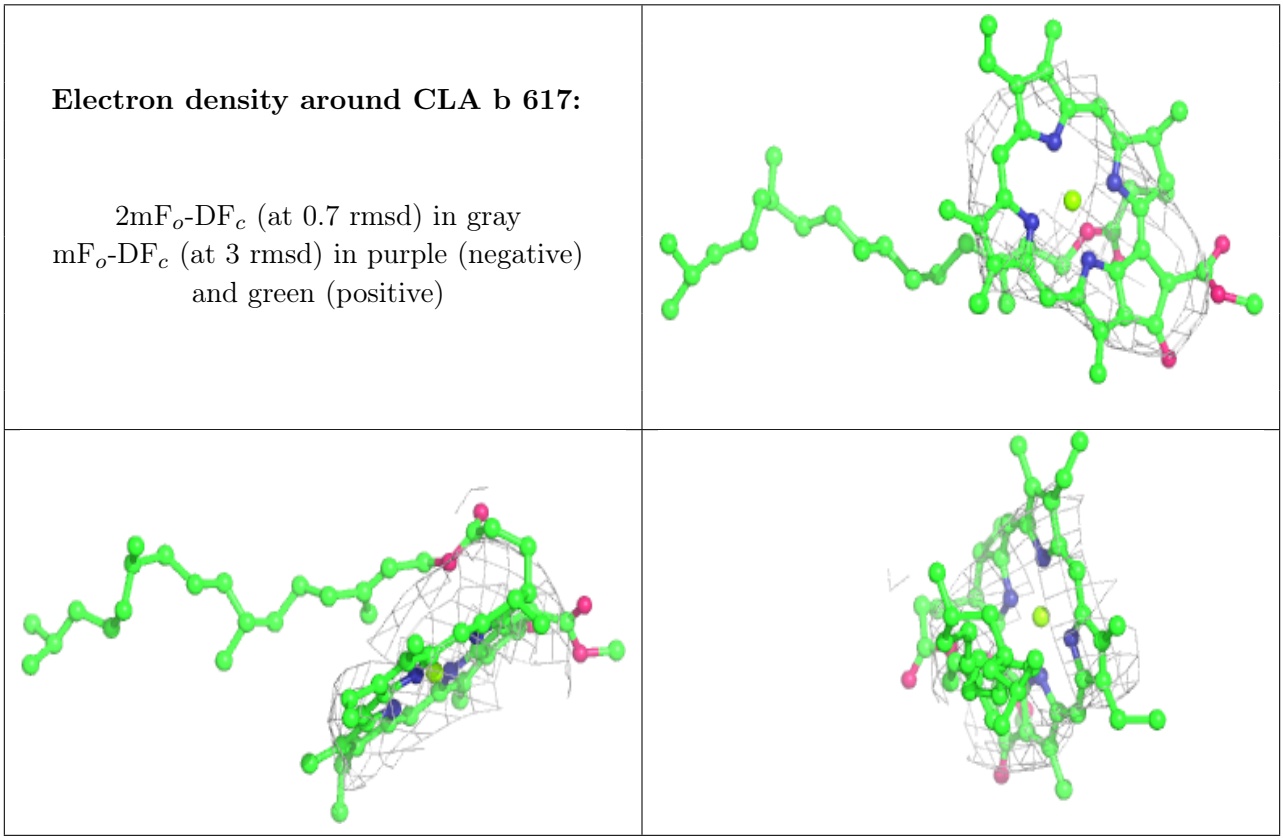
Electron density around LMG d 406:

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



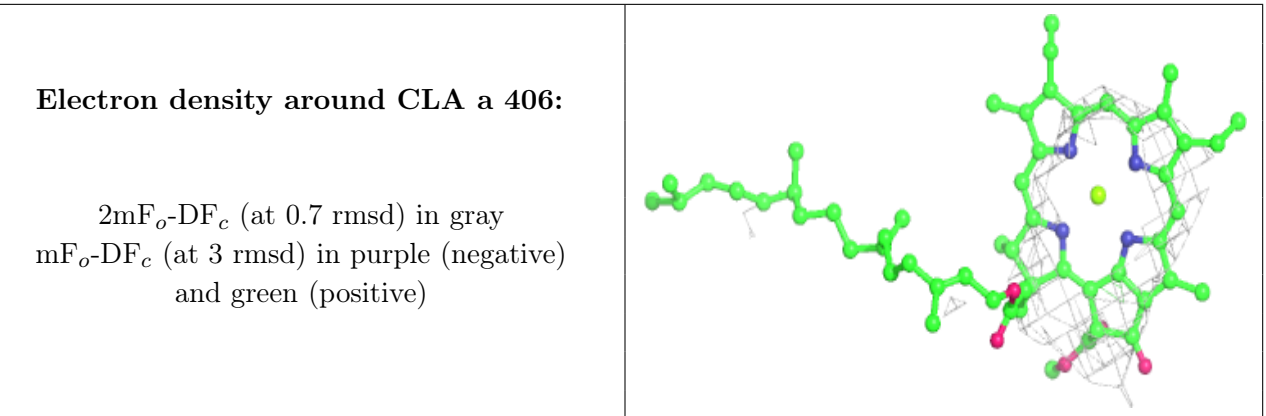
Electron density around CLA b 617:

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



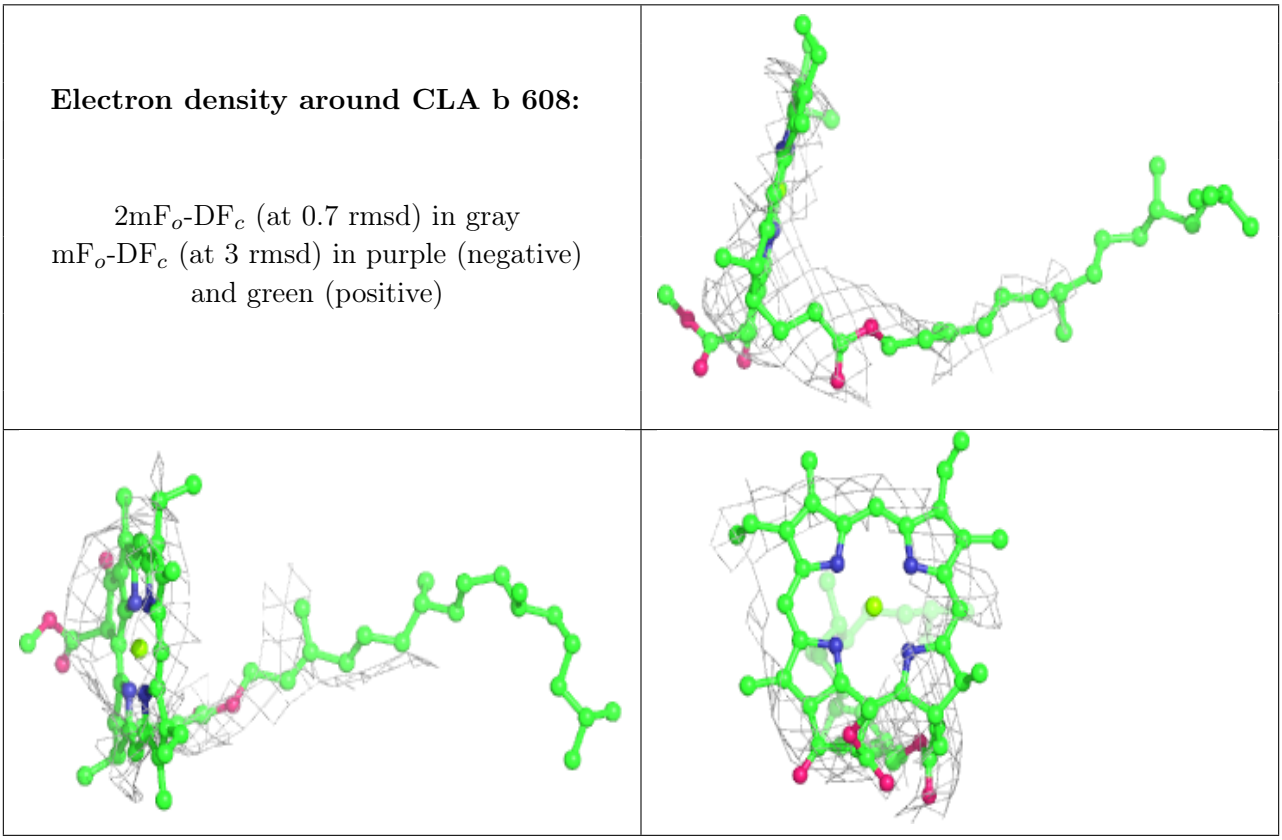
Electron density around CLA a 406:

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



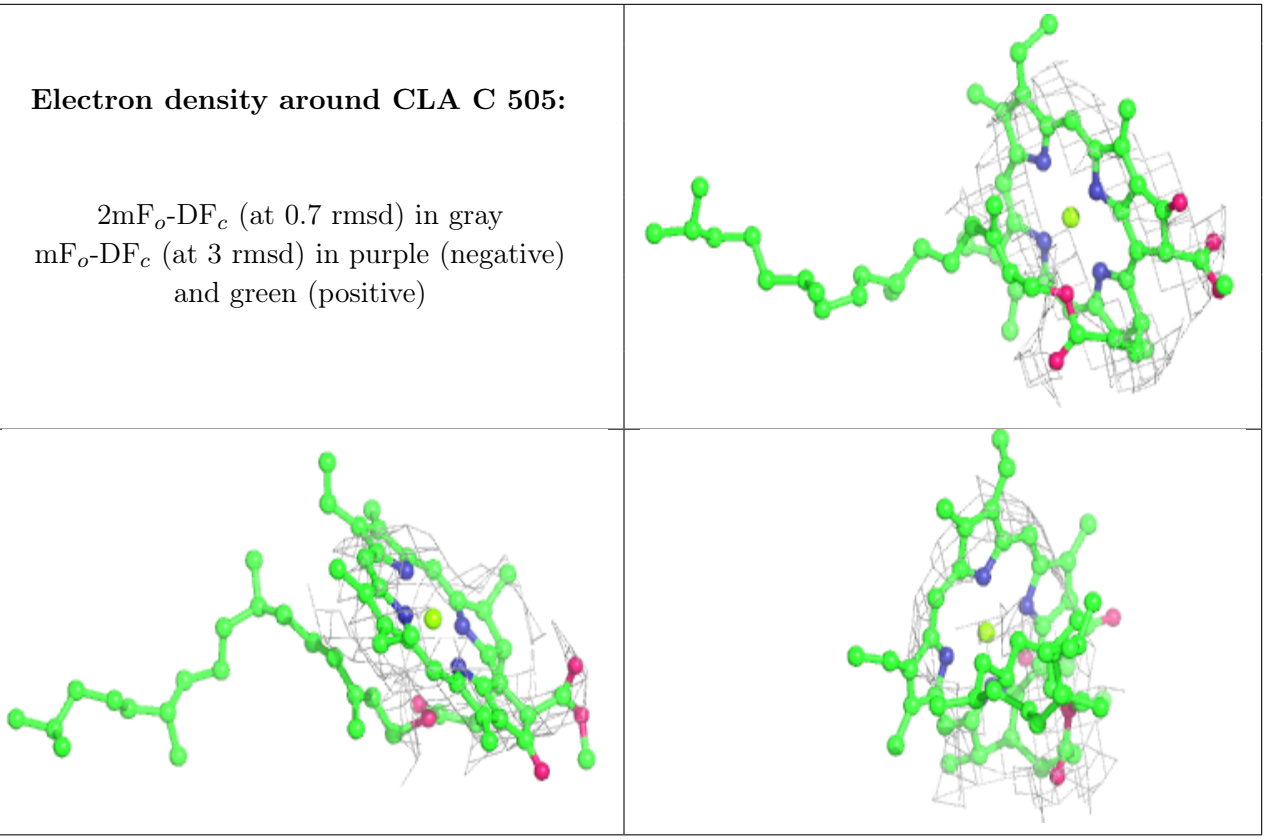
Electron density around CLA b 608:

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



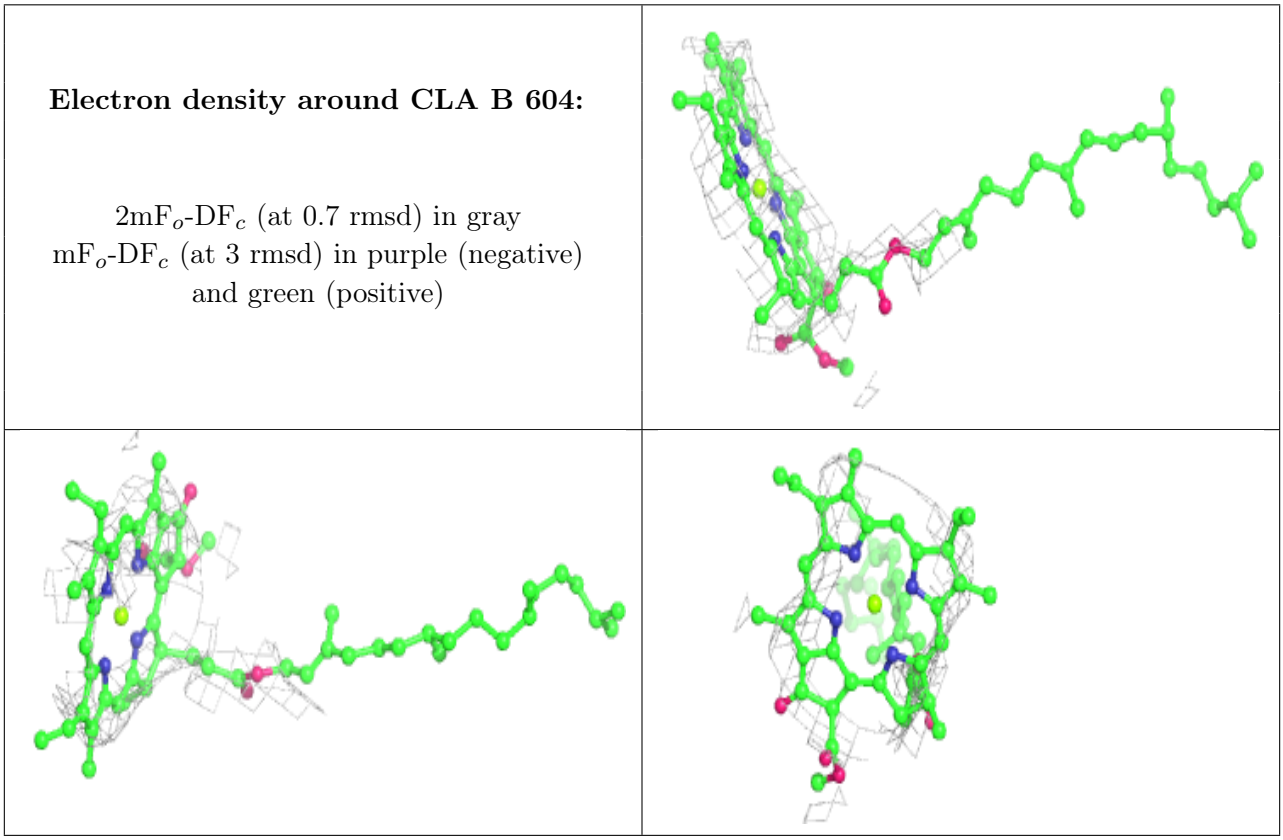
Electron density around CLA C 505:

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



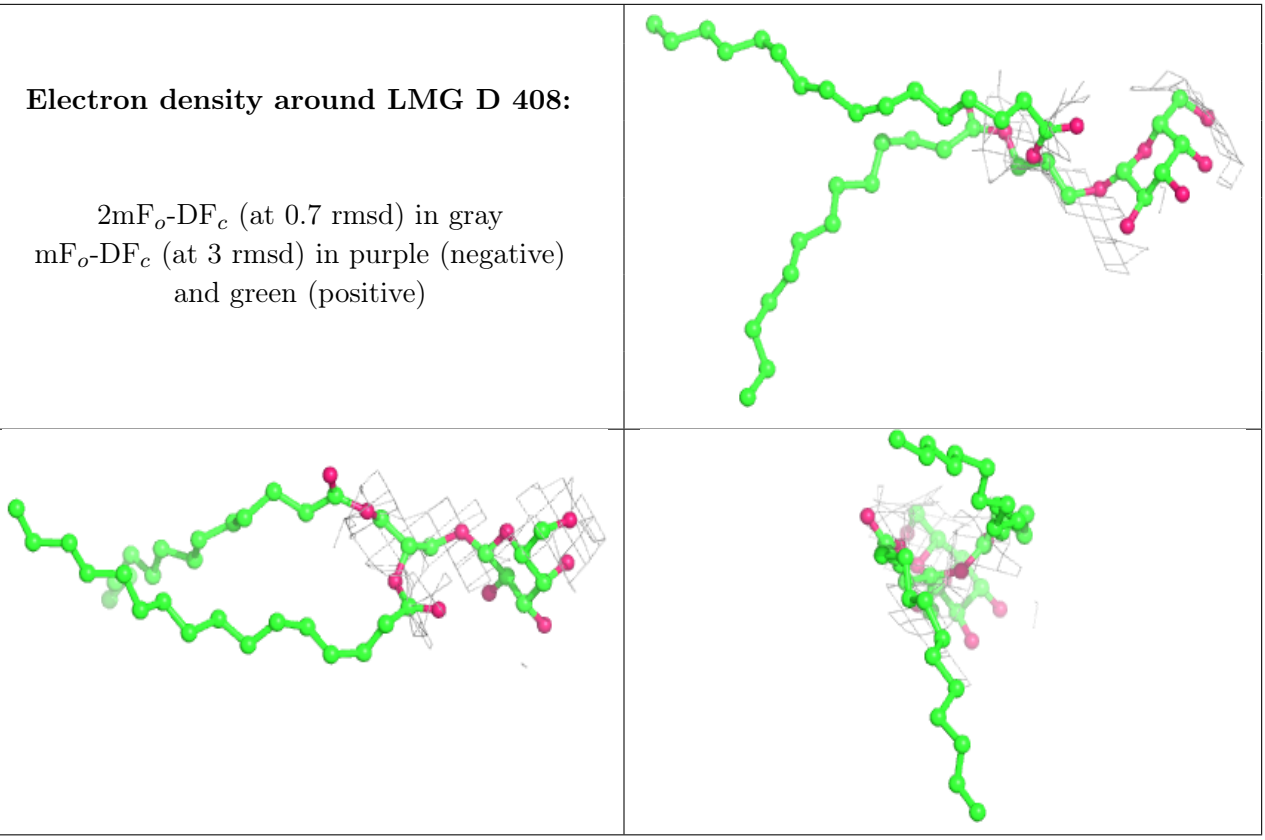
Electron density around CLA B 604:

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



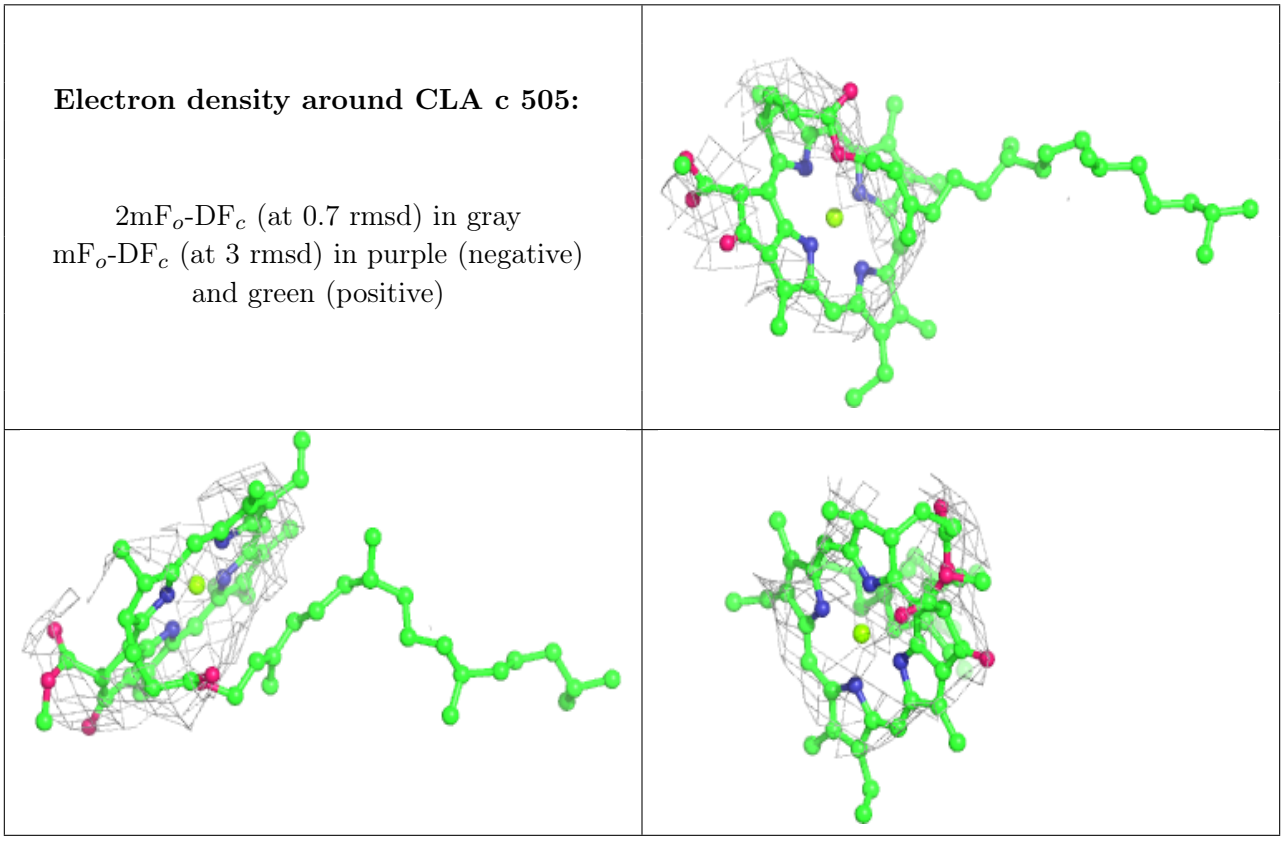
Electron density around LMG D 408:

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



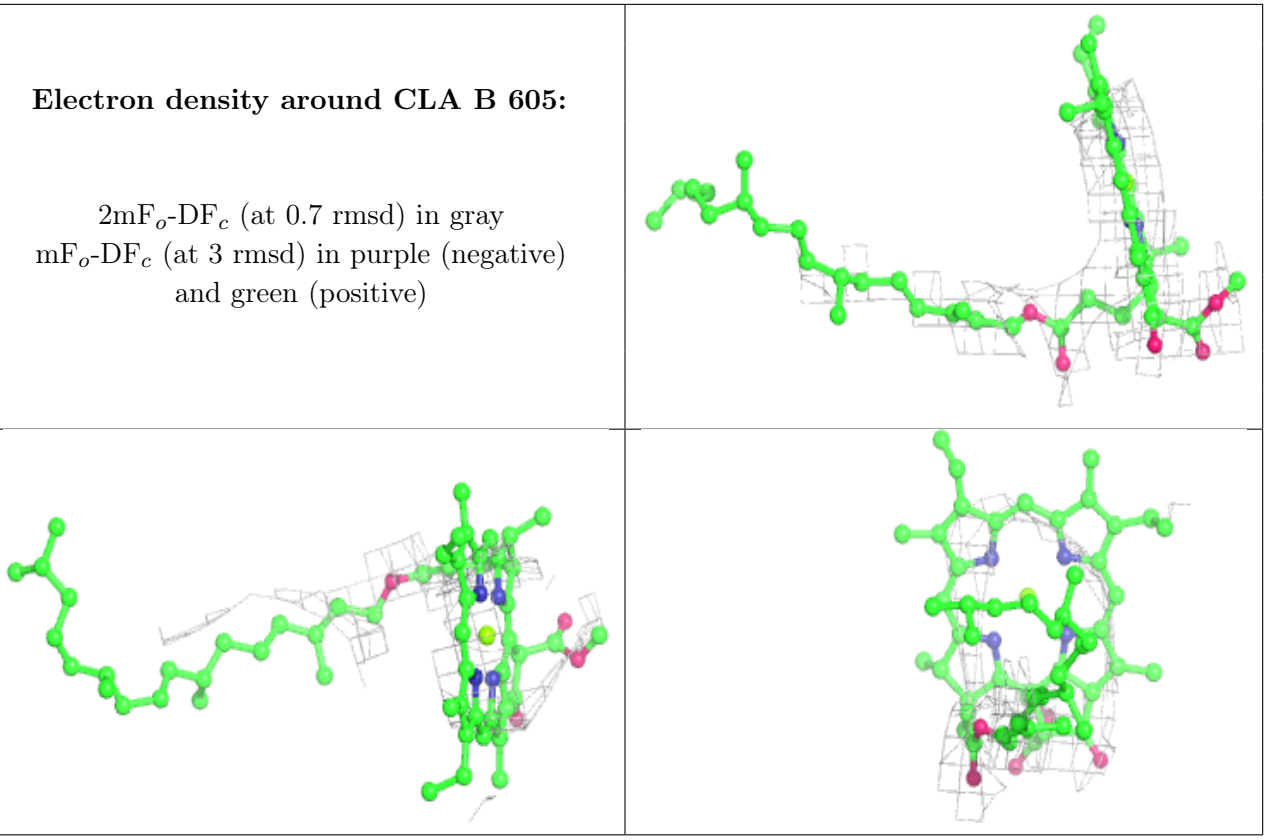
Electron density around CLA c 505:

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



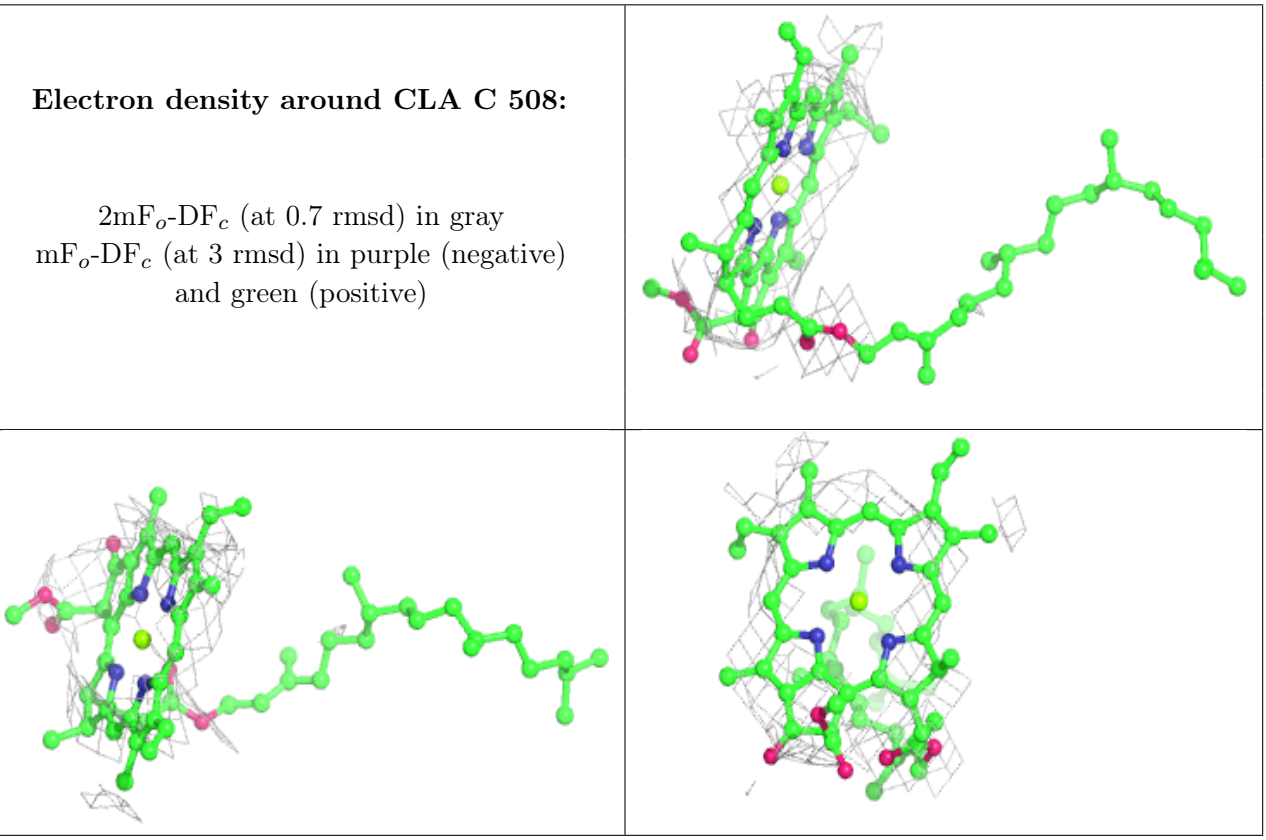
Electron density around CLA B 605:

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



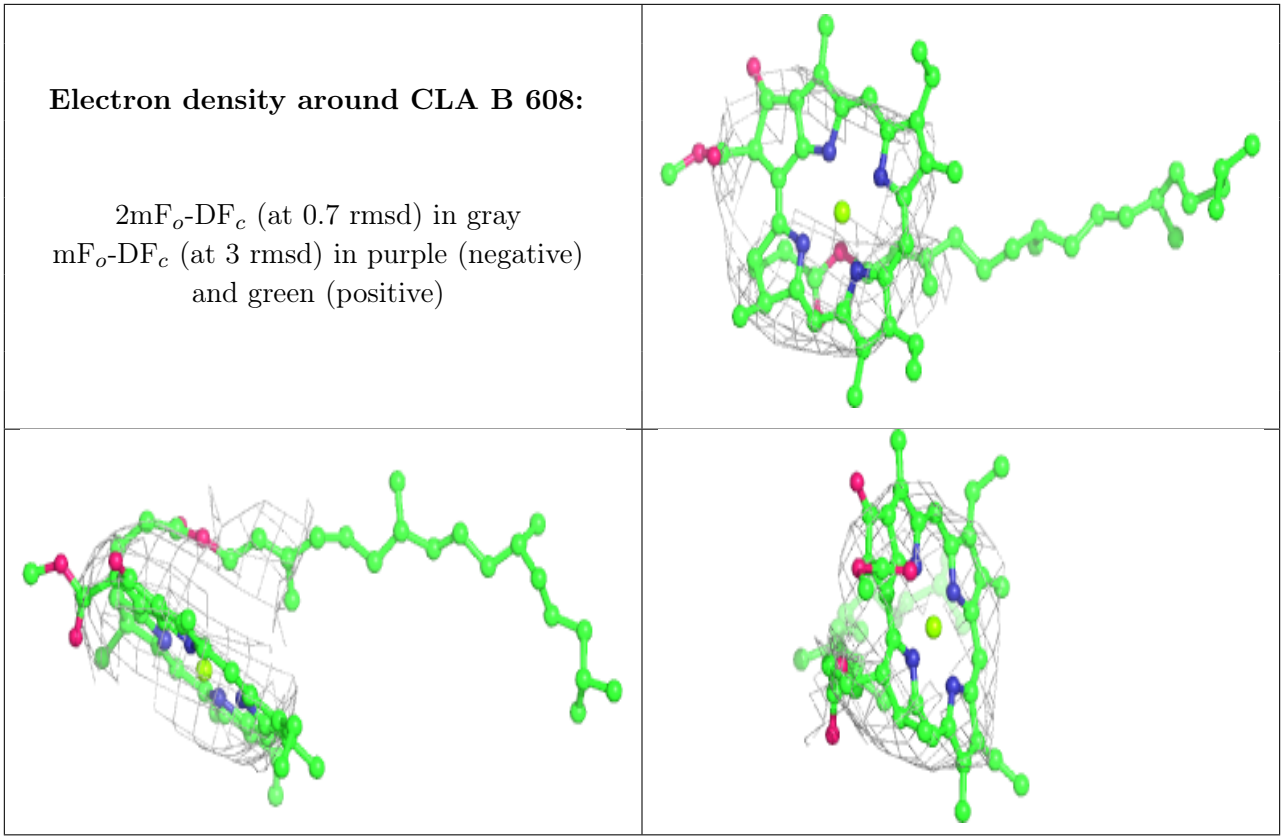
Electron density around CLA C 508:

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



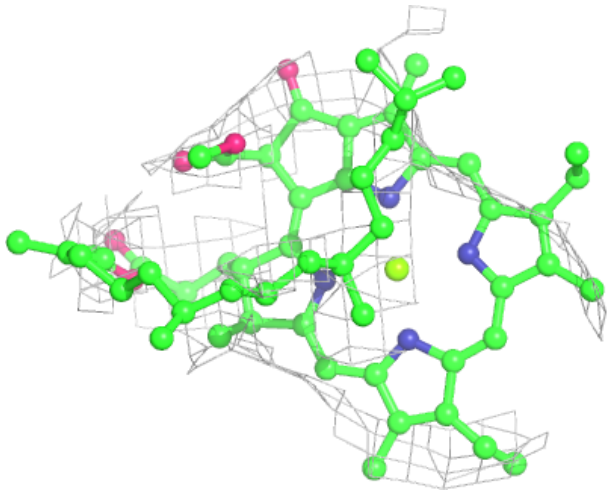
Electron density around CLA B 608:

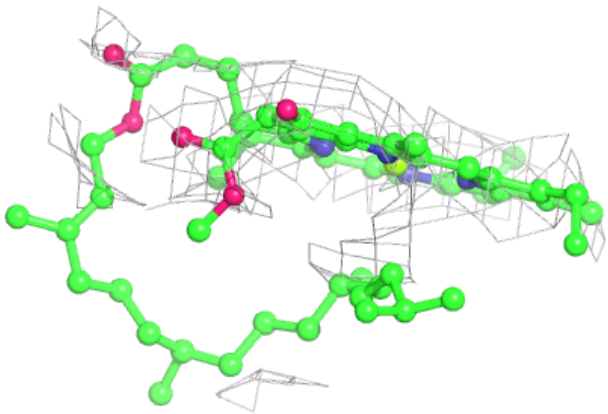
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

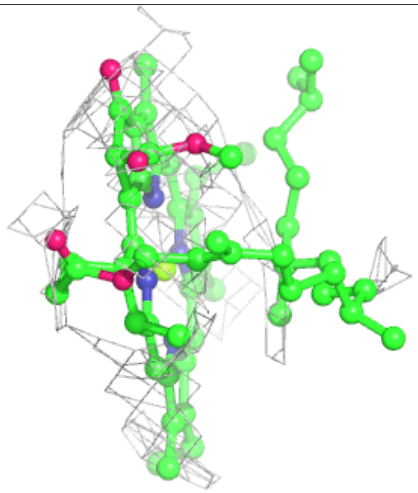


Electron density around CLA C 510:

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

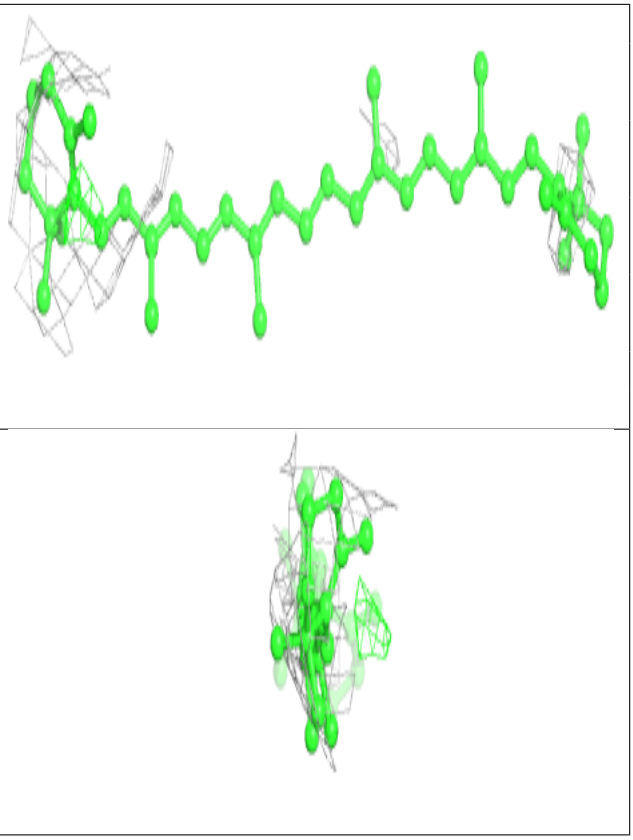






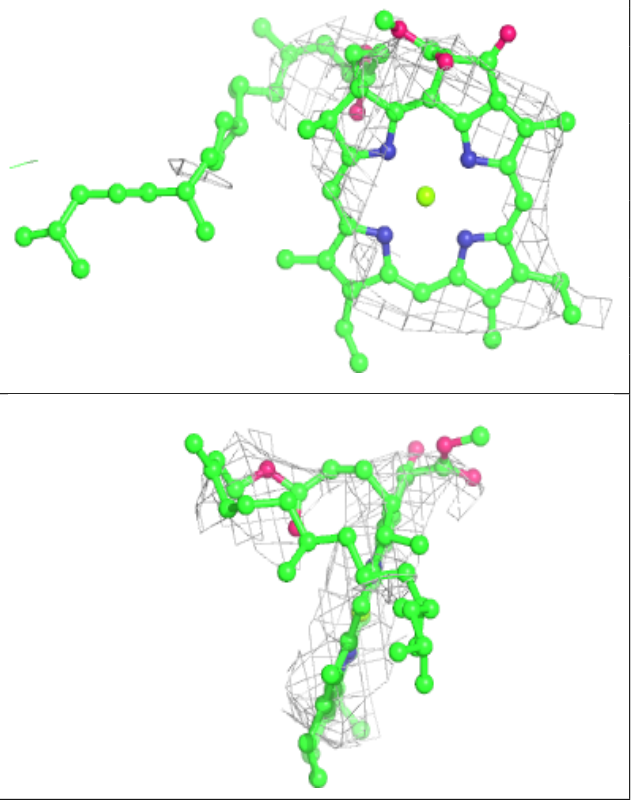
Electron density around BCR T 102:

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



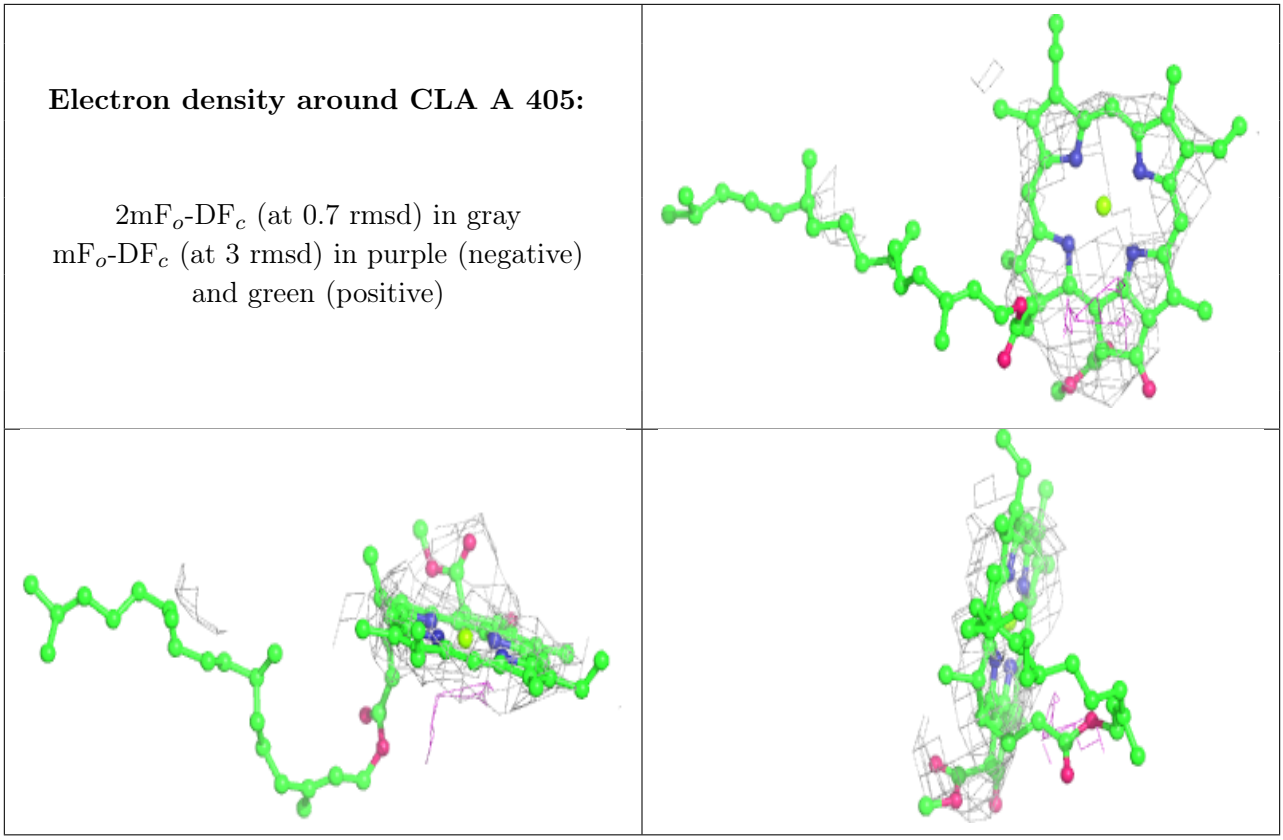
Electron density around CLA a 405:

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



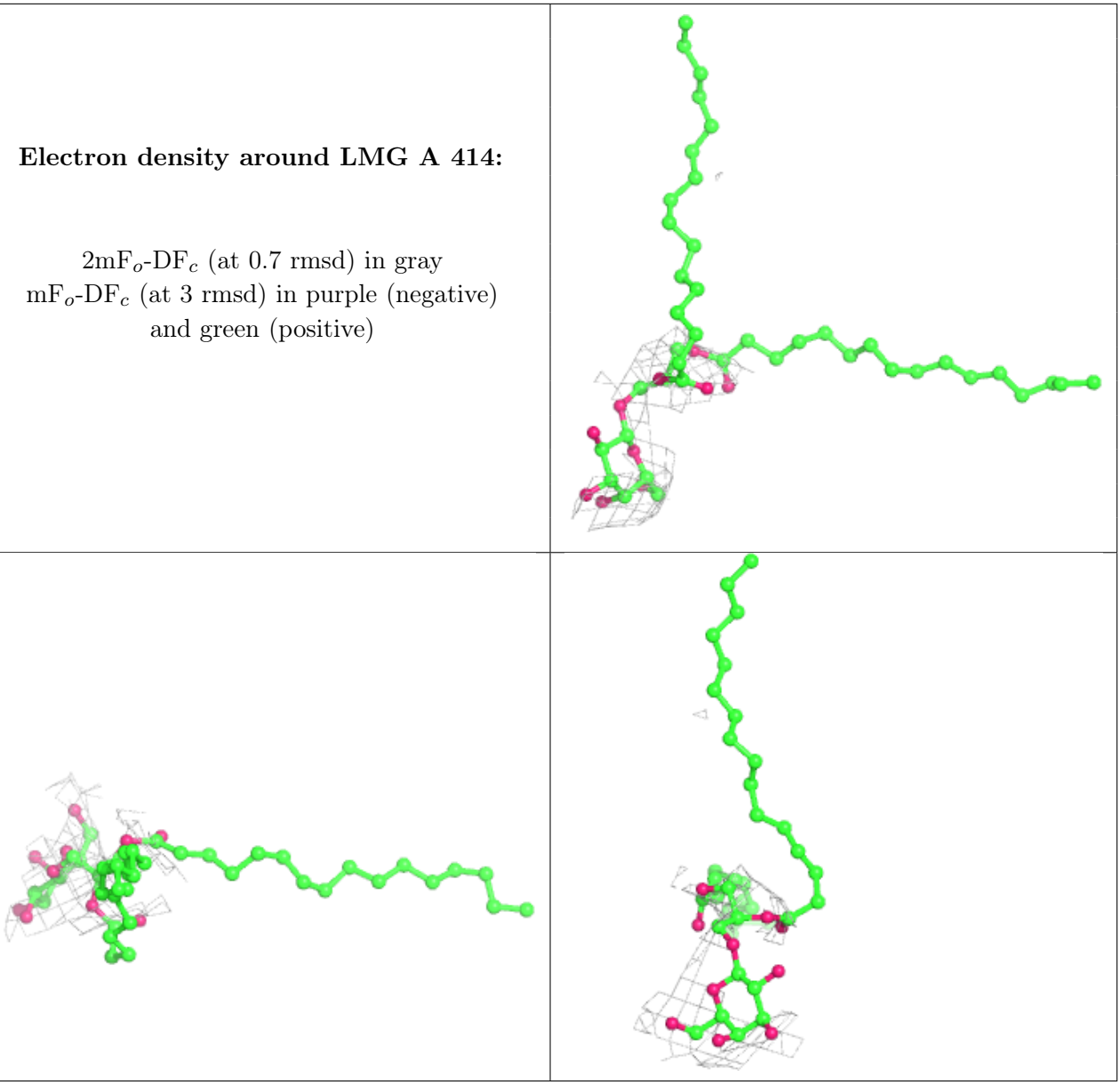
Electron density around CLA A 405:

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



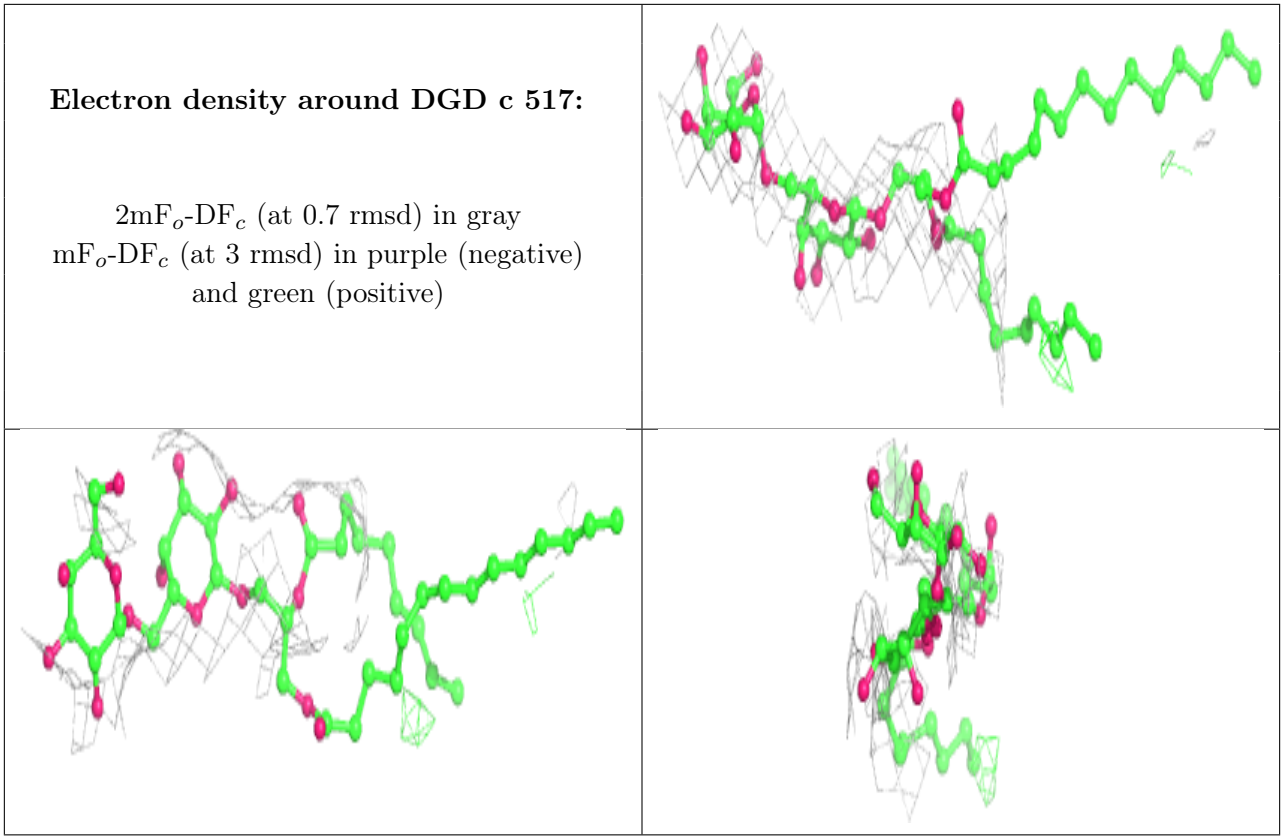
Electron density around LMG A 414:

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



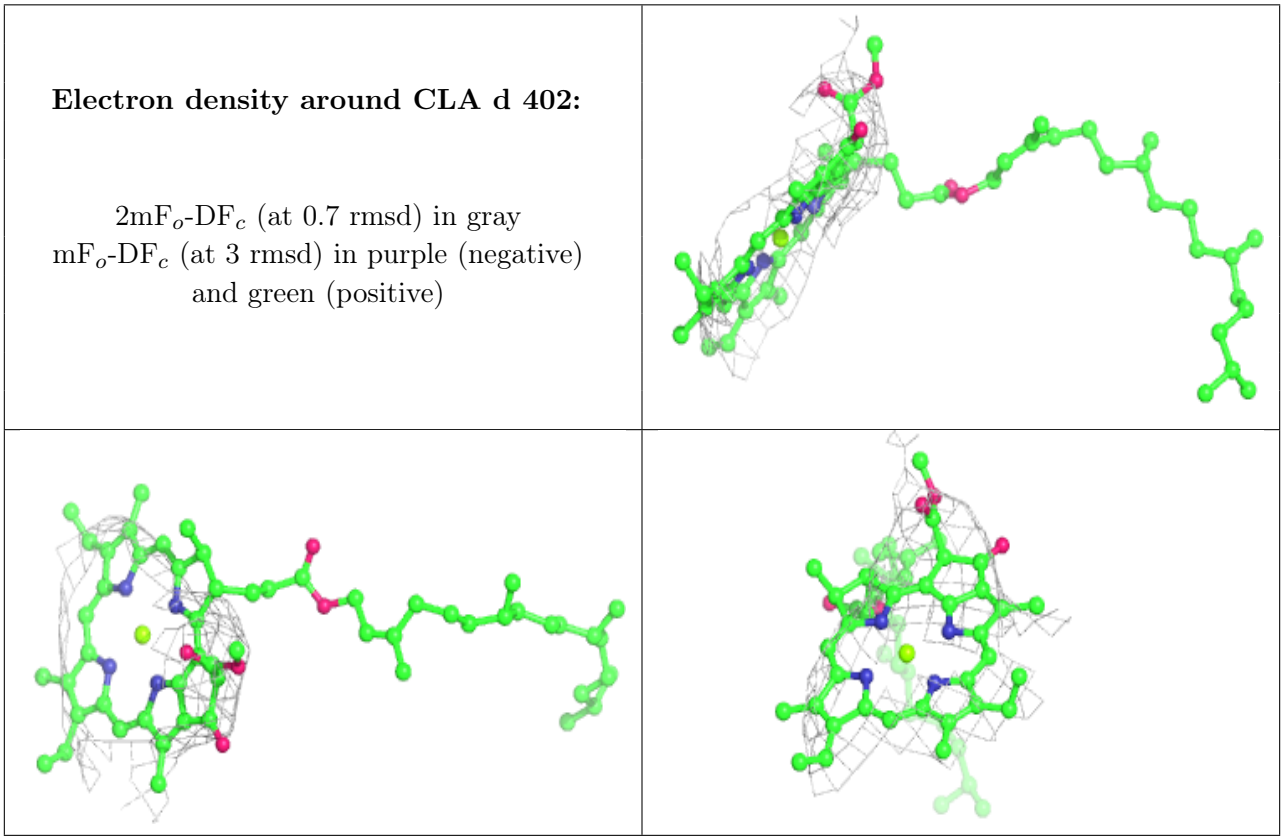
Electron density around DGD c 517:

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



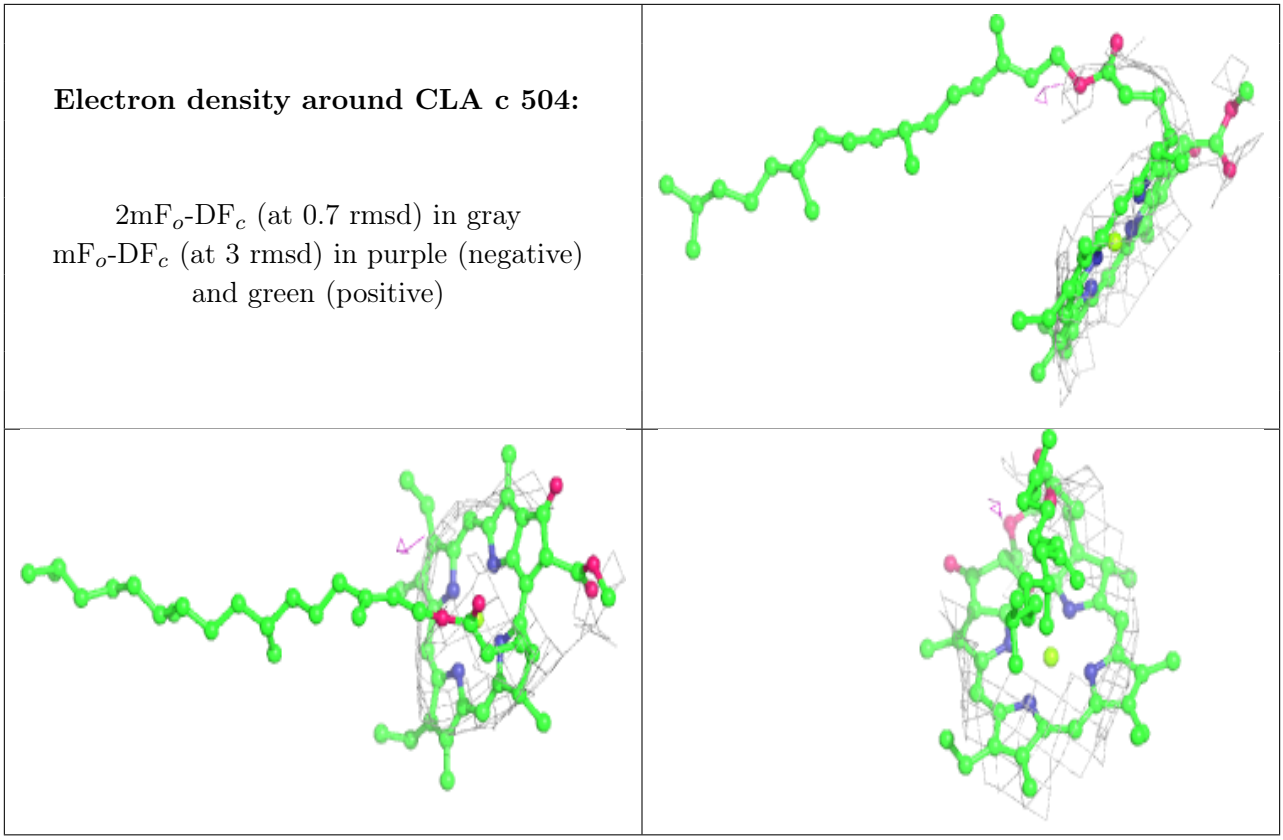
Electron density around CLA d 402:

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



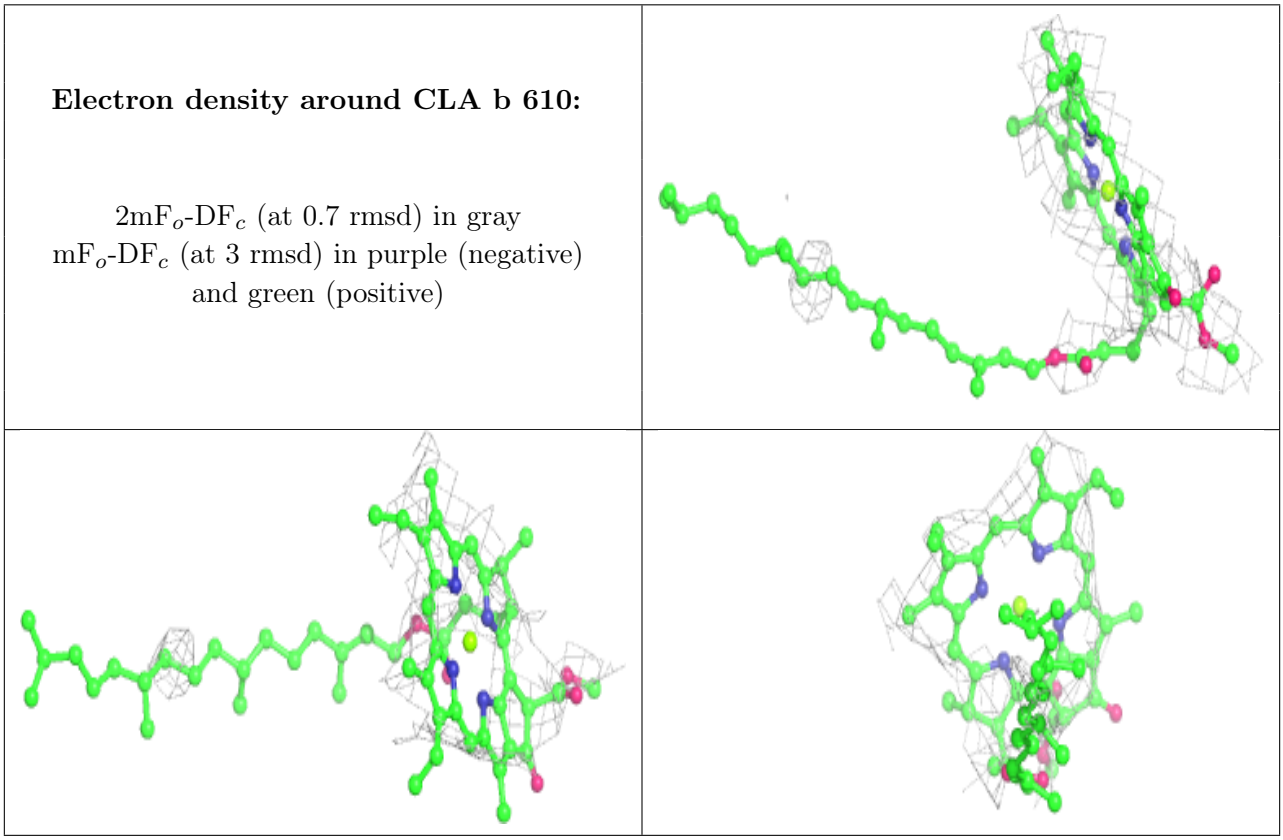
Electron density around CLA c 504:

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



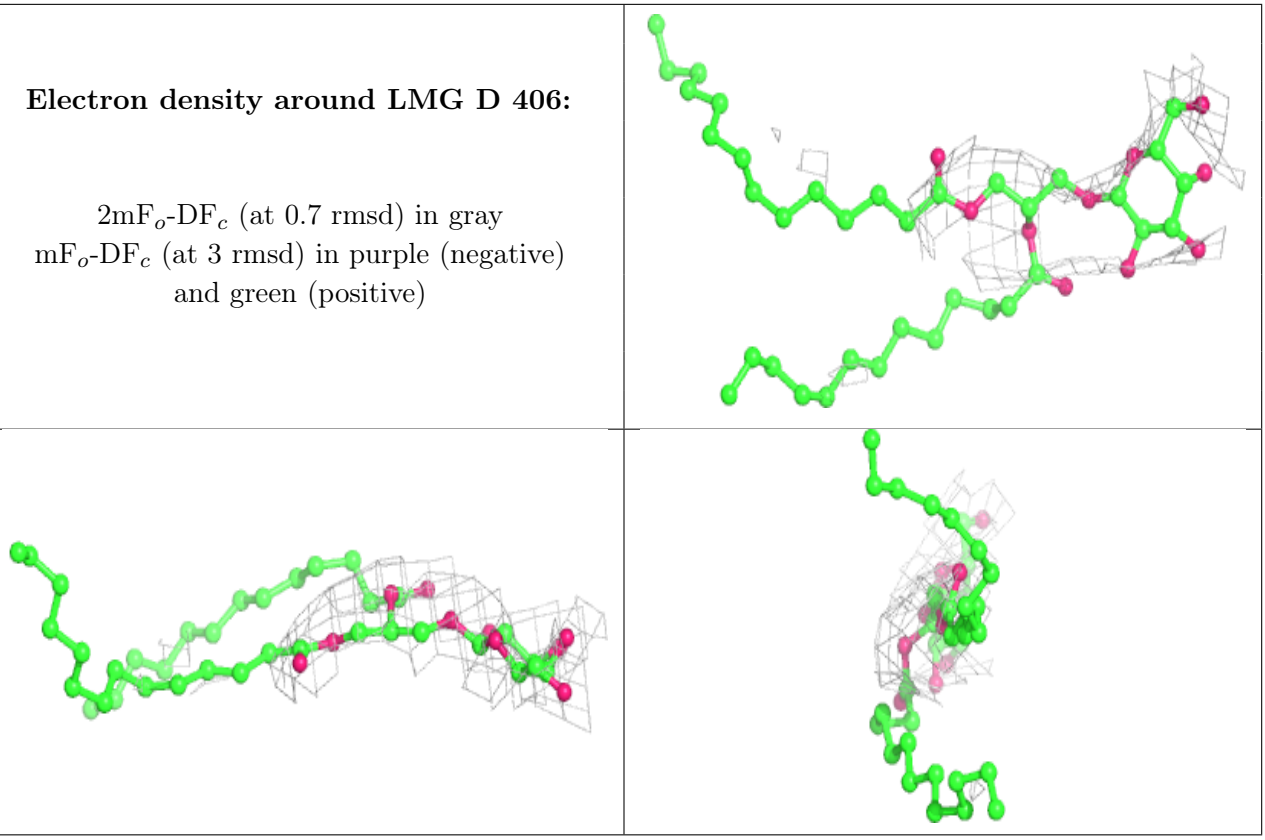
Electron density around CLA b 610:

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



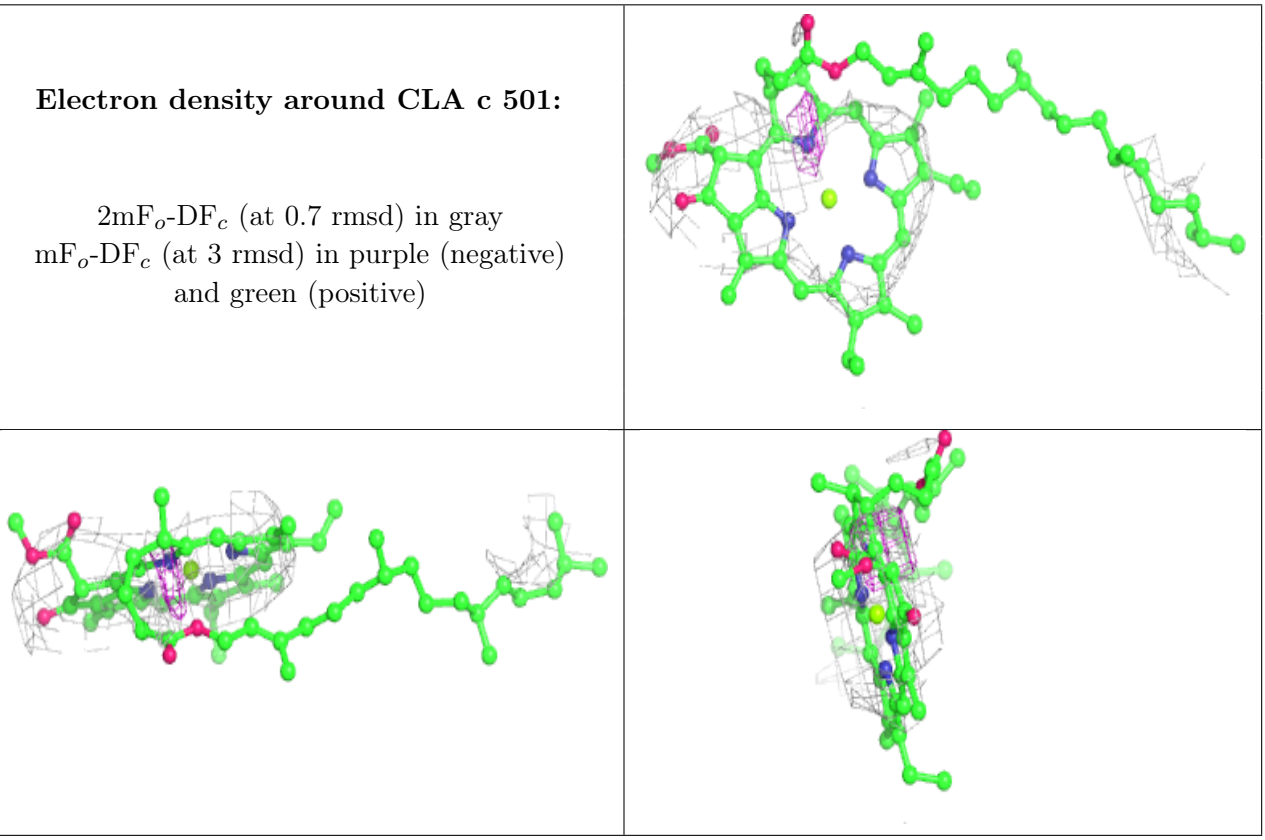
Electron density around LMG D 406:

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



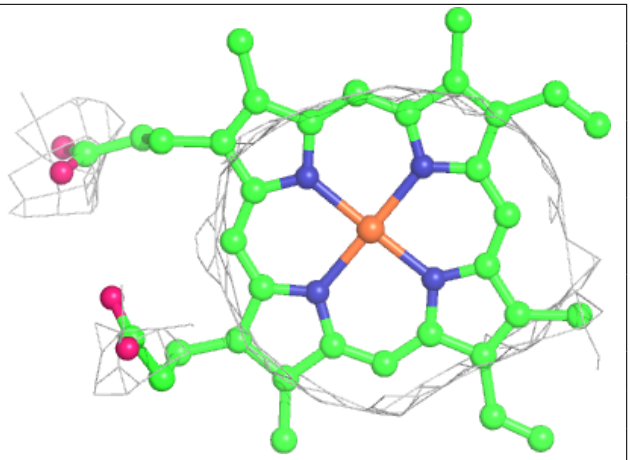
Electron density around CLA c 501:

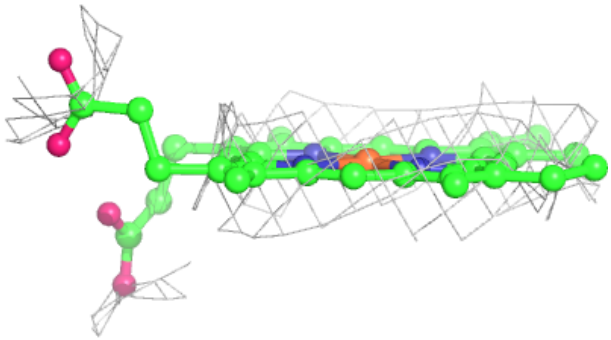
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

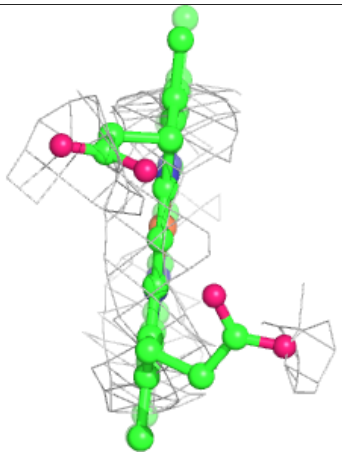


Electron density around HEM F 101:

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

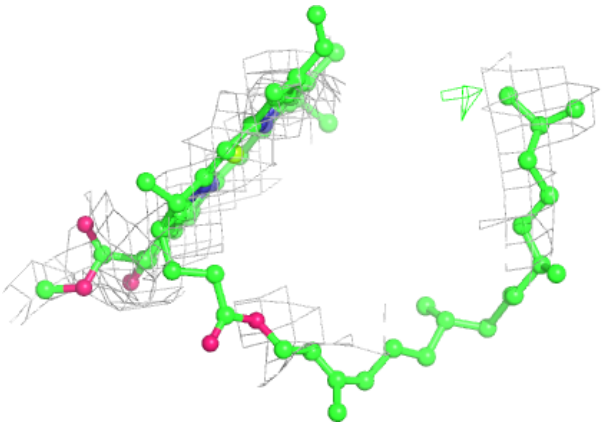


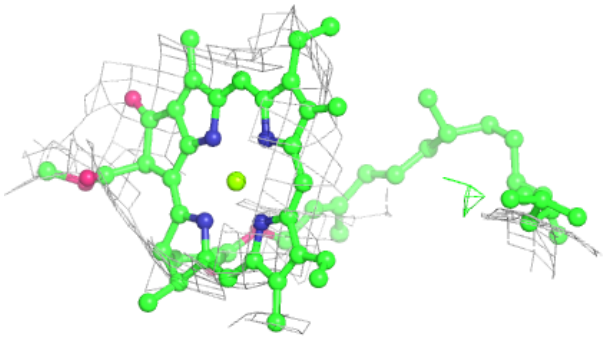


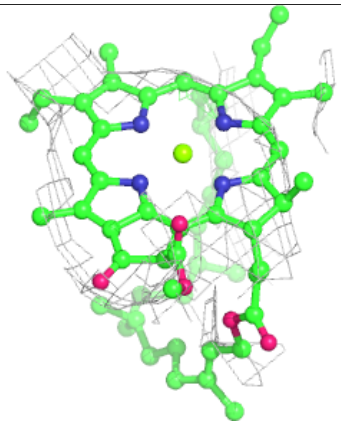


Electron density around CLA b 614:

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

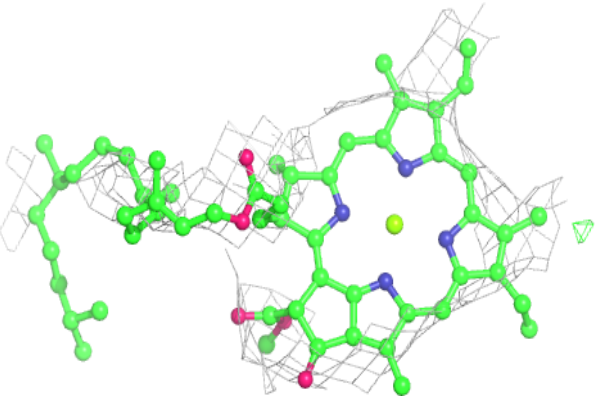


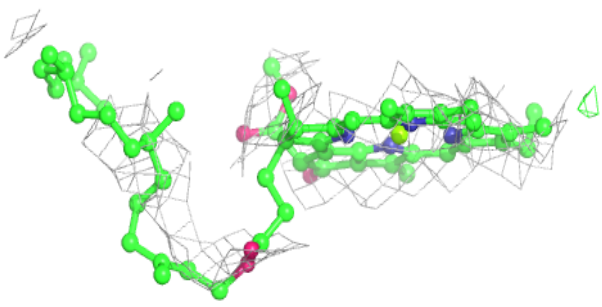


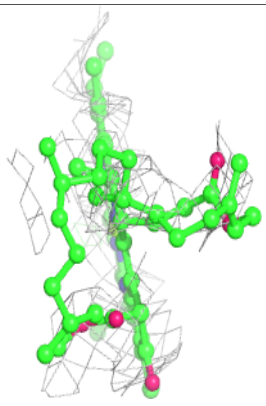


Electron density around CLA b 615:

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

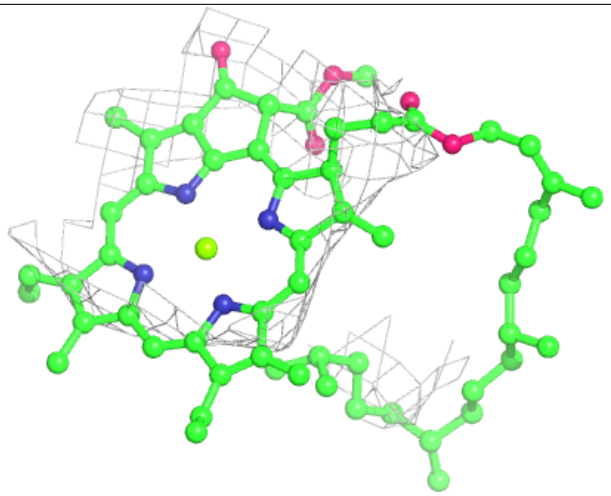


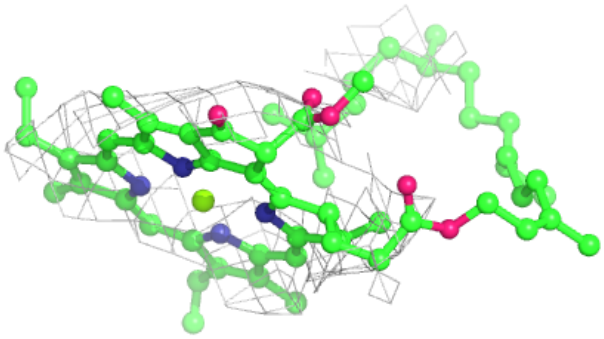


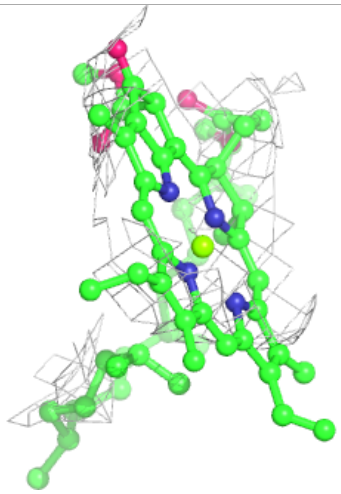


Electron density around CLA B 615:

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

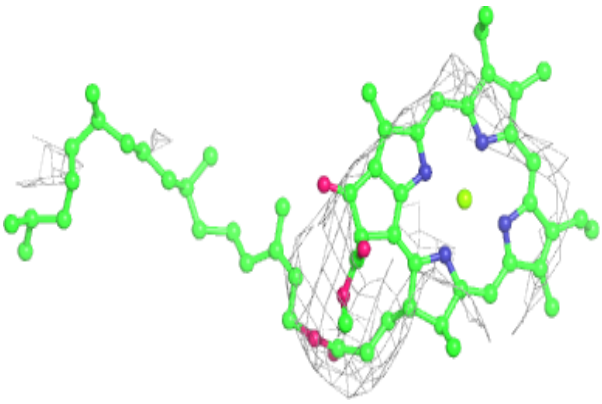


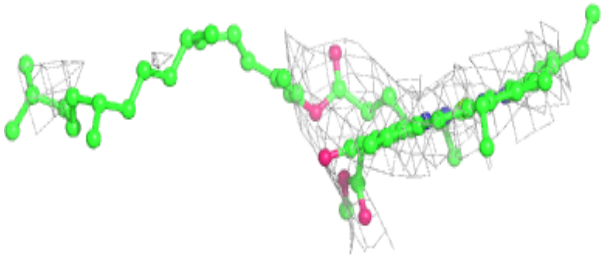


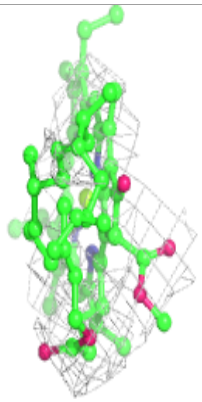


Electron density around CLA B 602:

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

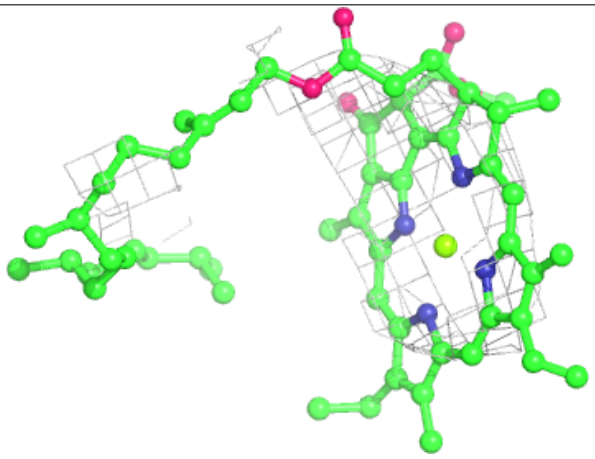


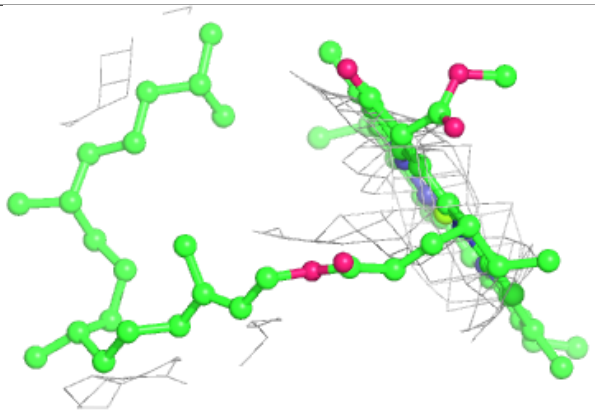


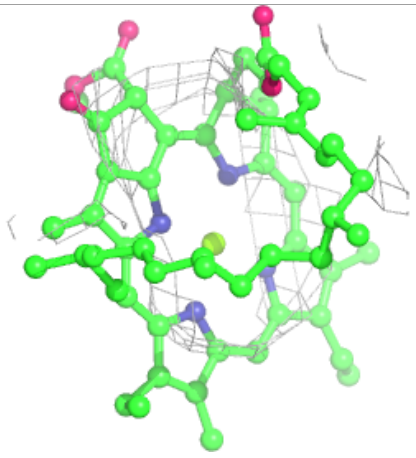


Electron density around CLA c 503:

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

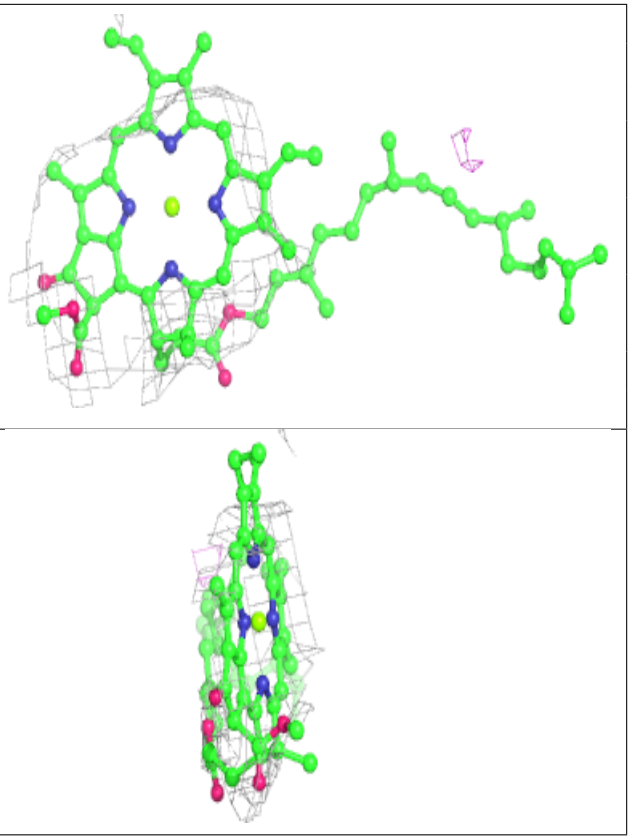


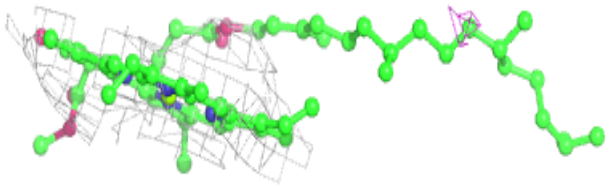




Electron density around CLA B 603:

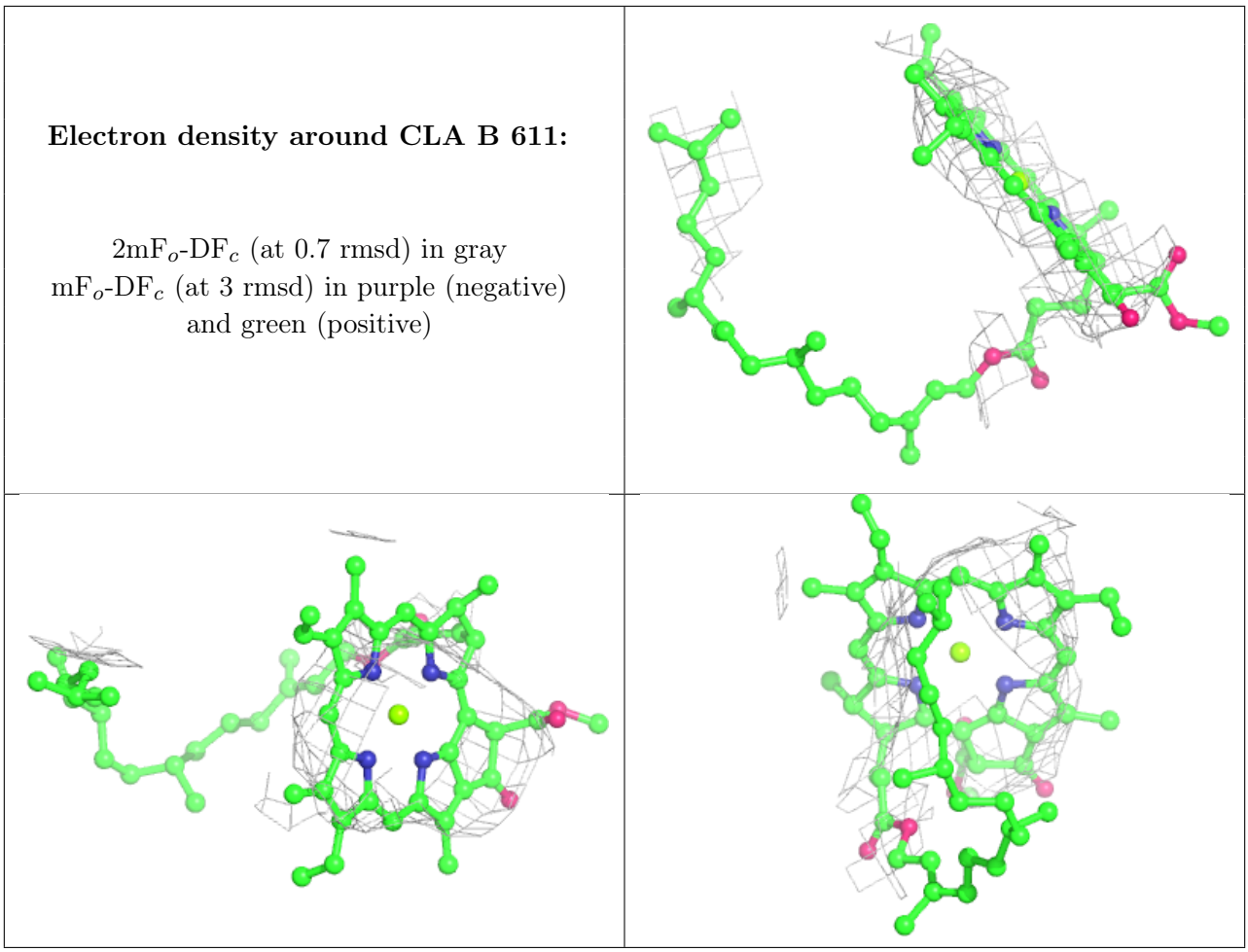
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





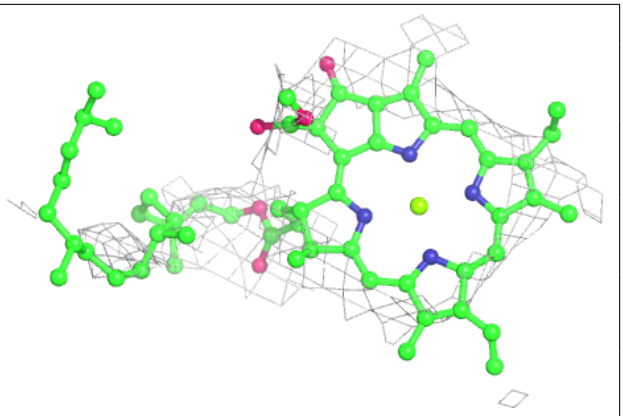
Electron density around CLA B 611:

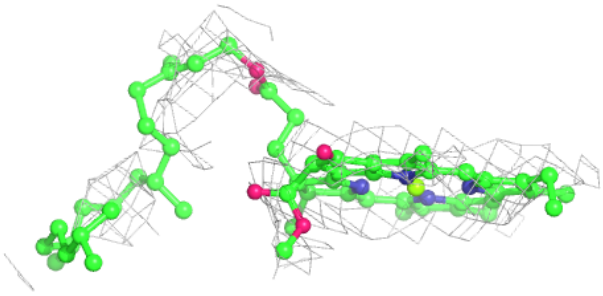
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

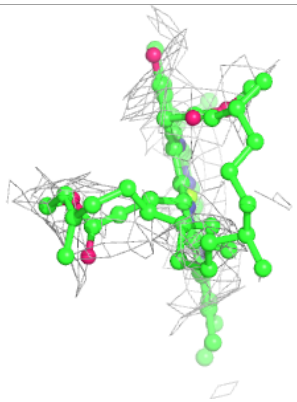


Electron density around CLA B 612:

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

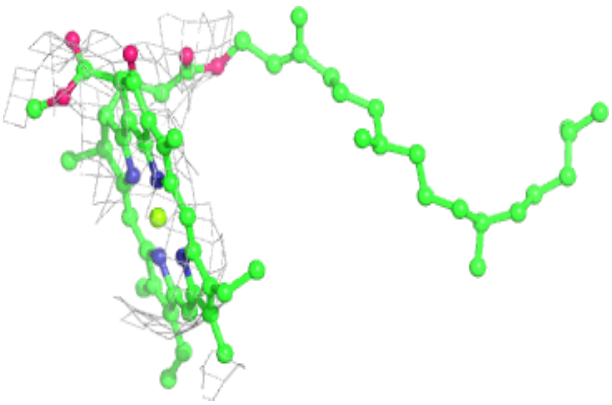


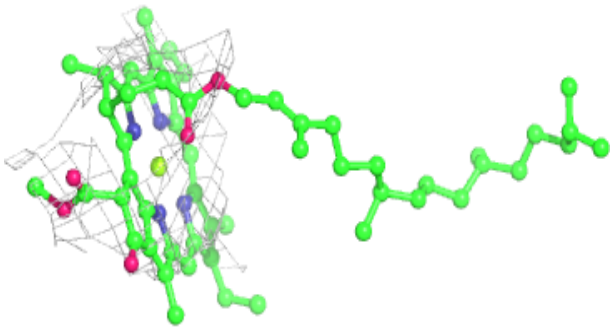


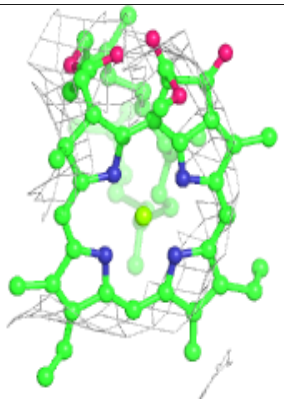


Electron density around CLA c 508:

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

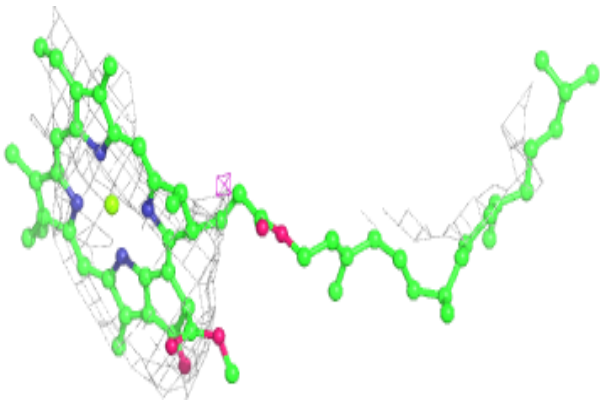


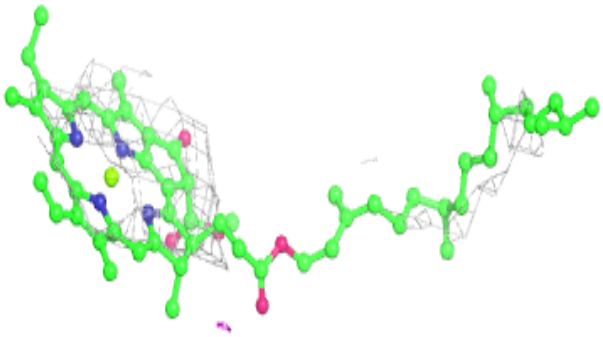


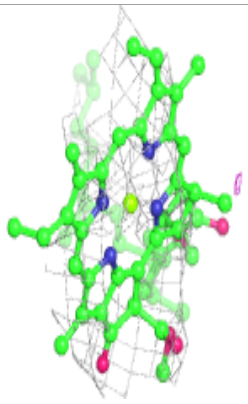


Electron density around CLA A 403:

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

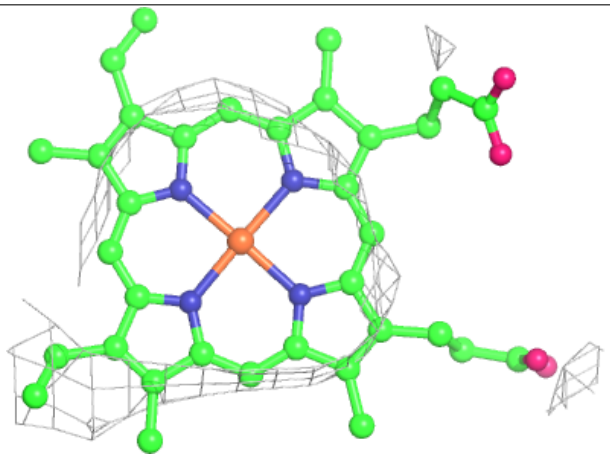


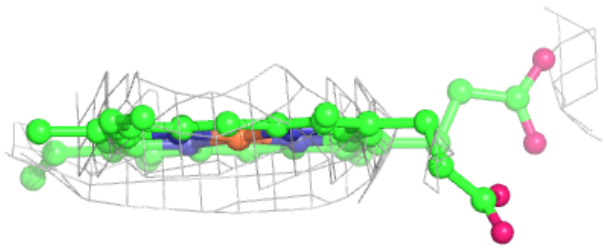


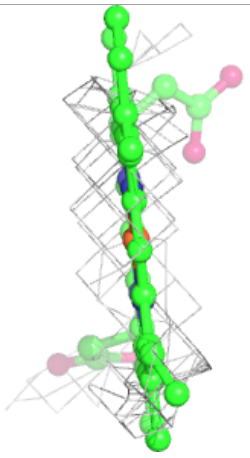


Electron density around HEM v 201:

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

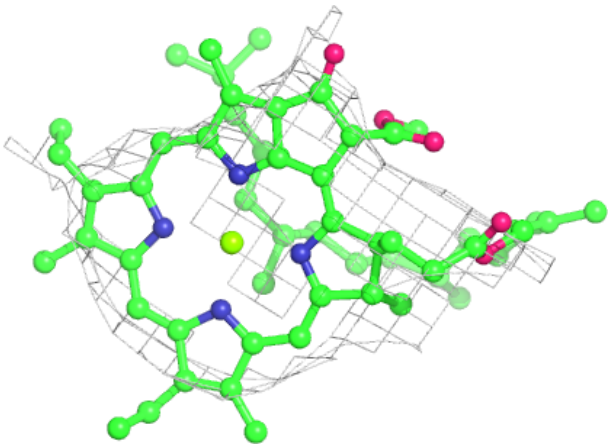


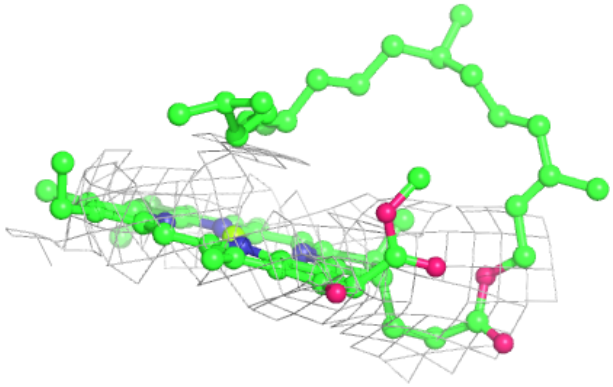


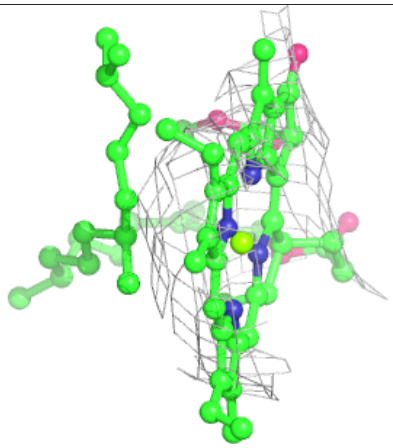


Electron density around CLA c 510:

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

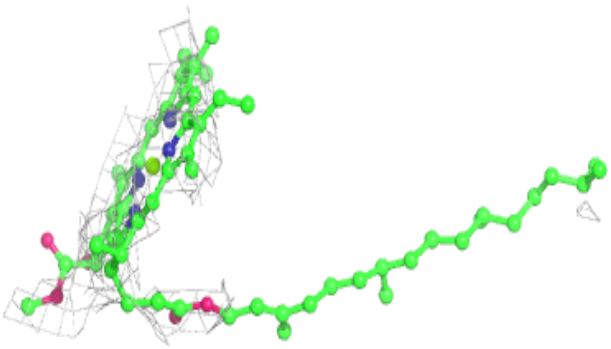


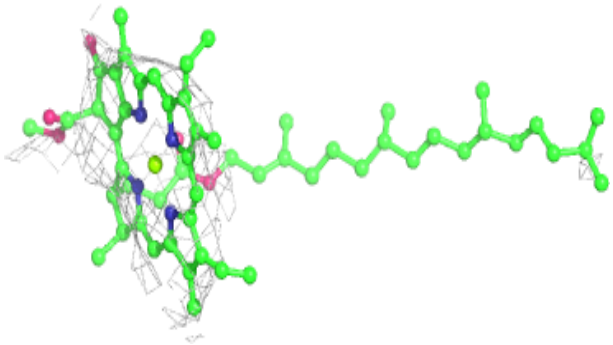


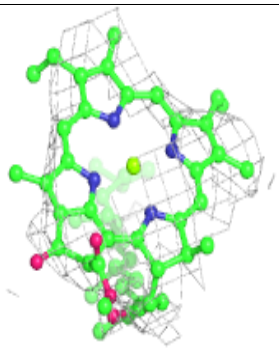


Electron density around CLA B 607:

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

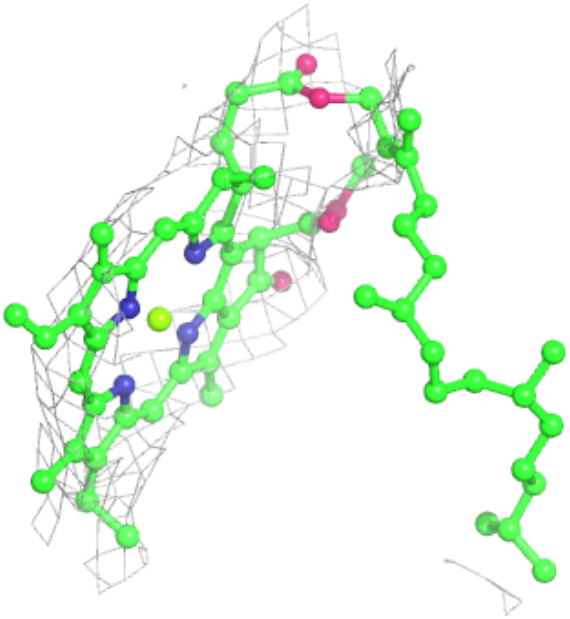


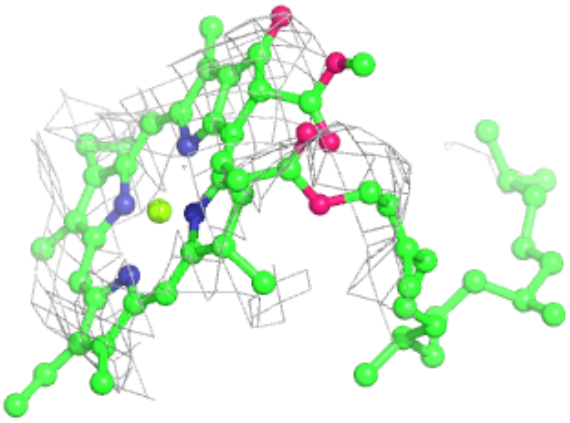


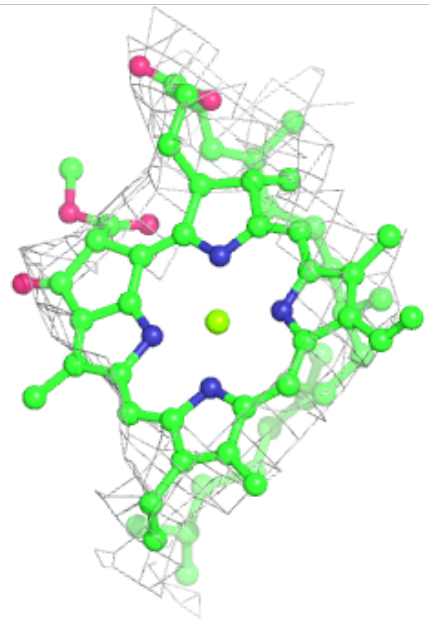


Electron density around CLA B 613:

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

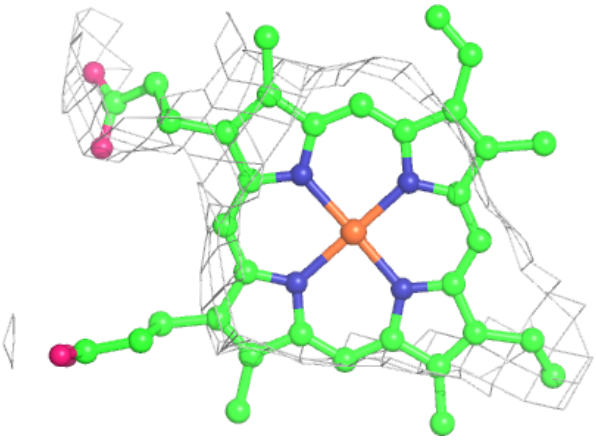


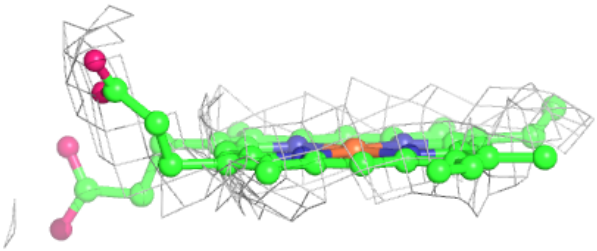


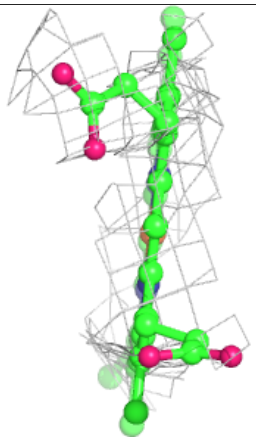


Electron density around HEM V 201:

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

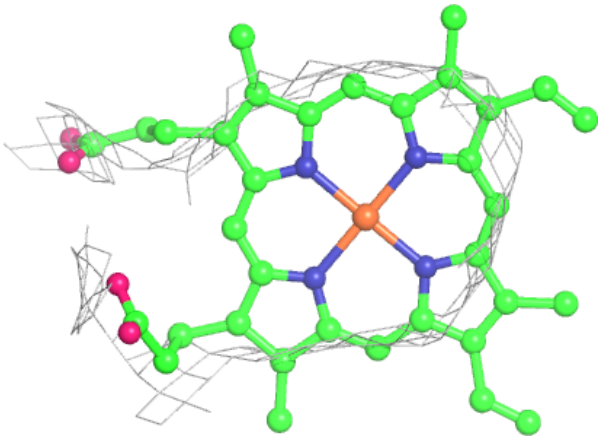


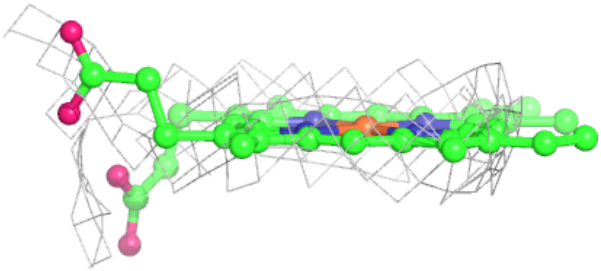


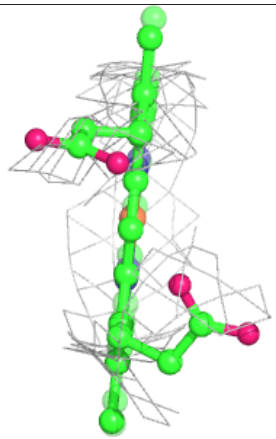


Electron density around HEM f 101:

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

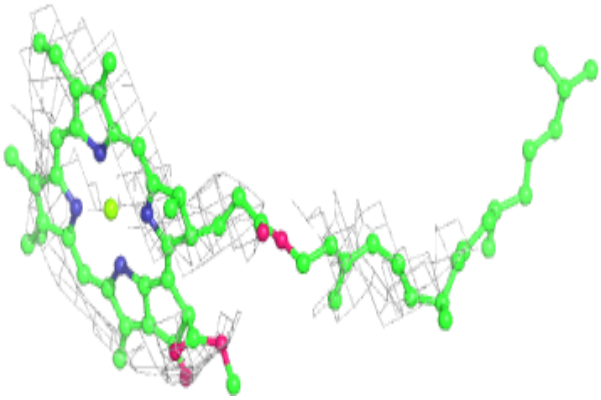


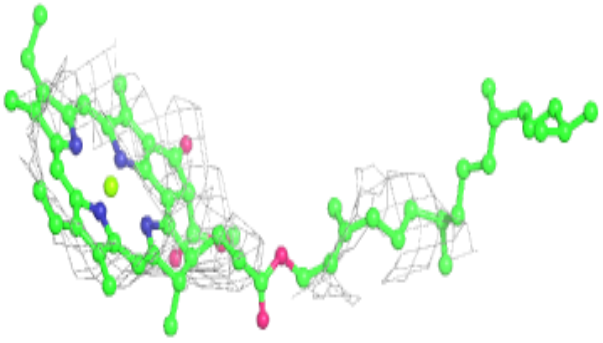


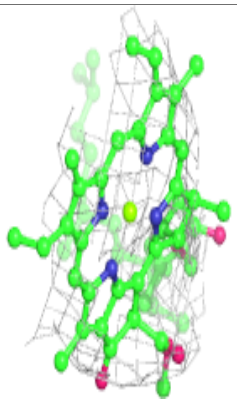


Electron density around CLA a 404:

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

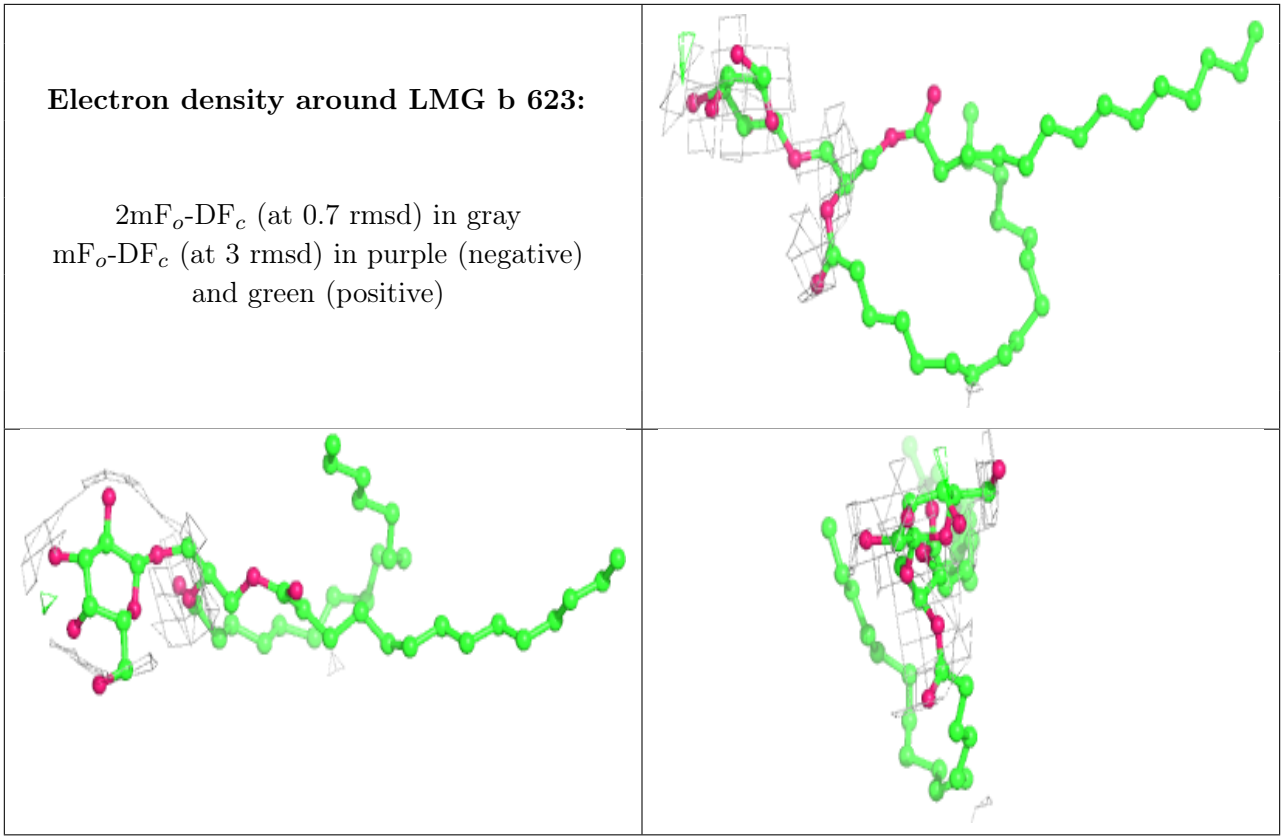






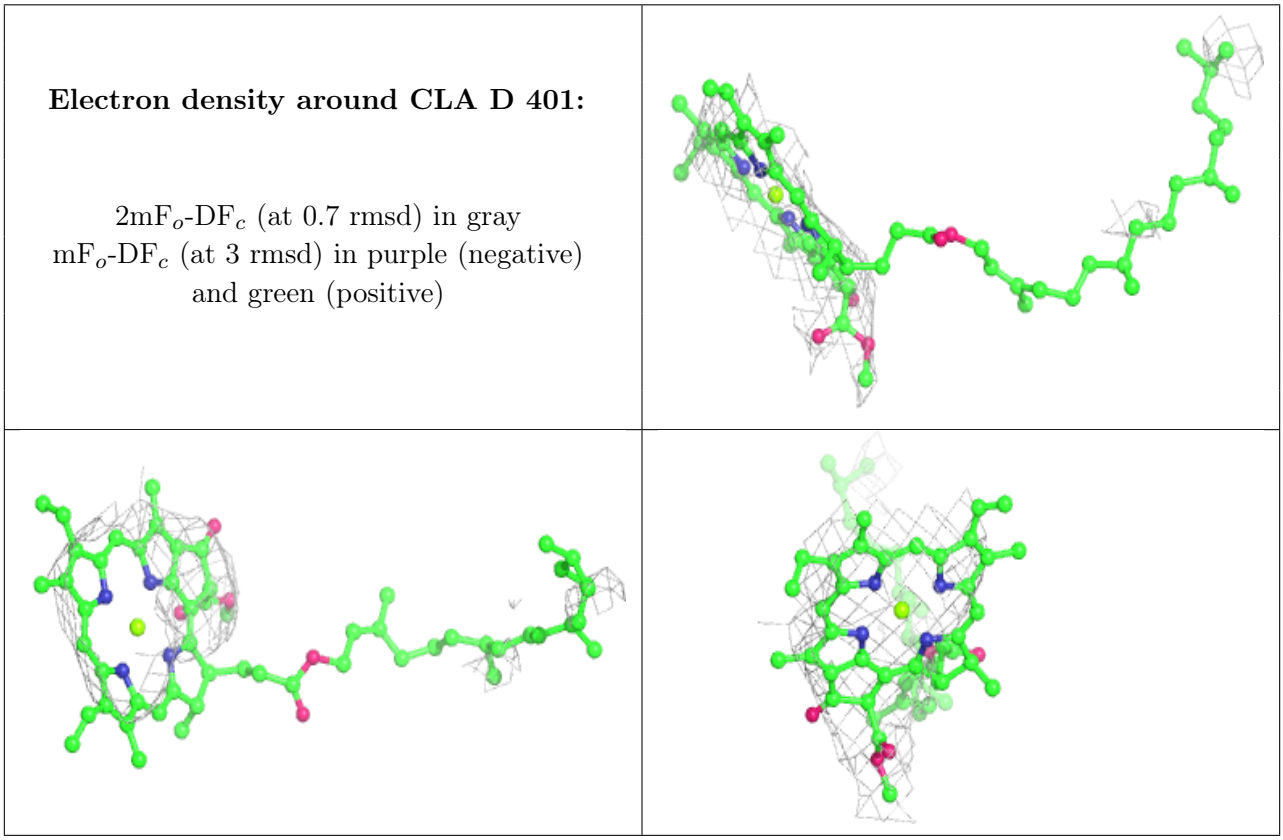
Electron density around LMG b 623:

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



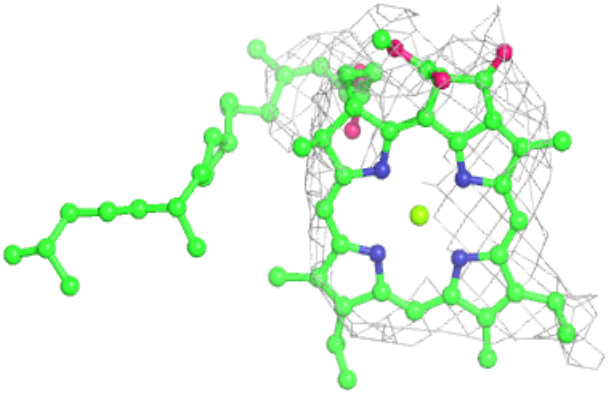
Electron density around CLA D 401:

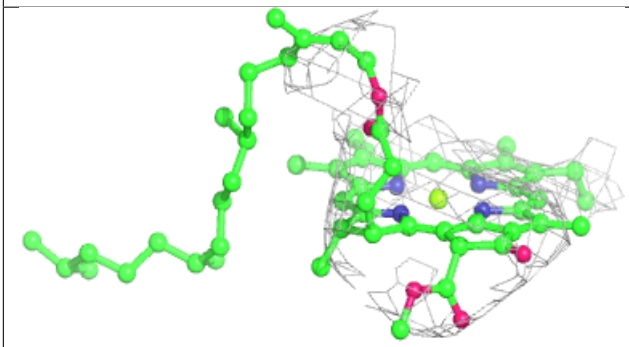
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

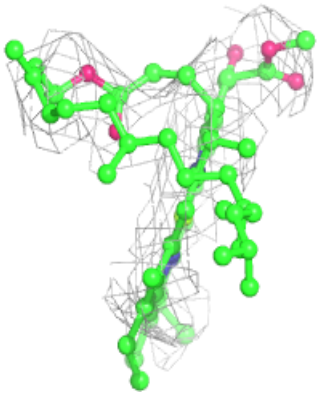


Electron density around CLA A 404:

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

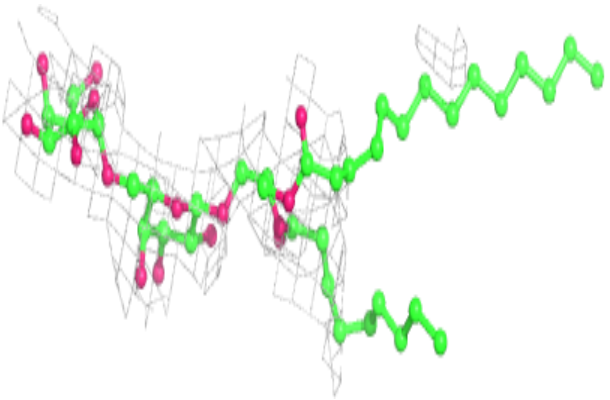


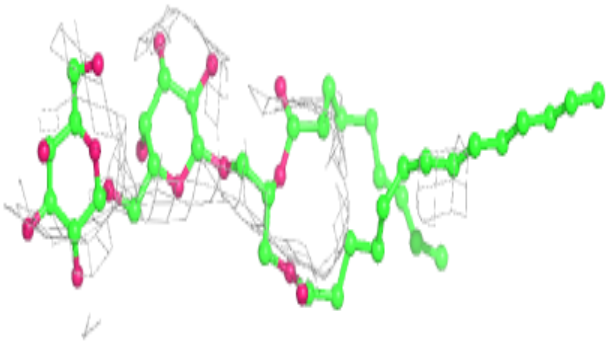


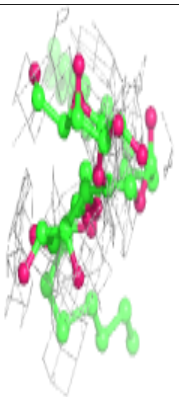


Electron density around DGD C 516:

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

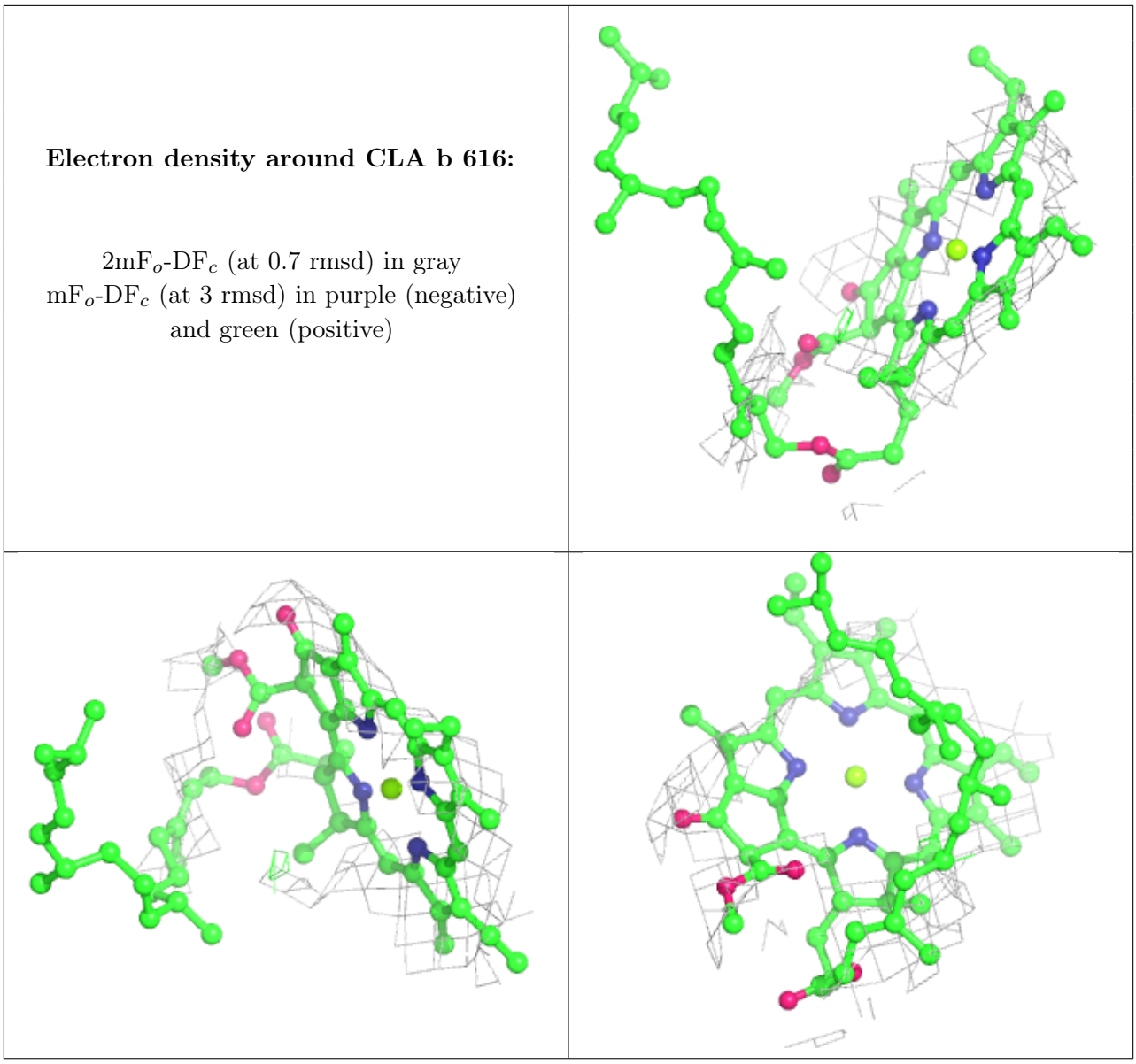






Electron density around CLA b 616:

$2mF_o$-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.