Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 12:11 AM EDT

PDB ID	:	4TNJ
Title	:	RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 A resolution
Authors	:	Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on	:	2014-06-04
Resolution	:	4.50 Å(reported)

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

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

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

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

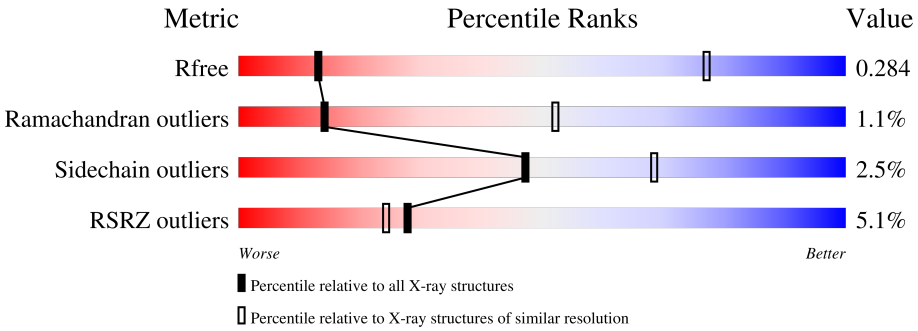
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1

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 4.50 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	1055 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	344	8% 95%
1	a	344	8% 95%

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buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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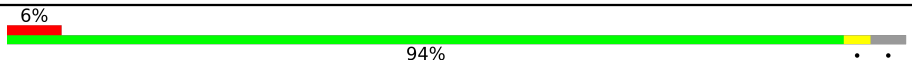
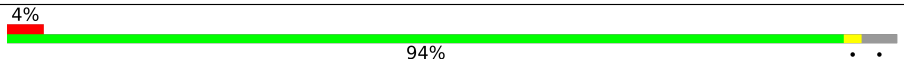
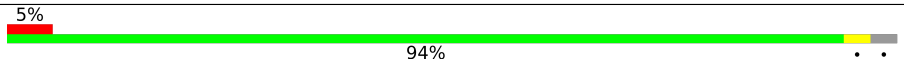
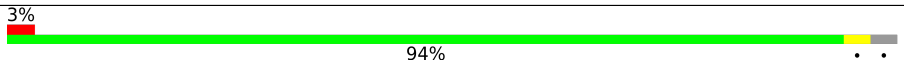
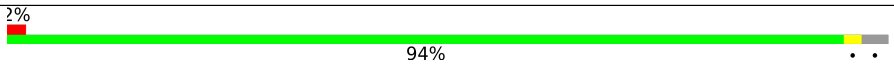
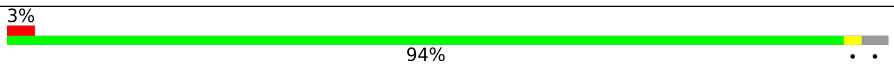
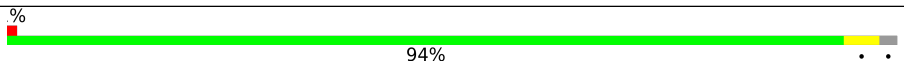
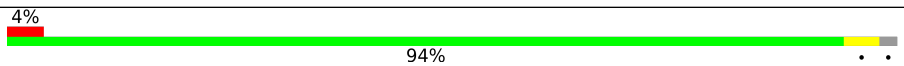
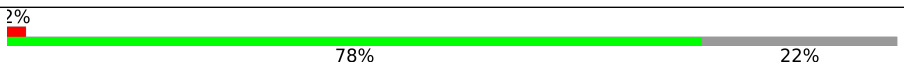
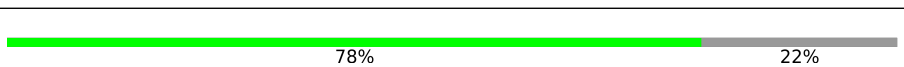
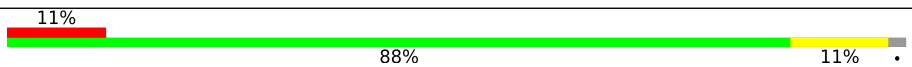
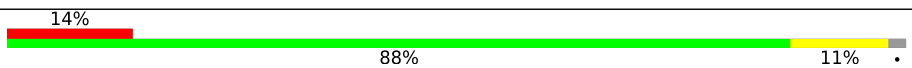
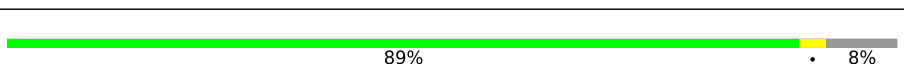
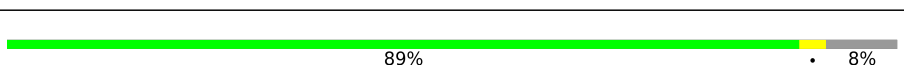
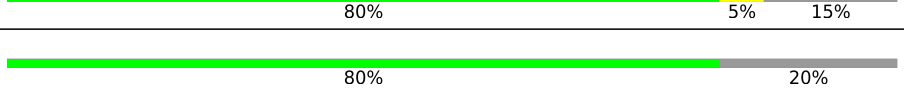
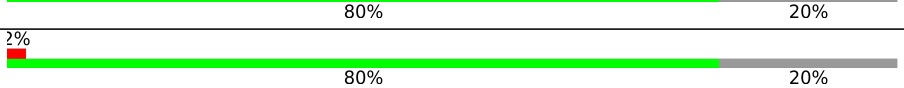
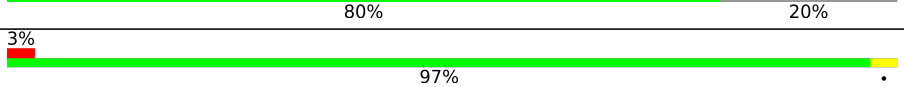
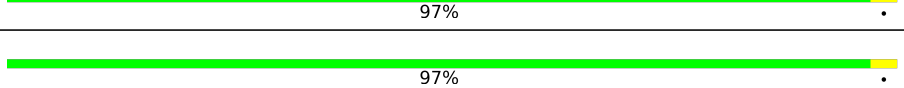
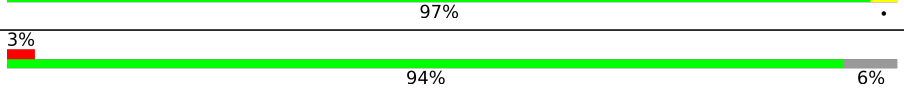
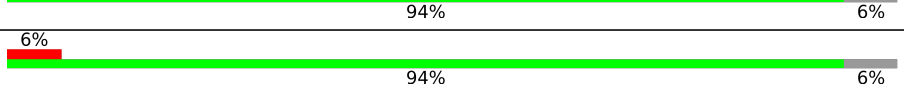
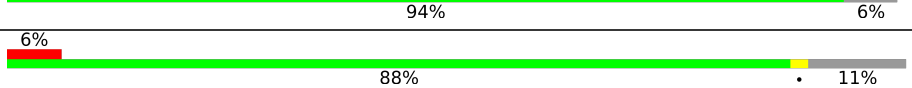
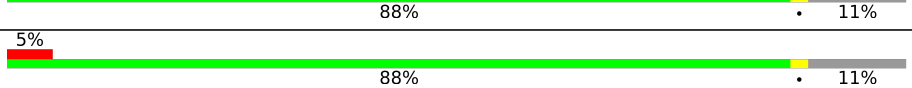
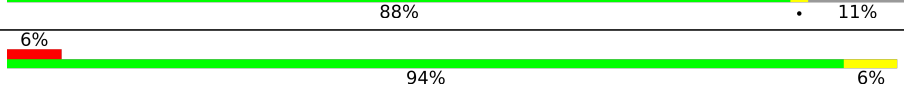
Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	t	32	9% 94% 6%
15	U	134	5% 70% 28%
15	u	134	7% 70% 28%
16	V	163	83% 16%
16	v	163	6% 83% 16%
17	g	46	2% 54% 7% 39%
17	y	46	54% 7% 39%
18	X	41	2% 85% 5% 10%
18	x	41	17% 85% 5% 10%
19	G	28	100%
19	Y	28	100%
20	Z	62	2% 95% 5%
20	z	62	8% 95% 5%

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
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	520	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	X
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	521	-	-	-	X
24	BCR	D	411	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	J	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	f	102	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	D	409	-	-	-	X
25	DGD	a	411	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	408	-	-	-	X
26	LHG	C	519	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	I	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	a	413	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	i	101	-	-	-	X
27	LMG	m	101	-	-	-	X
28	CL	A	411	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	d	402	-	-	-	X
31	LMT	B	622	-	-	-	X
31	LMT	B	623	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	102	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	M	103	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	626	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	409	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	d	401	-	-	-	X
35	CA	o	301	-	-	-	X

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 50244 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
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	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	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

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

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

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

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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 Y.

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

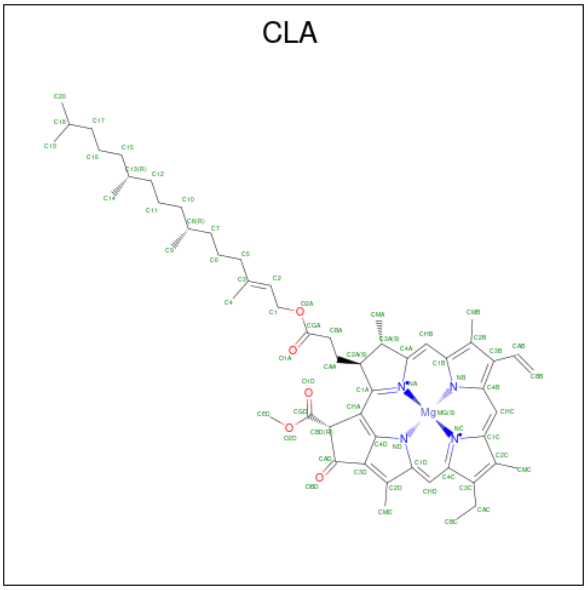
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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



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

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

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

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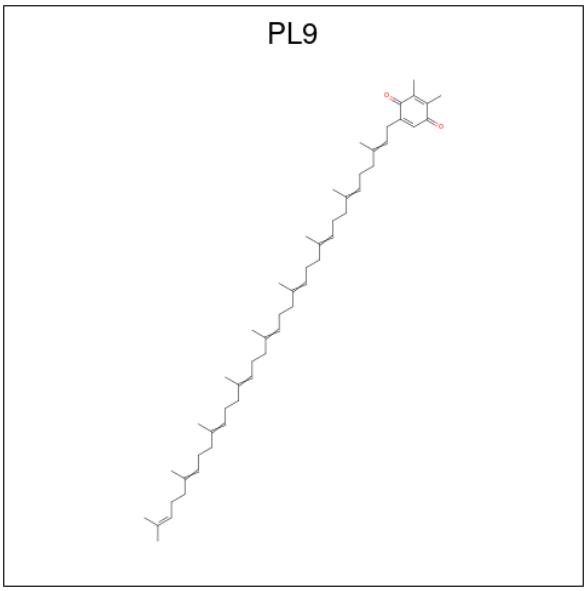
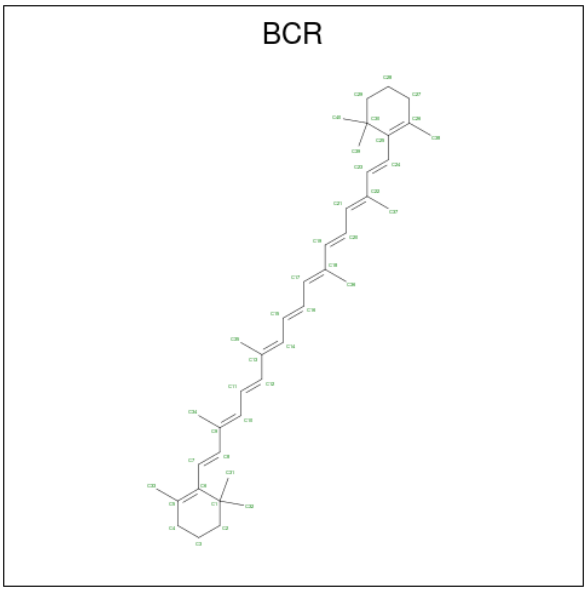
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N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

- Molecule 23 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
23	A	1	Total C O 45 43 2	0	0
23	D	1	Total C O 55 53 2	0	0
23	J	1	Total C O 35 33 2	0	0
23	a	1	Total C O 45 43 2	0	0
23	d	1	Total C O 55 53 2	0	0
23	j	1	Total C O 35 33 2	0	0

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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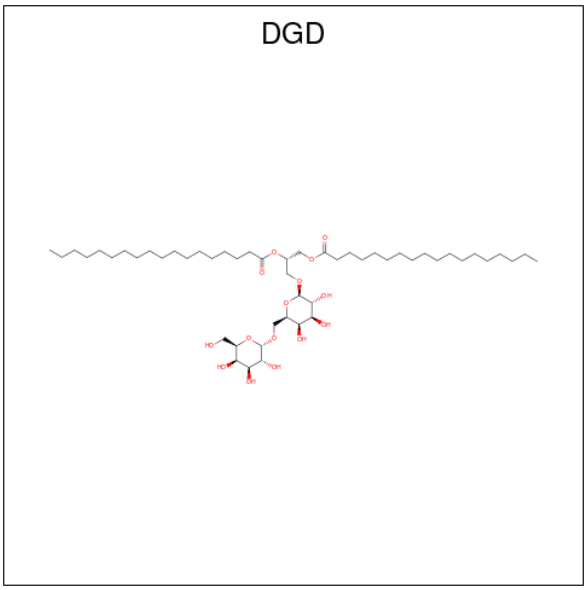
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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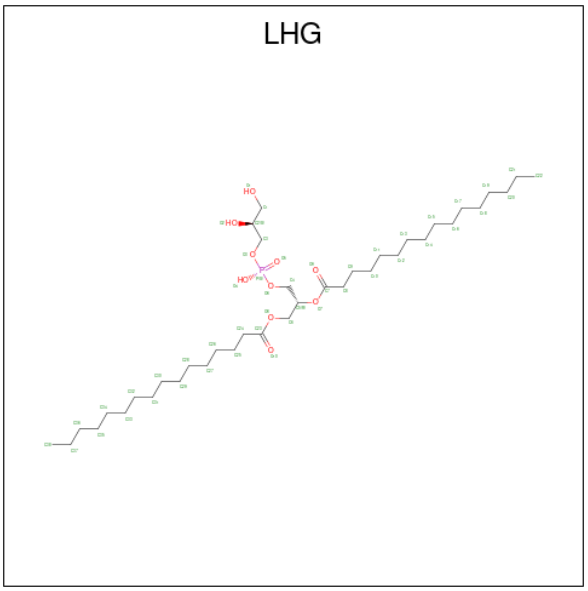
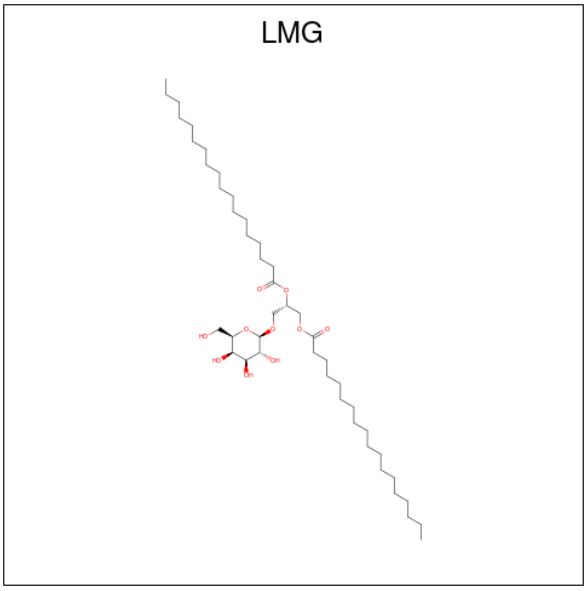
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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

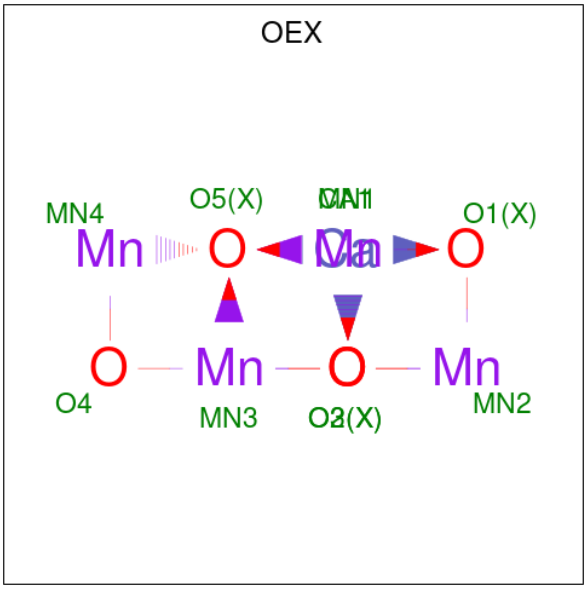


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 51 41 10	0	0
27	A	1	Total C O 42 32 10	0	0
27	B	1	Total C O 49 39 10	0	0
27	B	1	Total C O 49 39 10	0	0
27	C	1	Total C O 45 35 10	0	0
27	C	1	Total C O 48 38 10	0	0
27	D	1	Total C O 48 38 10	0	0
27	D	1	Total C O 46 36 10	0	0
27	E	1	Total C O 44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

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

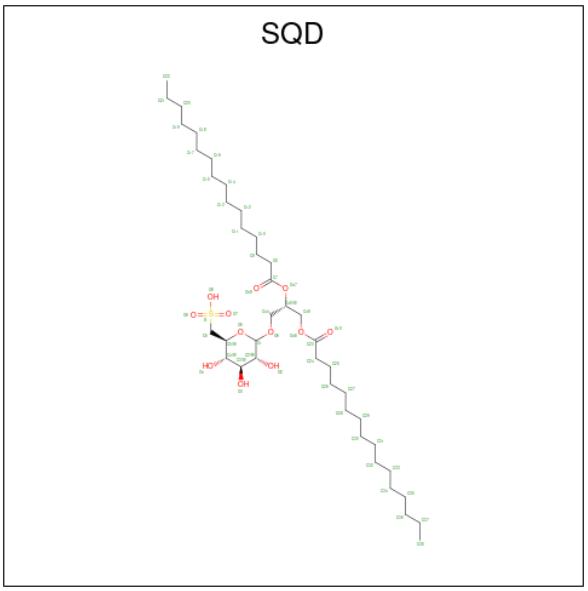
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Cl 1 1	0	0
28	a	1	Total Cl 1 1	0	0

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



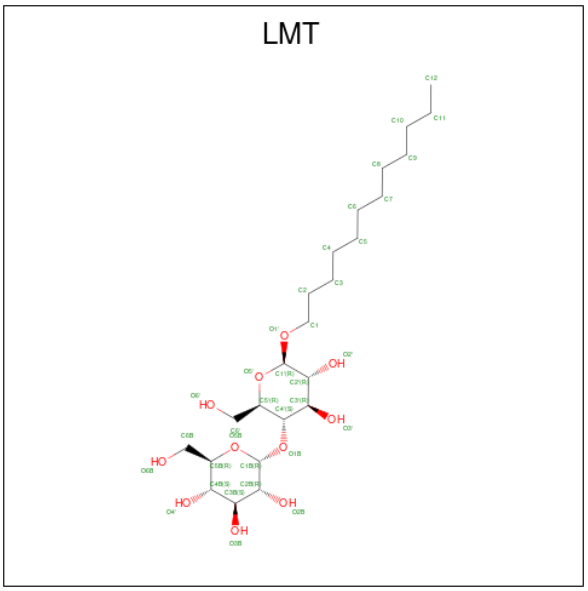
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Ca Mn O 10 1 4 5	0	0
29	a	1	Total Ca Mn O 10 1 4 5	0	0

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



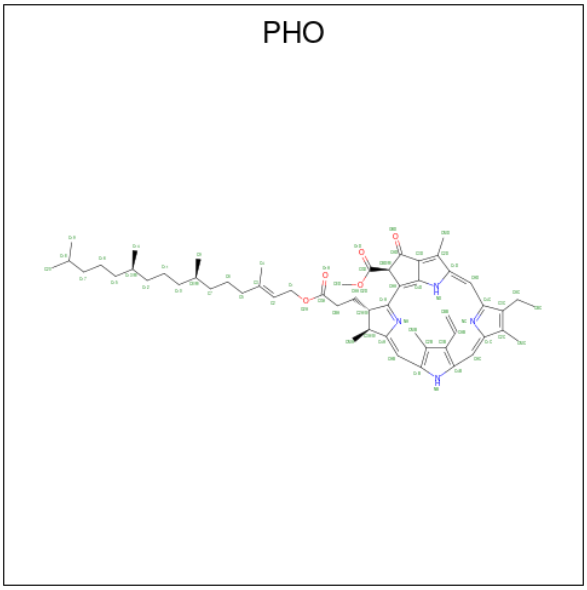
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			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 DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



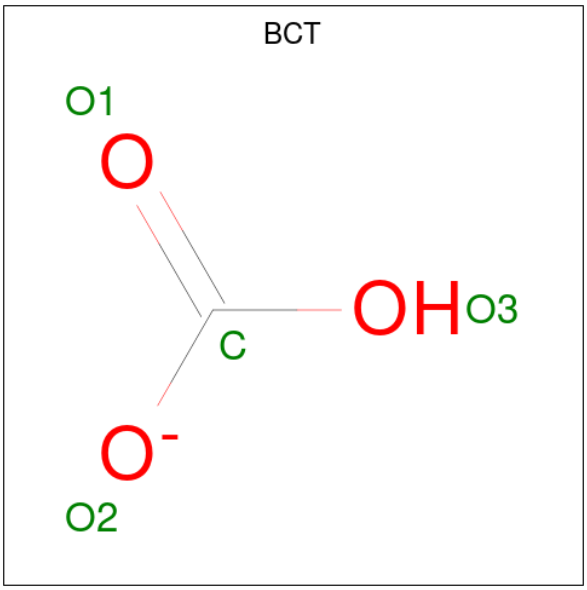
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total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

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



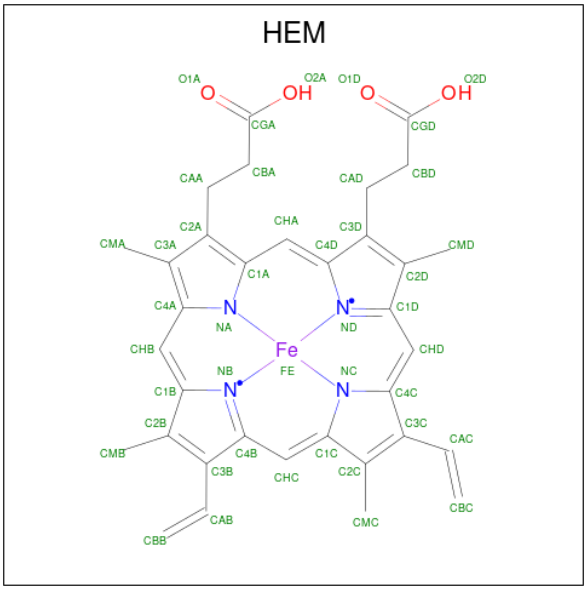
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 4 1 3	0	0
33	d	1	Total C O 4 1 3	0	0

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



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

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

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

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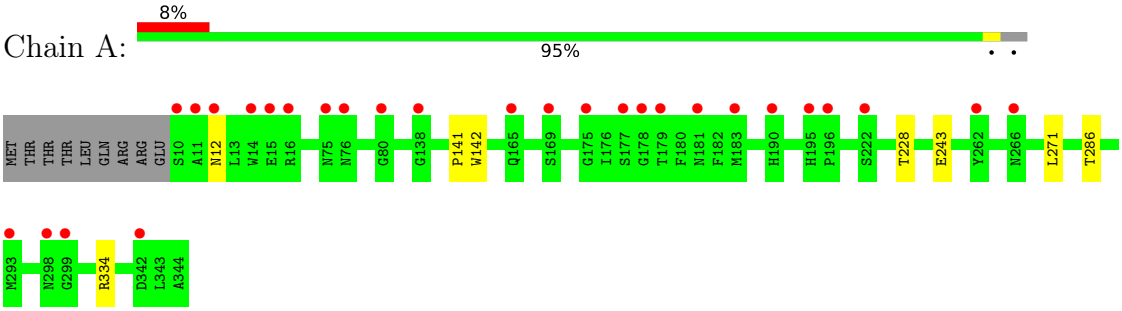
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total	Ca	0	0
			1	1		

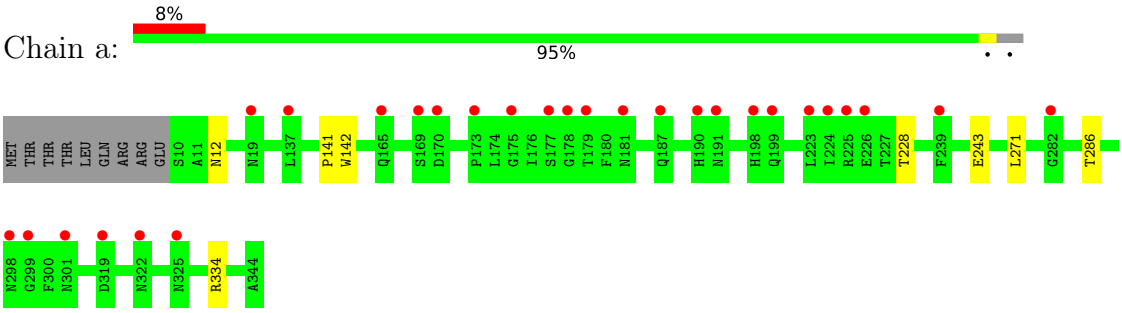
3 Residue-property plots (i)

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.

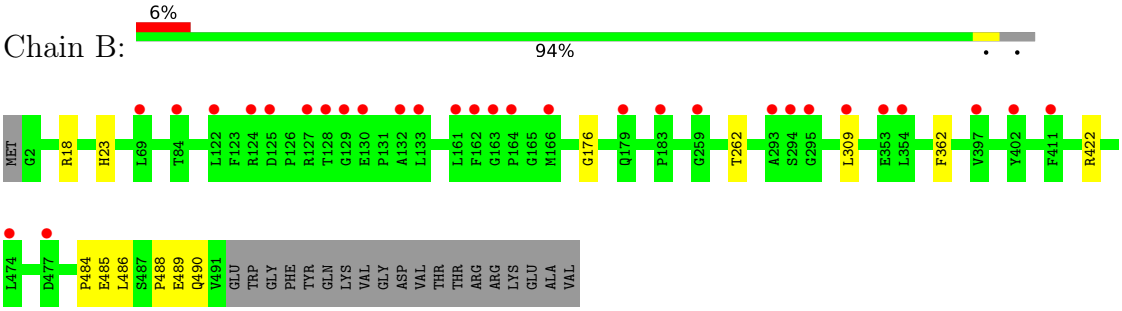
• Molecule 1: Photosystem Q(B) protein 1



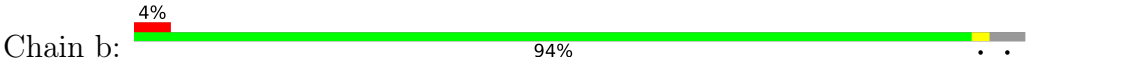
• Molecule 1: Photosystem Q(B) protein 1



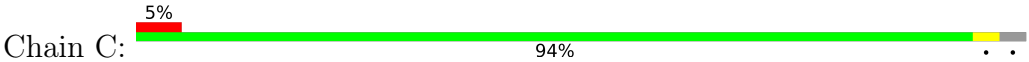
• Molecule 2: Photosystem II core light harvesting protein

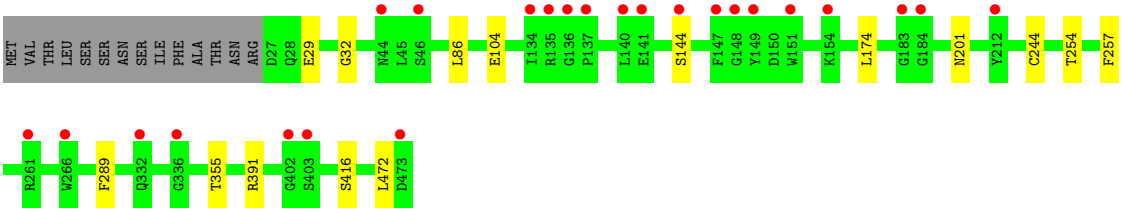


• Molecule 2: Photosystem II core light harvesting protein

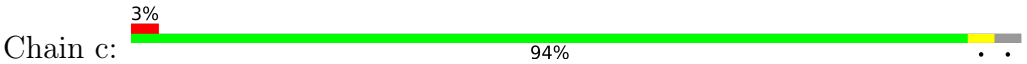


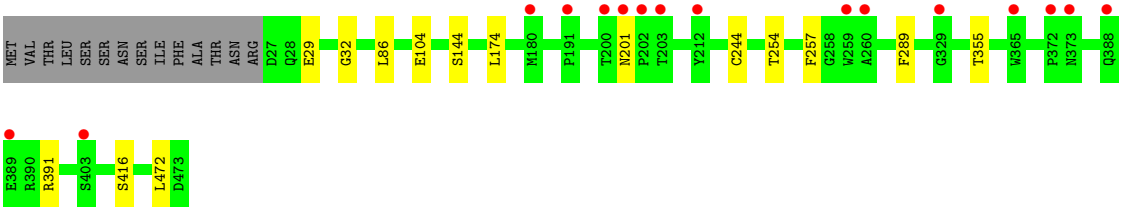
• Molecule 3: Photosystem II CP43 protein



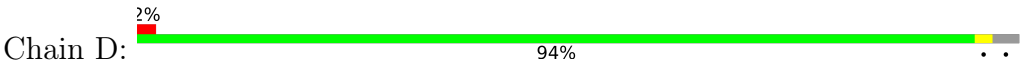


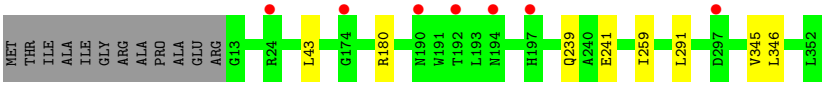
• Molecule 3: Photosystem II CP43 protein



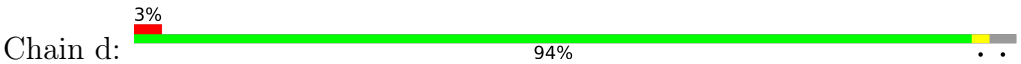


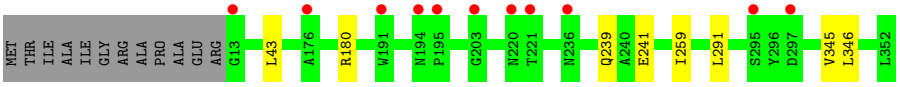
• Molecule 4: Photosystem II D2 protein



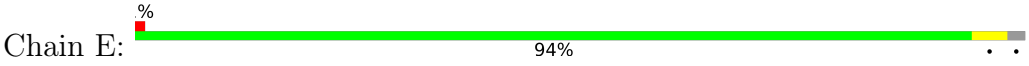


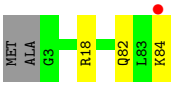
• Molecule 4: Photosystem II D2 protein





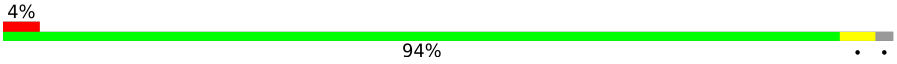
• Molecule 5: Cytochrome b559 subunit alpha

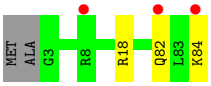




• Molecule 5: Cytochrome b559 subunit alpha

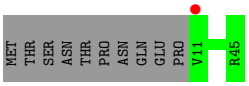
Chain e:





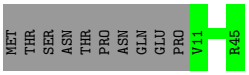
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



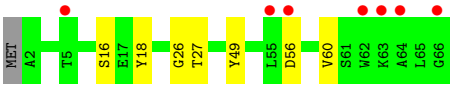
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



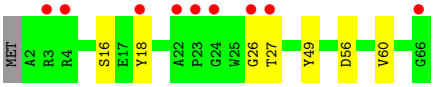
• Molecule 7: Photosystem II reaction center protein H

Chain H:



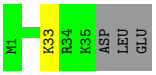
• Molecule 7: Photosystem II reaction center protein H

Chain h:



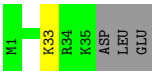
• Molecule 8: Photosystem II reaction center protein I

Chain I:



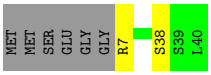
• Molecule 8: Photosystem II reaction center protein I

Chain i:



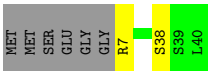
• Molecule 9: Photosystem II reaction center protein J

Chain J:



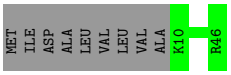
• Molecule 9: Photosystem II reaction center protein J

Chain j:



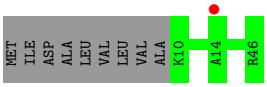
• Molecule 10: Photosystem II reaction center protein K

Chain K:



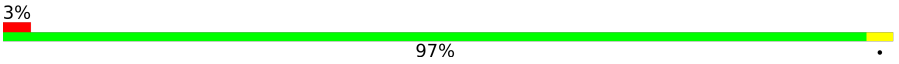
• Molecule 10: Photosystem II reaction center protein K

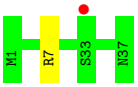
Chain k:



• Molecule 11: Photosystem II reaction center protein L

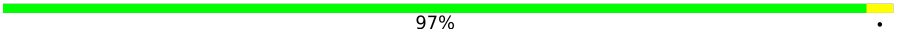
Chain L:





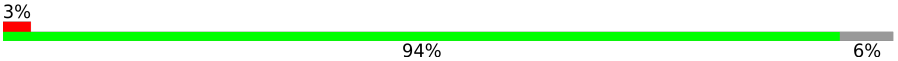
• Molecule 11: Photosystem II reaction center protein L

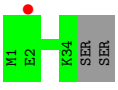
Chain l:



• Molecule 12: Photosystem II reaction center protein M

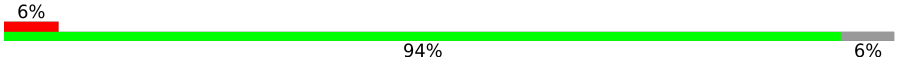
Chain M:

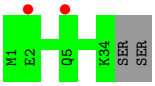




• Molecule 12: Photosystem II reaction center protein M

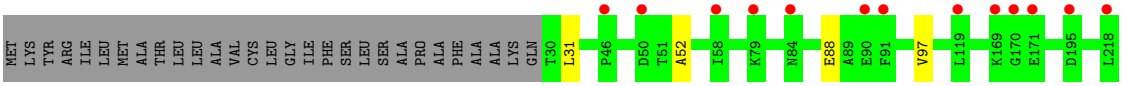
Chain m:

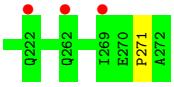




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

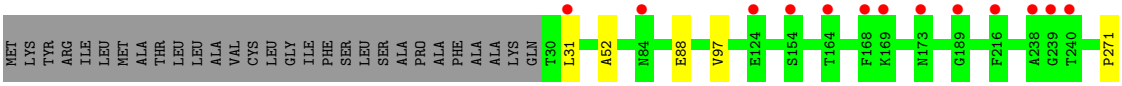
Chain O:





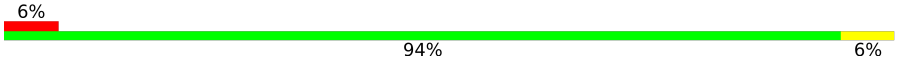
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

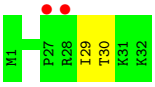
Chain o:



• Molecule 14: Photosystem II reaction center protein T

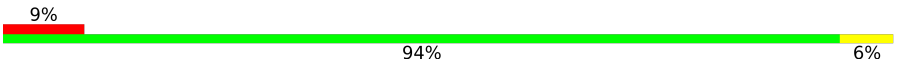
Chain T:

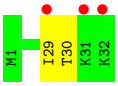




• Molecule 14: Photosystem II reaction center protein T

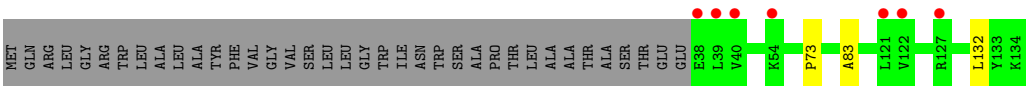
Chain t:





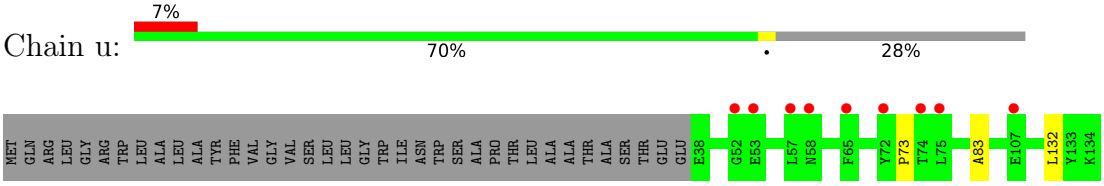
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



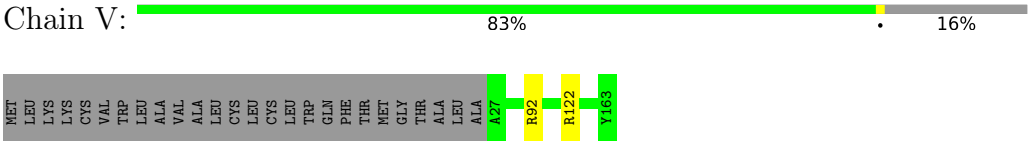
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



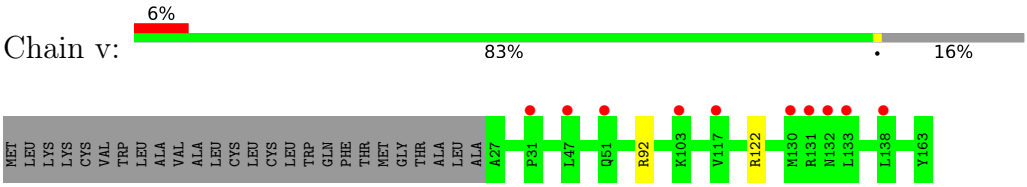
• Molecule 16: Cytochrome c-550

Chain V:



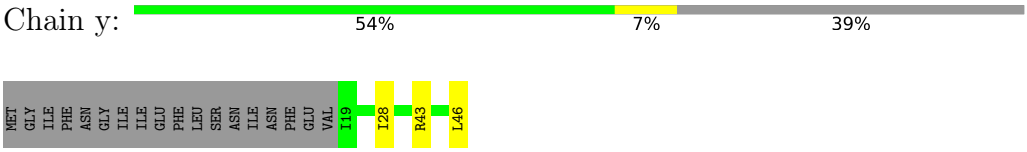
• Molecule 16: Cytochrome c-550

Chain v:



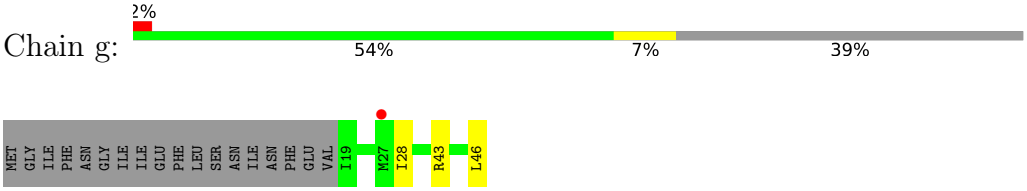
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



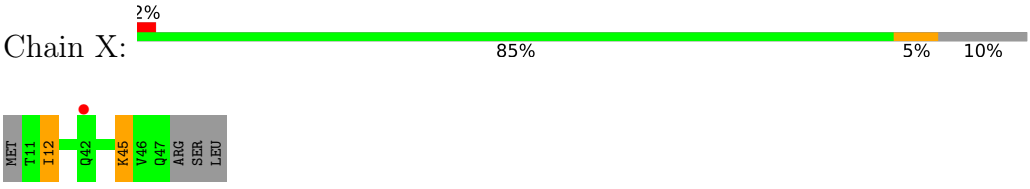
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



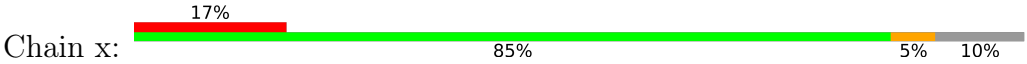
• Molecule 18: Photosystem II reaction center X protein

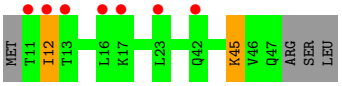
Chain X:



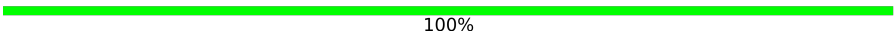
• Molecule 18: Photosystem II reaction center X protein

Chain x:



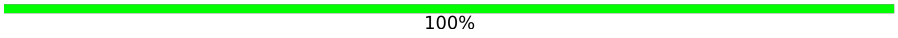


• Molecule 19: Photosystem II reaction center protein Y

Chain Y: 

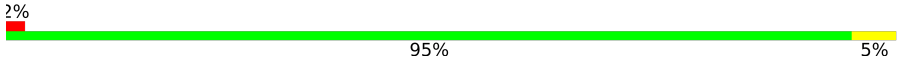
There are no outlier residues recorded for this chain.

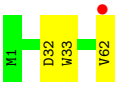
• Molecule 19: Photosystem II reaction center protein Y

Chain G: 

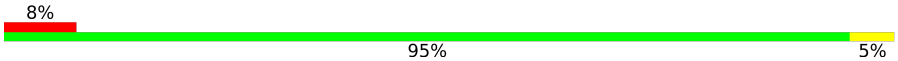
There are no outlier residues recorded for this chain.

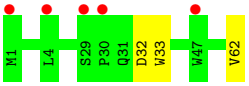
• Molecule 20: Photosystem II reaction center protein Z

Chain Z: 



• Molecule 20: Photosystem II reaction center protein Z

Chain z: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 4.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.276 , 0.284 0.277 , 0.284	Depositor DCC
R_{free} test set	2668 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	153.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 115.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å^2)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.23	0/3556	0.41	0/4842
3	c	0.23	0/3556	0.41	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.43	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.46	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.25	0/293	0.43	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.49	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.25	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.44	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.26	0/273	0.44	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.25	0/490	0.44	0/669
All	All	0.23	0/41950	0.42	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	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	19	60
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
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%)	208 (86%)	30 (12%)	3 (1%)	13	50
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	13	50
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	39
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	39
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	27
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	27
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
All	All	5138/5618 (92%)	4673 (91%)	410 (8%)	55 (1%)	14	52

All (55) 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
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
7	H	26	GLY
9	J	38	SER
13	O	52	ALA
14	T	30	THR
17	y	43	ARG
18	X	12	ILE
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
7	h	26	GLY
9	j	38	SER
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
2	b	489	GLU
4	d	239	GLN
13	o	88	GLU
1	A	142	TRP
2	B	489	GLU
3	C	32	GLY
5	E	82	GLN
1	a	334	ARG
3	c	32	GLY

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Mol	Chain	Res	Type
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
3	C	144	SER
7	H	16	SER
15	U	73	PRO
1	a	142	TRP
3	c	144	SER
7	h	16	SER
15	u	73	PRO
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY

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	271/280 (97%)	267 (98%)	4 (2%)	65 80
1	a	271/280 (97%)	267 (98%)	4 (2%)	65 80
2	B	390/407 (96%)	381 (98%)	9 (2%)	50 70
2	b	390/407 (96%)	381 (98%)	9 (2%)	50 70
3	C	347/362 (96%)	336 (97%)	11 (3%)	39 62
3	c	347/362 (96%)	336 (97%)	11 (3%)	39 62
4	D	275/283 (97%)	268 (98%)	7 (2%)	47 68
4	d	275/283 (97%)	268 (98%)	7 (2%)	47 68
5	E	72/73 (99%)	70 (97%)	2 (3%)	43 65
5	e	72/73 (99%)	70 (97%)	2 (3%)	43 65
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 40
7	h	53/55 (96%)	49 (92%)	4 (8%)	13 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	63
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	63
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	55
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	55
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	61
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	61
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	84
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	84
16	V	116/138 (84%)	114 (98%)	2 (2%)	60	78
16	v	116/138 (84%)	114 (98%)	2 (2%)	60	78
17	g	20/37 (54%)	18 (90%)	2 (10%)	7	28
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	28
18	X	30/34 (88%)	28 (93%)	2 (7%)	16	43
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	43
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	58
All	All	4244/4594 (92%)	4140 (98%)	104 (2%)	47	68

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG

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Mol	Chain	Res	Type
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
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	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG
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	92	ARG
16	V	122	ARG
17	y	28	ILE

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Mol	Chain	Res	Type
17	y	46	LEU
18	X	12	ILE
18	X	45	LYS
20	Z	33	TRP
20	Z	62	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	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
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	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	472	LEU
4	d	43	LEU
4	d	180	ARG
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL

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Mol	Chain	Res	Type
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	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	45	LYS
20	z	33	TRP
20	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	118	HIS
4	D	117	HIS
4	d	117	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
27	LMG	C	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
26	LHG	c	519	-	36,36,48	0.73	2 (5%)	39,42,54	1.26	4 (10%)
24	BCR	b	621	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
31	LMT	b	627	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
24	BCR	C	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	9 (16%)
22	CLA	c	505	-	65,73,73	1.52	5 (7%)	76,113,113	1.40	6 (7%)
22	CLA	b	619	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	7 (9%)
22	CLA	C	512	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	A	402	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
24	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	9 (16%)
27	LMG	A	410	-	51,51,55	0.74	0	59,59,63	1.36	5 (8%)
25	DGD	A	408	-	57,57,67	0.93	0	71,71,81	1.41	7 (9%)
22	CLA	a	404	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	8 (10%)
27	LMG	a	402	-	42,42,55	0.84	0	50,50,63	1.25	3 (6%)
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	59,62,65	1.74	10 (16%)
22	CLA	c	506	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	7 (9%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
24	BCR	g	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
22	CLA	b	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	8 (10%)
22	CLA	c	508	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
24	BCR	b	623	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.44	12 (15%)
30	SQD	f	103	-	44,45,54	1.04	4 (9%)	53,56,65	1.63	11 (20%)
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	53,56,65	1.64	10 (18%)
31	LMT	B	627	-	36,36,36	1.13	5 (13%)	47,47,47	0.95	1 (2%)
22	CLA	a	408	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	6 (7%)
22	CLA	C	504	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	7 (9%)
29	OEX	A	412	3,1	0,15,15	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	PL9	A	406	-	45,45,55	0.98	4 (8%)	56,57,69	1.56	10 (17%)
22	CLA	a	406	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
22	CLA	c	509	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	8 (10%)
25	DGD	c	516	-	63,63,67	0.92	1 (1%)	77,77,81	1.45	12 (15%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	8 (10%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.28	6 (8%)
30	SQD	D	403	-	42,43,54	1.04	3 (7%)	51,54,65	1.78	10 (19%)
25	DGD	D	409	-	64,64,67	0.91	0	78,78,81	1.33	9 (11%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.27	6 (11%)
22	CLA	b	618	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
25	DGD	b	601	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
24	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
27	LMG	d	407	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
22	CLA	b	614	-	65,73,73	1.55	6 (9%)	76,113,113	1.39	6 (7%)
25	DGD	b	624	-	59,59,67	0.91	1 (1%)	73,73,81	1.33	6 (8%)
24	BCR	a	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	7 (12%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.30	4 (7%)
24	BCR	C	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	9 (16%)
22	CLA	c	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
27	LMG	b	628	-	49,49,55	0.76	0	57,57,63	1.31	4 (7%)
32	PHO	D	402	-	51,69,69	1.01	3 (5%)	47,99,99	1.10	4 (8%)
32	PHO	D	401	-	51,69,69	1.01	4 (7%)	47,99,99	1.11	5 (10%)
22	CLA	c	520	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	C	505	-	65,73,73	1.52	5 (7%)	76,113,113	1.40	7 (9%)
27	LMG	B	624	-	49,49,55	0.76	0	57,57,63	1.32	5 (8%)
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
22	CLA	B	614	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
24	BCR	y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
30	SQD	d	402	-	42,43,54	1.05	3 (7%)	51,54,65	1.79	10 (19%)
31	LMT	I	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	D	405	-	65,73,73	1.51	5 (7%)	76,113,113	1.32	7 (9%)
23	PL9	d	406	-	55,55,55	1.02	2 (3%)	68,69,69	1.53	14 (20%)
31	LMT	d	409	-	32,32,36	1.18	5 (15%)	43,43,47	0.98	2 (4%)
22	CLA	C	510	3	65,73,73	1.50	5 (7%)	76,113,113	1.43	7 (9%)
22	CLA	b	617	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LMT	b	626	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
24	BCR	f	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	5 (8%)
22	CLA	B	602	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	C	506	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	7 (9%)
22	CLA	A	403	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
22	CLA	c	503	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	B	611	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
26	LHG	a	412	-	38,38,48	0.68	1 (2%)	41,44,54	1.19	3 (7%)
27	LMG	M	101	-	42,42,55	0.86	0	50,50,63	1.24	4 (8%)
27	LMG	d	410	-	46,46,55	0.80	1 (2%)	54,54,63	1.31	4 (7%)
22	CLA	b	613	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
22	CLA	d	405	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	8 (10%)
22	CLA	C	507	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	8 (10%)
24	BCR	D	411	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	7 (12%)
22	CLA	B	601	-	65,73,73	1.53	5 (7%)	76,113,113	1.37	7 (9%)
22	CLA	A	404	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.35	10 (17%)
22	CLA	B	615	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	7 (9%)
27	LMG	b	625	-	49,49,55	0.78	1 (2%)	57,57,63	1.31	6 (10%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
30	SQD	A	414	-	53,54,54	0.96	5 (9%)	62,65,65	1.57	9 (14%)
31	LMT	B	622	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
31	LMT	B	628	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	1 (2%)
24	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.58	12 (21%)
22	CLA	C	509	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
30	SQD	b	602	-	46,47,54	1.02	4 (8%)	55,58,65	1.79	10 (18%)
31	LMT	M	102	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	b	610	-	65,73,73	1.51	5 (7%)	76,113,113	1.35	8 (10%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.30	5 (9%)
33	BCT	D	404	21	2,3,3	1.24	0	2,3,3	4.17	1 (50%)
31	LMT	B	623	-	36,36,36	1.10	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	b	615	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
31	LMT	b	603	-	36,36,36	1.13	5 (13%)	47,47,47	0.94	1 (2%)
22	CLA	b	607	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	9 (11%)
30	SQD	A	413	-	50,51,54	0.97	4 (8%)	59,62,65	1.72	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	607	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	7 (9%)
22	CLA	B	606	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	9 (11%)
24	BCR	H	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	3 (5%)
26	LHG	A	409	-	38,38,48	0.69	0	41,44,54	1.18	3 (7%)
22	CLA	B	610	-	65,73,73	1.54	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	c	511	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)
22	CLA	b	612	-	65,73,73	1.52	5 (7%)	76,113,113	1.31	7 (9%)
27	LMG	D	412	-	46,46,55	0.79	1 (2%)	54,54,63	1.31	4 (7%)
22	CLA	C	520	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
22	CLA	d	404	-	65,73,73	1.52	5 (7%)	76,113,113	1.34	7 (9%)
22	CLA	a	405	-	65,73,73	1.51	5 (7%)	76,113,113	1.42	8 (10%)
27	LMG	C	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
24	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)
23	PL9	D	407	-	55,55,55	1.03	3 (5%)	68,69,69	1.52	13 (19%)
22	CLA	B	604	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	7 (9%)
26	LHG	C	519	-	36,36,48	0.71	0	39,42,54	1.25	4 (10%)
23	PL9	a	409	-	45,45,55	1.02	3 (6%)	56,57,69	1.55	10 (17%)
22	CLA	h	101	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	6 (7%)
25	DGD	d	408	-	64,64,67	0.92	2 (3%)	78,78,81	1.34	9 (11%)
22	CLA	c	512	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	8 (10%)
25	DGD	C	517	-	67,67,67	0.88	1 (1%)	81,81,81	1.41	10 (12%)
34	HEM	V	201	16	41,50,50	2.03	8 (19%)	45,82,82	1.56	4 (8%)
22	CLA	D	406	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	C	503	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	6 (7%)
22	CLA	B	612	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
22	CLA	b	611	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
22	CLA	b	605	-	65,73,73	1.53	5 (7%)	76,113,113	1.37	6 (7%)
25	DGD	c	517	-	67,67,67	0.88	0	81,81,81	1.40	10 (12%)
34	HEM	v	201	16	41,50,50	2.03	9 (21%)	45,82,82	1.59	4 (8%)
22	CLA	B	603	-	65,73,73	1.49	6 (9%)	76,113,113	1.43	9 (11%)
23	PL9	J	101	-	35,35,55	1.02	1 (2%)	44,45,69	1.56	7 (15%)
27	LMG	a	413	-	51,51,55	0.74	1 (1%)	59,59,63	1.34	7 (11%)
22	CLA	C	511	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
24	BCR	c	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
23	PL9	j	101	-	35,35,55	1.00	1 (2%)	44,45,69	1.56	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	BCT	d	403	21	2,3,3	1.24	0	2,3,3	4.15	1 (50%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
22	CLA	b	608	-	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
22	CLA	C	508	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
24	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
32	PHO	d	401	-	51,69,69	1.01	4 (7%)	47,99,99	1.12	5 (10%)
31	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.02	1 (2%)
22	CLA	c	507	-	65,73,73	1.50	5 (7%)	76,113,113	1.43	9 (11%)
24	BCR	x	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	2 (3%)
24	BCR	b	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	B	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.36	6 (7%)
22	CLA	B	608	-	65,73,73	1.52	5 (7%)	76,113,113	1.33	7 (9%)
30	SQD	a	401	-	53,54,54	0.96	4 (7%)	62,65,65	1.56	9 (14%)
22	CLA	C	502	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
31	LMT	i	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.98	2 (4%)
31	LMT	D	410	-	32,32,36	1.18	5 (15%)	43,43,47	1.00	2 (4%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.26	4 (7%)
22	CLA	c	504	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	7 (9%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	8 (14%)
31	LMT	M	103	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	2 (4%)
22	CLA	A	405	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	6 (7%)
24	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	6 (10%)
22	CLA	B	609	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	7 (9%)
30	SQD	B	626	-	46,47,54	1.02	4 (8%)	55,58,65	1.77	10 (18%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
25	DGD	a	411	-	57,57,67	0.94	1 (1%)	71,71,81	1.39	7 (9%)
34	HEM	f	101	5,6	41,50,50	1.96	6 (14%)	45,82,82	1.70	6 (13%)
25	DGD	C	515	-	54,54,67	0.98	2 (3%)	68,68,81	1.27	6 (8%)
27	LMG	m	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
22	CLA	H	101	-	65,73,73	1.51	5 (7%)	76,113,113	1.34	7 (9%)
22	CLA	c	502	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
24	BCR	B	616	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	8 (14%)
27	LMG	A	415	-	42,42,55	0.83	0	50,50,63	1.25	4 (8%)
32	PHO	a	407	-	51,69,69	1.01	3 (5%)	47,99,99	1.09	4 (8%)
22	CLA	b	616	-	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	606	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
34	HEM	F	101	5,6	41,50,50	1.97	6 (14%)	45,82,82	1.69	6 (13%)
24	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.57	12 (21%)
22	CLA	C	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
22	CLA	B	605	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
22	CLA	c	510	3	65,73,73	1.51	5 (7%)	76,113,113	1.41	7 (9%)
29	OEX	a	414	3,1	0,15,15	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
27	LMG	C	522	-	-	20/43/63/70	0/1/1/1
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	b	621	-	-	9/29/63/63	0/2/2/2
31	LMT	b	627	-	-	2/21/61/61	0/2/2/2
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	c	505	-	1/1/15/20	17/37/115/115	-
22	CLA	b	619	-	1/1/15/20	19/37/115/115	-
22	CLA	C	512	-	1/1/15/20	17/37/115/115	-
22	CLA	A	402	-	1/1/15/20	8/37/115/115	-
24	BCR	b	622	-	-	3/29/63/63	0/2/2/2
27	LMG	A	410	-	-	26/46/66/70	0/1/1/1
25	DGD	A	408	-	-	15/45/85/95	0/2/2/2
22	CLA	a	404	-	1/1/15/20	8/37/115/115	-
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
22	CLA	c	506	-	1/1/15/20	13/37/115/115	-
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
24	BCR	g	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	609	-	1/1/15/20	15/37/115/115	-
22	CLA	c	508	-	1/1/15/20	15/37/115/115	-
24	BCR	b	623	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	C	516	-	-	20/51/91/95	0/2/2/2
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
30	SQD	F	102	-	-	10/40/60/69	0/1/1/1
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
22	CLA	a	408	-	1/1/15/20	8/37/115/115	-
22	CLA	C	504	-	1/1/15/20	19/37/115/115	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
22	CLA	a	406	-	1/1/15/20	9/37/115/115	-
22	CLA	c	509	-	1/1/15/20	16/37/115/115	-
25	DGD	c	516	-	-	20/51/91/95	0/2/2/2
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
25	DGD	c	515	-	-	20/42/82/95	0/2/2/2
30	SQD	D	403	-	-	13/38/58/69	0/1/1/1
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
22	CLA	b	618	-	1/1/15/20	9/37/115/115	-
25	DGD	b	601	-	-	18/41/81/95	0/2/2/2
24	BCR	B	617	-	-	9/29/63/63	0/2/2/2
27	LMG	d	407	-	-	20/43/63/70	0/1/1/1
22	CLA	b	614	-	1/1/15/20	9/37/115/115	-
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
27	LMG	E	101	-	-	18/39/59/70	0/1/1/1
24	BCR	C	521	-	-	6/29/63/63	0/2/2/2
22	CLA	c	501	-	1/1/15/20	13/37/115/115	-
27	LMG	b	628	-	-	24/44/64/70	0/1/1/1
32	PHO	D	402	-	-	12/37/103/103	0/5/6/6
32	PHO	D	401	-	-	12/37/103/103	0/5/6/6
22	CLA	c	520	-	1/1/15/20	10/37/115/115	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
27	LMG	B	624	-	-	24/44/64/70	0/1/1/1
27	LMG	c	518	-	-	21/40/60/70	0/1/1/1
22	CLA	B	614	-	1/1/15/20	10/37/115/115	-
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	d	402	-	-	13/38/58/69	0/1/1/1
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
22	CLA	D	405	-	1/1/15/20	14/37/115/115	-
23	PL9	d	406	-	-	11/53/73/73	0/1/1/1
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
22	CLA	C	510	3	1/1/15/20	15/37/115/115	-
22	CLA	b	617	-	1/1/15/20	15/37/115/115	-
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
24	BCR	f	102	-	-	7/29/63/63	0/2/2/2
22	CLA	B	602	-	1/1/15/20	15/37/115/115	-
22	CLA	C	506	-	1/1/15/20	13/37/115/115	-
22	CLA	A	403	-	1/1/15/20	14/37/115/115	-
22	CLA	c	503	-	1/1/15/20	14/37/115/115	-
22	CLA	B	611	-	1/1/15/20	13/37/115/115	-
26	LHG	a	412	-	-	12/43/43/53	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
27	LMG	d	410	-	-	15/41/61/70	0/1/1/1
22	CLA	b	613	-	1/1/15/20	18/37/115/115	-
22	CLA	d	405	-	1/1/15/20	6/37/115/115	-
22	CLA	C	507	-	1/1/15/20	15/37/115/115	-
24	BCR	D	411	-	-	6/29/63/63	0/2/2/2
22	CLA	B	601	-	1/1/15/20	16/37/115/115	-
22	CLA	A	404	-	1/1/15/20	10/37/115/115	-
24	BCR	c	513	-	-	6/29/63/63	0/2/2/2
22	CLA	B	615	-	1/1/15/20	18/37/115/115	-
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
30	SQD	A	414	-	-	11/49/69/69	0/1/1/1
31	LMT	B	622	-	-	3/21/61/61	0/2/2/2
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
22	CLA	C	509	-	1/1/15/20	16/37/115/115	-
30	SQD	b	602	-	-	15/42/62/69	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	610	-	1/1/15/20	9/37/115/115	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
31	LMT	B	623	-	-	4/21/61/61	0/2/2/2
22	CLA	b	615	-	1/1/15/20	13/37/115/115	-
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
22	CLA	b	607	-	1/1/15/20	7/37/115/115	-
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
22	CLA	B	607	-	1/1/15/20	12/37/115/115	-
22	CLA	B	606	-	1/1/15/20	9/37/115/115	-
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
26	LHG	A	409	-	-	14/43/43/53	-
22	CLA	B	610	-	1/1/15/20	10/37/115/115	-
22	CLA	c	511	-	1/1/15/20	19/37/115/115	-
22	CLA	b	612	-	1/1/15/20	11/37/115/115	-
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1
22	CLA	C	520	-	1/1/15/20	12/37/115/115	-
22	CLA	d	404	-	1/1/15/20	12/37/115/115	-
22	CLA	a	405	-	1/1/15/20	14/37/115/115	-
27	LMG	C	518	-	-	21/40/60/70	0/1/1/1
24	BCR	c	521	-	-	6/29/63/63	0/2/2/2
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
22	CLA	B	604	-	1/1/15/20	14/37/115/115	-
26	LHG	C	519	-	-	16/41/41/53	-
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
22	CLA	h	101	-	1/1/15/20	19/37/115/115	-
25	DGD	d	408	-	-	35/52/92/95	0/2/2/2
22	CLA	c	512	-	1/1/15/20	21/37/115/115	-
25	DGD	C	517	-	-	22/55/95/95	0/2/2/2
34	HEM	V	201	16	-	4/12/54/54	-
22	CLA	D	406	-	-	6/37/115/115	-
22	CLA	C	503	-	1/1/15/20	15/37/115/115	-
22	CLA	B	612	-	1/1/15/20	15/37/115/115	-
22	CLA	b	611	-	1/1/15/20	12/37/115/115	-
22	CLA	b	605	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	c	517	-	-	21/55/95/95	0/2/2/2
34	HEM	v	201	16	-	4/12/54/54	-
22	CLA	B	603	-	1/1/15/20	7/37/115/115	-
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
27	LMG	a	413	-	-	25/46/66/70	0/1/1/1
22	CLA	C	511	-	1/1/15/20	19/37/115/115	-
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/15/20	15/37/115/115	-
22	CLA	C	508	-	1/1/15/20	16/37/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
32	PHO	d	401	-	-	11/37/103/103	0/5/6/6
31	LMT	b	604	-	-	4/21/61/61	0/2/2/2
22	CLA	c	507	-	1/1/15/20	14/37/115/115	-
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
22	CLA	B	613	-	1/1/15/20	16/37/115/115	-
22	CLA	B	608	-	1/1/15/20	11/37/115/115	-
30	SQD	a	401	-	-	13/49/69/69	0/1/1/1
22	CLA	C	502	-	1/1/15/20	9/37/115/115	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
27	LMG	I	101	-	-	17/38/58/70	0/1/1/1
22	CLA	c	504	-	1/1/15/20	19/37/115/115	-
24	BCR	B	618	-	-	3/29/63/63	0/2/2/2
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	A	405	-	1/1/15/20	8/37/115/115	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
22	CLA	B	609	-	1/1/15/20	18/37/115/115	-
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
27	LMG	B	621	-	-	16/44/64/70	0/1/1/1
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
34	HEM	f	101	5,6	-	2/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
22	CLA	H	101	-	1/1/15/20	19/37/115/115	-
22	CLA	c	502	-	1/1/15/20	11/37/115/115	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
32	PHO	a	407	-	-	12/37/103/103	0/5/6/6
22	CLA	b	616	-	1/1/15/20	15/37/115/115	-
22	CLA	b	606	-	1/1/15/20	13/37/115/115	-
34	HEM	F	101	5,6	-	2/12/54/54	-
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
22	CLA	C	501	-	1/1/15/20	15/37/115/115	-
22	CLA	B	605	-	1/1/15/20	12/37/115/115	-
22	CLA	c	510	3	1/1/15/20	17/37/115/115	-

All (615) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3D-C2D	8.30	1.54	1.36
34	V	201	HEM	C3D-C2D	8.29	1.54	1.36
34	F	101	HEM	C3D-C2D	8.05	1.53	1.36
34	f	101	HEM	C3D-C2D	7.98	1.53	1.36
22	A	402	CLA	C4B-NB	7.79	1.42	1.35
22	B	601	CLA	C4B-NB	7.74	1.42	1.35
22	a	404	CLA	C4B-NB	7.74	1.42	1.35
22	b	605	CLA	C4B-NB	7.74	1.42	1.35
22	c	508	CLA	C4B-NB	7.72	1.42	1.35
22	c	509	CLA	C4B-NB	7.70	1.42	1.35
22	C	509	CLA	C4B-NB	7.69	1.42	1.35
22	b	614	CLA	C4B-NB	7.69	1.42	1.35
22	b	619	CLA	C4B-NB	7.68	1.42	1.35
22	C	508	CLA	C4B-NB	7.68	1.42	1.35
22	C	505	CLA	C4B-NB	7.65	1.42	1.35
22	c	511	CLA	C4B-NB	7.65	1.42	1.35
22	B	610	CLA	C4B-NB	7.63	1.42	1.35
22	a	405	CLA	C4B-NB	7.62	1.42	1.35
22	B	615	CLA	C4B-NB	7.62	1.42	1.35
22	c	505	CLA	C4B-NB	7.62	1.42	1.35
22	c	520	CLA	C4B-NB	7.61	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	C4B-NB	7.60	1.42	1.35
22	c	512	CLA	C4B-NB	7.60	1.42	1.35
22	b	612	CLA	C4B-NB	7.60	1.42	1.35
22	d	405	CLA	C4B-NB	7.60	1.42	1.35
22	d	404	CLA	C4B-NB	7.60	1.42	1.35
22	b	610	CLA	C4B-NB	7.59	1.42	1.35
22	C	507	CLA	C4B-NB	7.59	1.42	1.35
22	B	606	CLA	C4B-NB	7.57	1.42	1.35
22	b	618	CLA	C4B-NB	7.57	1.42	1.35
22	D	406	CLA	C4B-NB	7.56	1.42	1.35
22	B	608	CLA	C4B-NB	7.56	1.42	1.35
22	C	512	CLA	C4B-NB	7.56	1.42	1.35
22	c	503	CLA	C4B-NB	7.56	1.42	1.35
22	H	101	CLA	C4B-NB	7.55	1.41	1.35
22	c	507	CLA	C4B-NB	7.54	1.41	1.35
22	B	604	CLA	C4B-NB	7.54	1.41	1.35
22	C	511	CLA	C4B-NB	7.53	1.41	1.35
22	B	614	CLA	C4B-NB	7.53	1.41	1.35
22	C	510	CLA	C4B-NB	7.53	1.41	1.35
22	c	510	CLA	C4B-NB	7.53	1.41	1.35
22	A	403	CLA	C4B-NB	7.53	1.41	1.35
22	a	408	CLA	C4B-NB	7.52	1.41	1.35
22	B	607	CLA	C4B-NB	7.50	1.41	1.35
22	C	503	CLA	C4B-NB	7.49	1.41	1.35
22	a	406	CLA	C4B-NB	7.49	1.41	1.35
22	b	608	CLA	C4B-NB	7.48	1.41	1.35
22	h	101	CLA	C4B-NB	7.48	1.41	1.35
22	B	609	CLA	C4B-NB	7.48	1.41	1.35
22	b	615	CLA	C4B-NB	7.47	1.41	1.35
22	A	405	CLA	C4B-NB	7.47	1.41	1.35
22	D	405	CLA	C4B-NB	7.47	1.41	1.35
22	b	611	CLA	C4B-NB	7.45	1.41	1.35
22	b	613	CLA	C4B-NB	7.45	1.41	1.35
22	C	520	CLA	C4B-NB	7.45	1.41	1.35
22	b	617	CLA	C4B-NB	7.43	1.41	1.35
22	C	501	CLA	C4B-NB	7.43	1.41	1.35
22	b	616	CLA	C4B-NB	7.42	1.41	1.35
22	B	611	CLA	C4B-NB	7.41	1.41	1.35
22	C	502	CLA	C4B-NB	7.41	1.41	1.35
22	b	609	CLA	C4B-NB	7.41	1.41	1.35
22	B	605	CLA	C4B-NB	7.40	1.41	1.35
22	C	504	CLA	C4B-NB	7.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	501	CLA	C4B-NB	7.39	1.41	1.35
22	B	612	CLA	C4B-NB	7.39	1.41	1.35
22	b	607	CLA	C4B-NB	7.38	1.41	1.35
22	c	506	CLA	C4B-NB	7.38	1.41	1.35
22	c	502	CLA	C4B-NB	7.37	1.41	1.35
22	C	506	CLA	C4B-NB	7.37	1.41	1.35
22	A	404	CLA	C4B-NB	7.36	1.41	1.35
22	B	613	CLA	C4B-NB	7.34	1.41	1.35
22	B	602	CLA	C4B-NB	7.33	1.41	1.35
22	B	603	CLA	C4B-NB	7.33	1.41	1.35
22	b	606	CLA	C4B-NB	7.30	1.41	1.35
34	v	201	HEM	C3C-C2C	-4.58	1.34	1.40
34	V	201	HEM	C3C-C2C	-4.54	1.34	1.40
22	h	101	CLA	C1D-ND	4.10	1.42	1.37
22	b	605	CLA	C1D-ND	4.09	1.42	1.37
22	c	510	CLA	C1D-ND	4.08	1.42	1.37
22	B	601	CLA	C1D-ND	4.08	1.42	1.37
22	c	503	CLA	C1D-ND	4.08	1.42	1.37
22	C	501	CLA	C1D-ND	4.07	1.42	1.37
22	d	405	CLA	C1D-ND	4.06	1.42	1.37
22	C	512	CLA	C1D-ND	4.04	1.42	1.37
22	d	404	CLA	C1D-ND	4.03	1.42	1.37
22	B	608	CLA	C1D-ND	4.03	1.42	1.37
22	D	405	CLA	C1D-ND	4.03	1.42	1.37
22	c	505	CLA	C1D-ND	4.02	1.42	1.37
22	C	510	CLA	C1D-ND	4.02	1.42	1.37
22	b	608	CLA	C1D-ND	4.02	1.42	1.37
22	H	101	CLA	C1D-ND	4.02	1.42	1.37
22	c	501	CLA	C1D-ND	4.01	1.42	1.37
22	C	505	CLA	C1D-ND	4.01	1.42	1.37
22	b	612	CLA	C1D-ND	4.01	1.42	1.37
22	c	512	CLA	C1D-ND	4.01	1.42	1.37
22	D	406	CLA	C1D-ND	4.00	1.42	1.37
22	b	618	CLA	C1D-ND	4.00	1.42	1.37
22	C	503	CLA	C1D-ND	3.99	1.42	1.37
22	A	403	CLA	C1D-ND	3.98	1.42	1.37
22	B	604	CLA	C1D-ND	3.98	1.42	1.37
22	a	405	CLA	C1D-ND	3.98	1.42	1.37
22	A	405	CLA	C1D-ND	3.98	1.42	1.37
22	C	506	CLA	C1D-ND	3.98	1.42	1.37
22	b	613	CLA	C1D-ND	3.97	1.42	1.37
22	a	408	CLA	C1D-ND	3.97	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	C1D-ND	3.96	1.42	1.37
22	b	609	CLA	C1D-ND	3.96	1.42	1.37
22	c	508	CLA	C1D-ND	3.96	1.42	1.37
22	c	506	CLA	C1D-ND	3.95	1.42	1.37
22	c	502	CLA	C1D-ND	3.94	1.42	1.37
22	b	606	CLA	C1D-ND	3.94	1.42	1.37
22	C	502	CLA	C1D-ND	3.93	1.42	1.37
22	B	614	CLA	C1D-ND	3.93	1.42	1.37
22	C	511	CLA	C1D-ND	3.93	1.42	1.37
22	a	406	CLA	C1D-ND	3.93	1.42	1.37
22	B	613	CLA	C1D-ND	3.92	1.42	1.37
22	B	603	CLA	C1D-ND	3.92	1.42	1.37
22	B	606	CLA	C1D-ND	3.91	1.42	1.37
22	c	504	CLA	C1D-ND	3.91	1.42	1.37
22	B	605	CLA	C1D-ND	3.91	1.42	1.37
22	b	607	CLA	C1D-ND	3.90	1.42	1.37
22	c	520	CLA	C1D-ND	3.90	1.42	1.37
22	C	520	CLA	C1D-ND	3.90	1.42	1.37
22	C	504	CLA	C1D-ND	3.90	1.42	1.37
22	B	612	CLA	C1D-ND	3.90	1.42	1.37
22	b	611	CLA	C1D-ND	3.89	1.42	1.37
22	B	602	CLA	C1D-ND	3.88	1.42	1.37
22	c	511	CLA	C1D-ND	3.87	1.42	1.37
22	b	610	CLA	C1D-ND	3.87	1.42	1.37
22	B	607	CLA	C1D-ND	3.86	1.42	1.37
22	c	507	CLA	C1D-ND	3.86	1.42	1.37
34	f	101	HEM	C3C-CAC	3.85	1.55	1.47
22	A	404	CLA	C1D-ND	3.85	1.42	1.37
22	b	617	CLA	C1D-ND	3.85	1.42	1.37
22	B	609	CLA	C1D-ND	3.85	1.42	1.37
22	B	615	CLA	C1D-ND	3.85	1.42	1.37
22	a	404	CLA	C1D-ND	3.83	1.42	1.37
22	b	619	CLA	C1D-ND	3.82	1.42	1.37
22	C	507	CLA	C1D-ND	3.82	1.42	1.37
34	F	101	HEM	C3C-CAC	3.79	1.55	1.47
22	C	508	CLA	C1D-ND	3.78	1.42	1.37
22	A	402	CLA	C1D-ND	3.78	1.42	1.37
22	B	610	CLA	C1D-ND	3.76	1.42	1.37
22	c	509	CLA	C1D-ND	3.76	1.42	1.37
22	C	509	CLA	C1D-ND	3.76	1.42	1.37
34	V	201	HEM	C3C-CAC	3.75	1.55	1.47
34	F	101	HEM	C3C-C2C	-3.74	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3C-CAC	3.72	1.55	1.47
22	b	614	CLA	C1D-ND	3.71	1.42	1.37
34	f	101	HEM	C3C-C2C	-3.68	1.35	1.40
23	d	406	PL9	C7-C3	-3.66	1.47	1.51
24	H	102	BCR	C1-C6	-3.61	1.48	1.53
24	y	101	BCR	C1-C6	-3.60	1.48	1.53
24	D	411	BCR	C1-C6	-3.55	1.48	1.53
22	b	615	CLA	C1D-ND	3.52	1.42	1.37
24	g	101	BCR	C1-C6	-3.52	1.48	1.53
24	f	102	BCR	C1-C6	-3.51	1.48	1.53
24	x	101	BCR	C1-C6	-3.49	1.49	1.53
22	B	611	CLA	C1D-ND	3.49	1.42	1.37
22	b	614	CLA	CMB-C2B	-3.48	1.44	1.51
23	D	407	PL9	C7-C3	-3.41	1.47	1.51
22	B	610	CLA	CMB-C2B	-3.40	1.44	1.51
24	C	513	BCR	C1-C6	-3.36	1.49	1.53
23	J	101	PL9	C7-C3	-3.33	1.47	1.51
24	B	616	BCR	C1-C6	-3.33	1.49	1.53
24	b	620	BCR	C1-C6	-3.33	1.49	1.53
24	C	514	BCR	C1-C6	-3.29	1.49	1.53
24	c	513	BCR	C1-C6	-3.28	1.49	1.53
24	c	514	BCR	C1-C6	-3.27	1.49	1.53
22	B	613	CLA	CHC-C1C	3.27	1.43	1.35
22	h	101	CLA	CHC-C1C	3.25	1.43	1.35
23	a	409	PL9	C7-C3	-3.25	1.48	1.51
22	B	608	CLA	CHC-C1C	3.24	1.43	1.35
22	b	612	CLA	CHC-C1C	3.22	1.43	1.35
22	H	101	CLA	CHC-C1C	3.22	1.43	1.35
24	b	622	BCR	C30-C25	-3.22	1.49	1.53
23	j	101	PL9	C7-C3	-3.22	1.48	1.51
22	B	607	CLA	CHC-C1C	3.20	1.43	1.35
22	b	611	CLA	CHC-C1C	3.20	1.43	1.35
22	a	404	CLA	CHC-C1C	3.20	1.43	1.35
22	c	502	CLA	CHC-C1C	3.20	1.43	1.35
22	d	405	CLA	CHC-C1C	3.20	1.43	1.35
22	C	512	CLA	CHC-C1C	3.19	1.43	1.35
22	D	405	CLA	CHC-C1C	3.19	1.43	1.35
22	b	606	CLA	CHC-C1C	3.19	1.43	1.35
22	c	512	CLA	CHC-C1C	3.19	1.43	1.35
22	c	507	CLA	CHC-C1C	3.18	1.43	1.35
24	y	101	BCR	C30-C25	-3.18	1.49	1.53
22	d	404	CLA	CHC-C1C	3.18	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	617	CLA	CHC-C1C	3.17	1.43	1.35
30	A	414	SQD	O48-C23	3.17	1.42	1.33
30	a	401	SQD	O48-C23	3.17	1.42	1.33
22	c	511	CLA	CHC-C1C	3.17	1.43	1.35
22	C	509	CLA	CHC-C1C	3.17	1.43	1.35
22	C	505	CLA	CHC-C1C	3.17	1.43	1.35
22	c	509	CLA	CHC-C1C	3.17	1.43	1.35
30	d	402	SQD	O48-C23	3.17	1.42	1.33
22	C	504	CLA	CHC-C1C	3.16	1.43	1.35
22	b	616	CLA	CHC-C1C	3.16	1.43	1.35
22	C	511	CLA	CHC-C1C	3.16	1.43	1.35
24	b	621	BCR	C1-C6	-3.15	1.49	1.53
22	B	609	CLA	CHC-C1C	3.15	1.43	1.35
22	c	505	CLA	CHC-C1C	3.15	1.43	1.35
22	B	602	CLA	CHC-C1C	3.15	1.43	1.35
22	a	406	CLA	CHC-C1C	3.15	1.43	1.35
22	C	510	CLA	CHC-C1C	3.15	1.43	1.35
24	g	101	BCR	C30-C25	-3.15	1.49	1.53
22	B	614	CLA	CHC-C1C	3.15	1.43	1.35
30	b	602	SQD	O48-C23	3.15	1.42	1.33
22	A	402	CLA	CHC-C1C	3.14	1.43	1.35
22	b	618	CLA	CHC-C1C	3.14	1.43	1.35
22	C	508	CLA	CHC-C1C	3.14	1.43	1.35
22	a	408	CLA	CHC-C1C	3.14	1.43	1.35
22	c	510	CLA	CHC-C1C	3.14	1.43	1.35
22	B	605	CLA	CHC-C1C	3.14	1.43	1.35
22	C	506	CLA	CHC-C1C	3.14	1.43	1.35
22	c	504	CLA	CHC-C1C	3.14	1.43	1.35
22	b	613	CLA	CHC-C1C	3.14	1.43	1.35
22	B	604	CLA	CHC-C1C	3.14	1.43	1.35
22	C	502	CLA	CHC-C1C	3.13	1.43	1.35
22	b	607	CLA	CHC-C1C	3.13	1.43	1.35
22	b	608	CLA	CHC-C1C	3.13	1.43	1.35
30	f	103	SQD	O48-C23	3.13	1.42	1.33
24	B	618	BCR	C30-C25	-3.13	1.49	1.53
22	A	404	CLA	CHC-C1C	3.13	1.43	1.35
30	B	626	SQD	O48-C23	3.13	1.42	1.33
22	B	603	CLA	CHC-C1C	3.13	1.43	1.35
22	B	612	CLA	CHC-C1C	3.13	1.43	1.35
22	c	503	CLA	CHC-C1C	3.13	1.43	1.35
22	c	508	CLA	CHC-C1C	3.12	1.43	1.35
30	a	415	SQD	O48-C23	3.12	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	619	BCR	C30-C25	-3.12	1.49	1.53
30	D	403	SQD	O48-C23	3.12	1.42	1.33
22	D	406	CLA	CHC-C1C	3.11	1.42	1.35
22	B	606	CLA	CHC-C1C	3.11	1.42	1.35
22	c	520	CLA	CHC-C1C	3.11	1.42	1.35
22	A	403	CLA	CHC-C1C	3.11	1.42	1.35
22	B	601	CLA	CHC-C1C	3.11	1.42	1.35
30	F	102	SQD	O48-C23	3.10	1.42	1.33
22	C	520	CLA	CHC-C1C	3.10	1.42	1.35
24	C	521	BCR	C30-C25	-3.10	1.49	1.53
22	C	507	CLA	CHC-C1C	3.10	1.42	1.35
24	b	623	BCR	C30-C25	-3.10	1.49	1.53
22	b	609	CLA	CHC-C1C	3.10	1.42	1.35
24	a	410	BCR	C1-C6	-3.10	1.49	1.53
22	C	501	CLA	CHC-C1C	3.10	1.42	1.35
30	A	413	SQD	O48-C23	3.10	1.42	1.33
24	b	620	BCR	C30-C25	-3.10	1.49	1.53
22	b	619	CLA	CHC-C1C	3.10	1.42	1.35
22	C	503	CLA	CHC-C1C	3.09	1.42	1.35
22	c	506	CLA	CHC-C1C	3.09	1.42	1.35
24	B	617	BCR	C1-C6	-3.09	1.49	1.53
22	b	610	CLA	CHC-C1C	3.09	1.42	1.35
22	B	615	CLA	CHC-C1C	3.08	1.42	1.35
22	b	615	CLA	CHC-C1C	3.08	1.42	1.35
24	c	521	BCR	C30-C25	-3.08	1.49	1.53
24	a	410	BCR	C30-C25	-3.07	1.49	1.53
22	b	605	CLA	CHC-C1C	3.07	1.42	1.35
24	A	407	BCR	C30-C25	-3.07	1.49	1.53
24	B	616	BCR	C30-C25	-3.07	1.49	1.53
24	b	623	BCR	C1-C6	-3.06	1.49	1.53
24	D	411	BCR	C30-C25	-3.06	1.49	1.53
22	c	501	CLA	CHC-C1C	3.05	1.42	1.35
22	B	611	CLA	CHC-C1C	3.05	1.42	1.35
22	a	405	CLA	CHC-C1C	3.05	1.42	1.35
22	A	405	CLA	CHC-C1C	3.05	1.42	1.35
24	B	618	BCR	C1-C6	-3.04	1.49	1.53
24	f	102	BCR	C30-C25	-3.04	1.49	1.53
24	B	619	BCR	C1-C6	-3.03	1.49	1.53
24	b	622	BCR	C1-C6	-3.03	1.49	1.53
34	V	201	HEM	CAB-C3B	3.03	1.55	1.47
24	A	407	BCR	C1-C6	-3.03	1.49	1.53
34	v	201	HEM	CAB-C3B	3.01	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	J	102	BCR	C30-C25	-3.00	1.49	1.53
24	j	102	BCR	C30-C25	-2.99	1.49	1.53
24	x	101	BCR	C30-C25	-2.98	1.49	1.53
23	A	406	PL9	C7-C3	-2.98	1.48	1.51
24	C	513	BCR	C30-C25	-2.97	1.49	1.53
22	B	615	CLA	C4D-ND	-2.96	1.33	1.37
24	j	102	BCR	C1-C6	-2.96	1.49	1.53
24	J	102	BCR	C1-C6	-2.95	1.49	1.53
34	F	101	HEM	FE-ND	2.95	2.11	1.96
30	A	414	SQD	O47-C7	2.93	1.42	1.34
22	a	405	CLA	C4D-ND	-2.93	1.33	1.37
24	c	514	BCR	C30-C25	-2.93	1.49	1.53
24	C	514	BCR	C30-C25	-2.93	1.49	1.53
24	C	521	BCR	C1-C6	-2.93	1.49	1.53
22	b	619	CLA	C4D-ND	-2.92	1.33	1.37
30	D	403	SQD	O47-C7	2.92	1.42	1.34
25	b	601	DGD	C1E-C2E	2.92	1.60	1.52
30	d	402	SQD	O47-C7	2.91	1.42	1.34
24	H	102	BCR	C30-C25	-2.90	1.49	1.53
30	F	102	SQD	O47-C7	2.90	1.42	1.34
22	B	610	CLA	CHC-C1C	2.90	1.42	1.35
30	a	401	SQD	O47-C7	2.90	1.42	1.34
30	A	413	SQD	O47-C7	2.89	1.42	1.34
30	a	415	SQD	O47-C7	2.89	1.42	1.34
22	B	606	CLA	C4D-ND	-2.88	1.33	1.37
22	C	508	CLA	C4D-ND	-2.88	1.33	1.37
22	A	404	CLA	C4D-ND	-2.88	1.33	1.37
22	b	610	CLA	C4D-ND	-2.88	1.33	1.37
22	b	615	CLA	C4D-ND	-2.88	1.33	1.37
22	B	611	CLA	C4D-ND	-2.88	1.33	1.37
24	c	521	BCR	C1-C6	-2.87	1.49	1.53
22	A	402	CLA	C4D-ND	-2.87	1.33	1.37
22	B	613	CLA	C4D-ND	-2.86	1.33	1.37
34	f	101	HEM	FE-ND	2.86	2.11	1.96
22	b	614	CLA	C4D-ND	-2.85	1.33	1.37
22	B	612	CLA	C4D-ND	-2.85	1.33	1.37
34	F	101	HEM	CAB-C3B	2.85	1.55	1.47
22	B	602	CLA	C4D-ND	-2.85	1.33	1.37
22	A	403	CLA	C4D-ND	-2.85	1.33	1.37
34	V	201	HEM	FE-ND	2.84	2.10	1.96
22	B	607	CLA	C4D-ND	-2.84	1.33	1.37
30	b	602	SQD	O47-C7	2.84	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	625	DGD	C1E-C2E	2.84	1.60	1.52
22	c	509	CLA	C4D-ND	-2.84	1.33	1.37
22	C	504	CLA	C4D-ND	-2.84	1.33	1.37
22	b	617	CLA	C4D-ND	-2.83	1.33	1.37
30	B	626	SQD	O47-C7	2.83	1.42	1.34
30	f	103	SQD	O47-C7	2.83	1.42	1.34
22	b	614	CLA	CHC-C1C	2.83	1.42	1.35
22	B	605	CLA	C4D-ND	-2.82	1.33	1.37
22	C	506	CLA	C4D-ND	-2.82	1.33	1.37
22	D	405	CLA	C4D-ND	-2.82	1.33	1.37
34	f	101	HEM	CAB-C3B	2.81	1.55	1.47
22	c	507	CLA	C4D-ND	-2.81	1.33	1.37
22	B	614	CLA	C4D-ND	-2.81	1.33	1.37
22	B	608	CLA	C4D-ND	-2.80	1.33	1.37
22	c	502	CLA	C4D-ND	-2.80	1.33	1.37
22	b	611	CLA	C4D-ND	-2.80	1.33	1.37
22	C	505	CLA	C4D-ND	-2.80	1.33	1.37
22	b	606	CLA	C4D-ND	-2.80	1.33	1.37
22	C	520	CLA	C4D-ND	-2.80	1.33	1.37
22	h	101	CLA	C4D-ND	-2.80	1.33	1.37
22	C	509	CLA	C4D-ND	-2.79	1.33	1.37
22	c	505	CLA	C4D-ND	-2.79	1.33	1.37
22	C	511	CLA	C4D-ND	-2.79	1.33	1.37
22	c	504	CLA	C4D-ND	-2.79	1.33	1.37
22	C	507	CLA	C4D-ND	-2.79	1.33	1.37
22	a	404	CLA	C4D-ND	-2.79	1.33	1.37
22	b	616	CLA	C4D-ND	-2.79	1.33	1.37
22	B	604	CLA	C4D-ND	-2.79	1.33	1.37
22	B	610	CLA	C4D-ND	-2.79	1.33	1.37
22	a	406	CLA	C4D-ND	-2.78	1.33	1.37
22	c	506	CLA	C4D-ND	-2.78	1.33	1.37
22	a	408	CLA	C4D-ND	-2.77	1.33	1.37
22	c	520	CLA	C4D-ND	-2.77	1.33	1.37
22	d	405	CLA	C4D-ND	-2.77	1.33	1.37
22	b	608	CLA	C4D-ND	-2.77	1.33	1.37
22	B	601	CLA	C4D-ND	-2.77	1.33	1.37
22	C	501	CLA	C4D-ND	-2.76	1.33	1.37
22	b	618	CLA	C4D-ND	-2.76	1.33	1.37
22	b	607	CLA	C4D-ND	-2.76	1.33	1.37
22	c	501	CLA	C4D-ND	-2.76	1.33	1.37
24	c	513	BCR	C30-C25	-2.76	1.50	1.53
22	B	609	CLA	C4D-ND	-2.76	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	C4D-ND	-2.75	1.33	1.37
22	H	101	CLA	C4D-ND	-2.75	1.33	1.37
22	B	603	CLA	C4D-ND	-2.75	1.33	1.37
22	A	405	CLA	C4D-ND	-2.75	1.33	1.37
22	C	510	CLA	C4D-ND	-2.75	1.33	1.37
24	B	617	BCR	C30-C25	-2.75	1.50	1.53
22	b	609	CLA	C4D-ND	-2.74	1.33	1.37
22	b	612	CLA	C4D-ND	-2.74	1.33	1.37
22	d	404	CLA	C4D-ND	-2.74	1.33	1.37
34	v	201	HEM	FE-ND	2.74	2.10	1.96
22	C	503	CLA	C4D-ND	-2.73	1.33	1.37
24	b	621	BCR	C30-C25	-2.73	1.50	1.53
22	D	406	CLA	C4D-ND	-2.73	1.33	1.37
22	c	511	CLA	C4D-ND	-2.73	1.33	1.37
22	b	613	CLA	C4D-ND	-2.72	1.33	1.37
23	a	409	PL9	C3-C4	-2.72	1.45	1.49
32	D	402	PHO	CAC-C3C	-2.70	1.47	1.52
22	c	508	CLA	C4D-ND	-2.70	1.34	1.37
22	c	510	CLA	C4D-ND	-2.69	1.34	1.37
22	c	512	CLA	C4D-ND	-2.69	1.34	1.37
32	d	401	PHO	CAC-C3C	-2.69	1.47	1.52
22	b	605	CLA	C4D-ND	-2.68	1.34	1.37
22	c	503	CLA	C4D-ND	-2.68	1.34	1.37
22	C	512	CLA	C4D-ND	-2.68	1.34	1.37
32	D	401	PHO	CAC-C3C	-2.63	1.47	1.52
32	a	407	PHO	CAC-C3C	-2.63	1.47	1.52
31	b	627	LMT	O3'-C3'	-2.59	1.36	1.43
22	c	507	CLA	CMB-C2B	-2.58	1.46	1.51
22	C	507	CLA	CMB-C2B	-2.58	1.46	1.51
31	M	102	LMT	O3'-C3'	-2.58	1.36	1.43
31	B	623	LMT	O3'-C3'	-2.57	1.36	1.43
31	D	410	LMT	O3'-C3'	-2.56	1.36	1.43
31	d	409	LMT	O3'-C3'	-2.56	1.37	1.43
23	D	407	PL9	C3-C4	-2.54	1.45	1.49
31	M	103	LMT	O3'-C3'	-2.53	1.37	1.43
25	C	515	DGD	O2G-C2G	-2.52	1.40	1.46
31	b	603	LMT	O3'-C3'	-2.52	1.37	1.43
23	d	406	PL9	C3-C4	-2.51	1.45	1.49
31	I	102	LMT	O3'-C3'	-2.51	1.37	1.43
23	A	406	PL9	C3-C4	-2.51	1.45	1.49
31	b	626	LMT	O3'-C3'	-2.50	1.37	1.43
31	B	622	LMT	O3'-C3'	-2.49	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	CMB-C2B	-2.48	1.46	1.51
31	B	627	LMT	O3'-C3'	-2.48	1.37	1.43
31	b	604	LMT	O3'-C3'	-2.48	1.37	1.43
31	i	102	LMT	O3'-C3'	-2.47	1.37	1.43
22	A	403	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	603	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.46	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.45	1.46	1.51
22	A	404	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.43	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.43	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.42	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.41	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.41	1.46	1.51
22	d	404	CLA	CMB-C2B	-2.41	1.46	1.51
22	h	101	CLA	CMB-C2B	-2.41	1.46	1.51
34	f	101	HEM	FE-NB	2.41	2.08	1.96
22	c	502	CLA	CMB-C2B	-2.41	1.46	1.51
31	B	628	LMT	O3'-C3'	-2.41	1.37	1.43
22	b	609	CLA	CMB-C2B	-2.40	1.46	1.51
22	a	408	CLA	CMB-C2B	-2.40	1.46	1.51
31	I	102	LMT	O2'-C2'	-2.40	1.37	1.43
22	A	405	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.40	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.39	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.38	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.38	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.38	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.37	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.37	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.37	1.46	1.51
34	v	201	HEM	FE-NB	2.37	2.08	1.96
22	D	406	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	625	DGD	C4D-C5D	2.37	1.58	1.53
22	B	612	CLA	CMB-C2B	-2.36	1.46	1.51
31	i	102	LMT	O2'-C2'	-2.36	1.37	1.43
22	b	616	CLA	CMB-C2B	-2.36	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.36	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.36	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.36	1.46	1.51
31	M	102	LMT	O3B-C3B	-2.35	1.37	1.43
22	c	511	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	613	CLA	CMB-C2B	-2.35	1.46	1.51
31	B	628	LMT	O3B-C3B	-2.33	1.37	1.43
34	F	101	HEM	FE-NB	2.32	2.08	1.96
31	b	604	LMT	O3B-C3B	-2.31	1.37	1.43
31	b	627	LMT	O3B-C3B	-2.31	1.37	1.43
30	b	602	SQD	O2-C2	-2.30	1.37	1.43
31	I	102	LMT	O2B-C2B	-2.30	1.37	1.43
31	M	103	LMT	O3B-C3B	-2.29	1.37	1.43
31	B	627	LMT	O2'-C2'	-2.29	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	603	LMT	O3B-C3B	-2.29	1.37	1.43
31	B	622	LMT	O3B-C3B	-2.28	1.37	1.43
25	c	515	DGD	O2G-C2G	-2.28	1.40	1.46
30	B	626	SQD	O2-C2	-2.28	1.37	1.43
31	B	623	LMT	O3B-C3B	-2.28	1.37	1.43
31	I	102	LMT	O3B-C3B	-2.27	1.37	1.43
22	B	611	CLA	CMD-C2D	-2.27	1.46	1.50
31	i	102	LMT	O2B-C2B	-2.26	1.37	1.43
31	D	410	LMT	O3B-C3B	-2.26	1.37	1.43
31	d	409	LMT	O3B-C3B	-2.26	1.37	1.43
31	b	603	LMT	O2'-C2'	-2.25	1.37	1.43
31	M	102	LMT	O2'-C2'	-2.25	1.37	1.43
34	V	201	HEM	FE-NB	2.25	2.08	1.96
22	b	614	CLA	C3B-C2B	-2.24	1.37	1.40
31	b	626	LMT	O3B-C3B	-2.24	1.37	1.43
27	b	625	LMG	C4-C5	2.24	1.57	1.53
31	M	103	LMT	O2'-C2'	-2.24	1.37	1.43
22	b	615	CLA	CMD-C2D	-2.23	1.46	1.50
31	i	102	LMT	O3B-C3B	-2.23	1.37	1.43
25	b	601	DGD	C4D-C5D	2.23	1.57	1.53
31	B	627	LMT	O3B-C3B	-2.23	1.37	1.43
31	b	626	LMT	O2'-C2'	-2.22	1.37	1.43
31	b	604	LMT	O2'-C2'	-2.22	1.37	1.43
31	B	622	LMT	O2'-C2'	-2.21	1.37	1.43
23	a	409	PL9	C53-C6	-2.20	1.46	1.50
31	b	627	LMT	O2'-C2'	-2.20	1.37	1.43
25	C	516	DGD	O2G-C2G	-2.20	1.41	1.46
31	B	628	LMT	O2'-C2'	-2.20	1.37	1.43
31	b	603	LMT	O2B-C2B	-2.20	1.37	1.43
31	B	627	LMT	O2B-C2B	-2.20	1.37	1.43
23	D	407	PL9	C6-C1	-2.19	1.44	1.48
25	B	625	DGD	C3G-C2G	2.19	1.57	1.50
31	M	102	LMT	O2B-C2B	-2.18	1.37	1.43
23	A	406	PL9	C53-C6	-2.18	1.46	1.50
31	M	103	LMT	O2B-C2B	-2.17	1.37	1.43
22	c	504	CLA	CMD-C2D	-2.17	1.46	1.50
22	B	610	CLA	C3B-C2B	-2.16	1.37	1.40
31	B	623	LMT	O2'-C2'	-2.16	1.37	1.43
25	b	601	DGD	C3G-C2G	2.15	1.57	1.50
27	D	412	LMG	O7-C8	-2.15	1.41	1.46
31	b	626	LMT	O2B-C2B	-2.14	1.37	1.43
31	M	102	LMT	O4'-C4B	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	402	SQD	O2-C2	-2.14	1.37	1.43
30	b	602	SQD	O3-C3	-2.14	1.37	1.43
27	B	621	LMG	C4-C5	2.13	1.57	1.53
30	B	626	SQD	O3-C3	-2.13	1.38	1.43
31	D	410	LMT	O2B-C2B	-2.13	1.38	1.43
31	d	409	LMT	O2'-C2'	-2.13	1.38	1.43
22	c	509	CLA	CMD-C2D	-2.13	1.46	1.50
31	B	628	LMT	O4'-C4B	-2.13	1.38	1.43
30	f	103	SQD	O2-C2	-2.13	1.38	1.43
31	B	628	LMT	O2B-C2B	-2.13	1.38	1.43
22	C	504	CLA	CMD-C2D	-2.12	1.46	1.50
26	a	412	LHG	O7-C5	-2.12	1.41	1.46
31	D	410	LMT	O2'-C2'	-2.12	1.38	1.43
31	b	603	LMT	O4'-C4B	-2.12	1.38	1.43
25	c	516	DGD	O2G-C2G	-2.12	1.41	1.46
30	D	403	SQD	O2-C2	-2.11	1.38	1.43
30	F	102	SQD	O2-C2	-2.11	1.38	1.43
26	c	519	LHG	P-O6	2.11	1.67	1.59
30	A	413	SQD	O2-C2	-2.11	1.38	1.43
31	B	622	LMT	O2B-C2B	-2.11	1.38	1.43
32	D	402	PHO	CMC-C2C	-2.11	1.46	1.51
31	d	409	LMT	O2B-C2B	-2.11	1.38	1.43
31	M	103	LMT	O4'-C4B	-2.11	1.38	1.43
22	C	509	CLA	CMD-C2D	-2.10	1.46	1.50
25	d	408	DGD	C1D-C2D	2.10	1.58	1.52
31	b	604	LMT	O2B-C2B	-2.10	1.38	1.43
22	B	607	CLA	CMD-C2D	-2.10	1.46	1.50
27	d	410	LMG	O7-C8	-2.10	1.41	1.46
31	d	409	LMT	O4'-C4B	-2.10	1.38	1.43
25	b	624	DGD	O2G-C2G	-2.10	1.41	1.46
30	a	401	SQD	O3-C3	-2.09	1.38	1.43
30	A	414	SQD	O3-C3	-2.09	1.38	1.43
31	b	604	LMT	O4'-C4B	-2.09	1.38	1.43
30	a	415	SQD	O2-C2	-2.09	1.38	1.43
22	b	611	CLA	CMD-C2D	-2.08	1.46	1.50
25	B	620	DGD	O2G-C2G	-2.07	1.41	1.46
30	A	414	SQD	O2-C2	-2.07	1.38	1.43
34	v	201	HEM	CAA-C2A	2.07	1.55	1.52
31	B	627	LMT	O4'-C4B	-2.07	1.38	1.43
22	B	603	CLA	CMD-C2D	-2.07	1.46	1.50
31	I	102	LMT	O4'-C4B	-2.07	1.38	1.43
32	a	407	PHO	CMC-C2C	-2.07	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	f	103	SQD	O3-C3	-2.07	1.38	1.43
30	a	401	SQD	O2-C2	-2.06	1.38	1.43
32	D	401	PHO	CMC-C2C	-2.06	1.46	1.51
22	A	402	CLA	CMD-C2D	-2.06	1.46	1.50
31	B	623	LMT	O2B-C2B	-2.06	1.38	1.43
32	d	401	PHO	CMC-C2C	-2.06	1.46	1.51
32	d	401	PHO	CMD-C2D	-2.06	1.46	1.51
31	D	410	LMT	O4'-C4B	-2.05	1.38	1.43
31	B	622	LMT	O4'-C4B	-2.05	1.38	1.43
22	a	404	CLA	CMD-C2D	-2.05	1.46	1.50
25	C	515	DGD	O1G-C1G	-2.05	1.40	1.45
31	b	626	LMT	O4'-C4B	-2.05	1.38	1.43
22	b	607	CLA	CMD-C2D	-2.05	1.46	1.50
23	A	406	PL9	C6-C1	-2.04	1.44	1.48
32	D	402	PHO	CMD-C2D	-2.04	1.46	1.51
30	F	102	SQD	O3-C3	-2.04	1.38	1.43
34	V	201	HEM	CMB-C2B	2.04	1.55	1.50
31	b	627	LMT	O2B-C2B	-2.03	1.38	1.43
32	a	407	PHO	CMD-C2D	-2.03	1.46	1.51
32	D	401	PHO	CMB-C2B	-2.02	1.46	1.51
22	B	604	CLA	CMD-C2D	-2.02	1.46	1.50
32	d	401	PHO	CMB-C2B	-2.02	1.46	1.51
31	i	102	LMT	O4'-C4B	-2.02	1.38	1.43
32	D	401	PHO	CMD-C2D	-2.02	1.46	1.51
31	b	627	LMT	O4'-C4B	-2.02	1.38	1.43
31	B	623	LMT	O4'-C4B	-2.02	1.38	1.43
22	A	404	CLA	CMD-C2D	-2.02	1.46	1.50
22	C	508	CLA	CMD-C2D	-2.02	1.46	1.50
34	v	201	HEM	CMD-C2D	2.01	1.55	1.50
34	V	201	HEM	CAA-C2A	2.01	1.55	1.52
22	b	608	CLA	CMD-C2D	-2.01	1.46	1.50
24	C	514	BCR	C38-C26	-2.01	1.47	1.50
25	C	517	DGD	C1G-C2G	2.01	1.56	1.50
25	d	408	DGD	O1G-C1G	-2.01	1.40	1.45
22	a	406	CLA	CMD-C2D	-2.01	1.46	1.50
30	a	415	SQD	O3-C3	-2.01	1.38	1.43
26	c	519	LHG	O7-C5	-2.01	1.41	1.46
22	c	503	CLA	CMD-C2D	-2.01	1.46	1.50
34	v	201	HEM	CMB-C2B	2.01	1.55	1.50
22	A	405	CLA	CMD-C2D	-2.01	1.46	1.50
30	A	413	SQD	O3-C3	-2.01	1.38	1.43
27	a	413	LMG	C7-C8	2.00	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	BCR	C38-C26	-2.00	1.47	1.50
22	B	602	CLA	CMD-C2D	-2.00	1.46	1.50
22	b	619	CLA	CMC-C2C	-2.00	1.46	1.50
25	a	411	DGD	O1G-C1G	-2.00	1.40	1.45
30	A	414	SQD	O4-C4	-2.00	1.38	1.43
30	F	102	SQD	O4-C4	-2.00	1.38	1.43

All (1150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	C4A-NA-C1A	7.20	109.94	106.71
22	c	504	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	C	510	CLA	C4A-NA-C1A	7.11	109.90	106.71
22	B	603	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	B	611	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	b	609	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	b	615	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	b	607	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	a	405	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	A	403	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	c	520	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	C	501	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	c	503	CLA	C4A-NA-C1A	6.78	109.76	106.71
22	C	503	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	b	616	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	c	510	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	C	520	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	b	618	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	605	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	c	501	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	c	511	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	B	615	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	C	512	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	c	512	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	C	506	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	C	511	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	B	614	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	B	604	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	b	619	CLA	C4A-NA-C1A	6.58	109.66	106.71
22	B	606	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	B	612	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	b	608	CLA	C4A-NA-C1A	6.56	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	C	505	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	a	406	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	d	404	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	A	405	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	B	609	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	b	617	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	B	607	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	D	405	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	c	505	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	a	408	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	c	508	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	h	101	CLA	C4A-NA-C1A	6.43	109.59	106.71
22	B	602	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	C	507	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	B	613	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	c	507	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	b	610	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	b	611	CLA	C4A-NA-C1A	6.32	109.55	106.71
34	v	201	HEM	C4D-ND-C1D	6.32	111.60	105.07
22	C	502	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	d	405	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	C	508	CLA	C4A-NA-C1A	6.31	109.55	106.71
22	c	502	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	B	601	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	B	608	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	H	101	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	D	406	CLA	C4A-NA-C1A	6.25	109.51	106.71
22	A	404	CLA	C4A-NA-C1A	6.18	109.48	106.71
22	b	605	CLA	C4A-NA-C1A	6.16	109.47	106.71
22	b	606	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	b	613	CLA	C4A-NA-C1A	6.15	109.47	106.71
34	V	201	HEM	C4D-ND-C1D	6.13	111.41	105.07
22	C	509	CLA	C4A-NA-C1A	6.11	109.45	106.71
22	a	404	CLA	C4A-NA-C1A	6.08	109.44	106.71
22	A	402	CLA	C4A-NA-C1A	6.07	109.44	106.71
22	c	509	CLA	C4A-NA-C1A	6.04	109.42	106.71
34	f	101	HEM	C4D-ND-C1D	6.04	111.31	105.07
22	b	612	CLA	C4A-NA-C1A	6.02	109.41	106.71
34	F	101	HEM	C4D-ND-C1D	5.99	111.27	105.07
23	j	101	PL9	C7-C3-C4	5.66	121.48	116.88
23	J	101	PL9	C7-C3-C4	5.58	121.41	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	602	SQD	O6-C1-C2	5.56	116.99	108.30
33	D	404	BCT	O2-C-O1	5.56	133.96	119.55
33	d	403	BCT	O2-C-O1	5.53	133.89	119.55
30	A	413	SQD	O9-S-C6	5.40	113.36	106.94
23	A	406	PL9	C7-C3-C4	5.38	121.25	116.88
30	B	626	SQD	O6-C1-C2	5.37	116.68	108.30
22	b	614	CLA	C4A-NA-C1A	5.36	109.11	106.71
22	B	610	CLA	C4A-NA-C1A	5.34	109.11	106.71
23	d	406	PL9	C7-C3-C4	5.31	121.19	116.88
23	D	407	PL9	C7-C3-C4	5.24	121.14	116.88
30	a	415	SQD	O6-C1-C2	5.22	116.45	108.30
30	a	415	SQD	O9-S-C6	5.17	113.08	106.94
23	a	409	PL9	C7-C3-C4	5.14	121.06	116.88
30	A	413	SQD	O6-C1-C2	4.91	115.97	108.30
25	A	408	DGD	O3G-C3G-C2G	-4.64	99.69	110.90
25	a	411	DGD	O3G-C3G-C2G	-4.64	99.70	110.90
22	B	610	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
30	D	403	SQD	O6-C1-C2	4.47	115.28	108.30
22	b	614	CLA	CMB-C2B-C1B	-4.44	121.63	128.46
30	A	414	SQD	O7-S-C6	4.44	112.21	106.94
30	d	402	SQD	O6-C1-C2	4.43	115.22	108.30
30	b	602	SQD	O7-S-C6	4.42	112.20	106.94
25	C	517	DGD	O3G-C3G-C2G	-4.37	100.36	110.90
30	a	401	SQD	O7-S-C6	4.34	112.09	106.94
30	d	402	SQD	O5-C5-C4	4.33	117.55	109.69
30	f	103	SQD	O7-S-C6	4.31	112.06	106.94
30	D	403	SQD	O5-C5-C4	4.25	117.40	109.69
30	B	626	SQD	O7-S-C6	4.23	111.96	106.94
26	a	412	LHG	O4-P-O5	4.18	132.92	112.24
22	C	507	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
22	c	507	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
26	C	519	LHG	O4-P-O5	4.16	132.83	112.24
26	c	519	LHG	O4-P-O5	4.16	132.82	112.24
26	A	409	LHG	O4-P-O5	4.16	132.80	112.24
30	b	602	SQD	O9-S-C6	4.14	111.86	106.94
22	B	612	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
30	B	626	SQD	O9-S-C6	4.11	111.82	106.94
30	F	102	SQD	O7-S-C6	4.11	111.82	106.94
25	c	517	DGD	O3G-C3G-C2G	-4.10	101.01	110.90
22	b	616	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
30	d	402	SQD	O9-S-C6	4.07	111.78	106.94
30	D	403	SQD	O9-S-C6	4.02	111.72	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	602	SQD	O5-C5-C4	4.02	116.99	109.69
30	B	626	SQD	O5-C5-C4	4.02	116.99	109.69
30	A	414	SQD	O5-C5-C4	3.97	116.91	109.69
30	A	413	SQD	O47-C7-C8	3.94	119.99	111.50
30	a	415	SQD	O47-C7-C8	3.92	119.94	111.50
27	d	407	LMG	C1-C2-C3	-3.88	101.92	110.00
22	b	611	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
22	B	607	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
27	D	408	LMG	C1-C2-C3	-3.83	102.02	110.00
25	c	516	DGD	O5D-C6D-C5D	-3.82	101.98	109.05
30	D	403	SQD	O7-S-C6	3.82	111.47	106.94
30	D	403	SQD	O9-S-O7	-3.79	100.83	113.95
30	d	402	SQD	O9-S-O7	-3.79	100.84	113.95
30	f	103	SQD	O9-S-O7	-3.78	100.86	113.95
30	F	102	SQD	O9-S-O7	-3.77	100.89	113.95
24	C	513	BCR	C2-C1-C6	3.77	116.28	110.48
30	a	401	SQD	O5-C5-C4	3.75	116.50	109.69
30	A	413	SQD	O9-S-O7	-3.75	100.98	113.95
24	c	513	BCR	C2-C1-C6	3.73	116.23	110.48
30	a	415	SQD	O9-S-O7	-3.73	101.04	113.95
23	j	101	PL9	C7-C3-C2	-3.73	118.40	123.30
22	c	510	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
30	b	602	SQD	O9-S-O7	-3.72	101.07	113.95
30	a	401	SQD	O9-S-C6	3.72	111.36	106.94
30	B	626	SQD	O9-S-O7	-3.72	101.09	113.95
34	V	201	HEM	C4C-CHD-C1D	3.71	127.46	122.56
22	B	602	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
30	a	415	SQD	O5-C5-C4	3.70	116.42	109.69
23	J	101	PL9	C7-C3-C2	-3.70	118.44	123.30
30	a	401	SQD	O9-S-O7	-3.70	101.16	113.95
30	a	415	SQD	O7-S-C6	3.70	111.33	106.94
22	b	617	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	B	609	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	B	613	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	b	615	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	d	408	DGD	O6D-C1D-O3G	-3.67	101.28	109.97
22	B	611	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
30	A	414	SQD	O9-S-O7	-3.66	101.27	113.95
30	B	626	SQD	O47-C7-C8	3.66	119.39	111.50
30	A	413	SQD	O7-S-C6	3.66	111.29	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	102	SQD	O8-S-C6	3.66	111.57	105.74
30	b	602	SQD	O47-C7-C8	3.65	119.37	111.50
22	C	512	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
30	f	103	SQD	O8-S-C6	3.65	111.55	105.74
22	C	506	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	A	402	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
25	D	409	DGD	O6D-C1D-O3G	-3.63	101.37	109.97
22	c	506	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	A	405	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	c	512	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
22	C	505	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
22	c	502	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
34	v	201	HEM	C4C-CHD-C1D	3.61	127.33	122.56
30	f	103	SQD	O5-C5-C4	3.61	116.25	109.69
22	a	408	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
30	d	402	SQD	O7-S-C6	3.61	111.23	106.94
25	c	516	DGD	O3G-C3G-C2G	-3.60	102.22	110.90
24	J	102	BCR	C11-C10-C9	-3.60	122.18	127.31
25	C	516	DGD	O3G-C3G-C2G	-3.59	102.23	110.90
22	C	510	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
30	F	102	SQD	O5-C5-C4	3.58	116.20	109.69
22	b	613	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	c	503	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
23	d	406	PL9	C7-C3-C2	-3.57	118.61	123.30
22	a	404	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
30	A	413	SQD	O5-C5-C4	3.55	116.14	109.69
25	C	516	DGD	O5D-C6D-C5D	-3.55	102.48	109.05
22	C	502	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	c	511	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
24	J	102	BCR	C3-C4-C5	-3.51	107.82	114.08
22	b	605	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
23	D	407	PL9	C7-C3-C2	-3.49	118.71	123.30
22	B	601	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	A	406	PL9	C7-C3-C2	-3.48	118.73	123.30
22	C	520	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
30	A	414	SQD	O47-C7-C8	3.47	118.98	111.50
22	B	614	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
30	A	414	SQD	O9-S-C6	3.46	111.06	106.94
22	B	612	CLA	CMB-C2B-C3B	3.46	131.15	124.68
22	c	520	CLA	CMB-C2B-C1B	-3.46	123.15	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	509	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	d	405	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	b	618	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	A	403	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	C	509	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	A	404	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
24	j	102	BCR	C3-C4-C5	-3.43	107.94	114.08
22	D	406	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
25	c	515	DGD	O3G-C3G-C2G	-3.42	102.64	110.90
22	B	603	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
25	C	515	DGD	O3G-C3G-C2G	-3.42	102.65	110.90
22	a	405	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	B	605	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
30	D	403	SQD	O47-C7-C8	3.41	118.84	111.50
24	j	102	BCR	C24-C23-C22	-3.40	121.09	126.23
22	b	616	CLA	CMB-C2B-C3B	3.40	131.04	124.68
30	a	401	SQD	C44-O6-C1	3.40	120.38	113.74
22	b	607	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
24	j	102	BCR	C11-C10-C9	-3.39	122.48	127.31
30	F	102	SQD	O6-C1-C2	3.38	113.57	108.30
22	b	608	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
22	b	609	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
30	F	102	SQD	O47-C7-C8	3.37	118.77	111.50
23	a	409	PL9	C7-C3-C2	-3.36	118.88	123.30
30	d	402	SQD	C3-C4-C5	3.35	116.22	110.24
25	B	620	DGD	O3G-C3G-C2G	-3.35	102.82	110.90
22	d	404	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
22	h	101	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
30	f	103	SQD	O47-C7-C8	3.34	118.69	111.50
22	H	101	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
22	D	405	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	C	508	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	c	507	CLA	CMB-C2B-C3B	3.33	130.90	124.68
22	b	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
30	d	402	SQD	O47-C7-C8	3.31	118.63	111.50
22	a	406	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
30	d	402	SQD	O8-S-C6	3.28	110.97	105.74
30	a	401	SQD	O47-C7-C8	3.27	118.56	111.50
22	C	507	CLA	CMB-C2B-C3B	3.27	130.79	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	BCR	C2-C1-C6	3.27	115.51	110.48
22	b	619	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
24	J	102	BCR	C2-C1-C6	3.26	115.50	110.48
24	j	102	BCR	C2-C1-C6	3.26	115.50	110.48
22	B	603	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	b	624	DGD	O3G-C3G-C2G	-3.24	103.07	110.90
22	c	503	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
22	b	611	CLA	CMB-C2B-C3B	3.24	130.75	124.68
22	B	606	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	B	608	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
22	b	606	CLA	CMB-C2B-C3B	3.22	130.71	124.68
22	b	612	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
25	d	408	DGD	O3G-C3G-C2G	-3.21	103.16	110.90
30	A	414	SQD	C44-O6-C1	3.20	120.00	113.74
24	J	102	BCR	C24-C23-C22	-3.20	121.39	126.23
22	b	606	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
22	B	607	CLA	CMB-C2B-C3B	3.20	130.66	124.68
22	b	609	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	613	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	c	507	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	602	CLA	CMB-C2B-C3B	3.19	130.64	124.68
25	b	624	DGD	O6D-C1D-O3G	-3.17	102.46	109.97
22	B	605	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
30	D	403	SQD	O8-S-C6	3.17	110.79	105.74
30	a	415	SQD	C3-C4-C5	3.17	115.89	110.24
22	b	617	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	C	506	CLA	CMB-C2B-C3B	3.15	130.58	124.68
22	B	613	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	c	516	DGD	O6D-C1D-O3G	-3.14	102.53	109.97
30	D	403	SQD	C3-C4-C5	3.14	115.84	110.24
22	c	506	CLA	CMB-C2B-C3B	3.14	130.55	124.68
34	F	101	HEM	C4B-CHC-C1C	3.13	126.68	122.56
24	a	410	BCR	C2-C1-C6	3.12	115.29	110.48
22	c	510	CLA	CMB-C2B-C3B	3.12	130.52	124.68
22	C	502	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
30	F	102	SQD	O9-S-C6	3.11	110.64	106.94
22	a	408	CLA	CMB-C2B-C3B	3.11	130.50	124.68
25	D	409	DGD	O3G-C3G-C2G	-3.11	103.40	110.90
31	B	628	LMT	C1'-O5'-C5'	-3.11	107.59	113.69
30	f	103	SQD	O6-C1-C2	3.11	113.15	108.30
22	b	617	CLA	CMB-C2B-C3B	3.11	130.49	124.68
34	f	101	HEM	C4B-CHC-C1C	3.10	126.65	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	620	DGD	O6D-C1D-O3G	-3.10	102.64	109.97
22	C	504	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	C	503	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	B	618	BCR	C2-C1-C6	3.09	115.24	110.48
22	C	512	CLA	CMB-C2B-C3B	3.09	130.46	124.68
30	A	413	SQD	C3-C4-C5	3.09	115.75	110.24
22	A	405	CLA	CMB-C2B-C3B	3.08	130.44	124.68
22	B	604	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	A	408	DGD	O6D-C1D-O3G	-3.07	102.70	109.97
22	B	610	CLA	CMB-C2B-C3B	3.07	130.42	124.68
22	C	505	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	b	607	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	C	504	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
22	b	610	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	c	505	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	b	622	BCR	C2-C1-C6	3.05	115.18	110.48
22	c	504	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	B	609	CLA	CMB-C2B-C3B	3.05	130.39	124.68
22	c	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
24	b	621	BCR	C15-C14-C13	-3.05	122.96	127.31
22	c	502	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	c	512	CLA	CMB-C2B-C3B	3.04	130.37	124.68
24	J	102	BCR	C7-C8-C9	-3.04	121.64	126.23
22	C	503	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	b	615	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	C	510	CLA	CMB-C2B-C3B	3.04	130.36	124.68
25	c	517	DGD	C1D-C2D-C3D	-3.03	103.68	110.00
22	c	502	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
24	g	101	BCR	C33-C5-C6	-3.03	121.13	124.53
22	B	606	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	B	611	CLA	CMB-C2B-C3B	3.02	130.34	124.68
22	C	505	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	B	608	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	C	516	DGD	O6D-C1D-O3G	-3.01	102.84	109.97
22	C	507	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	b	612	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	c	503	CLA	CMB-C2B-C3B	3.01	130.30	124.68
22	b	605	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
24	b	622	BCR	C24-C23-C22	-3.00	121.71	126.23
22	c	505	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	b	613	CLA	CMB-C2B-C3B	2.99	130.28	124.68
22	B	602	CLA	O2D-CGD-O1D	-2.99	117.99	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	j	102	BCR	C7-C8-C9	-2.98	121.73	126.23
24	B	617	BCR	C15-C16-C17	-2.98	117.37	123.47
22	b	611	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
34	f	101	HEM	C1B-NB-C4B	2.98	108.15	105.07
31	b	604	LMT	C1'-O5'-C5'	-2.97	107.85	113.69
25	c	515	DGD	O6D-C1D-O3G	-2.97	102.94	109.97
24	y	101	BCR	C33-C5-C6	-2.96	121.20	124.53
25	B	625	DGD	O5D-C1E-C2E	2.96	112.93	108.30
22	b	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	C	511	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	C	517	DGD	C1D-C2D-C3D	-2.96	103.83	110.00
24	j	102	BCR	C15-C14-C13	-2.96	123.09	127.31
34	F	101	HEM	C1B-NB-C4B	2.96	108.13	105.07
24	B	619	BCR	C2-C1-C6	2.95	115.03	110.48
22	C	510	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	H	101	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	C	502	CLA	CMB-C2B-C3B	2.95	130.19	124.68
24	f	102	BCR	C29-C30-C25	2.94	115.01	110.48
22	a	406	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	a	404	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	B	625	DGD	C1D-C2D-C3D	-2.94	103.88	110.00
24	H	102	BCR	C33-C5-C6	-2.94	121.23	124.53
22	c	511	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	d	405	CLA	CMB-C2B-C3B	2.93	130.17	124.68
22	c	511	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	b	623	BCR	C2-C1-C6	2.93	114.99	110.48
25	b	601	DGD	C1D-C2D-C3D	-2.92	103.91	110.00
22	C	506	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	b	608	CLA	CMB-C2B-C3B	2.92	130.13	124.68
22	B	601	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	D	406	CLA	CMB-C2B-C3B	2.91	130.13	124.68
22	B	607	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	b	613	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	C	515	DGD	O6D-C1D-O3G	-2.91	103.08	109.97
30	B	626	SQD	C3-C4-C5	2.91	115.43	110.24
25	a	411	DGD	O6D-C1D-O3G	-2.91	103.08	109.97
22	c	506	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	B	604	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	A	403	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	B	612	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	D	406	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	c	512	CLA	O2D-CGD-O1D	-2.90	118.18	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	520	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
24	b	621	BCR	C15-C16-C17	-2.89	117.54	123.47
22	A	402	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	b	616	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	b	614	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	C	501	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	b	628	LMG	O6-C1-O1	-2.89	103.14	109.97
24	c	521	BCR	C2-C1-C6	2.89	114.92	110.48
32	a	407	PHO	CMB-C2B-C3B	2.88	130.07	124.68
22	D	405	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	b	602	SQD	C3-C4-C5	2.88	115.37	110.24
22	b	618	CLA	CMB-C2B-C3B	2.87	130.06	124.68
22	d	404	CLA	CMB-C2B-C3B	2.87	130.06	124.68
24	x	101	BCR	C33-C5-C6	-2.87	121.30	124.53
32	D	402	PHO	CMB-C2B-C3B	2.87	130.05	124.68
22	B	614	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	B	605	CLA	CMB-C2B-C3B	2.87	130.05	124.68
22	c	510	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	b	601	DGD	O5D-C1E-C2E	2.87	112.78	108.30
22	C	520	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	B	614	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	A	404	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	C	517	DGD	CDB-CCB-CBB	-2.86	99.90	114.42
22	B	603	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	c	517	DGD	CDB-CCB-CBB	-2.86	99.92	114.42
24	D	411	BCR	C33-C5-C6	-2.86	121.32	124.53
22	A	404	CLA	CMB-C2B-C3B	2.86	130.02	124.68
24	B	617	BCR	C15-C14-C13	-2.85	123.24	127.31
22	C	520	CLA	CMB-C2B-C3B	2.85	130.01	124.68
22	d	405	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
32	D	402	PHO	O1D-CGD-CBD	2.84	129.47	124.74
30	f	103	SQD	C44-O6-C1	2.84	119.29	113.74
24	D	411	BCR	C29-C30-C25	2.84	114.86	110.48
22	C	511	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
31	B	623	LMT	C3'-C4'-C5'	-2.84	104.42	110.93
34	f	101	HEM	C4C-CHD-C1D	2.84	126.30	122.56
22	c	501	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	d	404	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	b	609	CLA	CMB-C2B-C3B	2.84	129.98	124.68
22	c	501	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
31	i	102	LMT	O1'-C1'-C2'	2.83	112.73	108.30
27	B	624	LMG	O6-C1-O1	-2.83	103.26	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	h	101	CLA	CMB-C2B-C3B	2.83	129.98	124.68
25	c	516	DGD	CDB-CCB-CBB	-2.83	100.05	114.42
22	C	501	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
22	b	607	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	c	509	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	H	101	CLA	CMB-C2B-C3B	2.82	129.96	124.68
25	b	601	DGD	O3G-C3G-C2G	-2.82	104.09	110.90
24	f	102	BCR	C33-C5-C6	-2.82	121.36	124.53
24	J	102	BCR	C15-C14-C13	-2.82	123.29	127.31
23	J	101	PL9	C7-C8-C9	-2.82	122.10	126.79
22	A	403	CLA	CMB-C2B-C3B	2.82	129.95	124.68
30	f	103	SQD	O9-S-C6	2.82	110.29	106.94
22	b	610	CLA	CMB-C2B-C3B	2.82	129.94	124.68
22	b	618	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	B	617	BCR	C33-C5-C6	-2.81	121.37	124.53
22	B	609	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	C	509	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	D	405	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	a	408	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	D	402	PHO	O2D-CGD-O1D	-2.81	118.34	123.84
22	h	101	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	C	516	DGD	CDB-CCB-CBB	-2.81	100.18	114.42
32	a	407	PHO	O1D-CGD-CBD	2.81	129.41	124.74
32	d	401	PHO	O1D-CGD-CBD	2.81	129.41	124.74
23	d	406	PL9	C40-C39-C41	2.80	119.98	115.27
25	C	517	DGD	O5D-C6D-C5D	-2.80	103.87	109.05
22	c	520	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	A	402	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	b	612	CLA	CMB-C2B-C3B	2.79	129.91	124.68
22	C	512	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	b	620	BCR	C33-C5-C6	-2.79	121.40	124.53
22	b	605	CLA	CMB-C2B-C3B	2.78	129.88	124.68
30	d	402	SQD	C44-O6-C1	2.78	119.17	113.74
24	J	102	BCR	C27-C26-C25	2.78	126.76	122.73
24	y	101	BCR	C7-C8-C9	-2.77	122.04	126.23
34	F	101	HEM	C3B-C2B-C1B	2.77	108.54	106.49
22	b	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	I	102	LMT	O1'-C1'-C2'	2.77	112.63	108.30
22	B	608	CLA	CMB-C2B-C3B	2.77	129.86	124.68
26	a	412	LHG	O8-C23-C24	2.77	120.60	111.91
23	d	406	PL9	C7-C8-C9	-2.77	122.18	126.79
24	B	616	BCR	C33-C5-C6	-2.77	121.42	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	601	CLA	CMB-C2B-C3B	2.77	129.85	124.68
22	a	405	CLA	CMB-C2B-C3B	2.77	129.85	124.68
24	C	521	BCR	C2-C1-C6	2.77	114.74	110.48
31	b	627	LMT	C3'-C4'-C5'	-2.76	104.59	110.93
22	c	509	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	B	606	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	a	405	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	B	618	BCR	C29-C30-C25	2.75	114.72	110.48
22	c	508	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	D	407	PL9	C22-C23-C24	-2.75	121.03	127.66
23	D	407	PL9	C7-C8-C9	-2.75	122.22	126.79
32	D	401	PHO	CMB-C2B-C3B	2.75	129.81	124.68
22	A	405	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
34	F	101	HEM	C4C-CHD-C1D	2.75	126.18	122.56
25	B	625	DGD	O3G-C3G-C2G	-2.74	104.28	110.90
34	f	101	HEM	C3B-C2B-C1B	2.74	108.52	106.49
24	b	621	BCR	C33-C5-C6	-2.74	121.45	124.53
23	j	101	PL9	C7-C8-C9	-2.74	122.23	126.79
26	A	409	LHG	O8-C23-C24	2.74	120.51	111.91
22	a	406	CLA	CMB-C2B-C3B	2.74	129.80	124.68
24	y	101	BCR	C27-C26-C25	2.73	126.70	122.73
24	C	514	BCR	C15-C16-C17	-2.73	117.88	123.47
24	b	622	BCR	C29-C30-C25	2.73	114.69	110.48
22	C	508	CLA	CMB-C2B-C3B	2.73	129.79	124.68
25	b	601	DGD	C3G-C2G-C1G	-2.73	105.33	111.79
22	a	404	CLA	CMB-C2B-C3B	2.73	129.78	124.68
24	b	621	BCR	C28-C27-C26	-2.73	109.21	114.08
22	b	609	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	A	403	CLA	CHB-C4A-NA	2.72	128.28	124.51
32	D	401	PHO	O2D-CGD-O1D	-2.72	118.52	123.84
25	D	409	DGD	CDB-CCB-CBB	-2.72	100.62	114.42
24	c	521	BCR	C15-C16-C17	-2.72	117.91	123.47
22	C	509	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
32	D	401	PHO	O1D-CGD-CBD	2.72	129.26	124.74
25	c	517	DGD	C1D-O6D-C5D	-2.71	108.36	113.69
24	y	101	BCR	C38-C26-C25	-2.71	121.48	124.53
30	D	403	SQD	C44-O6-C1	2.71	119.03	113.74
25	C	517	DGD	C1D-O6D-C5D	-2.71	108.37	113.69
22	b	619	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	a	405	CLA	CHB-C4A-NA	2.71	128.25	124.51
32	d	401	PHO	O2D-CGD-O1D	-2.71	118.55	123.84
23	D	407	PL9	C40-C39-C41	2.70	119.82	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	CMB-C2B-C3B	2.70	129.73	124.68
25	d	408	DGD	CDB-CCB-CBB	-2.70	100.71	114.42
23	A	406	PL9	C22-C23-C24	-2.70	121.17	127.66
22	C	504	CLA	CMB-C2B-C3B	2.70	129.72	124.68
24	B	617	BCR	C28-C27-C26	-2.69	109.27	114.08
24	g	101	BCR	C27-C26-C25	2.69	126.64	122.73
25	c	517	DGD	O5D-C6D-C5D	-2.69	104.06	109.05
32	a	407	PHO	O2D-CGD-O1D	-2.69	118.58	123.84
27	C	518	LMG	O6-C1-O1	-2.69	103.60	109.97
22	B	610	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	B	625	DGD	C3G-C2G-C1G	-2.69	105.43	111.79
24	c	514	BCR	C28-C27-C26	-2.69	109.28	114.08
24	g	101	BCR	C38-C26-C25	-2.68	121.51	124.53
24	B	618	BCR	C24-C23-C22	-2.67	122.19	126.23
23	a	409	PL9	C22-C23-C24	-2.67	121.23	127.66
24	c	514	BCR	C11-C10-C9	-2.67	123.50	127.31
24	j	102	BCR	C27-C26-C25	2.67	126.61	122.73
27	c	518	LMG	O6-C1-O1	-2.67	103.66	109.97
24	C	514	BCR	C28-C27-C26	-2.67	109.32	114.08
22	C	510	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	d	406	PL9	C22-C23-C24	-2.66	121.25	127.66
24	g	101	BCR	C7-C8-C9	-2.65	122.22	126.23
24	C	521	BCR	C15-C16-C17	-2.65	118.04	123.47
27	E	101	LMG	C1-C2-C3	-2.65	104.47	110.00
22	b	619	CLA	CMB-C2B-C3B	2.65	129.64	124.68
22	C	506	CLA	CHB-C4A-NA	2.65	128.17	124.51
27	I	101	LMG	O6-C1-O1	-2.65	103.71	109.97
22	c	504	CLA	CMB-C2B-C3B	2.64	129.62	124.68
24	b	623	BCR	C7-C8-C9	-2.64	122.25	126.23
22	B	603	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	c	506	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	b	622	BCR	C11-C10-C9	-2.63	123.56	127.31
22	B	605	CLA	CHB-C4A-NA	2.63	128.14	124.51
24	B	618	BCR	C11-C10-C9	-2.62	123.56	127.31
27	i	101	LMG	O6-C1-O1	-2.62	103.76	109.97
34	v	201	HEM	C4B-CHC-C1C	2.62	126.02	122.56
24	j	102	BCR	C33-C5-C6	-2.62	121.59	124.53
23	J	101	PL9	C22-C23-C24	-2.62	121.35	127.66
22	b	608	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	B	626	SQD	C4-C3-C2	2.61	115.38	110.82
32	d	401	PHO	CMB-C2B-C3B	2.61	129.55	124.68
22	B	603	CLA	C1-C2-C3	-2.61	121.54	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	520	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	J	102	BCR	C33-C5-C6	-2.60	121.61	124.53
22	C	512	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	b	607	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	B	626	SQD	O8-S-C6	2.60	109.88	105.74
23	j	101	PL9	C22-C23-C24	-2.60	121.41	127.66
22	b	607	CLA	C1-C2-C3	-2.60	121.55	126.04
26	c	519	LHG	O8-C23-C24	2.60	120.05	111.91
22	a	406	CLA	CHB-C4A-NA	2.60	128.10	124.51
30	b	602	SQD	C4-C3-C2	2.59	115.35	110.82
24	c	514	BCR	C15-C16-C17	-2.59	118.17	123.47
30	a	401	SQD	O8-S-C6	2.59	109.87	105.74
26	C	519	LHG	O8-C23-C24	2.59	120.04	111.91
24	j	102	BCR	C15-C16-C17	-2.59	118.17	123.47
22	C	505	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	C	520	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	a	409	PL9	C7-C8-C9	-2.58	122.49	126.79
22	c	512	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	C	513	BCR	C24-C23-C22	-2.58	122.34	126.23
31	M	102	LMT	C1'-O5'-C5'	-2.57	108.64	113.69
24	c	513	BCR	C7-C8-C9	-2.57	122.35	126.23
22	B	615	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	J	102	BCR	C35-C13-C14	-2.57	119.33	122.92
30	a	415	SQD	O8-S-C6	2.57	109.83	105.74
22	C	504	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	C	513	BCR	C15-C16-C17	-2.56	118.22	123.47
31	b	626	LMT	C1'-O5'-C5'	-2.56	108.67	113.69
24	c	514	BCR	C15-C14-C13	-2.56	123.66	127.31
22	c	508	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	C	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	c	510	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	A	408	DGD	O5D-C6D-C5D	-2.55	104.33	109.05
24	B	618	BCR	C15-C14-C13	-2.55	123.68	127.31
22	b	618	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	B	619	BCR	C7-C8-C9	-2.54	122.40	126.23
22	b	615	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	C	503	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	d	408	DGD	C3D-C4D-C5D	-2.54	105.72	110.24
22	c	511	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	B	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	b	625	LMG	C1-C2-C3	-2.53	104.72	110.00
31	B	622	LMT	C1'-O5'-C5'	-2.53	108.72	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	505	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	c	508	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	C	514	BCR	C29-C30-C25	2.52	114.37	110.48
25	c	516	DGD	O6E-C1E-O5D	-2.52	104.00	109.97
24	c	514	BCR	C29-C30-C25	2.52	114.36	110.48
25	d	408	DGD	C3G-C2G-C1G	-2.52	105.83	111.79
25	D	409	DGD	CFB-CEB-CDB	-2.51	101.67	114.42
22	c	503	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	b	615	CLA	CHB-C4A-NA	2.51	127.98	124.51
27	M	101	LMG	C1-C2-C3	-2.51	104.77	110.00
24	C	514	BCR	C33-C5-C6	-2.51	121.72	124.53
24	c	513	BCR	C11-C10-C9	-2.50	123.74	127.31
24	C	513	BCR	C15-C14-C13	-2.50	123.74	127.31
24	b	623	BCR	C3-C4-C5	-2.50	109.61	114.08
22	B	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	B	621	LMG	C1-C2-C3	-2.50	104.79	110.00
24	c	521	BCR	C15-C14-C13	-2.50	123.74	127.31
22	a	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	C	514	BCR	C15-C14-C13	-2.49	123.75	127.31
22	d	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	c	501	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	511	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	b	602	SQD	O8-S-C6	2.49	109.70	105.74
24	a	410	BCR	C33-C5-C6	-2.49	121.73	124.53
22	c	504	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	C	521	BCR	C15-C14-C13	-2.48	123.76	127.31
27	d	410	LMG	C38-C37-C36	-2.48	101.83	114.42
22	B	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	v	201	HEM	C1B-NB-C4B	2.48	107.63	105.07
24	b	622	BCR	C15-C14-C13	-2.48	123.77	127.31
22	A	404	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	A	413	SQD	O8-S-C6	2.48	109.69	105.74
27	D	412	LMG	C38-C37-C36	-2.48	101.85	114.42
22	B	606	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
22	D	406	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	B	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	b	616	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	d	407	LMG	C38-C37-C36	-2.47	101.88	114.42
25	d	408	DGD	CFB-CEB-CDB	-2.47	101.88	114.42
23	a	409	PL9	C41-C39-C40	2.47	120.06	114.60
24	B	619	BCR	C3-C4-C5	-2.47	109.67	114.08
23	A	406	PL9	C7-C8-C9	-2.47	122.68	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	BCR	C33-C5-C6	-2.47	121.76	124.53
22	b	611	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	B	611	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	h	101	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	B	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	A	408	DGD	CBB-CAB-C9B	-2.46	101.94	114.42
22	C	508	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
30	A	414	SQD	O8-S-C6	2.46	109.66	105.74
22	c	505	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	B	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	F	102	SQD	C3-C4-C5	2.46	114.62	110.24
27	A	410	LMG	C40-C39-C38	-2.46	101.96	114.42
24	c	513	BCR	C15-C14-C13	-2.46	123.81	127.31
24	C	513	BCR	C8-C7-C6	-2.45	120.31	127.20
22	c	501	CLA	CMB-C2B-C3B	2.45	129.27	124.68
22	B	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	a	408	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	C	508	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	M	102	LMT	C3'-C4'-C5'	-2.45	105.32	110.93
24	j	102	BCR	C35-C13-C14	-2.45	119.50	122.92
27	a	402	LMG	O6-C1-O1	-2.45	104.18	109.97
31	D	410	LMT	C1'-O5'-C5'	-2.44	108.89	113.69
24	y	101	BCR	C1-C6-C5	-2.44	119.17	122.61
25	a	411	DGD	CBB-CAB-C9B	-2.44	102.02	114.42
24	B	618	BCR	C15-C16-C17	-2.44	118.47	123.47
22	B	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	D	408	LMG	O6-C1-C2	-2.44	105.18	110.35
22	b	606	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	A	402	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	D	403	SQD	O48-C23-C24	2.44	119.56	111.91
22	a	408	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	B	611	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	B	619	BCR	C27-C26-C25	2.43	126.27	122.73
22	b	610	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	c	507	CLA	CHB-C4A-NA	2.43	127.88	124.51
30	a	401	SQD	C1-O5-C5	2.43	118.46	113.69
24	c	513	BCR	C8-C7-C6	-2.43	120.37	127.20
24	B	616	BCR	C11-C10-C9	-2.43	123.84	127.31
22	b	606	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	a	405	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
24	c	521	BCR	C27-C26-C25	2.43	126.26	122.73
22	c	502	CLA	CHB-C4A-NA	2.43	127.87	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	408	LMG	C38-C37-C36	-2.42	102.12	114.42
22	b	610	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	C	502	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	A	403	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
24	A	407	BCR	C33-C5-C6	-2.42	121.81	124.53
22	C	505	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	C	501	CLA	CMB-C2B-C3B	2.42	129.20	124.68
22	a	406	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
24	c	513	BCR	C15-C16-C17	-2.42	118.52	123.47
24	C	514	BCR	C11-C10-C9	-2.42	123.86	127.31
27	C	522	LMG	C40-C39-C38	-2.42	102.15	114.42
27	A	410	LMG	C1-C2-C3	-2.42	104.96	110.00
27	c	522	LMG	C40-C39-C38	-2.41	102.17	114.42
26	c	519	LHG	C11-C10-C9	-2.41	102.17	114.42
22	B	615	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	C	504	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
31	b	603	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
22	A	404	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	B	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	b	617	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	c	516	DGD	C3G-C2G-C1G	-2.41	106.09	111.79
30	F	102	SQD	C44-O6-C1	2.41	118.44	113.74
24	C	521	BCR	C27-C26-C25	2.41	126.23	122.73
23	a	409	PL9	C20-C19-C21	2.41	119.32	115.27
25	a	411	DGD	O5D-C6D-C5D	-2.41	104.60	109.05
24	b	621	BCR	C29-C30-C25	2.40	114.18	110.48
27	a	413	LMG	C40-C39-C38	-2.40	102.22	114.42
25	B	620	DGD	CBB-CAB-C9B	-2.40	102.22	114.42
25	C	516	DGD	O6E-C1E-O5D	-2.40	104.28	109.97
24	B	617	BCR	C29-C30-C25	2.40	114.18	110.48
31	M	103	LMT	C1'-O5'-C5'	-2.40	108.97	113.69
34	V	201	HEM	C1B-NB-C4B	2.40	107.55	105.07
27	B	624	LMG	C38-C37-C36	-2.40	102.23	114.42
24	b	623	BCR	C27-C26-C25	2.40	126.22	122.73
23	A	406	PL9	C41-C39-C40	2.40	119.90	114.60
22	A	402	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
25	b	624	DGD	CBB-CAB-C9B	-2.40	102.26	114.42
22	A	405	CLA	CHB-C4A-NA	2.40	127.83	124.51
27	e	101	LMG	O6-C1-O1	-2.40	104.30	109.97
24	c	513	BCR	C3-C4-C5	-2.40	109.80	114.08
31	M	103	LMT	C3'-C4'-C5'	-2.39	105.44	110.93
24	C	513	BCR	C3-C4-C5	-2.39	109.81	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	619	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	a	404	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
25	C	517	DGD	CFB-CEB-CDB	-2.39	102.30	114.42
22	C	511	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
25	c	516	DGD	CFB-CEB-CDB	-2.39	102.31	114.42
22	b	612	CLA	CHB-C4A-NA	2.39	127.81	124.51
27	A	415	LMG	O6-C1-O1	-2.39	104.33	109.97
22	B	608	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
27	b	628	LMG	C38-C37-C36	-2.38	102.33	114.42
25	c	517	DGD	CFB-CEB-CDB	-2.38	102.33	114.42
27	e	101	LMG	C1-C2-C3	-2.38	105.04	110.00
23	d	406	PL9	C20-C19-C21	2.38	119.28	115.27
24	A	407	BCR	C27-C26-C25	2.38	126.19	122.73
27	c	522	LMG	O6-C1-O1	-2.38	104.34	109.97
24	b	622	BCR	C15-C16-C17	-2.38	118.60	123.47
23	a	409	PL9	C27-C28-C29	-2.38	121.93	127.66
30	d	402	SQD	O48-C23-C24	2.38	119.37	111.91
22	C	506	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	b	612	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	c	511	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
25	B	620	DGD	C1D-C2D-C3D	-2.37	105.06	110.00
22	b	608	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	a	401	SQD	O48-C23-C24	2.37	119.35	111.91
22	B	601	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
24	b	620	BCR	C11-C10-C9	-2.37	123.93	127.31
25	c	515	DGD	C3G-C2G-C1G	-2.37	106.19	111.79
30	A	414	SQD	C1-O5-C5	2.37	118.33	113.69
22	b	611	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	C	509	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	j	102	BCR	C29-C30-C25	2.36	114.12	110.48
24	J	102	BCR	C29-C30-C25	2.36	114.12	110.48
22	c	506	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
24	C	521	BCR	C24-C23-C22	-2.36	122.67	126.23
22	C	507	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	D	407	PL9	C27-C28-C29	-2.36	121.98	127.66
31	B	627	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
22	h	101	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
24	g	101	BCR	C1-C6-C5	-2.36	119.29	122.61
31	i	102	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
22	B	602	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	a	413	LMG	C1-C2-C3	-2.36	105.09	110.00
22	A	405	CLA	C1B-CHB-C4A	-2.35	125.45	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	522	LMG	O6-C1-O1	-2.35	104.40	109.97
26	C	519	LHG	C11-C10-C9	-2.35	102.47	114.42
22	c	509	CLA	CHB-C4A-NA	2.35	127.77	124.51
24	a	410	BCR	C27-C26-C25	2.35	126.15	122.73
22	b	613	CLA	CHB-C4A-NA	2.35	127.76	124.51
31	d	409	LMT	C3'-C4'-C5'	-2.35	105.54	110.93
22	c	507	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
27	A	410	LMG	O3-C3-C2	-2.35	104.92	110.35
24	b	620	BCR	C2-C1-C6	2.35	114.10	110.48
23	J	101	PL9	C20-C19-C21	2.35	119.22	115.27
22	d	405	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
27	A	410	LMG	C38-C37-C36	-2.35	102.52	114.42
25	C	516	DGD	C3D-C4D-C5D	-2.34	106.06	110.24
24	b	623	BCR	C11-C10-C9	-2.34	123.97	127.31
22	B	605	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	612	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	D	409	DGD	C3G-C2G-C1G	-2.34	106.26	111.79
22	H	101	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	C	515	DGD	C3G-C2G-C1G	-2.34	106.26	111.79
22	C	520	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
23	D	407	PL9	C20-C19-C21	2.33	119.19	115.27
22	B	603	CLA	O1D-CGD-CBD	2.33	129.25	124.48
24	C	521	BCR	C33-C5-C6	-2.33	121.92	124.53
25	C	516	DGD	CFB-CEB-CDB	-2.33	102.61	114.42
22	H	101	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
25	C	516	DGD	C3G-C2G-C1G	-2.32	106.29	111.79
30	A	414	SQD	O48-C23-C24	2.32	119.19	111.91
30	a	415	SQD	O48-C23-C24	2.32	119.19	111.91
22	B	601	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	B	616	BCR	C2-C1-C6	2.32	114.05	110.48
27	D	412	LMG	C1-C2-C3	-2.31	105.17	110.00
24	c	513	BCR	C24-C23-C22	-2.31	122.74	126.23
27	C	518	LMG	C38-C37-C36	-2.31	102.68	114.42
25	b	601	DGD	O6D-C1D-O3G	-2.31	104.50	109.97
27	m	101	LMG	C1-C2-C3	-2.31	105.18	110.00
23	A	406	PL9	C20-C19-C21	2.31	119.16	115.27
25	D	409	DGD	C3D-C4D-C5D	-2.31	106.12	110.24
24	B	616	BCR	C15-C14-C13	-2.31	124.01	127.31
25	c	515	DGD	O5D-C6D-C5D	-2.31	104.77	109.05
22	b	614	CLA	C1-C2-C3	-2.31	122.05	126.04
27	b	625	LMG	C40-C39-C38	-2.31	102.70	114.42
27	a	413	LMG	C38-C37-C36	-2.31	102.72	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	621	LMG	C40-C39-C38	-2.31	102.72	114.42
22	B	608	CLA	C1-C2-C3	-2.30	122.06	126.04
22	d	405	CLA	C1-C2-C3	-2.30	122.06	126.04
22	b	605	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
31	d	409	LMT	C1'-O5'-C5'	-2.30	109.17	113.69
27	E	101	LMG	O6-C1-O1	-2.30	104.53	109.97
22	b	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	B	621	LMG	O6-C1-O1	-2.30	104.53	109.97
22	B	613	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
24	J	102	BCR	C15-C16-C17	-2.30	118.77	123.47
23	A	406	PL9	C27-C28-C29	-2.30	122.12	127.66
25	C	515	DGD	C1D-C2D-C3D	-2.30	105.21	110.00
24	C	521	BCR	C11-C10-C9	-2.30	124.03	127.31
27	c	518	LMG	C38-C37-C36	-2.30	102.77	114.42
24	B	619	BCR	C38-C26-C25	-2.29	121.95	124.53
27	d	410	LMG	O6-C1-O1	-2.29	104.54	109.97
27	m	101	LMG	O2-C2-C1	-2.29	104.47	110.05
25	c	516	DGD	C3D-C4D-C5D	-2.29	106.15	110.24
23	D	407	PL9	C37-C38-C39	-2.29	122.14	127.66
22	B	604	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	D	406	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	A	413	SQD	O48-C23-C24	2.29	119.09	111.91
22	B	609	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	D	407	PL9	C32-C33-C34	-2.29	122.15	127.66
23	d	406	PL9	C37-C38-C39	-2.29	122.15	127.66
24	B	616	BCR	C27-C26-C25	2.29	126.05	122.73
23	d	406	PL9	C27-C28-C29	-2.29	122.16	127.66
24	b	623	BCR	C38-C26-C25	-2.29	121.96	124.53
27	b	625	LMG	C38-C37-C36	-2.28	102.83	114.42
22	B	607	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	c	512	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	c	520	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	c	507	CLA	O2D-CGD-CBD	2.28	115.31	111.27
25	b	624	DGD	C1D-C2D-C3D	-2.28	105.26	110.00
22	c	502	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
22	c	512	CLA	CHD-C1D-ND	-2.27	122.36	124.45
22	C	512	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	c	509	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	B	615	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	a	405	CLA	CHD-C1D-ND	-2.27	122.37	124.45
22	B	610	CLA	C1-C2-C3	-2.27	122.12	126.04
24	c	521	BCR	C33-C5-C6	-2.27	121.98	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	515	DGD	O5D-C6D-C5D	-2.27	104.85	109.05
31	D	410	LMT	C3'-C4'-C5'	-2.27	105.73	110.93
25	a	411	DGD	C1D-C2D-C3D	-2.26	105.28	110.00
22	b	616	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
27	B	624	LMG	O2-C2-C1	-2.26	104.55	110.05
27	c	522	LMG	C38-C37-C36	-2.26	102.95	114.42
27	d	407	LMG	O6-C1-C2	-2.26	105.56	110.35
24	b	623	BCR	C24-C23-C22	-2.26	122.82	126.23
22	b	605	CLA	CHB-C4A-NA	2.26	127.63	124.51
23	d	406	PL9	C32-C33-C34	-2.26	122.23	127.66
22	C	507	CLA	CHD-C1D-ND	-2.25	122.38	124.45
27	D	412	LMG	O3-C3-C2	-2.25	105.14	110.35
27	i	101	LMG	O2-C2-C1	-2.25	104.58	110.05
34	V	201	HEM	C4B-CHC-C1C	2.25	125.53	122.56
24	b	620	BCR	C27-C26-C25	2.25	126.00	122.73
27	C	522	LMG	C38-C37-C36	-2.25	103.02	114.42
22	c	504	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
24	b	622	BCR	C7-C8-C9	-2.24	122.84	126.23
25	A	408	DGD	C3G-C2G-C1G	-2.24	106.48	111.79
22	C	507	CLA	C1-C2-C3	-2.24	122.16	126.04
27	D	412	LMG	O6-C1-O1	-2.24	104.66	109.97
25	B	620	DGD	C3G-C2G-C1G	-2.24	106.49	111.79
30	f	103	SQD	C3-C4-C5	2.24	114.23	110.24
22	C	509	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
30	a	415	SQD	C4-C3-C2	2.24	114.73	110.82
22	b	613	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
31	I	102	LMT	C1'-O5'-C5'	-2.24	109.30	113.69
23	d	406	PL9	O1-C4-C3	-2.24	118.26	120.72
27	b	628	LMG	O3-C3-C2	-2.24	105.18	110.35
27	a	402	LMG	O1-C7-C8	-2.23	105.51	110.90
24	b	620	BCR	C15-C14-C13	-2.23	124.12	127.31
23	j	101	PL9	C20-C19-C21	2.23	119.03	115.27
27	B	621	LMG	C38-C37-C36	-2.23	103.09	114.42
22	B	603	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
32	d	401	PHO	CMC-C2C-C3C	2.23	129.15	124.94
27	C	522	LMG	O2-C2-C1	-2.23	104.63	110.05
22	c	503	CLA	O2D-CGD-CBD	2.22	115.22	111.27
27	B	624	LMG	O3-C3-C2	-2.22	105.21	110.35
24	B	618	BCR	C7-C8-C9	-2.22	122.88	126.23
22	B	606	CLA	CHD-C1D-ND	-2.22	122.41	124.45
24	g	101	BCR	C3-C2-C1	-2.22	106.66	114.60
24	a	410	BCR	C38-C26-C25	-2.22	122.03	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	618	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	C	512	CLA	CHD-C1D-ND	-2.22	122.42	124.45
22	C	501	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
24	A	407	BCR	C15-C14-C13	-2.22	124.14	127.31
22	C	511	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
27	b	625	LMG	O6-C1-O1	-2.22	104.72	109.97
25	B	625	DGD	O6D-C1D-O3G	-2.21	104.73	109.97
27	d	410	LMG	O3-C3-C2	-2.21	105.23	110.35
22	b	617	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
27	d	410	LMG	C1-C2-C3	-2.21	105.39	110.00
22	C	502	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	D	411	BCR	C11-C10-C9	-2.21	124.16	127.31
30	B	626	SQD	O48-C23-C24	2.21	118.84	111.91
24	a	410	BCR	C15-C16-C17	-2.21	118.95	123.47
27	e	101	LMG	O1-C7-C8	-2.21	105.58	110.90
27	a	413	LMG	O3-C3-C2	-2.21	105.25	110.35
22	b	610	CLA	CHD-C1D-ND	-2.20	122.43	124.45
24	C	513	BCR	C27-C26-C25	2.20	125.93	122.73
27	c	522	LMG	O2-C2-C1	-2.20	104.69	110.05
24	f	102	BCR	C15-C16-C17	-2.20	118.96	123.47
22	d	404	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	C	507	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
31	B	623	LMT	C1'-O5'-C5'	-2.20	109.37	113.69
23	d	406	PL9	O2-C1-C2	-2.20	116.74	121.78
25	c	516	DGD	CBB-CAB-C9B	-2.20	103.26	114.42
27	m	101	LMG	C1-O6-C5	-2.20	109.37	113.69
22	c	510	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
27	b	628	LMG	O2-C2-C1	-2.20	104.71	110.05
24	c	513	BCR	C27-C26-C25	2.20	125.92	122.73
22	D	405	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	C	514	BCR	C38-C26-C25	-2.20	122.06	124.53
25	a	411	DGD	C3G-C2G-C1G	-2.20	106.59	111.79
23	j	101	PL9	O2-C1-C2	-2.20	116.75	121.78
24	A	407	BCR	C38-C26-C25	-2.20	122.06	124.53
25	C	516	DGD	CBB-CAB-C9B	-2.20	103.28	114.42
22	C	510	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
24	A	407	BCR	C15-C16-C17	-2.19	118.98	123.47
22	b	607	CLA	O1D-CGD-CBD	2.19	128.97	124.48
25	c	517	DGD	C3G-O3G-C1D	2.19	118.02	113.74
27	I	101	LMG	O2-C2-C1	-2.19	104.72	110.05
22	B	614	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	b	615	CLA	C1B-CHB-C4A	-2.19	125.78	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	508	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
24	y	101	BCR	C3-C2-C1	-2.19	106.78	114.60
22	d	404	CLA	O1D-CGD-CBD	2.19	128.96	124.48
27	A	415	LMG	O1-C7-C8	-2.19	105.62	110.90
22	a	404	CLA	CHD-C1D-ND	-2.19	122.45	124.45
22	D	405	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
27	M	101	LMG	O2-C2-C1	-2.18	104.74	110.05
24	c	521	BCR	C24-C23-C22	-2.18	122.94	126.23
24	c	514	BCR	C38-C26-C25	-2.18	122.08	124.53
24	c	521	BCR	C11-C10-C9	-2.18	124.20	127.31
22	b	619	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
32	a	407	PHO	CMC-C2C-C3C	2.18	129.05	124.94
22	B	604	CLA	CHD-C1D-ND	-2.18	122.45	124.45
27	D	408	LMG	O6-C1-O1	-2.18	104.82	109.97
23	D	407	PL9	O1-C4-C3	-2.18	118.32	120.72
22	c	520	CLA	CHD-C1D-ND	-2.18	122.45	124.45
22	C	503	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
22	c	501	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	d	404	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	b	607	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
23	J	101	PL9	O2-C1-C2	-2.17	116.81	121.78
22	c	508	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
22	B	603	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	B	605	CLA	O1D-CGD-CBD	2.17	128.92	124.48
22	D	405	CLA	O1D-CGD-CBD	2.17	128.92	124.48
22	A	403	CLA	CHD-C1D-ND	-2.17	122.46	124.45
25	C	517	DGD	CBB-CAB-C9B	-2.17	103.43	114.42
27	c	518	LMG	O7-C10-O9	-2.16	118.47	123.70
24	C	514	BCR	C24-C23-C22	-2.16	122.97	126.23
24	f	102	BCR	C11-C10-C9	-2.16	124.22	127.31
22	b	618	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	x	101	BCR	C29-C30-C25	2.16	113.81	110.48
25	c	516	DGD	O3D-C3D-C4D	-2.16	105.35	110.35
27	C	522	LMG	O3-C3-C2	-2.16	105.36	110.35
25	a	411	DGD	CAB-C9B-C8B	-2.16	103.46	114.42
25	c	515	DGD	C1D-C2D-C3D	-2.16	105.50	110.00
25	b	601	DGD	CBB-CAB-C9B	-2.16	103.48	114.42
22	c	502	CLA	C1-C2-C3	-2.15	122.32	126.04
25	C	516	DGD	O3D-C3D-C4D	-2.15	105.37	110.35
22	c	507	CLA	C1-C2-C3	-2.15	122.32	126.04
25	A	408	DGD	CAB-C9B-C8B	-2.15	103.49	114.42
27	a	402	LMG	O3-C3-C2	-2.15	105.37	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	609	CLA	CHD-C1D-ND	-2.15	122.48	124.45
27	B	621	LMG	O3-C3-C2	-2.15	105.38	110.35
22	c	503	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
22	B	611	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	D	411	BCR	C7-C8-C9	-2.15	122.99	126.23
23	j	101	PL9	O2-C1-C6	2.15	124.31	120.59
24	g	101	BCR	C15-C16-C17	-2.15	119.07	123.47
22	B	602	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
24	B	619	BCR	C24-C23-C22	-2.15	122.99	126.23
26	a	412	LHG	C27-C26-C25	-2.15	103.53	114.42
23	d	406	PL9	C36-C34-C33	-2.15	116.78	121.12
27	i	101	LMG	O1-C7-C8	-2.15	105.72	110.90
27	I	101	LMG	O3-C3-C2	-2.14	105.39	110.35
25	B	625	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
30	b	602	SQD	O48-C23-C24	2.14	118.64	111.91
25	c	517	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
25	C	516	DGD	CAB-C9B-C8B	-2.14	103.55	114.42
22	c	506	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
30	f	103	SQD	C1-O5-C5	2.14	117.89	113.69
27	i	101	LMG	O3-C3-C2	-2.14	105.40	110.35
22	B	611	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	c	511	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	C	501	CLA	CHD-C1D-ND	-2.14	122.49	124.45
27	C	518	LMG	O3-C3-C2	-2.14	105.41	110.35
23	a	409	PL9	O1-C4-C3	-2.14	118.37	120.72
27	c	522	LMG	O3-C3-C2	-2.14	105.41	110.35
22	D	406	CLA	C1-C2-C3	-2.14	122.35	126.04
24	H	102	BCR	C16-C15-C14	-2.13	119.10	123.47
22	c	509	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
23	J	101	PL9	O2-C1-C6	2.13	124.28	120.59
27	b	625	LMG	O3-C3-C2	-2.13	105.42	110.35
25	b	624	DGD	C3G-C2G-C1G	-2.13	106.75	111.79
24	b	622	BCR	C33-C5-C6	-2.13	122.14	124.53
24	C	513	BCR	C7-C8-C9	-2.13	123.02	126.23
22	C	509	CLA	CHD-C1D-ND	-2.13	122.50	124.45
27	C	518	LMG	O7-C10-O9	-2.13	118.56	123.70
32	D	401	PHO	CMC-C2C-C3C	2.13	128.95	124.94
24	D	411	BCR	C15-C16-C17	-2.12	119.12	123.47
22	b	615	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	C	508	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	a	410	BCR	C24-C23-C22	-2.12	123.03	126.23
27	C	518	LMG	O2-C2-C1	-2.12	104.90	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	BCR	C15-C16-C17	-2.12	119.14	123.47
31	b	627	LMT	C1'-O5'-C5'	-2.12	109.53	113.69
22	c	507	CLA	CHD-C1D-ND	-2.12	122.51	124.45
24	a	410	BCR	C15-C14-C13	-2.12	124.29	127.31
34	f	101	HEM	CHC-C4B-C3B	2.12	127.81	124.57
22	B	615	CLA	CHD-C1D-ND	-2.12	122.51	124.45
22	B	610	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
25	b	601	DGD	CAB-C9B-C8B	-2.11	103.69	114.42
27	e	101	LMG	O3-C3-C2	-2.11	105.46	110.35
22	d	405	CLA	CHD-C1D-ND	-2.11	122.51	124.45
25	C	517	DGD	CAB-C9B-C8B	-2.11	103.70	114.42
25	C	517	DGD	C3G-O3G-C1D	2.11	117.86	113.74
22	B	614	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	c	518	LMG	O3-C3-C2	-2.11	105.47	110.35
22	C	502	CLA	C1-C2-C3	-2.11	122.39	126.04
24	b	623	BCR	C15-C14-C13	-2.11	124.30	127.31
24	y	101	BCR	C15-C16-C17	-2.11	119.15	123.47
27	d	407	LMG	O6-C1-O1	-2.11	104.98	109.97
24	B	619	BCR	C11-C10-C9	-2.11	124.30	127.31
22	A	402	CLA	CHD-C1D-ND	-2.11	122.52	124.45
22	c	508	CLA	CHD-C1D-ND	-2.11	122.52	124.45
24	c	514	BCR	C24-C23-C22	-2.11	123.05	126.23
27	M	101	LMG	O3-C3-C2	-2.11	105.48	110.35
34	F	101	HEM	CHC-C4B-C3B	2.10	127.79	124.57
24	H	102	BCR	C29-C30-C25	2.10	113.72	110.48
30	A	413	SQD	C4-C3-C2	2.10	114.49	110.82
24	f	102	BCR	C27-C26-C25	2.10	125.78	122.73
22	b	614	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
23	D	407	PL9	O2-C1-C2	-2.10	116.97	121.78
27	c	518	LMG	O2-C2-C1	-2.10	104.94	110.05
22	b	610	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	A	415	LMG	O3-C3-C2	-2.10	105.50	110.35
24	b	621	BCR	C35-C13-C14	-2.10	119.98	122.92
22	C	506	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	I	101	LMG	O7-C10-O9	-2.09	118.64	123.70
25	B	625	DGD	CAB-C9B-C8B	-2.09	103.81	114.42
22	C	520	CLA	CHD-C1D-ND	-2.09	122.53	124.45
30	F	102	SQD	O48-C23-C24	2.09	118.47	111.91
22	B	601	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	a	409	PL9	O2-C1-C6	2.09	124.21	120.59
22	D	406	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	j	102	BCR	C20-C21-C22	-2.09	124.33	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	DGD	C1D-C2D-C3D	-2.09	105.65	110.00
27	A	415	LMG	O7-C10-O9	-2.09	118.66	123.70
27	B	621	LMG	O2-C2-C1	-2.09	104.98	110.05
25	c	517	DGD	CAB-C9B-C8B	-2.08	103.84	114.42
22	b	616	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
22	B	605	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	d	406	PL9	O2-C1-C6	2.08	124.20	120.59
27	b	625	LMG	O2-C2-C1	-2.08	104.99	110.05
22	a	406	CLA	CHD-C1D-ND	-2.08	122.54	124.45
26	A	409	LHG	C27-C26-C25	-2.08	103.86	114.42
25	b	624	DGD	CAB-C9B-C8B	-2.08	103.86	114.42
27	i	101	LMG	O1-C1-C2	-2.08	105.05	108.30
22	c	501	CLA	CHD-C1D-ND	-2.08	122.54	124.45
25	d	408	DGD	C5B-C4B-C3B	-2.08	103.86	114.42
22	C	501	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
32	D	401	PHO	O2A-CGA-O1A	-2.08	118.34	123.59
22	b	608	CLA	CHD-C1D-ND	-2.08	122.54	124.45
24	C	514	BCR	C7-C8-C9	-2.08	123.09	126.23
22	b	607	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	B	609	CLA	CHD-C1D-ND	-2.08	122.55	124.45
25	C	516	DGD	C1D-C2D-C3D	-2.07	105.67	110.00
22	C	504	CLA	O1D-CGD-CBD	2.07	128.73	124.48
25	B	620	DGD	C4E-C3E-C2E	-2.07	107.20	110.82
22	B	606	CLA	C1-C2-C3	-2.07	122.46	126.04
25	c	516	DGD	CAB-C9B-C8B	-2.07	103.91	114.42
23	d	406	PL9	C31-C32-C33	-2.07	105.07	111.88
22	b	616	CLA	CHD-C1D-ND	-2.07	122.55	124.45
24	B	616	BCR	C38-C26-C25	-2.07	122.20	124.53
22	B	606	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
24	B	618	BCR	C33-C5-C6	-2.07	122.20	124.53
27	E	101	LMG	O1-C7-C8	-2.07	105.91	110.90
27	M	101	LMG	C1-O6-C5	-2.07	109.63	113.69
22	C	520	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
27	E	101	LMG	O3-C3-C2	-2.07	105.57	110.35
22	C	505	CLA	CHD-C1D-ND	-2.07	122.56	124.45
22	B	612	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
27	m	101	LMG	O3-C3-C2	-2.06	105.58	110.35
22	c	512	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	A	406	PL9	O2-C1-C2	-2.06	117.06	121.78
23	a	409	PL9	O2-C1-C2	-2.06	117.06	121.78
25	D	409	DGD	CAB-C9B-C8B	-2.06	103.96	114.42
27	B	624	LMG	O1-C1-C2	-2.06	105.08	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	g	101	BCR	C15-C14-C13	-2.06	124.37	127.31
25	D	409	DGD	C5B-C4B-C3B	-2.06	103.96	114.42
24	C	513	BCR	C11-C10-C9	-2.06	124.37	127.31
24	D	411	BCR	C27-C26-C25	2.06	125.72	122.73
22	b	606	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	c	508	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	c	504	CLA	O1D-CGD-CBD	2.06	128.69	124.48
24	C	521	BCR	C38-C26-C25	-2.05	122.22	124.53
24	b	622	BCR	C27-C26-C25	2.05	125.71	122.73
25	c	516	DGD	C1D-O6D-C5D	-2.05	109.67	113.69
22	b	606	CLA	O2D-CGD-CBD	2.05	114.91	111.27
23	A	406	PL9	O2-C1-C6	2.05	124.14	120.59
22	B	607	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	c	501	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	b	620	BCR	C15-C16-C17	-2.04	119.28	123.47
24	C	513	BCR	C38-C26-C25	-2.04	122.23	124.53
22	a	405	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	H	101	CLA	C1-C2-C3	-2.04	122.52	126.04
22	C	512	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	d	408	DGD	CAB-C9B-C8B	-2.04	104.08	114.42
24	b	621	BCR	C24-C23-C22	-2.04	123.16	126.23
22	b	613	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
24	B	616	BCR	C7-C8-C9	-2.04	123.16	126.23
25	C	517	DGD	C5B-C4B-C3B	-2.04	104.09	114.42
23	A	406	PL9	O1-C4-C3	-2.03	118.48	120.72
27	a	413	LMG	O2-C2-C1	-2.03	105.10	110.05
30	f	103	SQD	O48-C23-C24	2.03	118.29	111.91
22	B	610	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	D	407	PL9	C12-C13-C14	-2.03	122.77	127.66
27	a	413	LMG	O7-C10-O9	-2.03	118.79	123.70
32	D	402	PHO	CMC-C2C-C3C	2.03	128.77	124.94
22	b	618	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	b	609	CLA	O1D-CGD-CBD	2.03	128.64	124.48
22	c	509	CLA	CHD-C1D-ND	-2.03	122.59	124.45
27	A	410	LMG	O7-C10-O9	-2.03	118.80	123.70
22	A	403	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	a	406	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	c	520	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	B	612	CLA	CHD-C1D-ND	-2.03	122.59	124.45
22	a	404	CLA	C1-C2-C3	-2.03	122.54	126.04
25	d	408	DGD	CBB-CAB-C9B	-2.03	104.14	114.42
32	d	401	PHO	O2A-CGA-O1A	-2.03	118.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	613	CLA	CHD-C1D-ND	-2.03	122.59	124.45
23	D	407	PL9	O2-C1-C6	2.02	124.10	120.59
27	e	101	LMG	O7-C10-O9	-2.02	118.81	123.70
25	c	517	DGD	C5B-C4B-C3B	-2.02	104.15	114.42
26	C	519	LHG	C27-C26-C25	-2.02	104.16	114.42
27	i	101	LMG	O7-C10-O9	-2.02	118.82	123.70
24	J	102	BCR	C34-C9-C10	-2.02	120.09	122.92
25	C	515	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
27	a	413	LMG	O1-C1-C2	-2.02	105.15	108.30
25	D	409	DGD	CBB-CAB-C9B	-2.02	104.18	114.42
22	B	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
25	c	515	DGD	C5B-C4B-C3B	-2.02	104.19	114.42
24	B	617	BCR	C38-C26-C25	-2.02	122.26	124.53
22	C	510	CLA	CHD-C1D-ND	-2.02	122.60	124.45
24	C	521	BCR	C7-C8-C9	-2.01	123.19	126.23
22	b	612	CLA	C1-C2-C3	-2.01	122.56	126.04
25	B	620	DGD	CAB-C9B-C8B	-2.01	104.21	114.42
26	c	519	LHG	C27-C26-C25	-2.01	104.21	114.42
24	B	617	BCR	C24-C23-C22	-2.01	123.20	126.23
24	D	411	BCR	C24-C23-C22	-2.01	123.20	126.23
24	c	513	BCR	C38-C26-C25	-2.01	122.27	124.53
25	B	620	DGD	C5B-C4B-C3B	-2.01	104.24	114.42
27	C	518	LMG	O1-C7-C8	-2.01	106.06	110.90
22	b	619	CLA	CHD-C1D-ND	-2.00	122.61	124.45
27	c	518	LMG	O1-C7-C8	-2.00	106.07	110.90
22	c	510	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	404	CLA	ND
22	A	405	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	609	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	C	501	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	508	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	520	CLA	ND
22	D	405	CLA	ND
22	H	101	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	CLA	ND
22	a	408	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	608	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	b	617	CLA	ND
22	b	618	CLA	ND
22	b	619	CLA	ND
22	c	501	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	520	CLA	ND
22	d	404	CLA	ND
22	d	405	CLA	ND
22	h	101	CLA	ND

All (2140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	402	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	A	404	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C2-C3-C5-C6
22	B	602	CLA	C4-C3-C5-C6
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	604	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	609	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CHA-CBD-CGD-O1D
22	B	613	CLA	CHA-CBD-CGD-O2D
22	B	613	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	C6-C7-C8-C9
22	C	511	CLA	C1A-C2A-CAA-CBA
22	D	405	CLA	C2-C3-C5-C6
22	D	405	CLA	C4-C3-C5-C6
22	H	101	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C3A-C2A-CAA-CBA
22	H	101	CLA	C2-C3-C5-C6
22	H	101	CLA	C4-C3-C5-C6
22	H	101	CLA	C6-C7-C8-C9
22	a	404	CLA	CBD-CGD-O2D-CED
22	a	405	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
22	b	605	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C2A-CAA-CBA-CGA
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	613	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CHA-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O2D
22	b	619	CLA	C3A-C2A-CAA-CBA
22	b	619	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	C1A-C2A-CAA-CBA
22	c	504	CLA	C3A-C2A-CAA-CBA
22	c	504	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	C1A-C2A-CAA-CBA
22	d	404	CLA	C2-C3-C5-C6
22	d	404	CLA	C4-C3-C5-C6
22	h	101	CLA	C1A-C2A-CAA-CBA
22	h	101	CLA	C2-C3-C5-C6
22	h	101	CLA	C4-C3-C5-C6
22	h	101	CLA	C6-C7-C8-C9
23	A	406	PL9	C7-C8-C9-C10
23	A	406	PL9	C7-C8-C9-C11
23	A	406	PL9	C12-C13-C14-C15
23	A	406	PL9	C12-C13-C14-C16
23	A	406	PL9	C17-C18-C19-C20
23	A	406	PL9	C17-C18-C19-C21
23	A	406	PL9	C22-C23-C24-C25
23	A	406	PL9	C24-C26-C27-C28
23	A	406	PL9	C27-C28-C29-C30
23	A	406	PL9	C27-C28-C29-C31
23	A	406	PL9	C30-C29-C31-C32
23	A	406	PL9	C37-C38-C39-C41
23	D	407	PL9	C27-C28-C29-C31
23	D	407	PL9	C34-C36-C37-C38
23	J	101	PL9	C12-C13-C14-C16
23	J	101	PL9	C22-C23-C24-C25
23	J	101	PL9	C22-C23-C24-C26
23	a	409	PL9	C7-C8-C9-C11
23	a	409	PL9	C12-C13-C14-C15
23	a	409	PL9	C12-C13-C14-C16
23	a	409	PL9	C17-C18-C19-C21
23	a	409	PL9	C22-C23-C24-C25
23	a	409	PL9	C24-C26-C27-C28
23	a	409	PL9	C27-C28-C29-C30
23	a	409	PL9	C27-C28-C29-C31
23	a	409	PL9	C30-C29-C31-C32
23	a	409	PL9	C37-C38-C39-C41
23	d	406	PL9	C27-C28-C29-C31
23	d	406	PL9	C34-C36-C37-C38
23	j	101	PL9	C12-C13-C14-C16
23	j	101	PL9	C22-C23-C24-C25
23	j	101	PL9	C22-C23-C24-C26

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Mol	Chain	Res	Type	Atoms
24	B	616	BCR	C1-C6-C7-C8
24	B	617	BCR	C21-C22-C23-C24
24	B	617	BCR	C37-C22-C23-C24
24	B	617	BCR	C23-C24-C25-C26
24	C	513	BCR	C1-C6-C7-C8
24	C	513	BCR	C6-C7-C8-C9
24	C	521	BCR	C7-C8-C9-C34
24	D	411	BCR	C1-C6-C7-C8
24	D	411	BCR	C7-C8-C9-C10
24	H	102	BCR	C7-C8-C9-C34
24	H	102	BCR	C21-C22-C23-C24
24	H	102	BCR	C37-C22-C23-C24
24	J	102	BCR	C1-C6-C7-C8
24	J	102	BCR	C21-C22-C23-C24
24	J	102	BCR	C37-C22-C23-C24
24	y	101	BCR	C7-C8-C9-C10
24	b	620	BCR	C1-C6-C7-C8
24	b	621	BCR	C21-C22-C23-C24
24	b	621	BCR	C23-C24-C25-C26
24	b	623	BCR	C23-C24-C25-C30
24	c	513	BCR	C6-C7-C8-C9
24	c	521	BCR	C7-C8-C9-C10
24	c	521	BCR	C7-C8-C9-C34
24	f	102	BCR	C1-C6-C7-C8
24	f	102	BCR	C7-C8-C9-C10
24	f	102	BCR	C37-C22-C23-C24
24	j	102	BCR	C1-C6-C7-C8
24	j	102	BCR	C21-C22-C23-C24
24	g	101	BCR	C7-C8-C9-C10
24	x	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C21-C22-C23-C24
24	x	101	BCR	C37-C22-C23-C24
25	A	408	DGD	C2D-C1D-O3G-C3G
25	B	620	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	O1B-C1B-O2G-C2G
25	B	625	DGD	O2G-C2G-C3G-O3G
25	B	625	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	O6E-C1E-O5D-C6D
25	C	515	DGD	C2B-C1B-O2G-C2G
25	C	515	DGD	O1B-C1B-O2G-C2G
25	C	515	DGD	C2E-C1E-O5D-C6D
25	C	516	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
25	C	516	DGD	C2D-C1D-O3G-C3G
25	C	516	DGD	O6D-C1D-O3G-C3G
25	C	517	DGD	C2D-C1D-O3G-C3G
25	C	517	DGD	O6D-C1D-O3G-C3G
25	D	409	DGD	O1B-C1B-O2G-C2G
25	D	409	DGD	O6D-C1D-O3G-C3G
25	a	411	DGD	C2D-C1D-O3G-C3G
25	b	601	DGD	O1B-C1B-O2G-C2G
25	b	601	DGD	O2G-C2G-C3G-O3G
25	b	601	DGD	C2E-C1E-O5D-C6D
25	b	601	DGD	O6E-C1E-O5D-C6D
25	b	624	DGD	C2E-C1E-O5D-C6D
25	c	515	DGD	C2B-C1B-O2G-C2G
25	c	515	DGD	O1B-C1B-O2G-C2G
25	c	515	DGD	C2E-C1E-O5D-C6D
25	c	516	DGD	O1B-C1B-O2G-C2G
25	c	516	DGD	C2D-C1D-O3G-C3G
25	c	516	DGD	O6D-C1D-O3G-C3G
25	c	517	DGD	C2D-C1D-O3G-C3G
25	c	517	DGD	O6D-C1D-O3G-C3G
25	d	408	DGD	O6D-C1D-O3G-C3G
26	A	409	LHG	C1-C2-C3-O3
26	C	519	LHG	C4-O6-P-O4
26	a	412	LHG	C1-C2-C3-O3
26	c	519	LHG	C3-O3-P-O6
26	c	519	LHG	C4-O6-P-O4
27	B	621	LMG	C11-C10-O7-C8
27	B	624	LMG	O1-C7-C8-O7
27	B	624	LMG	C11-C10-O7-C8
27	B	624	LMG	O10-C28-O8-C9
27	C	518	LMG	C2-C1-O1-C7
27	C	518	LMG	O6-C1-O1-C7
27	C	518	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
27	C	522	LMG	C2-C1-O1-C7
27	C	522	LMG	O6-C1-O1-C7
27	D	408	LMG	C2-C1-O1-C7
27	D	408	LMG	O6-C1-O1-C7
27	D	412	LMG	O9-C10-O7-C8
27	D	412	LMG	C11-C10-O7-C8
27	E	101	LMG	C2-C1-O1-C7
27	E	101	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	O9-C10-O7-C8
27	b	625	LMG	C11-C10-O7-C8
27	b	628	LMG	O1-C7-C8-O7
27	b	628	LMG	C11-C10-O7-C8
27	c	518	LMG	C2-C1-O1-C7
27	c	518	LMG	O6-C1-O1-C7
27	c	518	LMG	O9-C10-O7-C8
27	c	518	LMG	C11-C10-O7-C8
27	c	522	LMG	C2-C1-O1-C7
27	c	522	LMG	O6-C1-O1-C7
27	d	407	LMG	C2-C1-O1-C7
27	d	407	LMG	O6-C1-O1-C7
27	d	410	LMG	O9-C10-O7-C8
27	d	410	LMG	C11-C10-O7-C8
27	e	101	LMG	C2-C1-O1-C7
27	e	101	LMG	O6-C1-O1-C7
27	m	101	LMG	O9-C10-O7-C8
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O8
30	A	413	SQD	C5-C6-S-O9
30	A	414	SQD	C24-C23-O48-C46
30	B	626	SQD	O5-C5-C6-S
30	D	403	SQD	C2-C1-O6-C44
30	D	403	SQD	O5-C1-O6-C44
30	D	403	SQD	O49-C7-O47-C45
30	D	403	SQD	C8-C7-O47-C45
30	a	401	SQD	C24-C23-O48-C46
30	a	415	SQD	C2-C1-O6-C44
30	a	415	SQD	C5-C6-S-O7
30	a	415	SQD	C5-C6-S-O8
30	a	415	SQD	C5-C6-S-O9
30	b	602	SQD	O5-C5-C6-S
30	d	402	SQD	C2-C1-O6-C44
30	d	402	SQD	O5-C1-O6-C44
30	d	402	SQD	O49-C7-O47-C45
30	d	402	SQD	C8-C7-O47-C45
22	B	603	CLA	O1D-CGD-O2D-CED
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	b	619	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	A	402	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	C	520	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	520	CLA	CBD-CGD-O2D-CED
27	E	101	LMG	O10-C28-O8-C9
27	e	101	LMG	O10-C28-O8-C9
30	A	414	SQD	O10-C23-O48-C46
30	a	401	SQD	O10-C23-O48-C46
31	B	628	LMT	C3'-C4'-O1B-C1B
31	b	604	LMT	C3'-C4'-O1B-C1B
22	b	605	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	C8-C9-O8-C28
22	B	609	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
27	a	413	LMG	C29-C28-O8-C9
27	d	407	LMG	C29-C28-O8-C9
30	F	102	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
30	f	103	SQD	C24-C23-O48-C46
23	A	406	PL9	C37-C38-C39-C40
23	a	409	PL9	C37-C38-C39-C40
22	B	605	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
32	a	407	PHO	CBD-CGD-O2D-CED
27	A	410	LMG	O10-C28-O8-C9
27	C	518	LMG	O10-C28-O8-C9
27	D	408	LMG	O10-C28-O8-C9
27	a	413	LMG	O10-C28-O8-C9
27	b	628	LMG	O10-C28-O8-C9
27	c	518	LMG	O10-C28-O8-C9
27	d	407	LMG	O10-C28-O8-C9
30	F	102	SQD	O10-C23-O48-C46
30	f	103	SQD	O10-C23-O48-C46
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
32	D	402	PHO	CBD-CGD-O2D-CED
25	d	408	DGD	O1B-C1B-O2G-C2G
27	A	415	LMG	O9-C10-O7-C8
27	B	621	LMG	O9-C10-O7-C8
27	B	624	LMG	O9-C10-O7-C8
27	I	101	LMG	O9-C10-O7-C8
27	a	402	LMG	O9-C10-O7-C8
27	b	625	LMG	O9-C10-O7-C8
27	b	628	LMG	O9-C10-O7-C8
27	i	101	LMG	O9-C10-O7-C8
31	B	627	LMT	C3'-C4'-O1B-C1B
31	b	603	LMT	C3'-C4'-O1B-C1B
27	c	518	LMG	C8-C9-O8-C28
22	A	404	CLA	C3-C5-C6-C7
22	B	607	CLA	C3-C5-C6-C7
22	B	613	CLA	C3-C5-C6-C7
22	a	406	CLA	C3-C5-C6-C7
22	b	611	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	d	401	PHO	C3-C5-C6-C7
27	A	410	LMG	C29-C28-O8-C9
27	C	518	LMG	C29-C28-O8-C9
27	D	408	LMG	C29-C28-O8-C9
27	c	518	LMG	C29-C28-O8-C9
27	c	522	LMG	C29-C28-O8-C9
27	I	101	LMG	O6-C5-C6-O5
25	B	625	DGD	C2B-C1B-O2G-C2G
25	C	516	DGD	C2B-C1B-O2G-C2G
25	b	601	DGD	C2B-C1B-O2G-C2G
25	c	516	DGD	C2B-C1B-O2G-C2G
27	M	101	LMG	C11-C10-O7-C8
27	a	402	LMG	C11-C10-O7-C8
27	m	101	LMG	C11-C10-O7-C8
30	F	102	SQD	C8-C7-O47-C45
23	J	101	PL9	C27-C28-C29-C31
23	j	101	PL9	C27-C28-C29-C31
22	C	520	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
22	c	520	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
25	A	408	DGD	O6E-C5E-C6E-O5E
27	i	101	LMG	O6-C5-C6-O5
25	b	624	DGD	C4D-C5D-C6D-O5D
25	B	620	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	O6E-C5E-C6E-O5E
22	B	604	CLA	C4-C3-C5-C6
22	b	608	CLA	C4-C3-C5-C6
22	b	611	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	O1D-CGD-O2D-CED
31	i	102	LMT	C3'-C4'-O1B-C1B
25	D	409	DGD	C2A-C1A-O1G-C1G
25	d	408	DGD	C2A-C1A-O1G-C1G
27	B	624	LMG	C29-C28-O8-C9
27	C	522	LMG	C29-C28-O8-C9
27	b	628	LMG	C29-C28-O8-C9
31	I	102	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
22	C	508	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
25	B	620	DGD	C4D-C5D-C6D-O5D
23	J	101	PL9	C7-C8-C9-C10
23	a	409	PL9	C17-C18-C19-C20
23	j	101	PL9	C7-C8-C9-C10
22	c	512	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
22	C	501	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
27	e	101	LMG	O9-C10-O7-C8
23	A	406	PL9	C22-C23-C24-C26
23	J	101	PL9	C7-C8-C9-C11
23	a	409	PL9	C22-C23-C24-C26
23	j	101	PL9	C7-C8-C9-C11
25	C	516	DGD	C4E-C5E-C6E-O5E
25	c	516	DGD	C4E-C5E-C6E-O5E
25	D	409	DGD	O1A-C1A-O1G-C1G
25	d	408	DGD	O1A-C1A-O1G-C1G
27	C	522	LMG	O10-C28-O8-C9
22	b	614	CLA	O1D-CGD-O2D-CED
25	a	411	DGD	O6E-C5E-C6E-O5E
27	b	628	LMG	O6-C5-C6-O5
22	B	611	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
26	A	409	LHG	O2-C2-C3-O3
26	a	412	LHG	O2-C2-C3-O3
22	C	508	CLA	C3-C5-C6-C7
22	H	101	CLA	C3-C5-C6-C7
32	D	401	PHO	C3-C5-C6-C7
27	E	101	LMG	C29-C28-O8-C9
27	e	101	LMG	C29-C28-O8-C9
27	I	101	LMG	C4-C5-C6-O5
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
25	D	409	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
27	A	415	LMG	C11-C10-O7-C8
27	D	408	LMG	C11-C10-O7-C8
27	d	407	LMG	C11-C10-O7-C8
30	f	103	SQD	C8-C7-O47-C45
25	C	515	DGD	O6E-C5E-C6E-O5E
25	c	515	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	C4E-C5E-C6E-O5E
27	i	101	LMG	C4-C5-C6-O5
27	B	624	LMG	O6-C5-C6-O5
22	c	508	CLA	C3-C5-C6-C7
22	B	615	CLA	CBA-CGA-O2A-C1
25	C	516	DGD	O6E-C5E-C6E-O5E
25	c	516	DGD	O6E-C5E-C6E-O5E
27	c	522	LMG	O10-C28-O8-C9
27	C	518	LMG	O6-C5-C6-O5
32	D	401	PHO	C4-C3-C5-C6
32	d	401	PHO	C4-C3-C5-C6
25	A	408	DGD	C4E-C5E-C6E-O5E
32	D	401	PHO	C2-C3-C5-C6
32	d	401	PHO	C2-C3-C5-C6
22	B	601	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	B	606	CLA	O1D-CGD-O2D-CED
27	c	518	LMG	O6-C5-C6-O5
25	B	620	DGD	C4E-C5E-C6E-O5E
25	B	620	DGD	O6E-C1E-O5D-C6D
25	C	515	DGD	O6E-C1E-O5D-C6D
25	b	624	DGD	O6E-C1E-O5D-C6D
25	c	515	DGD	O6E-C1E-O5D-C6D
27	A	415	LMG	O6-C1-O1-C7
27	a	402	LMG	O6-C1-O1-C7
32	d	401	PHO	CBA-CGA-O2A-C1
25	C	515	DGD	C4E-C5E-C6E-O5E
25	c	515	DGD	C4E-C5E-C6E-O5E
22	B	615	CLA	O1A-CGA-O2A-C1
25	d	408	DGD	C2B-C1B-O2G-C2G
27	i	101	LMG	C11-C10-O7-C8
23	a	409	PL9	C7-C8-C9-C10
22	c	509	CLA	CBD-CGD-O2D-CED
27	E	101	LMG	O9-C10-O7-C8
27	d	407	LMG	O9-C10-O7-C8
32	d	401	PHO	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	CBA-CGA-O2A-C1
22	b	619	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
32	D	401	PHO	CBA-CGA-O2A-C1
27	C	518	LMG	C4-C5-C6-O5
27	c	518	LMG	C4-C5-C6-O5
22	B	605	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	C15-C16-C17-C18
22	B	611	CLA	C5-C6-C7-C8
22	b	610	CLA	C15-C16-C17-C18
25	a	411	DGD	C4E-C5E-C6E-O5E
34	V	201	HEM	C2D-C3D-CAD-CBD
22	B	615	CLA	C5-C6-C7-C8
27	C	518	LMG	C10-C11-C12-C13
25	D	409	DGD	C2D-C1D-O3G-C3G
25	d	408	DGD	C2D-C1D-O3G-C3G
25	C	516	DGD	O2G-C2G-C3G-O3G
25	c	516	DGD	O2G-C2G-C3G-O3G
27	m	101	LMG	O1-C7-C8-O7
30	b	602	SQD	O10-C23-O48-C46
32	D	401	PHO	O1A-CGA-O2A-C1
27	b	628	LMG	C4-C5-C6-O5
22	b	608	CLA	C2-C3-C5-C6
22	B	607	CLA	C6-C7-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C9
22	a	405	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	b	613	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
22	c	510	CLA	C6-C7-C8-C9
22	A	404	CLA	C10-C11-C12-C13
22	b	615	CLA	C5-C6-C7-C8
22	b	615	CLA	C13-C15-C16-C17
22	b	619	CLA	C5-C6-C7-C8
32	a	407	PHO	C15-C16-C17-C18
22	b	613	CLA	C2A-CAA-CBA-CGA
24	D	411	BCR	C37-C22-C23-C24
24	y	101	BCR	C7-C8-C9-C34
24	b	621	BCR	C37-C22-C23-C24
24	j	102	BCR	C37-C22-C23-C24
24	g	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	B	617	BCR	C7-C8-C9-C10
24	b	621	BCR	C7-C8-C9-C10
27	I	101	LMG	C11-C10-O7-C8
25	d	408	DGD	C1B-C2B-C3B-C4B
27	A	415	LMG	C28-C29-C30-C31
27	B	621	LMG	C10-C11-C12-C13
27	b	625	LMG	C10-C11-C12-C13
22	b	619	CLA	O1A-CGA-O2A-C1
22	B	611	CLA	C13-C15-C16-C17
22	c	503	CLA	C10-C11-C12-C13
22	b	609	CLA	O1D-CGD-O2D-CED
32	a	407	PHO	O1D-CGD-O2D-CED
27	c	522	LMG	O6-C5-C6-O5
22	h	101	CLA	C3-C5-C6-C7
22	B	603	CLA	C13-C15-C16-C17
22	B	609	CLA	C8-C10-C11-C12
22	C	520	CLA	C15-C16-C17-C18
22	a	406	CLA	C10-C11-C12-C13
22	b	619	CLA	C10-C11-C12-C13
22	c	520	CLA	C13-C15-C16-C17
22	c	520	CLA	C15-C16-C17-C18
32	D	402	PHO	C15-C16-C17-C18
22	B	608	CLA	C13-C15-C16-C17
22	B	615	CLA	C10-C11-C12-C13
22	C	501	CLA	C15-C16-C17-C18
22	C	503	CLA	C10-C11-C12-C13
22	C	504	CLA	C10-C11-C12-C13
22	C	505	CLA	C15-C16-C17-C18
22	C	507	CLA	C10-C11-C12-C13
22	C	508	CLA	C5-C6-C7-C8
22	C	520	CLA	C13-C15-C16-C17
22	D	405	CLA	C13-C15-C16-C17
22	D	405	CLA	C15-C16-C17-C18
22	b	607	CLA	C13-C15-C16-C17
22	b	612	CLA	C13-C15-C16-C17
22	b	613	CLA	C8-C10-C11-C12
22	c	504	CLA	C10-C11-C12-C13
22	c	505	CLA	C5-C6-C7-C8
22	c	505	CLA	C15-C16-C17-C18
22	c	507	CLA	C10-C11-C12-C13
22	c	508	CLA	C5-C6-C7-C8
22	d	404	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	d	404	CLA	C15-C16-C17-C18
23	D	407	PL9	C27-C28-C29-C30
25	C	515	DGD	C1B-C2B-C3B-C4B
25	D	409	DGD	C1B-C2B-C3B-C4B
27	C	518	LMG	C28-C29-C30-C31
27	D	412	LMG	C10-C11-C12-C13
27	c	518	LMG	C28-C29-C30-C31
27	d	410	LMG	C10-C11-C12-C13
22	C	501	CLA	C8-C10-C11-C12
22	C	505	CLA	C13-C15-C16-C17
22	C	509	CLA	C15-C16-C17-C18
22	b	610	CLA	C13-C15-C16-C17
22	b	614	CLA	C15-C16-C17-C18
22	c	505	CLA	C13-C15-C16-C17
22	c	509	CLA	C15-C16-C17-C18
27	c	522	LMG	C4-C5-C6-O5
22	B	601	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
22	b	605	CLA	C13-C15-C16-C17
22	c	501	CLA	C15-C16-C17-C18
22	c	510	CLA	C5-C6-C7-C8
25	c	515	DGD	C1B-C2B-C3B-C4B
27	C	522	LMG	C10-C11-C12-C13
27	c	518	LMG	C10-C11-C12-C13
27	c	522	LMG	C10-C11-C12-C13
27	c	522	LMG	C11-C10-O7-C8
22	b	611	CLA	C15-C16-C17-C18
22	c	506	CLA	C5-C6-C7-C8
22	C	512	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C10-C8-C7
22	A	402	CLA	C3-C5-C6-C7
22	C	512	CLA	O1A-CGA-O2A-C1
22	A	402	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	O1D-CGD-O2D-CED
32	D	402	PHO	O1D-CGD-O2D-CED
22	A	403	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C5-C6-C7-C8
22	C	507	CLA	C15-C16-C17-C18
22	C	512	CLA	C15-C16-C17-C18
22	a	405	CLA	C15-C16-C17-C18
22	c	501	CLA	C10-C11-C12-C13
22	c	507	CLA	C15-C16-C17-C18
27	I	101	LMG	O6-C1-O1-C7
27	i	101	LMG	O6-C1-O1-C7
30	A	413	SQD	O5-C1-O6-C44
30	a	415	SQD	O5-C1-O6-C44
22	A	404	CLA	C15-C16-C17-C18
23	D	407	PL9	C29-C31-C32-C33
23	d	406	PL9	C29-C31-C32-C33
25	b	624	DGD	C1B-C2B-C3B-C4B
24	j	102	BCR	C18-C19-C20-C21
27	D	408	LMG	O9-C10-O7-C8
22	a	404	CLA	C3-C5-C6-C7
22	B	607	CLA	C15-C16-C17-C18
22	B	610	CLA	C15-C16-C17-C18
22	C	506	CLA	C5-C6-C7-C8
22	a	406	CLA	C15-C16-C17-C18
22	c	501	CLA	C8-C10-C11-C12
22	c	512	CLA	C15-C16-C17-C18
22	B	604	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
30	B	626	SQD	O10-C23-O48-C46
22	B	607	CLA	C5-C6-C7-C8
22	C	510	CLA	C5-C6-C7-C8
22	C	511	CLA	O1D-CGD-O2D-CED
27	C	522	LMG	C11-C10-O7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
26	C	519	LHG	C3-O3-P-O6
26	C	519	LHG	C4-O6-P-O3
26	c	519	LHG	C4-O6-P-O3
27	a	402	LMG	C28-C29-C30-C31
27	I	101	LMG	C29-C28-O8-C9
22	b	619	CLA	C13-C15-C16-C17
25	C	515	DGD	C1A-C2A-C3A-C4A
30	a	415	SQD	C7-C8-C9-C10
25	C	517	DGD	O1B-C1B-O2G-C2G
25	c	517	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	O9-C10-O7-C8
22	B	604	CLA	C2-C3-C5-C6
22	C	501	CLA	C10-C11-C12-C13
22	b	618	CLA	C13-C15-C16-C17
22	c	520	CLA	C10-C11-C12-C13
22	C	511	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	CBA-CGA-O2A-C1
22	c	511	CLA	CBA-CGA-O2A-C1
22	c	520	CLA	CBA-CGA-O2A-C1
30	b	602	SQD	C24-C23-O48-C46
31	b	604	LMT	O1'-C1-C2-C3
25	b	601	DGD	C5B-C6B-C7B-C8B
22	B	615	CLA	C13-C15-C16-C17
22	C	520	CLA	C10-C11-C12-C13
22	b	611	CLA	C5-C6-C7-C8
22	b	619	CLA	C3-C5-C6-C7
25	B	620	DGD	C3B-C4B-C5B-C6B
25	C	516	DGD	C2A-C3A-C4A-C5A
25	D	409	DGD	C4B-C5B-C6B-C7B
25	D	409	DGD	C5B-C6B-C7B-C8B
25	b	624	DGD	C3B-C4B-C5B-C6B
25	c	515	DGD	C3B-C4B-C5B-C6B
27	A	410	LMG	C34-C35-C36-C37
27	I	101	LMG	C14-C15-C16-C17
27	b	625	LMG	C31-C32-C33-C34
27	i	101	LMG	C12-C13-C14-C15
30	b	602	SQD	C11-C10-C9-C8
31	I	102	LMT	C6-C7-C8-C9
31	i	102	LMT	C6-C7-C8-C9
22	b	611	CLA	O1D-CGD-O2D-CED
25	B	625	DGD	C5B-C6B-C7B-C8B
25	D	409	DGD	CEB-CFB-CGB-CHB
25	a	411	DGD	C8B-C9B-CAB-CBB
25	b	601	DGD	C9B-CAB-CBB-CCB
25	b	624	DGD	C6B-C7B-C8B-C9B
27	A	415	LMG	C30-C31-C32-C33
27	B	621	LMG	C31-C32-C33-C34
27	C	518	LMG	C29-C30-C31-C32
27	I	101	LMG	C12-C13-C14-C15
27	c	518	LMG	C29-C30-C31-C32
30	F	102	SQD	C12-C13-C14-C15
30	f	103	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C9-C8-O7-C10
27	e	101	LMG	C7-C8-O7-C10
27	C	522	LMG	O9-C10-O7-C8
30	F	102	SQD	O49-C7-O47-C45
25	A	408	DGD	C8B-C9B-CAB-CBB
25	C	515	DGD	C3B-C4B-C5B-C6B
25	c	516	DGD	C2A-C3A-C4A-C5A
25	d	408	DGD	C5B-C6B-C7B-C8B
25	d	408	DGD	CCB-CDB-CEB-CFB
25	d	408	DGD	CEB-CFB-CGB-CHB
27	C	522	LMG	C12-C13-C14-C15
27	c	522	LMG	C12-C13-C14-C15
27	i	101	LMG	C16-C17-C18-C19
30	B	626	SQD	C9-C10-C11-C12
27	C	522	LMG	O6-C5-C6-O5
25	B	620	DGD	C7A-C8A-C9A-CAA
25	B	625	DGD	C9B-CAB-CBB-CCB
25	D	409	DGD	CCB-CDB-CEB-CFB
25	c	516	DGD	C4A-C5A-C6A-C7A
25	d	408	DGD	C4B-C5B-C6B-C7B
27	a	402	LMG	C32-C33-C34-C35
27	a	413	LMG	C34-C35-C36-C37
27	d	407	LMG	C14-C15-C16-C17
30	A	413	SQD	C14-C15-C16-C17
22	b	616	CLA	C5-C6-C7-C8
25	B	620	DGD	C6B-C7B-C8B-C9B
25	c	515	DGD	C3A-C4A-C5A-C6A
27	A	415	LMG	C18-C19-C20-C21
27	a	402	LMG	C30-C31-C32-C33
30	a	415	SQD	C14-C15-C16-C17
31	B	628	LMT	O1'-C1-C2-C3
27	d	410	LMG	O6-C5-C6-O5
22	c	512	CLA	O1D-CGD-O2D-CED
24	H	102	BCR	C11-C10-C9-C8
24	j	102	BCR	C20-C21-C22-C23
24	x	101	BCR	C11-C10-C9-C8
25	D	409	DGD	C2E-C1E-O5D-C6D
25	d	408	DGD	C2E-C1E-O5D-C6D
27	I	101	LMG	C2-C1-O1-C7
27	i	101	LMG	C2-C1-O1-C7
27	B	624	LMG	C4-C5-C6-O5
25	C	515	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
25	b	624	DGD	C7A-C8A-C9A-CAA
27	A	410	LMG	C33-C34-C35-C36
27	A	415	LMG	C15-C16-C17-C18
22	b	608	CLA	O1A-CGA-O2A-C1
22	B	611	CLA	O1D-CGD-O2D-CED
22	c	509	CLA	C4-C3-C5-C6
25	D	409	DGD	C7B-C8B-C9B-CAB
25	d	408	DGD	C7B-C8B-C9B-CAB
27	A	410	LMG	C31-C32-C33-C34
27	B	624	LMG	C18-C19-C20-C21
27	D	408	LMG	C14-C15-C16-C17
27	D	408	LMG	C19-C20-C21-C22
27	a	402	LMG	C18-C19-C20-C21
27	a	413	LMG	C31-C32-C33-C34
27	a	413	LMG	C33-C34-C35-C36
30	B	626	SQD	C11-C10-C9-C8
30	b	602	SQD	C9-C10-C11-C12
22	A	403	CLA	C6-C7-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16
22	H	101	CLA	C11-C12-C13-C14
22	a	404	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C12-C13-C14
22	b	612	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
25	B	620	DGD	C1B-C2B-C3B-C4B
27	A	415	LMG	C32-C33-C34-C35
27	B	624	LMG	C31-C32-C33-C34
27	I	101	LMG	C16-C17-C18-C19
27	b	628	LMG	C31-C32-C33-C34
27	d	407	LMG	C19-C20-C21-C22
27	i	101	LMG	C14-C15-C16-C17
30	F	102	SQD	C11-C12-C13-C14
30	a	415	SQD	C27-C28-C29-C30
27	D	412	LMG	O6-C5-C6-O5
22	B	605	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C2A-CAA-CBA-CGA
22	c	520	CLA	C2A-CAA-CBA-CGA
27	C	522	LMG	C4-C5-C6-O5
24	B	617	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	b	621	BCR	C7-C8-C9-C34
25	C	515	DGD	C4A-C5A-C6A-C7A
25	C	515	DGD	C2B-C3B-C4B-C5B
25	C	517	DGD	CBA-CCA-CDA-CEA
25	C	517	DGD	C9B-CAB-CBB-CCB
25	c	517	DGD	C9B-CAB-CBB-CCB
30	f	103	SQD	C11-C12-C13-C14
24	C	521	BCR	C7-C8-C9-C10
30	b	602	SQD	C8-C7-O47-C45
25	a	411	DGD	C5B-C6B-C7B-C8B
27	b	628	LMG	C18-C19-C20-C21
30	A	413	SQD	C27-C28-C29-C30
27	B	624	LMG	C28-C29-C30-C31
27	E	101	LMG	C28-C29-C30-C31
22	b	615	CLA	O1D-CGD-O2D-CED
25	B	625	DGD	C4A-C5A-C6A-C7A
25	C	517	DGD	CAB-CBB-CCB-CDB
25	D	409	DGD	C5A-C6A-C7A-C8A
25	b	601	DGD	C4A-C5A-C6A-C7A
25	c	515	DGD	C4A-C5A-C6A-C7A
25	c	515	DGD	C2B-C3B-C4B-C5B
25	c	517	DGD	CAB-CBB-CCB-CDB
27	m	101	LMG	C29-C30-C31-C32
27	M	101	LMG	O6-C5-C6-O5
27	a	402	LMG	O6-C5-C6-O5
25	D	409	DGD	O6E-C1E-O5D-C6D
27	B	624	LMG	O6-C1-O1-C7
27	b	628	LMG	O6-C1-O1-C7
22	c	503	CLA	C5-C6-C7-C8
25	A	408	DGD	C5B-C6B-C7B-C8B
27	i	101	LMG	C13-C14-C15-C16
25	C	516	DGD	C4A-C5A-C6A-C7A
27	A	410	LMG	C14-C15-C16-C17
27	I	101	LMG	C13-C14-C15-C16
31	B	628	LMT	C7-C8-C9-C10
25	B	625	DGD	C1A-C2A-C3A-C4A
25	c	517	DGD	C1A-C2A-C3A-C4A
27	b	628	LMG	C28-C29-C30-C31
22	C	503	CLA	C5-C6-C7-C8
22	H	101	CLA	C5-C6-C7-C8
22	B	604	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	d	408	DGD	C5A-C6A-C7A-C8A
27	a	413	LMG	C14-C15-C16-C17
27	d	407	LMG	C32-C33-C34-C35
27	i	101	LMG	C29-C28-O8-C9
27	m	101	LMG	C29-C28-O8-C9
30	B	626	SQD	C24-C23-O48-C46
25	b	624	DGD	O6D-C5D-C6D-O5D
22	B	606	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	C3A-C2A-CAA-CBA
22	a	405	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
22	h	101	CLA	C3A-C2A-CAA-CBA
31	B	622	LMT	C1-C2-C3-C4
25	b	624	DGD	C5B-C6B-C7B-C8B
25	c	517	DGD	CBA-CCA-CDA-CEA
27	c	518	LMG	C12-C13-C14-C15
31	b	604	LMT	C7-C8-C9-C10
22	C	511	CLA	O1A-CGA-O2A-C1
26	a	412	LHG	C25-C26-C27-C28
27	A	410	LMG	C30-C31-C32-C33
27	D	408	LMG	C32-C33-C34-C35
27	E	101	LMG	C15-C16-C17-C18
27	a	413	LMG	C30-C31-C32-C33
27	C	518	LMG	C12-C13-C14-C15
27	D	408	LMG	C15-C16-C17-C18
27	a	402	LMG	C15-C16-C17-C18
27	d	407	LMG	C15-C16-C17-C18
34	V	201	HEM	C4D-C3D-CAD-CBD
25	B	620	DGD	O6D-C5D-C6D-O5D
22	C	509	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C3-C5-C6-C7
25	B	625	DGD	C2B-C3B-C4B-C5B
27	C	518	LMG	C34-C35-C36-C37
22	C	509	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
22	C	520	CLA	CBA-CGA-O2A-C1
22	C	509	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C33-C34-C36-C37
23	a	409	PL9	C33-C34-C36-C37
25	c	516	DGD	CAB-CBB-CCB-CDB
25	B	620	DGD	C5B-C6B-C7B-C8B
25	b	624	DGD	C4B-C5B-C6B-C7B
27	M	101	LMG	C29-C30-C31-C32
27	e	101	LMG	C15-C16-C17-C18
30	D	403	SQD	C9-C10-C11-C12
30	d	402	SQD	C9-C10-C11-C12
31	b	626	LMT	C1-C2-C3-C4
27	A	415	LMG	C31-C32-C33-C34
27	B	624	LMG	C30-C31-C32-C33
27	b	628	LMG	C30-C31-C32-C33
27	b	628	LMG	C36-C37-C38-C39
22	c	520	CLA	O1A-CGA-O2A-C1
25	c	515	DGD	C1A-C2A-C3A-C4A
25	C	515	DGD	C2A-C3A-C4A-C5A
27	c	518	LMG	C34-C35-C36-C37
26	A	409	LHG	O9-C7-O7-C5
30	f	103	SQD	O49-C7-O47-C45
22	C	508	CLA	C2-C1-O2A-CGA
22	c	508	CLA	C2-C1-O2A-CGA
25	b	601	DGD	C2B-C3B-C4B-C5B
27	A	410	LMG	C15-C16-C17-C18
22	H	101	CLA	C13-C15-C16-C17
25	B	620	DGD	C4B-C5B-C6B-C7B
26	C	519	LHG	C24-C25-C26-C27
30	b	602	SQD	C11-C12-C13-C14
31	b	627	LMT	C2B-C1B-O1B-C4'
25	C	516	DGD	C1A-C2A-C3A-C4A
26	a	412	LHG	C23-C24-C25-C26
22	c	506	CLA	CBD-CGD-O2D-CED
24	B	616	BCR	C5-C6-C7-C8
24	B	617	BCR	C23-C24-C25-C30
24	C	513	BCR	C5-C6-C7-C8
24	C	514	BCR	C23-C24-C25-C26
24	C	514	BCR	C23-C24-C25-C30
24	D	411	BCR	C5-C6-C7-C8
24	H	102	BCR	C1-C6-C7-C8
24	H	102	BCR	C5-C6-C7-C8
24	J	102	BCR	C5-C6-C7-C8
24	y	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	y	101	BCR	C23-C24-C25-C30
24	b	620	BCR	C5-C6-C7-C8
24	b	621	BCR	C23-C24-C25-C30
24	b	623	BCR	C23-C24-C25-C26
24	c	513	BCR	C1-C6-C7-C8
24	c	513	BCR	C5-C6-C7-C8
24	c	514	BCR	C23-C24-C25-C26
24	c	514	BCR	C23-C24-C25-C30
24	f	102	BCR	C5-C6-C7-C8
24	j	102	BCR	C5-C6-C7-C8
24	g	101	BCR	C23-C24-C25-C26
24	g	101	BCR	C23-C24-C25-C30
24	x	101	BCR	C1-C6-C7-C8
24	x	101	BCR	C5-C6-C7-C8
25	A	408	DGD	C3B-C4B-C5B-C6B
26	c	519	LHG	C24-C25-C26-C27
22	b	607	CLA	C8-C10-C11-C12
22	h	101	CLA	C5-C6-C7-C8
25	c	517	DGD	C2B-C1B-O2G-C2G
30	B	626	SQD	C8-C7-O47-C45
25	C	516	DGD	CAB-CBB-CCB-CDB
27	D	412	LMG	C17-C18-C19-C20
30	F	102	SQD	C10-C11-C12-C13
30	f	103	SQD	C10-C11-C12-C13
22	C	506	CLA	CBD-CGD-O2D-CED
25	b	601	DGD	C1A-C2A-C3A-C4A
27	e	101	LMG	C28-C29-C30-C31
30	A	413	SQD	C7-C8-C9-C10
26	A	409	LHG	C25-C26-C27-C28
23	d	406	PL9	C47-C48-C49-C51
22	B	603	CLA	C8-C10-C11-C12
22	C	505	CLA	C10-C11-C12-C13
25	D	409	DGD	CAB-CBB-CCB-CDB
27	A	415	LMG	C17-C18-C19-C20
27	a	402	LMG	C31-C32-C33-C34
22	C	512	CLA	C4-C3-C5-C6
23	j	101	PL9	C15-C14-C16-C17
22	A	404	CLA	C6-C7-C8-C10
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C11-C10-C8-C7
22	C	512	CLA	C2-C3-C5-C6
22	C	512	CLA	C12-C13-C15-C16
22	b	605	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C12-C13-C15
22	c	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C11-C10-C8-C7
22	c	512	CLA	C2-C3-C5-C6
22	c	512	CLA	C11-C10-C8-C7
22	c	512	CLA	C12-C13-C15-C16
32	D	402	PHO	C11-C10-C8-C7
32	a	407	PHO	C11-C10-C8-C7
22	c	502	CLA	C3-C5-C6-C7
22	c	509	CLA	C3-C5-C6-C7
25	D	409	DGD	C6B-C7B-C8B-C9B
22	C	511	CLA	C13-C15-C16-C17
22	C	512	CLA	C13-C15-C16-C17
22	h	101	CLA	C13-C15-C16-C17
22	b	605	CLA	C16-C17-C18-C20
31	B	623	LMT	C2B-C1B-O1B-C4'
26	a	412	LHG	O9-C7-O7-C5
25	C	517	DGD	C1A-C2A-C3A-C4A
25	c	516	DGD	C1A-C2A-C3A-C4A
22	D	406	CLA	CBA-CGA-O2A-C1
22	b	614	CLA	CBA-CGA-O2A-C1
22	d	405	CLA	CBA-CGA-O2A-C1
26	C	519	LHG	C24-C23-O8-C6
27	M	101	LMG	C29-C28-O8-C9
25	C	515	DGD	C4B-C5B-C6B-C7B
22	c	501	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	C10-C11-C12-C13
25	D	409	DGD	C2A-C3A-C4A-C5A
25	d	408	DGD	C2A-C3A-C4A-C5A
25	d	408	DGD	CAB-CBB-CCB-CDB
22	C	520	CLA	O1A-CGA-O2A-C1
27	c	518	LMG	C36-C37-C38-C39
30	B	626	SQD	C12-C13-C14-C15
22	D	406	CLA	C15-C16-C17-C18
22	c	505	CLA	C10-C11-C12-C13
25	D	409	DGD	C3A-C4A-C5A-C6A
27	D	408	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
30	B	626	SQD	C11-C12-C13-C14
22	C	509	CLA	C3-C5-C6-C7
25	c	515	DGD	C2A-C3A-C4A-C5A
25	d	408	DGD	C3A-C4A-C5A-C6A
26	a	412	LHG	C30-C31-C32-C33
27	B	624	LMG	C36-C37-C38-C39
27	C	518	LMG	C36-C37-C38-C39
31	B	622	LMT	O1'-C1-C2-C3
22	B	612	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C19
25	d	408	DGD	O6E-C1E-O5D-C6D
22	a	408	CLA	C10-C11-C12-C13
22	b	605	CLA	C10-C11-C12-C13
27	D	412	LMG	C31-C32-C33-C34
27	b	625	LMG	C13-C14-C15-C16
27	d	410	LMG	C17-C18-C19-C20
25	C	517	DGD	C2B-C1B-O2G-C2G
26	A	409	LHG	C8-C7-O7-C5
26	a	412	LHG	C8-C7-O7-C5
27	E	101	LMG	C11-C10-O7-C8
27	e	101	LMG	C11-C10-O7-C8
26	A	409	LHG	C30-C31-C32-C33
27	D	412	LMG	C34-C35-C36-C37
22	c	511	CLA	C13-C15-C16-C17
23	D	407	PL9	C47-C48-C49-C51
27	C	522	LMG	C16-C17-C18-C19
27	a	413	LMG	C15-C16-C17-C18
30	b	602	SQD	C12-C13-C14-C15
22	a	405	CLA	C3-C5-C6-C7
27	d	410	LMG	C31-C32-C33-C34
27	A	410	LMG	O1-C7-C8-O7
27	I	101	LMG	O1-C7-C8-O7
27	M	101	LMG	O1-C7-C8-O7
27	i	101	LMG	O1-C7-C8-O7
30	A	413	SQD	O47-C45-C46-O48
30	A	414	SQD	O6-C44-C45-O47
30	a	401	SQD	O6-C44-C45-O47
30	a	415	SQD	O47-C45-C46-O48
27	e	101	LMG	O6-C5-C6-O5
27	m	101	LMG	O6-C5-C6-O5
27	d	410	LMG	C34-C35-C36-C37
25	a	411	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
27	B	624	LMG	C17-C18-C19-C20
22	A	405	CLA	C10-C11-C12-C13
22	c	512	CLA	C13-C15-C16-C17
23	d	406	PL9	C35-C34-C36-C37
22	C	504	CLA	C2-C3-C5-C6
22	A	402	CLA	C11-C12-C13-C14
22	A	404	CLA	C6-C7-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	C	503	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	605	CLA	C6-C7-C8-C9
22	b	606	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	c	510	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
22	d	404	CLA	C14-C13-C15-C16
32	D	402	PHO	C11-C10-C8-C9
32	a	407	PHO	C11-C10-C8-C9
27	B	624	LMG	C15-C16-C17-C18
22	C	501	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
22	C	520	CLA	C2A-CAA-CBA-CGA
25	c	515	DGD	C4B-C5B-C6B-C7B
34	v	201	HEM	C4D-C3D-CAD-CBD
34	v	201	HEM	C2D-C3D-CAD-CBD
22	d	405	CLA	C15-C16-C17-C18
25	A	408	DGD	C4B-C5B-C6B-C7B
25	c	517	DGD	C3B-C4B-C5B-C6B
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	D	405	CLA	C1A-C2A-CAA-CBA
22	b	619	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C1A-C2A-CAA-CBA
22	B	612	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C20
25	C	517	DGD	C3B-C4B-C5B-C6B
27	a	413	LMG	C4-C5-C6-O5
22	a	408	CLA	C13-C15-C16-C17
25	d	408	DGD	C6B-C7B-C8B-C9B
27	E	101	LMG	O6-C5-C6-O5
22	C	502	CLA	C3-C5-C6-C7
25	A	408	DGD	C1B-C2B-C3B-C4B
25	a	411	DGD	C1B-C2B-C3B-C4B
27	B	621	LMG	C34-C35-C36-C37
27	b	625	LMG	C34-C35-C36-C37
27	B	621	LMG	C13-C14-C15-C16
27	c	522	LMG	C16-C17-C18-C19
27	d	407	LMG	C13-C14-C15-C16
30	a	401	SQD	C10-C11-C12-C13
22	C	504	CLA	CBA-CGA-O2A-C1
27	B	624	LMG	C32-C33-C34-C35
27	b	628	LMG	C17-C18-C19-C20
31	b	626	LMT	O1'-C1-C2-C3
22	b	614	CLA	O1A-CGA-O2A-C1
25	D	409	DGD	C8B-C9B-CAB-CBB
26	c	519	LHG	C25-C26-C27-C28
27	b	628	LMG	C32-C33-C34-C35
30	A	413	SQD	C17-C18-C19-C20
22	C	503	CLA	C8-C10-C11-C12
22	c	502	CLA	C13-C15-C16-C17
22	B	613	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
22	c	509	CLA	O1D-CGD-O2D-CED
22	A	403	CLA	C3-C5-C6-C7
25	A	408	DGD	C1G-C2G-C3G-O3G
25	C	517	DGD	O1G-C1G-C2G-C3G
25	c	517	DGD	O1G-C1G-C2G-C3G
25	d	408	DGD	C8B-C9B-CAB-CBB
27	B	621	LMG	C7-C8-C9-O8
27	B	624	LMG	O1-C7-C8-C9
27	C	522	LMG	C7-C8-C9-O8
27	D	408	LMG	O1-C7-C8-C9
27	I	101	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	I	101	LMG	C18-C19-C20-C21
27	M	101	LMG	C7-C8-C9-O8
27	a	413	LMG	O1-C7-C8-C9
27	b	625	LMG	C7-C8-C9-O8
27	b	628	LMG	O1-C7-C8-C9
27	c	522	LMG	C7-C8-C9-O8
27	d	407	LMG	O1-C7-C8-C9
27	e	101	LMG	C18-C19-C20-C21
27	i	101	LMG	O1-C7-C8-C9
27	m	101	LMG	C7-C8-C9-O8
30	A	414	SQD	O6-C44-C45-C46
30	B	626	SQD	C44-C45-C46-O48
30	b	602	SQD	C44-C45-C46-O48
22	c	508	CLA	CBA-CGA-O2A-C1
25	a	411	DGD	C4B-C5B-C6B-C7B
27	i	101	LMG	C31-C32-C33-C34
30	a	415	SQD	C17-C18-C19-C20
27	A	410	LMG	C8-C7-O1-C1
27	D	408	LMG	C8-C7-O1-C1
27	d	407	LMG	C8-C7-O1-C1
30	D	403	SQD	C45-C44-O6-C1
30	d	402	SQD	C45-C44-O6-C1
27	E	101	LMG	C17-C18-C19-C20
27	i	101	LMG	C18-C19-C20-C21
22	A	405	CLA	C5-C6-C7-C8
27	c	522	LMG	C17-C18-C19-C20
27	E	101	LMG	O7-C10-C11-C12
26	A	409	LHG	C23-C24-C25-C26
27	d	407	LMG	C28-C29-C30-C31
25	D	409	DGD	CDB-CEB-CFB-CGB
25	d	408	DGD	CDB-CEB-CFB-CGB
27	A	415	LMG	C11-C12-C13-C14
32	d	401	PHO	CBD-CGD-O2D-CED
31	I	102	LMT	C5'-C4'-O1B-C1B
22	b	607	CLA	C15-C16-C17-C18
22	D	406	CLA	O1A-CGA-O2A-C1
27	A	410	LMG	C11-C10-O7-C8
22	c	503	CLA	C8-C10-C11-C12
24	b	621	BCR	C20-C21-C22-C37
22	C	504	CLA	C4-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
22	d	405	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	C24-C23-O8-C6
26	c	519	LHG	C11-C10-C9-C8
30	A	413	SQD	C10-C11-C12-C13
31	i	102	LMT	C5'-C4'-O1B-C1B
25	D	409	DGD	C1G-C2G-O2G-C1B
25	d	408	DGD	C1G-C2G-O2G-C1B
27	E	101	LMG	C7-C8-O7-C10
27	c	518	LMG	C9-C8-O7-C10
31	B	623	LMT	O5B-C1B-O1B-C4'
22	a	408	CLA	C5-C6-C7-C8
22	b	613	CLA	C2-C1-O2A-CGA
26	C	519	LHG	C11-C10-C9-C8
30	A	414	SQD	C10-C11-C12-C13
27	A	415	LMG	O6-C5-C6-O5
25	D	409	DGD	CBA-CCA-CDA-CEA
27	a	402	LMG	C17-C18-C19-C20
27	A	410	LMG	C4-C5-C6-O5
31	b	627	LMT	O5B-C1B-O1B-C4'
24	J	102	BCR	C20-C21-C22-C23
27	B	624	LMG	C2-C1-O1-C7
27	b	628	LMG	C2-C1-O1-C7
27	A	410	LMG	C8-C9-O8-C28
25	C	515	DGD	O2G-C2G-C3G-O3G
25	c	517	DGD	O1G-C1G-C2G-O2G
27	a	413	LMG	O1-C7-C8-O7
27	m	101	LMG	O7-C8-C9-O8
25	d	408	DGD	CBA-CCA-CDA-CEA
25	B	625	DGD	O6D-C5D-C6D-O5D
25	c	516	DGD	O6D-C5D-C6D-O5D
22	B	603	CLA	C15-C16-C17-C18
22	C	504	CLA	C15-C16-C17-C18
22	c	508	CLA	O1A-CGA-O2A-C1
27	i	101	LMG	C17-C18-C19-C20
23	D	407	PL9	C15-C14-C16-C17
27	C	522	LMG	C34-C35-C36-C37
22	B	602	CLA	C11-C12-C13-C15
22	B	605	CLA	C12-C13-C15-C16
22	B	607	CLA	C6-C7-C8-C10
22	B	610	CLA	C11-C10-C8-C7
22	B	612	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C11-C10-C8-C7
22	C	502	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C6-C7-C8-C10
22	C	509	CLA	C11-C10-C8-C7
22	D	405	CLA	C12-C13-C15-C16
22	H	101	CLA	C11-C12-C13-C15
22	a	406	CLA	C6-C7-C8-C10
22	b	616	CLA	C11-C10-C8-C7
22	b	618	CLA	C11-C10-C8-C7
22	b	618	CLA	C12-C13-C15-C16
22	b	619	CLA	C12-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C12-C13-C15
22	c	504	CLA	C2-C3-C5-C6
22	c	504	CLA	C6-C7-C8-C10
22	c	504	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
22	c	510	CLA	C12-C13-C15-C16
22	d	404	CLA	C12-C13-C15-C16
22	h	101	CLA	C6-C7-C8-C10
32	D	402	PHO	C12-C13-C15-C16
32	a	407	PHO	C12-C13-C15-C16
27	b	628	LMG	C15-C16-C17-C18
22	B	602	CLA	C6-C7-C8-C9
22	B	608	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C14
22	C	502	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C12-C13-C14
22	C	504	CLA	C6-C7-C8-C9
22	C	504	CLA	C14-C13-C15-C16
22	C	505	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	D	405	CLA	C14-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	606	CLA	C6-C7-C8-C9
22	b	618	CLA	C11-C10-C8-C9
22	b	618	CLA	C14-C13-C15-C16
22	c	502	CLA	C11-C12-C13-C14
22	c	502	CLA	C14-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C9
22	c	504	CLA	C14-C13-C15-C16
22	c	505	CLA	C14-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16
32	D	402	PHO	C14-C13-C15-C16
32	a	407	PHO	C14-C13-C15-C16
25	D	409	DGD	CAA-CBA-CCA-CDA
22	B	610	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	CBA-CGA-O2A-C1
22	B	615	CLA	C15-C16-C17-C18
22	c	501	CLA	C13-C15-C16-C17
25	c	517	DGD	CFA-CGA-CHA-CIA
27	E	101	LMG	C19-C20-C21-C22
22	C	504	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C16-C17-C18-C20
25	D	409	DGD	C1A-C2A-C3A-C4A
25	C	516	DGD	O6D-C5D-C6D-O5D
22	A	405	CLA	C13-C15-C16-C17
22	B	613	CLA	C15-C16-C17-C18
27	a	413	LMG	C11-C10-O7-C8
27	D	412	LMG	C38-C39-C40-C41
27	a	402	LMG	C11-C12-C13-C14
27	d	410	LMG	C38-C39-C40-C41
22	C	510	CLA	CBA-CGA-O2A-C1
27	e	101	LMG	C19-C20-C21-C22
22	C	502	CLA	C13-C15-C16-C17
22	b	617	CLA	C5-C6-C7-C8
27	B	624	LMG	C19-C20-C21-C22
22	B	609	CLA	C16-C17-C18-C20
22	B	613	CLA	C16-C17-C18-C19
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
22	B	604	CLA	C5-C6-C7-C8
23	D	407	PL9	C24-C26-C27-C28
27	C	522	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
27	E	101	LMG	C18-C19-C20-C21
22	c	504	CLA	C15-C16-C17-C18
27	B	621	LMG	C17-C18-C19-C20
25	b	601	DGD	O6D-C5D-C6D-O5D
23	A	406	PL9	C35-C34-C36-C37
23	D	407	PL9	C35-C34-C36-C37
23	J	101	PL9	C27-C28-C29-C30
27	b	625	LMG	C17-C18-C19-C20
27	b	628	LMG	C19-C20-C21-C22
25	c	516	DGD	C4D-C5D-C6D-O5D
22	b	617	CLA	C16-C17-C18-C20
27	I	101	LMG	C31-C32-C33-C34
22	b	617	CLA	C15-C16-C17-C18
22	b	619	CLA	C8-C10-C11-C12
22	b	613	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	CBA-CGA-O2A-C1
27	D	408	LMG	C28-C29-C30-C31
27	b	628	LMG	C13-C14-C15-C16
22	A	402	CLA	C3A-C2A-CAA-CBA
22	a	404	CLA	C3A-C2A-CAA-CBA
22	B	604	CLA	C15-C16-C17-C18
25	D	409	DGD	C3B-C4B-C5B-C6B
25	c	516	DGD	C3A-C4A-C5A-C6A
25	C	516	DGD	C4D-C5D-C6D-O5D
25	C	517	DGD	CFA-CGA-CHA-CIA
25	B	625	DGD	C5A-C6A-C7A-C8A
25	d	408	DGD	CAA-CBA-CCA-CDA
22	C	508	CLA	C15-C16-C17-C18
25	B	625	DGD	C1G-C2G-C3G-O3G
25	C	516	DGD	C1G-C2G-C3G-O3G
25	D	409	DGD	C1G-C2G-C3G-O3G
25	a	411	DGD	C1G-C2G-C3G-O3G
25	c	516	DGD	C1G-C2G-C3G-O3G
25	d	408	DGD	C1G-C2G-C3G-O3G
27	A	410	LMG	O1-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
27	M	101	LMG	O1-C7-C8-C9
27	c	518	LMG	O1-C7-C8-C9
27	m	101	LMG	O1-C7-C8-C9
30	a	401	SQD	O6-C44-C45-C46
30	A	414	SQD	C9-C10-C11-C12
30	a	415	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	I	101	LMG	O10-C28-O8-C9
27	m	101	LMG	C30-C31-C32-C33
30	a	415	SQD	C10-C11-C12-C13
27	a	413	LMG	O6-C5-C6-O5
23	j	101	PL9	C27-C28-C29-C30
27	D	412	LMG	C19-C20-C21-C22
22	c	511	CLA	C3-C5-C6-C7
27	I	101	LMG	C17-C18-C19-C20
30	A	413	SQD	C31-C32-C33-C34
23	d	406	PL9	C15-C14-C16-C17
26	C	519	LHG	C25-C26-C27-C28
27	D	408	LMG	C29-C30-C31-C32
27	e	101	LMG	C17-C18-C19-C20
22	B	613	CLA	C5-C6-C7-C8
22	b	608	CLA	C10-C11-C12-C13
26	c	519	LHG	O10-C23-O8-C6
22	c	512	CLA	C2A-CAA-CBA-CGA
25	d	408	DGD	C3B-C4B-C5B-C6B
23	d	406	PL9	C27-C28-C29-C30
22	c	504	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C16-C17-C18-C19
22	C	508	CLA	O1A-CGA-O2A-C1
26	C	519	LHG	O10-C23-O8-C6
25	c	516	DGD	C4B-C5B-C6B-C7B
27	c	522	LMG	C34-C35-C36-C37
25	C	517	DGD	O1G-C1G-C2G-O2G
25	c	515	DGD	O2G-C2G-C3G-O3G
27	C	518	LMG	O1-C7-C8-O7
27	C	522	LMG	O7-C8-C9-O8
27	M	101	LMG	O7-C8-C9-O8
27	c	518	LMG	O1-C7-C8-O7
27	c	522	LMG	O7-C8-C9-O8
30	D	403	SQD	O6-C44-C45-O47
30	b	602	SQD	O47-C45-C46-O48
30	d	402	SQD	O6-C44-C45-O47
22	c	506	CLA	O1D-CGD-O2D-CED
30	f	103	SQD	C29-C30-C31-C32
22	B	615	CLA	C8-C10-C11-C12
27	d	410	LMG	C19-C20-C21-C22
30	b	602	SQD	O49-C7-O47-C45
22	B	609	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	a	405	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
32	D	401	PHO	C2-C1-O2A-CGA
31	B	628	LMT	C2-C3-C4-C5
22	b	608	CLA	C15-C16-C17-C18
22	B	605	CLA	C14-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C9
22	D	405	CLA	C6-C7-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
32	d	401	PHO	C6-C7-C8-C9
25	C	517	DGD	CDB-CEB-CFB-CGB
25	D	409	DGD	C2B-C3B-C4B-C5B
25	b	601	DGD	C5A-C6A-C7A-C8A
27	A	410	LMG	O6-C5-C6-O5
22	a	405	CLA	C5-C6-C7-C8
22	b	608	CLA	C5-C6-C7-C8
22	b	613	CLA	C5-C6-C7-C8
22	b	619	CLA	C15-C16-C17-C18
26	A	409	LHG	C2-C3-O3-P
22	B	610	CLA	O1A-CGA-O2A-C1
25	C	516	DGD	C3A-C4A-C5A-C6A
27	c	518	LMG	C13-C14-C15-C16
22	B	609	CLA	C16-C17-C18-C19
22	b	613	CLA	C16-C17-C18-C19
22	C	511	CLA	C3-C5-C6-C7
24	A	407	BCR	C1-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C26
24	A	407	BCR	C23-C24-C25-C30
24	B	619	BCR	C1-C6-C7-C8
24	B	619	BCR	C5-C6-C7-C8
24	B	619	BCR	C23-C24-C25-C26
24	B	619	BCR	C23-C24-C25-C30
24	C	513	BCR	C23-C24-C25-C26
24	C	513	BCR	C23-C24-C25-C30
24	C	521	BCR	C23-C24-C25-C26
24	C	521	BCR	C23-C24-C25-C30
24	a	410	BCR	C1-C6-C7-C8
24	a	410	BCR	C5-C6-C7-C8
24	a	410	BCR	C23-C24-C25-C26
24	a	410	BCR	C23-C24-C25-C30
24	b	623	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	623	BCR	C5-C6-C7-C8
24	c	513	BCR	C23-C24-C25-C26
24	c	513	BCR	C23-C24-C25-C30
25	d	408	DGD	C4E-C5E-C6E-O5E
22	C	506	CLA	O1D-CGD-O2D-CED
24	J	102	BCR	C7-C8-C9-C10
24	c	514	BCR	C7-C8-C9-C10
22	B	609	CLA	C10-C11-C12-C13
22	c	511	CLA	C5-C6-C7-C8
25	d	408	DGD	C1A-C2A-C3A-C4A
34	F	101	HEM	C3D-CAD-CBD-CGD
27	b	625	LMG	C28-C29-C30-C31
32	D	402	PHO	C10-C11-C12-C13
27	B	624	LMG	C20-C21-C22-C23
25	b	624	DGD	C5A-C6A-C7A-C8A
22	C	511	CLA	C5-C6-C7-C8
27	d	407	LMG	C29-C30-C31-C32
22	A	403	CLA	C12-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	B	608	CLA	C12-C13-C15-C16
22	B	609	CLA	C11-C12-C13-C15
22	B	612	CLA	C11-C12-C13-C15
22	B	614	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	C	501	CLA	C11-C12-C13-C15
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C6-C7-C8-C10
22	C	504	CLA	C12-C13-C15-C16
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C10
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C15
22	C	511	CLA	C12-C13-C15-C16
22	H	101	CLA	C6-C7-C8-C10
22	a	405	CLA	C12-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	C6-C7-C8-C10
22	b	614	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C12-C13-C15
22	b	619	CLA	C11-C10-C8-C7
22	c	501	CLA	C11-C12-C13-C15
22	c	502	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
31	B	627	LMT	C5'-C4'-O1B-C1B
22	C	511	CLA	C16-C17-C18-C19
30	b	602	SQD	C10-C11-C12-C13
27	d	407	LMG	C36-C37-C38-C39
22	b	615	CLA	C10-C11-C12-C13
22	C	510	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	C2A-CAA-CBA-CGA
31	b	603	LMT	C4'-C5'-C6'-O6'
24	B	617	BCR	C20-C21-C22-C37
30	B	626	SQD	C10-C11-C12-C13
31	b	603	LMT	C5'-C4'-O1B-C1B
25	C	516	DGD	C4B-C5B-C6B-C7B
30	B	626	SQD	C17-C18-C19-C20
22	B	611	CLA	C10-C11-C12-C13
27	A	410	LMG	C20-C21-C22-C23
30	A	413	SQD	C15-C16-C17-C18
30	a	415	SQD	C15-C16-C17-C18
22	A	404	CLA	C5-C6-C7-C8
22	C	506	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
32	D	401	PHO	CAD-CBD-CGD-O2D
32	d	401	PHO	CAD-CBD-CGD-O2D
22	b	617	CLA	C16-C17-C18-C19
27	C	518	LMG	C13-C14-C15-C16
27	A	410	LMG	O6-C1-O1-C7
25	b	601	DGD	C1G-C2G-C3G-O3G
26	a	412	LHG	C2-C3-O3-P
30	A	413	SQD	C44-C45-C46-O48
30	a	415	SQD	C44-C45-C46-O48
32	D	401	PHO	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	b	628	LMG	C20-C21-C22-C23
22	C	507	CLA	C5-C6-C7-C8
22	b	613	CLA	C10-C11-C12-C13
32	D	401	PHO	C5-C6-C7-C8
34	F	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4B-C3B-CAB-CBB
25	c	517	DGD	CDB-CEB-CFB-CGB
30	B	626	SQD	O49-C7-O47-C45
22	A	404	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	B	611	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CHA-CBD-CGD-O1D
22	b	617	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	c	505	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O2D
27	e	101	LMG	O7-C10-C11-C12
22	c	510	CLA	O1A-CGA-O2A-C1
27	i	101	LMG	O10-C28-O8-C9
25	d	408	DGD	C2B-C3B-C4B-C5B
30	A	414	SQD	C32-C33-C34-C35
30	F	102	SQD	C29-C30-C31-C32
25	a	411	DGD	O2G-C2G-C3G-O3G
27	B	621	LMG	O7-C8-C9-O8
27	b	625	LMG	O7-C8-C9-O8
30	B	626	SQD	O47-C45-C46-O48
22	B	603	CLA	CBA-CGA-O2A-C1
27	c	522	LMG	C35-C36-C37-C38
22	b	613	CLA	O1A-CGA-O2A-C1
27	B	621	LMG	C28-C29-C30-C31
23	A	406	PL9	C4-C3-C7-C8
23	a	409	PL9	C4-C3-C7-C8
27	A	410	LMG	C29-C30-C31-C32
22	c	508	CLA	C15-C16-C17-C18
22	B	608	CLA	C11-C12-C13-C14
22	B	608	CLA	C14-C13-C15-C16
22	C	501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C14-C13-C15-C16
22	b	618	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C10-C8-C9
25	d	408	DGD	C4A-C5A-C6A-C7A
30	D	403	SQD	C5-C6-S-O8
30	d	402	SQD	C5-C6-S-O8
32	d	401	PHO	O1D-CGD-O2D-CED
25	D	409	DGD	C4A-C5A-C6A-C7A
22	B	605	CLA	CBA-CGA-O2A-C1
24	f	102	BCR	C7-C8-C9-C34
24	C	514	BCR	C7-C8-C9-C10
24	H	102	BCR	C7-C8-C9-C10
24	j	102	BCR	C7-C8-C9-C10
22	A	402	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
32	d	401	PHO	C5-C6-C7-C8
22	b	607	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	O2-C2-C3-O3
30	D	403	SQD	C10-C11-C12-C13
27	C	522	LMG	C35-C36-C37-C38
26	C	519	LHG	C3-O3-P-O5
26	C	519	LHG	C4-O6-P-O5
26	c	519	LHG	C3-O3-P-O5
26	c	519	LHG	C4-O6-P-O5
22	A	403	CLA	C5-C6-C7-C8
22	B	604	CLA	C10-C11-C12-C13
27	B	624	LMG	C16-C17-C18-C19
25	D	409	DGD	C4E-C5E-C6E-O5E
22	c	506	CLA	C3-C5-C6-C7
27	c	518	LMG	C32-C33-C34-C35
27	D	408	LMG	C31-C32-C33-C34
27	a	413	LMG	C20-C21-C22-C23
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
30	a	401	SQD	C5-C6-S-O9
27	a	413	LMG	C10-C11-C12-C13
32	a	407	PHO	C10-C11-C12-C13
25	c	515	DGD	C5A-C6A-C7A-C8A
27	d	407	LMG	C31-C32-C33-C34
26	c	519	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	C8-C10-C11-C12
23	a	409	PL9	C35-C34-C36-C37
23	D	407	PL9	C32-C33-C34-C36
22	A	405	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	609	CLA	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	C	512	CLA	C3A-C2A-CAA-CBA
22	D	406	CLA	C11-C10-C8-C7
22	H	101	CLA	C11-C10-C8-C7
22	b	611	CLA	C11-C12-C13-C15
22	b	612	CLA	C12-C13-C15-C16
22	b	613	CLA	C11-C12-C13-C15
22	b	613	CLA	C12-C13-C15-C16
22	c	505	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
22	c	520	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C10-C8-C7
22	h	101	CLA	C11-C10-C8-C7
26	C	519	LHG	O6-C4-C5-O7
26	c	519	LHG	O6-C4-C5-O7
32	a	407	PHO	C6-C7-C8-C10
27	a	413	LMG	C16-C17-C18-C19
31	b	604	LMT	C2-C3-C4-C5
22	A	405	CLA	C16-C17-C18-C19
27	e	101	LMG	O1-C7-C8-C9
30	D	403	SQD	O6-C44-C45-C46
30	d	402	SQD	O6-C44-C45-C46
25	A	408	DGD	O2G-C2G-C3G-O3G
25	D	409	DGD	O2G-C2G-C3G-O3G
25	d	408	DGD	O2G-C2G-C3G-O3G
25	B	620	DGD	CAB-CBB-CCB-CDB
22	B	603	CLA	O1A-CGA-O2A-C1
22	B	605	CLA	O1A-CGA-O2A-C1
25	b	624	DGD	CCA-CDA-CEA-CFA
27	a	413	LMG	C8-C7-O1-C1
22	a	408	CLA	C16-C17-C18-C19
22	C	506	CLA	C3-C5-C6-C7
27	b	625	LMG	C12-C13-C14-C15
30	a	401	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	O1A-C1A-O1G-C1G
27	m	101	LMG	O10-C28-O8-C9
22	b	615	CLA	C4-C3-C5-C6
22	B	609	CLA	C5-C6-C7-C8
32	D	402	PHO	C13-C15-C16-C17
32	a	407	PHO	C13-C15-C16-C17
22	A	403	CLA	C14-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C9
22	B	609	CLA	C11-C12-C13-C14
22	B	612	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C10-C8-C9
22	C	507	CLA	C14-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C9
22	C	511	CLA	C14-C13-C15-C16
22	a	405	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C12-C13-C14
22	b	619	CLA	C11-C10-C8-C9
22	b	619	CLA	C11-C12-C13-C14
22	c	501	CLA	C11-C12-C13-C14
22	c	507	CLA	C14-C13-C15-C16
22	c	511	CLA	C14-C13-C15-C16
22	d	404	CLA	C6-C7-C8-C9
32	D	401	PHO	C6-C7-C8-C9
23	d	406	PL9	C24-C26-C27-C28
27	B	624	LMG	C10-C11-C12-C13
22	C	508	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
27	B	621	LMG	C12-C13-C14-C15
24	c	513	BCR	C11-C12-C13-C35
22	b	609	CLA	C13-C15-C16-C17
22	h	101	CLA	CBA-CGA-O2A-C1
30	d	402	SQD	C10-C11-C12-C13
27	b	628	LMG	C16-C17-C18-C19
22	B	611	CLA	C4-C3-C5-C6
22	C	511	CLA	CAA-CBA-CGA-O2A
27	C	518	LMG	C32-C33-C34-C35
27	a	402	LMG	C16-C17-C18-C19
30	a	401	SQD	C32-C33-C34-C35
30	f	103	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
23	d	406	PL9	C13-C14-C16-C17
25	c	516	DGD	C6A-C7A-C8A-C9A
25	c	517	DGD	C8B-C9B-CAB-CBB
27	E	101	LMG	C31-C32-C33-C34
32	D	401	PHO	O1D-CGD-O2D-CED
30	a	415	SQD	C11-C10-C9-C8
22	c	510	CLA	C3-C5-C6-C7
22	c	511	CLA	CAA-CBA-CGA-O2A
25	b	624	DGD	CAB-CBB-CCB-CDB
27	a	413	LMG	C29-C30-C31-C32
25	C	517	DGD	C3G-C2G-O2G-C1B
25	c	517	DGD	C3G-C2G-O2G-C1B
26	A	409	LHG	C6-C5-O7-C7
26	a	412	LHG	C6-C5-O7-C7
27	m	101	LMG	C9-C8-O7-C10
26	C	519	LHG	O6-C4-C5-C6
26	c	519	LHG	O6-C4-C5-C6
22	b	617	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	O1A-CGA-O2A-C1
22	A	403	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
22	b	616	CLA	C2-C1-O2A-CGA
32	d	401	PHO	C2-C1-O2A-CGA
27	A	410	LMG	C10-C11-C12-C13
30	b	602	SQD	C17-C18-C19-C20
27	M	101	LMG	O10-C28-O8-C9
22	a	406	CLA	C5-C6-C7-C8
25	C	515	DGD	C5A-C6A-C7A-C8A
27	A	410	LMG	C38-C39-C40-C41
22	h	101	CLA	O1A-CGA-O2A-C1
23	D	407	PL9	C20-C19-C21-C22
23	d	406	PL9	C20-C19-C21-C22
27	B	624	LMG	C13-C14-C15-C16
24	A	407	BCR	C5-C6-C7-C8
24	B	617	BCR	C1-C6-C7-C8
24	C	514	BCR	C1-C6-C7-C8
24	C	514	BCR	C5-C6-C7-C8
24	C	521	BCR	C1-C6-C7-C8
24	C	521	BCR	C5-C6-C7-C8
24	c	514	BCR	C1-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	c	521	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	c	521	BCR	C23-C24-C25-C26
24	c	521	BCR	C23-C24-C25-C30
24	g	101	BCR	C5-C6-C7-C8
22	b	616	CLA	C10-C11-C12-C13
27	D	412	LMG	C16-C17-C18-C19
30	A	413	SQD	C11-C10-C9-C8
25	c	515	DGD	O6D-C1D-O3G-C3G
22	d	405	CLA	C2A-CAA-CBA-CGA
27	D	408	LMG	O1-C7-C8-O7
27	d	407	LMG	O1-C7-C8-O7
26	A	409	LHG	C3-O3-P-O6
26	a	412	LHG	C3-O3-P-O6
22	b	606	CLA	C16-C17-C18-C19
25	C	517	DGD	C8B-C9B-CAB-CBB
27	M	101	LMG	C31-C32-C33-C34
27	m	101	LMG	C31-C32-C33-C34
22	B	612	CLA	C10-C11-C12-C13
22	C	504	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C10-C8-C7
22	c	508	CLA	C6-C7-C8-C10
22	B	607	CLA	C11-C12-C13-C14
22	B	610	CLA	C11-C10-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C10-C8-C9
22	b	611	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C12-C13-C14
22	b	619	CLA	C14-C13-C15-C16
22	c	505	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
32	a	407	PHO	C6-C7-C8-C9
25	B	620	DGD	C5A-C6A-C7A-C8A
25	c	515	DGD	C5B-C6B-C7B-C8B
27	c	522	LMG	C32-C33-C34-C35
30	a	401	SQD	C12-C13-C14-C15
27	A	415	LMG	C12-C13-C14-C15
27	A	415	LMG	C16-C17-C18-C19
27	C	522	LMG	C32-C33-C34-C35
22	c	504	CLA	C8-C10-C11-C12
22	A	405	CLA	C16-C17-C18-C20
22	B	609	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	b	617	CLA	C2C-C3C-CAC-CBC
22	b	608	CLA	C8-C10-C11-C12
27	b	625	LMG	C15-C16-C17-C18
26	c	519	LHG	C1-C2-C3-O3
23	d	406	PL9	C32-C33-C34-C36
27	a	413	LMG	C35-C36-C37-C38
27	c	522	LMG	C30-C31-C32-C33
27	d	410	LMG	C16-C17-C18-C19
27	A	410	LMG	C16-C17-C18-C19
34	f	101	HEM	C3D-CAD-CBD-CGD
25	C	515	DGD	C5B-C6B-C7B-C8B
27	a	413	LMG	C11-C12-C13-C14
22	b	616	CLA	C8-C10-C11-C12
25	A	408	DGD	O6E-C1E-O5D-C6D
25	C	516	DGD	O6E-C1E-O5D-C6D
25	b	601	DGD	O6D-C1D-O3G-C3G
25	b	624	DGD	O1A-C1A-O1G-C1G
22	b	616	CLA	C13-C15-C16-C17
25	C	516	DGD	C7B-C8B-C9B-CAB
22	a	408	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C20
22	A	403	CLA	C4-C3-C5-C6
23	D	407	PL9	C40-C39-C41-C42
23	J	101	PL9	C15-C14-C16-C17
27	M	101	LMG	C30-C31-C32-C33
23	D	407	PL9	C13-C14-C16-C17
26	C	519	LHG	O2-C2-C3-O3
27	M	101	LMG	C16-C17-C18-C19
22	A	402	CLA	C2-C1-O2A-CGA
27	B	624	LMG	C29-C30-C31-C32
27	B	621	LMG	C15-C16-C17-C18
22	c	512	CLA	C3A-C2A-CAA-CBA
22	b	606	CLA	C15-C16-C17-C18
22	B	602	CLA	C16-C17-C18-C19
27	e	101	LMG	C31-C32-C33-C34
22	B	610	CLA	C4-C3-C5-C6
27	D	408	LMG	C18-C19-C20-C21
22	B	614	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	D	406	CLA	C11-C10-C8-C9
22	b	612	CLA	C11-C12-C13-C14
22	c	520	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	C11-C10-C8-C9
22	h	101	CLA	C11-C12-C13-C14
22	B	605	CLA	C13-C15-C16-C17
25	c	516	DGD	C7B-C8B-C9B-CAB
27	D	408	LMG	C36-C37-C38-C39
30	A	414	SQD	C12-C13-C14-C15
22	B	602	CLA	C15-C16-C17-C18
27	d	410	LMG	O1-C7-C8-C9
25	d	408	DGD	CBB-CCB-CDB-CEB
25	B	625	DGD	O6D-C1D-O3G-C3G
25	C	515	DGD	O6D-C1D-O3G-C3G
25	a	411	DGD	O6E-C1E-O5D-C6D
25	c	516	DGD	O6E-C1E-O5D-C6D
27	M	101	LMG	O6-C1-O1-C7
27	m	101	LMG	O6-C1-O1-C7
30	F	102	SQD	C9-C10-C11-C12
30	a	415	SQD	C12-C13-C14-C15
27	A	410	LMG	C35-C36-C37-C38
27	C	522	LMG	C30-C31-C32-C33
27	M	101	LMG	C9-C8-O7-C10
22	a	405	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	C	512	CLA	C1A-C2A-CAA-CBA
22	d	404	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C12-C13-C15
22	C	520	CLA	C6-C7-C8-C10
22	D	405	CLA	C11-C10-C8-C7
22	H	101	CLA	C12-C13-C15-C16
22	b	605	CLA	C12-C13-C15-C16
22	b	609	CLA	C6-C7-C8-C10
22	c	505	CLA	C6-C7-C8-C10
27	a	413	LMG	C38-C39-C40-C41
22	B	609	CLA	O1A-CGA-O2A-C1
25	D	409	DGD	CBB-CCB-CDB-CEB
22	B	604	CLA	C8-C10-C11-C12
22	B	612	CLA	C13-C15-C16-C17
25	b	601	DGD	C2A-C3A-C4A-C5A
30	F	102	SQD	C24-C25-C26-C27
27	A	410	LMG	C17-C18-C19-C20
27	b	625	LMG	C29-C28-O8-C9
25	b	624	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C16-C17-C18-C19
22	B	612	CLA	C8-C10-C11-C12
30	a	401	SQD	C26-C27-C28-C29
27	a	413	LMG	C8-C9-O8-C28
27	b	628	LMG	C29-C30-C31-C32
30	f	103	SQD	C9-C10-C11-C12
31	B	623	LMT	C6-C7-C8-C9
30	A	413	SQD	C12-C13-C14-C15
27	a	402	LMG	C12-C13-C14-C15
27	e	101	LMG	C30-C31-C32-C33
27	e	101	LMG	C14-C15-C16-C17
22	C	501	CLA	C13-C15-C16-C17
22	C	503	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
25	B	620	DGD	CCA-CDA-CEA-CFA
22	b	617	CLA	C4C-C3C-CAC-CBC
22	B	612	CLA	C2-C1-O2A-CGA
22	B	610	CLA	C2-C3-C5-C6
22	B	611	CLA	C2-C3-C5-C6
25	B	620	DGD	C7B-C8B-C9B-CAB
22	A	403	CLA	C11-C10-C8-C9
22	C	503	CLA	C6-C7-C8-C9
22	c	503	CLA	C6-C7-C8-C9
25	d	408	DGD	O6E-C5E-C6E-O5E
27	A	410	LMG	C11-C12-C13-C14
25	c	517	DGD	CBB-CCB-CDB-CEB
26	A	409	LHG	C27-C28-C29-C30
22	D	406	CLA	C2A-CAA-CBA-CGA
22	c	510	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C16-C17-C18-C20
24	B	617	BCR	C5-C6-C7-C8
24	B	618	BCR	C1-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C30
24	D	411	BCR	C23-C24-C25-C30
24	b	621	BCR	C1-C6-C7-C8
24	b	622	BCR	C1-C6-C7-C8
24	b	622	BCR	C23-C24-C25-C30
24	c	521	BCR	C5-C6-C7-C8
24	f	102	BCR	C23-C24-C25-C30
24	g	101	BCR	C1-C6-C7-C8
25	a	411	DGD	C2A-C3A-C4A-C5A
30	f	103	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	f	102	BCR	C21-C22-C23-C24
24	x	101	BCR	C7-C8-C9-C10
22	B	607	CLA	C13-C15-C16-C17
22	b	615	CLA	C2-C3-C5-C6
25	B	625	DGD	C2G-C3G-O3G-C1D
25	b	601	DGD	C2G-C3G-O3G-C1D
27	d	410	LMG	C8-C7-O1-C1
27	m	101	LMG	C17-C18-C19-C20
25	A	408	DGD	C2A-C3A-C4A-C5A
22	b	609	CLA	C16-C17-C18-C19
22	c	509	CLA	C13-C15-C16-C17
22	b	609	CLA	CBA-CGA-O2A-C1
22	b	618	CLA	CBA-CGA-O2A-C1
27	D	408	LMG	C34-C35-C36-C37
22	C	510	CLA	C4-C3-C5-C6
31	B	622	LMT	C4-C5-C6-C7
22	C	503	CLA	C6-C7-C8-C10
22	b	612	CLA	C11-C12-C13-C15
22	b	614	CLA	C2-C3-C5-C6
22	b	615	CLA	C6-C7-C8-C10
22	h	101	CLA	C11-C12-C13-C15
32	D	402	PHO	C6-C7-C8-C10
25	C	516	DGD	C2E-C1E-O5D-C6D
25	c	516	DGD	C2E-C1E-O5D-C6D
22	C	509	CLA	C16-C17-C18-C19
27	b	625	LMG	O1-C7-C8-O7
27	e	101	LMG	O1-C7-C8-O7
22	c	507	CLA	C5-C6-C7-C8
22	b	616	CLA	CAA-CBA-CGA-O2A
26	C	519	LHG	O7-C7-C8-C9
27	a	413	LMG	O7-C10-C11-C12
22	b	618	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	C2C-C3C-CAC-CBC
22	b	606	CLA	C16-C17-C18-C20
27	B	621	LMG	C29-C28-O8-C9
22	B	612	CLA	CAA-CBA-CGA-O2A
26	c	519	LHG	O7-C7-C8-C9
22	c	510	CLA	C4-C3-C5-C6
25	B	625	DGD	C2A-C3A-C4A-C5A
25	D	409	DGD	C8A-C9A-CAA-CBA
30	a	415	SQD	C16-C17-C18-C19
22	b	609	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	C16-C17-C18-C20
25	b	601	DGD	C4E-C5E-C6E-O5E
22	A	405	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C12-C13-C14
22	H	101	CLA	C11-C10-C8-C9
22	a	405	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	609	CLA	C6-C7-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	508	CLA	C11-C10-C8-C9
22	h	101	CLA	C11-C10-C8-C9
22	C	520	CLA	C3A-C2A-CAA-CBA
22	D	405	CLA	C3A-C2A-CAA-CBA
22	d	404	CLA	CAA-CBA-CGA-O2A
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	B	611	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	b	608	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	c	501	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
26	A	409	LHG	C4-C5-O7-C7
26	a	412	LHG	C4-C5-O7-C7
22	c	509	CLA	C16-C17-C18-C20
22	B	611	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
25	C	517	DGD	O1G-C1A-C2A-C3A
27	A	410	LMG	O7-C10-C11-C12
27	C	522	LMG	O8-C28-C29-C30
27	a	402	LMG	O7-C10-C11-C12
27	E	101	LMG	C33-C34-C35-C36
30	A	413	SQD	C16-C17-C18-C19
22	c	510	CLA	C2-C3-C5-C6
25	c	517	DGD	O1G-C1A-C2A-C3A
24	D	411	BCR	C21-C22-C23-C24
27	m	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	C	515	DGD	C1G-C2G-C3G-O3G
25	c	515	DGD	C1G-C2G-C3G-O3G
27	E	101	LMG	O1-C7-C8-C9
27	c	518	LMG	C7-C8-C9-O8
27	A	415	LMG	O7-C10-C11-C12
27	D	412	LMG	C36-C37-C38-C39
27	d	410	LMG	C11-C12-C13-C14
27	E	101	LMG	C30-C31-C32-C33
22	B	615	CLA	O2A-C1-C2-C3
22	C	511	CLA	O2A-C1-C2-C3
22	b	619	CLA	O2A-C1-C2-C3
22	c	511	CLA	O2A-C1-C2-C3
32	D	402	PHO	O2A-C1-C2-C3
32	a	407	PHO	O2A-C1-C2-C3
27	B	621	LMG	C35-C36-C37-C38
25	B	625	DGD	CAB-CBB-CCB-CDB
27	c	522	LMG	O8-C28-C29-C30
22	c	512	CLA	C16-C17-C18-C20
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	CHA-CBD-CGD-O1D
22	C	512	CLA	CHA-CBD-CGD-O2D
22	H	101	CLA	CHA-CBD-CGD-O1D
22	H	101	CLA	CHA-CBD-CGD-O2D
22	a	406	CLA	CHA-CBD-CGD-O1D
22	a	406	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CHA-CBD-CGD-O1D
22	c	512	CLA	CHA-CBD-CGD-O2D
22	h	101	CLA	CHA-CBD-CGD-O1D
22	h	101	CLA	CHA-CBD-CGD-O2D
34	V	201	HEM	CAA-CBA-CGA-O2A
25	C	517	DGD	C4A-C5A-C6A-C7A
22	C	509	CLA	C13-C15-C16-C17
22	B	613	CLA	C4C-C3C-CAC-CBC
27	M	101	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	A	408	DGD	C2E-C1E-O5D-C6D
25	a	411	DGD	C2E-C1E-O5D-C6D
26	C	519	LHG	C11-C12-C13-C14
22	C	501	CLA	C16-C17-C18-C20
30	A	414	SQD	O47-C7-C8-C9
30	a	401	SQD	O47-C7-C8-C9
27	B	621	LMG	O1-C7-C8-O7
27	d	410	LMG	O1-C7-C8-O7
26	C	519	LHG	C7-C8-C9-C10
25	C	517	DGD	CBB-CCB-CDB-CEB
22	c	501	CLA	CAA-CBA-CGA-O2A
26	c	519	LHG	C11-C12-C13-C14
32	D	401	PHO	C13-C15-C16-C17
22	H	101	CLA	CBA-CGA-O2A-C1
27	b	628	LMG	C10-C11-C12-C13
30	A	413	SQD	C8-C7-O47-C45
22	C	501	CLA	CAA-CBA-CGA-O2A
22	D	405	CLA	CAA-CBA-CGA-O2A
30	f	103	SQD	C15-C16-C17-C18
25	c	517	DGD	C4A-C5A-C6A-C7A
22	B	601	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C12-C13-C15
22	B	611	CLA	C6-C7-C8-C10
22	C	506	CLA	C11-C12-C13-C15
22	a	408	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C12-C13-C15
22	c	503	CLA	C6-C7-C8-C10
22	c	507	CLA	C11-C12-C13-C15
22	c	512	CLA	C11-C12-C13-C15
22	b	611	CLA	C13-C15-C16-C17
22	c	509	CLA	CAA-CBA-CGA-O2A
30	d	402	SQD	O47-C7-C8-C9
34	v	201	HEM	CAA-CBA-CGA-O2A
22	B	601	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C10-C8-C9
22	B	611	CLA	C6-C7-C8-C9
22	B	614	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C12-C13-C14
22	C	520	CLA	C6-C7-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	615	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	618	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
30	D	403	SQD	O49-C7-C8-C9
25	C	517	DGD	C4B-C5B-C6B-C7B
22	C	502	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	CAA-CBA-CGA-O2A
22	B	602	CLA	C16-C17-C18-C20
22	B	605	CLA	C16-C17-C18-C19
22	C	509	CLA	C16-C17-C18-C20
22	H	101	CLA	O1A-CGA-O2A-C1
22	C	510	CLA	C2A-CAA-CBA-CGA
22	H	101	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	CAA-CBA-CGA-O2A
22	C	509	CLA	CAA-CBA-CGA-O2A
25	c	517	DGD	C4B-C5B-C6B-C7B
22	c	502	CLA	CBA-CGA-O2A-C1
22	C	501	CLA	C16-C17-C18-C19
22	C	509	CLA	CAA-CBA-CGA-O1A
22	A	404	CLA	CBA-CGA-O2A-C1
25	B	620	DGD	C4A-C5A-C6A-C7A
22	B	601	CLA	C1A-C2A-CAA-CBA
22	C	520	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
25	a	411	DGD	C4A-C5A-C6A-C7A
22	b	616	CLA	CAA-CBA-CGA-O1A
22	c	509	CLA	CAA-CBA-CGA-O1A
30	A	414	SQD	O49-C7-C8-C9
25	C	517	DGD	O2G-C1B-C2B-C3B
22	C	511	CLA	C2-C1-O2A-CGA
22	c	511	CLA	C2-C1-O2A-CGA
31	B	623	LMT	O5'-C5'-C6'-O6'
27	c	522	LMG	O10-C28-C29-C30
30	d	402	SQD	O49-C7-C8-C9
25	d	408	DGD	C8A-C9A-CAA-CBA
27	a	413	LMG	C17-C18-C19-C20
27	C	518	LMG	C7-C8-C9-O8
27	i	101	LMG	C7-C8-C9-O8
22	B	602	CLA	C2A-CAA-CBA-CGA
22	B	611	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	d	410	LMG	O9-C10-C11-C12
22	c	501	CLA	CAA-CBA-CGA-O1A
22	d	404	CLA	CAA-CBA-CGA-O1A
25	A	408	DGD	O6D-C5D-C6D-O5D
22	A	404	CLA	O1A-CGA-O2A-C1
22	C	502	CLA	O1A-CGA-O2A-C1
25	c	515	DGD	C2D-C1D-O3G-C3G
22	B	602	CLA	C8-C10-C11-C12
26	A	409	LHG	C3-O3-P-O5
26	a	412	LHG	C3-O3-P-O5
25	d	408	DGD	C9B-CAB-CBB-CCB
22	B	612	CLA	CAA-CBA-CGA-O1A
22	C	501	CLA	CAA-CBA-CGA-O1A
22	D	405	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
27	D	412	LMG	O9-C10-C11-C12
22	h	101	CLA	CAA-CBA-CGA-O2A
27	D	408	LMG	O7-C10-C11-C12
34	V	201	HEM	CAA-CBA-CGA-O1A
24	B	618	BCR	C23-C24-C25-C26
24	b	621	BCR	C5-C6-C7-C8
24	b	622	BCR	C23-C24-C25-C26
27	D	412	LMG	C32-C33-C34-C35
27	d	407	LMG	C34-C35-C36-C37
22	c	508	CLA	C8-C10-C11-C12
22	C	506	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	C16-C17-C18-C19
25	D	409	DGD	O6E-C5E-C6E-O5E
30	a	401	SQD	O49-C7-C8-C9
22	A	405	CLA	C4-C3-C5-C6
22	a	408	CLA	C4-C3-C5-C6
22	B	610	CLA	C16-C17-C18-C19
22	B	608	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	a	406	CLA	CAD-CBD-CGD-O1D
22	b	612	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
27	M	101	LMG	C7-C8-O7-C10
30	A	414	SQD	C5-C6-S-O9
30	D	403	SQD	O5-C5-C6-S
30	d	402	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
25	A	408	DGD	C4D-C5D-C6D-O5D
22	a	408	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	d	404	CLA	C11-C10-C8-C9
32	D	402	PHO	C6-C7-C8-C9
25	C	517	DGD	CEA-CFA-CGA-CHA
25	C	516	DGD	C6A-C7A-C8A-C9A
34	v	201	HEM	CAA-CBA-CGA-O1A
26	A	409	LHG	C24-C25-C26-C27
22	D	405	CLA	C3-C5-C6-C7
22	b	615	CLA	C3-C5-C6-C7
22	b	605	CLA	CAA-CBA-CGA-O2A
25	c	517	DGD	O2G-C1B-C2B-C3B
27	m	101	LMG	O8-C28-C29-C30
30	D	403	SQD	O47-C7-C8-C9
30	A	413	SQD	C9-C10-C11-C12
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	613	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
30	b	602	SQD	C15-C16-C17-C18
27	a	413	LMG	O9-C10-C11-C12
22	C	508	CLA	C8-C10-C11-C12
22	A	403	CLA	C2-C3-C5-C6
22	B	602	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	a	405	CLA	C2-C3-C5-C6
22	b	606	CLA	C11-C10-C8-C7
22	b	619	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C12-C13-C15
22	d	404	CLA	C11-C10-C8-C7
22	h	101	CLA	C12-C13-C15-C16
27	A	410	LMG	O9-C10-C11-C12
27	a	402	LMG	O9-C10-C11-C12
22	B	609	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
22	c	504	CLA	CAA-CBA-CGA-O2A
27	M	101	LMG	O8-C28-C29-C30
25	b	601	DGD	CAB-CBB-CCB-CDB
22	c	502	CLA	C16-C17-C18-C19
25	B	620	DGD	O2G-C1B-C2B-C3B
25	b	624	DGD	O2G-C1B-C2B-C3B
27	d	407	LMG	O7-C10-C11-C12

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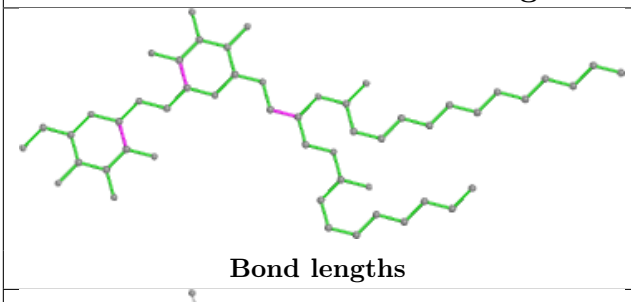
Mol	Chain	Res	Type	Atoms
27	B	621	LMG	O6-C1-O1-C7
22	B	609	CLA	C13-C15-C16-C17
27	C	522	LMG	O10-C28-C29-C30
25	c	517	DGD	C5B-C6B-C7B-C8B
30	a	401	SQD	C25-C26-C27-C28
31	B	627	LMT	C4'-C5'-C6'-O6'
22	B	601	CLA	CAA-CBA-CGA-O2A
30	b	602	SQD	O47-C7-C8-C9
25	C	517	DGD	O1A-C1A-C2A-C3A
22	C	508	CLA	C10-C11-C12-C13
30	a	415	SQD	C24-C25-C26-C27
22	B	613	CLA	CAA-CBA-CGA-O1A
22	C	504	CLA	CAA-CBA-CGA-O1A
22	b	613	CLA	CAA-CBA-CGA-O1A
22	c	504	CLA	CAA-CBA-CGA-O1A
30	A	413	SQD	O49-C7-C8-C9
27	D	412	LMG	C12-C13-C14-C15

There are no ring outliers.

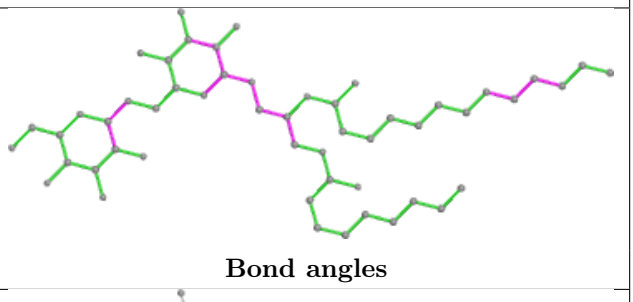
No monomer is involved in short contacts.

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.

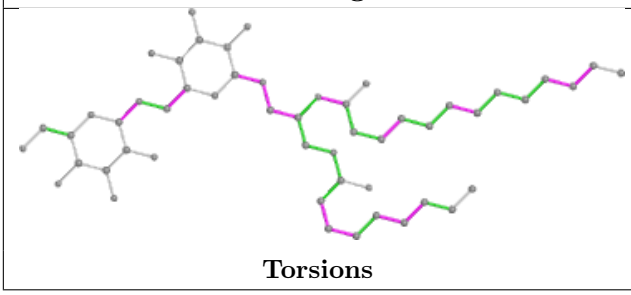
Ligand DGD B 625



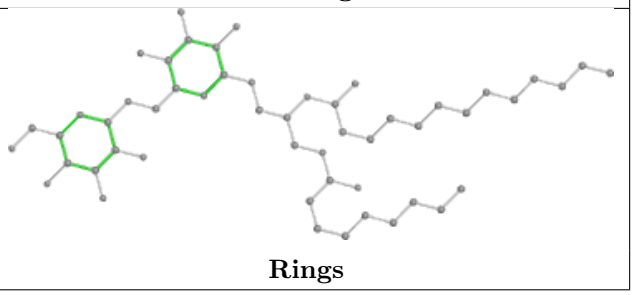
Bond lengths



Bond angles

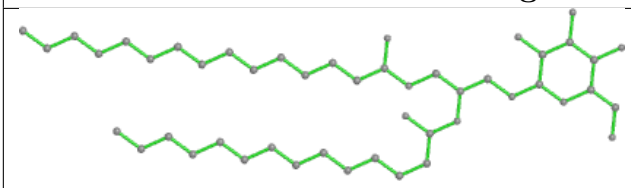


Torsions

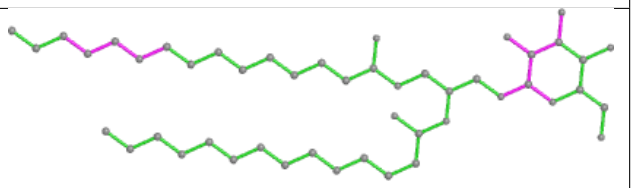


Rings

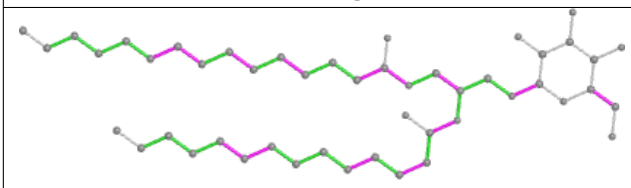
Ligand LMG C 522



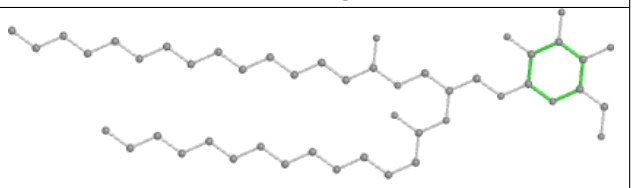
Bond lengths



Bond angles

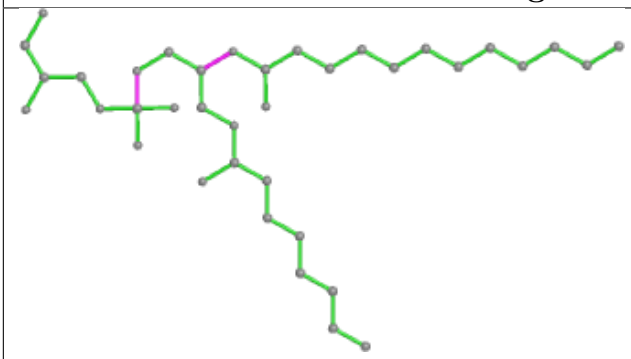


Torsions

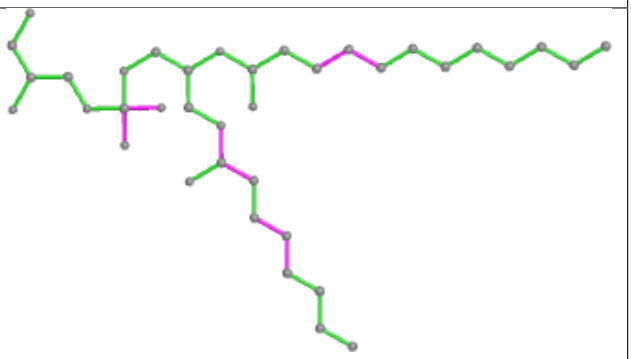


Rings

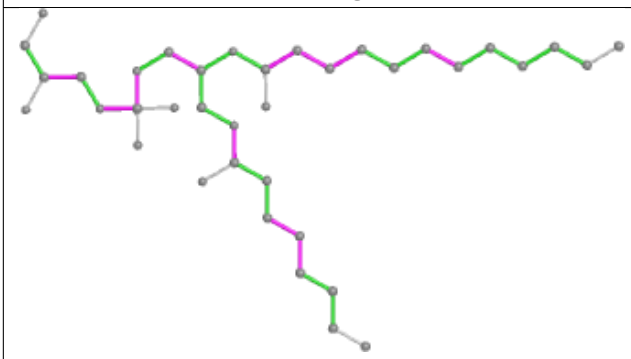
Ligand LHG c 519



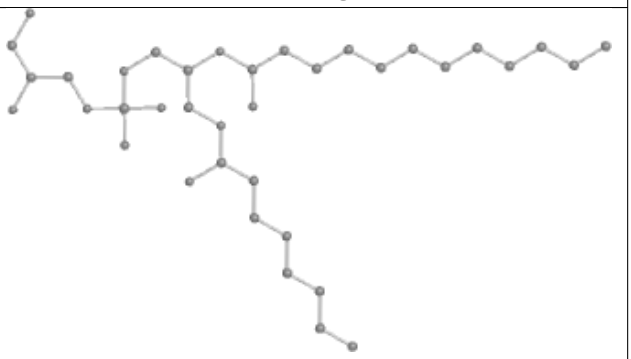
Bond lengths



Bond angles

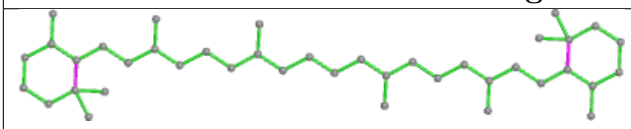


Torsions

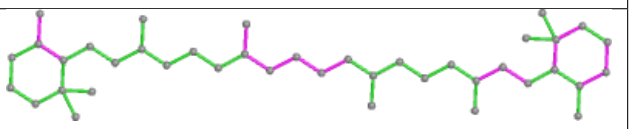


Rings

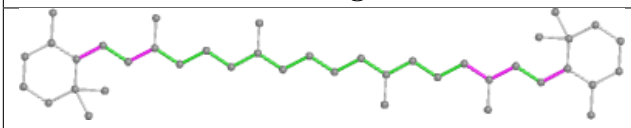
Ligand BCR b 621



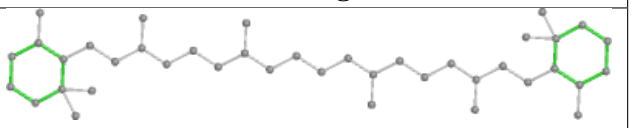
Bond lengths



Bond angles

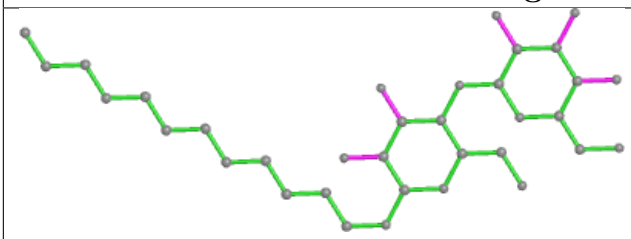


Torsions

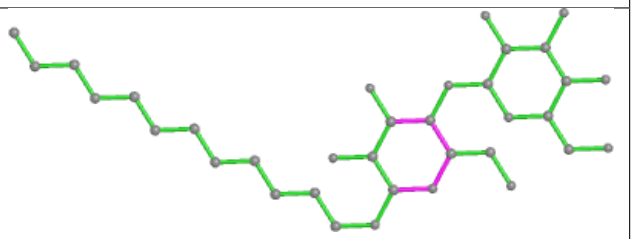


Rings

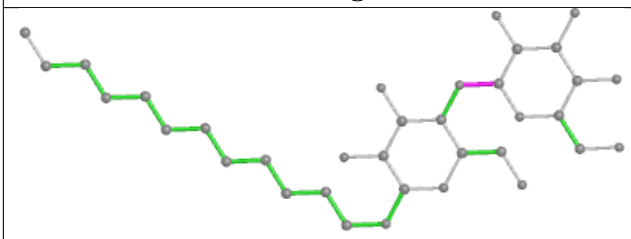
Ligand LMT b 627



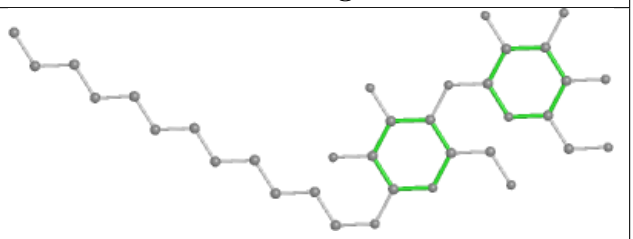
Bond lengths



Bond angles

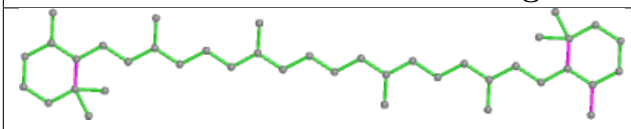


Torsions



Rings

Ligand BCR C 514



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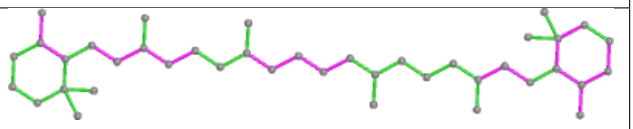
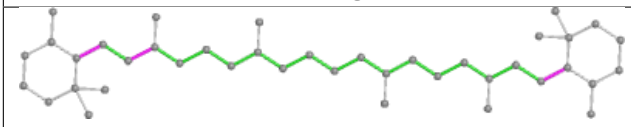


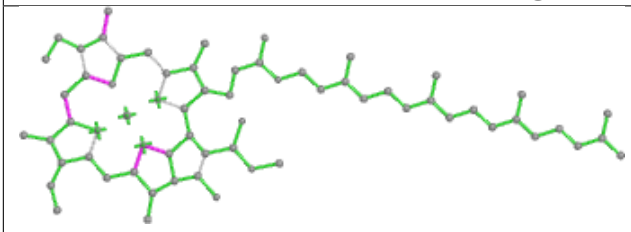
Bond angles



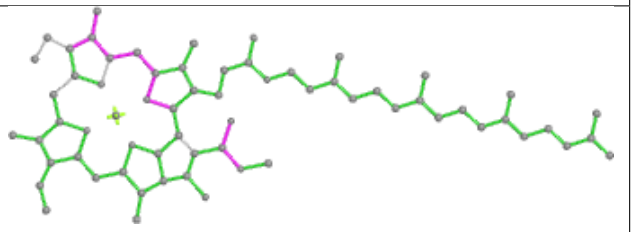
Torsions

Rings

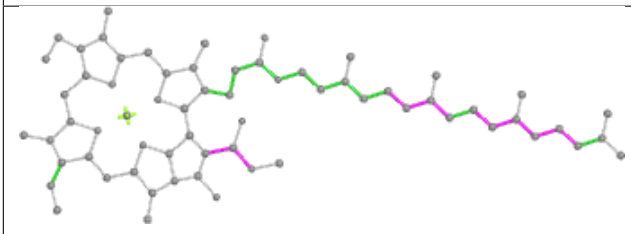
Ligand CLA c 505



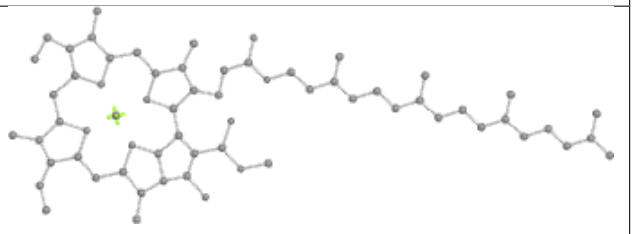
Bond lengths



Bond angles

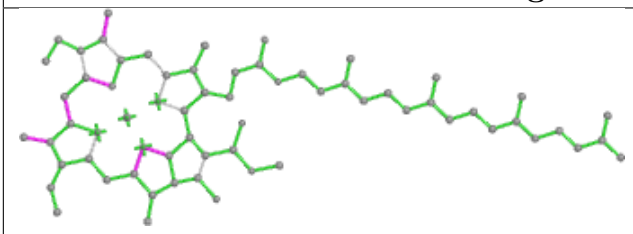


Torsions

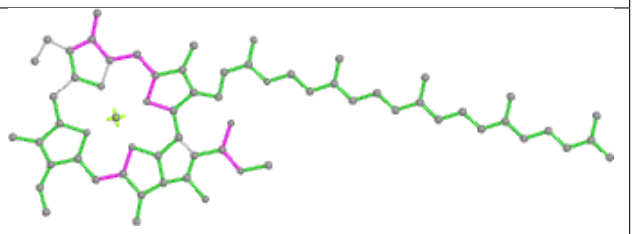


Rings

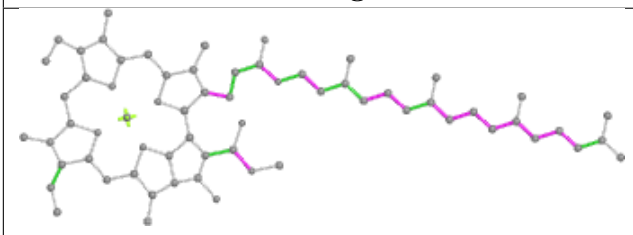
Ligand CLA b 619



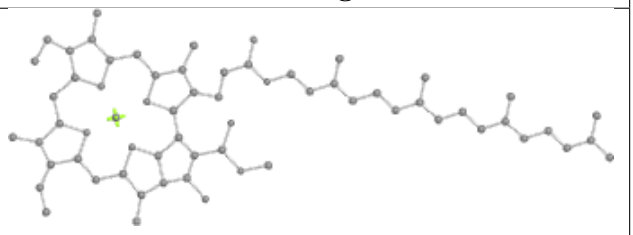
Bond lengths



Bond angles

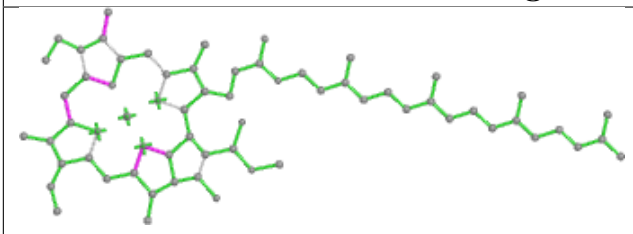


Torsions

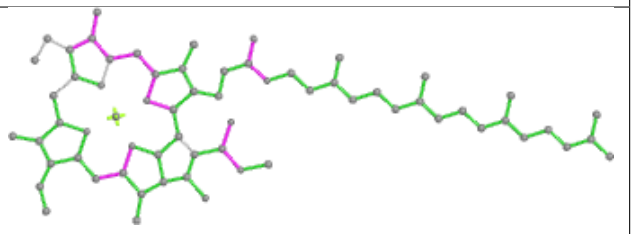


Rings

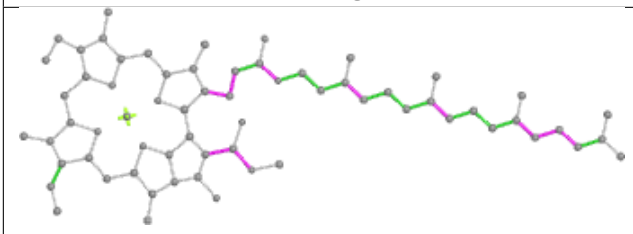
Ligand CLA C 512



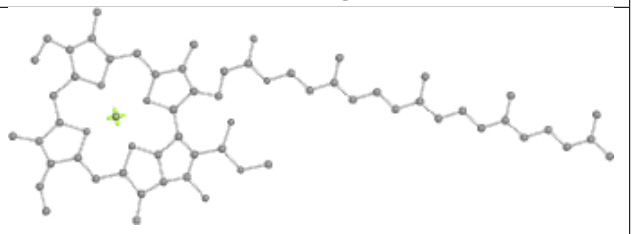
Bond lengths



Bond angles

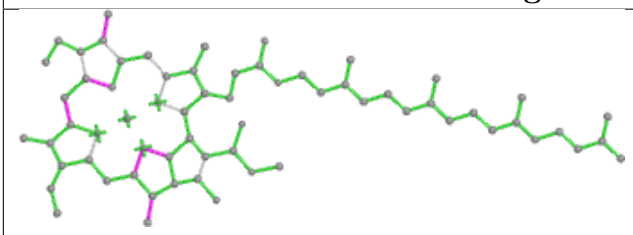


Torsions

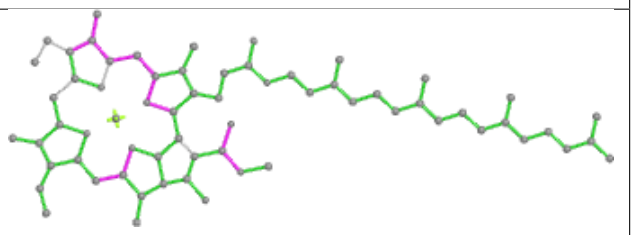


Rings

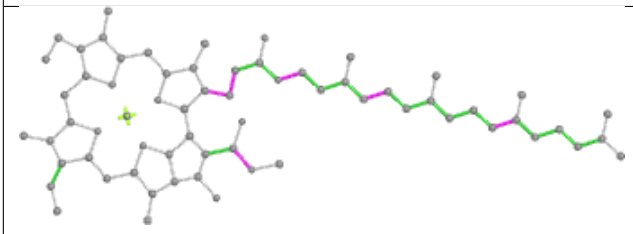
Ligand CLA A 402



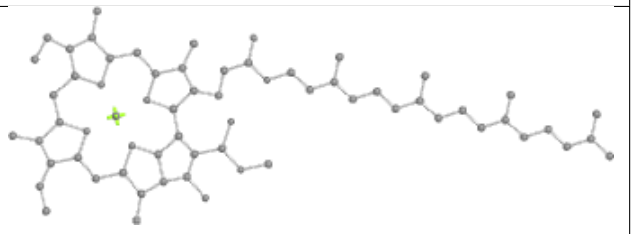
Bond lengths



Bond angles

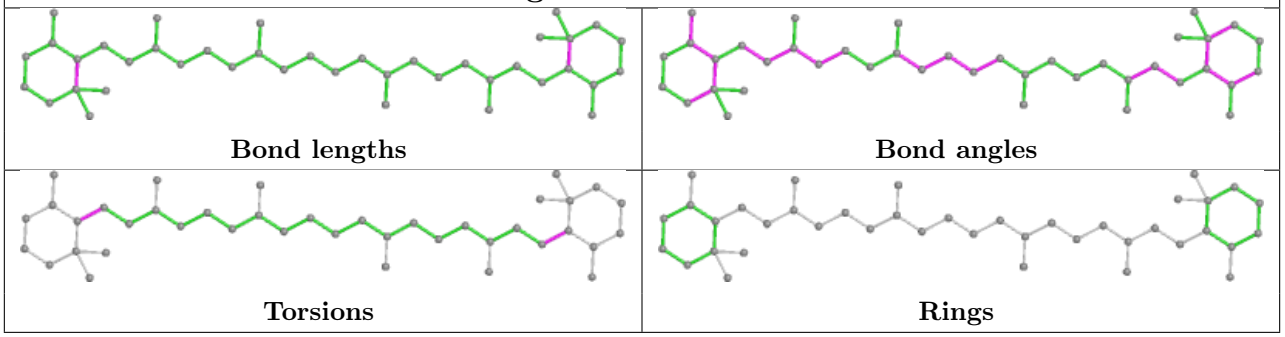


Torsions

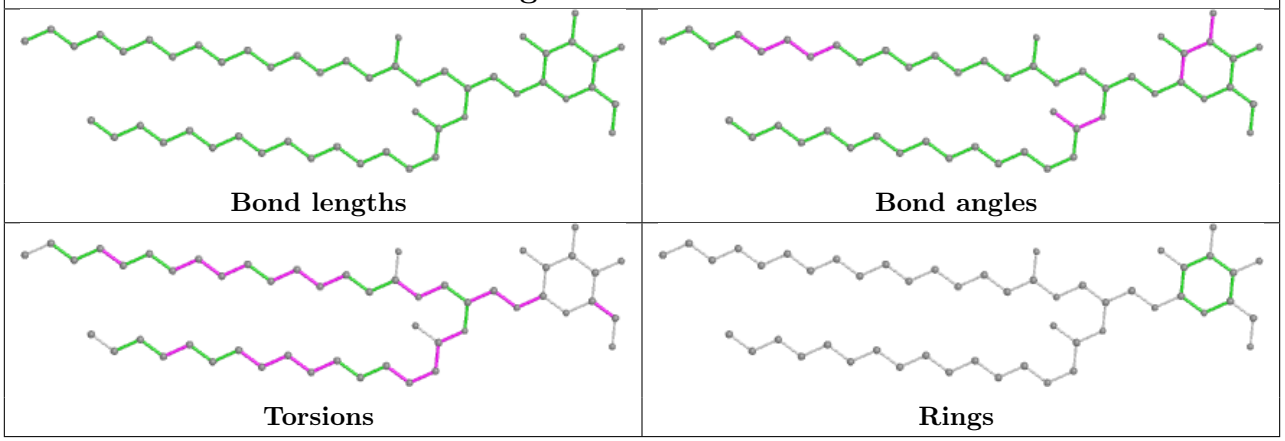


Rings

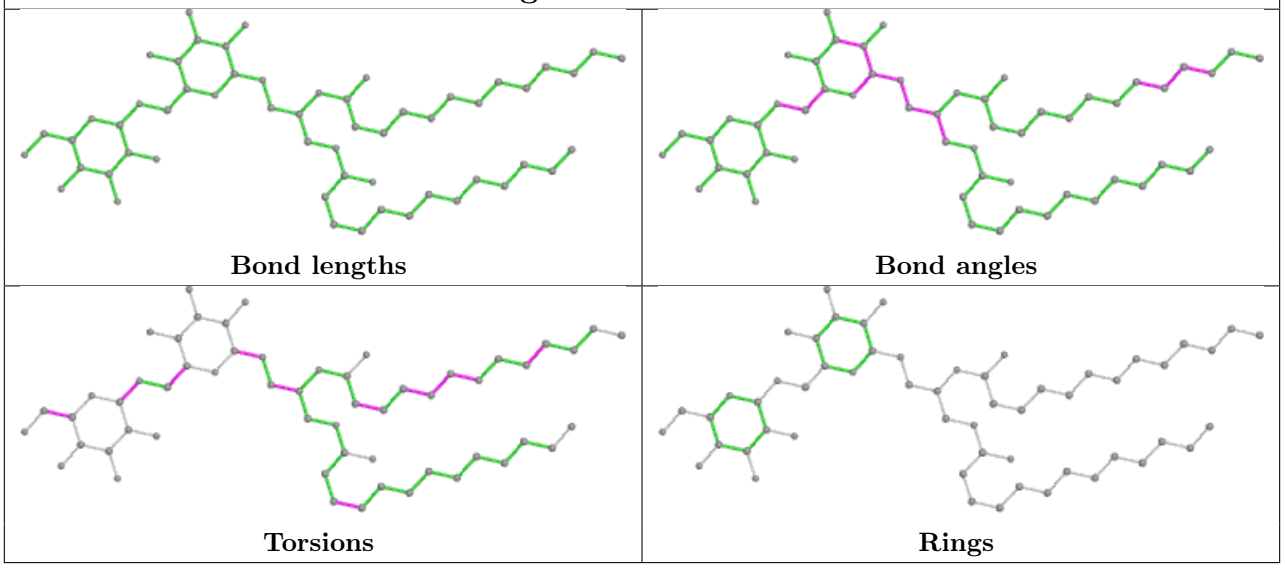
Ligand BCR b 622



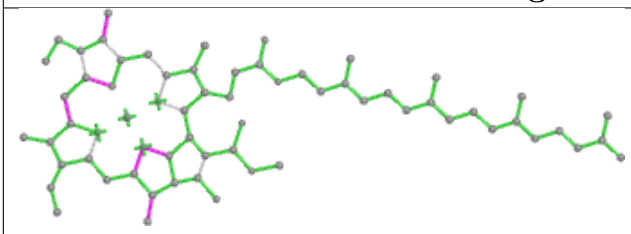
Ligand LMG A 410



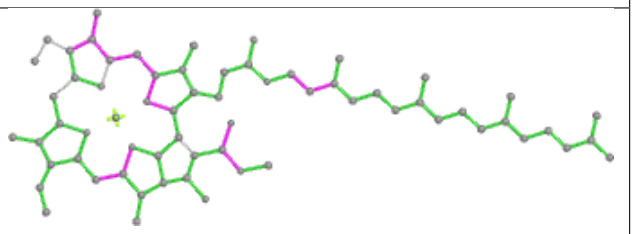
Ligand DGD A 408



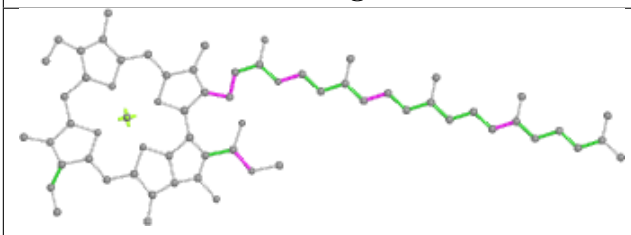
Ligand CLA a 404



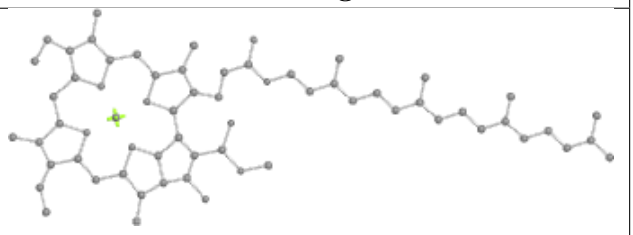
Bond lengths



Bond angles

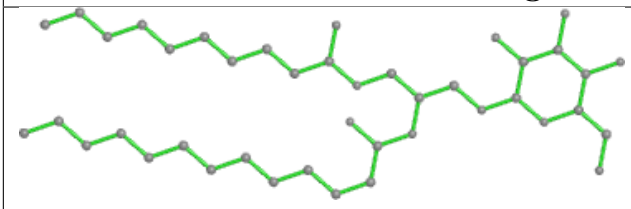


Torsions

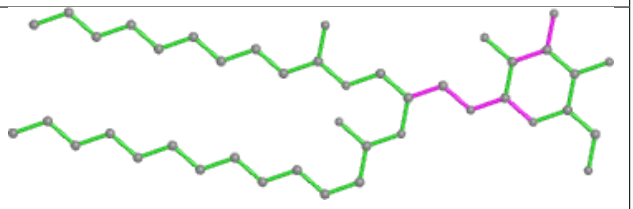


Rings

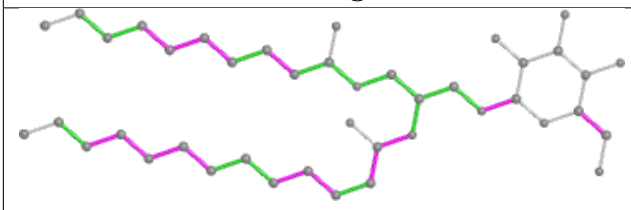
Ligand LMG a 402



Bond lengths



Bond angles



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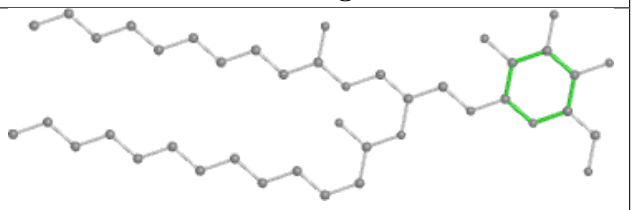
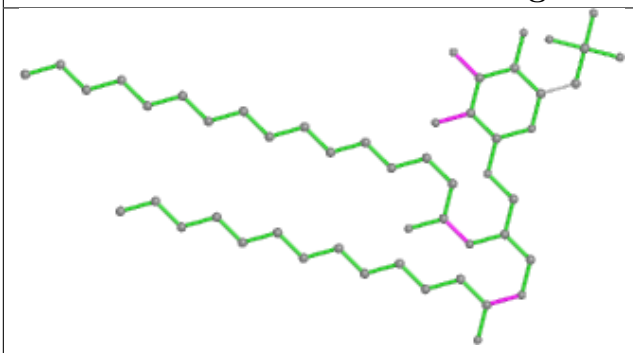
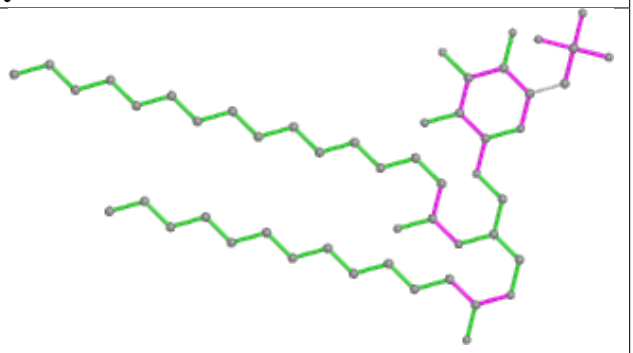


Rings

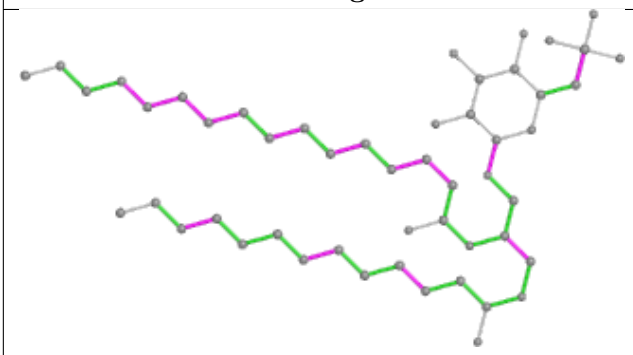
Ligand SQD a 415



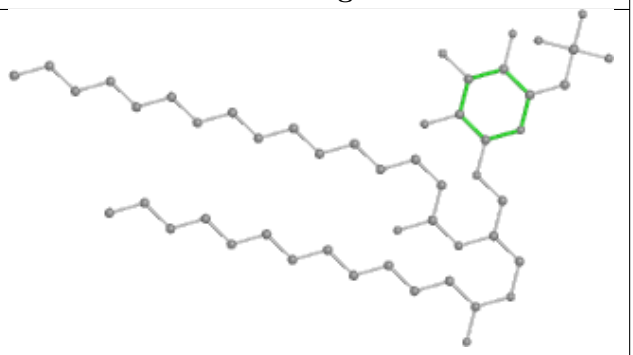
Bond lengths



Bond angles

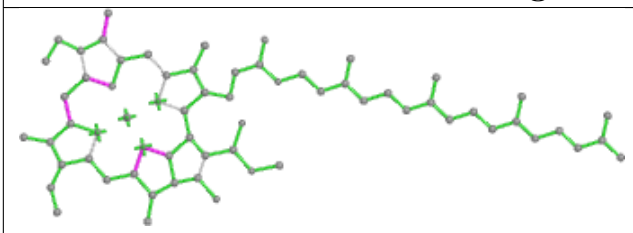


Torsions

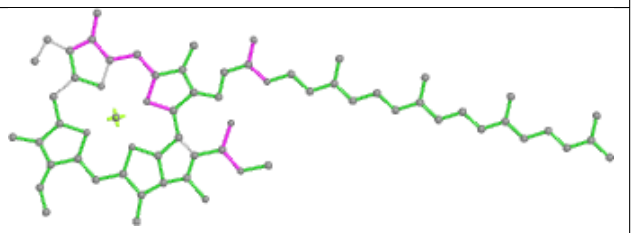


Rings

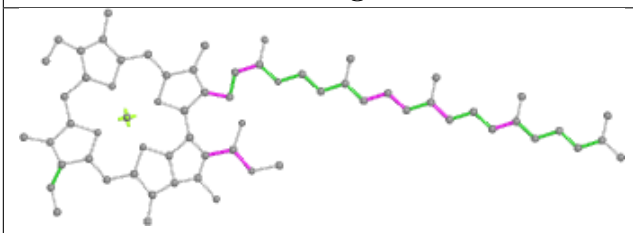
Ligand CLA c 506



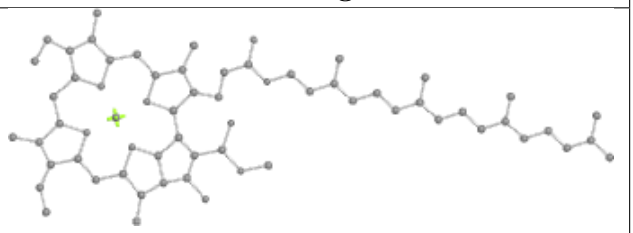
Bond lengths



Bond angles

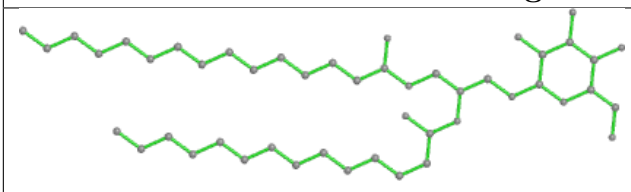


Torsions

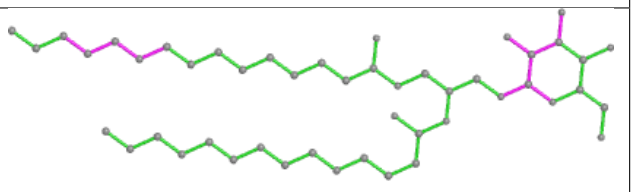


Rings

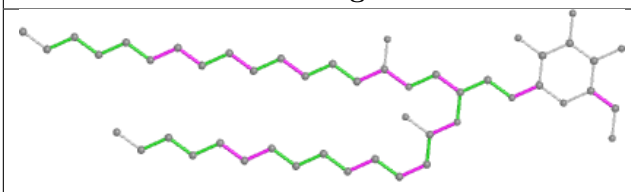
Ligand LMG c 522



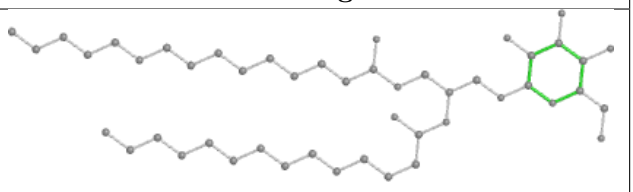
Bond lengths



Bond angles

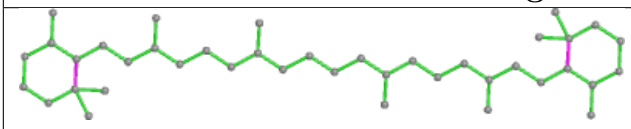


Torsions

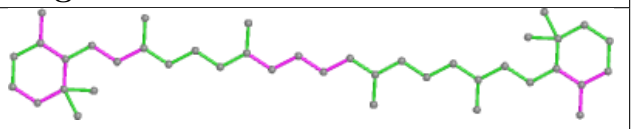


Rings

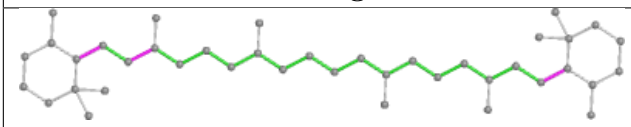
Ligand BCR g 101



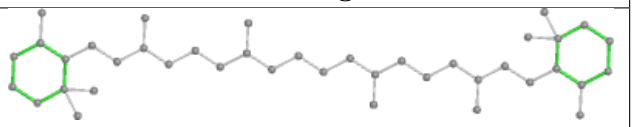
Bond lengths



Bond angles

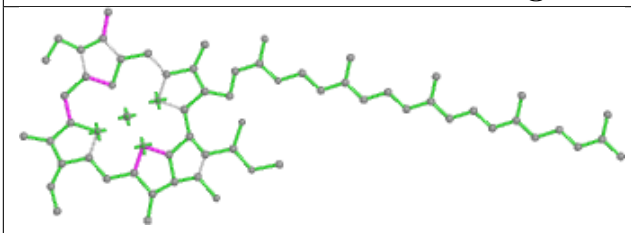


Torsions

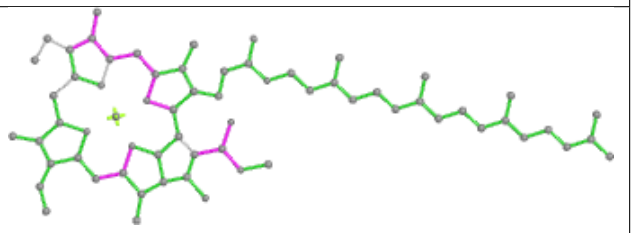


Rings

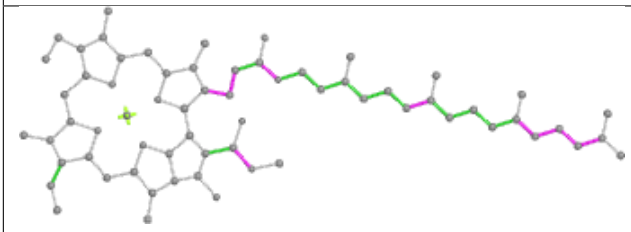
Ligand CLA b 609



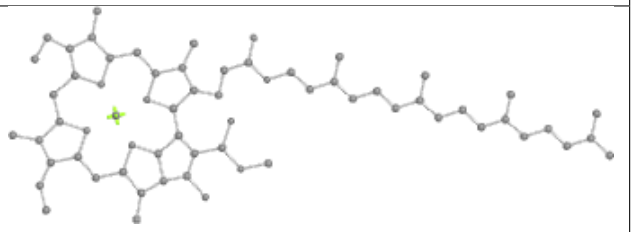
Bond lengths



Bond angles

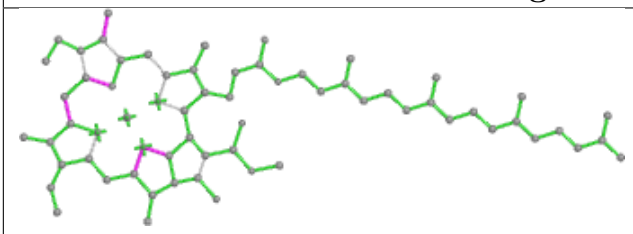


Torsions

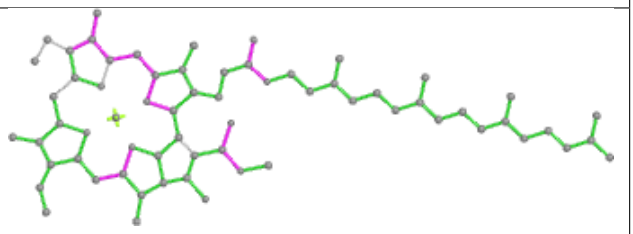


Rings

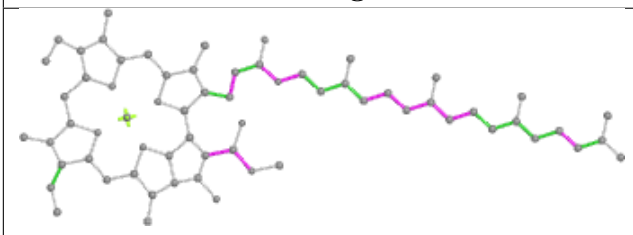
Ligand CLA c 508



Bond lengths



Bond angles



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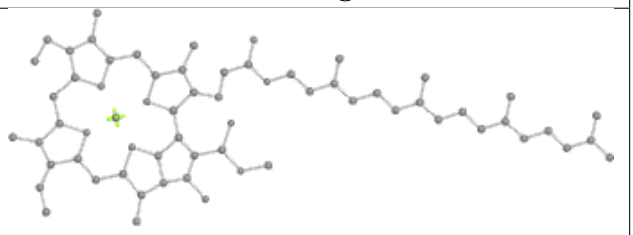
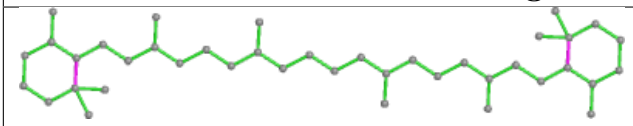


Rings

Ligand BCR b 623



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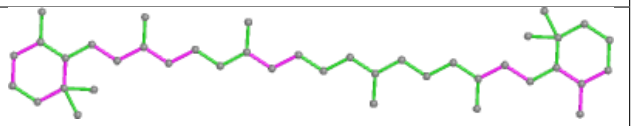
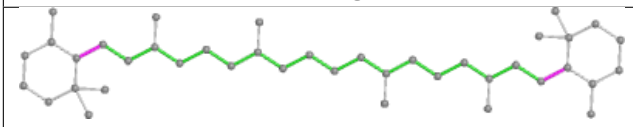


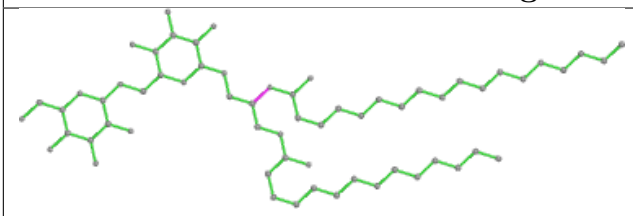
Bond angles



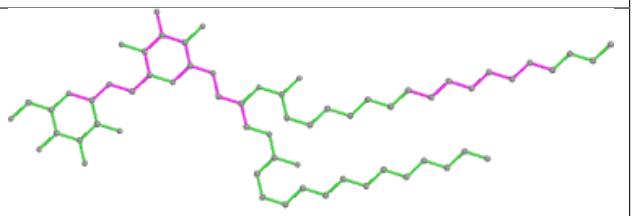
Torsions

Rings

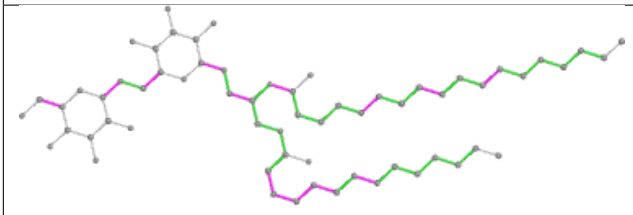
Ligand DGD C 516



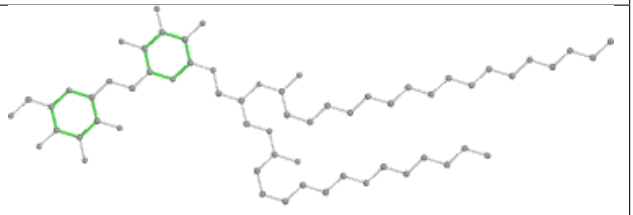
Bond lengths



Bond angles

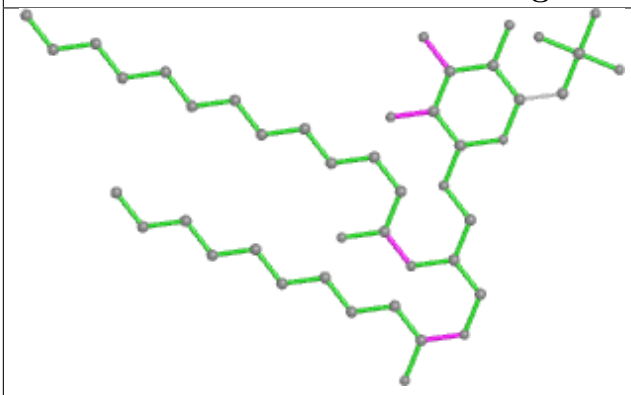


Torsions

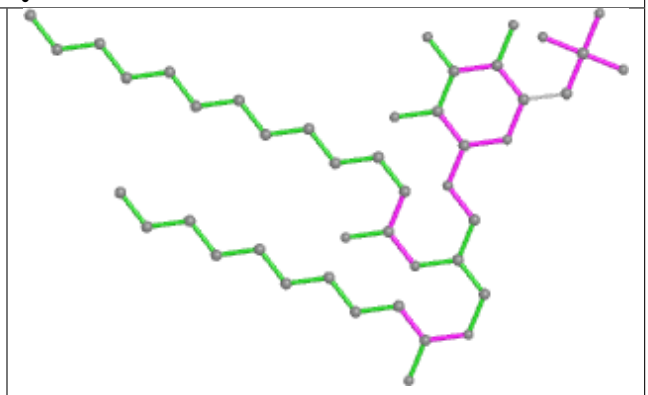


Rings

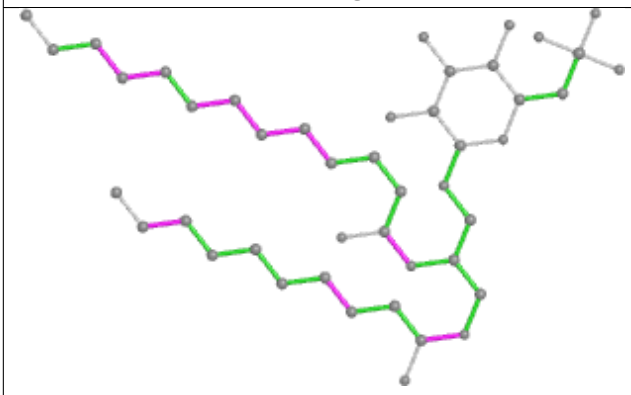
Ligand SQD f 103



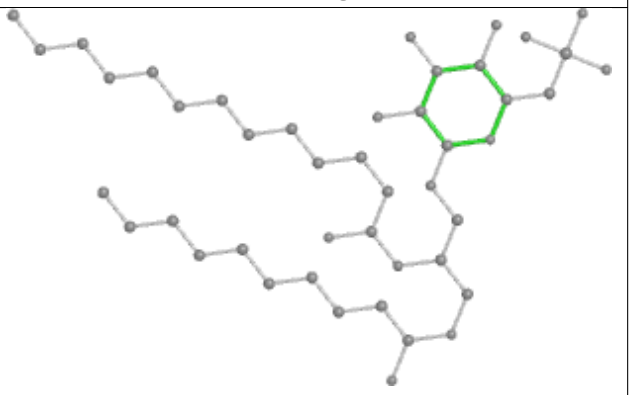
Bond lengths



Bond angles

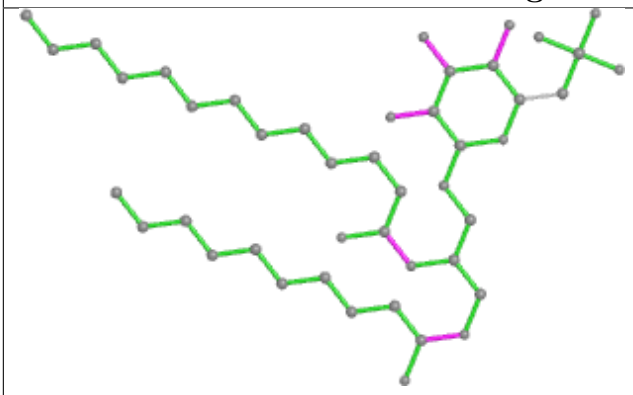


Torsions

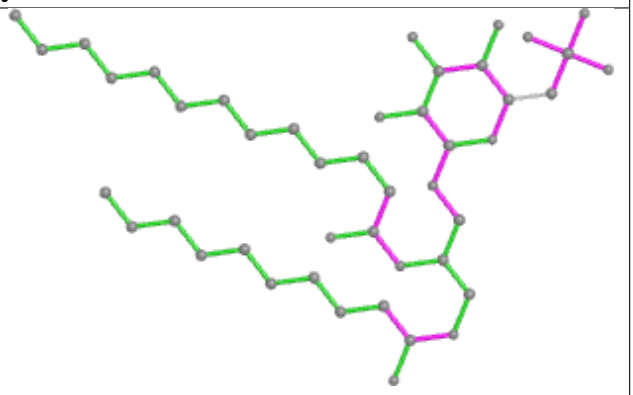


Rings

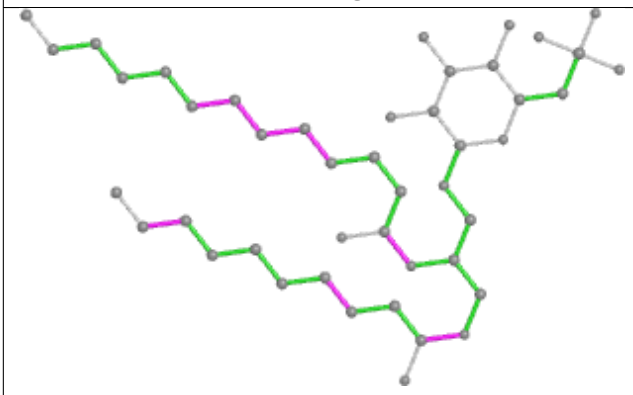
Ligand SQD F 102



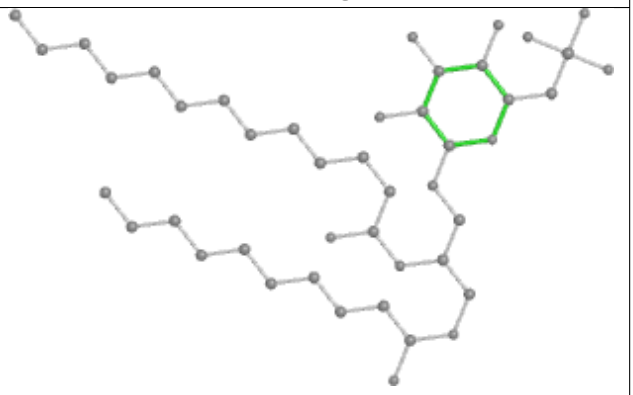
Bond lengths



Bond angles

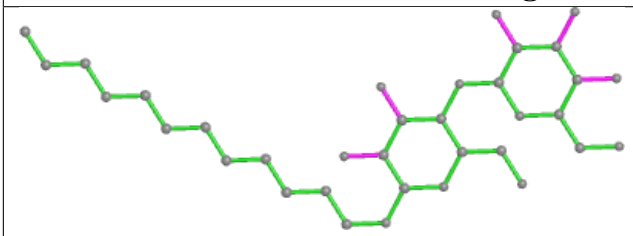


Torsions

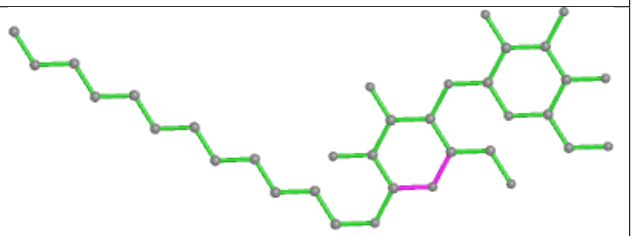


Rings

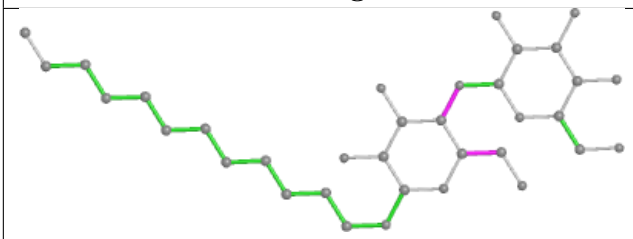
Ligand LMT B 627



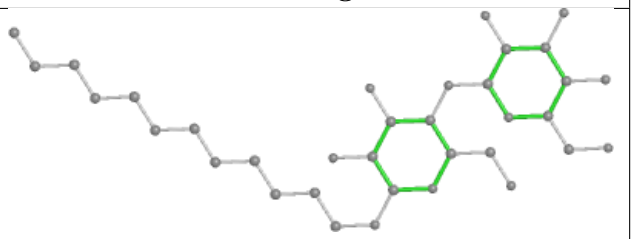
Bond lengths



Bond angles

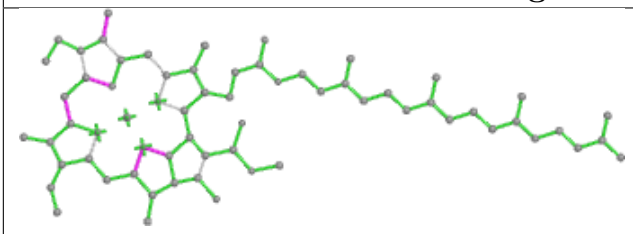


Torsions

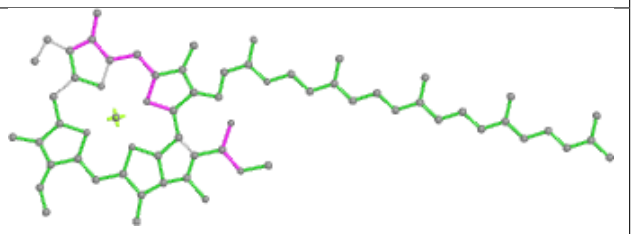


Rings

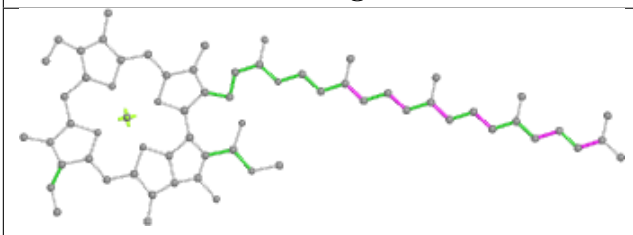
Ligand CLA a 408



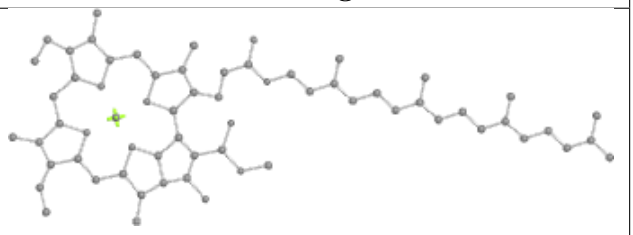
Bond lengths



Bond angles

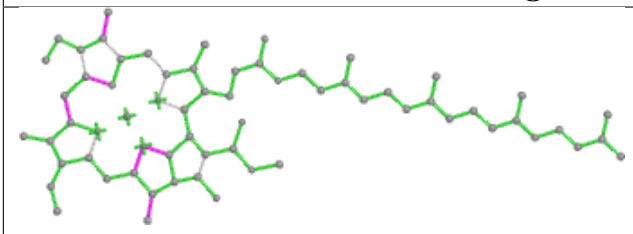


Torsions

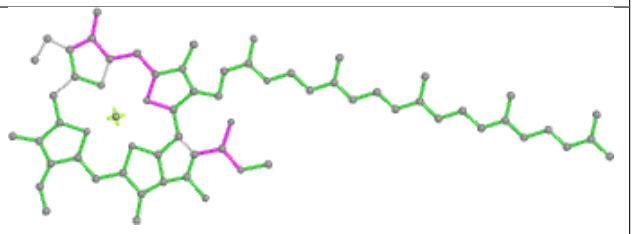


Rings

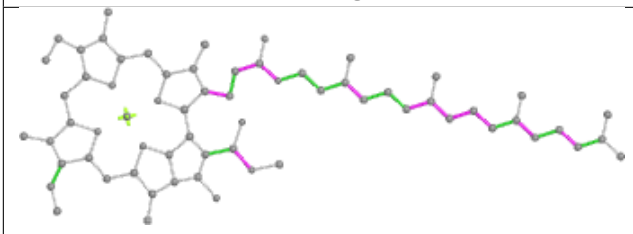
Ligand CLA C 504



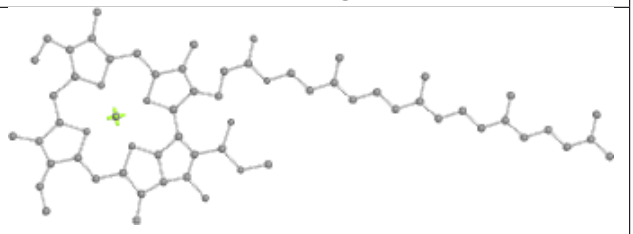
Bond lengths



Bond angles

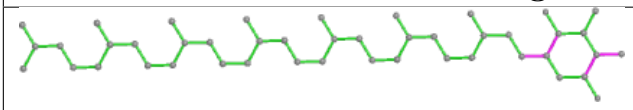


Torsions

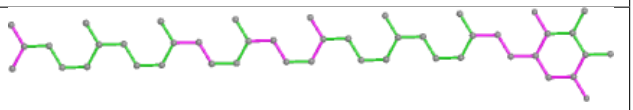


Rings

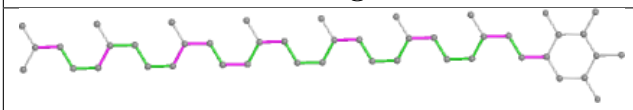
Ligand PL9 A 406



Bond lengths



Bond angles



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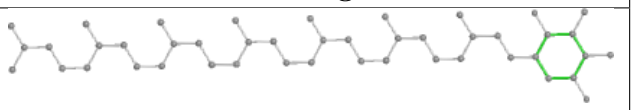
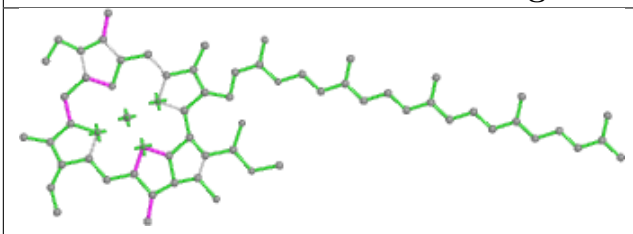


Rings

Ligand CLA a 406



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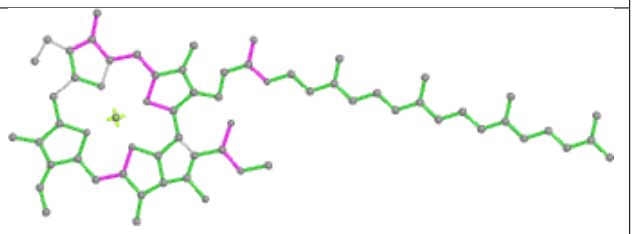
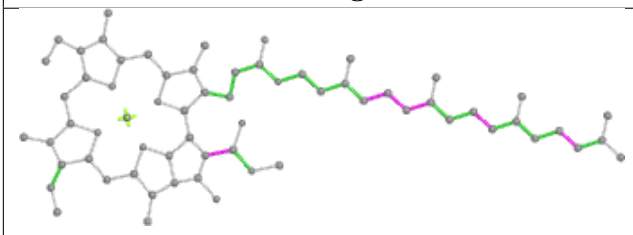


Bond angles



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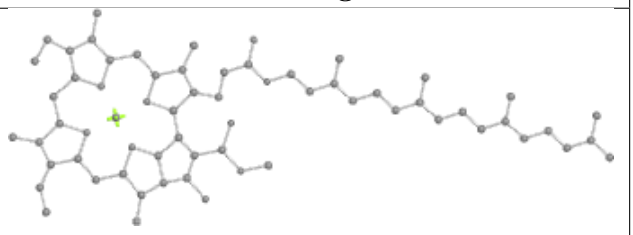
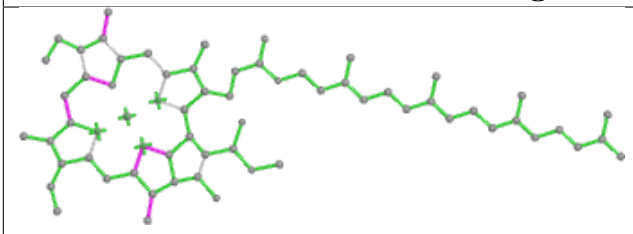
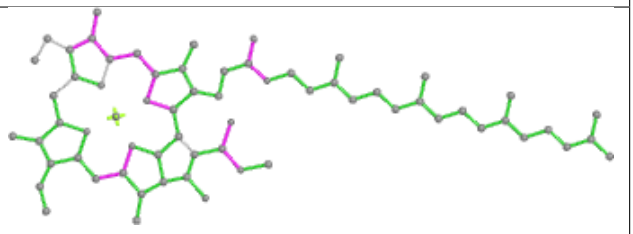


Rings

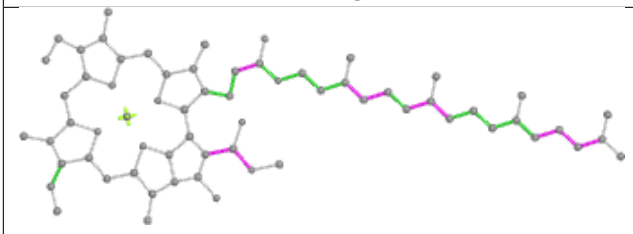
Ligand CLA c 509



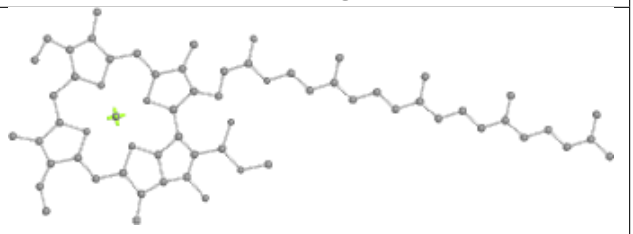
Bond lengths



Bond angles

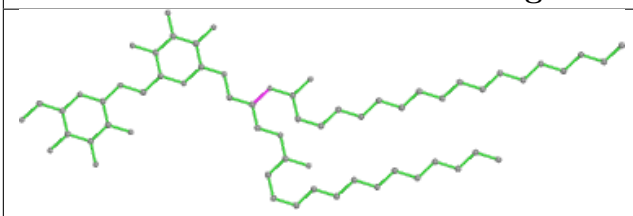


Torsions

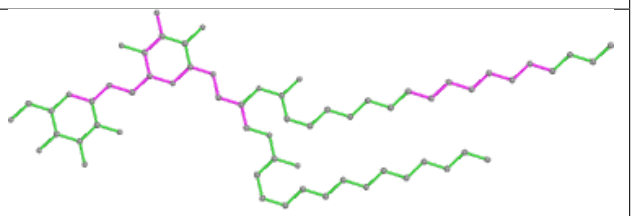


Rings

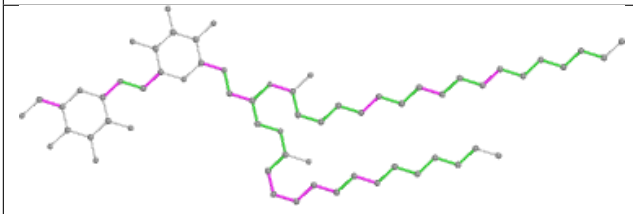
Ligand DGD c 516



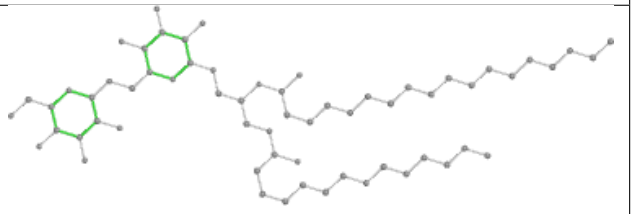
Bond lengths



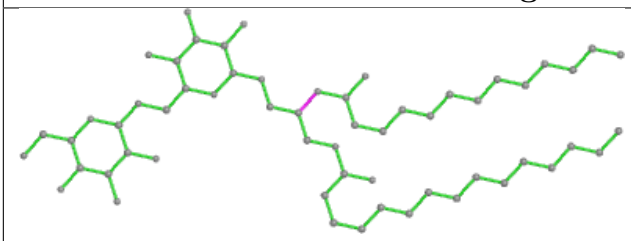
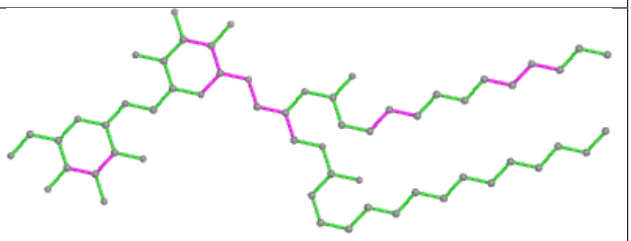
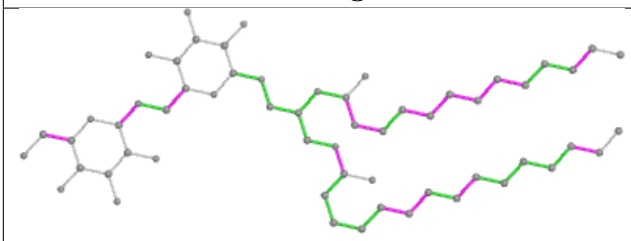
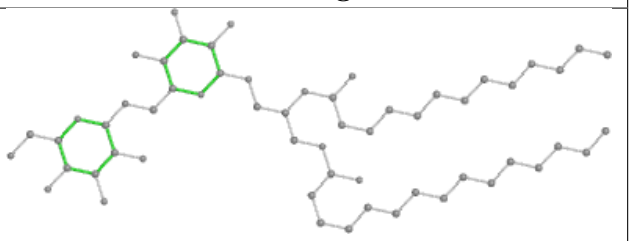
Bond angles

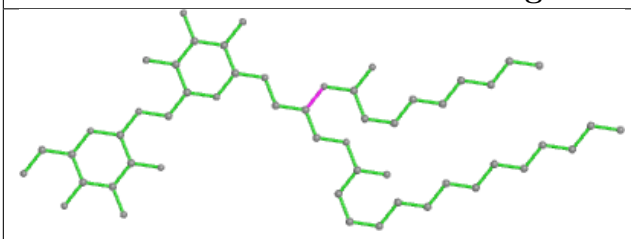
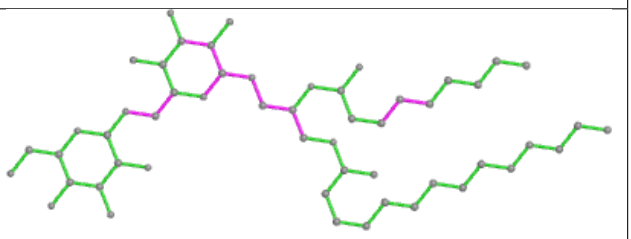
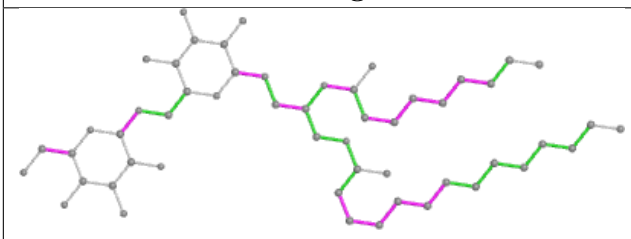
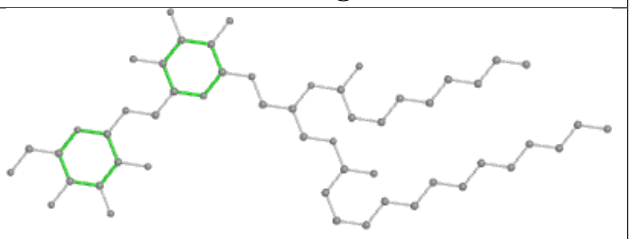


Torsions

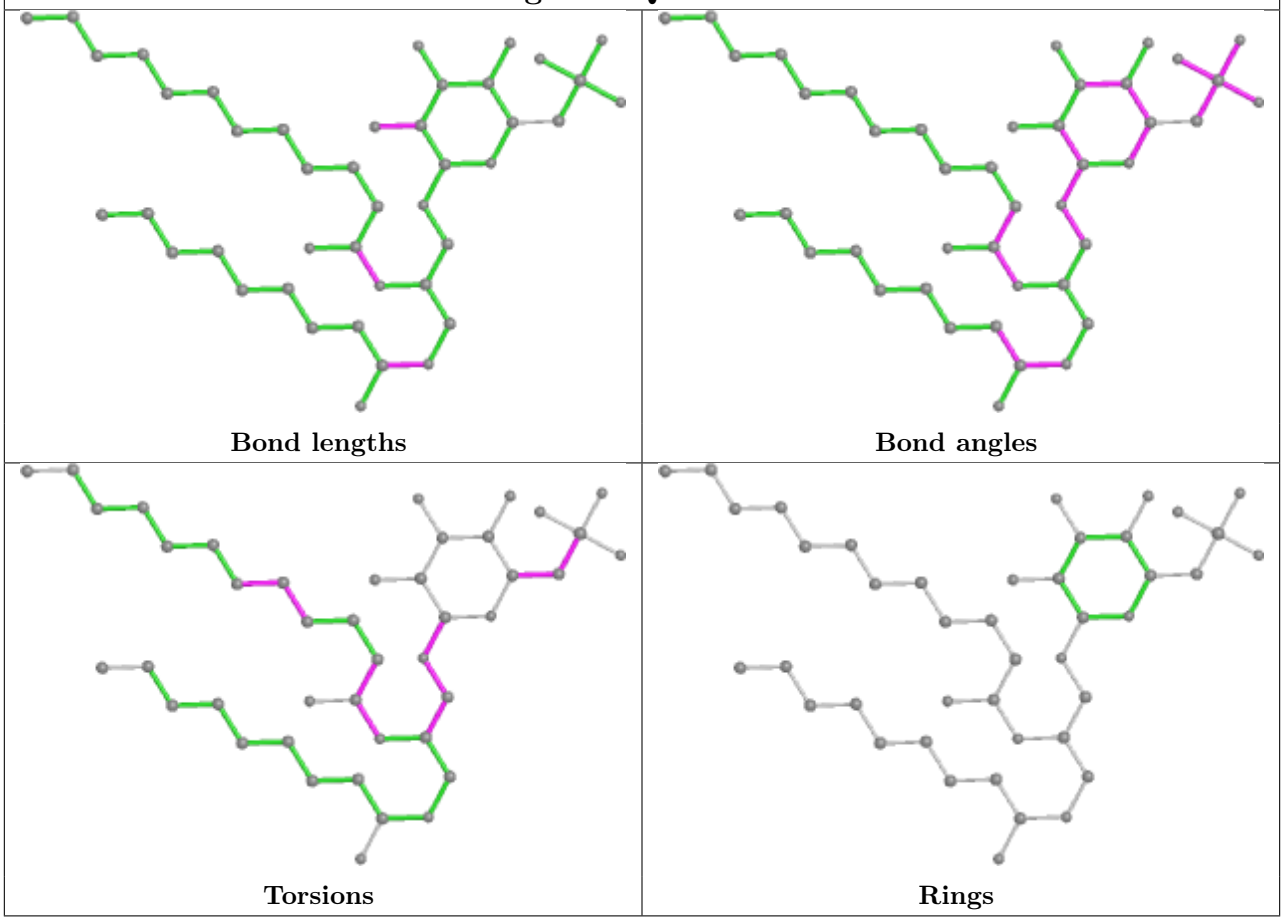


Rings

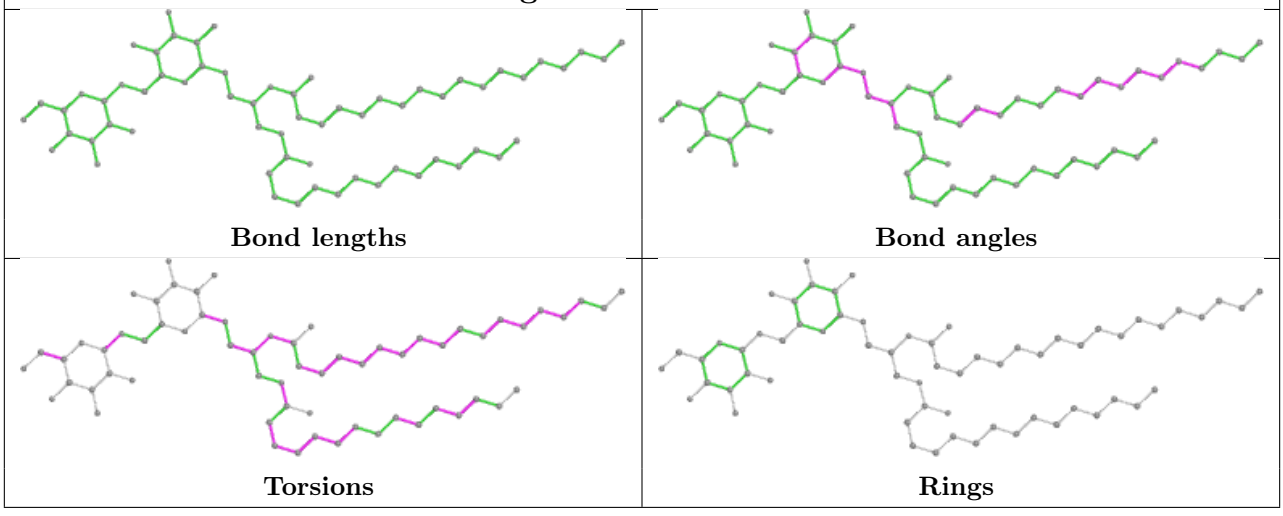
Ligand DGD B 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD c 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

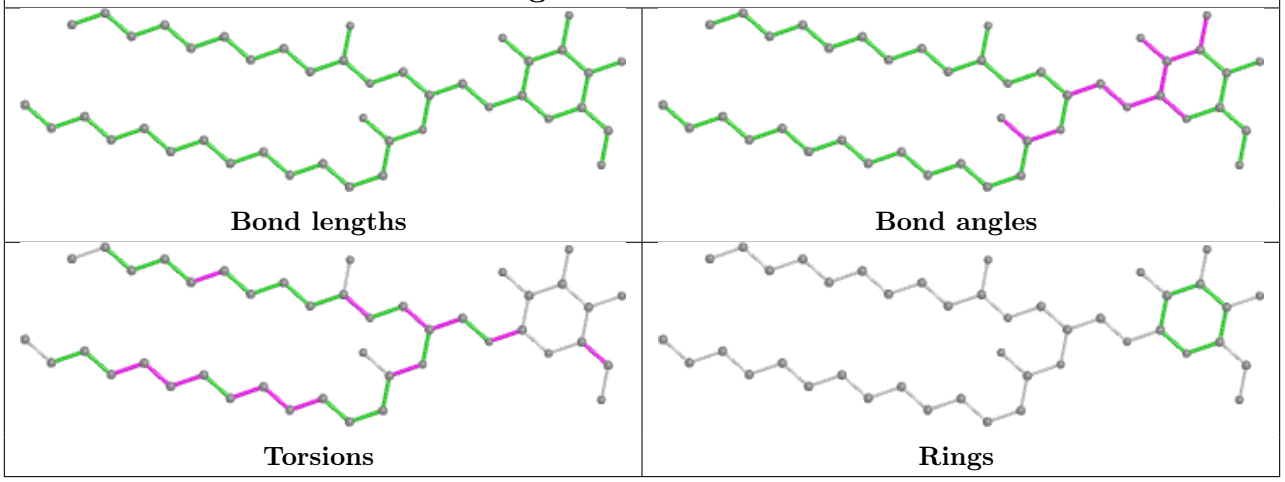
Ligand SQD D 403



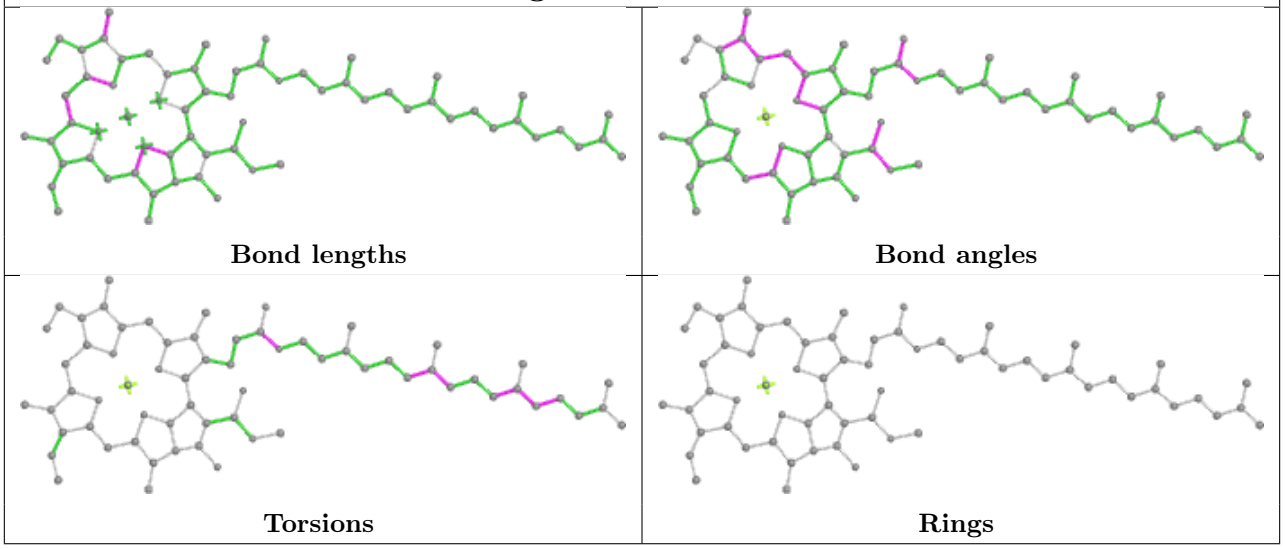
Ligand DGD D 409



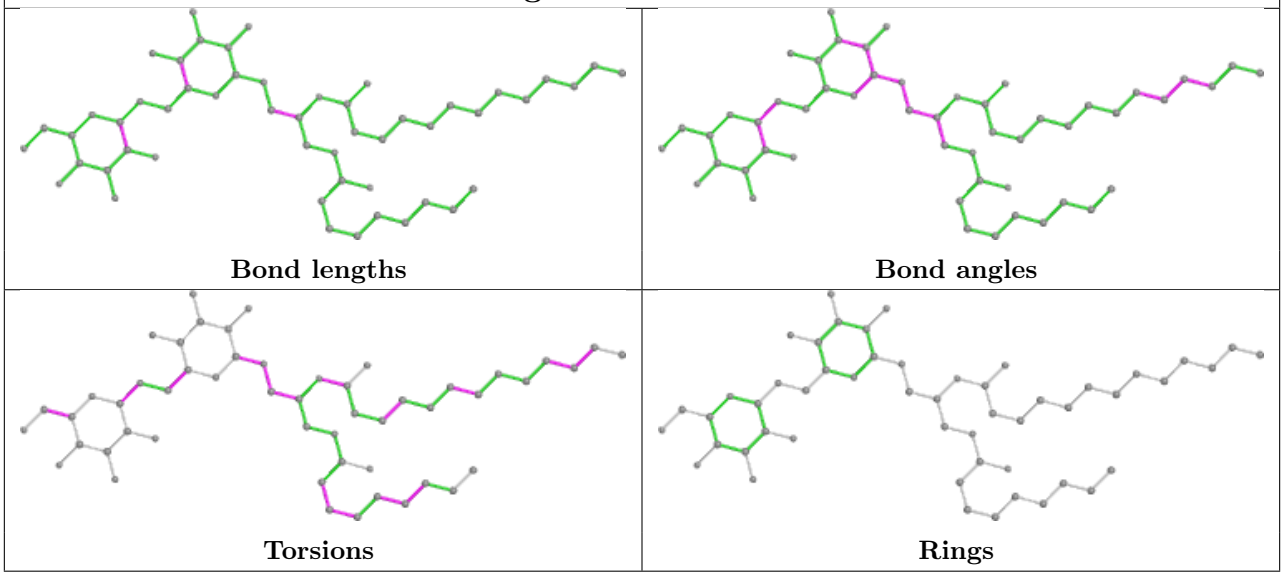
Ligand LMG i 101



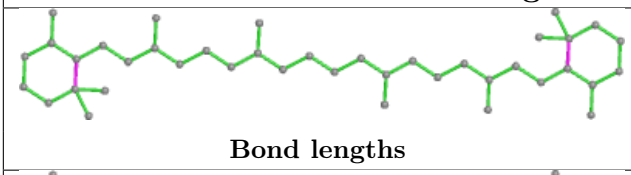
Ligand CLA b 618



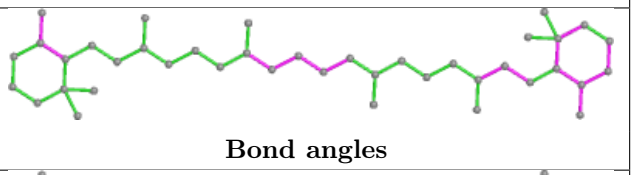
Ligand DGD b 601



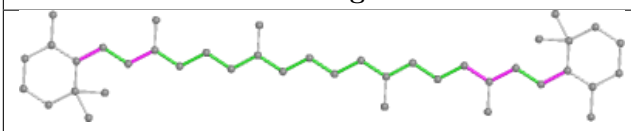
Ligand BCR B 617



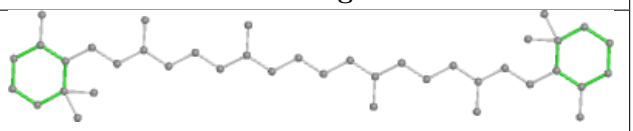
Bond lengths



Bond angles

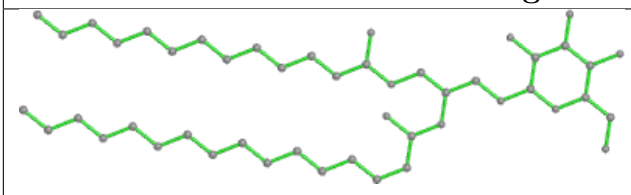


Torsions

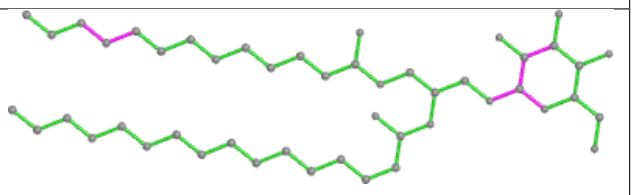


Rings

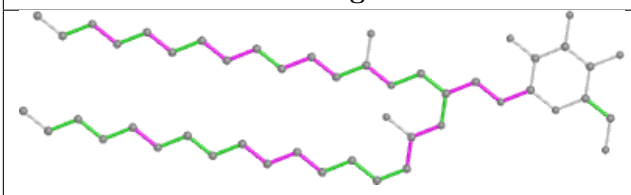
Ligand LMG d 407



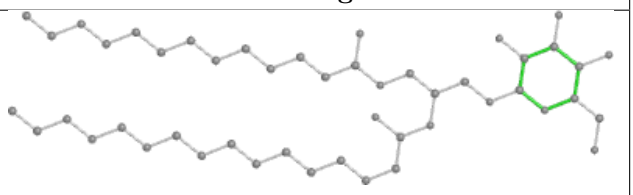
Bond lengths



Bond angles

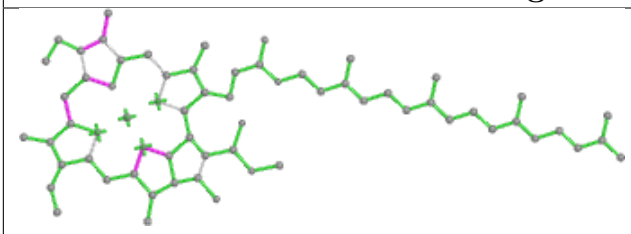


Torsions

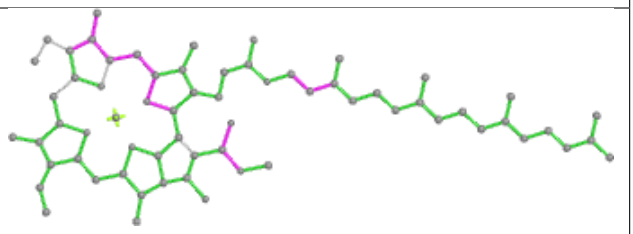


Rings

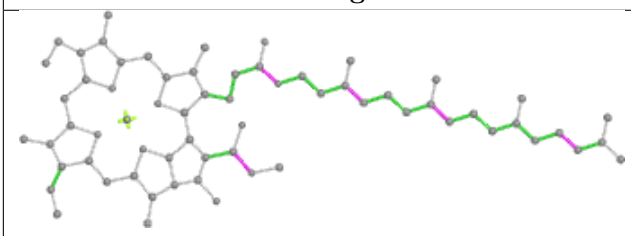
Ligand CLA b 614



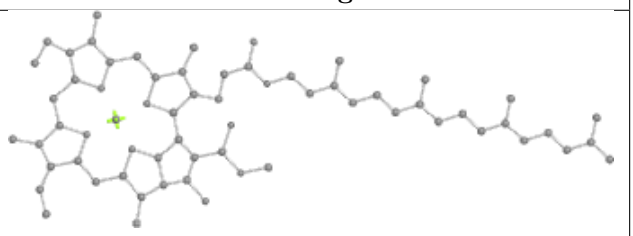
Bond lengths



Bond angles

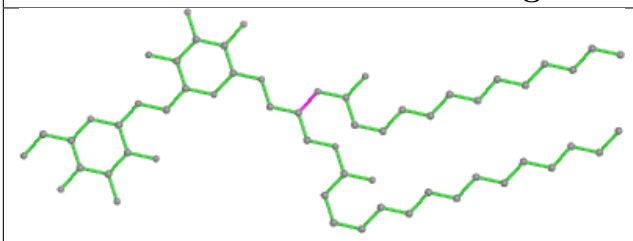


Torsions

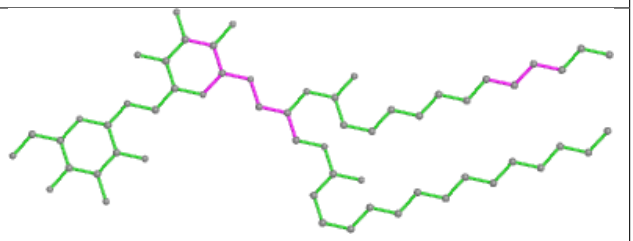


Rings

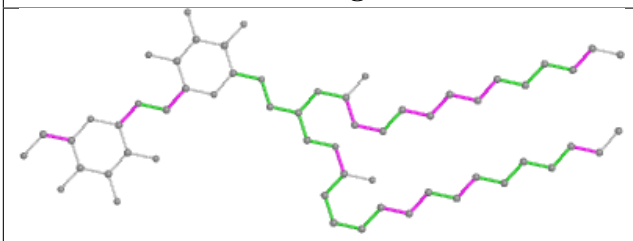
Ligand DGD b 624



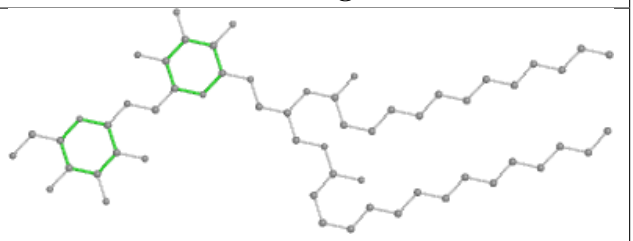
Bond lengths



Bond angles

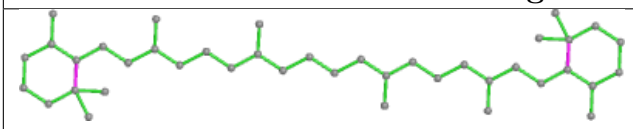


Torsions

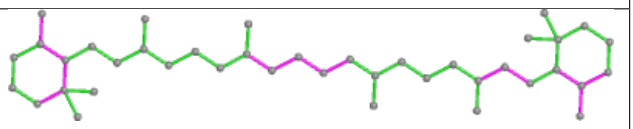


Rings

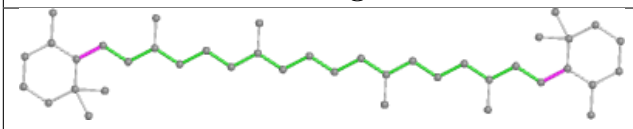
Ligand BCR a 410



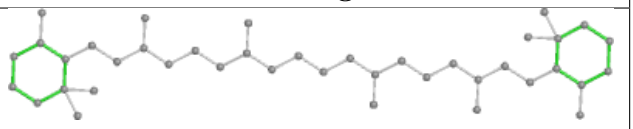
Bond lengths



Bond angles

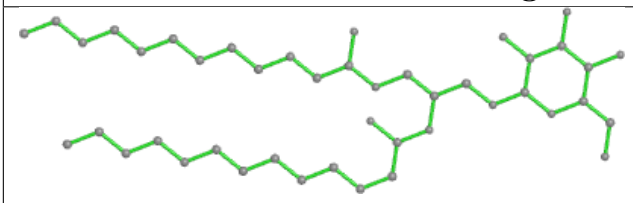


Torsions

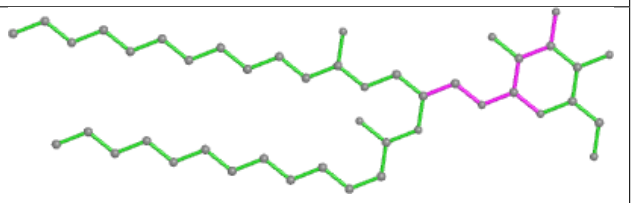


Rings

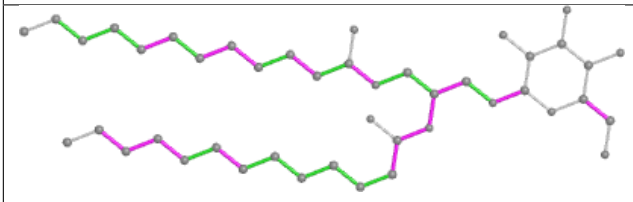
Ligand LMG E 101



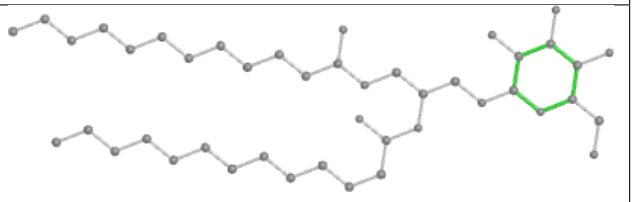
Bond lengths



Bond angles

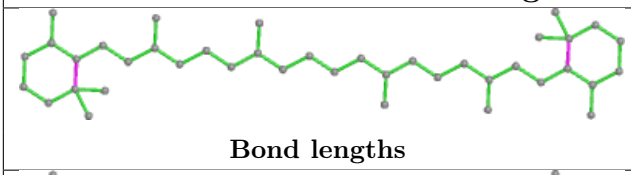


Torsions

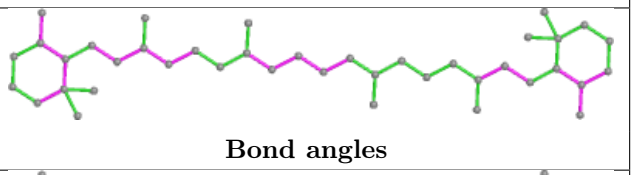


Rings

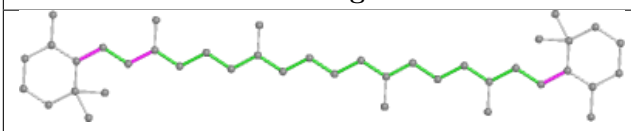
Ligand BCR C 521



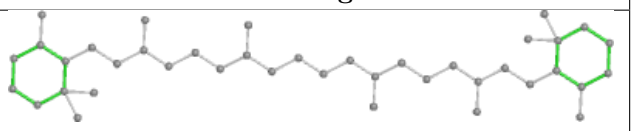
Bond lengths



Bond angles

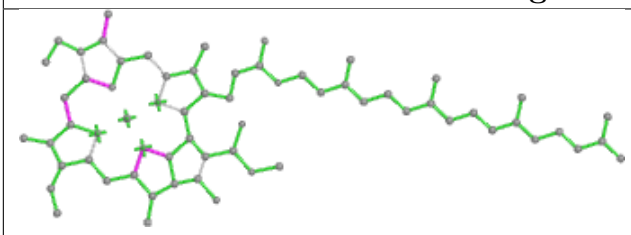


Torsions

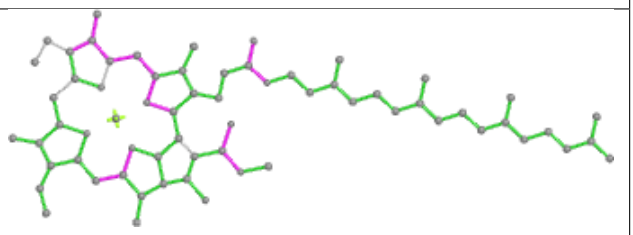


Rings

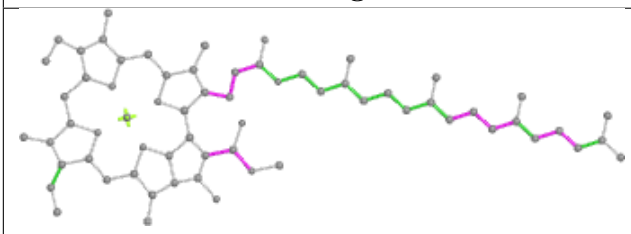
Ligand CLA c 501



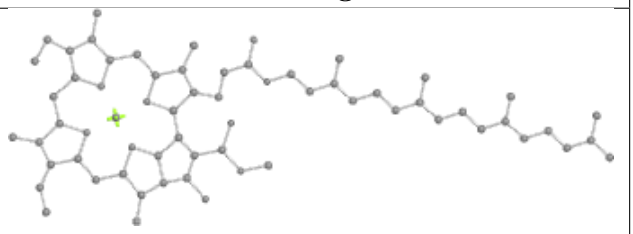
Bond lengths



Bond angles

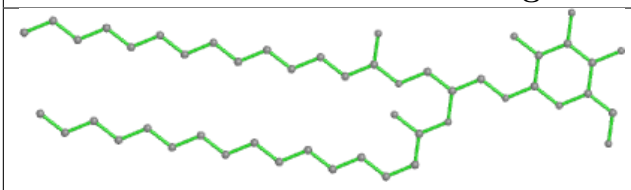


Torsions

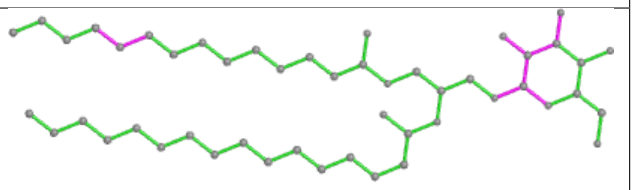


Rings

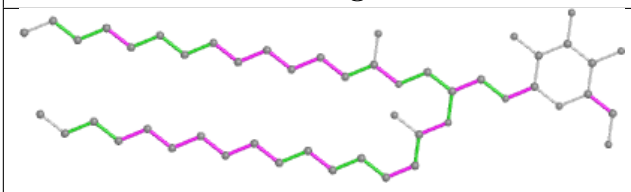
Ligand LMG b 628



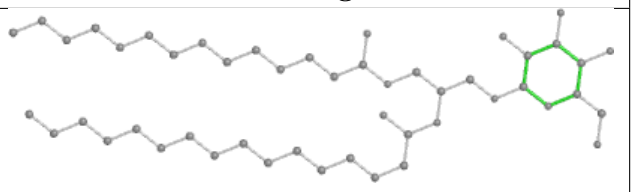
Bond lengths



Bond angles

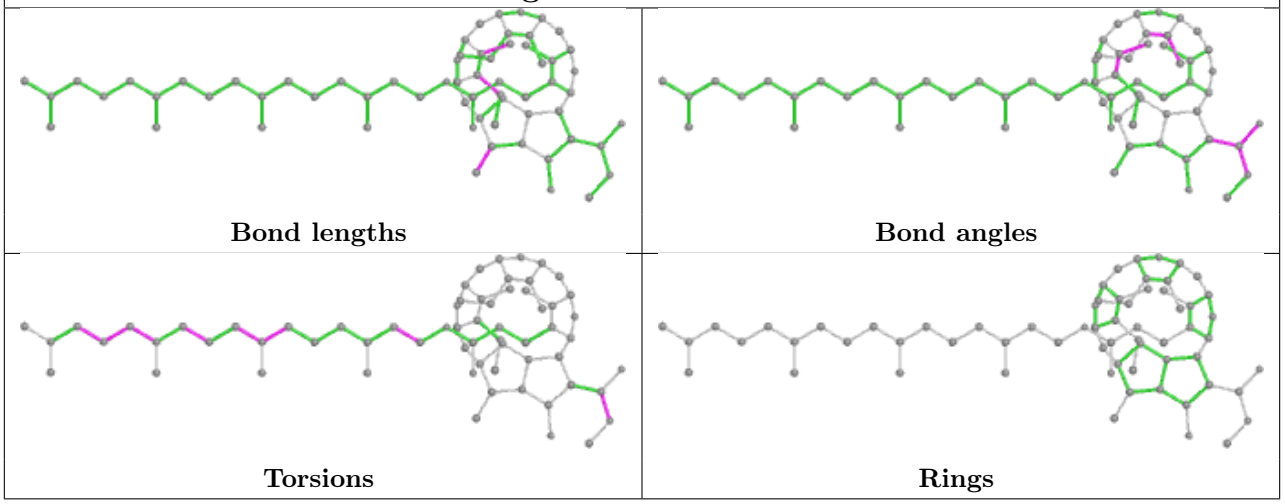


Torsions

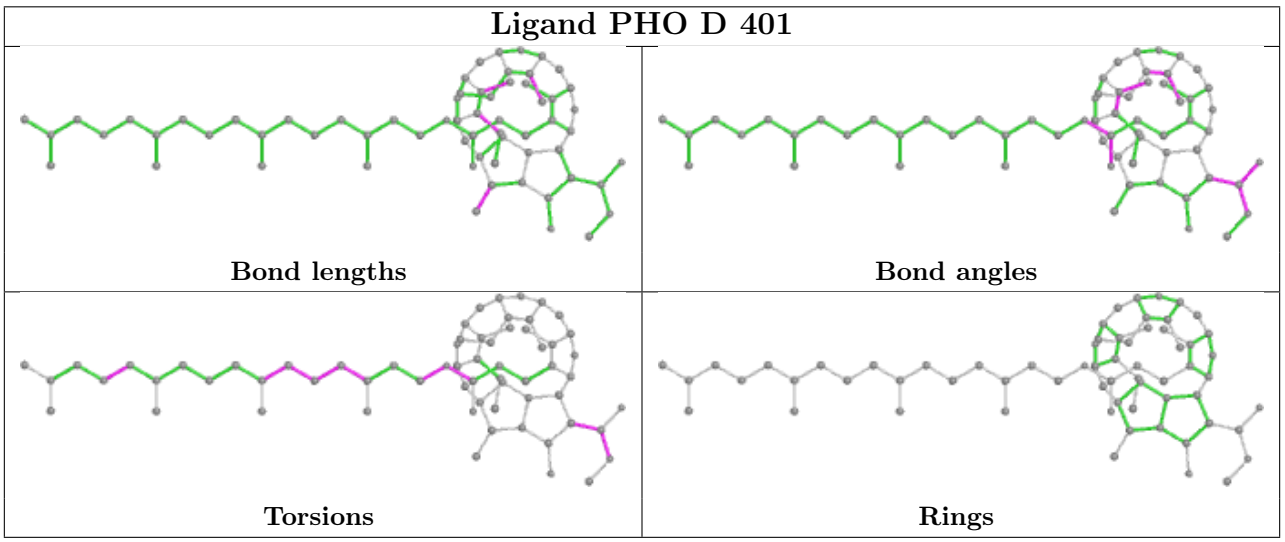


Rings

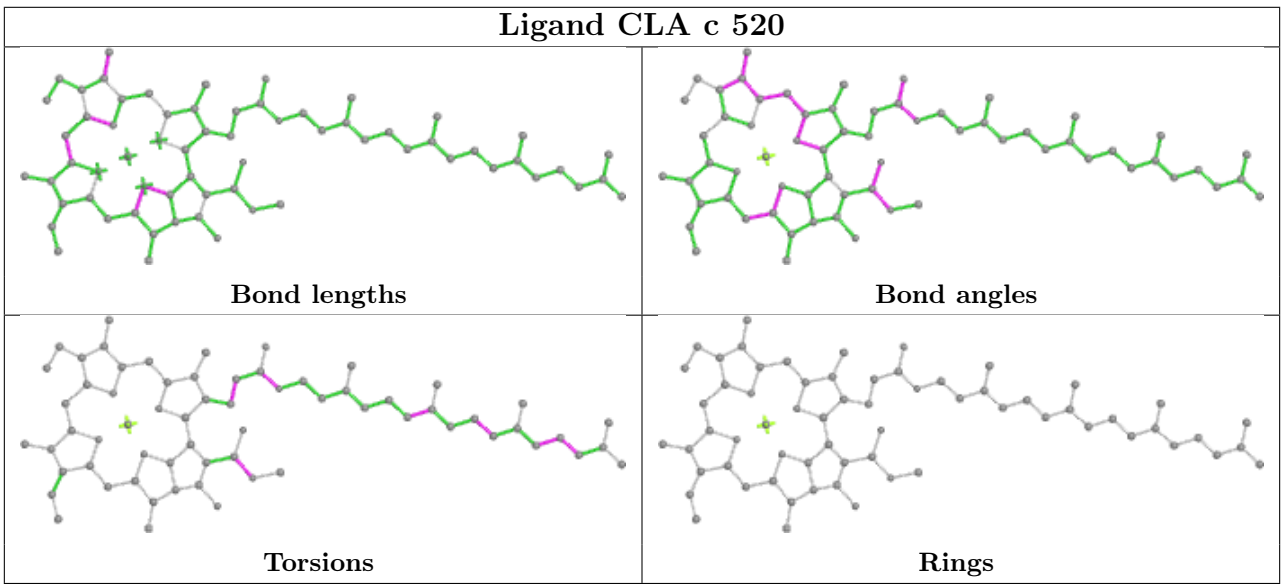
Ligand PHO D 402



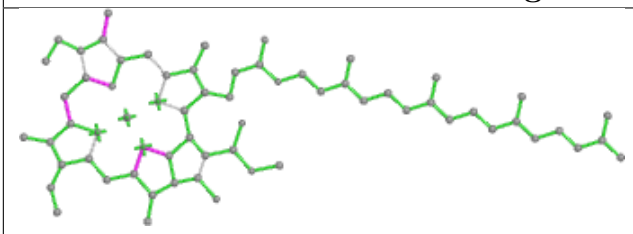
Ligand PHO D 401



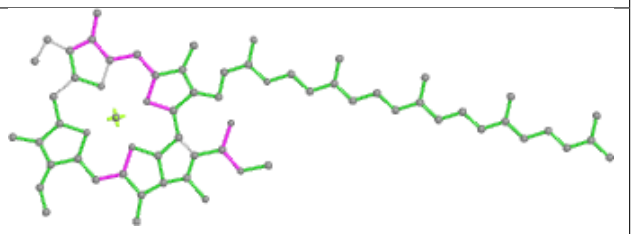
Ligand CLA c 520



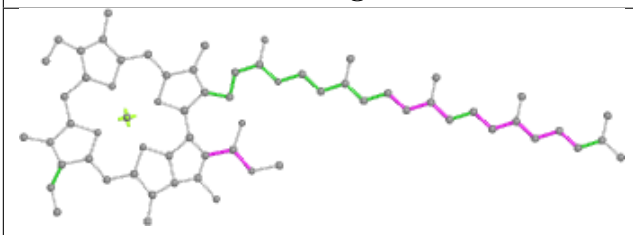
Ligand CLA C 505



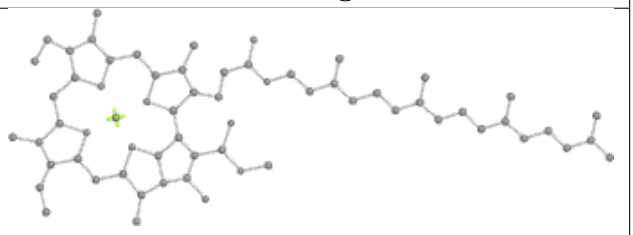
Bond lengths



Bond angles

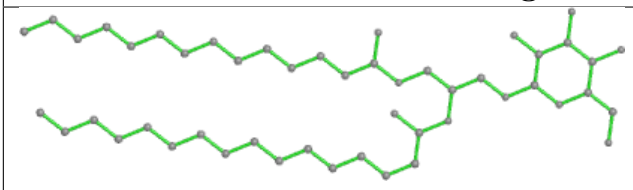


Torsions

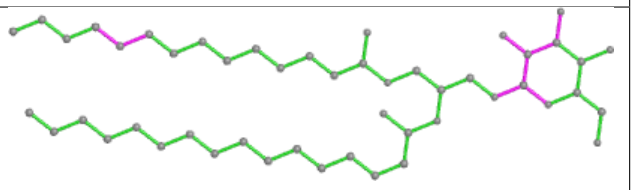


Rings

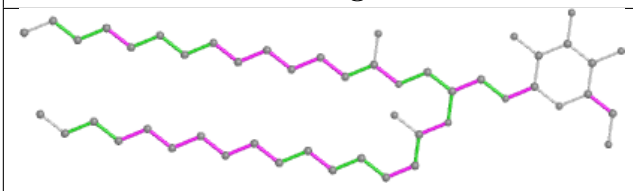
Ligand LMG B 624



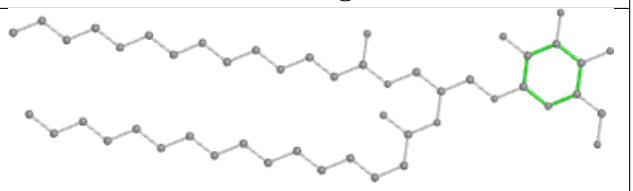
Bond lengths



Bond angles

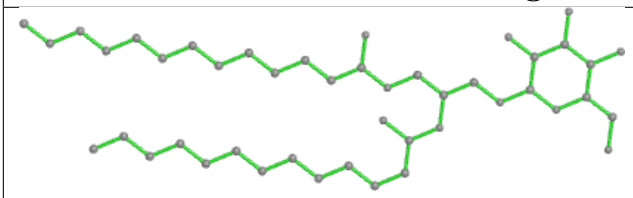


Torsions

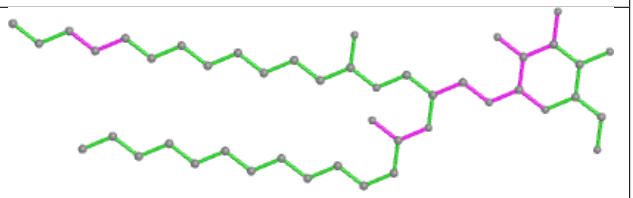


Rings

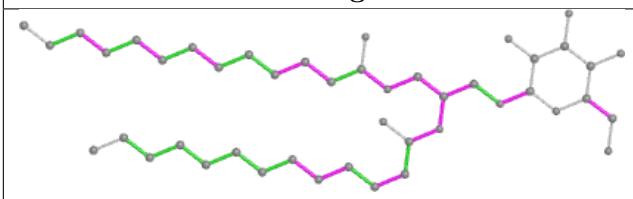
Ligand LMG c 518



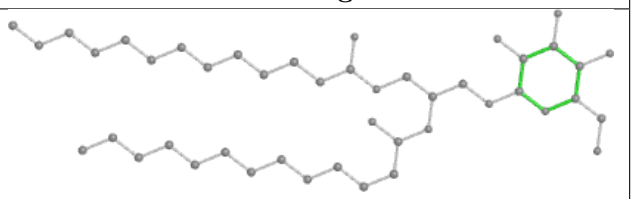
Bond lengths



Bond angles

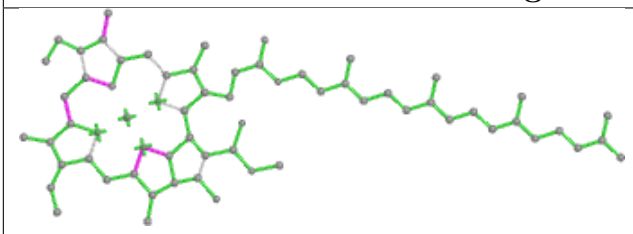


Torsions

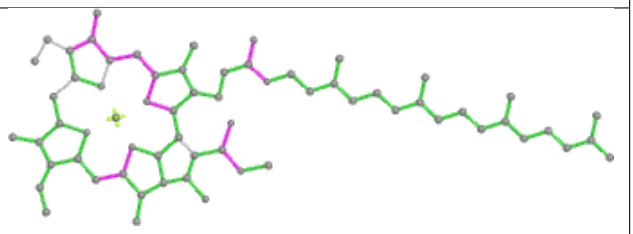


Rings

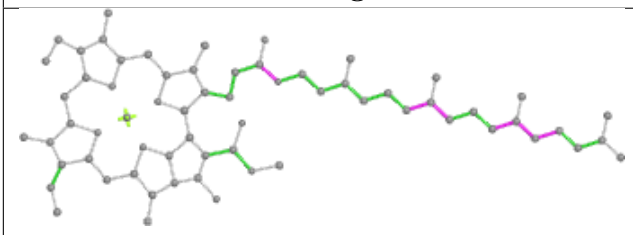
Ligand CLA B 614



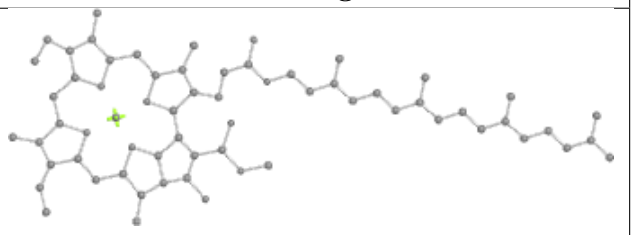
Bond lengths



Bond angles

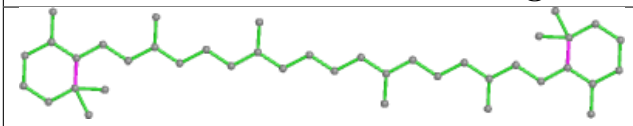


Torsions

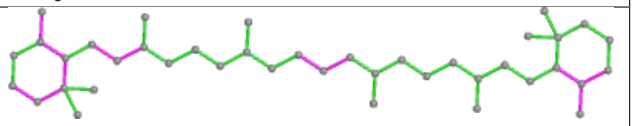


Rings

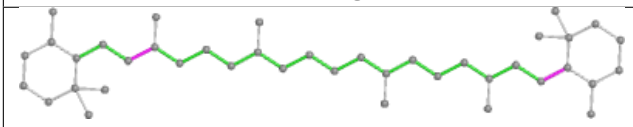
Ligand BCR y 101



Bond lengths



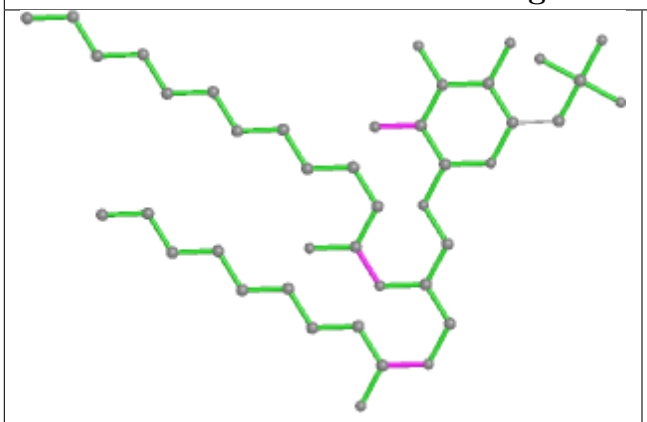
Bond angles



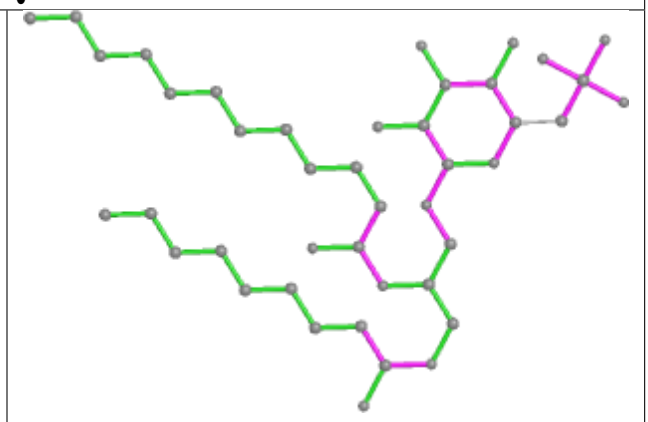
Torsions

Rings

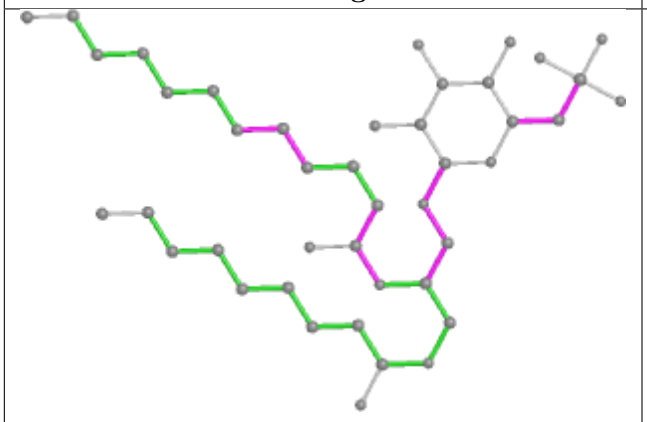
Ligand SQD d 402



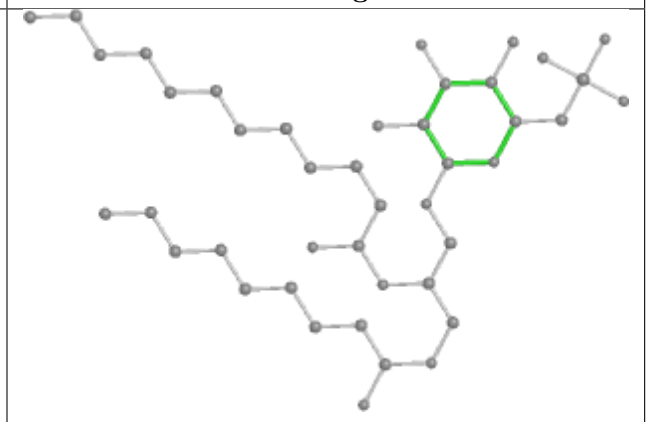
Bond lengths



Bond angles

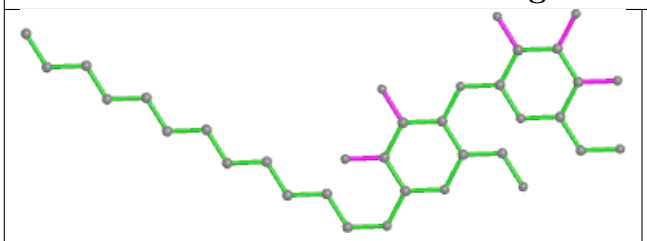


Torsions

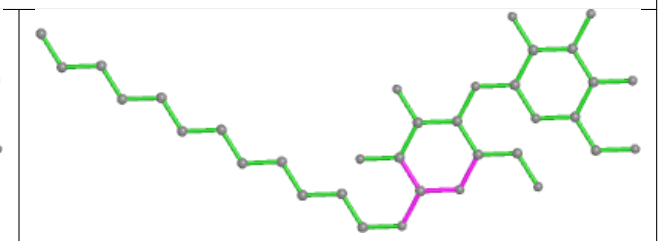


Rings

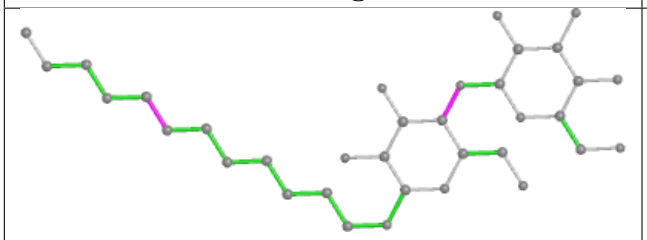
Ligand LMT I 102



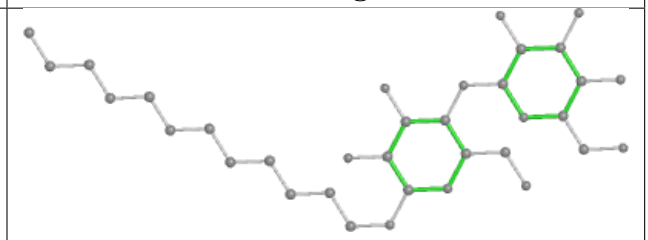
Bond lengths



Bond angles

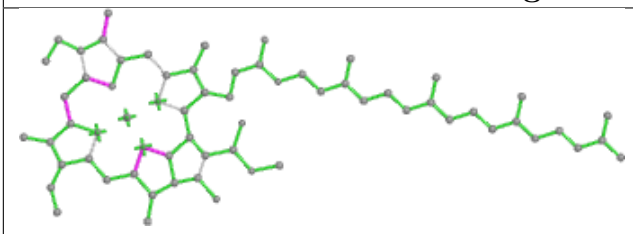


Torsions

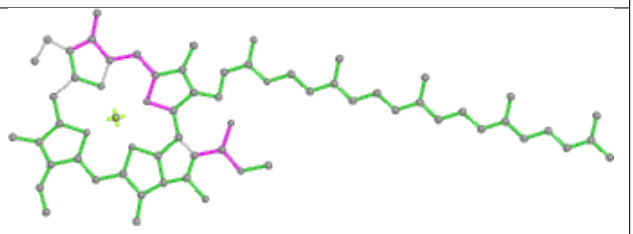


Rings

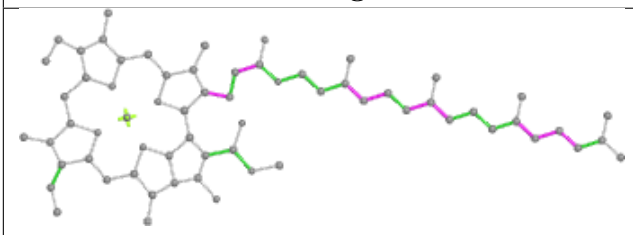
Ligand CLA D 405



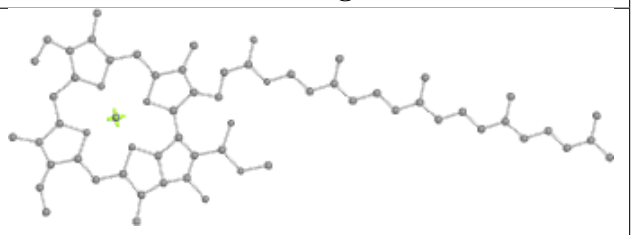
Bond lengths



Bond angles

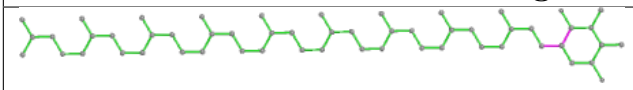


Torsions

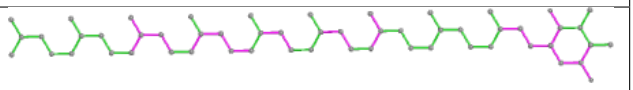


Rings

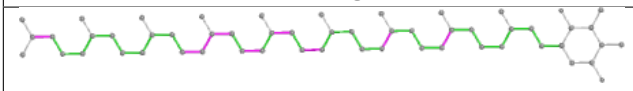
Ligand PL9 d 406



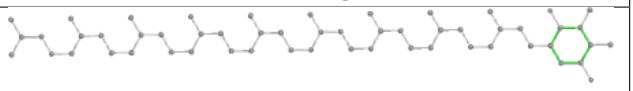
Bond lengths



Bond angles

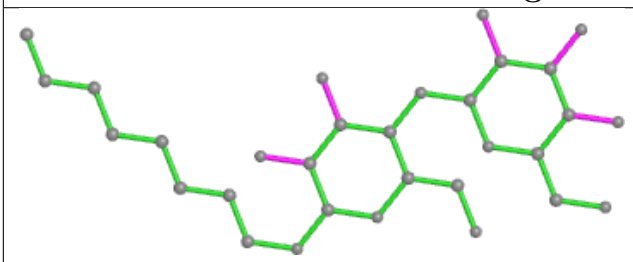


Torsions



Rings

Ligand LMT d 409



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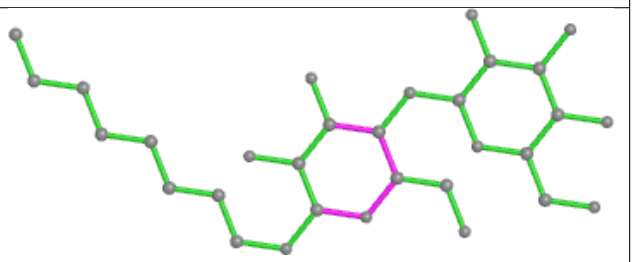
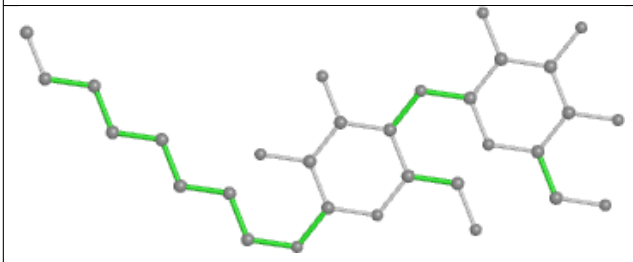


Bond angles



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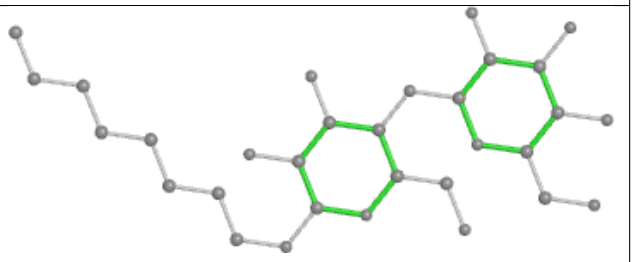
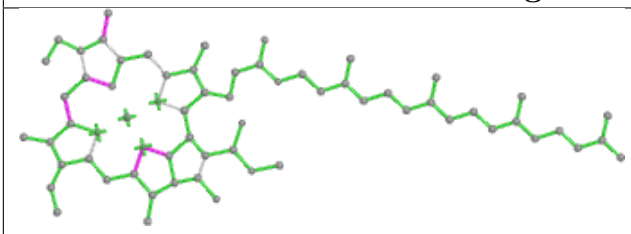


Rings

Ligand CLA C 510



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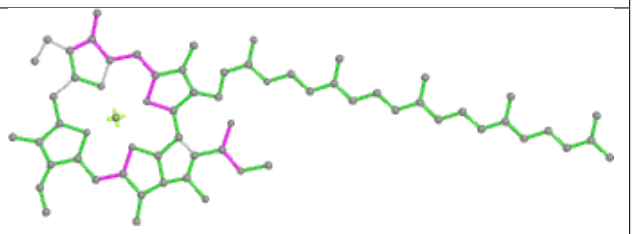

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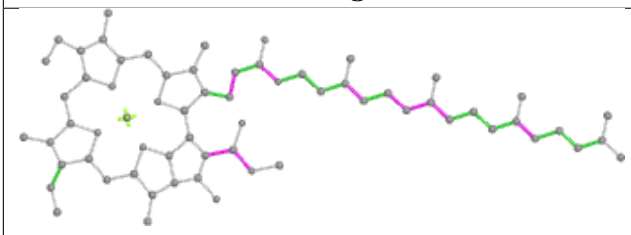
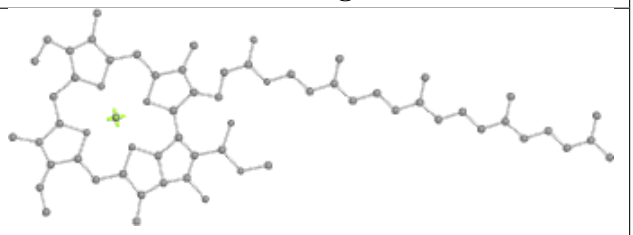
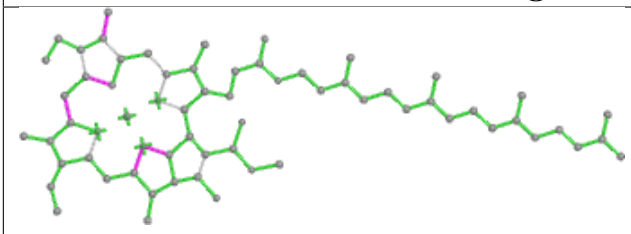


Torsions



Rings

Ligand CLA b 617



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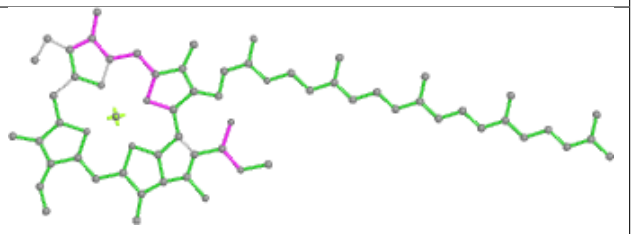
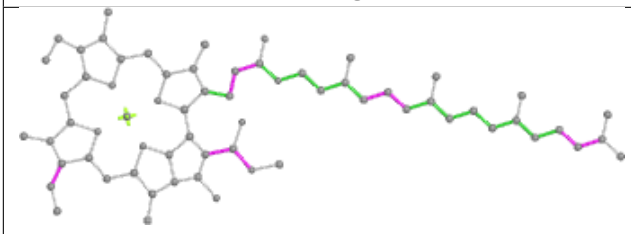
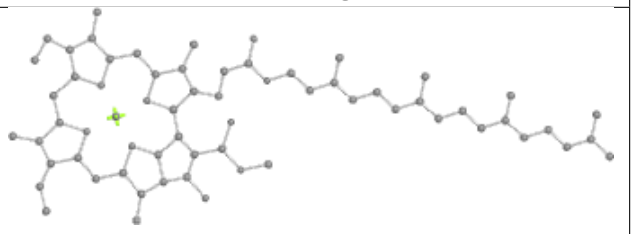


Bond angles

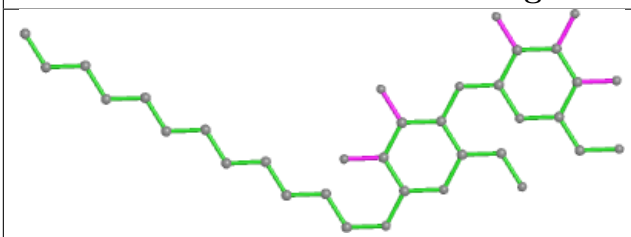


Torsions

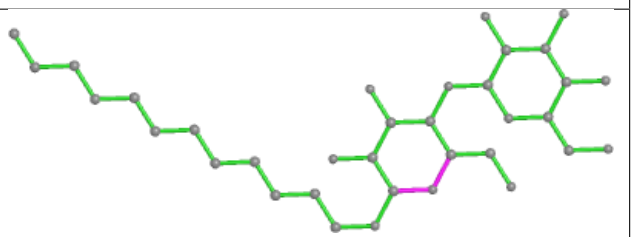


Rings

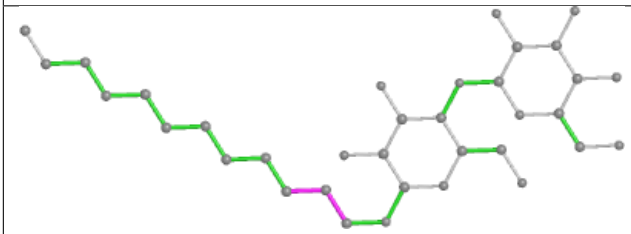
Ligand LMT b 626



Bond lengths



Bond angles



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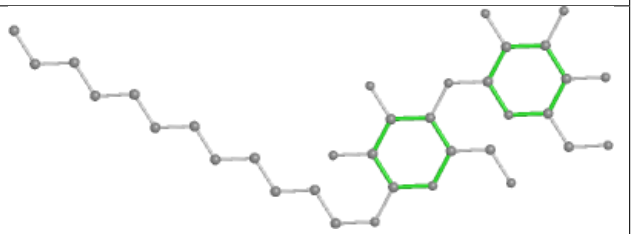
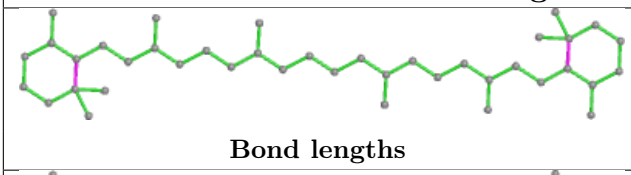


Rings

Ligand BCR f 102



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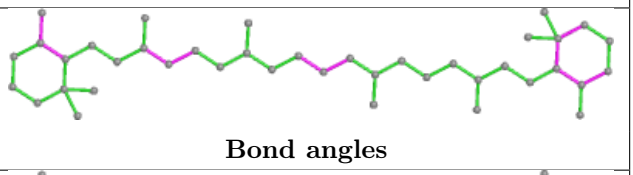
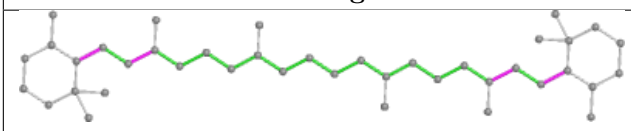


Bond angles



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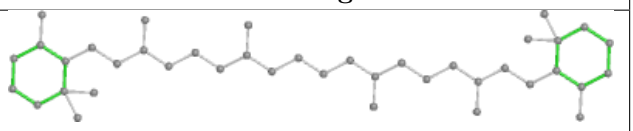
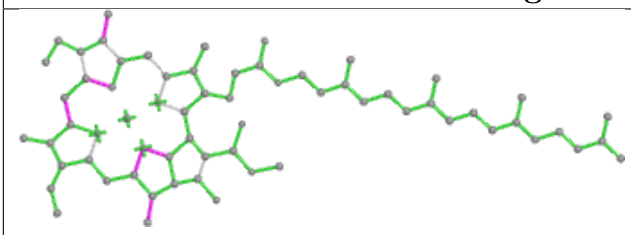


Rings

Ligand CLA B 602



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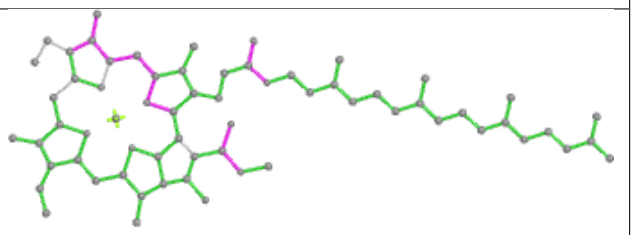
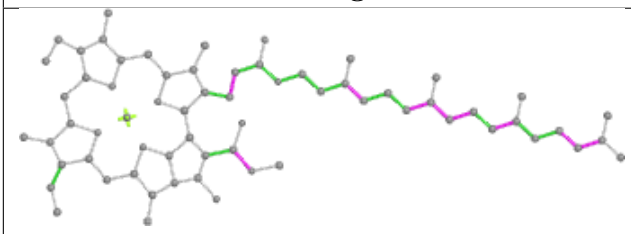


Bond angles



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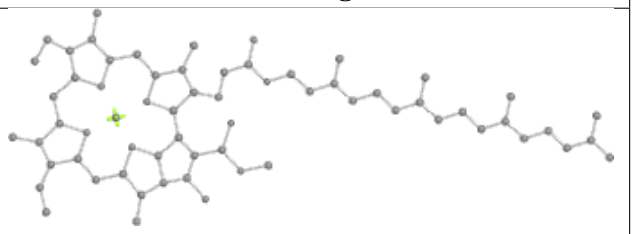
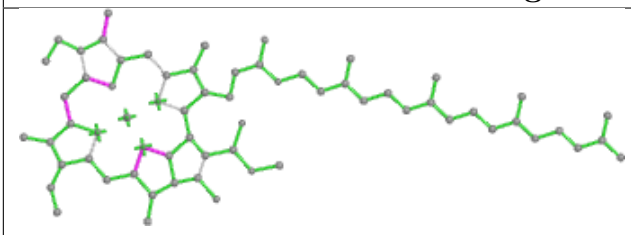


Rings

Ligand CLA C 506



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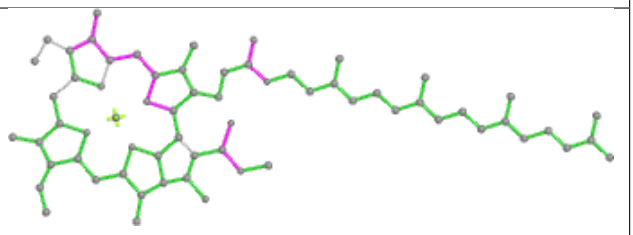
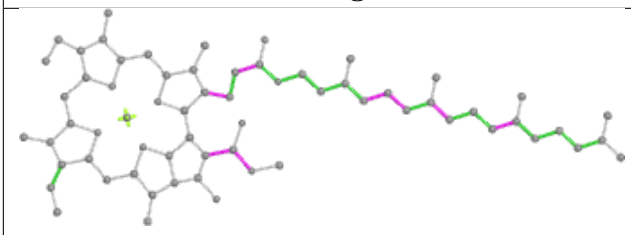


Bond angles



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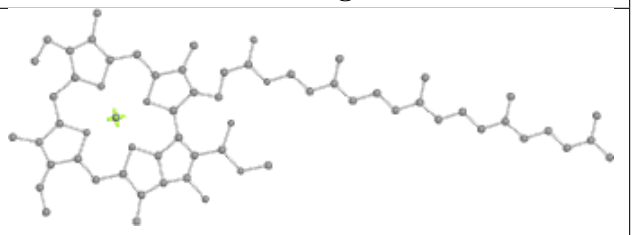
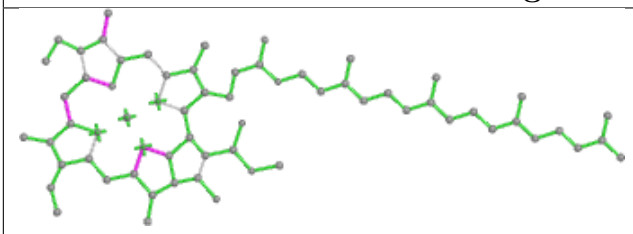


Rings

Ligand CLA A 403



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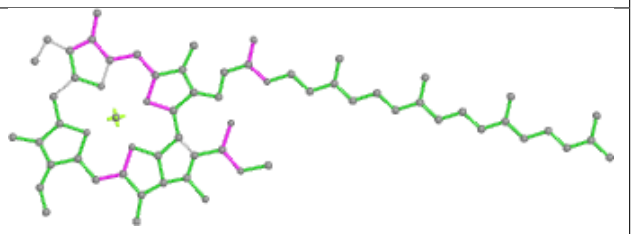
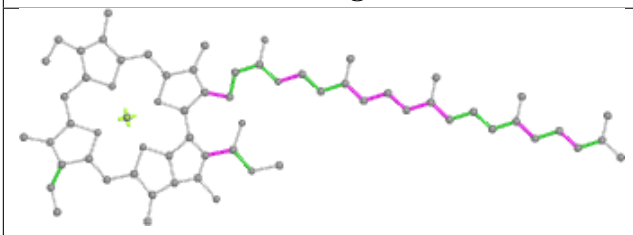


Bond angles



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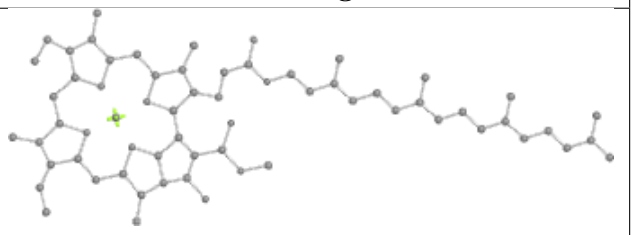
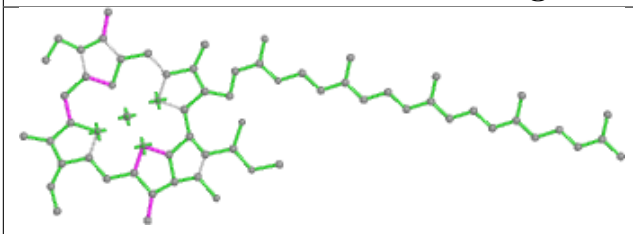


Rings

Ligand CLA c 503



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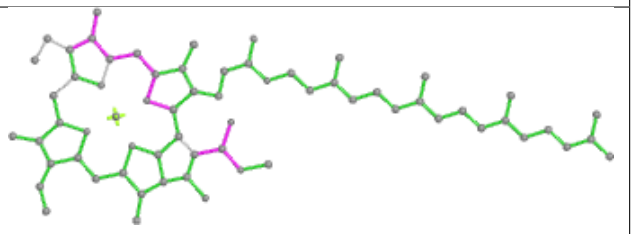
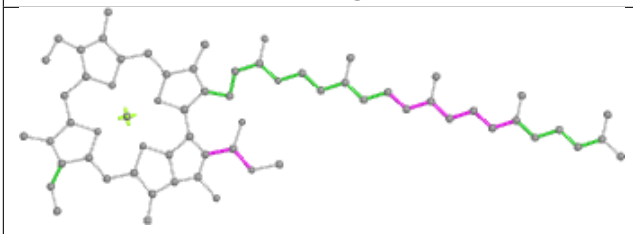


Bond angles



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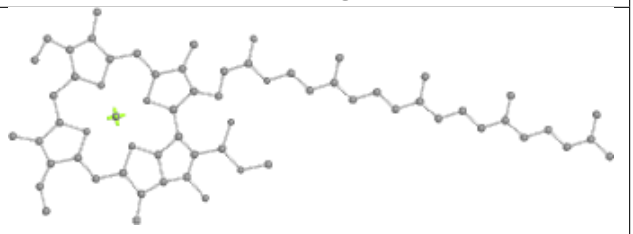
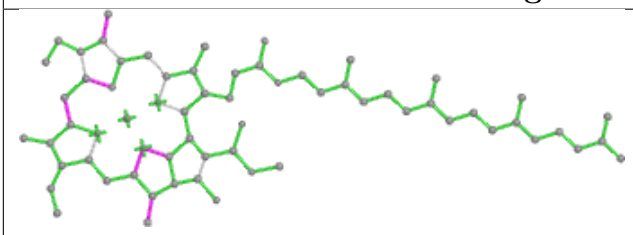


Rings

Ligand CLA B 611



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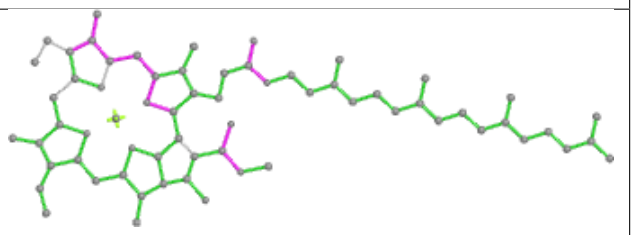
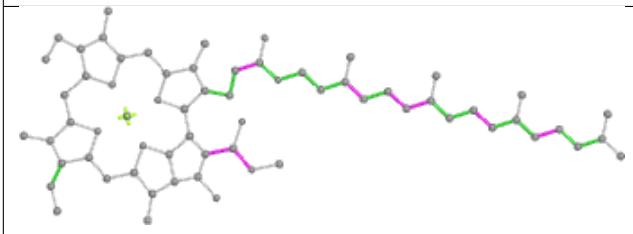


Bond angles



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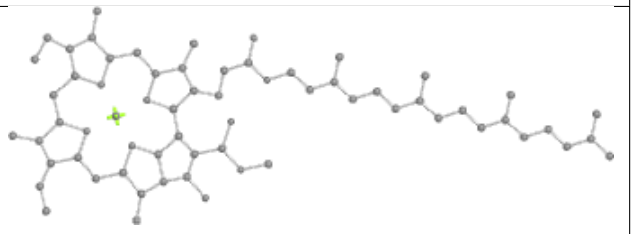
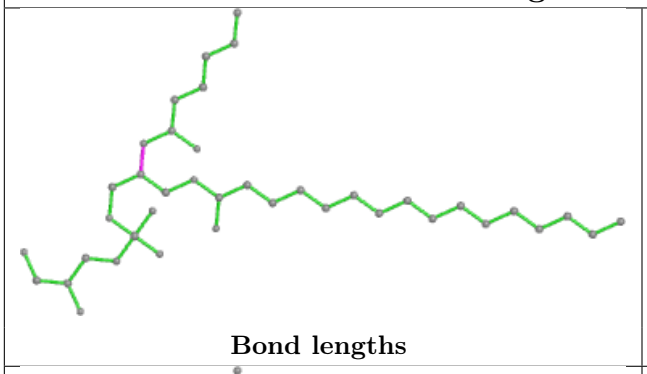


Rings

Ligand LHG a 412



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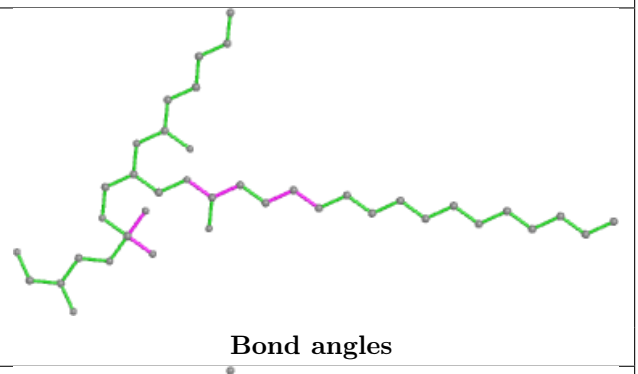
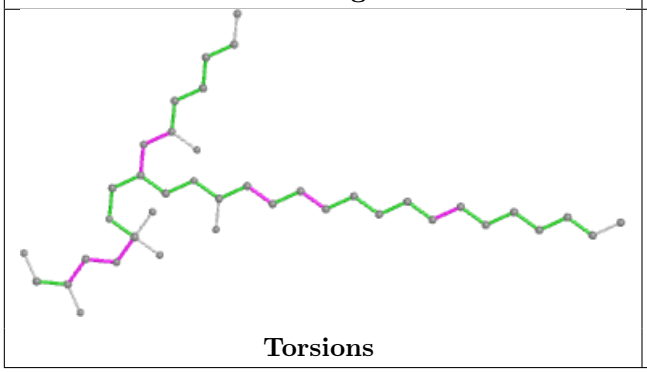


Bond angles



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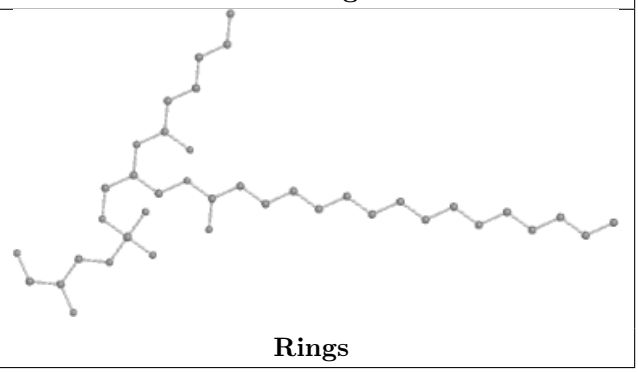
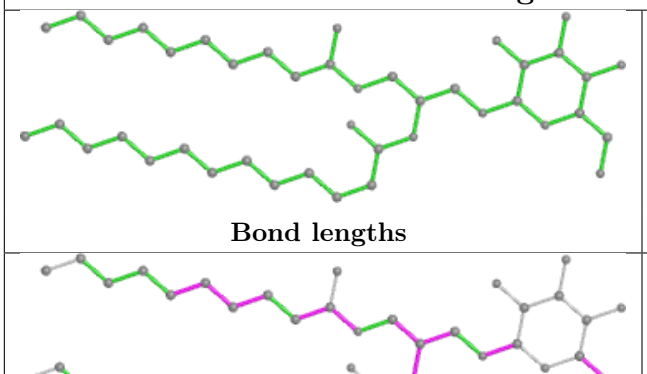
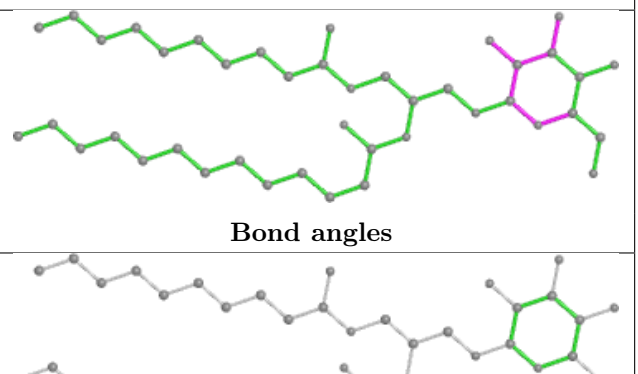


Rings

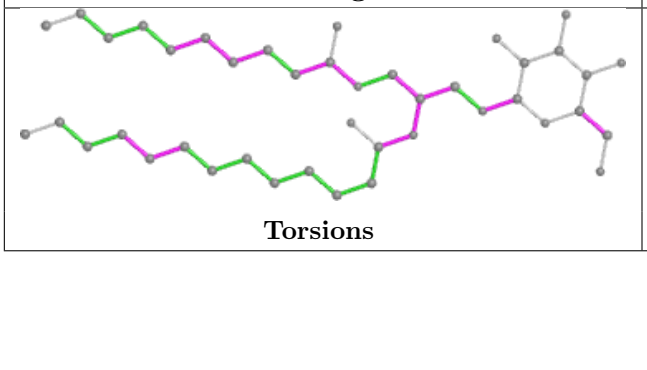
Ligand LMG M 101



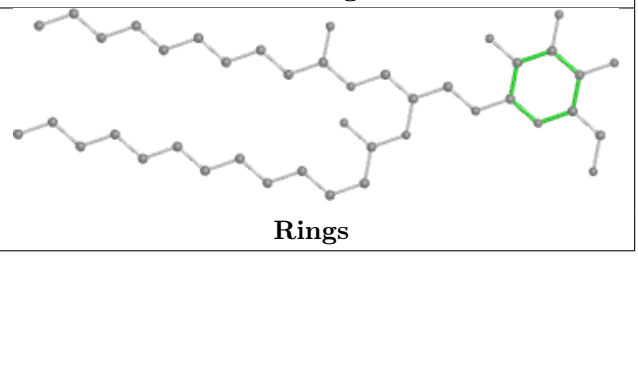
Bond lengths



Bond angles

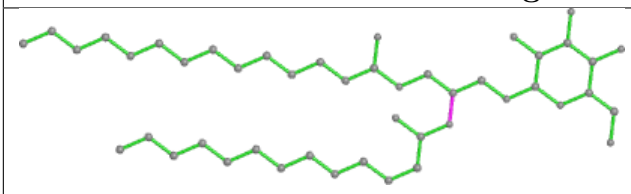


Torsions



Rings

Ligand LMG d 410



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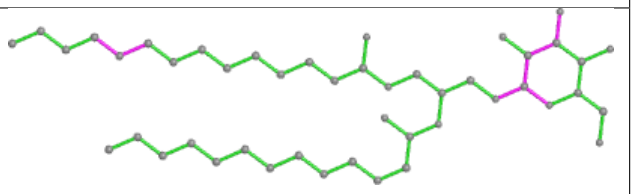
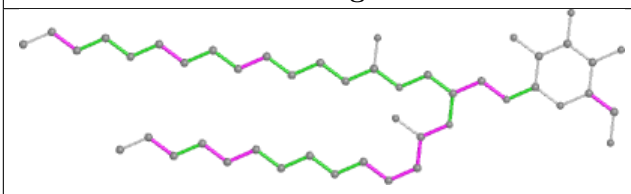
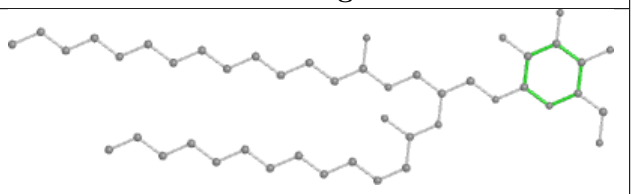


Bond angles

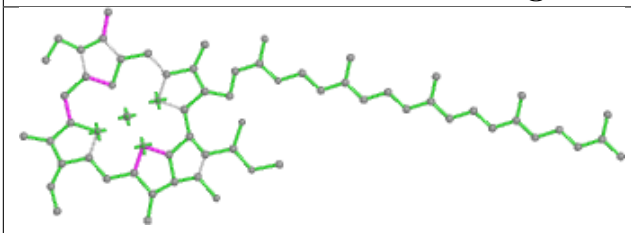


Torsions

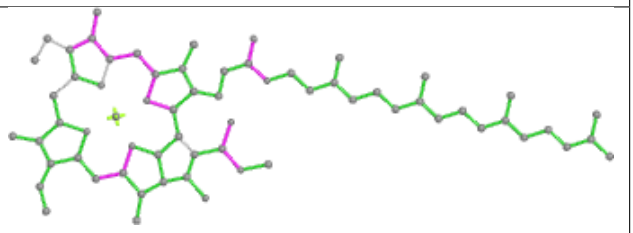


Rings

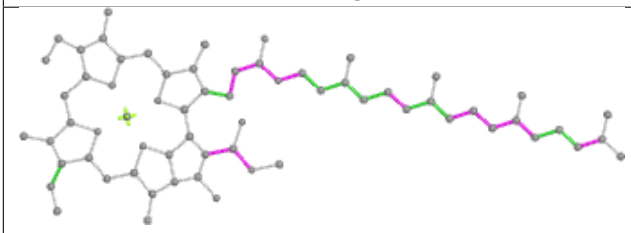
Ligand CLA b 613



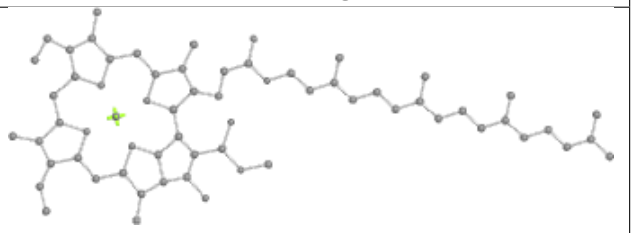
Bond lengths



Bond angles

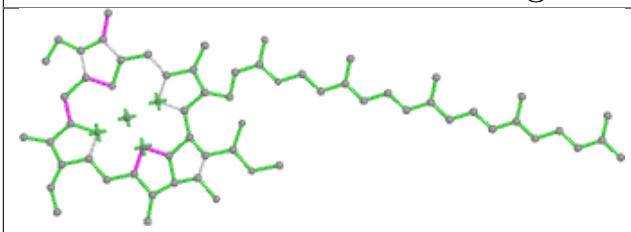


Torsions

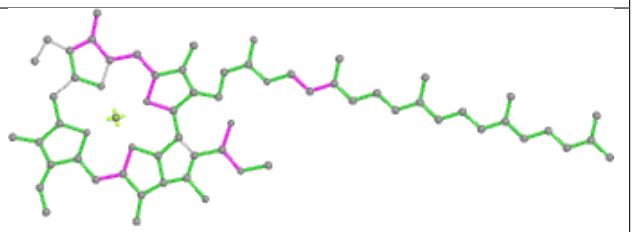


Rings

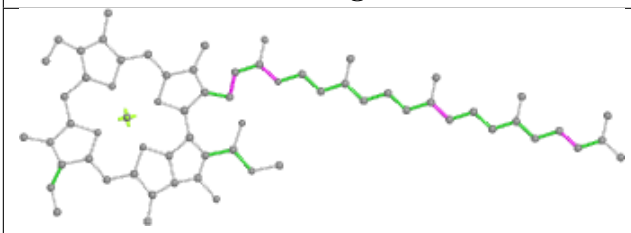
Ligand CLA d 405



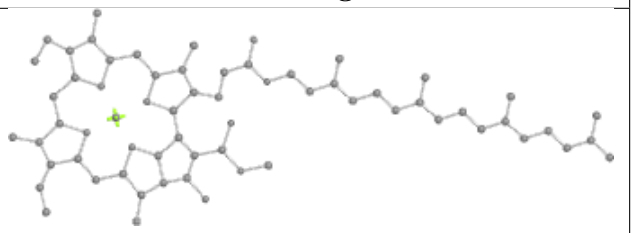
Bond lengths



Bond angles

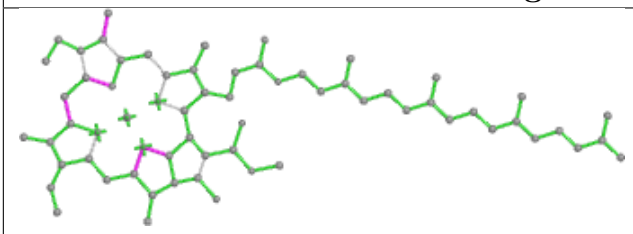


Torsions

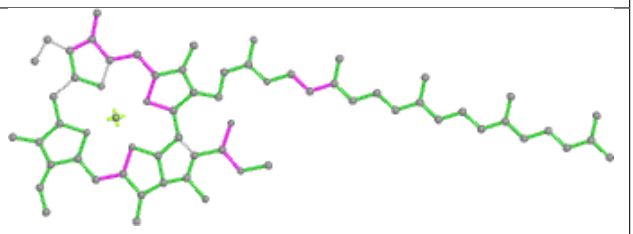


Rings

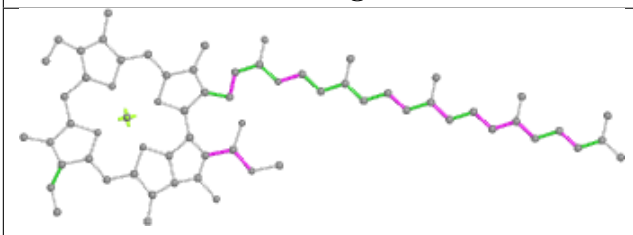
Ligand CLA C 507



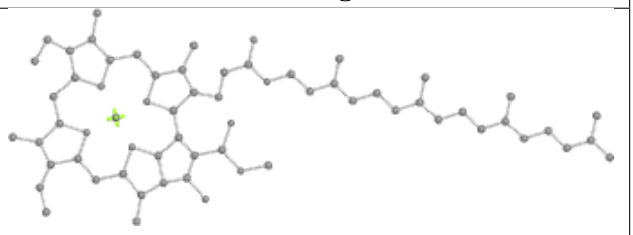
Bond lengths



Bond angles

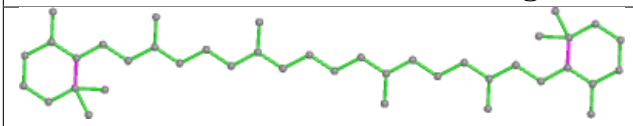


Torsions

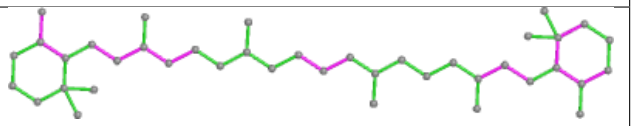


Rings

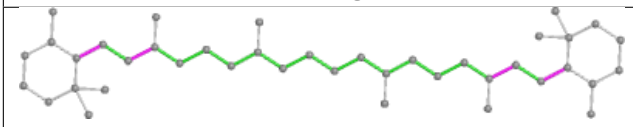
Ligand BCR D 411



Bond lengths



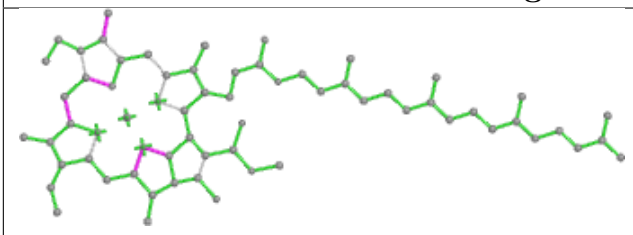
Bond angles



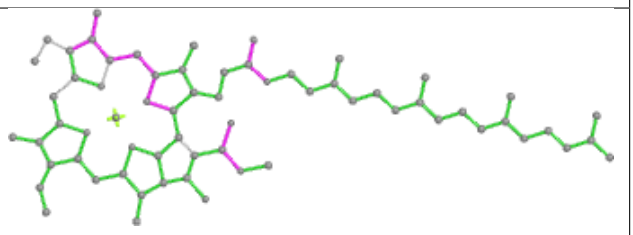
Torsions

Rings

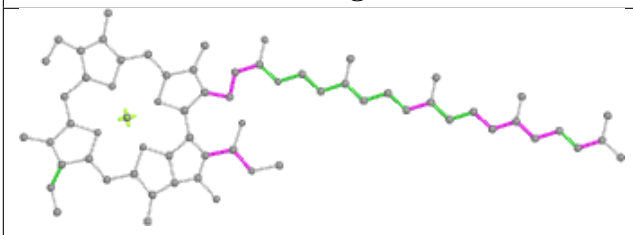
Ligand CLA B 601



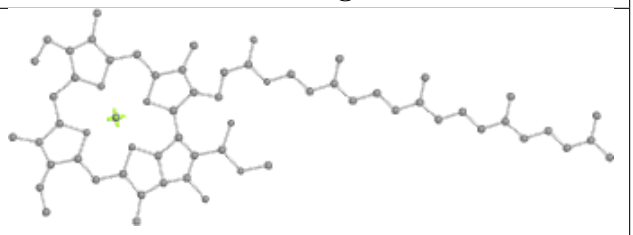
Bond lengths



Bond angles

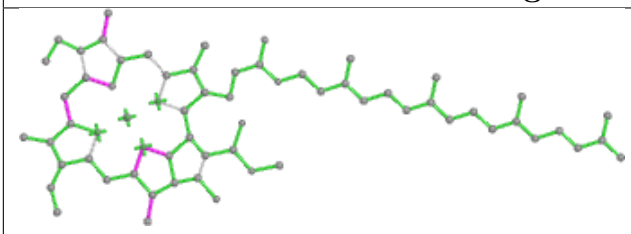


Torsions

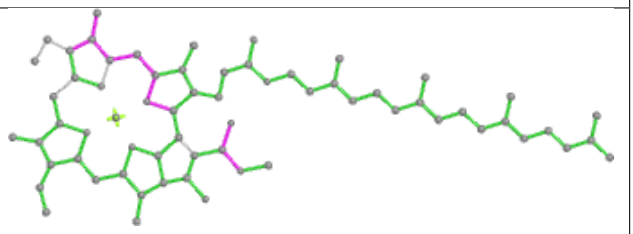


Rings

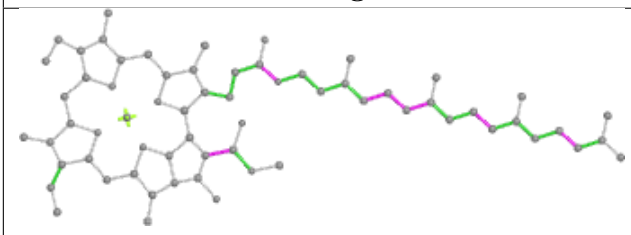
Ligand CLA A 404



Bond lengths



Bond angles



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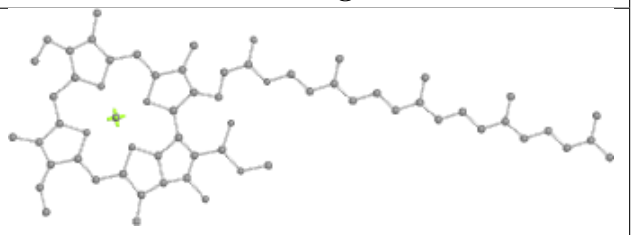
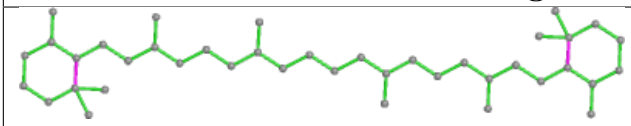


Rings

Ligand BCR c 513



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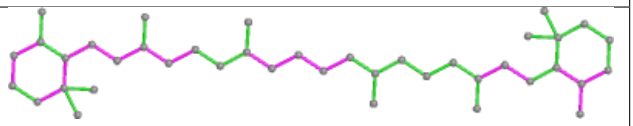
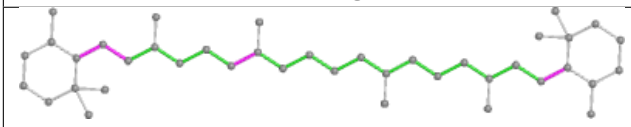


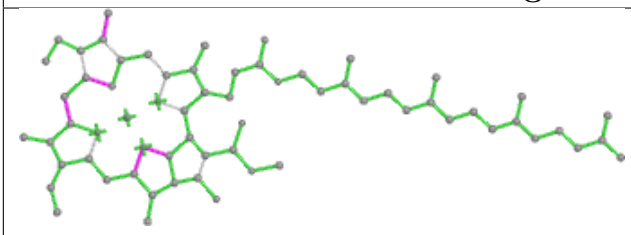
Bond angles



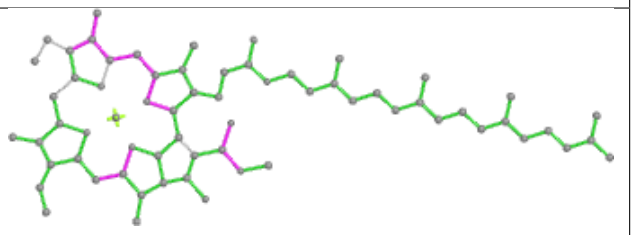
Torsions

Rings

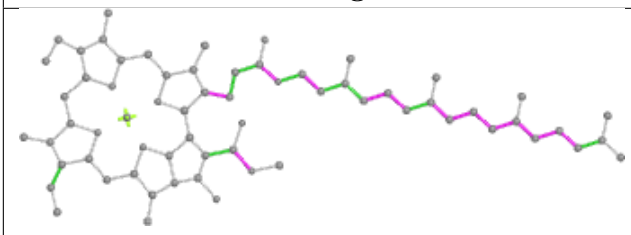
Ligand CLA B 615



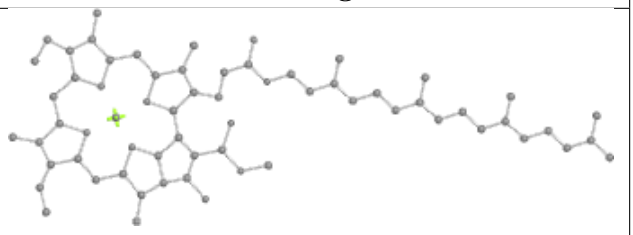
Bond lengths



Bond angles

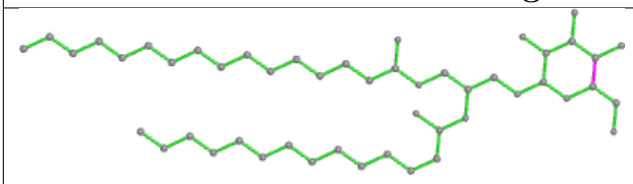


Torsions

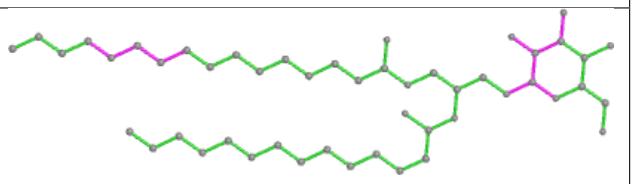


Rings

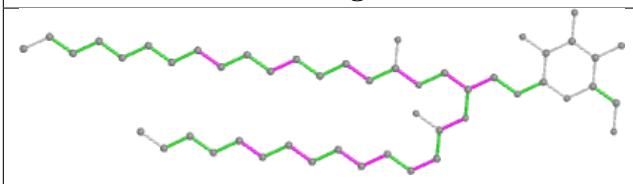
Ligand LMG b 625



Bond lengths



Bond angles



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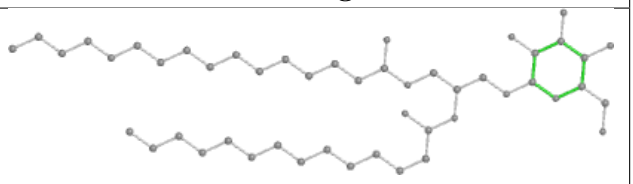
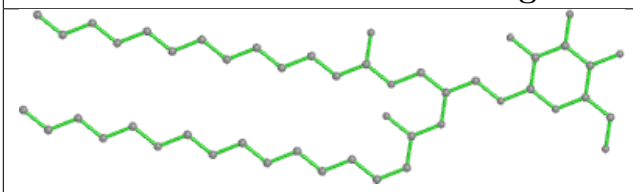
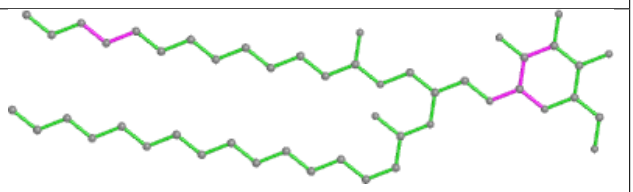


Rings

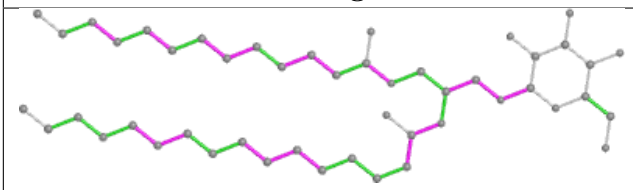
Ligand LMG D 408



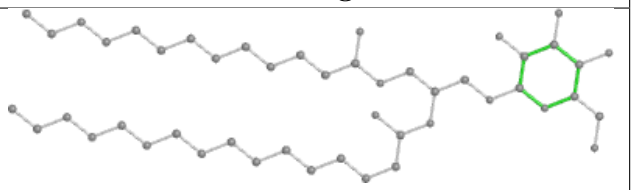
Bond lengths



Bond angles

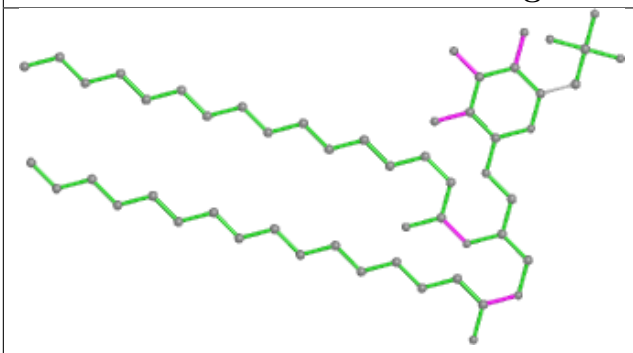


Torsions

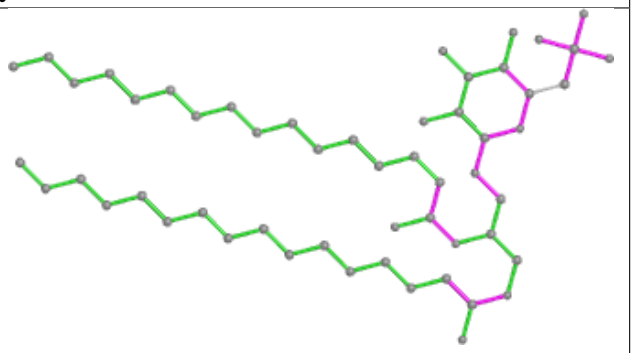


Rings

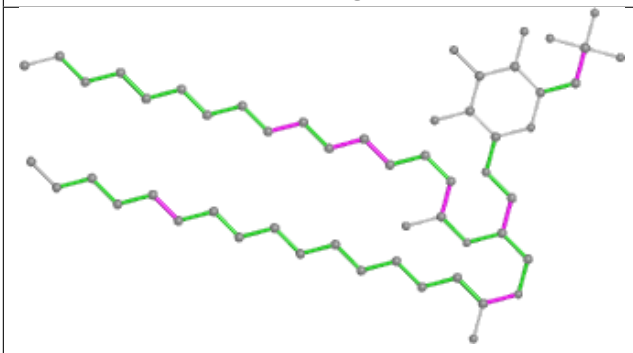
Ligand SQD A 414



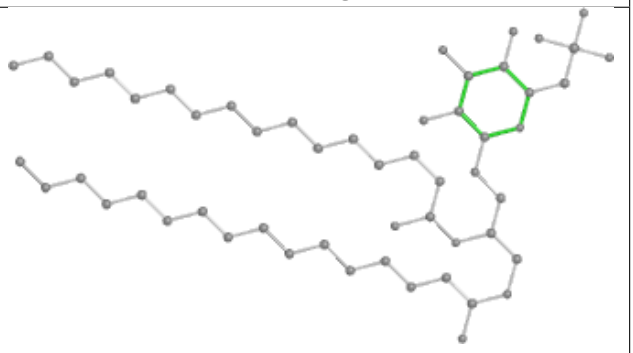
Bond lengths



Bond angles

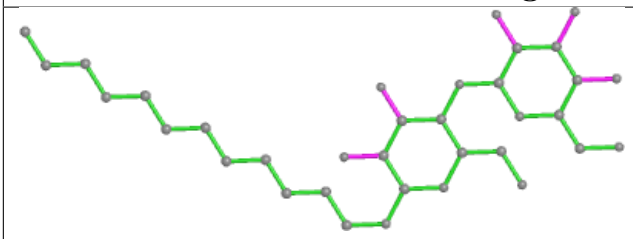


Torsions

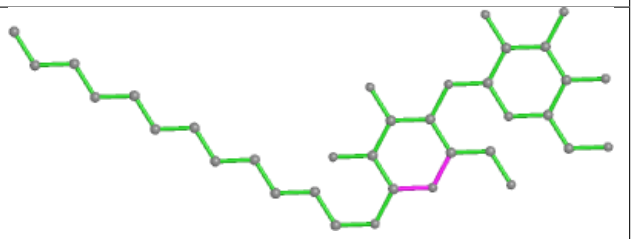


Rings

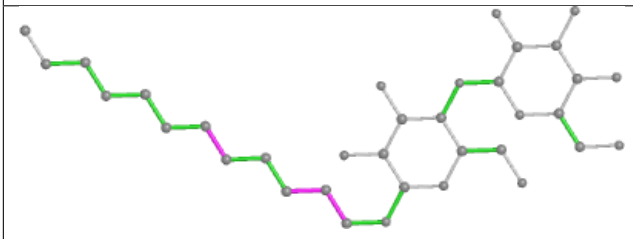
Ligand LMT B 622



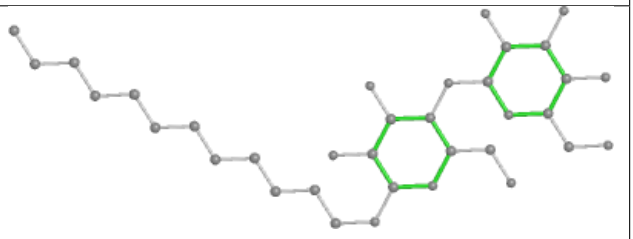
Bond lengths



Bond angles

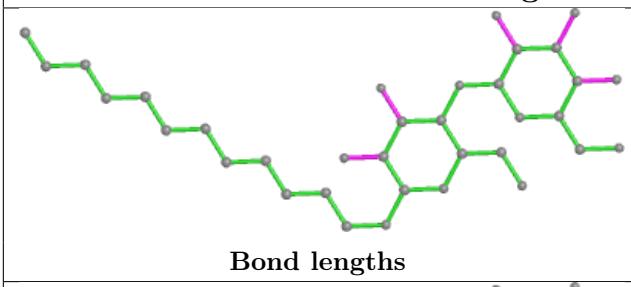


Torsions

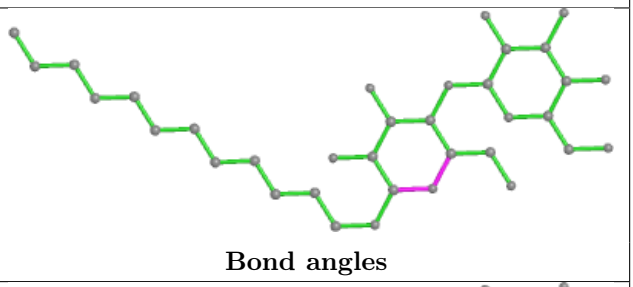


Rings

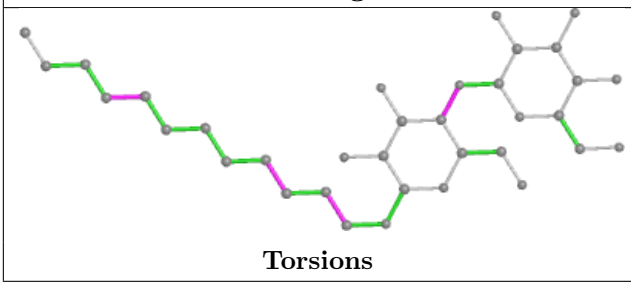
Ligand LMT B 628



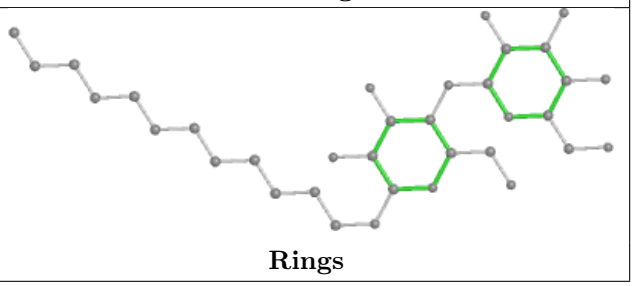
Bond lengths



Bond angles

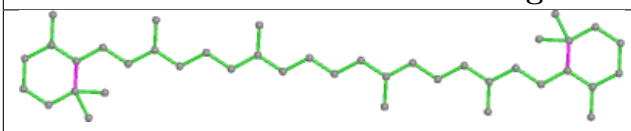


Torsions

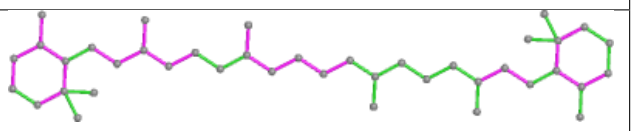


Rings

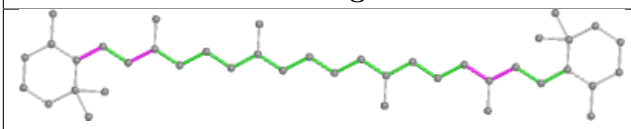
Ligand BCR J 102



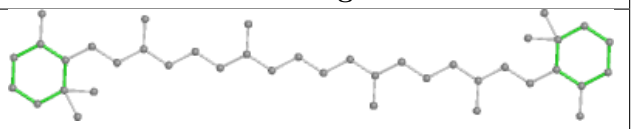
Bond lengths



Bond angles

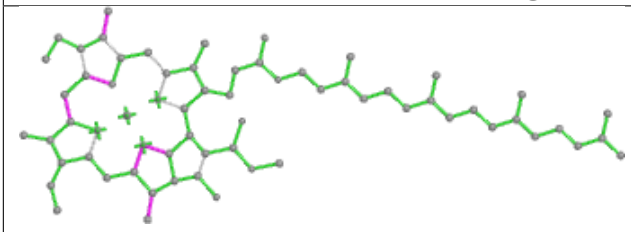


Torsions

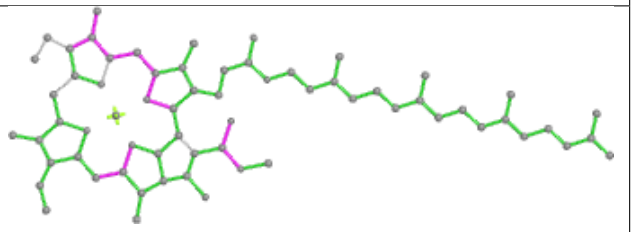


Rings

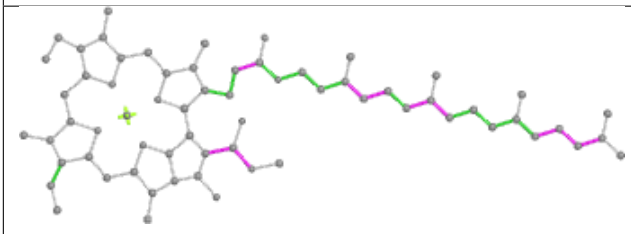
Ligand CLA C 509



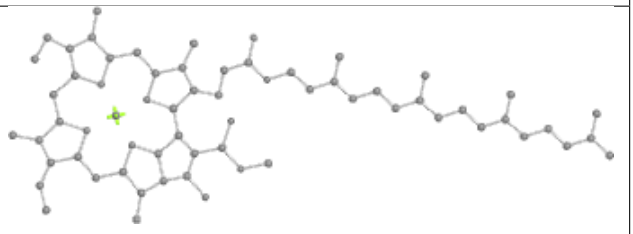
Bond lengths



Bond angles

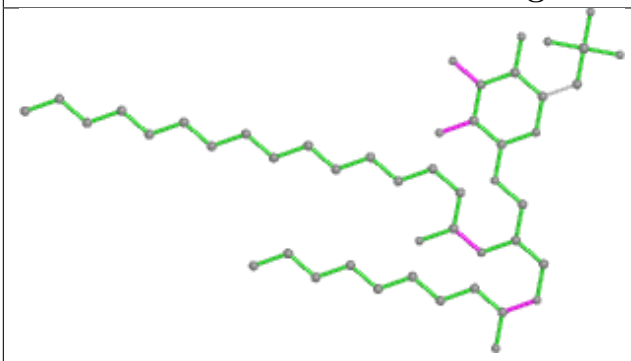


Torsions

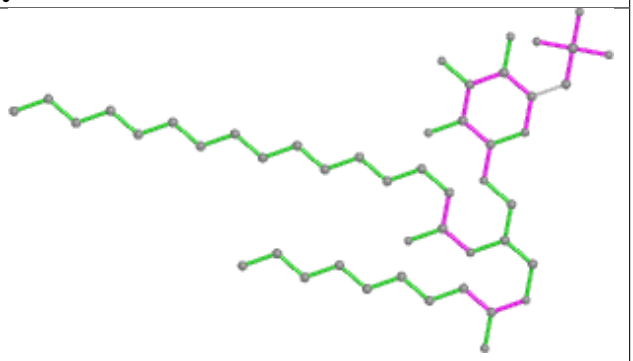


Rings

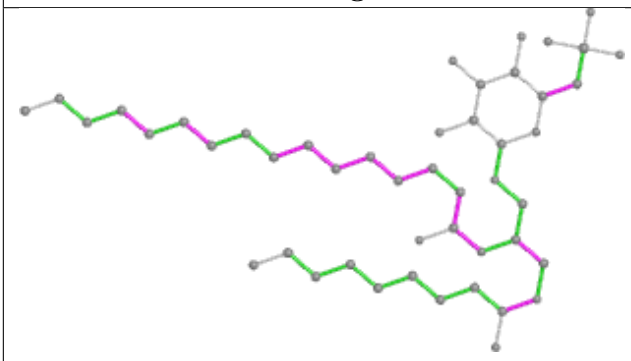
Ligand SQD b 602



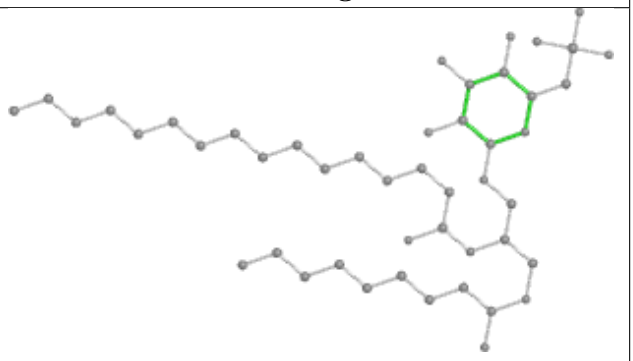
Bond lengths



Bond angles

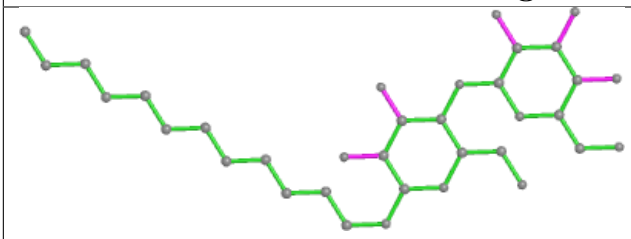


Torsions



Rings

Ligand LMT M 102



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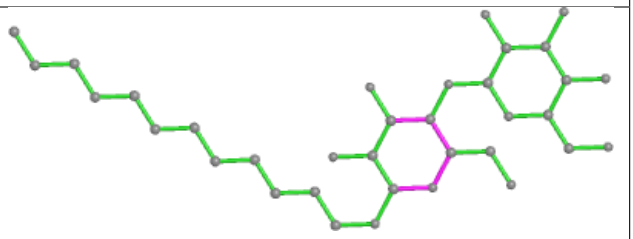

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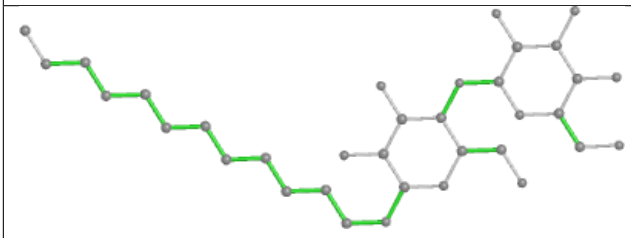

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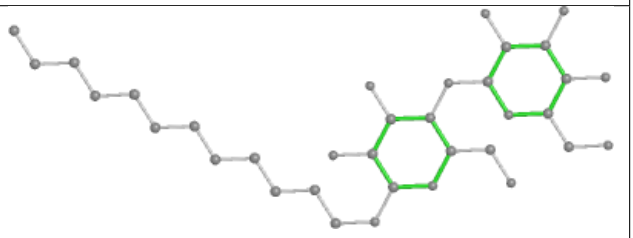
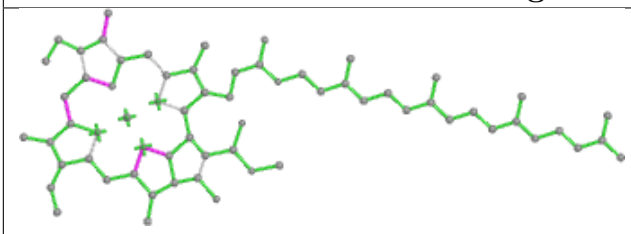


Rings

Ligand CLA b 610



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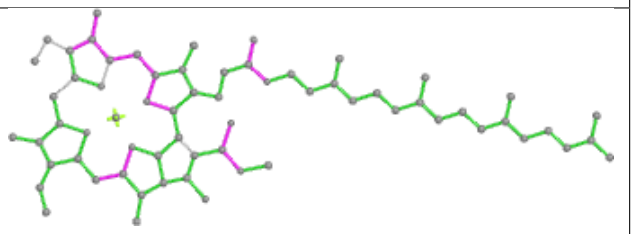
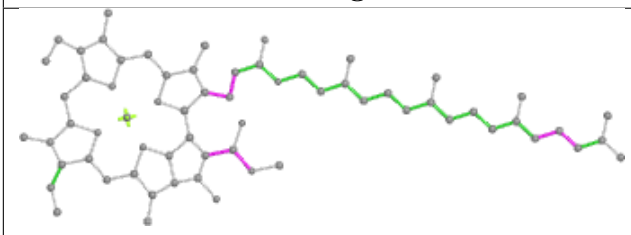


Bond angles



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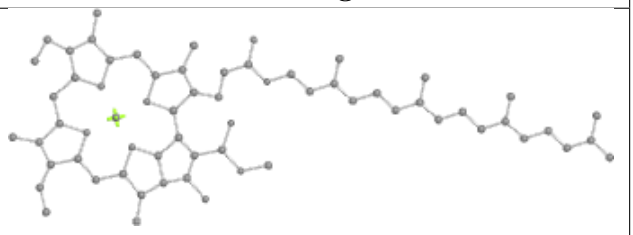
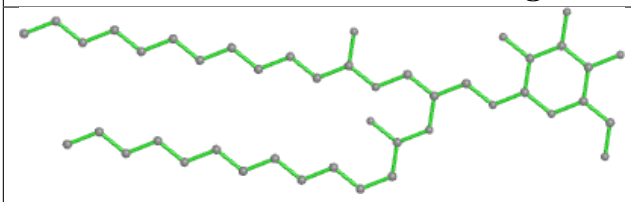


Rings

Ligand LMG e 101



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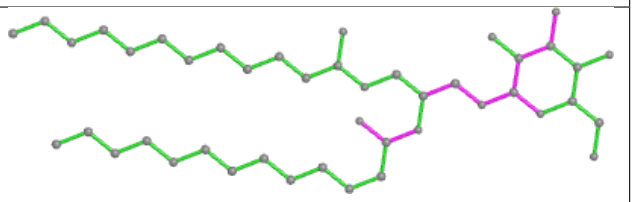
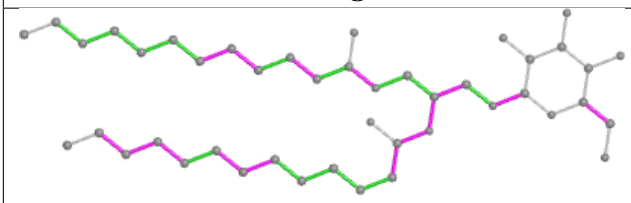
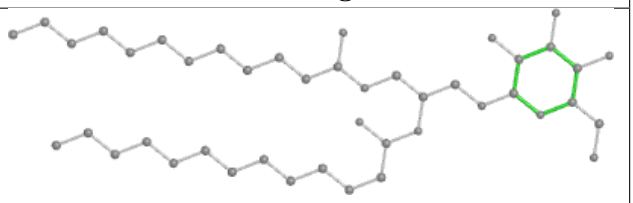


Bond angles

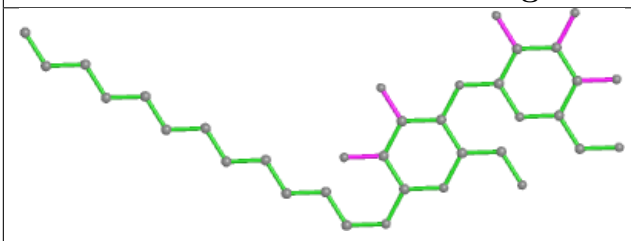


Torsions



Rings

Ligand LMT B 623



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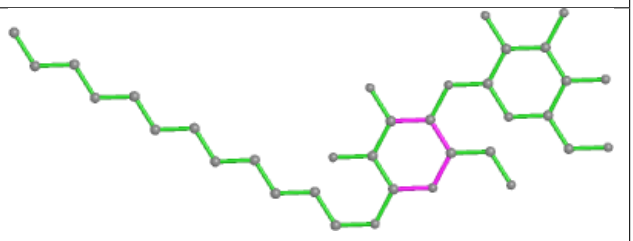
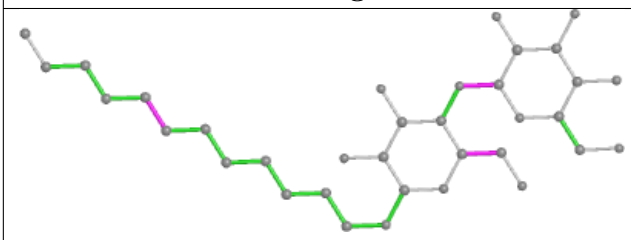


Bond angles



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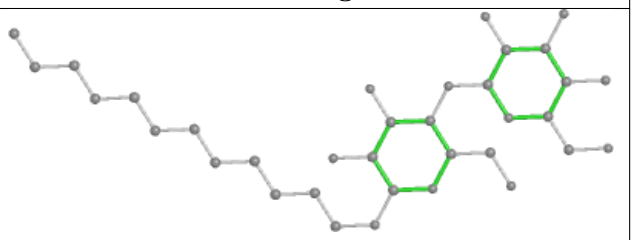
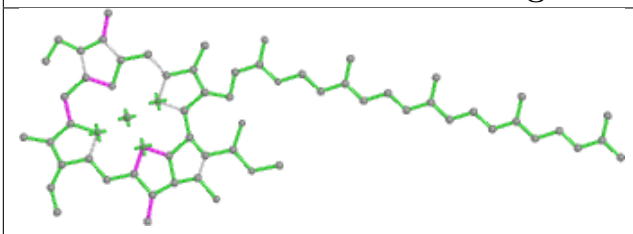


Rings

Ligand CLA b 615



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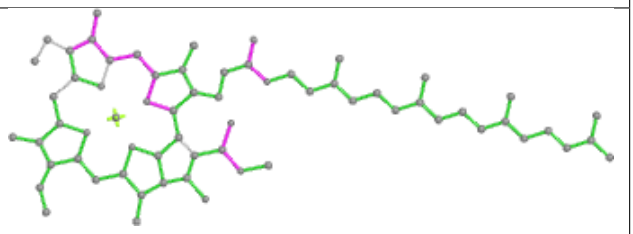
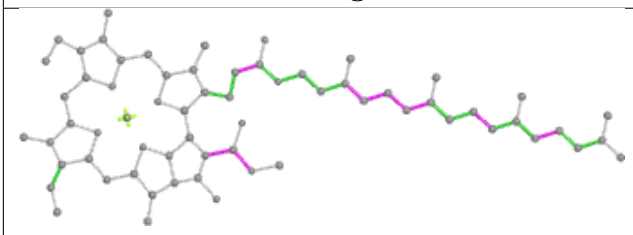


Bond angles



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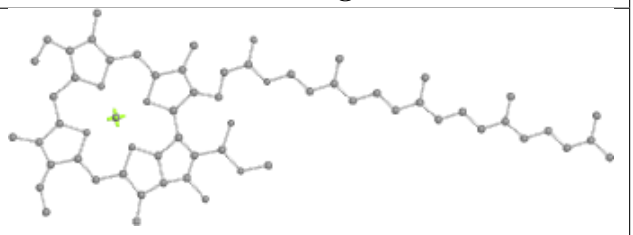
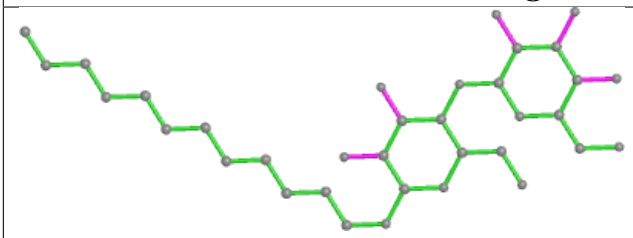


Rings

Ligand LMT b 603



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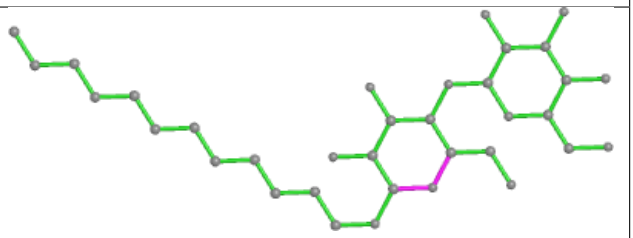
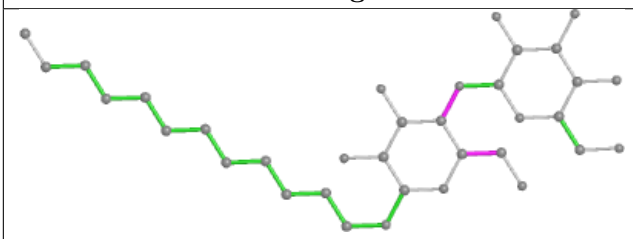


Bond angles



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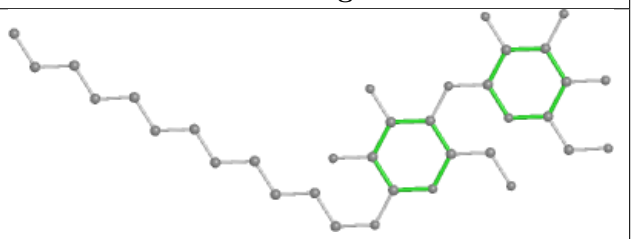
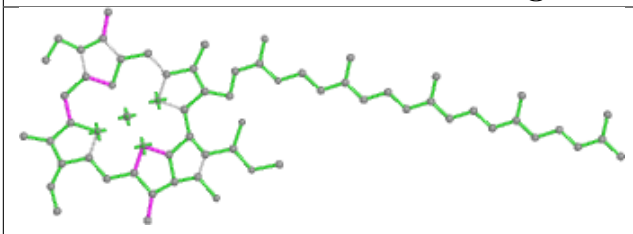


Rings

Ligand CLA b 607



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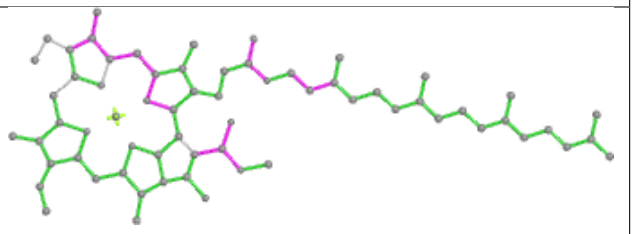
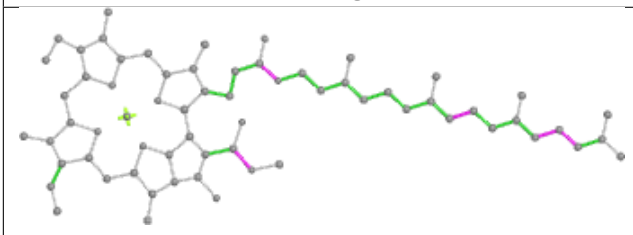


Bond angles



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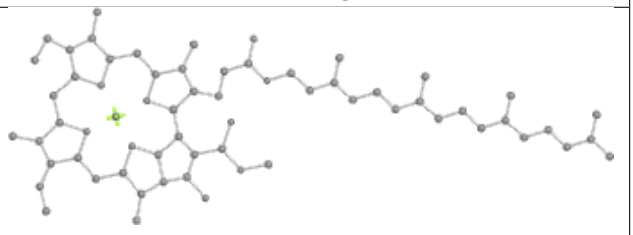
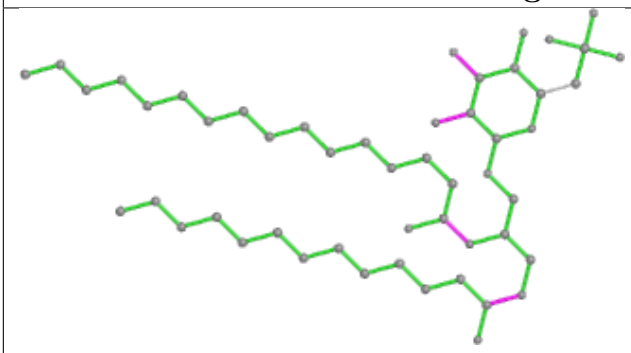


Rings

Ligand SQD A 413



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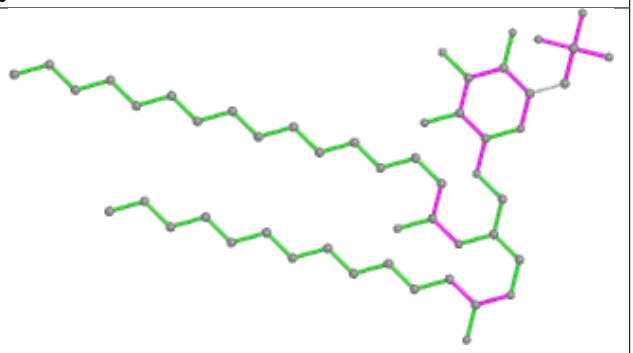
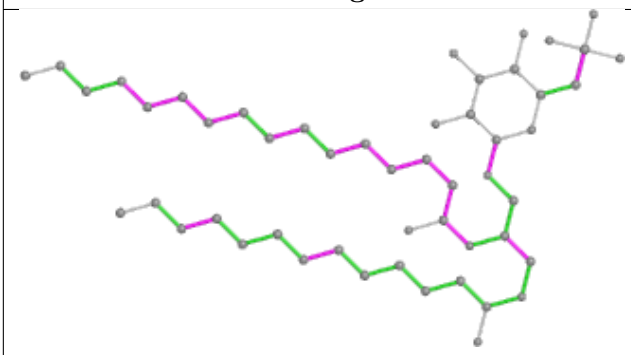


Bond angles



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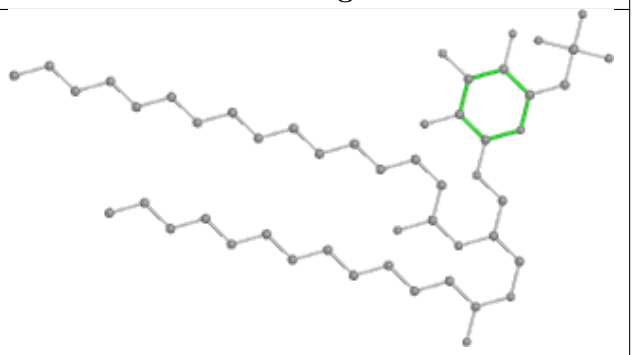
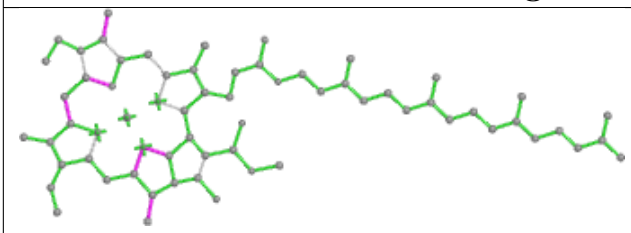


Rings

Ligand CLA B 607



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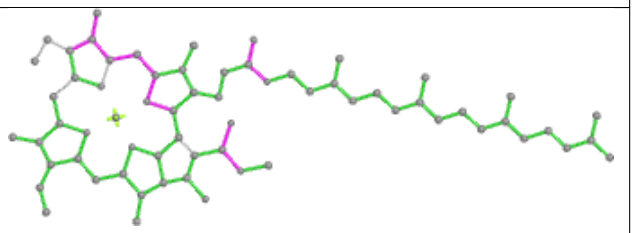
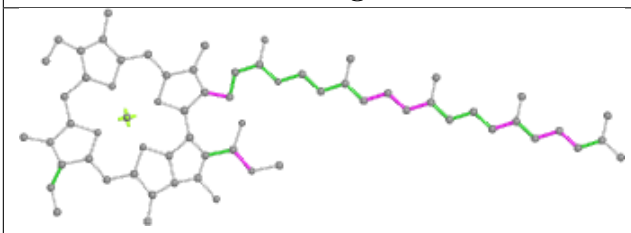


Bond angles



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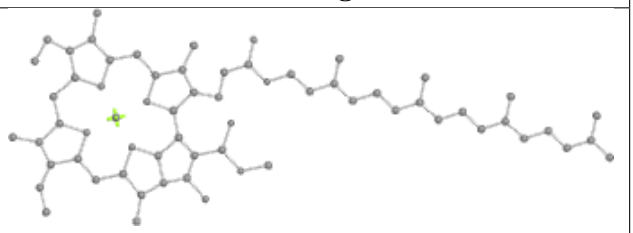
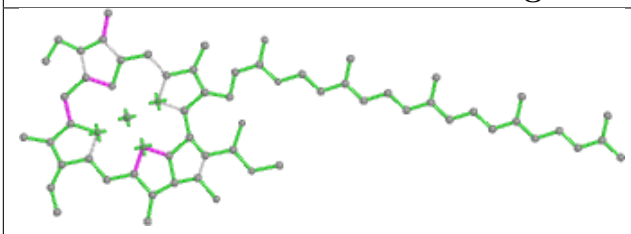


Rings

Ligand CLA B 606



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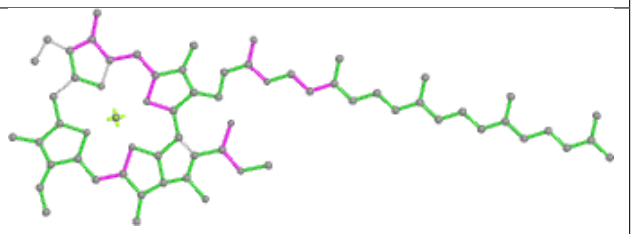
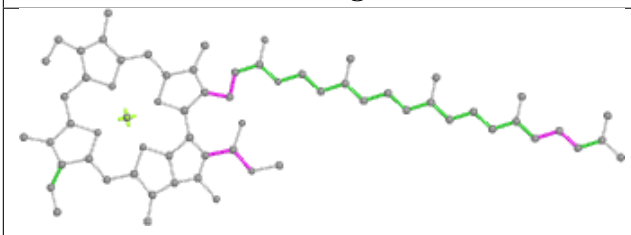


Bond angles



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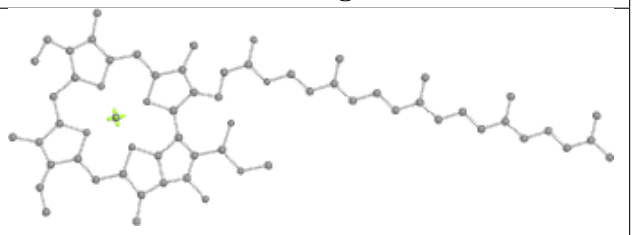
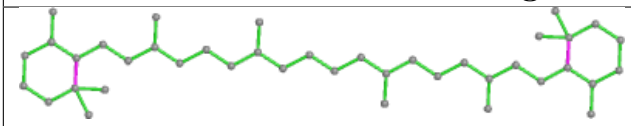


Rings

Ligand BCR H 102



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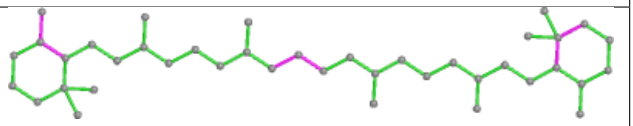
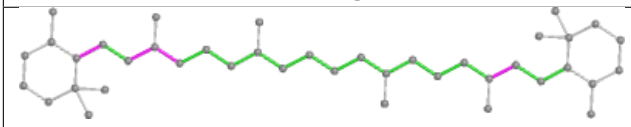


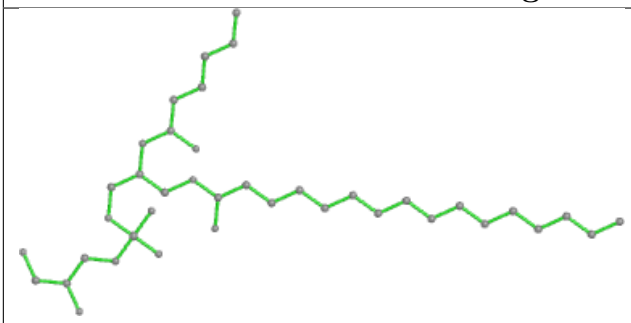
Bond angles



Torsions

Rings

Ligand LHG A 409



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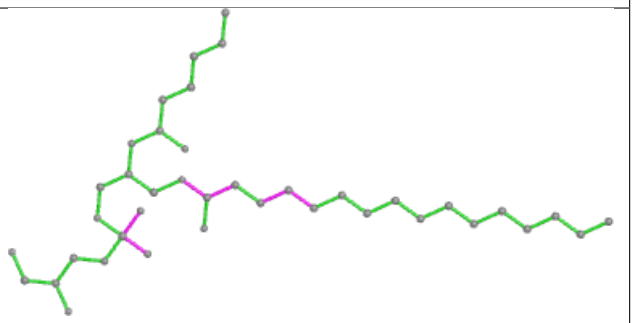
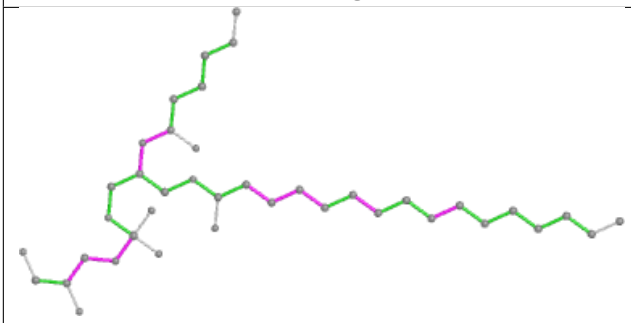
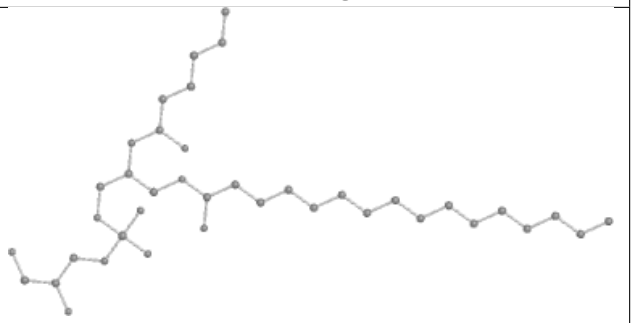


Bond angles

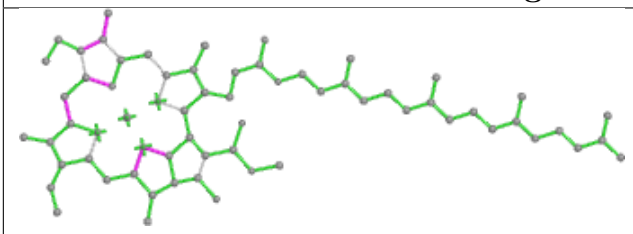


Torsions

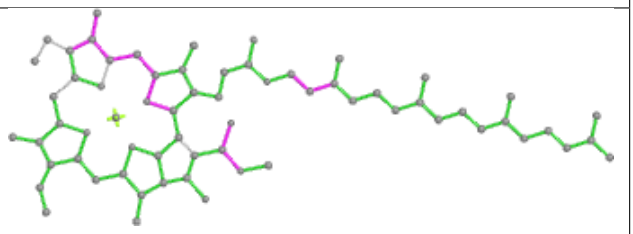


Rings

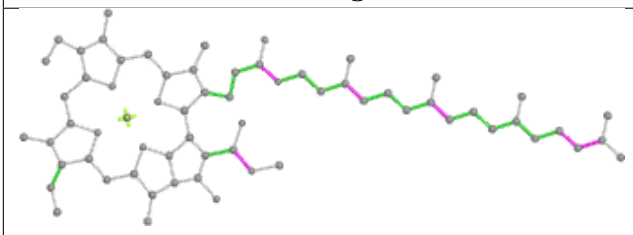
Ligand CLA B 610



Bond lengths



Bond angles



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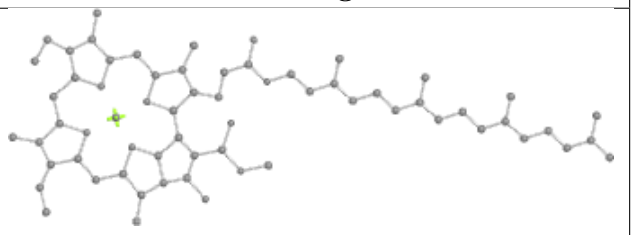
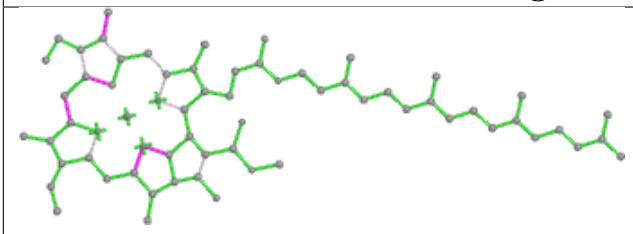
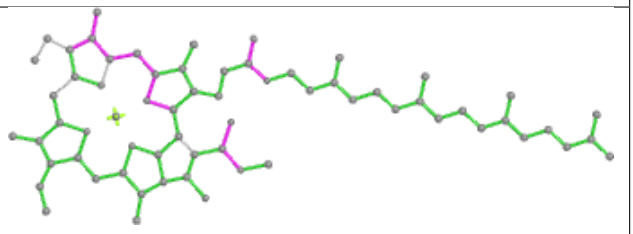


Rings

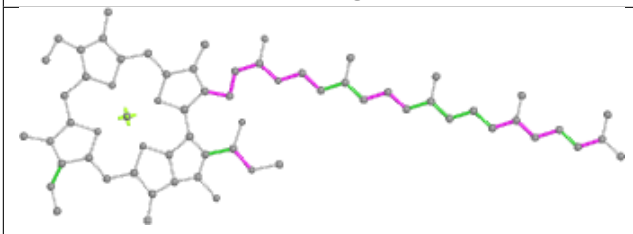
Ligand CLA c 511



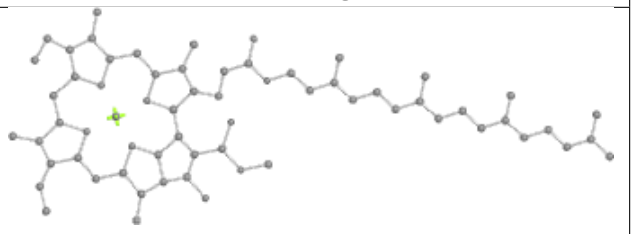
Bond lengths



Bond angles

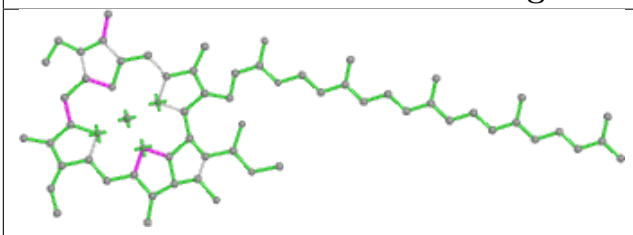


Torsions

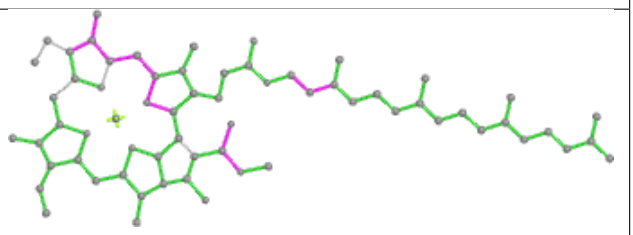


Rings

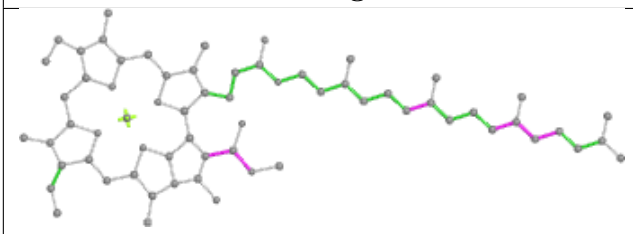
Ligand CLA b 612



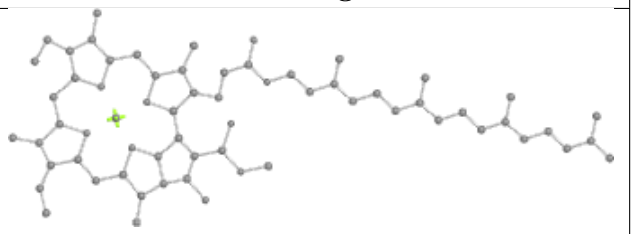
Bond lengths



Bond angles

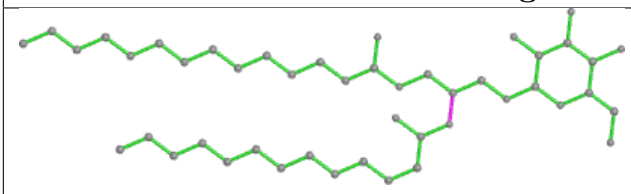


Torsions



Rings

Ligand LMG D 412



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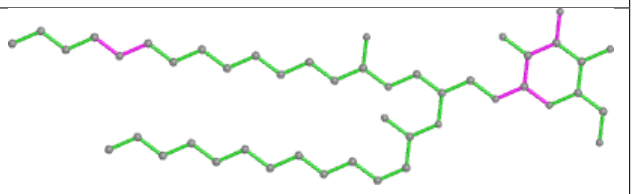
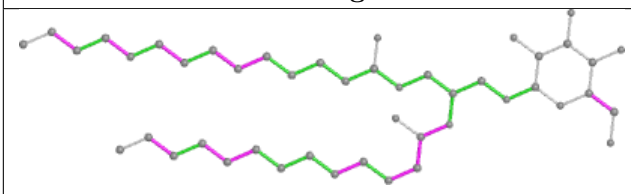


Bond angles



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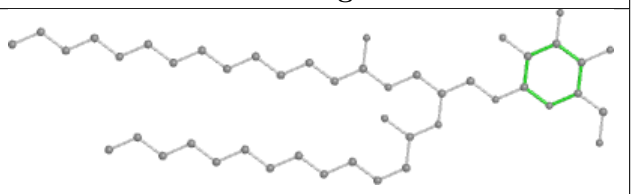
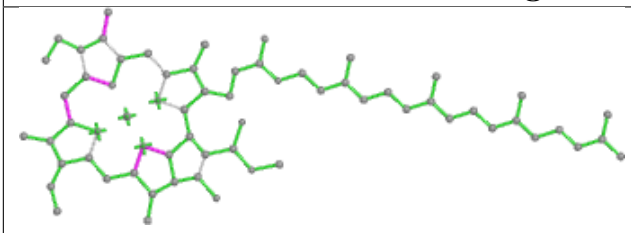


Rings

Ligand CLA C 520



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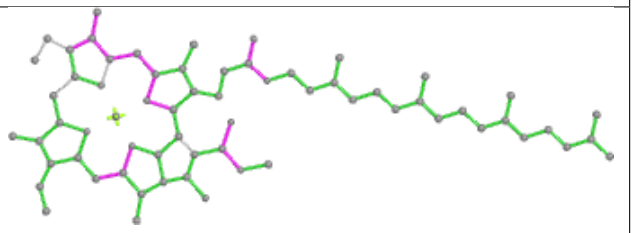
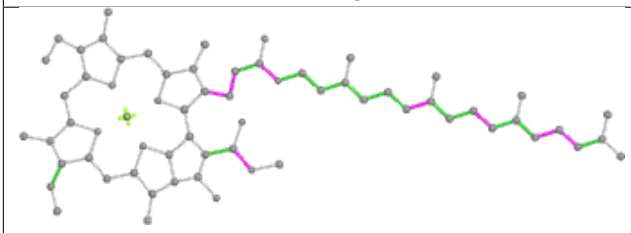
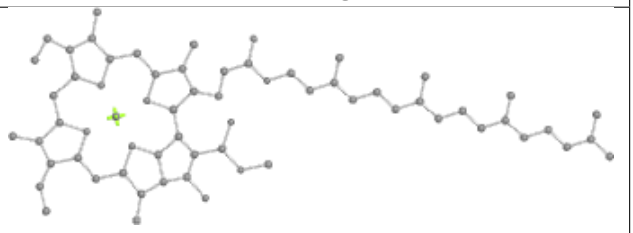


Bond angles

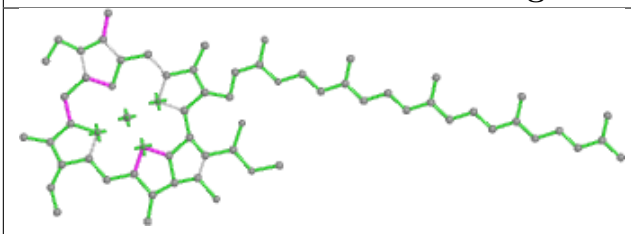


Torsions



Rings

Ligand CLA d 404



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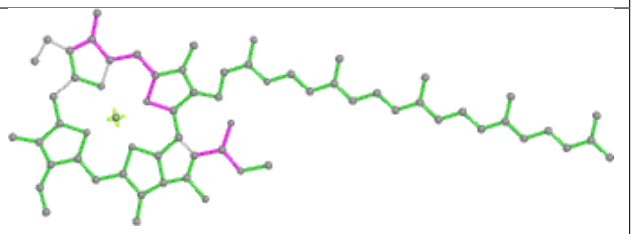
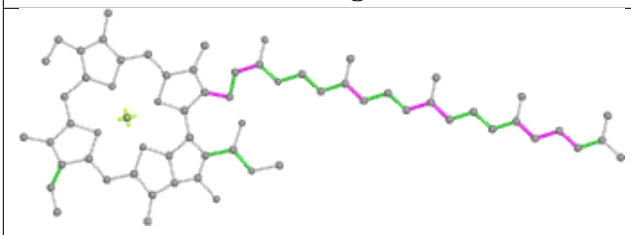
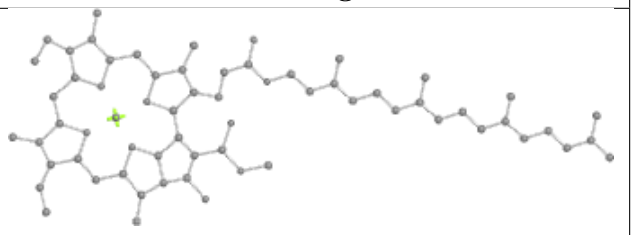


Bond angles

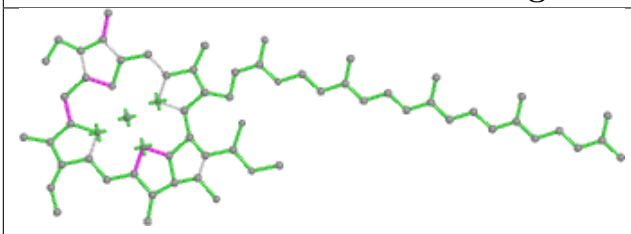


Torsions



Rings

Ligand CLA a 405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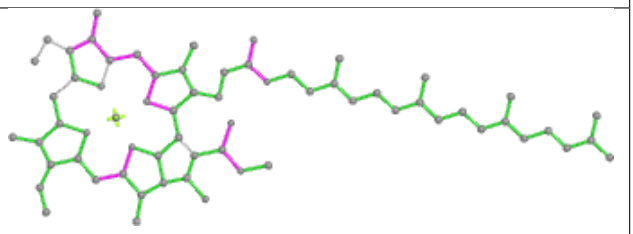
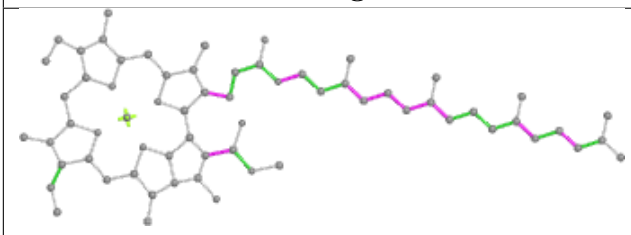

Bond angles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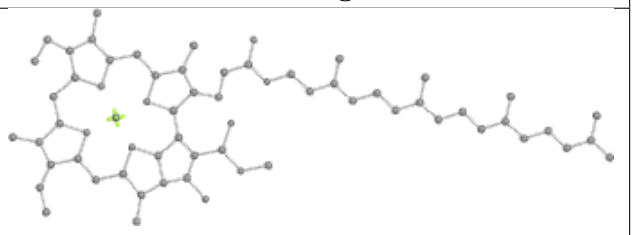
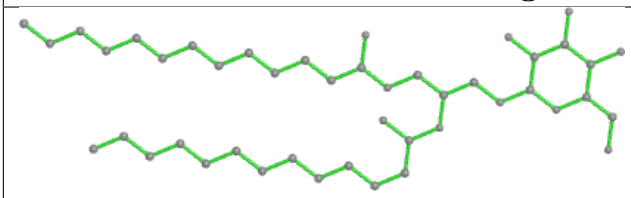

Rings

Ligand LMG C 518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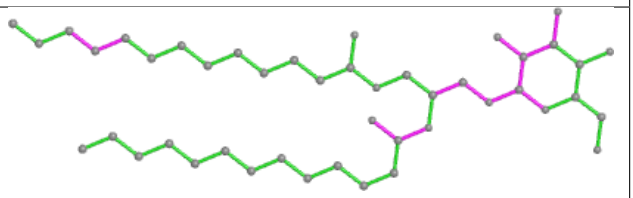
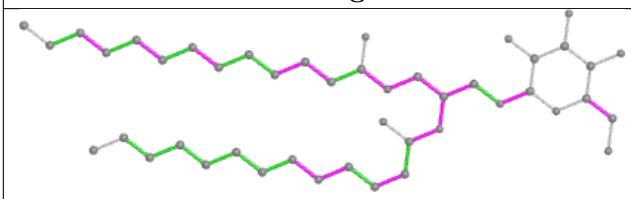

Bond angles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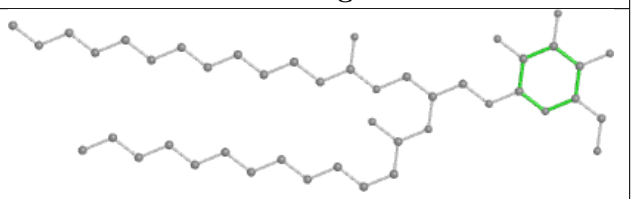
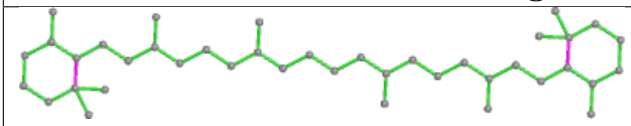
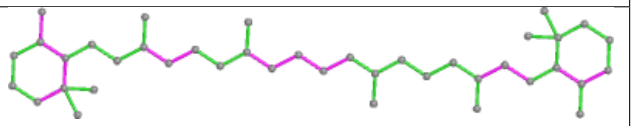
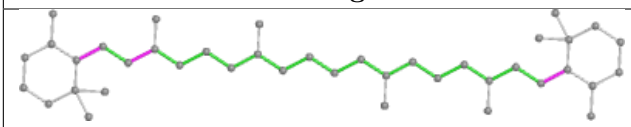

Rings

Ligand BCR c 521


Bond lengths


Bond angles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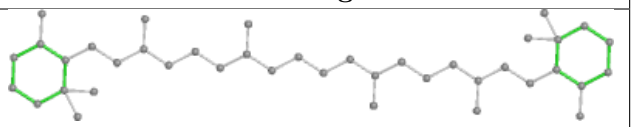
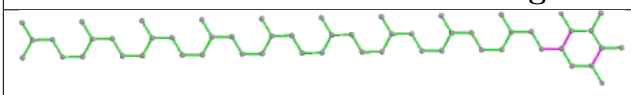

Rings

Ligand PL9 D 407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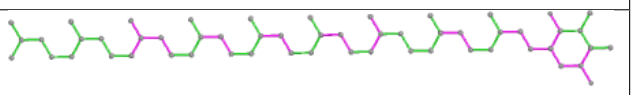
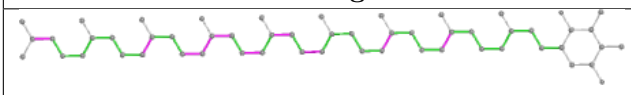

Bond angles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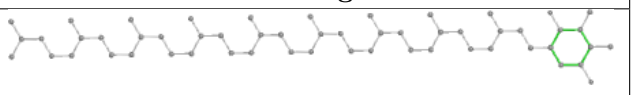
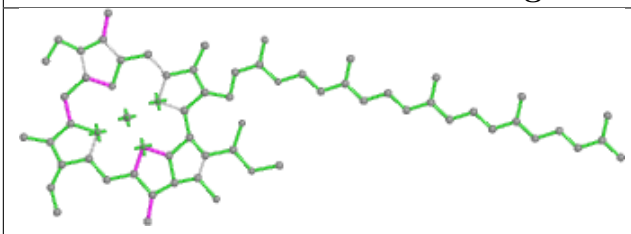
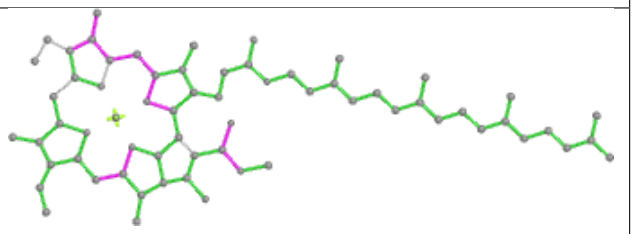

Rings

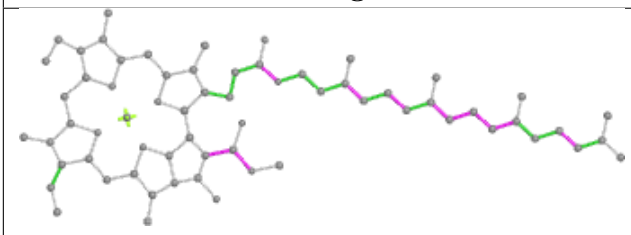
Ligand CLA B 604



Bond lengths



Bond angles



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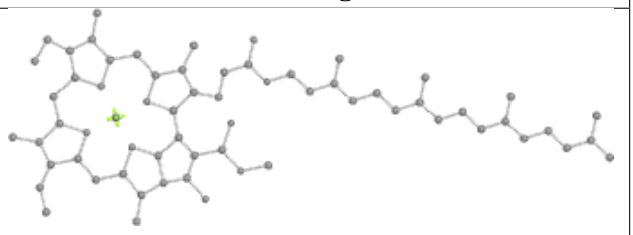
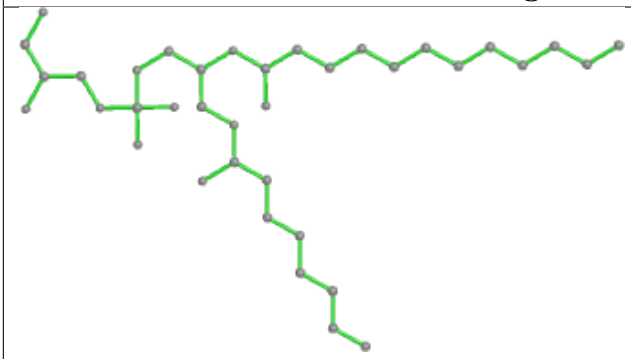


Rings

Ligand LHG C 519



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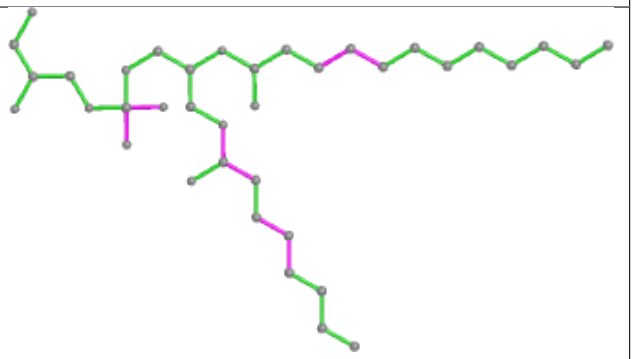
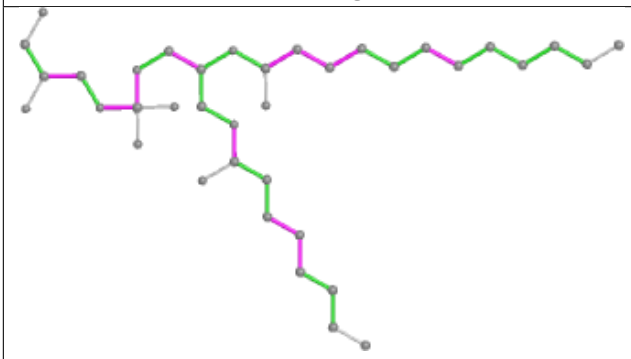
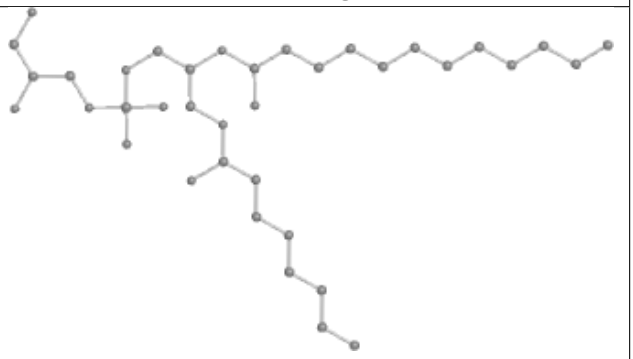


Bond angles

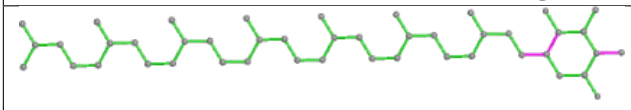


Torsions



Rings

Ligand PL9 a 409



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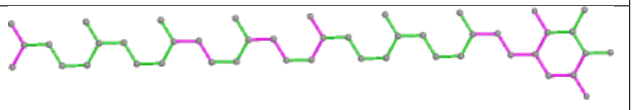
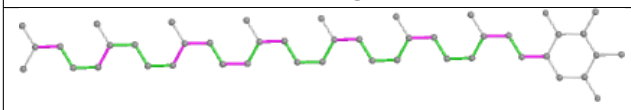


Bond angles



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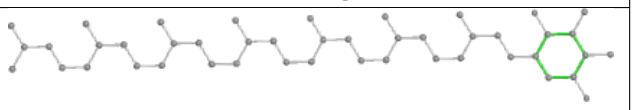
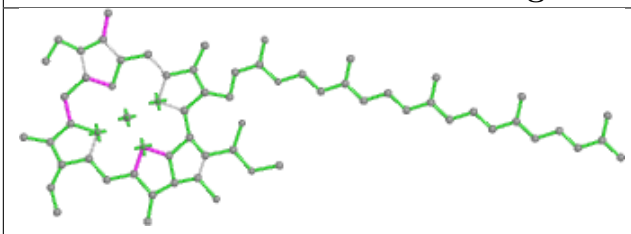
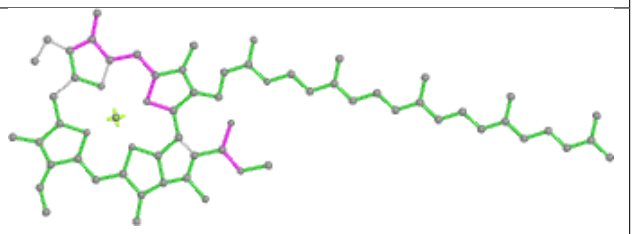


Rings

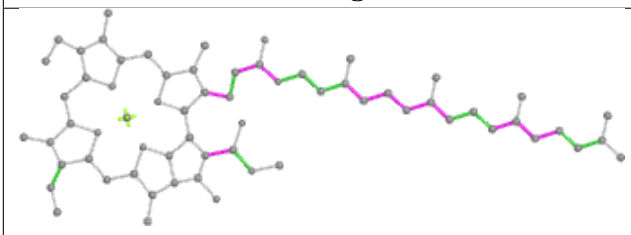
Ligand CLA h 101



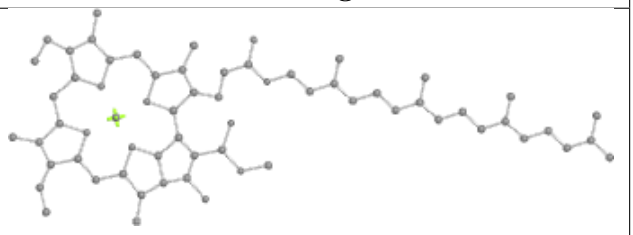
Bond lengths



Bond angles

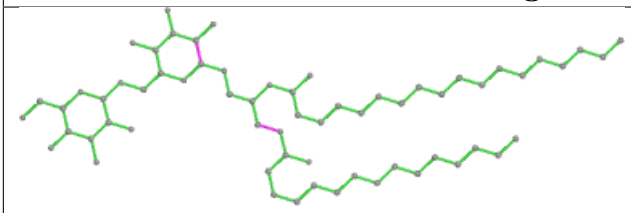


Torsions

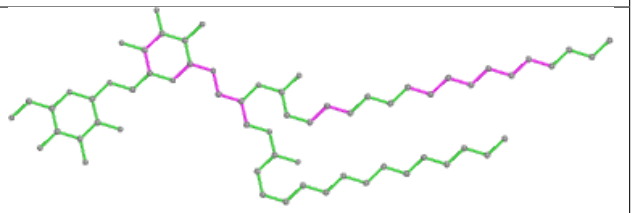


Rings

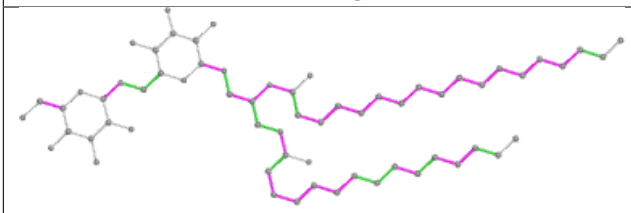
Ligand DGD d 408



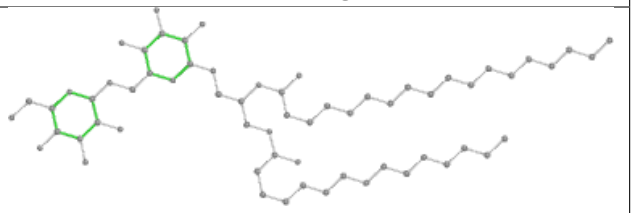
Bond lengths



Bond angles

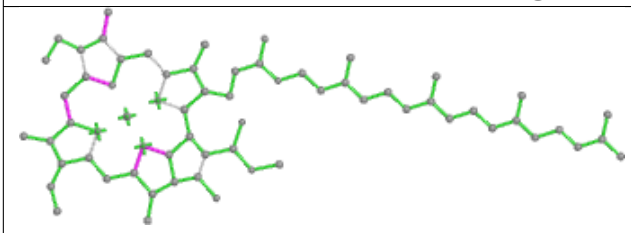


Torsions

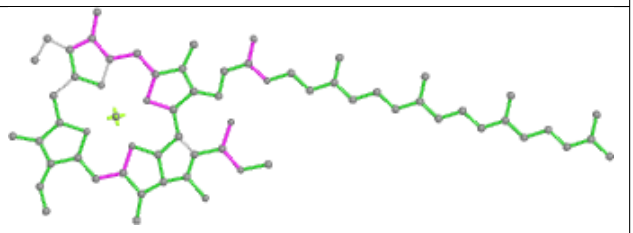


Rings

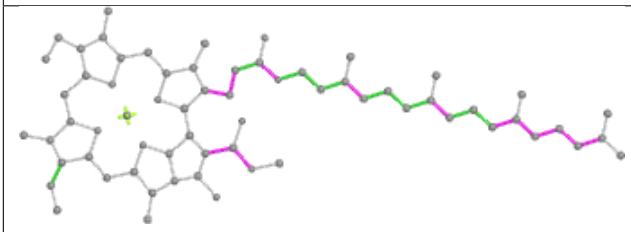
Ligand CLA c 512



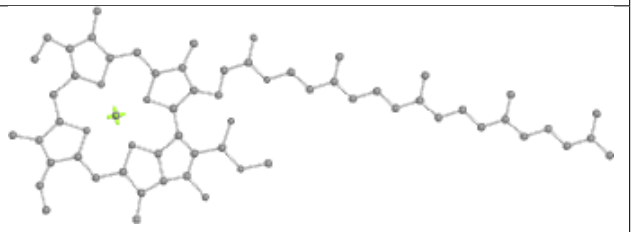
Bond lengths



Bond angles

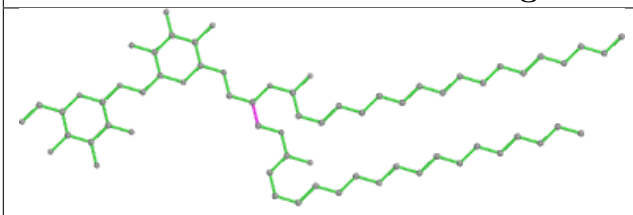


Torsions

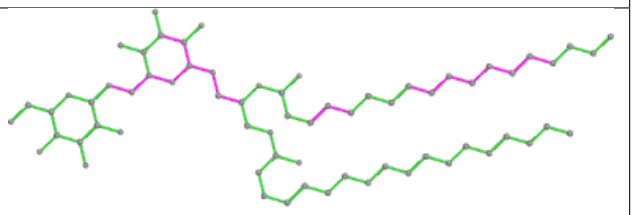


Rings

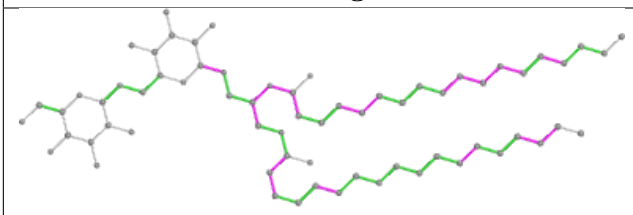
Ligand DGD C 517



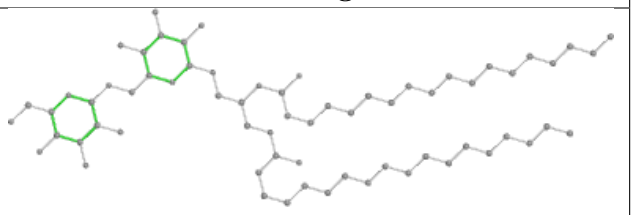
Bond lengths



Bond angles

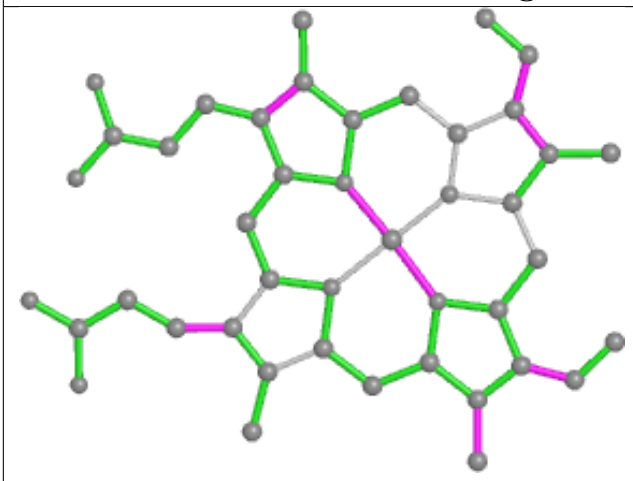


Torsions

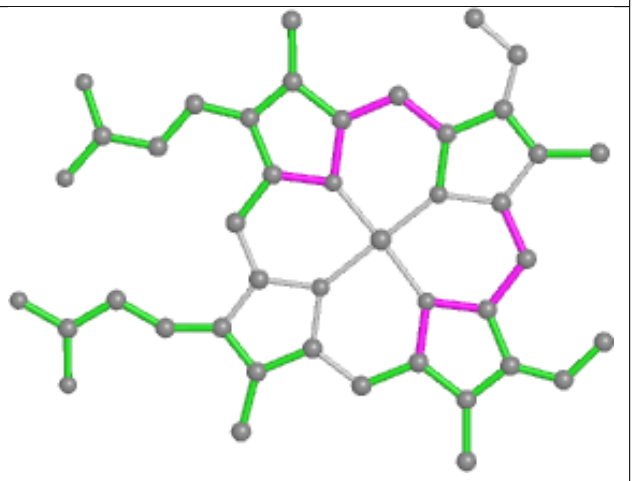


Rings

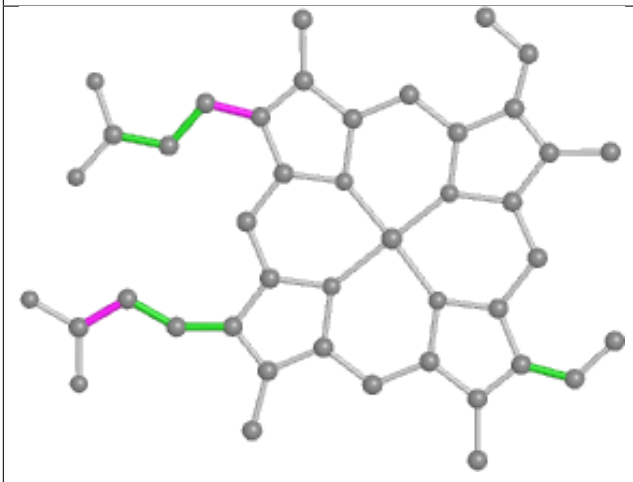
Ligand HEM V 201



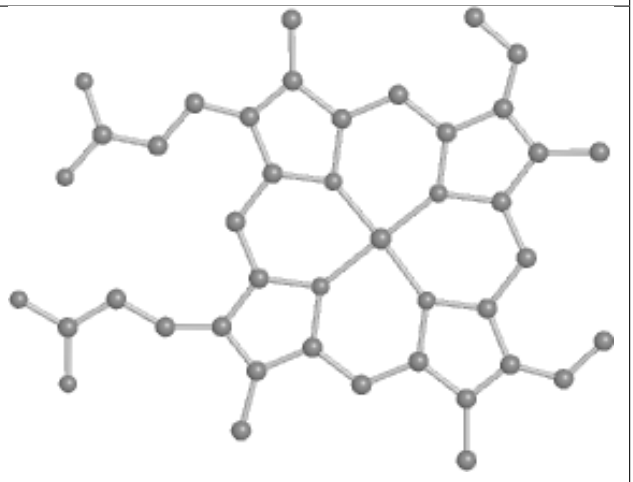
Bond lengths



Bond angles

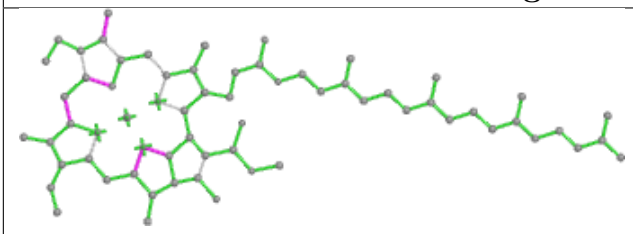


Torsions

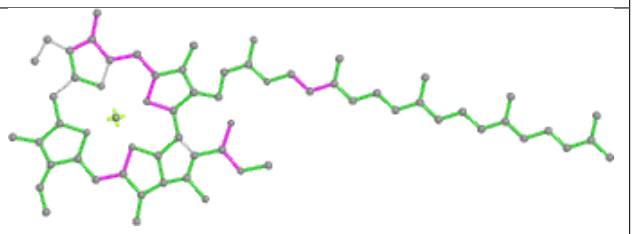


Rings

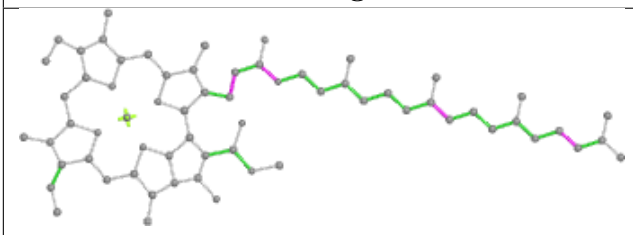
Ligand CLA D 406



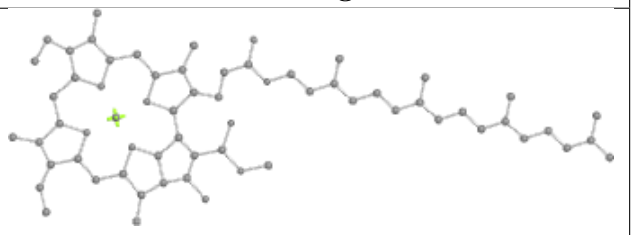
Bond lengths



Bond angles

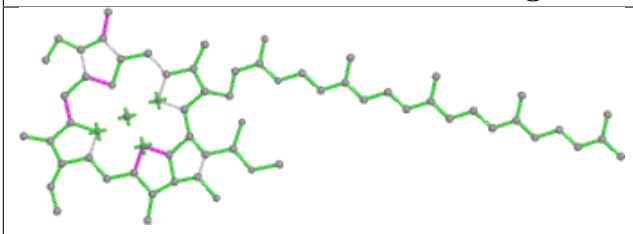


Torsions

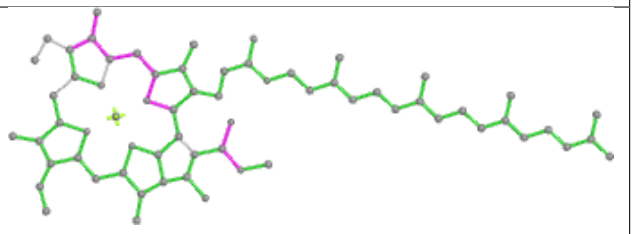


Rings

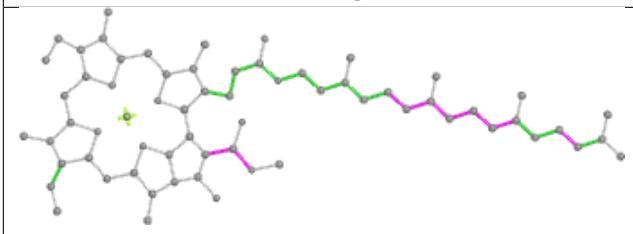
Ligand CLA C 503



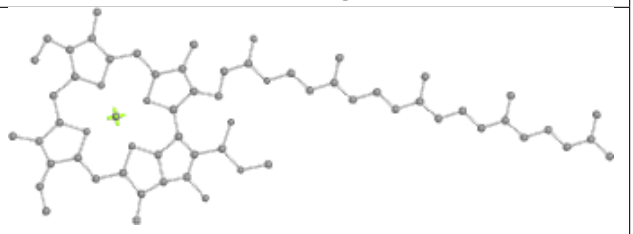
Bond lengths



Bond angles

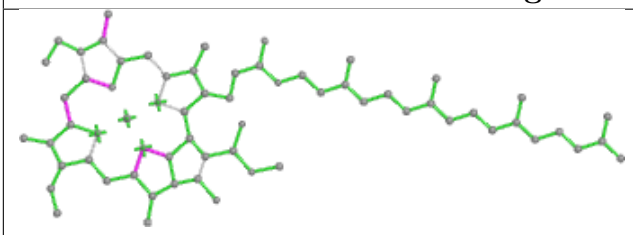


Torsions

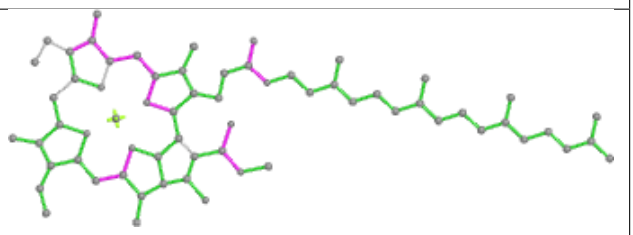


Rings

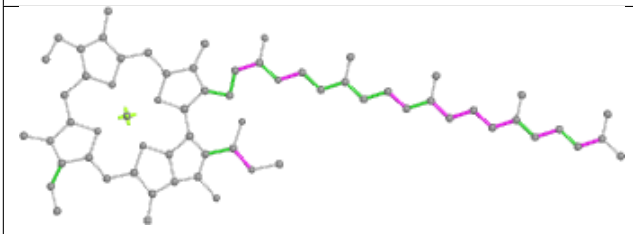
Ligand CLA B 612



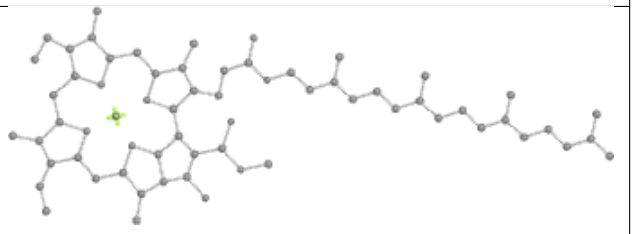
Bond lengths



Bond angles

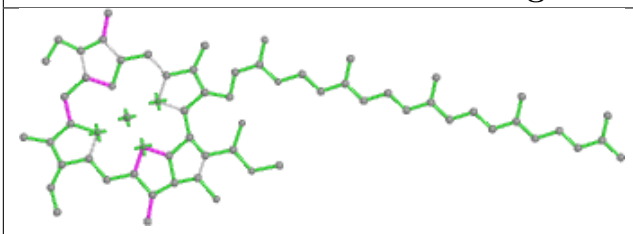


Torsions

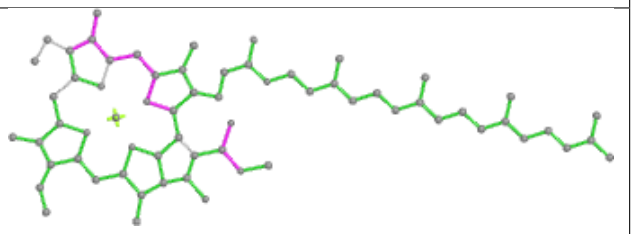


Rings

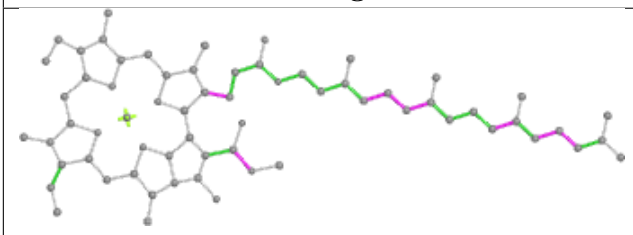
Ligand CLA b 611



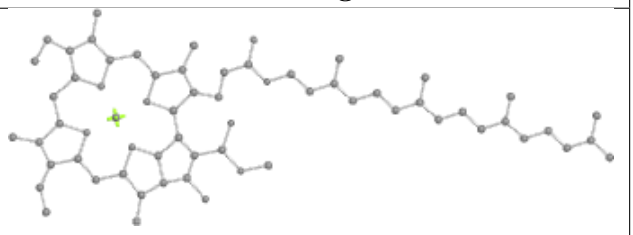
Bond lengths



Bond angles

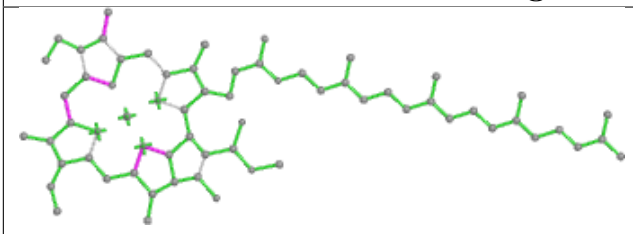


Torsions

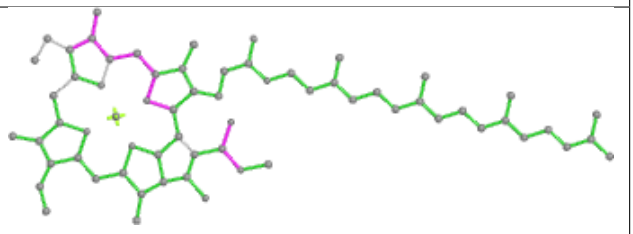


Rings

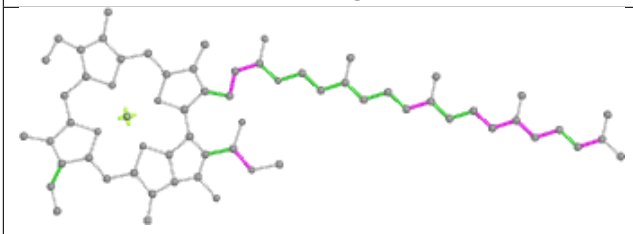
Ligand CLA b 605



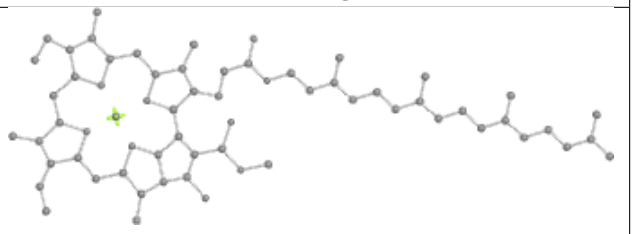
Bond lengths



Bond angles

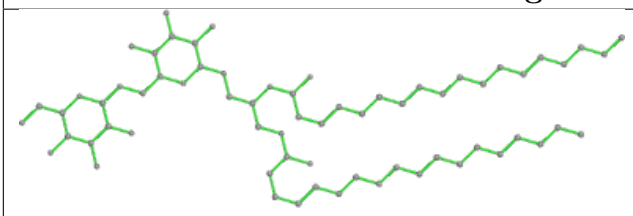


Torsions

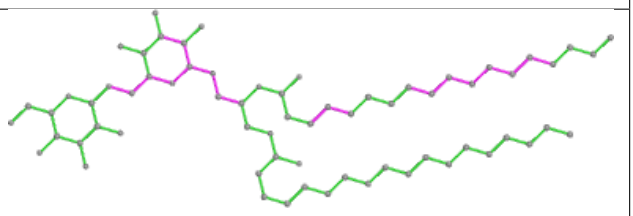


Rings

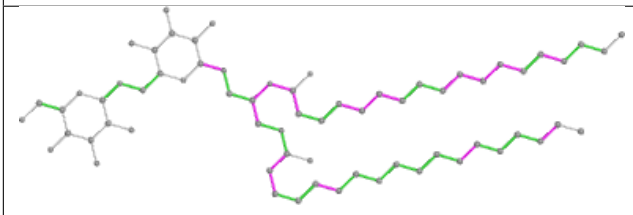
Ligand DGD c 517



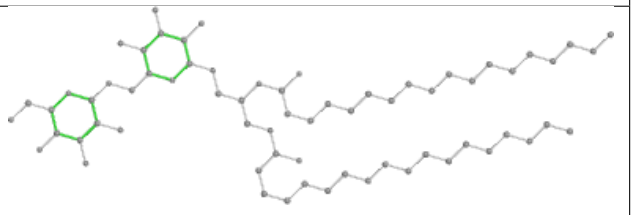
Bond lengths



Bond angles

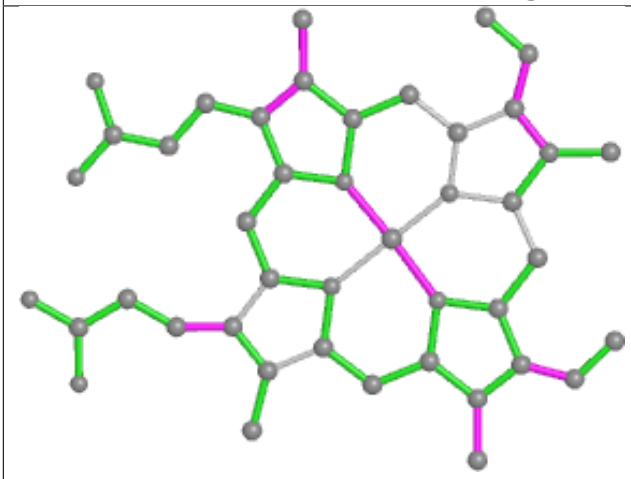


Torsions

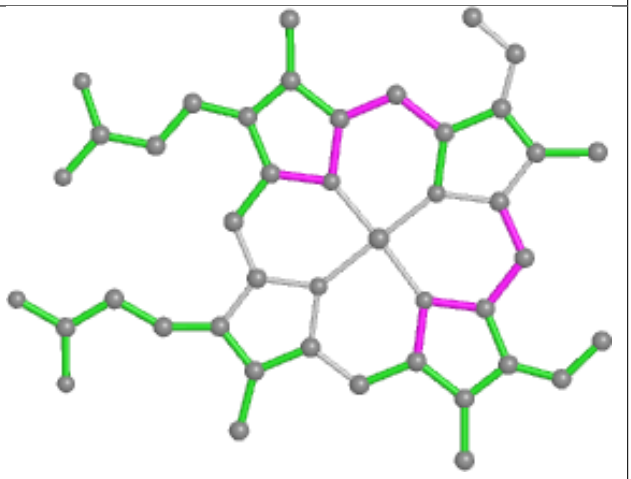


Rings

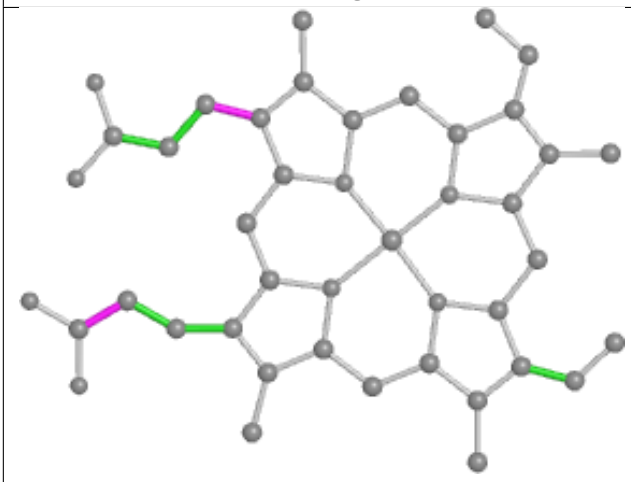
Ligand HEM v 201



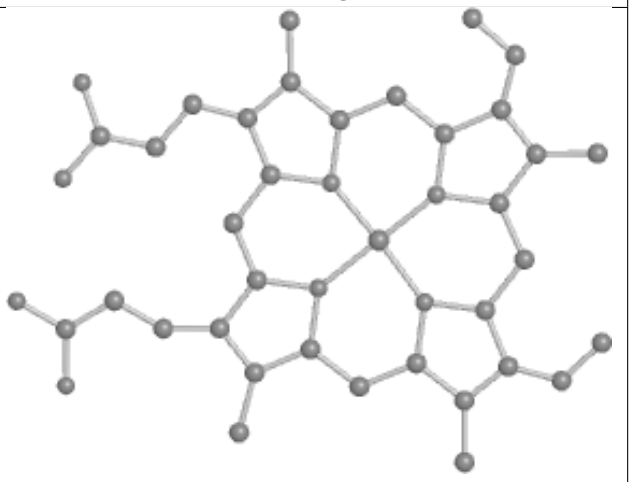
Bond lengths



Bond angles

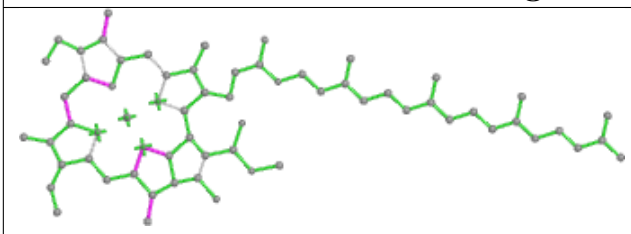


Torsions

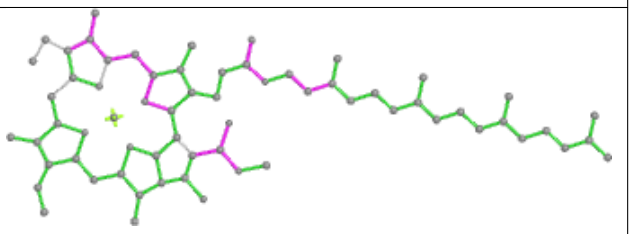


Rings

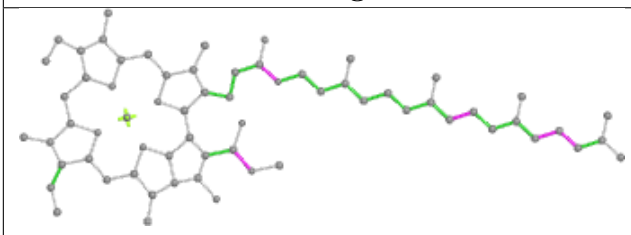
Ligand CLA B 603



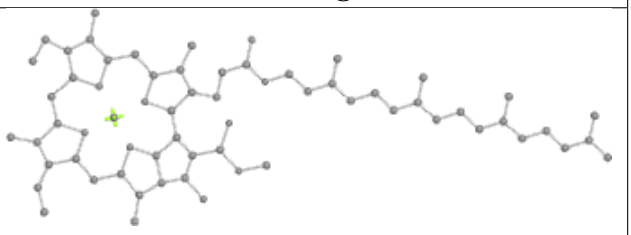
Bond lengths



Bond angles

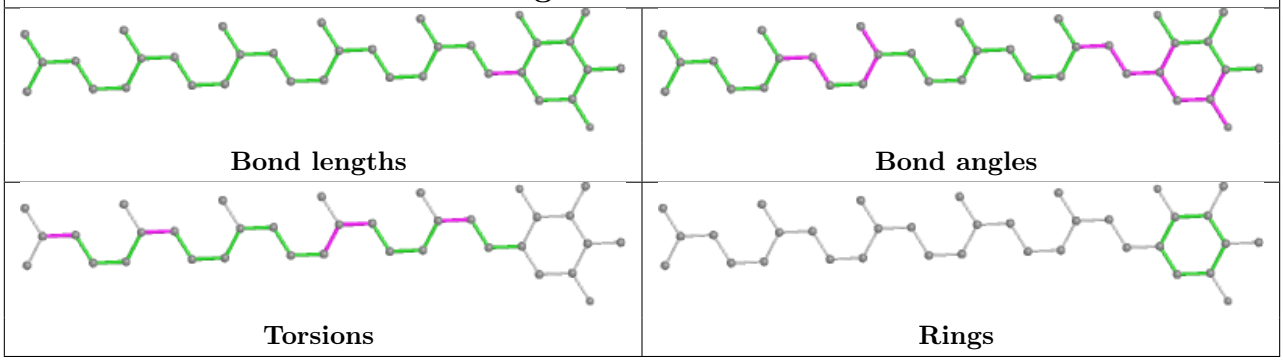


Torsions

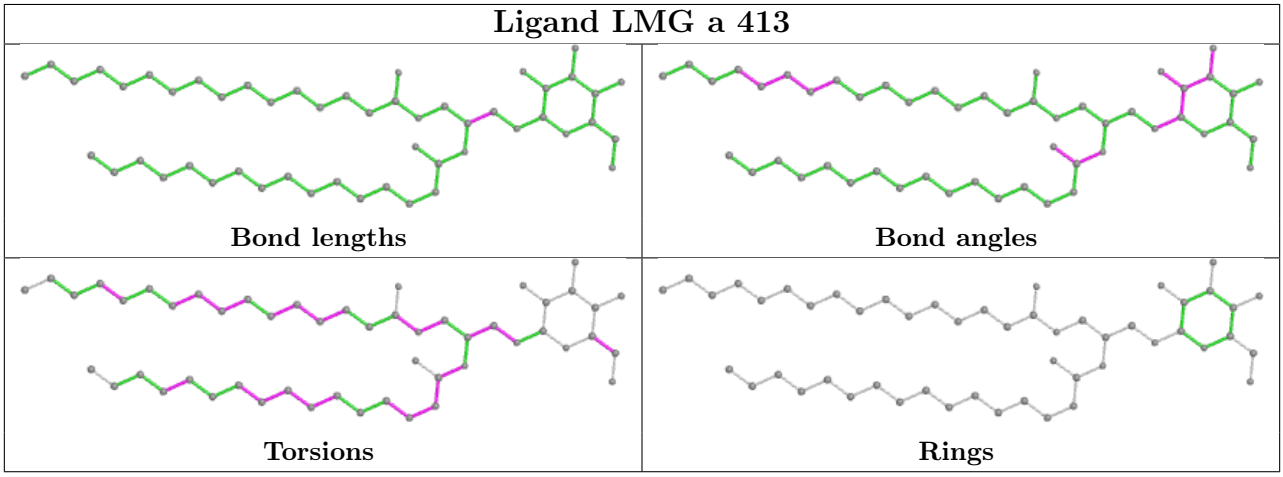


Rings

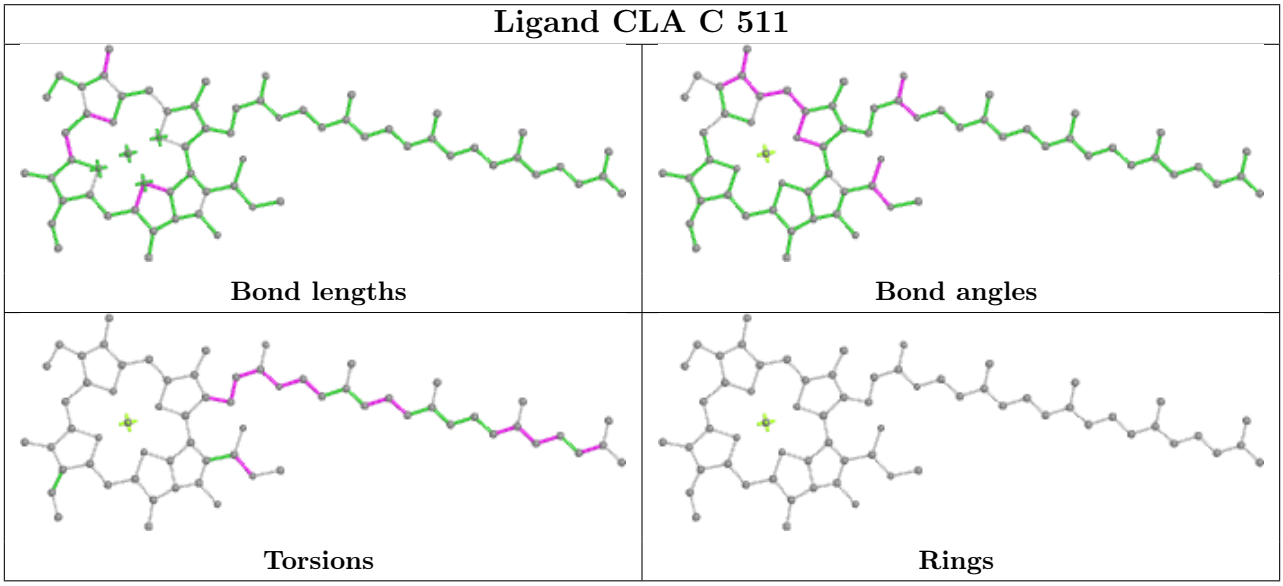
Ligand PL9 J 101



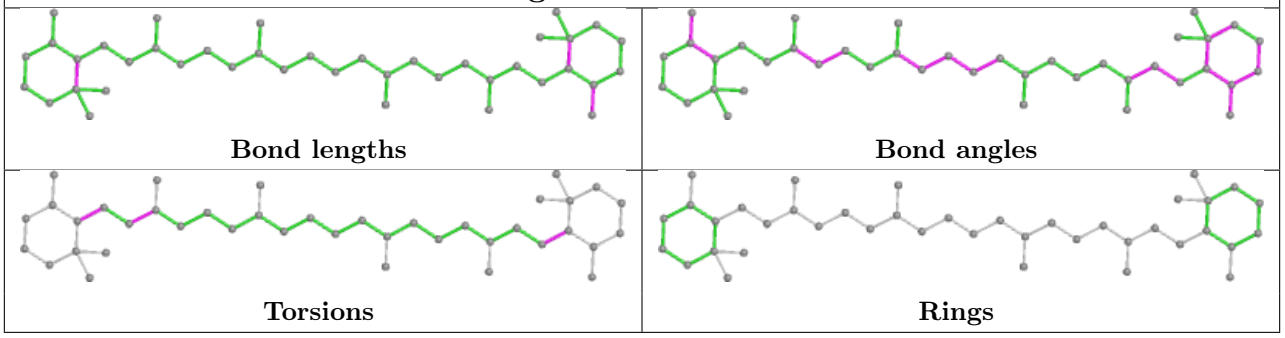
Ligand LMG a 413



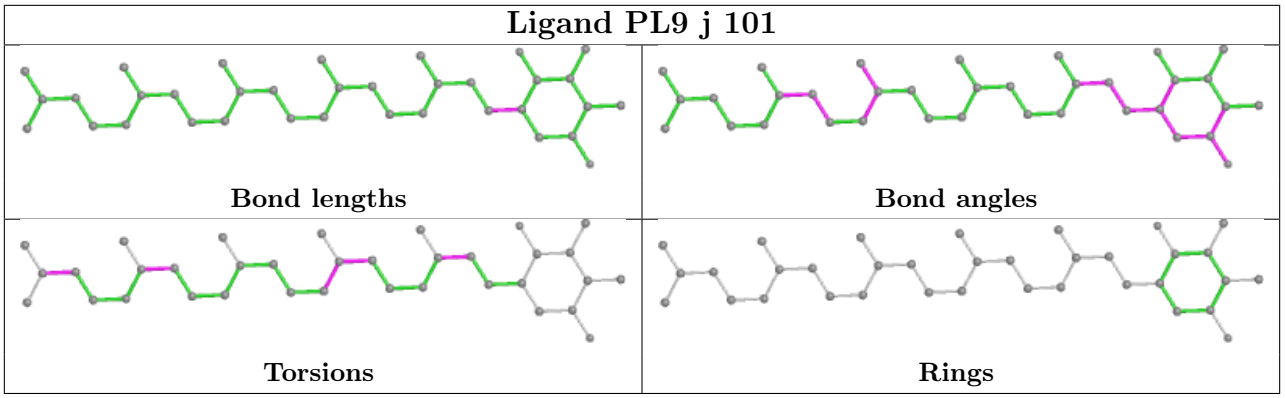
Ligand CLA C 511



Ligand BCR c 514



Ligand PL9 j 101



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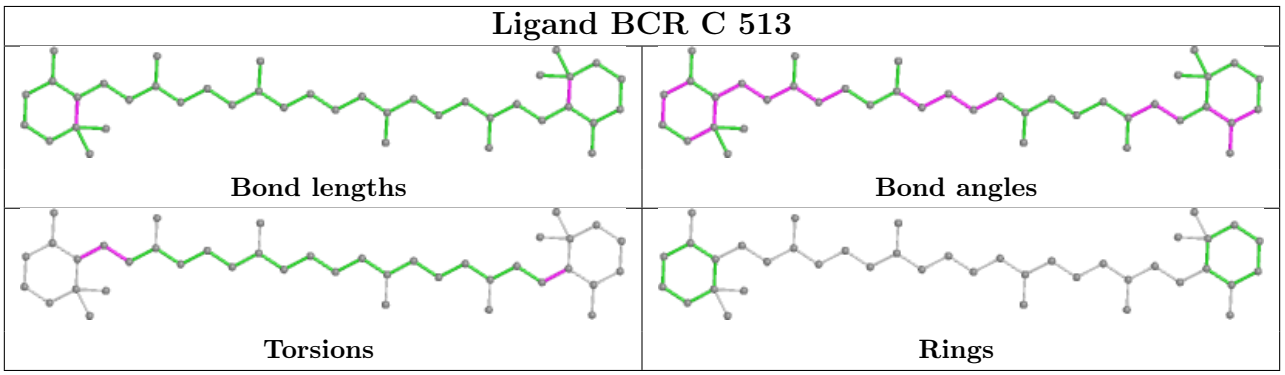
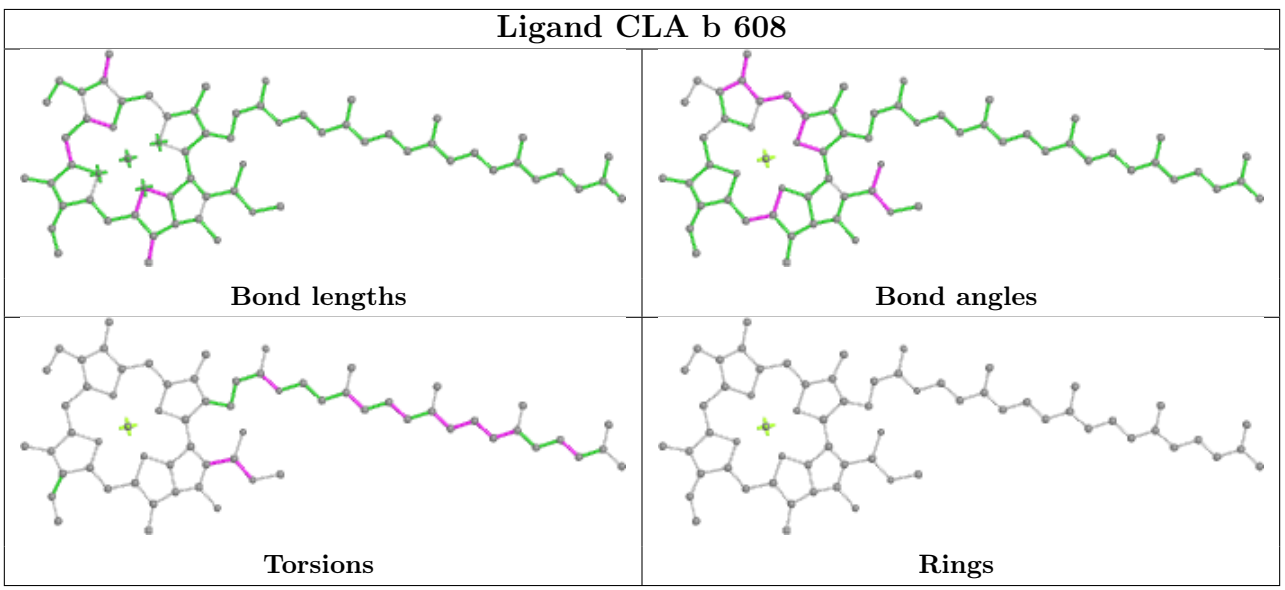
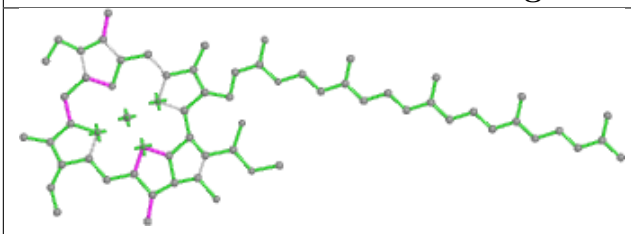


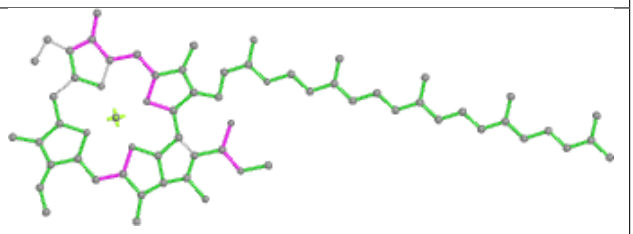
Ligand CLA b 608



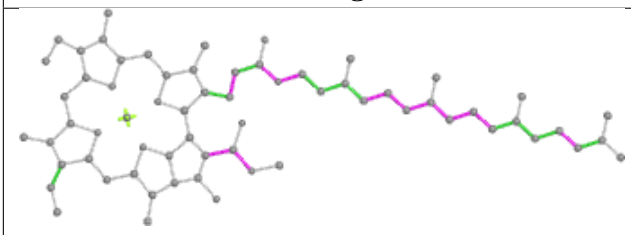
Ligand CLA C 508



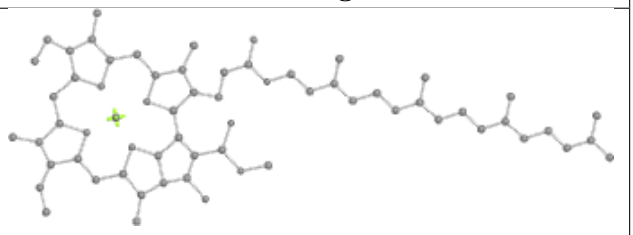
Bond lengths



Bond angles

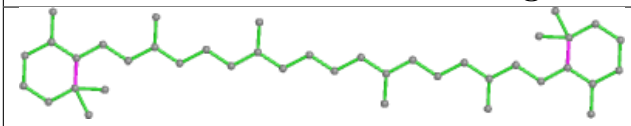


Torsions

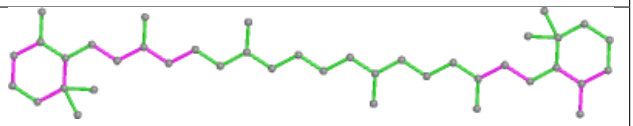


Rings

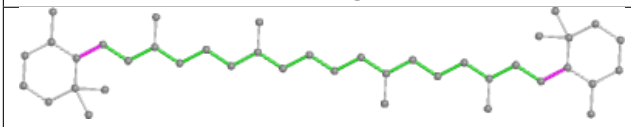
Ligand BCR B 619



Bond lengths



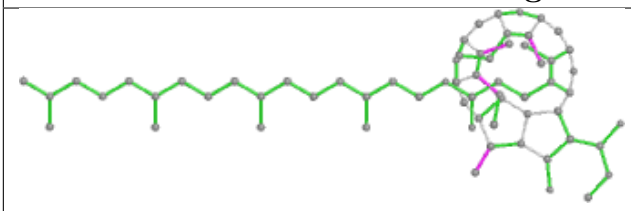
Bond angles



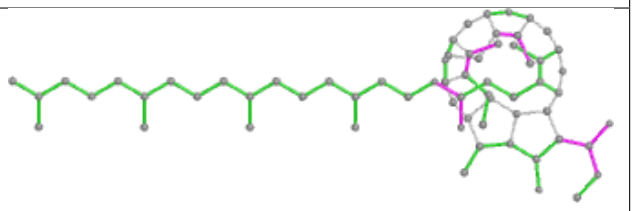
Torsions

Rings

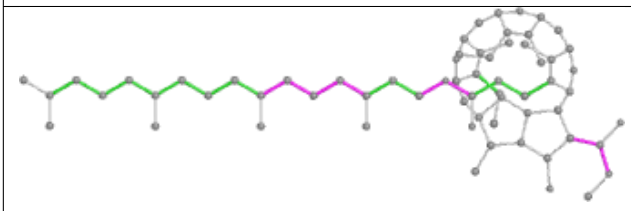
Ligand PHO d 401



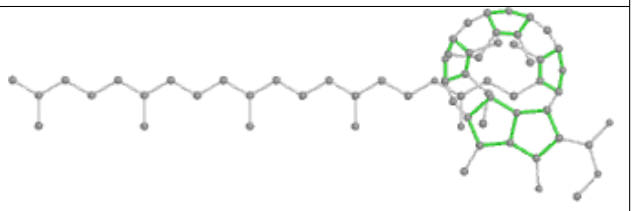
Bond lengths



Bond angles

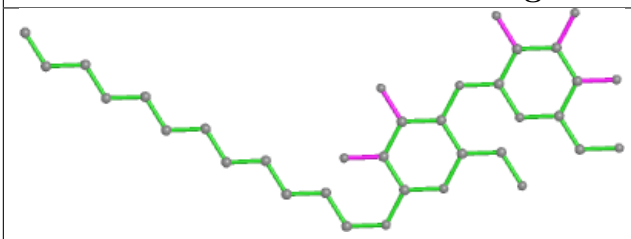


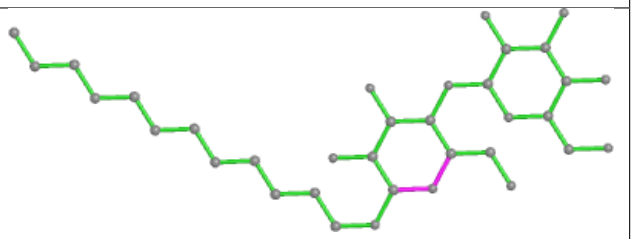
Torsions

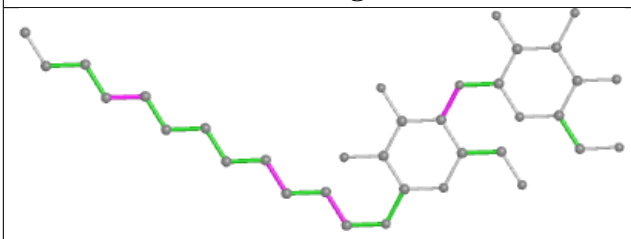


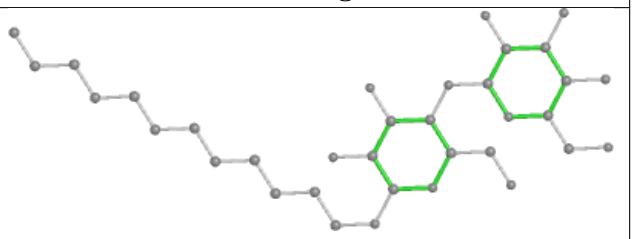
Rings

Ligand LMT b 604

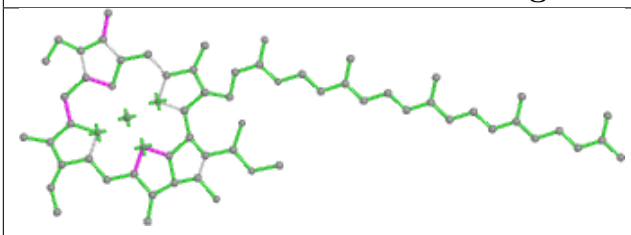

Bond lengths

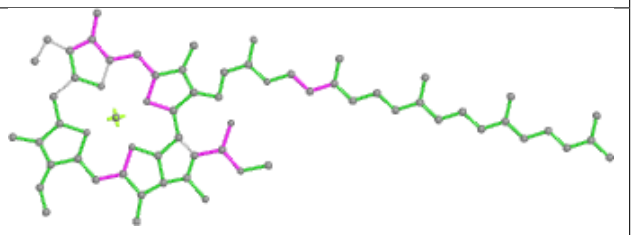

Bond angles

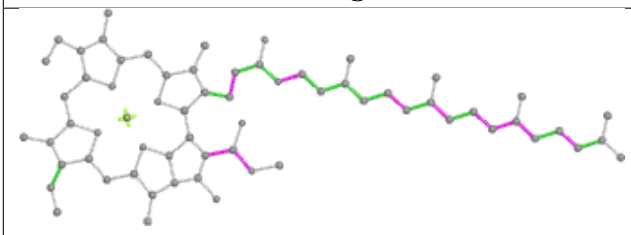

Torsions

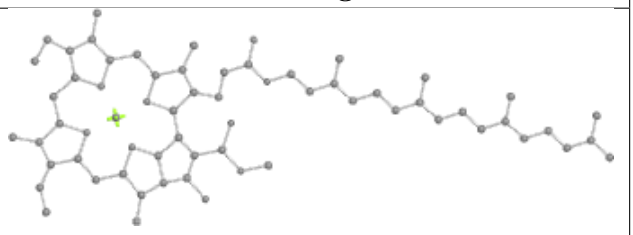

Rings

Ligand CLA c 507

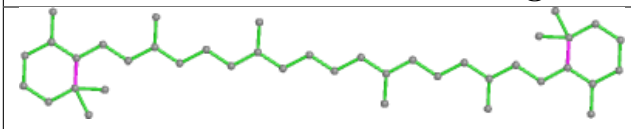

Bond lengths

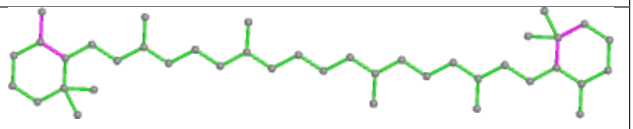

Bond angles

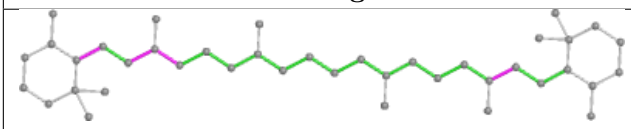

Torsions

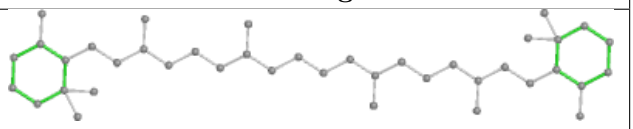

Rings

Ligand BCR x 101

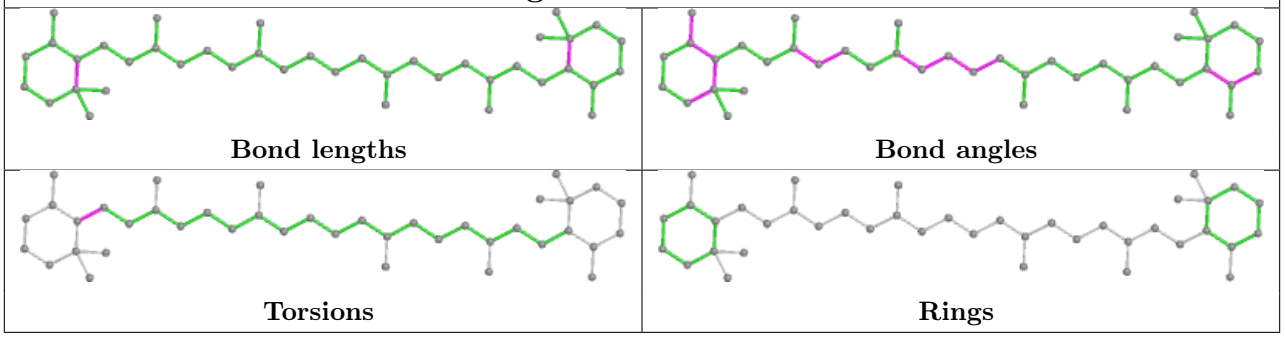

Bond lengths


Bond angles


Torsions


Rings

Ligand BCR b 620



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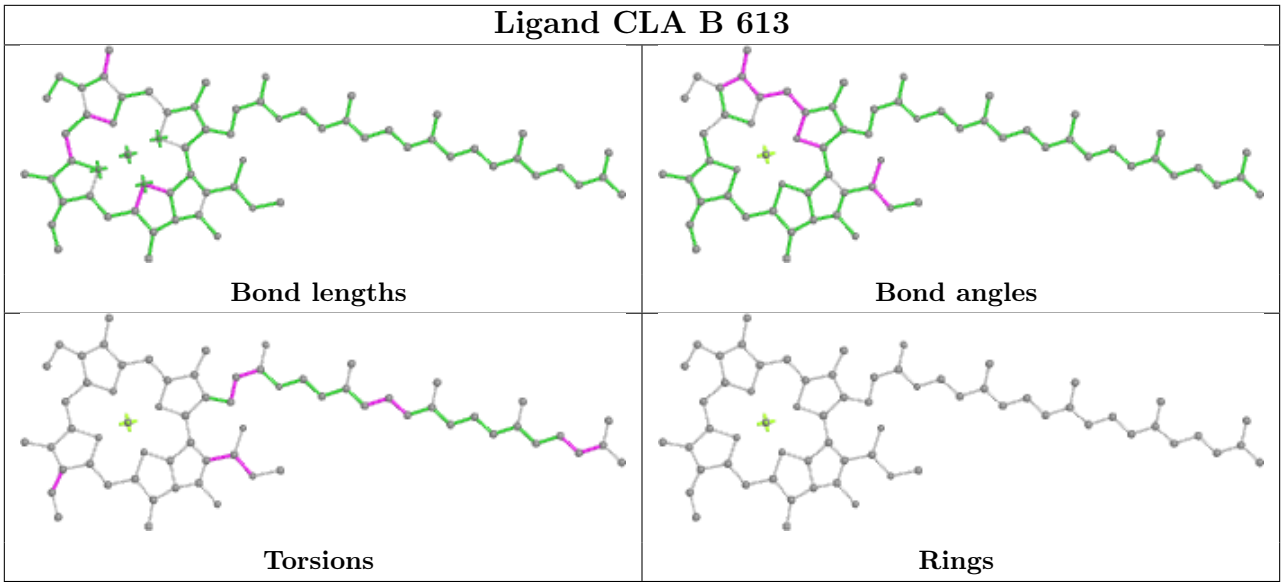

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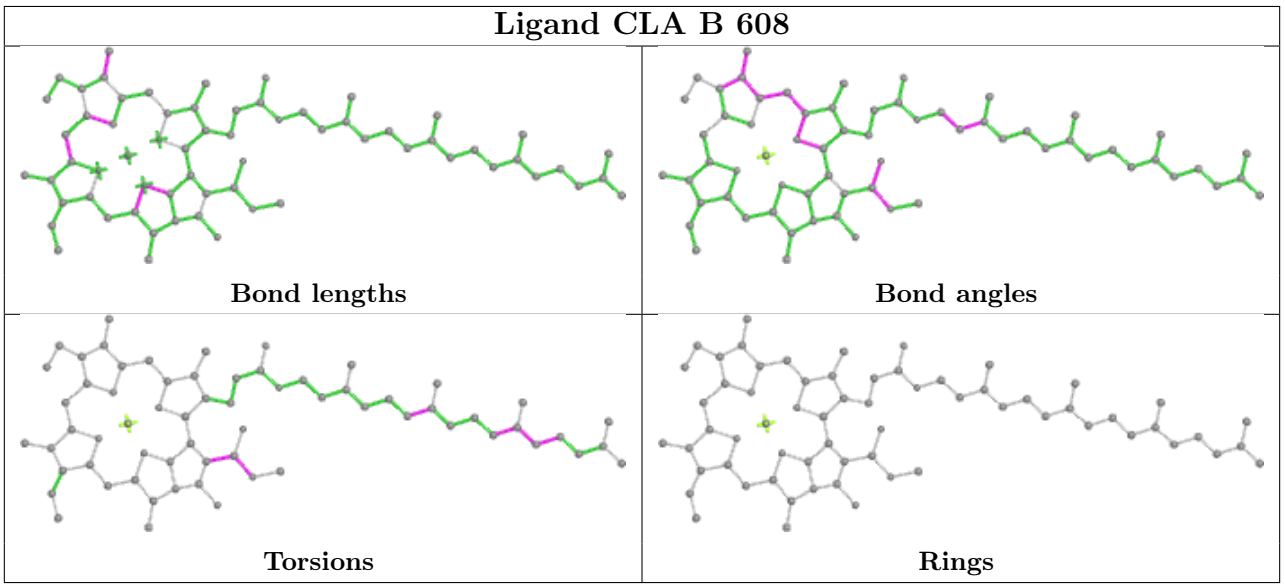
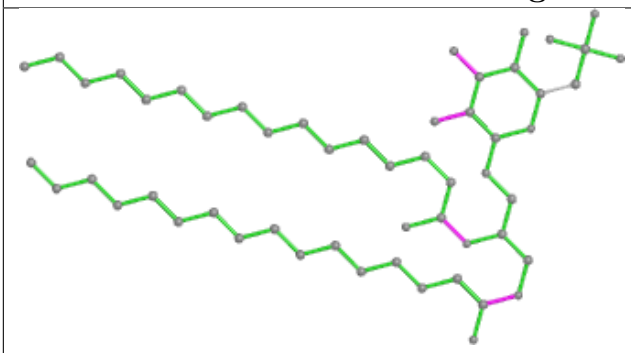
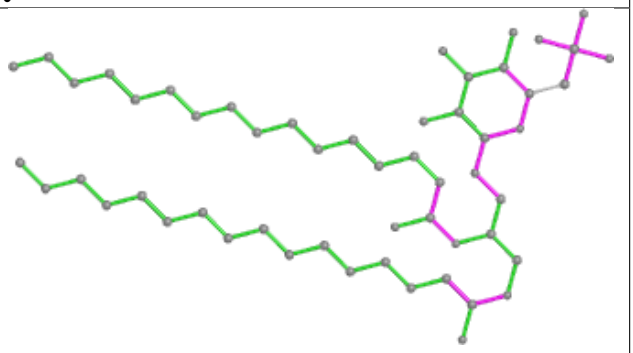


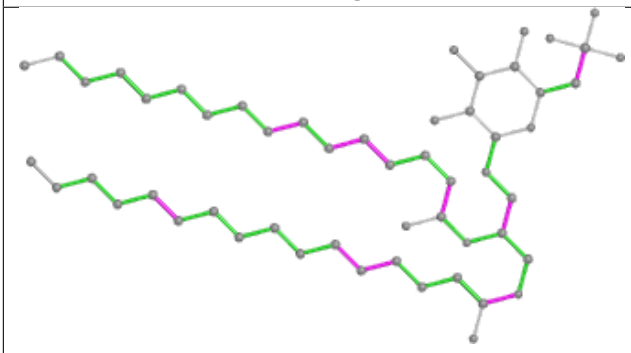
Ligand SQD a 401



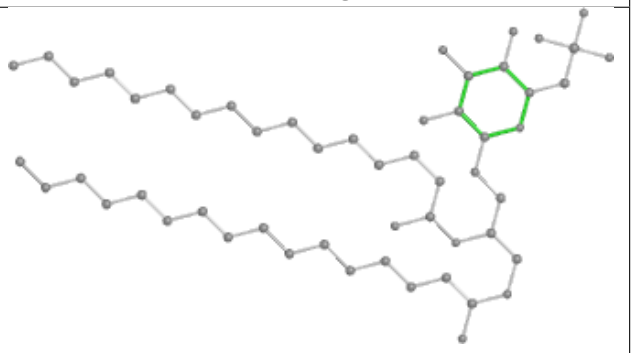
Bond lengths



Bond angles

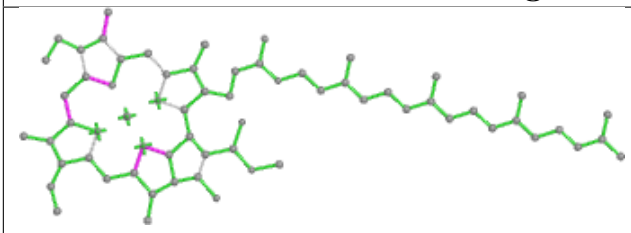


Torsions

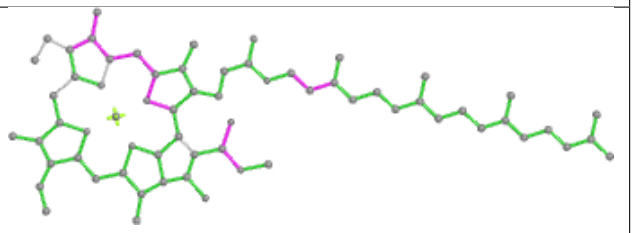


Rings

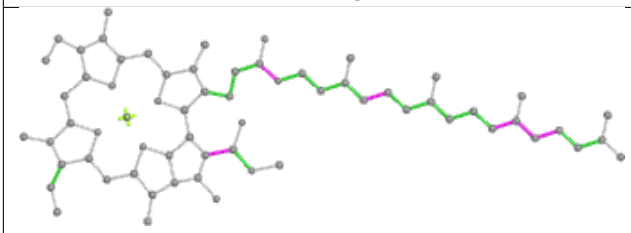
Ligand CLA C 502



Bond lengths



Bond angles



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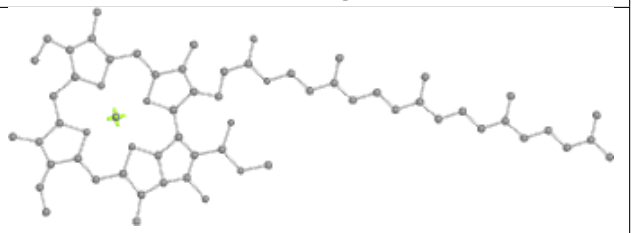
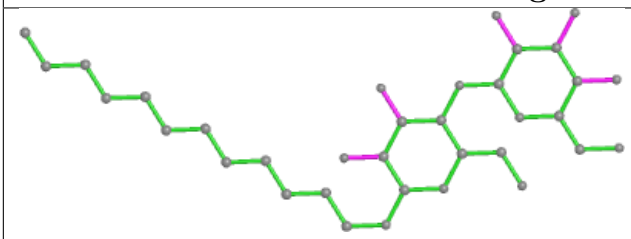


Rings

Ligand LMT i 102



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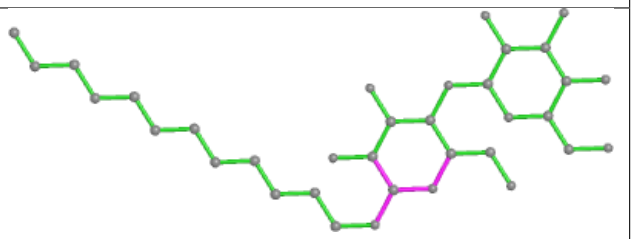
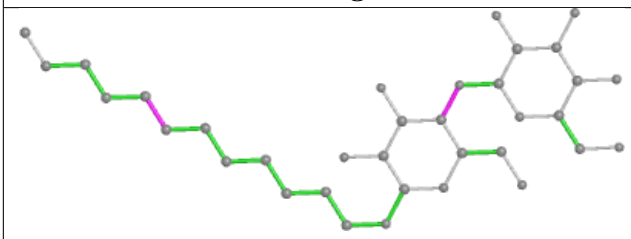


Bond angles



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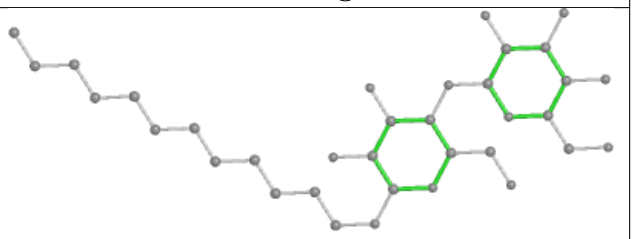
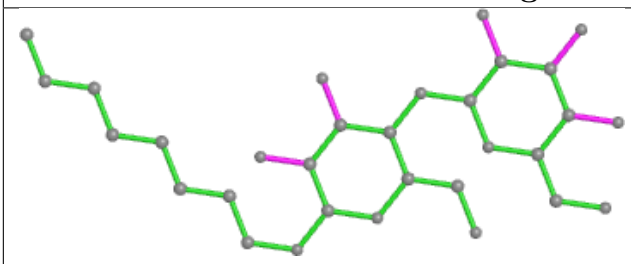
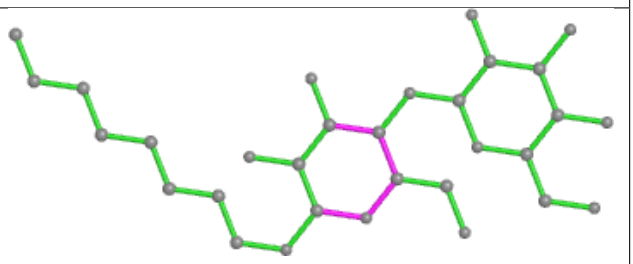


Rings

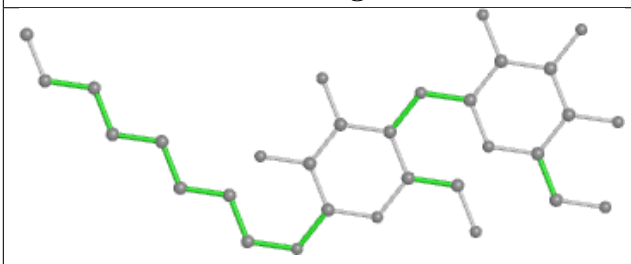
Ligand LMT D 410



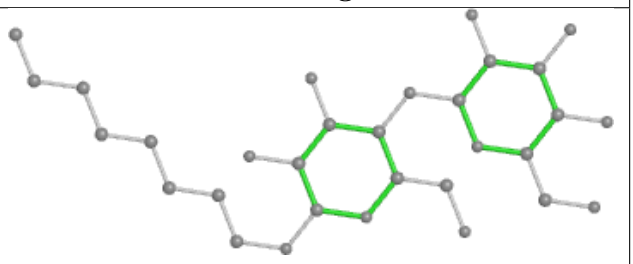
Bond lengths



Bond angles

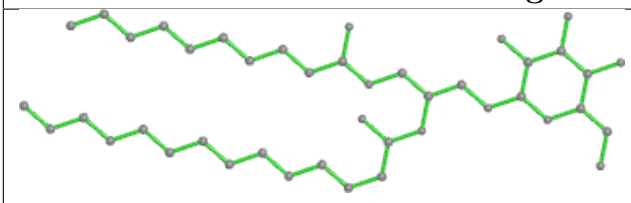


Torsions

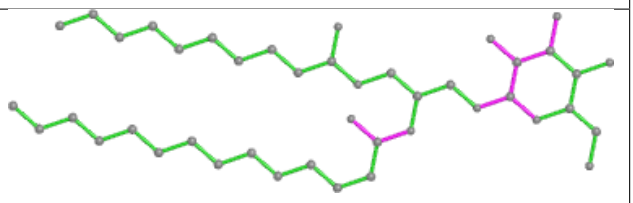


Rings

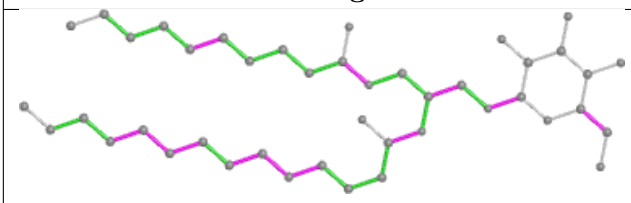
Ligand LMG I 101



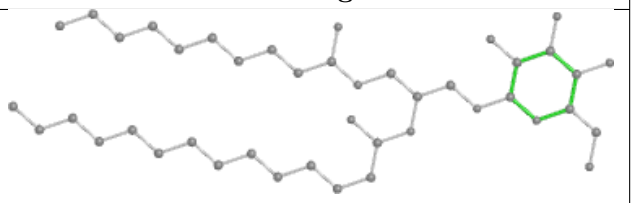
Bond lengths



Bond angles

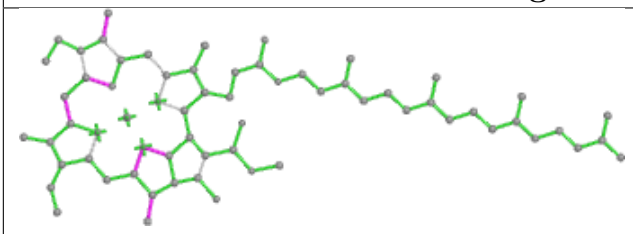


Torsions

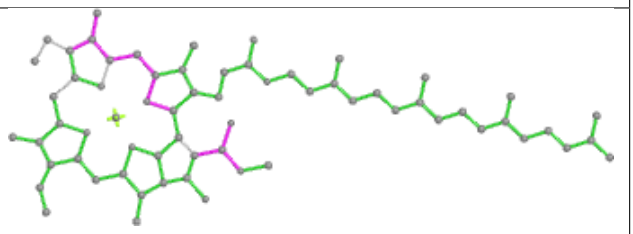


Rings

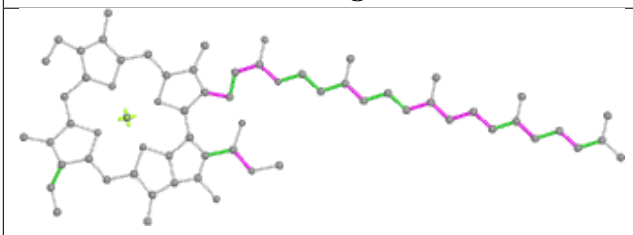
Ligand CLA c 504



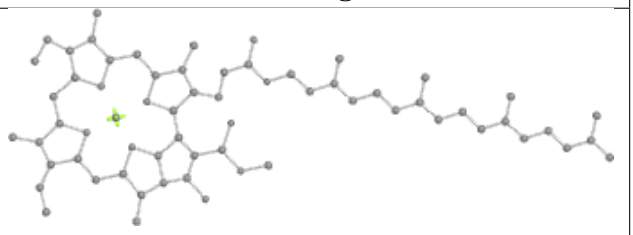
Bond lengths



Bond angles

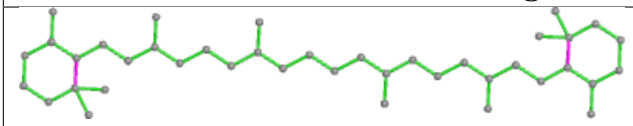


Torsions

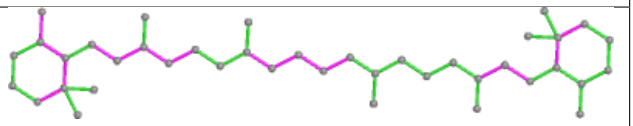


Rings

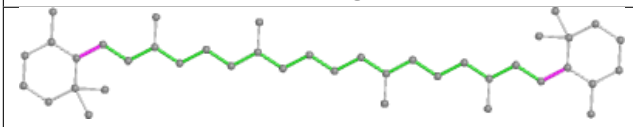
Ligand BCR B 618



Bond lengths



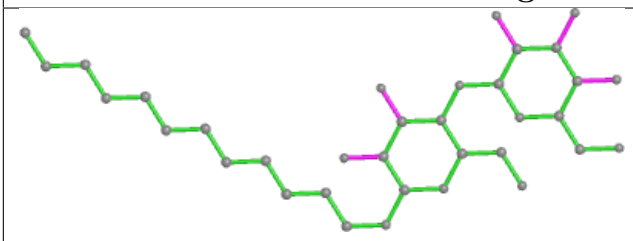
Bond angles



Torsions

Rings

Ligand LMT M 103



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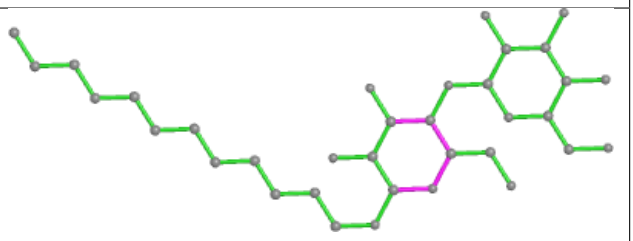
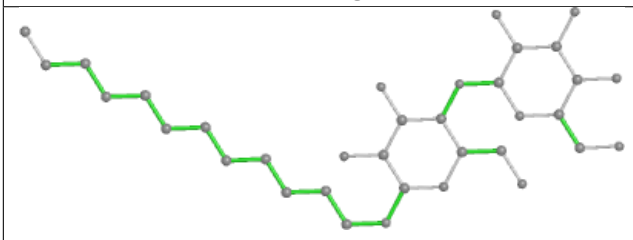


Bond angles



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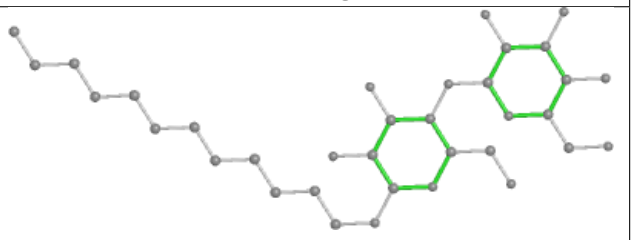
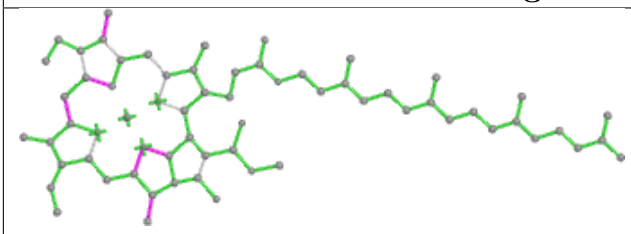
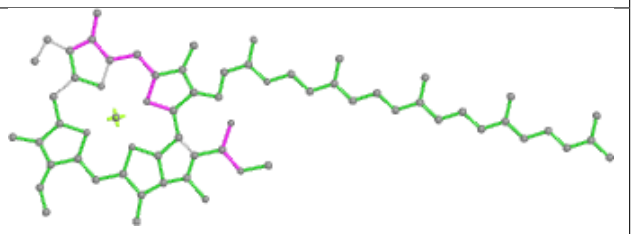


Rings

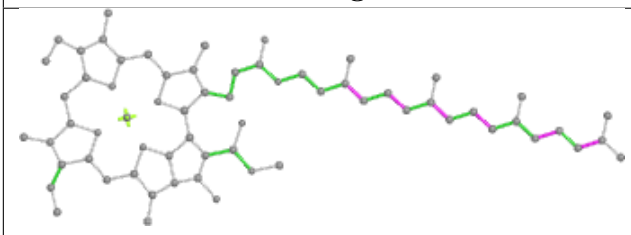
Ligand CLA A 405



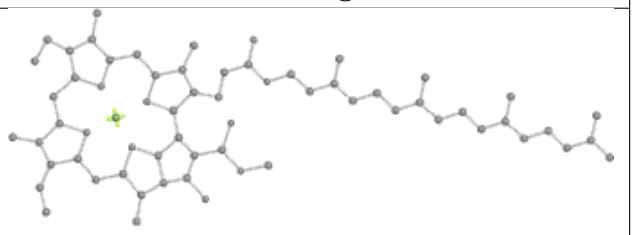
Bond lengths



Bond angles

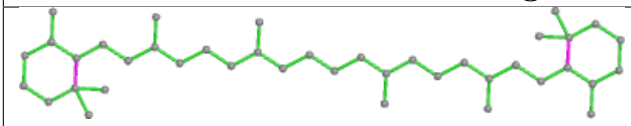


Torsions

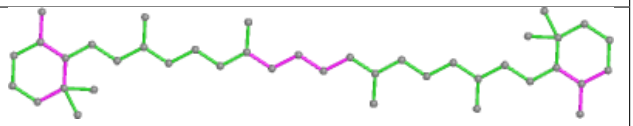


Rings

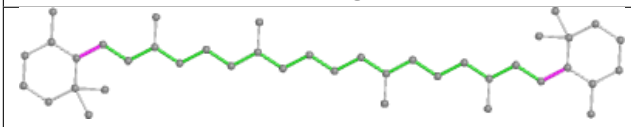
Ligand BCR A 407



Bond lengths



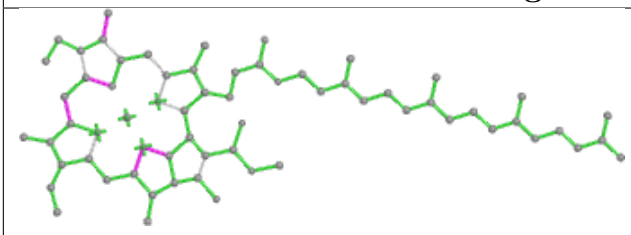
Bond angles



Torsions

Rings

Ligand CLA B 609



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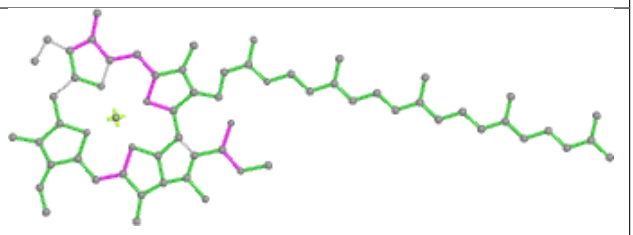
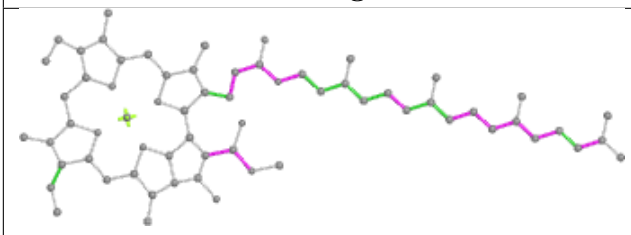
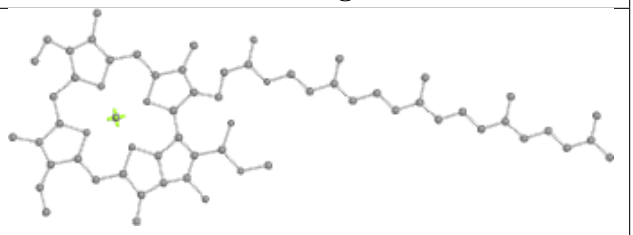


Bond angles

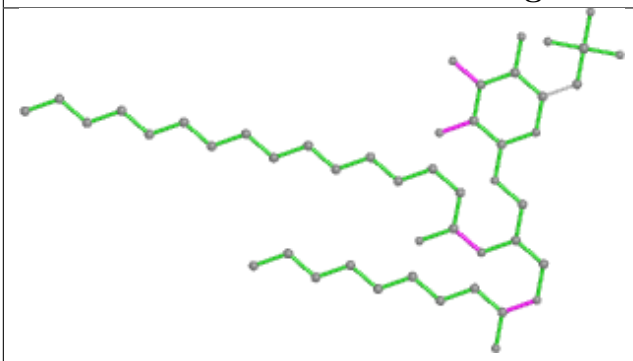


Torsions

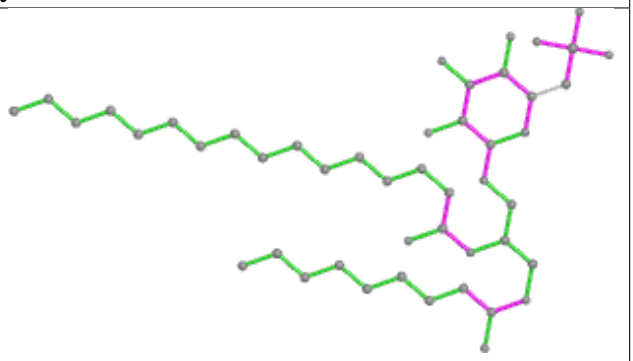


Rings

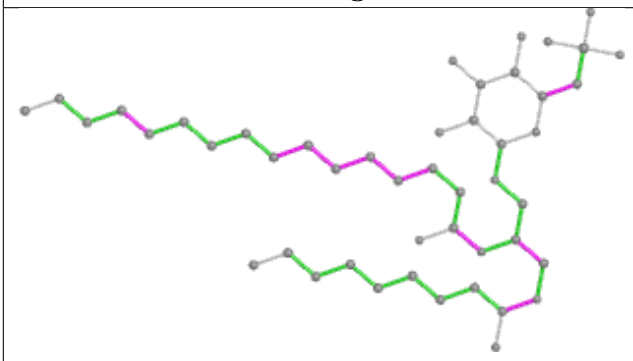
Ligand SQD B 626



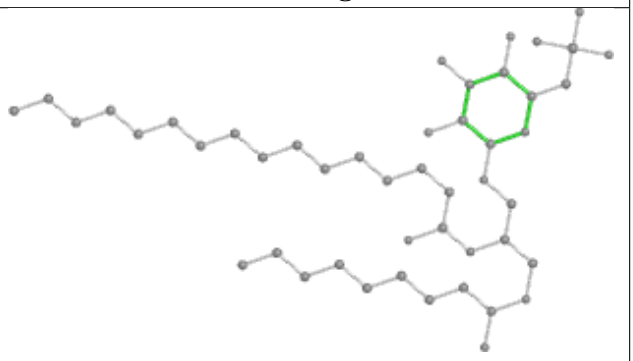
Bond lengths



Bond angles

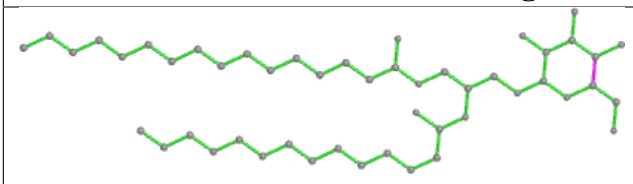


Torsions

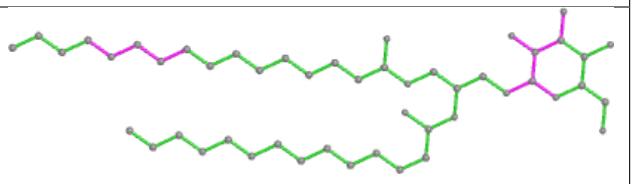


Rings

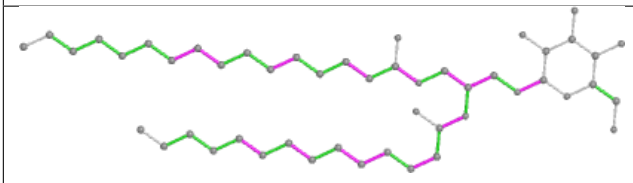
Ligand LMG B 621



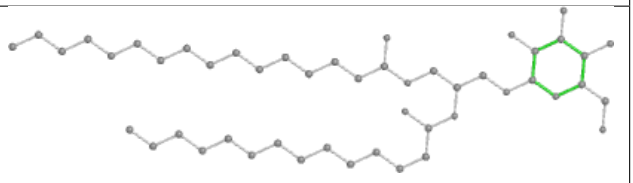
Bond lengths



Bond angles

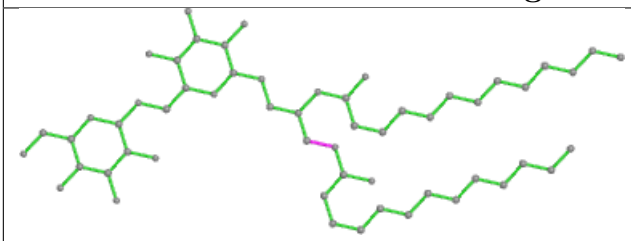


Torsions

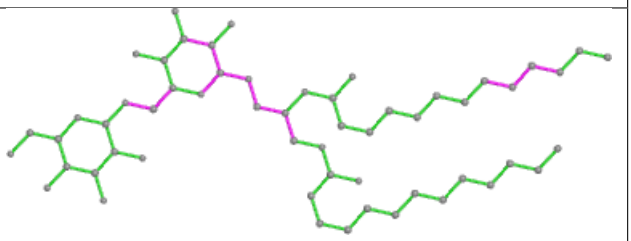


Rings

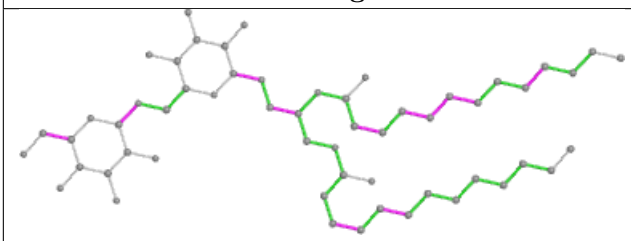
Ligand DGD a 411



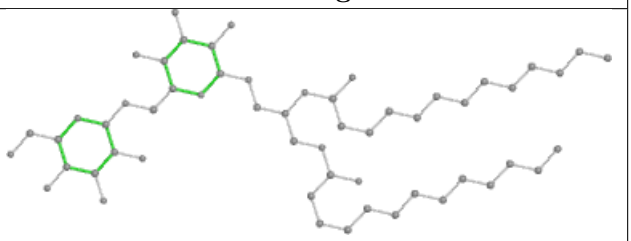
Bond lengths



Bond angles

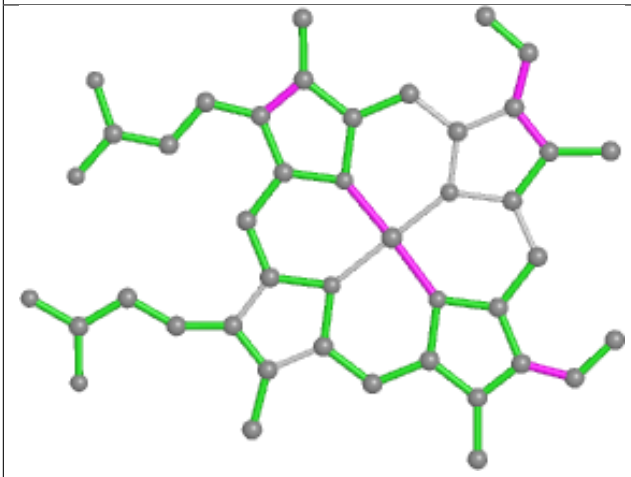


Torsions



Rings

Ligand HEM f 101



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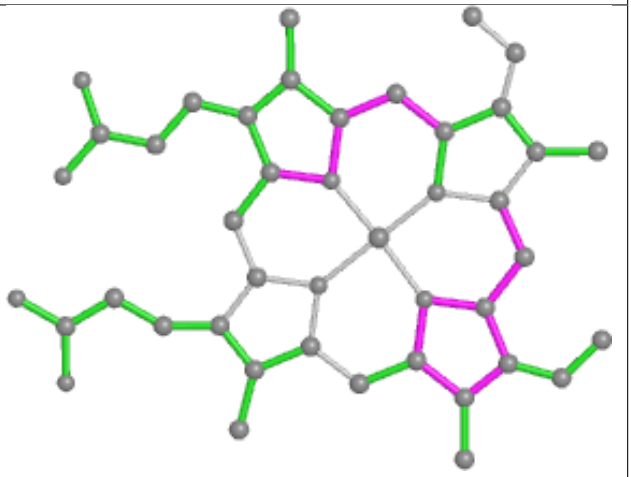
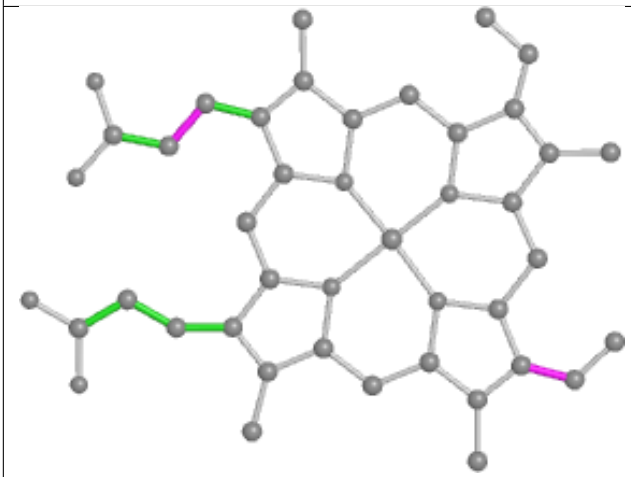
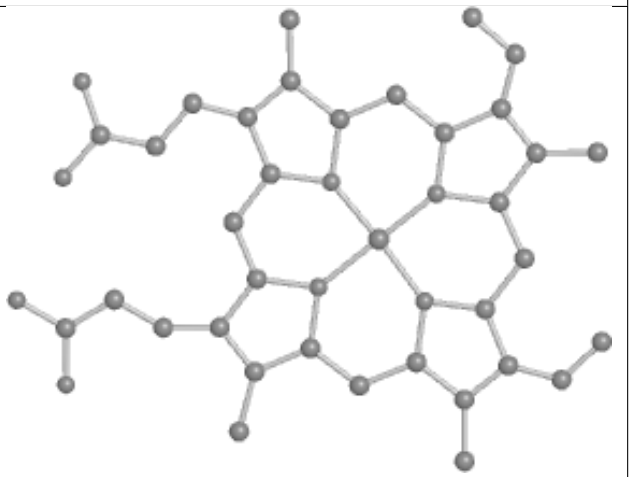


Bond angles

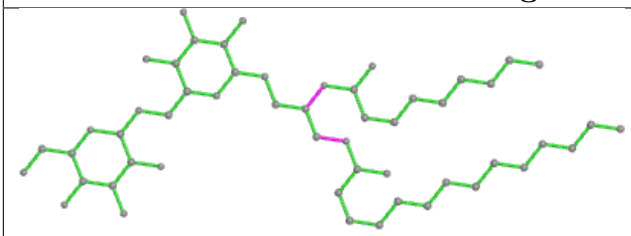


Torsions



Rings

Ligand DGD C 515



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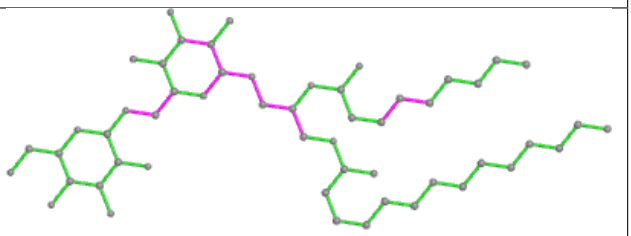
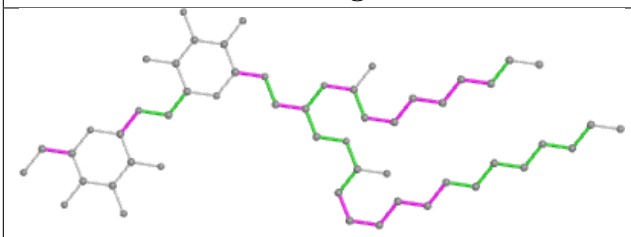


Bond angles



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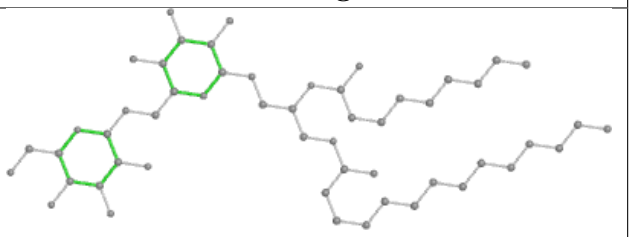
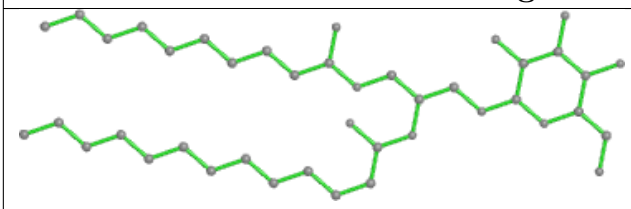


Rings

Ligand LMG m 101



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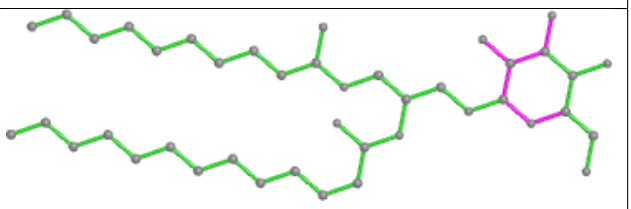
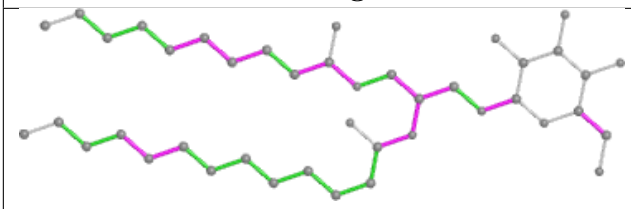


Bond angles



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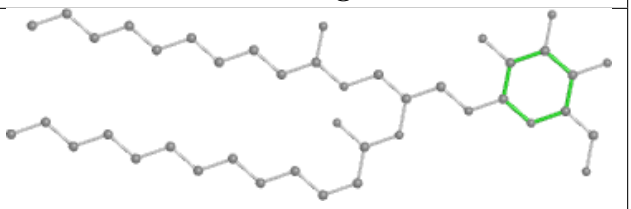
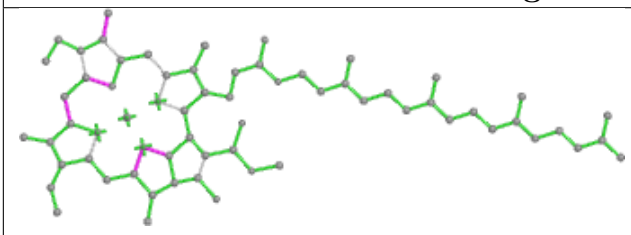


Rings

Ligand CLA H 101



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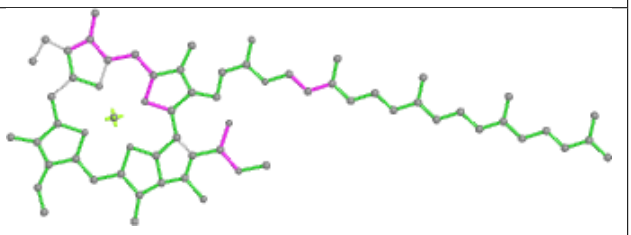
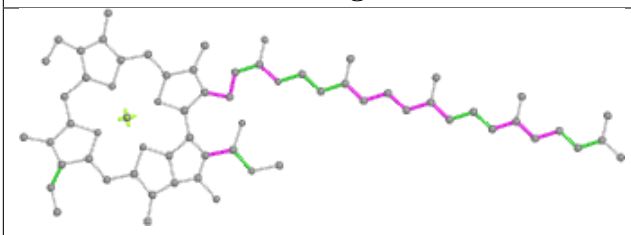


Bond angles



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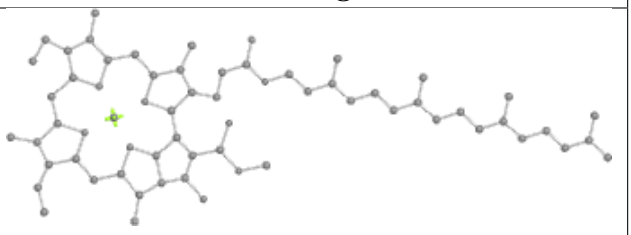
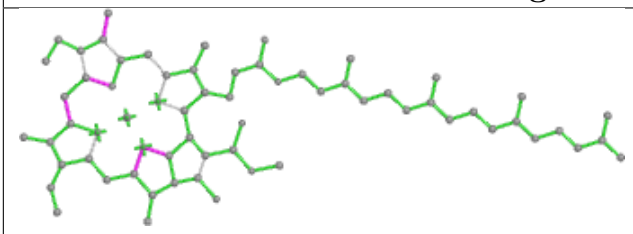
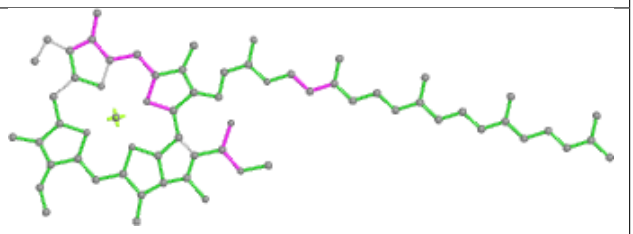


Rings

Ligand CLA c 502


Bond lengths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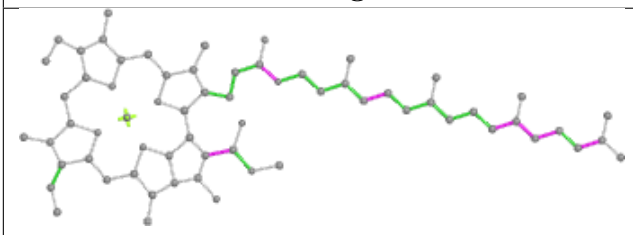
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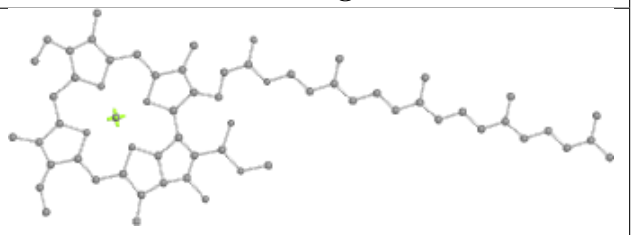
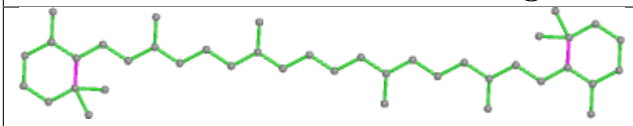

Rings

Ligand BCR B 616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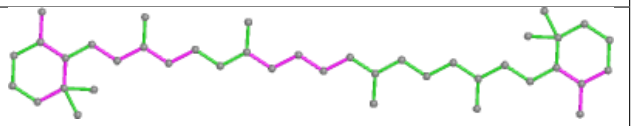
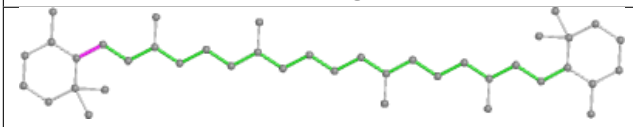
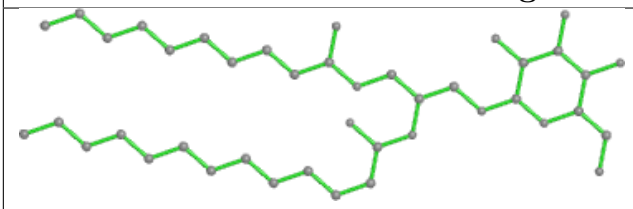

Bond angles


Torsions


Rings

Ligand LMG A 415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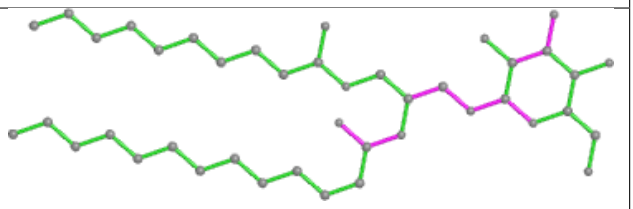
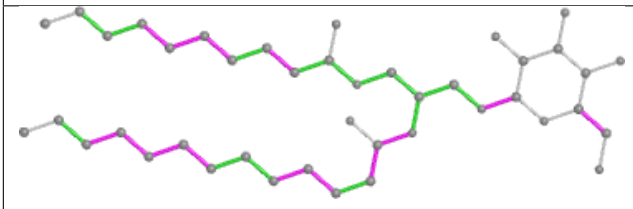
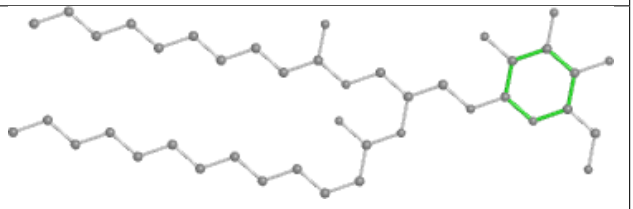
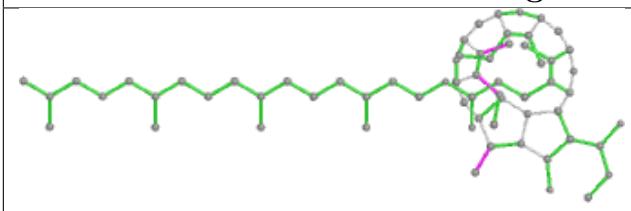

Bond angles


Torsions


Rings

Ligand PHO a 407



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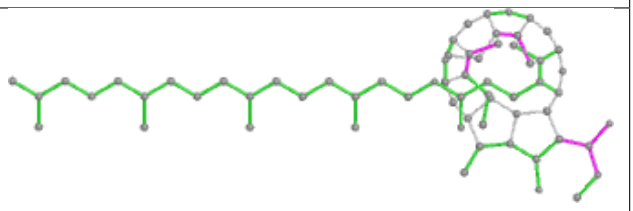
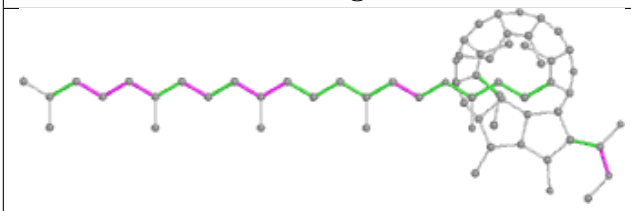


Bond angles



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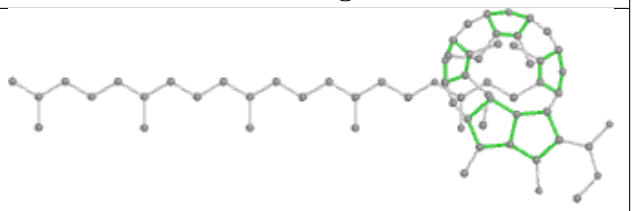
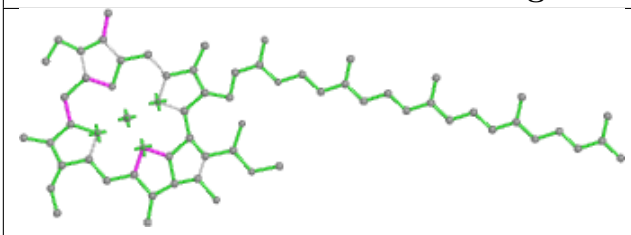


Rings

Ligand CLA b 616



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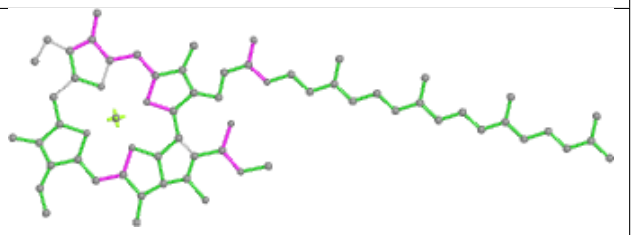
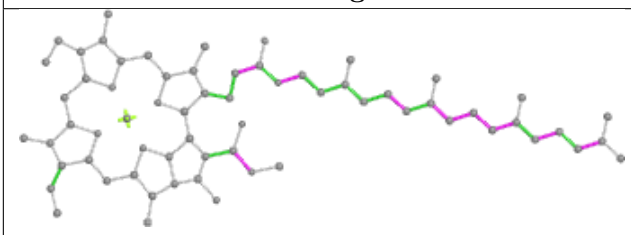


Bond angles



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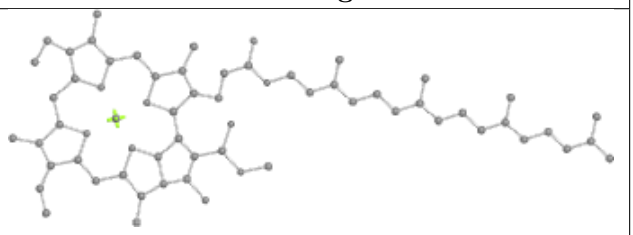
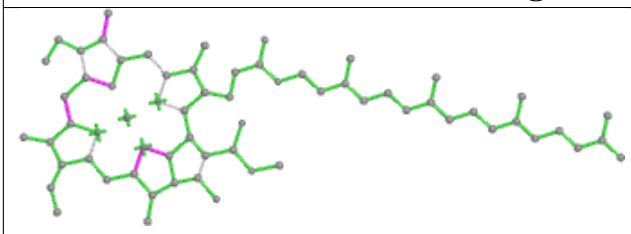
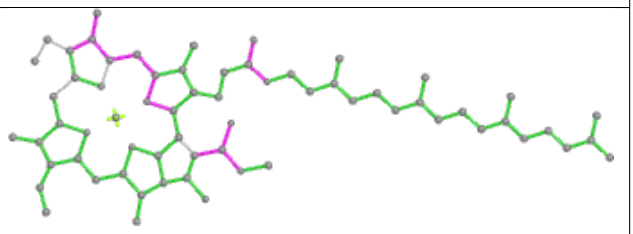


Rings

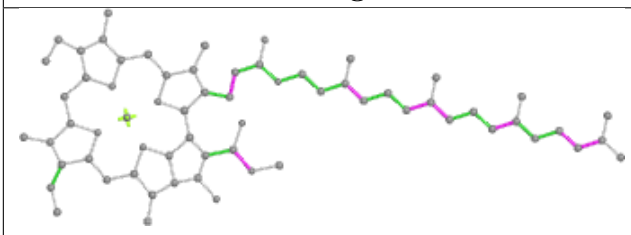
Ligand CLA b 606



Bond lengths



Bond angles



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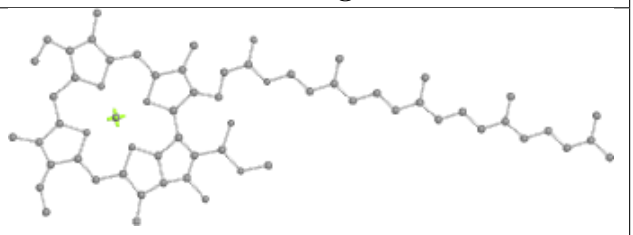
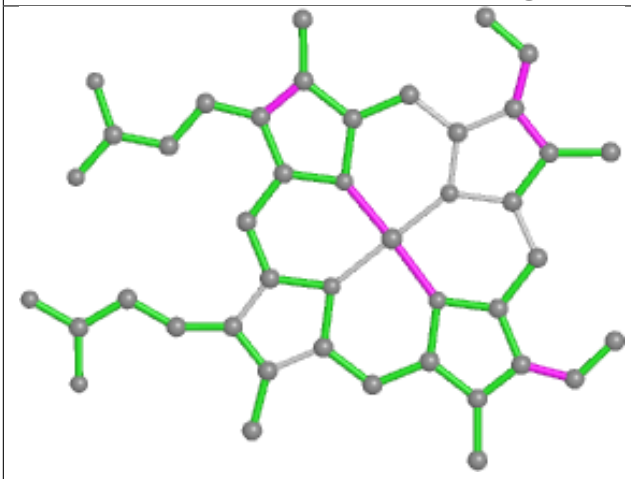
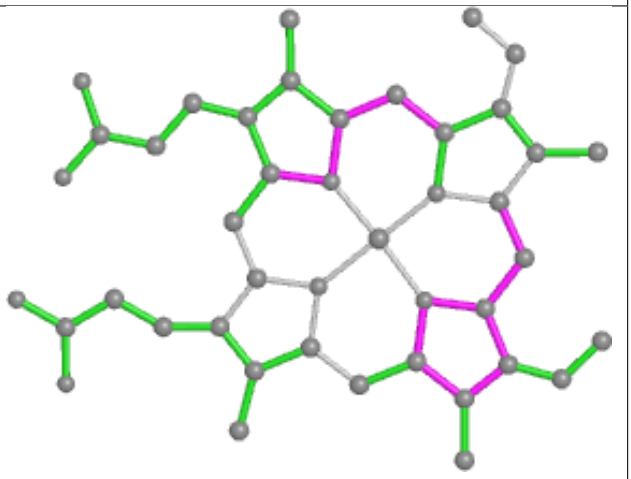


Rings

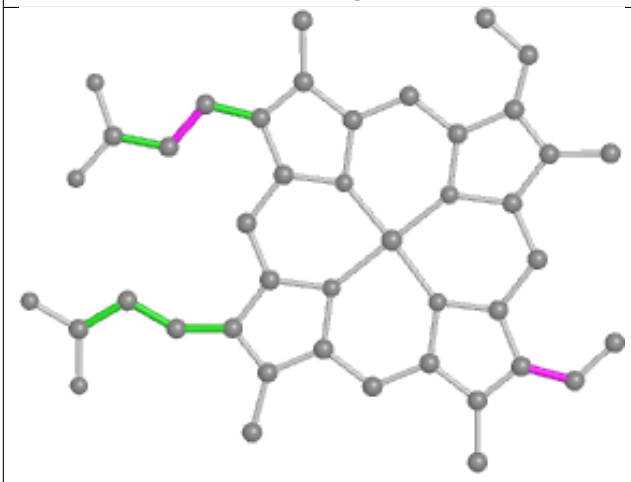
Ligand HEM F 101



Bond lengths



Bond angles



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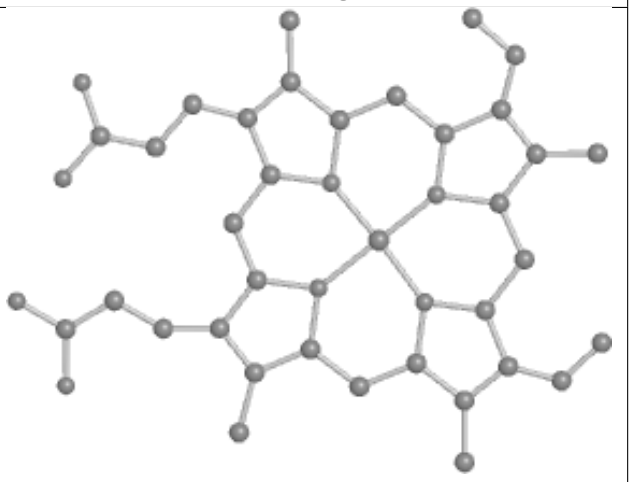
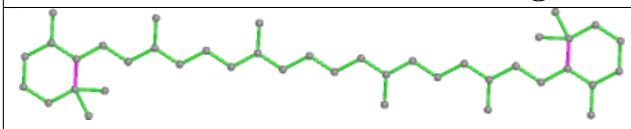
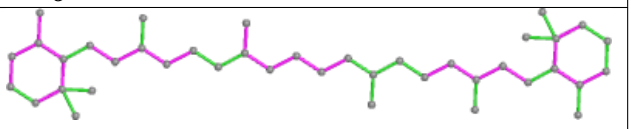


Rings

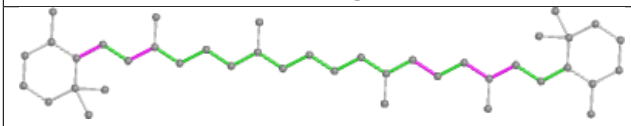
Ligand BCR j 102



Bond lengths



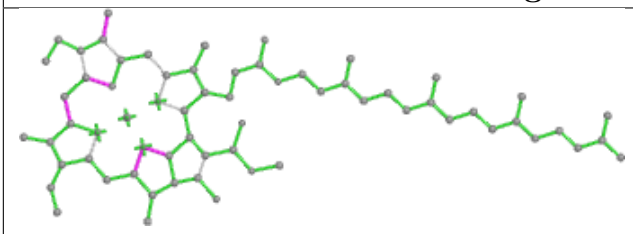
Bond angles



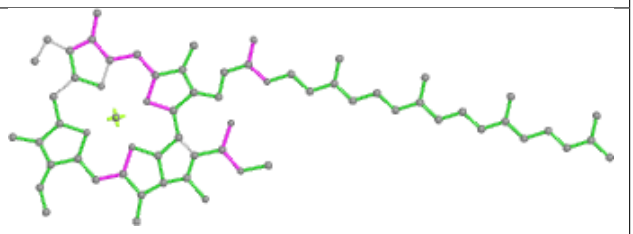
Torsions

Rings

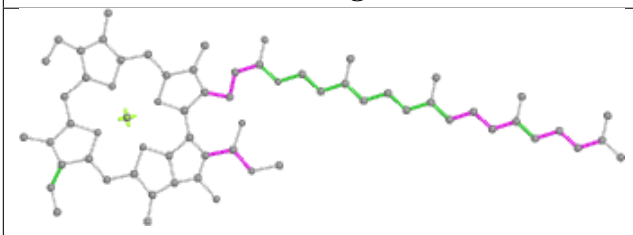
Ligand CLA C 501



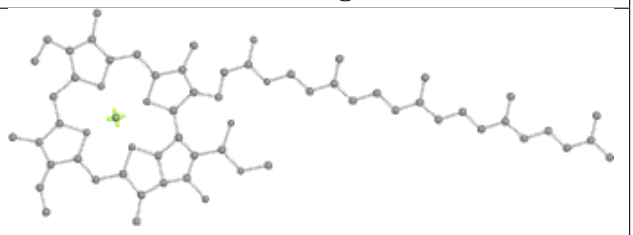
Bond lengths



Bond angles

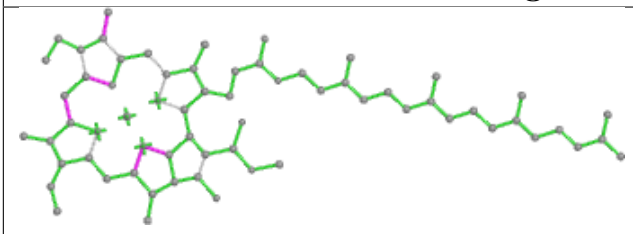


Torsions

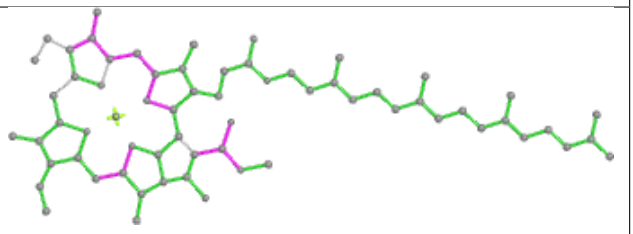


Rings

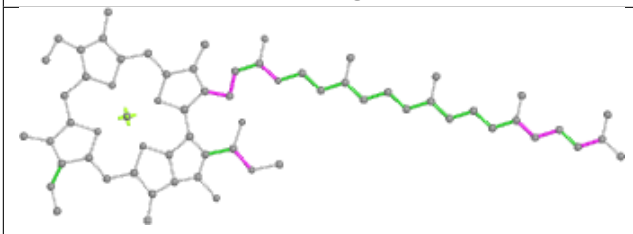
Ligand CLA B 605



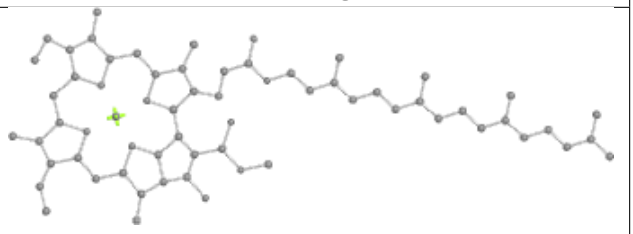
Bond lengths



Bond angles

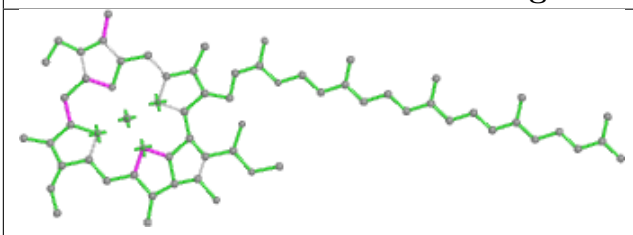


Torsions

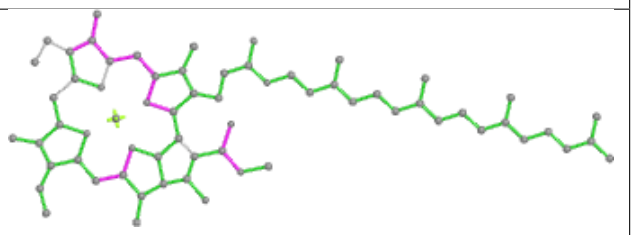


Rings

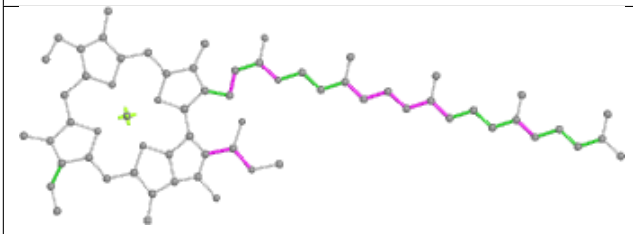
Ligand CLA c 510



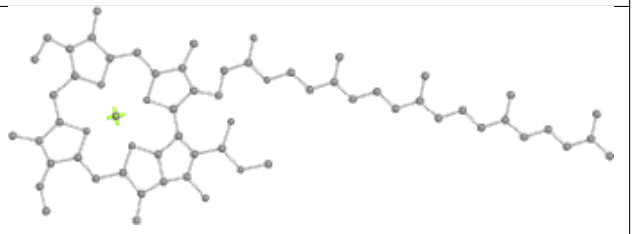
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/344 (97%)	0.43	28 (8%) 11 10	172, 174, 175, 176	0
1	a	335/344 (97%)	0.45	28 (8%) 11 10	172, 174, 175, 176	0
2	B	490/510 (96%)	0.22	30 (6%) 21 17	172, 174, 175, 176	0
2	b	490/510 (96%)	0.27	19 (3%) 39 31	172, 174, 175, 176	0
3	C	447/461 (96%)	0.25	24 (5%) 25 22	172, 174, 175, 176	0
3	c	447/461 (96%)	0.13	16 (3%) 42 35	173, 174, 175, 176	0
4	D	340/352 (96%)	0.17	7 (2%) 63 54	171, 174, 175, 176	0
4	d	340/352 (96%)	0.17	11 (3%) 47 38	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.07	1 (1%) 79 70	172, 174, 175, 175	0
5	e	82/84 (97%)	0.03	3 (3%) 41 33	173, 174, 175, 177	0
6	F	35/45 (77%)	-0.14	1 (2%) 51 41	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.45	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.42	7 (10%) 5 6	173, 174, 175, 176	0
7	h	65/66 (98%)	0.71	9 (13%) 2 3	173, 174, 175, 176	0
8	I	35/38 (92%)	0.24	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	-0.12	0 100 100	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.11	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	-0.43	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.31	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	0.15	1 (2%) 54 45	174, 174, 175, 176	0
11	L	37/37 (100%)	0.35	1 (2%) 54 45	172, 174, 175, 175	0
11	l	37/37 (100%)	0.16	0 100 100	173, 174, 175, 176	0
12	M	34/36 (94%)	0.21	1 (2%) 51 41	172, 174, 174, 176	0
12	m	34/36 (94%)	0.11	2 (5%) 22 19	173, 173, 174, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.47	16 (6%) 18 15	172, 174, 175, 176	0
13	o	243/272 (89%)	0.47	13 (5%) 26 23	172, 174, 175, 176	0
14	T	32/32 (100%)	0.27	2 (6%) 20 16	173, 174, 176, 176	0
14	t	32/32 (100%)	0.34	3 (9%) 8 8	173, 174, 175, 176	0
15	U	97/134 (72%)	0.46	7 (7%) 15 13	172, 174, 174, 175	0
15	u	97/134 (72%)	0.63	9 (9%) 8 8	173, 174, 175, 175	0
16	V	137/163 (84%)	0.05	0 100 100	172, 174, 175, 175	0
16	v	137/163 (84%)	0.49	10 (7%) 15 12	173, 174, 175, 176	0
17	g	28/46 (60%)	0.32	1 (3%) 42 35	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.06	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	0.31	1 (2%) 54 45	173, 174, 175, 176	0
18	x	37/41 (90%)	0.84	7 (18%) 1 2	173, 174, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.26	1 (1%) 72 62	173, 174, 175, 176	0
20	z	62/62 (100%)	0.88	5 (8%) 12 11	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.27	264 (5%) 28 24	171, 174, 175, 177	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.6
1	a	224	ILE	5.2
5	e	84	LYS	5.0
15	U	38	GLU	4.9
3	C	135	ARG	4.6
13	O	90	GLU	4.3
5	E	84	LYS	4.3
3	C	332	GLN	4.3
14	t	31	LYS	4.3
1	a	191	ASN	4.3
1	a	165	GLN	4.2
4	d	295	SER	4.1
7	h	66	GLY	4.1
7	h	23	PRO	3.9
1	A	299	GLY	3.9
1	A	175	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	b	217	ILE	3.8
3	c	200	THR	3.8
14	t	32	LYS	3.7
7	H	56	ASP	3.7
18	x	42	GLN	3.7
13	o	169	LYS	3.7
15	U	39	LEU	3.7
1	a	225	ARG	3.7
20	z	1	MET	3.7
7	h	26	GLY	3.6
18	x	12	ILE	3.6
15	u	53	GLU	3.6
10	k	14	ALA	3.5
1	A	190	HIS	3.5
2	B	69	LEU	3.5
3	C	184	GLY	3.5
1	A	293	MET	3.5
5	e	82	GLN	3.4
3	C	136	GLY	3.4
15	u	58	ASN	3.4
2	B	295	GLY	3.3
2	B	162	PHE	3.3
1	a	175	GLY	3.3
3	C	137	PRO	3.3
14	T	28	ARG	3.3
7	H	66	GLY	3.3
3	C	147	PHE	3.3
1	a	282	GLY	3.2
1	A	177	SER	3.2
3	c	201	ASN	3.2
7	H	5	THR	3.2
7	h	4	ARG	3.2
3	C	402	GLY	3.2
3	C	140	LEU	3.1
4	D	190	ASN	3.1
16	v	51	GLN	3.1
1	a	223	LEU	3.1
2	B	309	LEU	3.1
2	b	411	PHE	3.1
1	A	15	GLU	3.1
1	a	226	GLU	3.1
2	B	179	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	b	379	ALA	3.0
7	H	63	LYS	3.0
1	A	266	ASN	3.0
3	c	202	PRO	3.0
3	c	372	PRO	3.0
14	T	27	PRO	3.0
1	a	325	ASN	3.0
16	v	47	LEU	3.0
1	a	178	GLY	3.0
7	h	24	GLY	3.0
15	u	74	THR	3.0
2	b	303	SER	3.0
1	a	190	HIS	3.0
1	A	179	THR	3.0
18	X	42	GLN	2.9
2	B	259	GLY	2.9
2	B	474	LEU	2.9
1	A	298	ASN	2.9
7	H	64	ALA	2.9
13	o	124	GLU	2.9
15	U	40	VAL	2.9
15	u	107	GLU	2.9
1	A	138	GLY	2.8
3	C	149	TYR	2.8
2	B	164	PRO	2.8
3	c	403	SER	2.8
13	O	170	GLY	2.8
13	o	31	LEU	2.8
2	b	301	ALA	2.8
1	a	299	GLY	2.8
16	v	131	ARG	2.8
18	x	17	LYS	2.8
13	O	222	GLN	2.8
7	h	3	ARG	2.8
1	A	196	PRO	2.8
2	b	482	ILE	2.8
13	o	240	THR	2.8
2	b	218	LEU	2.8
4	D	24	ARG	2.7
1	A	195	HIS	2.7
1	A	181	ASN	2.7
4	d	221	THR	2.7

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Mol	Chain	Res	Type	RSRZ
15	u	65	PHE	2.7
13	O	262	GLN	2.7
2	B	132	ALA	2.7
1	a	181	ASN	2.7
3	C	44	ASN	2.7
13	O	218	LEU	2.6
16	v	133	LEU	2.6
1	a	239	PHE	2.6
2	B	294	SER	2.6
12	m	5	GLN	2.6
13	O	79	LYS	2.6
13	O	46	PRO	2.6
3	c	329	GLY	2.6
3	C	266	TRP	2.6
15	u	57	LEU	2.6
2	B	477	ASP	2.6
4	D	174	GLY	2.6
1	a	19	ASN	2.5
3	C	183	GLY	2.5
15	u	72	TYR	2.5
3	C	151	TRP	2.5
1	a	198	HIS	2.5
3	C	473	ASP	2.5
13	O	269	ILE	2.5
13	o	154	SER	2.5
3	c	260	ALA	2.5
2	B	127	ARG	2.5
4	d	236	ASN	2.5
2	b	119	ASP	2.5
2	b	120	LEU	2.5
13	O	84	ASN	2.5
1	a	187	GLN	2.5
1	A	10	SER	2.5
13	o	173	ASN	2.4
13	O	195	ASP	2.4
6	F	11	VAL	2.4
13	o	189	GLY	2.4
2	b	490	GLN	2.4
20	z	4	LEU	2.4
2	B	129	GLY	2.4
16	v	138	LEU	2.4
2	B	161	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
11	L	33	SER	2.4
2	B	402	TYR	2.4
18	x	16	LEU	2.4
2	B	84	THR	2.4
7	h	18	TYR	2.4
1	A	14	TRP	2.4
2	b	402	TYR	2.4
20	z	47	TRP	2.4
15	u	75	LEU	2.4
1	a	319	ASP	2.4
4	d	195	PRO	2.4
13	o	84	ASN	2.4
13	o	168	PHE	2.3
13	O	58	ILE	2.3
15	u	52	GLY	2.3
16	v	130	MET	2.3
2	B	128	THR	2.3
1	a	170	ASP	2.3
1	A	178	GLY	2.3
3	c	203	THR	2.3
1	A	222	SER	2.3
2	B	293	ALA	2.3
13	O	169	LYS	2.3
13	O	91	PHE	2.3
1	a	137	LEU	2.3
12	M	2	GLU	2.3
7	h	27	THR	2.3
1	a	199	GLN	2.3
2	B	397	VAL	2.3
3	c	259	TRP	2.3
1	A	165	GLN	2.3
3	C	148	GLY	2.3
4	d	194	ASN	2.3
2	b	302	TRP	2.3
5	e	8	ARG	2.3
16	v	31	PRO	2.3
12	m	2	GLU	2.3
4	d	203	GLY	2.3
1	A	80	GLY	2.3
2	b	133	LEU	2.2
13	o	239	GLY	2.2
17	g	27	MET	2.2

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Mol	Chain	Res	Type	RSRZ
15	U	127	ARG	2.2
3	C	46	SER	2.2
20	Z	62	VAL	2.2
3	c	180	MET	2.2
15	U	121	LEU	2.2
4	d	176	ALA	2.2
3	C	144	SER	2.2
1	A	169	SER	2.2
4	d	13	GLY	2.2
2	B	130	GLU	2.2
13	O	119	LEU	2.2
3	C	154	LYS	2.2
1	A	262	TYR	2.2
16	v	103	LYS	2.2
13	o	238	ALA	2.2
2	b	216	HIS	2.2
3	c	373	ASN	2.2
2	B	122	LEU	2.2
1	a	298	ASN	2.2
1	a	301	ASN	2.2
1	a	177	SER	2.2
1	A	16	ARG	2.2
7	H	62	TRP	2.2
7	H	55	LEU	2.2
3	C	134	ILE	2.2
3	c	191	PRO	2.2
3	c	388	GLN	2.2
4	d	220	ASN	2.2
3	C	261	ARG	2.2
20	z	30	PRO	2.1
1	a	169	SER	2.1
3	C	336	GLY	2.1
15	U	122	VAL	2.1
4	D	297	ASP	2.1
3	c	365	TRP	2.1
2	B	411	PHE	2.1
2	b	420	TYR	2.1
2	B	124	ARG	2.1
13	O	171	GLU	2.1
2	B	354	LEU	2.1
3	C	403	SER	2.1
2	B	125	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	75	ASN	2.1
3	C	141	GLU	2.1
1	a	179	THR	2.1
18	x	13	THR	2.1
1	A	183	MET	2.1
2	b	339	ALA	2.1
3	c	212	TYR	2.1
4	D	194	ASN	2.1
16	v	117	VAL	2.1
1	A	76	ASN	2.1
4	d	297	ASP	2.1
4	D	192	THR	2.1
16	v	132	ASN	2.1
20	z	29	SER	2.1
13	o	216	PHE	2.1
1	a	173	PRO	2.1
1	a	322	ASN	2.1
18	x	23	LEU	2.1
2	B	183	PRO	2.1
15	U	54	LYS	2.1
3	C	212	TYR	2.0
2	B	163	GLY	2.0
13	O	50	ASP	2.0
2	B	166	MET	2.0
7	h	22	ALA	2.0
4	D	197	HIS	2.0
14	t	29	ILE	2.0
13	o	164	THR	2.0
1	A	11	ALA	2.0
3	c	389	GLU	2.0
2	B	133	LEU	2.0
2	b	403	GLY	2.0
4	d	191	TRP	2.0
2	b	137	LYS	2.0
2	b	304	ALA	2.0
1	A	12	ASN	2.0
1	A	342	ASP	2.0
2	B	353	GLU	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
35	CA	o	301	1/1	0.32	0.68	180,180,180,180	0
31	LMT	I	102	35/35	0.40	0.94	173,175,176,178	0
23	PL9	J	101	35/55	0.43	0.54	172,175,176,176	0
23	PL9	j	101	35/55	0.49	0.37	173,175,175,176	0
24	BCR	J	102	40/40	0.50	0.44	172,174,176,177	0
31	LMT	i	102	35/35	0.52	1.29	173,175,176,177	0
35	CA	O	301	1/1	0.53	0.38	177,177,177,177	0
31	LMT	d	409	31/35	0.53	0.66	172,175,177,177	0
31	LMT	b	627	35/35	0.54	1.22	173,175,177,177	0
31	LMT	b	626	35/35	0.59	0.69	172,175,176,177	0
22	CLA	b	605	65/65	0.61	1.14	172,175,176,176	0
27	LMG	A	415	42/55	0.62	0.53	171,174,176,177	0
27	LMG	C	518	45/55	0.62	1.09	171,174,175,175	0
22	CLA	B	601	65/65	0.62	0.85	172,175,176,177	0
24	BCR	j	102	40/40	0.63	0.34	173,175,177,178	0
27	LMG	E	101	44/55	0.63	0.56	170,174,176,177	0
24	BCR	f	102	40/40	0.63	0.47	171,173,175,175	0
31	LMT	D	410	31/35	0.64	0.93	174,175,176,176	0
24	BCR	g	101	40/40	0.64	0.78	173,174,175,175	0
27	LMG	a	402	42/55	0.65	0.49	171,174,176,176	0
26	LHG	C	519	37/49	0.65	0.48	172,174,179,183	0
22	CLA	b	619	65/65	0.65	0.77	172,174,175,175	0
25	DGD	d	408	63/66	0.66	0.77	172,175,177,178	0
27	LMG	I	101	43/55	0.66	1.04	172,174,177,177	0
22	CLA	c	502	65/65	0.66	0.54	173,174,175,175	0
31	LMT	B	628	35/35	0.66	0.46	172,174,177,178	0
24	BCR	D	411	40/40	0.67	0.44	171,173,174,175	0
24	BCR	c	514	40/40	0.67	0.71	172,173,175,175	0
31	LMT	B	622	35/35	0.67	0.88	171,175,177,177	0
23	PL9	D	407	55/55	0.68	0.39	171,173,174,175	0
23	PL9	d	406	55/55	0.68	0.39	172,173,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	BCR	H	102	40/40	0.69	0.94	173,174,175,176	0
27	LMG	a	413	51/55	0.69	0.42	172,173,175,176	0
23	PL9	A	406	45/55	0.69	0.43	172,174,175,175	0
22	CLA	C	502	65/65	0.70	0.53	173,174,174,175	0
25	DGD	D	409	63/66	0.70	0.81	172,174,176,178	0
31	LMT	b	604	35/35	0.70	0.47	172,174,176,176	0
27	LMG	c	518	45/55	0.71	1.01	172,174,176,176	0
25	DGD	A	408	56/66	0.71	0.45	172,174,175,176	0
24	BCR	x	101	40/40	0.71	0.86	173,174,175,175	0
32	PHO	d	401	64/64	0.72	0.42	172,173,174,174	0
24	BCR	B	616	40/40	0.72	0.43	172,173,174,175	0
25	DGD	b	601	52/66	0.72	0.47	172,174,176,177	0
25	DGD	a	411	56/66	0.73	0.44	173,174,175,176	0
24	BCR	a	410	40/40	0.73	0.68	172,173,174,175	0
30	SQD	A	413	51/54	0.73	0.37	172,174,175,176	0
27	LMG	M	101	42/55	0.73	0.53	173,174,176,176	0
27	LMG	C	522	48/55	0.73	0.36	172,174,174,175	0
22	CLA	a	408	65/65	0.74	0.82	173,174,175,175	0
27	LMG	i	101	43/55	0.74	0.80	172,174,177,178	0
26	LHG	c	519	37/49	0.74	0.35	172,174,178,181	0
24	BCR	B	617	40/40	0.75	0.44	172,173,174,174	0
27	LMG	e	101	44/55	0.75	0.39	171,174,175,176	0
30	SQD	d	402	43/54	0.75	0.83	172,174,176,178	0
22	CLA	B	613	65/65	0.76	0.46	172,174,174,175	0
31	LMT	B	627	35/35	0.76	0.55	172,175,177,177	0
23	PL9	a	409	45/55	0.76	0.38	171,173,174,175	0
28	CL	A	411	1/1	0.76	0.42	172,172,172,172	0
25	DGD	B	625	52/66	0.76	0.56	172,175,177,177	0
31	LMT	M	103	35/35	0.76	0.47	172,173,175,176	0
25	DGD	b	624	58/66	0.76	0.40	171,173,174,175	0
31	LMT	M	102	35/35	0.77	0.46	172,174,175,175	0
22	CLA	C	506	65/65	0.77	0.73	172,174,175,175	0
25	DGD	C	517	66/66	0.77	0.34	172,173,174,175	0
24	BCR	y	101	40/40	0.77	1.00	173,173,174,175	0
35	CA	k	101	1/1	0.77	0.20	172,172,172,172	0
22	CLA	C	507	65/65	0.77	0.40	173,174,175,177	0
27	LMG	b	625	49/55	0.78	0.34	172,174,175,175	0
27	LMG	D	412	46/55	0.78	0.40	172,174,175,175	0
22	CLA	h	101	65/65	0.78	0.53	171,174,175,175	0
24	BCR	b	622	40/40	0.78	0.36	171,172,173,173	0
27	LMG	m	101	42/55	0.78	0.45	170,174,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	LMG	B	624	49/55	0.78	0.31	171,173,174,175	0
24	BCR	C	514	40/40	0.78	0.83	172,173,175,175	0
22	CLA	c	512	65/65	0.78	0.68	172,174,176,176	0
24	BCR	A	407	40/40	0.79	0.48	171,173,174,174	0
30	SQD	B	626	47/54	0.79	0.46	170,174,176,178	0
30	SQD	F	102	45/54	0.79	0.69	172,175,177,178	0
32	PHO	D	402	64/64	0.79	0.37	171,173,175,175	0
22	CLA	C	505	65/65	0.79	0.45	172,174,175,176	0
24	BCR	C	521	40/40	0.79	0.82	172,174,175,176	0
31	LMT	B	623	35/35	0.79	0.50	173,174,177,177	0
27	LMG	A	410	51/55	0.79	0.35	171,173,174,175	0
30	SQD	b	602	47/54	0.80	0.38	171,174,176,178	0
25	DGD	c	517	66/66	0.80	0.35	172,173,175,176	0
24	BCR	B	619	40/40	0.80	0.83	172,173,174,175	0
24	BCR	b	623	40/40	0.80	0.76	171,173,174,174	0
22	CLA	b	609	65/65	0.81	0.55	172,174,175,175	0
31	LMT	b	603	35/35	0.81	0.44	172,174,175,176	0
22	CLA	b	613	65/65	0.81	0.67	172,174,175,175	0
35	CA	K	101	1/1	0.81	0.35	177,177,177,177	0
24	BCR	c	521	40/40	0.81	1.26	172,174,175,175	0
27	LMG	c	522	48/55	0.81	0.29	172,174,175,176	0
22	CLA	B	603	65/65	0.81	0.49	171,173,175,175	0
30	SQD	D	403	43/54	0.82	0.41	172,174,177,180	0
22	CLA	b	607	65/65	0.82	0.43	172,173,175,176	0
22	CLA	c	503	65/65	0.82	0.57	172,174,175,175	0
22	CLA	b	617	65/65	0.82	0.45	173,173,175,176	0
22	CLA	b	618	65/65	0.82	0.66	172,174,175,175	0
22	CLA	C	520	65/65	0.82	0.33	172,174,175,176	0
25	DGD	C	515	53/66	0.83	0.36	172,173,174,174	0
22	CLA	a	405	65/65	0.83	0.58	170,172,174,175	0
26	LHG	a	412	39/49	0.83	0.28	171,174,176,177	0
22	CLA	C	510	65/65	0.83	0.46	172,173,175,175	0
24	BCR	B	618	40/40	0.83	0.32	171,172,174,174	0
24	BCR	c	513	40/40	0.83	0.87	172,173,175,175	0
22	CLA	C	512	65/65	0.83	0.88	172,174,176,177	0
22	CLA	A	405	65/65	0.83	0.62	172,174,175,176	0
22	CLA	c	508	65/65	0.84	0.56	172,174,175,175	0
22	CLA	C	504	65/65	0.84	0.41	171,173,175,175	0
25	DGD	B	620	58/66	0.84	0.33	171,173,175,176	0
32	PHO	D	401	64/64	0.84	0.40	171,173,174,175	0
30	SQD	a	401	54/54	0.84	0.58	172,174,176,178	0
22	CLA	d	404	65/65	0.84	0.45	172,173,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	B	610	65/65	0.84	0.34	172,174,174,175	0
30	SQD	f	103	45/54	0.84	0.52	172,174,176,178	0
25	DGD	C	516	62/66	0.84	0.29	171,174,175,176	0
22	CLA	b	612	65/65	0.84	0.66	171,174,175,176	0
30	SQD	A	414	54/54	0.85	0.40	171,174,176,179	0
24	BCR	b	621	40/40	0.85	0.33	171,173,174,174	0
26	LHG	A	409	39/49	0.85	0.28	172,173,175,176	0
22	CLA	a	406	65/65	0.85	0.36	172,174,175,176	0
22	CLA	c	505	65/65	0.85	0.45	172,174,175,175	0
30	SQD	a	415	51/54	0.85	0.29	173,174,175,176	0
22	CLA	B	607	65/65	0.85	0.42	172,174,174,175	0
22	CLA	C	509	65/65	0.85	0.34	173,173,174,174	0
22	CLA	c	501	65/65	0.85	0.45	172,174,175,175	0
22	CLA	b	606	65/65	0.85	0.61	172,173,174,174	0
27	LMG	d	407	48/55	0.86	0.28	171,173,175,175	0
22	CLA	C	503	65/65	0.86	0.41	172,174,175,176	0
25	DGD	c	515	53/66	0.86	0.36	171,174,175,177	0
22	CLA	B	605	65/65	0.86	0.72	172,173,175,176	0
21	FE2	a	403	1/1	0.86	0.18	175,175,175,175	0
24	BCR	C	513	40/40	0.86	0.77	172,173,174,174	0
22	CLA	c	506	65/65	0.86	0.55	173,174,175,175	0
32	PHO	a	407	64/64	0.86	0.26	173,174,175,175	0
22	CLA	B	615	65/65	0.86	0.66	172,174,175,175	0
22	CLA	c	510	65/65	0.86	0.53	173,174,175,176	0
22	CLA	H	101	65/65	0.86	0.35	172,174,175,175	0
22	CLA	B	609	65/65	0.86	0.53	172,174,175,175	0
22	CLA	d	405	65/65	0.86	0.45	172,174,175,175	0
22	CLA	A	404	65/65	0.87	0.47	170,173,174,175	0
22	CLA	c	520	65/65	0.87	0.36	173,174,174,175	0
22	CLA	B	604	65/65	0.87	0.67	172,173,175,175	0
25	DGD	c	516	62/66	0.87	0.30	172,174,175,175	0
22	CLA	C	501	65/65	0.87	0.40	172,174,174,175	0
22	CLA	C	508	65/65	0.87	0.86	172,174,175,175	0
22	CLA	c	509	65/65	0.87	0.32	172,173,175,175	0
27	LMG	D	408	48/55	0.87	0.28	170,173,175,175	0
22	CLA	D	406	65/65	0.87	0.64	172,174,175,176	0
22	CLA	a	404	65/65	0.88	0.54	172,173,174,176	0
34	HEM	V	201	43/43	0.88	0.45	172,173,175,175	0
22	CLA	b	608	65/65	0.88	0.51	172,173,175,176	0
22	CLA	b	614	65/65	0.88	0.30	172,173,174,175	0
22	CLA	B	606	65/65	0.88	0.34	172,173,174,175	0
27	LMG	B	621	49/55	0.88	0.26	172,173,174,174	0

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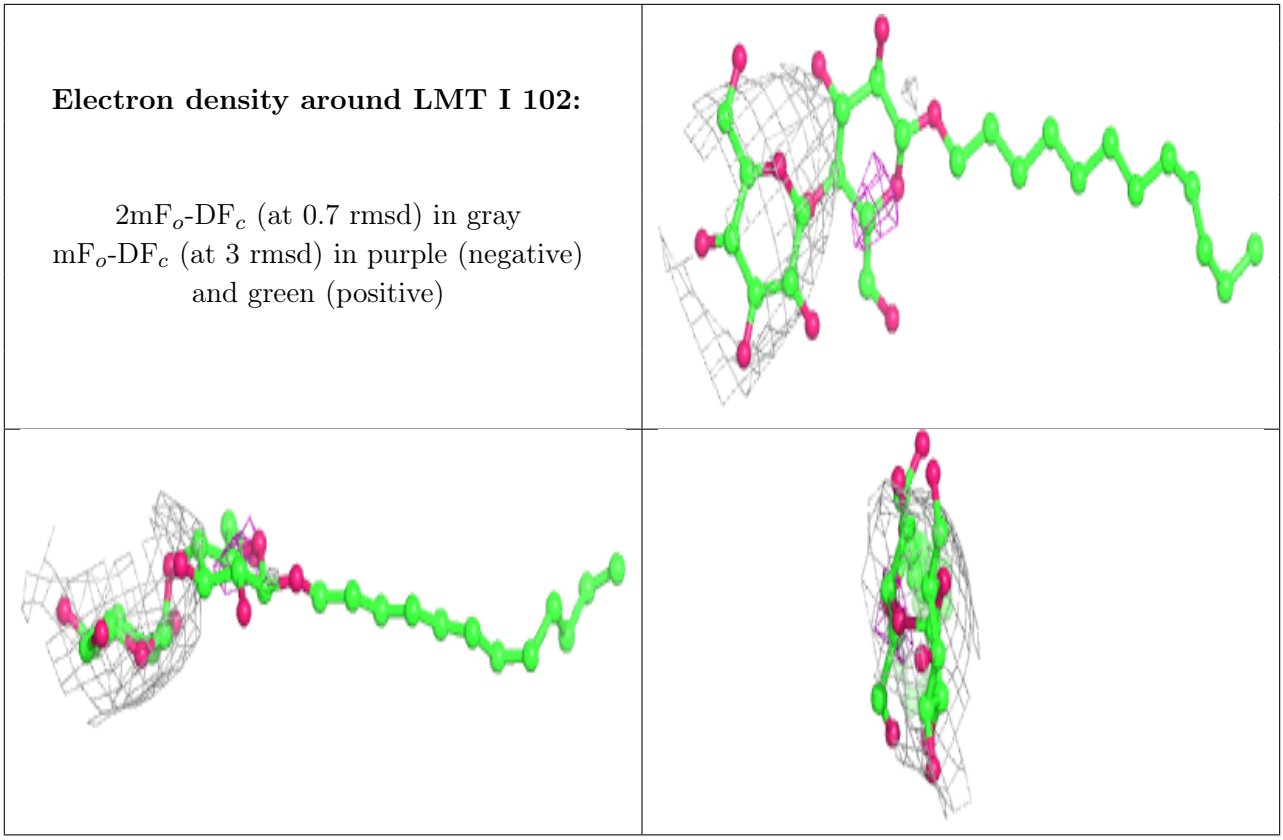
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	D	405	65/65	0.89	0.36	172,173,174,175	0
22	CLA	c	511	65/65	0.89	0.62	172,174,175,176	0
22	CLA	c	504	65/65	0.89	0.33	172,174,175,175	0
22	CLA	B	614	65/65	0.89	0.62	172,174,175,175	0
22	CLA	b	610	65/65	0.90	0.33	172,173,175,175	0
24	BCR	b	620	40/40	0.90	0.32	172,173,174,175	0
34	HEM	v	201	43/43	0.90	0.55	171,174,175,175	0
22	CLA	A	402	65/65	0.90	0.42	172,173,174,175	0
22	CLA	C	511	65/65	0.90	0.92	172,174,175,175	0
22	CLA	B	608	65/65	0.90	0.50	172,174,175,175	0
22	CLA	B	612	65/65	0.90	0.28	171,173,175,175	0
28	CL	a	416	1/1	0.91	0.33	173,173,173,173	0
22	CLA	c	507	65/65	0.91	0.24	172,174,175,176	0
33	BCT	d	403	4/4	0.91	0.92	174,174,175,176	0
34	HEM	F	101	43/43	0.91	0.48	173,174,175,176	0
27	LMG	d	410	46/55	0.91	0.23	172,173,175,175	0
21	FE2	A	401	1/1	0.92	0.18	170,170,170,170	0
22	CLA	B	602	65/65	0.92	0.52	171,173,174,175	0
22	CLA	B	611	65/65	0.92	0.36	171,173,174,174	0
22	CLA	b	615	65/65	0.92	0.40	172,173,174,175	0
22	CLA	b	611	65/65	0.92	0.31	172,174,175,175	0
29	OEX	A	412	10/10	0.93	0.42	165,169,172,173	0
27	LMG	b	628	49/55	0.93	0.23	172,174,175,175	0
34	HEM	f	101	43/43	0.93	0.34	173,174,175,175	0
22	CLA	A	403	65/65	0.93	0.54	171,173,174,175	0
33	BCT	D	404	4/4	0.95	0.25	173,174,174,174	0
22	CLA	b	616	65/65	0.95	0.29	171,173,174,175	0
29	OEX	a	414	10/10	0.96	0.45	168,171,173,177	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.

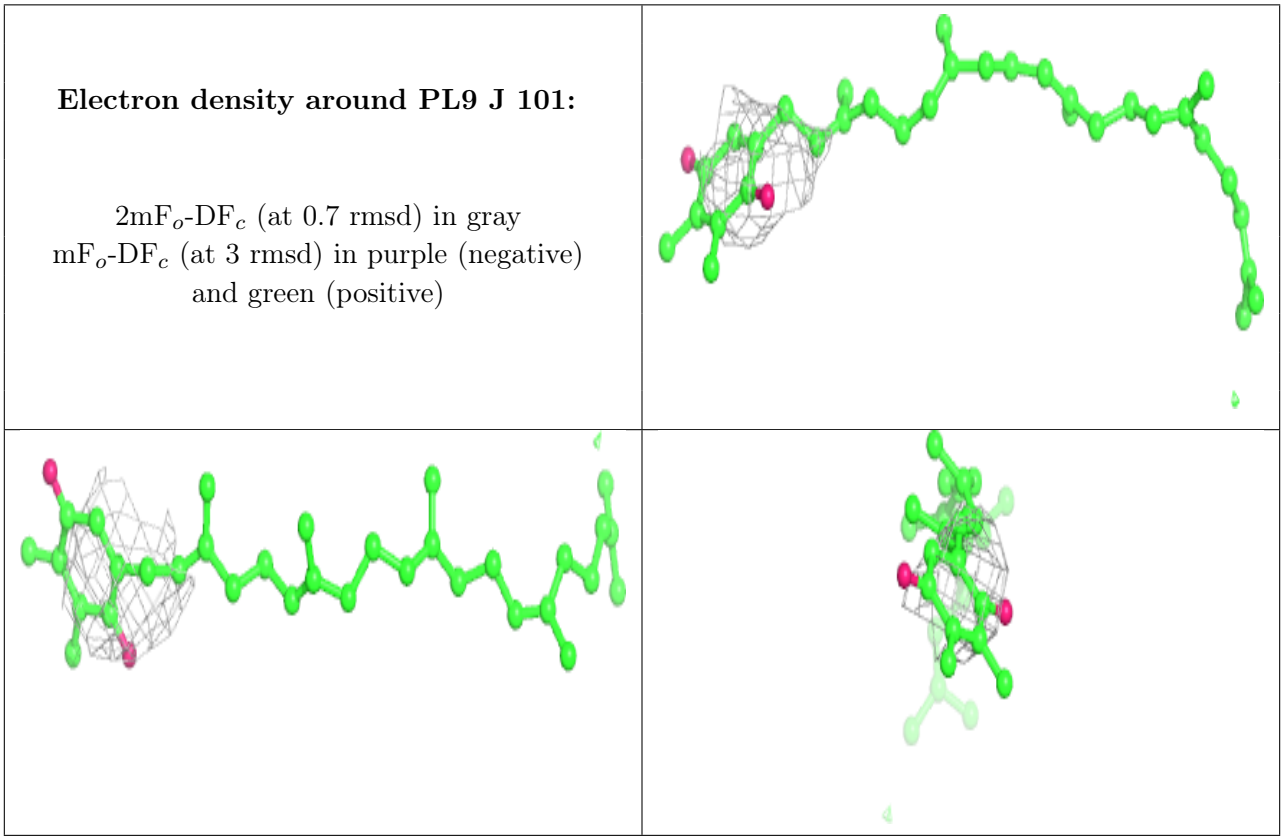
Electron density around LMT I 102:

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



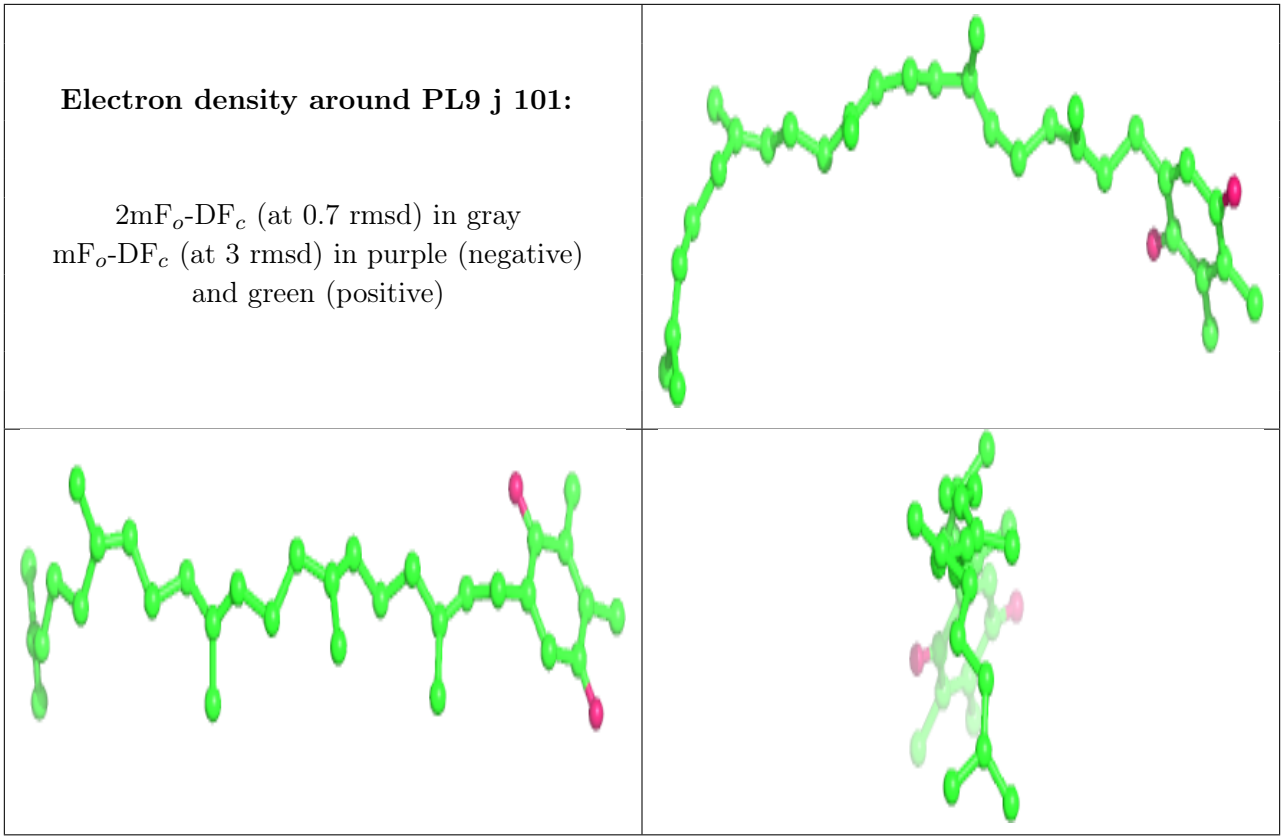
Electron density around PL9 J 101:

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



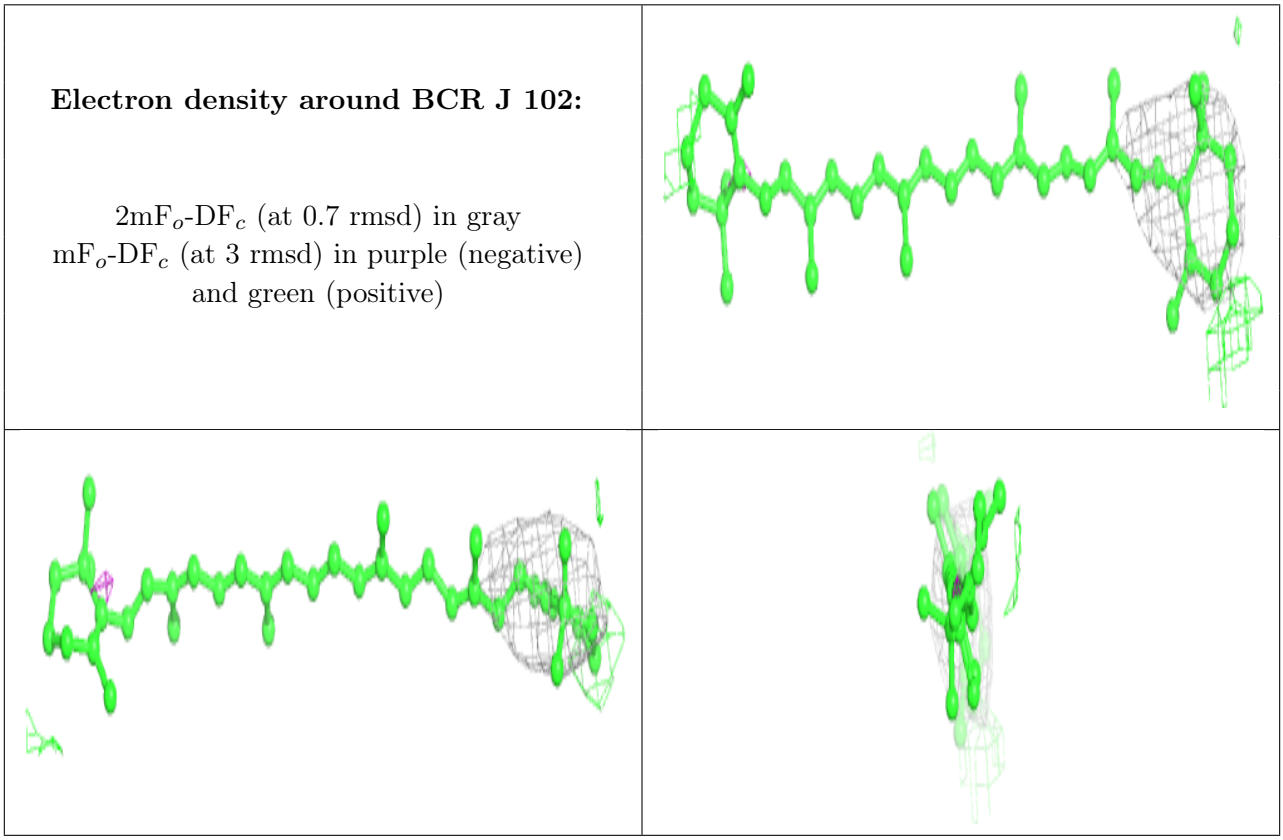
Electron density around PL9 j 101:

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



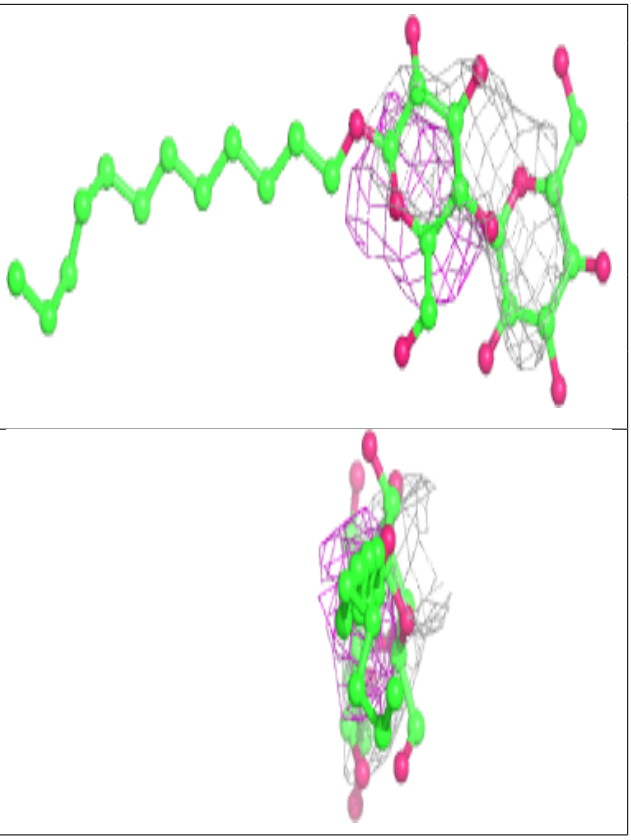
Electron density around BCR J 102:

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



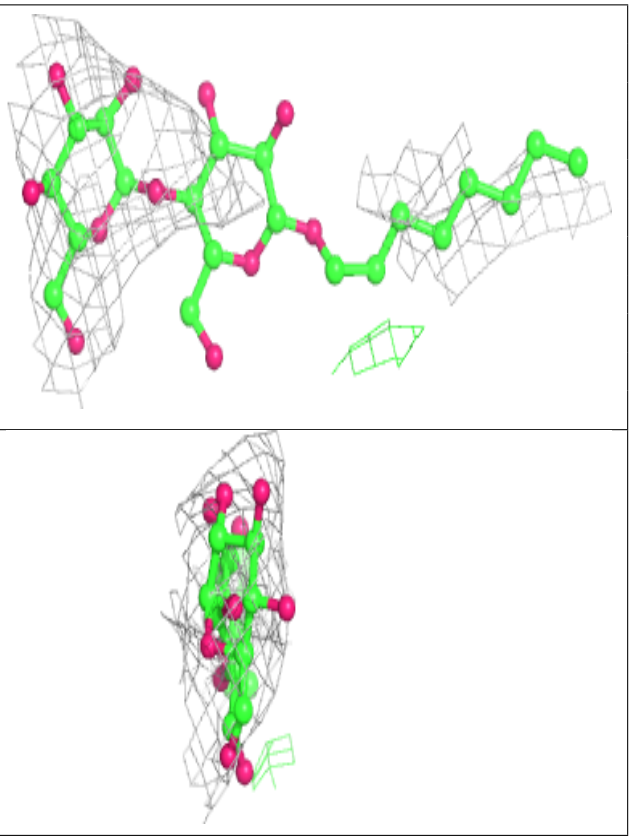
Electron density around LMT i 102:

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



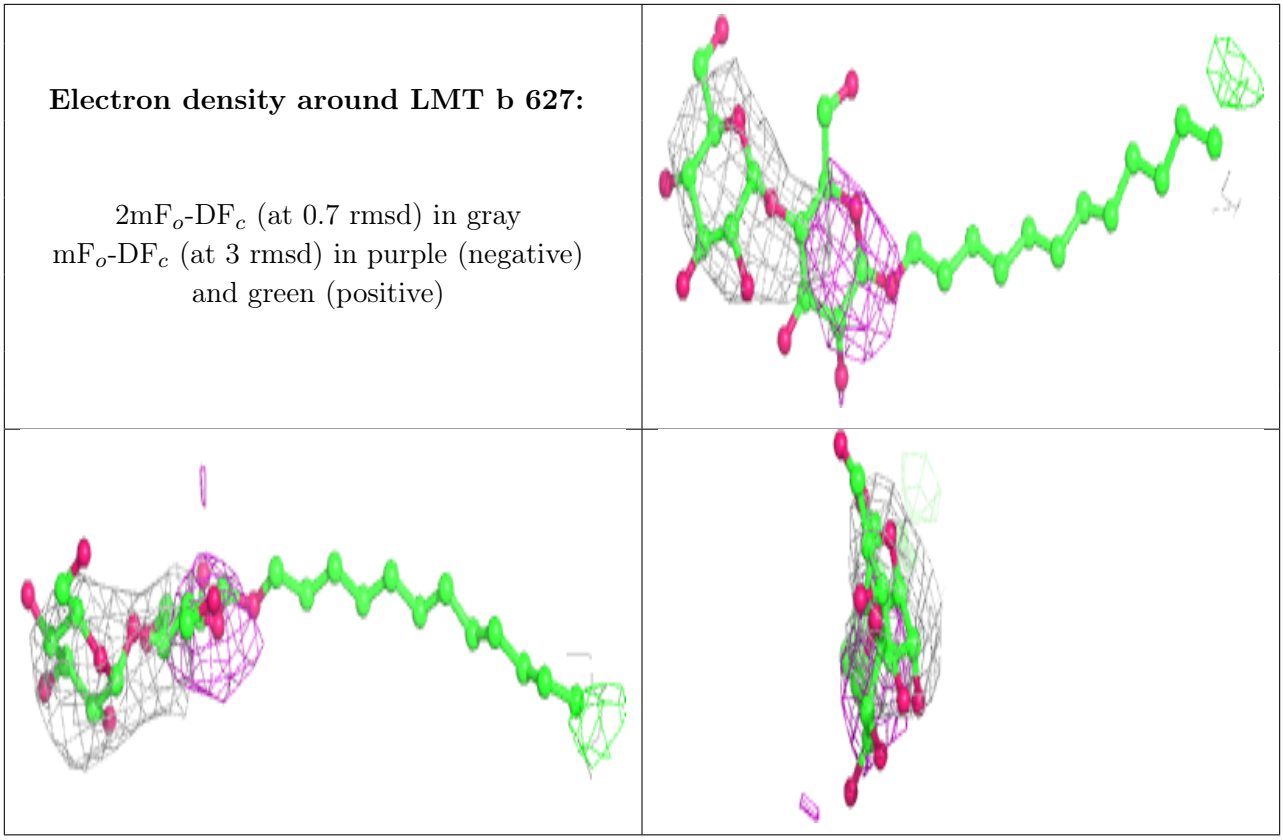
Electron density around LMT d 409:

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



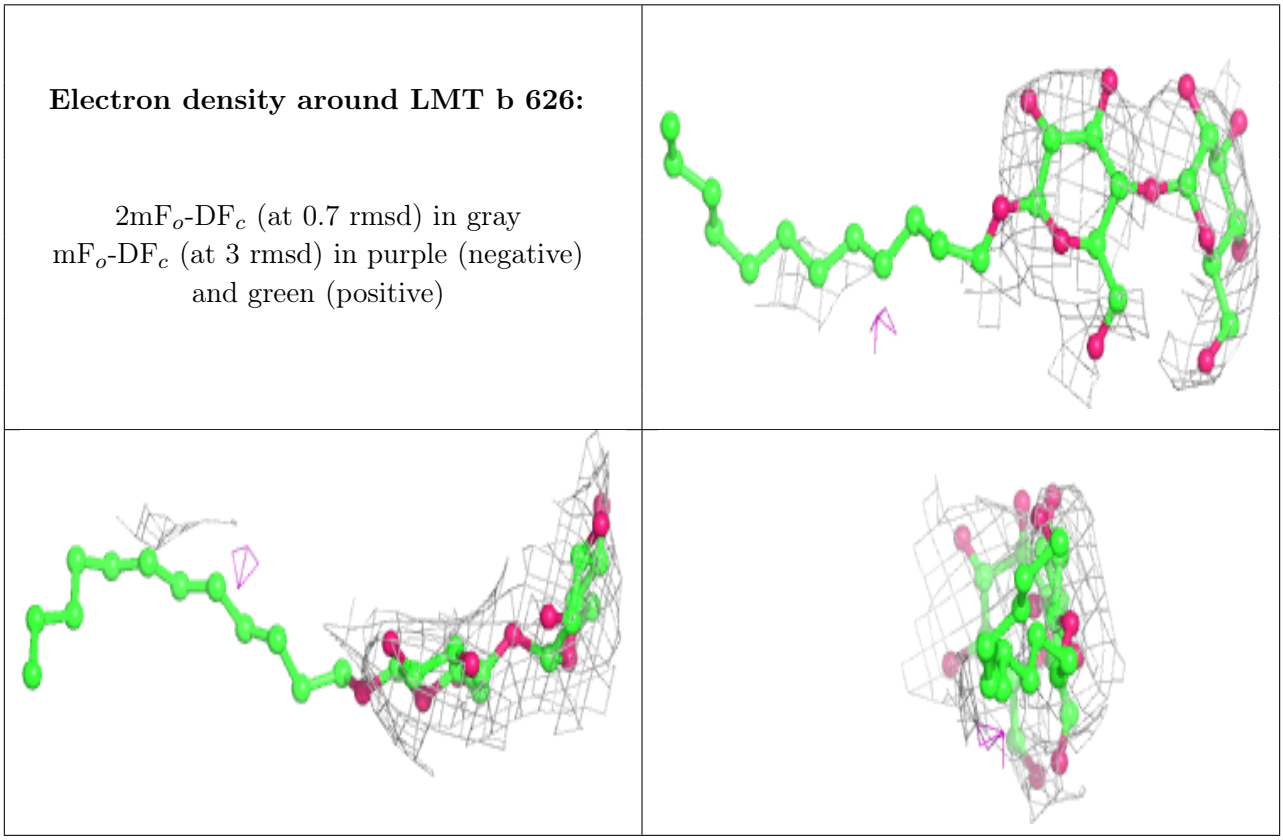
Electron density around LMT b 627:

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



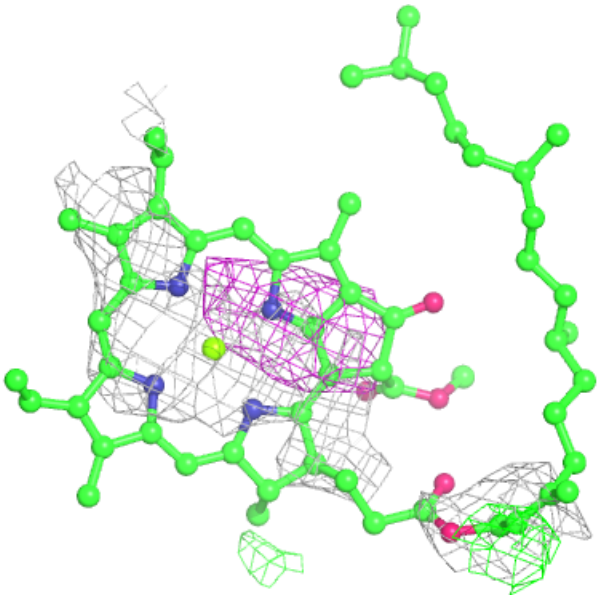
Electron density around LMT b 626:

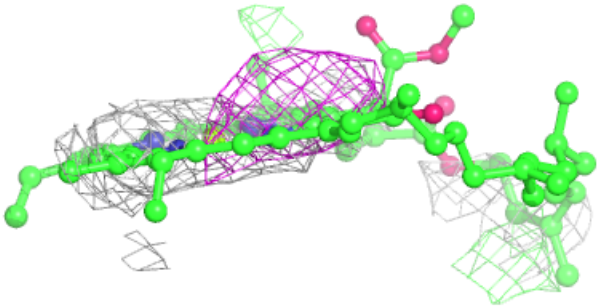
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

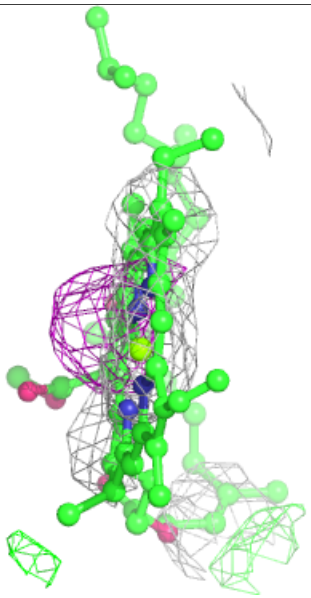


Electron density around CLA b 605:

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

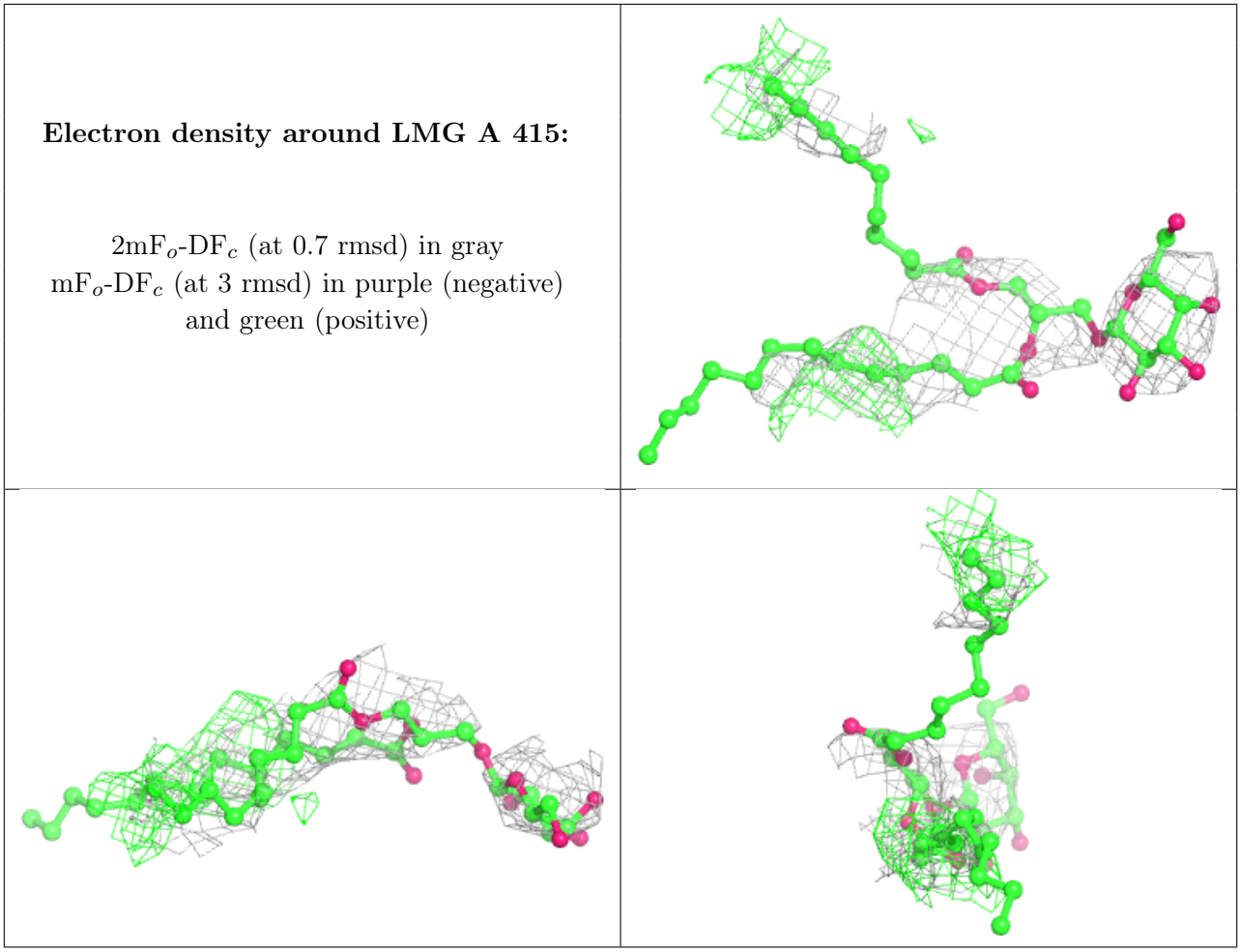






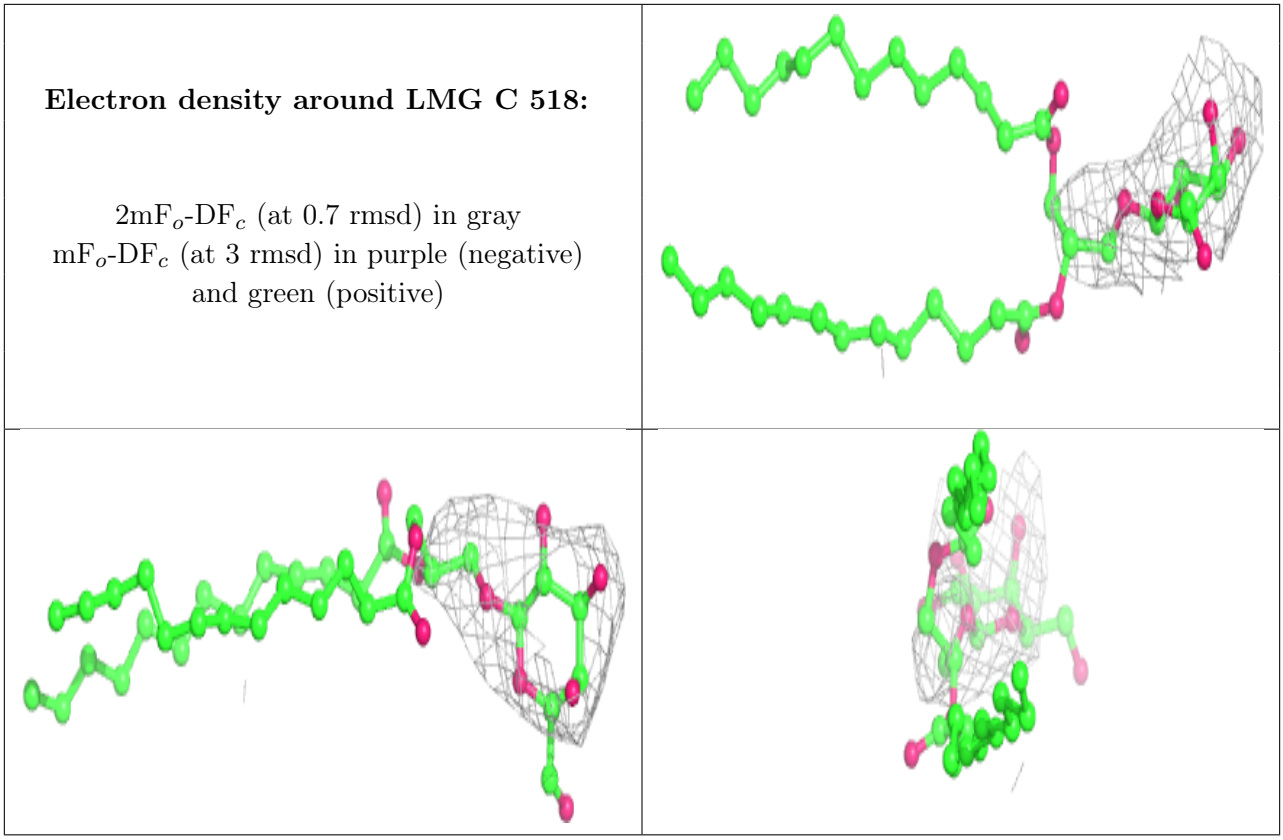
Electron density around LMG A 415:

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



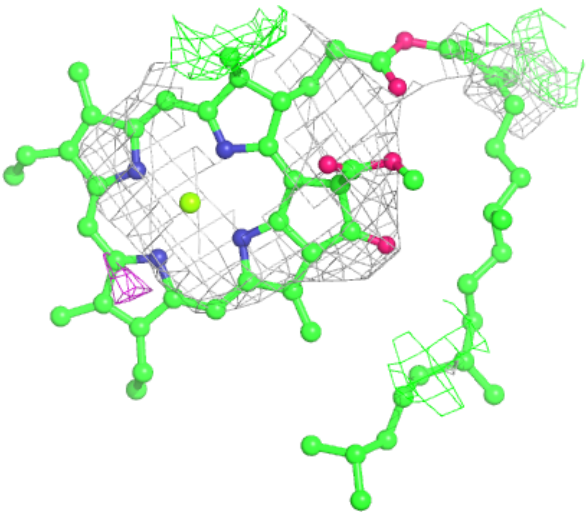
Electron density around LMG C 518:

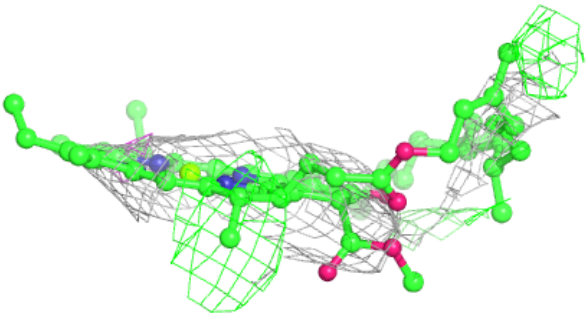
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

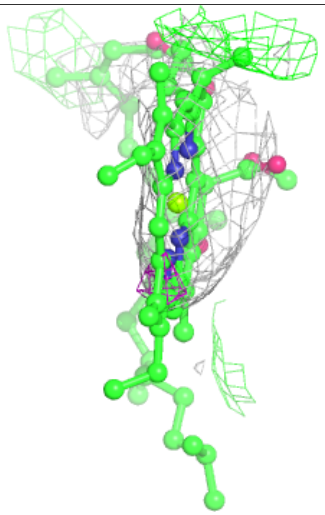


Electron density around CLA B 601:

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

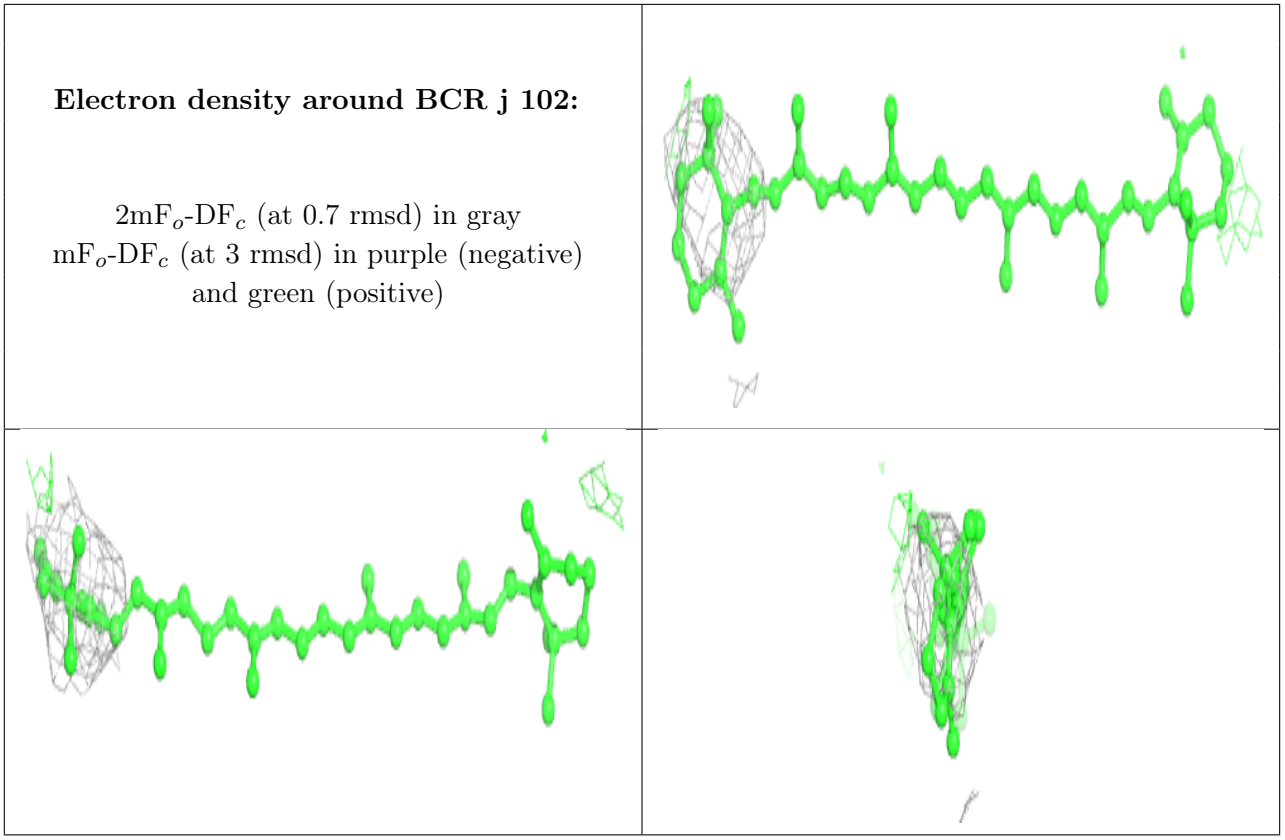






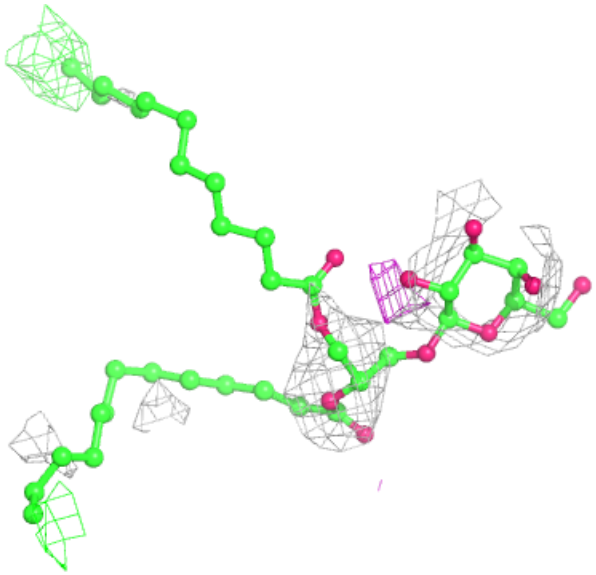
Electron density around BCR j 102:

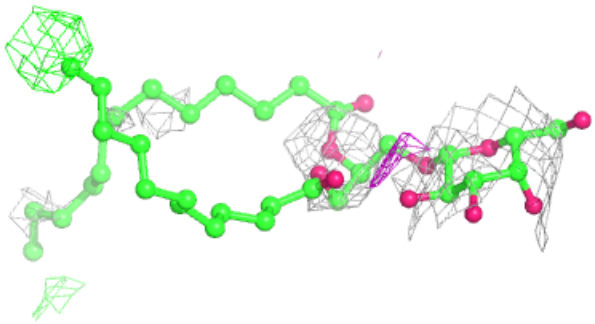
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG E 101:

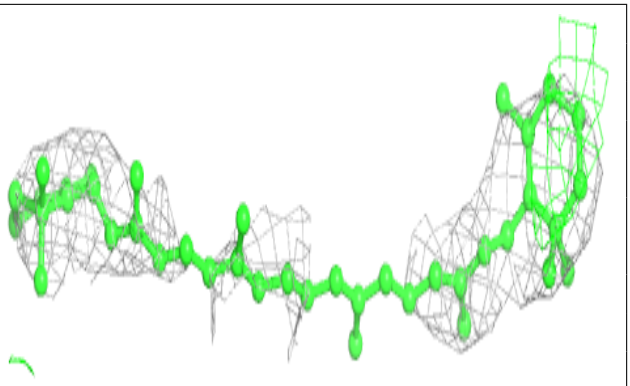
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

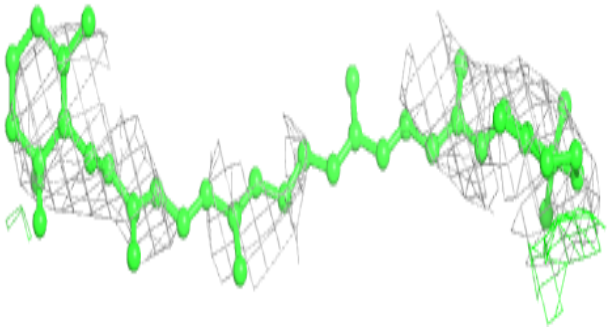


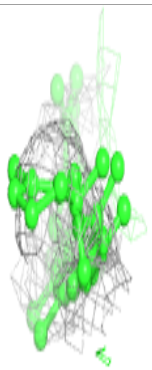


Electron density around BCR f 102:

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

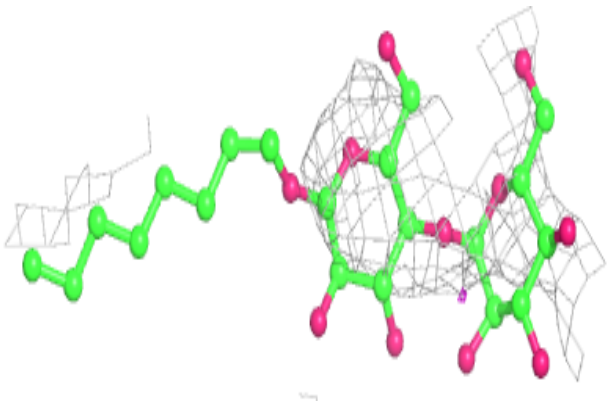


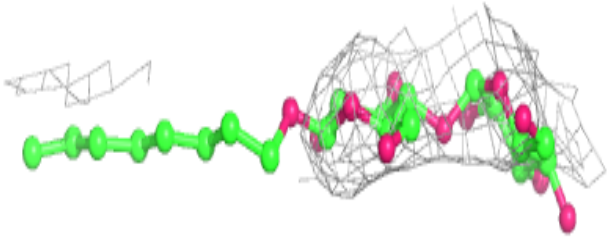


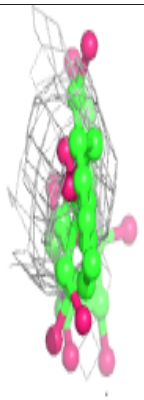


Electron density around LMT D 410:

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

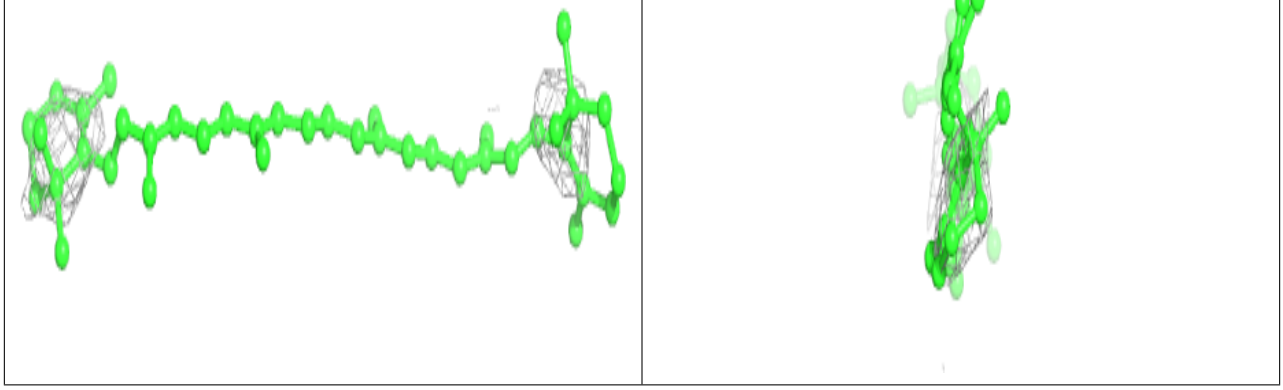






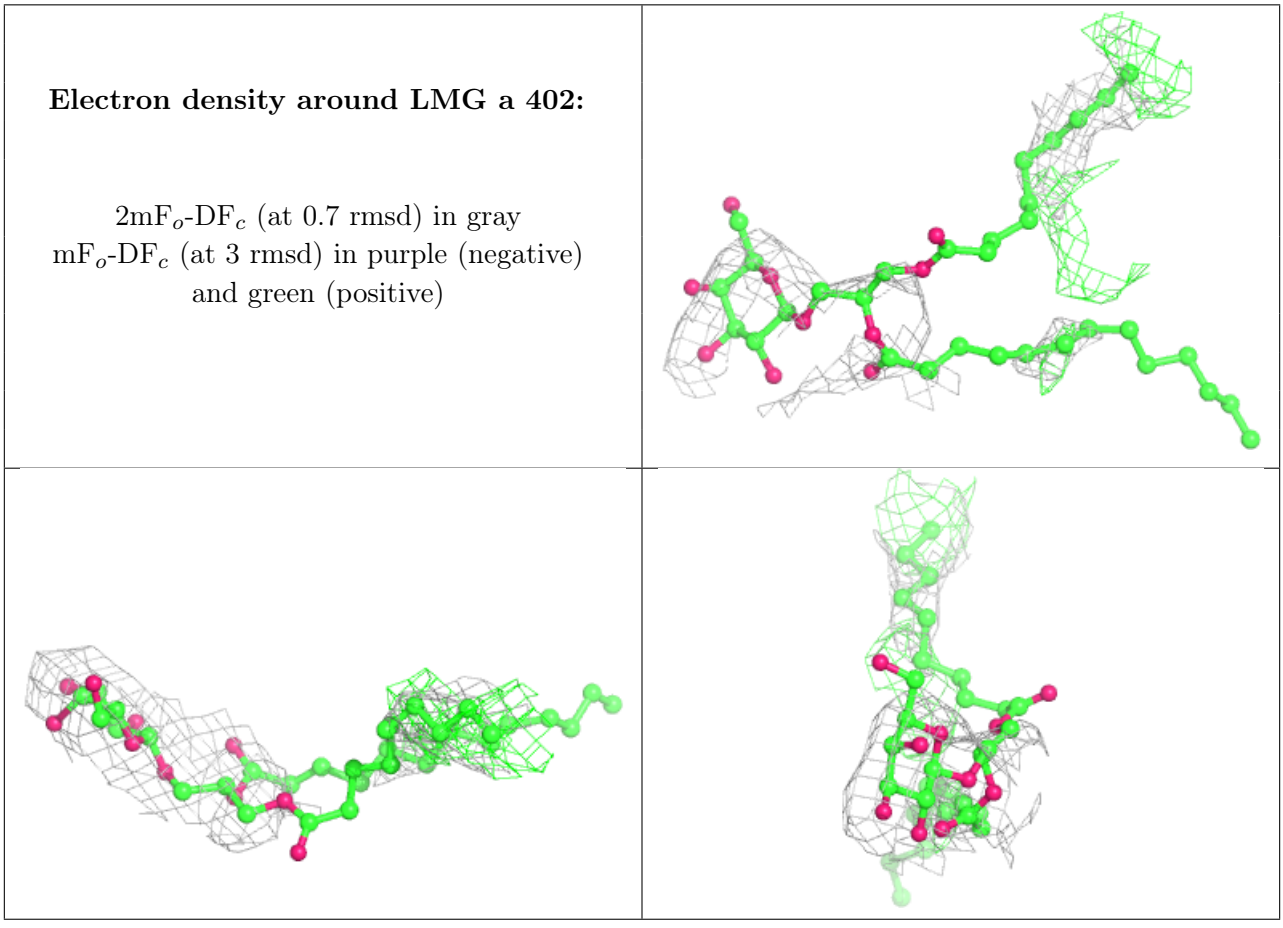
Electron density around BCR g 101:

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



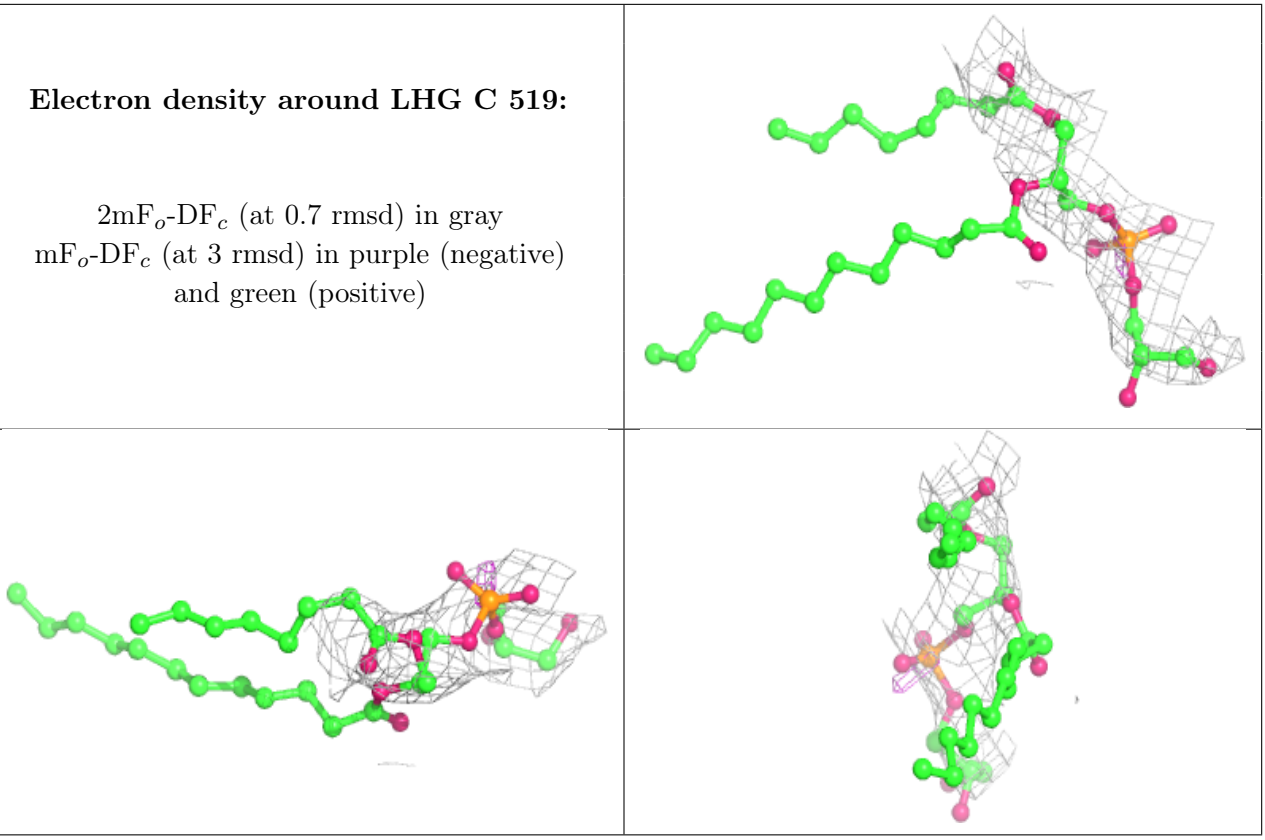
Electron density around LMG a 402:

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



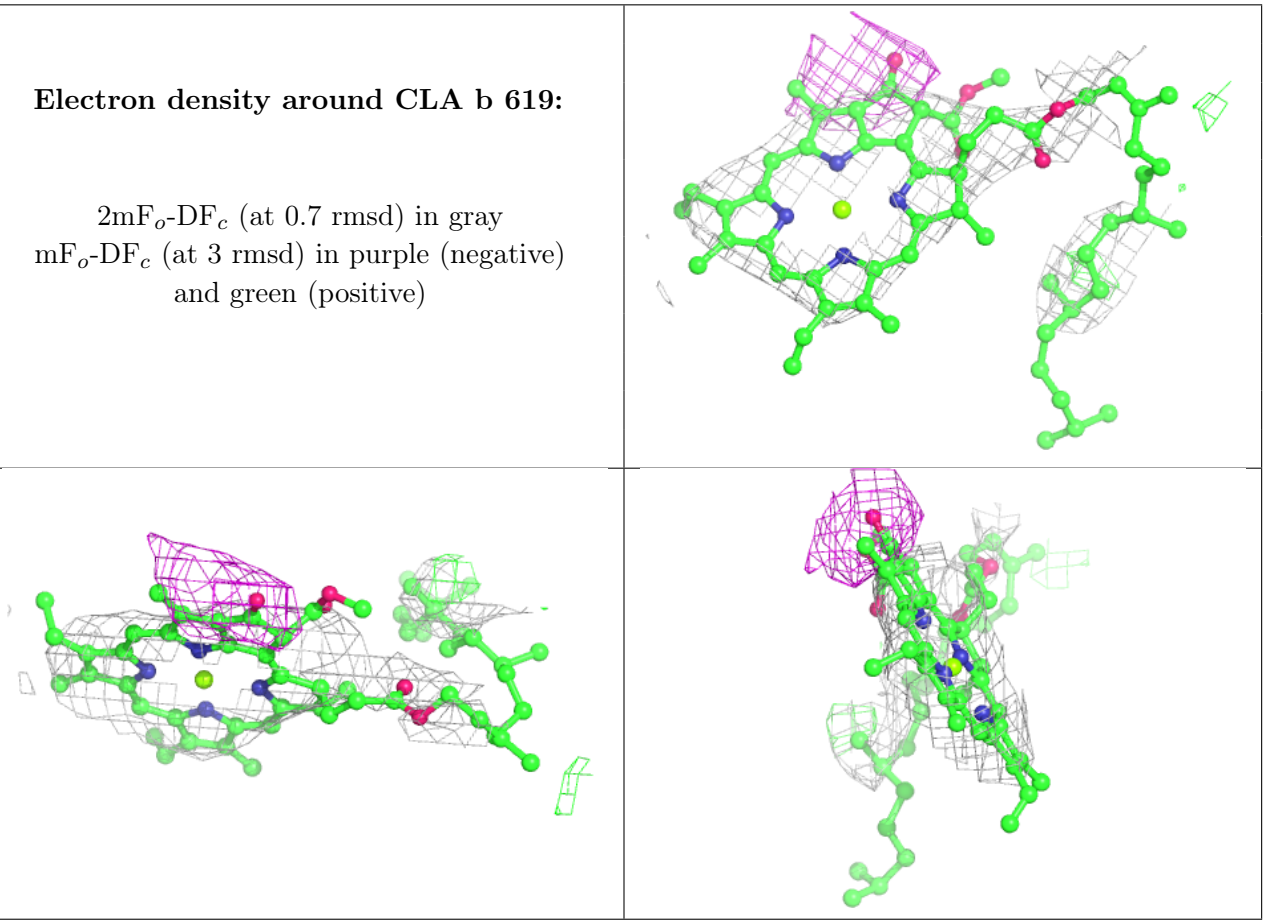
Electron density around LHG C 519:

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



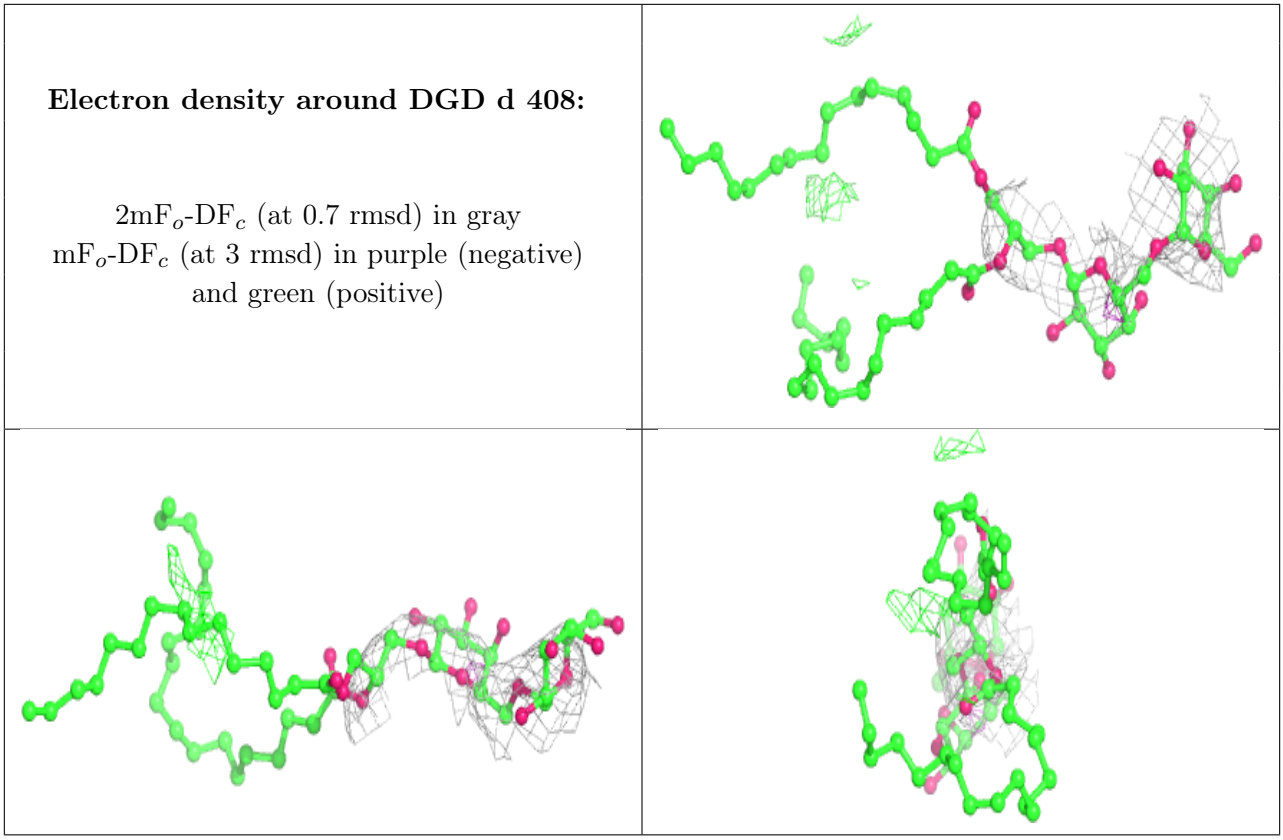
Electron density around CLA b 619:

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



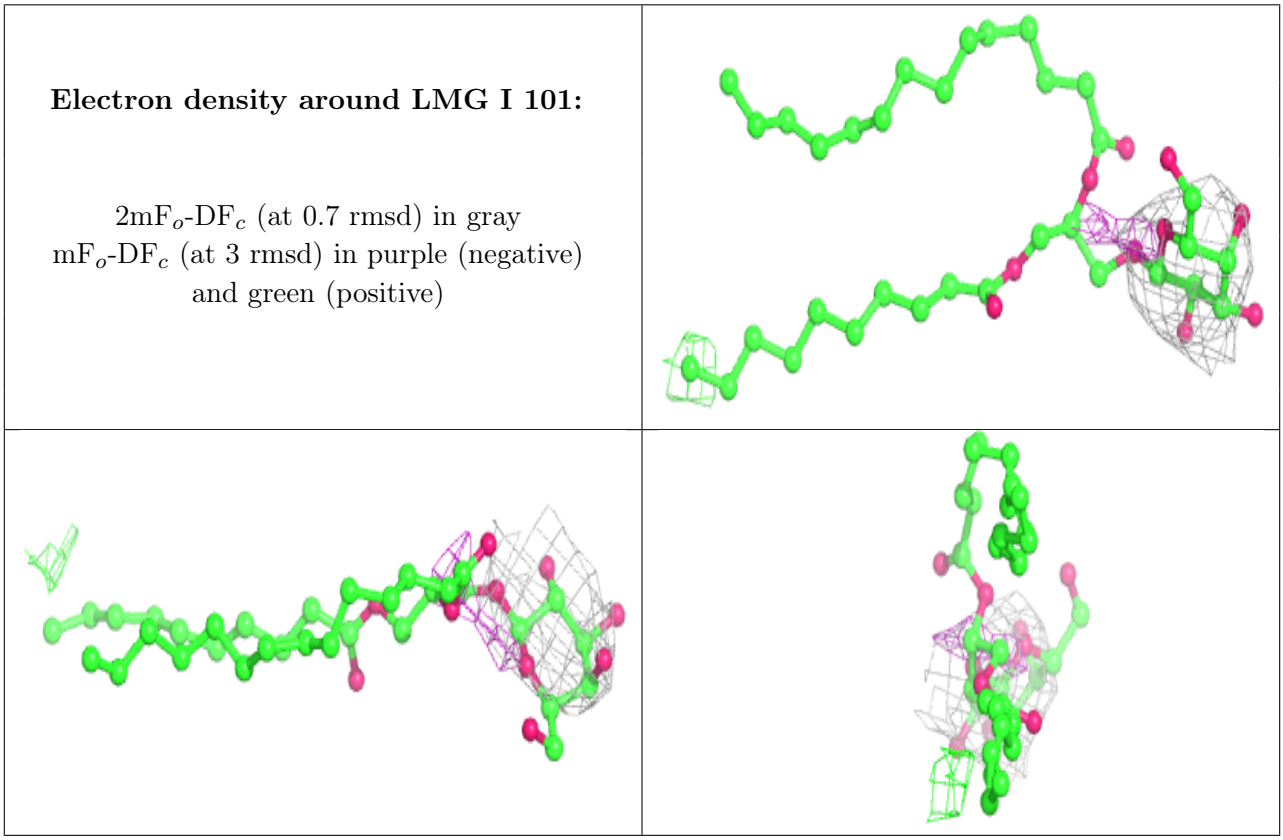
Electron density around DGD d 408:

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



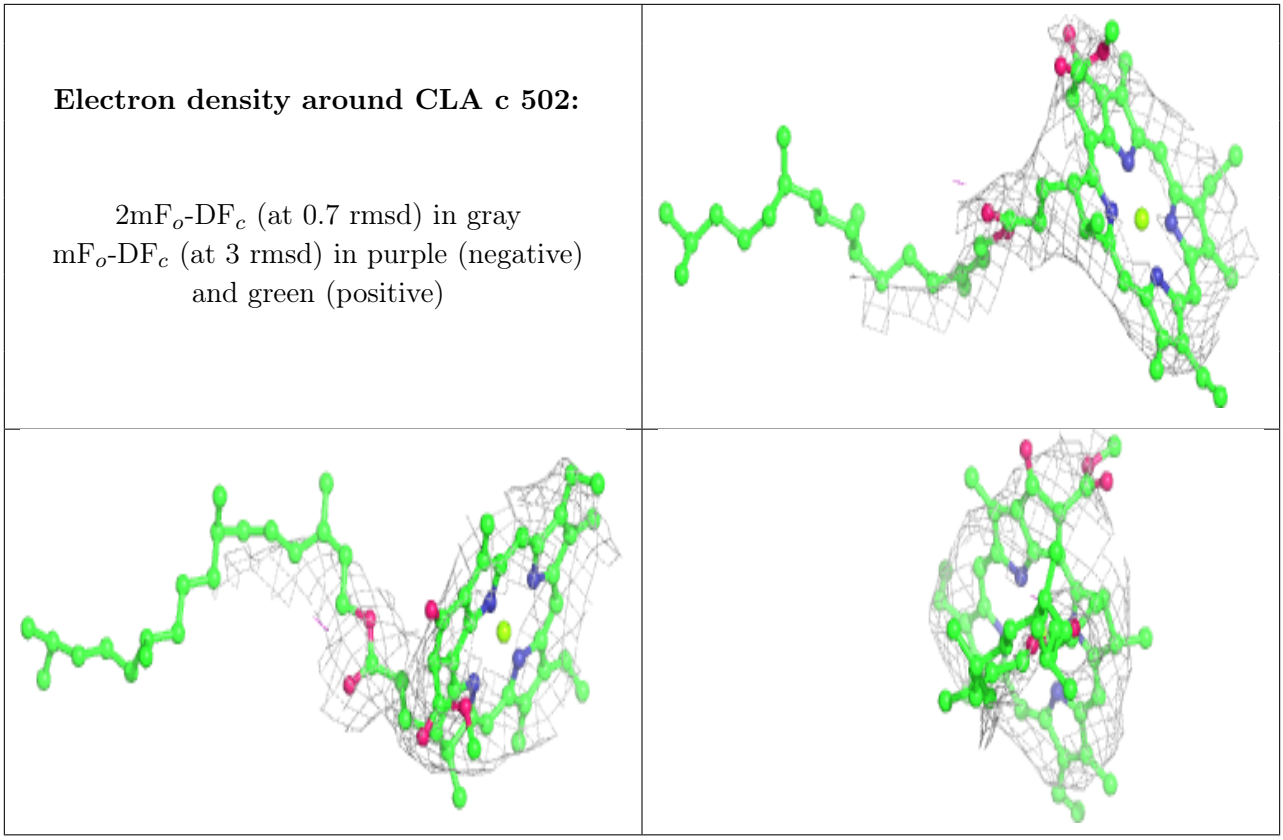
Electron density around LMG I 101:

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



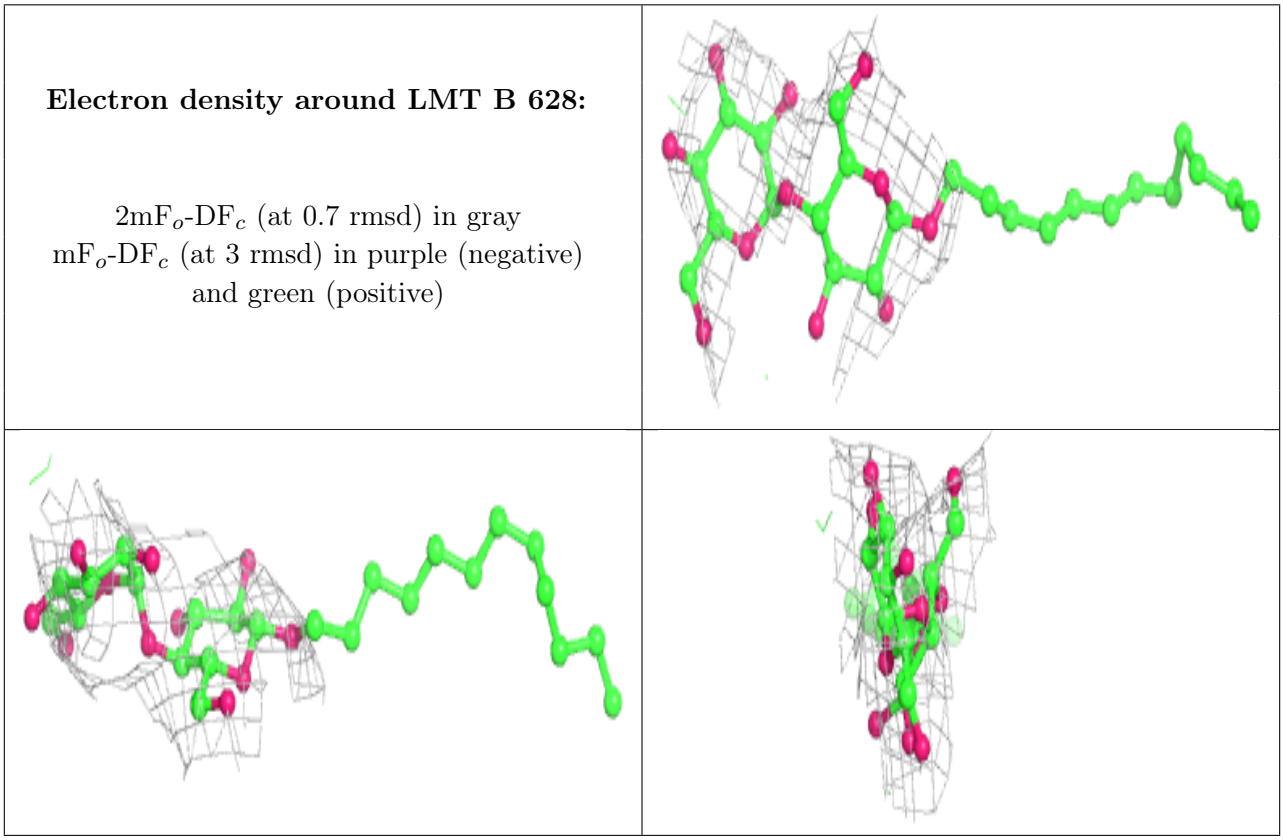
Electron density around CLA c 502:

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



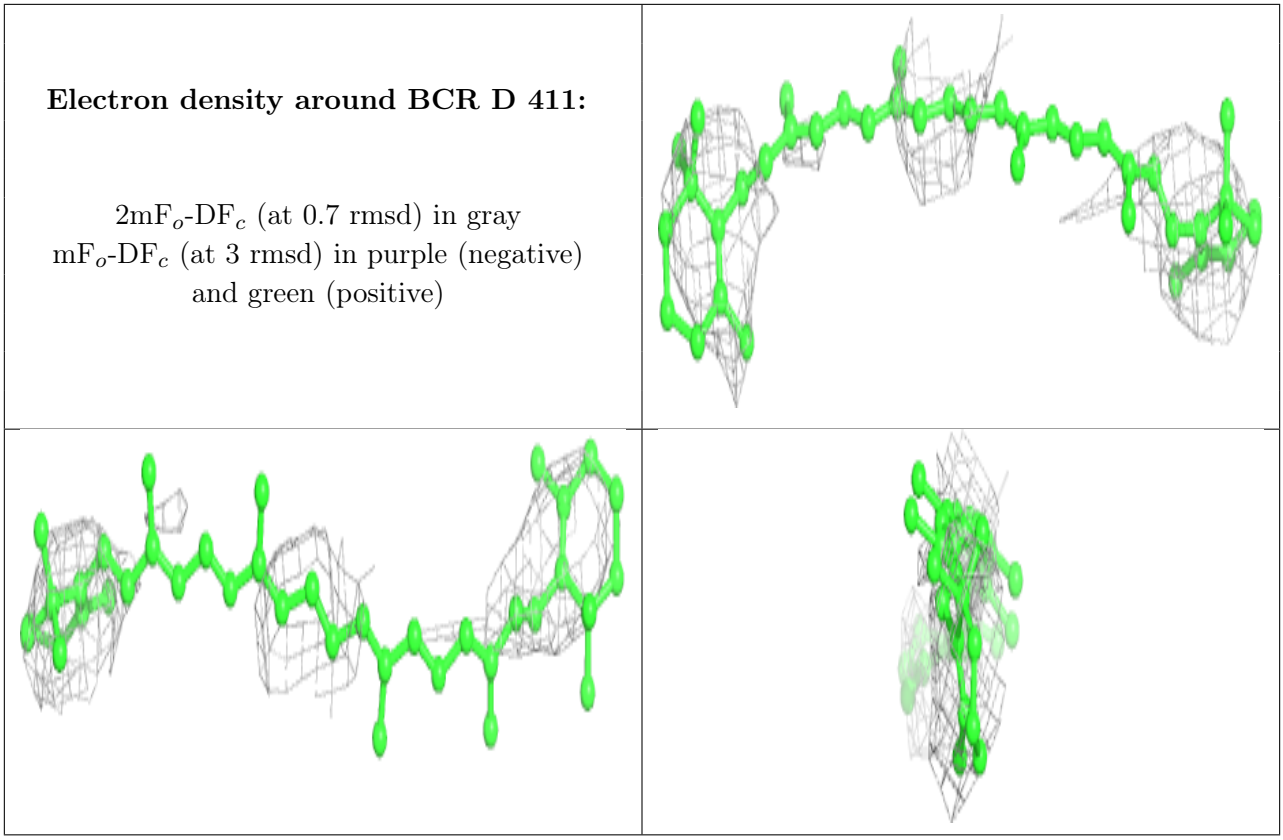
Electron density around LMT B 628:

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



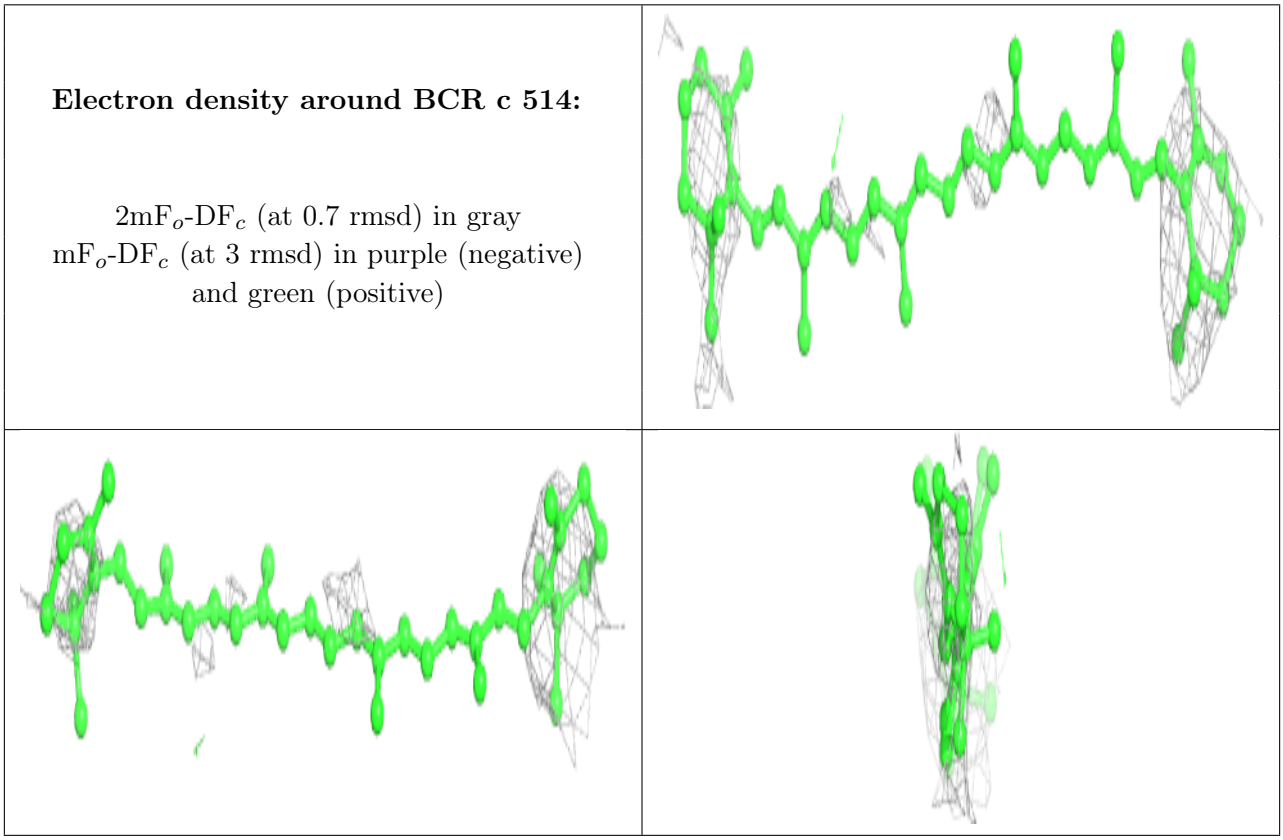
Electron density around BCR D 411:

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



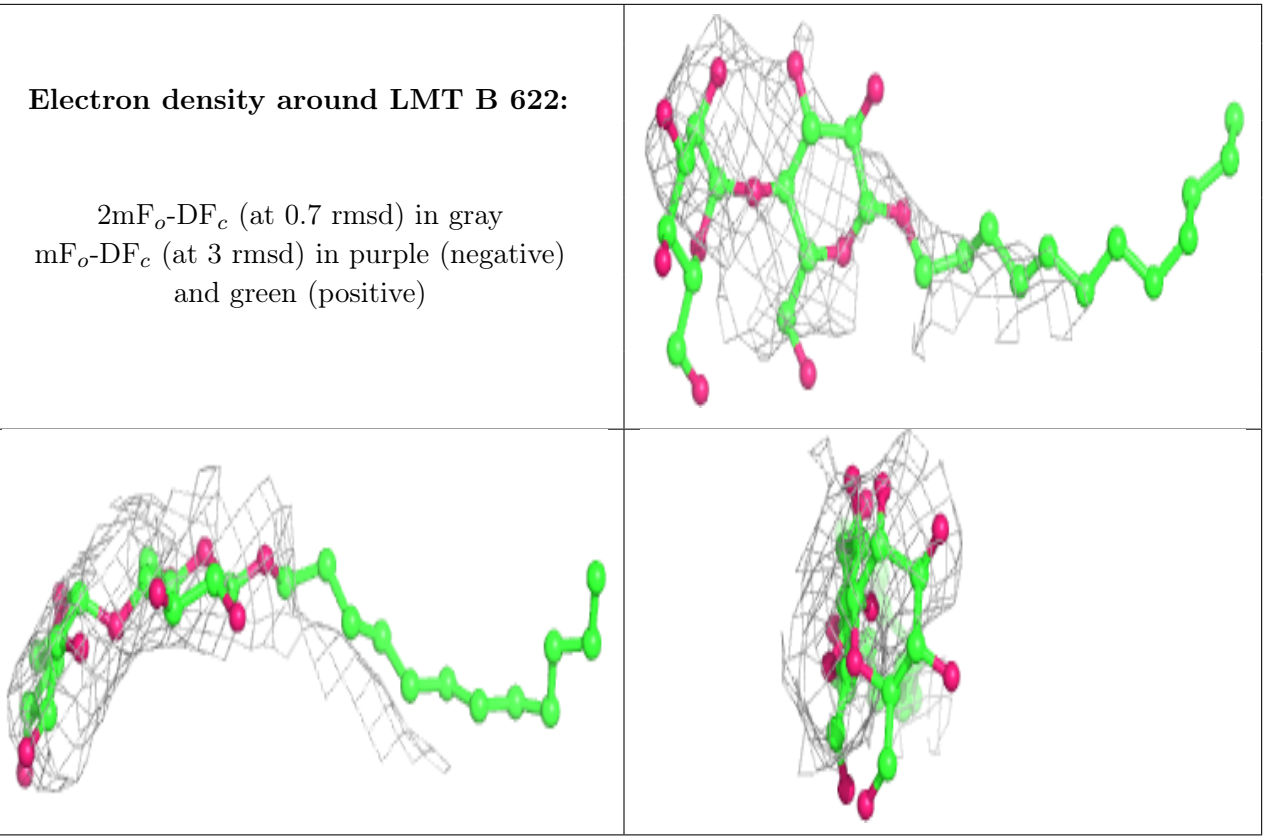
Electron density around BCR c 514:

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



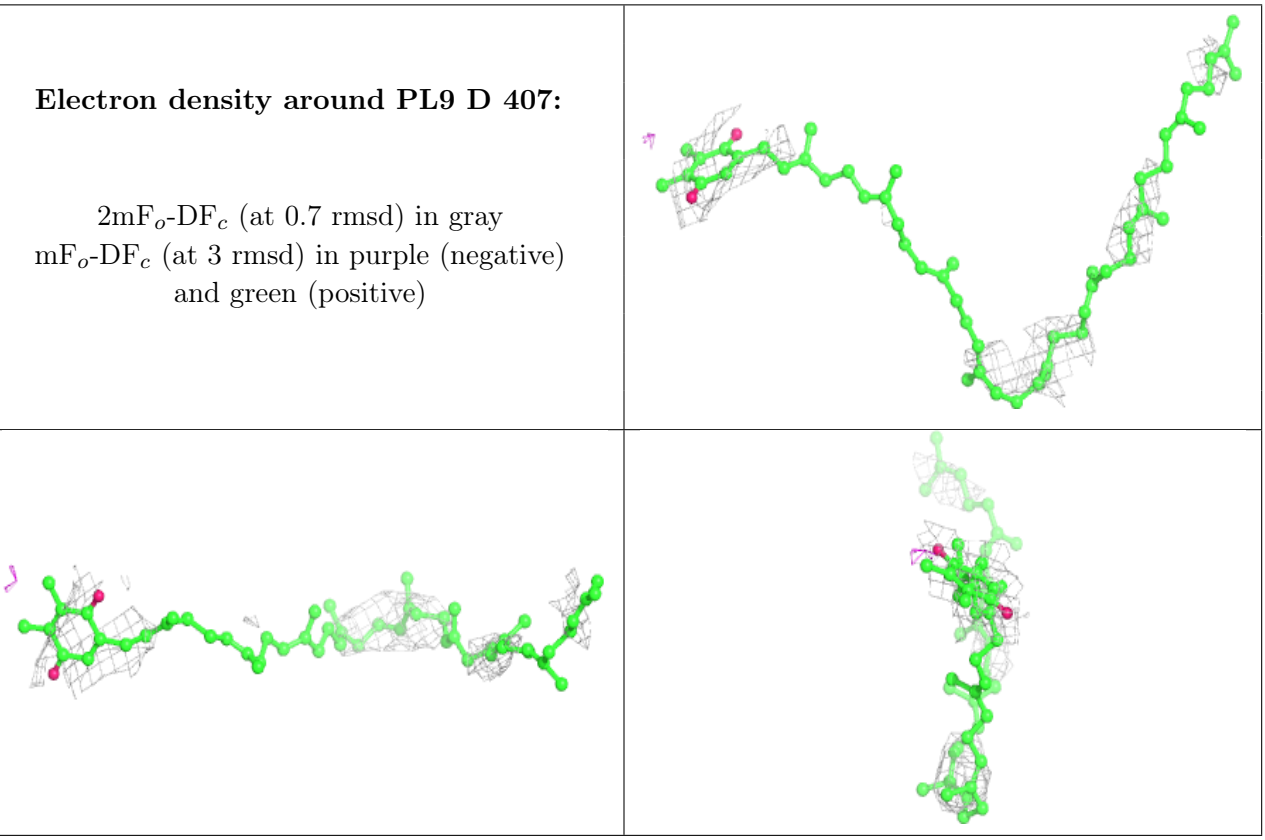
Electron density around LMT B 622:

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



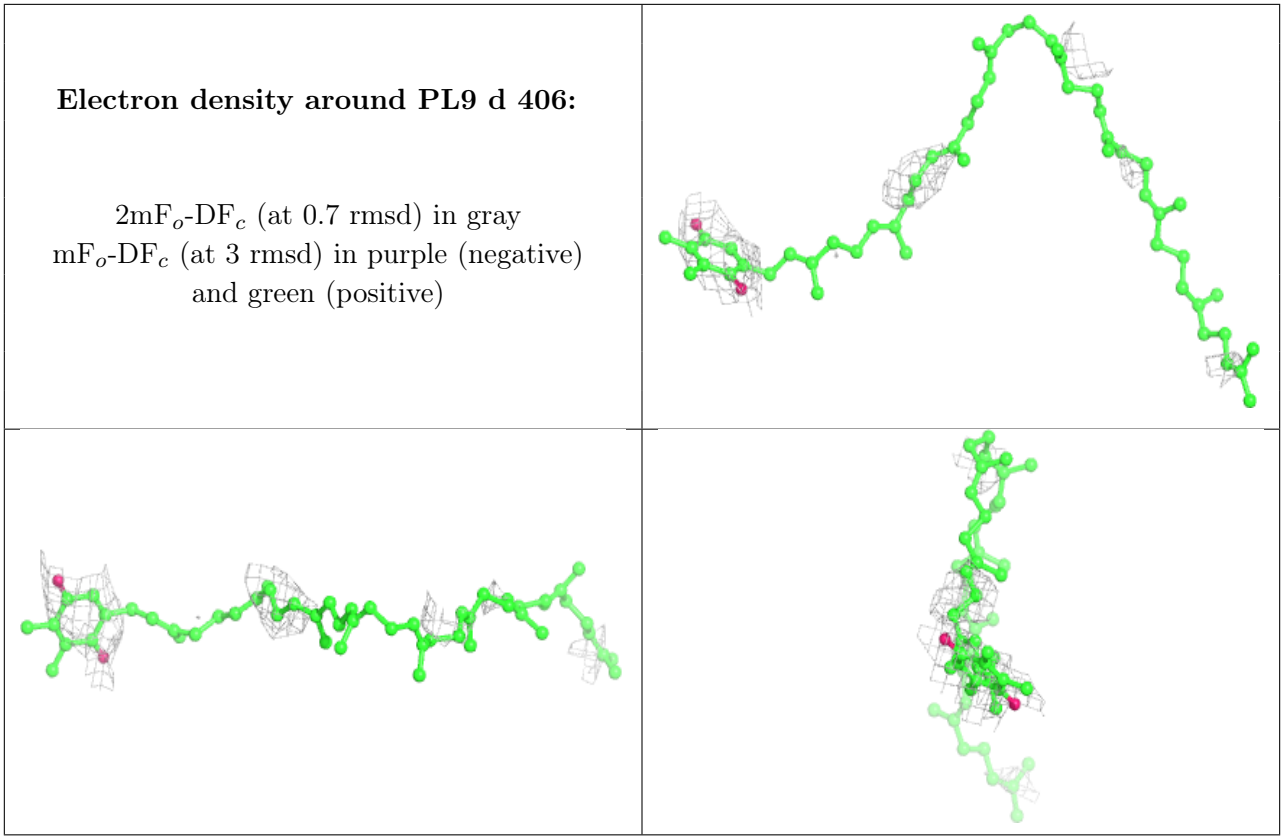
Electron density around PL9 D 407:

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



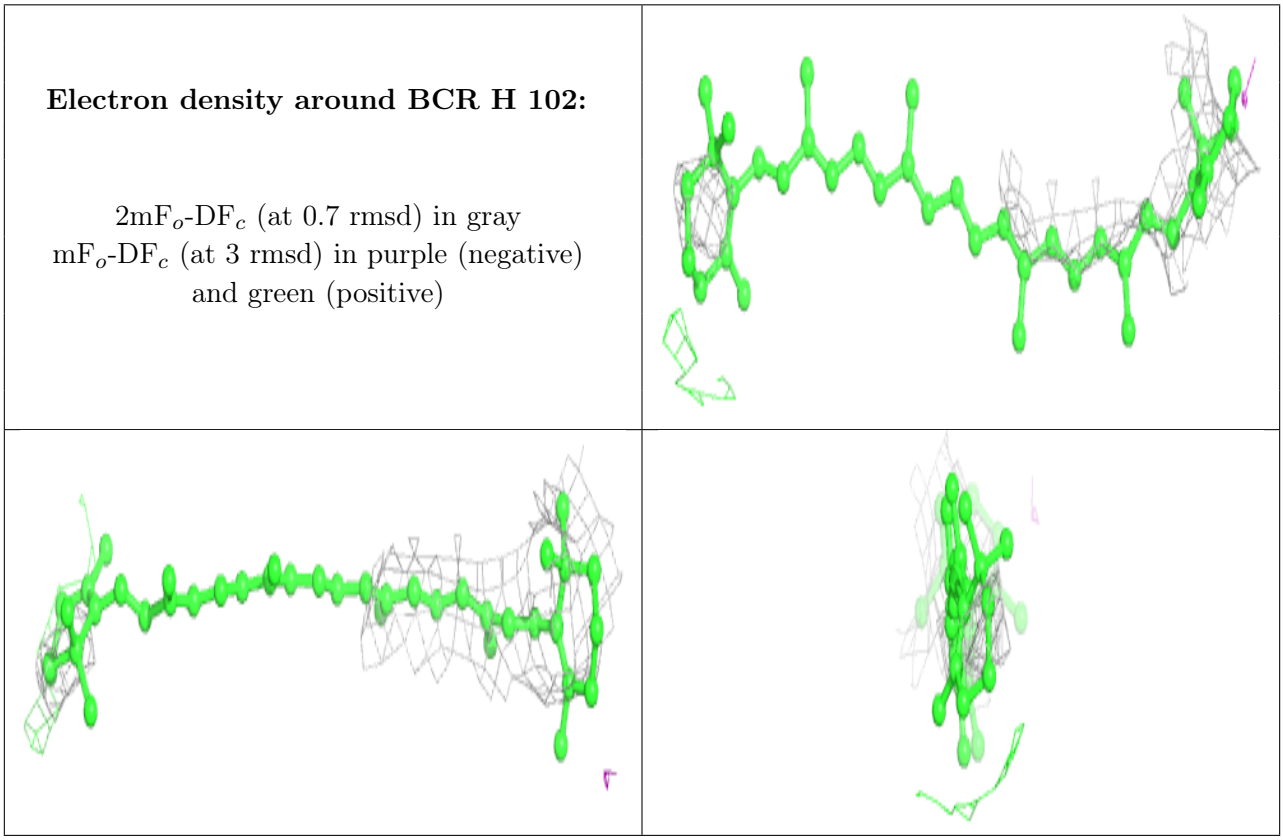
Electron density around PL9 d 406:

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



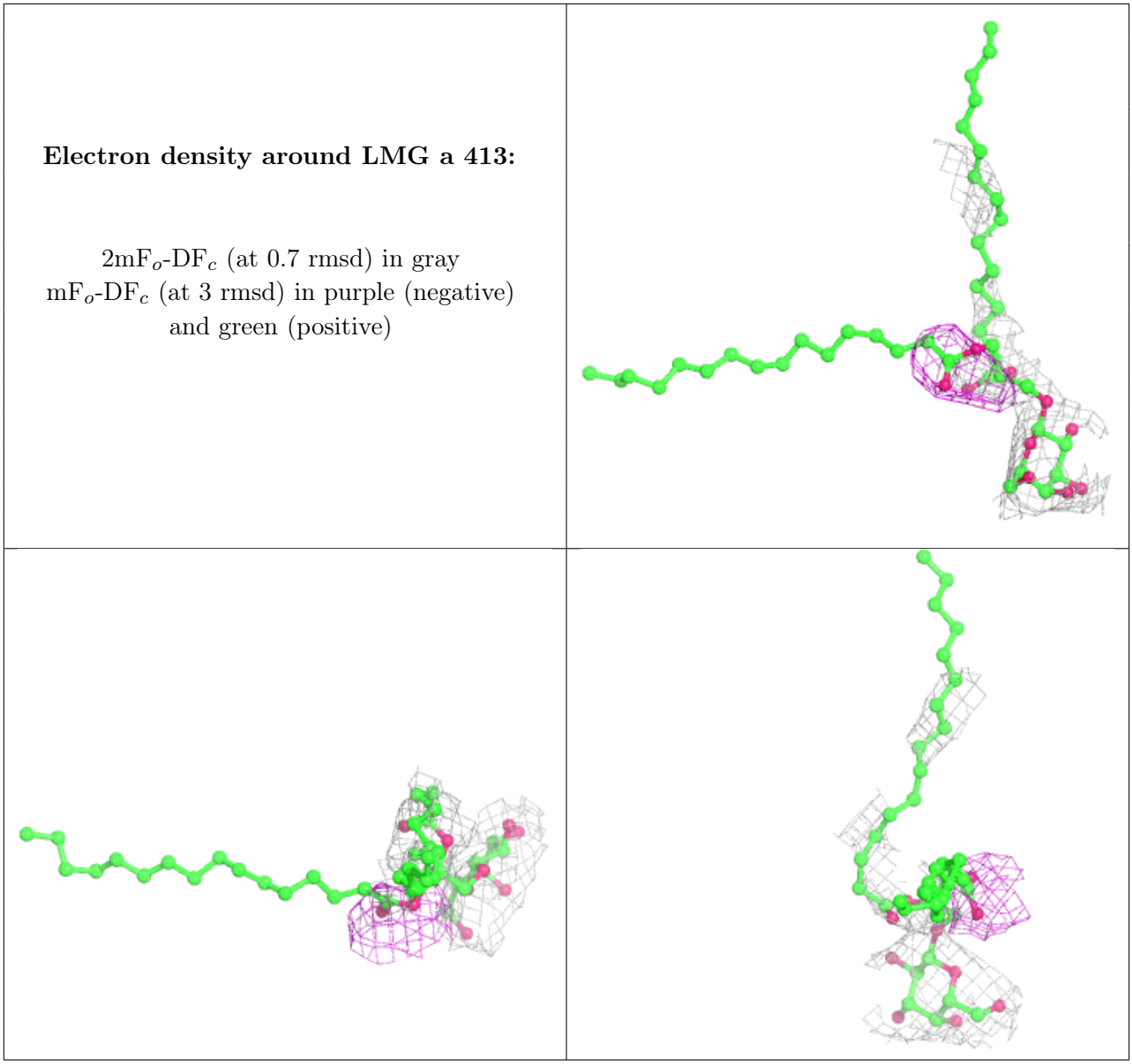
Electron density around BCR H 102:

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



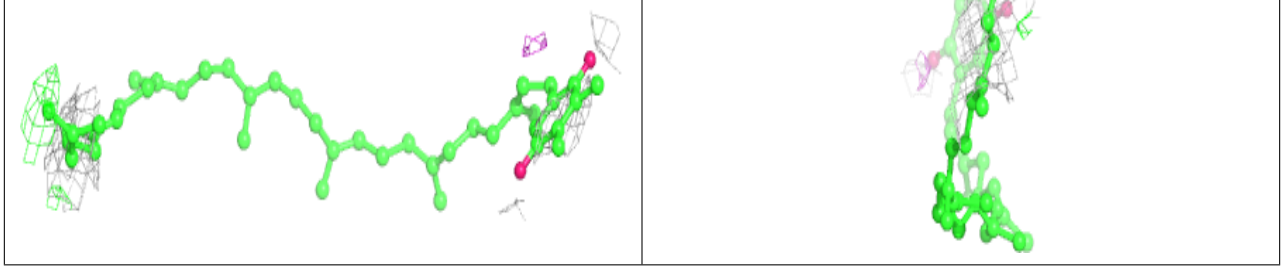
Electron density around LMG a 413:

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



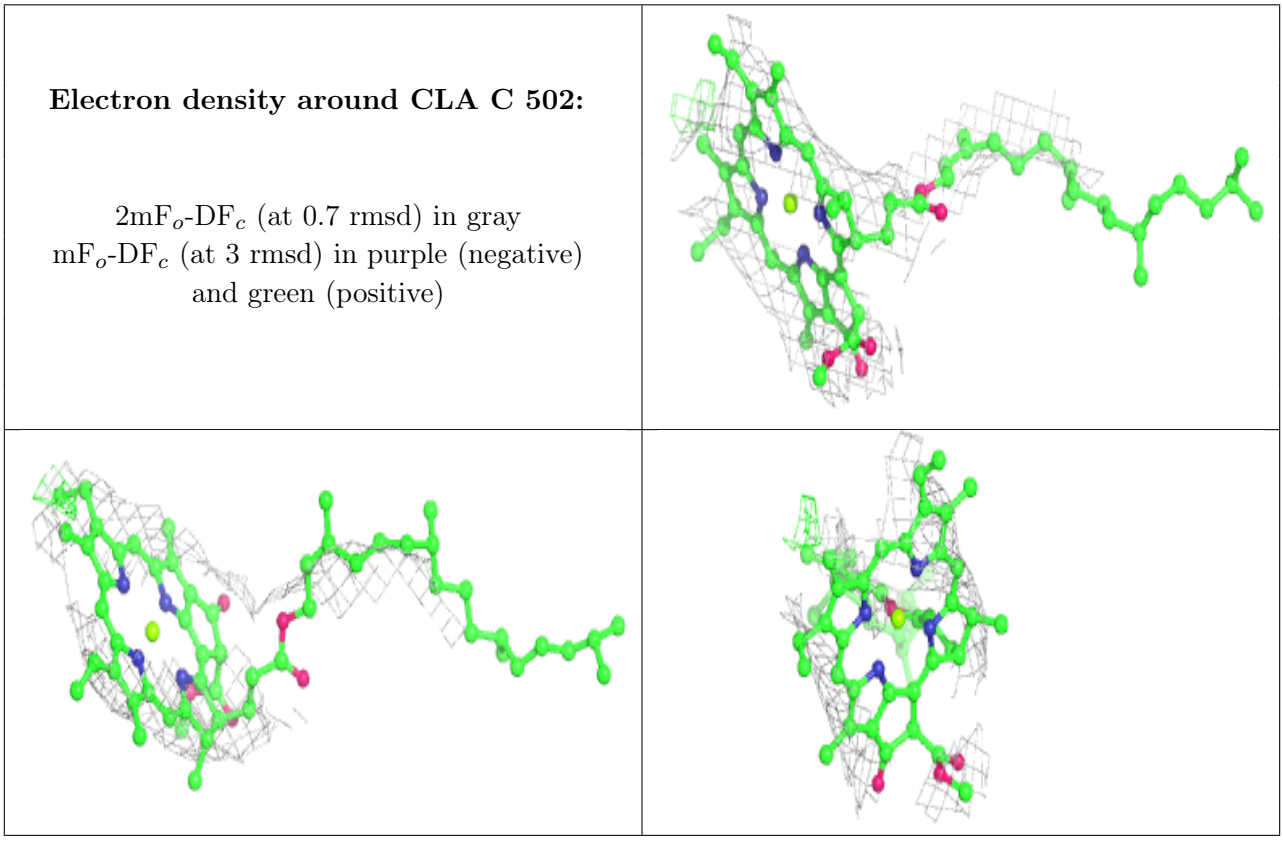
Electron density around PL9 A 406:

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



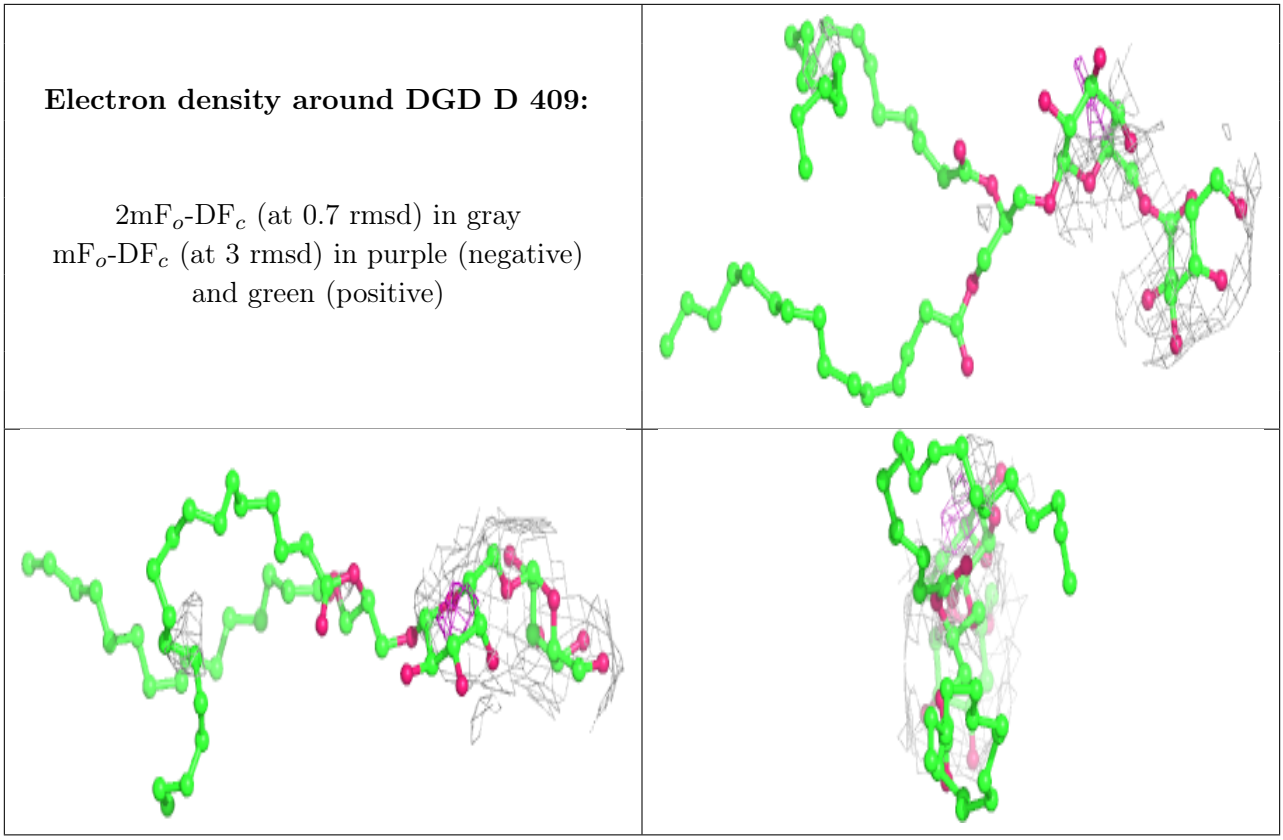
Electron density around CLA C 502:

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



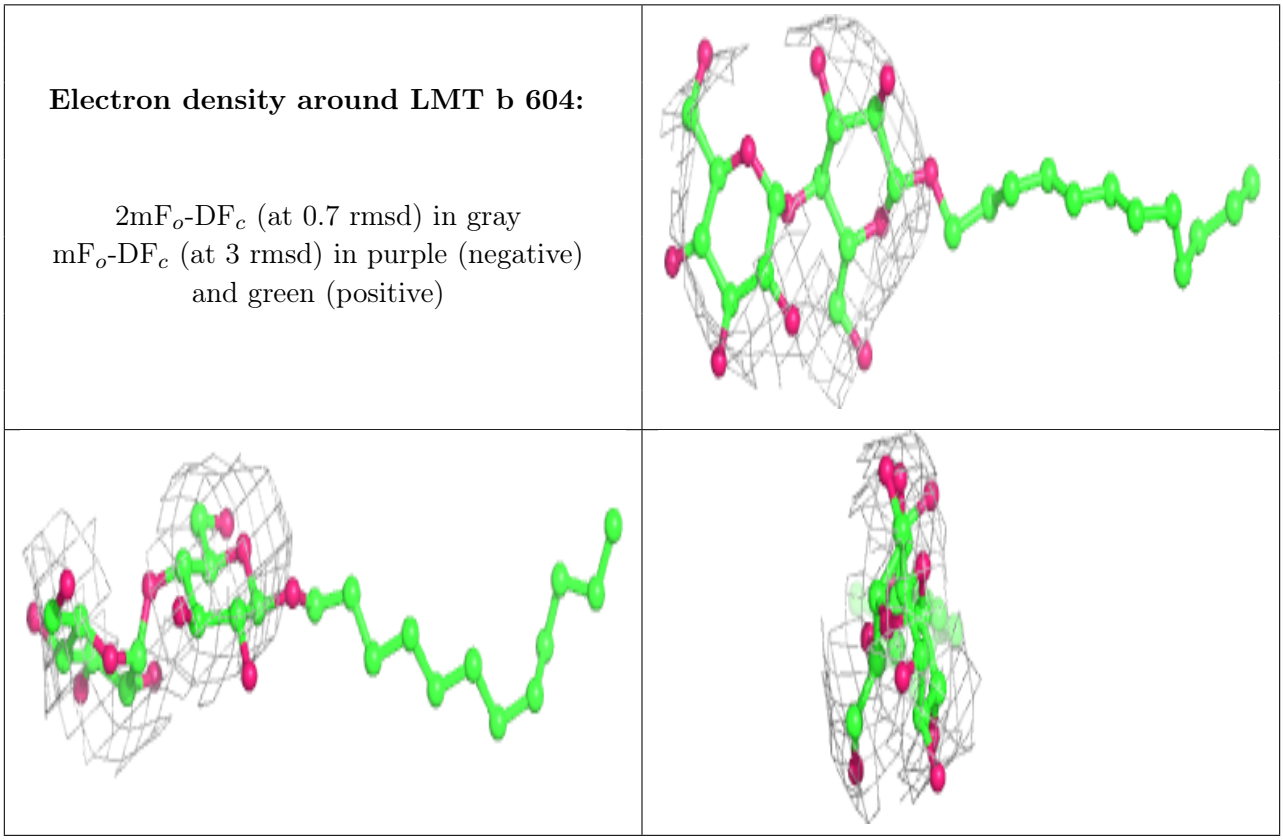
Electron density around DGD D 409:

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



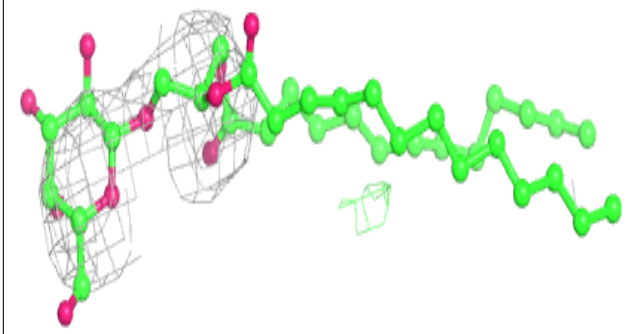
Electron density around LMT b 604:

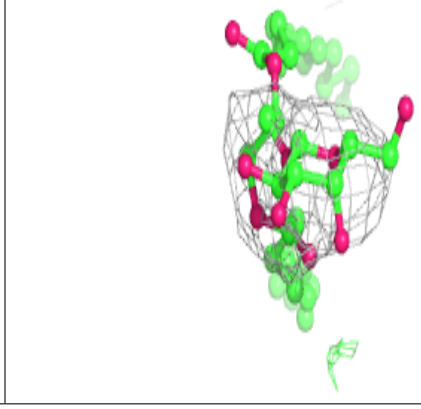
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG c 518:

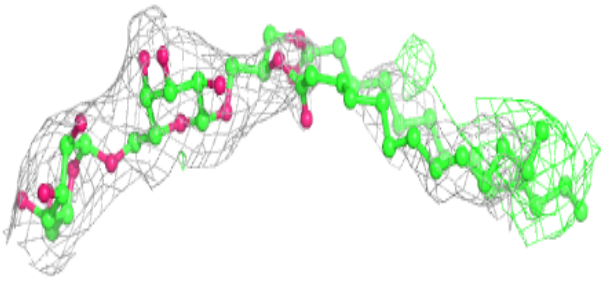
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

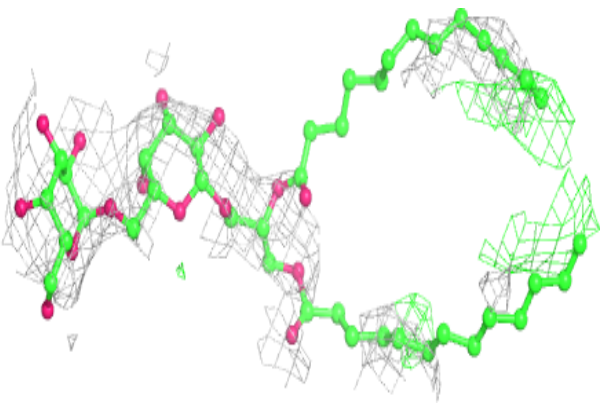


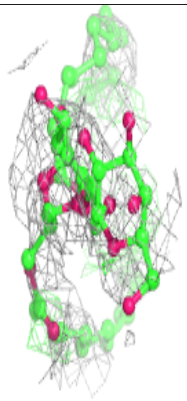


Electron density around DGD A 408:

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

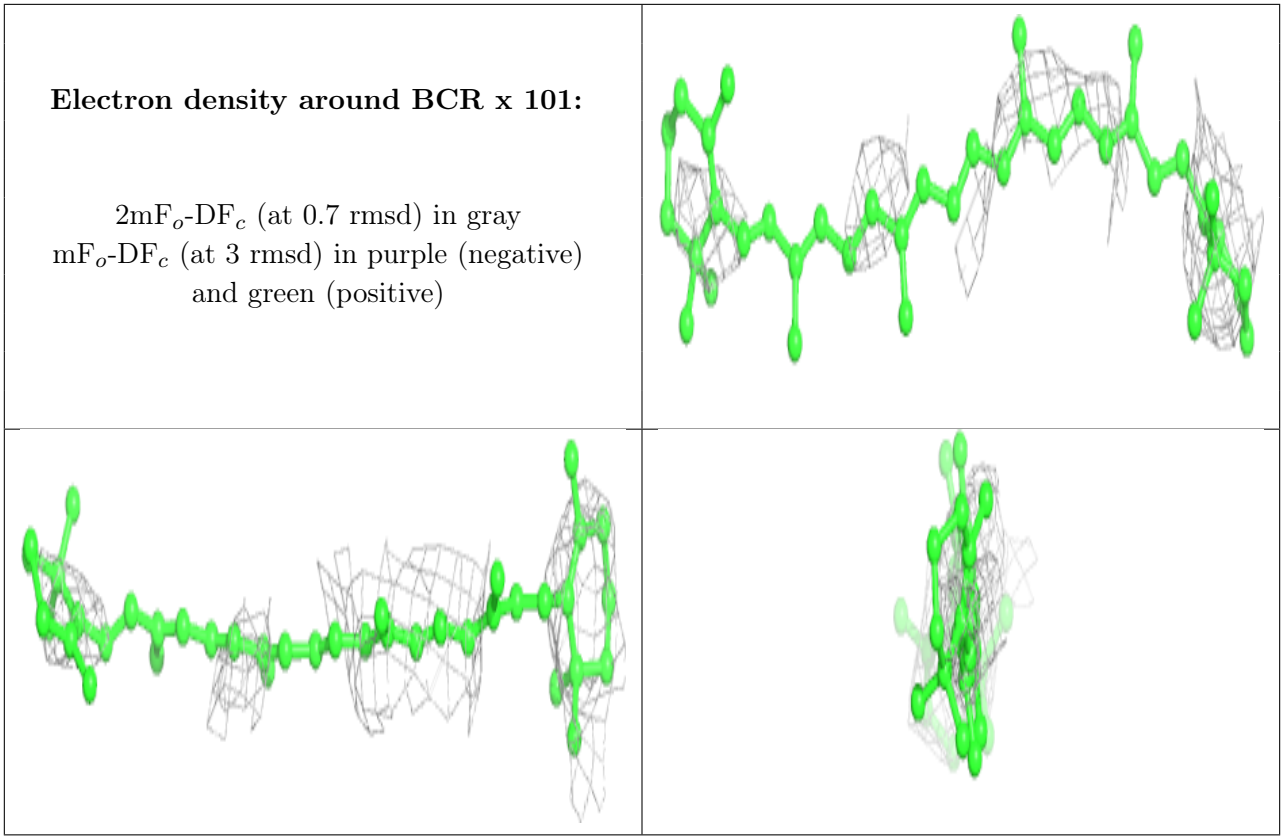






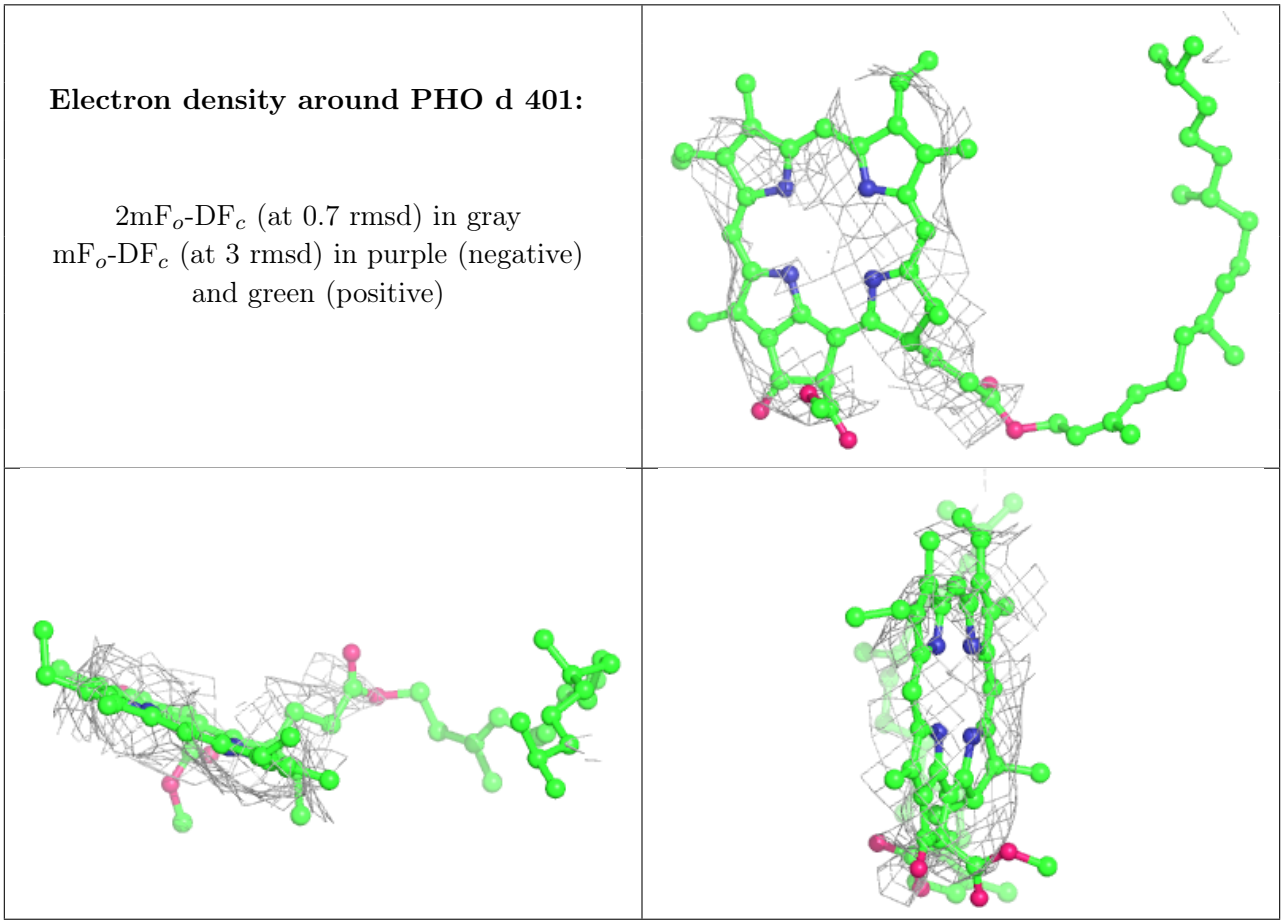
Electron density around BCR x 101:

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



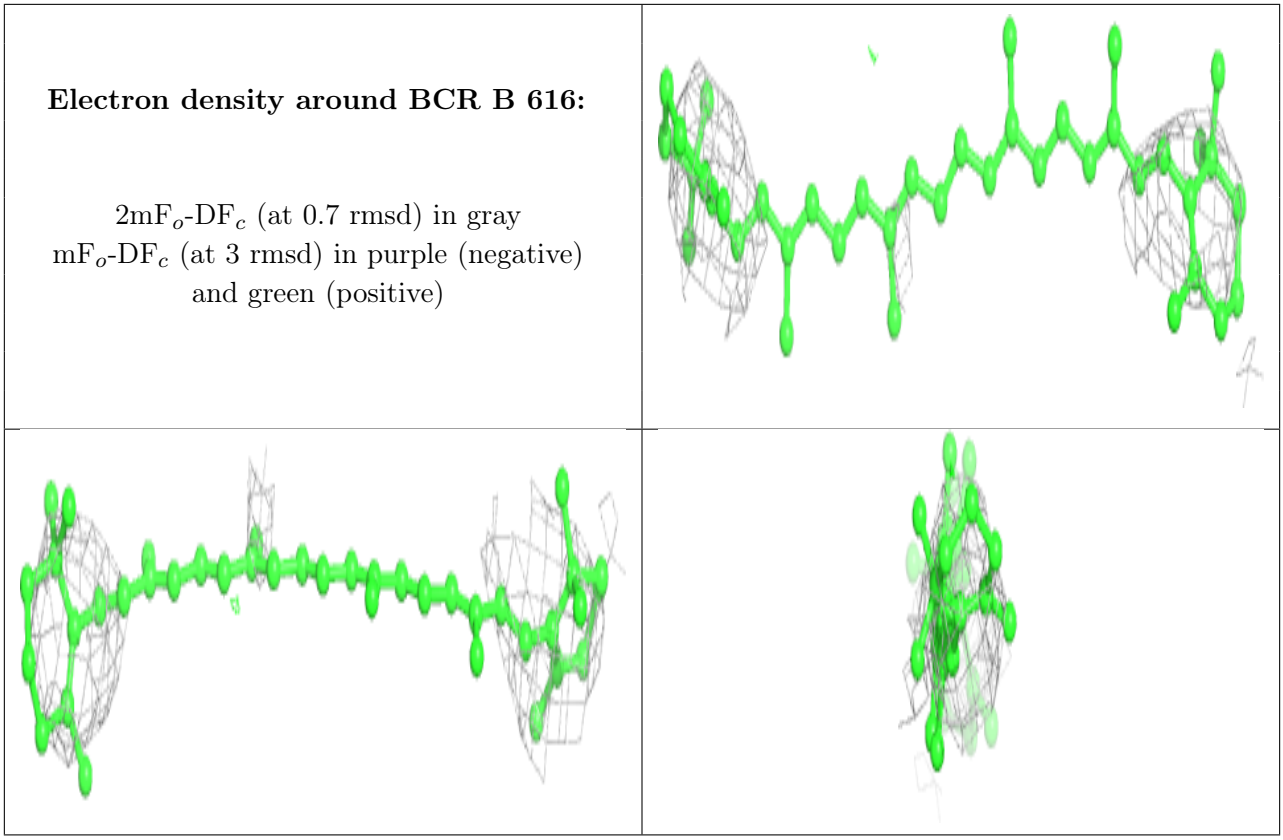
Electron density around PHO d 401:

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



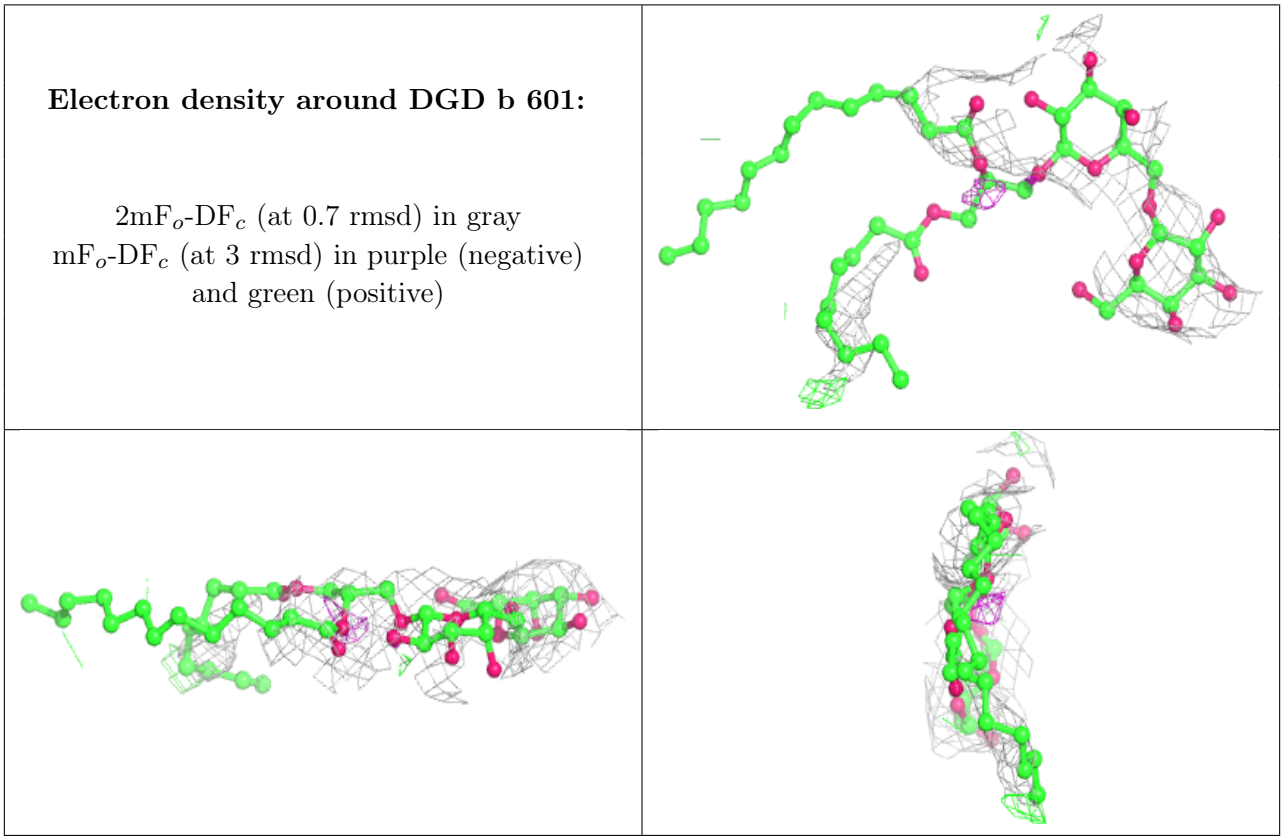
Electron density around BCR B 616:

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



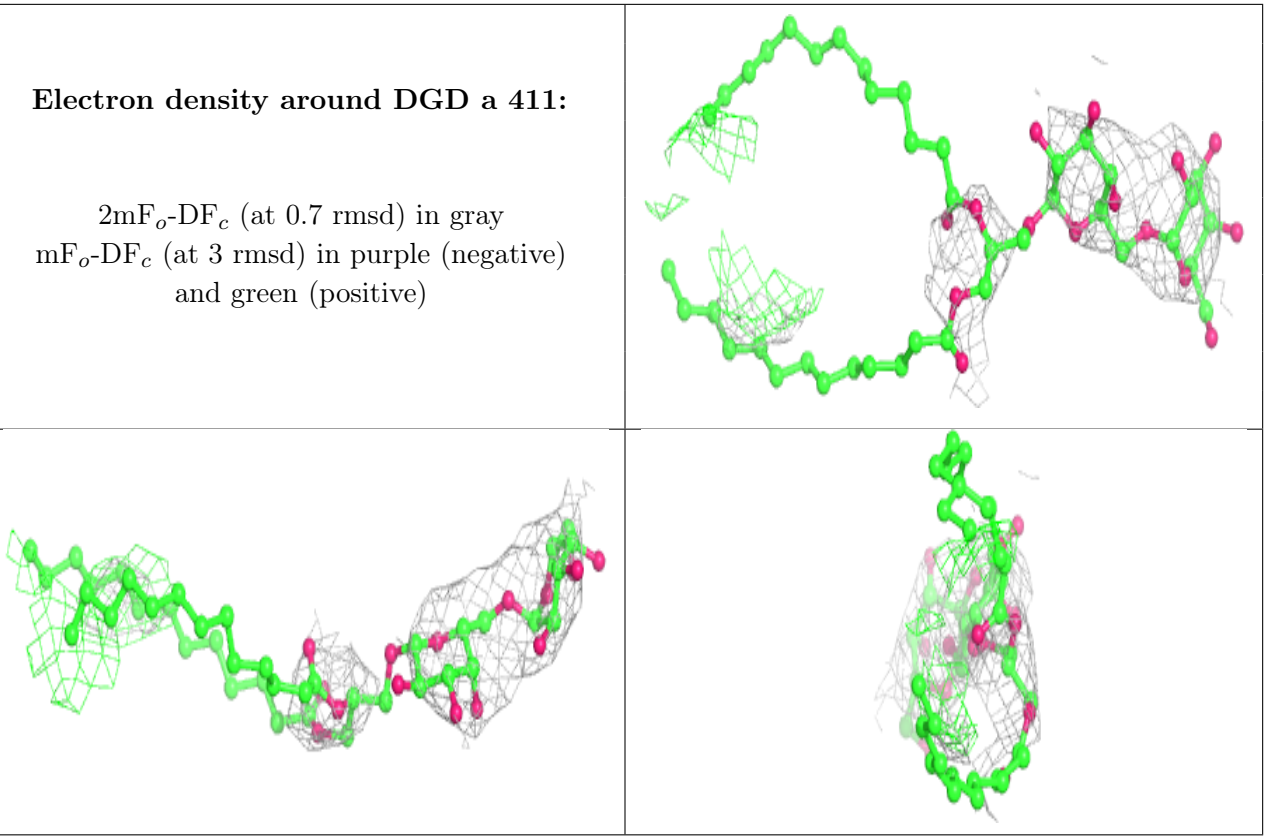
Electron density around DGD b 601:

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



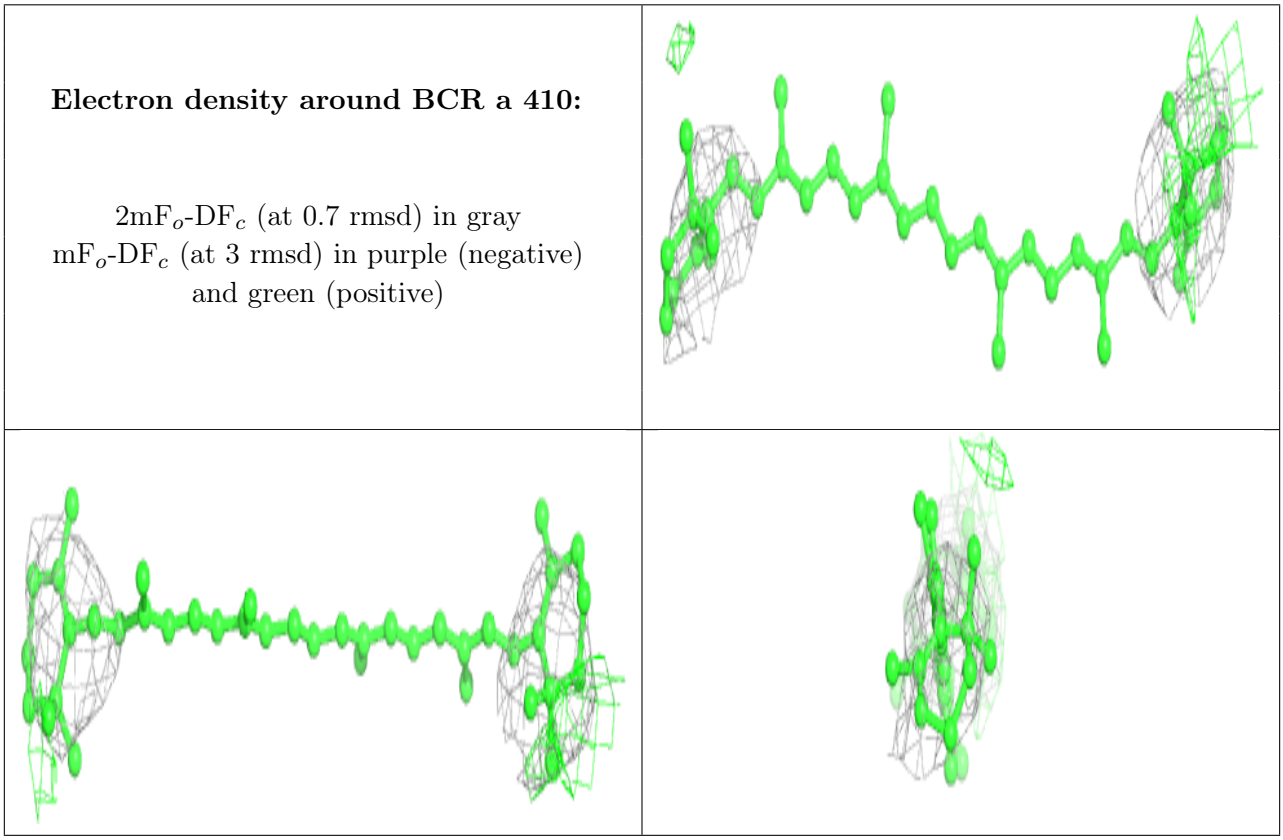
Electron density around DGD a 411:

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



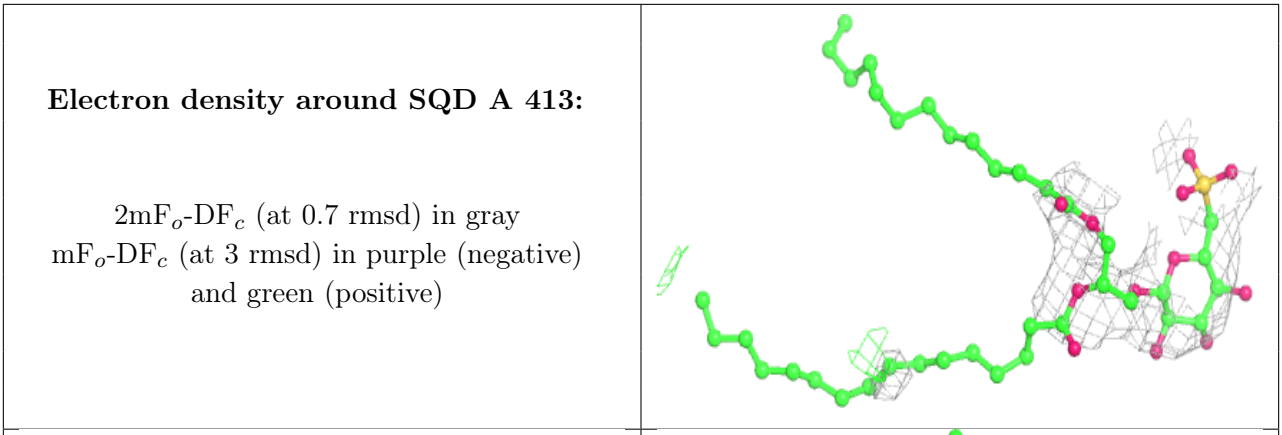
Electron density around BCR a 410:

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



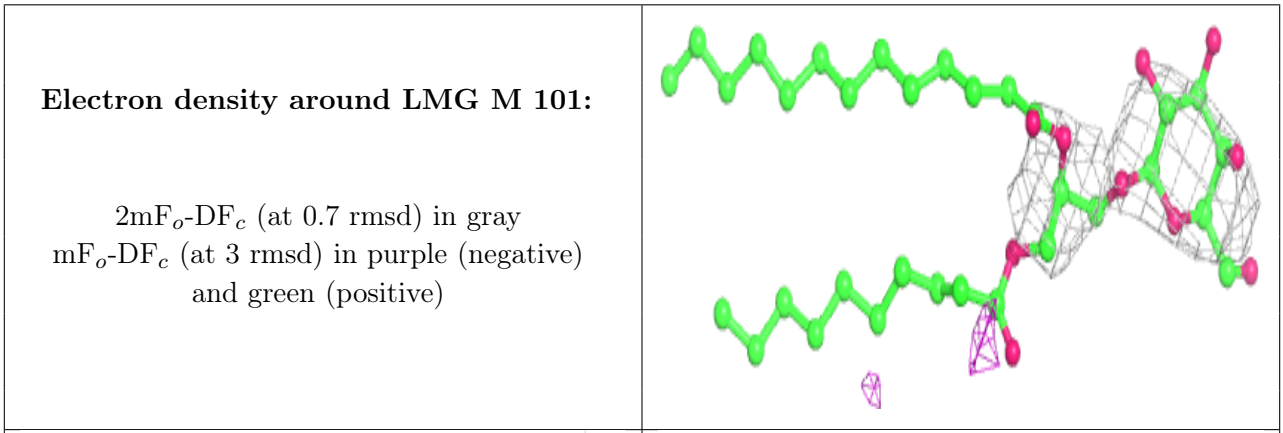
Electron density around SQD A 413:

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



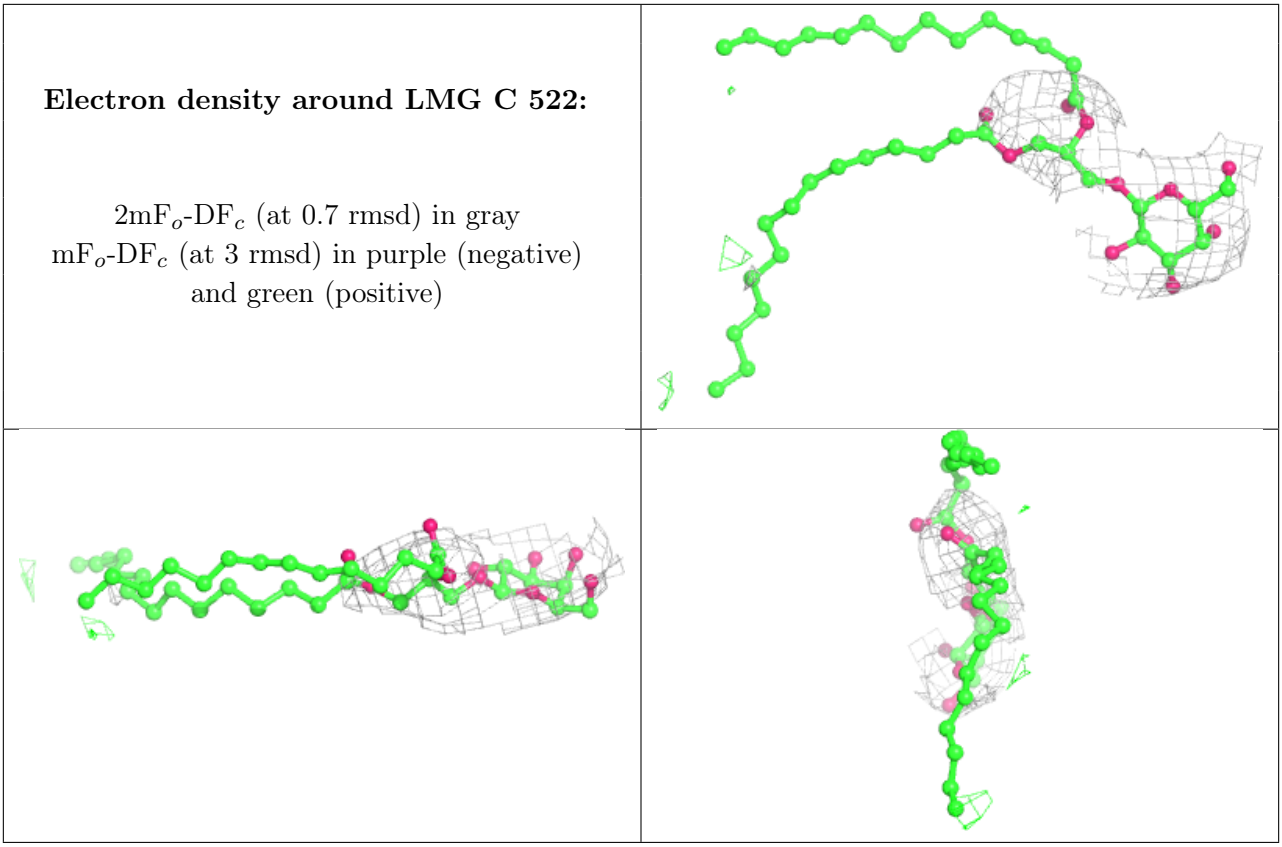
Electron density around LMG M 101:

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



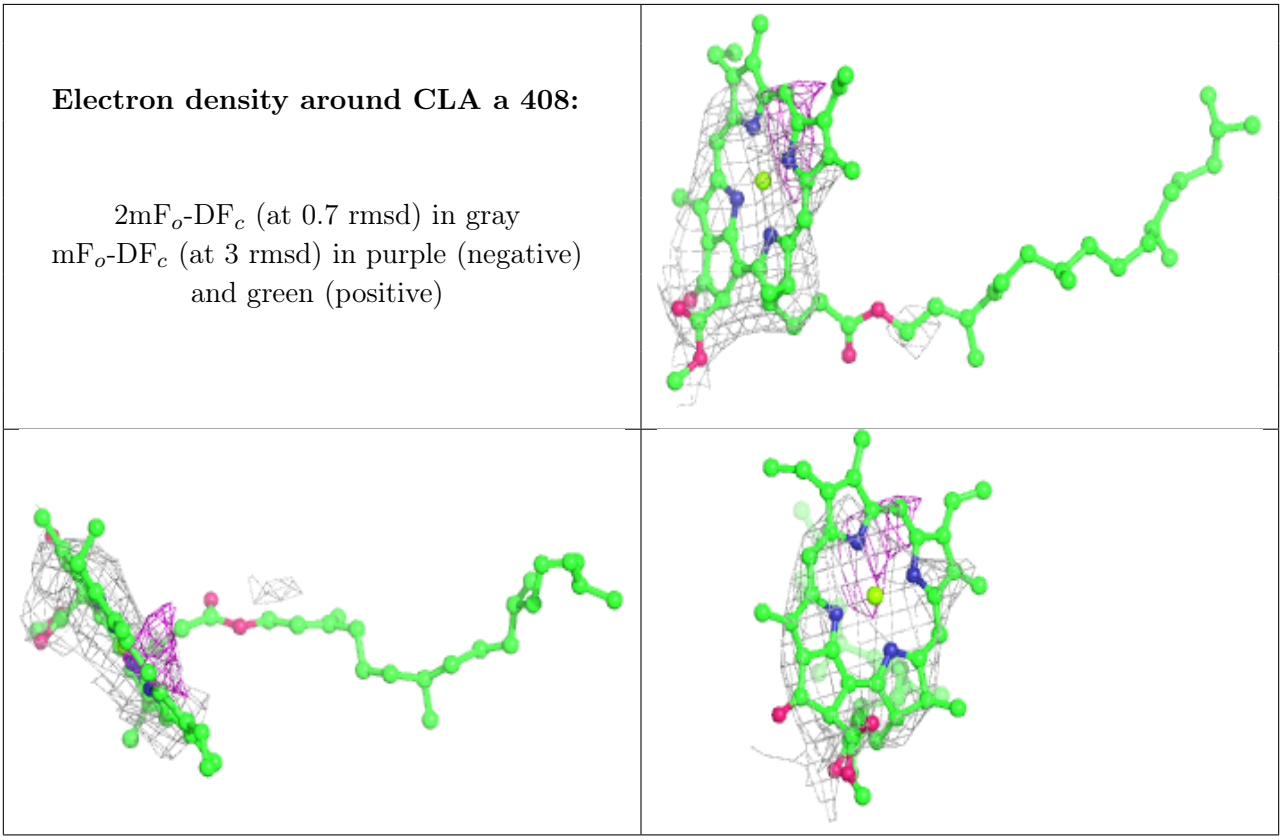
Electron density around LMG C 522:

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



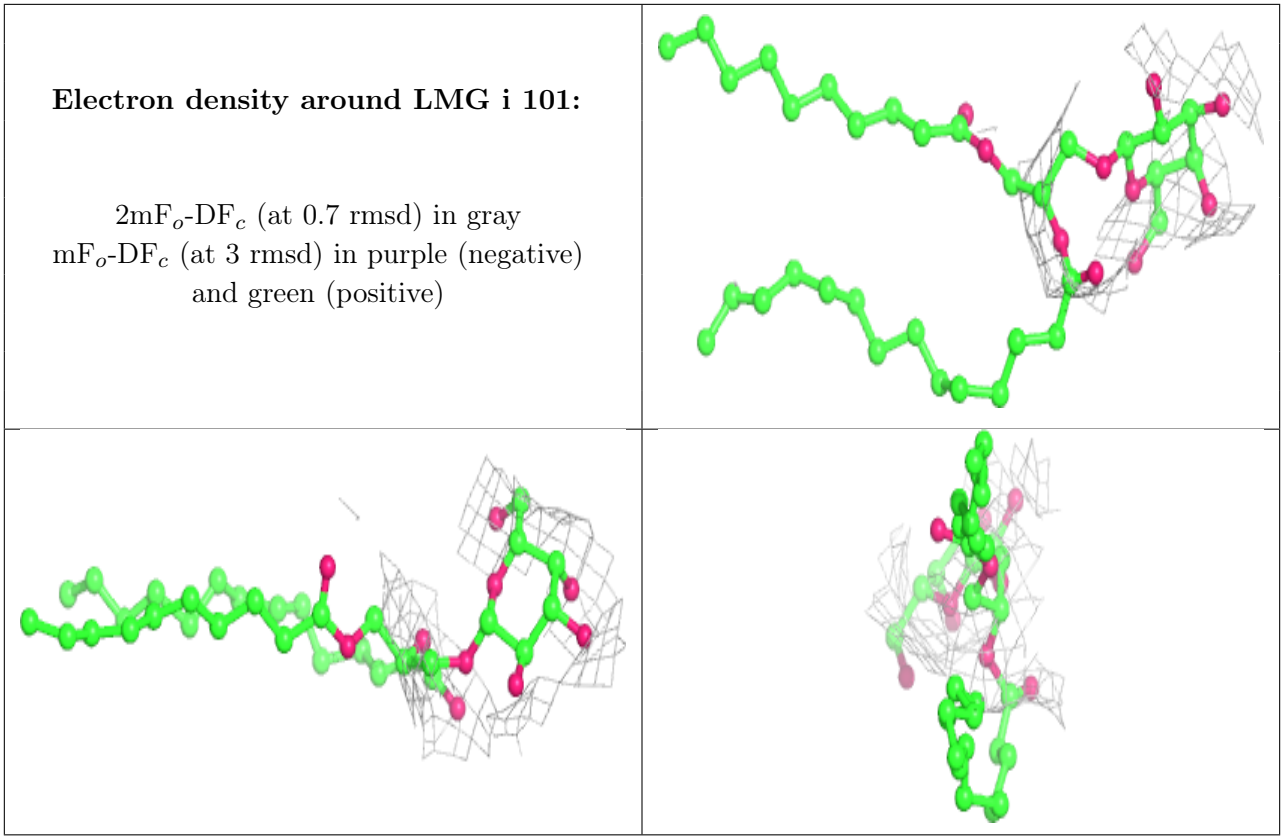
Electron density around CLA a 408:

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



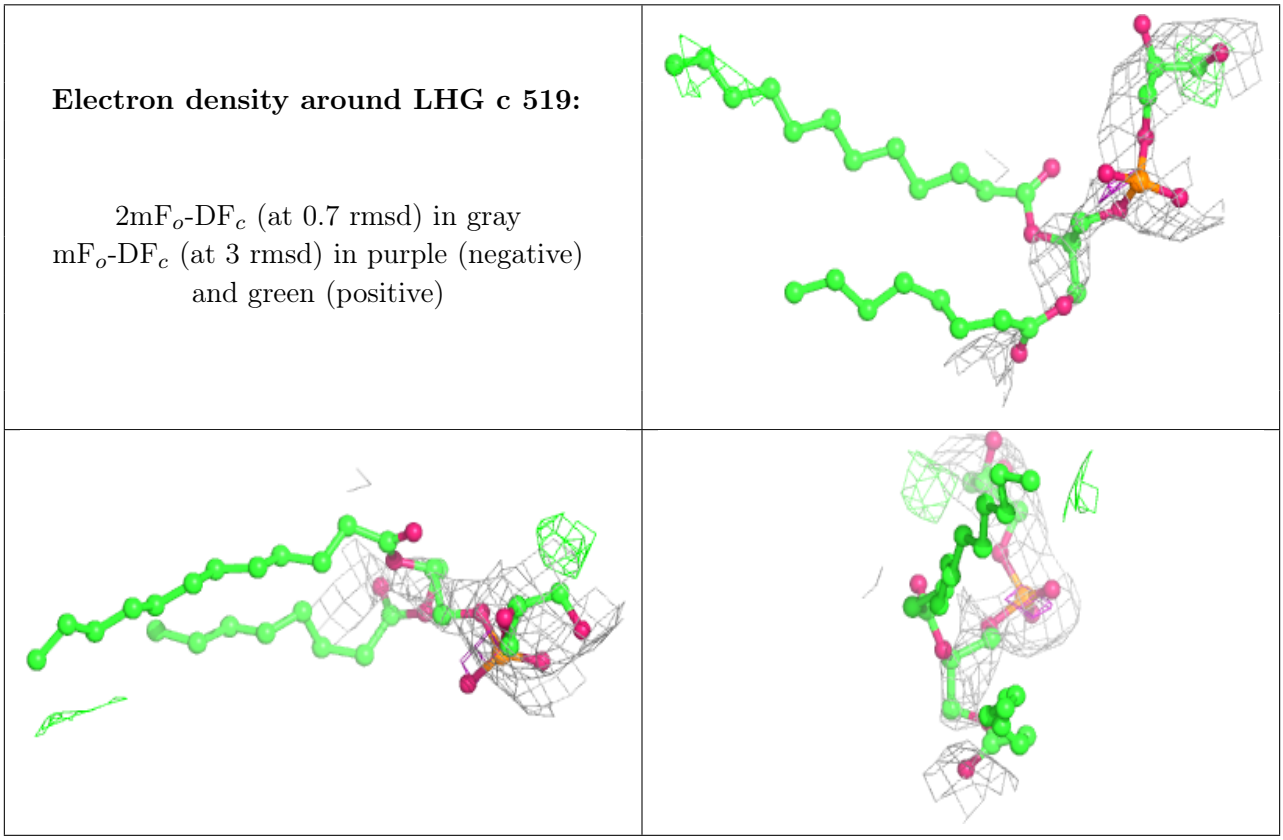
Electron density around LMG i 101:

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



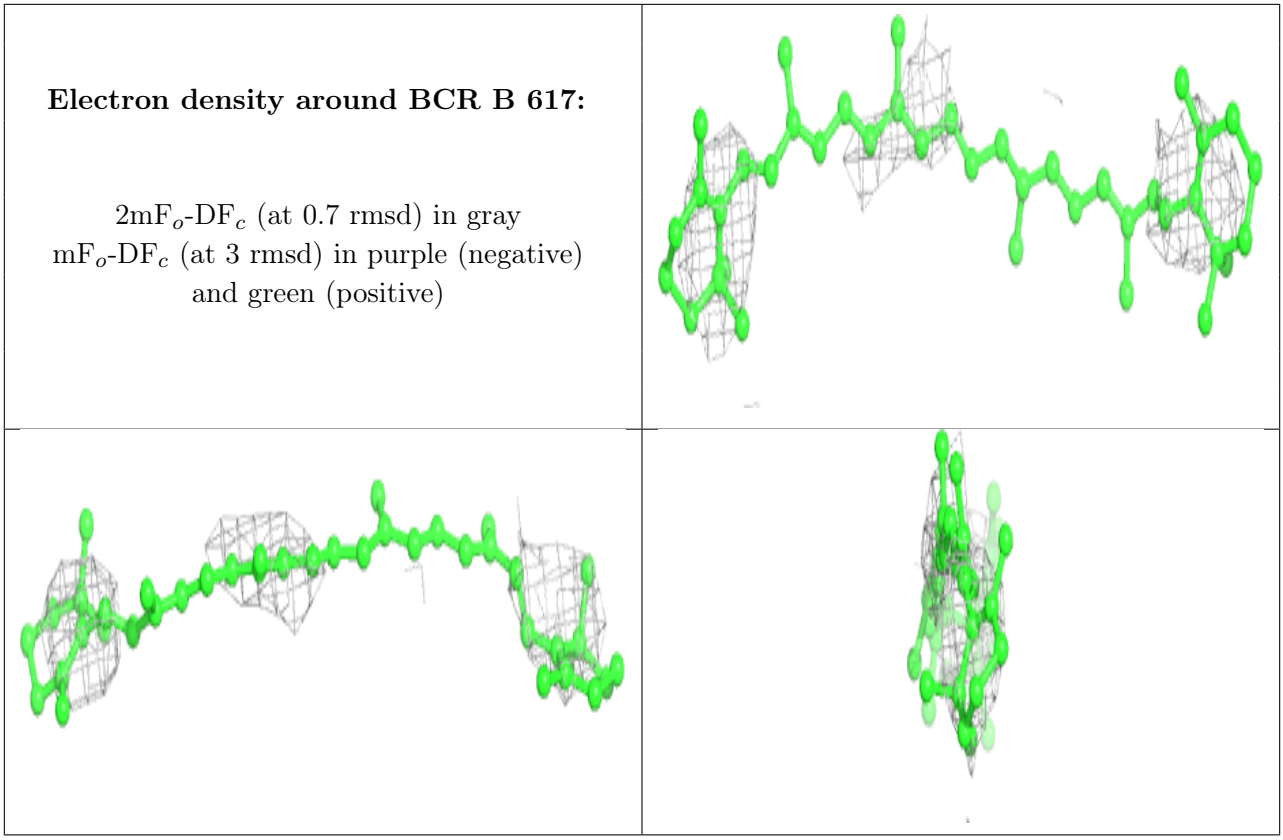
Electron density around LHG c 519:

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



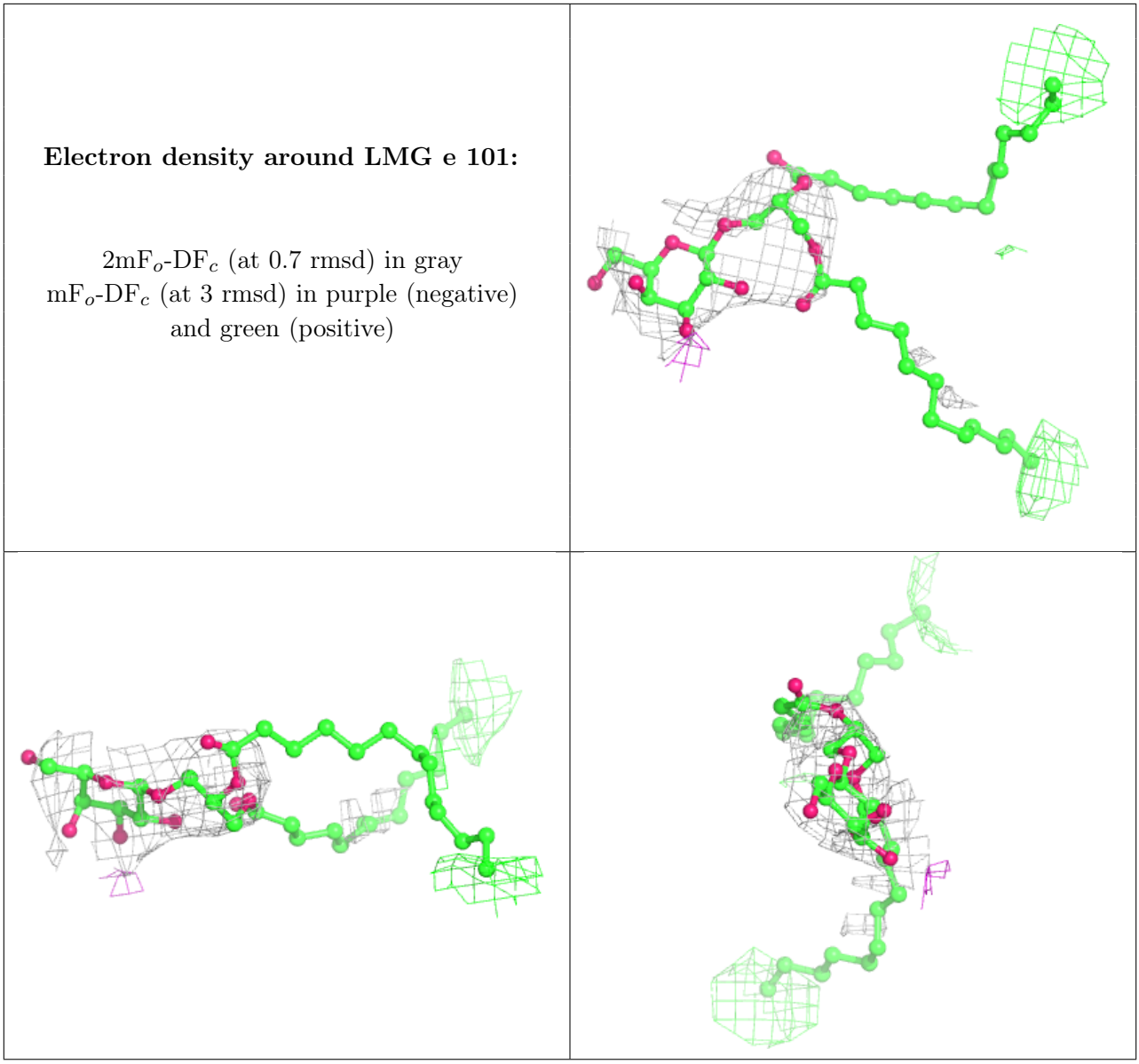
Electron density around BCR B 617:

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



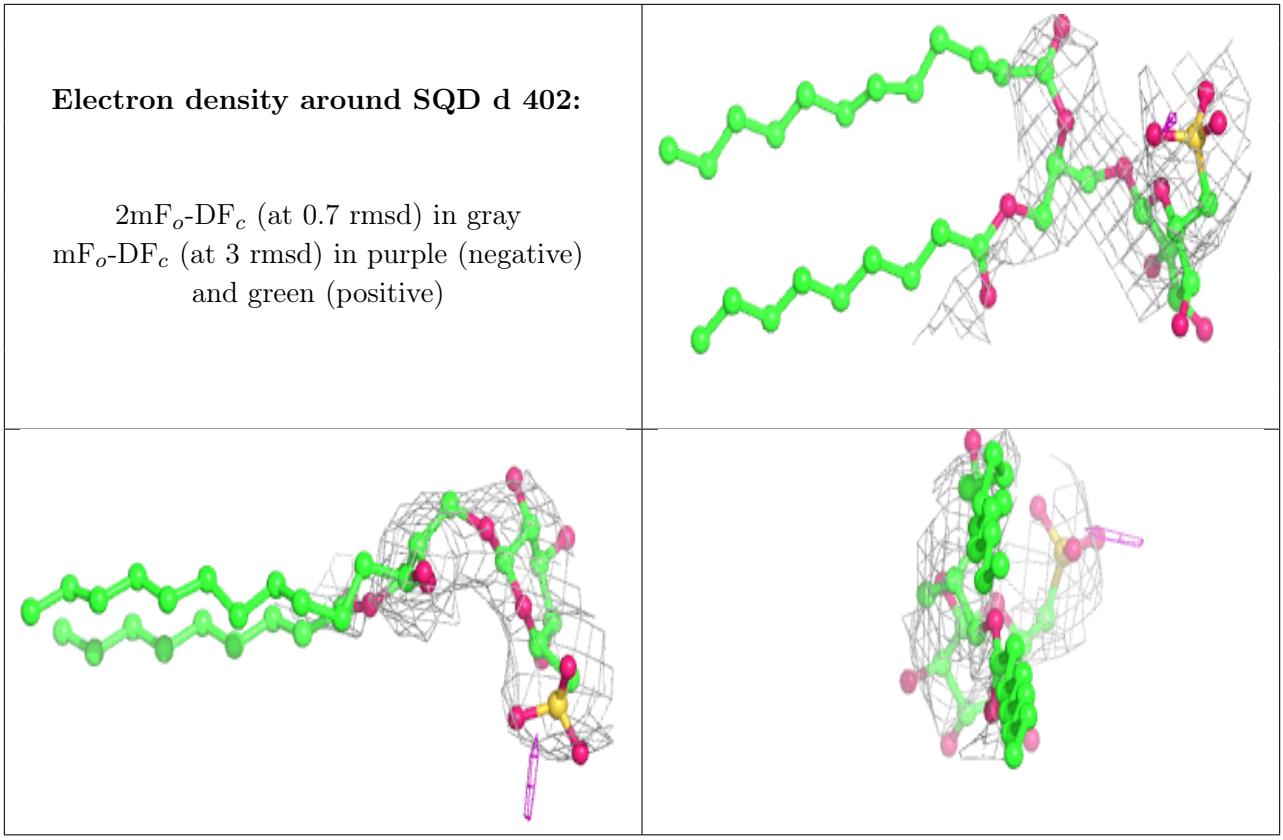
Electron density around LMG e 101:

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



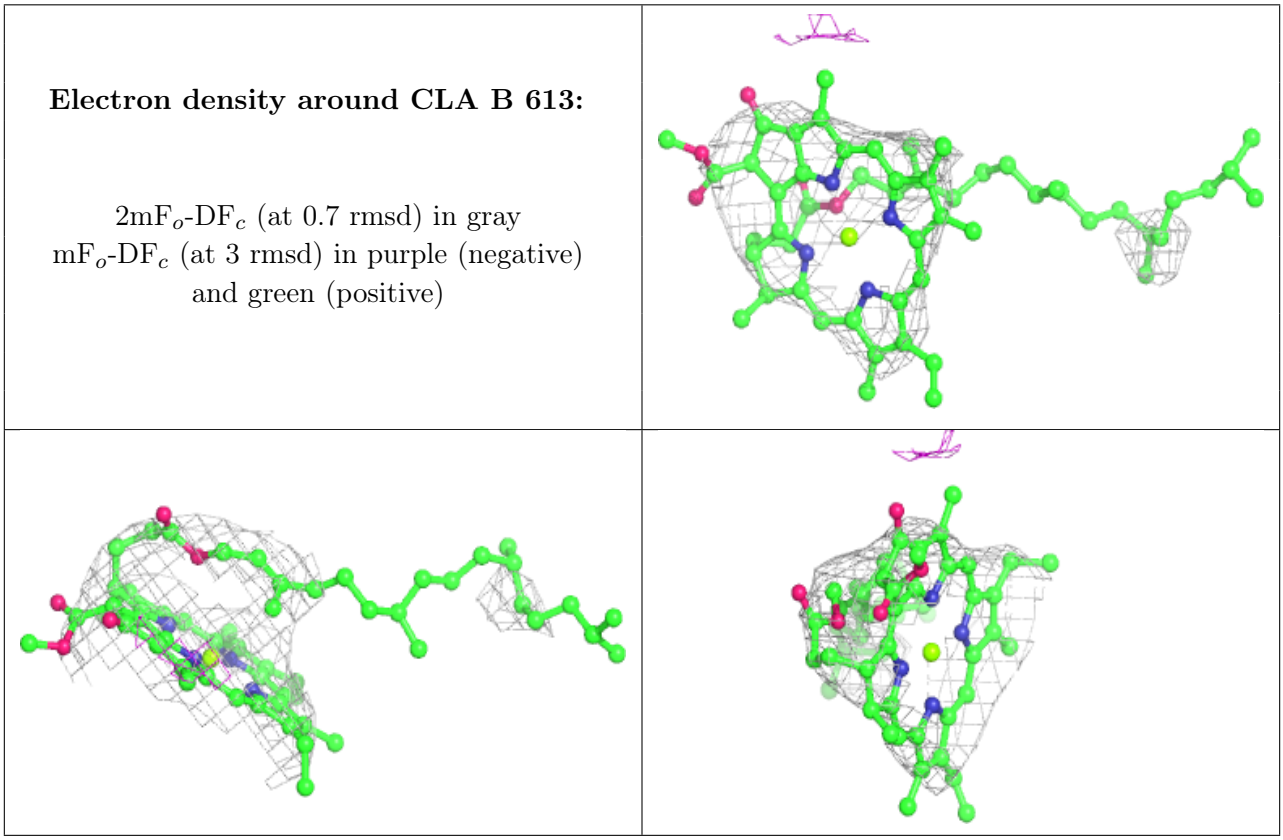
Electron density around SQD d 402:

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



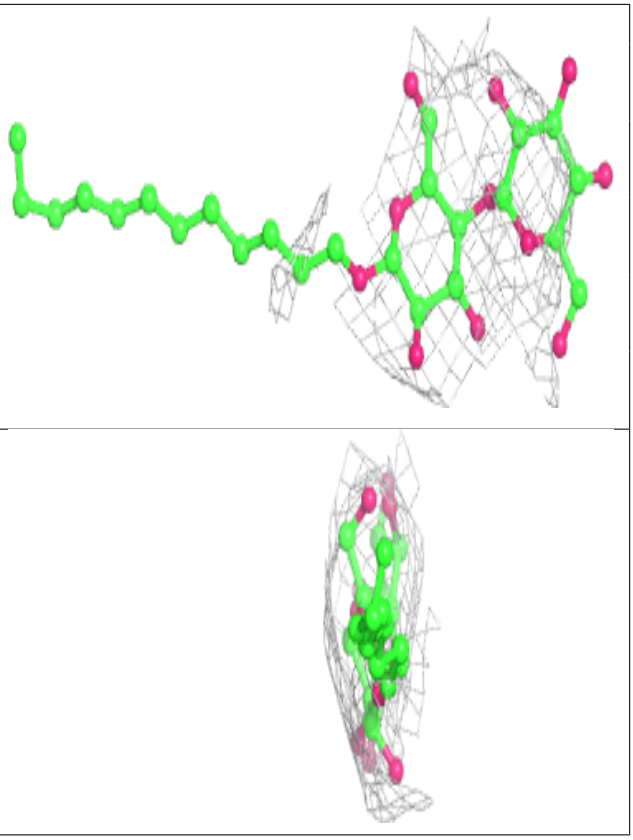
Electron density around CLA B 613:

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



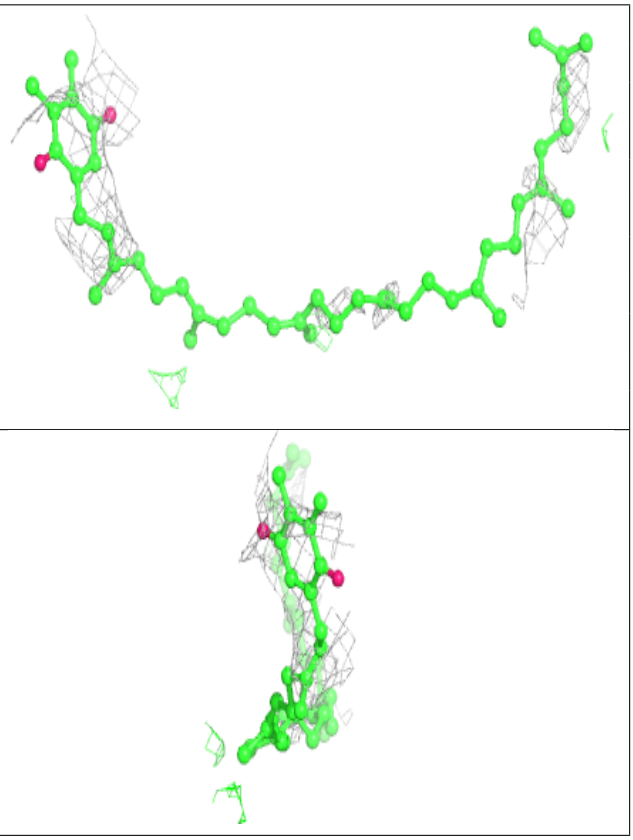
Electron density around LMT B 627:

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



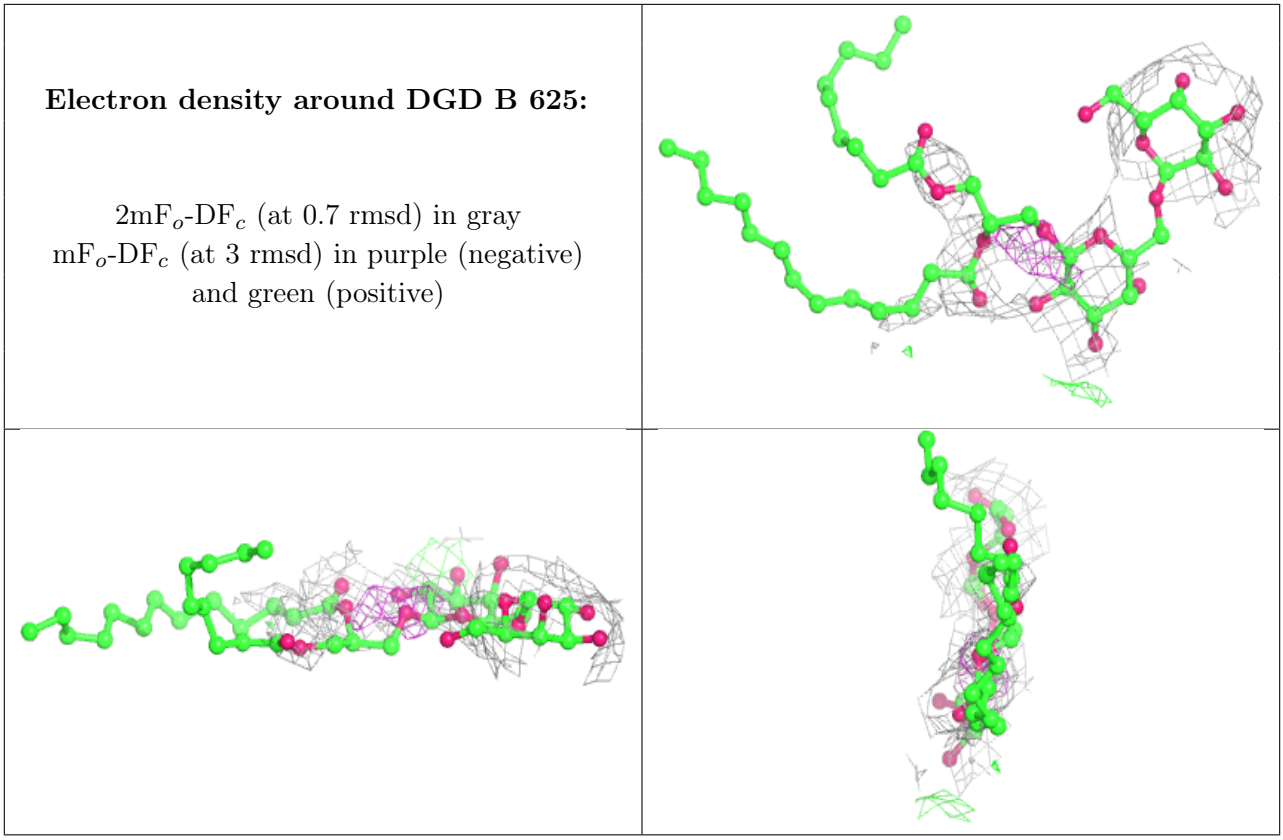
Electron density around PL9 a 409:

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



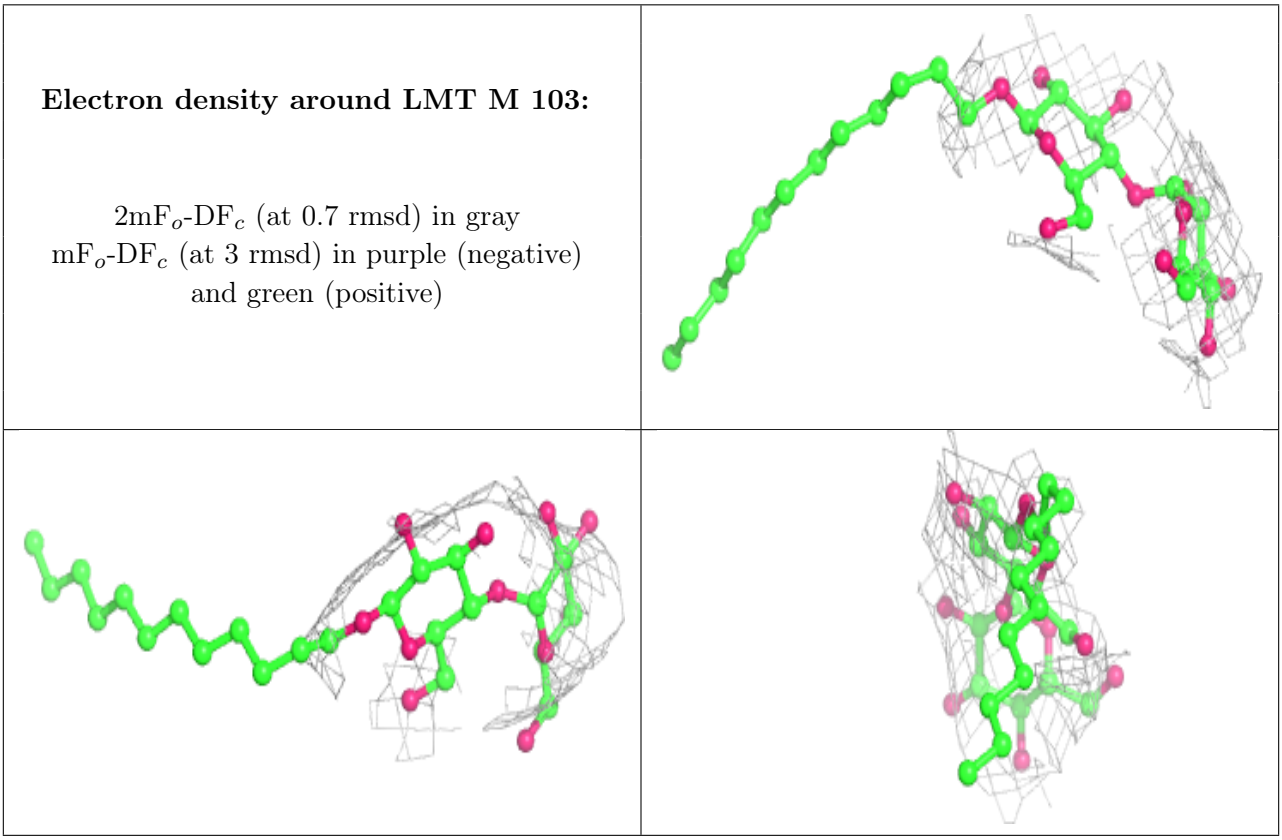
Electron density around DGD B 625:

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



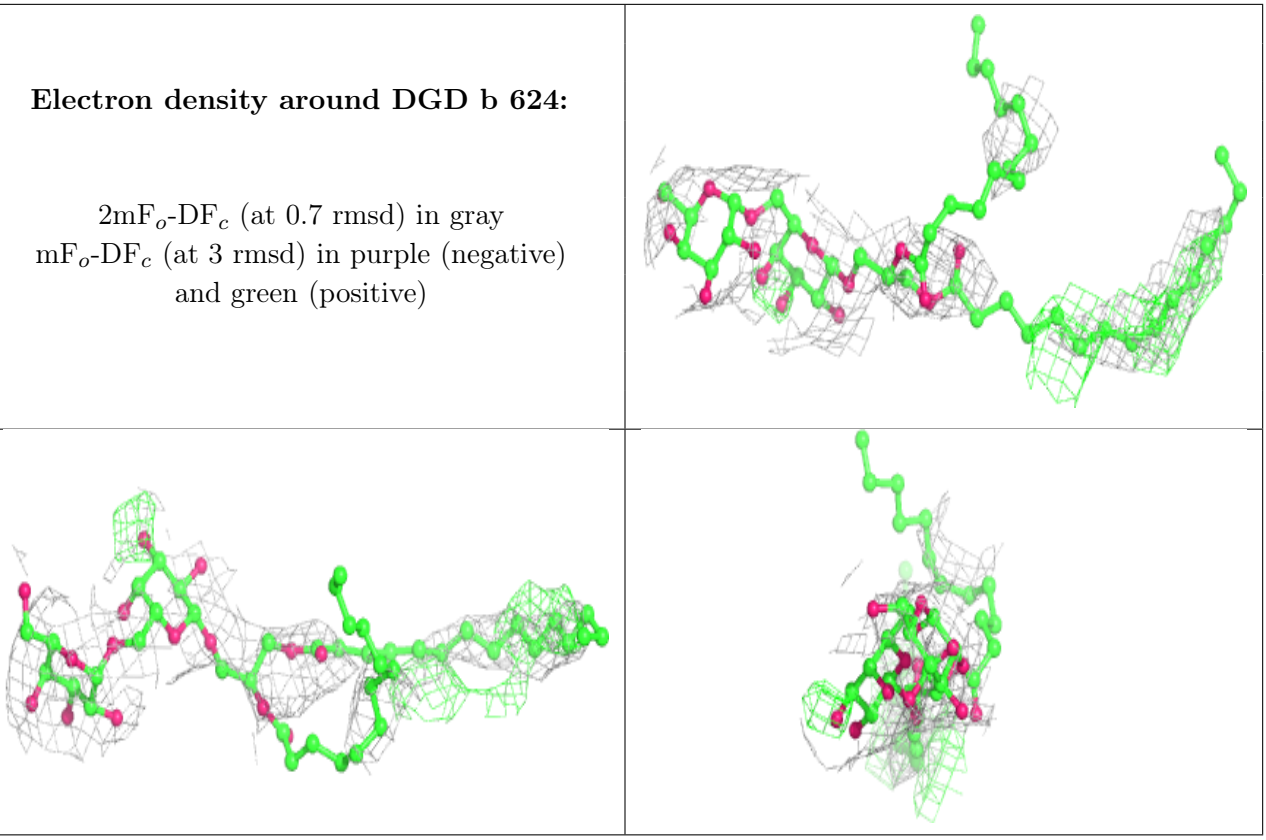
Electron density around LMT M 103:

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



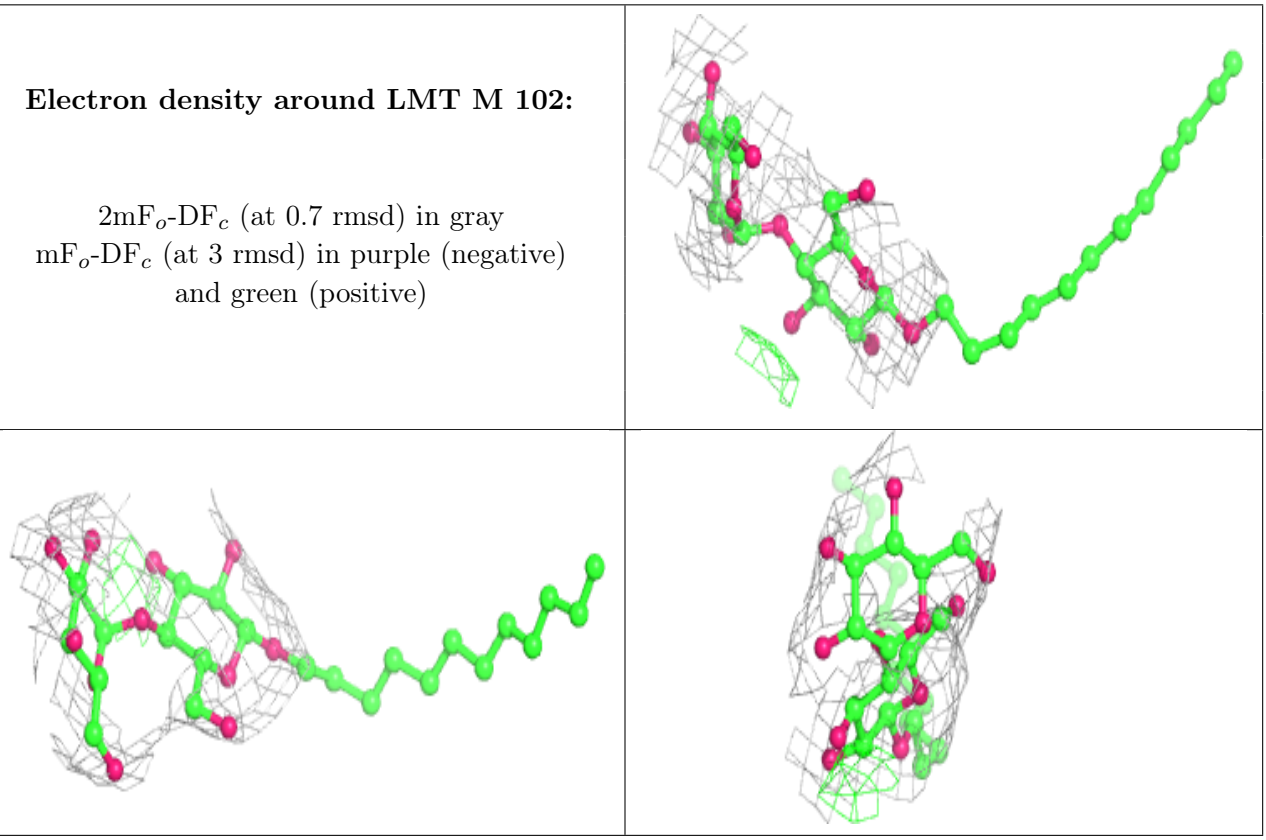
Electron density around DGD b 624:

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



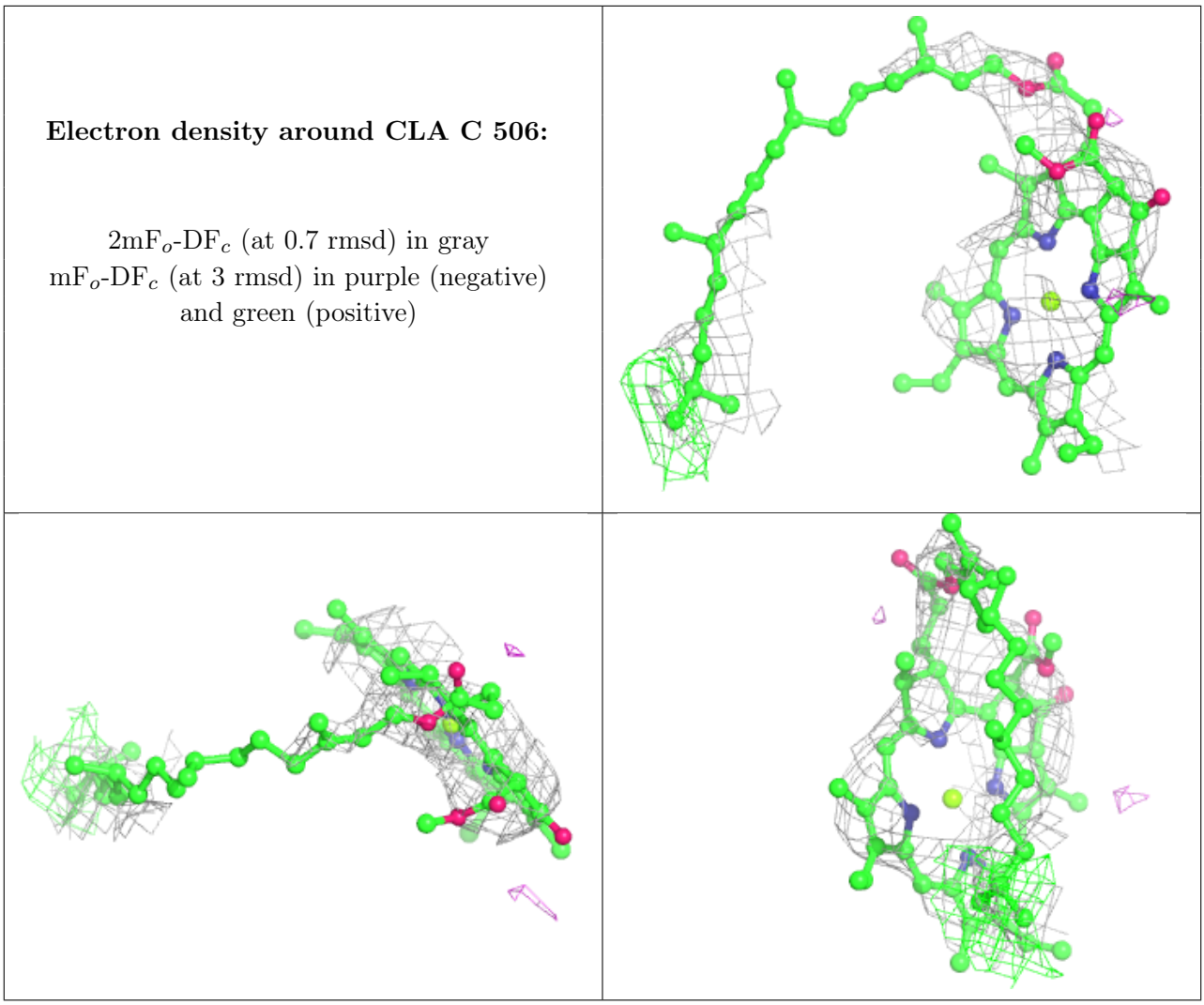
Electron density around LMT M 102:

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



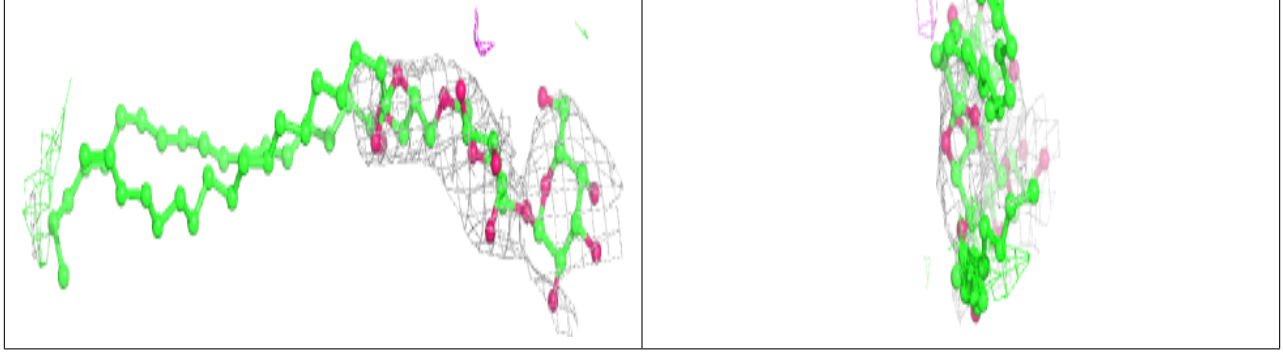
Electron density around CLA C 506:

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



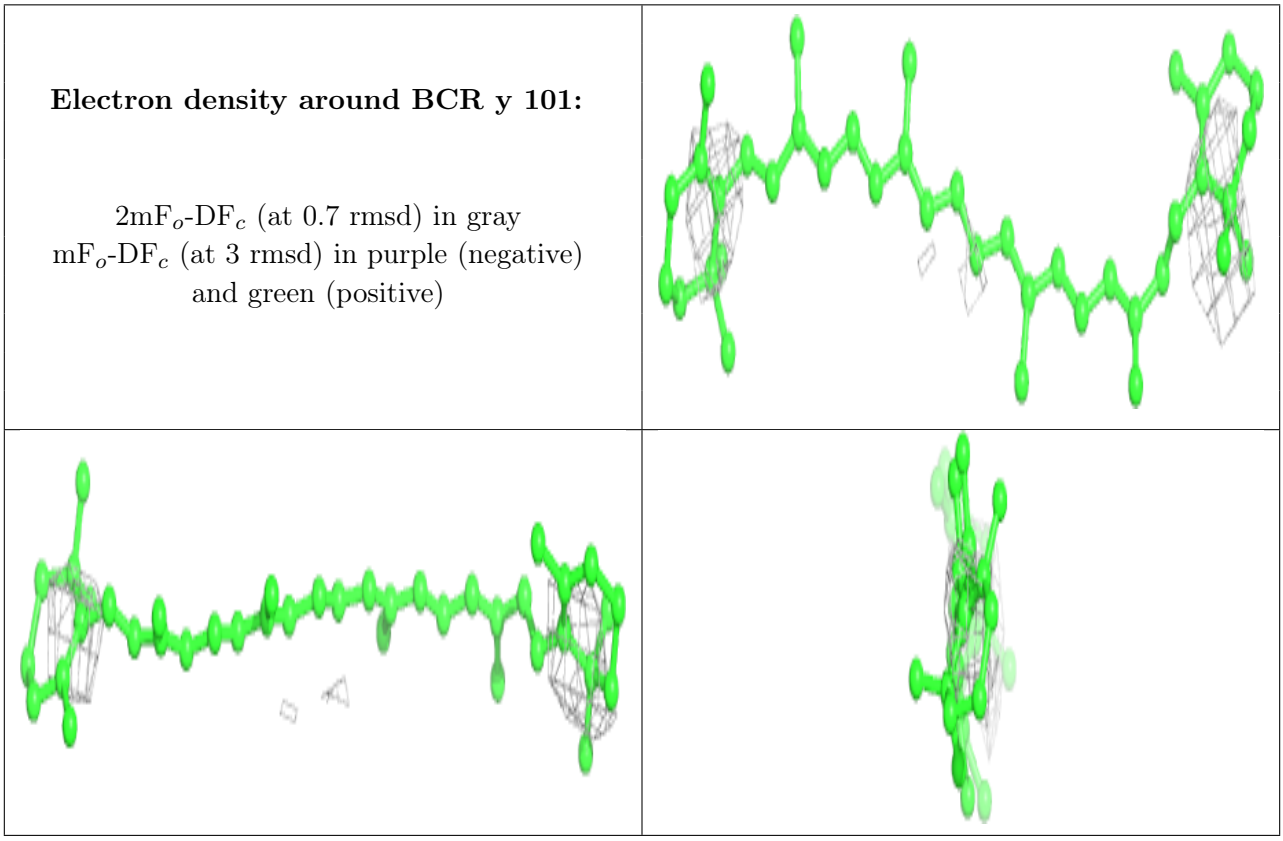
Electron density around DGD C 517:

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



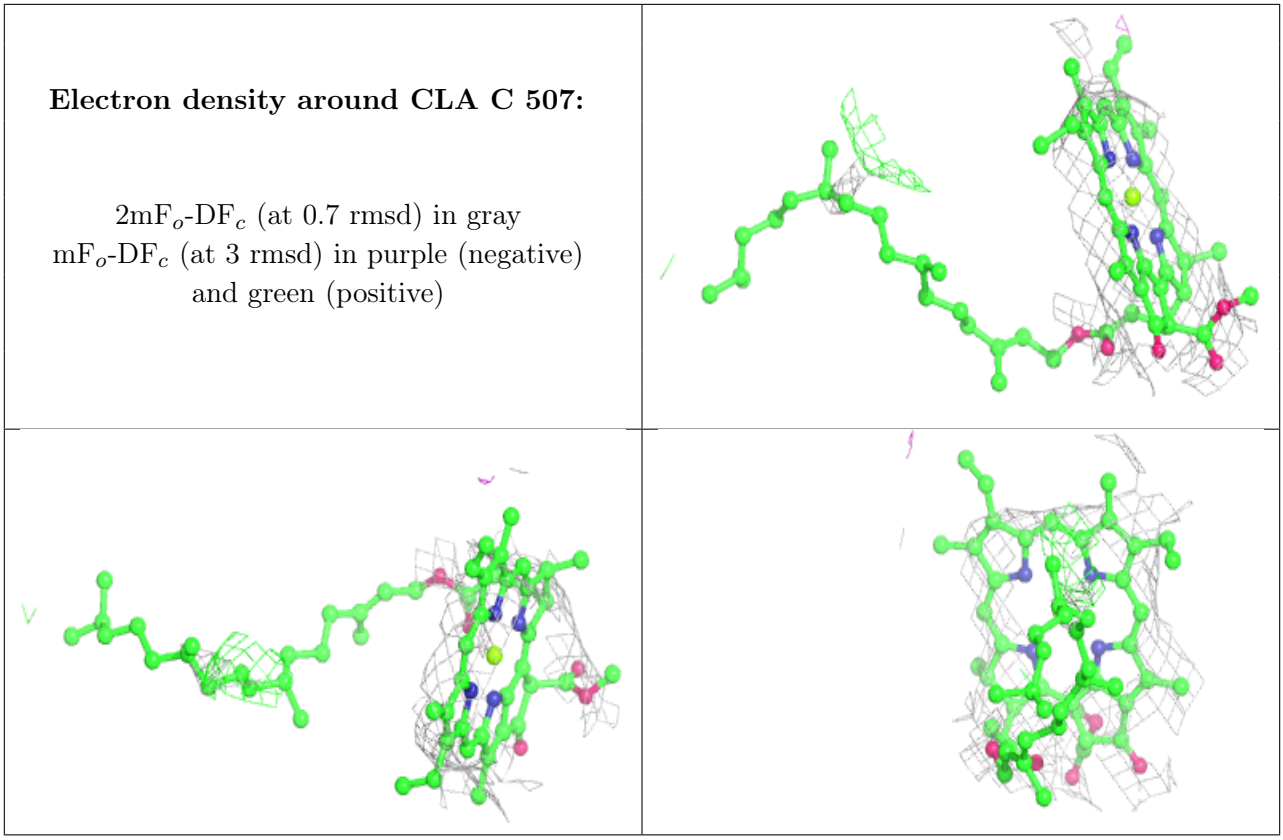
Electron density around BCR y 101:

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



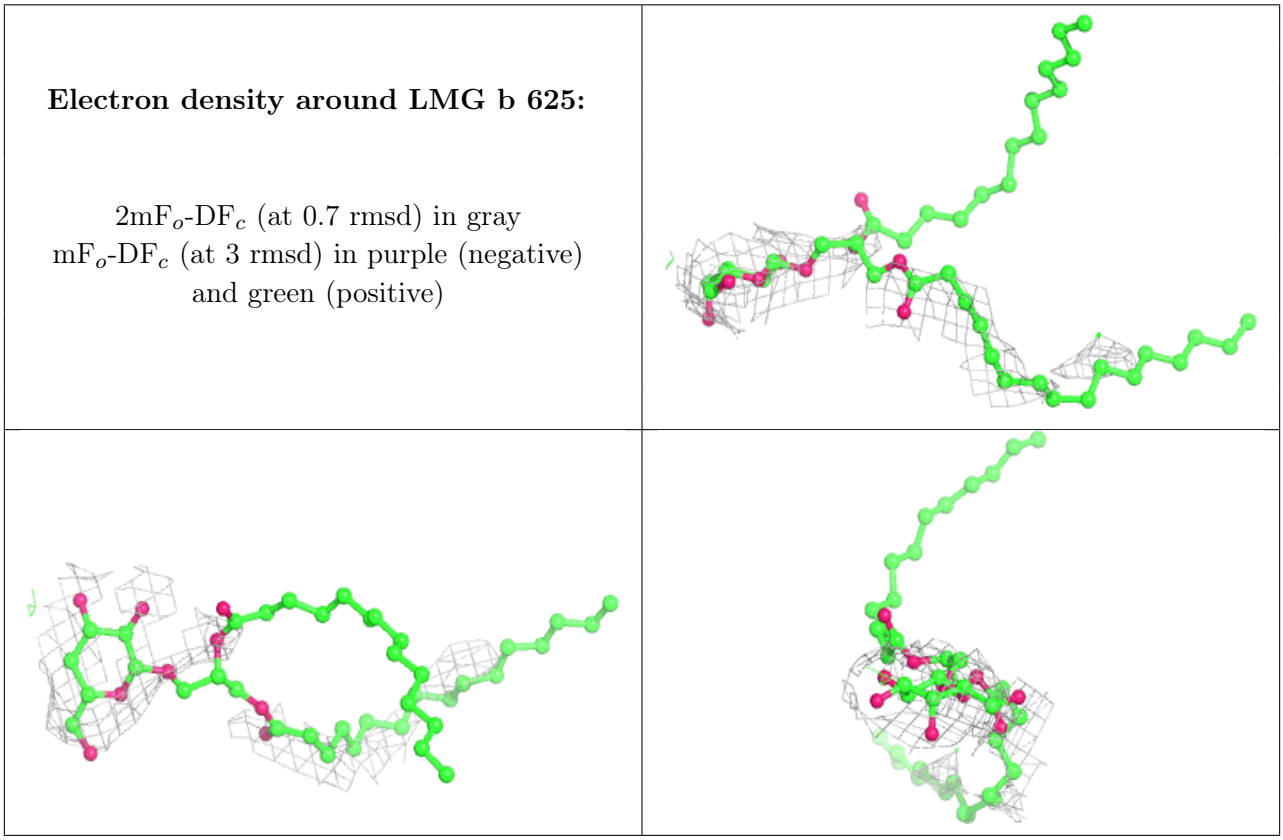
Electron density around CLA C 507:

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



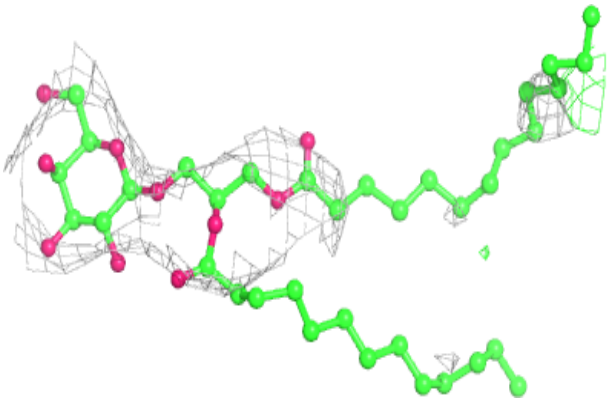
Electron density around LMG b 625:

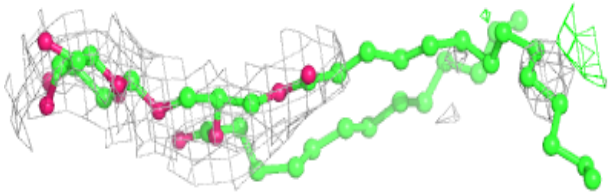
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

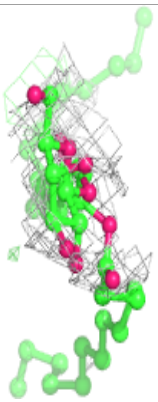


Electron density around LMG D 412:

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

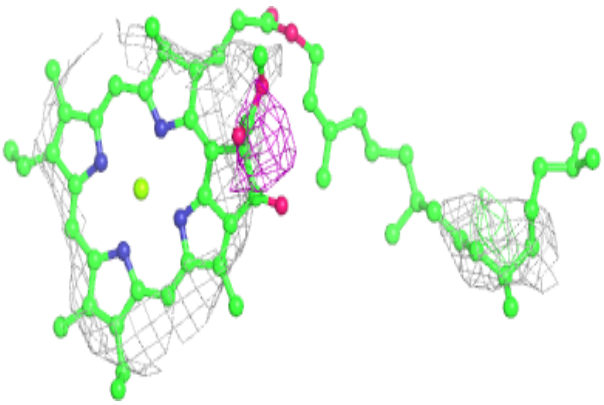


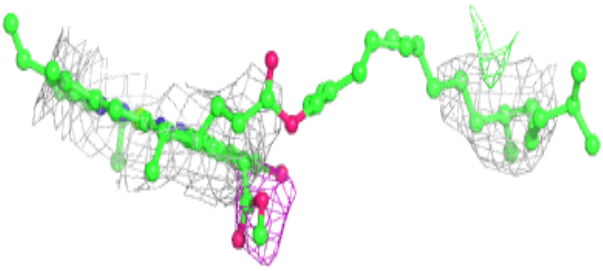


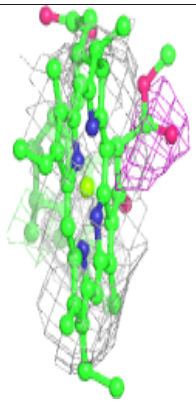


Electron density around CLA h 101:

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

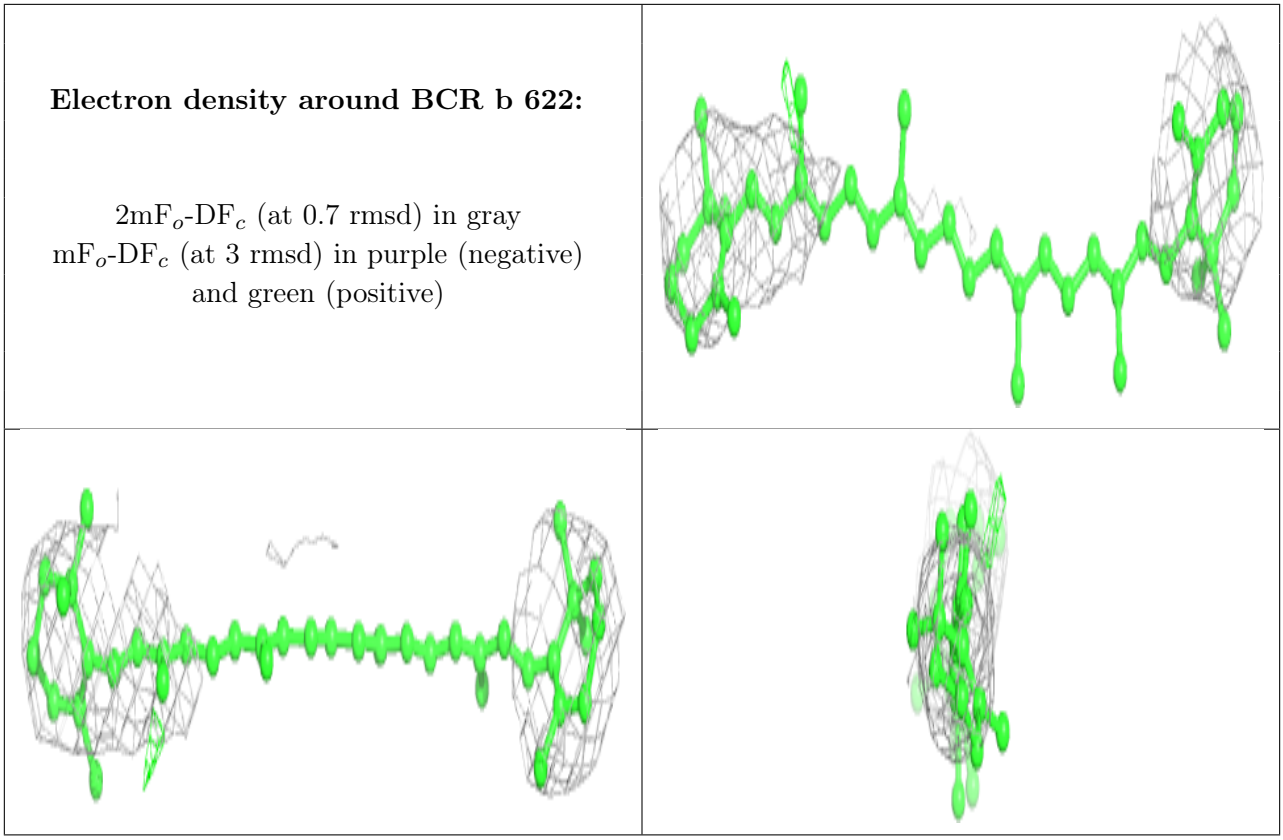






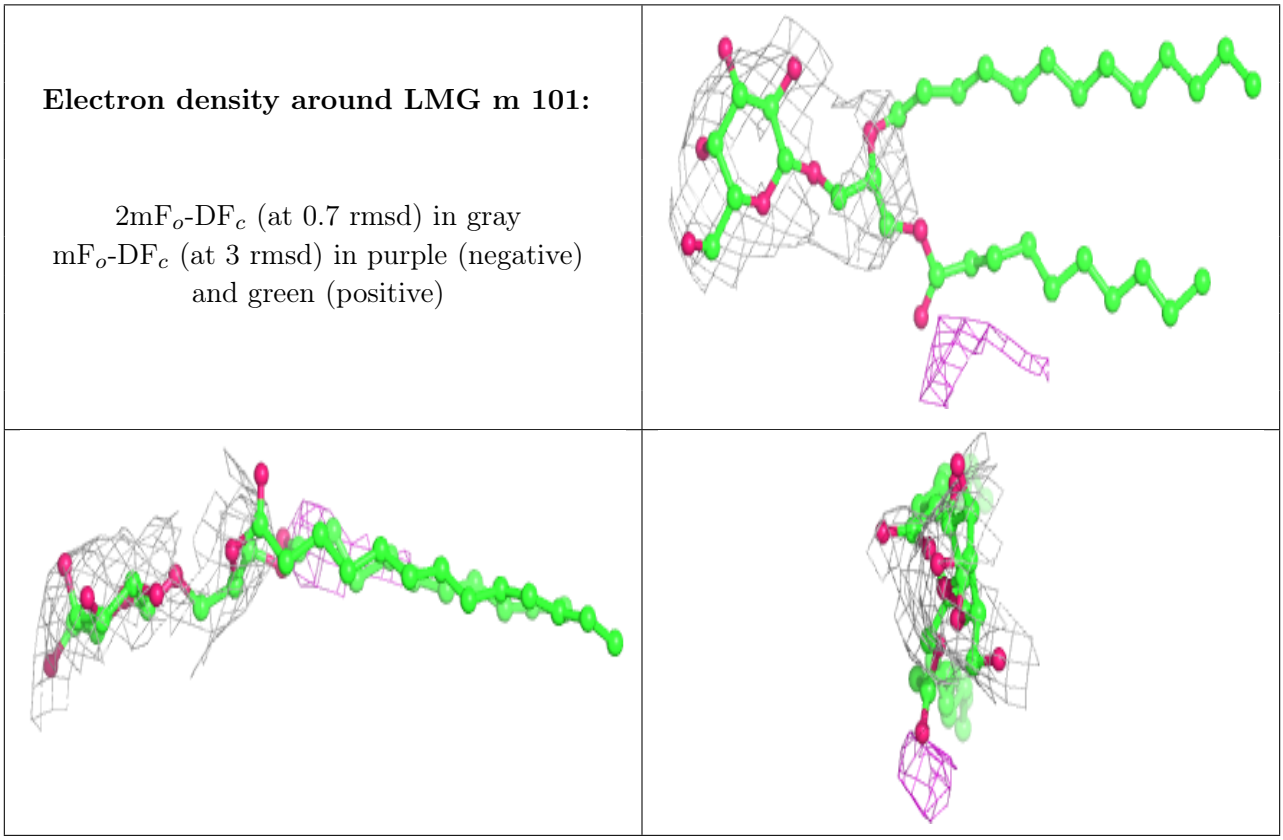
Electron density around BCR b 622:

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



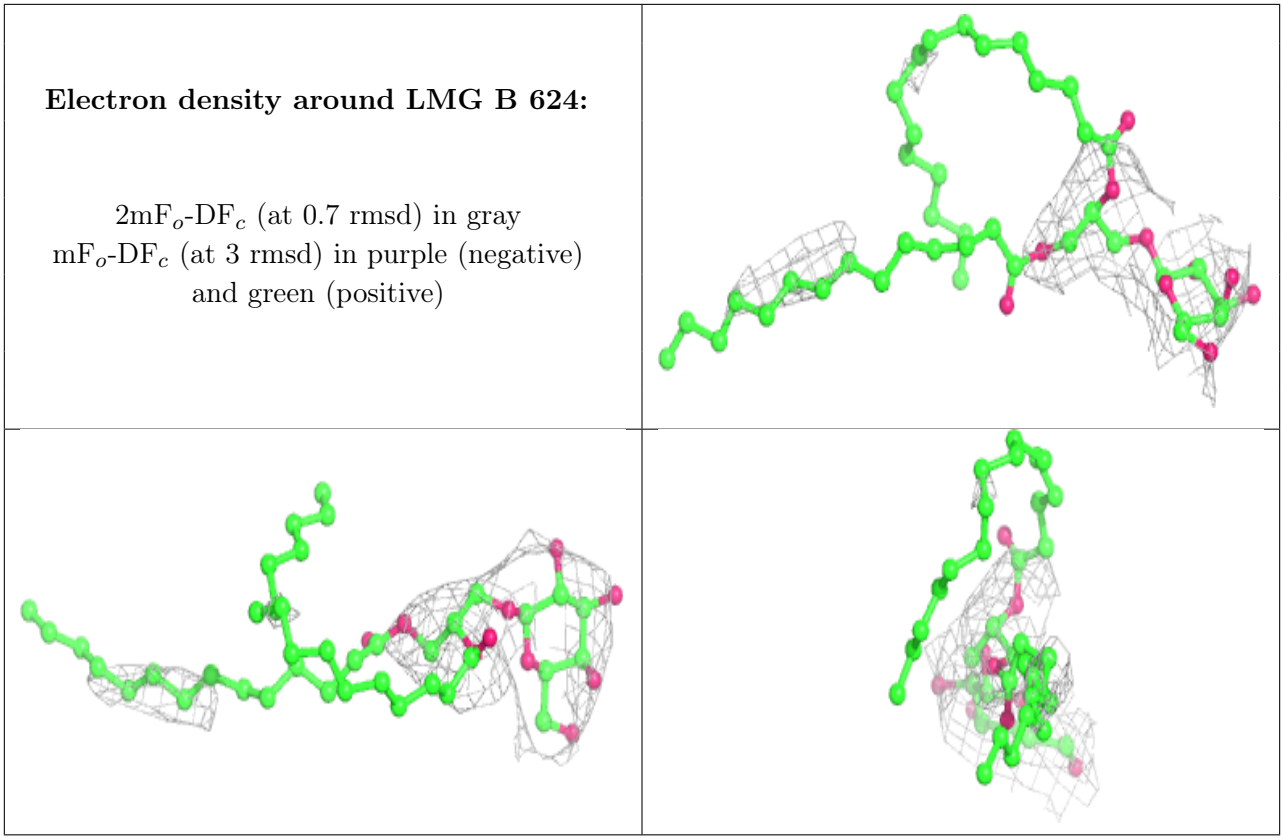
Electron density around LMG m 101:

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



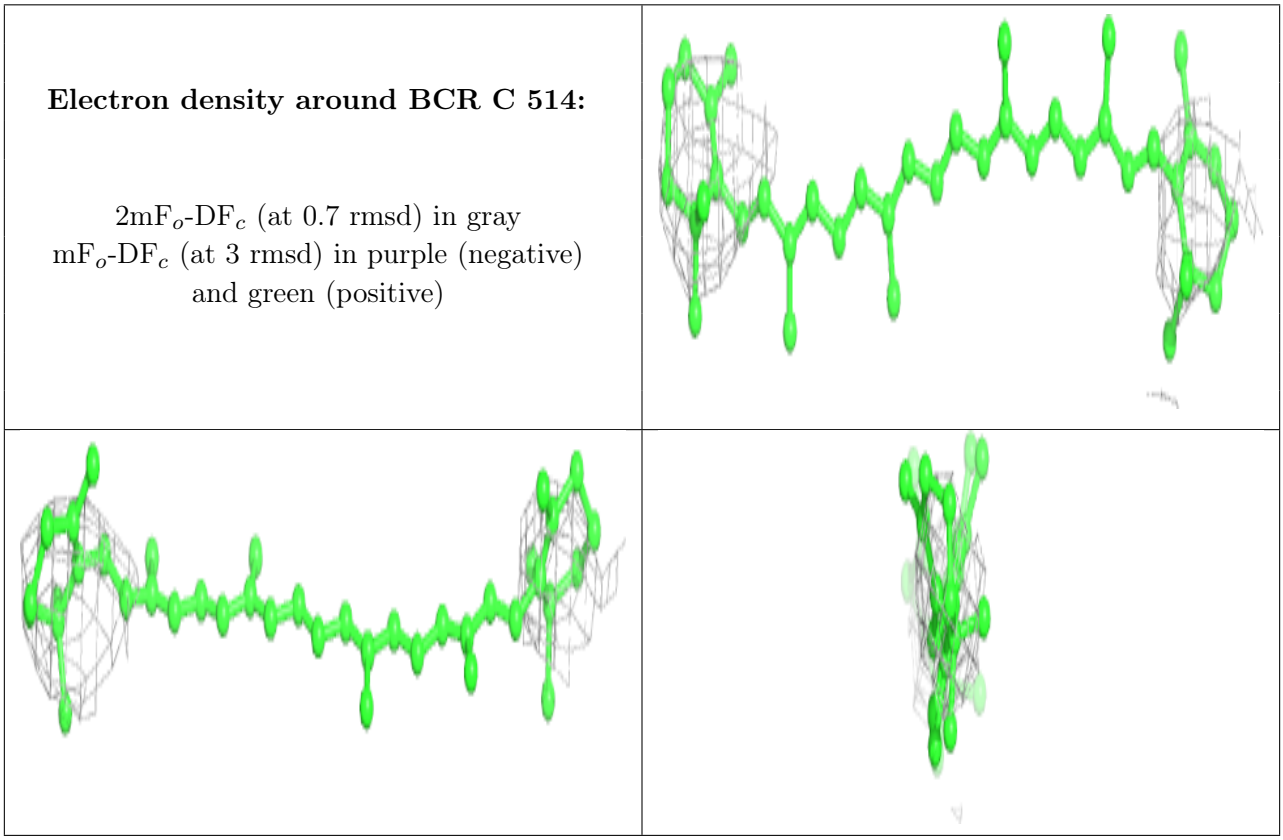
Electron density around LMG B 624:

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



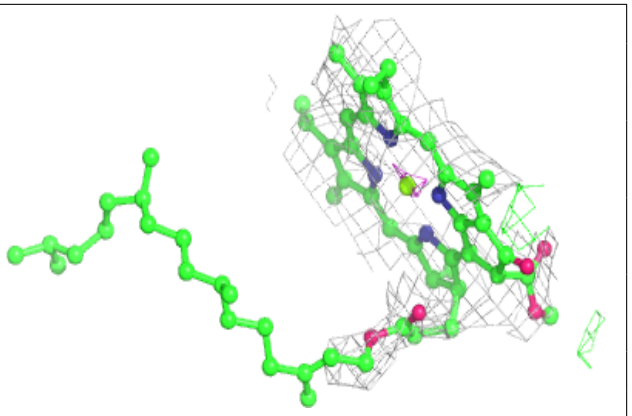
Electron density around BCR C 514:

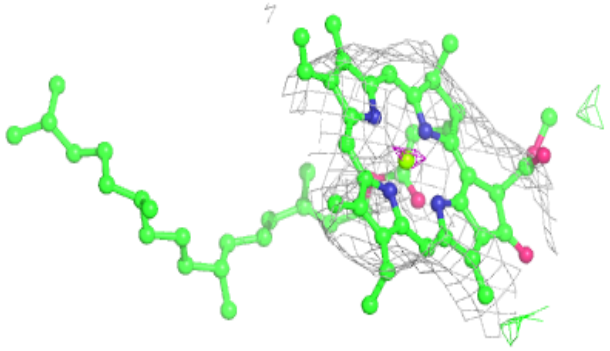
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

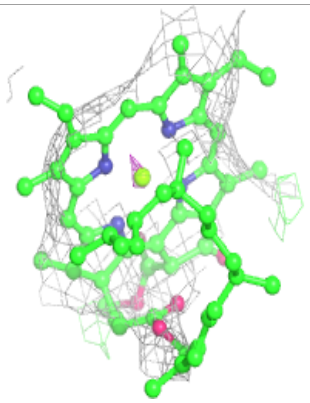


Electron density around CLA c 512:

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

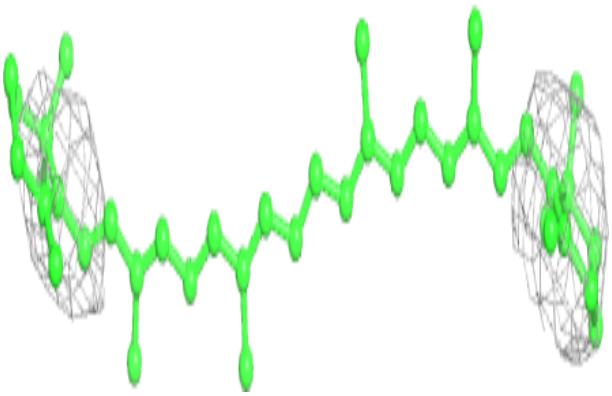


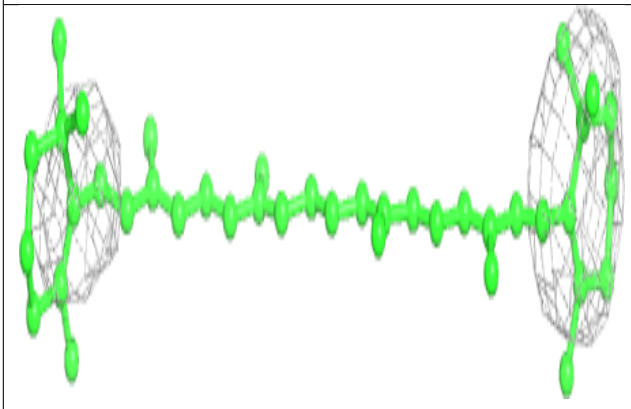


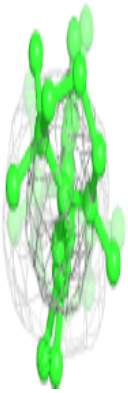


Electron density around BCR A 407:

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

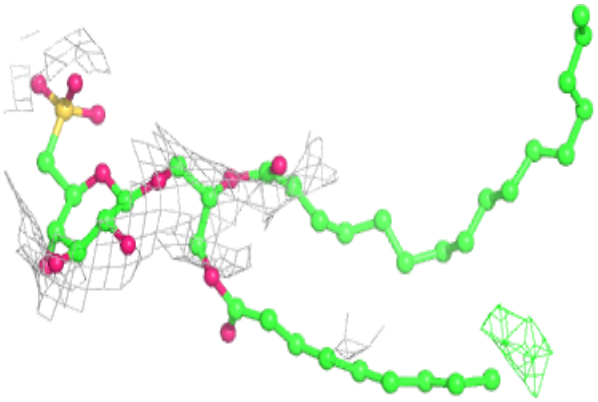


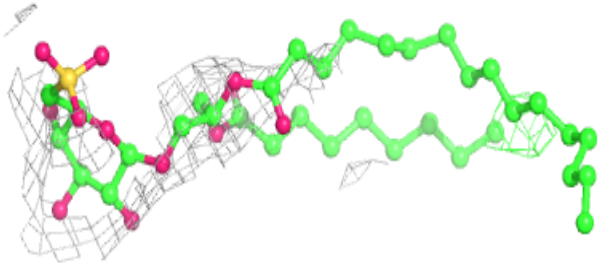


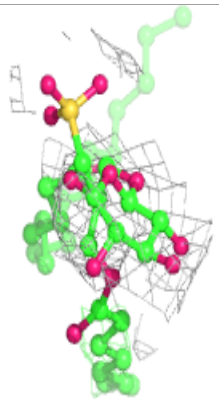


Electron density around SQD B 626:

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

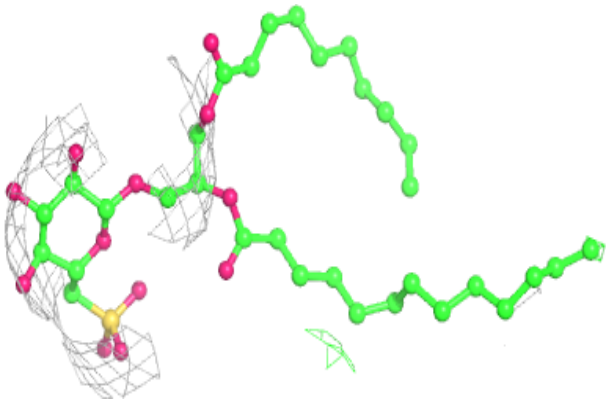


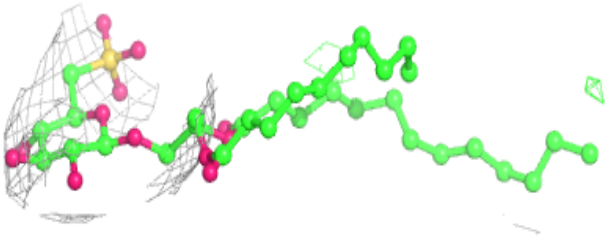


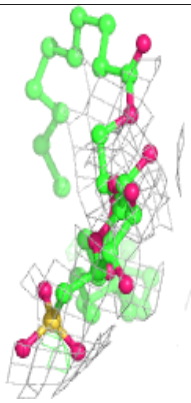


Electron density around SQD F 102:

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

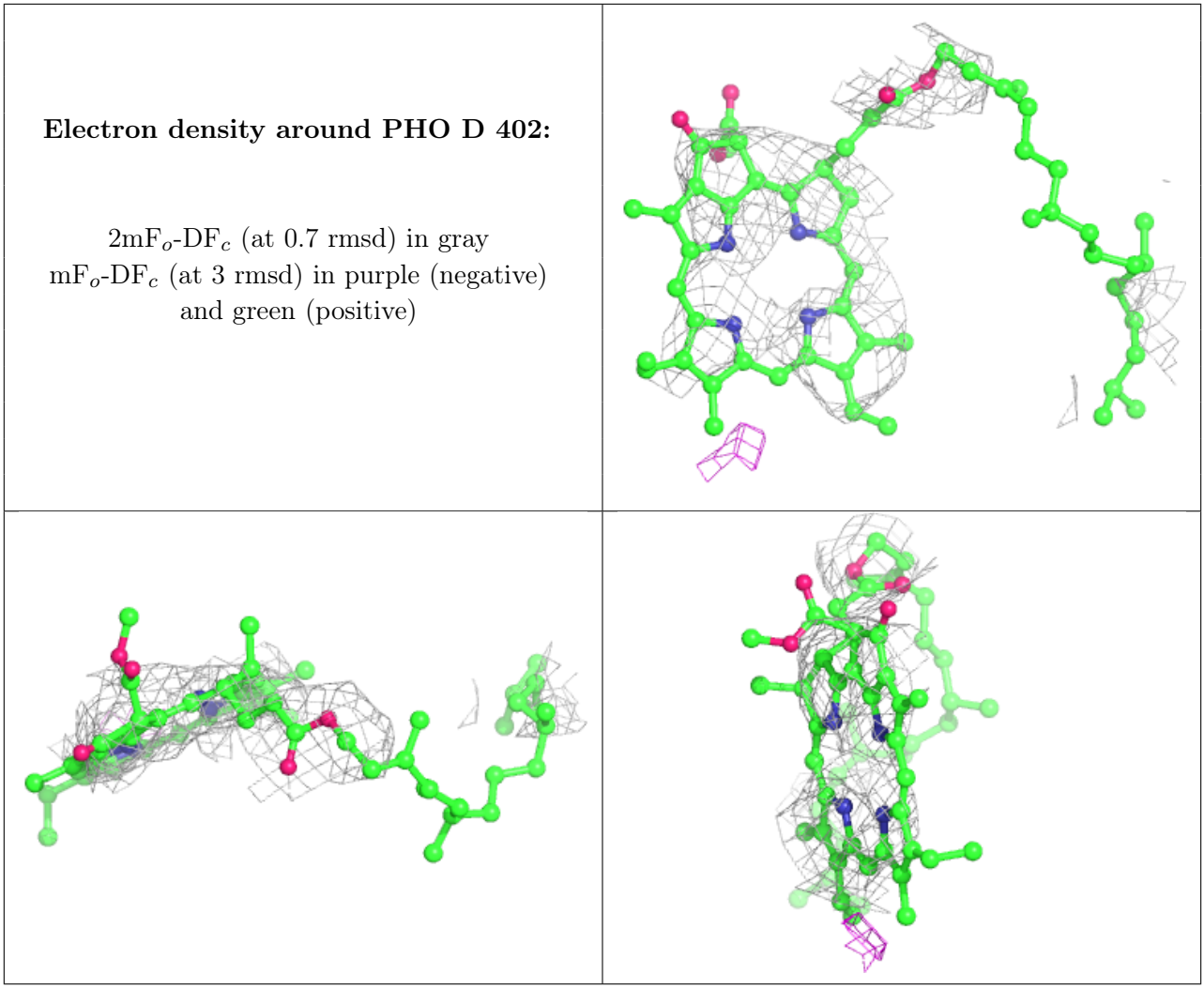






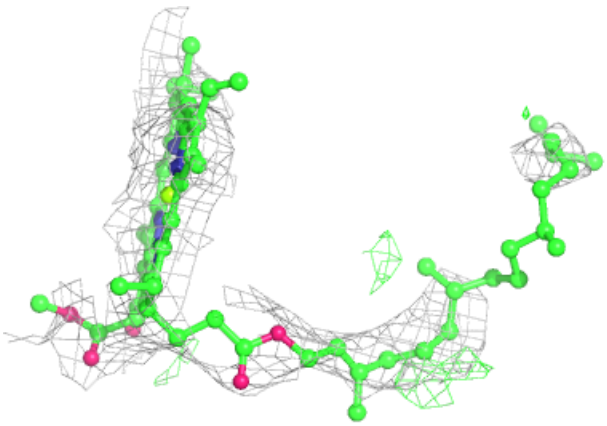
Electron density around PHO D 402:

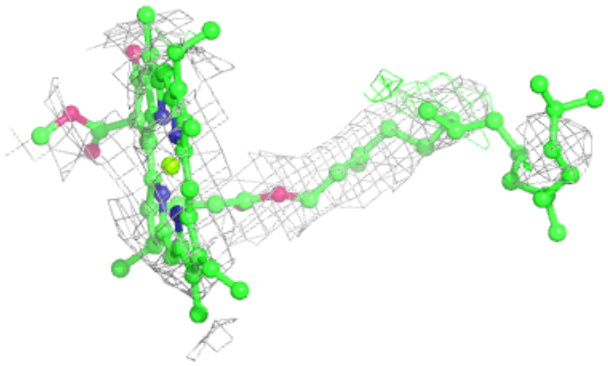
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

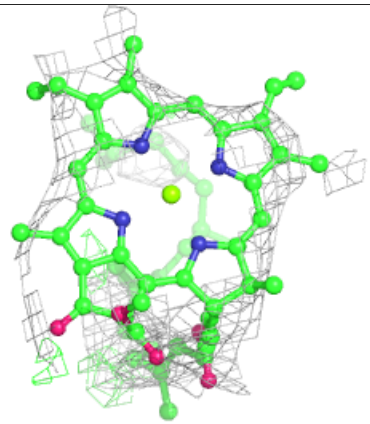


Electron density around CLA C 505:

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

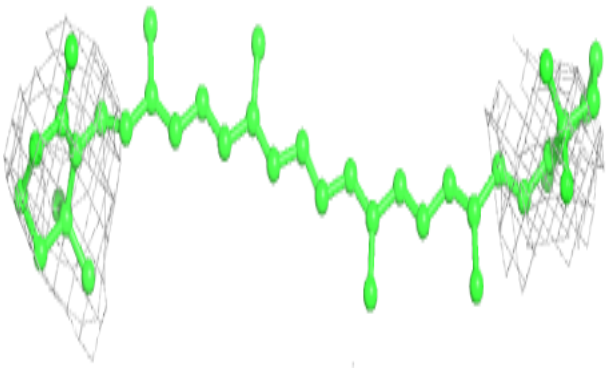


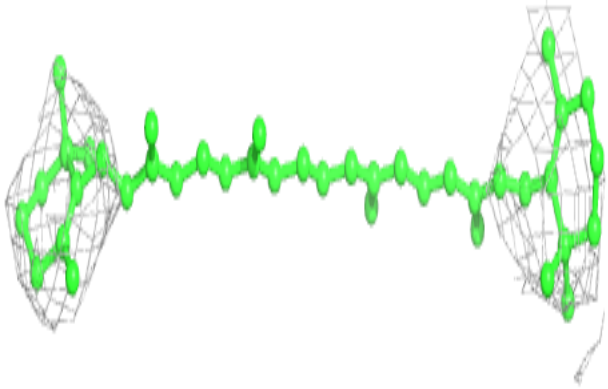


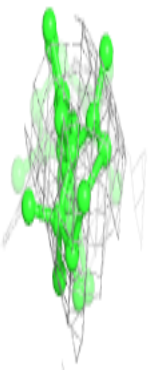


Electron density around BCR C 521:

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

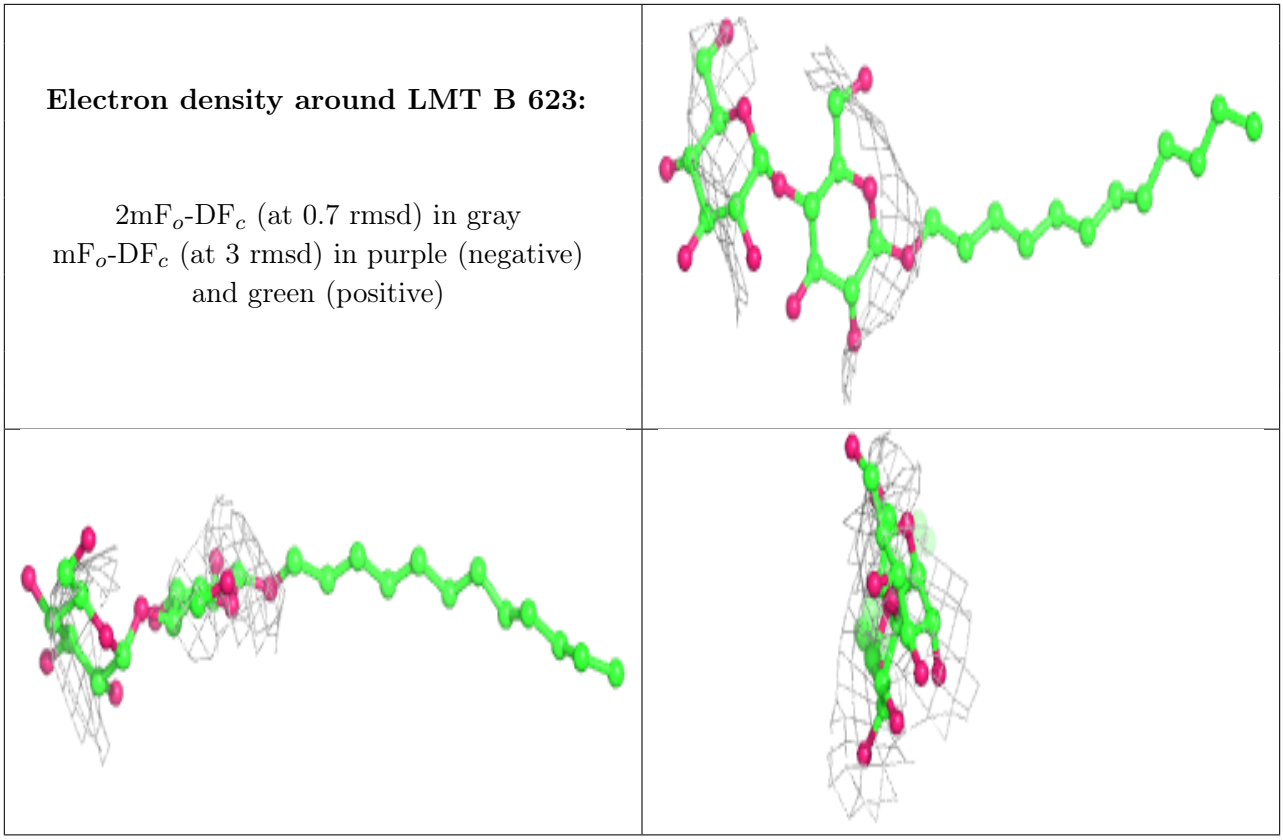






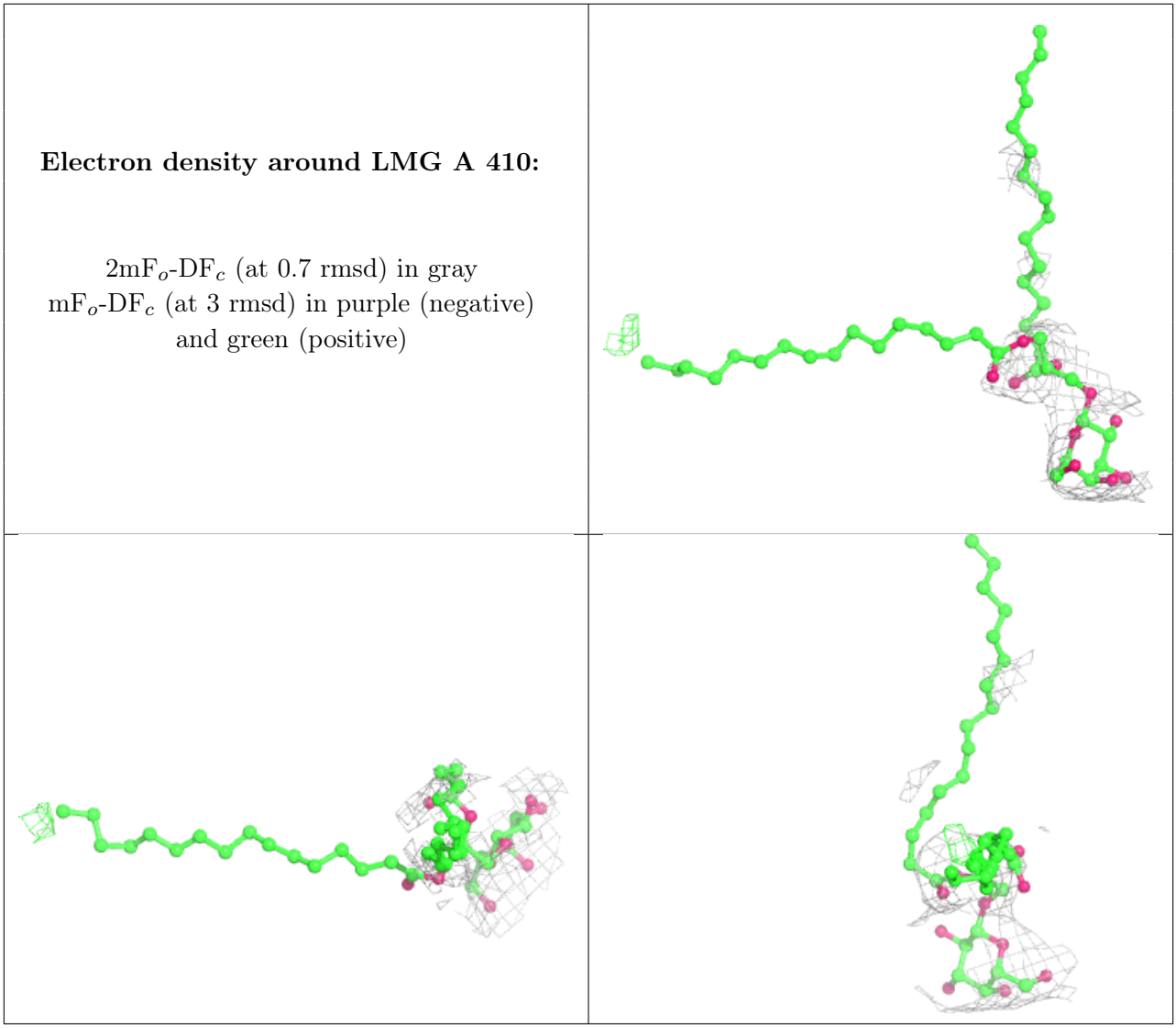
Electron density around LMT B 623:

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



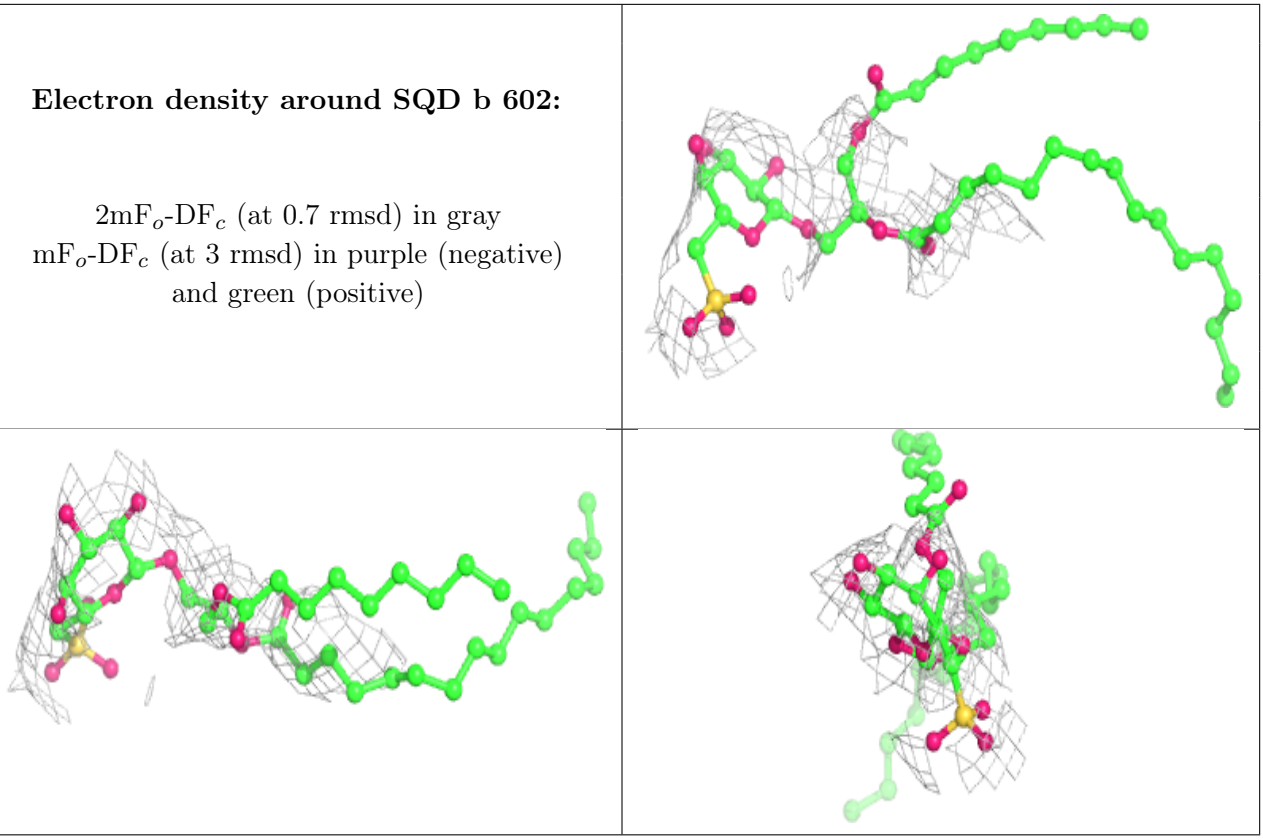
Electron density around LMG A 410:

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



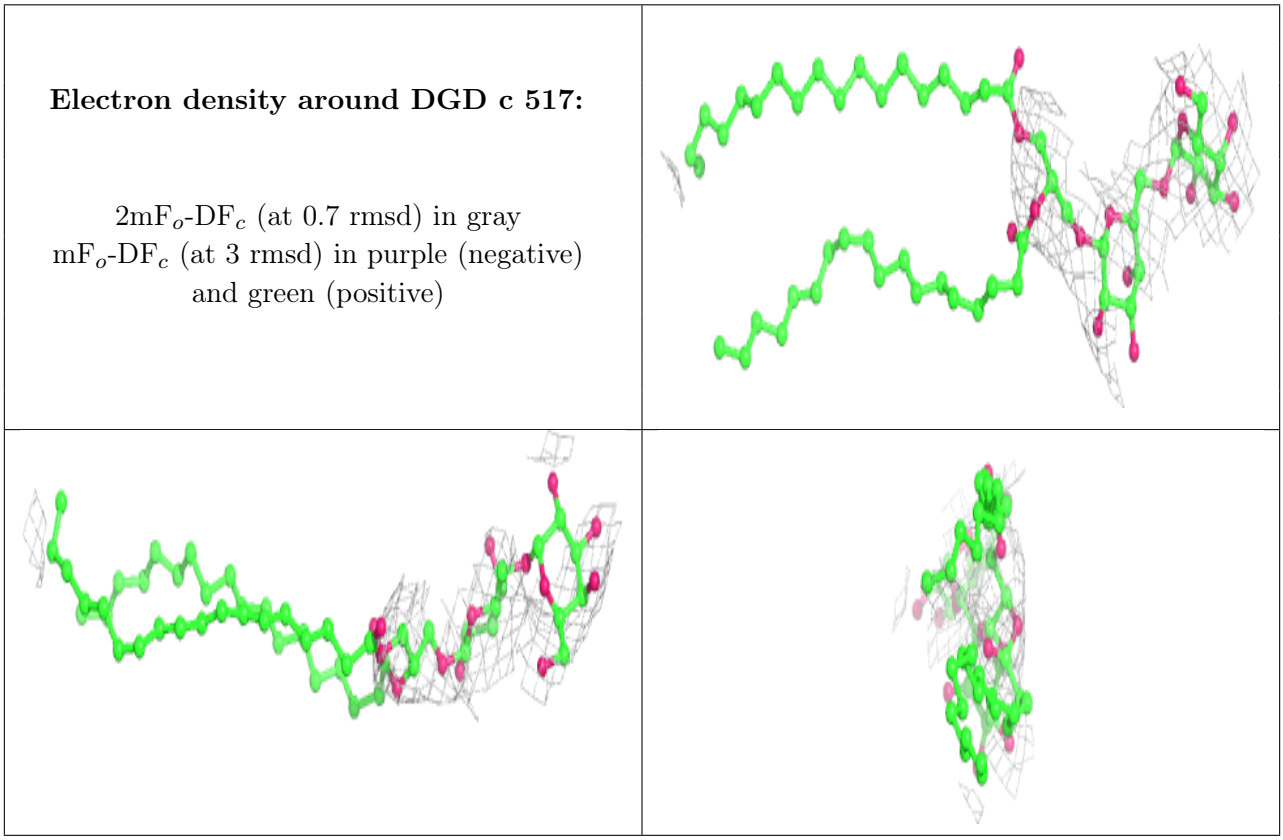
Electron density around SQD b 602:

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



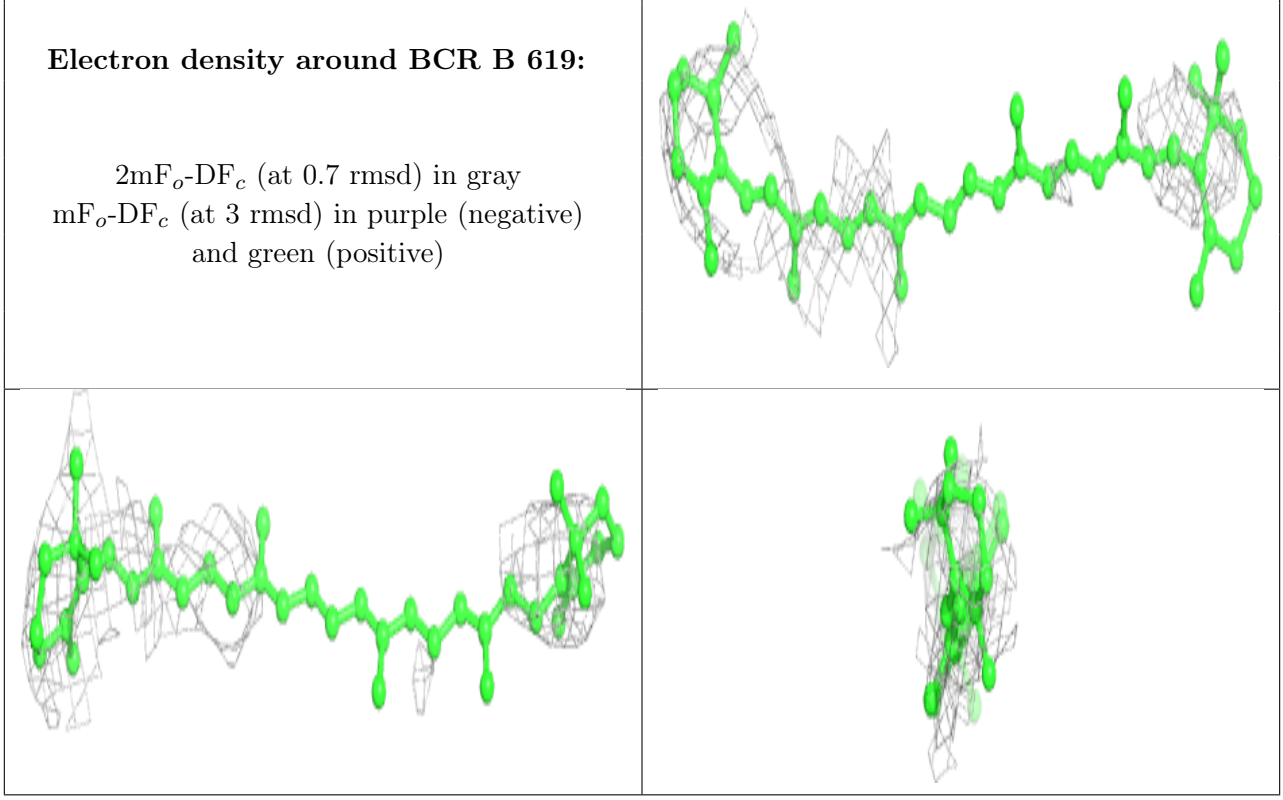
Electron density around DGD c 517:

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



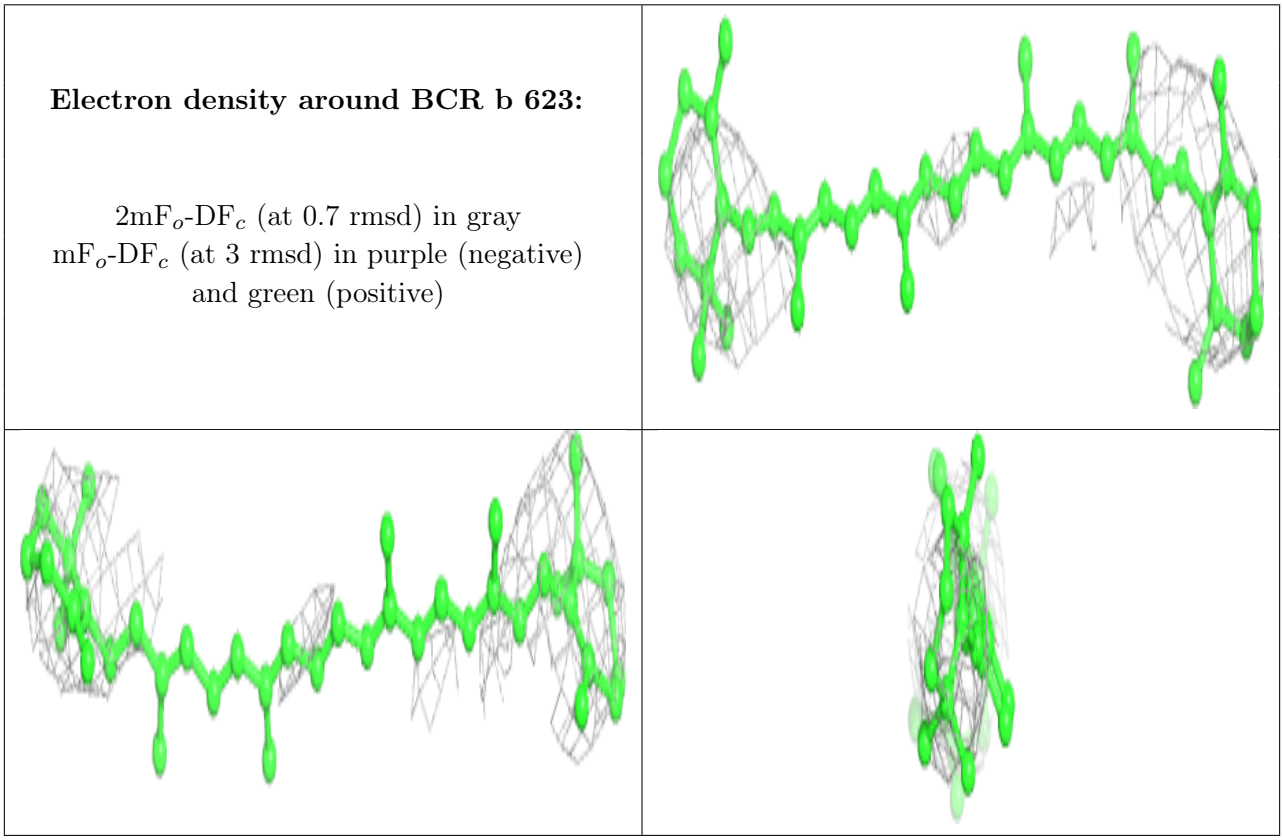
Electron density around BCR B 619:

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



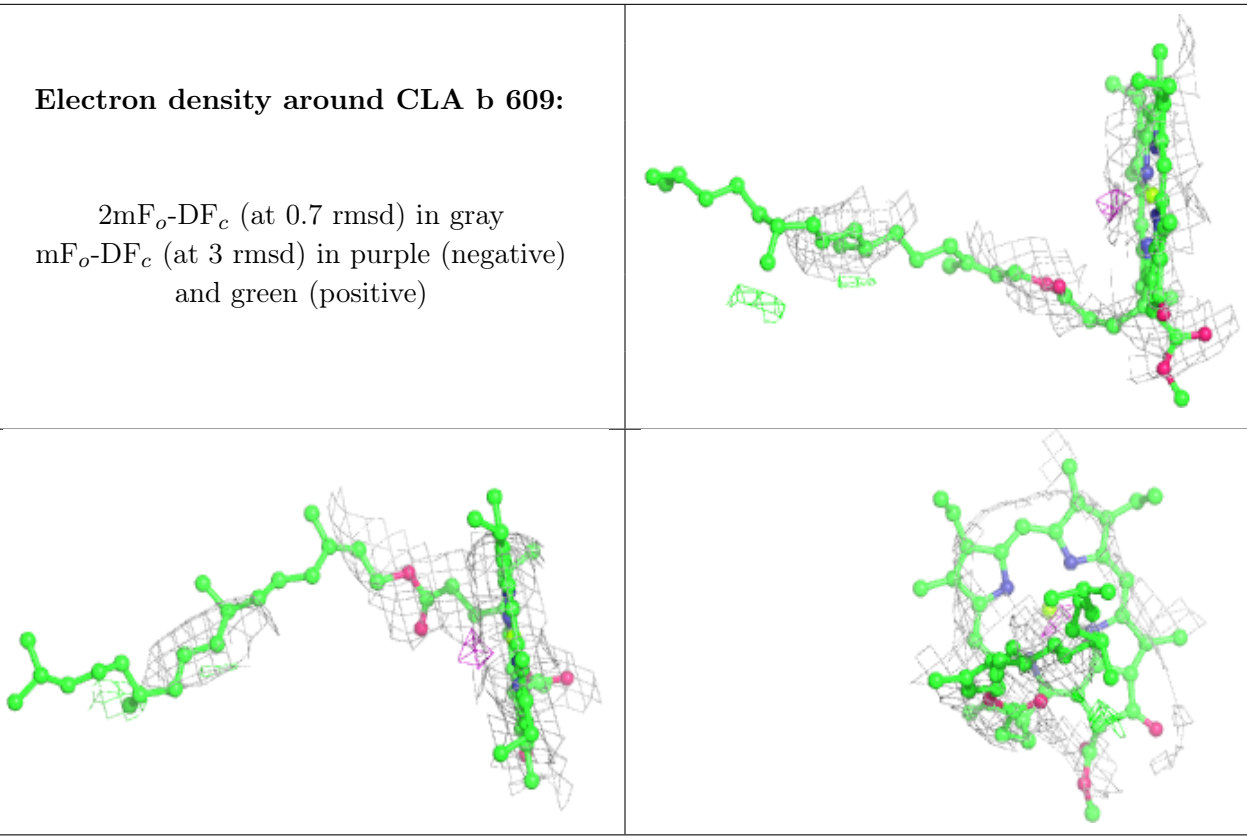
Electron density around BCR b 623:

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



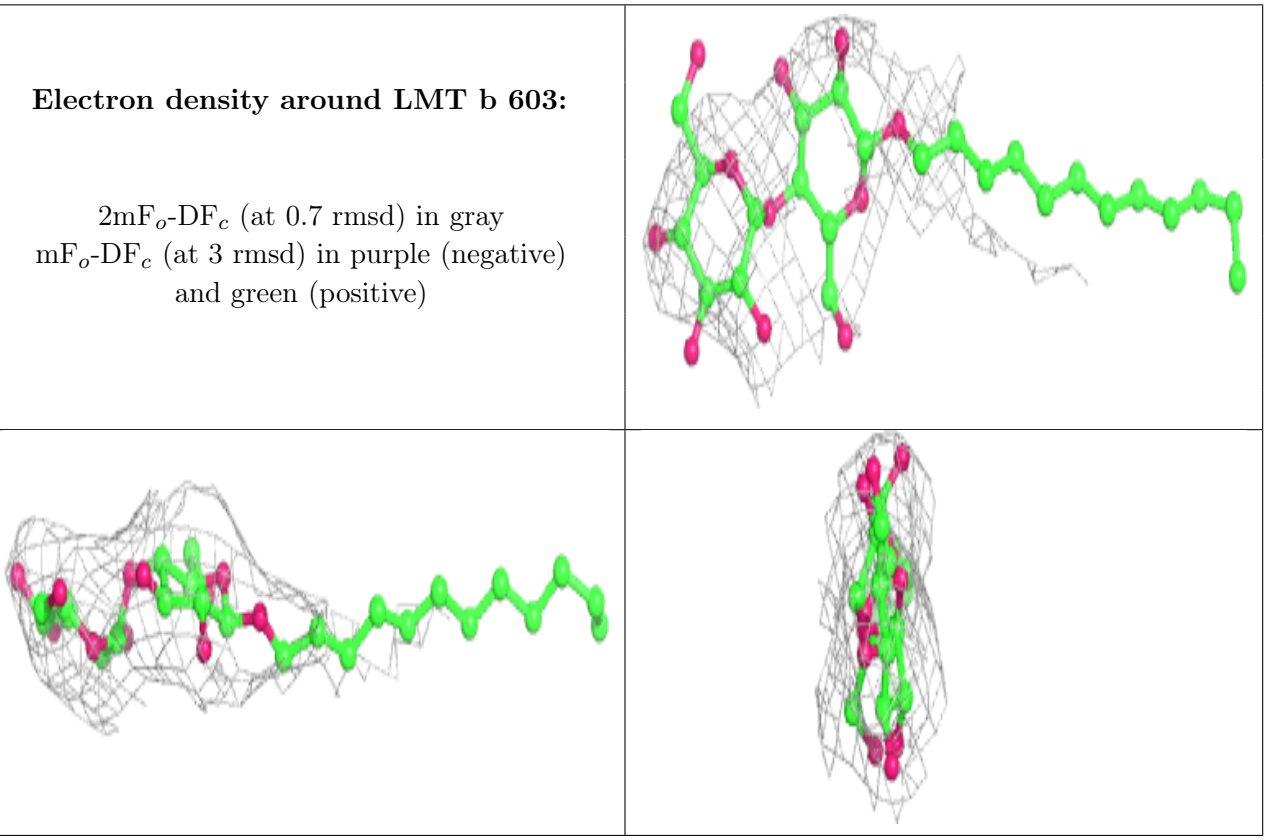
Electron density around CLA b 609:

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



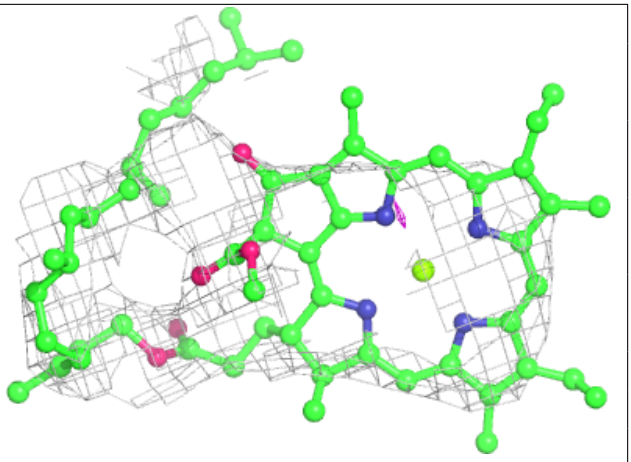
Electron density around LMT b 603:

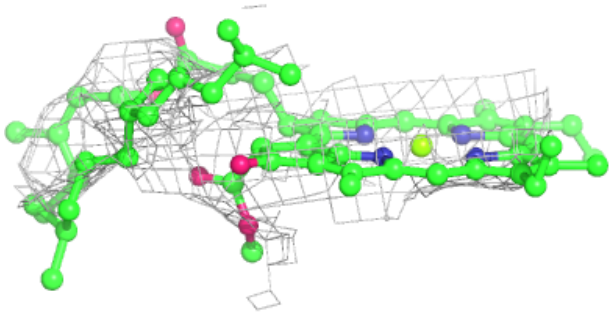
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

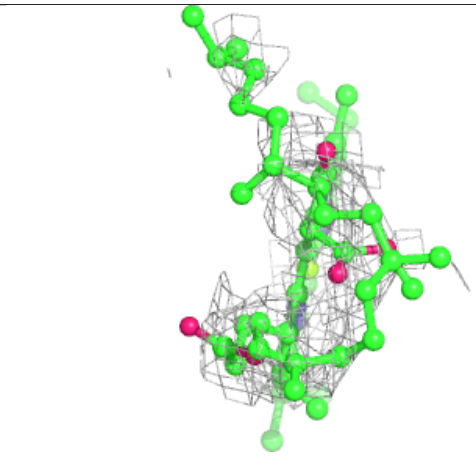


Electron density around CLA b 613:

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

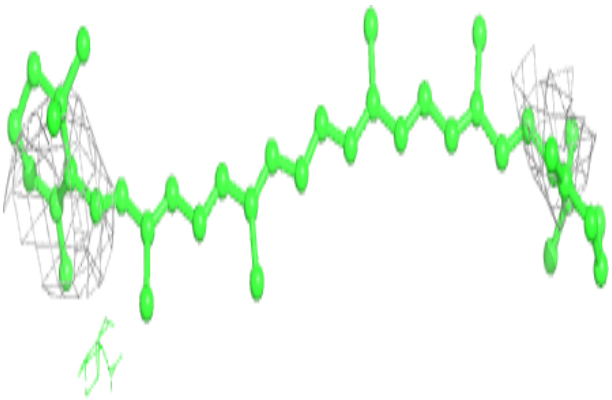


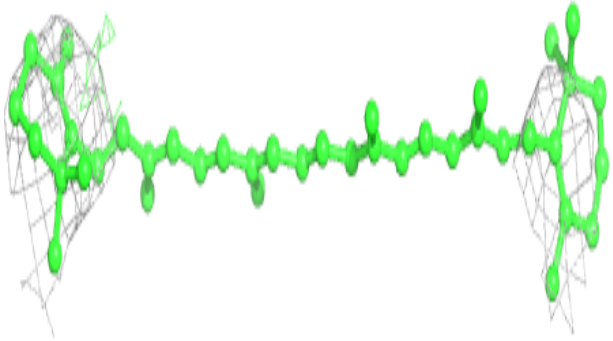


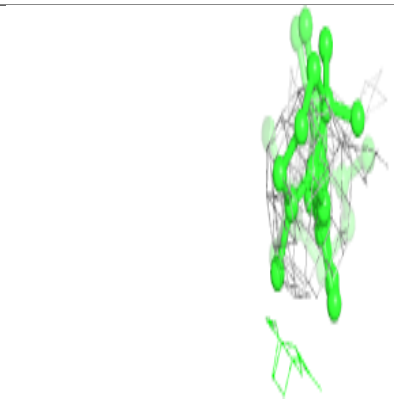


Electron density around BCR c 521:

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

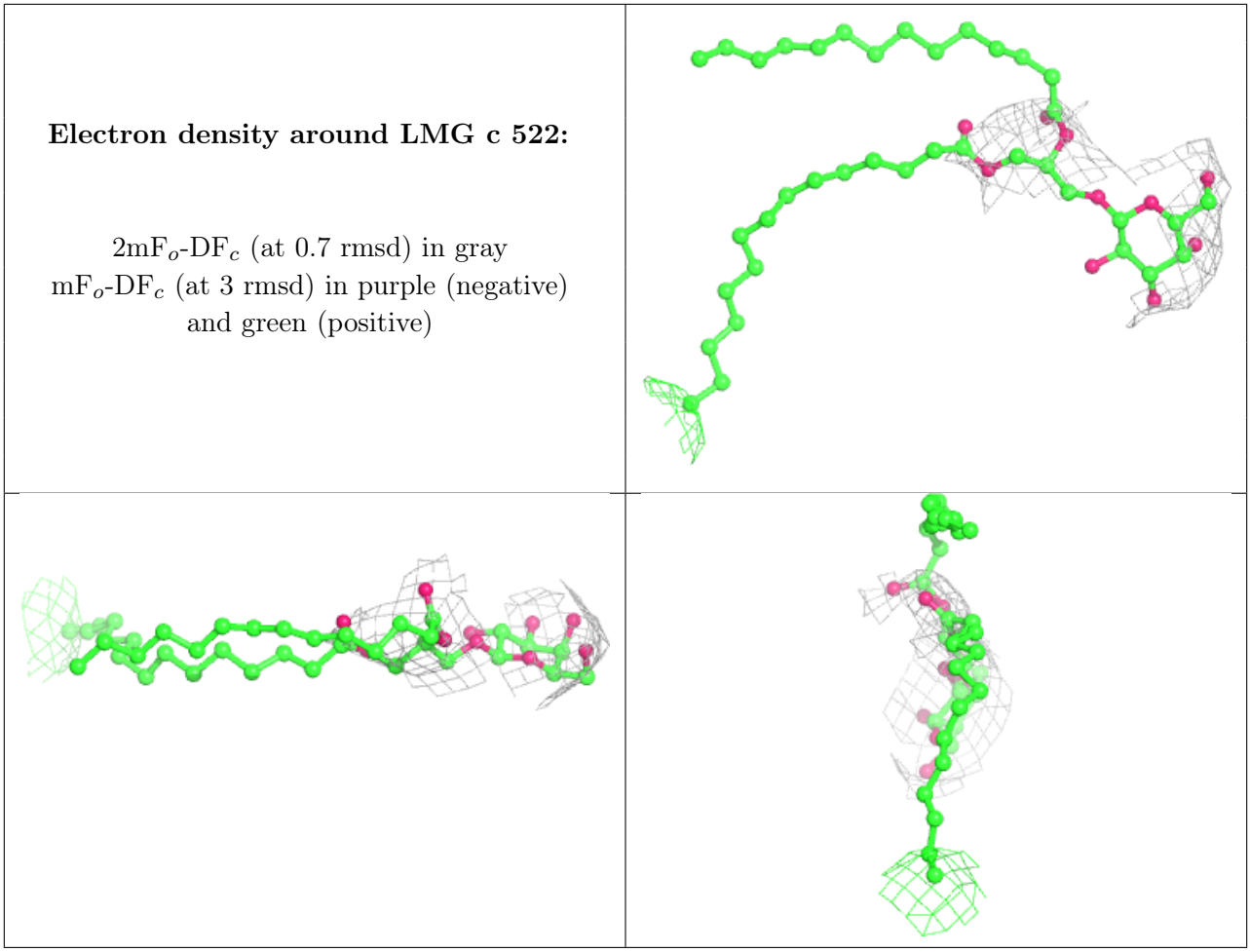






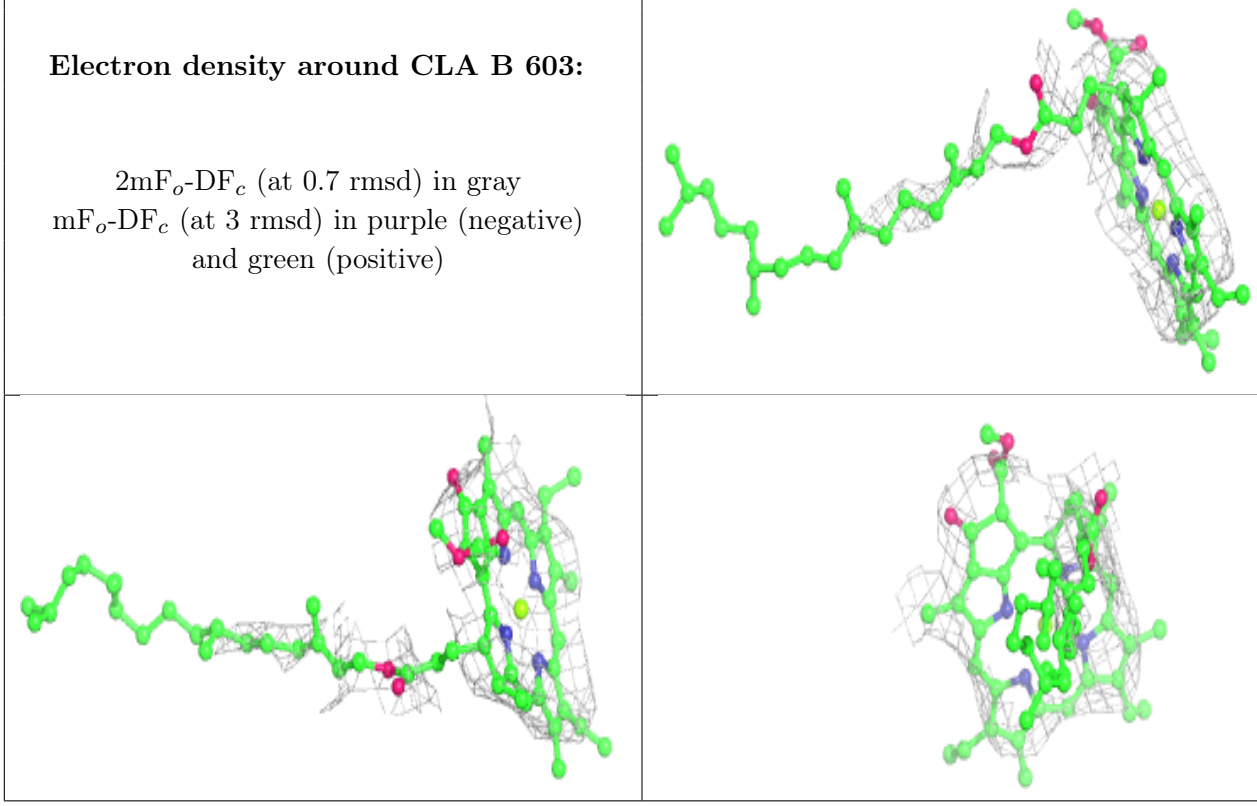
Electron density around LMG c 522:

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



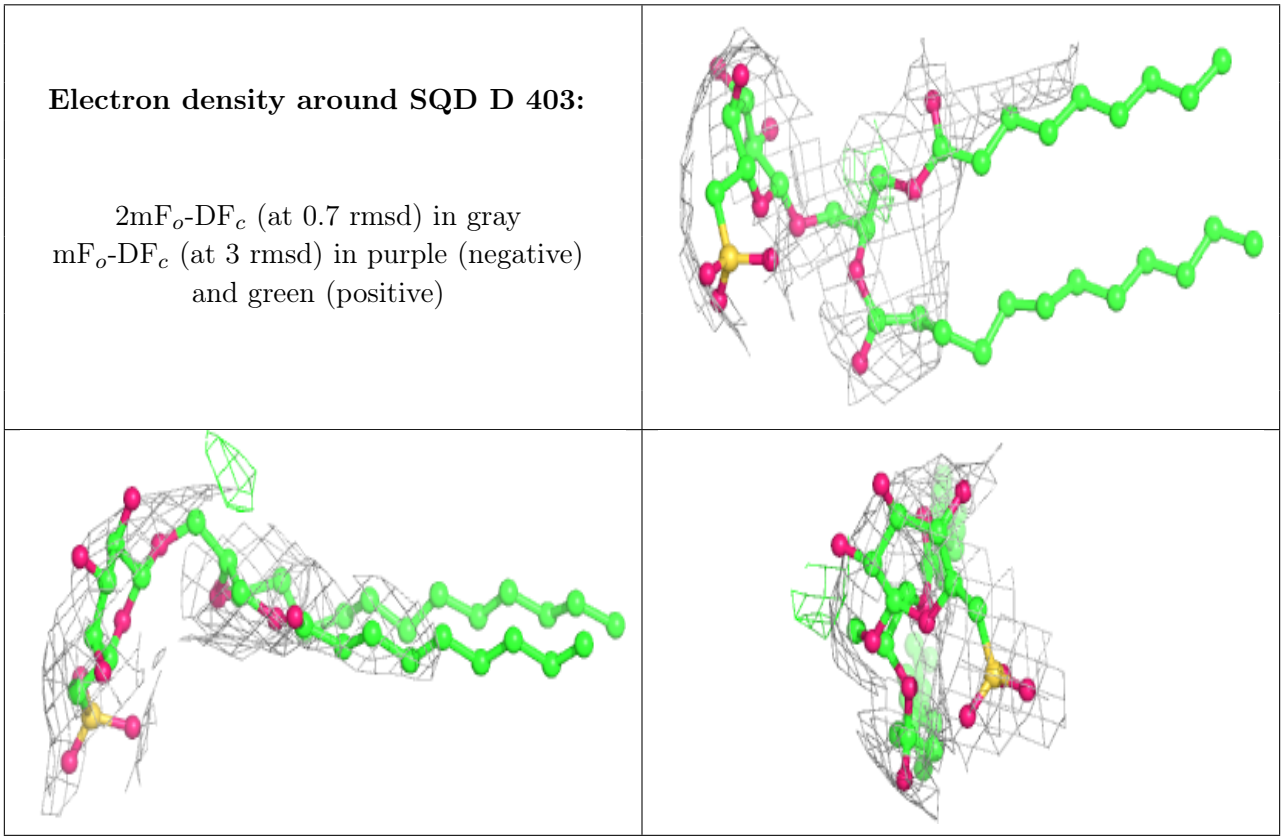
Electron density around CLA B 603:

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



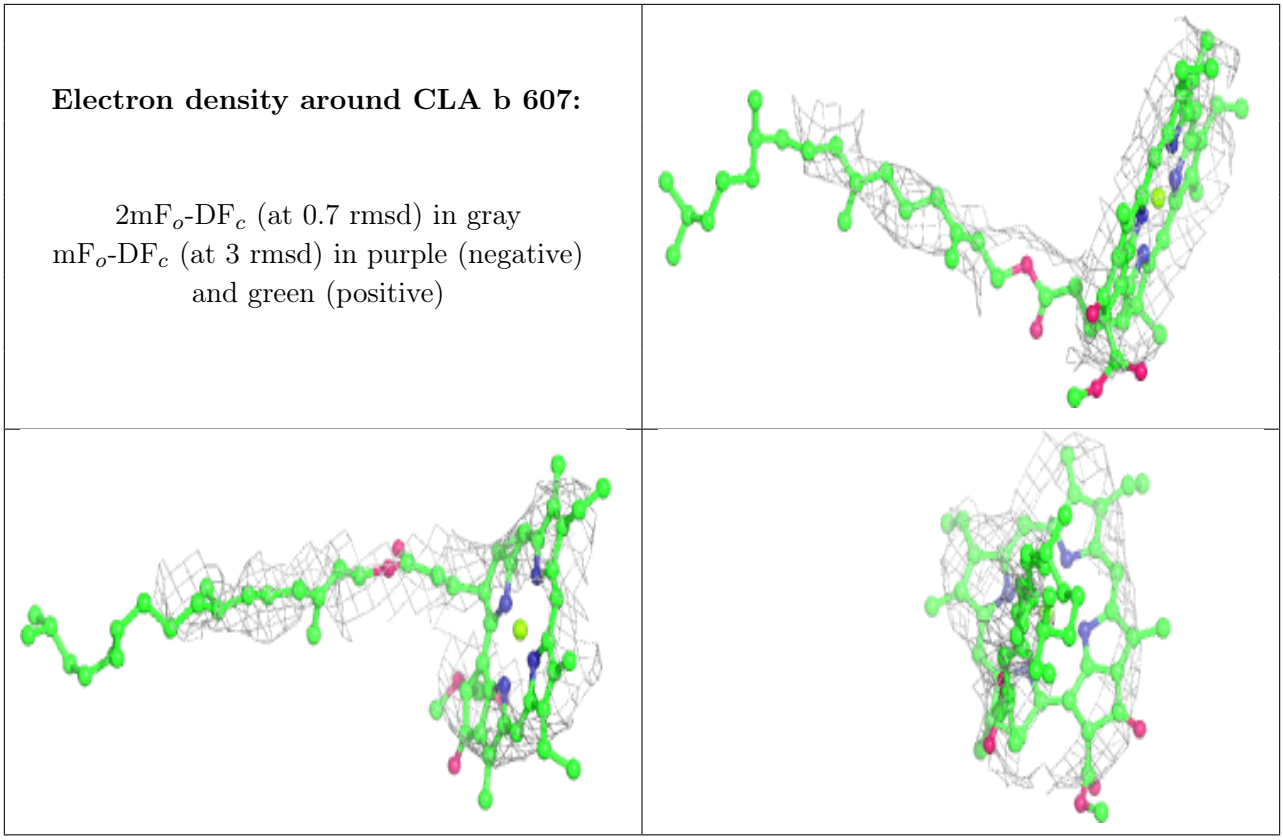
Electron density around SQD D 403:

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



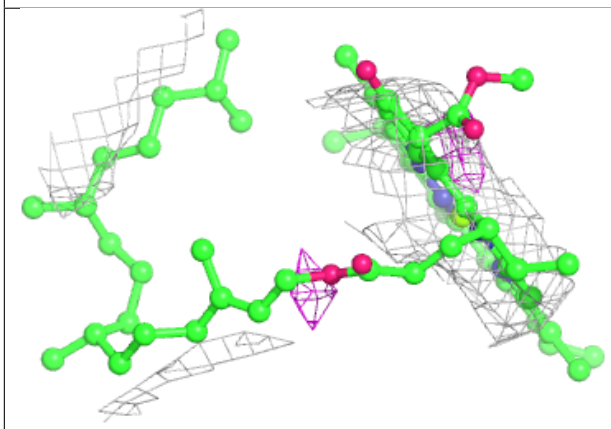
Electron density around CLA b 607:

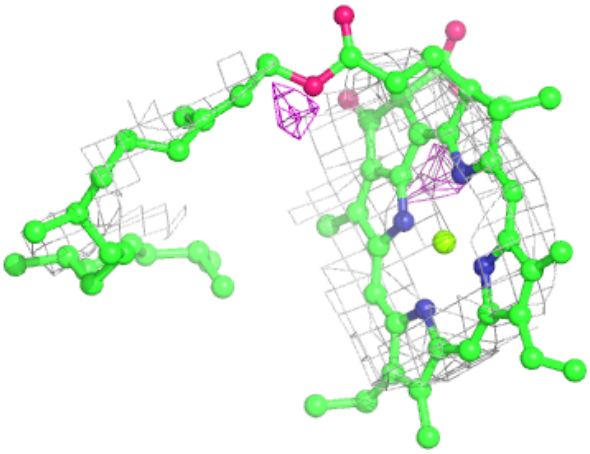
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

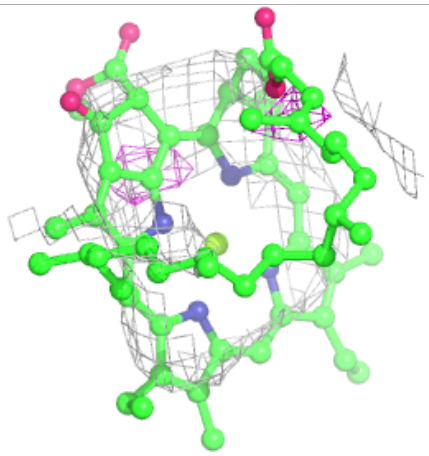


Electron density around CLA c 503:

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

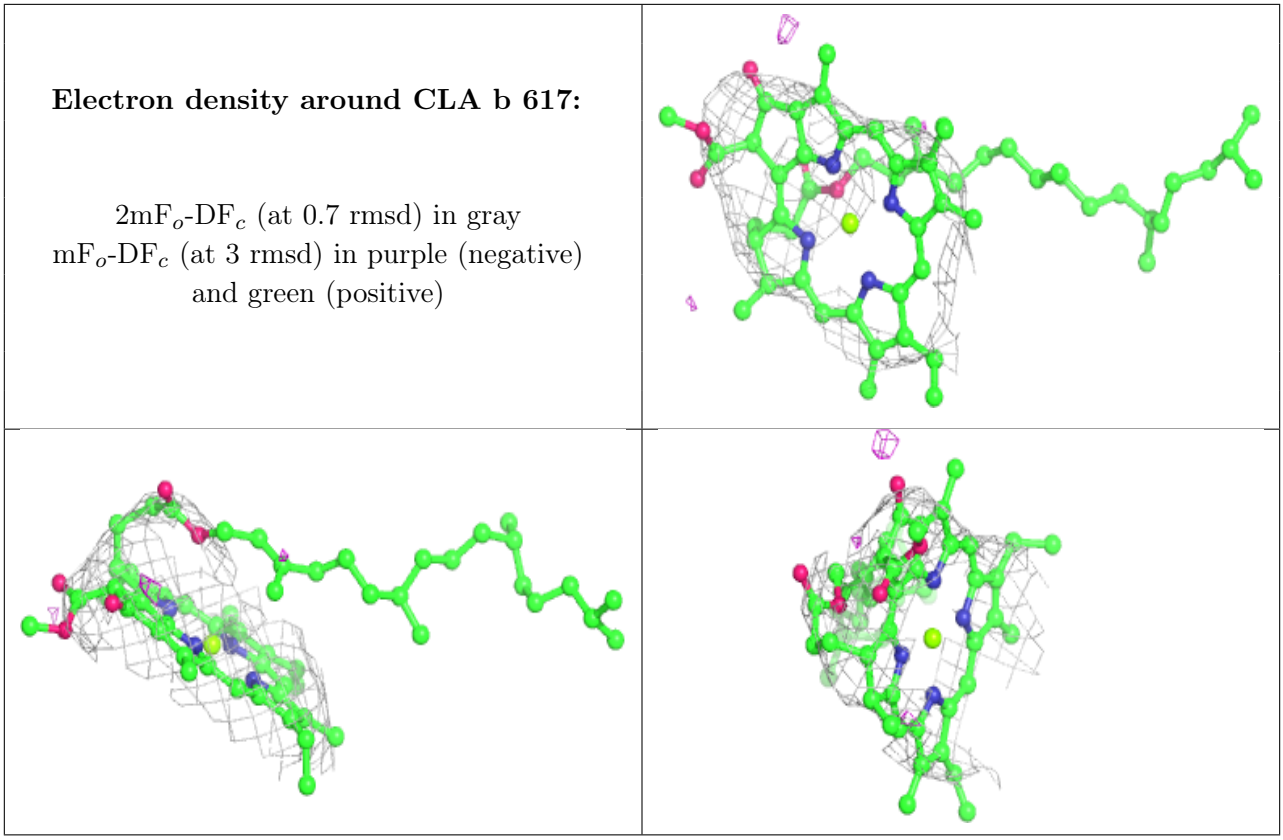






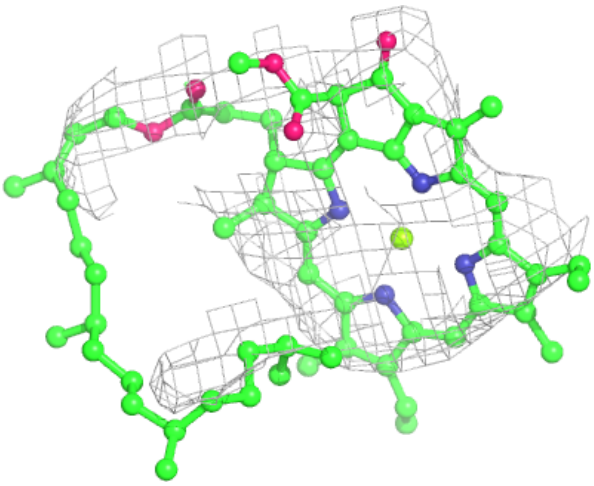
Electron density around CLA b 617:

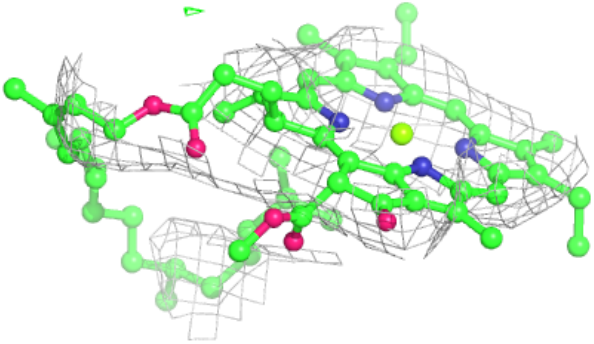
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

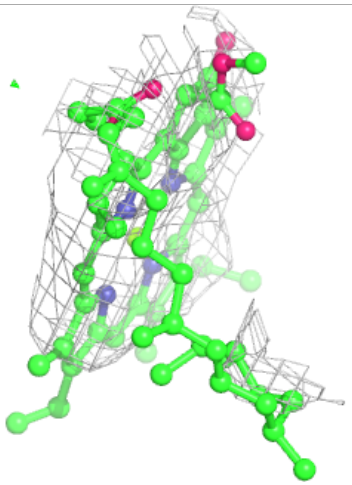


Electron density around CLA b 618:

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

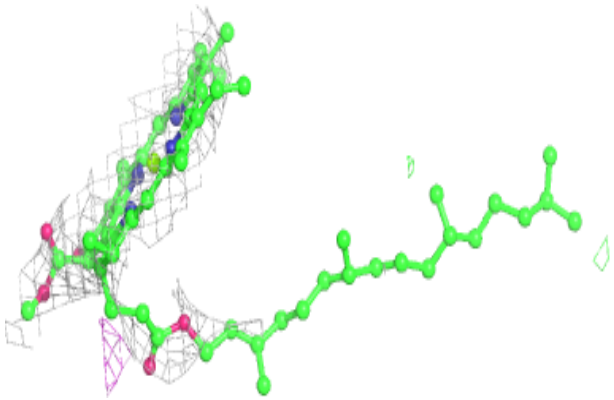


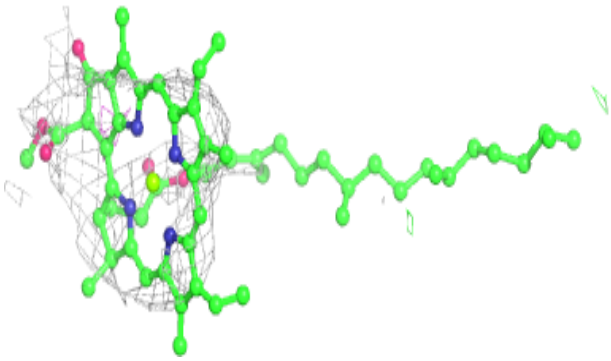


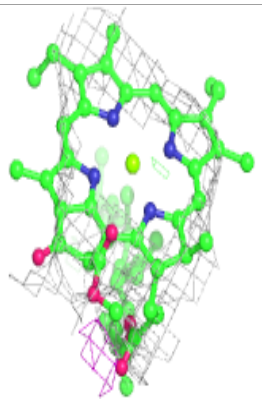


Electron density around CLA C 520:

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

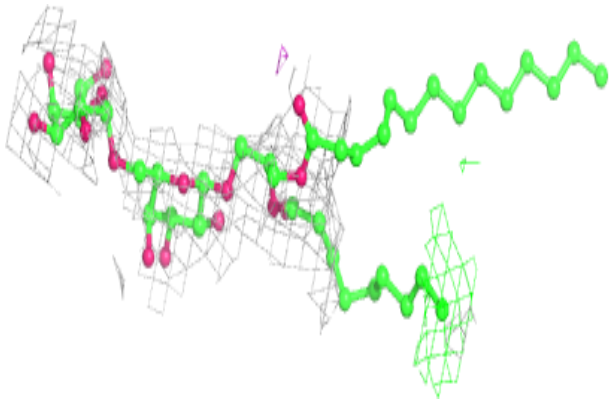


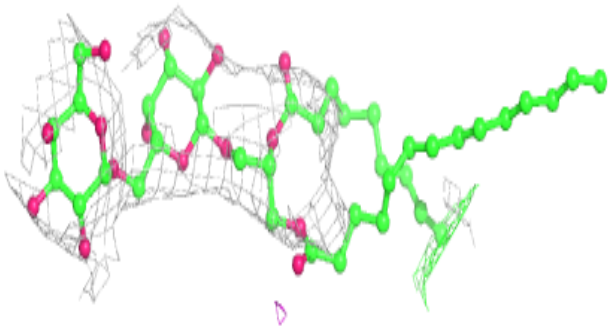


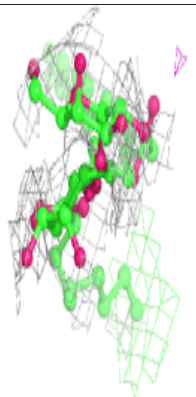


Electron density around DGD C 515:

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

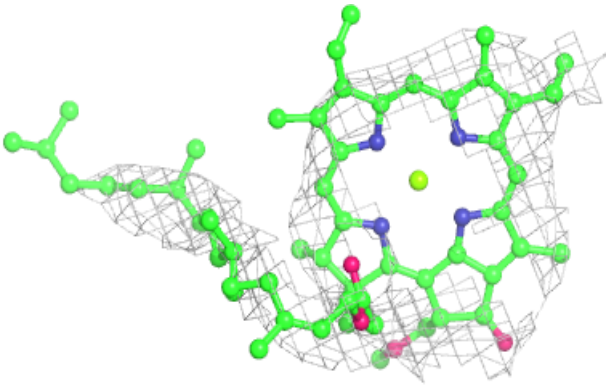


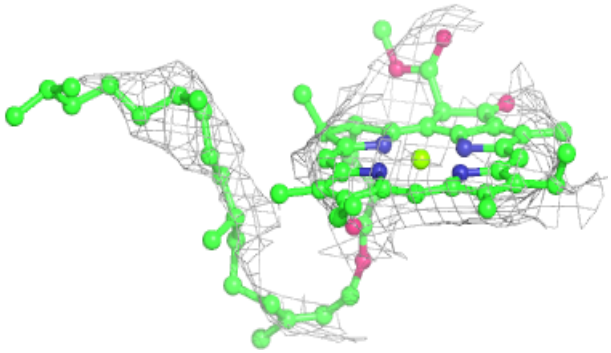


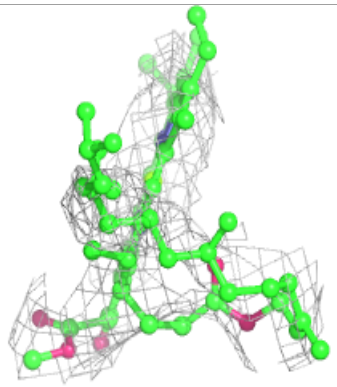


Electron density around CLA a 405:

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

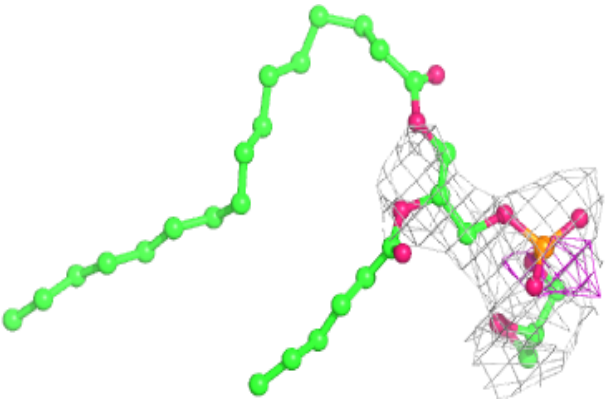


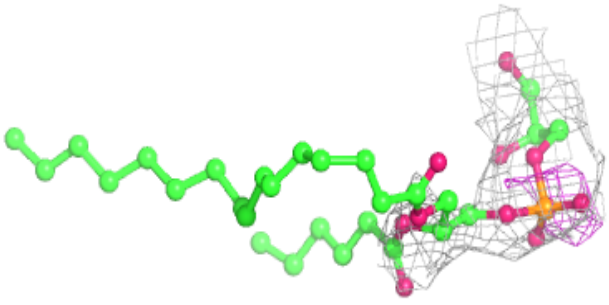




Electron density around LHG a 412:

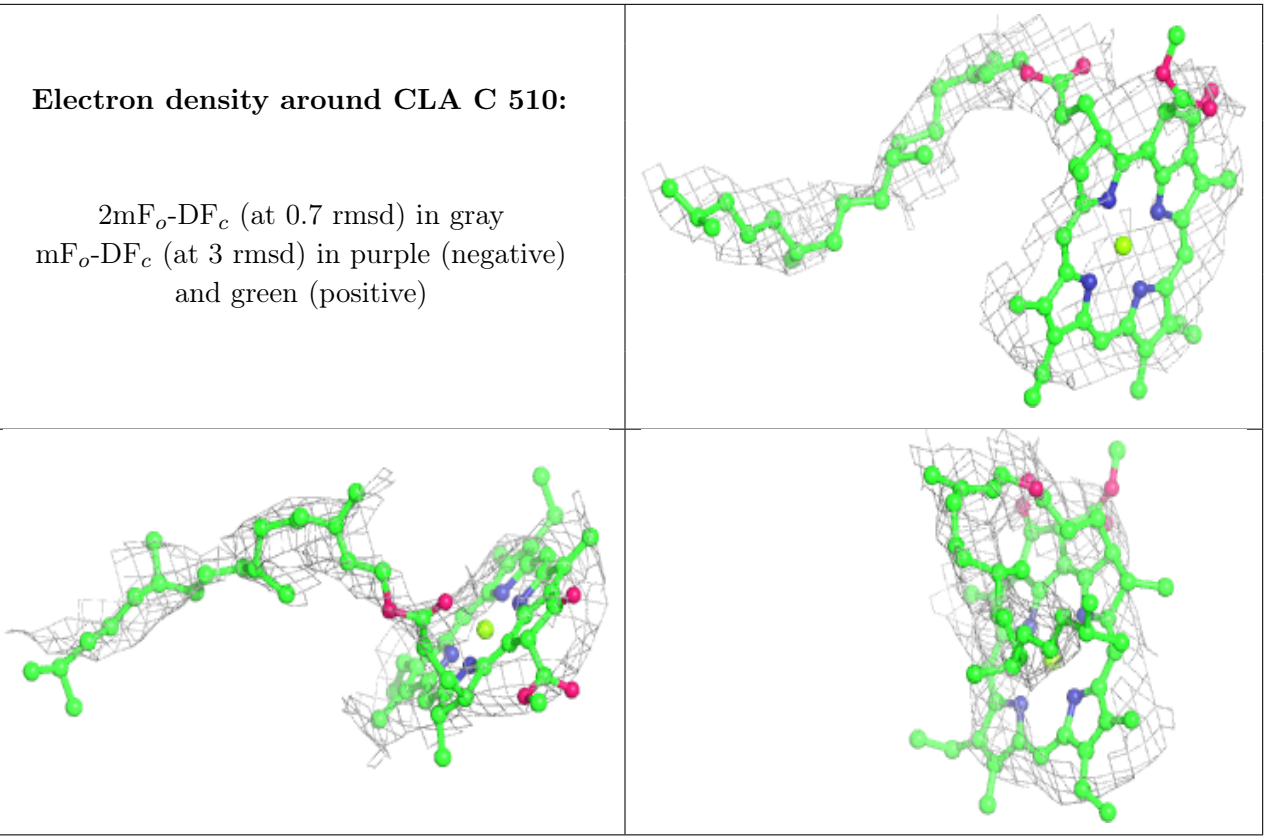
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





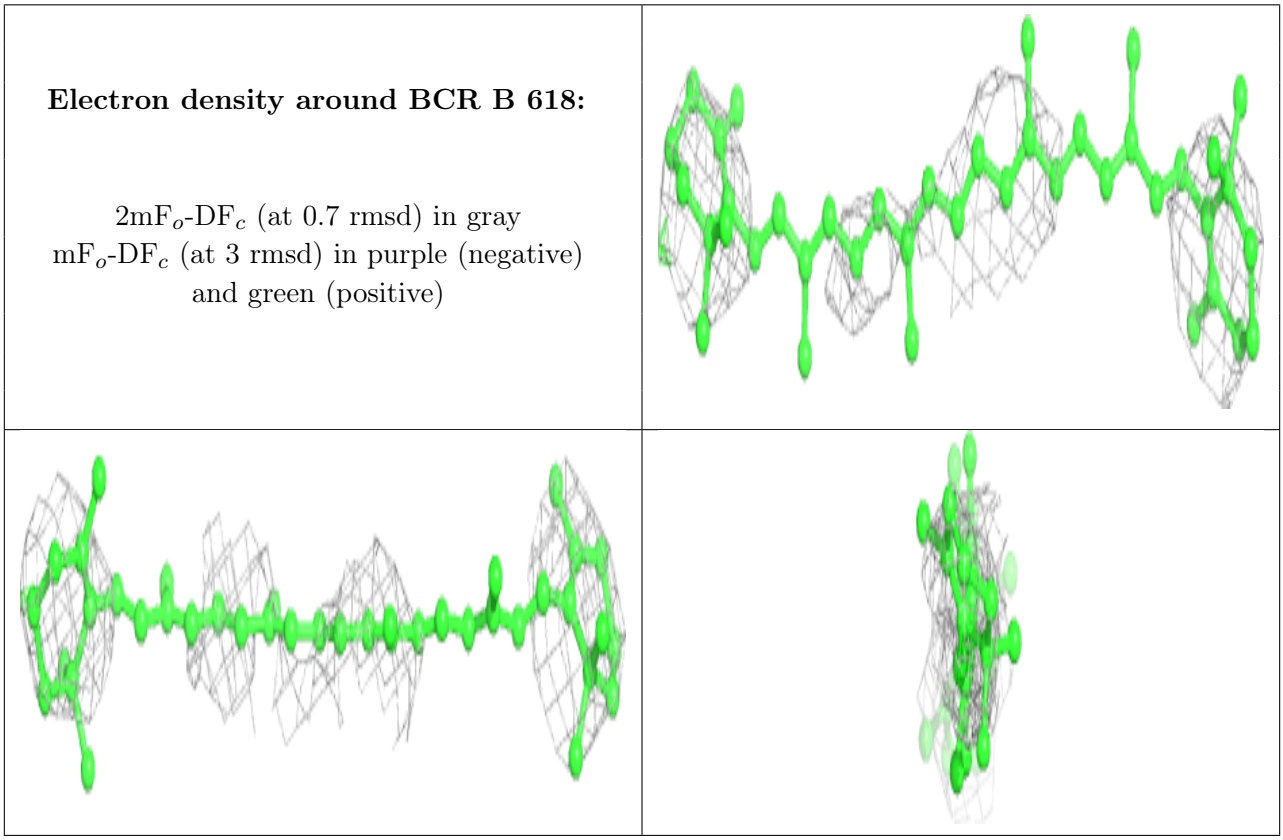
Electron density around CLA C 510:

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



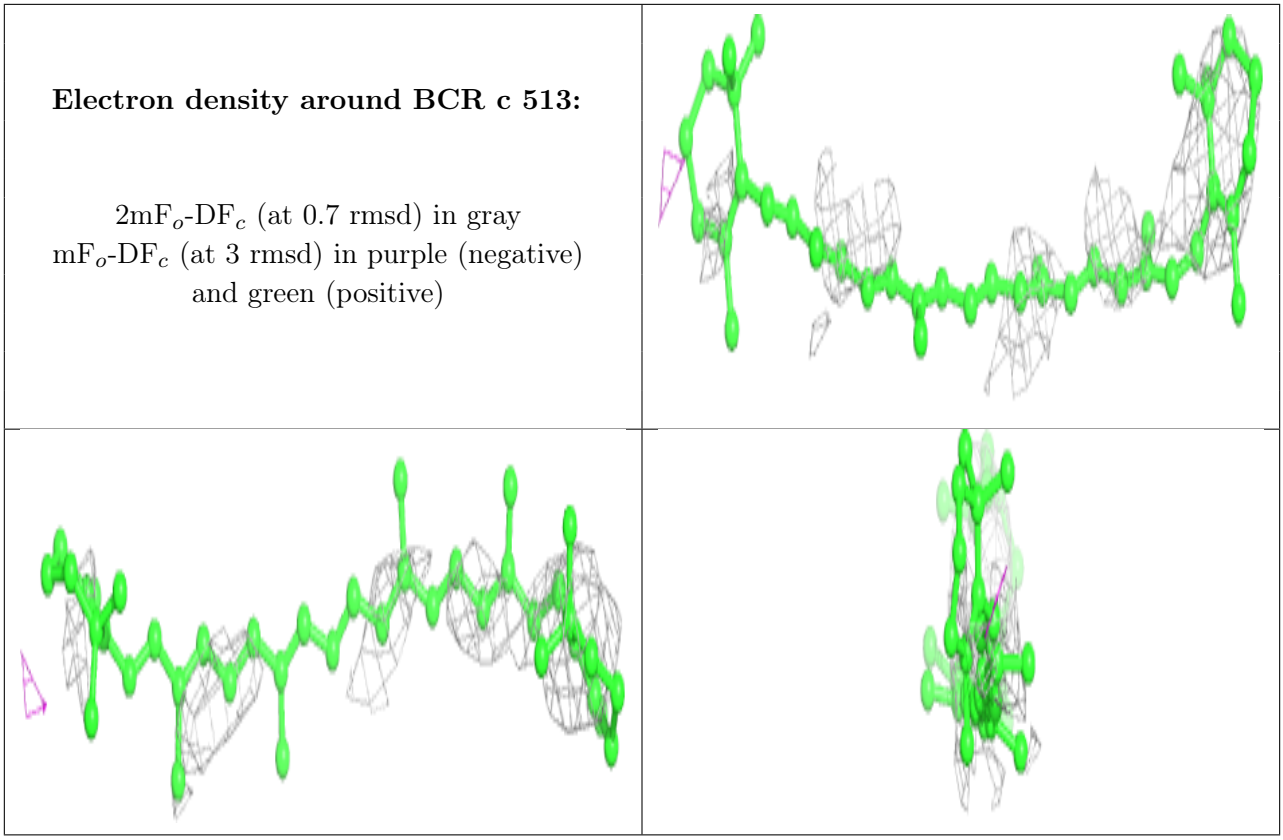
Electron density around BCR B 618:

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



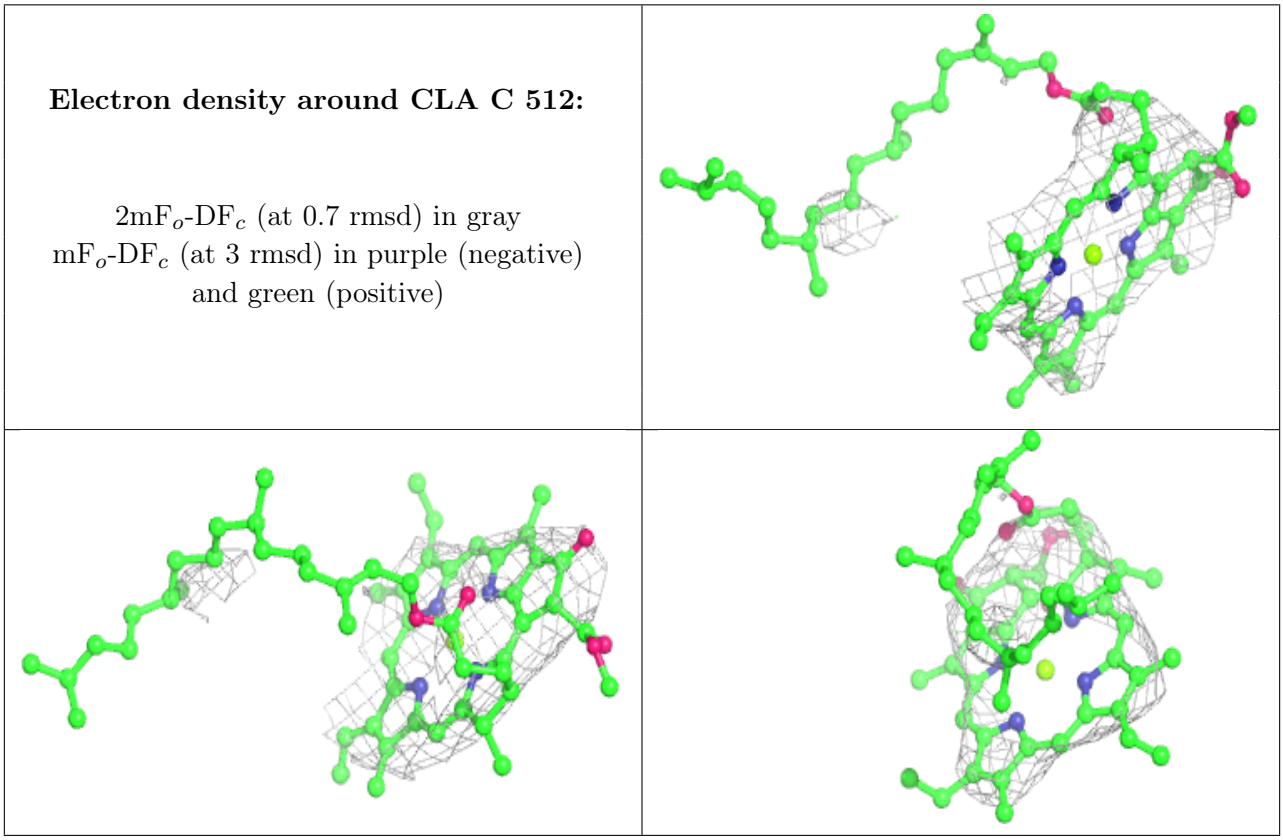
Electron density around BCR c 513:

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



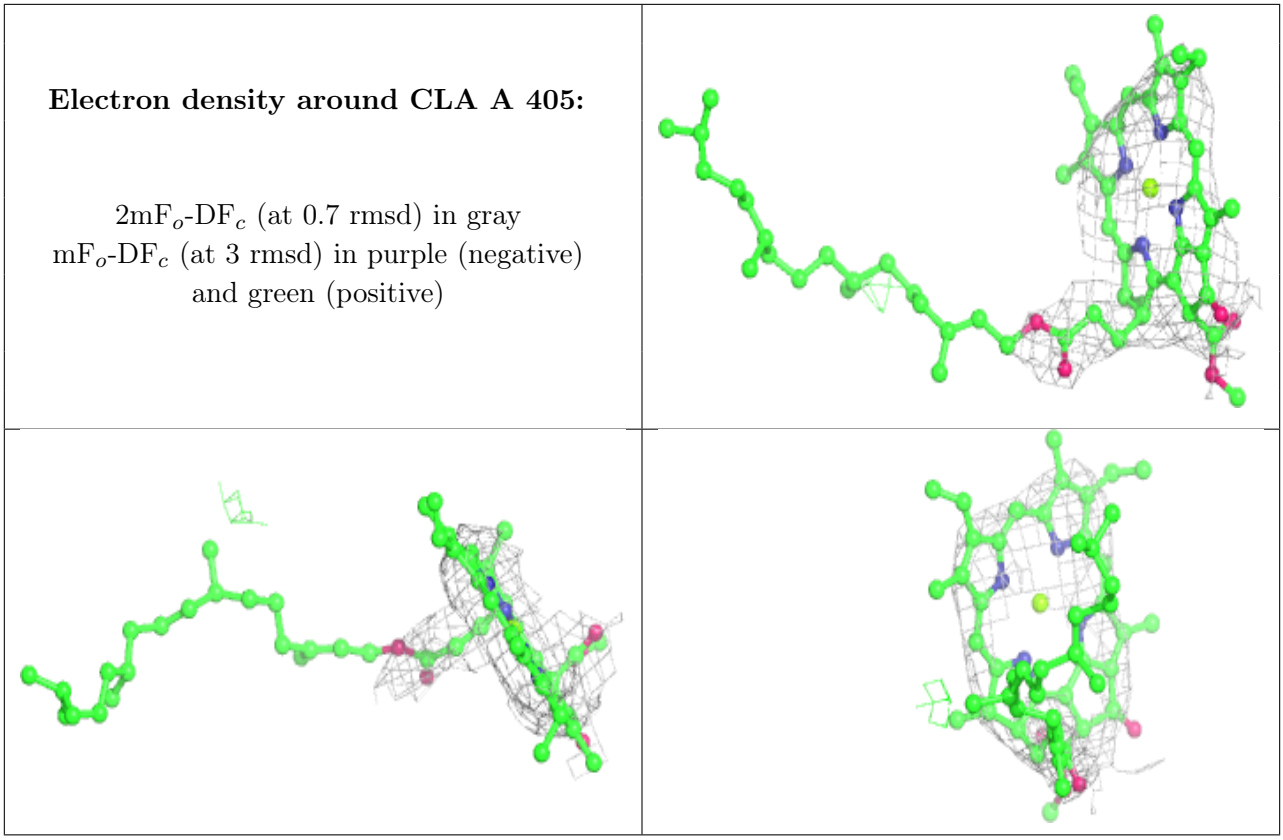
Electron density around CLA C 512:

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



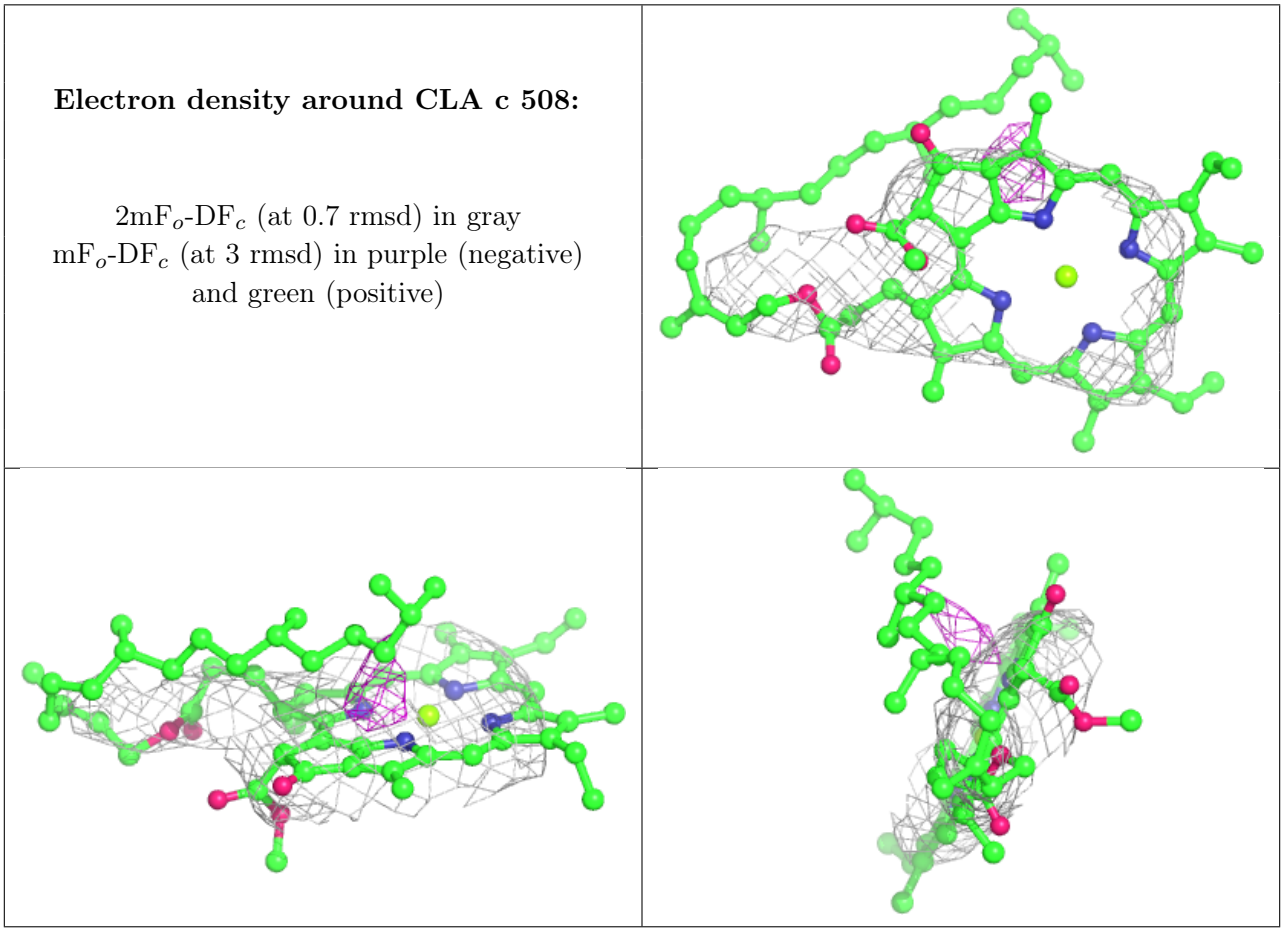
Electron density around CLA A 405:

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



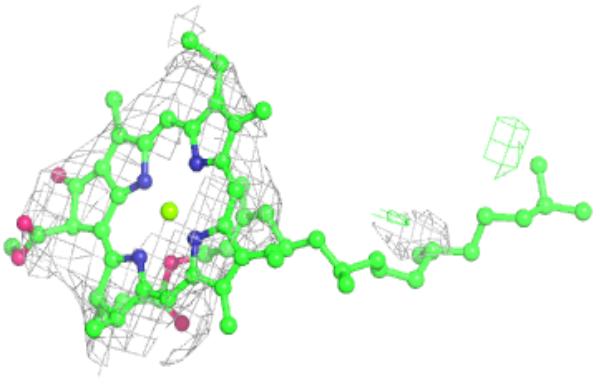
Electron density around CLA c 508:

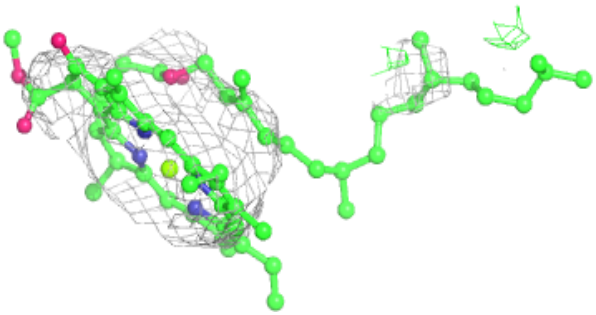
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

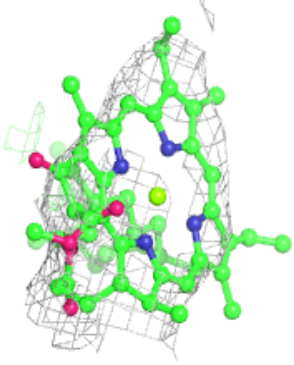


Electron density around CLA C 504:

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

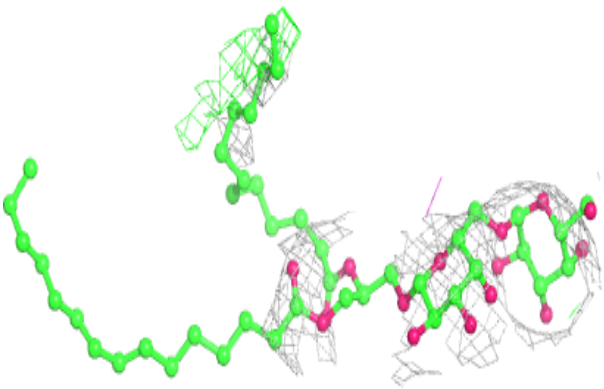


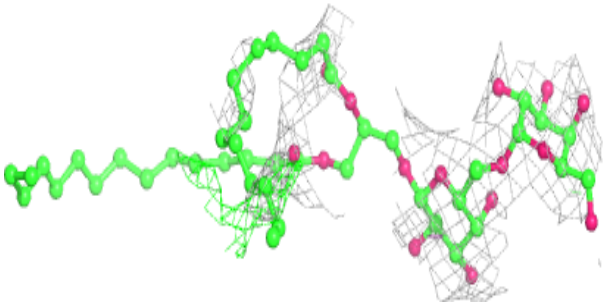


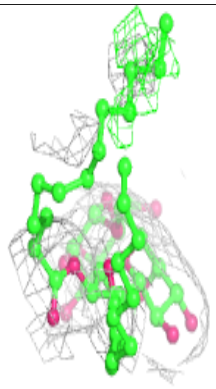


Electron density around DGD B 620:

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

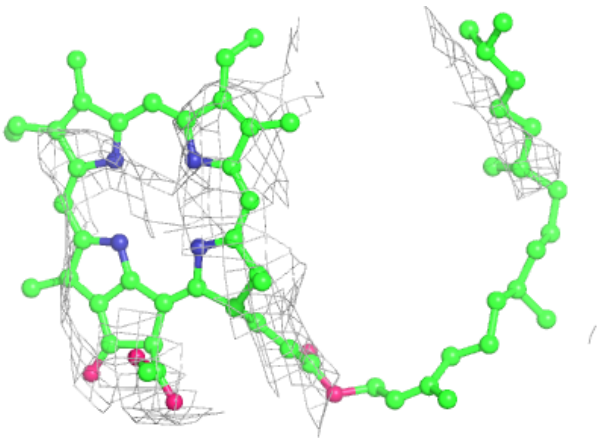


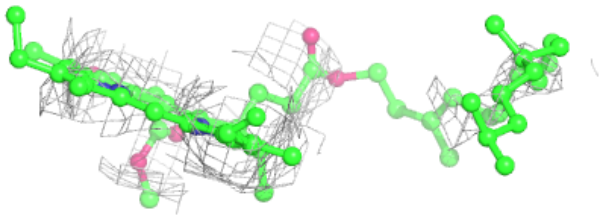


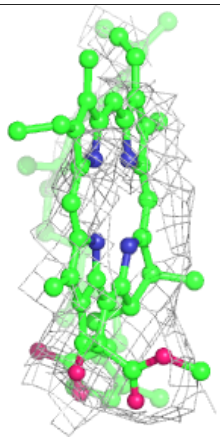


Electron density around PHO D 401:

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

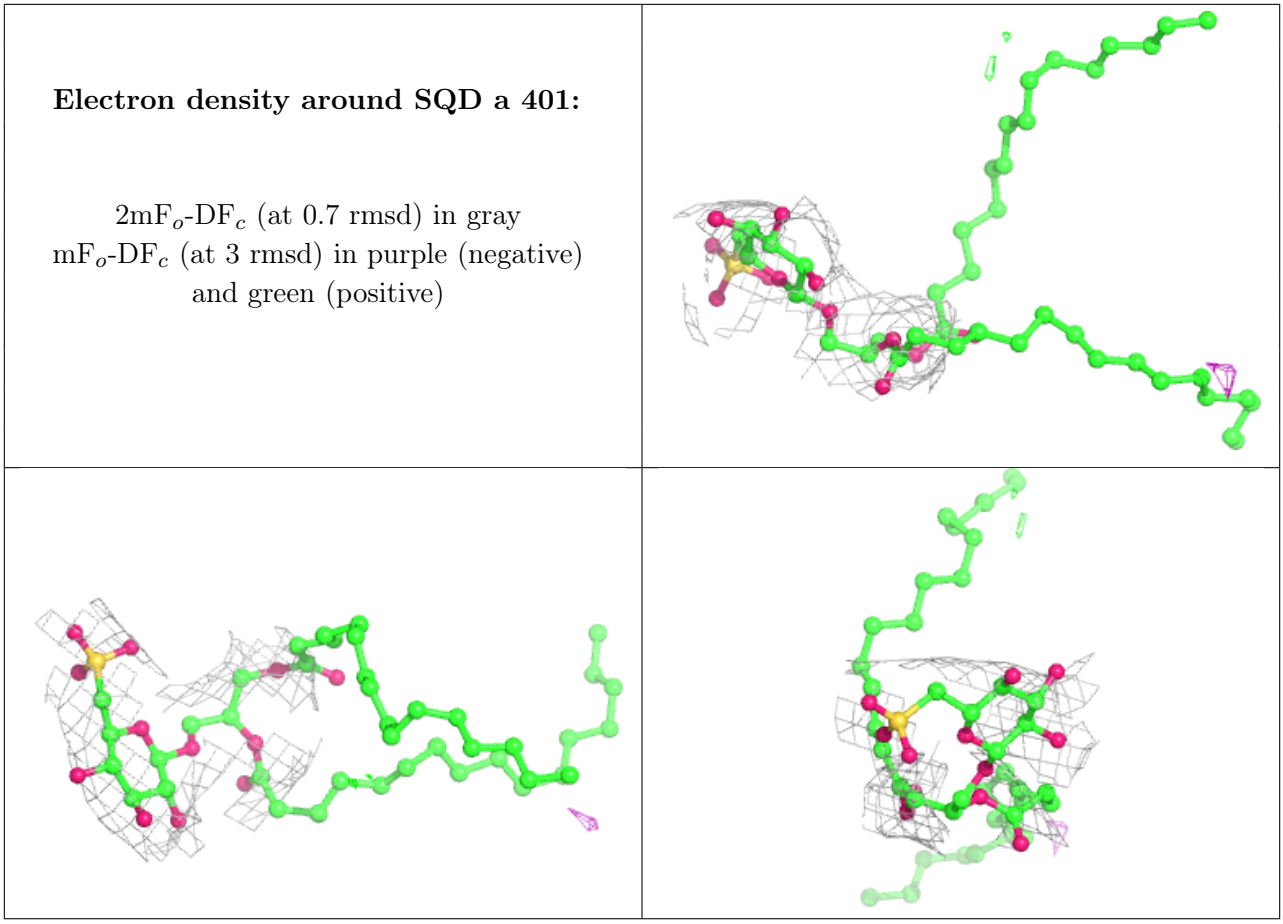






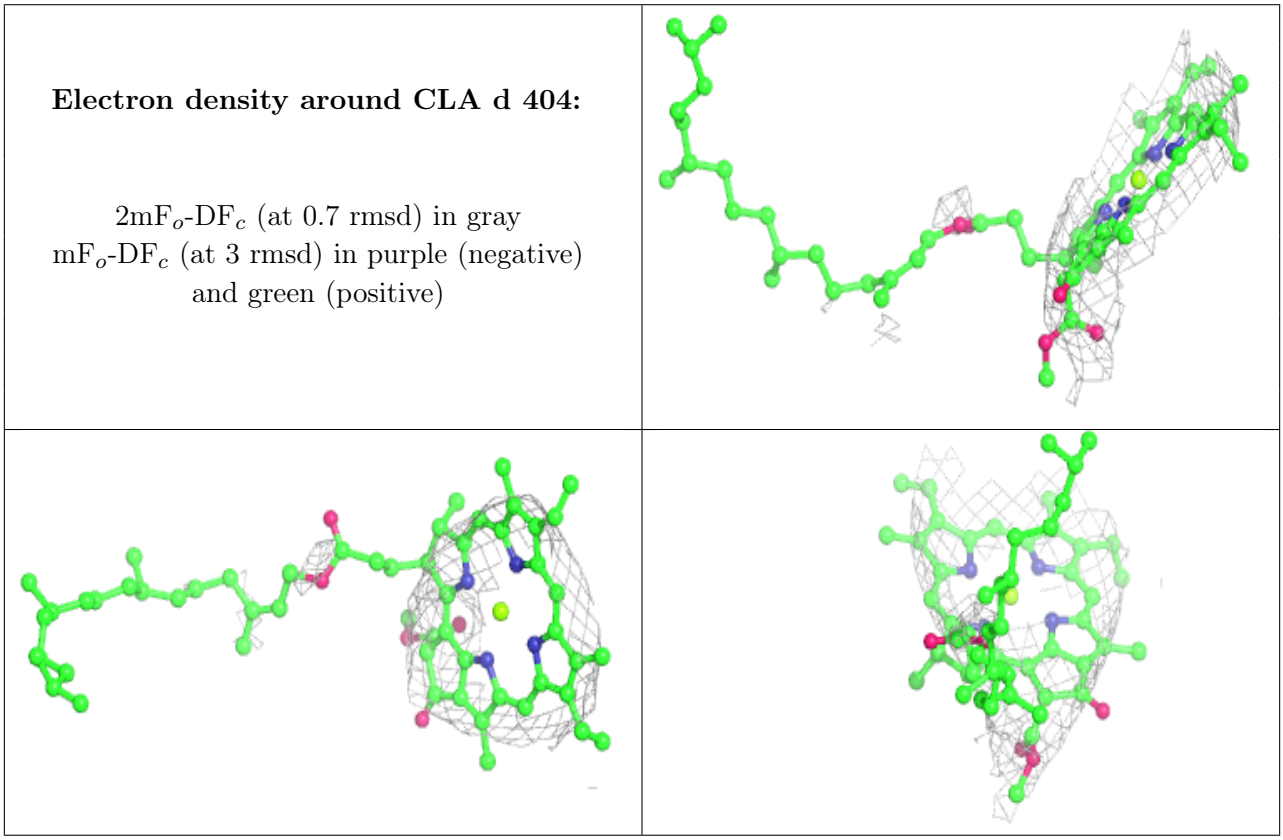
Electron density around SQD a 401:

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



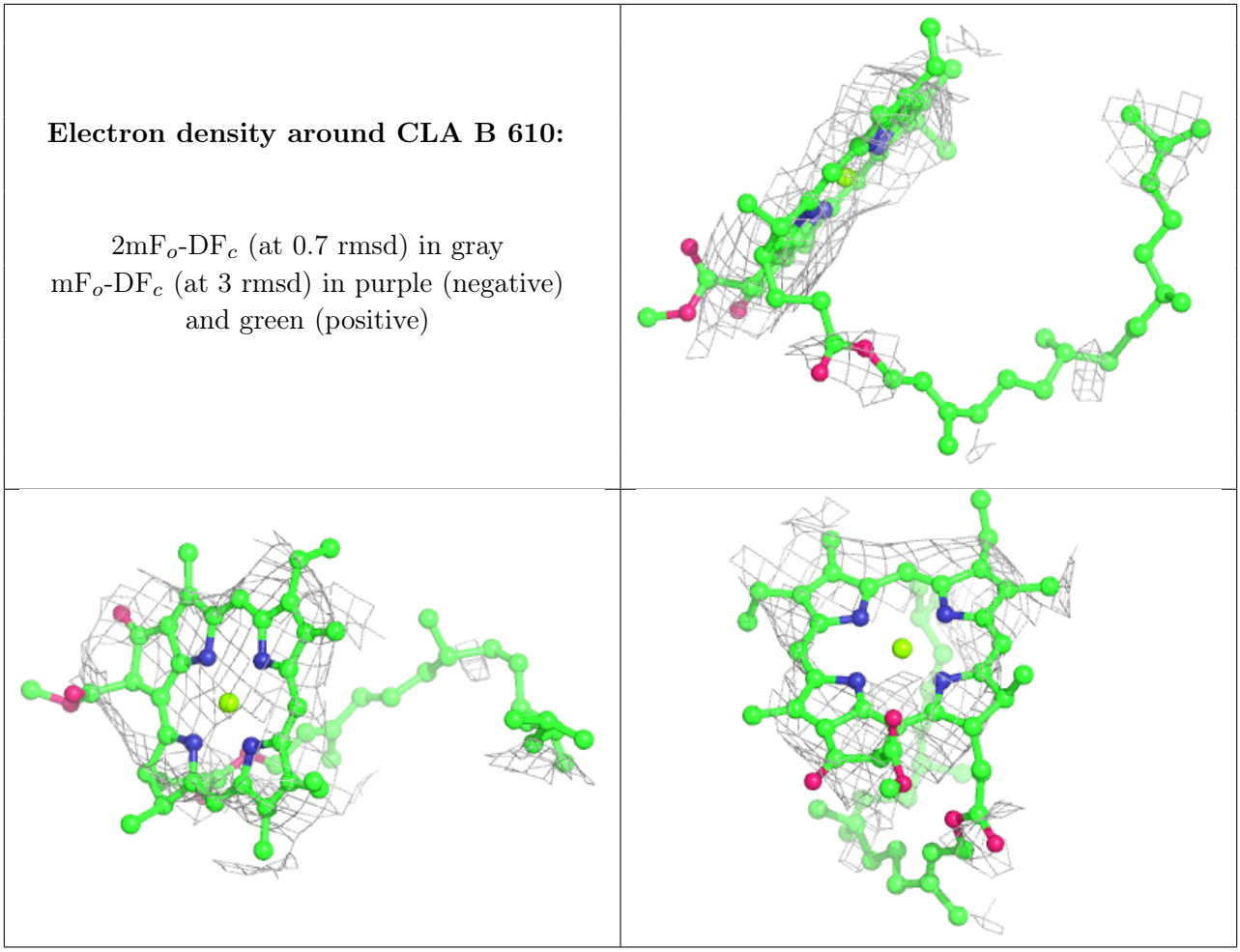
Electron density around CLA d 404:

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



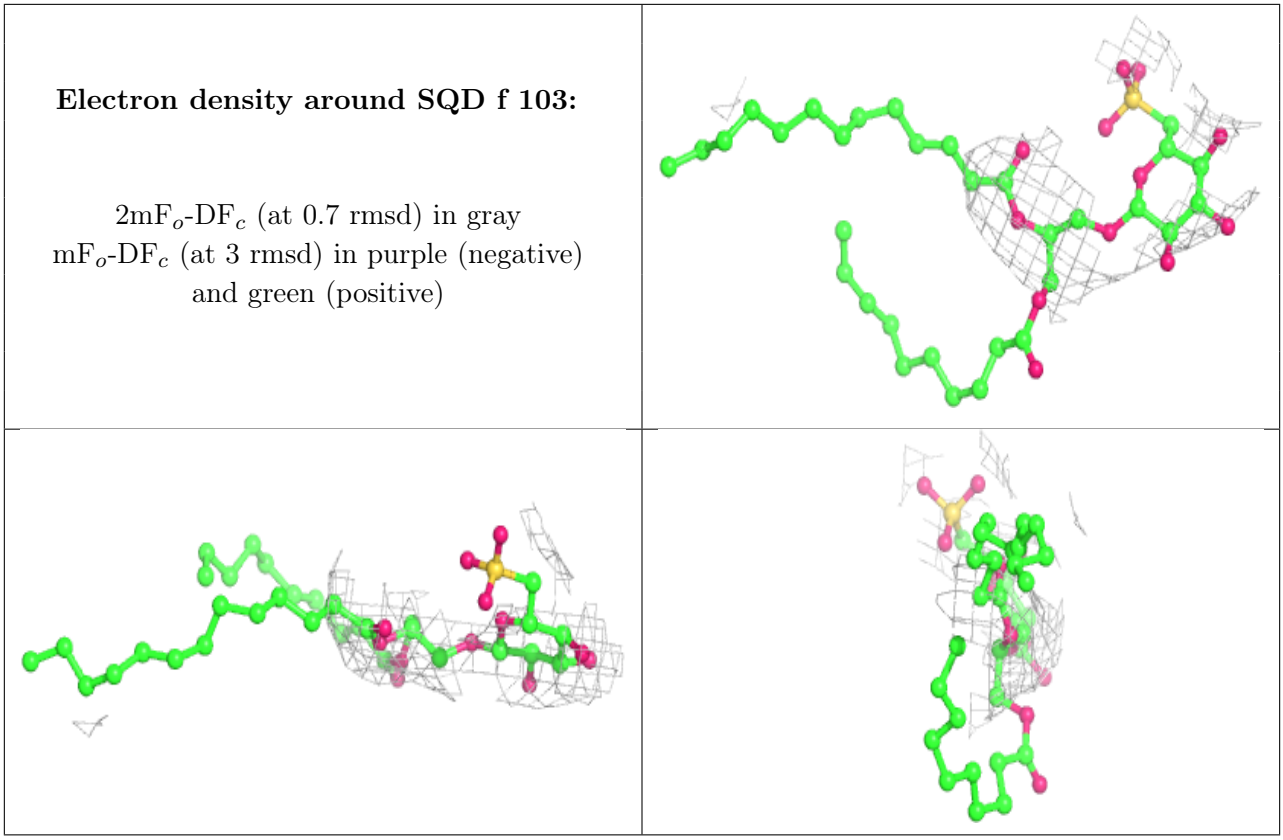
Electron density around CLA B 610:

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



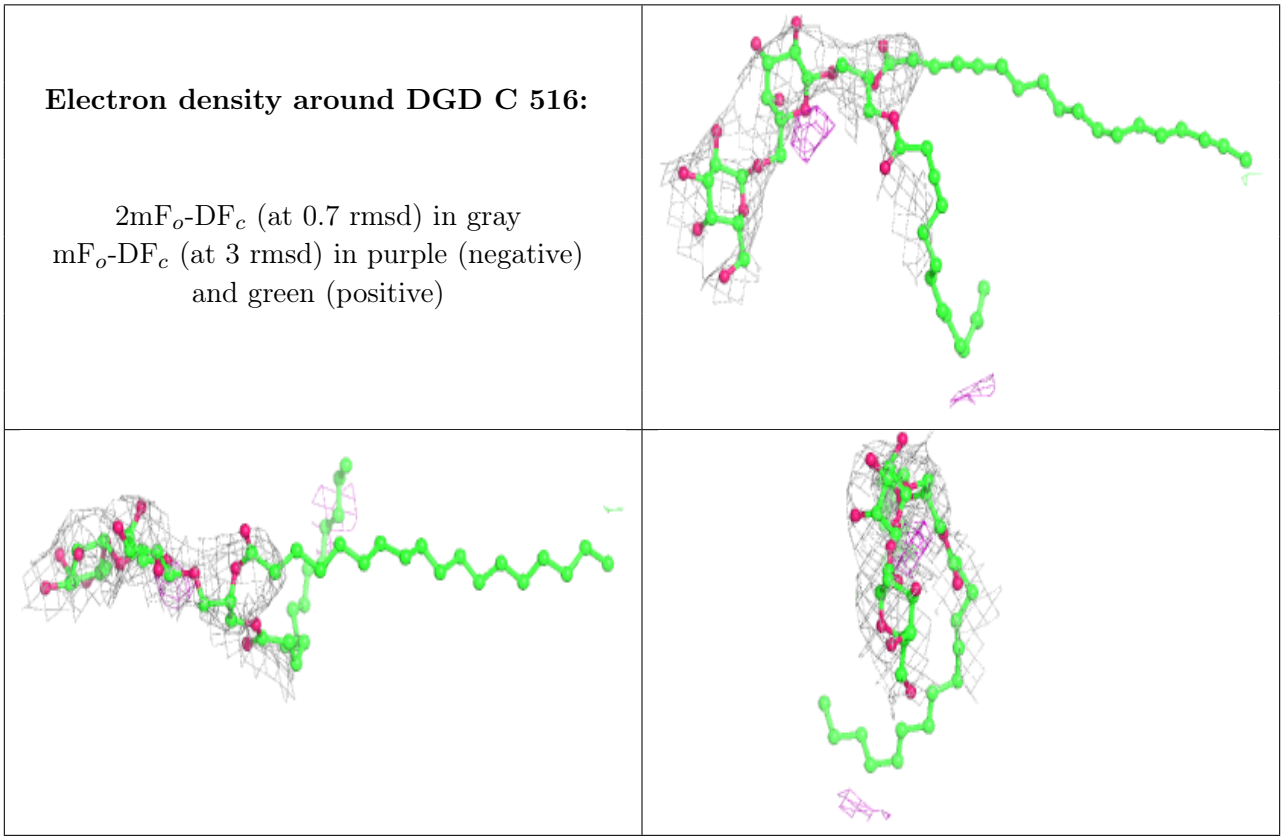
Electron density around SQD f 103:

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



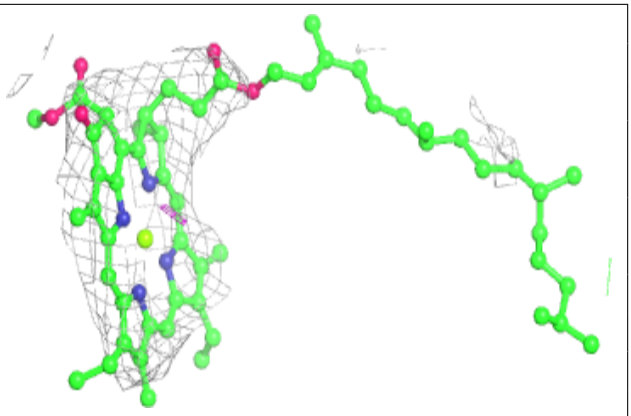
Electron density around DGD C 516:

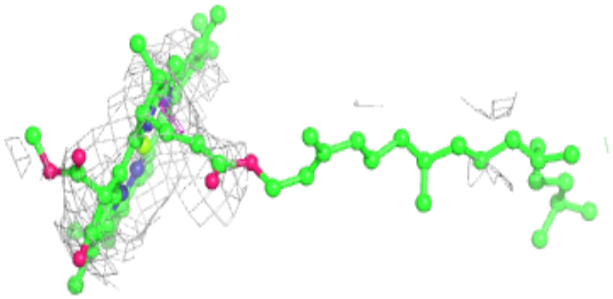
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

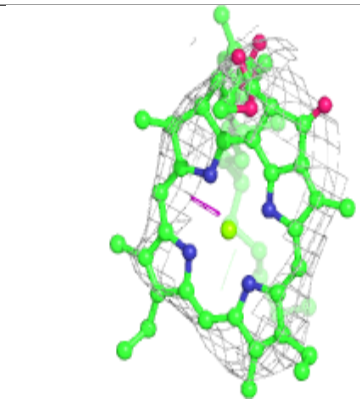


Electron density around CLA b 612:

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

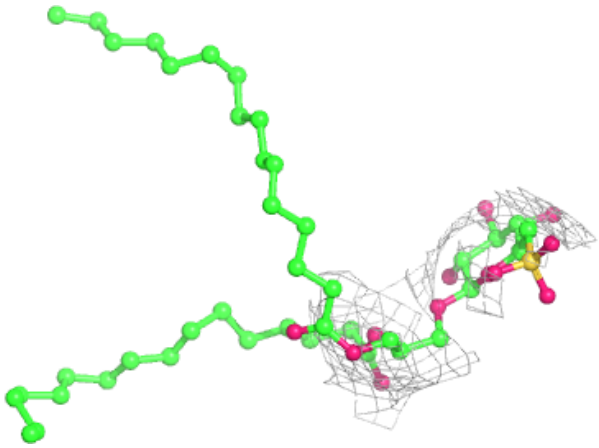


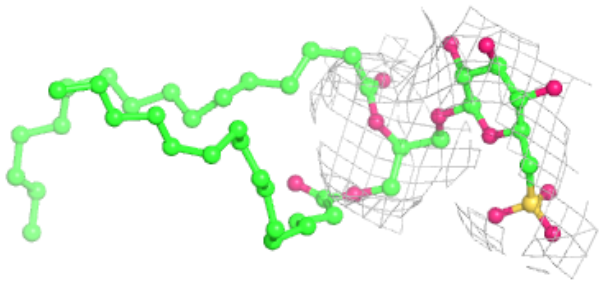


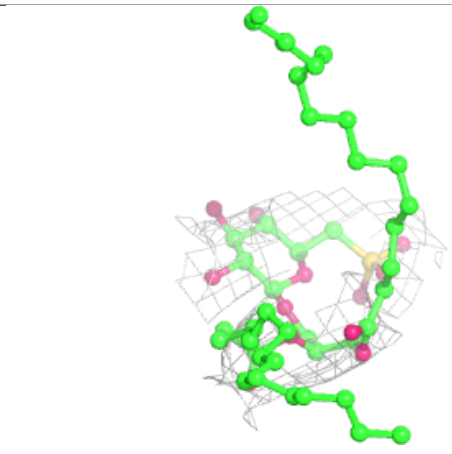


Electron density around SQD A 414:

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

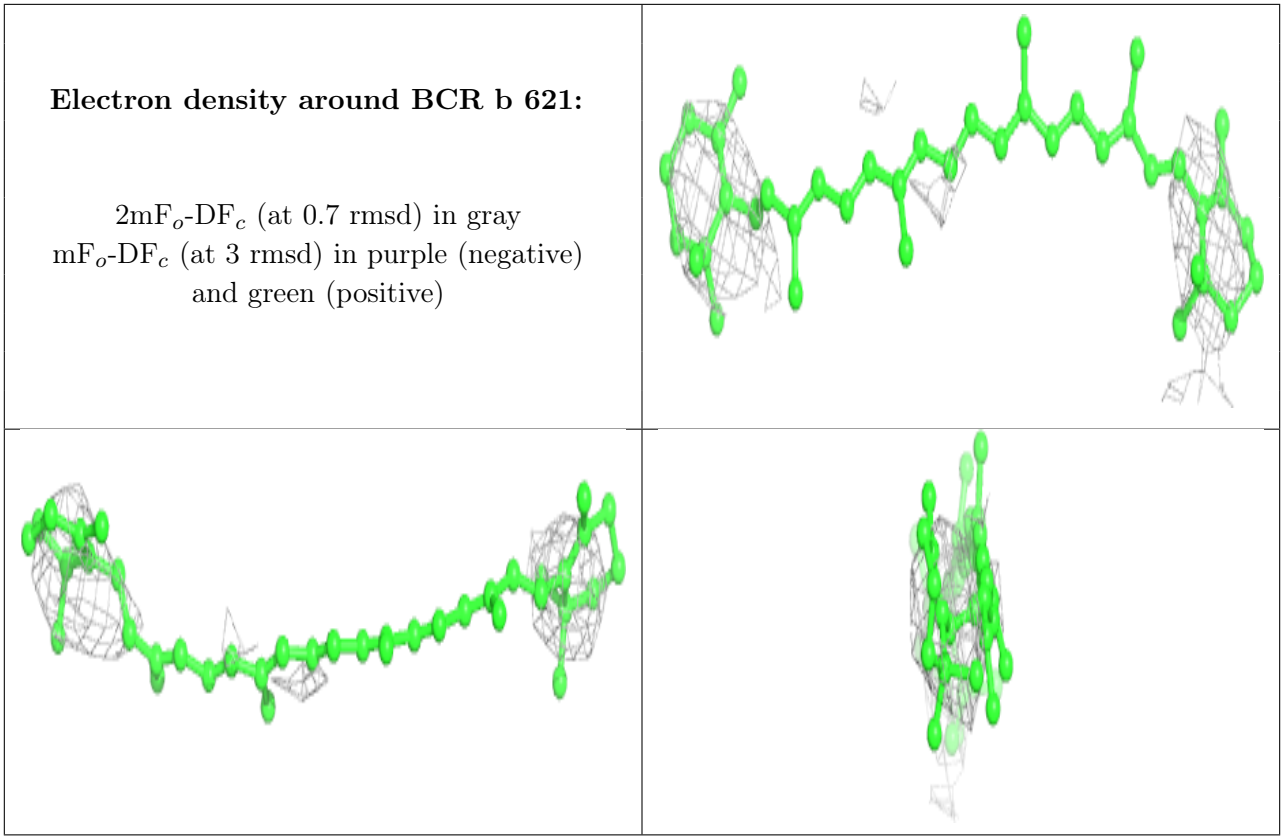






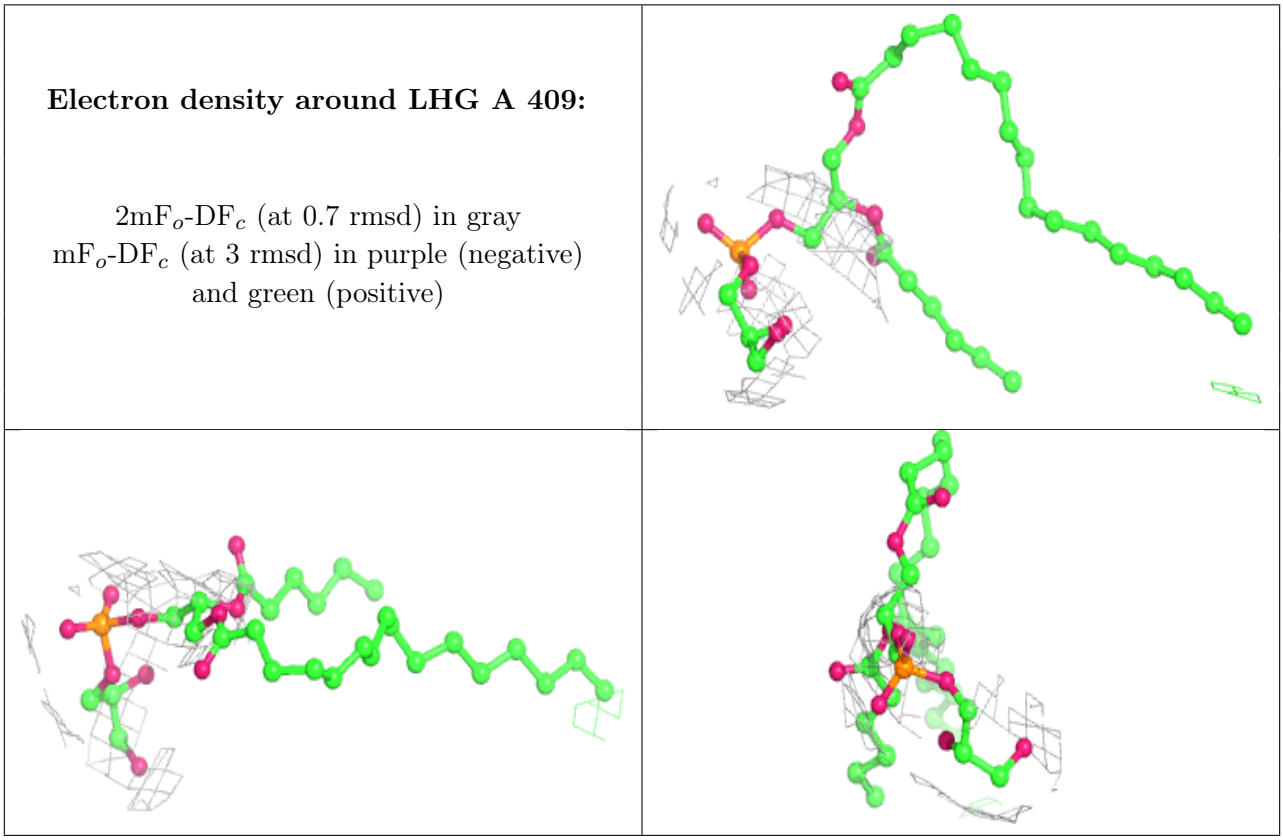
Electron density around BCR b 621:

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



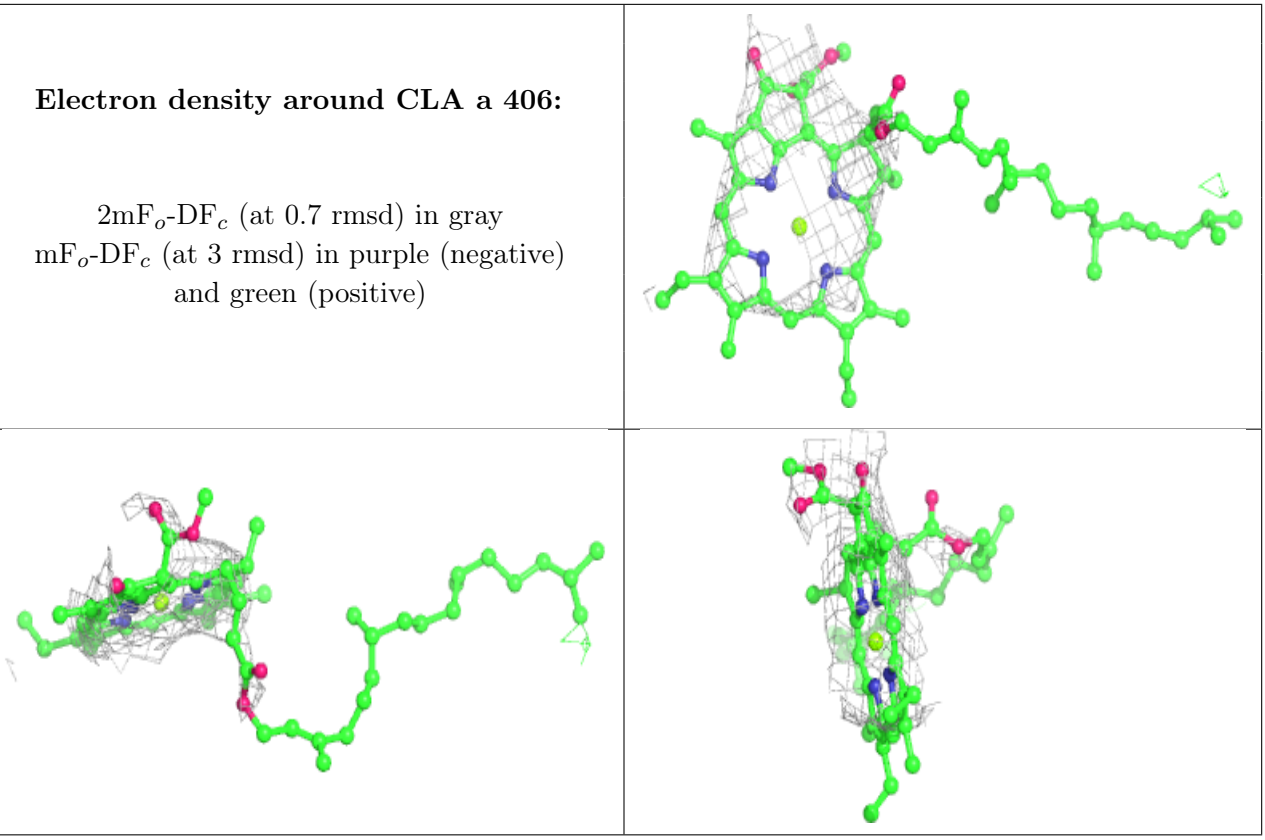
Electron density around LHG A 409:

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



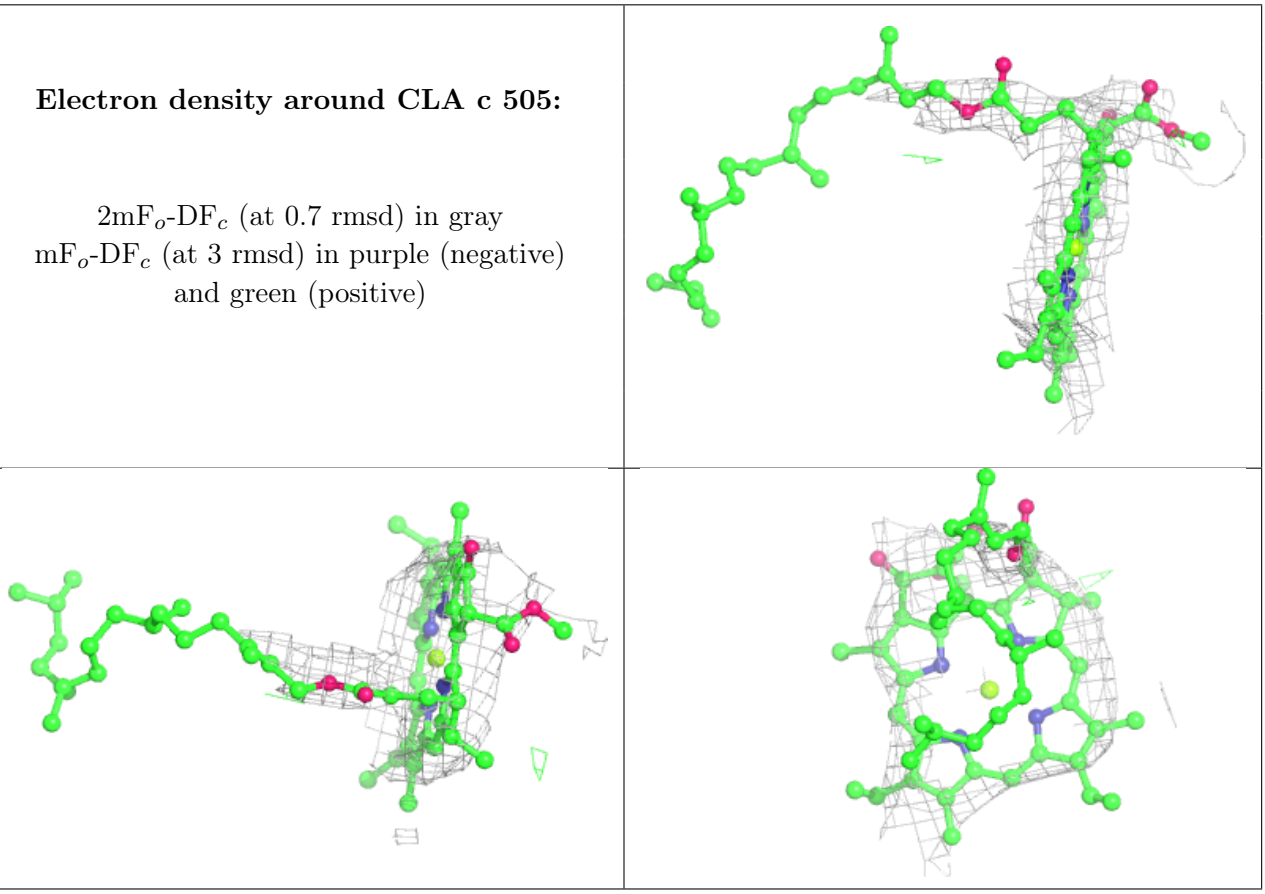
Electron density around CLA a 406:

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



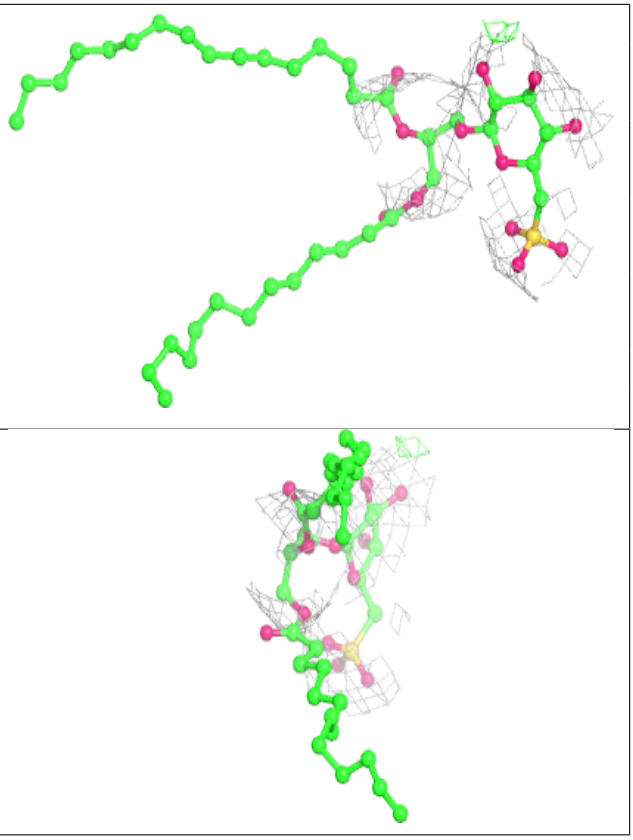
Electron density around CLA c 505:

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



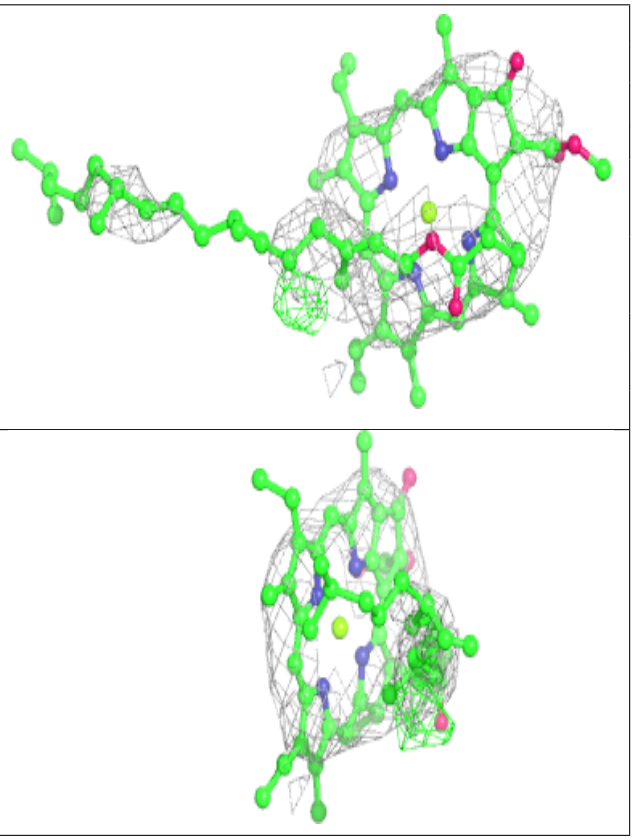
Electron density around SQD a 415:

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



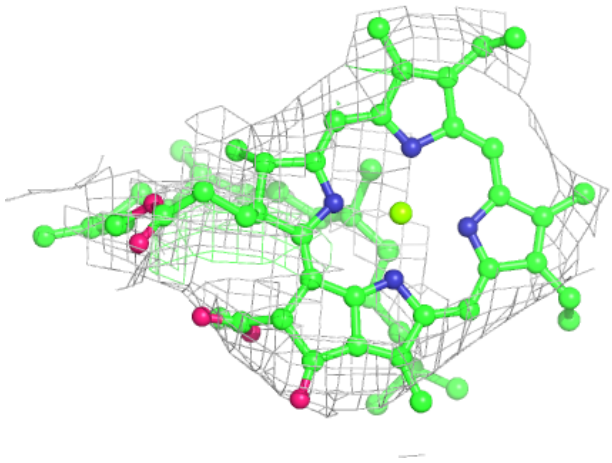
Electron density around CLA B 607:

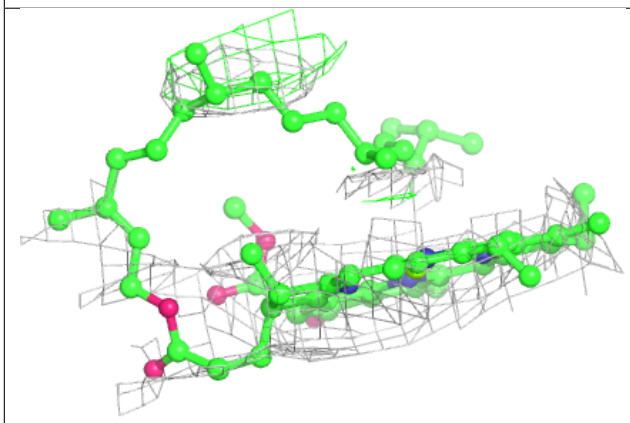
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

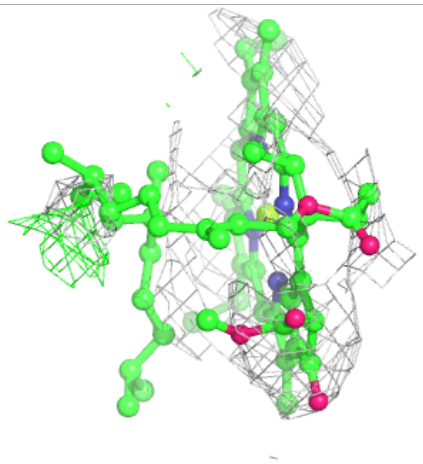


Electron density around CLA C 509:

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

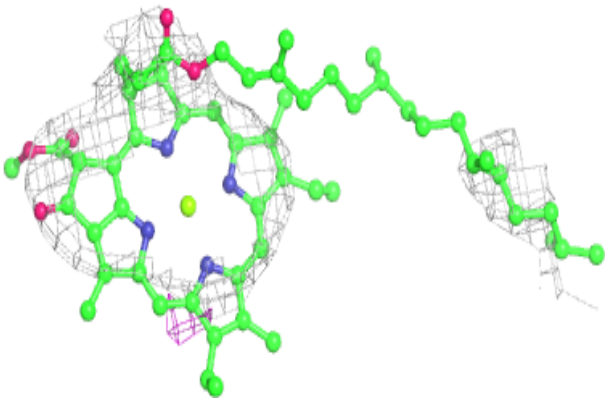


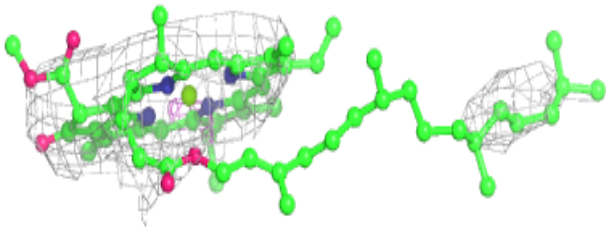


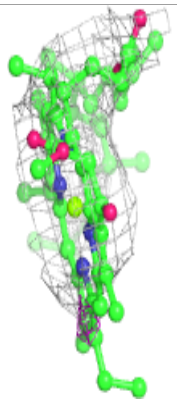


Electron density around CLA c 501:

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

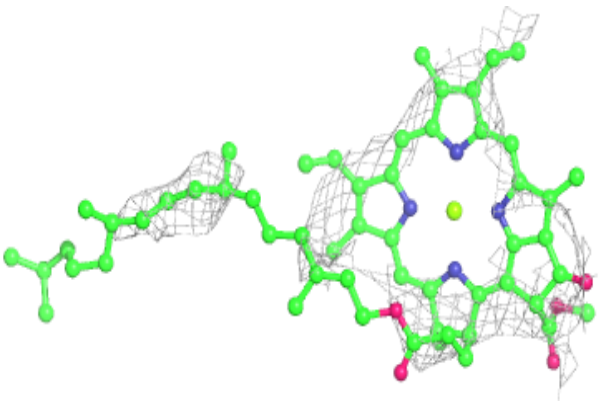


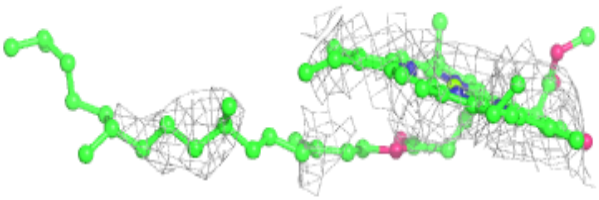


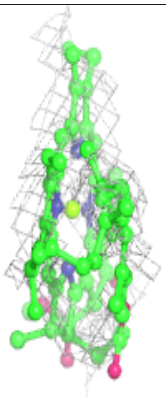


Electron density around CLA b 606:

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

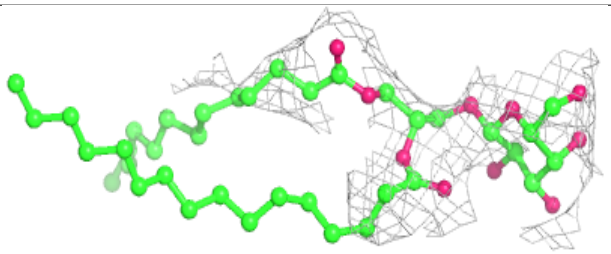


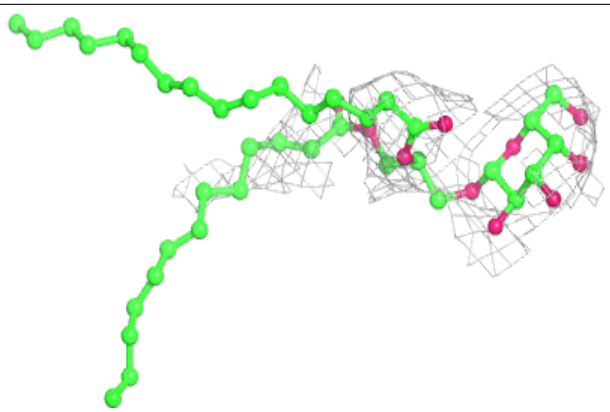


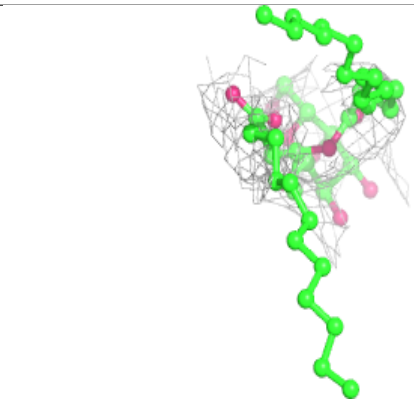


Electron density around LMG d 407:

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

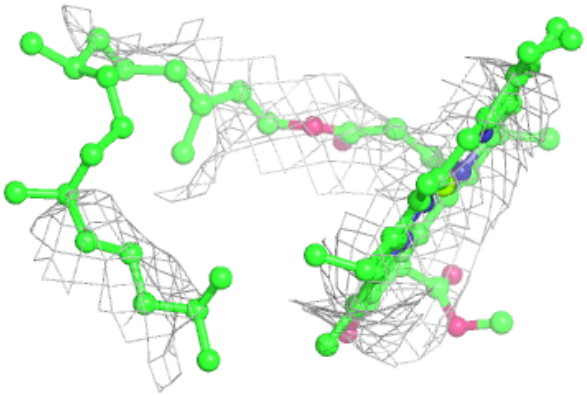


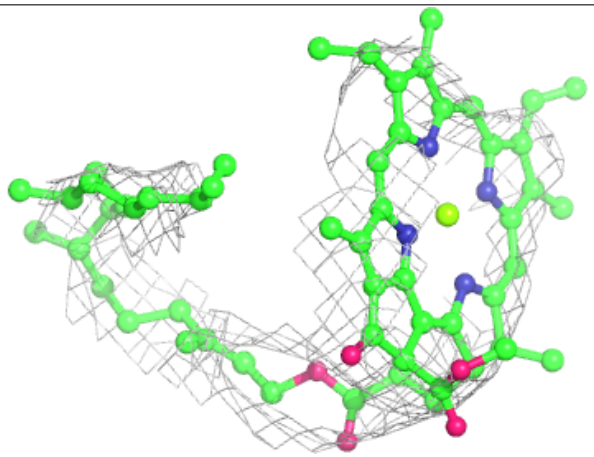


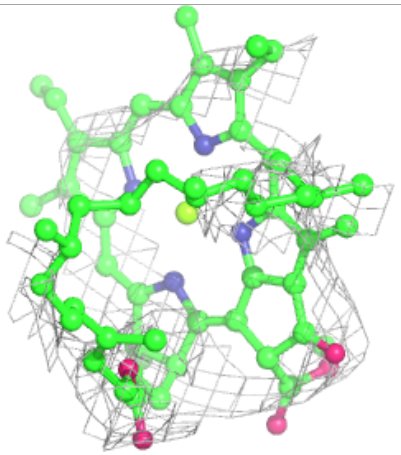


Electron density around CLA C 503:

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

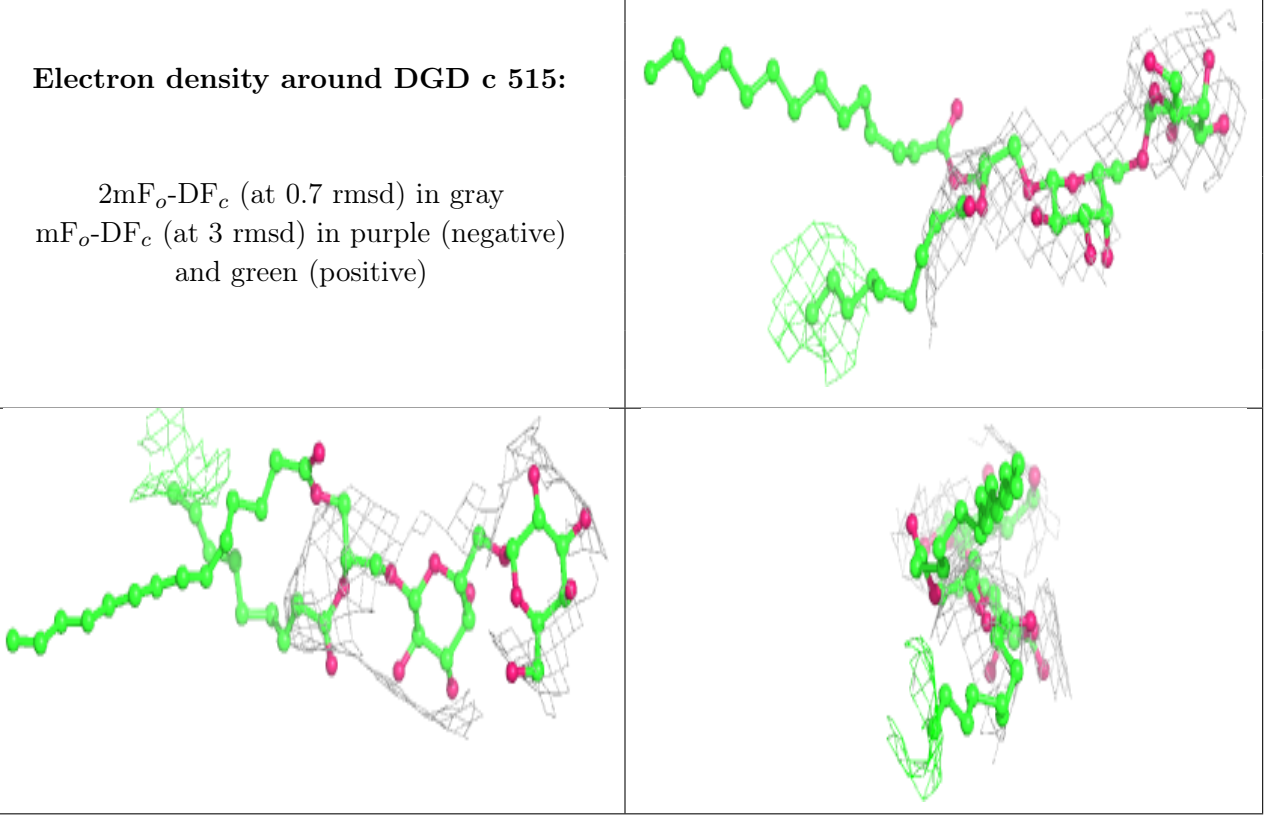






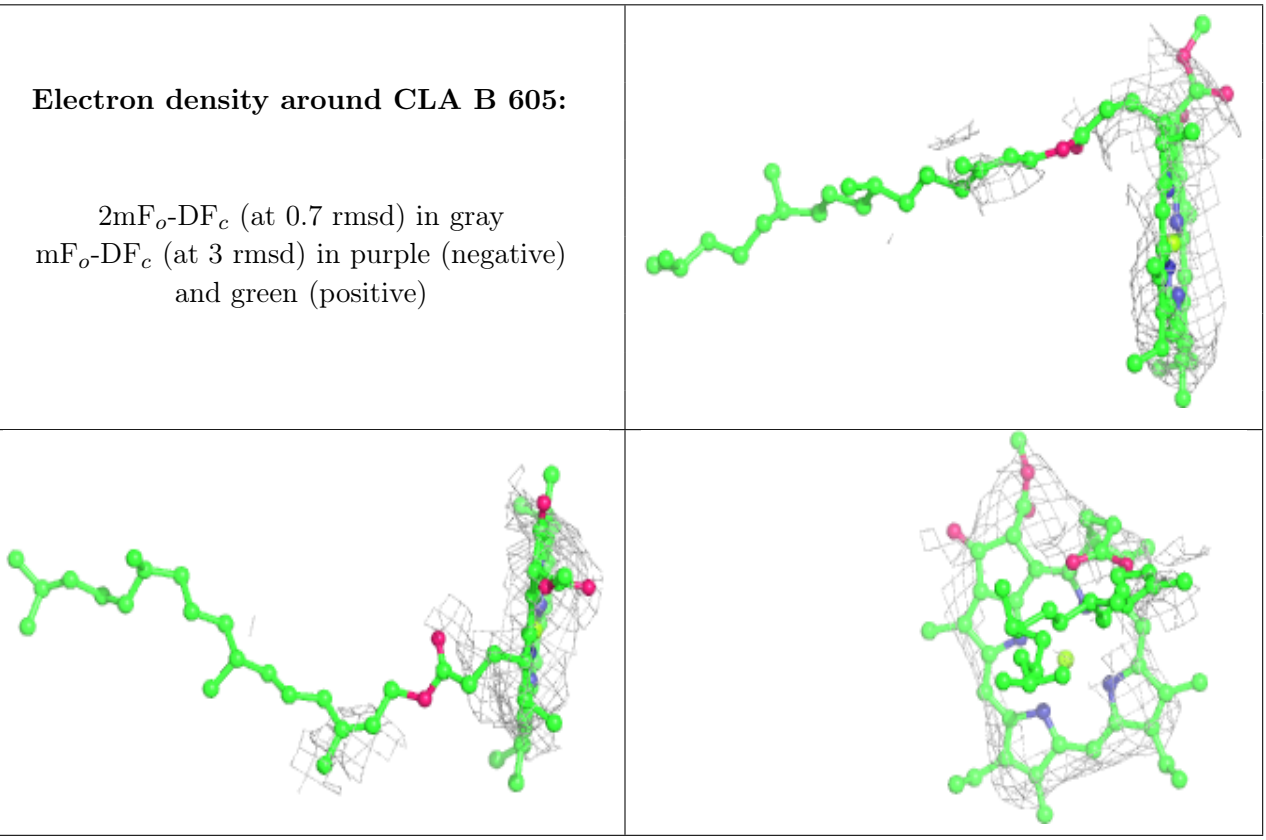
Electron density around DGD c 515:

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



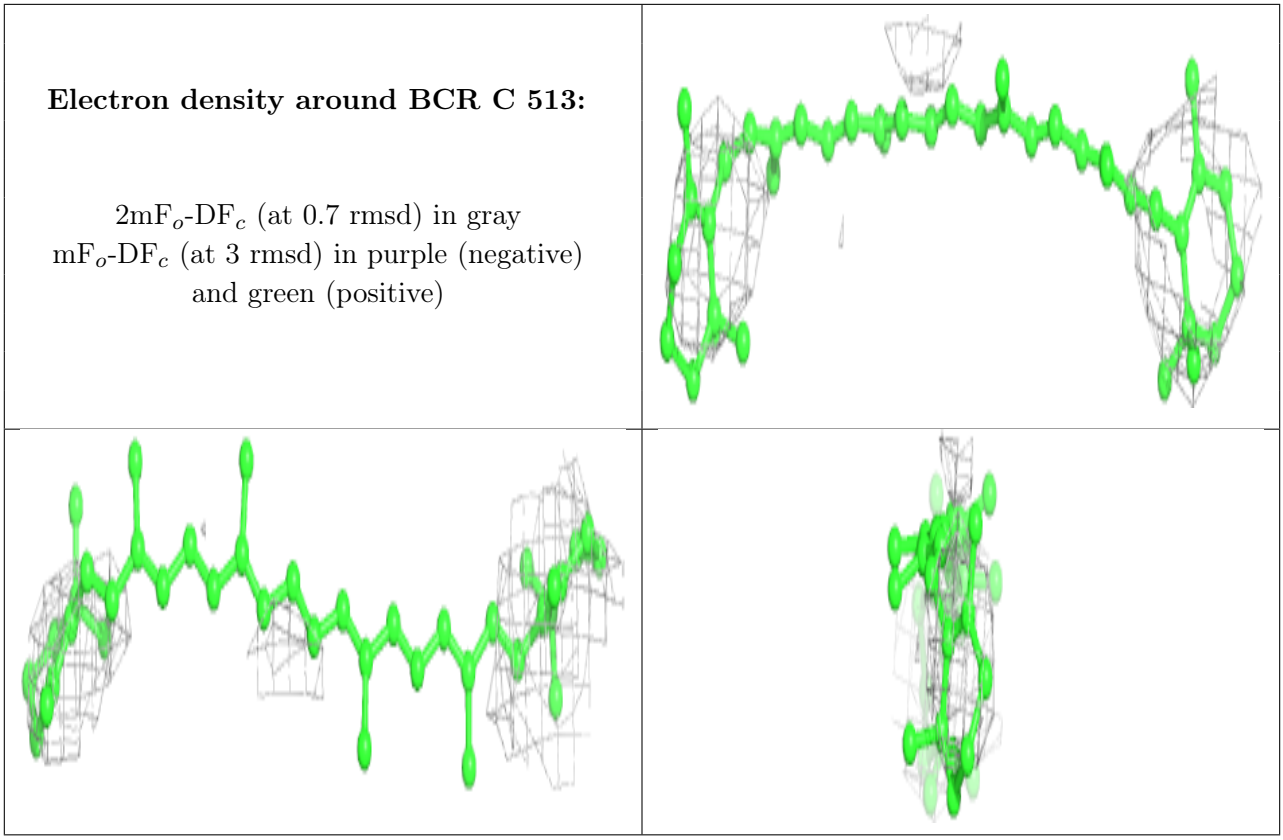
Electron density around CLA B 605:

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



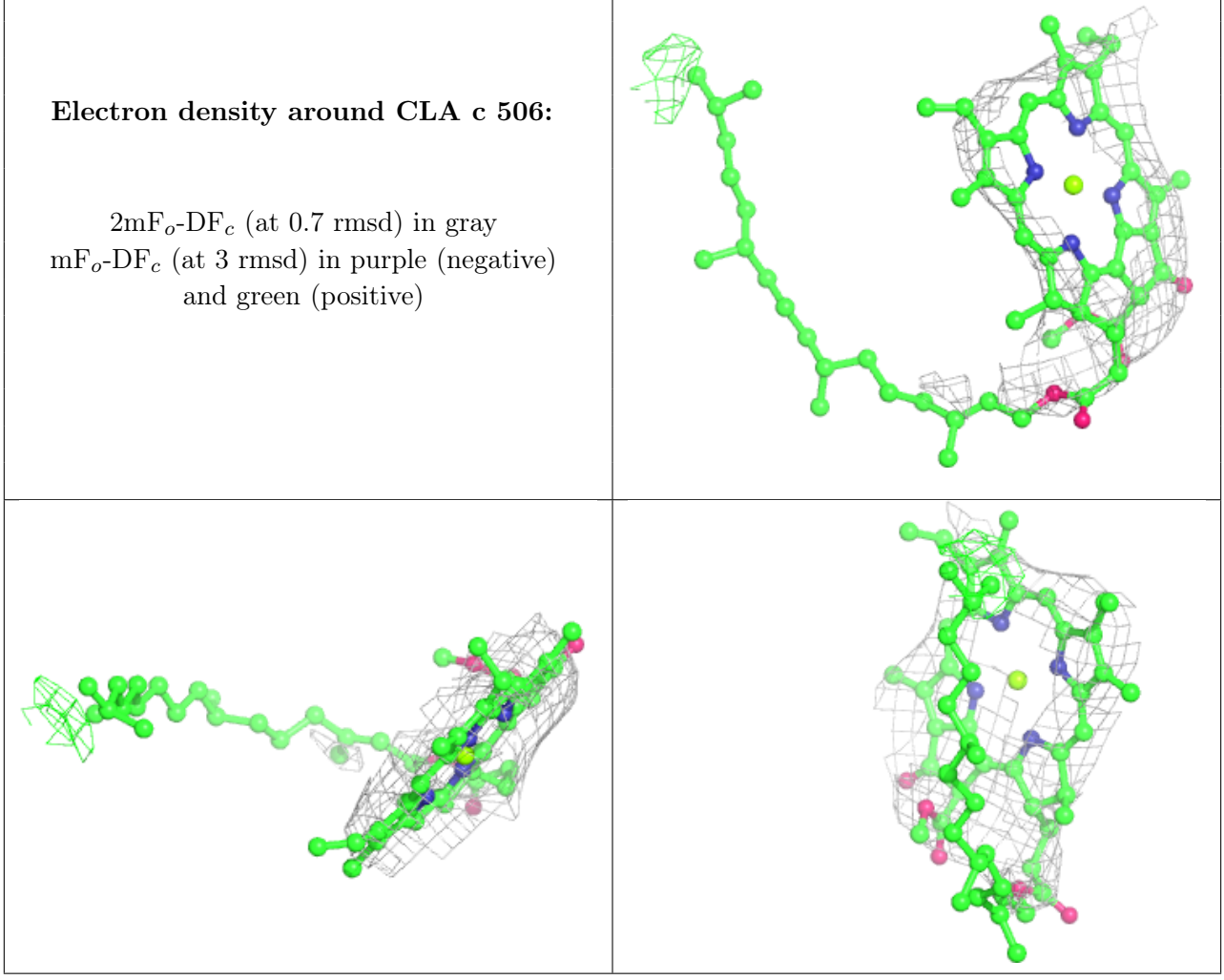
Electron density around BCR C 513:

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



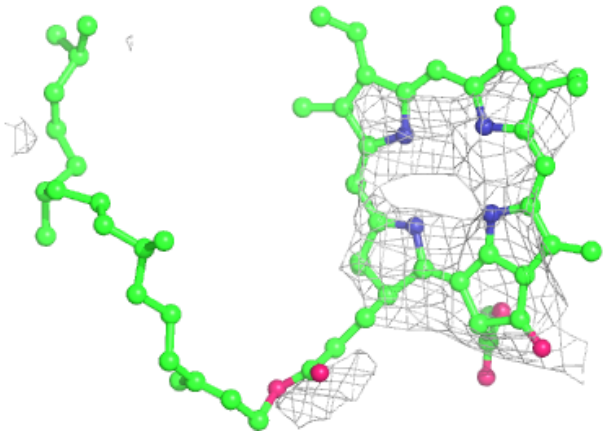
Electron density around CLA c 506:

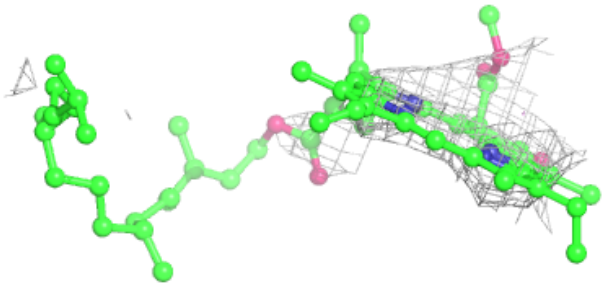
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

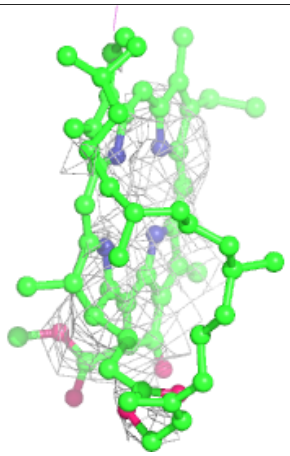


Electron density around PHO a 407:

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

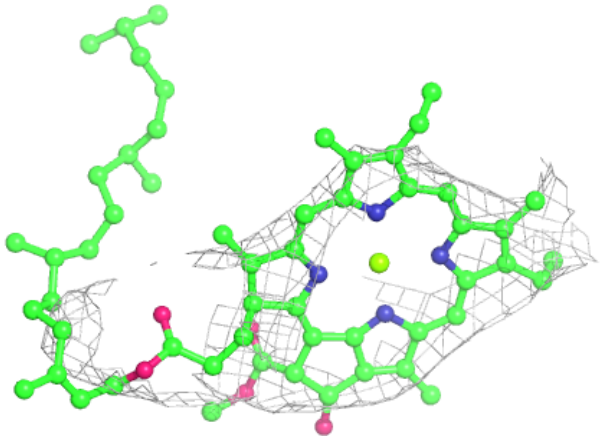


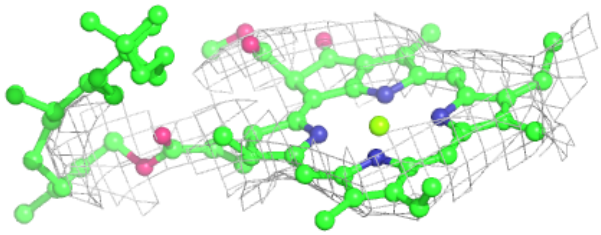


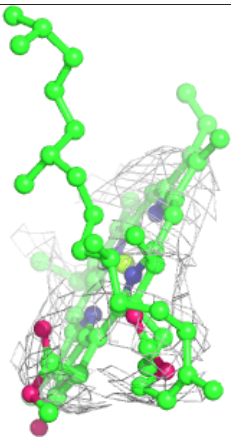


Electron density around CLA B 615:

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

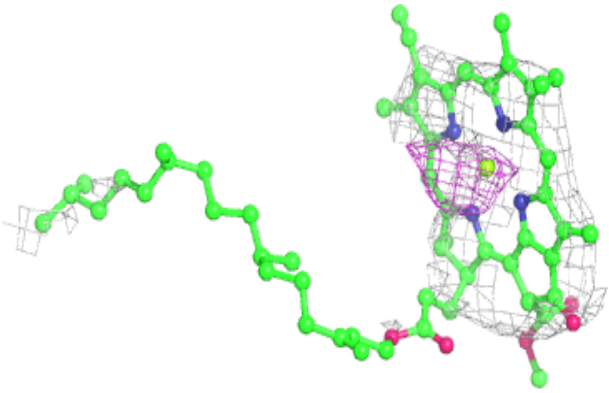


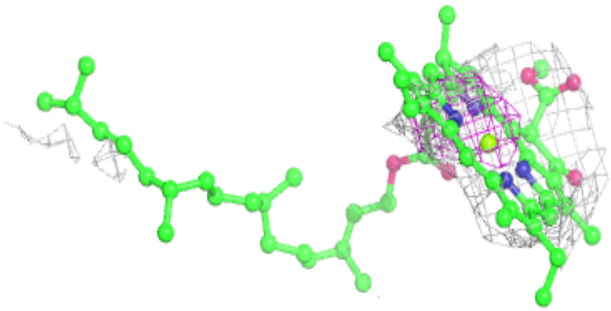


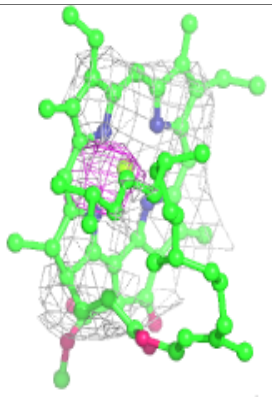


Electron density around CLA c 510:

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

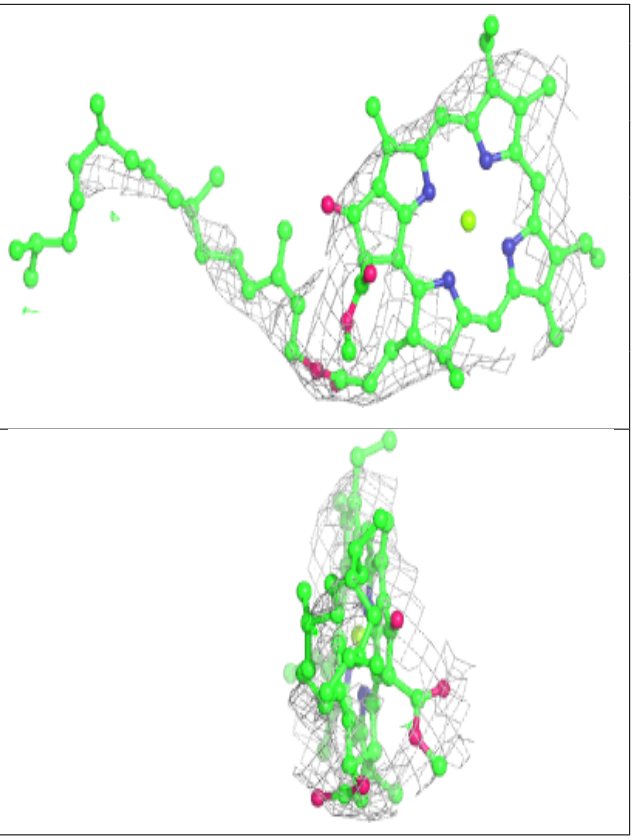


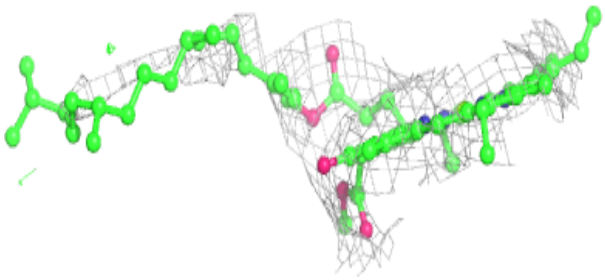




Electron density around CLA H 101:

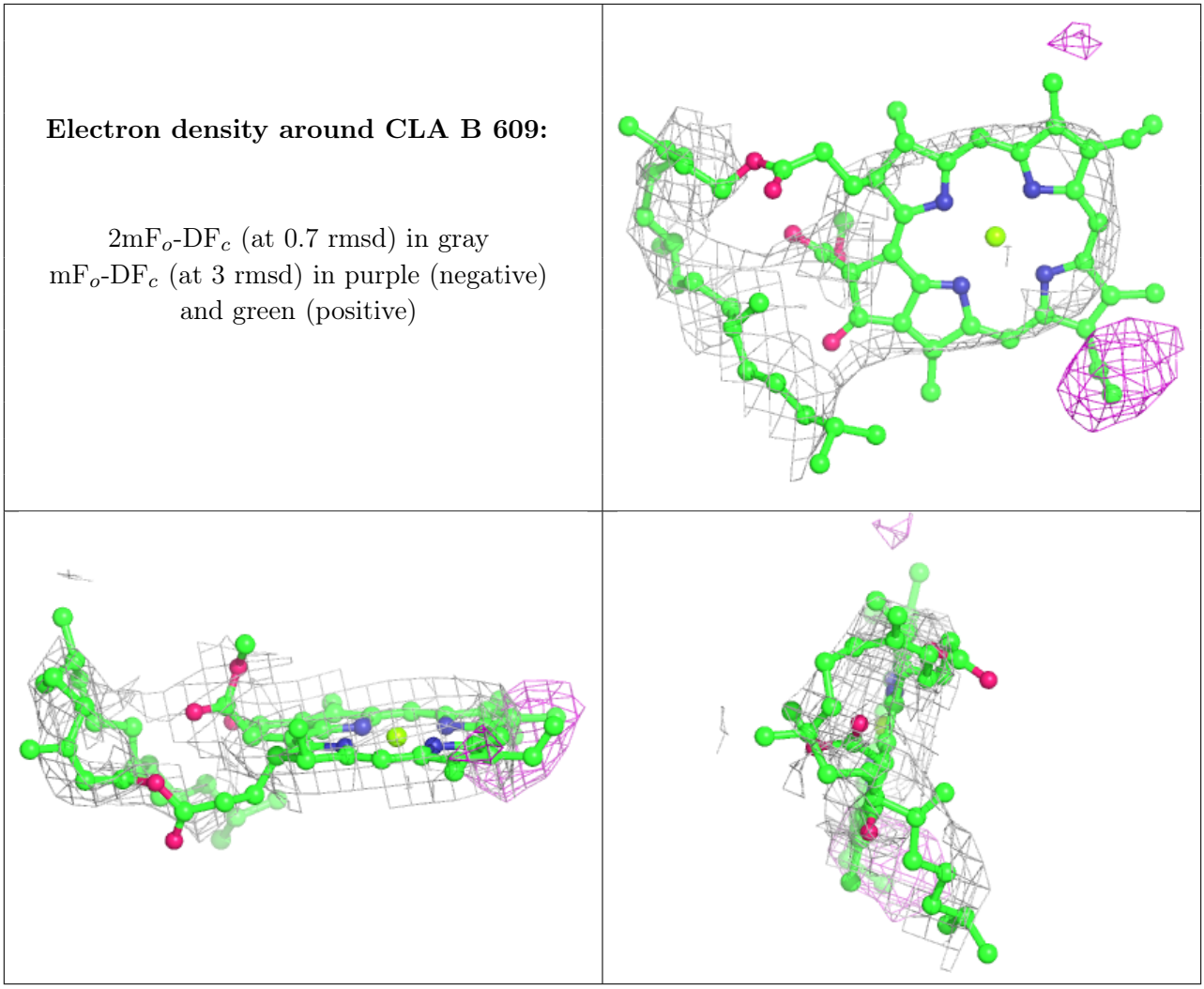
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





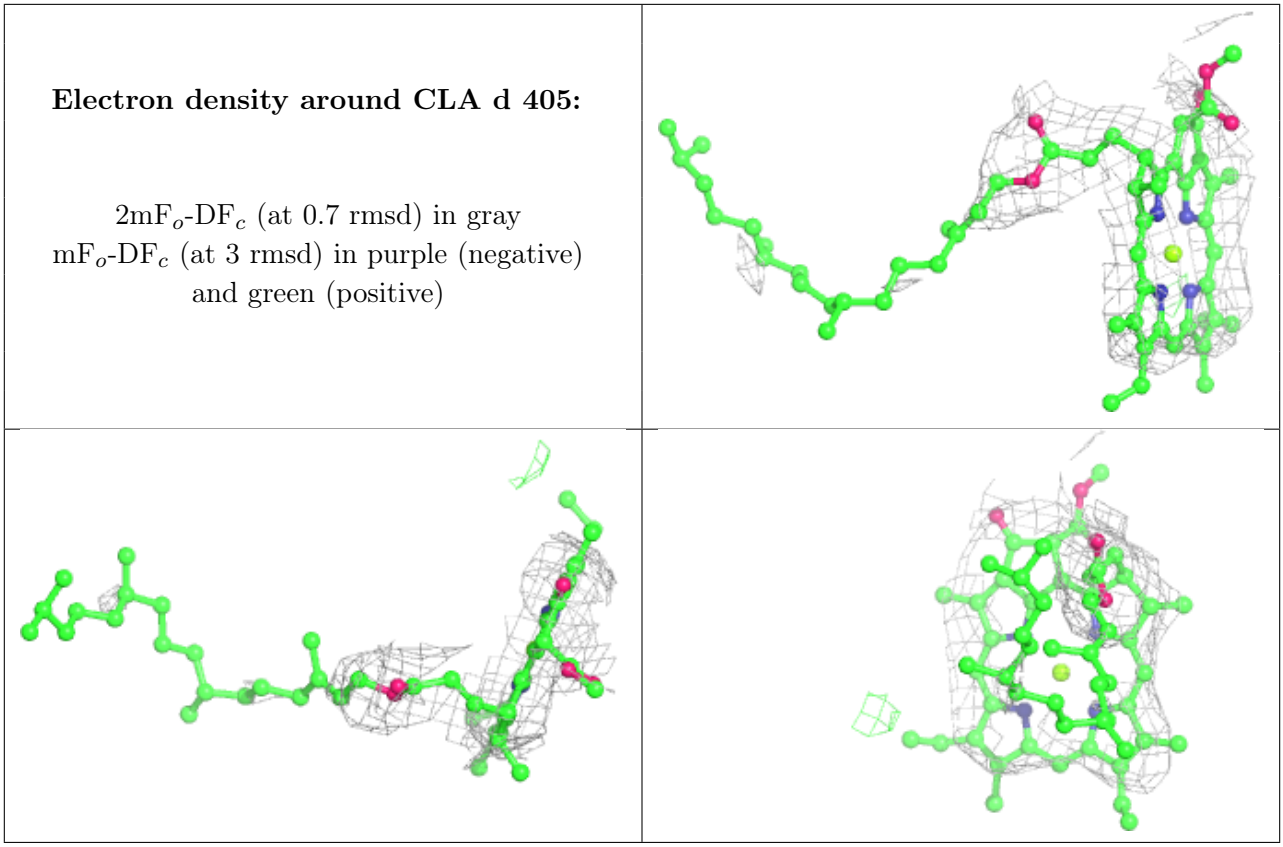
Electron density around CLA B 609:

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



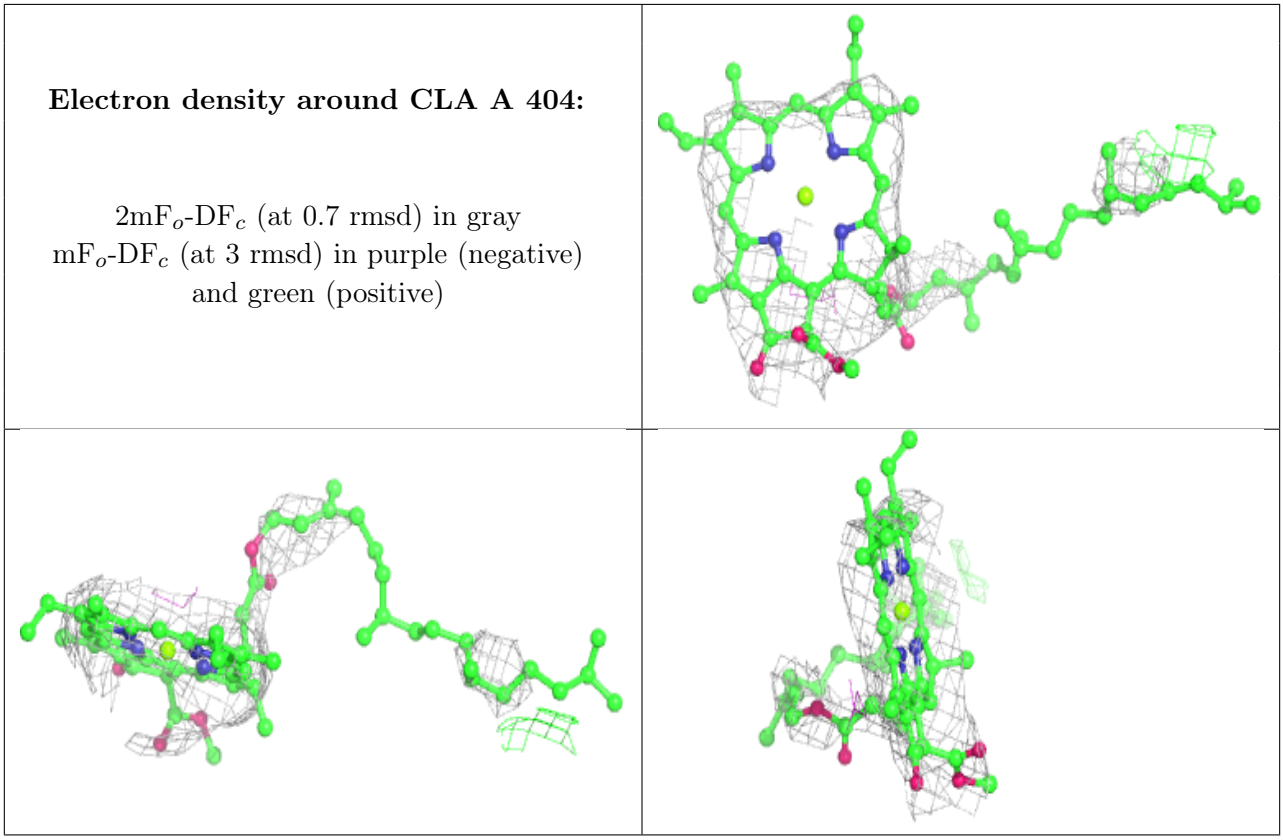
Electron density around CLA d 405:

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



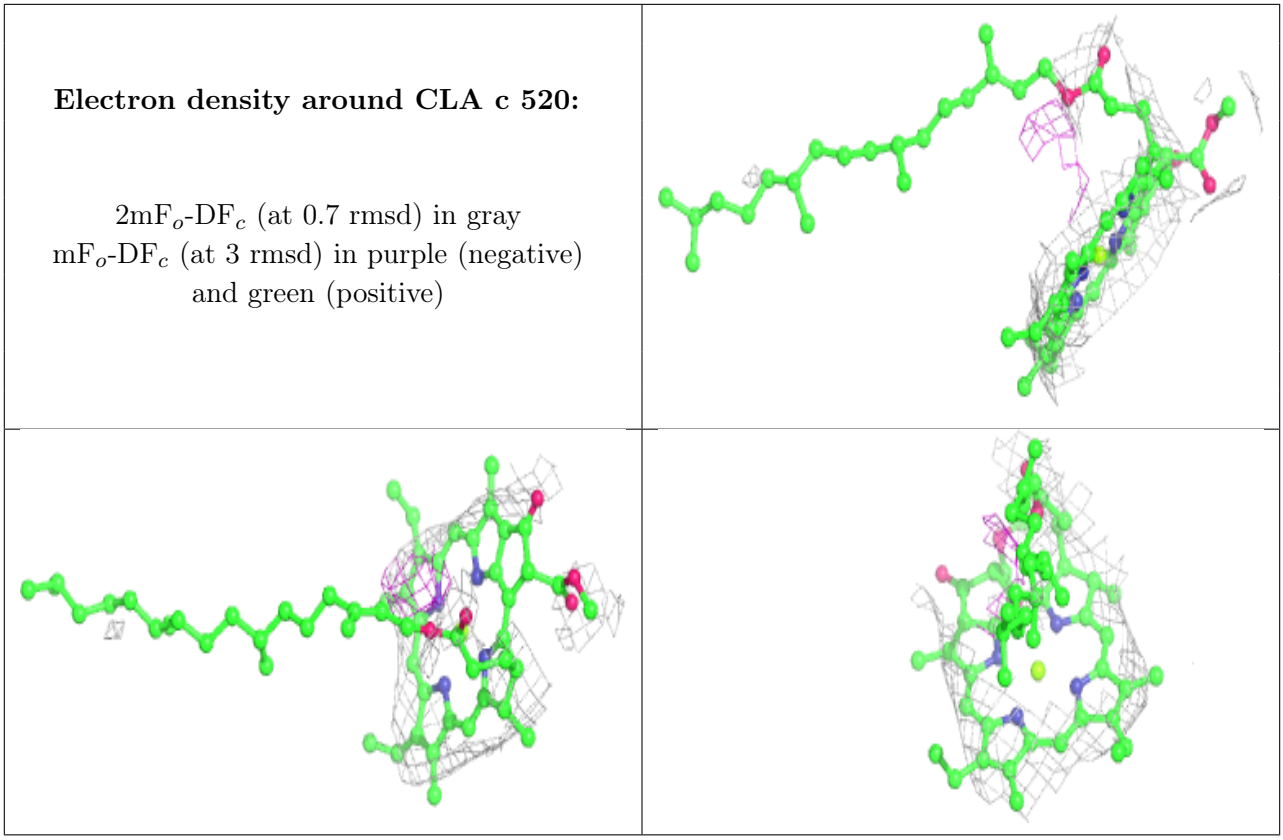
Electron density around CLA A 404:

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



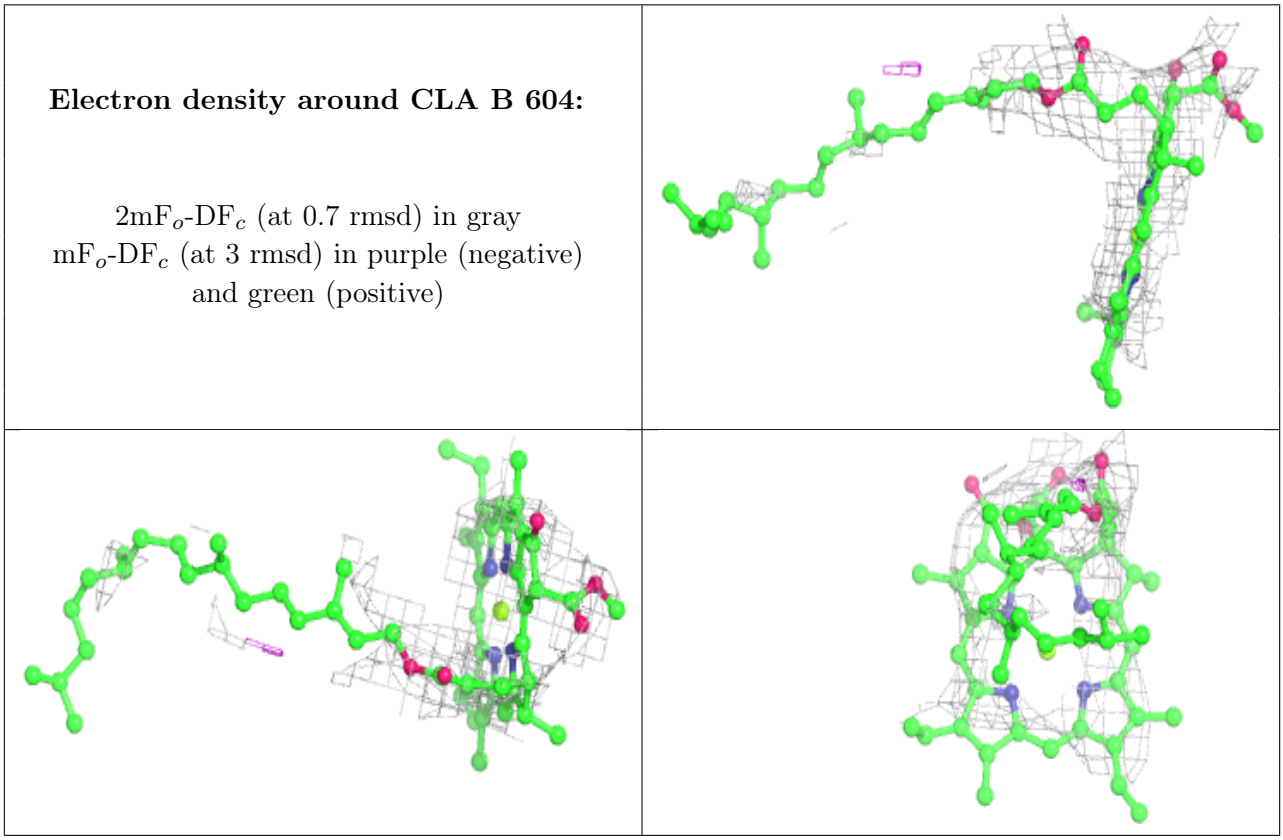
Electron density around CLA c 520:

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



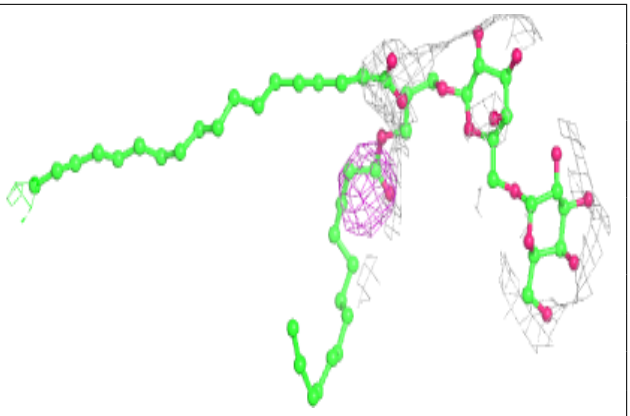
Electron density around CLA B 604:

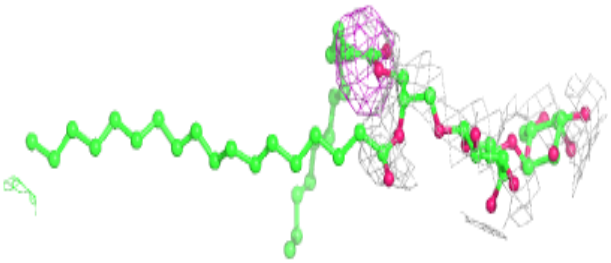
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

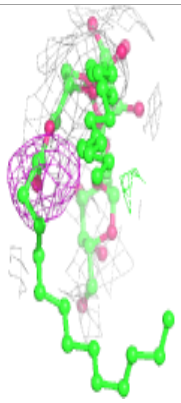


Electron density around DGD c 516:

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

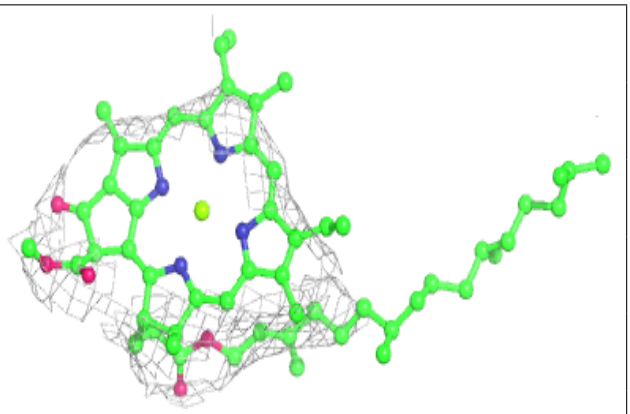


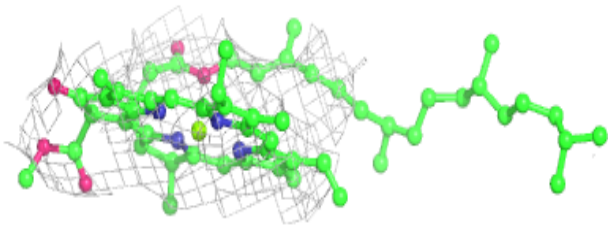


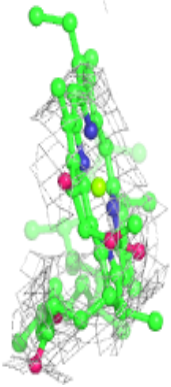


Electron density around CLA C 501:

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

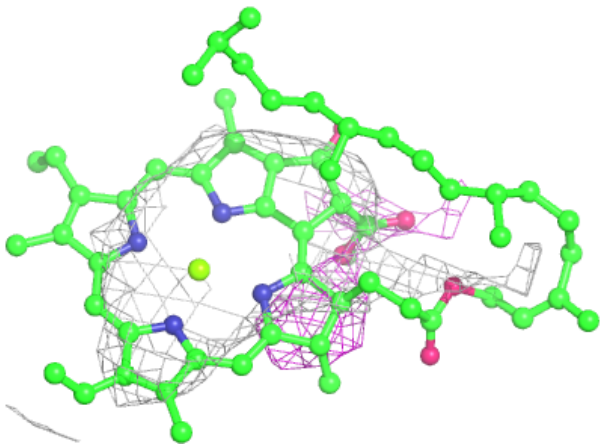


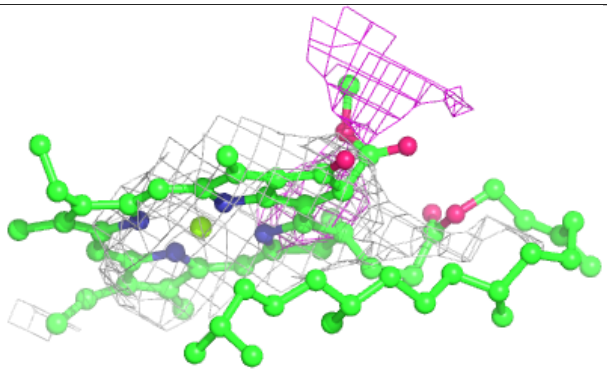


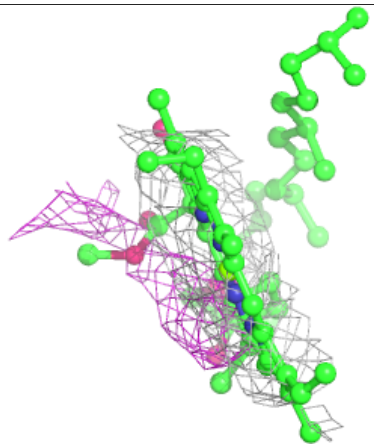


Electron density around CLA C 508:

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

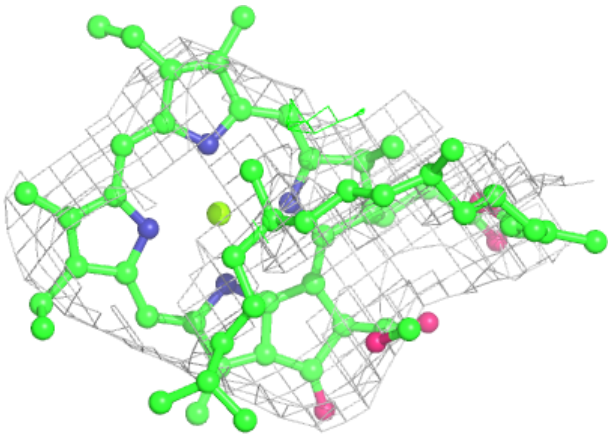


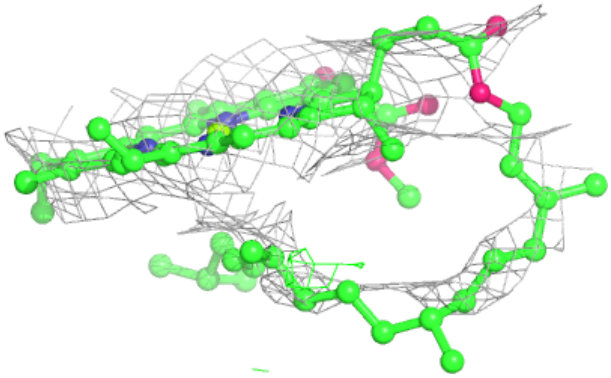


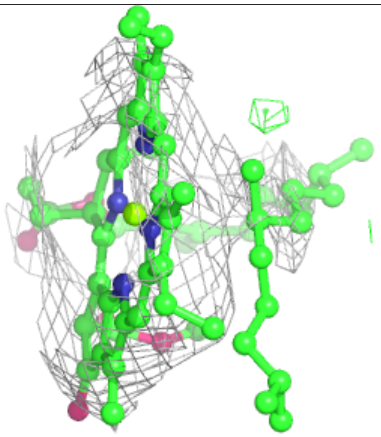


Electron density around CLA c 509:

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

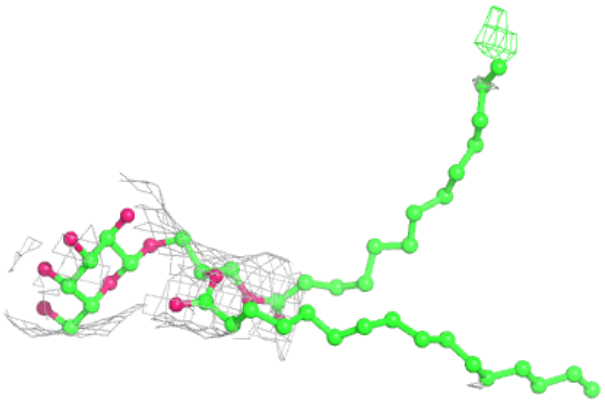


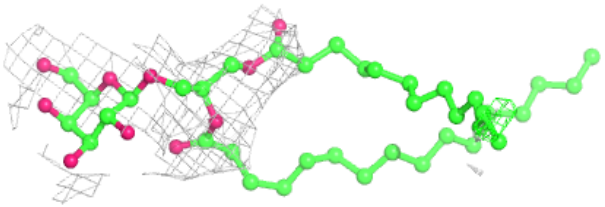


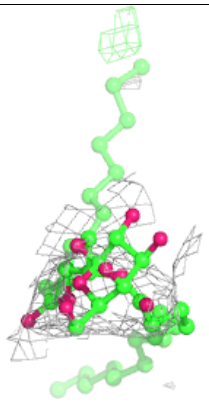


Electron density around LMG D 408:

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

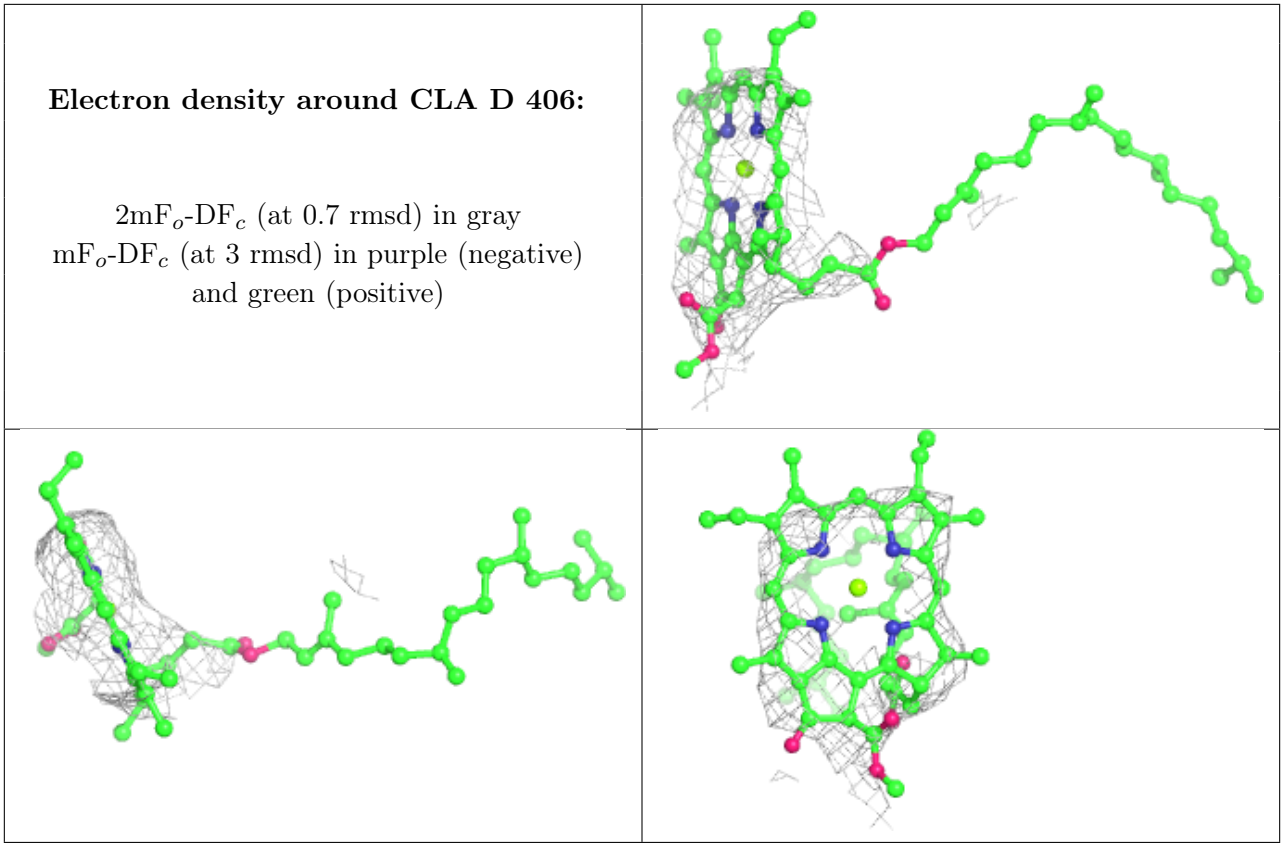






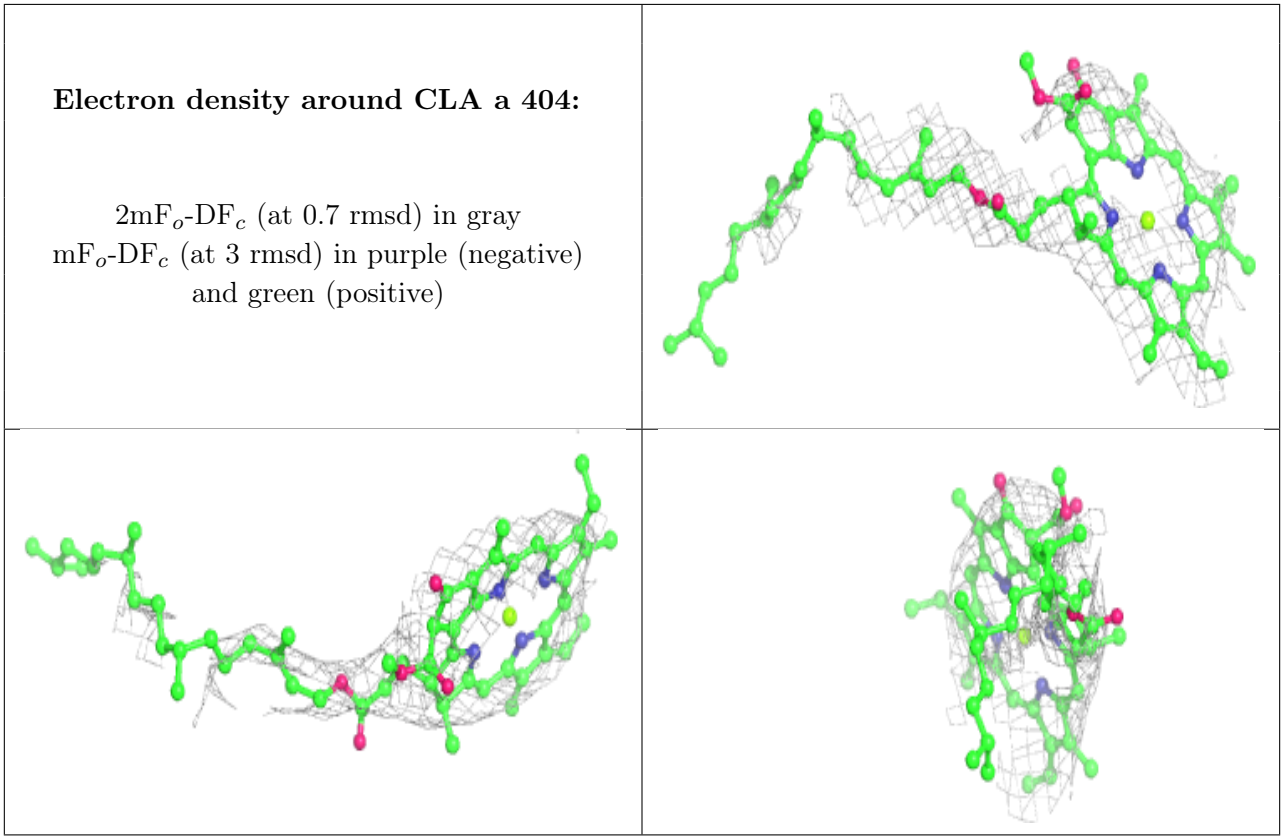
Electron density around CLA D 406:

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



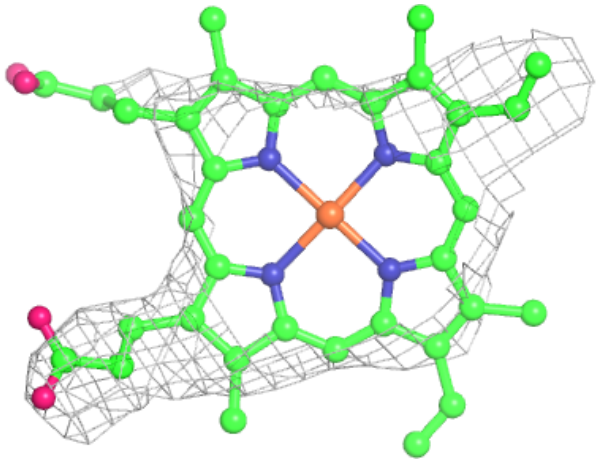
Electron density around CLA a 404:

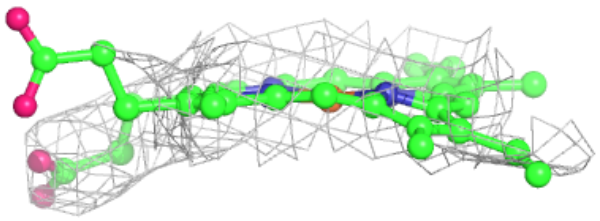
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

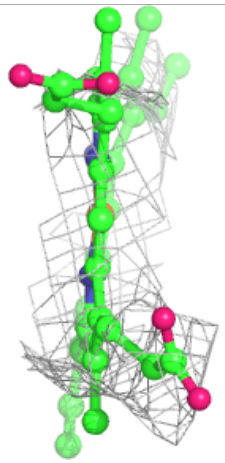


Electron density around HEM V 201:

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

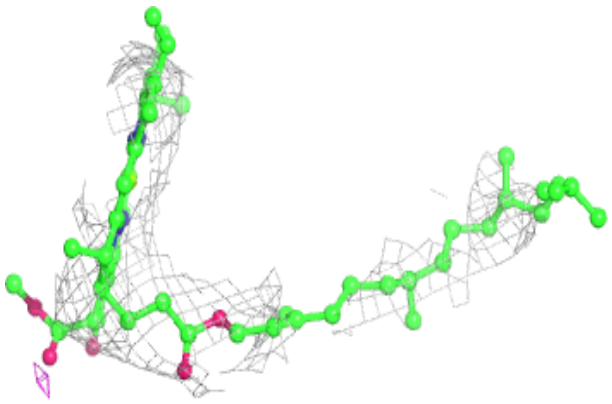


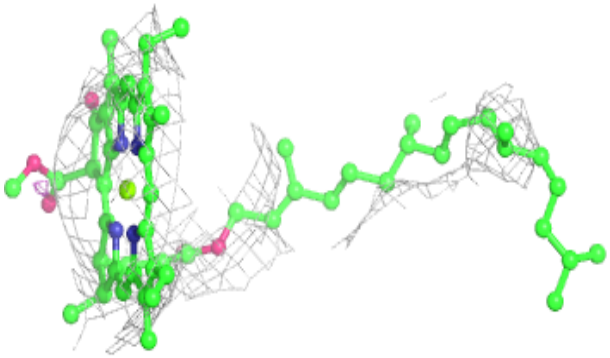


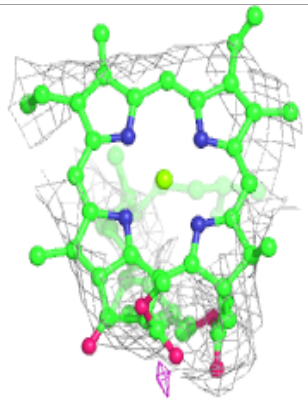


Electron density around CLA b 608:

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

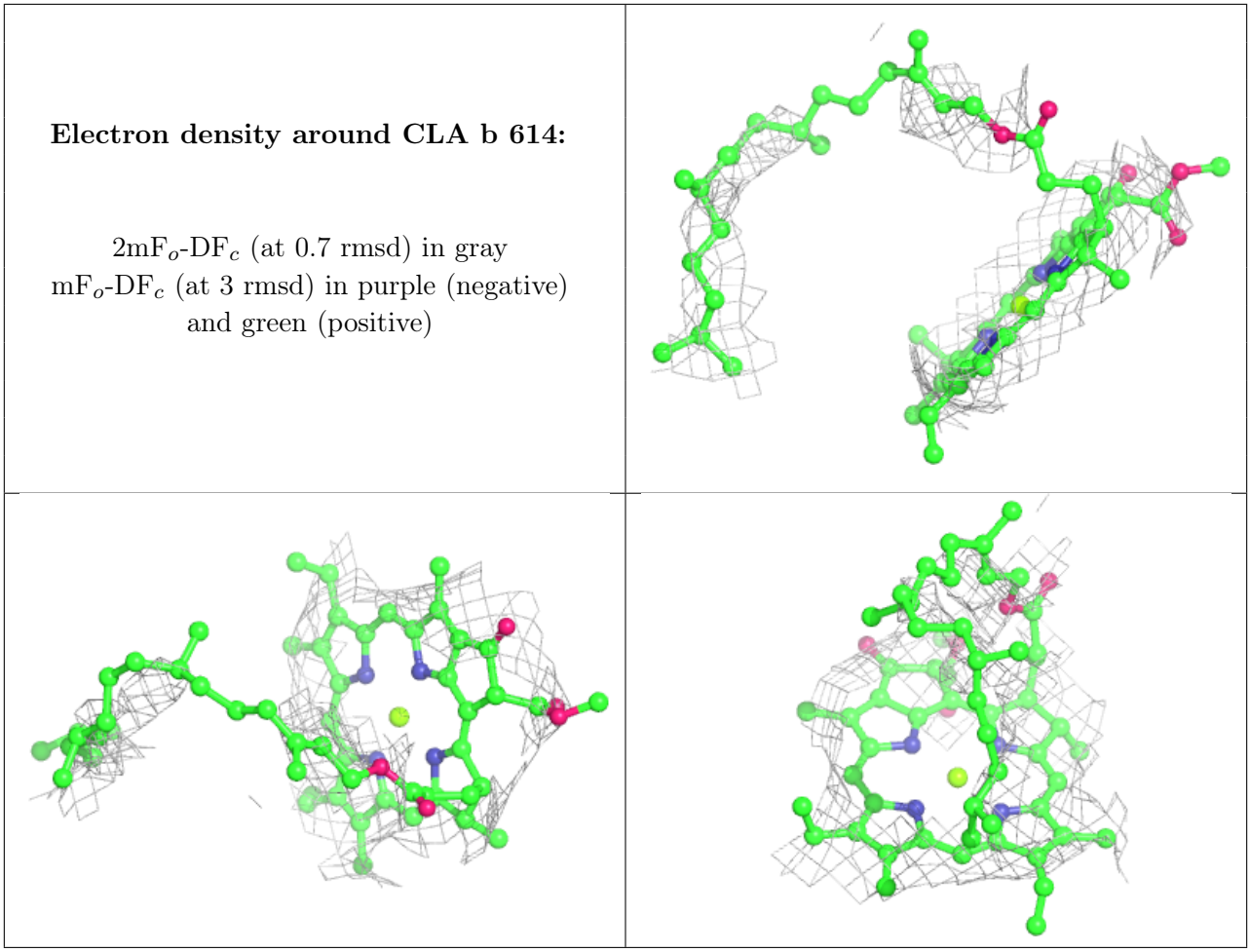






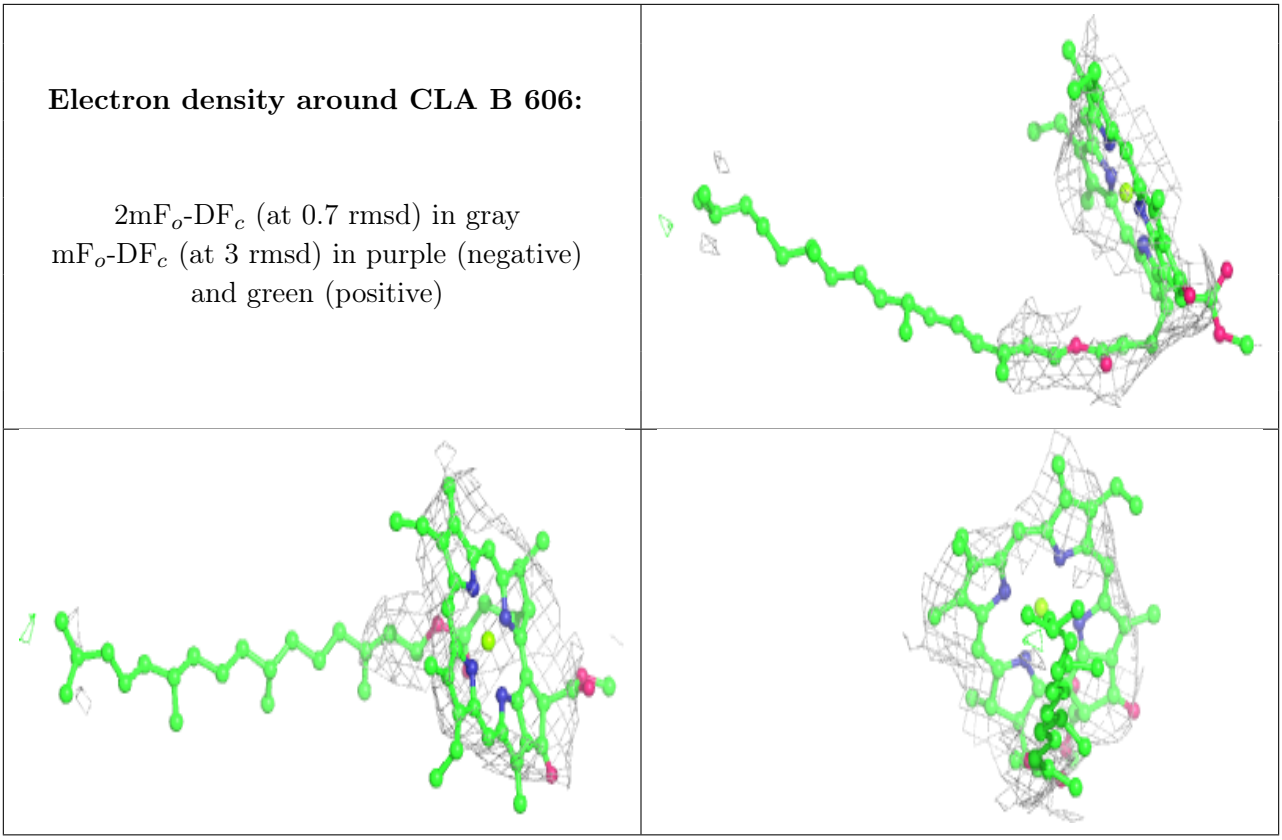
Electron density around CLA b 614:

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



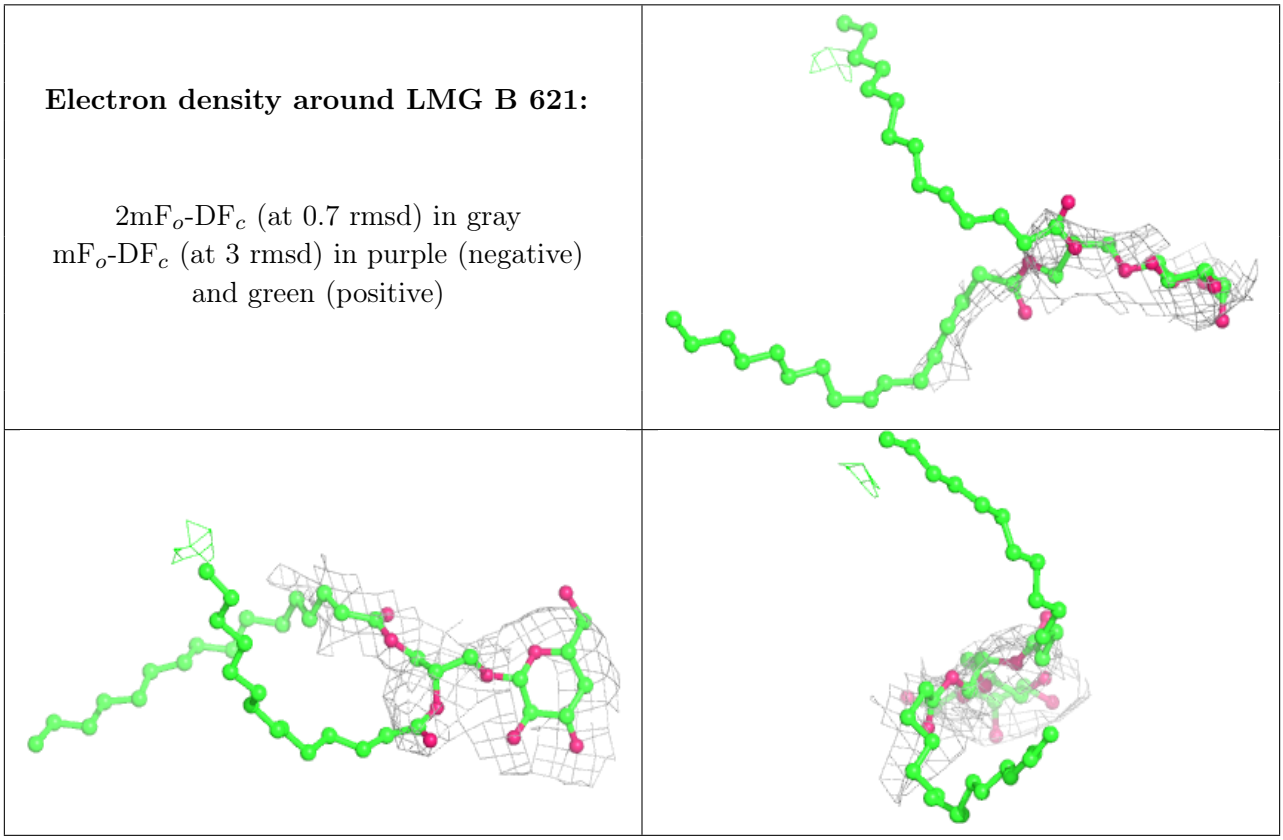
Electron density around CLA B 606:

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



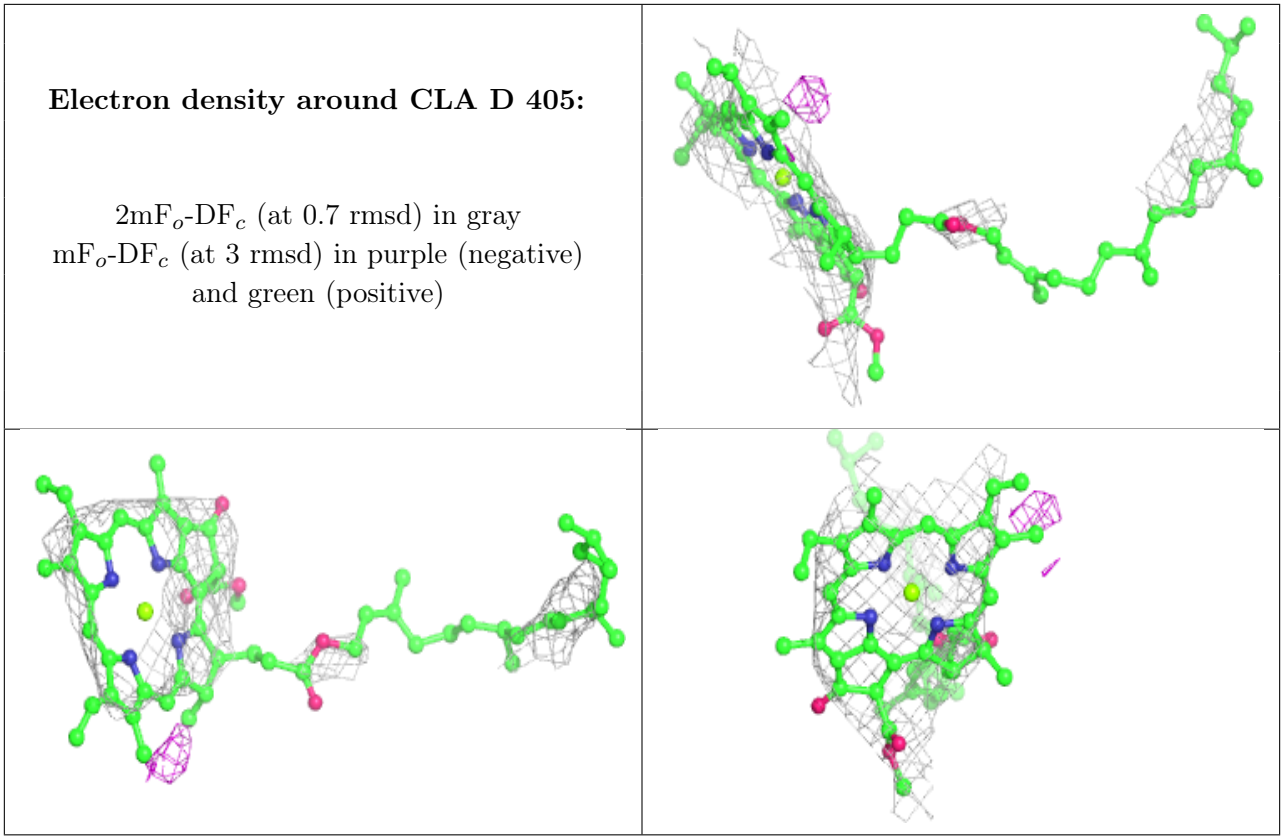
Electron density around LMG B 621:

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



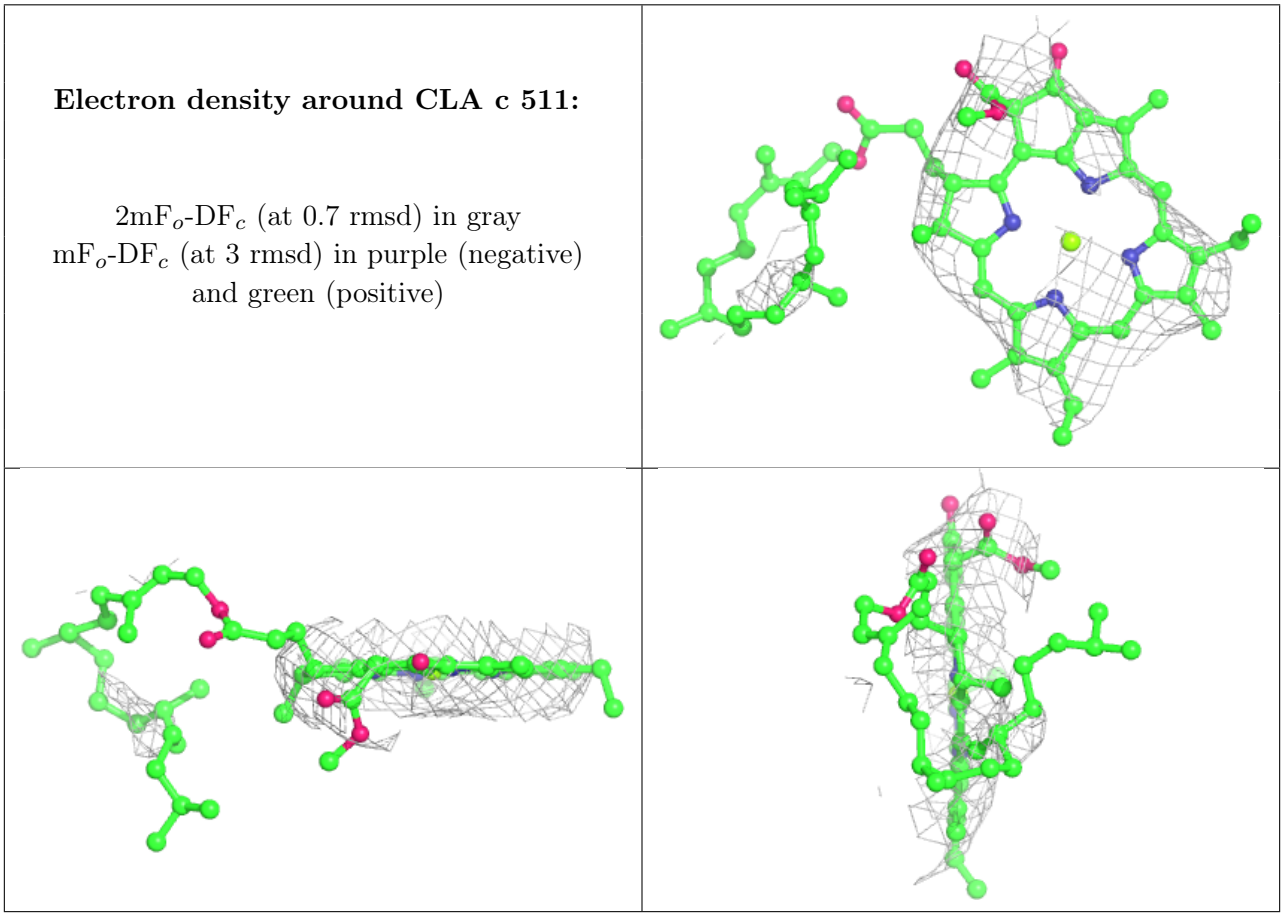
Electron density around CLA D 405:

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



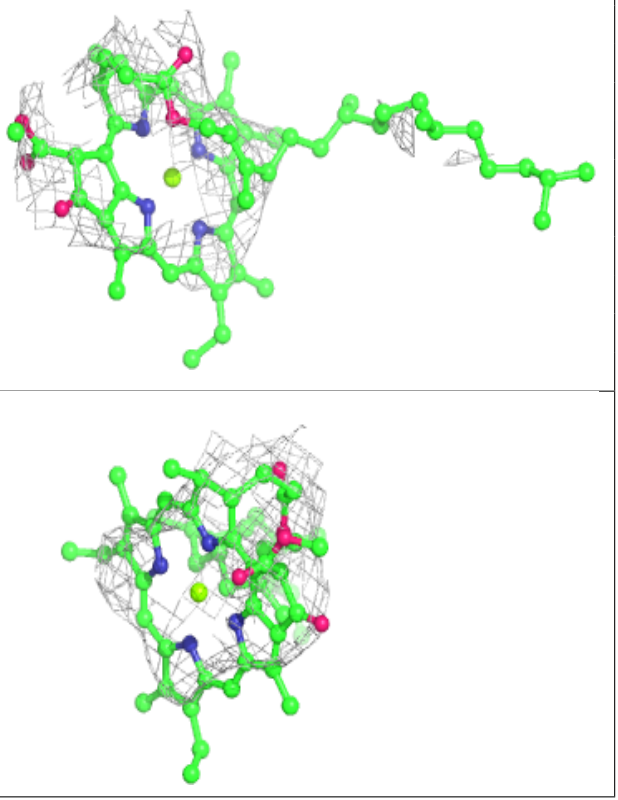
Electron density around CLA c 511:

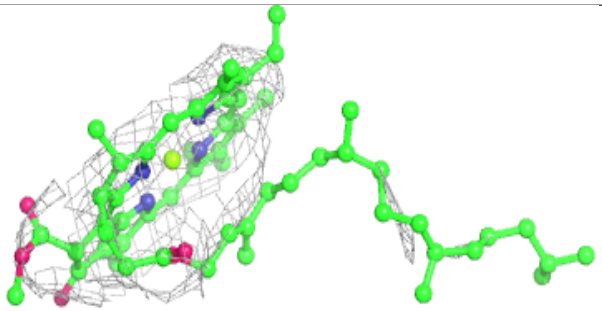
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA c 504:

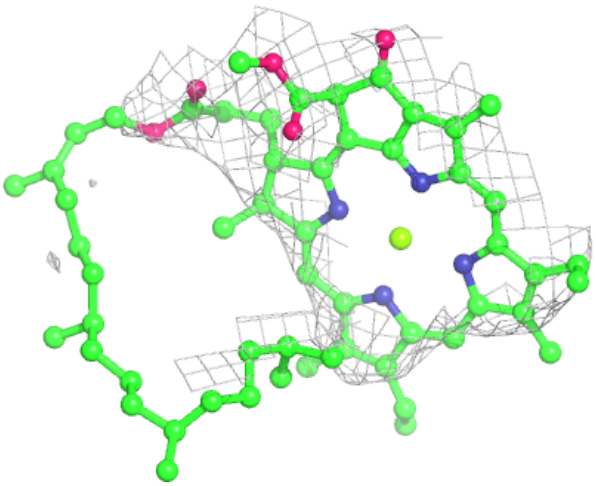
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

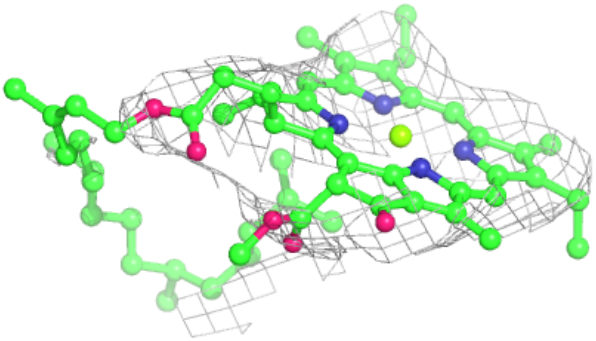


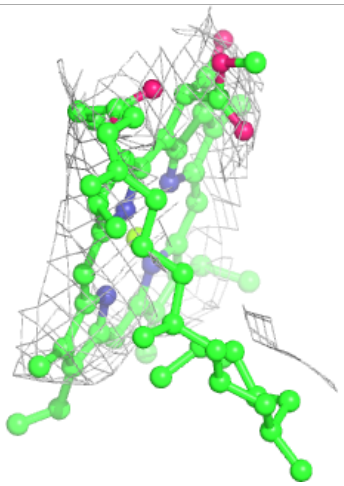


Electron density around CLA B 614:

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

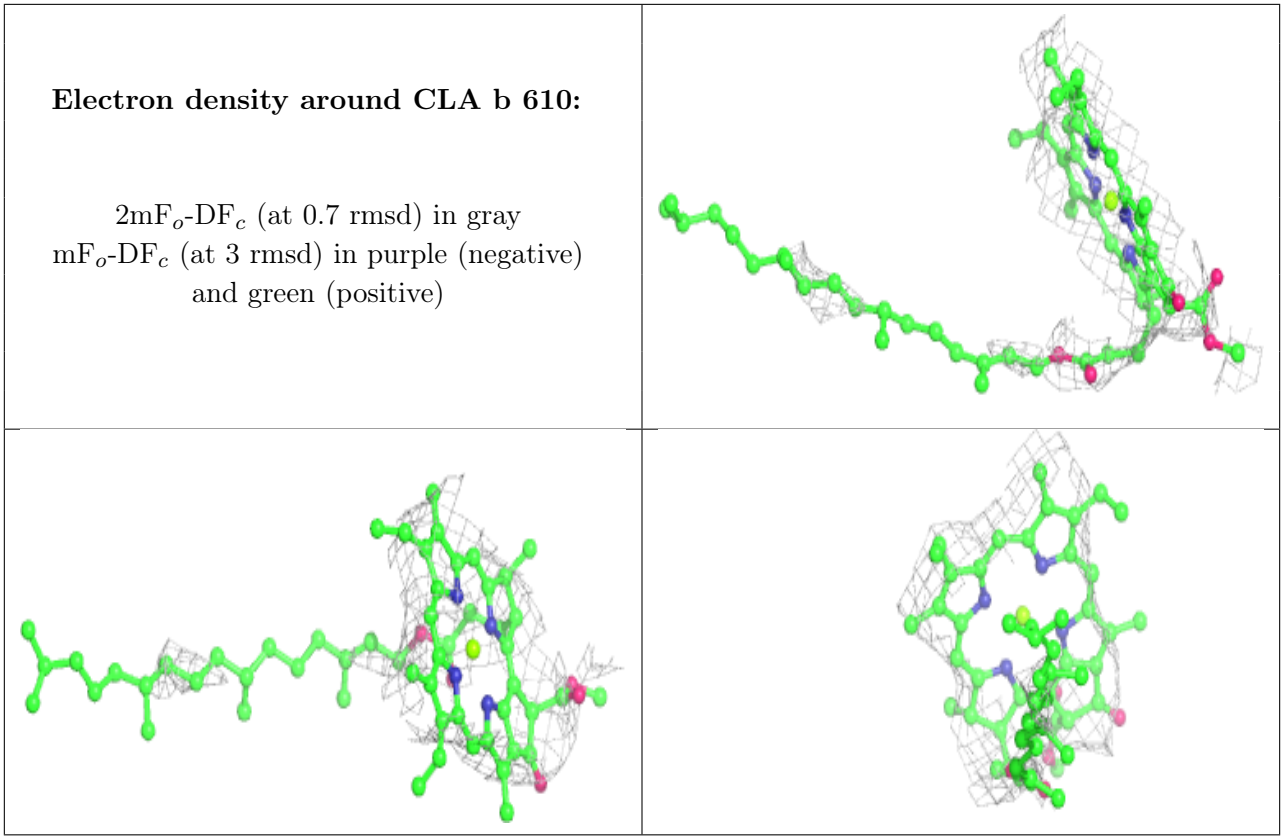






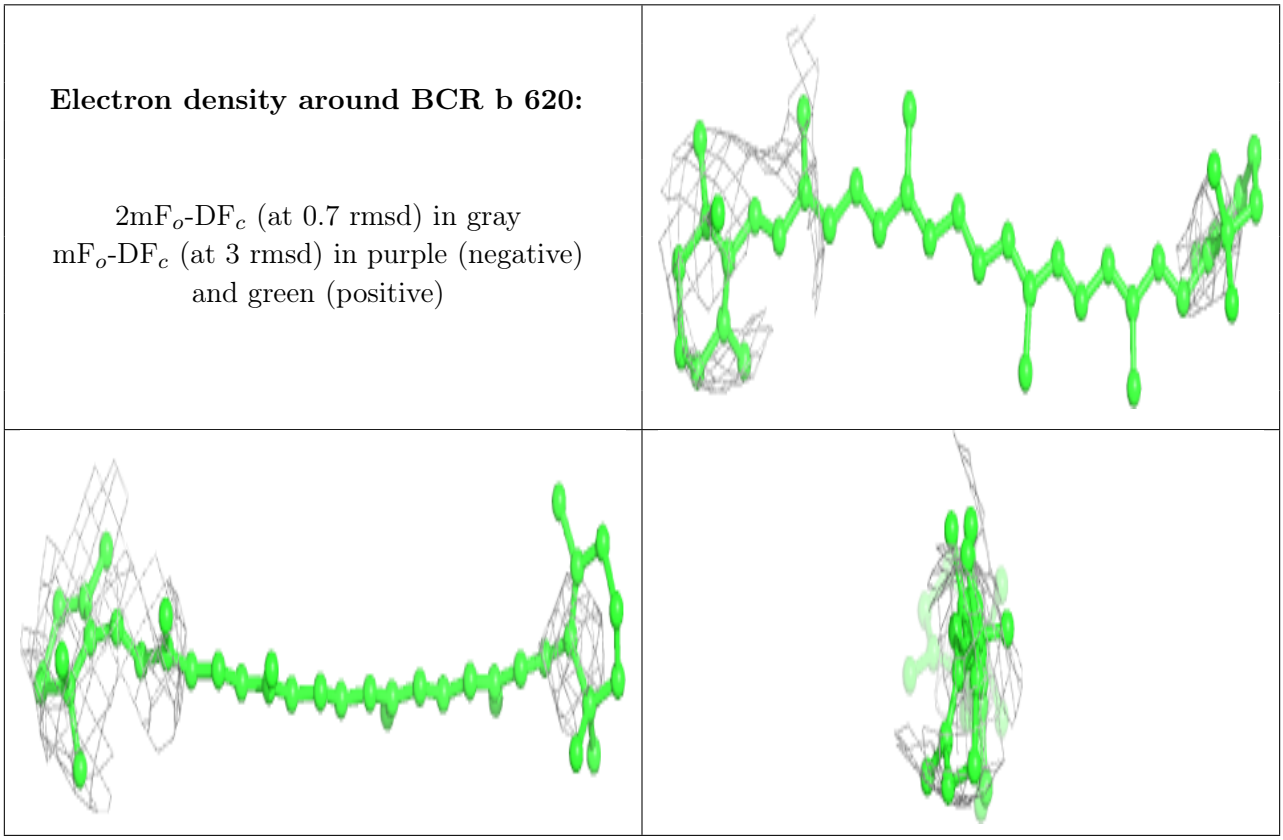
Electron density around CLA b 610:

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



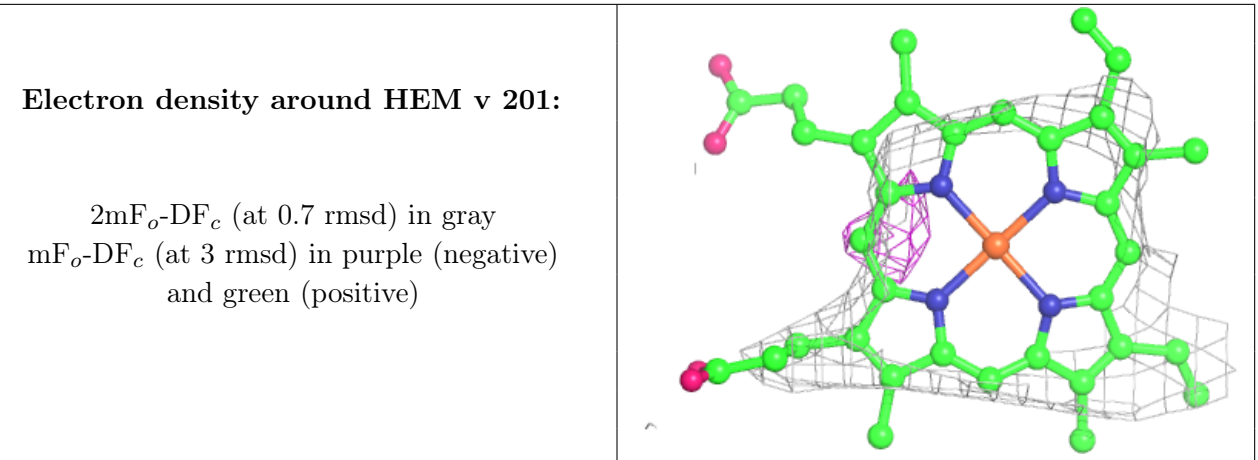
Electron density around BCR b 620:

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



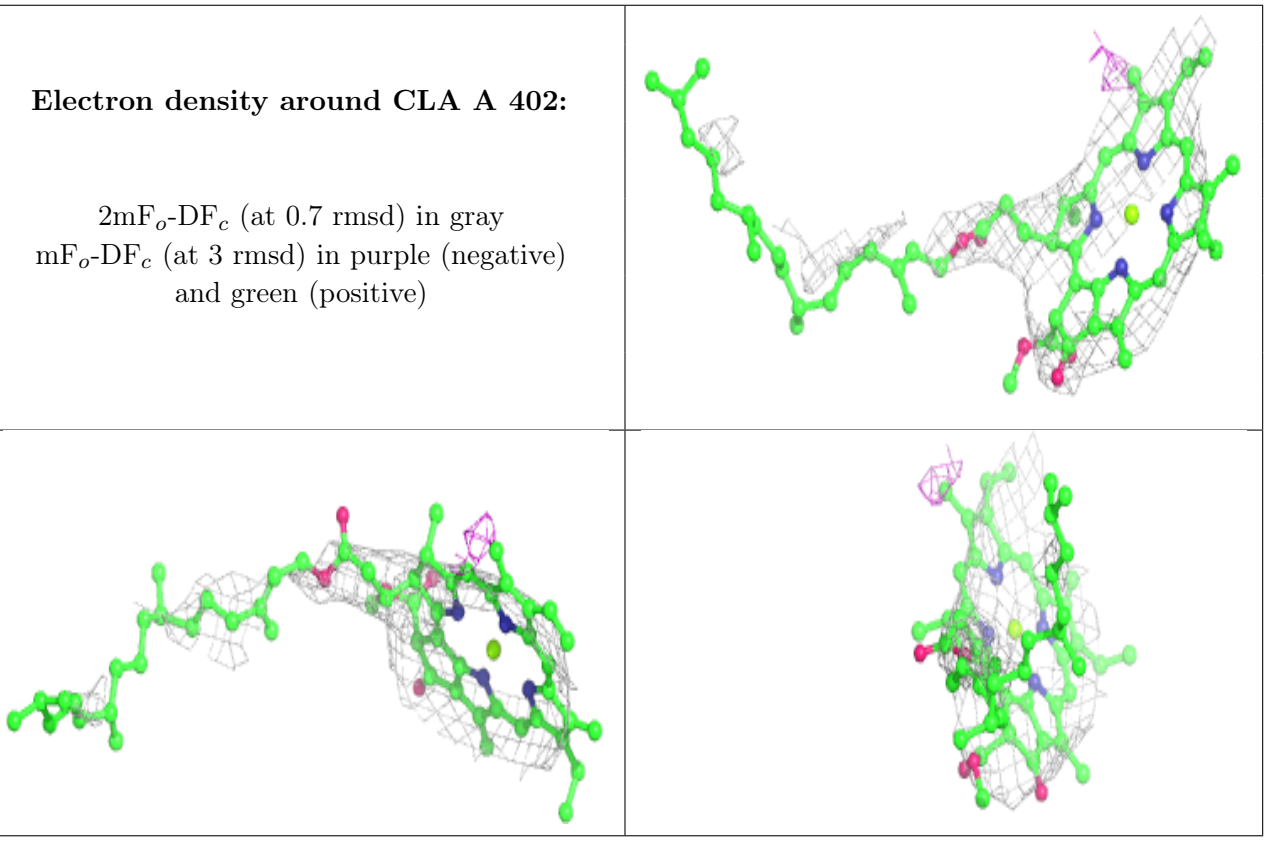
Electron density around HEM v 201:

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



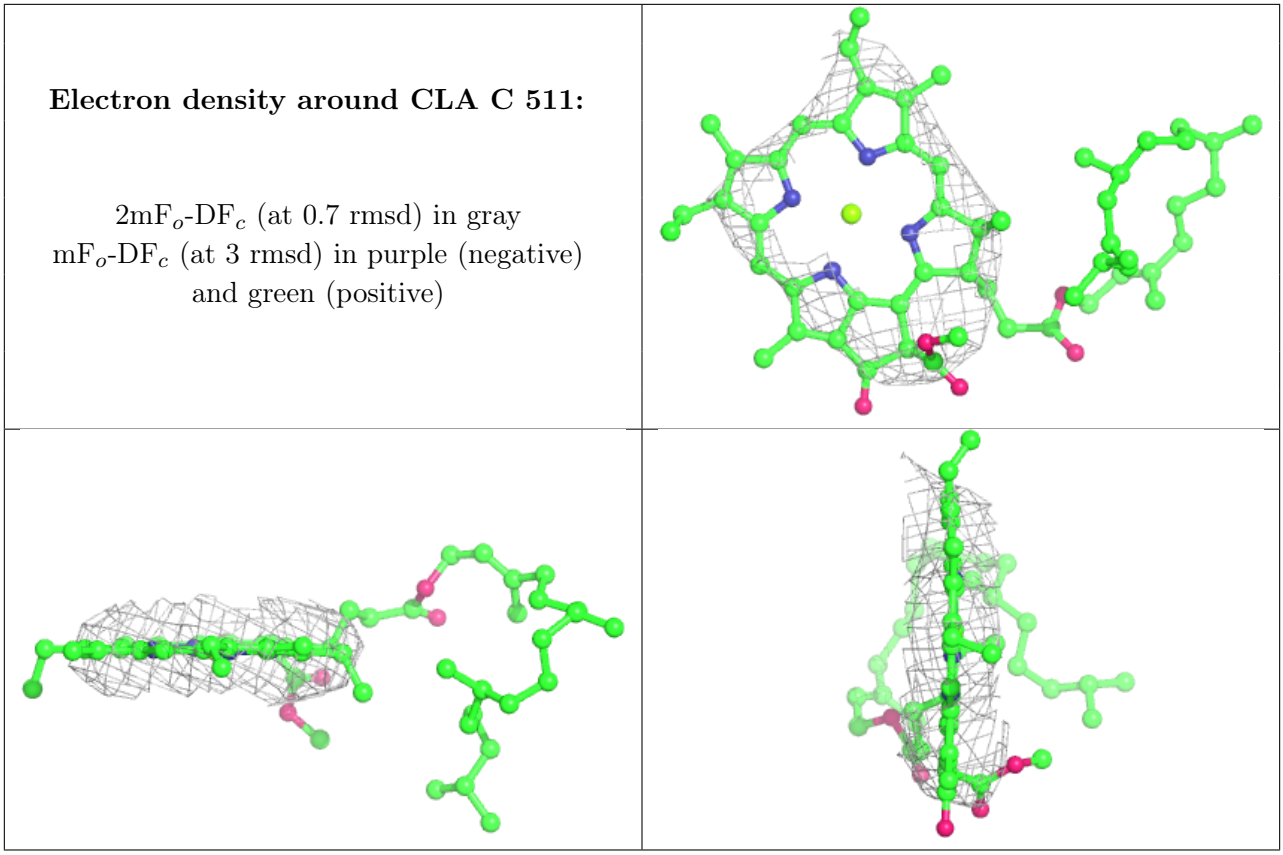
Electron density around CLA A 402:

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



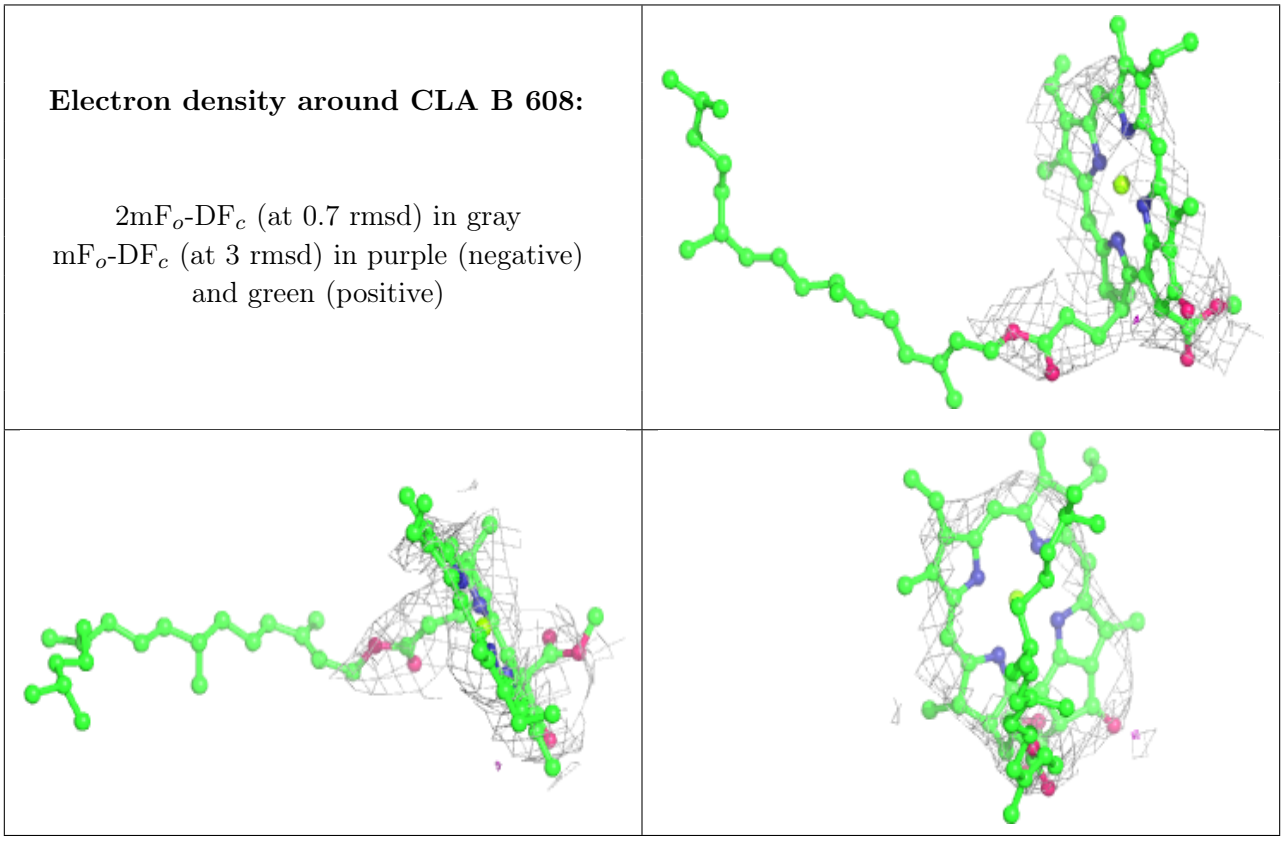
Electron density around CLA C 511:

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



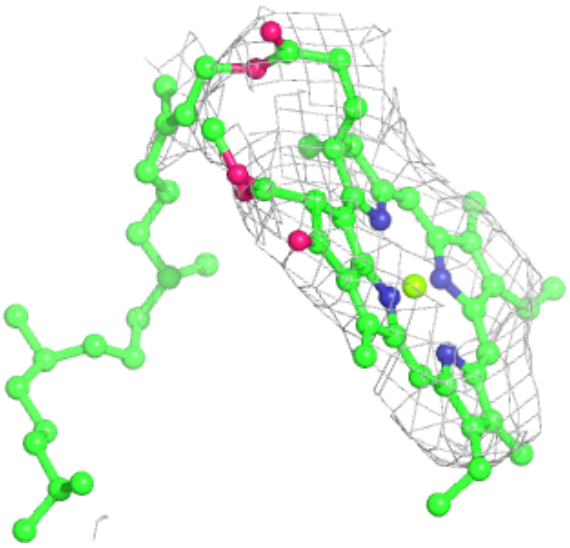
Electron density around CLA B 608:

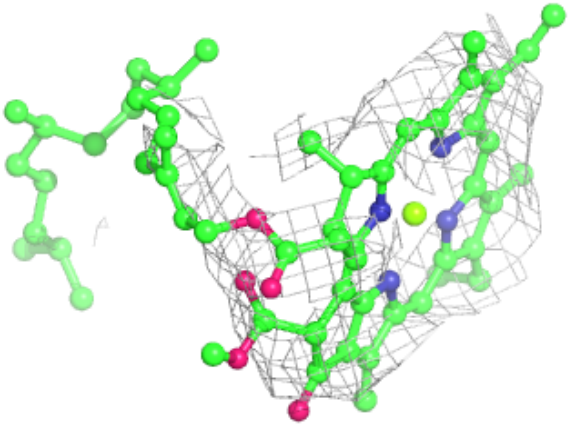
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

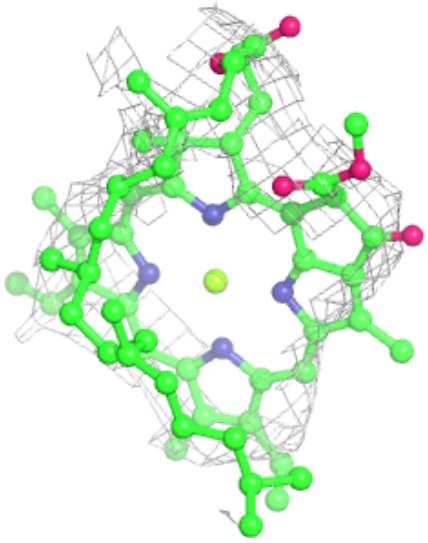


Electron density around CLA B 612:

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

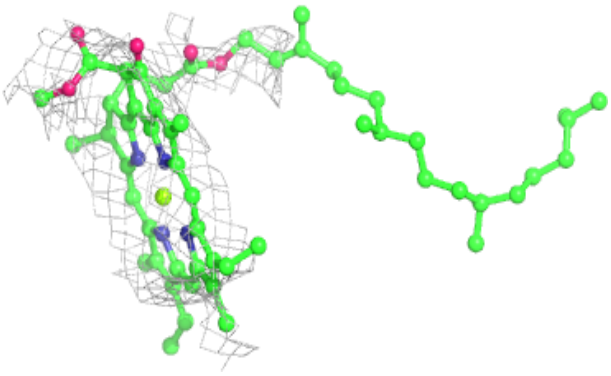


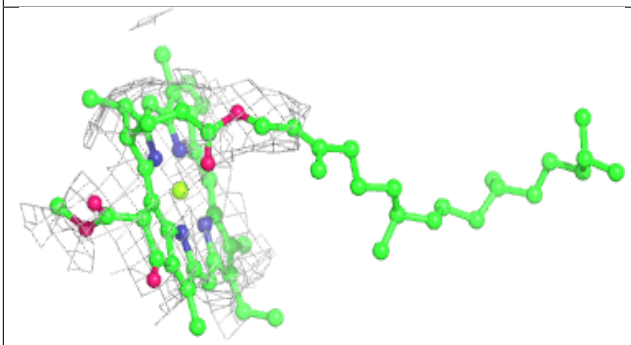


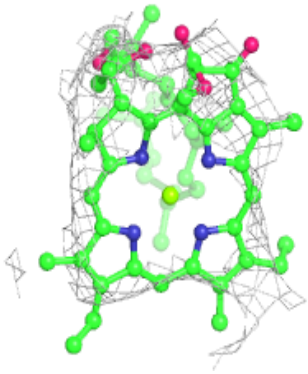


Electron density around CLA c 507:

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

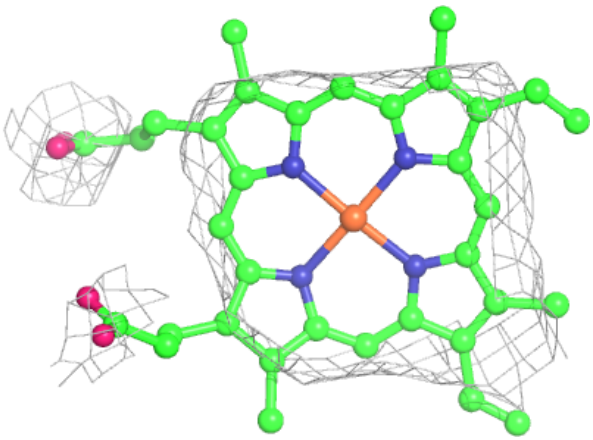


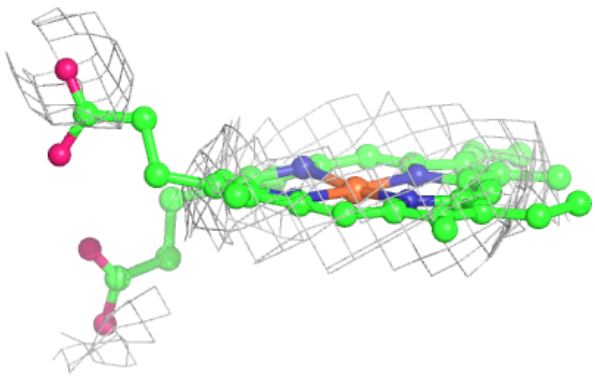


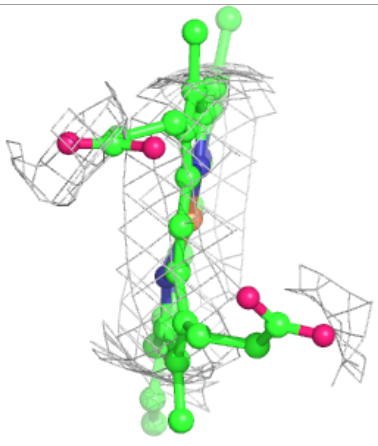


Electron density around HEM F 101:

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

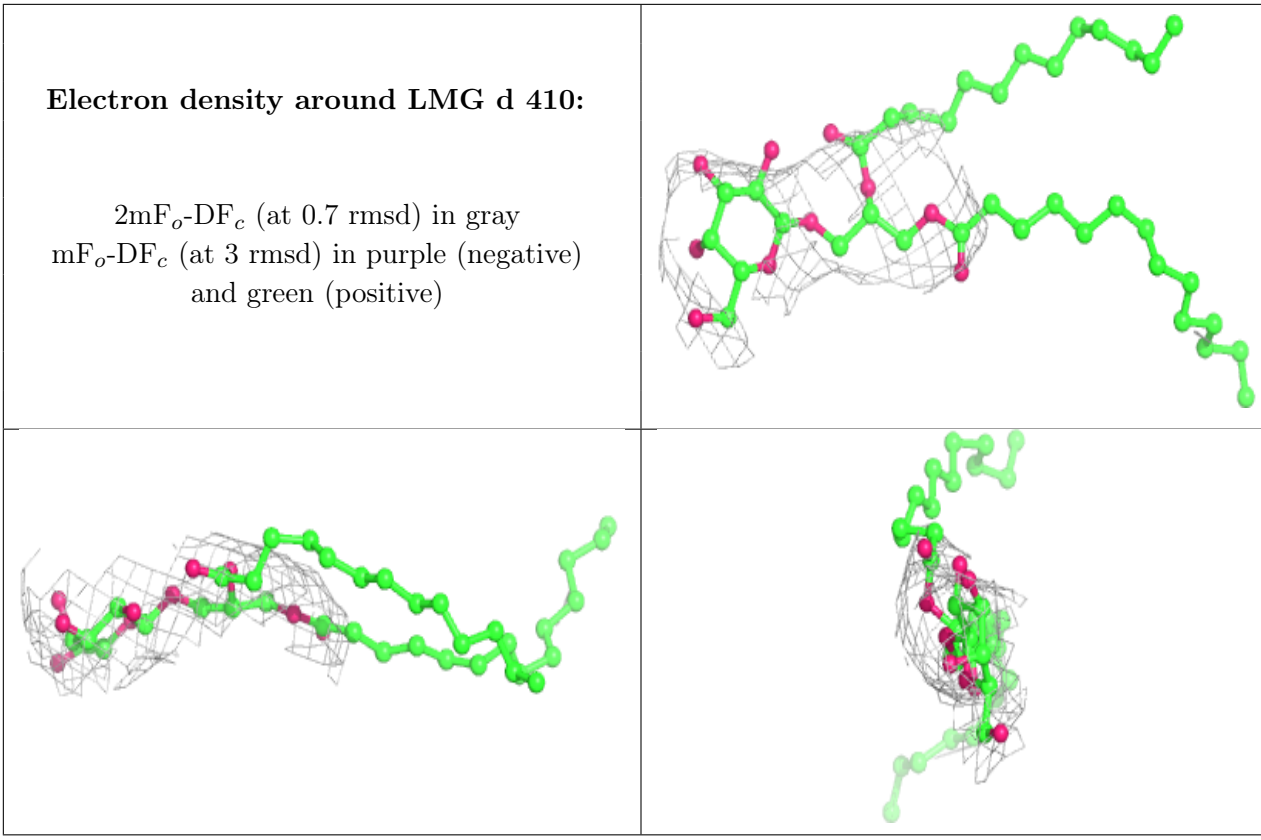






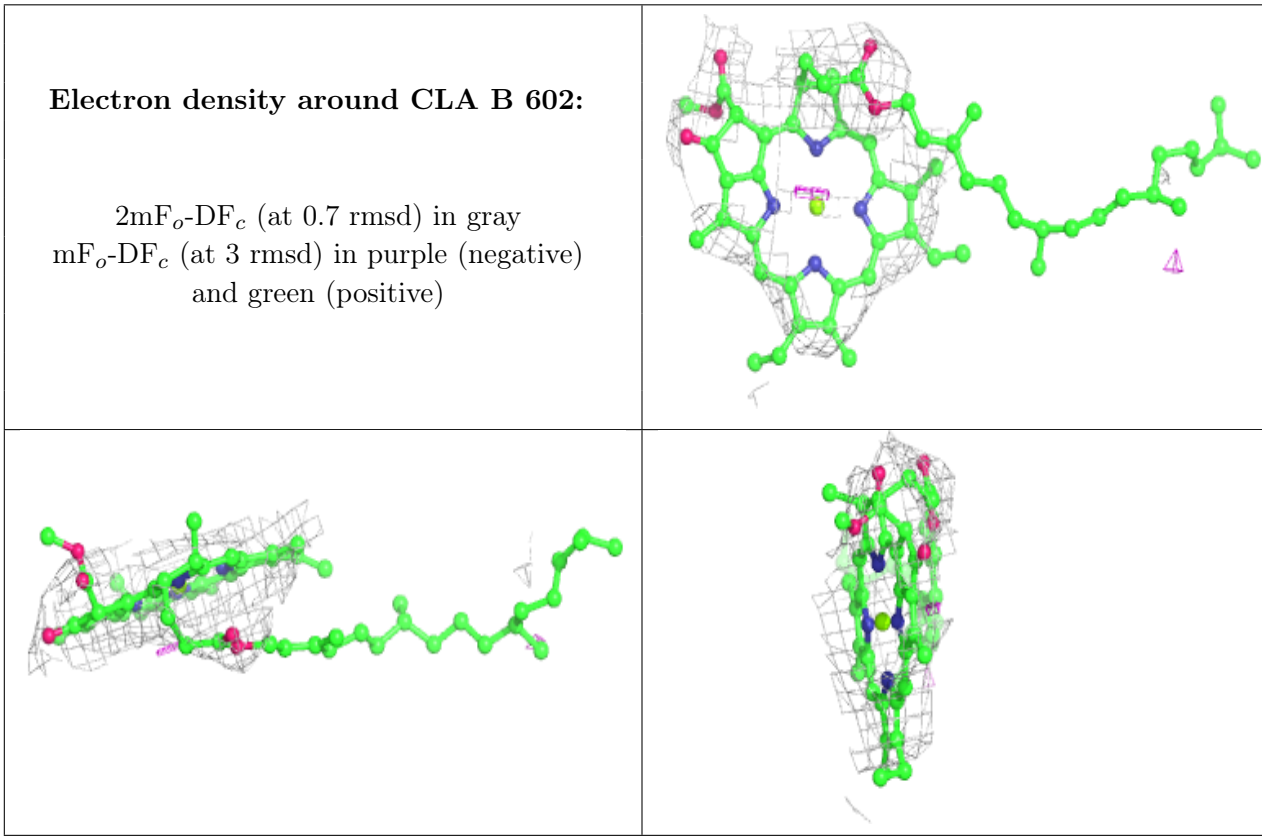
Electron density around LMG d 410:

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



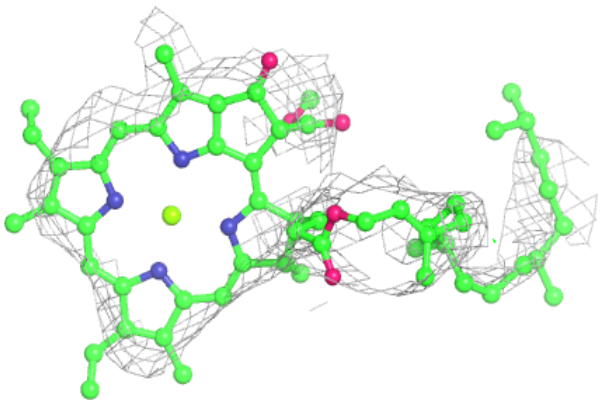
Electron density around CLA B 602:

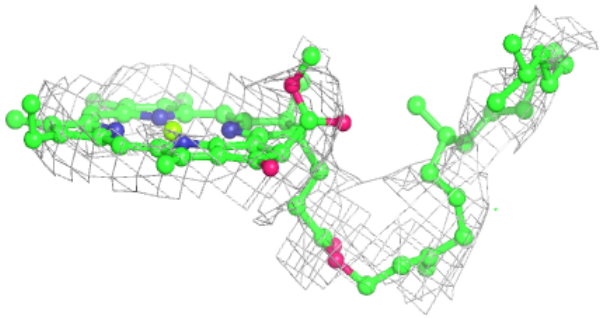
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

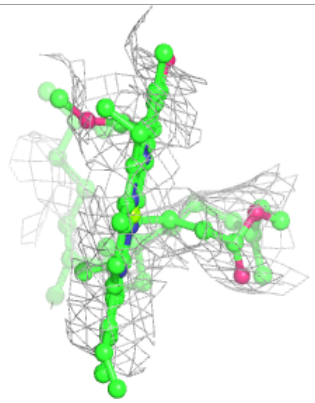


Electron density around CLA B 611:

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

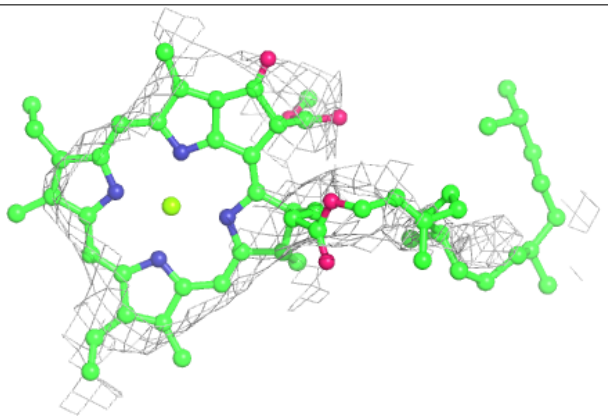


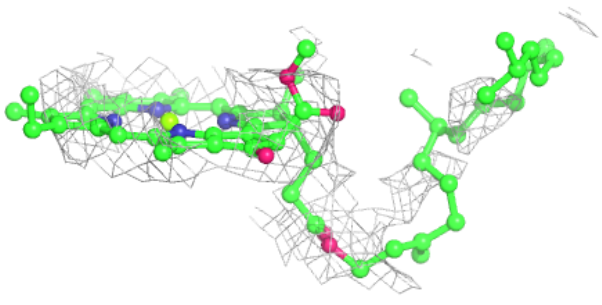


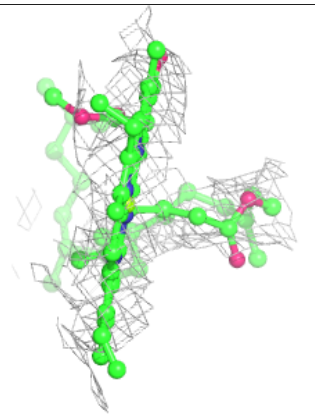


Electron density around CLA b 615:

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

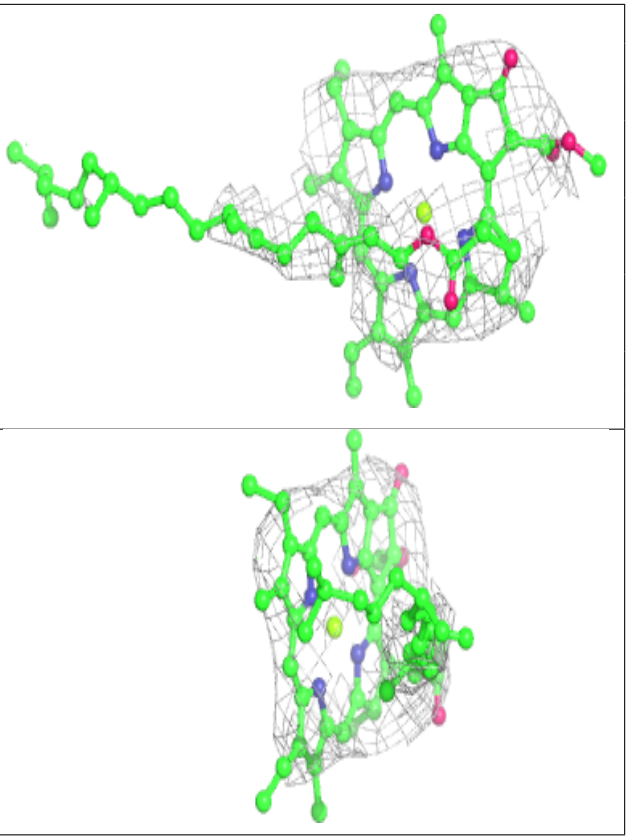






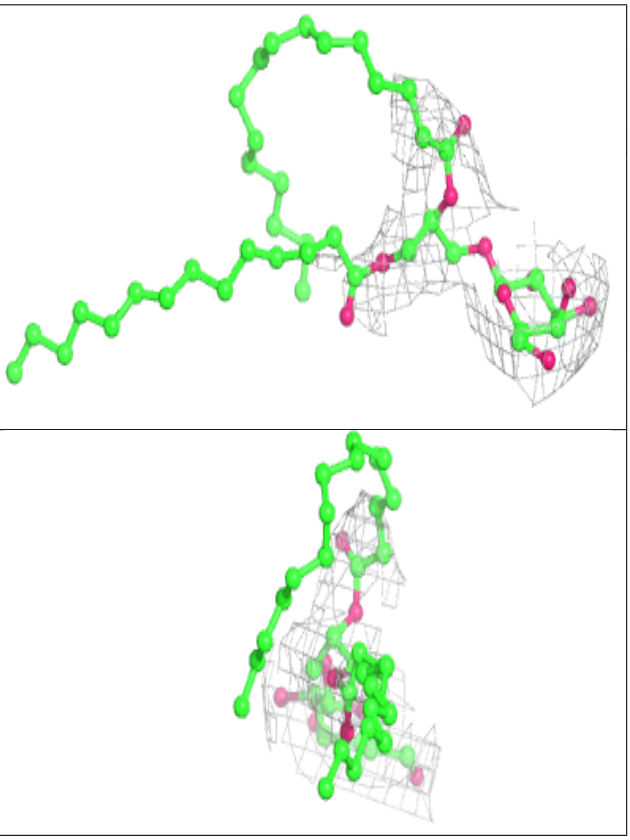
Electron density around CLA b 611:

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



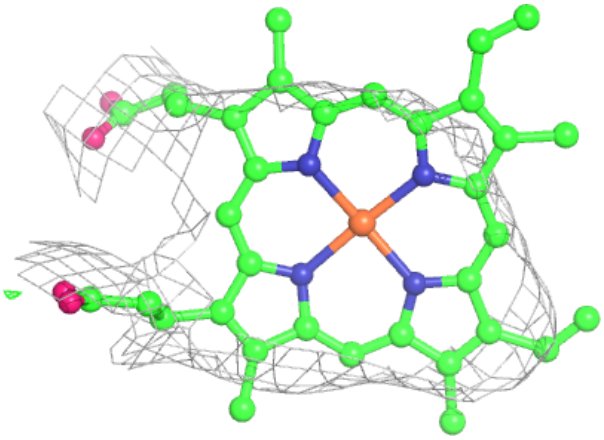
Electron density around LMG b 628:

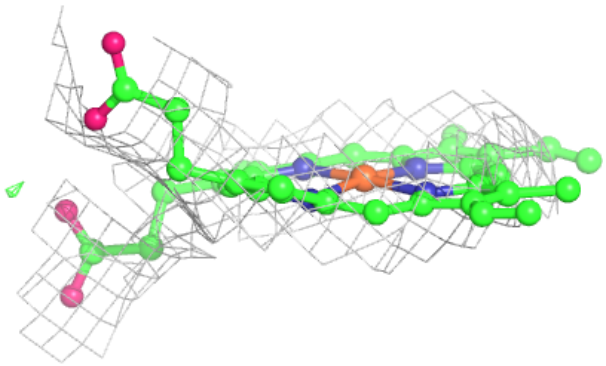
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

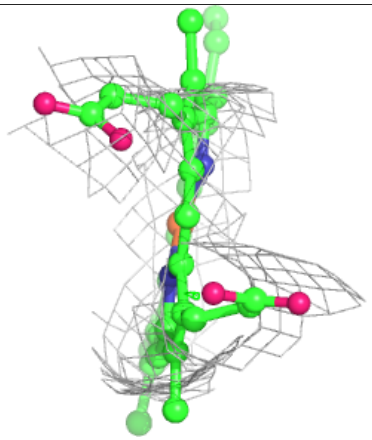


Electron density around HEM f 101:

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

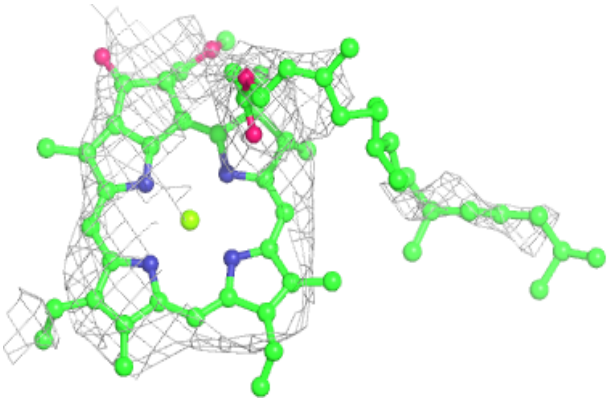


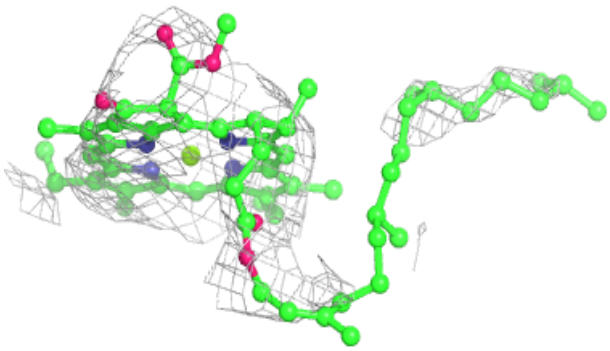


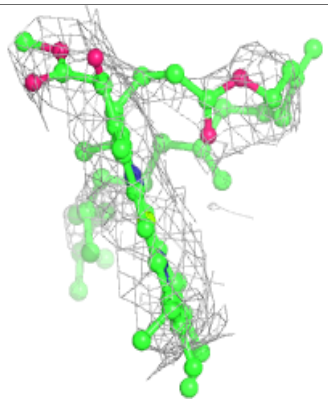


Electron density around CLA A 403:

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

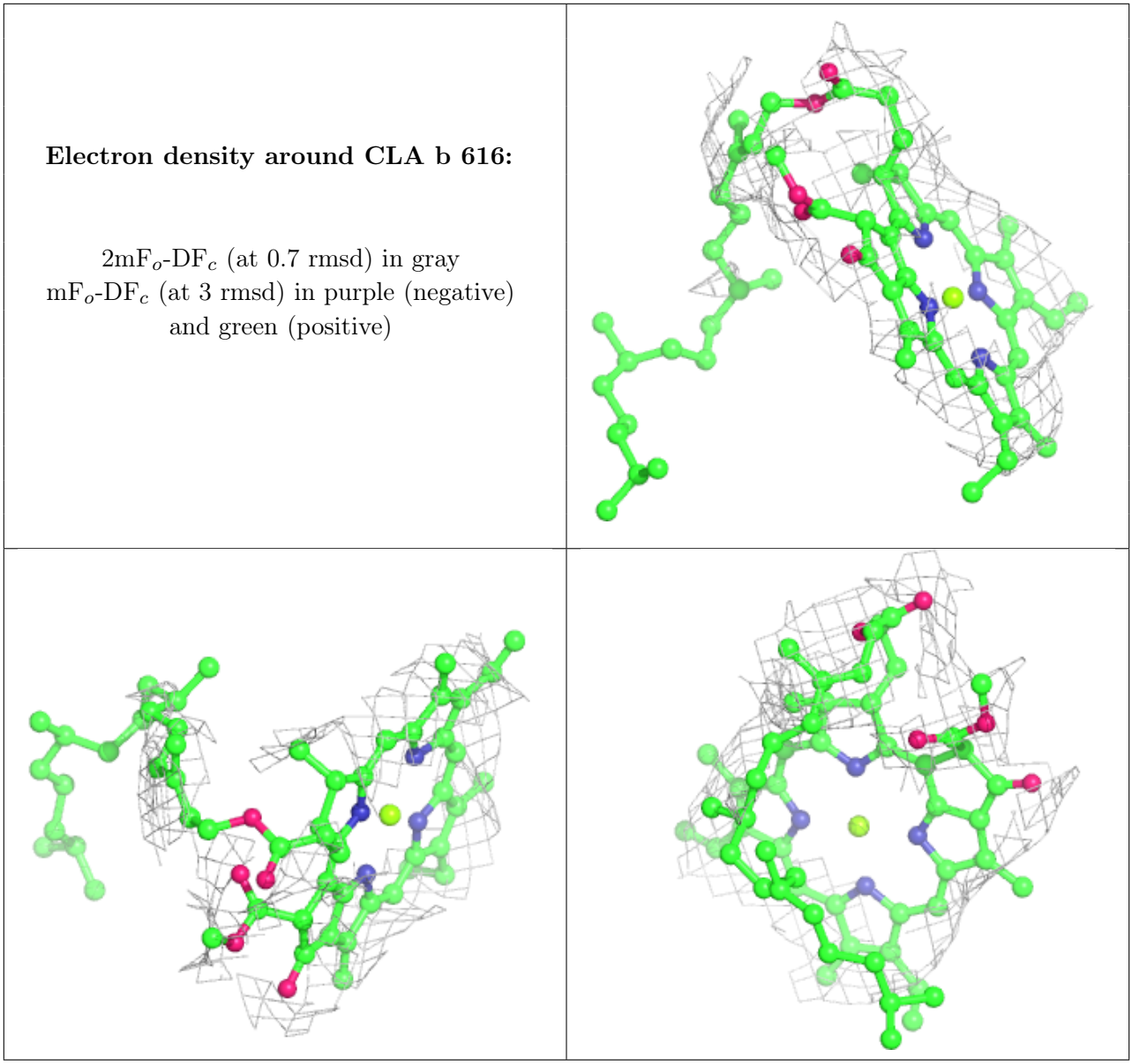






Electron density around CLA b 616:

$2mF_o$-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 (i)

There are no such residues in this entry.