Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 06:46 AM EDT

PDB ID	:	4TNK
Title	:	RT XFEL structure of Photosystem II 250 microsec after the third illumination at 5.2 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	:	5.20 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:

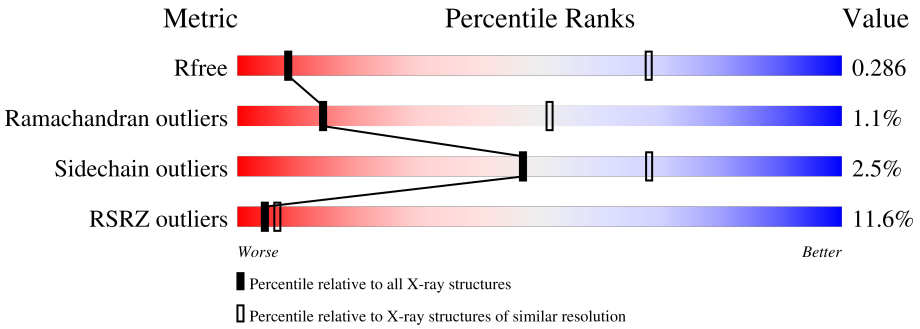
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1

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 5.20 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	1167 (6.60-3.80)
Ramachandran outliers	138981	1173 (6.60-3.80)
Sidechain outliers	138945	1148 (6.60-3.80)
RSRZ outliers	127900	1008 (6.64-3.74)

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	12% 95%
1	a	344	18% 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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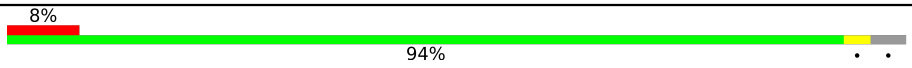
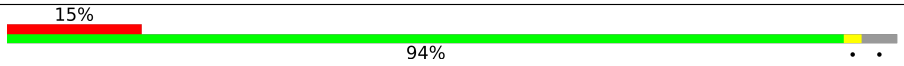
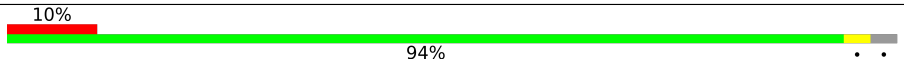
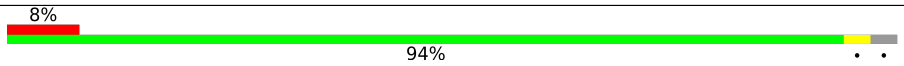
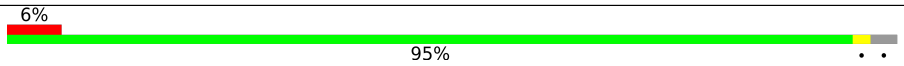
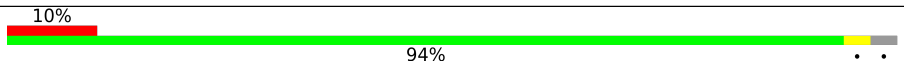
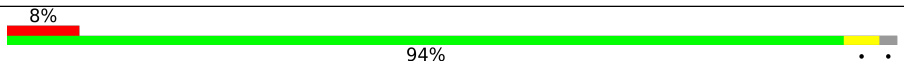
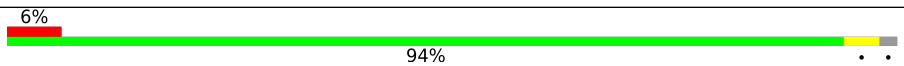
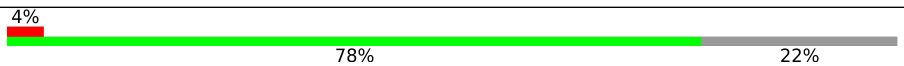
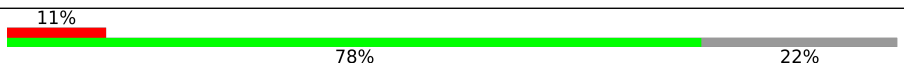
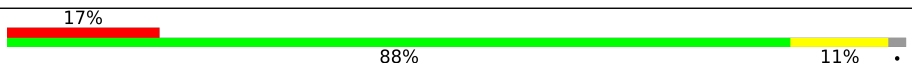
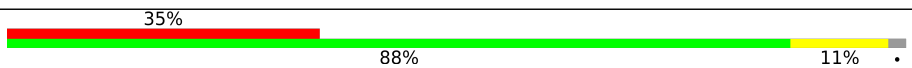
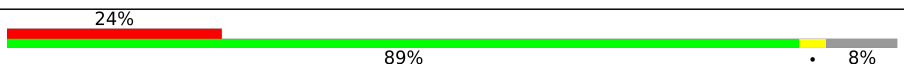
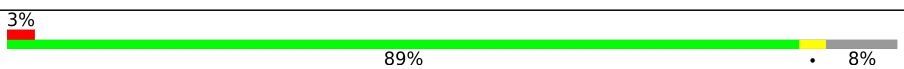
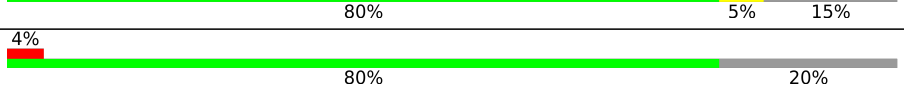
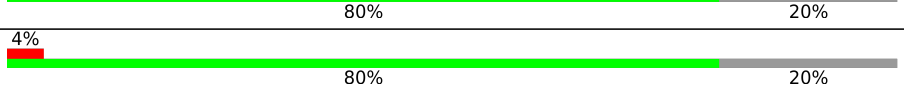
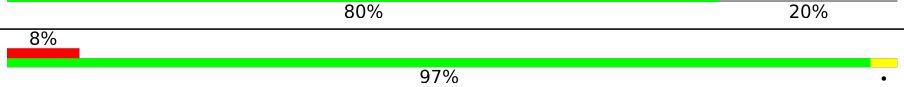
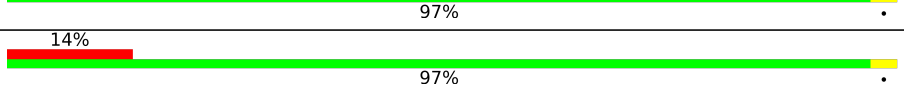
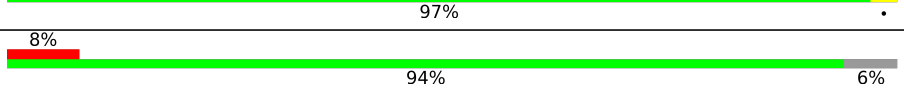
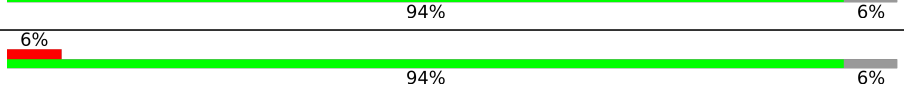
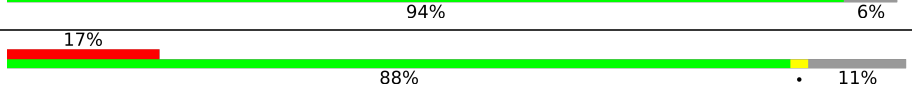
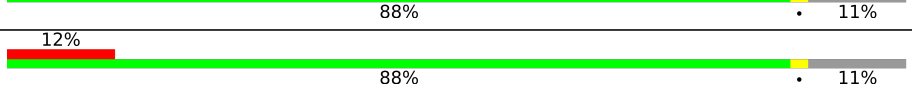
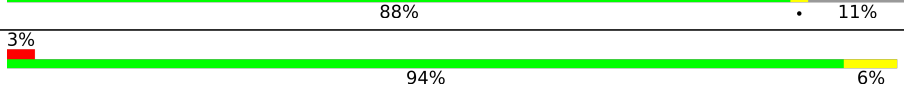
Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	

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Mol	Chain	Length	Quality of chain
14	t	32	9% 94% 6%
15	U	134	6% 70% 28%
15	u	134	14% 70% 28%
16	V	163	6% 83% 16%
16	v	163	12% 83% 16%
17	g	46	4% 54% 7% 39%
17	y	46	4% 54% 7% 39%
18	X	41	17% 85% 5% 10%
18	x	41	15% 85% 5% 10%
19	G	28	100%
19	Y	28	100%
20	Z	62	2% 95% 5%
20	z	62	5% 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	406	X	-	-	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	-	-	X
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	519	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	403	X	-	-	X
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	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	-	-	X
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	X
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	X
22	CLA	b	620	X	-	-	X
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	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	-	-	X
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	405	X	-	-	X
23	PHO	d	401	-	-	-	X
24	PL9	A	407	-	-	-	X
24	PL9	D	405	-	-	-	X
24	PL9	J	101	-	-	-	X
24	PL9	a	407	-	-	-	X
24	PL9	d	407	-	-	-	X
24	PL9	j	101	-	-	-	X
25	BCR	A	408	-	-	-	X
25	BCR	B	616	-	-	-	X
25	BCR	B	619	-	-	-	X
25	BCR	C	513	-	-	-	X
25	BCR	C	520	-	-	-	X
25	BCR	F	102	-	-	-	X
25	BCR	H	102	-	-	-	X
25	BCR	b	624	-	-	-	X
25	BCR	c	513	-	-	-	X
25	BCR	c	514	-	-	-	X
25	BCR	c	521	-	-	-	X
25	BCR	g	101	-	-	-	X
25	BCR	i	101	-	-	-	X
25	BCR	x	101	-	-	-	X
26	DGD	A	409	-	-	-	X
26	DGD	B	626	-	-	-	X
26	DGD	C	516	-	-	-	X
26	DGD	D	407	-	-	-	X
26	DGD	a	408	-	-	-	X
26	DGD	b	601	-	-	-	X
26	DGD	d	410	-	-	-	X
28	CL	A	411	-	-	-	X
30	SQD	B	622	-	-	-	X
30	SQD	B	627	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	b	602	-	-	-	X
30	SQD	d	403	-	-	-	X
31	LMG	C	517	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	b	627	-	-	-	X
31	LMG	c	518	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	102	-	-	-	X
31	LMG	m	101	-	-	-	X
32	LMT	B	623	-	-	-	X
32	LMT	B	624	-	-	-	X
32	LMT	B	628	-	-	-	X
32	LMT	D	408	-	-	-	X
32	LMT	I	102	-	-	-	X
32	LMT	M	102	-	-	-	X
32	LMT	b	603	-	-	-	X
32	LMT	b	628	-	-	-	X
32	LMT	b	629	-	-	-	X
32	LMT	d	411	-	-	-	X
32	LMT	i	103	-	-	-	X
35	CA	K	102	-	-	-	X
35	CA	O	301	-	-	-	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 666	C 434	N 108	O 124	0	0	0
5	e	82	Total 666	C 434	N 108	O 124	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

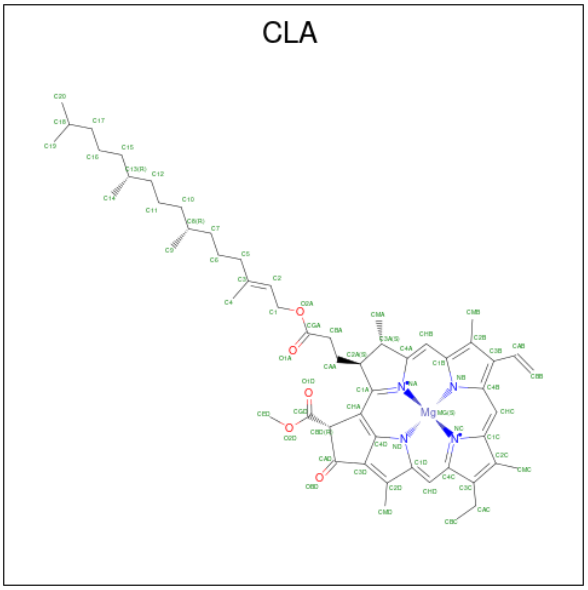
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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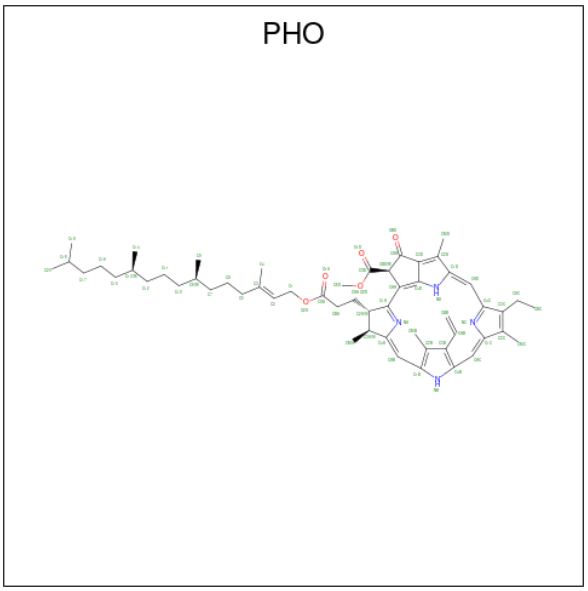
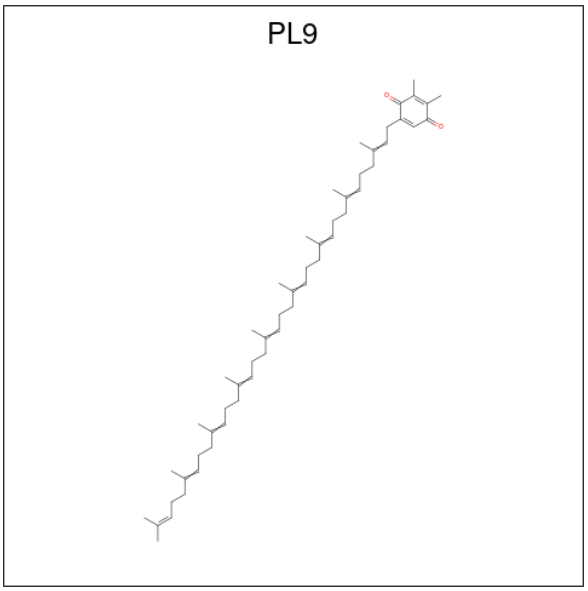
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



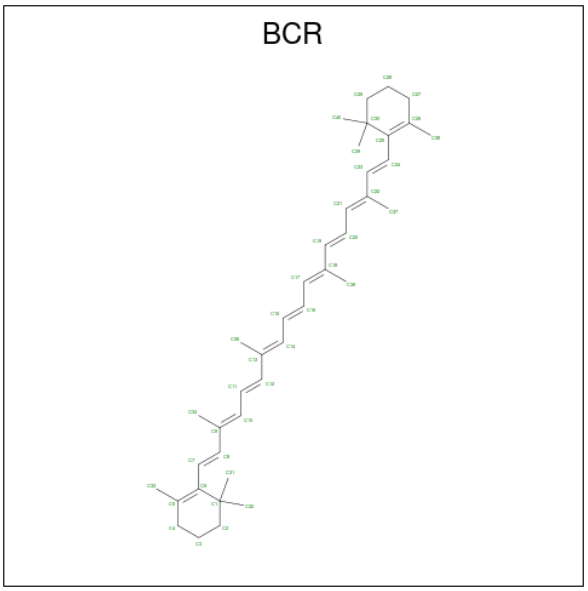
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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
24	A	1	Total C O 45 43 2	0	0
24	D	1	Total C O 55 53 2	0	0
24	J	1	Total C O 35 33 2	0	0
24	a	1	Total C O 45 43 2	0	0
24	d	1	Total C O 55 53 2	0	0
24	j	1	Total C O 35 33 2	0	0

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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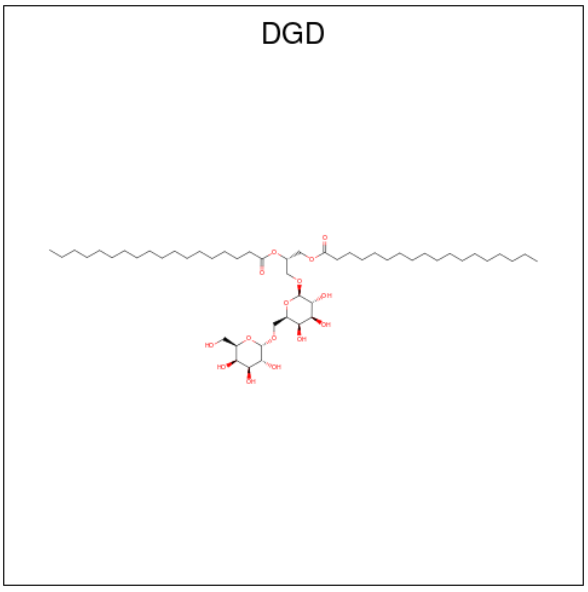
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	i	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	g	1	Total C 40 40	0	0
25	x	1	Total C 40 40	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

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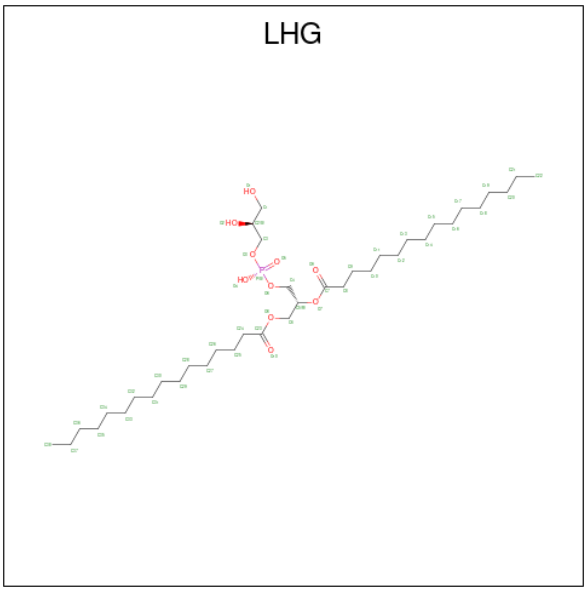
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			58	43	15		
26	B	1	Total	C	O	0	0
			52	37	15		
26	C	1	Total	C	O	0	0
			53	38	15		
26	C	1	Total	C	O	0	0
			62	47	15		
26	C	1	Total	C	O	0	0
			66	51	15		
26	D	1	Total	C	O	0	0
			63	48	15		
26	a	1	Total	C	O	0	0
			56	41	15		
26	b	1	Total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

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).

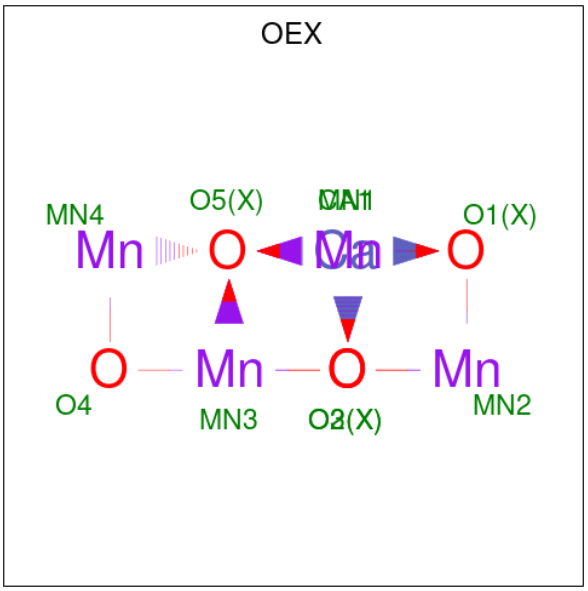


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O P 39 28 10 1	0	0
27	C	1	Total C O P 37 26 10 1	0	0
27	a	1	Total C O P 39 28 10 1	0	0
27	c	1	Total C O P 37 26 10 1	0	0

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

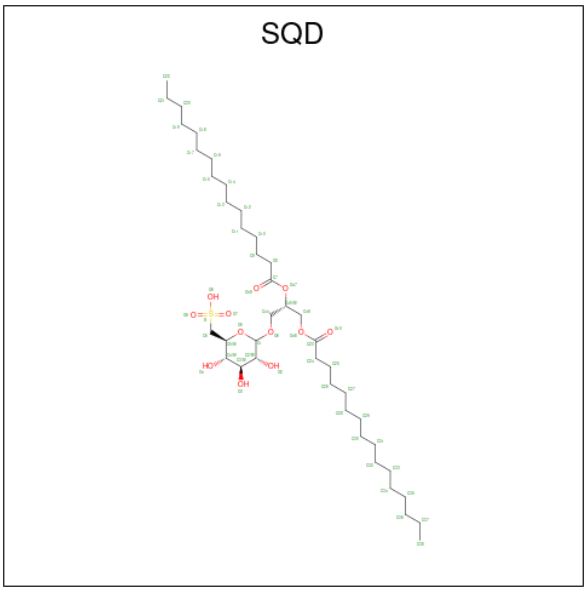
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Cl 1 1	0	0
28	a	1	Total Cl 1 1	0	0

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

- 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		

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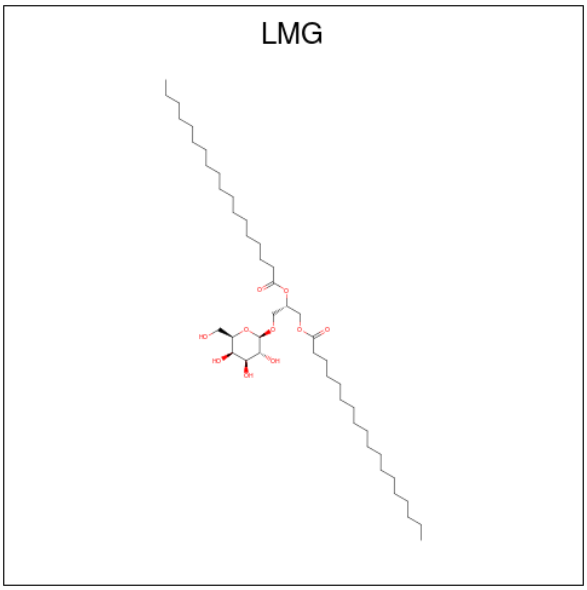
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		

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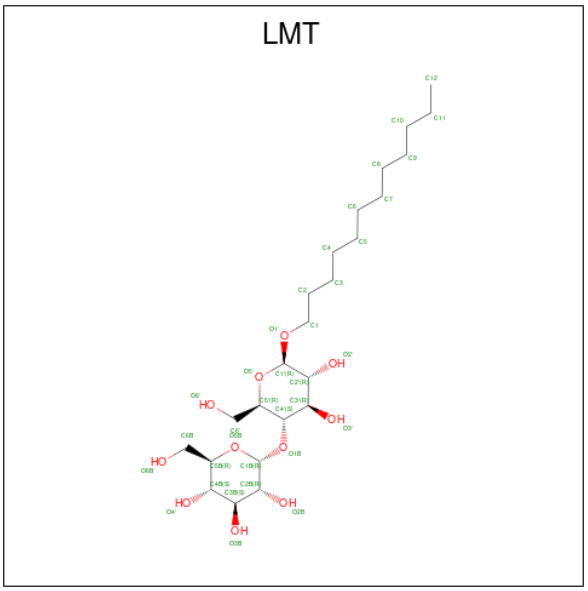
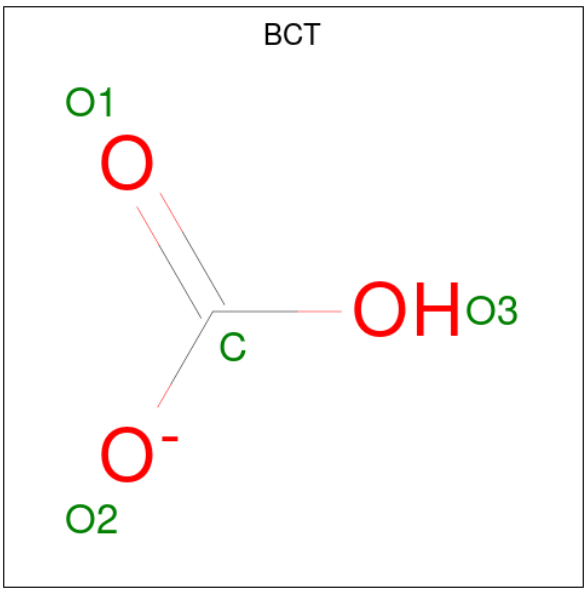
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	C	1	Total C O 45 35 10	0	0
31	C	1	Total C O 48 38 10	0	0
31	D	1	Total C O 48 38 10	0	0
31	D	1	Total C O 46 36 10	0	0
31	E	1	Total C O 44 34 10	0	0
31	I	1	Total C O 43 33 10	0	0
31	L	1	Total C O 51 41 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	a	1	Total C O 42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

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



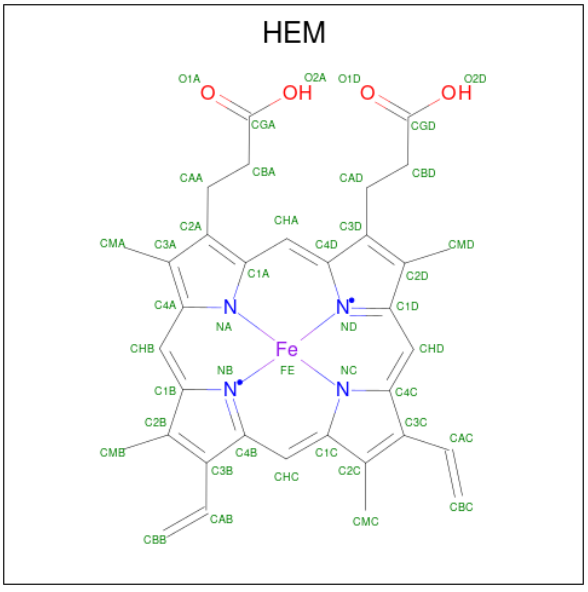
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	D	1	Total C O 31 20 11	0	0
32	I	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	b	1	Total C O 35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

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

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

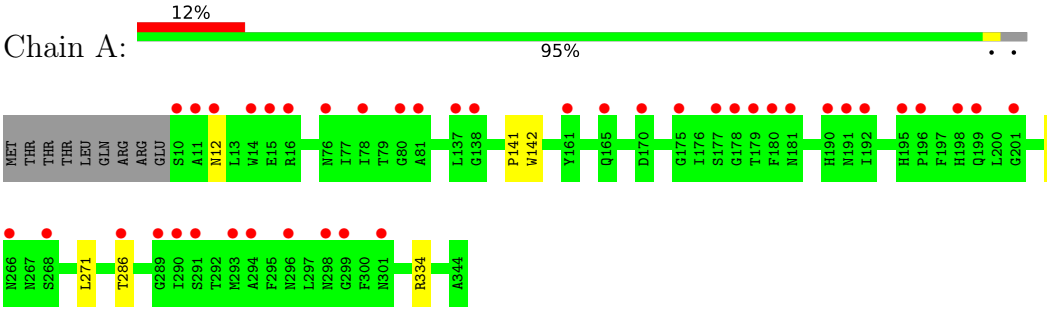
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

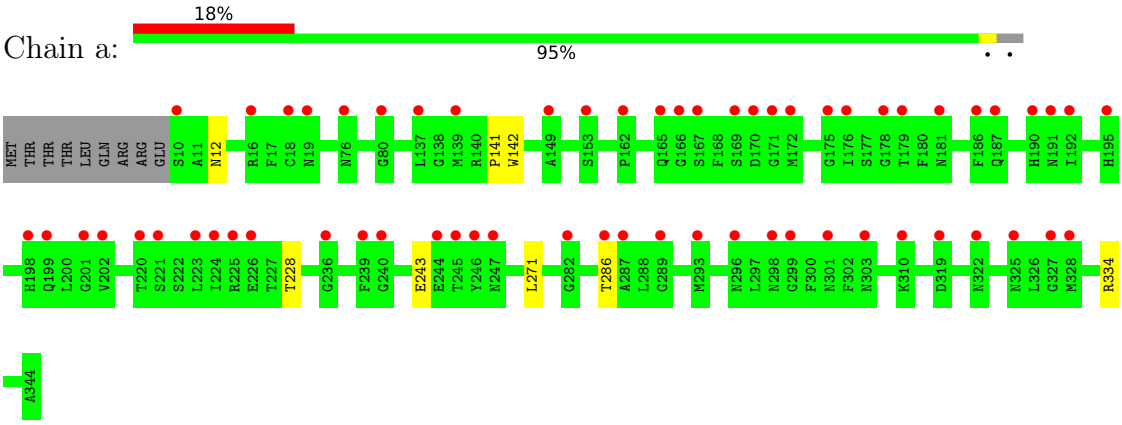
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



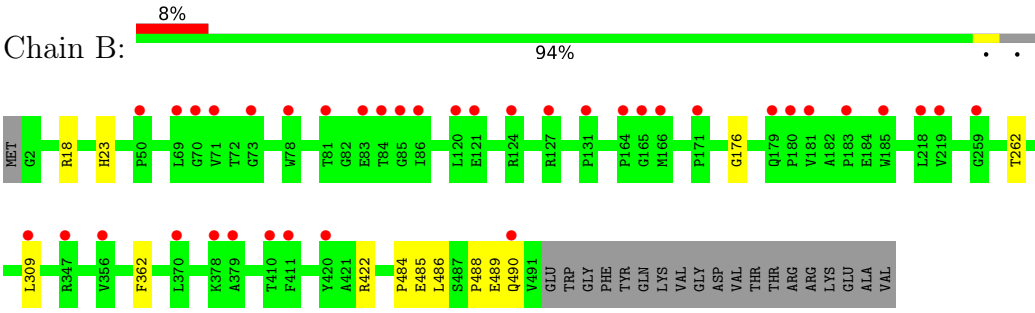
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



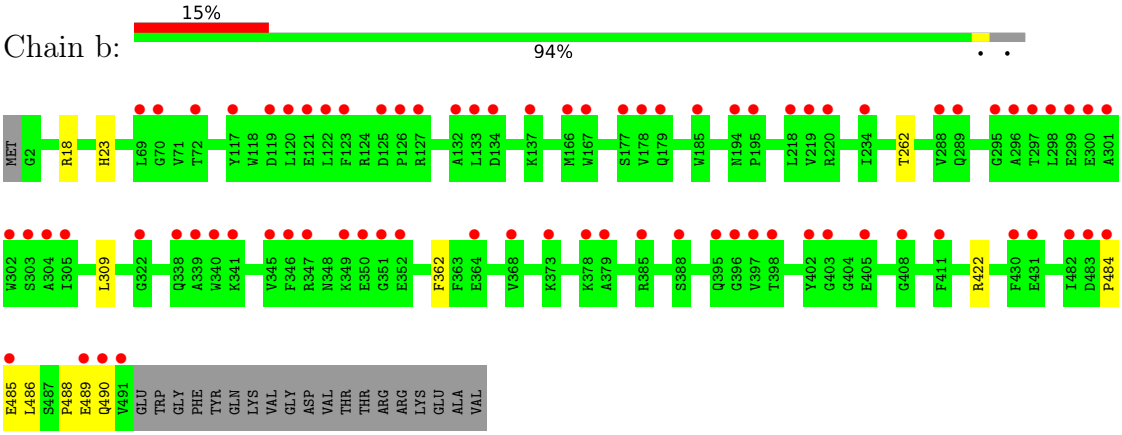
• Molecule 2: Photosystem II core light harvesting protein

Chain B:



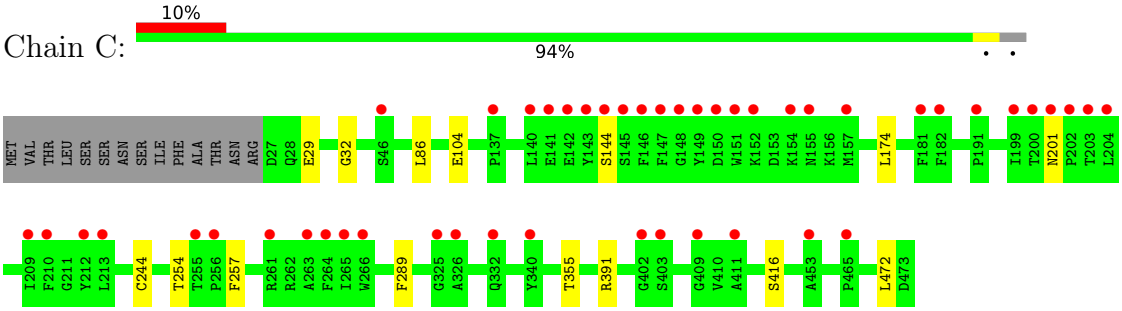
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



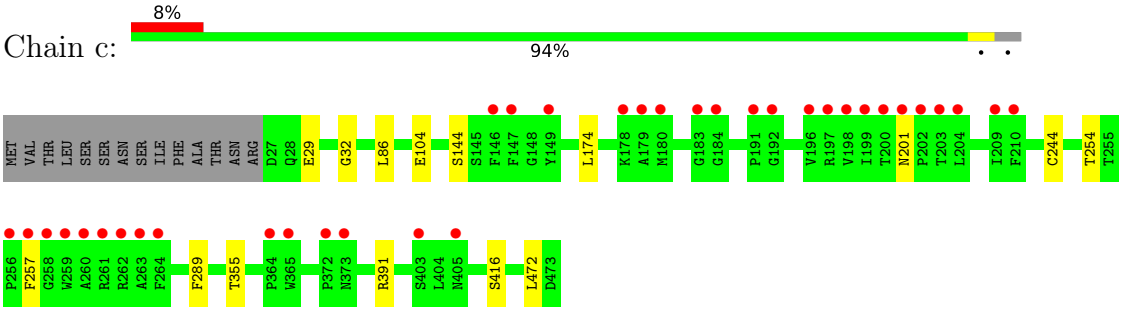
• Molecule 3: Photosystem II CP43 protein

Chain C:



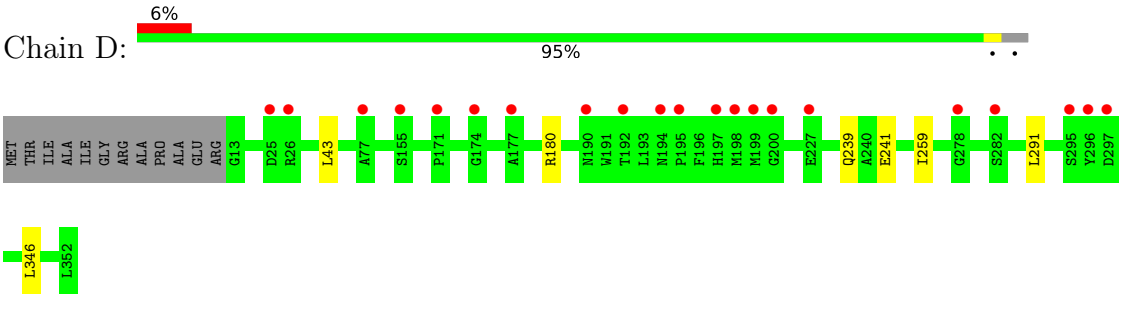
• Molecule 3: Photosystem II CP43 protein

Chain c:



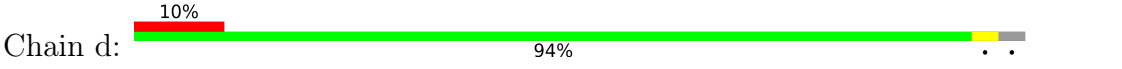
• Molecule 4: Photosystem II D2 protein

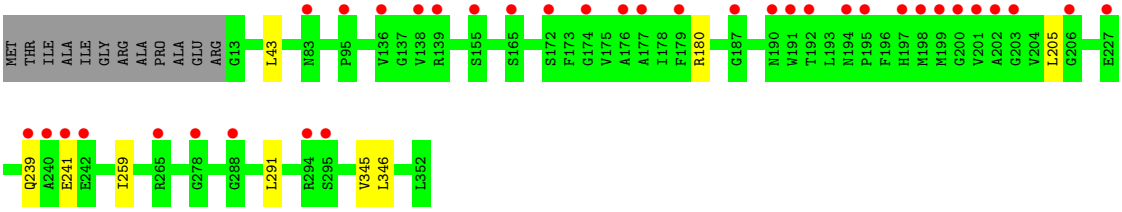
Chain D:



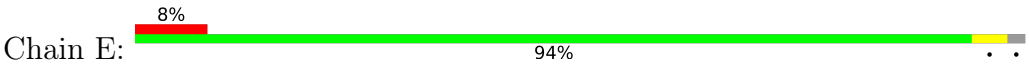
• Molecule 4: Photosystem II D2 protein

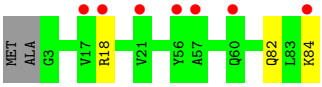
Chain d:



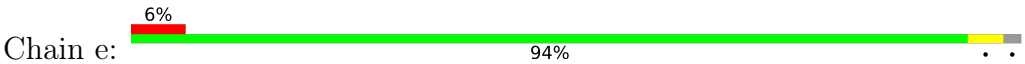


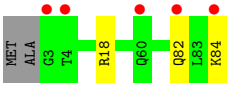
• Molecule 5: Cytochrome b559 subunit alpha



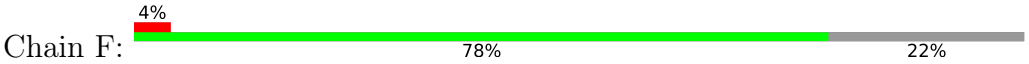


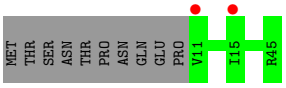
• Molecule 5: Cytochrome b559 subunit alpha



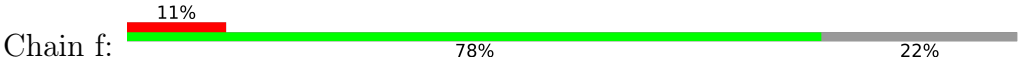


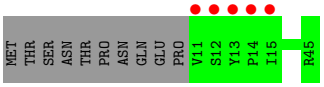
• Molecule 6: Cytochrome b559 subunit beta



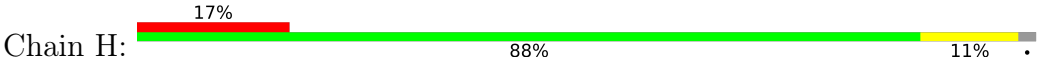


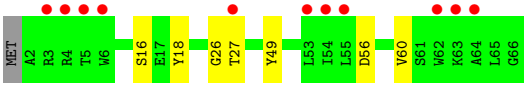
• Molecule 6: Cytochrome b559 subunit beta



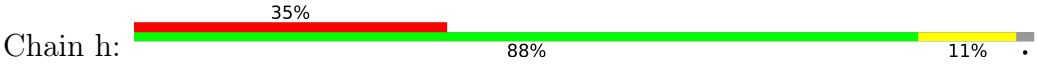


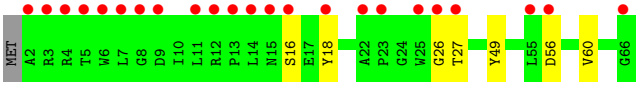
• Molecule 7: Photosystem II reaction center protein H



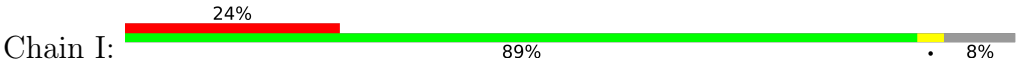


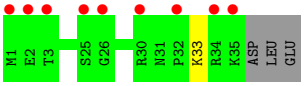
• Molecule 7: Photosystem II reaction center protein H



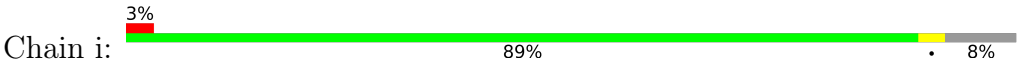


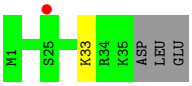
• Molecule 8: Photosystem II reaction center protein I



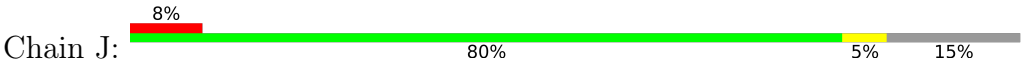


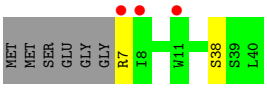
• Molecule 8: Photosystem II reaction center protein I



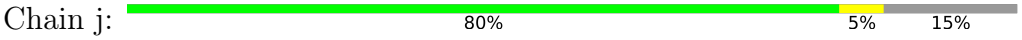


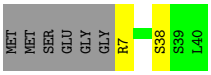
• Molecule 9: Photosystem II reaction center protein J



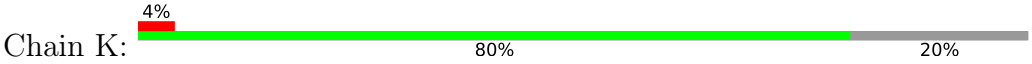


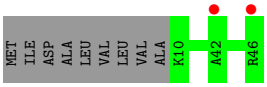
• Molecule 9: Photosystem II reaction center protein J



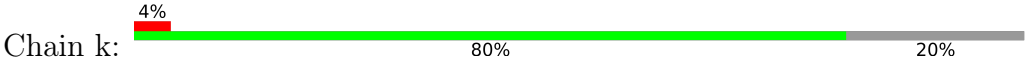


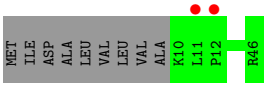
• Molecule 10: Photosystem II reaction center protein K





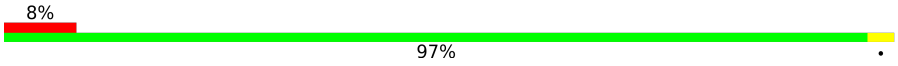
• Molecule 10: Photosystem II reaction center protein K

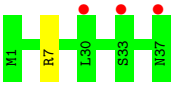




• Molecule 11: Photosystem II reaction center protein L

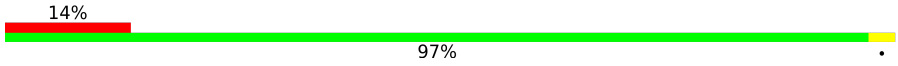
Chain L:

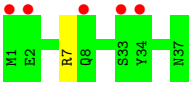




• Molecule 11: Photosystem II reaction center protein L

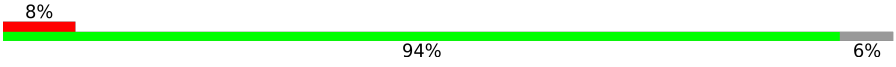
Chain l:

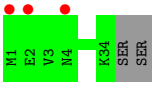




• Molecule 12: Photosystem II reaction center protein M

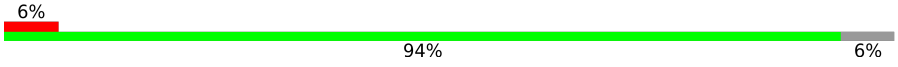
Chain M:

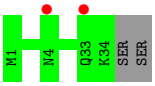




• Molecule 12: Photosystem II reaction center protein M

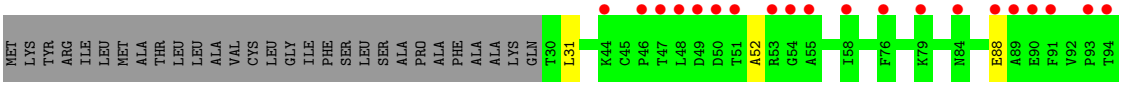
Chain m:

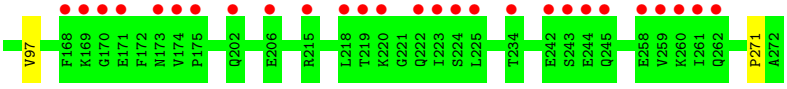




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

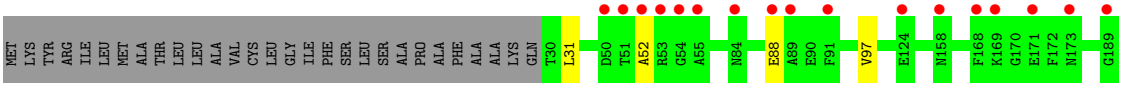
Chain O:

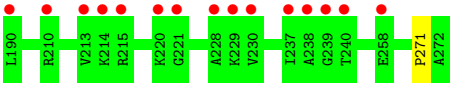




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

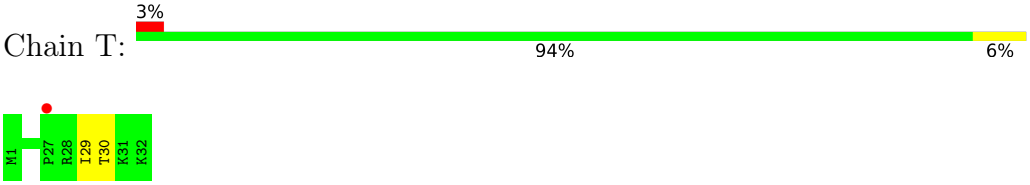
Chain o:





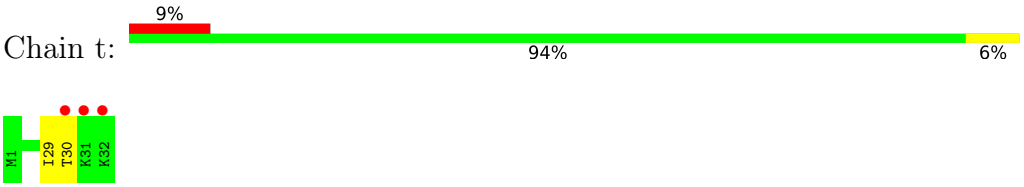
• Molecule 14: Photosystem II reaction center protein T

Chain T:



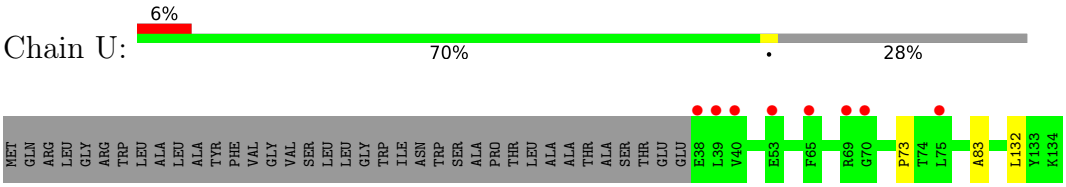
• Molecule 14: Photosystem II reaction center protein T

Chain t:



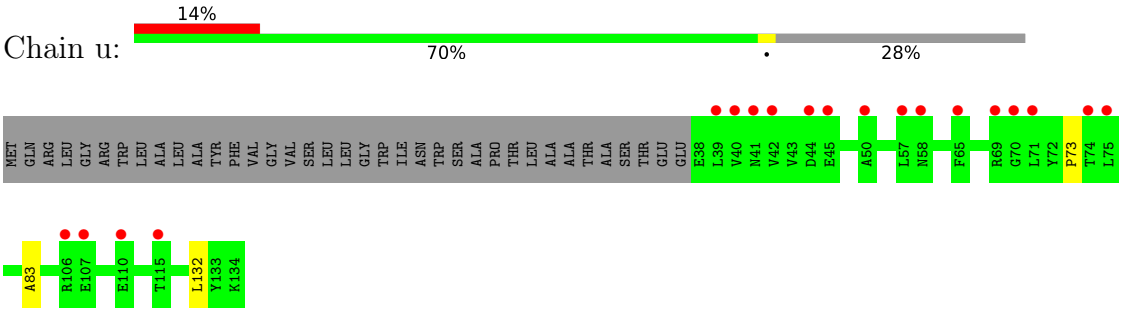
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



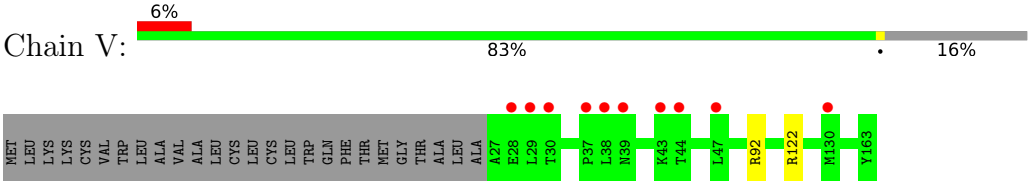
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



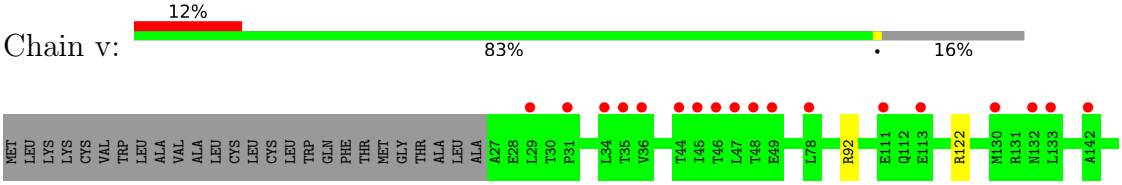
• Molecule 16: Cytochrome c-550

Chain V:



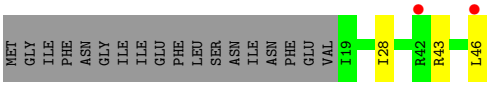
• Molecule 16: Cytochrome c-550

Chain v:



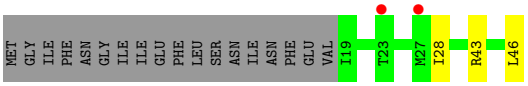
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



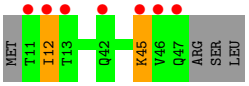
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:



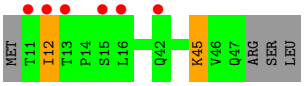
• Molecule 18: Photosystem II reaction center X protein

Chain X:



• Molecule 18: Photosystem II reaction center X protein

Chain x:



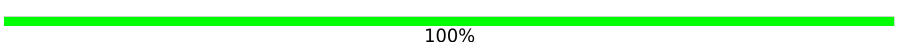
• Molecule 19: Photosystem II reaction center protein Y

Chain Y:

There are no outlier residues recorded for this chain.

• Molecule 19: Photosystem II reaction center protein Y

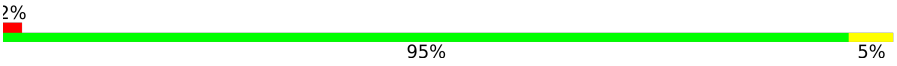
Chain G:

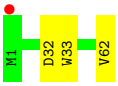


There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Z

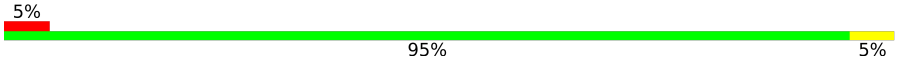
Chain Z:

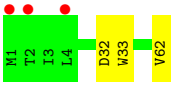




• Molecule 20: Photosystem II reaction center protein Z

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	132.62Å 229.30Å 306.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.41 – 5.20 68.41 – 5.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (68.41-5.20) 97.9 (68.41-5.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.271 , 0.289 0.275 , 0.286	Depositor DCC
R_{free} test set	1753 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	176.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 157.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.15$	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)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.25	0/2713	0.42	0/3700
1	a	0.24	0/2713	0.42	0/3700
2	B	0.24	0/3986	0.41	0/5433
2	b	0.24	0/3986	0.41	0/5433
3	C	0.23	0/3556	0.42	0/4842
3	c	0.23	0/3556	0.42	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	0.44	0/933
5	e	0.23	0/685	0.43	0/933
6	F	0.23	0/291	0.40	0/397
6	f	0.23	0/291	0.41	0/397
7	H	0.24	0/520	0.46	0/709
7	h	0.23	0/520	0.46	0/709
8	I	0.25	0/293	0.44	0/395
8	i	0.26	0/293	0.44	0/395
9	J	0.21	0/255	0.41	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.27	0/303	0.49	0/416
10	k	0.27	0/303	0.49	0/416
11	L	0.23	0/311	0.40	0/422
11	l	0.22	0/311	0.40	0/422
12	M	0.24	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.23	0/1876	0.44	0/2548
13	o	0.23	0/1876	0.44	0/2548
14	T	0.25	0/284	0.41	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.23	0/785	0.43	0/1064
15	u	0.23	0/785	0.44	0/1064
16	V	0.22	0/1081	0.42	0/1468
16	v	0.22	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	0.27	0/273	0.44	0/370
18	x	0.26	0/273	0.45	0/370
20	Z	0.25	0/490	0.45	0/669
20	z	0.24	0/490	0.45	0/669
All	All	0.24	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%)	311 (93%)	18 (5%)	4 (1%)	13	50
1	a	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	13	50
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	19	59
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%)	316 (94%)	21 (6%)	1 (0%)	41	76
4	d	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
5	e	80/84 (95%)	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	22
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	22
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
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%)	207 (86%)	31 (13%)	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	29
14	t	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	4	29
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	37
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	37
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	26
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	26
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	19
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	19
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	42
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	42
All	All	5138/5618 (92%)	4677 (91%)	406 (8%)	55 (1%)	14	51

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

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Mol	Chain	Res	Type
1	a	334	ARG
13	o	271	PRO
15	u	73	PRO
7	H	16	SER
15	U	73	PRO
3	c	144	SER
7	h	16	SER
7	h	26	GLY
3	C	144	SER
15	U	83	ALA
1	a	142	TRP
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	61
3	c	347/362 (96%)	336 (97%)	11 (3%)	39	61
4	D	275/283 (97%)	269 (98%)	6 (2%)	52	71
4	d	275/283 (97%)	267 (97%)	8 (3%)	42	64
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	39
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	62
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	54
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	54
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76	86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	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	27
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	27
18	X	30/34 (88%)	28 (93%)	2 (7%)	16	42
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	42
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	57
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	57
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	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
17	y	46	LEU

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Mol	Chain	Res	Type
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	205	LEU
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	266	ASN
4	D	117	HIS
4	D	332	GLN
1	a	241	GLN
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	$\#\|Z\| > 2$
32	LMT	b	628	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	1 (2%)
22	CLA	a	406	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	6 (7%)
30	SQD	f	103	-	44,45,54	1.02	3 (6%)	53,56,65	1.70	11 (20%)
22	CLA	B	604	-	65,73,73	1.51	5 (7%)	76,113,113	1.43	7 (9%)
24	PL9	D	405	-	55,55,55	1.16	3 (5%)	68,69,69	1.54	13 (19%)
31	LMG	b	627	-	42,42,55	0.87	1 (2%)	50,50,63	1.23	4 (8%)
22	CLA	b	618	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
22	CLA	C	512	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	9 (11%)
24	PL9	j	101	-	35,35,55	1.11	2 (5%)	44,45,69	1.59	8 (18%)
27	LHG	A	410	-	38,38,48	0.70	1 (2%)	41,44,54	1.20	3 (7%)
25	BCR	A	408	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	7 (12%)
30	SQD	A	413	-	50,51,54	0.96	3 (6%)	59,62,65	1.78	10 (16%)
31	LMG	d	408	-	49,49,55	0.77	0	57,57,63	1.34	7 (12%)
22	CLA	C	505	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	7 (9%)
24	PL9	d	407	-	55,55,55	1.10	5 (9%)	68,69,69	1.54	13 (19%)
31	LMG	B	621	-	49,49,55	0.79	1 (2%)	57,57,63	1.31	7 (12%)
32	LMT	d	411	-	32,32,36	1.18	5 (15%)	43,43,47	1.02	2 (4%)
22	CLA	b	615	-	65,73,73	1.55	6 (9%)	76,113,113	1.46	8 (10%)
32	LMT	B	624	-	36,36,36	1.11	4 (11%)	47,47,47	1.01	2 (4%)
31	LMG	e	101	-	44,44,55	0.77	0	52,52,63	1.28	3 (5%)
23	PHO	D	401	-	51,69,69	1.01	3 (5%)	47,99,99	1.12	4 (8%)
30	SQD	a	412	-	50,51,54	0.96	3 (6%)	59,62,65	1.76	11 (18%)
31	LMG	l	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.33	6 (10%)
22	CLA	b	617	-	65,73,73	1.49	5 (7%)	76,113,113	1.41	8 (10%)
26	DGD	b	601	-	53,53,67	1.05	4 (7%)	67,67,81	1.32	7 (10%)
32	LMT	B	628	-	36,36,36	1.13	5 (13%)	47,47,47	1.01	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	a	403	-	65,73,73	1.52	6 (9%)	76,113,113	1.39	8 (10%)
22	CLA	B	615	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	7 (9%)
22	CLA	B	613	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
22	CLA	b	605	-	65,73,73	1.53	6 (9%)	76,113,113	1.38	7 (9%)
22	CLA	D	404	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	8 (10%)
32	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.04	1 (2%)
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	8 (14%)
22	CLA	D	403	-	65,73,73	1.49	6 (9%)	76,113,113	1.33	7 (9%)
26	DGD	C	514	-	54,54,67	0.98	2 (3%)	68,68,81	1.26	5 (7%)
31	LMG	c	522	-	48,48,55	0.78	0	56,56,63	1.29	5 (8%)
22	CLA	b	607	-	65,73,73	1.48	5 (7%)	76,113,113	1.32	7 (9%)
23	PHO	A	405	-	51,69,69	1.01	4 (7%)	47,99,99	1.11	5 (10%)
32	LMT	D	408	-	32,32,36	1.18	5 (15%)	43,43,47	1.02	2 (4%)
30	SQD	A	414	-	53,54,54	0.95	3 (5%)	62,65,65	1.57	9 (14%)
26	DGD	C	515	-	63,63,67	0.93	1 (1%)	77,77,81	1.42	12 (15%)
22	CLA	C	502	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
31	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.29	3 (5%)
22	CLA	A	404	-	65,73,73	1.48	6 (9%)	76,113,113	1.38	6 (7%)
22	CLA	C	506	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	8 (10%)
22	CLA	C	511	-	65,73,73	1.51	5 (7%)	76,113,113	1.40	7 (9%)
26	DGD	b	625	-	59,59,67	0.92	0	73,73,81	1.36	7 (9%)
31	LMG	d	409	-	48,48,55	0.78	0	56,56,63	1.40	5 (8%)
22	CLA	a	405	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	7 (9%)
25	BCR	g	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.31	8 (14%)
25	BCR	b	623	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	10 (17%)
29	OEX	a	411	3,1	0,15,15	-	-	-		
22	CLA	c	510	3	65,73,73	1.52	5 (7%)	76,113,113	1.38	7 (9%)
26	DGD	c	515	-	54,54,67	0.97	1 (1%)	68,68,81	1.29	5 (7%)
25	BCR	H	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	6 (10%)
22	CLA	B	601	-	65,73,73	1.54	5 (7%)	76,113,113	1.37	7 (9%)
22	CLA	c	503	-	65,73,73	1.52	5 (7%)	76,113,113	1.42	7 (9%)
22	CLA	c	512	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	7 (9%)
25	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	8 (14%)
32	LMT	I	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.05	2 (4%)
25	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	b	611	-	65,73,73	1.51	5 (7%)	76,113,113	1.33	7 (9%)
22	CLA	b	612	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	6 (7%)
22	CLA	b	616	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
22	CLA	b	610	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	8 (10%)
22	CLA	B	610	-	65,73,73	1.55	7 (10%)	76,113,113	1.49	8 (10%)
22	CLA	c	511	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	7 (9%)
30	SQD	F	103	-	44,45,54	1.04	3 (6%)	53,56,65	1.70	11 (20%)
31	LMG	C	521	-	48,48,55	0.77	0	56,56,63	1.30	5 (8%)
22	CLA	c	502	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	6 (7%)
32	LMT	M	102	-	36,36,36	1.15	6 (16%)	47,47,47	1.02	2 (4%)
31	LMG	D	409	-	46,46,55	0.79	1 (2%)	54,54,63	1.32	4 (7%)
22	CLA	a	404	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
24	PL9	A	407	-	45,45,55	1.00	4 (8%)	56,57,69	1.56	9 (16%)
29	OEX	A	412	3,1	0,15,15	-	-	-		
32	LMT	M	103	-	36,36,36	1.13	5 (13%)	47,47,47	1.00	2 (4%)
25	BCR	C	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	8 (14%)
26	DGD	c	517	-	67,67,67	0.90	2 (2%)	81,81,81	1.40	9 (11%)
22	CLA	d	405	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
25	BCR	x	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	3 (5%)
23	PHO	d	401	-	51,69,69	1.02	4 (7%)	47,99,99	1.15	5 (10%)
22	CLA	C	501	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	8 (10%)
26	DGD	B	620	-	59,59,67	0.94	0	73,73,81	1.34	7 (9%)
24	PL9	a	407	-	45,45,55	1.04	3 (6%)	56,57,69	1.59	9 (16%)
30	SQD	B	622	-	42,43,54	1.05	3 (7%)	51,54,65	1.81	11 (21%)
22	CLA	B	614	-	65,73,73	1.51	5 (7%)	76,113,113	1.39	8 (10%)
22	CLA	B	606	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
23	PHO	d	402	-	51,69,69	1.00	4 (7%)	47,99,99	1.10	4 (8%)
31	LMG	M	101	-	42,42,55	0.87	0	50,50,63	1.23	4 (8%)
32	LMT	B	623	-	36,36,36	1.13	5 (13%)	47,47,47	1.01	1 (2%)
27	LHG	C	518	-	36,36,48	0.71	0	39,42,54	1.28	4 (10%)
32	LMT	b	629	-	36,36,36	1.11	5 (13%)	47,47,47	1.03	2 (4%)
22	CLA	H	101	-	65,73,73	1.52	5 (7%)	76,113,113	1.35	6 (7%)
31	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.29	6 (11%)
31	LMG	m	101	-	42,42,55	0.87	2 (4%)	50,50,63	1.23	4 (8%)
25	BCR	b	621	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LMG	C	517	-	45,45,55	0.77	0	53,53,63	1.30	6 (11%)
25	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.54	13 (23%)
25	BCR	i	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
26	DGD	D	407	-	64,64,67	0.98	4 (6%)	78,78,81	1.33	8 (10%)
22	CLA	C	510	3	65,73,73	1.50	5 (7%)	76,113,113	1.44	7 (9%)
22	CLA	b	609	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	7 (9%)
22	CLA	B	612	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
26	DGD	a	408	-	57,57,67	0.97	0	71,71,81	1.39	8 (11%)
25	BCR	C	520	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	9 (16%)
31	LMG	i	102	-	43,43,55	0.84	1 (2%)	51,51,63	1.25	3 (5%)
22	CLA	A	406	-	65,73,73	1.51	5 (7%)	76,113,113	1.36	7 (9%)
33	BCT	d	404	21	2,3,3	1.25	0	2,3,3	4.36	2 (100%)
34	HEM	F	101	6,5	41,50,50	1.95	5 (12%)	45,82,82	1.64	7 (15%)
30	SQD	d	403	-	42,43,54	1.04	3 (7%)	51,54,65	1.77	11 (21%)
22	CLA	c	505	-	65,73,73	1.52	5 (7%)	76,113,113	1.41	6 (7%)
22	CLA	B	609	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	7 (9%)
30	SQD	b	602	-	46,47,54	1.02	4 (8%)	55,58,65	1.83	10 (18%)
22	CLA	b	614	-	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
22	CLA	A	402	-	65,73,73	1.51	6 (9%)	76,113,113	1.36	8 (10%)
27	LHG	c	519	-	36,36,48	0.75	2 (5%)	39,42,54	1.27	4 (10%)
25	BCR	b	624	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
25	BCR	y	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.25	7 (12%)
32	LMT	i	103	-	36,36,36	1.10	5 (13%)	47,47,47	1.02	2 (4%)
30	SQD	a	401	-	53,54,54	0.95	3 (5%)	62,65,65	1.58	10 (16%)
32	LMT	b	603	-	36,36,36	1.13	5 (13%)	47,47,47	0.98	1 (2%)
31	LMG	I	101	-	43,43,55	0.85	1 (2%)	51,51,63	1.25	5 (9%)
22	CLA	d	406	-	65,73,73	1.52	5 (7%)	76,113,113	1.38	7 (9%)
22	CLA	b	606	-	65,73,73	1.50	5 (7%)	76,113,113	1.34	6 (7%)
25	BCR	B	616	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	8 (14%)
25	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	8 (14%)
22	CLA	C	504	-	65,73,73	1.48	6 (9%)	76,113,113	1.44	9 (11%)
31	LMG	L	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.35	5 (8%)
26	DGD	c	516	-	63,63,67	0.93	2 (3%)	77,77,81	1.44	11 (14%)
22	CLA	C	519	-	65,73,73	1.48	5 (7%)	76,113,113	1.35	7 (9%)
22	CLA	B	602	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	509	-	65,73,73	1.51	6 (9%)	76,113,113	1.33	7 (9%)
22	CLA	C	507	-	65,73,73	1.51	5 (7%)	76,113,113	1.45	9 (11%)
25	BCR	F	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	7 (12%)
34	HEM	V	201	16	41,50,50	2.03	9 (21%)	45,82,82	1.49	4 (8%)
22	CLA	b	613	-	65,73,73	1.53	5 (7%)	76,113,113	1.31	7 (9%)
31	LMG	B	625	-	49,49,55	0.77	0	57,57,63	1.33	6 (10%)
25	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	8 (14%)
22	CLA	b	619	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
31	LMG	b	626	-	49,49,55	0.80	1 (2%)	57,57,63	1.33	8 (14%)
33	BCT	D	402	21	2,3,3	1.24	0	2,3,3	4.33	2 (100%)
25	BCR	b	622	-	41,41,41	1.08	2 (4%)	56,56,56	1.35	10 (17%)
22	CLA	C	503	-	65,73,73	1.50	5 (7%)	76,113,113	1.42	8 (10%)
22	CLA	c	520	-	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
22	CLA	b	620	-	65,73,73	1.51	7 (10%)	76,113,113	1.35	8 (10%)
31	LMG	D	406	-	48,48,55	0.78	0	56,56,63	1.39	4 (7%)
22	CLA	C	508	-	65,73,73	1.52	6 (9%)	76,113,113	1.35	8 (10%)
22	CLA	B	611	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	7 (9%)
31	LMG	d	412	-	46,46,55	0.80	1 (2%)	54,54,63	1.29	6 (11%)
22	CLA	B	605	-	65,73,73	1.48	5 (7%)	76,113,113	1.44	8 (10%)
26	DGD	B	626	-	53,53,67	1.06	3 (5%)	67,67,81	1.31	7 (10%)
22	CLA	c	509	-	65,73,73	1.53	6 (9%)	76,113,113	1.38	8 (10%)
25	BCR	K	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
22	CLA	c	507	-	65,73,73	1.51	5 (7%)	76,113,113	1.45	9 (11%)
22	CLA	B	607	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	6 (7%)
25	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.61	13 (23%)
31	LMG	a	402	-	42,42,55	0.88	2 (4%)	50,50,63	1.23	3 (6%)
25	BCR	f	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	7 (12%)
32	LMT	B	629	-	36,36,36	1.15	6 (16%)	47,47,47	1.03	1 (2%)
27	LHG	a	409	-	38,38,48	0.68	1 (2%)	41,44,54	1.21	3 (7%)
34	HEM	v	201	16	41,50,50	2.04	9 (21%)	45,82,82	1.61	4 (8%)
22	CLA	c	508	-	65,73,73	1.52	5 (7%)	76,113,113	1.37	8 (10%)
25	BCR	B	618	-	41,41,41	1.12	2 (4%)	56,56,56	1.40	9 (16%)
22	CLA	b	608	-	65,73,73	1.49	6 (9%)	76,113,113	1.44	9 (11%)
22	CLA	B	608	-	65,73,73	1.54	5 (7%)	76,113,113	1.34	7 (9%)
24	PL9	J	101	-	35,35,55	1.05	2 (5%)	44,45,69	1.62	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	DGD	C	516	-	67,67,67	0.88	0	81,81,81	1.43	10 (12%)
22	CLA	B	603	-	65,73,73	1.51	6 (9%)	76,113,113	1.43	9 (11%)
30	SQD	B	627	-	46,47,54	1.01	3 (6%)	55,58,65	1.81	10 (18%)
34	HEM	f	101	6,5	41,50,50	1.93	6 (14%)	45,82,82	1.71	8 (17%)
22	CLA	c	501	-	65,73,73	1.52	5 (7%)	76,113,113	1.36	8 (10%)
26	DGD	A	409	-	57,57,67	0.96	1 (1%)	71,71,81	1.43	7 (9%)
22	CLA	c	504	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	8 (10%)
22	CLA	A	403	-	65,73,73	1.51	5 (7%)	76,113,113	1.41	8 (10%)
26	DGD	d	410	-	64,64,67	0.95	2 (3%)	78,78,81	1.36	9 (11%)
22	CLA	c	506	-	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)

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
32	LMT	b	628	-	-	3/21/61/61	0/2/2/2
22	CLA	a	406	-	1/1/15/20	8/37/115/115	-
30	SQD	f	103	-	-	10/40/60/69	0/1/1/1
22	CLA	B	604	-	1/1/15/20	15/37/115/115	-
24	PL9	D	405	-	-	12/53/73/73	0/1/1/1
31	LMG	b	627	-	-	15/37/57/70	0/1/1/1
22	CLA	b	618	-	1/1/15/20	16/37/115/115	-
22	CLA	C	512	-	1/1/15/20	20/37/115/115	-
24	PL9	j	101	-	-	8/29/49/73	0/1/1/1
27	LHG	A	410	-	-	12/43/43/53	-
25	BCR	A	408	-	-	4/29/63/63	0/2/2/2
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
31	LMG	d	408	-	-	25/44/64/70	0/1/1/1
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
24	PL9	d	407	-	-	11/53/73/73	0/1/1/1
31	LMG	B	621	-	-	15/44/64/70	0/1/1/1
32	LMT	d	411	-	-	1/17/57/61	0/2/2/2
22	CLA	b	615	-	1/1/15/20	11/37/115/115	-
32	LMT	B	624	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	e	101	-	-	20/39/59/70	0/1/1/1
23	PHO	D	401	-	-	10/37/103/103	0/5/6/6
30	SQD	a	412	-	-	21/46/66/69	0/1/1/1
31	LMG	l	101	-	-	27/46/66/70	0/1/1/1
22	CLA	b	617	-	1/1/15/20	15/37/115/115	-
26	DGD	b	601	-	-	18/41/81/95	0/2/2/2
32	LMT	B	628	-	-	2/21/61/61	0/2/2/2
22	CLA	a	403	-	1/1/15/20	8/37/115/115	-
22	CLA	B	615	-	1/1/15/20	18/37/115/115	-
22	CLA	B	613	-	1/1/15/20	17/37/115/115	-
22	CLA	b	605	-	1/1/15/20	16/37/115/115	-
22	CLA	D	404	-	-	6/37/115/115	-
32	LMT	b	604	-	-	5/21/61/61	0/2/2/2
25	BCR	B	619	-	-	5/29/63/63	0/2/2/2
22	CLA	D	403	-	1/1/15/20	13/37/115/115	-
26	DGD	C	514	-	-	19/42/82/95	0/2/2/2
31	LMG	c	522	-	-	19/43/63/70	0/1/1/1
22	CLA	b	607	-	1/1/15/20	13/37/115/115	-
23	PHO	A	405	-	-	11/37/103/103	0/5/6/6
32	LMT	D	408	-	-	2/17/57/61	0/2/2/2
30	SQD	A	414	-	-	14/49/69/69	0/1/1/1
26	DGD	C	515	-	-	20/51/91/95	0/2/2/2
22	CLA	C	502	-	1/1/15/20	11/37/115/115	-
31	LMG	E	101	-	-	16/39/59/70	0/1/1/1
22	CLA	A	404	-	1/1/15/20	10/37/115/115	-
22	CLA	C	506	-	1/1/15/20	12/37/115/115	-
22	CLA	C	511	-	1/1/15/20	18/37/115/115	-
26	DGD	b	625	-	-	18/47/87/95	0/2/2/2
31	LMG	d	409	-	-	21/43/63/70	0/1/1/1
22	CLA	a	405	-	1/1/15/20	8/37/115/115	-
25	BCR	g	101	-	-	5/29/63/63	0/2/2/2
25	BCR	b	623	-	-	4/29/63/63	0/2/2/2
22	CLA	c	510	3	1/1/15/20	15/37/115/115	-
26	DGD	c	515	-	-	19/42/82/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	H	102	-	-	9/29/63/63	0/2/2/2
22	CLA	B	601	-	1/1/15/20	15/37/115/115	-
22	CLA	c	503	-	1/1/15/20	17/37/115/115	-
22	CLA	c	512	-	1/1/15/20	18/37/115/115	-
25	BCR	B	617	-	-	8/29/63/63	0/2/2/2
32	LMT	I	102	-	-	3/21/61/61	0/2/2/2
25	BCR	c	513	-	-	5/29/63/63	0/2/2/2
22	CLA	b	611	-	1/1/15/20	8/37/115/115	-
22	CLA	b	612	-	1/1/15/20	13/37/115/115	-
22	CLA	b	616	-	1/1/15/20	12/37/115/115	-
22	CLA	b	610	-	1/1/15/20	12/37/115/115	-
22	CLA	B	610	-	1/1/15/20	10/37/115/115	-
22	CLA	c	511	-	1/1/15/20	18/37/115/115	-
30	SQD	F	103	-	-	11/40/60/69	0/1/1/1
31	LMG	C	521	-	-	20/43/63/70	0/1/1/1
22	CLA	c	502	-	1/1/15/20	10/37/115/115	-
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
31	LMG	D	409	-	-	15/41/61/70	0/1/1/1
22	CLA	a	404	-	1/1/15/20	15/37/115/115	-
24	PL9	A	407	-	-	18/41/61/73	0/1/1/1
32	LMT	M	103	-	-	0/21/61/61	0/2/2/2
25	BCR	C	513	-	-	5/29/63/63	0/2/2/2
26	DGD	c	517	-	-	22/55/95/95	0/2/2/2
22	CLA	d	405	-	1/1/15/20	12/37/115/115	-
25	BCR	x	101	-	-	7/29/63/63	0/2/2/2
23	PHO	d	401	-	-	9/37/103/103	0/5/6/6
22	CLA	C	501	-	1/1/15/20	13/37/115/115	-
26	DGD	B	620	-	-	18/47/87/95	0/2/2/2
24	PL9	a	407	-	-	18/41/61/73	0/1/1/1
30	SQD	B	622	-	-	14/38/58/69	0/1/1/1
22	CLA	B	614	-	1/1/15/20	9/37/115/115	-
22	CLA	B	606	-	1/1/15/20	8/37/115/115	-
23	PHO	d	402	-	-	14/37/103/103	0/5/6/6
31	LMG	M	101	-	-	18/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	B	623	-	-	2/21/61/61	0/2/2/2
27	LHG	C	518	-	-	14/41/41/53	-
32	LMT	b	629	-	-	3/21/61/61	0/2/2/2
22	CLA	H	101	-	1/1/15/20	19/37/115/115	-
31	LMG	c	518	-	-	22/40/60/70	0/1/1/1
31	LMG	m	101	-	-	17/37/57/70	0/1/1/1
25	BCR	b	621	-	-	2/29/63/63	0/2/2/2
31	LMG	C	517	-	-	22/40/60/70	0/1/1/1
25	BCR	j	102	-	-	7/29/63/63	0/2/2/2
25	BCR	i	101	-	-	4/29/63/63	0/2/2/2
26	DGD	D	407	-	-	36/52/92/95	0/2/2/2
22	CLA	C	510	3	1/1/15/20	17/37/115/115	-
22	CLA	b	609	-	1/1/15/20	15/37/115/115	-
22	CLA	B	612	-	1/1/15/20	15/37/115/115	-
26	DGD	a	408	-	-	14/45/85/95	0/2/2/2
25	BCR	C	520	-	-	6/29/63/63	0/2/2/2
31	LMG	i	102	-	-	18/38/58/70	0/1/1/1
22	CLA	A	406	-	1/1/15/20	8/37/115/115	-
34	HEM	F	101	6,5	-	2/12/54/54	-
30	SQD	d	403	-	-	16/38/58/69	0/1/1/1
22	CLA	c	505	-	1/1/15/20	17/37/115/115	-
22	CLA	B	609	-	1/1/15/20	18/37/115/115	-
30	SQD	b	602	-	-	14/42/62/69	0/1/1/1
22	CLA	b	614	-	1/1/15/20	18/37/115/115	-
22	CLA	A	402	-	1/1/15/20	8/37/115/115	-
27	LHG	c	519	-	-	17/41/41/53	-
25	BCR	b	624	-	-	5/29/63/63	0/2/2/2
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
32	LMT	i	103	-	-	4/21/61/61	0/2/2/2
30	SQD	a	401	-	-	15/49/69/69	0/1/1/1
32	LMT	b	603	-	-	3/21/61/61	0/2/2/2
31	LMG	I	101	-	-	19/38/58/70	0/1/1/1
22	CLA	d	406	-	-	6/37/115/115	-
22	CLA	b	606	-	1/1/15/20	20/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	616	-	-	3/29/63/63	0/2/2/2
25	BCR	c	521	-	-	6/29/63/63	0/2/2/2
22	CLA	C	504	-	1/1/15/20	18/37/115/115	-
31	LMG	L	101	-	-	26/46/66/70	0/1/1/1
26	DGD	c	516	-	-	21/51/91/95	0/2/2/2
22	CLA	C	519	-	1/1/15/20	12/37/115/115	-
22	CLA	B	602	-	1/1/15/20	14/37/115/115	-
22	CLA	C	509	-	1/1/15/20	13/37/115/115	-
22	CLA	C	507	-	1/1/15/20	14/37/115/115	-
25	BCR	F	102	-	-	6/29/63/63	0/2/2/2
34	HEM	V	201	16	-	4/12/54/54	-
22	CLA	b	613	-	1/1/15/20	11/37/115/115	-
31	LMG	B	625	-	-	24/44/64/70	0/1/1/1
25	BCR	c	514	-	-	5/29/63/63	0/2/2/2
22	CLA	b	619	-	1/1/15/20	10/37/115/115	-
31	LMG	b	626	-	-	14/44/64/70	0/1/1/1
25	BCR	b	622	-	-	7/29/63/63	0/2/2/2
22	CLA	C	503	-	1/1/15/20	15/37/115/115	-
22	CLA	c	520	-	1/1/15/20	10/37/115/115	-
22	CLA	b	620	-	1/1/15/20	19/37/115/115	-
31	LMG	D	406	-	-	21/43/63/70	0/1/1/1
22	CLA	C	508	-	1/1/15/20	15/37/115/115	-
22	CLA	B	611	-	1/1/15/20	13/37/115/115	-
31	LMG	d	412	-	-	14/41/61/70	0/1/1/1
22	CLA	B	605	-	1/1/15/20	16/37/115/115	-
26	DGD	B	626	-	-	18/41/81/95	0/2/2/2
22	CLA	c	509	-	1/1/15/20	16/37/115/115	-
25	BCR	K	101	-	-	5/29/63/63	0/2/2/2
22	CLA	c	507	-	1/1/15/20	14/37/115/115	-
22	CLA	B	607	-	1/1/15/20	12/37/115/115	-
25	BCR	J	102	-	-	6/29/63/63	0/2/2/2
31	LMG	a	402	-	-	16/37/57/70	0/1/1/1
25	BCR	f	102	-	-	6/29/63/63	0/2/2/2
32	LMT	B	629	-	-	4/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LHG	a	409	-	-	11/43/43/53	-
34	HEM	v	201	16	-	4/12/54/54	-
22	CLA	c	508	-	1/1/15/20	16/37/115/115	-
25	BCR	B	618	-	-	3/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/15/20	5/37/115/115	-
22	CLA	B	608	-	1/1/15/20	11/37/115/115	-
24	PL9	J	101	-	-	9/29/49/73	0/1/1/1
26	DGD	C	516	-	-	23/55/95/95	0/2/2/2
22	CLA	B	603	-	1/1/15/20	9/37/115/115	-
30	SQD	B	627	-	-	16/42/62/69	0/1/1/1
34	HEM	f	101	6,5	-	2/12/54/54	-
22	CLA	c	501	-	1/1/15/20	13/37/115/115	-
26	DGD	A	409	-	-	16/45/85/95	0/2/2/2
22	CLA	c	504	-	1/1/15/20	19/37/115/115	-
22	CLA	A	403	-	1/1/15/20	14/37/115/115	-
26	DGD	d	410	-	-	36/52/92/95	0/2/2/2
22	CLA	c	506	-	1/1/15/20	13/37/115/115	-

All (630) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3D-C2D	8.27	1.54	1.36
34	V	201	HEM	C3D-C2D	8.25	1.54	1.36
34	F	101	HEM	C3D-C2D	8.02	1.53	1.36
22	c	509	CLA	C4B-NB	7.98	1.42	1.35
34	f	101	HEM	C3D-C2D	7.90	1.53	1.36
22	A	402	CLA	C4B-NB	7.84	1.42	1.35
22	a	403	CLA	C4B-NB	7.83	1.42	1.35
22	B	601	CLA	C4B-NB	7.82	1.42	1.35
22	b	605	CLA	C4B-NB	7.81	1.42	1.35
22	C	508	CLA	C4B-NB	7.80	1.42	1.35
22	c	508	CLA	C4B-NB	7.80	1.42	1.35
22	c	512	CLA	C4B-NB	7.78	1.42	1.35
22	B	614	CLA	C4B-NB	7.77	1.42	1.35
22	b	620	CLA	C4B-NB	7.74	1.42	1.35
22	C	509	CLA	C4B-NB	7.74	1.42	1.35
22	B	615	CLA	C4B-NB	7.72	1.42	1.35
22	c	511	CLA	C4B-NB	7.70	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	C4B-NB	7.69	1.42	1.35
22	c	503	CLA	C4B-NB	7.69	1.42	1.35
22	d	406	CLA	C4B-NB	7.69	1.42	1.35
22	C	507	CLA	C4B-NB	7.68	1.42	1.35
22	B	610	CLA	C4B-NB	7.67	1.42	1.35
22	c	510	CLA	C4B-NB	7.67	1.42	1.35
22	c	507	CLA	C4B-NB	7.66	1.42	1.35
22	b	615	CLA	C4B-NB	7.66	1.42	1.35
22	B	608	CLA	C4B-NB	7.65	1.42	1.35
22	c	520	CLA	C4B-NB	7.63	1.42	1.35
22	b	616	CLA	C4B-NB	7.62	1.42	1.35
22	C	511	CLA	C4B-NB	7.61	1.42	1.35
22	H	101	CLA	C4B-NB	7.60	1.42	1.35
22	A	403	CLA	C4B-NB	7.59	1.42	1.35
22	c	501	CLA	C4B-NB	7.58	1.42	1.35
22	B	604	CLA	C4B-NB	7.58	1.42	1.35
22	a	405	CLA	C4B-NB	7.58	1.42	1.35
22	A	406	CLA	C4B-NB	7.58	1.42	1.35
22	b	611	CLA	C4B-NB	7.57	1.42	1.35
22	b	619	CLA	C4B-NB	7.56	1.42	1.35
22	C	505	CLA	C4B-NB	7.55	1.41	1.35
22	b	613	CLA	C4B-NB	7.54	1.41	1.35
22	D	404	CLA	C4B-NB	7.52	1.41	1.35
22	d	405	CLA	C4B-NB	7.52	1.41	1.35
22	B	611	CLA	C4B-NB	7.50	1.41	1.35
22	C	512	CLA	C4B-NB	7.50	1.41	1.35
22	b	610	CLA	C4B-NB	7.49	1.41	1.35
22	b	612	CLA	C4B-NB	7.48	1.41	1.35
22	C	503	CLA	C4B-NB	7.48	1.41	1.35
22	C	510	CLA	C4B-NB	7.47	1.41	1.35
22	C	501	CLA	C4B-NB	7.46	1.41	1.35
22	b	617	CLA	C4B-NB	7.46	1.41	1.35
22	B	603	CLA	C4B-NB	7.45	1.41	1.35
22	c	504	CLA	C4B-NB	7.44	1.41	1.35
22	b	614	CLA	C4B-NB	7.43	1.41	1.35
22	b	609	CLA	C4B-NB	7.43	1.41	1.35
22	D	403	CLA	C4B-NB	7.41	1.41	1.35
22	c	502	CLA	C4B-NB	7.38	1.41	1.35
22	C	502	CLA	C4B-NB	7.38	1.41	1.35
22	a	404	CLA	C4B-NB	7.38	1.41	1.35
22	a	406	CLA	C4B-NB	7.37	1.41	1.35
22	b	608	CLA	C4B-NB	7.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C4B-NB	7.36	1.41	1.35
22	c	506	CLA	C4B-NB	7.35	1.41	1.35
22	A	404	CLA	C4B-NB	7.32	1.41	1.35
22	B	609	CLA	C4B-NB	7.32	1.41	1.35
22	C	506	CLA	C4B-NB	7.32	1.41	1.35
22	B	605	CLA	C4B-NB	7.31	1.41	1.35
22	b	618	CLA	C4B-NB	7.31	1.41	1.35
22	C	519	CLA	C4B-NB	7.30	1.41	1.35
22	B	607	CLA	C4B-NB	7.29	1.41	1.35
22	B	612	CLA	C4B-NB	7.25	1.41	1.35
22	C	504	CLA	C4B-NB	7.24	1.41	1.35
22	b	606	CLA	C4B-NB	7.21	1.41	1.35
22	B	602	CLA	C4B-NB	7.20	1.41	1.35
22	b	607	CLA	C4B-NB	7.18	1.41	1.35
22	B	613	CLA	C4B-NB	7.18	1.41	1.35
34	V	201	HEM	C3C-C2C	-4.65	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.55	1.34	1.40
22	c	510	CLA	C1D-ND	4.19	1.42	1.37
22	B	608	CLA	C1D-ND	4.16	1.42	1.37
22	b	609	CLA	C1D-ND	4.15	1.42	1.37
22	c	501	CLA	C1D-ND	4.13	1.42	1.37
24	D	405	PL9	C7-C3	-4.12	1.47	1.51
22	C	510	CLA	C1D-ND	4.12	1.42	1.37
22	C	501	CLA	C1D-ND	4.12	1.42	1.37
22	a	406	CLA	C1D-ND	4.11	1.42	1.37
22	d	406	CLA	C1D-ND	4.09	1.42	1.37
22	B	601	CLA	C1D-ND	4.09	1.42	1.37
22	C	512	CLA	C1D-ND	4.08	1.42	1.37
22	C	503	CLA	C1D-ND	4.08	1.42	1.37
22	c	503	CLA	C1D-ND	4.08	1.42	1.37
22	c	506	CLA	C1D-ND	4.06	1.42	1.37
22	b	606	CLA	C1D-ND	4.06	1.42	1.37
22	b	605	CLA	C1D-ND	4.05	1.42	1.37
22	b	613	CLA	C1D-ND	4.05	1.42	1.37
22	H	101	CLA	C1D-ND	4.05	1.42	1.37
22	c	512	CLA	C1D-ND	4.04	1.42	1.37
22	A	406	CLA	C1D-ND	4.03	1.42	1.37
22	B	604	CLA	C1D-ND	4.02	1.42	1.37
22	C	506	CLA	C1D-ND	4.01	1.42	1.37
22	A	403	CLA	C1D-ND	4.00	1.42	1.37
22	D	404	CLA	C1D-ND	3.99	1.42	1.37
22	c	508	CLA	C1D-ND	3.98	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	C1D-ND	3.98	1.42	1.37
22	B	602	CLA	C1D-ND	3.98	1.42	1.37
22	C	511	CLA	C1D-ND	3.97	1.42	1.37
22	b	607	CLA	C1D-ND	3.96	1.42	1.37
22	c	505	CLA	C1D-ND	3.96	1.42	1.37
22	b	618	CLA	C1D-ND	3.96	1.42	1.37
22	B	613	CLA	C1D-ND	3.95	1.42	1.37
22	B	607	CLA	C1D-ND	3.95	1.42	1.37
22	b	610	CLA	C1D-ND	3.94	1.42	1.37
22	c	502	CLA	C1D-ND	3.94	1.42	1.37
22	c	504	CLA	C1D-ND	3.94	1.42	1.37
22	b	619	CLA	C1D-ND	3.94	1.42	1.37
22	C	519	CLA	C1D-ND	3.93	1.42	1.37
22	b	608	CLA	C1D-ND	3.92	1.42	1.37
22	b	612	CLA	C1D-ND	3.92	1.42	1.37
22	c	511	CLA	C1D-ND	3.91	1.42	1.37
22	b	614	CLA	C1D-ND	3.91	1.42	1.37
22	C	504	CLA	C1D-ND	3.90	1.42	1.37
22	c	520	CLA	C1D-ND	3.90	1.42	1.37
22	C	502	CLA	C1D-ND	3.89	1.42	1.37
22	B	614	CLA	C1D-ND	3.89	1.42	1.37
22	a	405	CLA	C1D-ND	3.89	1.42	1.37
22	C	505	CLA	C1D-ND	3.88	1.42	1.37
22	B	612	CLA	C1D-ND	3.88	1.42	1.37
22	B	605	CLA	C1D-ND	3.88	1.42	1.37
22	c	507	CLA	C1D-ND	3.87	1.42	1.37
22	b	617	CLA	C1D-ND	3.87	1.42	1.37
22	a	404	CLA	C1D-ND	3.85	1.42	1.37
22	b	611	CLA	C1D-ND	3.85	1.42	1.37
22	C	507	CLA	C1D-ND	3.84	1.42	1.37
34	f	101	HEM	C3C-CAC	3.84	1.55	1.47
22	B	615	CLA	C1D-ND	3.84	1.42	1.37
34	F	101	HEM	C3C-C2C	-3.84	1.35	1.40
22	d	405	CLA	C1D-ND	3.83	1.42	1.37
22	a	403	CLA	C1D-ND	3.83	1.42	1.37
22	B	606	CLA	C1D-ND	3.83	1.42	1.37
22	B	609	CLA	C1D-ND	3.83	1.42	1.37
22	D	403	CLA	C1D-ND	3.82	1.42	1.37
22	A	404	CLA	C1D-ND	3.81	1.42	1.37
22	b	620	CLA	C1D-ND	3.80	1.42	1.37
22	C	508	CLA	C1D-ND	3.79	1.42	1.37
22	A	402	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	C1D-ND	3.79	1.42	1.37
22	b	615	CLA	C1D-ND	3.77	1.42	1.37
34	F	101	HEM	C3C-CAC	3.76	1.55	1.47
34	V	201	HEM	C3C-CAC	3.73	1.55	1.47
34	v	201	HEM	C3C-CAC	3.73	1.55	1.47
24	d	407	PL9	C7-C3	-3.72	1.47	1.51
22	C	509	CLA	C1D-ND	3.70	1.42	1.37
24	j	101	PL9	C7-C3	-3.70	1.47	1.51
22	B	610	CLA	C1D-ND	3.70	1.42	1.37
34	f	101	HEM	C3C-C2C	-3.69	1.35	1.40
25	F	102	BCR	C1-C6	-3.61	1.48	1.53
22	b	615	CLA	CMB-C2B	-3.60	1.44	1.51
22	B	610	CLA	CMB-C2B	-3.60	1.44	1.51
25	H	102	BCR	C1-C6	-3.59	1.48	1.53
25	x	101	BCR	C1-C6	-3.55	1.48	1.53
22	b	616	CLA	C1D-ND	3.54	1.42	1.37
25	f	102	BCR	C1-C6	-3.53	1.48	1.53
25	g	101	BCR	C30-C25	-3.43	1.49	1.53
25	B	616	BCR	C1-C6	-3.43	1.49	1.53
22	B	608	CLA	CHC-C1C	3.39	1.43	1.35
22	B	611	CLA	C1D-ND	3.39	1.42	1.37
25	y	101	BCR	C1-C6	-3.37	1.49	1.53
25	b	621	BCR	C1-C6	-3.37	1.49	1.53
22	b	613	CLA	CHC-C1C	3.34	1.43	1.35
25	C	513	BCR	C1-C6	-3.32	1.49	1.53
22	b	606	CLA	CHC-C1C	3.31	1.43	1.35
25	c	514	BCR	C1-C6	-3.31	1.49	1.53
22	b	612	CLA	CHC-C1C	3.30	1.43	1.35
25	b	623	BCR	C30-C25	-3.30	1.49	1.53
22	B	613	CLA	CHC-C1C	3.30	1.43	1.35
25	J	102	BCR	C30-C25	-3.29	1.49	1.53
25	y	101	BCR	C30-C25	-3.29	1.49	1.53
25	g	101	BCR	C1-C6	-3.29	1.49	1.53
30	b	602	SQD	O48-C23	3.29	1.43	1.33
25	b	622	BCR	C1-C6	-3.27	1.49	1.53
22	H	101	CLA	CHC-C1C	3.27	1.43	1.35
22	c	512	CLA	CHC-C1C	3.26	1.43	1.35
22	B	607	CLA	CHC-C1C	3.26	1.43	1.35
22	b	607	CLA	CHC-C1C	3.25	1.43	1.35
25	B	618	BCR	C30-C25	-3.25	1.49	1.53
25	j	102	BCR	C30-C25	-3.23	1.49	1.53
22	d	406	CLA	CHC-C1C	3.23	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	CHC-C1C	3.23	1.43	1.35
25	c	513	BCR	C1-C6	-3.23	1.49	1.53
25	b	624	BCR	C30-C25	-3.23	1.49	1.53
22	b	618	CLA	CHC-C1C	3.22	1.43	1.35
22	C	511	CLA	CHC-C1C	3.22	1.43	1.35
25	K	101	BCR	C1-C6	-3.22	1.49	1.53
22	c	511	CLA	CHC-C1C	3.22	1.43	1.35
25	C	520	BCR	C30-C25	-3.21	1.49	1.53
24	a	407	PL9	C7-C3	-3.21	1.48	1.51
30	B	622	SQD	O48-C23	3.20	1.42	1.33
22	a	405	CLA	CHC-C1C	3.20	1.43	1.35
30	B	627	SQD	O48-C23	3.20	1.42	1.33
22	c	509	CLA	CHC-C1C	3.20	1.43	1.35
22	B	603	CLA	CHC-C1C	3.19	1.43	1.35
25	F	102	BCR	C30-C25	-3.18	1.49	1.53
25	B	619	BCR	C30-C25	-3.17	1.49	1.53
22	b	608	CLA	CHC-C1C	3.17	1.43	1.35
22	c	507	CLA	CHC-C1C	3.17	1.43	1.35
22	c	506	CLA	CHC-C1C	3.17	1.43	1.35
22	c	505	CLA	CHC-C1C	3.17	1.43	1.35
22	B	602	CLA	CHC-C1C	3.17	1.43	1.35
22	D	404	CLA	CHC-C1C	3.16	1.43	1.35
24	J	101	PL9	C7-C3	-3.16	1.48	1.51
22	d	405	CLA	CHC-C1C	3.16	1.43	1.35
30	a	401	SQD	O48-C23	3.16	1.42	1.33
22	C	502	CLA	CHC-C1C	3.15	1.43	1.35
22	C	512	CLA	CHC-C1C	3.15	1.43	1.35
22	a	406	CLA	CHC-C1C	3.15	1.43	1.35
22	B	612	CLA	CHC-C1C	3.15	1.43	1.35
22	c	503	CLA	CHC-C1C	3.15	1.43	1.35
22	c	510	CLA	CHC-C1C	3.14	1.43	1.35
22	C	509	CLA	CHC-C1C	3.14	1.43	1.35
25	B	616	BCR	C30-C25	-3.14	1.49	1.53
30	F	103	SQD	O48-C23	3.14	1.42	1.33
22	A	404	CLA	CHC-C1C	3.14	1.43	1.35
22	c	508	CLA	CHC-C1C	3.13	1.43	1.35
30	A	414	SQD	O48-C23	3.13	1.42	1.33
22	b	617	CLA	CHC-C1C	3.13	1.43	1.35
22	B	604	CLA	CHC-C1C	3.13	1.43	1.35
22	B	614	CLA	CHC-C1C	3.13	1.43	1.35
22	A	403	CLA	CHC-C1C	3.13	1.43	1.35
22	c	501	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	i	101	BCR	C1-C6	-3.13	1.49	1.53
22	b	616	CLA	CHC-C1C	3.12	1.43	1.35
22	C	505	CLA	CHC-C1C	3.12	1.43	1.35
22	B	609	CLA	CHC-C1C	3.12	1.43	1.35
30	a	412	SQD	O48-C23	3.12	1.42	1.33
22	C	519	CLA	CHC-C1C	3.12	1.43	1.35
22	B	605	CLA	CHC-C1C	3.12	1.43	1.35
30	f	103	SQD	O48-C23	3.12	1.42	1.33
22	b	619	CLA	CHC-C1C	3.12	1.43	1.35
22	D	403	CLA	CHC-C1C	3.11	1.43	1.35
25	A	408	BCR	C30-C25	-3.11	1.49	1.53
25	b	624	BCR	C1-C6	-3.11	1.49	1.53
22	a	403	CLA	CHC-C1C	3.10	1.42	1.35
22	B	606	CLA	CHC-C1C	3.10	1.42	1.35
22	A	406	CLA	CHC-C1C	3.10	1.42	1.35
25	c	521	BCR	C30-C25	-3.10	1.49	1.53
22	C	501	CLA	CHC-C1C	3.09	1.42	1.35
22	b	614	CLA	CHC-C1C	3.09	1.42	1.35
22	b	610	CLA	CHC-C1C	3.09	1.42	1.35
22	C	510	CLA	CHC-C1C	3.09	1.42	1.35
22	C	508	CLA	CHC-C1C	3.09	1.42	1.35
25	B	617	BCR	C1-C6	-3.09	1.49	1.53
25	i	101	BCR	C30-C25	-3.08	1.49	1.53
22	C	503	CLA	CHC-C1C	3.08	1.42	1.35
25	f	102	BCR	C30-C25	-3.08	1.49	1.53
30	d	403	SQD	O48-C23	3.08	1.42	1.33
22	b	605	CLA	CHC-C1C	3.07	1.42	1.35
22	c	520	CLA	CHC-C1C	3.07	1.42	1.35
22	C	507	CLA	CHC-C1C	3.07	1.42	1.35
22	A	402	CLA	CHC-C1C	3.07	1.42	1.35
25	B	619	BCR	C1-C6	-3.07	1.49	1.53
22	a	404	CLA	C4D-ND	-3.06	1.33	1.37
22	b	611	CLA	CHC-C1C	3.06	1.42	1.35
25	B	618	BCR	C1-C6	-3.06	1.49	1.53
22	C	506	CLA	CHC-C1C	3.06	1.42	1.35
22	B	601	CLA	CHC-C1C	3.05	1.42	1.35
25	b	621	BCR	C30-C25	-3.05	1.49	1.53
22	b	609	CLA	CHC-C1C	3.05	1.42	1.35
30	A	413	SQD	O48-C23	3.05	1.42	1.33
22	c	504	CLA	CHC-C1C	3.05	1.42	1.35
25	A	408	BCR	C1-C6	-3.05	1.49	1.53
22	B	611	CLA	C4D-ND	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	623	BCR	C1-C6	-3.04	1.49	1.53
22	B	615	CLA	C4D-ND	-3.04	1.33	1.37
22	C	504	CLA	CHC-C1C	3.04	1.42	1.35
22	B	615	CLA	CHC-C1C	3.03	1.42	1.35
25	C	513	BCR	C30-C25	-3.02	1.49	1.53
22	b	620	CLA	CHC-C1C	3.01	1.42	1.35
34	V	201	HEM	CAB-C3B	3.01	1.55	1.47
22	B	611	CLA	CHC-C1C	3.01	1.42	1.35
22	b	616	CLA	C4D-ND	-3.00	1.33	1.37
34	v	201	HEM	CAB-C3B	2.99	1.55	1.47
25	K	101	BCR	C30-C25	-2.98	1.49	1.53
22	D	403	CLA	C4D-ND	-2.98	1.33	1.37
22	b	606	CLA	C4D-ND	-2.98	1.33	1.37
22	B	612	CLA	C4D-ND	-2.97	1.33	1.37
25	C	520	BCR	C1-C6	-2.96	1.49	1.53
22	b	620	CLA	C4D-ND	-2.95	1.33	1.37
22	C	519	CLA	C4D-ND	-2.95	1.33	1.37
22	d	405	CLA	C4D-ND	-2.95	1.33	1.37
22	B	613	CLA	C4D-ND	-2.94	1.33	1.37
22	C	505	CLA	C4D-ND	-2.94	1.33	1.37
30	B	622	SQD	O47-C7	2.93	1.42	1.34
22	a	404	CLA	CHC-C1C	2.93	1.42	1.35
24	D	405	PL9	C3-C4	-2.93	1.44	1.49
22	b	612	CLA	C4D-ND	-2.93	1.33	1.37
22	C	504	CLA	C4D-ND	-2.93	1.33	1.37
22	C	508	CLA	C4D-ND	-2.93	1.33	1.37
22	B	606	CLA	C4D-ND	-2.92	1.33	1.37
34	F	101	HEM	FE-ND	2.92	2.11	1.96
22	B	605	CLA	C4D-ND	-2.91	1.33	1.37
22	B	607	CLA	C4D-ND	-2.91	1.33	1.37
30	d	403	SQD	O47-C7	2.90	1.42	1.34
22	A	404	CLA	C4D-ND	-2.90	1.33	1.37
30	a	412	SQD	O47-C7	2.89	1.42	1.34
22	b	607	CLA	C4D-ND	-2.89	1.33	1.37
30	A	414	SQD	O47-C7	2.88	1.42	1.34
30	a	401	SQD	O47-C7	2.88	1.42	1.34
22	C	509	CLA	C4D-ND	-2.88	1.33	1.37
22	b	617	CLA	C4D-ND	-2.88	1.33	1.37
25	c	521	BCR	C1-C6	-2.88	1.49	1.53
25	c	514	BCR	C30-C25	-2.88	1.49	1.53
24	A	407	PL9	C7-C3	-2.87	1.48	1.51
25	H	102	BCR	C30-C25	-2.87	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	601	DGD	C1E-C2E	2.87	1.60	1.52
34	v	201	HEM	FE-ND	2.86	2.11	1.96
30	A	413	SQD	O47-C7	2.86	1.42	1.34
22	a	405	CLA	C4D-ND	-2.86	1.33	1.37
30	F	103	SQD	O47-C7	2.86	1.42	1.34
30	B	627	SQD	O47-C7	2.86	1.42	1.34
22	c	505	CLA	C4D-ND	-2.86	1.33	1.37
25	x	101	BCR	C30-C25	-2.86	1.49	1.53
22	b	611	CLA	C4D-ND	-2.85	1.33	1.37
30	b	602	SQD	O47-C7	2.84	1.42	1.34
25	c	513	BCR	C30-C25	-2.84	1.49	1.53
26	B	626	DGD	C1E-C2E	2.84	1.60	1.52
22	C	506	CLA	C4D-ND	-2.84	1.33	1.37
22	A	403	CLA	C4D-ND	-2.83	1.33	1.37
34	f	101	HEM	CAB-C3B	2.83	1.55	1.47
22	b	610	CLA	C4D-ND	-2.83	1.33	1.37
22	c	509	CLA	C4D-ND	-2.82	1.33	1.37
22	b	613	CLA	C4D-ND	-2.81	1.33	1.37
22	c	506	CLA	C4D-ND	-2.81	1.33	1.37
22	A	402	CLA	C4D-ND	-2.81	1.33	1.37
22	b	615	CLA	CHC-C1C	2.80	1.42	1.35
34	V	201	HEM	FE-ND	2.80	2.10	1.96
22	A	406	CLA	C4D-ND	-2.80	1.33	1.37
22	B	602	CLA	C4D-ND	-2.80	1.33	1.37
22	b	608	CLA	C4D-ND	-2.79	1.33	1.37
22	B	614	CLA	C4D-ND	-2.79	1.33	1.37
22	d	406	CLA	C4D-ND	-2.79	1.33	1.37
22	C	511	CLA	C4D-ND	-2.78	1.33	1.37
22	c	511	CLA	C4D-ND	-2.77	1.33	1.37
34	F	101	HEM	CAB-C3B	2.77	1.55	1.47
22	D	404	CLA	C4D-ND	-2.77	1.33	1.37
22	c	507	CLA	C4D-ND	-2.77	1.33	1.37
22	B	604	CLA	C4D-ND	-2.77	1.33	1.37
22	C	507	CLA	C4D-ND	-2.76	1.33	1.37
30	f	103	SQD	O47-C7	2.76	1.42	1.34
34	f	101	HEM	FE-ND	2.76	2.10	1.96
23	D	401	PHO	CAC-C3C	-2.76	1.47	1.52
22	c	504	CLA	C4D-ND	-2.75	1.33	1.37
22	B	610	CLA	CHC-C1C	2.75	1.42	1.35
23	d	401	PHO	CAC-C3C	-2.75	1.47	1.52
22	H	101	CLA	C4D-ND	-2.74	1.33	1.37
22	c	508	CLA	C4D-ND	-2.74	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	514	DGD	O2G-C2G	-2.74	1.39	1.46
22	b	619	CLA	C4D-ND	-2.73	1.33	1.37
22	B	603	CLA	C4D-ND	-2.73	1.33	1.37
22	B	609	CLA	C4D-ND	-2.73	1.33	1.37
25	B	617	BCR	C30-C25	-2.72	1.50	1.53
22	c	502	CLA	C4D-ND	-2.72	1.33	1.37
22	a	406	CLA	C4D-ND	-2.72	1.34	1.37
22	b	618	CLA	C4D-ND	-2.72	1.34	1.37
22	C	503	CLA	C4D-ND	-2.71	1.34	1.37
22	c	520	CLA	C4D-ND	-2.71	1.34	1.37
22	C	502	CLA	C4D-ND	-2.71	1.34	1.37
22	B	601	CLA	C4D-ND	-2.70	1.34	1.37
22	B	608	CLA	C4D-ND	-2.70	1.34	1.37
22	c	512	CLA	C4D-ND	-2.70	1.34	1.37
25	b	622	BCR	C30-C25	-2.70	1.50	1.53
22	b	614	CLA	C4D-ND	-2.69	1.34	1.37
25	j	102	BCR	C1-C6	-2.69	1.50	1.53
22	c	501	CLA	C4D-ND	-2.67	1.34	1.37
22	b	605	CLA	C4D-ND	-2.67	1.34	1.37
25	J	102	BCR	C1-C6	-2.67	1.50	1.53
22	a	403	CLA	C4D-ND	-2.67	1.34	1.37
24	d	407	PL9	C3-C4	-2.67	1.45	1.49
22	b	615	CLA	C4D-ND	-2.66	1.34	1.37
23	A	405	PHO	CAC-C3C	-2.64	1.47	1.52
22	C	507	CLA	CMB-C2B	-2.62	1.46	1.51
22	C	510	CLA	C4D-ND	-2.62	1.34	1.37
22	C	512	CLA	C4D-ND	-2.62	1.34	1.37
32	b	629	LMT	O3'-C3'	-2.61	1.36	1.43
22	c	507	CLA	CMB-C2B	-2.60	1.46	1.51
22	C	501	CLA	C4D-ND	-2.59	1.34	1.37
22	c	503	CLA	C4D-ND	-2.56	1.34	1.37
32	b	603	LMT	O3'-C3'	-2.56	1.36	1.43
32	d	411	LMT	O3'-C3'	-2.56	1.36	1.43
32	M	103	LMT	O3'-C3'	-2.56	1.36	1.43
23	d	402	PHO	CAC-C3C	-2.56	1.47	1.52
22	c	510	CLA	C4D-ND	-2.55	1.34	1.37
32	b	628	LMT	O3'-C3'	-2.55	1.37	1.43
32	B	624	LMT	O3'-C3'	-2.55	1.37	1.43
22	B	607	CLA	CMB-C2B	-2.53	1.46	1.51
32	B	623	LMT	O3'-C3'	-2.53	1.37	1.43
32	M	102	LMT	O3'-C3'	-2.52	1.37	1.43
32	D	408	LMT	O3'-C3'	-2.52	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	FE-NB	2.52	2.09	1.96
22	B	603	CLA	CMB-C2B	-2.51	1.46	1.51
22	b	609	CLA	C4D-ND	-2.51	1.34	1.37
22	a	403	CLA	CMB-C2B	-2.51	1.46	1.51
32	I	102	LMT	O3'-C3'	-2.51	1.37	1.43
24	A	407	PL9	C3-C4	-2.50	1.45	1.49
22	B	610	CLA	C4D-ND	-2.50	1.34	1.37
22	b	612	CLA	CMB-C2B	-2.50	1.46	1.51
32	B	628	LMT	O3'-C3'	-2.50	1.37	1.43
24	a	407	PL9	C3-C4	-2.49	1.45	1.49
22	A	403	CLA	CMB-C2B	-2.49	1.46	1.51
22	A	406	CLA	CMB-C2B	-2.48	1.46	1.51
32	i	103	LMT	O3'-C3'	-2.48	1.37	1.43
22	C	501	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.47	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.46	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.45	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.45	1.46	1.51
31	b	626	LMG	C4-C5	2.45	1.58	1.53
22	C	502	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.45	1.46	1.51
26	B	626	DGD	C4D-C5D	2.45	1.58	1.53
22	c	504	CLA	CMB-C2B	-2.45	1.46	1.51
22	a	404	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	614	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	519	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.42	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.42	1.46	1.51
22	d	406	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.41	1.46	1.51
22	D	404	CLA	CMB-C2B	-2.40	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.40	1.46	1.51
32	B	629	LMT	O3'-C3'	-2.40	1.37	1.43
32	b	604	LMT	O3'-C3'	-2.40	1.37	1.43
22	C	506	CLA	CMB-C2B	-2.39	1.46	1.51
22	A	404	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.39	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.39	1.46	1.51
24	j	101	PL9	C3-C4	-2.38	1.45	1.49
22	C	510	CLA	CMB-C2B	-2.38	1.46	1.51
32	I	102	LMT	O2'-C2'	-2.38	1.37	1.43
22	c	506	CLA	CMB-C2B	-2.38	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	611	CLA	CMD-C2D	-2.37	1.45	1.50
22	b	607	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.37	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.36	1.46	1.51
24	D	405	PL9	C6-C1	-2.36	1.44	1.48
22	B	612	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.35	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.35	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.35	1.46	1.51
22	D	403	CLA	CMB-C2B	-2.34	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.34	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.32	1.46	1.51
31	B	621	LMG	C4-C5	2.32	1.57	1.53
32	B	629	LMT	O3B-C3B	-2.32	1.37	1.43
22	b	620	CLA	CMB-C2B	-2.30	1.46	1.51
32	D	408	LMT	O3B-C3B	-2.30	1.37	1.43
32	b	604	LMT	O3B-C3B	-2.30	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CMB-C2B	-2.29	1.46	1.51
31	I	101	LMG	C4-C5	2.29	1.57	1.53
32	M	103	LMT	O3B-C3B	-2.29	1.37	1.43
32	b	629	LMT	O3B-C3B	-2.29	1.37	1.43
32	i	103	LMT	O2'-C2'	-2.29	1.37	1.43
31	D	409	LMG	O7-C8	-2.28	1.40	1.46
31	b	627	LMG	C4-C5	2.28	1.57	1.53
26	b	601	DGD	C4D-C5D	2.28	1.57	1.53
32	B	623	LMT	O2'-C2'	-2.28	1.37	1.43
32	b	603	LMT	O3B-C3B	-2.27	1.37	1.43
32	B	629	LMT	O2'-C2'	-2.27	1.37	1.43
32	B	628	LMT	O2B-C2B	-2.26	1.37	1.43
32	b	628	LMT	O3B-C3B	-2.26	1.37	1.43
22	b	616	CLA	CMD-C2D	-2.26	1.46	1.50
32	I	102	LMT	O3B-C3B	-2.25	1.37	1.43
32	B	624	LMT	O3B-C3B	-2.25	1.37	1.43
32	b	603	LMT	O2'-C2'	-2.25	1.37	1.43
32	d	411	LMT	O3B-C3B	-2.25	1.37	1.43
32	M	102	LMT	O3B-C3B	-2.24	1.37	1.43
32	b	628	LMT	O2'-C2'	-2.24	1.37	1.43
32	B	628	LMT	O3B-C3B	-2.24	1.37	1.43
32	i	103	LMT	O2B-C2B	-2.24	1.37	1.43
34	f	101	HEM	FE-NB	2.23	2.07	1.96
32	i	103	LMT	O3B-C3B	-2.23	1.37	1.43
34	V	201	HEM	FE-NB	2.22	2.07	1.96
32	I	102	LMT	O2B-C2B	-2.22	1.37	1.43
32	b	628	LMT	O2B-C2B	-2.22	1.37	1.43
32	M	102	LMT	O2'-C2'	-2.21	1.37	1.43
24	a	407	PL9	C53-C6	-2.21	1.46	1.50
32	B	624	LMT	O2'-C2'	-2.21	1.37	1.43
32	b	629	LMT	O2'-C2'	-2.21	1.37	1.43
32	b	604	LMT	O2'-C2'	-2.21	1.37	1.43
32	B	623	LMT	O3B-C3B	-2.20	1.37	1.43
25	g	101	BCR	C33-C5	-2.20	1.47	1.50
22	c	504	CLA	CMD-C2D	-2.20	1.46	1.50
32	D	408	LMT	O2B-C2B	-2.19	1.37	1.43
22	c	509	CLA	CMD-C2D	-2.19	1.46	1.50
32	M	103	LMT	O2'-C2'	-2.19	1.37	1.43
26	d	410	DGD	C1D-C2D	2.19	1.58	1.52
32	B	629	LMT	O2B-C2B	-2.18	1.37	1.43
32	b	603	LMT	O2B-C2B	-2.18	1.37	1.43
31	a	402	LMG	C4-C5	2.18	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	628	LMT	O2'-C2'	-2.17	1.37	1.43
27	a	409	LHG	O7-C5	-2.17	1.41	1.46
30	b	602	SQD	O2-C2	-2.17	1.37	1.43
24	d	407	PL9	C31-C29	-2.16	1.46	1.51
24	d	407	PL9	C6-C1	-2.16	1.44	1.48
22	B	610	CLA	C3B-C2B	-2.16	1.37	1.40
32	M	103	LMT	O2B-C2B	-2.16	1.37	1.43
32	B	623	LMT	O2B-C2B	-2.16	1.37	1.43
34	v	201	HEM	CAA-C2A	2.15	1.55	1.52
22	C	504	CLA	CMD-C2D	-2.15	1.46	1.50
26	B	626	DGD	C3G-C2G	2.15	1.57	1.50
27	c	519	LHG	O7-C5	-2.15	1.41	1.46
32	d	411	LMT	O2B-C2B	-2.14	1.37	1.43
32	M	102	LMT	O1'-C1'	-2.14	1.36	1.40
27	c	519	LHG	P-O6	2.14	1.68	1.59
30	B	627	SQD	O2-C2	-2.14	1.37	1.43
25	y	101	BCR	C33-C5	-2.14	1.47	1.50
22	b	615	CLA	C3B-C2B	-2.13	1.37	1.40
31	m	101	LMG	C4-C5	2.13	1.57	1.53
30	a	412	SQD	O2-C2	-2.13	1.38	1.43
30	A	413	SQD	O2-C2	-2.13	1.38	1.43
32	b	604	LMT	O2B-C2B	-2.13	1.38	1.43
24	A	407	PL9	C53-C6	-2.13	1.46	1.50
22	C	509	CLA	CMD-C2D	-2.13	1.46	1.50
26	D	407	DGD	O5D-C6D	-2.13	1.39	1.43
22	b	612	CLA	CMD-C2D	-2.13	1.46	1.50
26	c	515	DGD	O2G-C2G	-2.12	1.41	1.46
26	C	514	DGD	O1G-C1G	-2.12	1.40	1.45
32	d	411	LMT	O4'-C4B	-2.12	1.38	1.43
26	b	601	DGD	C3G-C2G	2.12	1.57	1.50
26	c	516	DGD	O2G-C2G	-2.12	1.41	1.46
32	d	411	LMT	O2'-C2'	-2.12	1.38	1.43
23	d	401	PHO	CMC-C2C	-2.12	1.46	1.51
31	l	101	LMG	C7-C8	2.11	1.57	1.50
23	D	401	PHO	CMC-C2C	-2.11	1.46	1.51
30	A	414	SQD	O3-C3	-2.11	1.38	1.43
22	B	607	CLA	CMD-C2D	-2.11	1.46	1.50
32	D	408	LMT	O4'-C4B	-2.11	1.38	1.43
32	b	629	LMT	O4'-C4B	-2.11	1.38	1.43
32	M	102	LMT	O2B-C2B	-2.11	1.38	1.43
32	I	102	LMT	O4'-C4B	-2.10	1.38	1.43
26	D	407	DGD	C1G-C2G	2.10	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	401	SQD	O3-C3	-2.09	1.38	1.43
23	d	402	PHO	CMC-C2C	-2.09	1.46	1.51
31	a	402	LMG	O7-C8	-2.09	1.41	1.46
22	B	603	CLA	CMD-C2D	-2.08	1.46	1.50
30	F	103	SQD	O2-C2	-2.08	1.38	1.43
32	b	629	LMT	O2B-C2B	-2.08	1.38	1.43
32	B	628	LMT	O4'-C4B	-2.08	1.38	1.43
32	b	604	LMT	O4'-C4B	-2.08	1.38	1.43
32	b	603	LMT	O4'-C4B	-2.08	1.38	1.43
32	D	408	LMT	O2'-C2'	-2.08	1.38	1.43
22	D	403	CLA	CMD-C2D	-2.08	1.46	1.50
26	b	601	DGD	C1G-C2G	2.07	1.57	1.50
26	c	516	DGD	O5D-C6D	-2.07	1.40	1.43
23	d	401	PHO	CMB-C2B	-2.07	1.46	1.51
23	A	405	PHO	CMC-C2C	-2.06	1.46	1.51
22	d	405	CLA	CMD-C2D	-2.06	1.46	1.50
32	M	103	LMT	O4'-C4B	-2.06	1.38	1.43
24	A	407	PL9	C6-C1	-2.06	1.44	1.48
26	c	517	DGD	C1G-C2G	2.06	1.57	1.50
30	f	103	SQD	O2-C2	-2.06	1.38	1.43
26	C	515	DGD	O2G-C2G	-2.06	1.41	1.46
32	M	102	LMT	O4'-C4B	-2.05	1.38	1.43
26	D	407	DGD	C1D-C2D	2.05	1.58	1.52
32	b	628	LMT	O4'-C4B	-2.05	1.38	1.43
30	B	622	SQD	O2-C2	-2.05	1.38	1.43
22	A	404	CLA	CMD-C2D	-2.05	1.46	1.50
30	b	602	SQD	O3-C3	-2.05	1.38	1.43
22	a	403	CLA	CMD-C2D	-2.05	1.46	1.50
34	V	201	HEM	CAA-C2A	2.04	1.55	1.52
23	D	401	PHO	CMD-C2D	-2.04	1.46	1.51
30	d	403	SQD	O2-C2	-2.04	1.38	1.43
31	L	101	LMG	C7-C8	2.04	1.57	1.50
32	B	629	LMT	O4'-C4B	-2.04	1.38	1.43
22	b	608	CLA	CMD-C2D	-2.04	1.46	1.50
26	d	410	DGD	O5D-C6D	-2.03	1.40	1.43
23	d	401	PHO	CMD-C2D	-2.03	1.46	1.51
23	A	405	PHO	CMB-C2B	-2.03	1.46	1.51
31	d	412	LMG	O7-C8	-2.03	1.41	1.46
27	A	410	LHG	O7-C5	-2.03	1.41	1.46
34	V	201	HEM	CMB-C2B	2.03	1.55	1.50
22	B	615	CLA	CMC-C2C	-2.03	1.46	1.50
31	m	101	LMG	C7-C8	2.02	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	CMD-C2D	-2.02	1.46	1.50
23	A	405	PHO	CMD-C2D	-2.02	1.46	1.51
22	a	405	CLA	CMD-C2D	-2.02	1.46	1.50
32	B	629	LMT	O1'-C1'	-2.02	1.36	1.40
23	d	402	PHO	CMD-C2D	-2.02	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.01	1.46	1.50
22	b	620	CLA	CMC-C2C	-2.01	1.46	1.50
24	J	101	PL9	C3-C4	-2.01	1.46	1.49
32	i	103	LMT	O4'-C4B	-2.01	1.38	1.43
22	a	404	CLA	CMD-C2D	-2.01	1.46	1.50
34	v	201	HEM	CMB-C2B	2.01	1.55	1.50
22	B	610	CLA	C4B-CHC	-2.01	1.35	1.41
31	i	102	LMG	C4-C5	2.01	1.57	1.53
22	b	620	CLA	CMD-C2D	-2.01	1.46	1.50
22	B	606	CLA	CMD-C2D	-2.01	1.46	1.50
26	c	517	DGD	C3G-C2G	2.01	1.56	1.50
22	b	605	CLA	CMD-C2D	-2.01	1.46	1.50
26	A	409	DGD	C4E-C5E	2.01	1.57	1.53
24	d	407	PL9	C53-C6	-2.01	1.46	1.50
26	D	407	DGD	C3D-C2D	2.00	1.57	1.52
32	B	624	LMT	O4'-C4B	-2.00	1.38	1.43
34	v	201	HEM	CMD-C2D	2.00	1.55	1.50
32	B	623	LMT	O4'-C4B	-2.00	1.38	1.43
34	V	201	HEM	CMD-C2D	2.00	1.55	1.50
23	d	402	PHO	CMB-C2B	-2.00	1.46	1.51

All (1179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	C4A-NA-C1A	7.60	110.12	106.71
22	B	611	CLA	C4A-NA-C1A	7.55	110.10	106.71
22	B	605	CLA	C4A-NA-C1A	7.39	110.03	106.71
22	b	608	CLA	C4A-NA-C1A	7.34	110.01	106.71
22	C	501	CLA	C4A-NA-C1A	7.23	109.96	106.71
22	b	610	CLA	C4A-NA-C1A	7.23	109.95	106.71
22	C	503	CLA	C4A-NA-C1A	7.21	109.95	106.71
22	b	616	CLA	C4A-NA-C1A	7.20	109.94	106.71
22	C	511	CLA	C4A-NA-C1A	7.19	109.94	106.71
22	B	603	CLA	C4A-NA-C1A	7.19	109.94	106.71
22	c	503	CLA	C4A-NA-C1A	7.18	109.94	106.71
22	C	510	CLA	C4A-NA-C1A	7.14	109.92	106.71
22	c	501	CLA	C4A-NA-C1A	7.14	109.91	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	C4A-NA-C1A	7.13	109.91	106.71
22	C	507	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	B	604	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	c	504	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	C	512	CLA	C4A-NA-C1A	7.00	109.85	106.71
22	A	403	CLA	C4A-NA-C1A	6.96	109.84	106.71
22	C	506	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	B	614	CLA	C4A-NA-C1A	6.93	109.82	106.71
22	b	609	CLA	C4A-NA-C1A	6.92	109.82	106.71
22	c	520	CLA	C4A-NA-C1A	6.90	109.81	106.71
22	a	406	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	c	511	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	d	405	CLA	C4A-NA-C1A	6.87	109.79	106.71
22	c	507	CLA	C4A-NA-C1A	6.83	109.78	106.71
22	b	619	CLA	C4A-NA-C1A	6.83	109.78	106.71
22	b	620	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	d	406	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	b	617	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	B	613	CLA	C4A-NA-C1A	6.69	109.72	106.71
22	c	512	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	A	406	CLA	C4A-NA-C1A	6.68	109.71	106.71
22	H	101	CLA	C4A-NA-C1A	6.67	109.71	106.71
22	c	505	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	B	612	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	c	508	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	C	519	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	a	404	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	b	618	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	c	509	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	c	502	CLA	C4A-NA-C1A	6.52	109.64	106.71
22	B	606	CLA	C4A-NA-C1A	6.47	109.62	106.71
34	v	201	HEM	C4D-ND-C1D	6.42	111.70	105.07
22	A	404	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	C	508	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	D	403	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	b	612	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	a	403	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	b	606	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	c	510	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	B	608	CLA	C4A-NA-C1A	6.37	109.57	106.71
22	B	607	CLA	C4A-NA-C1A	6.36	109.56	106.71
22	C	509	CLA	C4A-NA-C1A	6.34	109.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	A	402	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	B	602	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	a	405	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	B	609	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	b	611	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	C	505	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	D	404	CLA	C4A-NA-C1A	6.22	109.50	106.71
30	b	602	SQD	O6-C1-C2	6.13	117.87	108.30
22	C	502	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	b	605	CLA	C4A-NA-C1A	6.08	109.44	106.71
22	B	601	CLA	C4A-NA-C1A	6.03	109.42	106.71
22	b	613	CLA	C4A-NA-C1A	6.01	109.41	106.71
34	f	101	HEM	C4D-ND-C1D	5.96	111.22	105.07
22	b	607	CLA	C4A-NA-C1A	5.89	109.36	106.71
24	J	101	PL9	C7-C3-C4	5.88	121.66	116.88
30	B	627	SQD	O6-C1-C2	5.86	117.45	108.30
34	F	101	HEM	C4D-ND-C1D	5.83	111.09	105.07
22	b	614	CLA	C4A-NA-C1A	5.81	109.32	106.71
34	V	201	HEM	C4D-ND-C1D	5.79	111.06	105.07
33	d	404	BCT	O2-C-O1	5.79	134.56	119.55
33	D	402	BCT	O2-C-O1	5.73	134.42	119.55
22	b	615	CLA	C4A-NA-C1A	5.68	109.26	106.71
22	B	610	CLA	CMB-C2B-C1B	-5.52	119.98	128.46
30	A	413	SQD	O6-C1-C2	5.48	116.86	108.30
30	a	412	SQD	O6-C1-C2	5.48	116.86	108.30
24	j	101	PL9	C7-C3-C4	5.46	121.32	116.88
22	B	610	CLA	C4A-NA-C1A	5.43	109.15	106.71
24	a	407	PL9	C7-C3-C4	5.42	121.28	116.88
24	A	407	PL9	C7-C3-C4	5.39	121.26	116.88
22	b	615	CLA	CMB-C2B-C1B	-5.37	120.20	128.46
24	d	407	PL9	C7-C3-C4	5.35	121.22	116.88
30	A	413	SQD	O9-S-C6	5.22	113.14	106.94
24	D	405	PL9	C7-C3-C4	5.22	121.12	116.88
30	a	412	SQD	O9-S-C6	4.77	112.61	106.94
30	B	622	SQD	O7-S-C6	4.73	112.56	106.94
26	A	409	DGD	O3G-C3G-C2G	-4.60	99.80	110.90
30	f	103	SQD	O7-S-C6	4.57	112.37	106.94
26	a	408	DGD	O3G-C3G-C2G	-4.45	100.16	110.90
30	a	401	SQD	O7-S-C6	4.39	112.16	106.94
26	C	516	DGD	O3G-C3G-C2G	-4.33	100.45	110.90
30	d	403	SQD	O5-C5-C4	4.29	117.49	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	B	622	SQD	O5-C5-C4	4.27	117.45	109.69
30	F	103	SQD	O7-S-C6	4.26	112.00	106.94
27	C	518	LHG	O4-P-O5	4.25	133.25	112.24
27	a	409	LHG	O4-P-O5	4.23	133.17	112.24
27	c	519	LHG	O4-P-O5	4.23	133.13	112.24
27	A	410	LHG	O4-P-O5	4.21	133.06	112.24
30	A	414	SQD	O7-S-C6	4.18	111.91	106.94
22	c	507	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
30	B	627	SQD	O9-S-C6	4.15	111.87	106.94
22	B	612	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
31	d	409	LMG	C1-C2-C3	-4.10	101.46	110.00
22	C	507	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
22	b	617	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
30	B	622	SQD	O6-C1-C2	4.08	114.67	108.30
30	b	602	SQD	O7-S-C6	4.07	111.78	106.94
31	D	406	LMG	C1-C2-C3	-4.06	101.54	110.00
30	d	403	SQD	O7-S-C6	4.04	111.74	106.94
26	c	517	DGD	O3G-C3G-C2G	-4.04	101.16	110.90
30	b	602	SQD	O9-S-C6	4.03	111.73	106.94
22	B	607	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
30	f	103	SQD	O9-S-O7	-3.90	100.46	113.95
30	d	403	SQD	O9-S-O7	-3.88	100.50	113.95
22	b	612	CLA	CMB-C2B-C1B	-3.88	122.49	128.46
30	A	414	SQD	O5-C5-C4	3.87	116.72	109.69
30	A	413	SQD	O47-C7-C8	3.86	119.83	111.50
30	F	103	SQD	O9-S-O7	-3.85	100.61	113.95
24	J	101	PL9	C7-C3-C2	-3.85	118.23	123.30
22	B	609	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
22	b	614	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
30	b	602	SQD	O47-C7-C8	3.83	119.75	111.50
30	B	622	SQD	O9-S-O7	-3.82	100.72	113.95
25	J	102	BCR	C11-C10-C9	-3.82	121.86	127.31
30	F	103	SQD	O5-C5-C4	3.82	116.62	109.69
30	B	627	SQD	O7-S-C6	3.80	111.46	106.94
30	a	412	SQD	O9-S-O7	-3.80	100.80	113.95
25	j	102	BCR	C2-C1-C6	3.80	116.33	110.48
25	c	513	BCR	C2-C1-C6	3.80	116.32	110.48
25	K	101	BCR	C2-C1-C6	3.79	116.31	110.48
30	f	103	SQD	O5-C5-C4	3.78	116.56	109.69
30	d	403	SQD	O6-C1-C2	3.78	114.20	108.30
30	B	627	SQD	O5-C5-C4	3.77	116.55	109.69
30	A	413	SQD	O9-S-O7	-3.77	100.90	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	401	SQD	O9-S-O7	-3.76	100.95	113.95
24	j	101	PL9	C7-C3-C2	-3.75	118.37	123.30
30	a	412	SQD	O47-C7-C8	3.74	119.57	111.50
22	B	613	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
30	b	602	SQD	O5-C5-C4	3.74	116.48	109.69
30	b	602	SQD	O9-S-O7	-3.73	101.04	113.95
30	B	627	SQD	O47-C7-C8	3.73	119.53	111.50
22	B	611	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
30	a	401	SQD	O5-C5-C4	3.72	116.44	109.69
30	a	412	SQD	O7-S-C6	3.72	111.36	106.94
30	F	103	SQD	O8-S-C6	3.70	111.64	105.74
25	J	102	BCR	C2-C1-C6	3.70	116.18	110.48
30	a	412	SQD	O5-C5-C4	3.70	116.41	109.69
30	f	103	SQD	O8-S-C6	3.70	111.64	105.74
30	B	627	SQD	O9-S-O7	-3.70	101.15	113.95
30	A	414	SQD	O9-S-O7	-3.69	101.17	113.95
22	c	506	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
30	a	401	SQD	C44-O6-C1	3.68	120.92	113.74
22	B	601	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
30	A	413	SQD	O5-C5-C4	3.67	116.35	109.69
22	b	618	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
26	d	410	DGD	O6D-C1D-O3G	-3.65	101.32	109.97
22	B	602	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	C	505	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
26	c	516	DGD	O5D-C6D-C5D	-3.64	102.32	109.05
22	b	605	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
22	c	512	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
26	c	516	DGD	O3G-C3G-C2G	-3.63	102.14	110.90
26	C	515	DGD	O3G-C3G-C2G	-3.63	102.15	110.90
30	d	403	SQD	O9-S-C6	3.62	111.25	106.94
30	A	413	SQD	O7-S-C6	3.62	111.25	106.94
22	c	510	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
22	A	406	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
22	b	616	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
24	d	407	PL9	C7-C3-C2	-3.62	118.54	123.30
22	C	510	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
22	C	508	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
22	C	512	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	c	502	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
26	D	407	DGD	O6D-C1D-O3G	-3.57	101.52	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	103	SQD	O9-S-C6	3.57	111.18	106.94
22	b	607	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
24	D	405	PL9	C7-C3-C2	-3.56	118.62	123.30
26	C	515	DGD	O5D-C6D-C5D	-3.56	102.47	109.05
22	c	503	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
24	a	407	PL9	C7-C3-C2	-3.54	118.64	123.30
22	C	502	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
22	c	509	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
25	j	102	BCR	C11-C10-C9	-3.54	122.26	127.31
22	C	503	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	B	612	CLA	CMB-C2B-C3B	3.53	131.28	124.68
22	B	605	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
22	C	509	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	b	625	DGD	O3G-C3G-C2G	-3.52	102.40	110.90
22	c	520	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
22	a	404	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	C	519	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
22	C	506	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
30	A	414	SQD	O9-S-C6	3.50	111.10	106.94
30	B	622	SQD	O47-C7-C8	3.50	119.04	111.50
22	D	404	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
22	b	609	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
22	a	406	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
30	F	103	SQD	O6-C1-C2	3.47	113.72	108.30
22	B	610	CLA	CMB-C2B-C3B	3.47	131.17	124.68
34	v	201	HEM	C4C-CHD-C1D	3.47	127.13	122.56
22	C	511	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
26	c	515	DGD	O3G-C3G-C2G	-3.45	102.58	110.90
22	A	402	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	a	403	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
34	V	201	HEM	C4C-CHD-C1D	3.44	127.10	122.56
30	a	401	SQD	O9-S-C6	3.44	111.03	106.94
24	A	407	PL9	C7-C3-C2	-3.44	118.78	123.30
26	B	620	DGD	O3G-C3G-C2G	-3.44	102.61	110.90
30	d	403	SQD	O47-C7-C8	3.43	118.90	111.50
22	c	511	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
30	d	403	SQD	O8-S-C6	3.42	111.18	105.74
30	F	103	SQD	O47-C7-C8	3.41	118.85	111.50
22	c	503	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
30	A	414	SQD	C44-O6-C1	3.41	120.39	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
22	b	618	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
22	D	403	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
22	b	617	CLA	CMB-C2B-C3B	3.38	130.99	124.68
22	d	406	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
22	b	619	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	B	606	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
25	B	617	BCR	C15-C16-C17	-3.35	116.61	123.47
30	A	414	SQD	O47-C7-C8	3.35	118.72	111.50
22	b	615	CLA	CMB-C2B-C3B	3.35	130.95	124.68
26	b	625	DGD	O6D-C1D-O3G	-3.34	102.06	109.97
30	f	103	SQD	O9-S-C6	3.34	110.91	106.94
22	A	403	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
22	B	603	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
25	A	408	BCR	C2-C1-C6	3.33	115.61	110.48
30	f	103	SQD	O6-C1-C2	3.33	113.50	108.30
22	c	507	CLA	CMB-C2B-C3B	3.32	130.90	124.68
22	b	608	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
26	C	514	DGD	O3G-C3G-C2G	-3.32	102.89	110.90
22	a	405	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
22	A	404	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
22	B	613	CLA	CMB-C2B-C3B	3.30	130.86	124.68
22	d	405	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
22	b	611	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
22	B	607	CLA	CMB-C2B-C3B	3.29	130.83	124.68
24	J	101	PL9	C7-C8-C9	-3.28	121.33	126.79
25	j	102	BCR	C7-C8-C9	-3.28	121.28	126.23
22	b	610	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
22	C	503	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
26	B	620	DGD	O6D-C1D-O3G	-3.26	102.26	109.97
22	B	603	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
22	B	613	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
30	B	622	SQD	O9-S-C6	3.23	110.78	106.94
30	B	627	SQD	C3-C4-C5	3.23	116.00	110.24
22	c	504	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
25	b	622	BCR	C15-C16-C17	-3.22	116.87	123.47
22	H	101	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
22	c	506	CLA	CMB-C2B-C3B	3.22	130.71	124.68
22	b	612	CLA	CMB-C2B-C3B	3.22	130.70	124.68
22	B	609	CLA	CMB-C2B-C3B	3.21	130.69	124.68
24	j	101	PL9	C7-C8-C9	-3.21	121.45	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	608	CLA	CMB-C2B-C1B	-3.21	123.54	128.46
22	b	620	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
26	c	516	DGD	O6D-C1D-O3G	-3.19	102.42	109.97
30	a	401	SQD	O47-C7-C8	3.19	118.38	111.50
30	f	103	SQD	O47-C7-C8	3.19	118.37	111.50
22	B	602	CLA	CMB-C2B-C3B	3.18	130.63	124.68
30	B	622	SQD	O8-S-C6	3.17	110.80	105.74
30	a	401	SQD	O8-S-C6	3.17	110.79	105.74
22	b	613	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
25	J	102	BCR	C7-C8-C9	-3.16	121.45	126.23
22	C	507	CLA	CMB-C2B-C3B	3.16	130.59	124.68
25	J	102	BCR	C24-C23-C22	-3.16	121.46	126.23
22	C	502	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
25	B	618	BCR	C2-C1-C6	3.15	115.33	110.48
22	b	607	CLA	CMB-C2B-C3B	3.15	130.56	124.68
30	B	627	SQD	O8-S-C6	3.14	110.75	105.74
22	c	505	CLA	CMB-C2B-C3B	3.14	130.55	124.68
22	b	614	CLA	CMB-C2B-C3B	3.14	130.54	124.68
30	B	622	SQD	C44-O6-C1	3.13	119.85	113.74
30	f	103	SQD	C44-O6-C1	3.13	119.85	113.74
22	C	507	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
32	b	604	LMT	C1'-O5'-C5'	-3.13	107.55	113.69
30	F	103	SQD	C44-O6-C1	3.12	119.84	113.74
22	C	505	CLA	CMB-C2B-C3B	3.11	130.50	124.68
32	B	629	LMT	C1'-O5'-C5'	-3.10	107.60	113.69
22	B	604	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
25	b	623	BCR	C24-C23-C22	-3.10	121.55	126.23
22	C	504	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	a	403	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
22	B	605	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
25	B	617	BCR	C33-C5-C6	-3.09	121.06	124.53
30	d	403	SQD	C3-C4-C5	3.08	115.73	110.24
25	i	101	BCR	C2-C1-C6	3.08	115.22	110.48
26	A	409	DGD	O6D-C1D-O3G	-3.07	102.69	109.97
25	b	622	BCR	C33-C5-C6	-3.07	121.09	124.53
22	B	608	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	B	606	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	C	506	CLA	CMB-C2B-C3B	3.05	130.39	124.68
22	B	611	CLA	CMB-C2B-C3B	3.05	130.39	124.68
26	c	517	DGD	O5D-C6D-C5D	-3.05	103.40	109.05
31	B	625	LMG	O6-C1-O1	-3.05	102.75	109.97
22	b	618	CLA	CMB-C2B-C3B	3.05	130.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	x	101	BCR	C33-C5-C6	-3.05	121.11	124.53
22	C	510	CLA	CMB-C2B-C3B	3.05	130.38	124.68
22	c	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
22	c	507	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
22	b	606	CLA	CMB-C2B-C3B	3.04	130.37	124.68
26	d	410	DGD	O3G-C3G-C2G	-3.04	103.56	110.90
30	B	622	SQD	C3-C4-C5	3.04	115.66	110.24
25	J	102	BCR	C35-C13-C14	-3.04	118.67	122.92
22	a	405	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	b	607	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
22	c	510	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	c	521	BCR	C15-C16-C17	-3.03	117.27	123.47
25	b	623	BCR	C2-C1-C6	3.02	115.14	110.48
26	C	515	DGD	O6D-C1D-O3G	-3.01	102.84	109.97
22	b	614	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
34	v	201	HEM	C4B-CHC-C1C	3.01	126.53	122.56
26	c	515	DGD	O6D-C1D-O3G	-3.01	102.86	109.97
25	F	102	BCR	C33-C5-C6	-3.00	121.16	124.53
22	a	406	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	H	102	BCR	C33-C5-C6	-3.00	121.16	124.53
22	b	613	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
25	C	513	BCR	C15-C16-C17	-2.99	117.34	123.47
30	a	412	SQD	O8-S-C6	2.99	110.51	105.74
22	A	406	CLA	CMB-C2B-C3B	2.99	130.28	124.68
32	i	103	LMT	O1'-C1'-C2'	2.99	112.97	108.30
24	d	407	PL9	C7-C8-C9	-2.99	121.81	126.79
22	b	612	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	B	602	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	c	512	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	A	403	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
22	C	505	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
22	c	510	CLA	CMB-C2B-C3B	2.99	130.27	124.68
26	C	516	DGD	CDB-CCB-CBB	-2.99	99.27	114.42
22	C	501	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
34	f	101	HEM	C1B-NB-C4B	2.98	108.16	105.07
22	b	605	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
22	b	616	CLA	CMB-C2B-C3B	2.98	130.25	124.68
23	d	402	PHO	CMB-C2B-C3B	2.98	130.25	124.68
25	j	102	BCR	C24-C23-C22	-2.98	121.74	126.23
22	c	520	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
26	C	516	DGD	O5D-C6D-C5D	-2.97	103.55	109.05
22	A	402	CLA	O2D-CGD-O1D	-2.97	118.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	505	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	D	404	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	B	605	CLA	CMB-C2B-C3B	2.97	130.23	124.68
30	a	412	SQD	C3-C4-C5	2.97	115.53	110.24
22	c	502	CLA	CMB-C2B-C3B	2.97	130.23	124.68
26	D	407	DGD	O3G-C3G-C2G	-2.96	103.75	110.90
25	f	102	BCR	C33-C5-C6	-2.96	121.20	124.53
22	b	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	b	610	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
26	c	517	DGD	CDB-CCB-CBB	-2.96	99.40	114.42
25	g	101	BCR	C38-C26-C25	-2.96	121.21	124.53
30	b	602	SQD	C4-C3-C2	2.96	115.98	110.82
26	b	601	DGD	O3G-C3G-C2G	-2.96	103.77	110.90
23	D	401	PHO	CMB-C2B-C3B	2.95	130.20	124.68
22	C	512	CLA	CMB-C2B-C3B	2.95	130.20	124.68
22	c	502	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
31	d	408	LMG	O6-C1-O1	-2.95	103.00	109.97
22	B	601	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
30	d	403	SQD	C44-O6-C1	2.94	119.49	113.74
22	D	403	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	c	512	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	B	618	BCR	C24-C23-C22	-2.94	121.79	126.23
22	C	502	CLA	CMB-C2B-C3B	2.94	130.17	124.68
30	A	413	SQD	O8-S-C6	2.94	110.42	105.74
22	A	404	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
26	B	626	DGD	O5D-C1E-C2E	2.93	112.88	108.30
32	M	102	LMT	C1'-O5'-C5'	-2.93	107.95	113.69
22	c	503	CLA	CMB-C2B-C3B	2.92	130.15	124.68
22	C	511	CLA	CMB-C2B-C3B	2.92	130.14	124.68
22	C	503	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	d	410	DGD	C3D-C4D-C5D	-2.92	105.03	110.24
22	b	609	CLA	CMB-C2B-C3B	2.92	130.13	124.68
25	b	624	BCR	C7-C8-C9	-2.91	121.83	126.23
22	C	519	CLA	CMB-C2B-C3B	2.91	130.13	124.68
22	c	508	CLA	CMB-C2B-C3B	2.91	130.13	124.68
24	d	407	PL9	C40-C39-C41	2.91	120.17	115.27
34	f	101	HEM	C3B-C2B-C1B	2.91	108.64	106.49
22	C	504	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
22	B	601	CLA	CMB-C2B-C3B	2.90	130.10	124.68
22	B	609	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	c	501	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	B	604	CLA	CMB-C2B-C3B	2.90	130.10	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	b	602	SQD	O8-S-C6	2.90	110.36	105.74
26	a	408	DGD	O6D-C1D-O3G	-2.89	103.12	109.97
30	A	414	SQD	O8-S-C6	2.89	110.35	105.74
26	A	409	DGD	O5D-C6D-C5D	-2.89	103.69	109.05
22	B	606	CLA	CMB-C2B-C3B	2.89	130.08	124.68
26	C	514	DGD	O6D-C1D-O3G	-2.88	103.14	109.97
22	B	610	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	B	626	DGD	O3G-C3G-C2G	-2.88	103.95	110.90
32	I	102	LMT	O1'-C1'-C2'	2.88	112.80	108.30
32	b	629	LMT	C3'-C4'-C5'	-2.88	104.32	110.93
25	J	102	BCR	C15-C14-C13	-2.88	123.20	127.31
22	C	510	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
32	B	624	LMT	C3'-C4'-C5'	-2.88	104.33	110.93
22	b	609	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	D	405	PL9	C7-C8-C9	-2.88	122.00	126.79
22	a	404	CLA	CMB-C2B-C3B	2.87	130.06	124.68
22	c	511	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	b	601	DGD	O5D-C1E-C2E	2.87	112.79	108.30
22	C	506	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	c	509	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	b	611	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	c	511	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	c	506	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
22	b	619	CLA	CMB-C2B-C3B	2.86	130.02	124.68
25	J	102	BCR	C27-C26-C25	2.86	126.88	122.73
34	f	101	HEM	C4B-CHC-C1C	2.86	126.33	122.56
26	c	516	DGD	CDB-CCB-CBB	-2.85	99.94	114.42
30	b	602	SQD	C3-C4-C5	2.85	115.32	110.24
22	B	607	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	C	508	CLA	CMB-C2B-C3B	2.85	130.00	124.68
23	d	402	PHO	O1D-CGD-CBD	2.84	129.48	124.74
25	b	624	BCR	C2-C1-C6	2.84	114.86	110.48
22	C	509	CLA	CMB-C2B-C3B	2.84	130.00	124.68
25	b	624	BCR	C3-C4-C5	-2.84	109.00	114.08
22	d	406	CLA	CMB-C2B-C3B	2.84	130.00	124.68
26	d	410	DGD	CDB-CCB-CBB	-2.84	100.02	114.42
25	B	619	BCR	C2-C1-C6	2.84	114.85	110.48
27	a	409	LHG	O8-C23-C24	2.84	120.81	111.91
25	F	102	BCR	C29-C30-C25	2.84	114.85	110.48
22	b	605	CLA	CMB-C2B-C3B	2.84	129.98	124.68
25	j	102	BCR	C27-C26-C25	2.83	126.85	122.73
30	B	627	SQD	C4-C3-C2	2.83	115.76	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	406	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	b	619	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
22	b	609	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	y	101	BCR	C38-C26-C25	-2.82	121.36	124.53
26	C	516	DGD	C1D-C2D-C3D	-2.82	104.12	110.00
25	B	619	BCR	C7-C8-C9	-2.82	121.97	126.23
23	d	401	PHO	CMB-C2B-C3B	2.82	129.96	124.68
25	b	623	BCR	C15-C16-C17	-2.82	117.70	123.47
26	D	407	DGD	CDB-CCB-CBB	-2.81	100.14	114.42
26	C	515	DGD	CDB-CCB-CBB	-2.81	100.14	114.42
34	F	101	HEM	C1B-NB-C4B	2.81	107.98	105.07
22	d	405	CLA	CMB-C2B-C3B	2.81	129.94	124.68
25	f	102	BCR	C29-C30-C25	2.81	114.81	110.48
25	B	618	BCR	C11-C10-C9	-2.81	123.30	127.31
26	c	517	DGD	C1D-O6D-C5D	-2.81	108.18	113.69
22	C	519	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	b	608	CLA	CMB-C2B-C3B	2.81	129.93	124.68
27	A	410	LHG	O8-C23-C24	2.80	120.71	111.91
22	A	404	CLA	CMB-C2B-C3B	2.80	129.91	124.68
32	B	628	LMT	C1'-O5'-C5'	-2.80	108.20	113.69
25	g	101	BCR	C27-C26-C25	2.80	126.79	122.73
22	C	511	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
22	b	617	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
31	i	102	LMG	O6-C1-O1	-2.79	103.36	109.97
22	b	613	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	B	614	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	b	621	BCR	C33-C5-C6	-2.79	121.40	124.53
34	f	101	HEM	C4C-CHD-C1D	2.79	126.24	122.56
22	c	520	CLA	CMB-C2B-C3B	2.79	129.89	124.68
22	b	611	CLA	CMB-C2B-C3B	2.78	129.89	124.68
25	B	617	BCR	C28-C27-C26	-2.78	109.11	114.08
23	D	401	PHO	O1D-CGD-CBD	2.78	129.37	124.74
23	D	401	PHO	O2D-CGD-O1D	-2.78	118.41	123.84
25	y	101	BCR	C27-C26-C25	2.78	126.76	122.73
25	g	101	BCR	C7-C8-C9	-2.77	122.05	126.23
22	b	608	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	K	101	BCR	C24-C23-C22	-2.77	122.05	126.23
25	B	619	BCR	C3-C4-C5	-2.77	109.14	114.08
22	B	612	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	C	512	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
22	b	610	CLA	CMB-C2B-C3B	2.77	129.85	124.68
30	A	413	SQD	C3-C4-C5	2.77	115.17	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	CHB-C4A-NA	2.76	128.34	124.51
25	j	102	BCR	C35-C13-C14	-2.76	119.05	122.92
23	d	401	PHO	O2D-CGD-O1D	-2.76	118.44	123.84
25	B	617	BCR	C15-C14-C13	-2.76	123.37	127.31
31	C	517	LMG	O6-C1-O1	-2.76	103.45	109.97
25	b	622	BCR	C28-C27-C26	-2.76	109.16	114.08
22	a	405	CLA	CMB-C2B-C3B	2.76	129.83	124.68
23	d	401	PHO	O1D-CGD-CBD	2.75	129.32	124.74
22	B	608	CLA	CMB-C2B-C3B	2.75	129.83	124.68
22	b	615	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
25	c	521	BCR	C2-C1-C6	2.75	114.72	110.48
25	B	616	BCR	C33-C5-C6	-2.75	121.44	124.53
22	a	404	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
34	F	101	HEM	C4C-CHD-C1D	2.75	126.18	122.56
22	B	614	CLA	CMB-C2B-C3B	2.75	129.81	124.68
22	c	501	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
31	c	518	LMG	O6-C1-O1	-2.74	103.49	109.97
22	H	101	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	B	604	CLA	CHB-C4A-NA	2.74	128.29	124.51
22	B	605	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	A	407	PL9	C22-C23-C24	-2.73	121.09	127.66
30	A	413	SQD	C44-O6-C1	2.73	119.07	113.74
25	c	514	BCR	C15-C16-C17	-2.73	117.89	123.47
32	b	628	LMT	C1'-O5'-C5'	-2.73	108.34	113.69
34	F	101	HEM	C4B-CHC-C1C	2.72	126.15	122.56
23	A	405	PHO	O2D-CGD-O1D	-2.72	118.52	123.84
23	A	405	PHO	CMB-C2B-C3B	2.72	129.76	124.68
24	D	405	PL9	C40-C39-C41	2.71	119.83	115.27
24	A	407	PL9	C41-C39-C40	2.71	120.58	114.60
22	B	603	CLA	CMB-C2B-C3B	2.71	129.74	124.68
22	A	403	CLA	CMB-C2B-C3B	2.71	129.74	124.68
22	D	404	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
22	A	403	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	a	407	PL9	C22-C23-C24	-2.70	121.17	127.66
23	A	405	PHO	O1D-CGD-CBD	2.69	129.22	124.74
25	J	102	BCR	C3-C4-C5	-2.69	109.27	114.08
22	c	509	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
25	y	101	BCR	C7-C8-C9	-2.69	122.17	126.23
31	I	101	LMG	O6-C1-O1	-2.69	103.61	109.97
22	H	101	CLA	CMB-C2B-C3B	2.69	129.71	124.68
22	C	501	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	c	508	CLA	CHB-C4A-NA	2.69	128.23	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	606	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
25	B	618	BCR	C15-C16-C17	-2.69	117.97	123.47
22	C	511	CLA	CHB-C4A-NA	2.69	128.22	124.51
25	b	623	BCR	C29-C30-C25	2.68	114.61	110.48
22	C	506	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	C	520	BCR	C2-C1-C6	2.68	114.61	110.48
25	c	514	BCR	C11-C10-C9	-2.68	123.49	127.31
25	C	520	BCR	C15-C16-C17	-2.68	117.99	123.47
22	B	603	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	b	610	CLA	CHB-C4A-NA	2.67	128.21	124.51
26	B	626	DGD	C3G-C2G-C1G	-2.67	105.47	111.79
26	b	601	DGD	C1D-C2D-C3D	-2.67	104.44	110.00
32	B	623	LMT	C1'-O5'-C5'	-2.67	108.45	113.69
25	b	623	BCR	C11-C10-C9	-2.67	123.50	127.31
26	b	601	DGD	C3G-C2G-C1G	-2.67	105.48	111.79
25	b	622	BCR	C15-C14-C13	-2.66	123.51	127.31
22	C	501	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
22	B	615	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	b	606	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	D	403	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
22	c	501	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	c	517	DGD	C1D-C2D-C3D	-2.65	104.48	110.00
22	c	506	CLA	CHB-C4A-NA	2.65	128.18	124.51
22	c	511	CLA	CHB-C4A-NA	2.65	128.17	124.51
22	B	613	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	d	410	DGD	CFB-CEB-CDB	-2.63	101.08	114.42
34	F	101	HEM	C3B-C2B-C1B	2.63	108.44	106.49
25	J	102	BCR	C15-C16-C17	-2.63	118.09	123.47
22	b	620	CLA	CMB-C2B-C3B	2.62	129.59	124.68
32	d	411	LMT	C3'-C4'-C5'	-2.62	104.92	110.93
26	D	407	DGD	CFB-CEB-CDB	-2.62	101.13	114.42
22	b	619	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	B	618	BCR	C15-C14-C13	-2.62	123.57	127.31
22	B	612	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	A	402	CLA	CMB-C2B-C3B	2.61	129.57	124.68
22	a	406	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	c	512	CLA	CHB-C4A-NA	2.61	128.12	124.51
34	v	201	HEM	C1B-NB-C4B	2.61	107.77	105.07
22	b	608	CLA	C1-C2-C3	-2.61	121.53	126.04
31	D	409	LMG	C38-C37-C36	-2.61	101.18	114.42
22	C	504	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	b	606	CLA	CHB-C4A-NA	2.61	128.12	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	409	DGD	CBB-CAB-C9B	-2.61	101.20	114.42
22	a	406	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
32	D	408	LMT	C3'-C4'-C5'	-2.60	104.95	110.93
22	c	504	CLA	CMB-C2B-C3B	2.60	129.54	124.68
22	C	503	CLA	CHB-C4A-NA	2.60	128.10	124.51
25	C	513	BCR	C29-C30-C25	2.60	114.48	110.48
27	c	519	LHG	O8-C23-C24	2.59	120.05	111.91
22	C	519	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	c	514	BCR	C28-C27-C26	-2.59	109.45	114.08
25	J	102	BCR	C38-C26-C25	-2.59	121.62	124.53
22	d	406	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	c	505	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	c	521	BCR	C15-C14-C13	-2.58	123.62	127.31
22	A	406	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
22	a	403	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	B	606	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
24	d	407	PL9	C22-C23-C24	-2.58	121.45	127.66
22	B	608	CLA	CHB-C4A-NA	2.58	128.07	124.51
25	j	102	BCR	C38-C26-C25	-2.57	121.64	124.53
22	A	404	CLA	CHB-C4A-NA	2.57	128.07	124.51
26	C	516	DGD	C1D-O6D-C5D	-2.57	108.64	113.69
27	C	518	LHG	O8-C23-C24	2.57	119.97	111.91
24	D	405	PL9	C22-C23-C24	-2.57	121.47	127.66
24	a	407	PL9	C41-C39-C40	2.57	120.28	114.60
25	C	513	BCR	C28-C27-C26	-2.57	109.49	114.08
22	C	504	CLA	CMB-C2B-C3B	2.57	129.48	124.68
22	a	404	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	d	402	PHO	O2D-CGD-O1D	-2.57	118.82	123.84
25	b	622	BCR	C35-C13-C14	-2.56	119.33	122.92
31	d	412	LMG	C38-C37-C36	-2.56	101.42	114.42
26	B	626	DGD	C1D-C2D-C3D	-2.56	104.66	110.00
25	c	513	BCR	C24-C23-C22	-2.56	122.37	126.23
22	c	507	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	c	520	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	B	616	BCR	C11-C10-C9	-2.55	123.66	127.31
25	C	520	BCR	C27-C26-C25	2.55	126.43	122.73
26	b	625	DGD	CBB-CAB-C9B	-2.55	101.49	114.42
22	C	508	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	c	514	BCR	C15-C14-C13	-2.55	123.68	127.31
22	d	405	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
31	d	408	LMG	C38-C37-C36	-2.54	101.52	114.42
26	C	516	DGD	CFB-CEB-CDB	-2.54	101.53	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	615	CLA	C1-C2-C3	-2.54	121.65	126.04
24	J	101	PL9	C22-C23-C24	-2.54	121.55	127.66
22	B	609	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	c	513	BCR	C7-C8-C9	-2.54	122.40	126.23
25	c	514	BCR	C29-C30-C25	2.53	114.38	110.48
22	C	512	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	c	503	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	D	404	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	j	101	PL9	C22-C23-C24	-2.53	121.57	127.66
25	j	102	BCR	C3-C4-C5	-2.53	109.56	114.08
22	B	607	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	a	408	DGD	CBB-CAB-C9B	-2.53	101.60	114.42
25	B	618	BCR	C29-C30-C25	2.53	114.37	110.48
22	C	509	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
25	c	514	BCR	C33-C5-C6	-2.52	121.70	124.53
31	d	409	LMG	C38-C37-C36	-2.52	101.62	114.42
22	c	509	CLA	CHB-C4A-NA	2.52	128.00	124.51
25	B	616	BCR	C7-C8-C9	-2.52	122.43	126.23
22	b	620	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
26	C	515	DGD	O6E-C1E-O5D	-2.52	104.02	109.97
22	c	508	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
26	c	516	DGD	C3G-C2G-C1G	-2.51	105.84	111.79
22	B	611	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	C	507	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	b	616	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	b	618	CLA	CHB-C4A-NA	2.51	127.98	124.51
24	D	405	PL9	C20-C19-C21	2.51	119.49	115.27
22	B	603	CLA	C1-C2-C3	-2.50	121.72	126.04
22	c	502	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	C	518	LHG	C11-C10-C9	-2.50	101.73	114.42
25	K	101	BCR	C11-C10-C9	-2.50	123.74	127.31
25	C	513	BCR	C15-C14-C13	-2.50	123.74	127.31
30	a	412	SQD	O48-C23-C24	2.50	119.74	111.91
26	c	517	DGD	CFB-CEB-CDB	-2.50	101.76	114.42
25	C	513	BCR	C33-C5-C6	-2.50	121.73	124.53
25	i	101	BCR	C15-C16-C17	-2.50	118.36	123.47
22	b	613	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
31	b	627	LMG	O6-C1-O1	-2.49	104.07	109.97
31	B	625	LMG	C38-C37-C36	-2.49	101.77	114.42
31	a	402	LMG	O6-C1-O1	-2.49	104.07	109.97
22	C	504	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
22	c	505	CLA	C1B-CHB-C4A	-2.49	125.19	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	E	101	LMG	C1-C2-C3	-2.49	104.81	110.00
24	a	407	PL9	C7-C8-C9	-2.49	122.65	126.79
22	b	613	CLA	CHB-C4A-NA	2.49	127.95	124.51
32	M	103	LMT	C1'-O5'-C5'	-2.49	108.81	113.69
22	a	403	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	d	407	PL9	C37-C38-C39	-2.49	121.67	127.66
22	b	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	505	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	606	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	614	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	a	404	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
31	L	101	LMG	C40-C39-C38	-2.48	101.83	114.42
22	H	101	CLA	CHB-C4A-NA	2.48	127.94	124.51
32	b	603	LMT	C1'-O5'-C5'	-2.48	108.82	113.69
24	A	407	PL9	C7-C8-C9	-2.48	122.67	126.79
25	c	513	BCR	C15-C16-C17	-2.48	118.40	123.47
22	B	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
32	i	103	LMT	C1'-O5'-C5'	-2.48	108.83	113.69
31	D	406	LMG	C38-C37-C36	-2.47	101.88	114.42
26	C	515	DGD	C3G-C2G-C1G	-2.47	105.95	111.79
26	c	516	DGD	O6E-C1E-O5D	-2.47	104.13	109.97
22	B	610	CLA	C1-C2-C3	-2.46	121.78	126.04
25	c	521	BCR	C27-C26-C25	2.46	126.31	122.73
22	B	612	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
26	B	620	DGD	CBB-CAB-C9B	-2.46	101.94	114.42
30	a	412	SQD	C44-O6-C1	2.46	118.54	113.74
25	b	623	BCR	C15-C14-C13	-2.46	123.81	127.31
22	B	607	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	b	624	BCR	C11-C10-C9	-2.45	123.81	127.31
22	B	613	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
31	c	522	LMG	C40-C39-C38	-2.45	101.98	114.42
22	B	615	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	C	505	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
25	C	513	BCR	C11-C10-C9	-2.45	123.82	127.31
22	C	511	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
25	K	101	BCR	C15-C16-C17	-2.44	118.47	123.47
22	c	506	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	C	508	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	B	602	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
32	b	629	LMT	C1'-O5'-C5'	-2.44	108.90	113.69
31	b	626	LMG	C40-C39-C38	-2.44	102.05	114.42
25	B	619	BCR	C27-C26-C25	2.44	126.27	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	621	BCR	C15-C14-C13	-2.44	123.83	127.31
25	j	102	BCR	C15-C16-C17	-2.44	118.48	123.47
25	b	624	BCR	C27-C26-C25	2.43	126.26	122.73
22	b	611	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
22	c	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	b	609	CLA	CHD-C1D-ND	-2.43	122.22	124.45
22	b	610	CLA	CHD-C1D-ND	-2.43	122.22	124.45
30	a	401	SQD	C1-O5-C5	2.43	118.45	113.69
22	b	620	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	a	405	CLA	CHB-C4A-NA	2.42	127.86	124.51
30	d	403	SQD	O48-C23-C24	2.42	119.52	111.91
30	F	103	SQD	C1-O5-C5	2.42	118.45	113.69
25	i	101	BCR	C27-C26-C25	2.42	126.25	122.73
31	l	101	LMG	C40-C39-C38	-2.42	102.14	114.42
27	c	519	LHG	C11-C10-C9	-2.42	102.14	114.42
22	b	607	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
22	c	511	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
25	b	621	BCR	C2-C1-C6	2.41	114.20	110.48
22	A	404	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	b	611	CLA	CHB-C4A-NA	2.41	127.85	124.51
30	A	413	SQD	O48-C23-C24	2.41	119.47	111.91
25	A	408	BCR	C27-C26-C25	2.41	126.23	122.73
22	a	403	CLA	CHD-C1D-ND	-2.41	122.24	124.45
25	c	513	BCR	C11-C10-C9	-2.41	123.87	127.31
22	a	405	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	D	404	CLA	C1-C2-C3	-2.40	121.89	126.04
25	B	617	BCR	C29-C30-C25	2.40	114.18	110.48
26	c	515	DGD	C3G-C2G-C1G	-2.40	106.11	111.79
22	a	406	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	A	402	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	C	519	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	b	617	CLA	CHB-C4A-NA	2.40	127.83	124.51
31	C	521	LMG	C40-C39-C38	-2.40	102.26	114.42
25	K	101	BCR	C7-C8-C9	-2.39	122.62	126.23
22	b	612	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
30	B	627	SQD	O48-C23-C24	2.39	119.42	111.91
25	B	616	BCR	C2-C1-C6	2.39	114.16	110.48
25	B	617	BCR	C35-C13-C14	-2.39	119.58	122.92
25	A	408	BCR	C15-C14-C13	-2.39	123.90	127.31
24	d	407	PL9	C20-C19-C21	2.39	119.29	115.27
25	i	101	BCR	C33-C5-C6	-2.39	121.84	124.53
22	A	406	CLA	CHB-C4A-NA	2.39	127.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	504	CLA	CHB-C4A-NA	2.39	127.81	124.51
26	d	410	DGD	C3G-C2G-C1G	-2.39	106.14	111.79
24	D	405	PL9	C37-C38-C39	-2.38	121.92	127.66
26	B	620	DGD	C4E-C3E-C2E	-2.38	106.66	110.82
22	B	603	CLA	O1D-CGD-CBD	2.38	129.36	124.48
22	D	403	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	B	604	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
25	A	408	BCR	C33-C5-C6	-2.38	121.86	124.53
22	C	509	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	y	101	BCR	C1-C6-C5	-2.38	119.26	122.61
26	c	516	DGD	CFB-CEB-CDB	-2.38	102.36	114.42
22	B	605	CLA	CHD-C1D-ND	-2.38	122.27	124.45
32	M	103	LMT	C3'-C4'-C5'	-2.38	105.48	110.93
31	L	101	LMG	C38-C37-C36	-2.37	102.38	114.42
22	C	507	CLA	CHD-C1D-ND	-2.37	122.27	124.45
22	B	615	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
22	b	616	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
25	j	102	BCR	C15-C14-C13	-2.37	123.93	127.31
25	B	618	BCR	C7-C8-C9	-2.37	122.66	126.23
22	A	403	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
31	C	517	LMG	C38-C37-C36	-2.37	102.40	114.42
22	b	607	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	B	601	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
25	F	102	BCR	C15-C16-C17	-2.37	118.63	123.47
22	B	608	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
22	C	506	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
22	c	503	CLA	O2D-CGD-CBD	2.36	115.47	111.27
22	c	508	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
26	B	620	DGD	C3G-C2G-C1G	-2.36	106.20	111.79
26	b	625	DGD	C3G-C2G-C1G	-2.36	106.20	111.79
31	B	625	LMG	O3-C3-C2	-2.36	104.89	110.35
22	C	502	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	d	407	PL9	C32-C33-C34	-2.36	121.98	127.66
25	b	622	BCR	C29-C30-C25	2.36	114.11	110.48
25	b	623	BCR	C7-C8-C9	-2.35	122.68	126.23
22	c	509	CLA	CHD-C1D-ND	-2.35	122.29	124.45
24	a	407	PL9	C27-C28-C29	-2.35	122.00	127.66
24	a	407	PL9	C20-C19-C21	2.35	119.22	115.27
25	b	624	BCR	C38-C26-C25	-2.35	121.89	124.53
22	H	101	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
31	b	626	LMG	O6-C1-O1	-2.34	104.42	109.97
31	L	101	LMG	C1-C2-C3	-2.34	105.12	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	614	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	B	611	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
31	B	621	LMG	C40-C39-C38	-2.34	102.56	114.42
31	d	412	LMG	O6-C1-O1	-2.34	104.44	109.97
22	B	610	CLA	C3C-C4C-NC	-2.34	107.95	110.57
24	D	405	PL9	C32-C33-C34	-2.34	122.04	127.66
30	B	622	SQD	C4-C3-C2	2.33	114.90	110.82
24	J	101	PL9	C20-C19-C21	2.33	119.20	115.27
22	A	406	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	c	501	CLA	CMB-C2B-C3B	2.33	129.04	124.68
25	C	520	BCR	C11-C10-C9	-2.33	123.98	127.31
32	I	102	LMT	C1'-O5'-C5'	-2.33	109.11	113.69
22	B	605	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	c	504	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
25	B	619	BCR	C38-C26-C25	-2.33	121.92	124.53
24	D	405	PL9	C27-C28-C29	-2.33	122.06	127.66
25	g	101	BCR	C15-C16-C17	-2.33	118.71	123.47
30	B	622	SQD	O48-C23-C24	2.32	119.20	111.91
31	l	101	LMG	C38-C37-C36	-2.32	102.64	114.42
22	B	604	CLA	CHD-C1D-ND	-2.32	122.32	124.45
31	D	409	LMG	C1-C2-C3	-2.32	105.16	110.00
25	g	101	BCR	C1-C6-C5	-2.32	119.35	122.61
26	C	515	DGD	CFB-CEB-CDB	-2.31	102.68	114.42
30	F	103	SQD	C3-C4-C5	2.31	114.37	110.24
31	c	522	LMG	C38-C37-C36	-2.31	102.69	114.42
22	b	611	CLA	CHD-C1D-ND	-2.31	122.33	124.45
31	c	518	LMG	C38-C37-C36	-2.31	102.69	114.42
31	e	101	LMG	O6-C1-O1	-2.31	104.50	109.97
26	b	601	DGD	O6D-C1D-O3G	-2.31	104.51	109.97
25	b	621	BCR	C15-C16-C17	-2.31	118.75	123.47
26	a	408	DGD	O5D-C6D-C5D	-2.31	104.78	109.05
31	b	626	LMG	C38-C37-C36	-2.31	102.72	114.42
25	c	513	BCR	C15-C14-C13	-2.31	124.02	127.31
22	B	609	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
31	D	406	LMG	O6-C1-C2	-2.30	105.47	110.35
22	b	618	CLA	O2D-CGD-CBD	2.30	115.36	111.27
24	A	407	PL9	C20-C19-C21	2.30	119.15	115.27
22	A	402	CLA	CHD-C1D-ND	-2.30	122.34	124.45
30	A	414	SQD	C1-O5-C5	2.30	118.21	113.69
22	c	507	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
31	D	409	LMG	O3-C3-C2	-2.30	105.03	110.35
26	a	408	DGD	C3G-C2G-C1G	-2.30	106.35	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	616	BCR	C27-C26-C25	2.30	126.07	122.73
22	b	620	CLA	CHD-C1D-ND	-2.30	122.34	124.45
30	A	414	SQD	O48-C23-C24	2.30	119.11	111.91
22	B	608	CLA	C1-C2-C3	-2.30	122.07	126.04
31	m	101	LMG	C1-O6-C5	-2.29	109.18	113.69
24	D	405	PL9	O1-C4-C3	-2.29	118.19	120.72
31	d	408	LMG	O2-C2-C1	-2.29	104.48	110.05
22	d	406	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
24	d	407	PL9	C27-C28-C29	-2.29	122.14	127.66
26	B	626	DGD	O6D-C1D-O3G	-2.29	104.55	109.97
22	D	404	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
31	B	621	LMG	C1-C2-C3	-2.29	105.23	110.00
22	d	406	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	b	621	BCR	C27-C26-C25	2.29	126.05	122.73
31	d	408	LMG	O3-C3-C2	-2.29	105.06	110.35
23	d	401	PHO	CMC-C2C-C3C	2.29	129.25	124.94
22	b	609	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
22	b	614	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
25	H	102	BCR	C16-C15-C14	-2.28	118.80	123.47
22	b	605	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
30	d	403	SQD	C4-C3-C2	2.28	114.81	110.82
31	M	101	LMG	C1-O6-C5	-2.28	109.21	113.69
30	f	103	SQD	C3-C4-C5	2.28	114.30	110.24
25	f	102	BCR	C15-C16-C17	-2.28	118.81	123.47
25	C	513	BCR	C38-C26-C25	-2.28	121.97	124.53
25	x	101	BCR	C29-C30-C25	2.28	113.99	110.48
30	a	401	SQD	O48-C23-C24	2.28	119.05	111.91
25	y	101	BCR	C33-C5-C6	-2.28	121.97	124.53
26	c	516	DGD	C3D-C4D-C5D	-2.27	106.19	110.24
31	d	412	LMG	O3-C3-C2	-2.27	105.10	110.35
22	D	403	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	b	608	CLA	O1D-CGD-CBD	2.27	129.13	124.48
22	B	615	CLA	CHD-C1D-ND	-2.27	122.37	124.45
31	d	409	LMG	O6-C1-C2	-2.27	105.54	110.35
25	c	514	BCR	C38-C26-C25	-2.27	121.98	124.53
31	b	626	LMG	C1-C2-C3	-2.27	105.27	110.00
22	C	501	CLA	CMB-C2B-C3B	2.27	128.92	124.68
32	D	408	LMT	C1'-O5'-C5'	-2.27	109.24	113.69
31	L	101	LMG	O3-C3-C2	-2.27	105.11	110.35
22	B	603	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
31	C	521	LMG	C38-C37-C36	-2.26	102.94	114.42
25	C	520	BCR	C24-C23-C22	-2.26	122.82	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	503	CLA	O2D-CGD-CBD	2.26	115.29	111.27
25	C	513	BCR	C24-C23-C22	-2.26	122.82	126.23
31	B	625	LMG	O2-C2-C1	-2.26	104.56	110.05
22	B	605	CLA	O1D-CGD-CBD	2.26	129.10	124.48
31	l	101	LMG	O3-C3-C2	-2.26	105.13	110.35
22	c	509	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
22	B	606	CLA	C1-C2-C3	-2.26	122.14	126.04
22	C	502	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
30	f	103	SQD	C1-O5-C5	2.25	118.11	113.69
25	b	624	BCR	C24-C23-C22	-2.25	122.83	126.23
31	B	621	LMG	C38-C37-C36	-2.25	103.00	114.42
22	c	509	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
22	b	617	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
31	B	621	LMG	O6-C1-O1	-2.25	104.65	109.97
22	c	507	CLA	CHD-C1D-ND	-2.25	122.39	124.45
25	F	102	BCR	C11-C10-C9	-2.24	124.11	127.31
26	b	601	DGD	CBB-CAB-C9B	-2.24	103.04	114.42
25	c	521	BCR	C33-C5-C6	-2.24	122.01	124.53
22	B	611	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
22	B	601	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	B	614	CLA	CHD-C1D-ND	-2.24	122.40	124.45
31	E	101	LMG	O6-C1-O1	-2.24	104.67	109.97
25	C	520	BCR	C33-C5-C6	-2.24	122.02	124.53
22	c	512	CLA	CHD-C1D-ND	-2.24	122.40	124.45
25	A	408	BCR	C38-C26-C25	-2.24	122.02	124.53
31	l	101	LMG	C1-C2-C3	-2.24	105.34	110.00
22	C	508	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	A	402	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	C	511	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	b	608	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
31	D	406	LMG	O6-C1-O1	-2.23	104.69	109.97
31	m	101	LMG	C1-C2-C3	-2.23	105.35	110.00
26	b	601	DGD	CAB-C9B-C8B	-2.23	103.10	114.42
25	b	624	BCR	C15-C16-C17	-2.23	118.91	123.47
31	C	521	LMG	O6-C1-O1	-2.23	104.69	109.97
34	V	201	HEM	C1B-NB-C4B	2.23	107.37	105.07
26	a	408	DGD	CAB-C9B-C8B	-2.23	103.12	114.42
22	b	619	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
22	B	611	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
31	m	101	LMG	O2-C2-C1	-2.23	104.64	110.05
31	c	522	LMG	O6-C1-O1	-2.22	104.70	109.97
22	c	504	CLA	O1D-CGD-CBD	2.22	129.04	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	624	LMT	C1'-O5'-C5'	-2.22	109.32	113.69
22	a	403	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
22	C	509	CLA	CHD-C1D-ND	-2.22	122.41	124.45
31	b	626	LMG	O2-C2-C1	-2.22	104.65	110.05
26	A	409	DGD	C3G-C2G-C1G	-2.22	106.54	111.79
22	C	509	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	b	610	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
25	x	101	BCR	C15-C16-C17	-2.22	118.94	123.47
31	c	518	LMG	O1-C7-C8	-2.21	105.56	110.90
22	c	501	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	A	408	BCR	C15-C16-C17	-2.21	118.94	123.47
25	c	521	BCR	C24-C23-C22	-2.21	122.89	126.23
22	b	616	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	C	512	CLA	CHD-C1D-ND	-2.21	122.42	124.45
25	J	102	BCR	C20-C21-C22	-2.21	124.15	127.31
22	B	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
26	c	516	DGD	O3D-C3D-C4D	-2.21	105.24	110.35
22	C	510	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
26	c	516	DGD	CBB-CAB-C9B	-2.21	103.22	114.42
25	g	101	BCR	C3-C2-C1	-2.21	106.71	114.60
24	j	101	PL9	C20-C19-C21	2.21	118.98	115.27
31	e	101	LMG	O3-C3-C2	-2.21	105.25	110.35
31	L	101	LMG	O7-C10-O9	-2.21	118.37	123.70
25	i	101	BCR	C38-C26-C25	-2.20	122.05	124.53
25	H	102	BCR	C29-C30-C25	2.20	113.87	110.48
26	A	409	DGD	CAB-C9B-C8B	-2.20	103.25	114.42
31	B	621	LMG	O3-C3-C2	-2.20	105.26	110.35
31	e	101	LMG	C1-C2-C3	-2.20	105.42	110.00
22	C	504	CLA	O1D-CGD-CBD	2.20	128.98	124.48
22	c	502	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
22	b	605	CLA	CHB-C4A-NA	2.19	127.55	124.51
22	c	512	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
25	c	513	BCR	C27-C26-C25	2.19	125.91	122.73
25	g	101	BCR	C33-C5-C6	-2.19	122.07	124.53
22	c	520	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
31	C	521	LMG	O3-C3-C2	-2.19	105.29	110.35
22	d	405	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
22	b	618	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
31	I	101	LMG	O7-C10-O9	-2.19	118.42	123.70
22	b	619	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
25	F	102	BCR	C7-C8-C9	-2.19	122.93	126.23
31	d	409	LMG	O6-C1-O1	-2.19	104.80	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	f	102	BCR	C11-C10-C9	-2.18	124.19	127.31
31	C	517	LMG	O7-C10-O9	-2.18	118.43	123.70
22	C	512	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
25	C	520	BCR	C7-C8-C9	-2.18	122.94	126.23
26	B	626	DGD	CAB-C9B-C8B	-2.18	103.35	114.42
22	c	507	CLA	O2D-CGD-CBD	2.18	115.14	111.27
26	C	515	DGD	CBB-CAB-C9B	-2.18	103.35	114.42
31	a	402	LMG	O3-C3-C2	-2.18	105.31	110.35
31	C	521	LMG	O2-C2-C1	-2.18	104.75	110.05
22	C	508	CLA	CHD-C1D-ND	-2.18	122.45	124.45
22	b	620	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
24	j	101	PL9	O2-C1-C6	2.18	124.36	120.59
31	c	518	LMG	O2-C2-C1	-2.17	104.76	110.05
31	i	102	LMG	O3-C3-C2	-2.17	105.32	110.35
31	I	101	LMG	O2-C2-C1	-2.17	104.77	110.05
22	C	501	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	C	516	DGD	CBB-CAB-C9B	-2.17	103.40	114.42
30	b	602	SQD	O48-C23-C24	2.17	118.72	111.91
22	C	510	CLA	CHD-C1D-ND	-2.17	122.46	124.45
31	M	101	LMG	C1-C2-C3	-2.17	105.48	110.00
25	B	619	BCR	C24-C23-C22	-2.17	122.96	126.23
22	A	403	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	c	520	CLA	CHD-C1D-ND	-2.17	122.46	124.45
22	b	613	CLA	C1-C2-C3	-2.17	122.30	126.04
33	D	402	BCT	O3-C-O1	-2.17	113.93	119.55
24	a	407	PL9	O2-C1-C6	2.17	124.34	120.59
25	K	101	BCR	C15-C14-C13	-2.17	124.22	127.31
22	b	610	CLA	O1D-CGD-CBD	2.16	128.91	124.48
22	B	609	CLA	CHD-C1D-ND	-2.16	122.47	124.45
25	b	623	BCR	C33-C5-C6	-2.16	122.10	124.53
31	b	626	LMG	O3-C3-C2	-2.16	105.36	110.35
31	a	402	LMG	O1-C7-C8	-2.16	105.69	110.90
31	c	522	LMG	O2-C2-C1	-2.16	104.80	110.05
25	b	623	BCR	C27-C26-C25	2.16	125.86	122.73
32	d	411	LMT	C1'-O5'-C5'	-2.16	109.45	113.69
25	B	616	BCR	C38-C26-C25	-2.16	122.11	124.53
27	a	409	LHG	C27-C26-C25	-2.16	103.48	114.42
27	A	410	LHG	C27-C26-C25	-2.16	103.48	114.42
22	d	405	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
32	M	102	LMT	C3'-C4'-C5'	-2.15	105.99	110.93
25	B	617	BCR	C24-C23-C22	-2.15	122.98	126.23
24	A	407	PL9	C27-C28-C29	-2.15	122.48	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	616	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
22	c	511	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
31	D	409	LMG	O7-C10-O9	-2.15	118.51	123.70
31	c	518	LMG	O7-C10-O9	-2.15	118.51	123.70
24	j	101	PL9	O2-C1-C2	-2.15	116.86	121.78
25	i	101	BCR	C15-C14-C13	-2.15	124.25	127.31
25	K	101	BCR	C27-C26-C25	2.15	125.85	122.73
23	D	401	PHO	CMC-C2C-C3C	2.15	128.99	124.94
31	b	627	LMG	O1-C7-C8	-2.15	105.72	110.90
24	d	407	PL9	O1-C4-C3	-2.15	118.36	120.72
31	C	517	LMG	O3-C3-C2	-2.15	105.39	110.35
31	c	518	LMG	O3-C3-C2	-2.14	105.39	110.35
33	d	404	BCT	O3-C-O1	-2.14	113.99	119.55
26	C	516	DGD	C3G-O3G-C1D	2.14	117.92	113.74
25	F	102	BCR	C27-C26-C25	2.14	125.84	122.73
24	d	407	PL9	O2-C1-C2	-2.14	116.88	121.78
22	B	602	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
26	d	410	DGD	CAB-C9B-C8B	-2.14	103.57	114.42
31	c	522	LMG	O3-C3-C2	-2.14	105.41	110.35
22	a	404	CLA	CHD-C1D-ND	-2.14	122.49	124.45
31	I	101	LMG	O3-C3-C2	-2.14	105.41	110.35
31	l	101	LMG	O7-C10-O9	-2.14	118.54	123.70
22	D	403	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
22	b	615	CLA	C3C-C4C-NC	-2.14	108.18	110.57
26	B	626	DGD	CBB-CAB-C9B	-2.14	103.58	114.42
26	C	514	DGD	C5B-C4B-C3B	-2.13	103.59	114.42
25	y	101	BCR	C15-C16-C17	-2.13	119.10	123.47
22	d	405	CLA	CHB-C4A-NA	2.13	127.46	124.51
31	b	627	LMG	O7-C10-O9	-2.13	118.55	123.70
31	M	101	LMG	O2-C2-C1	-2.13	104.86	110.05
22	b	607	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
26	c	515	DGD	C1D-C2D-C3D	-2.13	105.55	110.00
31	C	517	LMG	O1-C7-C8	-2.13	105.76	110.90
23	A	405	PHO	CMC-C2C-C3C	2.13	128.96	124.94
22	c	508	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	D	405	PL9	O2-C1-C2	-2.13	116.90	121.78
26	c	516	DGD	CAB-C9B-C8B	-2.13	103.62	114.42
25	c	513	BCR	C8-C7-C6	-2.13	121.23	127.20
31	i	102	LMG	O2-C2-C1	-2.13	104.88	110.05
25	J	102	BCR	C33-C5-C6	-2.13	122.14	124.53
26	b	625	DGD	CAB-C9B-C8B	-2.13	103.63	114.42
26	b	625	DGD	C1D-C2D-C3D	-2.12	105.58	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	507	CLA	C1-C2-C3	-2.12	122.38	126.04
31	B	621	LMG	O2-C2-C1	-2.12	104.90	110.05
25	B	619	BCR	C11-C10-C9	-2.12	124.29	127.31
31	d	412	LMG	C1-C2-C3	-2.12	105.59	110.00
31	B	621	LMG	O7-C10-O9	-2.12	118.59	123.70
25	b	622	BCR	C24-C23-C22	-2.12	123.04	126.23
24	j	101	PL9	O1-C4-C3	-2.11	118.39	120.72
24	a	407	PL9	O2-C1-C2	-2.11	116.94	121.78
22	b	617	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
25	C	520	BCR	C38-C26-C25	-2.11	122.16	124.53
31	E	101	LMG	O3-C3-C2	-2.11	105.47	110.35
25	H	102	BCR	C15-C16-C17	-2.11	119.15	123.47
22	c	504	CLA	CBA-CAA-C2A	2.11	120.10	113.86
22	c	510	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
31	C	517	LMG	O2-C2-C1	-2.11	104.92	110.05
25	g	101	BCR	C24-C23-C22	-2.11	123.04	126.23
26	c	515	DGD	C5B-C4B-C3B	-2.11	103.71	114.42
26	D	407	DGD	C3D-C4D-C5D	-2.11	106.47	110.24
22	C	507	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
25	K	101	BCR	C3-C4-C5	-2.11	110.31	114.08
25	B	619	BCR	C33-C5-C6	-2.11	122.16	124.53
24	J	101	PL9	O2-C1-C2	-2.11	116.95	121.78
22	B	613	CLA	O2D-CGD-CBD	2.11	115.01	111.27
26	C	515	DGD	CAB-C9B-C8B	-2.11	103.74	114.42
22	C	501	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
25	j	102	BCR	C20-C21-C22	-2.10	124.31	127.31
34	f	101	HEM	CMC-C2C-C3C	2.10	128.62	124.68
26	c	517	DGD	CBB-CAB-C9B	-2.10	103.74	114.42
22	B	603	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
30	a	412	SQD	C4-C3-C2	2.10	114.50	110.82
31	b	627	LMG	O3-C3-C2	-2.10	105.49	110.35
22	C	519	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
26	C	515	DGD	O3D-C3D-C4D	-2.10	105.50	110.35
22	C	512	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	C	501	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
24	A	407	PL9	O2-C1-C2	-2.10	116.97	121.78
23	d	402	PHO	CMC-C2C-C3C	2.10	128.90	124.94
22	C	508	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	B	614	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	b	623	BCR	C20-C21-C22	-2.10	124.32	127.31
22	B	610	CLA	CHB-C4A-NA	2.10	127.41	124.51
22	C	503	CLA	C1B-CHB-C4A	-2.10	125.97	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	BCR	C24-C23-C22	-2.09	123.07	126.23
25	B	616	BCR	C15-C16-C17	-2.09	119.19	123.47
26	C	514	DGD	C3G-C2G-C1G	-2.09	106.84	111.79
26	D	407	DGD	CAB-C9B-C8B	-2.09	103.81	114.42
34	V	201	HEM	C4B-CHC-C1C	2.09	125.31	122.56
22	C	504	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	f	103	SQD	O48-C23-C24	2.09	118.46	111.91
22	c	506	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
30	F	103	SQD	O48-C23-C24	2.09	118.46	111.91
31	d	408	LMG	O1-C1-C2	-2.09	105.05	108.30
24	A	407	PL9	O2-C1-C6	2.09	124.20	120.59
22	B	601	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
25	K	101	BCR	C8-C7-C6	-2.08	121.35	127.20
24	J	101	PL9	O2-C1-C6	2.08	124.20	120.59
22	B	606	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	d	407	PL9	O2-C1-C6	2.08	124.19	120.59
25	y	101	BCR	C3-C2-C1	-2.08	107.16	114.60
26	C	515	DGD	C5B-C4B-C3B	-2.08	103.86	114.42
25	C	520	BCR	C15-C14-C13	-2.08	124.34	127.31
22	C	506	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
22	a	404	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
22	b	615	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
25	b	621	BCR	C11-C10-C9	-2.08	124.34	127.31
25	j	102	BCR	C29-C30-C25	2.08	113.68	110.48
27	c	519	LHG	C27-C26-C25	-2.08	103.89	114.42
25	H	102	BCR	C27-C26-C25	2.08	125.74	122.73
25	J	102	BCR	C29-C30-C25	2.07	113.67	110.48
25	b	624	BCR	C33-C5-C6	-2.07	122.20	124.53
26	C	516	DGD	CAB-C9B-C8B	-2.07	103.90	114.42
24	d	407	PL9	C36-C34-C33	-2.07	116.92	121.12
25	B	616	BCR	C15-C14-C13	-2.07	124.35	127.31
25	f	102	BCR	C27-C26-C25	2.07	125.74	122.73
22	b	605	CLA	C1-C2-C3	-2.07	122.46	126.04
31	M	101	LMG	O3-C3-C2	-2.07	105.57	110.35
25	c	521	BCR	C11-C10-C9	-2.07	124.36	127.31
25	B	618	BCR	C33-C5-C6	-2.07	122.21	124.53
31	d	412	LMG	O7-C10-O9	-2.07	118.71	123.70
34	F	101	HEM	CMC-C2C-C3C	2.07	128.54	124.68
26	d	410	DGD	C5B-C4B-C3B	-2.07	103.93	114.42
22	C	507	CLA	C1-C2-C3	-2.06	122.47	126.04
25	B	617	BCR	C8-C7-C6	-2.06	121.40	127.20
27	C	518	LHG	C27-C26-C25	-2.06	103.94	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	520	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
34	F	101	HEM	CHB-C1B-NB	2.06	126.93	124.38
34	f	101	HEM	CHB-C1B-NB	2.06	126.93	124.38
22	A	402	CLA	O1D-CGD-CBD	2.06	128.71	124.48
26	D	407	DGD	C5B-C4B-C3B	-2.06	103.95	114.42
26	C	514	DGD	O5D-C6D-C5D	-2.06	105.23	109.05
22	B	612	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	c	501	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
22	B	610	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	C	507	CLA	O2D-CGD-CBD	2.06	114.92	111.27
22	b	615	CLA	CHB-C4A-NA	2.06	127.36	124.51
26	D	407	DGD	CBB-CAB-C9B	-2.06	103.99	114.42
22	D	404	CLA	CHD-C1D-ND	-2.06	122.56	124.45
22	B	614	CLA	C1B-CHB-C4A	-2.06	126.05	130.12
25	c	513	BCR	C3-C4-C5	-2.05	110.42	114.08
26	d	410	DGD	CBB-CAB-C9B	-2.05	104.03	114.42
25	B	618	BCR	C27-C26-C25	2.05	125.70	122.73
31	d	412	LMG	C6-C5-C4	-2.04	108.22	113.00
22	c	501	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
30	a	401	SQD	C4-C3-C2	2.04	114.39	110.82
22	C	512	CLA	O1D-CGD-CBD	2.04	128.66	124.48
22	A	403	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
31	d	408	LMG	O7-C10-O9	-2.04	118.77	123.70
22	C	506	CLA	CHD-C1D-ND	-2.04	122.58	124.45
22	b	617	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	d	409	LMG	C4-C3-C2	-2.04	107.27	110.82
22	C	502	CLA	O2D-CGD-CBD	2.04	114.89	111.27
22	C	505	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	b	626	LMG	O1-C7-C8	-2.04	105.98	110.90
26	C	515	DGD	C3D-C4D-C5D	-2.04	106.61	110.24
23	d	401	PHO	O2A-CGA-O1A	-2.04	118.46	123.59
22	b	620	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
31	m	101	LMG	O3-C3-C2	-2.03	105.65	110.35
31	d	408	LMG	C22-C21-C20	-2.03	104.11	114.42
25	f	102	BCR	C38-C26-C25	-2.03	122.25	124.53
26	a	408	DGD	C5B-C4B-C3B	-2.03	104.11	114.42
22	b	614	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	A	409	DGD	C5B-C4B-C3B	-2.03	104.11	114.42
25	b	622	BCR	C7-C8-C9	-2.03	123.17	126.23
26	c	517	DGD	CAB-C9B-C8B	-2.03	104.13	114.42
22	c	503	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
26	a	408	DGD	C1D-C2D-C3D	-2.03	105.77	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	508	CLA	CHD-C1D-ND	-2.03	122.59	124.45
25	c	521	BCR	C38-C26-C25	-2.03	122.25	124.53
22	b	619	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	C	516	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
25	f	102	BCR	C24-C23-C22	-2.02	123.18	126.23
22	C	504	CLA	C1-C2-C3	-2.02	122.55	126.04
31	B	625	LMG	O7-C10-O9	-2.02	118.82	123.70
22	a	403	CLA	O1D-CGD-CBD	2.02	128.62	124.48
23	A	405	PHO	O2A-CGA-O1A	-2.02	118.50	123.59
31	b	626	LMG	O7-C10-O9	-2.02	118.82	123.70
24	D	405	PL9	C36-C34-C33	-2.02	117.03	121.12
22	b	608	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	C	503	CLA	CHD-C1D-ND	-2.02	122.60	124.45
31	B	625	LMG	C22-C21-C20	-2.01	104.20	114.42
26	c	517	DGD	C3G-O3G-C1D	2.01	117.67	113.74
25	H	102	BCR	C38-C26-C25	-2.01	122.27	124.53
24	D	405	PL9	O2-C1-C6	2.01	124.08	120.59
25	b	622	BCR	C8-C7-C6	-2.01	121.55	127.20
25	F	102	BCR	C38-C26-C25	-2.01	122.27	124.53
25	b	622	BCR	C38-C26-C25	-2.01	122.27	124.53
25	j	102	BCR	C33-C5-C6	-2.01	122.27	124.53
25	b	621	BCR	C38-C26-C25	-2.01	122.27	124.53
26	B	620	DGD	CAB-C9B-C8B	-2.01	104.21	114.42
22	c	510	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	c	514	BCR	C24-C23-C22	-2.01	123.20	126.23
22	A	406	CLA	CHD-C1D-ND	-2.01	122.61	124.45
22	a	405	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
31	I	101	LMG	O1-C7-C8	-2.01	106.06	110.90
26	b	625	DGD	C5B-C4B-C3B	-2.01	104.24	114.42
34	f	101	HEM	CHC-C4B-C3B	2.00	127.64	124.57
26	B	620	DGD	C5B-C4B-C3B	-2.00	104.26	114.42
31	l	101	LMG	O6-C1-O1	-2.00	105.23	109.97

All (68) 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	406	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND

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Mol	Chain	Res	Type	Atom
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
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	519	CLA	ND
22	D	403	CLA	ND
22	H	101	CLA	ND
22	a	403	CLA	ND
22	a	404	CLA	ND
22	a	405	CLA	ND
22	a	406	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

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Mol	Chain	Res	Type	Atom
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	b	620	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

All (2161) 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	B	601	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	604	CLA	C4-C3-C5-C6
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	C3A-C2A-CAA-CBA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	609	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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
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	CBD-CGD-O2D-CED
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	511	CLA	C1A-C2A-CAA-CBA
22	D	403	CLA	C2-C3-C5-C6
22	D	403	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
22	a	403	CLA	CBD-CGD-O2D-CED
22	a	404	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C3A-C2A-CAA-CBA
22	a	404	CLA	CHA-CBD-CGD-O1D
22	a	404	CLA	CHA-CBD-CGD-O2D
22	b	605	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	C1A-C2A-CAA-CBA
22	b	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
22	b	606	CLA	C6-C7-C8-C9
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	C2-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C1A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C2A-CAA-CBA-CGA
22	b	612	CLA	C1A-C2A-CAA-CBA
22	b	614	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	b	618	CLA	CHA-CBD-CGD-O1D
22	b	618	CLA	CAD-CBD-CGD-O1D
22	b	618	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	b	620	CLA	C1A-C2A-CAA-CBA
22	b	620	CLA	C3A-C2A-CAA-CBA
22	b	620	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	507	CLA	C2A-CAA-CBA-CGA
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	d	405	CLA	C2-C3-C5-C6
22	d	405	CLA	C4-C3-C5-C6
24	A	407	PL9	C7-C8-C9-C10
24	A	407	PL9	C7-C8-C9-C11
24	A	407	PL9	C12-C13-C14-C15
24	A	407	PL9	C12-C13-C14-C16
24	A	407	PL9	C17-C18-C19-C21
24	A	407	PL9	C22-C23-C24-C25
24	A	407	PL9	C24-C26-C27-C28
24	A	407	PL9	C27-C28-C29-C30
24	A	407	PL9	C27-C28-C29-C31
24	A	407	PL9	C30-C29-C31-C32
24	A	407	PL9	C37-C38-C39-C41
24	D	405	PL9	C27-C28-C29-C31
24	D	405	PL9	C34-C36-C37-C38
24	J	101	PL9	C7-C8-C9-C10
24	J	101	PL9	C12-C13-C14-C16
24	J	101	PL9	C22-C23-C24-C25
24	J	101	PL9	C22-C23-C24-C26
24	a	407	PL9	C7-C8-C9-C11
24	a	407	PL9	C12-C13-C14-C15
24	a	407	PL9	C12-C13-C14-C16
24	a	407	PL9	C22-C23-C24-C25
24	a	407	PL9	C24-C26-C27-C28
24	a	407	PL9	C27-C28-C29-C30
24	a	407	PL9	C27-C28-C29-C31
24	a	407	PL9	C30-C29-C31-C32
24	a	407	PL9	C37-C38-C39-C40
24	a	407	PL9	C37-C38-C39-C41
24	d	407	PL9	C27-C28-C29-C31
24	d	407	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
24	j	101	PL9	C7-C8-C9-C11
24	j	101	PL9	C12-C13-C14-C16
24	j	101	PL9	C22-C23-C24-C25
24	j	101	PL9	C22-C23-C24-C26
25	B	616	BCR	C1-C6-C7-C8
25	B	617	BCR	C7-C8-C9-C10
25	B	617	BCR	C21-C22-C23-C24
25	B	617	BCR	C23-C24-C25-C26
25	B	617	BCR	C23-C24-C25-C30
25	C	520	BCR	C7-C8-C9-C10
25	C	520	BCR	C7-C8-C9-C34
25	F	102	BCR	C1-C6-C7-C8
25	F	102	BCR	C7-C8-C9-C10
25	H	102	BCR	C7-C8-C9-C34
25	H	102	BCR	C21-C22-C23-C24
25	H	102	BCR	C37-C22-C23-C24
25	J	102	BCR	C1-C6-C7-C8
25	J	102	BCR	C21-C22-C23-C24
25	J	102	BCR	C37-C22-C23-C24
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C6-C7-C8-C9
25	K	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C7-C8-C9-C10
25	b	621	BCR	C1-C6-C7-C8
25	b	622	BCR	C21-C22-C23-C24
25	b	622	BCR	C23-C24-C25-C26
25	b	624	BCR	C23-C24-C25-C30
25	c	513	BCR	C6-C7-C8-C9
25	c	521	BCR	C7-C8-C9-C10
25	c	521	BCR	C7-C8-C9-C34
25	f	102	BCR	C1-C6-C7-C8
25	f	102	BCR	C7-C8-C9-C10
25	j	102	BCR	C1-C6-C7-C8
25	j	102	BCR	C21-C22-C23-C24
25	j	102	BCR	C37-C22-C23-C24
25	g	101	BCR	C7-C8-C9-C10
25	x	101	BCR	C7-C8-C9-C34
25	x	101	BCR	C21-C22-C23-C24
25	x	101	BCR	C37-C22-C23-C24
26	A	409	DGD	C2D-C1D-O3G-C3G
26	B	620	DGD	C2E-C1E-O5D-C6D
26	B	626	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
26	B	626	DGD	O2G-C2G-C3G-O3G
26	B	626	DGD	C2E-C1E-O5D-C6D
26	B	626	DGD	O6E-C1E-O5D-C6D
26	C	514	DGD	C2B-C1B-O2G-C2G
26	C	514	DGD	O1B-C1B-O2G-C2G
26	C	514	DGD	C2E-C1E-O5D-C6D
26	C	515	DGD	C2B-C1B-O2G-C2G
26	C	515	DGD	O1B-C1B-O2G-C2G
26	C	515	DGD	C2D-C1D-O3G-C3G
26	C	515	DGD	O6D-C1D-O3G-C3G
26	C	516	DGD	C2D-C1D-O3G-C3G
26	C	516	DGD	O6D-C1D-O3G-C3G
26	D	407	DGD	O1B-C1B-O2G-C2G
26	D	407	DGD	O6D-C1D-O3G-C3G
26	a	408	DGD	C2D-C1D-O3G-C3G
26	b	601	DGD	O1B-C1B-O2G-C2G
26	b	601	DGD	O2G-C2G-C3G-O3G
26	b	601	DGD	C2E-C1E-O5D-C6D
26	b	601	DGD	O6E-C1E-O5D-C6D
26	b	625	DGD	C2E-C1E-O5D-C6D
26	b	625	DGD	O6E-C1E-O5D-C6D
26	c	515	DGD	C2B-C1B-O2G-C2G
26	c	515	DGD	O1B-C1B-O2G-C2G
26	c	515	DGD	C2E-C1E-O5D-C6D
26	c	516	DGD	O1B-C1B-O2G-C2G
26	c	516	DGD	C2D-C1D-O3G-C3G
26	c	516	DGD	O6D-C1D-O3G-C3G
26	c	517	DGD	C2D-C1D-O3G-C3G
26	c	517	DGD	O6D-C1D-O3G-C3G
26	d	410	DGD	O6D-C1D-O3G-C3G
27	A	410	LHG	C1-C2-C3-O3
27	C	518	LHG	C4-O6-P-O4
27	C	518	LHG	C4-O6-P-O5
27	a	409	LHG	C1-C2-C3-O3
27	c	519	LHG	C4-O6-P-O4
27	c	519	LHG	C4-O6-P-O5
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	O10-C23-O48-C46
30	A	414	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
30	B	622	SQD	C2-C1-O6-C44
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	C8-C7-O47-C45
30	B	627	SQD	O5-C5-C6-S
30	a	401	SQD	C24-C23-O48-C46
30	a	412	SQD	C2-C1-O6-C44
30	a	412	SQD	C5-C6-S-O7
30	a	412	SQD	C5-C6-S-O8
30	a	412	SQD	C5-C6-S-O9
30	b	602	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
31	B	621	LMG	C11-C10-O7-C8
31	B	625	LMG	O1-C7-C8-O7
31	B	625	LMG	C11-C10-O7-C8
31	C	517	LMG	C2-C1-O1-C7
31	C	517	LMG	O6-C1-O1-C7
31	C	517	LMG	C9-C8-O7-C10
31	C	517	LMG	O9-C10-O7-C8
31	C	517	LMG	C11-C10-O7-C8
31	C	521	LMG	C2-C1-O1-C7
31	C	521	LMG	O6-C1-O1-C7
31	D	406	LMG	C2-C1-O1-C7
31	D	406	LMG	O6-C1-O1-C7
31	D	409	LMG	O9-C10-O7-C8
31	D	409	LMG	C11-C10-O7-C8
31	E	101	LMG	C2-C1-O1-C7
31	E	101	LMG	O6-C1-O1-C7
31	M	101	LMG	O9-C10-O7-C8
31	b	626	LMG	C11-C10-O7-C8
31	c	518	LMG	C2-C1-O1-C7
31	c	518	LMG	O6-C1-O1-C7
31	c	518	LMG	C9-C8-O7-C10
31	c	518	LMG	O9-C10-O7-C8
31	c	518	LMG	C11-C10-O7-C8
31	c	518	LMG	O10-C28-O8-C9
31	c	522	LMG	C2-C1-O1-C7
31	c	522	LMG	O6-C1-O1-C7
31	d	408	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
31	d	408	LMG	C11-C10-O7-C8
31	d	409	LMG	C2-C1-O1-C7
31	d	409	LMG	O6-C1-O1-C7
31	d	412	LMG	O9-C10-O7-C8
31	d	412	LMG	C11-C10-O7-C8
31	e	101	LMG	C2-C1-O1-C7
31	e	101	LMG	O6-C1-O1-C7
31	e	101	LMG	C7-C8-O7-C10
31	m	101	LMG	O9-C10-O7-C8
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	b	620	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	603	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	a	403	CLA	O1D-CGD-O2D-CED
22	B	602	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	510	CLA	CBD-CGD-O2D-CED
22	C	519	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	b	611	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
30	a	401	SQD	O10-C23-O48-C46
31	d	408	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
32	B	629	LMT	C3'-C4'-O1B-C1B
32	b	604	LMT	C3'-C4'-O1B-C1B
22	B	601	CLA	O1D-CGD-O2D-CED
26	b	625	DGD	C4D-C5D-C6D-O5D
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
30	F	103	SQD	C24-C23-O48-C46
30	f	103	SQD	C24-C23-O48-C46
31	d	409	LMG	C29-C28-O8-C9
31	l	101	LMG	C29-C28-O8-C9
24	A	407	PL9	C37-C38-C39-C40
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
22	b	618	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
23	d	402	PHO	CBD-CGD-O2D-CED
30	F	103	SQD	O10-C23-O48-C46
30	f	103	SQD	O10-C23-O48-C46
31	B	625	LMG	O10-C28-O8-C9
31	C	517	LMG	O10-C28-O8-C9
31	D	406	LMG	O10-C28-O8-C9
31	E	101	LMG	O10-C28-O8-C9
31	L	101	LMG	O10-C28-O8-C9
31	d	409	LMG	O10-C28-O8-C9
31	e	101	LMG	O10-C28-O8-C9
31	l	101	LMG	O10-C28-O8-C9
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	614	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
32	b	603	LMT	C3'-C4'-O1B-C1B
23	D	401	PHO	CBD-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
22	C	519	CLA	O1D-CGD-O2D-CED
26	d	410	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
31	B	621	LMG	O9-C10-O7-C8
31	B	625	LMG	O9-C10-O7-C8
31	I	101	LMG	O9-C10-O7-C8
31	a	402	LMG	O9-C10-O7-C8
31	b	626	LMG	O9-C10-O7-C8
31	b	627	LMG	O9-C10-O7-C8
31	d	408	LMG	O9-C10-O7-C8
31	d	409	LMG	O9-C10-O7-C8
31	i	102	LMG	O9-C10-O7-C8
26	C	515	DGD	C4E-C5E-C6E-O5E
26	D	407	DGD	O1A-C1A-O1G-C1G
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	405	CLA	C3-C5-C6-C7
22	b	612	CLA	C3-C5-C6-C7
22	b	618	CLA	C3-C5-C6-C7
31	C	517	LMG	C29-C28-O8-C9
31	D	406	LMG	C29-C28-O8-C9
31	L	101	LMG	C29-C28-O8-C9
31	c	518	LMG	C29-C28-O8-C9
32	B	628	LMT	C3'-C4'-O1B-C1B
26	B	626	DGD	C2B-C1B-O2G-C2G
26	b	601	DGD	C2B-C1B-O2G-C2G
26	c	516	DGD	C2B-C1B-O2G-C2G
30	F	103	SQD	C8-C7-O47-C45
31	M	101	LMG	C11-C10-O7-C8
31	m	101	LMG	C11-C10-O7-C8
22	B	602	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	C4-C3-C5-C6
22	B	604	CLA	C2-C3-C5-C6
22	b	609	CLA	C2-C3-C5-C6
22	B	606	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	b	611	CLA	O1D-CGD-O2D-CED
32	i	103	LMT	C3'-C4'-O1B-C1B
31	B	625	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
31	E	101	LMG	C29-C28-O8-C9
31	d	408	LMG	C29-C28-O8-C9
26	B	620	DGD	O6E-C5E-C6E-O5E
31	i	102	LMG	O6-C5-C6-O5
32	I	102	LMT	C3'-C4'-O1B-C1B
22	c	501	CLA	O1D-CGD-O2D-CED
26	B	620	DGD	C4D-C5D-C6D-O5D
24	J	101	PL9	C27-C28-C29-C31
24	j	101	PL9	C27-C28-C29-C31
24	A	407	PL9	C17-C18-C19-C20
24	a	407	PL9	C7-C8-C9-C10
24	a	407	PL9	C17-C18-C19-C20
24	j	101	PL9	C7-C8-C9-C10
22	c	512	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
31	c	522	LMG	O9-C10-O7-C8
24	A	407	PL9	C22-C23-C24-C26
24	J	101	PL9	C7-C8-C9-C11
24	a	407	PL9	C17-C18-C19-C21
24	a	407	PL9	C22-C23-C24-C26
26	c	516	DGD	C4E-C5E-C6E-O5E
31	d	408	LMG	C4-C5-C6-O5
26	d	410	DGD	O1A-C1A-O1G-C1G
31	c	522	LMG	O10-C28-O8-C9
22	c	520	CLA	O1D-CGD-O2D-CED
26	A	409	DGD	O6E-C5E-C6E-O5E
26	C	514	DGD	O6E-C5E-C6E-O5E
26	a	408	DGD	O6E-C5E-C6E-O5E
31	I	101	LMG	O6-C5-C6-O5
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	O1D-CGD-O2D-CED
27	A	410	LHG	O2-C2-C3-O3
27	a	409	LHG	O2-C2-C3-O3
22	C	508	CLA	C3-C5-C6-C7
22	H	101	CLA	C3-C5-C6-C7
23	A	405	PHO	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	d	401	PHO	C3-C5-C6-C7
23	A	405	PHO	CBA-CGA-O2A-C1
26	d	410	DGD	C2A-C1A-O1G-C1G
31	C	521	LMG	C29-C28-O8-C9
31	c	522	LMG	C29-C28-O8-C9
31	e	101	LMG	C29-C28-O8-C9
26	C	515	DGD	O6E-C5E-C6E-O5E
26	b	625	DGD	O6E-C5E-C6E-O5E
26	c	515	DGD	O6E-C5E-C6E-O5E
22	c	508	CLA	O1D-CGD-O2D-CED
26	D	407	DGD	C2B-C1B-O2G-C2G
26	d	410	DGD	C2B-C1B-O2G-C2G
30	f	103	SQD	C8-C7-O47-C45
31	a	402	LMG	C11-C10-O7-C8
31	b	627	LMG	C11-C10-O7-C8
31	d	409	LMG	C11-C10-O7-C8
22	b	612	CLA	CBD-CGD-O2D-CED
31	B	625	LMG	O6-C5-C6-O5
26	C	514	DGD	C4E-C5E-C6E-O5E
26	b	625	DGD	C4E-C5E-C6E-O5E
31	i	102	LMG	C4-C5-C6-O5
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	C3-C5-C6-C7
26	D	407	DGD	C2A-C1A-O1G-C1G
34	V	201	HEM	C2D-C3D-CAD-CBD
31	C	517	LMG	O6-C5-C6-O5
31	D	406	LMG	O9-C10-O7-C8
31	e	101	LMG	O9-C10-O7-C8
31	I	101	LMG	C4-C5-C6-O5
31	C	521	LMG	O10-C28-O8-C9
23	A	405	PHO	C4-C3-C5-C6
23	d	401	PHO	C4-C3-C5-C6
23	A	405	PHO	C2-C3-C5-C6
23	d	401	PHO	C2-C3-C5-C6
22	B	601	CLA	C2A-CAA-CBA-CGA
26	c	516	DGD	O6E-C5E-C6E-O5E
31	c	518	LMG	O6-C5-C6-O5
31	d	408	LMG	O6-C5-C6-O5
26	B	620	DGD	C4E-C5E-C6E-O5E
26	C	514	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
26	c	515	DGD	O6E-C1E-O5D-C6D
31	a	402	LMG	O6-C1-O1-C7
31	b	627	LMG	O6-C1-O1-C7
26	c	515	DGD	C4E-C5E-C6E-O5E
34	V	201	HEM	C4D-C3D-CAD-CBD
23	A	405	PHO	O1A-CGA-O2A-C1
31	D	406	LMG	C11-C10-O7-C8
22	C	511	CLA	O1D-CGD-O2D-CED
22	b	615	CLA	O1D-CGD-O2D-CED
22	b	618	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	O1D-CGD-O2D-CED
23	d	402	PHO	O1D-CGD-O2D-CED
22	B	605	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
22	b	620	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
23	d	401	PHO	CBA-CGA-O2A-C1
22	B	606	CLA	O1D-CGD-O2D-CED
31	C	517	LMG	C8-C9-O8-C28
22	A	404	CLA	C10-C11-C12-C13
22	b	613	CLA	C13-C15-C16-C17
31	c	522	LMG	O6-C5-C6-O5
22	B	615	CLA	O1A-CGA-O2A-C1
26	A	409	DGD	C4E-C5E-C6E-O5E
26	a	408	DGD	C4E-C5E-C6E-O5E
31	c	518	LMG	C4-C5-C6-O5
22	B	615	CLA	C5-C6-C7-C8
22	C	508	CLA	C5-C6-C7-C8
26	D	407	DGD	C2D-C1D-O3G-C3G
26	d	410	DGD	C2D-C1D-O3G-C3G
26	C	515	DGD	O2G-C2G-C3G-O3G
26	c	516	DGD	O2G-C2G-C3G-O3G
30	A	414	SQD	O6-C44-C45-O47
31	c	522	LMG	C4-C5-C6-O5
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	C	510	CLA	C6-C7-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C15-C16-C17-C18
22	b	616	CLA	C5-C6-C7-C8
22	c	505	CLA	C5-C6-C7-C8
23	D	401	PHO	C15-C16-C17-C18
22	b	614	CLA	C2A-CAA-CBA-CGA
25	B	619	BCR	C7-C8-C9-C34
25	F	102	BCR	C37-C22-C23-C24
25	y	101	BCR	C7-C8-C9-C34
25	b	622	BCR	C37-C22-C23-C24
25	f	102	BCR	C37-C22-C23-C24
25	g	101	BCR	C7-C8-C9-C34
25	b	622	BCR	C7-C8-C9-C10
31	C	521	LMG	C11-C10-O7-C8
31	c	522	LMG	C11-C10-O7-C8
26	D	407	DGD	C1B-C2B-C3B-C4B
31	c	518	LMG	C28-C29-C30-C31
23	d	401	PHO	O1A-CGA-O2A-C1
22	B	608	CLA	C13-C15-C16-C17
22	B	609	CLA	C8-C10-C11-C12
22	C	503	CLA	C10-C11-C12-C13
22	D	403	CLA	C15-C16-C17-C18
22	b	611	CLA	C15-C16-C17-C18
22	c	520	CLA	C15-C16-C17-C18
23	d	402	PHO	C15-C16-C17-C18
22	A	402	CLA	C3-C5-C6-C7
22	a	403	CLA	C3-C5-C6-C7
22	c	511	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	C15-C16-C17-C18
22	C	509	CLA	C15-C16-C17-C18
22	a	405	CLA	C10-C11-C12-C13
22	b	614	CLA	C8-C10-C11-C12
22	b	616	CLA	C13-C15-C16-C17
22	b	620	CLA	C5-C6-C7-C8
22	c	501	CLA	C15-C16-C17-C18
22	c	503	CLA	C10-C11-C12-C13
22	c	505	CLA	C15-C16-C17-C18
22	c	509	CLA	C15-C16-C17-C18
31	C	517	LMG	C28-C29-C30-C31
31	C	521	LMG	C10-C11-C12-C13
31	b	627	LMG	C28-C29-C30-C31
31	c	522	LMG	C10-C11-C12-C13
31	C	517	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C15-C16-C17-C18
22	B	601	CLA	C13-C15-C16-C17
22	B	611	CLA	C5-C6-C7-C8
22	B	615	CLA	C10-C11-C12-C13
22	D	403	CLA	C13-C15-C16-C17
22	b	605	CLA	C13-C15-C16-C17
22	b	608	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
22	b	620	CLA	C10-C11-C12-C13
22	c	504	CLA	C10-C11-C12-C13
22	c	507	CLA	C15-C16-C17-C18
22	c	508	CLA	C5-C6-C7-C8
22	d	405	CLA	C13-C15-C16-C17
22	d	405	CLA	C15-C16-C17-C18
22	C	512	CLA	O1D-CGD-O2D-CED
26	c	515	DGD	C1B-C2B-C3B-C4B
26	d	410	DGD	C1B-C2B-C3B-C4B
31	C	517	LMG	C10-C11-C12-C13
31	D	409	LMG	C10-C11-C12-C13
31	d	412	LMG	C10-C11-C12-C13
22	B	603	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
22	B	607	CLA	C15-C16-C17-C18
22	B	610	CLA	C15-C16-C17-C18
22	C	519	CLA	C13-C15-C16-C17
22	C	519	CLA	C15-C16-C17-C18
26	C	516	DGD	O1B-C1B-O2G-C2G
22	A	404	CLA	C15-C16-C17-C18
22	c	501	CLA	C8-C10-C11-C12
22	c	505	CLA	C13-C15-C16-C17
22	c	520	CLA	C13-C15-C16-C17
30	b	602	SQD	O10-C23-O48-C46
26	C	514	DGD	C1B-C2B-C3B-C4B
26	b	625	DGD	C1B-C2B-C3B-C4B
31	a	402	LMG	C28-C29-C30-C31
31	c	518	LMG	C10-C11-C12-C13
31	I	101	LMG	C11-C10-O7-C8
22	C	501	CLA	C15-C16-C17-C18
22	C	510	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C12-C13-C15
22	c	510	CLA	C11-C10-C8-C7
22	C	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	b	609	CLA	CBA-CGA-O2A-C1
22	b	610	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	C5-C6-C7-C8
22	C	501	CLA	C10-C11-C12-C13
22	C	505	CLA	C13-C15-C16-C17
22	C	506	CLA	C5-C6-C7-C8
22	C	507	CLA	C10-C11-C12-C13
22	a	405	CLA	C15-C16-C17-C18
22	c	507	CLA	C10-C11-C12-C13
22	b	620	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
26	B	620	DGD	O6E-C1E-O5D-C6D
30	A	413	SQD	O5-C1-O6-C44
30	a	412	SQD	O5-C1-O6-C44
31	I	101	LMG	O6-C1-O1-C7
31	i	102	LMG	O6-C1-O1-C7
22	C	512	CLA	C15-C16-C17-C18
22	c	506	CLA	C5-C6-C7-C8
23	D	401	PHO	O1D-CGD-O2D-CED
24	D	405	PL9	C29-C31-C32-C33
24	d	407	PL9	C29-C31-C32-C33
25	j	102	BCR	C18-C19-C20-C21
32	B	629	LMT	O1'-C1-C2-C3
31	E	101	LMG	O9-C10-O7-C8
31	c	518	LMG	C8-C9-O8-C28
22	b	606	CLA	C3-C5-C6-C7
22	B	614	CLA	C13-C15-C16-C17
22	C	501	CLA	C8-C10-C11-C12
22	C	504	CLA	C10-C11-C12-C13
22	C	507	CLA	C15-C16-C17-C18
22	C	510	CLA	C5-C6-C7-C8
22	b	615	CLA	C15-C16-C17-C18
31	i	102	LMG	C29-C28-O8-C9
22	A	406	CLA	C10-C11-C12-C13
22	b	612	CLA	C15-C16-C17-C18
22	b	619	CLA	C13-C15-C16-C17
22	b	620	CLA	C13-C15-C16-C17
22	c	510	CLA	C5-C6-C7-C8
26	b	625	DGD	O6D-C5D-C6D-O5D
31	i	102	LMG	C11-C10-O7-C8
22	B	607	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C5-C6-C7-C8
22	b	617	CLA	C5-C6-C7-C8
22	c	501	CLA	C10-C11-C12-C13
22	c	512	CLA	C15-C16-C17-C18
27	C	518	LHG	C3-O3-P-O6
27	C	518	LHG	C4-O6-P-O3
27	c	519	LHG	C3-O3-P-O6
27	c	519	LHG	C4-O6-P-O3
26	a	408	DGD	C1B-C2B-C3B-C4B
22	B	604	CLA	CBA-CGA-O2A-C1
22	C	511	CLA	CBA-CGA-O2A-C1
31	C	521	LMG	O6-C5-C6-O5
22	B	611	CLA	C13-C15-C16-C17
26	B	620	DGD	C1B-C2B-C3B-C4B
31	E	101	LMG	C28-C29-C30-C31
31	d	412	LMG	O6-C5-C6-O5
26	c	517	DGD	O1B-C1B-O2G-C2G
22	C	519	CLA	C10-C11-C12-C13
22	c	503	CLA	C5-C6-C7-C8
22	c	511	CLA	O1A-CGA-O2A-C1
31	M	101	LMG	O6-C5-C6-O5
30	B	627	SQD	C24-C23-O48-C46
22	b	606	CLA	C5-C6-C7-C8
32	b	604	LMT	O1'-C1-C2-C3
22	c	520	CLA	C10-C11-C12-C13
31	C	521	LMG	C4-C5-C6-O5
26	B	626	DGD	C5B-C6B-C7B-C8B
26	C	515	DGD	C2A-C3A-C4A-C5A
26	c	515	DGD	C3B-C4B-C5B-C6B
26	d	410	DGD	CEB-CFB-CGB-CHB
30	f	103	SQD	C12-C13-C14-C15
32	b	628	LMT	O1'-C1-C2-C3
22	c	509	CLA	CBD-CGD-O2D-CED
22	B	615	CLA	C3-C5-C6-C7
26	D	407	DGD	C4B-C5B-C6B-C7B
26	D	407	DGD	C5B-C6B-C7B-C8B
26	D	407	DGD	CCB-CDB-CEB-CFB
26	b	601	DGD	C5B-C6B-C7B-C8B
26	b	601	DGD	C9B-CAB-CBB-CCB
26	b	625	DGD	C3B-C4B-C5B-C6B
26	c	516	DGD	C2A-C3A-C4A-C5A
26	d	410	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
30	F	103	SQD	C12-C13-C14-C15
30	a	412	SQD	C14-C15-C16-C17
31	B	621	LMG	C31-C32-C33-C34
31	C	517	LMG	C29-C30-C31-C32
31	L	101	LMG	C34-C35-C36-C37
31	a	402	LMG	C30-C31-C32-C33
31	b	626	LMG	C31-C32-C33-C34
31	c	518	LMG	C29-C30-C31-C32
31	i	102	LMG	C12-C13-C14-C15
32	i	103	LMT	C6-C7-C8-C9
22	c	520	CLA	CBA-CGA-O2A-C1
30	b	602	SQD	C24-C23-O48-C46
26	B	620	DGD	C3B-C4B-C5B-C6B
26	B	626	DGD	C9B-CAB-CBB-CCB
26	b	625	DGD	C6B-C7B-C8B-C9B
26	c	515	DGD	C3A-C4A-C5A-C6A
26	d	410	DGD	C4B-C5B-C6B-C7B
22	b	616	CLA	O1D-CGD-O2D-CED
30	F	103	SQD	O49-C7-O47-C45
31	C	521	LMG	O9-C10-O7-C8
22	B	603	CLA	C8-C10-C11-C12
30	A	413	SQD	C7-C8-C9-C10
26	B	620	DGD	C6B-C7B-C8B-C9B
26	C	514	DGD	C3A-C4A-C5A-C6A
26	C	514	DGD	C3B-C4B-C5B-C6B
26	d	410	DGD	C5B-C6B-C7B-C8B
30	B	627	SQD	C9-C10-C11-C12
31	I	101	LMG	C12-C13-C14-C15
31	I	101	LMG	C14-C15-C16-C17
31	b	627	LMG	C30-C31-C32-C33
32	I	102	LMT	C6-C7-C8-C9
26	C	514	DGD	C2B-C3B-C4B-C5B
30	A	413	SQD	C14-C15-C16-C17
30	a	412	SQD	C27-C28-C29-C30
31	D	406	LMG	C14-C15-C16-C17
31	l	101	LMG	C33-C34-C35-C36
26	C	516	DGD	CBA-CCA-CDA-CEA
31	i	102	LMG	C16-C17-C18-C19
26	C	514	DGD	C1A-C2A-C3A-C4A
26	C	516	DGD	C1A-C2A-C3A-C4A
30	a	412	SQD	C7-C8-C9-C10
31	B	621	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	O1D-CGD-O2D-CED
25	H	102	BCR	C11-C10-C9-C8
25	J	102	BCR	C20-C21-C22-C23
25	j	102	BCR	C20-C21-C22-C23
25	x	101	BCR	C11-C10-C9-C8
26	D	407	DGD	C2E-C1E-O5D-C6D
26	d	410	DGD	C2E-C1E-O5D-C6D
31	I	101	LMG	C2-C1-O1-C7
31	d	408	LMG	C2-C1-O1-C7
31	i	102	LMG	C2-C1-O1-C7
31	I	101	LMG	C29-C28-O8-C9
26	B	620	DGD	C7A-C8A-C9A-CAA
26	D	407	DGD	C7B-C8B-C9B-CAB
26	D	407	DGD	CEB-CFB-CGB-CHB
31	B	625	LMG	C18-C19-C20-C21
31	d	408	LMG	C18-C19-C20-C21
22	b	612	CLA	C5-C6-C7-C8
22	b	609	CLA	O1A-CGA-O2A-C1
22	c	509	CLA	C4-C3-C5-C6
24	D	405	PL9	C27-C28-C29-C30
26	d	410	DGD	C7B-C8B-C9B-CAB
31	L	101	LMG	C31-C32-C33-C34
31	L	101	LMG	C33-C34-C35-C36
31	l	101	LMG	C34-C35-C36-C37
22	A	402	CLA	C11-C12-C13-C14
22	B	601	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16
22	a	404	CLA	C6-C7-C8-C9
22	b	613	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
26	A	409	DGD	C8B-C9B-CAB-CBB
26	C	514	DGD	C4A-C5A-C6A-C7A
26	a	408	DGD	C5B-C6B-C7B-C8B
26	a	408	DGD	C8B-C9B-CAB-CBB
26	c	516	DGD	C4A-C5A-C6A-C7A
30	A	413	SQD	C27-C28-C29-C30
30	F	103	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	b	602	SQD	C9-C10-C11-C12
30	f	103	SQD	C11-C12-C13-C14
31	B	625	LMG	C31-C32-C33-C34
31	C	521	LMG	C12-C13-C14-C15
31	I	101	LMG	C16-C17-C18-C19
31	b	627	LMG	C15-C16-C17-C18
31	b	627	LMG	C18-C19-C20-C21
31	b	627	LMG	C32-C33-C34-C35
31	c	522	LMG	C12-C13-C14-C15
31	d	408	LMG	C31-C32-C33-C34
31	d	409	LMG	C14-C15-C16-C17
22	a	404	CLA	C15-C16-C17-C18
22	b	608	CLA	C8-C10-C11-C12
31	D	409	LMG	O6-C5-C6-O5
22	A	402	CLA	C2A-CAA-CBA-CGA
31	L	101	LMG	C4-C5-C6-O5
25	B	617	BCR	C7-C8-C9-C34
25	b	622	BCR	C7-C8-C9-C34
26	c	517	DGD	C9B-CAB-CBB-CCB
22	b	620	CLA	C3-C5-C6-C7
26	c	517	DGD	CBA-CCA-CDA-CEA
31	l	101	LMG	C30-C31-C32-C33
31	m	101	LMG	C29-C30-C31-C32
31	d	408	LMG	C28-C29-C30-C31
26	C	516	DGD	C9B-CAB-CBB-CCB
26	C	516	DGD	CAB-CBB-CCB-CDB
26	b	601	DGD	C4A-C5A-C6A-C7A
26	b	625	DGD	C7A-C8A-C9A-CAA
26	c	515	DGD	C2B-C3B-C4B-C5B
27	A	410	LHG	C25-C26-C27-C28
30	B	627	SQD	C11-C10-C9-C8
30	b	602	SQD	C11-C10-C9-C8
31	D	406	LMG	C15-C16-C17-C18
31	a	402	LMG	C18-C19-C20-C21
31	a	402	LMG	C32-C33-C34-C35
31	b	627	LMG	C31-C32-C33-C34
31	c	518	LMG	C12-C13-C14-C15
31	d	408	LMG	C30-C31-C32-C33
31	d	408	LMG	C36-C37-C38-C39
31	d	409	LMG	C19-C20-C21-C22
31	i	102	LMG	C13-C14-C15-C16
31	i	102	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	l	101	LMG	C14-C15-C16-C17
26	D	407	DGD	O6E-C1E-O5D-C6D
31	B	625	LMG	O6-C1-O1-C7
31	d	408	LMG	O6-C1-O1-C7
22	C	503	CLA	C5-C6-C7-C8
26	A	409	DGD	C5B-C6B-C7B-C8B
26	c	515	DGD	C4A-C5A-C6A-C7A
26	c	517	DGD	CAB-CBB-CCB-CDB
31	B	625	LMG	C36-C37-C38-C39
31	I	101	LMG	C13-C14-C15-C16
26	B	626	DGD	C4A-C5A-C6A-C7A
26	D	407	DGD	C3A-C4A-C5A-C6A
32	B	629	LMT	C7-C8-C9-C10
26	C	515	DGD	C1A-C2A-C3A-C4A
26	b	601	DGD	C1A-C2A-C3A-C4A
22	H	101	CLA	C5-C6-C7-C8
30	B	627	SQD	O10-C23-O48-C46
26	B	620	DGD	C5B-C6B-C7B-C8B
31	M	101	LMG	C29-C30-C31-C32
31	l	101	LMG	C31-C32-C33-C34
32	b	604	LMT	C7-C8-C9-C10
31	b	627	LMG	O6-C5-C6-O5
26	d	410	DGD	C5A-C6A-C7A-C8A
31	D	406	LMG	C19-C20-C21-C22
31	D	409	LMG	C17-C18-C19-C20
31	e	101	LMG	C15-C16-C17-C18
22	B	611	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	C	504	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
22	b	606	CLA	C3A-C2A-CAA-CBA
22	b	612	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
31	B	625	LMG	C28-C29-C30-C31
22	B	604	CLA	O1A-CGA-O2A-C1
26	b	625	DGD	C4B-C5B-C6B-C7B
31	D	406	LMG	C13-C14-C15-C16
31	L	101	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C13-C15-C16-C17
26	A	409	DGD	C1G-C2G-C3G-O3G
26	C	515	DGD	C4A-C5A-C6A-C7A
26	D	407	DGD	C5A-C6A-C7A-C8A
31	L	101	LMG	C14-C15-C16-C17
31	d	409	LMG	C15-C16-C17-C18
31	e	101	LMG	C28-C29-C30-C31
32	B	623	LMT	C1-C2-C3-C4
32	b	628	LMT	C1-C2-C3-C4
27	a	409	LHG	C25-C26-C27-C28
31	c	518	LMG	C34-C35-C36-C37
22	C	511	CLA	O1A-CGA-O2A-C1
22	C	509	CLA	C4-C3-C5-C6
22	C	512	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
27	C	518	LHG	C24-C23-O8-C6
22	C	509	CLA	C2-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
24	a	407	PL9	C33-C34-C36-C37
30	B	627	SQD	C8-C7-O47-C45
31	D	406	LMG	C32-C33-C34-C35
26	b	601	DGD	C2B-C3B-C4B-C5B
31	a	402	LMG	C15-C16-C17-C18
31	d	409	LMG	C32-C33-C34-C35
31	L	101	LMG	O6-C5-C6-O5
26	b	625	DGD	C5B-C6B-C7B-C8B
31	E	101	LMG	C15-C16-C17-C18
32	b	629	LMT	C2B-C1B-O1B-C4'
31	m	101	LMG	O6-C5-C6-O5
30	B	622	SQD	C9-C10-C11-C12
31	a	402	LMG	C31-C32-C33-C34
31	c	518	LMG	C36-C37-C38-C39
30	f	103	SQD	O49-C7-O47-C45
24	D	405	PL9	C47-C48-C49-C51
30	a	412	SQD	C17-C18-C19-C20
22	c	520	CLA	O1A-CGA-O2A-C1
30	b	602	SQD	C12-C13-C14-C15
31	C	517	LMG	C12-C13-C14-C15
31	d	412	LMG	C31-C32-C33-C34
22	C	509	CLA	C3-C5-C6-C7
25	B	616	BCR	C5-C6-C7-C8
25	C	513	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	C	513	BCR	C23-C24-C25-C30
25	F	102	BCR	C5-C6-C7-C8
25	H	102	BCR	C1-C6-C7-C8
25	H	102	BCR	C5-C6-C7-C8
25	J	102	BCR	C5-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
25	b	621	BCR	C5-C6-C7-C8
25	b	622	BCR	C23-C24-C25-C30
25	b	624	BCR	C23-C24-C25-C26
25	c	513	BCR	C1-C6-C7-C8
25	c	513	BCR	C5-C6-C7-C8
25	c	514	BCR	C23-C24-C25-C26
25	c	514	BCR	C23-C24-C25-C30
25	f	102	BCR	C5-C6-C7-C8
25	i	101	BCR	C1-C6-C7-C8
25	i	101	BCR	C5-C6-C7-C8
25	g	101	BCR	C23-C24-C25-C26
25	g	101	BCR	C23-C24-C25-C30
25	x	101	BCR	C1-C6-C7-C8
25	x	101	BCR	C5-C6-C7-C8
26	A	409	DGD	C3B-C4B-C5B-C6B
30	d	403	SQD	C9-C10-C11-C12
31	L	101	LMG	C15-C16-C17-C18
22	b	615	CLA	CBA-CGA-O2A-C1
22	d	406	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	C10-C11-C12-C13
22	H	101	CLA	C13-C15-C16-C17
22	b	606	CLA	C13-C15-C16-C17
22	d	406	CLA	C15-C16-C17-C18
26	c	517	DGD	C2B-C1B-O2G-C2G
30	b	602	SQD	C8-C7-O47-C45
26	B	626	DGD	C2B-C3B-C4B-C5B
31	B	625	LMG	C30-C31-C32-C33
23	A	405	PHO	CBD-CGD-O2D-CED
26	c	517	DGD	C1A-C2A-C3A-C4A
26	B	620	DGD	C4B-C5B-C6B-C7B
26	D	407	DGD	C6B-C7B-C8B-C9B
26	C	516	DGD	C3B-C4B-C5B-C6B
26	c	516	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
31	d	409	LMG	C13-C14-C15-C16
24	d	407	PL9	C20-C19-C21-C22
22	b	612	CLA	O1D-CGD-O2D-CED
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	B	602	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	b	605	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	509	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	c	512	CLA	C11-C10-C8-C7
22	c	512	CLA	C12-C13-C15-C16
23	D	401	PHO	C11-C10-C8-C7
22	c	509	CLA	C3-C5-C6-C7
22	C	511	CLA	C13-C15-C16-C17
22	b	609	CLA	C15-C16-C17-C18
22	B	612	CLA	C16-C17-C18-C19
26	B	620	DGD	O6D-C5D-C6D-O5D
27	A	410	LHG	O9-C7-O7-C5
26	A	409	DGD	C1B-C2B-C3B-C4B
27	a	409	LHG	C23-C24-C25-C26
22	B	610	CLA	CBA-CGA-O2A-C1
22	C	519	CLA	CBA-CGA-O2A-C1
22	D	404	CLA	CBA-CGA-O2A-C1
31	m	101	LMG	C29-C28-O8-C9
22	B	605	CLA	C2A-CAA-CBA-CGA
22	a	403	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	C10-C11-C12-C13
32	B	624	LMT	C2B-C1B-O1B-C4'
26	C	514	DGD	C2A-C3A-C4A-C5A
31	d	412	LMG	C17-C18-C19-C20
31	C	517	LMG	C34-C35-C36-C37
31	b	627	LMG	C17-C18-C19-C20
26	c	515	DGD	C1A-C2A-C3A-C4A
31	b	626	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C15-C16-C17-C18
22	C	512	CLA	C13-C15-C16-C17
26	C	514	DGD	C4B-C5B-C6B-C7B
26	D	407	DGD	CAB-CBB-CCB-CDB
30	F	103	SQD	C10-C11-C12-C13
31	B	621	LMG	C34-C35-C36-C37
31	d	412	LMG	C34-C35-C36-C37
22	A	403	CLA	C3-C5-C6-C7
26	c	515	DGD	C2A-C3A-C4A-C5A
26	d	410	DGD	CAB-CBB-CCB-CDB
27	C	518	LHG	C24-C25-C26-C27
32	B	623	LMT	O1'-C1-C2-C3
22	b	617	CLA	C16-C17-C18-C19
26	d	410	DGD	O6E-C1E-O5D-C6D
31	B	625	LMG	C32-C33-C34-C35
26	B	626	DGD	C1A-C2A-C3A-C4A
26	c	516	DGD	C1A-C2A-C3A-C4A
26	d	410	DGD	C1A-C2A-C3A-C4A
26	C	516	DGD	C2B-C1B-O2G-C2G
27	A	410	LHG	C8-C7-O7-C5
27	a	409	LHG	C8-C7-O7-C5
31	E	101	LMG	C11-C10-O7-C8
31	e	101	LMG	C11-C10-O7-C8
26	d	410	DGD	C2A-C3A-C4A-C5A
31	b	626	LMG	C34-C35-C36-C37
31	l	101	LMG	C4-C5-C6-O5
22	a	406	CLA	C5-C6-C7-C8
27	a	409	LHG	O9-C7-O7-C5
22	D	404	CLA	C15-C16-C17-C18
30	A	413	SQD	O47-C45-C46-O48
30	a	401	SQD	O6-C44-C45-O47
30	a	412	SQD	O47-C45-C46-O48
31	I	101	LMG	O1-C7-C8-O7
31	M	101	LMG	O1-C7-C8-O7
31	i	102	LMG	O1-C7-C8-O7
31	m	101	LMG	O1-C7-C8-O7
31	C	517	LMG	C36-C37-C38-C39
31	i	102	LMG	C17-C18-C19-C20
26	D	407	DGD	C8B-C9B-CAB-CBB
27	A	410	LHG	C30-C31-C32-C33
27	c	519	LHG	C24-C25-C26-C27
27	c	519	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	e	101	LMG	O6-C5-C6-O5
22	c	511	CLA	C13-C15-C16-C17
24	A	407	PL9	C4-C3-C7-C8
30	B	627	SQD	C12-C13-C14-C15
22	A	403	CLA	C6-C7-C8-C9
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	B	612	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	a	405	CLA	C6-C7-C8-C9
22	b	605	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C12-C13-C14
22	b	617	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	510	CLA	C11-C10-C8-C9
23	D	401	PHO	C11-C10-C8-C9
22	A	406	CLA	C5-C6-C7-C8
22	C	501	CLA	C2A-CAA-CBA-CGA
22	c	520	CLA	C2A-CAA-CBA-CGA
26	C	515	DGD	CAB-CBB-CCB-CDB
26	D	407	DGD	C2A-C3A-C4A-C5A
31	C	521	LMG	C16-C17-C18-C19
31	M	101	LMG	C29-C28-O8-C9
25	b	624	BCR	C7-C8-C9-C34
22	C	509	CLA	O1D-CGD-O2D-CED
31	B	625	LMG	C4-C5-C6-O5
26	A	409	DGD	C4B-C5B-C6B-C7B
31	B	625	LMG	C17-C18-C19-C20
31	D	409	LMG	C31-C32-C33-C34
25	x	101	BCR	C7-C8-C9-C10
22	b	615	CLA	O1A-CGA-O2A-C1
22	d	406	CLA	O1A-CGA-O2A-C1
31	i	102	LMG	O10-C28-O8-C9
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	B	612	CLA	C16-C17-C18-C20
26	d	410	DGD	C6B-C7B-C8B-C9B
27	c	519	LHG	C11-C10-C9-C8
30	f	103	SQD	C10-C11-C12-C13
22	C	502	CLA	C13-C15-C16-C17
22	a	406	CLA	C10-C11-C12-C13
22	a	406	CLA	C13-C15-C16-C17
26	D	407	DGD	CDB-CEB-CFB-CGB
26	a	408	DGD	C4B-C5B-C6B-C7B
26	c	515	DGD	C4B-C5B-C6B-C7B
27	a	409	LHG	C30-C31-C32-C33
22	C	502	CLA	C3-C5-C6-C7
22	A	406	CLA	C13-C15-C16-C17
31	d	408	LMG	C17-C18-C19-C20
31	b	626	LMG	C28-C29-C30-C31
31	a	402	LMG	O6-C5-C6-O5
22	C	503	CLA	C8-C10-C11-C12
22	B	601	CLA	C16-C17-C18-C20
22	b	617	CLA	C16-C17-C18-C20
31	D	409	LMG	C34-C35-C36-C37
24	a	407	PL9	C35-C34-C36-C37
31	I	101	LMG	C18-C19-C20-C21
31	l	101	LMG	C15-C16-C17-C18
26	c	517	DGD	C3B-C4B-C5B-C6B
31	c	522	LMG	C16-C17-C18-C19
31	l	101	LMG	C11-C10-O7-C8
26	a	408	DGD	C3B-C4B-C5B-C6B
30	a	412	SQD	C10-C11-C12-C13
31	d	408	LMG	C32-C33-C34-C35
31	e	101	LMG	C18-C19-C20-C21
22	c	512	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C16-C17-C18-C20
26	a	408	DGD	C1G-C2G-C3G-O3G
26	c	517	DGD	O1G-C1G-C2G-C3G
30	A	413	SQD	C44-C45-C46-O48
30	A	414	SQD	O6-C44-C45-C46
30	B	627	SQD	C44-C45-C46-O48
30	a	412	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
30	b	602	SQD	C44-C45-C46-O48
31	B	621	LMG	C7-C8-C9-O8
31	B	625	LMG	O1-C7-C8-C9
31	M	101	LMG	C7-C8-C9-O8
31	b	626	LMG	C7-C8-C9-O8
31	c	522	LMG	C7-C8-C9-O8
31	d	408	LMG	O1-C7-C8-C9
31	i	102	LMG	O1-C7-C8-C9
31	m	101	LMG	C7-C8-C9-O8
27	c	519	LHG	C24-C23-O8-C6
30	a	401	SQD	C10-C11-C12-C13
22	C	519	CLA	O1A-CGA-O2A-C1
30	B	622	SQD	C45-C44-O6-C1
30	d	403	SQD	C45-C44-O6-C1
31	D	406	LMG	C8-C7-O1-C1
31	d	409	LMG	C8-C7-O1-C1
31	L	101	LMG	C8-C9-O8-C28
31	B	621	LMG	C13-C14-C15-C16
22	B	615	CLA	C15-C16-C17-C18
30	A	414	SQD	C10-C11-C12-C13
22	D	404	CLA	O1A-CGA-O2A-C1
26	C	516	DGD	CDB-CEB-CFB-CGB
26	d	410	DGD	C3A-C4A-C5A-C6A
22	c	502	CLA	C3-C5-C6-C7
22	c	505	CLA	C10-C11-C12-C13
30	A	413	SQD	C17-C18-C19-C20
31	E	101	LMG	O6-C5-C6-O5
31	i	102	LMG	C18-C19-C20-C21
24	d	407	PL9	C27-C28-C29-C30
22	B	613	CLA	C5-C6-C7-C8
30	A	413	SQD	C10-C11-C12-C13
30	b	602	SQD	C11-C12-C13-C14
31	C	521	LMG	C17-C18-C19-C20
26	D	407	DGD	CBA-CCA-CDA-CEA
22	C	504	CLA	C15-C16-C17-C18
22	c	502	CLA	C13-C15-C16-C17
22	C	504	CLA	C4-C3-C5-C6
24	D	405	PL9	C15-C14-C16-C17
31	b	626	LMG	C13-C14-C15-C16
27	A	410	LHG	C23-C24-C25-C26
27	C	518	LHG	C25-C26-C27-C28
26	c	517	DGD	CFA-CGA-CHA-CIA

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Mol	Chain	Res	Type	Atoms
32	I	102	LMT	C5'-C4'-O1B-C1B
26	D	407	DGD	C1G-C2G-O2G-C1B
26	d	410	DGD	C1G-C2G-O2G-C1B
31	E	101	LMG	C7-C8-O7-C10
22	B	615	CLA	C8-C10-C11-C12
22	b	608	CLA	C15-C16-C17-C18
22	C	508	CLA	C2-C1-O2A-CGA
22	c	508	CLA	C2-C1-O2A-CGA
26	c	516	DGD	O6D-C5D-C6D-O5D
22	a	404	CLA	C3-C5-C6-C7
26	d	410	DGD	CBA-CCA-CDA-CEA
32	i	103	LMT	C5'-C4'-O1B-C1B
26	B	626	DGD	C5A-C6A-C7A-C8A
30	B	627	SQD	C11-C12-C13-C14
31	d	408	LMG	C13-C14-C15-C16
22	C	508	CLA	CBA-CGA-O2A-C1
27	C	518	LHG	O6-C4-C5-O7
22	B	601	CLA	C16-C17-C18-C19
32	B	624	LMT	O5B-C1B-O1B-C4'
34	v	201	HEM	C4D-C3D-CAD-CBD
22	c	504	CLA	C15-C16-C17-C18
22	B	610	CLA	O1A-CGA-O2A-C1
26	d	410	DGD	C3B-C4B-C5B-C6B
30	b	602	SQD	C17-C18-C19-C20
22	b	605	CLA	C10-C11-C12-C13
26	C	514	DGD	O2G-C2G-C3G-O3G
31	L	101	LMG	O1-C7-C8-O7
31	c	518	LMG	O1-C7-C8-O7
31	l	101	LMG	O1-C7-C8-O7
26	c	516	DGD	C3A-C4A-C5A-C6A
31	I	101	LMG	C31-C32-C33-C34
26	B	626	DGD	O6D-C5D-C6D-O5D
22	B	604	CLA	C5-C6-C7-C8
26	d	410	DGD	C8B-C9B-CAB-CBB
31	I	101	LMG	C17-C18-C19-C20
22	c	504	CLA	C4-C3-C5-C6
22	c	512	CLA	C13-C15-C16-C17
22	B	602	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
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	505	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C10-C8-C7
22	C	512	CLA	C12-C13-C15-C16
22	D	403	CLA	C12-C13-C15-C16
22	H	101	CLA	C6-C7-C8-C10
22	a	405	CLA	C6-C7-C8-C10
22	b	606	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C12-C13-C15
22	b	612	CLA	C6-C7-C8-C10
22	b	617	CLA	C11-C10-C8-C7
22	b	619	CLA	C12-C13-C15-C16
22	b	620	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	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	c	511	CLA	C12-C13-C15-C16
22	d	405	CLA	C12-C13-C15-C16
23	D	401	PHO	C12-C13-C15-C16
23	d	402	PHO	C11-C10-C8-C7
34	v	201	HEM	C2D-C3D-CAD-CBD
22	c	511	CLA	C3-C5-C6-C7
26	b	601	DGD	C5A-C6A-C7A-C8A
22	B	602	CLA	C6-C7-C8-C9
22	B	605	CLA	C14-C13-C15-C16
22	B	608	CLA	C6-C7-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	507	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C14-C13-C15-C16
22	D	403	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C14
22	b	607	CLA	C6-C7-C8-C9
22	b	610	CLA	C14-C13-C15-C16
22	b	619	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
22	d	405	CLA	C14-C13-C15-C16
23	D	401	PHO	C14-C13-C15-C16
23	d	402	PHO	C11-C10-C8-C9
23	d	402	PHO	C14-C13-C15-C16
31	d	409	LMG	C28-C29-C30-C31
31	E	101	LMG	C18-C19-C20-C21
31	a	402	LMG	C17-C18-C19-C20
31	d	408	LMG	C19-C20-C21-C22
22	C	504	CLA	CBA-CGA-O2A-C1
22	c	508	CLA	CBA-CGA-O2A-C1
23	D	401	PHO	C10-C11-C12-C13
32	b	629	LMT	O5B-C1B-O1B-C4'
26	c	516	DGD	C4D-C5D-C6D-O5D
22	B	613	CLA	C16-C17-C18-C20
22	C	511	CLA	C16-C17-C18-C19
26	C	515	DGD	O6D-C5D-C6D-O5D
31	L	101	LMG	C11-C10-O7-C8
26	d	410	DGD	CDB-CEB-CFB-CGB
22	B	614	CLA	CBA-CGA-O2A-C1
31	C	521	LMG	C34-C35-C36-C37
31	D	406	LMG	C29-C30-C31-C32
31	E	101	LMG	C19-C20-C21-C22
22	b	618	CLA	C5-C6-C7-C8
22	c	503	CLA	C8-C10-C11-C12
31	B	625	LMG	C15-C16-C17-C18
31	E	101	LMG	O7-C10-C11-C12
22	b	614	CLA	C16-C17-C18-C20
27	c	519	LHG	O6-C4-C5-C6
24	D	405	PL9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	B	621	LMG	C17-C18-C19-C20
31	B	625	LMG	C19-C20-C21-C22
31	l	101	LMG	O6-C5-C6-O5
31	B	625	LMG	C13-C14-C15-C16
31	b	627	LMG	C11-C12-C13-C14
22	b	620	CLA	C8-C10-C11-C12
26	c	517	DGD	CDB-CEB-CFB-CGB
31	E	101	LMG	C17-C18-C19-C20
24	d	407	PL9	C15-C14-C16-C17
22	c	504	CLA	C2-C3-C5-C6
24	J	101	PL9	C27-C28-C29-C30
24	j	101	PL9	C27-C28-C29-C30
31	b	626	LMG	C17-C18-C19-C20
31	c	522	LMG	C17-C18-C19-C20
27	c	519	LHG	O10-C23-O8-C6
22	A	402	CLA	C3A-C2A-CAA-CBA
22	a	403	CLA	C3A-C2A-CAA-CBA
26	D	407	DGD	C3B-C4B-C5B-C6B
31	d	408	LMG	C15-C16-C17-C18
31	d	412	LMG	C19-C20-C21-C22
22	b	618	CLA	C15-C16-C17-C18
22	b	614	CLA	CBA-CGA-O2A-C1
31	e	101	LMG	C19-C20-C21-C22
26	B	626	DGD	C1G-C2G-C3G-O3G
26	C	515	DGD	C1G-C2G-C3G-O3G
26	C	516	DGD	O1G-C1G-C2G-C3G
26	D	407	DGD	C1G-C2G-C3G-O3G
26	c	516	DGD	C1G-C2G-C3G-O3G
30	a	401	SQD	O6-C44-C45-C46
31	C	517	LMG	O1-C7-C8-C9
31	C	521	LMG	C7-C8-C9-O8
31	D	406	LMG	O1-C7-C8-C9
31	I	101	LMG	O1-C7-C8-C9
31	L	101	LMG	O1-C7-C8-C9
31	c	518	LMG	O1-C7-C8-C9
31	d	409	LMG	O1-C7-C8-C9
31	l	101	LMG	O1-C7-C8-C9
31	m	101	LMG	O1-C7-C8-C9
31	D	409	LMG	C19-C20-C21-C22
26	D	407	DGD	C1A-C2A-C3A-C4A
24	D	405	PL9	C32-C33-C34-C36
26	c	516	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
30	b	602	SQD	C10-C11-C12-C13
22	C	511	CLA	C3-C5-C6-C7
31	D	406	LMG	C28-C29-C30-C31
31	D	409	LMG	C38-C39-C40-C41
31	b	626	LMG	C12-C13-C14-C15
22	A	403	CLA	C4-C3-C5-C6
24	D	405	PL9	C35-C34-C36-C37
24	J	101	PL9	C15-C14-C16-C17
27	C	518	LHG	C11-C10-C9-C8
22	c	509	CLA	O1D-CGD-O2D-CED
22	C	519	CLA	C2A-CAA-CBA-CGA
31	a	402	LMG	C11-C12-C13-C14
27	c	519	LHG	O6-C4-C5-O7
26	C	515	DGD	C4D-C5D-C6D-O5D
22	C	508	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	C16-C17-C18-C20
30	A	413	SQD	C31-C32-C33-C34
31	i	102	LMG	C31-C32-C33-C34
22	B	604	CLA	C10-C11-C12-C13
22	c	508	CLA	O1A-CGA-O2A-C1
26	C	516	DGD	O1G-C1G-C2G-O2G
26	c	517	DGD	O1G-C1G-C2G-O2G
30	B	622	SQD	O6-C44-C45-O47
30	B	627	SQD	O47-C45-C46-O48
30	b	602	SQD	O47-C45-C46-O48
30	d	403	SQD	O6-C44-C45-O47
31	C	517	LMG	O1-C7-C8-O7
31	c	522	LMG	O7-C8-C9-O8
22	c	504	CLA	CBA-CGA-O2A-C1
22	b	609	CLA	C10-C11-C12-C13
30	F	103	SQD	C29-C30-C31-C32
22	B	609	CLA	C16-C17-C18-C20
31	L	101	LMG	C20-C21-C22-C23
31	d	412	LMG	C38-C39-C40-C41
26	D	407	DGD	C4E-C5E-C6E-O5E
31	e	101	LMG	C17-C18-C19-C20
30	B	627	SQD	O49-C7-O47-C45
30	b	602	SQD	O49-C7-O47-C45
22	B	612	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
22	b	614	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	b	617	CLA	C2-C1-O2A-CGA
23	A	405	PHO	C2-C1-O2A-CGA
23	d	401	PHO	C2-C1-O2A-CGA
22	C	504	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	D	403	CLA	C6-C7-C8-C9
22	H	101	CLA	C11-C12-C13-C14
22	b	613	CLA	C14-C13-C15-C16
22	b	619	CLA	C11-C10-C8-C9
22	b	620	CLA	C11-C12-C13-C14
22	c	509	CLA	C11-C10-C8-C9
22	c	511	CLA	C11-C12-C13-C14
23	d	401	PHO	C6-C7-C8-C9
32	B	628	LMT	C5'-C4'-O1B-C1B
26	d	410	DGD	C4A-C5A-C6A-C7A
22	A	403	CLA	C5-C6-C7-C8
22	B	613	CLA	C15-C16-C17-C18
27	a	409	LHG	C2-C3-O3-P
30	a	412	SQD	C31-C32-C33-C34
31	B	625	LMG	C20-C21-C22-C23
22	B	613	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C19
25	A	408	BCR	C1-C6-C7-C8
25	A	408	BCR	C5-C6-C7-C8
25	A	408	BCR	C23-C24-C25-C26
25	A	408	BCR	C23-C24-C25-C30
25	B	619	BCR	C1-C6-C7-C8
25	B	619	BCR	C5-C6-C7-C8
25	B	619	BCR	C23-C24-C25-C30
25	b	624	BCR	C1-C6-C7-C8
25	b	624	BCR	C5-C6-C7-C8
25	c	513	BCR	C23-C24-C25-C26
25	c	513	BCR	C23-C24-C25-C30
25	c	521	BCR	C23-C24-C25-C26
25	i	101	BCR	C23-C24-C25-C26
25	i	101	BCR	C23-C24-C25-C30
25	j	102	BCR	C5-C6-C7-C8
31	I	101	LMG	O10-C28-O8-C9
23	A	405	PHO	O1D-CGD-O2D-CED
25	J	102	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	c	514	BCR	C7-C8-C9-C10
22	C	511	CLA	C5-C6-C7-C8
22	b	616	CLA	C10-C11-C12-C13
26	D	407	DGD	C4A-C5A-C6A-C7A
26	C	516	DGD	CFA-CGA-CHA-CIA
22	b	618	CLA	C16-C17-C18-C20
31	C	517	LMG	C13-C14-C15-C16
27	C	518	LHG	O6-C4-C5-C6
22	A	406	CLA	C11-C10-C8-C7
22	B	605	CLA	C12-C13-C15-C16
22	B	607	CLA	C6-C7-C8-C10
22	B	608	CLA	C12-C13-C15-C16
22	B	609	CLA	C11-C12-C13-C15
22	B	609	CLA	C12-C13-C15-C16
22	B	610	CLA	C11-C10-C8-C7
22	B	612	CLA	C11-C12-C13-C15
22	B	615	CLA	C11-C10-C8-C7
22	C	501	CLA	C11-C12-C13-C15
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C12-C13-C15-C16
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
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	a	404	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	b	609	CLA	C11-C10-C8-C7
22	b	610	CLA	C12-C13-C15-C16
22	b	613	CLA	C12-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C7
22	b	617	CLA	C11-C12-C13-C15
22	b	619	CLA	C11-C10-C8-C7
22	b	620	CLA	C11-C10-C8-C7
22	c	502	CLA	C12-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C10
22	c	505	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C10-C8-C7
22	c	510	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C11-C12-C13-C15
23	d	402	PHO	C12-C13-C15-C16
22	C	504	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	C16-C17-C18-C19
26	D	407	DGD	CAA-CBA-CCA-CDA
22	b	614	CLA	C10-C11-C12-C13
30	A	413	SQD	C15-C16-C17-C18
25	H	102	BCR	C16-C17-C18-C36
25	g	101	BCR	C20-C21-C22-C37
26	C	515	DGD	C4B-C5B-C6B-C7B
31	d	409	LMG	C29-C30-C31-C32
22	B	614	CLA	O1A-CGA-O2A-C1
22	B	609	CLA	C5-C6-C7-C8
22	B	609	CLA	C10-C11-C12-C13
22	a	404	CLA	C5-C6-C7-C8
22	a	405	CLA	C5-C6-C7-C8
22	B	605	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	CBA-CGA-O2A-C1
26	c	515	DGD	C5B-C6B-C7B-C8B
31	m	101	LMG	C30-C31-C32-C33
22	c	508	CLA	C15-C16-C17-C18
30	B	627	SQD	C10-C11-C12-C13
30	F	103	SQD	C24-C25-C26-C27
30	f	103	SQD	C29-C30-C31-C32
22	B	611	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	CAD-CBD-CGD-O2D
23	d	401	PHO	CAD-CBD-CGD-O2D
23	d	402	PHO	CAD-CBD-CGD-O2D
26	c	517	DGD	C3G-C2G-O2G-C1B
22	b	610	CLA	C13-C15-C16-C17
22	b	620	CLA	C15-C16-C17-C18
23	d	402	PHO	C10-C11-C12-C13
31	B	621	LMG	C29-C28-O8-C9
24	d	407	PL9	C35-C34-C36-C37
31	M	101	LMG	O6-C1-O1-C7
26	b	601	DGD	C1G-C2G-C3G-O3G
26	d	410	DGD	C1G-C2G-C3G-O3G
27	A	410	LHG	C2-C3-O3-P
22	c	504	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	B	604	CLA	C15-C16-C17-C18
26	b	625	DGD	CCA-CDA-CEA-CFA
26	c	516	DGD	C6A-C7A-C8A-C9A
30	A	414	SQD	C9-C10-C11-C12
34	F	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4B-C3B-CAB-CBB
22	B	613	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
22	c	510	CLA	C2A-CAA-CBA-CGA
31	B	621	LMG	C28-C29-C30-C31
22	B	609	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C19
30	B	627	SQD	C17-C18-C19-C20
22	A	404	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O2D
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	613	CLA	CHA-CBD-CGD-O1D
22	b	613	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
30	A	414	SQD	C32-C33-C34-C35
22	b	614	CLA	O1A-CGA-O2A-C1
31	B	625	LMG	C2-C1-O1-C7
22	b	614	CLA	C5-C6-C7-C8
32	b	603	LMT	C5'-C4'-O1B-C1B
26	c	515	DGD	O2G-C2G-C3G-O3G
31	C	521	LMG	O7-C8-C9-O8
31	M	101	LMG	O7-C8-C9-O8
31	m	101	LMG	O7-C8-C9-O8
26	C	515	DGD	C3A-C4A-C5A-C6A
24	d	407	PL9	C47-C48-C49-C51
27	C	518	LHG	O10-C23-O8-C6
22	b	618	CLA	C16-C17-C18-C19
26	b	601	DGD	O6D-C5D-C6D-O5D
30	f	103	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
24	a	407	PL9	C4-C3-C7-C8
22	A	403	CLA	C14-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C9
22	B	608	CLA	C11-C12-C13-C14
22	B	608	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	c	501	CLA	C11-C12-C13-C14
22	d	405	CLA	C6-C7-C8-C9
32	D	408	LMT	O5'-C5'-C6'-O6'
22	C	510	CLA	O1A-CGA-O2A-C1
26	d	410	DGD	CAA-CBA-CCA-CDA
30	B	622	SQD	C5-C6-S-O8
30	d	403	SQD	C5-C6-S-O8
26	D	407	DGD	C2B-C3B-C4B-C5B
22	b	609	CLA	C5-C6-C7-C8
25	j	102	BCR	C7-C8-C9-C10
22	A	402	CLA	C1A-C2A-CAA-CBA
22	a	403	CLA	C1A-C2A-CAA-CBA
22	b	607	CLA	C16-C17-C18-C19
22	A	404	CLA	C5-C6-C7-C8
22	b	619	CLA	CBA-CGA-O2A-C1
26	d	410	DGD	C2B-C3B-C4B-C5B
26	d	410	DGD	C4E-C5E-C6E-O5E
26	A	409	DGD	C2A-C3A-C4A-C5A
26	b	625	DGD	C5A-C6A-C7A-C8A
26	c	515	DGD	C5A-C6A-C7A-C8A
22	b	616	CLA	C4-C3-C5-C6
24	j	101	PL9	C15-C14-C16-C17
26	B	620	DGD	O1A-C1A-O1G-C1G
27	C	518	LHG	C3-O3-P-O5
27	c	519	LHG	C3-O3-P-O5
27	c	519	LHG	C7-C8-C9-C10
22	C	508	CLA	C15-C16-C17-C18
23	d	401	PHO	C5-C6-C7-C8
31	c	522	LMG	C35-C36-C37-C38
22	b	618	CLA	C2A-CAA-CBA-CGA
22	c	510	CLA	C3-C5-C6-C7
31	d	408	LMG	C20-C21-C22-C23
22	B	605	CLA	O1A-CGA-O2A-C1
22	B	608	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	C	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
30	A	414	SQD	C5-C6-S-O9
30	d	403	SQD	O5-C5-C6-S
30	d	403	SQD	C10-C11-C12-C13
31	C	521	LMG	C35-C36-C37-C38
31	c	522	LMG	C34-C35-C36-C37
31	b	627	LMG	C12-C13-C14-C15
31	B	621	LMG	C12-C13-C14-C15
22	c	509	CLA	C16-C17-C18-C19
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C12-C13-C15
22	C	509	CLA	C6-C7-C8-C10
22	D	404	CLA	C11-C10-C8-C7
22	b	605	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C7
22	b	612	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C12-C13-C15
22	b	614	CLA	C12-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C15
22	c	505	CLA	C11-C12-C13-C15
22	c	508	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
22	c	512	CLA	C3A-C2A-CAA-CBA
22	c	520	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C10-C8-C7
22	d	406	CLA	C11-C10-C8-C7
23	d	402	PHO	C6-C7-C8-C10
31	C	517	LMG	C32-C33-C34-C35
22	C	506	CLA	C3-C5-C6-C7
30	A	413	SQD	C11-C10-C9-C8
30	B	622	SQD	C10-C11-C12-C13
22	c	511	CLA	C5-C6-C7-C8
23	A	405	PHO	C5-C6-C7-C8
31	l	101	LMG	C10-C11-C12-C13
31	L	101	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	a	412	SQD	C12-C13-C14-C15
30	d	403	SQD	O6-C44-C45-C46
26	A	409	DGD	O2G-C2G-C3G-O3G
26	D	407	DGD	O2G-C2G-C3G-O3G
26	a	408	DGD	O2G-C2G-C3G-O3G
26	d	410	DGD	O2G-C2G-C3G-O3G
31	D	406	LMG	O1-C7-C8-O7
31	d	409	LMG	O1-C7-C8-O7
31	l	101	LMG	C16-C17-C18-C19
31	a	402	LMG	C16-C17-C18-C19
31	l	101	LMG	C35-C36-C37-C38
31	L	101	LMG	C8-C7-O1-C1
31	l	101	LMG	C8-C7-O1-C1
22	B	602	CLA	C15-C16-C17-C18
22	C	508	CLA	C10-C11-C12-C13
22	c	501	CLA	C13-C15-C16-C17
30	a	412	SQD	C15-C16-C17-C18
31	B	625	LMG	C10-C11-C12-C13
30	a	401	SQD	C26-C27-C28-C29
22	b	619	CLA	O1A-CGA-O2A-C1
31	b	626	LMG	C29-C28-O8-C9
32	b	603	LMT	C4'-C5'-C6'-O6'
26	B	620	DGD	C5A-C6A-C7A-C8A
32	b	604	LMT	C2-C3-C4-C5
22	A	406	CLA	C11-C10-C8-C9
22	B	610	CLA	C11-C10-C8-C9
22	B	611	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C10-C8-C9
22	C	501	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C10-C8-C9
22	C	511	CLA	C14-C13-C15-C16
22	a	404	CLA	C14-C13-C15-C16
22	b	609	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C10-C8-C9
22	b	617	CLA	C11-C12-C13-C14
22	b	620	CLA	C11-C10-C8-C9
22	b	620	CLA	C14-C13-C15-C16
23	A	405	PHO	C6-C7-C8-C9
22	c	506	CLA	C3-C5-C6-C7
22	B	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	d	407	PL9	C24-C26-C27-C28
22	C	508	CLA	C2A-CAA-CBA-CGA
31	e	101	LMG	O7-C10-C11-C12
23	d	402	PHO	C13-C15-C16-C17
31	L	101	LMG	C29-C30-C31-C32
31	c	518	LMG	C32-C33-C34-C35
22	B	602	CLA	C16-C17-C18-C19
22	a	406	CLA	C16-C17-C18-C19
31	L	101	LMG	C38-C39-C40-C41
31	e	101	LMG	C31-C32-C33-C34
31	d	409	LMG	C34-C35-C36-C37
26	C	516	DGD	C1B-C2B-C3B-C4B
26	C	516	DGD	C8B-C9B-CAB-CBB
22	B	612	CLA	C10-C11-C12-C13
22	C	511	CLA	CAA-CBA-CGA-O2A
31	C	521	LMG	C30-C31-C32-C33
26	C	516	DGD	C3G-C2G-O2G-C1B
27	A	410	LHG	C6-C5-O7-C7
22	c	508	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
26	C	514	DGD	C5B-C6B-C7B-C8B
26	d	410	DGD	CBB-CCB-CDB-CEB
30	f	103	SQD	C9-C10-C11-C12
26	C	515	DGD	C7B-C8B-C9B-CAB
31	B	625	LMG	C16-C17-C18-C19
31	d	409	LMG	C31-C32-C33-C34
22	B	613	CLA	C2C-C3C-CAC-CBC
31	l	101	LMG	C11-C12-C13-C14
25	B	617	BCR	C1-C6-C7-C8
25	B	619	BCR	C23-C24-C25-C26
25	C	513	BCR	C1-C6-C7-C8
25	C	520	BCR	C23-C24-C25-C26
25	C	520	BCR	C23-C24-C25-C30
25	c	514	BCR	C1-C6-C7-C8
25	c	521	BCR	C23-C24-C25-C30
22	b	616	CLA	C2-C3-C5-C6
24	d	407	PL9	C13-C14-C16-C17
31	L	101	LMG	C16-C17-C18-C19
31	l	101	LMG	C20-C21-C22-C23
34	F	101	HEM	C3D-CAD-CBD-CGD
30	a	401	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	D	409	LMG	C32-C33-C34-C35
31	d	409	LMG	C36-C37-C38-C39
26	C	515	DGD	O6E-C1E-O5D-C6D
26	c	515	DGD	O6D-C1D-O3G-C3G
31	B	621	LMG	O7-C8-C9-O8
31	b	626	LMG	O7-C8-C9-O8
26	D	407	DGD	C8A-C9A-CAA-CBA
27	A	410	LHG	C3-O3-P-O6
27	a	409	LHG	C3-O3-P-O6
22	c	511	CLA	CAA-CBA-CGA-O2A
30	B	622	SQD	O6-C44-C45-C46
31	M	101	LMG	O1-C7-C8-C9
31	d	412	LMG	O1-C7-C8-C9
22	B	611	CLA	C4-C3-C5-C6
22	B	608	CLA	C11-C12-C13-C15
22	B	611	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	H	101	CLA	C11-C10-C8-C7
22	H	101	CLA	C11-C12-C13-C15
22	b	620	CLA	C11-C12-C13-C15
22	B	607	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C12-C13-C14
22	B	615	CLA	C14-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C12-C13-C14
22	c	507	CLA	C14-C13-C15-C16
22	c	508	CLA	C11-C10-C8-C9
22	c	511	CLA	C14-C13-C15-C16
22	d	406	CLA	C11-C10-C8-C9
22	b	607	CLA	C16-C17-C18-C20
22	c	504	CLA	C8-C10-C11-C12
23	D	401	PHO	C13-C15-C16-C17
31	l	101	LMG	C17-C18-C19-C20
22	A	406	CLA	C16-C17-C18-C19
22	c	509	CLA	C16-C17-C18-C20
27	c	519	LHG	O2-C2-C3-O3
31	D	406	LMG	C31-C32-C33-C34
22	C	507	CLA	C5-C6-C7-C8
31	D	409	LMG	C16-C17-C18-C19
27	c	519	LHG	C1-C2-C3-O3
31	M	101	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
22	a	404	CLA	C4-C3-C5-C6
30	a	401	SQD	C9-C10-C11-C12
22	b	610	CLA	C16-C17-C18-C20
22	B	609	CLA	CBA-CGA-O2A-C1
22	b	606	CLA	CBA-CGA-O2A-C1
34	f	101	HEM	C3D-CAD-CBD-CGD
31	b	627	LMG	C16-C17-C18-C19
31	L	101	LMG	C35-C36-C37-C38
31	L	101	LMG	C10-C11-C12-C13
31	d	408	LMG	C16-C17-C18-C19
26	b	601	DGD	O6D-C1D-O3G-C3G
22	b	606	CLA	O1A-CGA-O2A-C1
22	B	607	CLA	C13-C15-C16-C17
22	c	502	CLA	C5-C6-C7-C8
31	c	518	LMG	C13-C14-C15-C16
22	b	618	CLA	C2C-C3C-CAC-CBC
30	A	414	SQD	C12-C13-C14-C15
24	D	405	PL9	C40-C39-C41-C42
32	b	629	LMT	O5'-C5'-C6'-O6'
31	e	101	LMG	C30-C31-C32-C33
22	B	609	CLA	O1A-CGA-O2A-C1
22	a	403	CLA	C2-C1-O2A-CGA
31	B	621	LMG	C15-C16-C17-C18
22	b	617	CLA	C10-C11-C12-C13
22	a	406	CLA	C16-C17-C18-C20
31	B	621	LMG	O1-C7-C8-O7
30	F	103	SQD	C9-C10-C11-C12
31	D	406	LMG	C11-C12-C13-C14
31	d	412	LMG	C16-C17-C18-C19
22	C	512	CLA	C3A-C2A-CAA-CBA
30	a	401	SQD	C12-C13-C14-C15
31	D	406	LMG	C36-C37-C38-C39
31	l	101	LMG	C29-C30-C31-C32
22	B	615	CLA	C11-C12-C13-C14
22	D	404	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
32	B	629	LMT	C2-C3-C4-C5
31	e	101	LMG	O1-C7-C8-C9
22	D	404	CLA	C2A-CAA-CBA-CGA
30	a	412	SQD	C16-C17-C18-C19
22	A	406	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	b	610	CLA	C16-C17-C18-C19
26	A	409	DGD	O6E-C1E-O5D-C6D
26	B	626	DGD	O6D-C1D-O3G-C3G
26	a	408	DGD	O6E-C1E-O5D-C6D
26	c	516	DGD	O6E-C1E-O5D-C6D
31	m	101	LMG	O6-C1-O1-C7
22	b	609	CLA	C8-C10-C11-C12
25	B	617	BCR	C37-C22-C23-C24
27	C	518	LHG	C7-C8-C9-C10
26	B	626	DGD	C2A-C3A-C4A-C5A
31	b	626	LMG	C15-C16-C17-C18
27	a	409	LHG	C6-C5-O7-C7
31	M	101	LMG	C9-C8-O7-C10
31	m	101	LMG	C9-C8-O7-C10
22	C	502	CLA	C5-C6-C7-C8
22	b	615	CLA	C4-C3-C5-C6
22	c	512	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C12-C13-C15
22	B	605	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	519	CLA	C6-C7-C8-C10
22	a	406	CLA	C11-C10-C8-C7
22	b	609	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C12-C13-C15
22	B	605	CLA	C13-C15-C16-C17
22	b	607	CLA	C15-C16-C17-C18
22	c	509	CLA	C13-C15-C16-C17
26	C	514	DGD	C5A-C6A-C7A-C8A
32	i	103	LMT	C7-C8-C9-C10
22	B	603	CLA	CBA-CGA-O2A-C1
22	c	502	CLA	CBA-CGA-O2A-C1
32	D	408	LMT	O5B-C5B-C6B-O6B
31	L	101	LMG	C13-C14-C15-C16
22	C	504	CLA	C8-C10-C11-C12
22	b	617	CLA	C8-C10-C11-C12
31	c	518	LMG	C17-C18-C19-C20
31	D	406	LMG	C34-C35-C36-C37
31	m	101	LMG	C17-C18-C19-C20
22	B	612	CLA	C13-C15-C16-C17
22	B	610	CLA	C4-C3-C5-C6
24	A	407	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
26	B	620	DGD	C7B-C8B-C9B-CAB
22	A	403	CLA	C2-C3-C5-C6
24	D	405	PL9	C13-C14-C16-C17
22	b	607	CLA	C8-C10-C11-C12
22	B	613	CLA	C4C-C3C-CAC-CBC
31	l	101	LMG	C39-C40-C41-C42
26	C	515	DGD	C2E-C1E-O5D-C6D
22	B	612	CLA	C8-C10-C11-C12
26	d	410	DGD	C8A-C9A-CAA-CBA
30	a	401	SQD	C17-C18-C19-C20
22	c	507	CLA	C5-C6-C7-C8
26	c	517	DGD	C5B-C6B-C7B-C8B
26	b	601	DGD	C2A-C3A-C4A-C5A
31	C	517	LMG	C17-C18-C19-C20
31	L	101	LMG	O6-C1-O1-C7
31	c	522	LMG	C30-C31-C32-C33
22	C	510	CLA	C4-C3-C5-C6
22	A	403	CLA	C2-C1-O2A-CGA
24	d	407	PL9	C42-C43-C44-C46
30	A	413	SQD	C16-C17-C18-C19
31	M	101	LMG	C17-C18-C19-C20
22	b	619	CLA	C11-C12-C13-C14
22	c	503	CLA	C6-C7-C8-C9
22	c	502	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	O1A-CGA-O2A-C1
26	b	625	DGD	C4A-C5A-C6A-C7A
30	F	103	SQD	C15-C16-C17-C18
34	V	201	HEM	CAA-CBA-CGA-O2A
22	b	618	CLA	C4C-C3C-CAC-CBC
25	B	616	BCR	C23-C24-C25-C30
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C30
25	C	520	BCR	C1-C6-C7-C8
25	F	102	BCR	C23-C24-C25-C30
25	H	102	BCR	C23-C24-C25-C30
25	b	622	BCR	C1-C6-C7-C8
25	b	623	BCR	C1-C6-C7-C8
25	b	623	BCR	C23-C24-C25-C30
25	c	514	BCR	C5-C6-C7-C8
25	c	521	BCR	C1-C6-C7-C8
25	f	102	BCR	C23-C24-C25-C30
31	D	409	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	M	101	LMG	C31-C32-C33-C34
22	B	611	CLA	C10-C11-C12-C13
22	b	617	CLA	C13-C15-C16-C17
31	m	101	LMG	C31-C32-C33-C34
22	c	510	CLA	C4-C3-C5-C6
25	C	513	BCR	C7-C8-C9-C10
31	e	101	LMG	C14-C15-C16-C17
22	B	611	CLA	C2-C3-C5-C6
30	A	414	SQD	C26-C27-C28-C29
31	D	409	LMG	C36-C37-C38-C39
22	B	609	CLA	C13-C15-C16-C17
26	B	626	DGD	C2G-C3G-O3G-C1D
26	b	601	DGD	C2G-C3G-O3G-C1D
31	D	409	LMG	C8-C7-O1-C1
26	B	620	DGD	CCA-CDA-CEA-CFA
26	a	408	DGD	C2A-C3A-C4A-C5A
22	C	510	CLA	C3-C5-C6-C7
31	m	101	LMG	C11-C12-C13-C14
22	C	506	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	C2A-CAA-CBA-CGA
22	H	101	CLA	C2A-CAA-CBA-CGA
22	d	406	CLA	C2A-CAA-CBA-CGA
30	d	403	SQD	C7-C8-C9-C10
26	B	626	DGD	CAB-CBB-CCB-CDB
31	l	101	LMG	O6-C1-O1-C7
26	c	516	DGD	C7B-C8B-C9B-CAB
31	E	101	LMG	C31-C32-C33-C34
26	b	601	DGD	C4E-C5E-C6E-O5E
22	b	606	CLA	C12-C13-C15-C16
22	c	503	CLA	C6-C7-C8-C10
26	c	517	DGD	C8B-C9B-CAB-CBB
26	A	409	DGD	C2E-C1E-O5D-C6D
26	a	408	DGD	C2E-C1E-O5D-C6D
31	e	101	LMG	C11-C12-C13-C14
31	d	408	LMG	C29-C30-C31-C32
27	C	518	LHG	O7-C7-C8-C9
26	c	517	DGD	CBB-CCB-CDB-CEB
31	m	101	LMG	C16-C17-C18-C19
26	D	407	DGD	O6E-C5E-C6E-O5E
22	d	405	CLA	CAA-CBA-CGA-O2A
27	c	519	LHG	O7-C7-C8-C9
31	L	101	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C4-C3-C5-C6
22	b	612	CLA	C4-C3-C5-C6
24	D	405	PL9	C20-C19-C21-C22
26	b	625	DGD	CAB-CBB-CCB-CDB
30	a	412	SQD	C11-C10-C9-C8
22	b	615	CLA	C2-C3-C5-C6
31	l	101	LMG	C38-C39-C40-C41
22	B	612	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
22	B	605	CLA	C6-C7-C8-C9
22	B	614	CLA	C6-C7-C8-C9
22	C	519	CLA	C6-C7-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	609	CLA	C11-C12-C13-C14
22	b	612	CLA	C11-C12-C13-C14
22	b	614	CLA	C11-C12-C13-C14
22	b	619	CLA	C6-C7-C8-C9
22	c	520	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C10-C8-C9
23	d	402	PHO	C6-C7-C8-C9
26	C	515	DGD	C6A-C7A-C8A-C9A
22	C	519	CLA	C3A-C2A-CAA-CBA
22	D	403	CLA	C3A-C2A-CAA-CBA
26	c	517	DGD	O1G-C1A-C2A-C3A
26	d	410	DGD	O6E-C5E-C6E-O5E
22	B	603	CLA	C2C-C3C-CAC-CBC
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	C	502	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	c	501	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
23	A	405	PHO	CAD-CBD-CGD-O2D
27	A	410	LHG	C4-C5-O7-C7
27	a	409	LHG	C4-C5-O7-C7
31	B	625	LMG	C29-C30-C31-C32
22	A	402	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	c	522	LMG	C32-C33-C34-C35
30	a	401	SQD	C23-C24-C25-C26
22	B	611	CLA	CAA-CBA-CGA-O2A
22	C	506	CLA	CAA-CBA-CGA-O2A
31	l	101	LMG	O7-C10-C11-C12
22	B	603	CLA	C4C-C3C-CAC-CBC
31	M	101	LMG	C16-C17-C18-C19
22	A	406	CLA	C4-C3-C5-C6
22	b	611	CLA	C4-C3-C5-C6
22	B	605	CLA	C16-C17-C18-C20
22	c	504	CLA	C3-C5-C6-C7
34	v	201	HEM	CAA-CBA-CGA-O2A
22	B	610	CLA	C2-C3-C5-C6
22	c	510	CLA	C2-C3-C5-C6
31	b	627	LMG	O7-C10-C11-C12
30	A	413	SQD	C12-C13-C14-C15
26	C	514	DGD	C1G-C2G-C3G-O3G
31	C	517	LMG	C7-C8-C9-O8
31	E	101	LMG	O1-C7-C8-C9
31	I	101	LMG	C7-C8-C9-O8
31	c	518	LMG	C7-C8-C9-O8
31	d	408	LMG	C7-C8-C9-O8
26	A	409	DGD	O6D-C5D-C6D-O5D
22	c	501	CLA	CAA-CBA-CGA-O2A
26	c	516	DGD	CEB-CFB-CGB-CHB
34	V	201	HEM	CAA-CBA-CGA-O1A
30	a	412	SQD	C32-C33-C34-C35
22	B	615	CLA	O2A-C1-C2-C3
22	C	511	CLA	O2A-C1-C2-C3
22	b	620	CLA	O2A-C1-C2-C3
22	c	511	CLA	O2A-C1-C2-C3
23	D	401	PHO	O2A-C1-C2-C3
23	d	402	PHO	O2A-C1-C2-C3
26	C	516	DGD	O1A-C1A-O1G-C1G
22	b	607	CLA	C2A-CAA-CBA-CGA
26	C	516	DGD	O1G-C1A-C2A-C3A
30	a	401	SQD	O47-C7-C8-C9
31	C	521	LMG	O8-C28-C29-C30
26	A	409	DGD	O1A-C1A-O1G-C1G
31	M	101	LMG	O10-C28-O8-C9
26	D	407	DGD	CBB-CCB-CDB-CEB
31	d	408	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	A	404	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	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	618	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	C	501	CLA	CAA-CBA-CGA-O2A
31	a	402	LMG	O7-C10-C11-C12
26	B	620	DGD	CAB-CBB-CCB-CDB
31	B	621	LMG	C35-C36-C37-C38
31	C	521	LMG	C32-C33-C34-C35
22	C	506	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C20
22	c	509	CLA	CAA-CBA-CGA-O2A
30	A	414	SQD	O47-C7-C8-C9
26	B	626	DGD	C4E-C5E-C6E-O5E
31	b	626	LMG	O1-C7-C8-O7
31	d	412	LMG	O1-C7-C8-O7
22	C	501	CLA	C13-C15-C16-C17
22	c	503	CLA	C15-C16-C17-C18
22	c	503	CLA	C2A-CAA-CBA-CGA
23	d	402	PHO	CHA-CBD-CGD-O1D
30	B	622	SQD	C7-C8-C9-C10
32	d	411	LMT	C1-C2-C3-C4
26	c	517	DGD	O2G-C1B-C2B-C3B
26	D	407	DGD	C6A-C7A-C8A-C9A
26	b	601	DGD	CAB-CBB-CCB-CDB
26	A	409	DGD	C4D-C5D-C6D-O5D
22	B	602	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C12-C13-C15
22	b	619	CLA	C11-C12-C13-C15
22	c	512	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	CAA-CBA-CGA-O2A
31	c	522	LMG	O8-C28-C29-C30
22	B	601	CLA	C14-C13-C15-C16
22	B	604	CLA	C11-C12-C13-C14
22	C	505	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C12-C13-C14
22	C	512	CLA	C11-C12-C13-C14
22	a	406	CLA	C11-C10-C8-C9
22	b	606	CLA	C11-C10-C8-C9
22	b	606	CLA	C11-C12-C13-C14
22	b	610	CLA	C6-C7-C8-C9
26	D	407	DGD	C9B-CAB-CBB-CCB
30	a	412	SQD	C24-C25-C26-C27
22	A	404	CLA	CBA-CGA-O2A-C1
30	B	622	SQD	O49-C7-C8-C9
22	C	502	CLA	C16-C17-C18-C20
22	A	404	CLA	O1A-CGA-O2A-C1
30	A	413	SQD	C8-C7-O47-C45
30	a	412	SQD	C8-C7-O47-C45
22	A	403	CLA	C2A-CAA-CBA-CGA
22	D	403	CLA	CAA-CBA-CGA-O2A
22	b	616	CLA	CAA-CBA-CGA-O2A
22	B	612	CLA	CAA-CBA-CGA-O1A
22	b	617	CLA	CAA-CBA-CGA-O1A
31	d	412	LMG	O9-C10-C11-C12
30	d	403	SQD	C12-C13-C14-C15
30	B	627	SQD	C15-C16-C17-C18
22	c	506	CLA	CAA-CBA-CGA-O1A
22	B	605	CLA	C15-C16-C17-C18
22	C	512	CLA	C1A-C2A-CAA-CBA
22	C	519	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C1A-C2A-CAA-CBA
22	d	405	CLA	C1A-C2A-CAA-CBA
22	d	405	CLA	CAA-CBA-CGA-O1A
34	v	201	HEM	CAA-CBA-CGA-O1A
31	a	402	LMG	C12-C13-C14-C15
26	b	625	DGD	O1A-C1A-O1G-C1G
26	c	517	DGD	C4A-C5A-C6A-C7A
26	d	410	DGD	C9B-CAB-CBB-CCB
22	H	101	CLA	CBA-CGA-O2A-C1
31	D	409	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	d	409	LMG	O9-C10-C11-C12
30	a	401	SQD	C25-C26-C27-C28
26	c	515	DGD	C1G-C2G-C3G-O3G
26	C	516	DGD	O2G-C1B-C2B-C3B
30	d	403	SQD	O47-C7-C8-C9
22	a	404	CLA	C2A-CAA-CBA-CGA
32	B	624	LMT	C6-C7-C8-C9
24	J	101	PL9	C2-C3-C7-C8
22	B	605	CLA	C16-C17-C18-C19
22	C	501	CLA	CAA-CBA-CGA-O1A
22	C	506	CLA	CAA-CBA-CGA-O1A
22	b	616	CLA	CAA-CBA-CGA-O1A
30	d	403	SQD	O49-C7-C8-C9
31	l	101	LMG	O9-C10-C11-C12
22	B	611	CLA	CAA-CBA-CGA-O1A
30	A	414	SQD	O49-C7-C8-C9
22	a	404	CLA	C2-C3-C5-C6
26	c	516	DGD	C2E-C1E-O5D-C6D
31	M	101	LMG	C2-C1-O1-C7
26	b	625	DGD	C7B-C8B-C9B-CAB
31	M	101	LMG	C11-C12-C13-C14
27	A	410	LHG	C3-O3-P-O5
30	A	414	SQD	C18-C19-C20-C21
30	B	627	SQD	C19-C20-C21-C22
22	c	501	CLA	CAA-CBA-CGA-O1A
31	a	402	LMG	O9-C10-C11-C12
26	C	514	DGD	O6D-C1D-O3G-C3G
31	m	101	LMG	O10-C28-O8-C9
32	b	628	LMT	C4-C5-C6-C7
22	B	605	CLA	C3-C5-C6-C7
25	B	617	BCR	C5-C6-C7-C8
25	B	618	BCR	C23-C24-C25-C26
25	C	513	BCR	C5-C6-C7-C8
25	C	520	BCR	C5-C6-C7-C8
25	H	102	BCR	C23-C24-C25-C26
25	b	623	BCR	C5-C6-C7-C8
25	b	623	BCR	C23-C24-C25-C26
25	c	521	BCR	C5-C6-C7-C8
22	c	508	CLA	C8-C10-C11-C12
22	H	101	CLA	O1A-CGA-O2A-C1
31	d	409	LMG	O7-C10-C11-C12
26	C	516	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	C16-C17-C18-C20
22	C	502	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C15-C16-C17-C18
30	b	602	SQD	C15-C16-C17-C18
30	A	413	SQD	C9-C10-C11-C12
26	d	410	DGD	C6A-C7A-C8A-C9A
22	C	501	CLA	CAD-CBD-CGD-O1D
22	C	512	CLA	CAD-CBD-CGD-O1D
30	B	622	SQD	O5-C5-C6-S
30	B	627	SQD	C5-C6-S-O9
30	a	401	SQD	C5-C6-S-O9
31	C	521	LMG	O10-C28-C29-C30
22	C	509	CLA	CAA-CBA-CGA-O2A
22	b	618	CLA	CAA-CBA-CGA-O2A
22	B	602	CLA	C11-C10-C8-C9
22	B	610	CLA	C11-C12-C13-C14
22	B	614	CLA	C11-C12-C13-C14
22	C	503	CLA	C6-C7-C8-C9
22	D	403	CLA	C11-C10-C8-C9
22	b	616	CLA	C6-C7-C8-C9
22	c	503	CLA	C14-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C12-C13-C14
22	c	506	CLA	CBD-CGD-O2D-CED
30	A	414	SQD	C25-C26-C27-C28
22	C	509	CLA	C13-C15-C16-C17
22	B	613	CLA	O1A-CGA-O2A-C1
26	c	517	DGD	C4B-C5B-C6B-C7B
22	B	609	CLA	CAA-CBA-CGA-O2A
26	B	620	DGD	O2G-C1B-C2B-C3B
30	B	622	SQD	O47-C7-C8-C9
30	d	403	SQD	C11-C10-C9-C8
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	606	CLA	CAA-CBA-CGA-O2A
22	c	504	CLA	CAA-CBA-CGA-O2A
22	a	404	CLA	C2C-C3C-CAC-CBC
22	b	612	CLA	C13-C15-C16-C17
22	C	503	CLA	C6-C7-C8-C10
22	C	510	CLA	C2-C3-C5-C6
22	D	403	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	H	101	CLA	C12-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C10
22	b	606	CLA	C11-C12-C13-C15
22	b	610	CLA	C6-C7-C8-C10
22	b	616	CLA	C6-C7-C8-C10
22	c	505	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C12-C13-C15
22	c	507	CLA	C11-C12-C13-C15
24	A	407	PL9	C28-C29-C31-C32
24	a	407	PL9	C28-C29-C31-C32
22	b	614	CLA	CAA-CBA-CGA-O1A
22	c	509	CLA	CAA-CBA-CGA-O1A
26	a	408	DGD	O6D-C5D-C6D-O5D
22	b	605	CLA	CAA-CBA-CGA-O2A
22	b	614	CLA	CAA-CBA-CGA-O2A
31	I	101	LMG	O7-C10-C11-C12
31	L	101	LMG	C39-C40-C41-C42
31	D	406	LMG	C12-C13-C14-C15
32	b	604	LMT	C11-C10-C9-C8
25	F	102	BCR	C21-C22-C23-C24
25	f	102	BCR	C21-C22-C23-C24
22	B	613	CLA	CAA-CBA-CGA-O1A
22	b	605	CLA	CAA-CBA-CGA-O1A
30	A	413	SQD	O49-C7-C8-C9
24	A	407	PL9	C2-C3-C7-C8
22	B	601	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
22	c	508	CLA	CAA-CBA-CGA-O2A
22	C	502	CLA	O1A-CGA-O2A-C1
30	a	401	SQD	O49-C7-C8-C9
30	a	412	SQD	O49-C7-C8-C9
26	C	516	DGD	C4A-C5A-C6A-C7A
31	d	412	LMG	C11-C12-C13-C14
26	C	516	DGD	C6A-C7A-C8A-C9A
22	D	403	CLA	CAA-CBA-CGA-O1A
26	C	516	DGD	O1A-C1A-C2A-C3A
26	c	517	DGD	O1A-C1A-C2A-C3A
22	b	606	CLA	C2A-CAA-CBA-CGA
31	e	101	LMG	C32-C33-C34-C35
31	l	101	LMG	C12-C13-C14-C15
27	c	519	LHG	C11-C12-C13-C14
22	b	618	CLA	CAA-CBA-CGA-O1A

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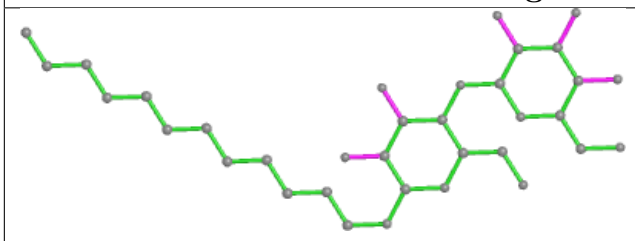
Mol	Chain	Res	Type	Atoms
31	i	102	LMG	O7-C10-C11-C12

There are no ring outliers.

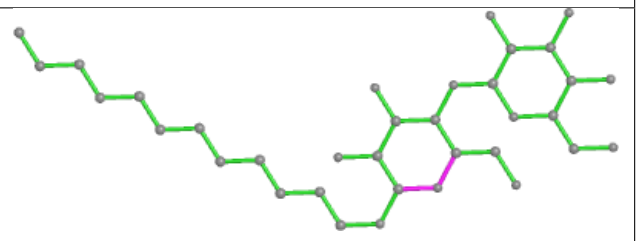
No monomer is involved in short contacts.

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.

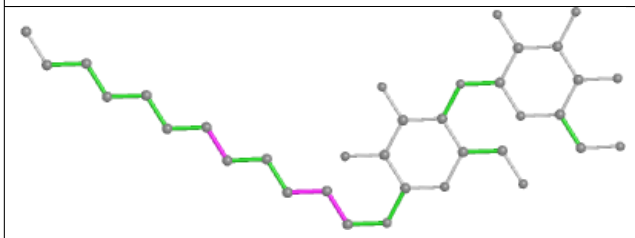
Ligand LMT b 628



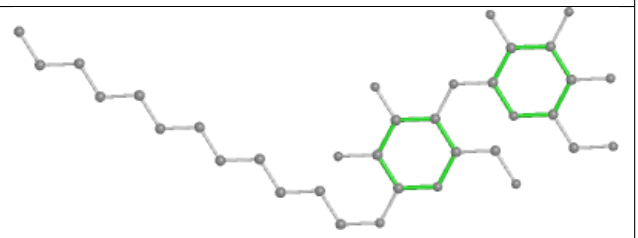
Bond lengths



Bond angles

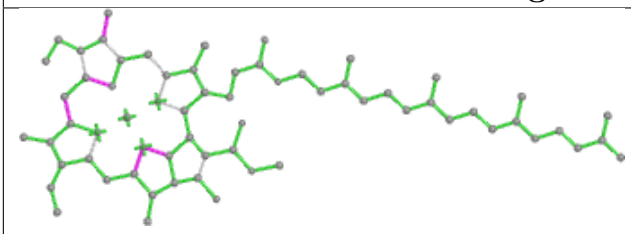


Torsions

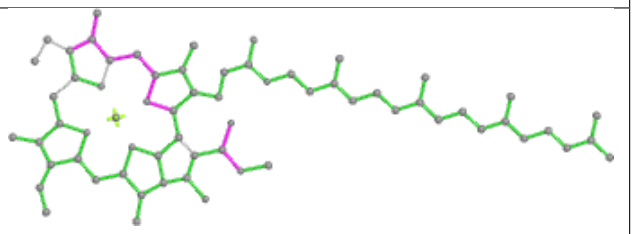


Rings

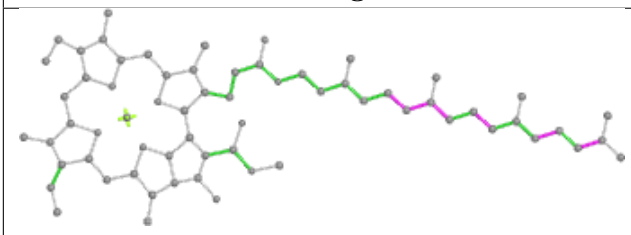
Ligand CLA a 406



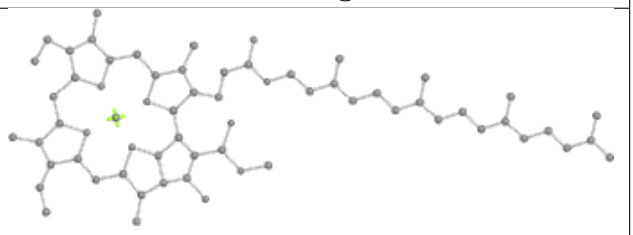
Bond lengths



Bond angles

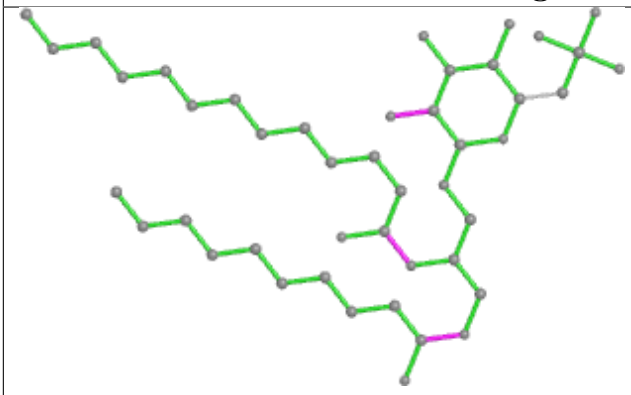


Torsions



Rings

Ligand SQD f 103



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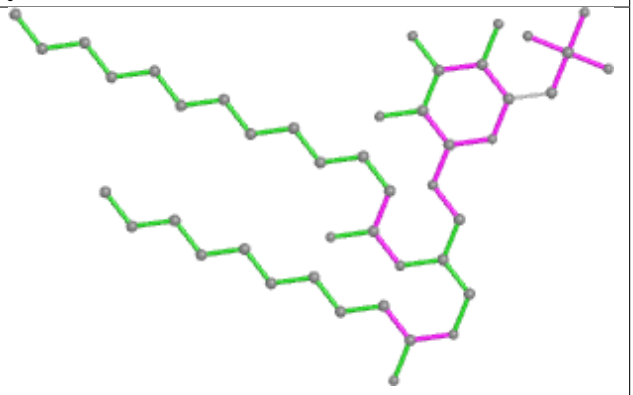
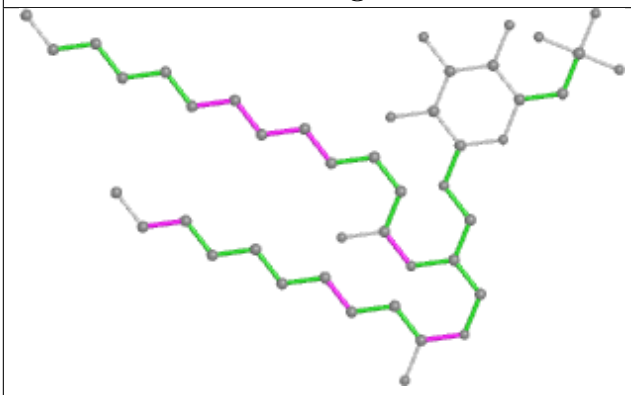
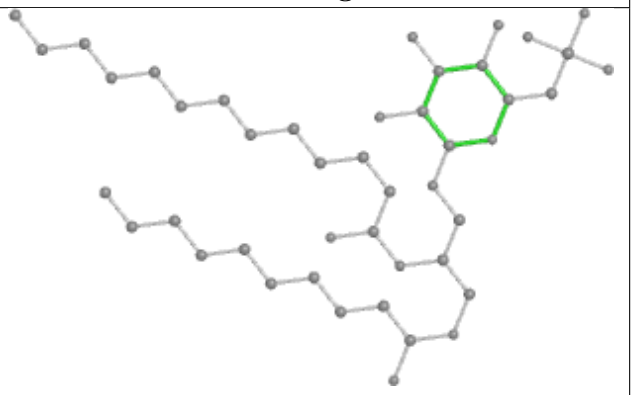


Bond angles

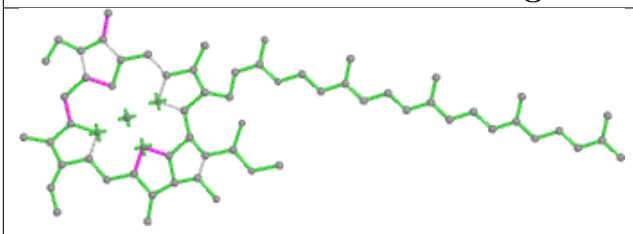


Torsions



Rings

Ligand CLA B 604



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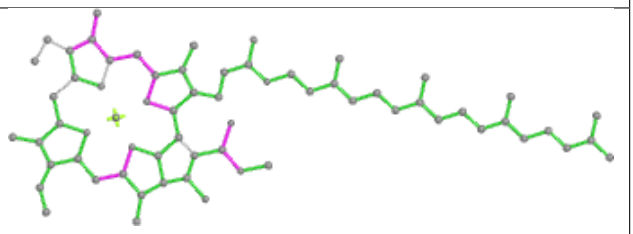
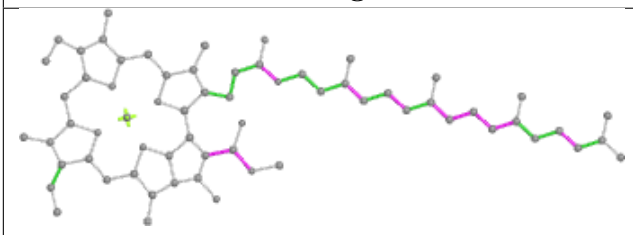


Bond angles



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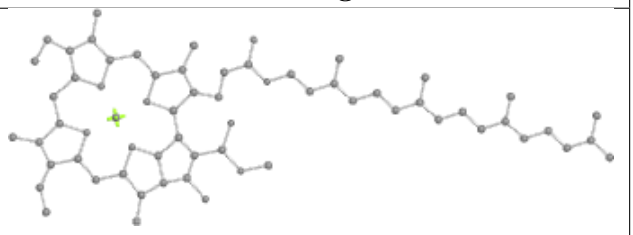
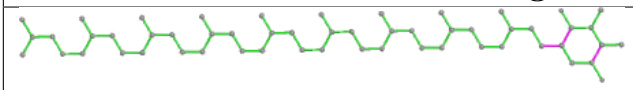


Rings

Ligand PL9 D 405



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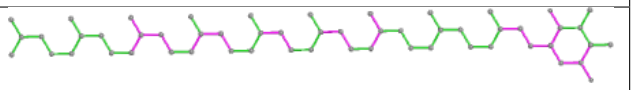
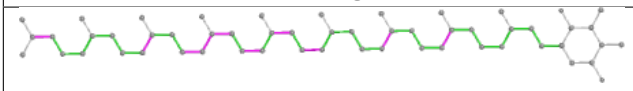


Bond angles



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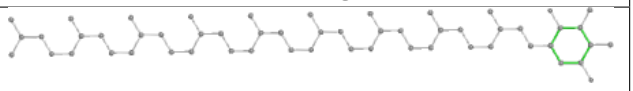
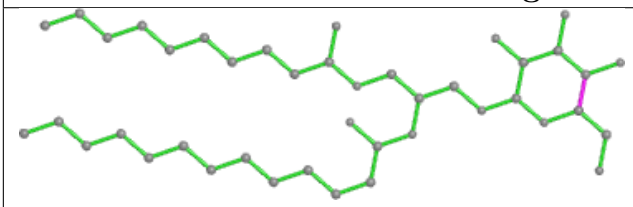


Rings

Ligand LMG b 627



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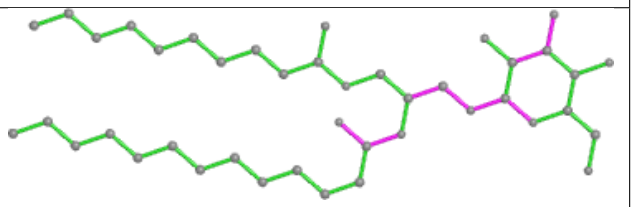
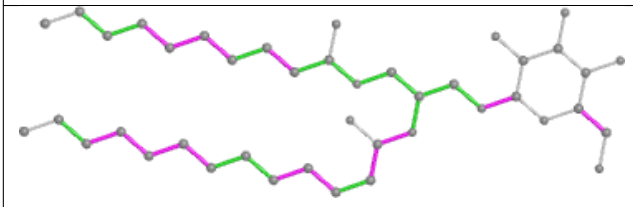


Bond angles



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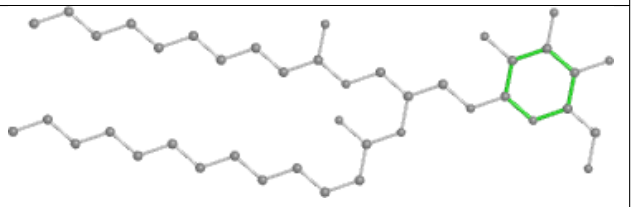
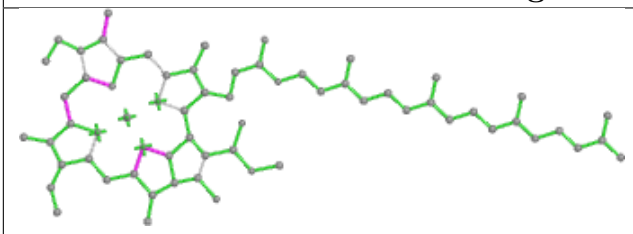


Rings

Ligand CLA b 618



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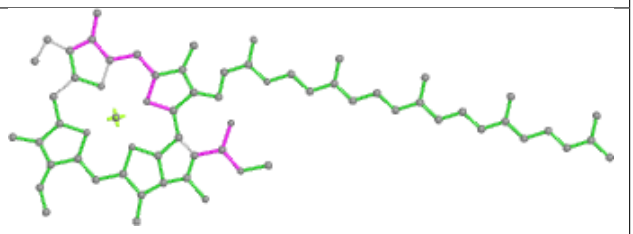

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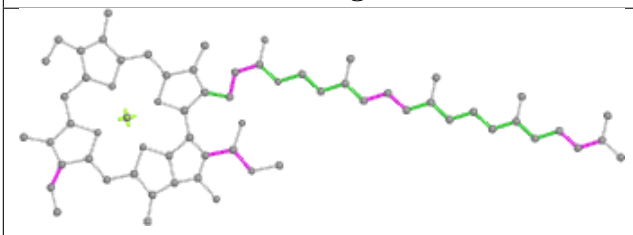

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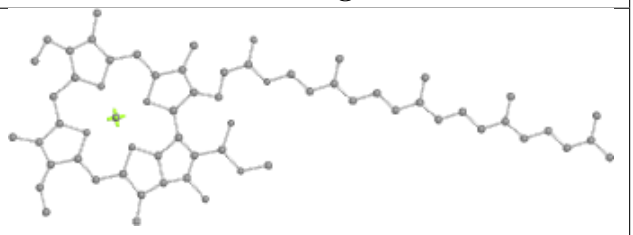
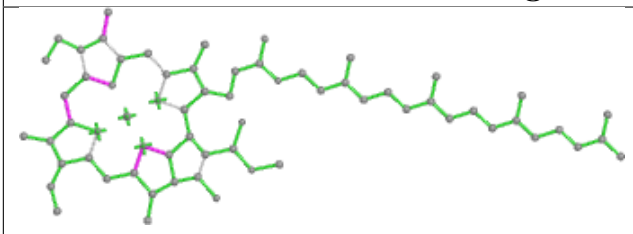


Rings

Ligand CLA C 512



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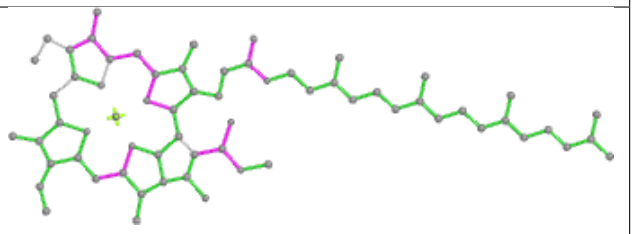
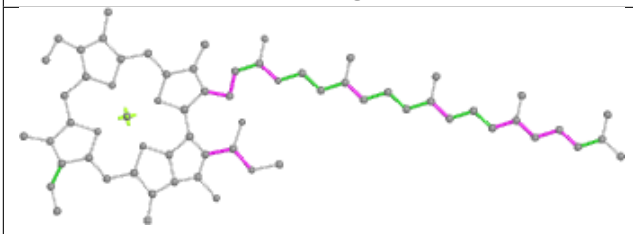


Bond angles



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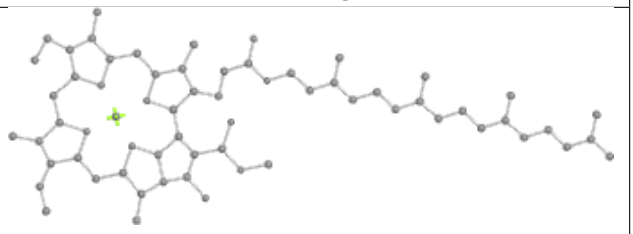
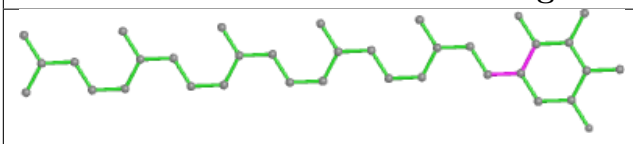


Rings

Ligand PL9 j 101



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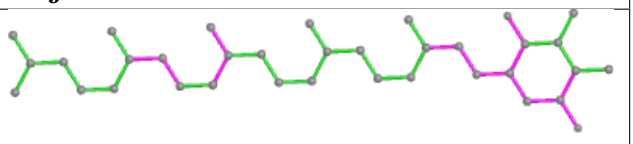
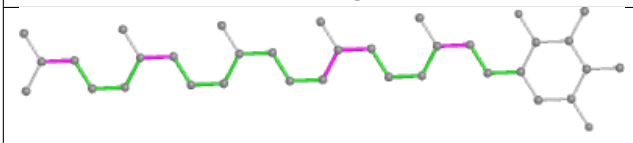


Bond angles



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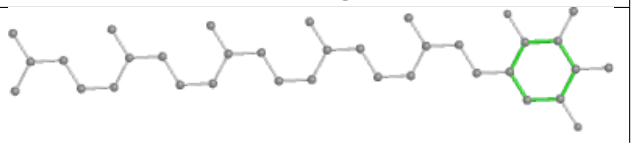
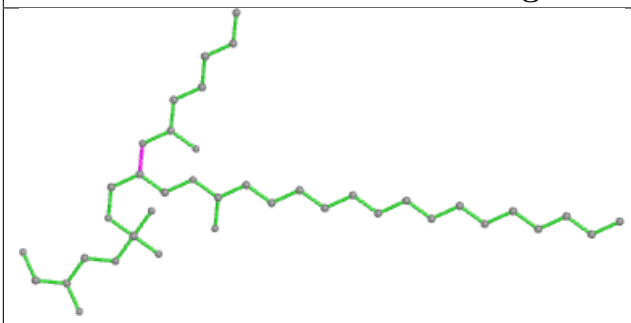


Rings

Ligand LHG A 410



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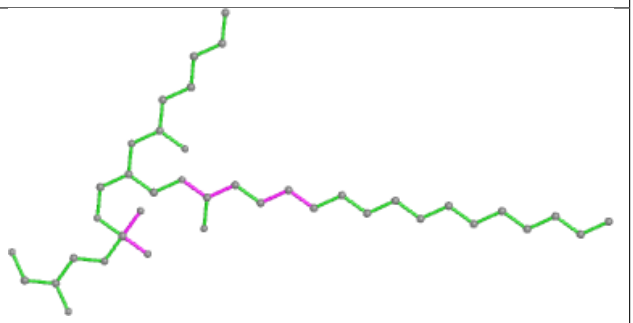
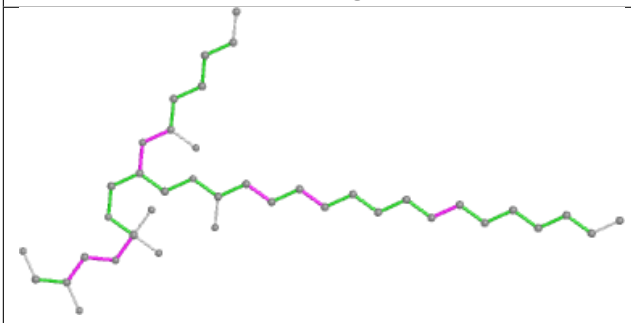


Bond angles



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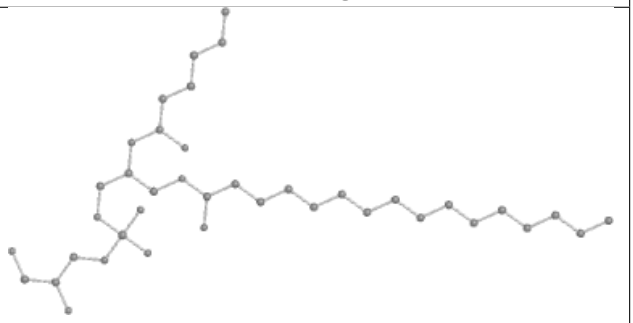
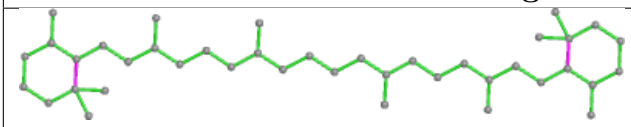


Rings

Ligand BCR A 408



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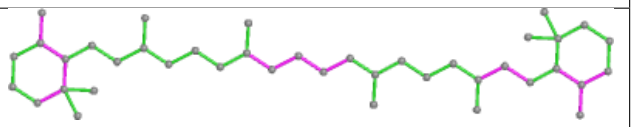
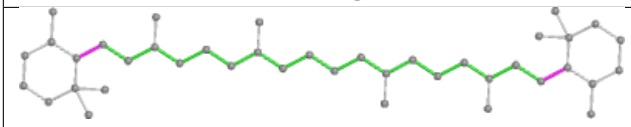


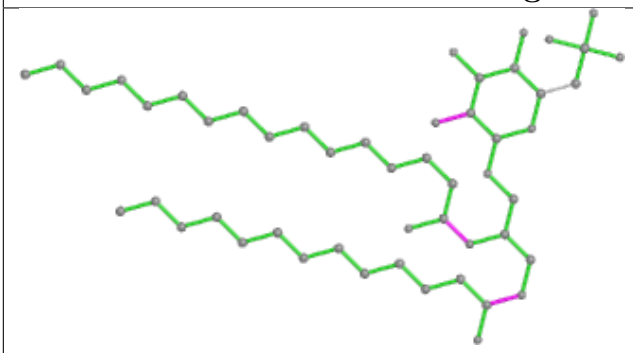
Bond angles



Torsions

Rings

Ligand SQD A 413



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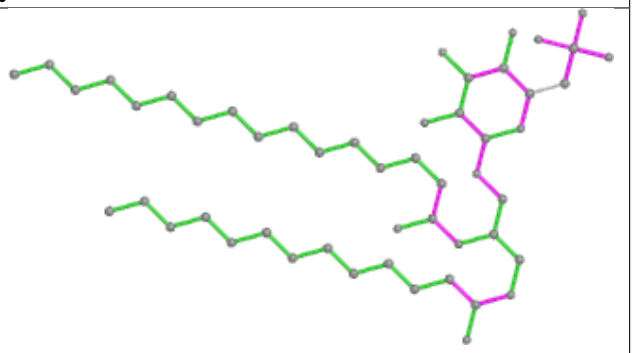
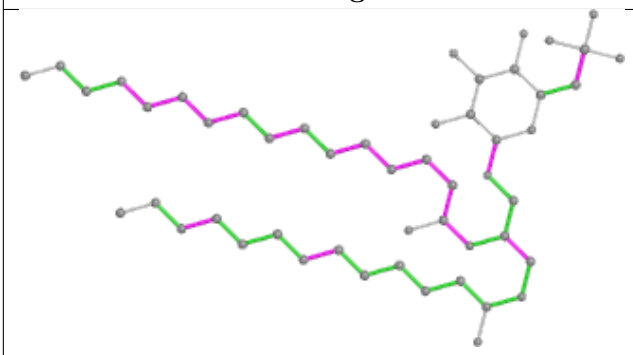


Bond angles



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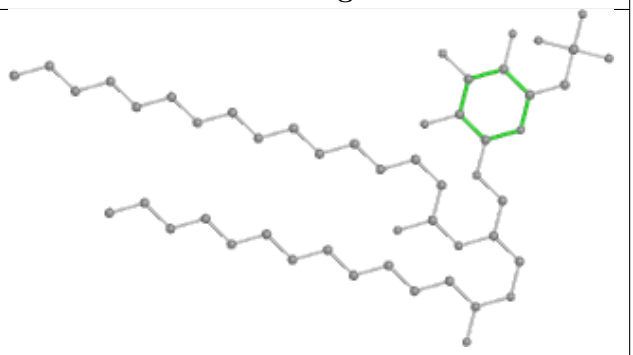
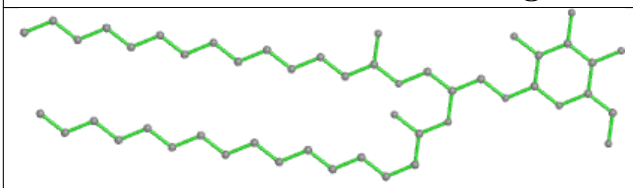


Rings

Ligand LMG d 408



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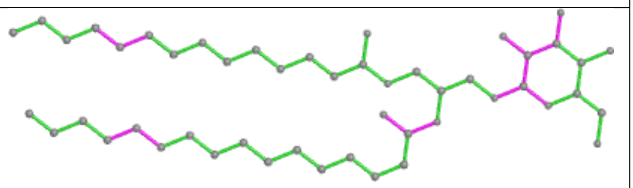
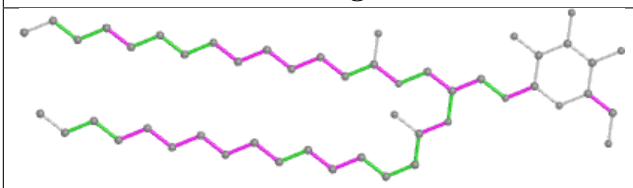
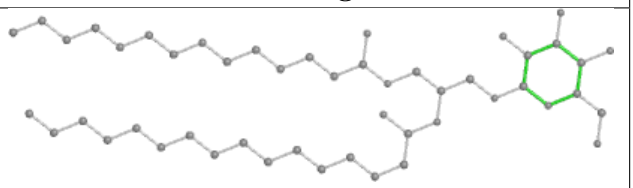


Bond angles

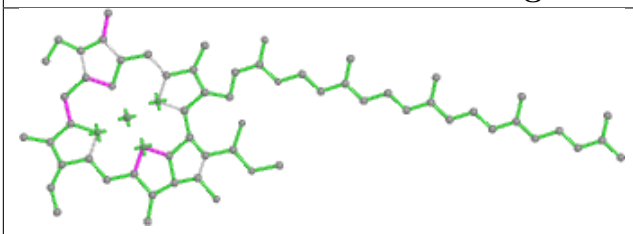


Torsions



Rings

Ligand CLA C 505



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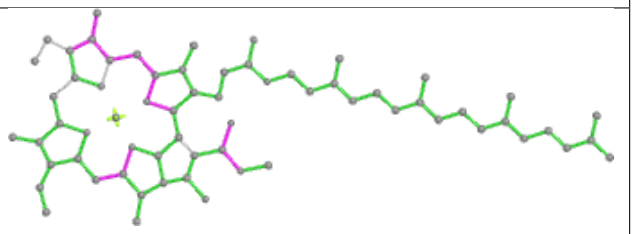
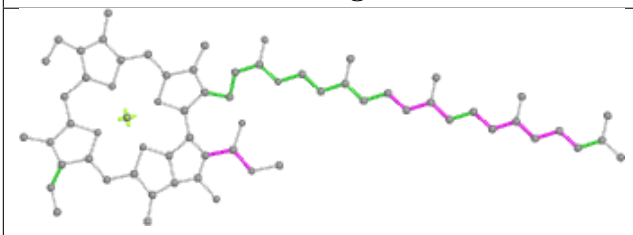


Bond angles



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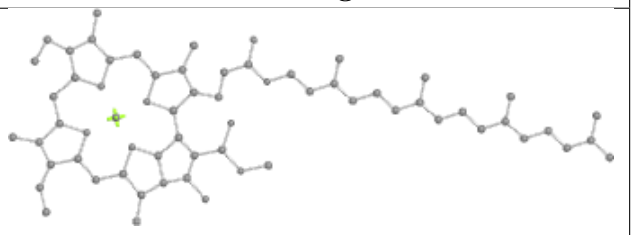
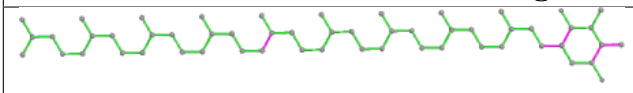


Rings

Ligand PL9 d 407



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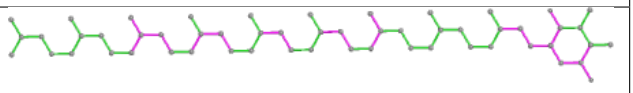
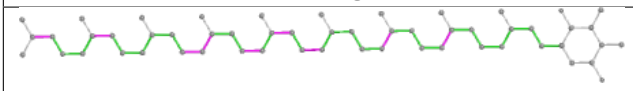
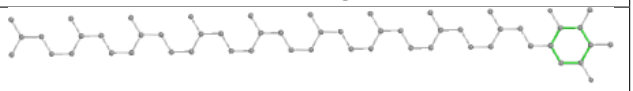


Bond angles

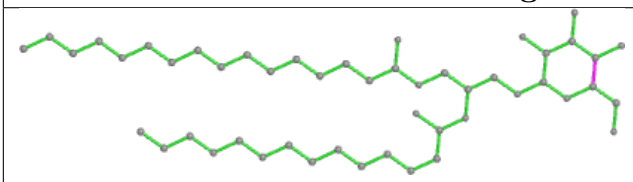


Torsions

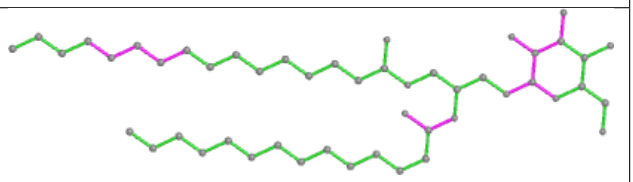


Rings

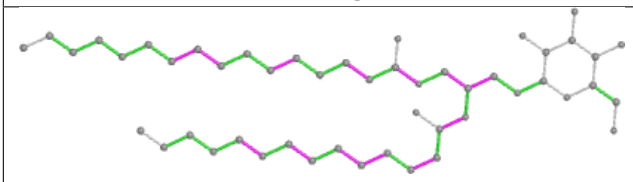
Ligand LMG B 621



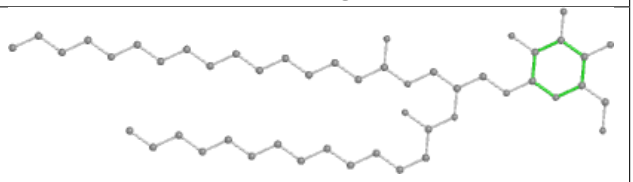
Bond lengths



Bond angles

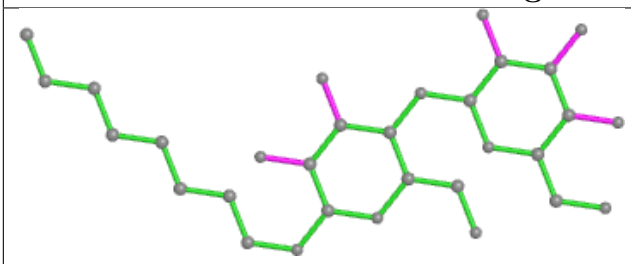


Torsions

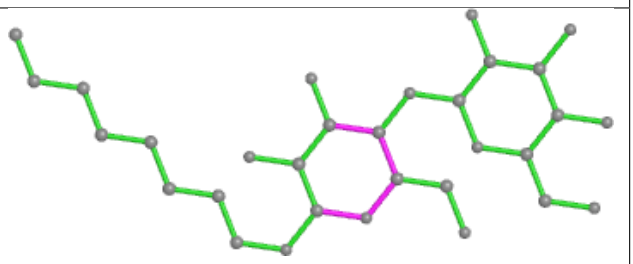


Rings

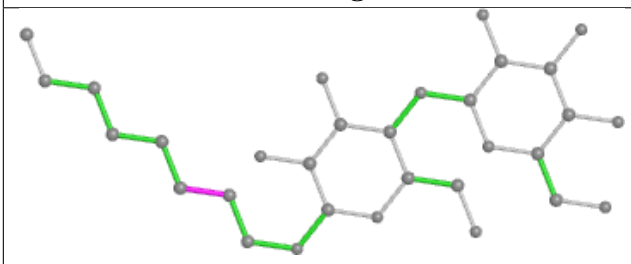
Ligand LMT d 411



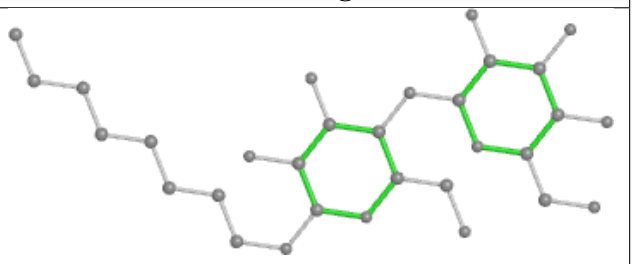
Bond lengths



Bond angles

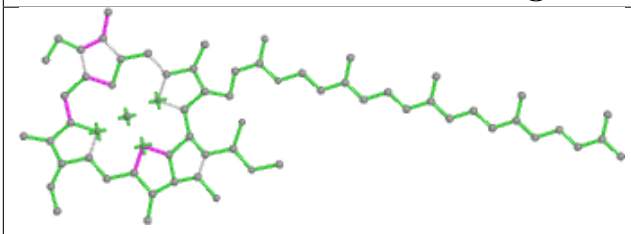


Torsions

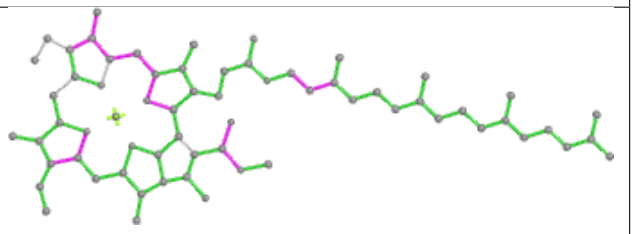


Rings

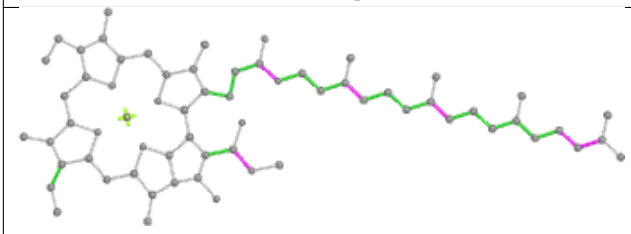
Ligand CLA b 615



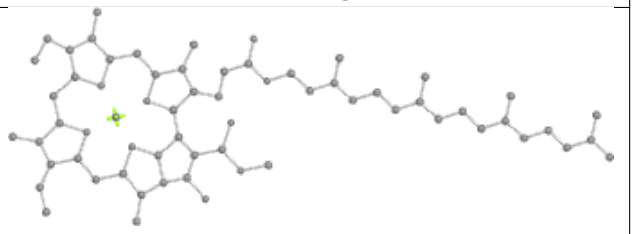
Bond lengths



Bond angles

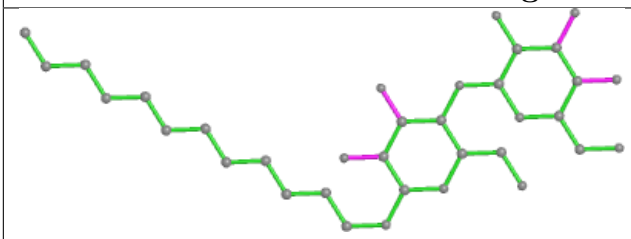


Torsions



Rings

Ligand LMT B 624



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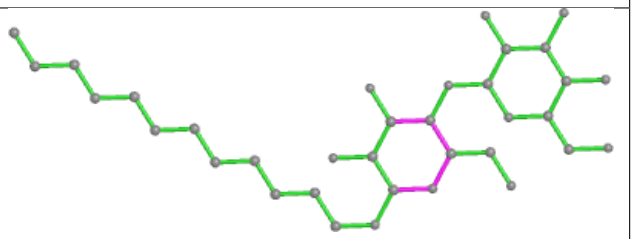
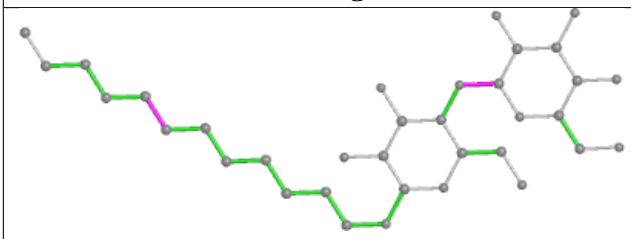
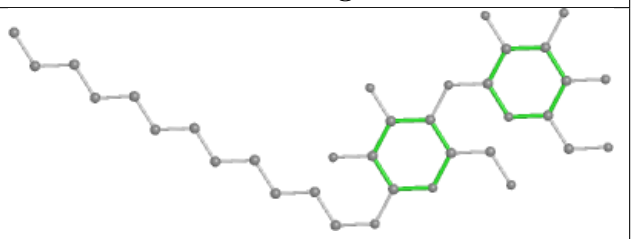


Bond angles

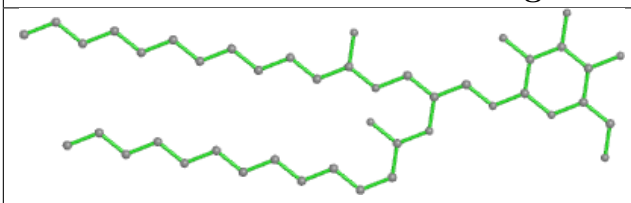


Torsions

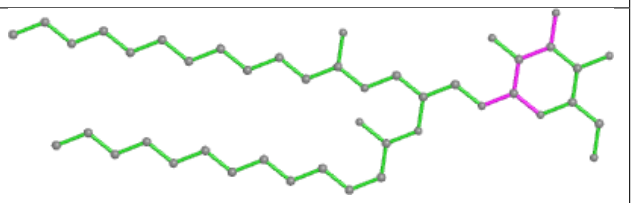


Rings

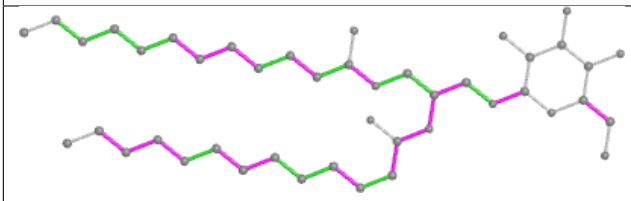
Ligand LMG e 101



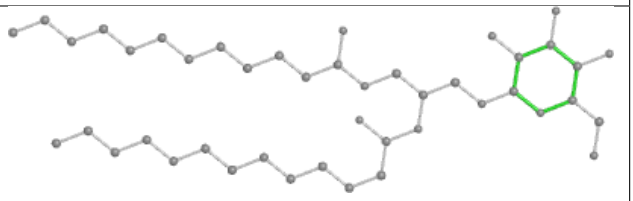
Bond lengths



Bond angles

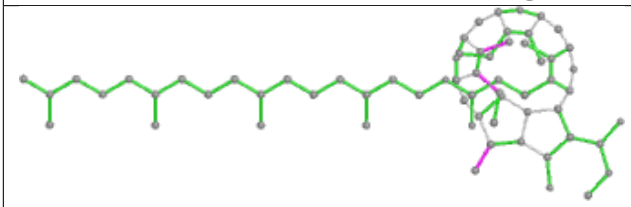


Torsions



Rings

Ligand PHO D 401



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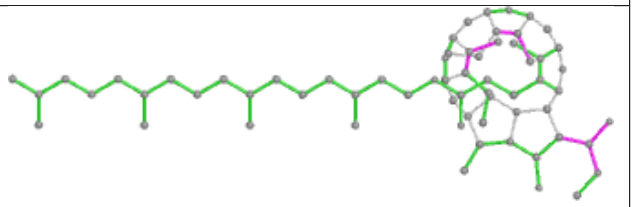
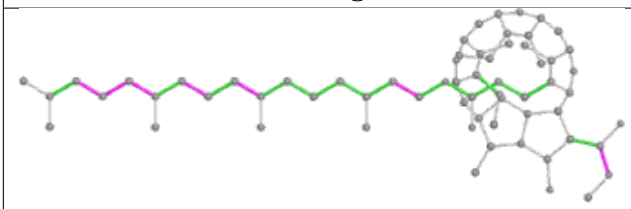


Bond angles



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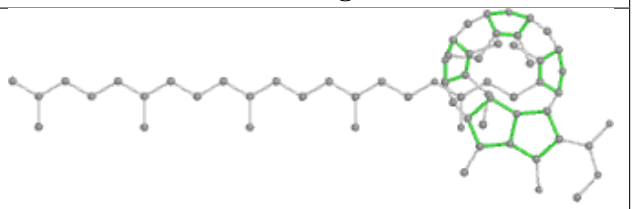
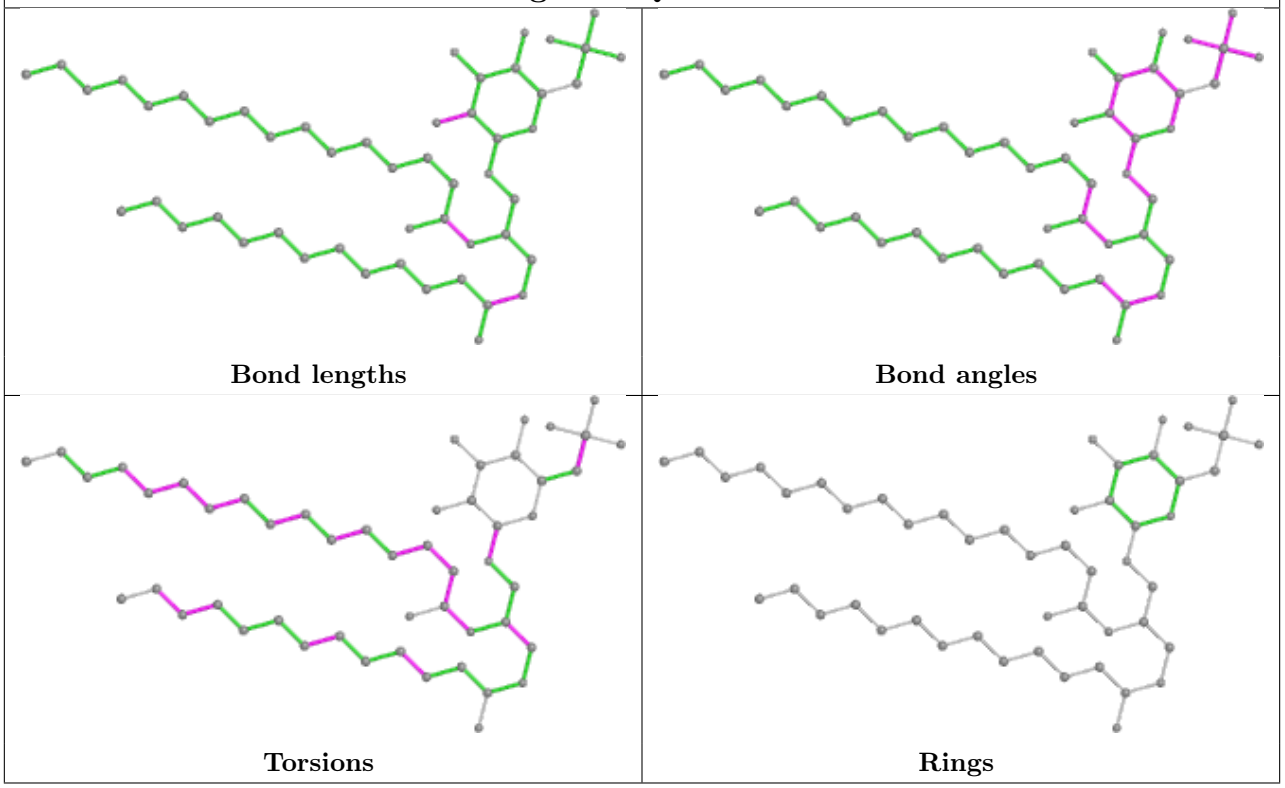
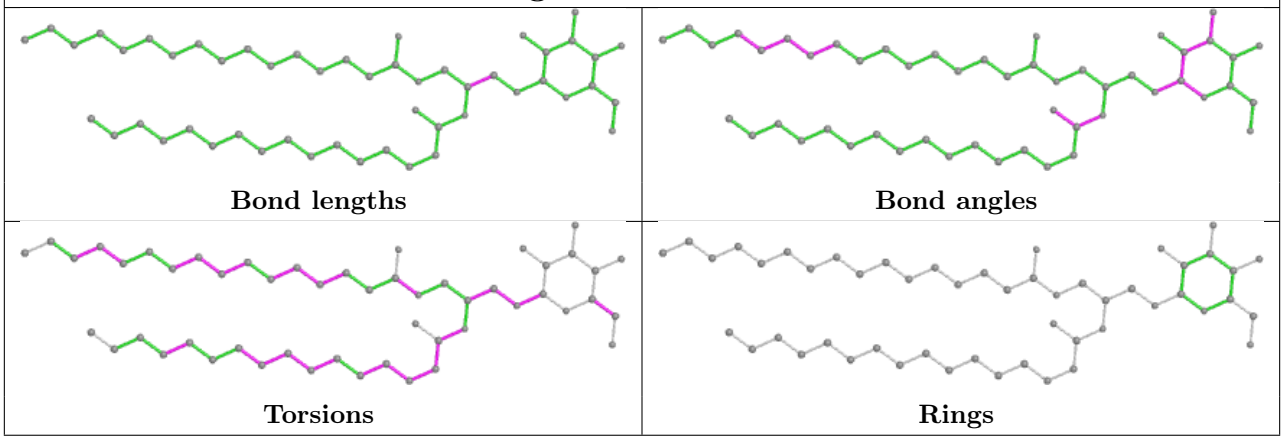


Rings

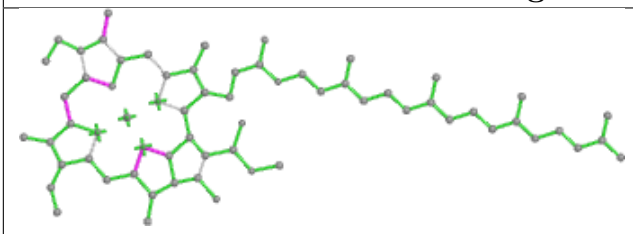
Ligand SQD a 412



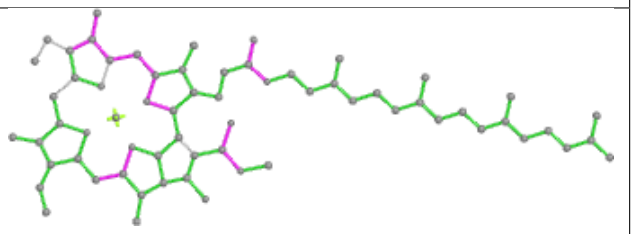
Ligand LMG l 101



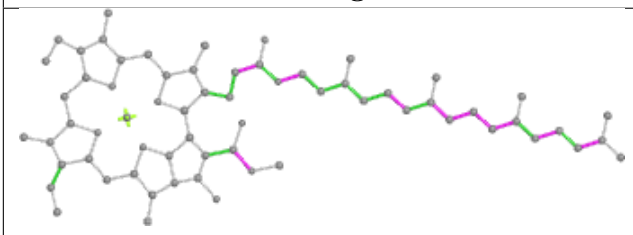
Ligand CLA b 617



Bond lengths



Bond angles



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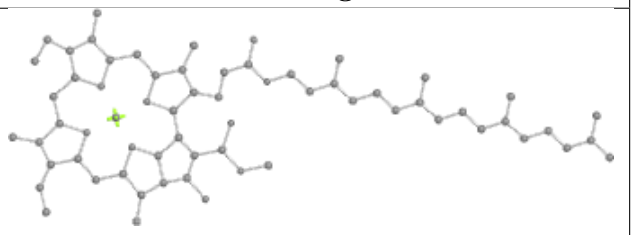
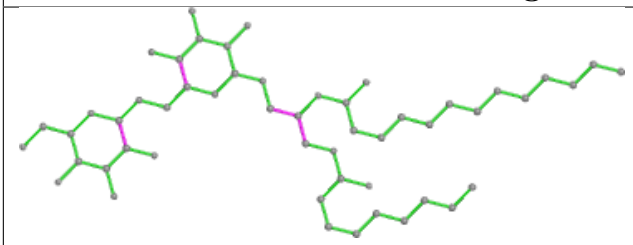
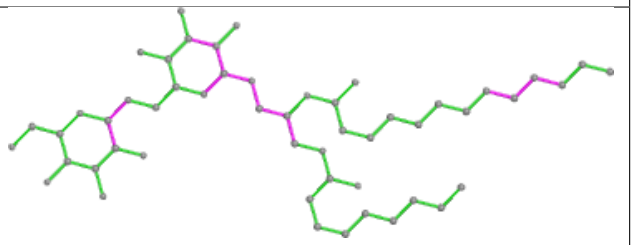


Rings

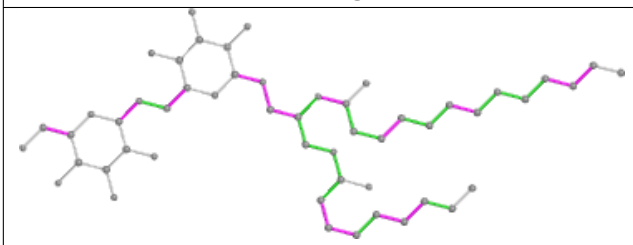
Ligand DGD b 601



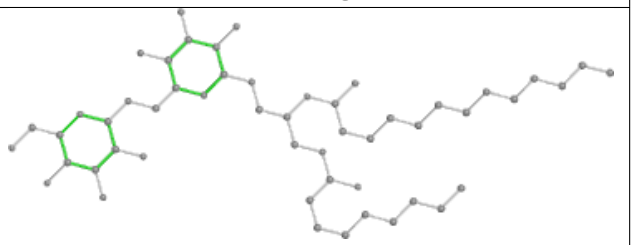
Bond lengths



Bond angles

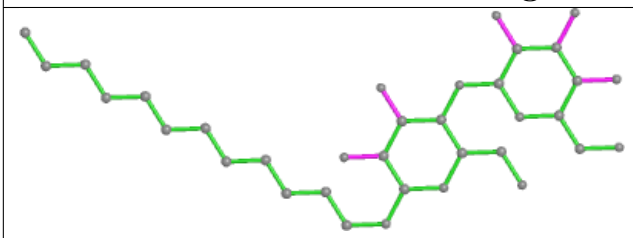


Torsions

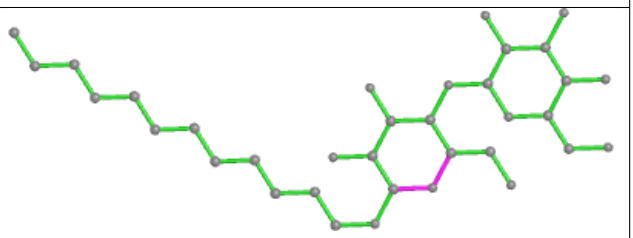


Rings

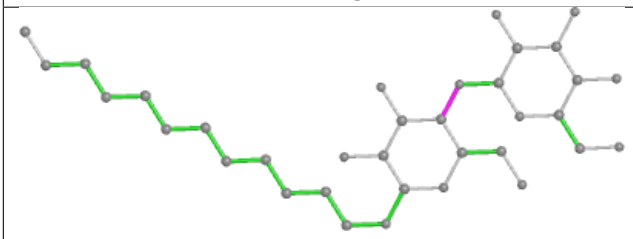
Ligand LMT B 628



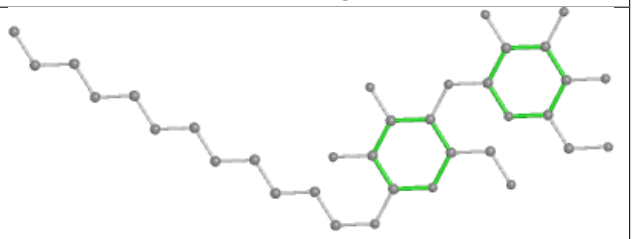
Bond lengths



Bond angles

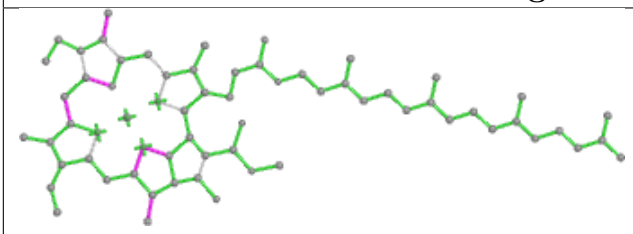


Torsions

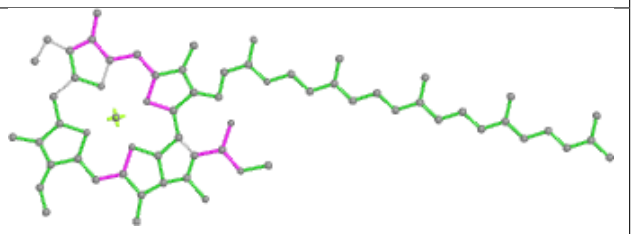


Rings

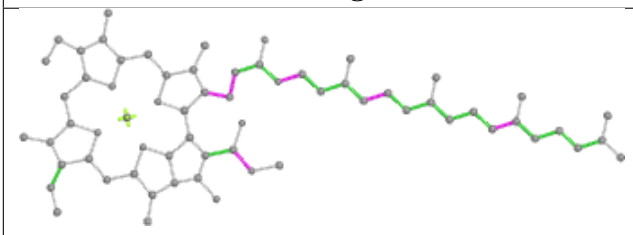
Ligand CLA a 403



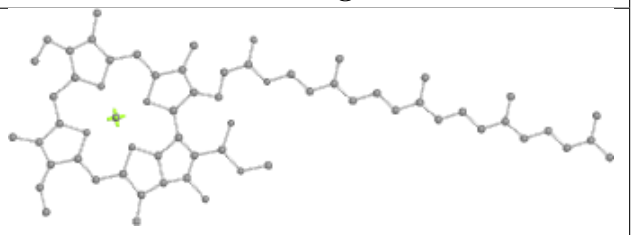
Bond lengths



Bond angles

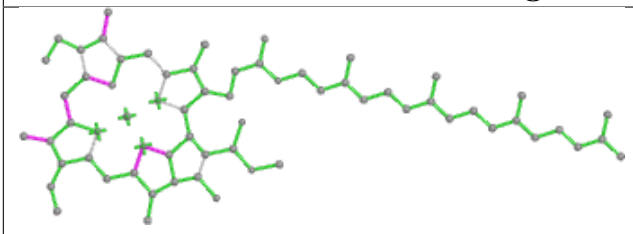


Torsions



Rings

Ligand CLA B 615



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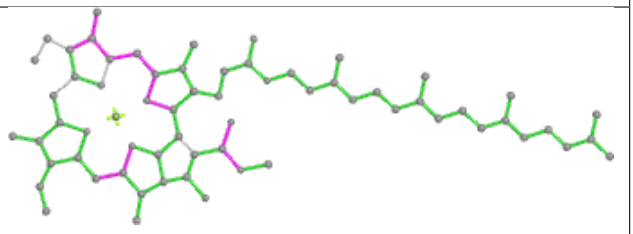
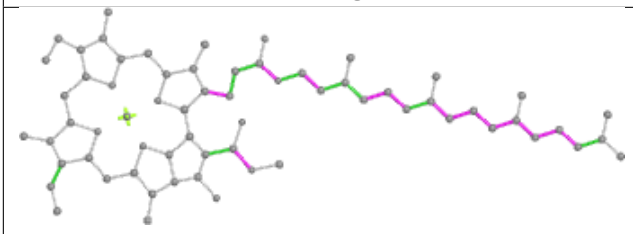
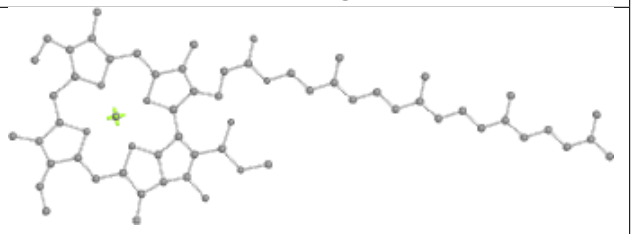


Bond angles

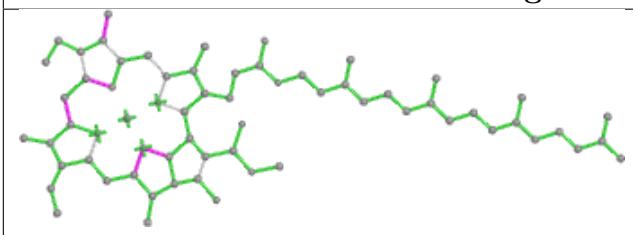


Torsions



Rings

Ligand CLA B 613



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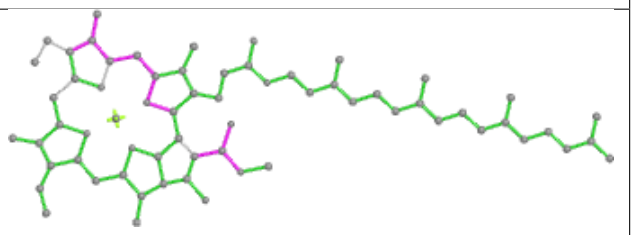
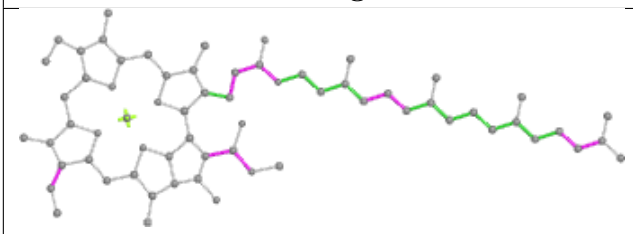
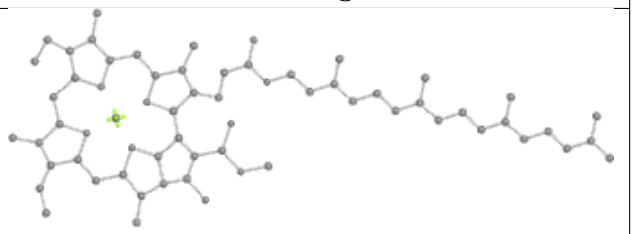


Bond angles

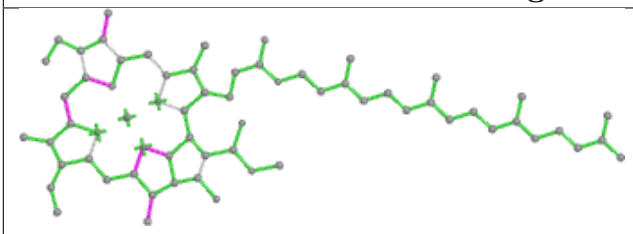


Torsions

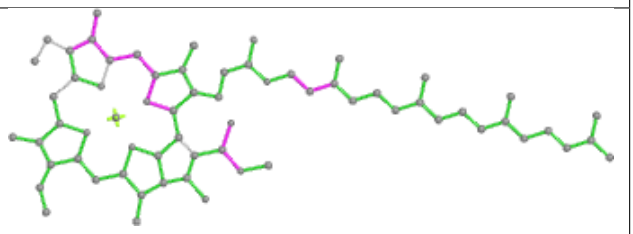


Rings

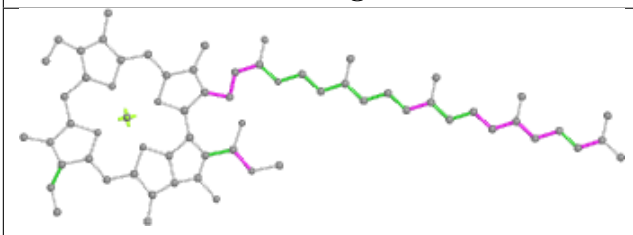
Ligand CLA b 605



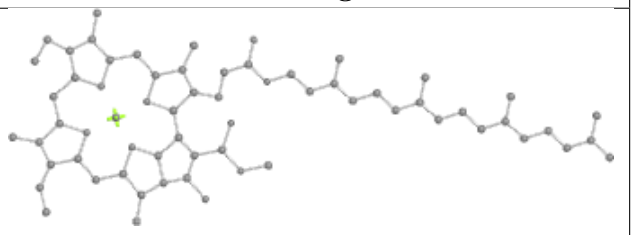
Bond lengths



Bond angles

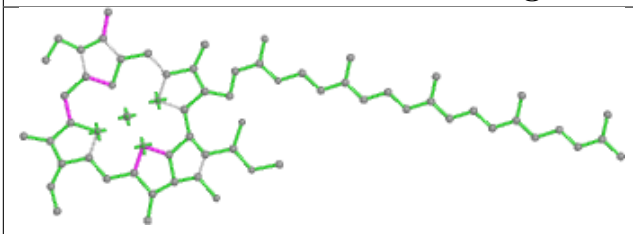


Torsions

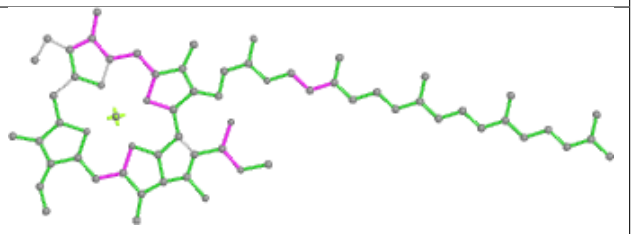


Rings

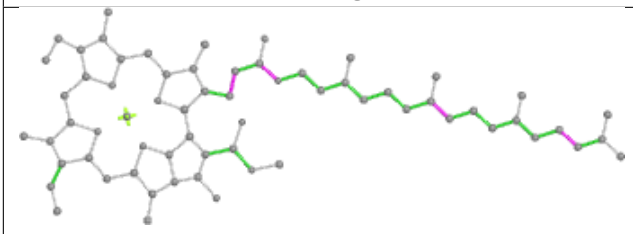
Ligand CLA D 404



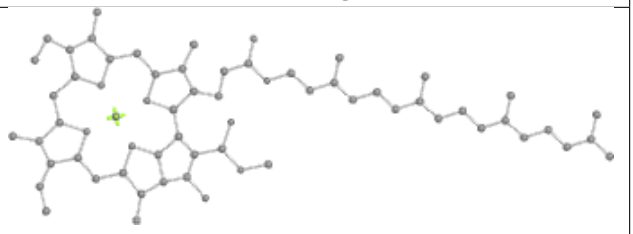
Bond lengths



Bond angles

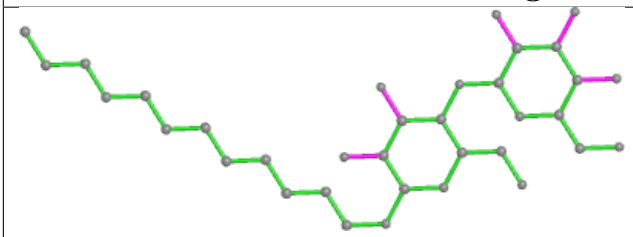


Torsions

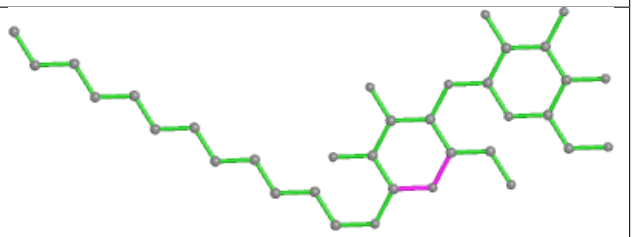


Rings

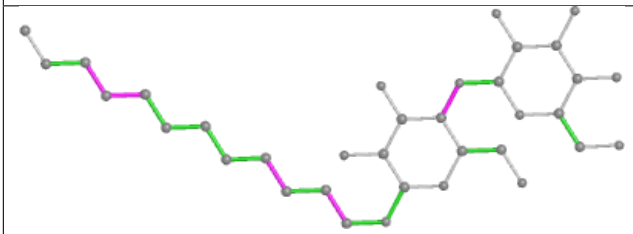
Ligand LMT b 604



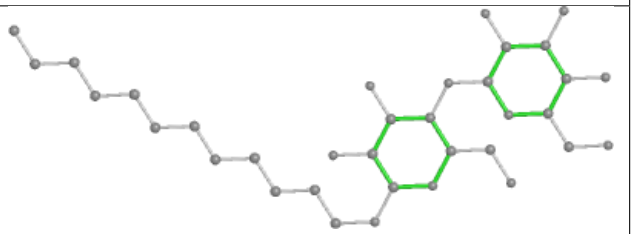
Bond lengths



Bond angles

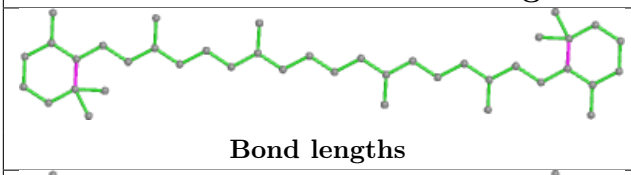


Torsions

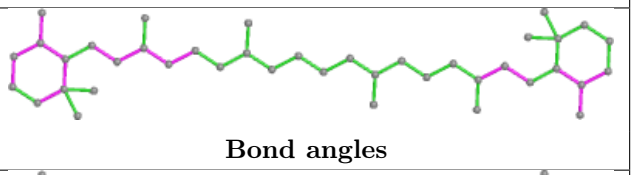


Rings

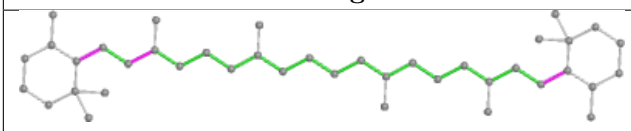
Ligand BCR B 619



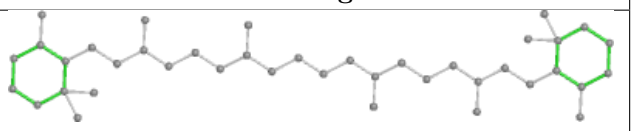
Bond lengths



Bond angles

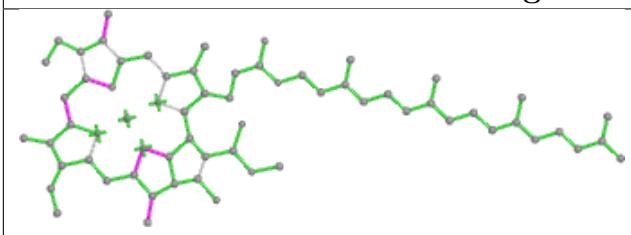


Torsions



Rings

Ligand CLA D 403



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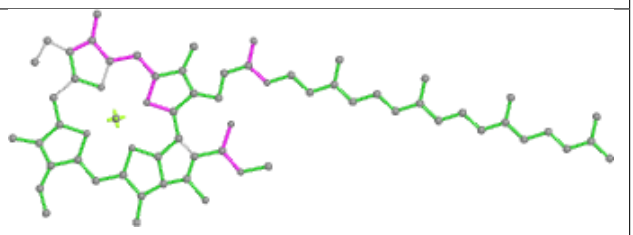
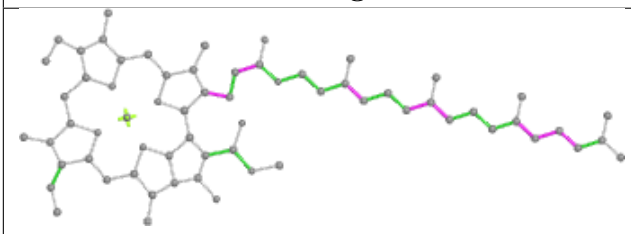


Bond angles



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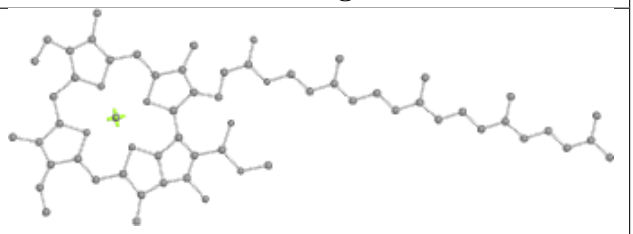
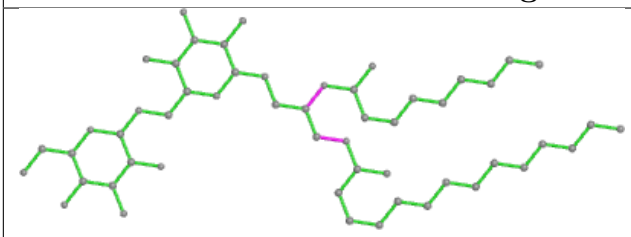


Rings

Ligand DGD C 514



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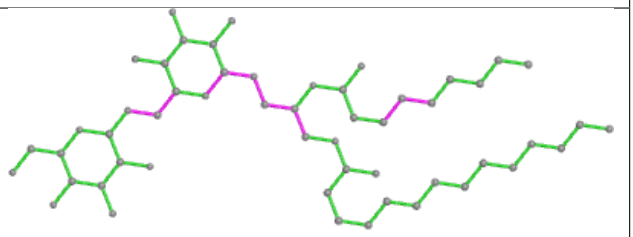
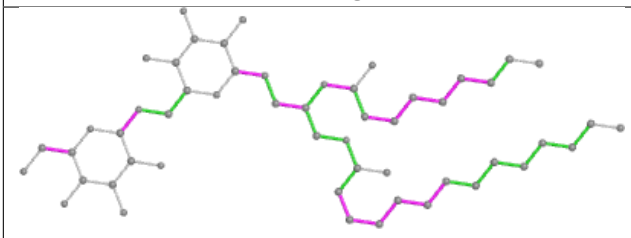


Bond angles



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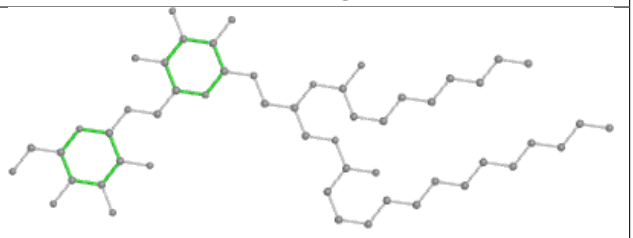
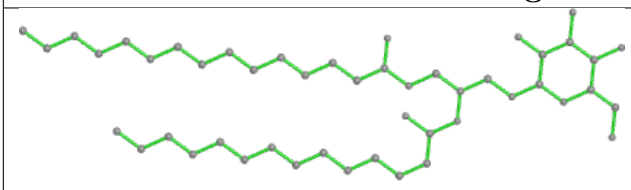


Rings

Ligand LMG c 522



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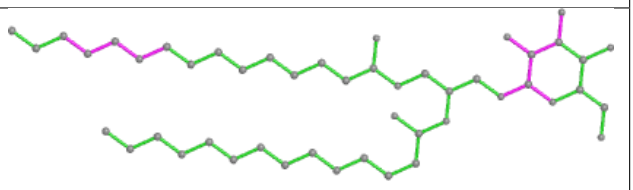
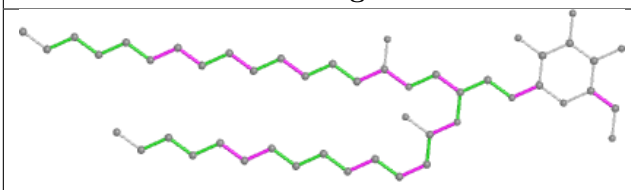


Bond angles



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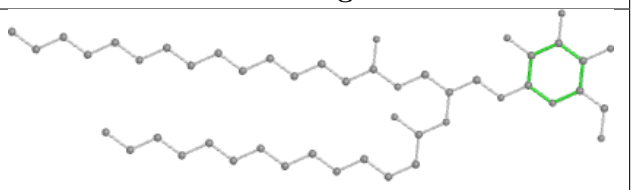
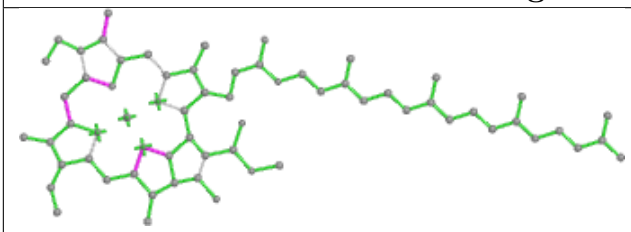


Rings

Ligand CLA b 607



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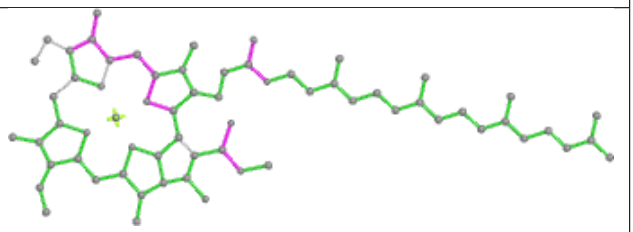
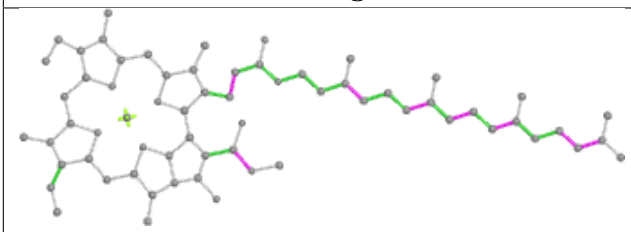


Bond angles



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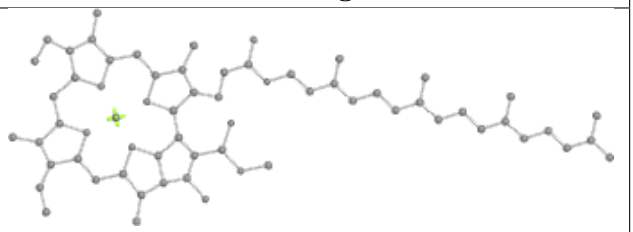
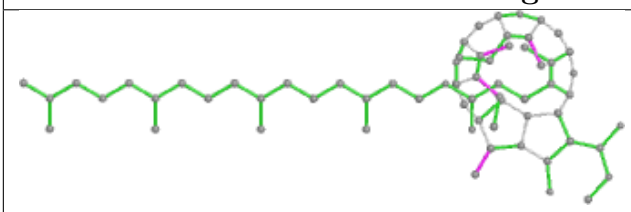


Rings

Ligand PHO A 405



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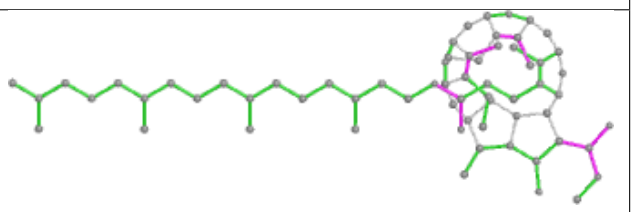
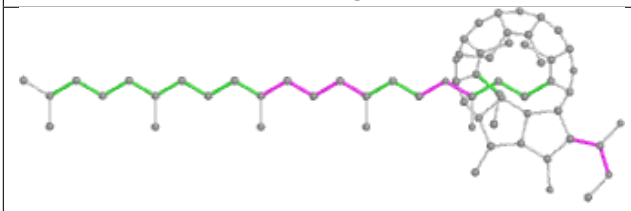


Bond angles



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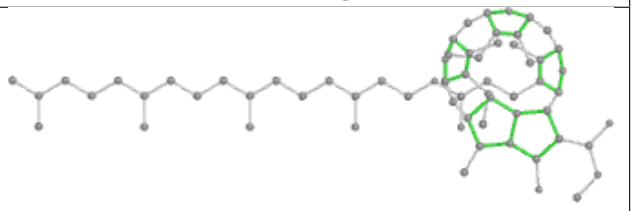
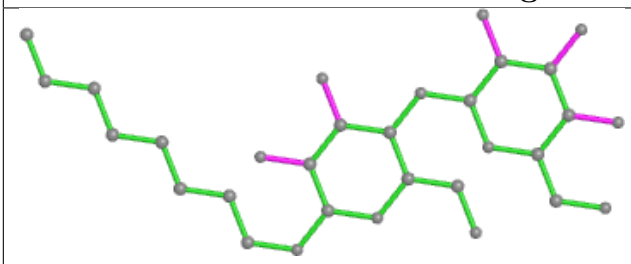


Rings

Ligand LMT D 408



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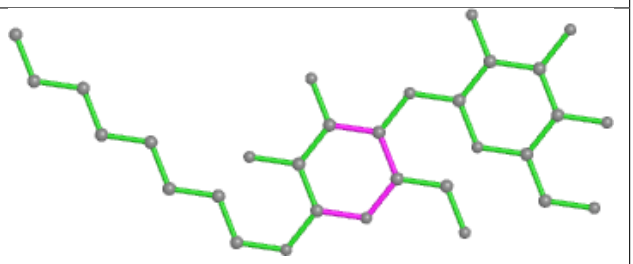
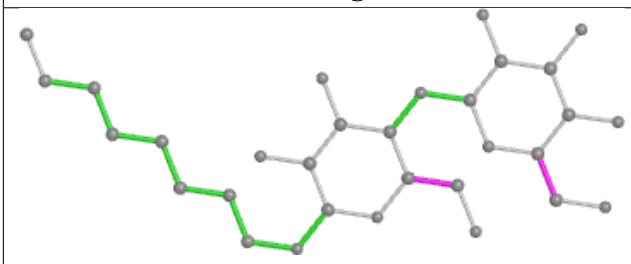


Bond angles



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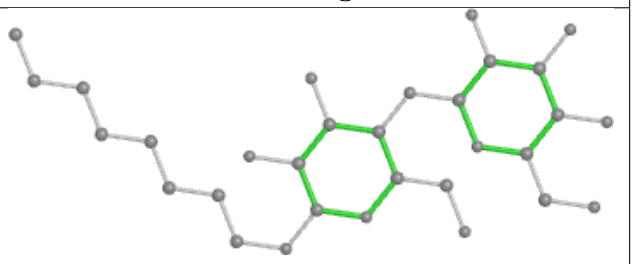
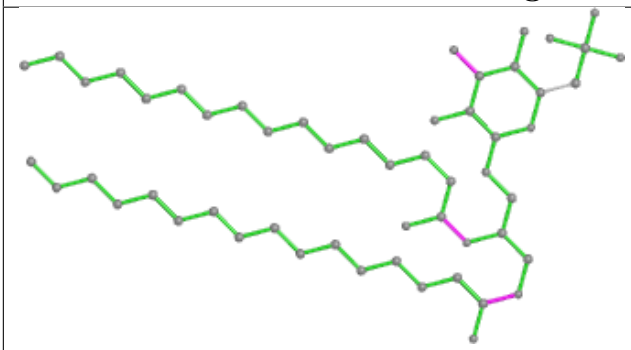


Rings

Ligand SQD A 414



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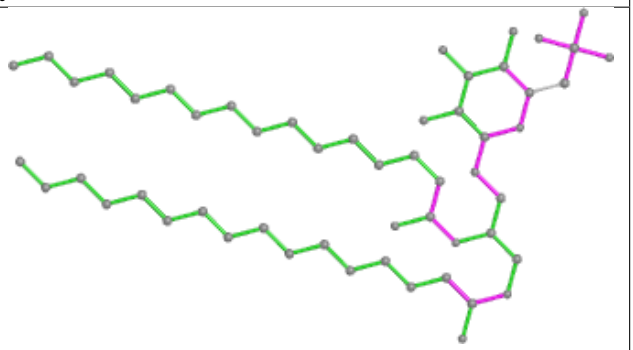
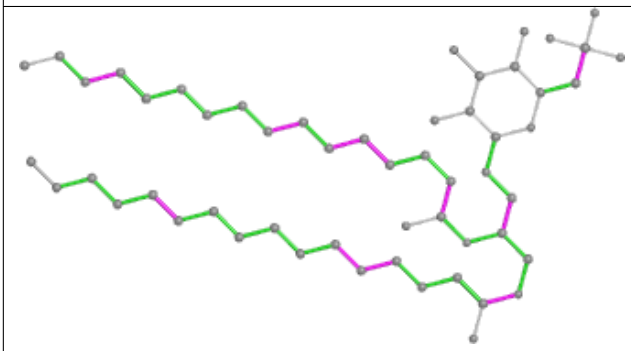
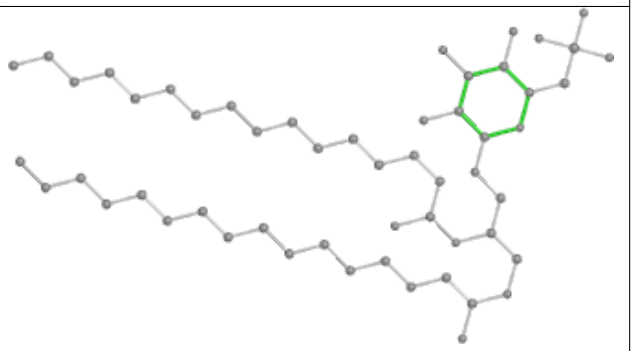


Bond angles

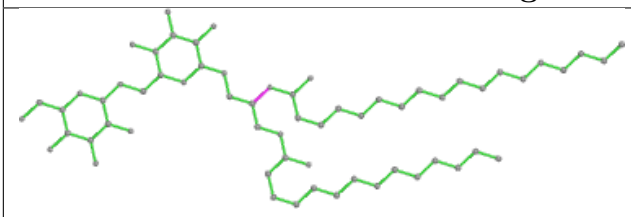


Torsions



Rings

Ligand DGD C 515



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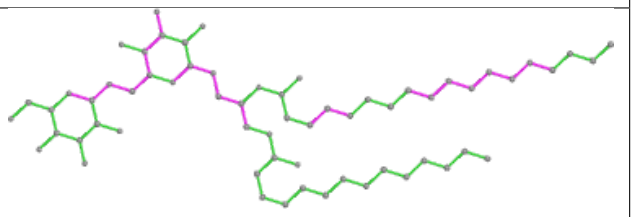
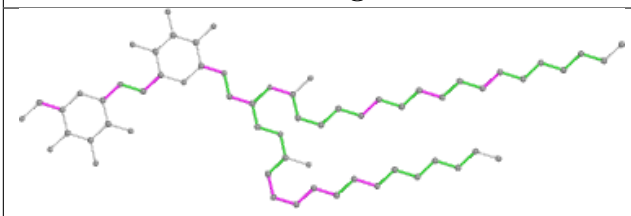
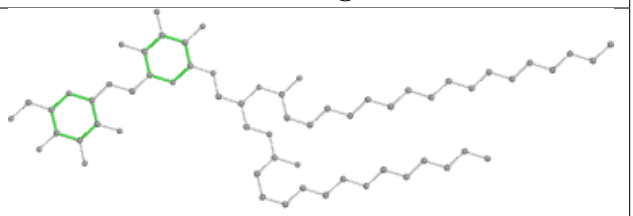


Bond angles

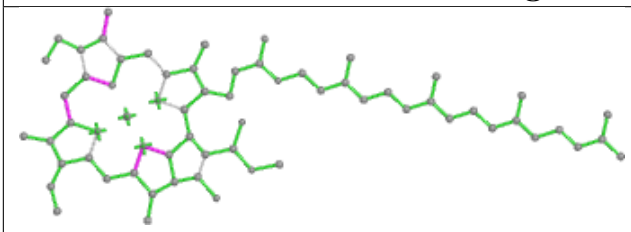


Torsions



Rings

Ligand CLA C 502



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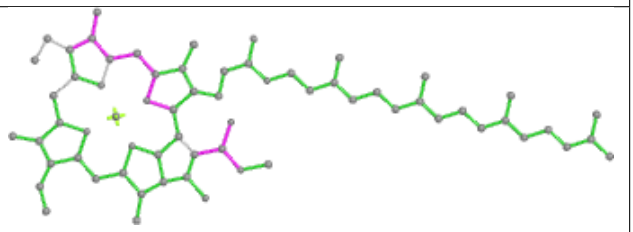
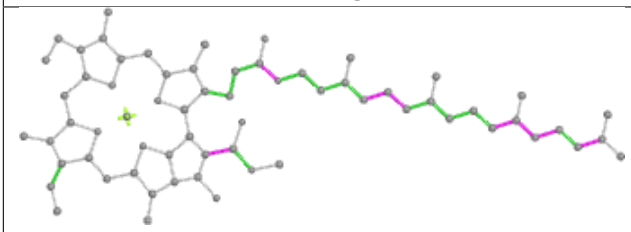
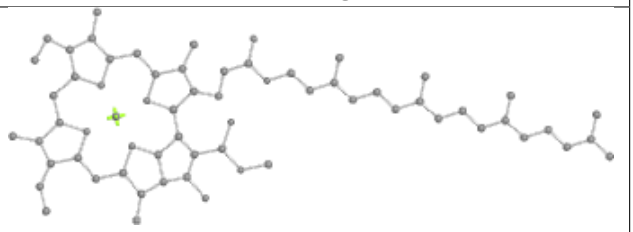


Bond angles

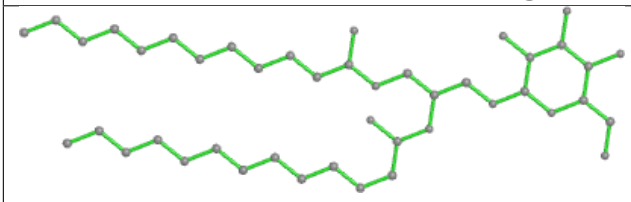


Torsions



Rings

Ligand LMG E 101



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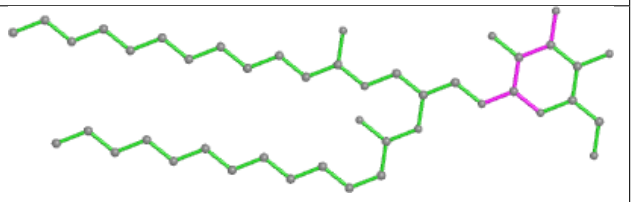
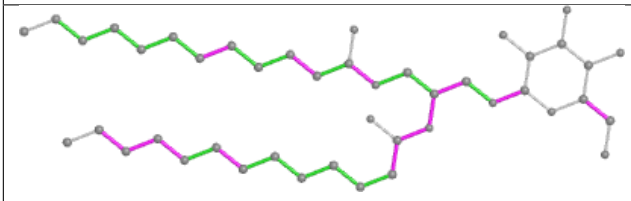
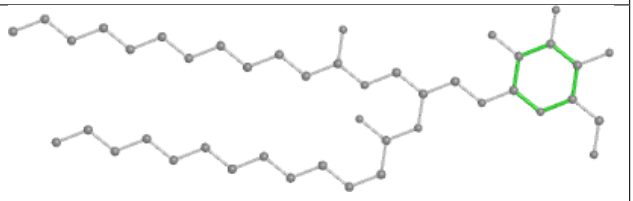


Bond angles

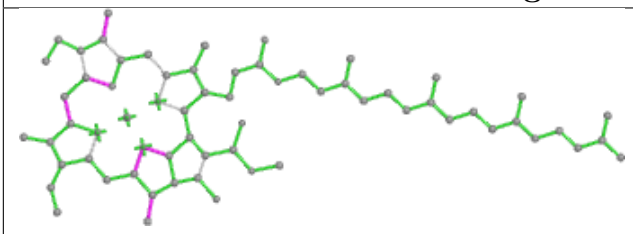


Torsions



Rings

Ligand CLA A 404



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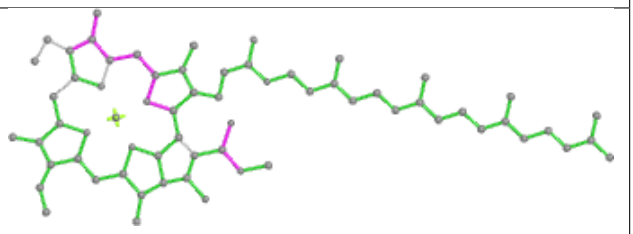
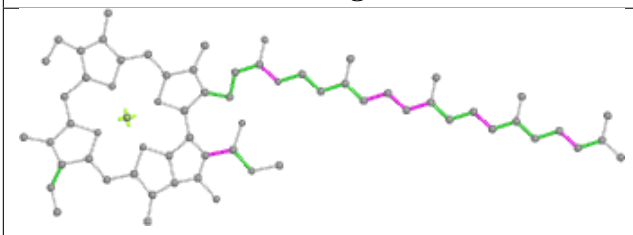
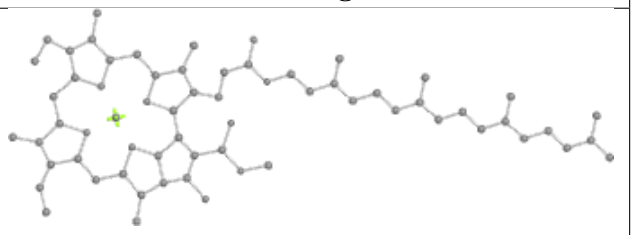


Bond angles

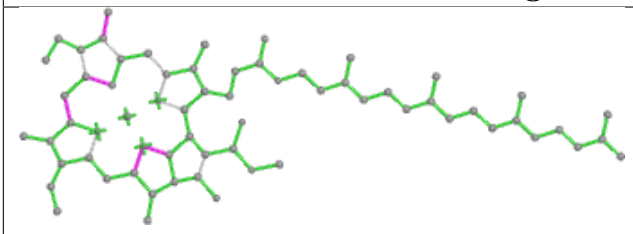


Torsions



Rings

Ligand CLA C 506



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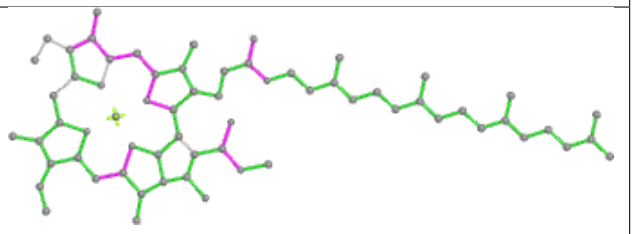
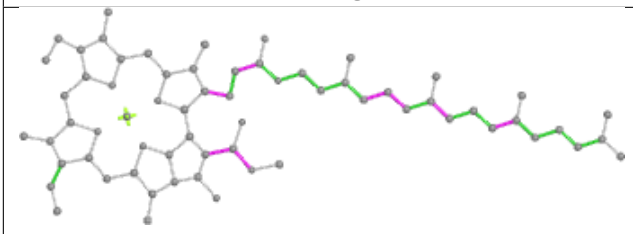
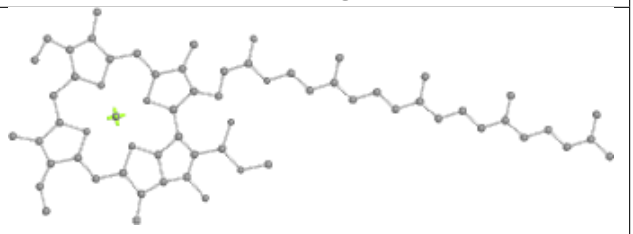


Bond angles

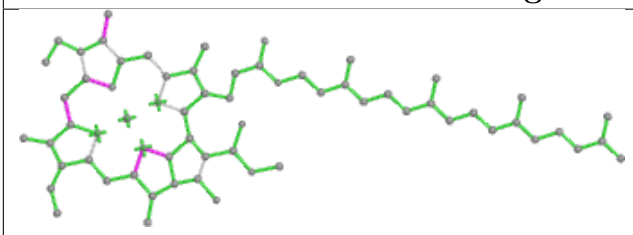


Torsions

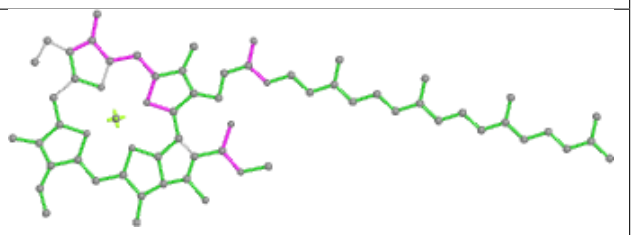


Rings

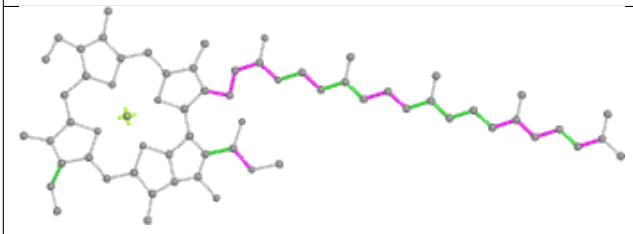
Ligand CLA C 511



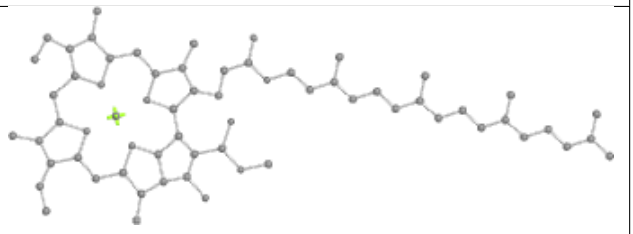
Bond lengths



Bond angles

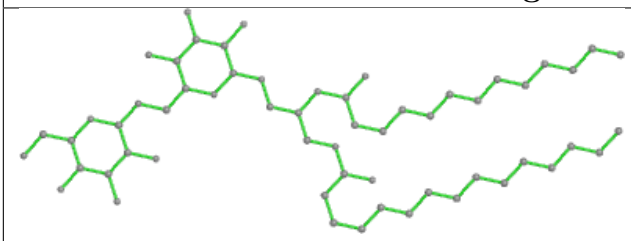


Torsions

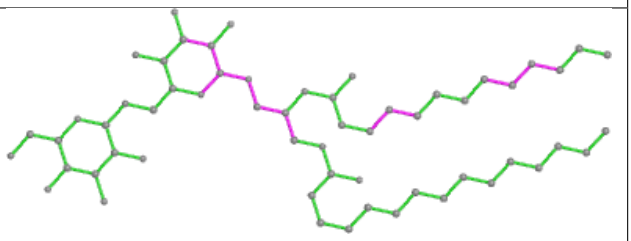


Rings

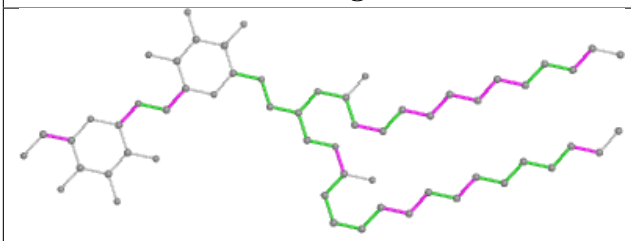
Ligand DGD b 625



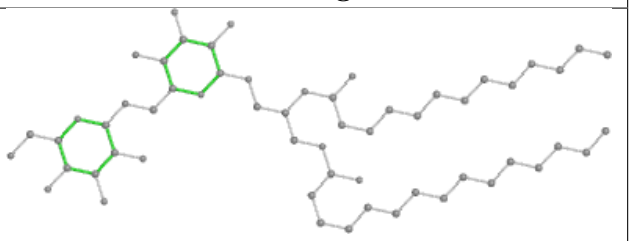
Bond lengths



Bond angles

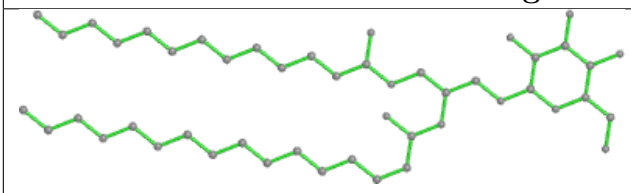


Torsions



Rings

Ligand LMG d 409



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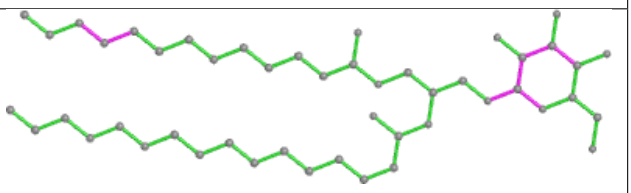
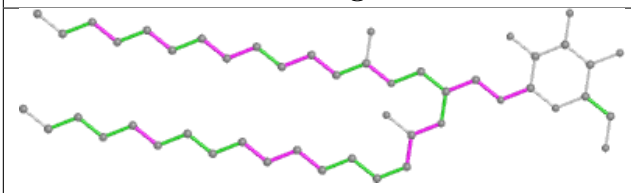
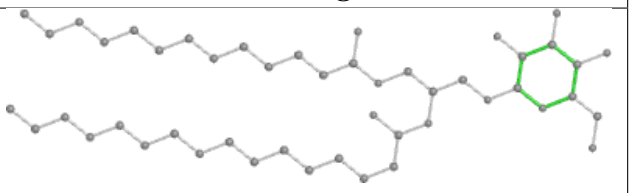


Bond angles

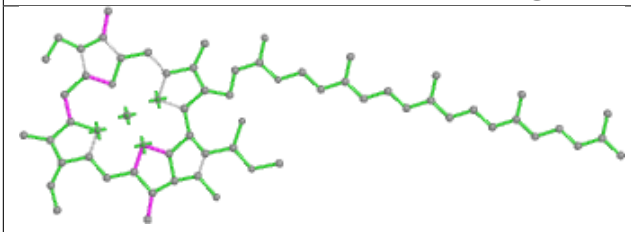


Torsions



Rings

Ligand CLA a 405



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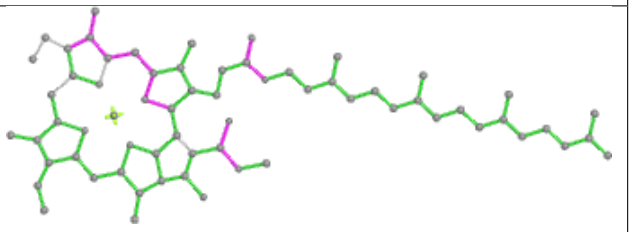
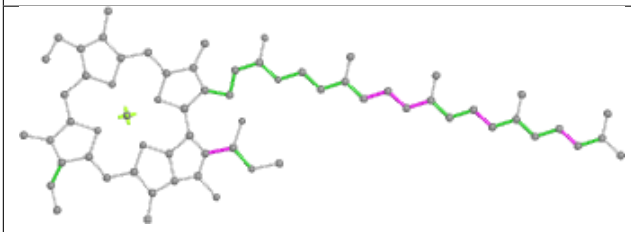
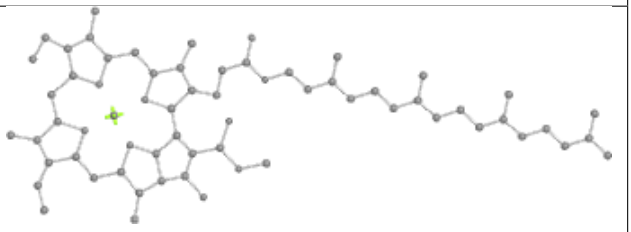


Bond angles

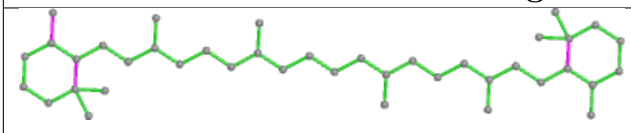


Torsions



Rings

Ligand BCR g 101



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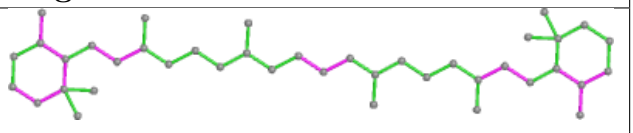
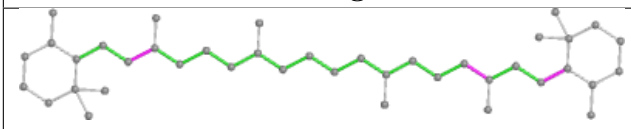
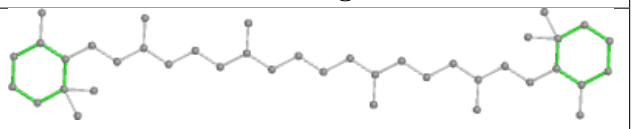


Bond angles

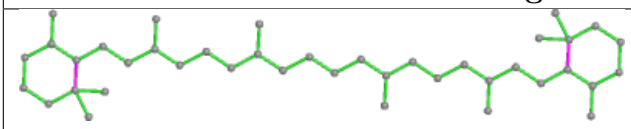


Torsions



Rings

Ligand BCR b 623



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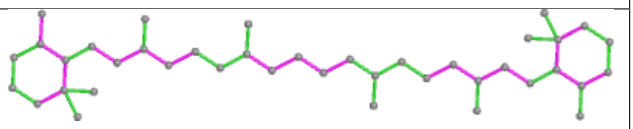
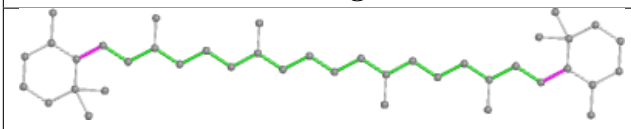
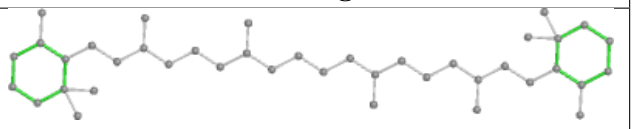


Bond angles

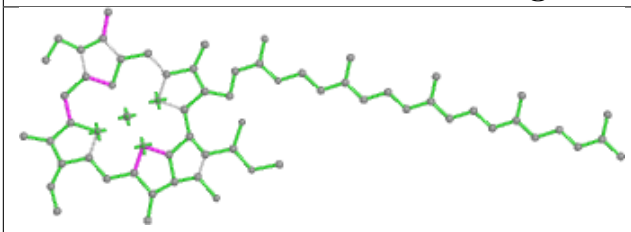


Torsions

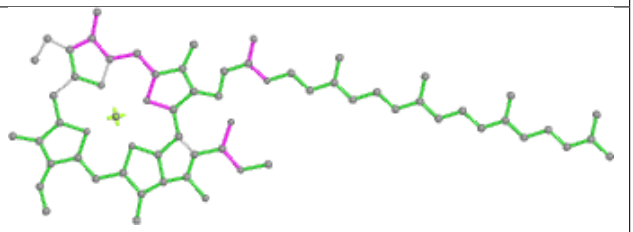


Rings

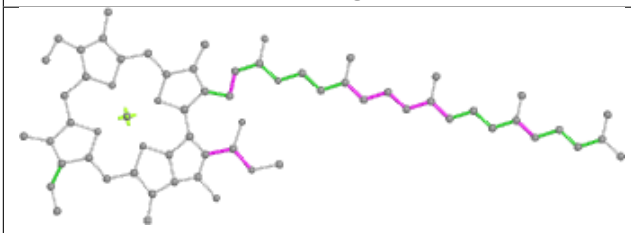
Ligand CLA c 510



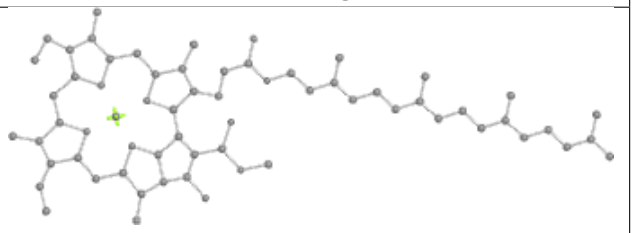
Bond lengths



Bond angles

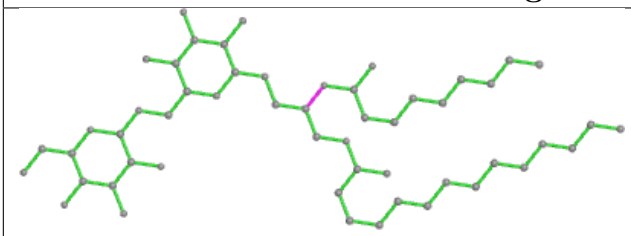


Torsions



Rings

Ligand DGD c 515



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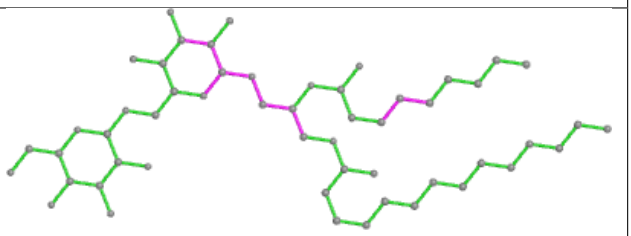
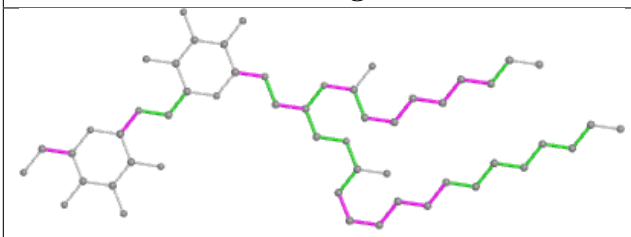
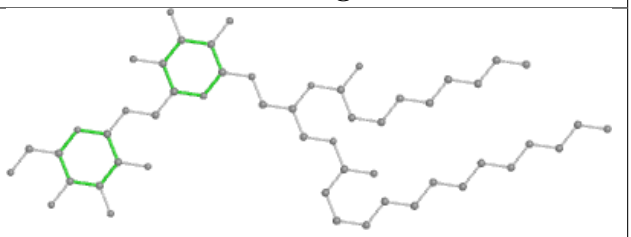


Bond angles

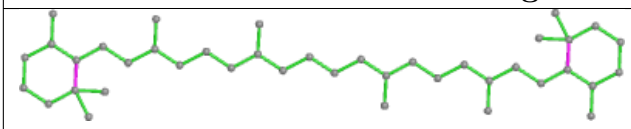


Torsions

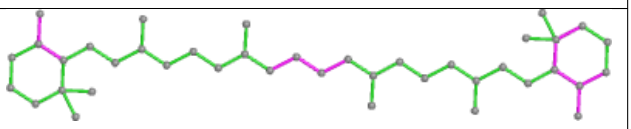


Rings

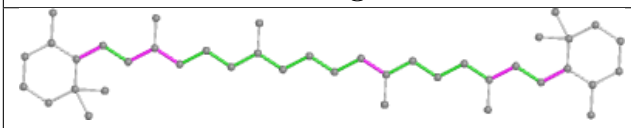
Ligand BCR H 102



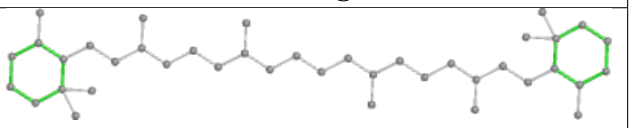
Bond lengths



Bond angles

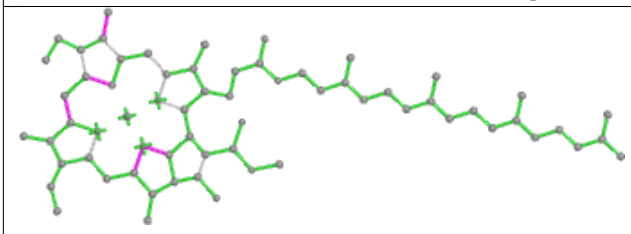


Torsions

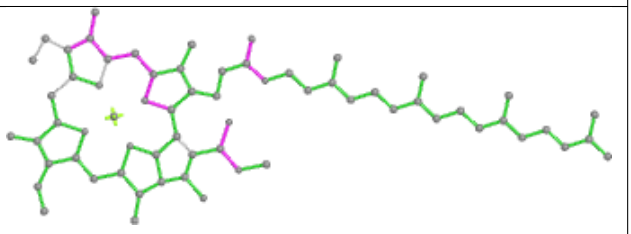


Rings

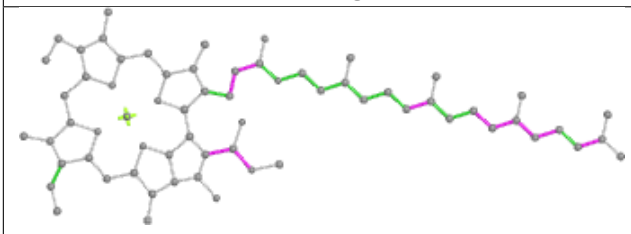
Ligand CLA B 601



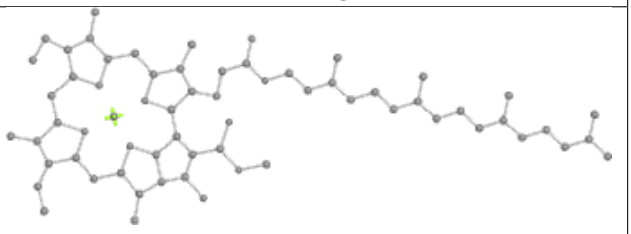
Bond lengths



Bond angles

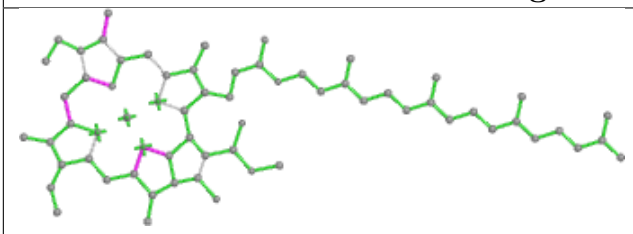


Torsions



Rings

Ligand CLA c 503



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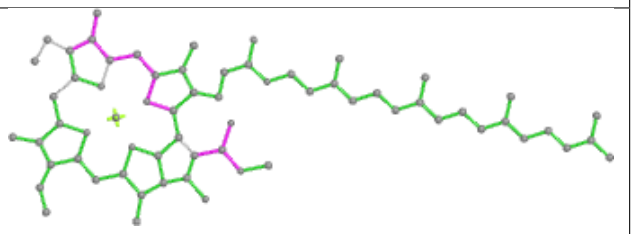
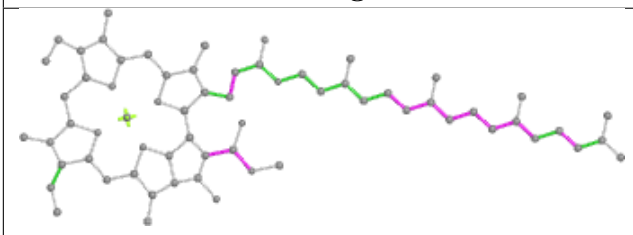
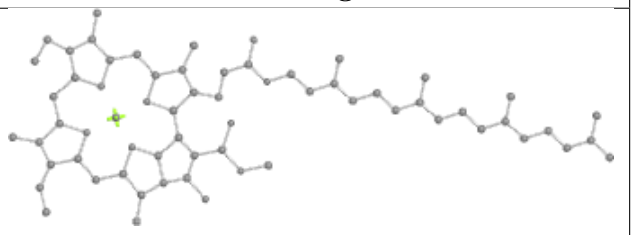


Bond angles

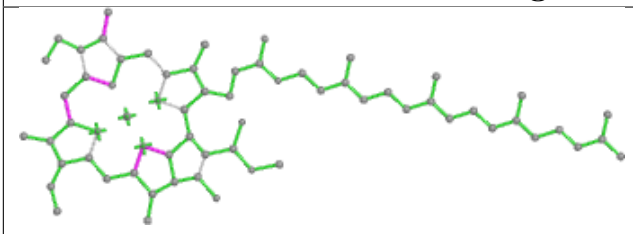


Torsions



Rings

Ligand CLA c 512



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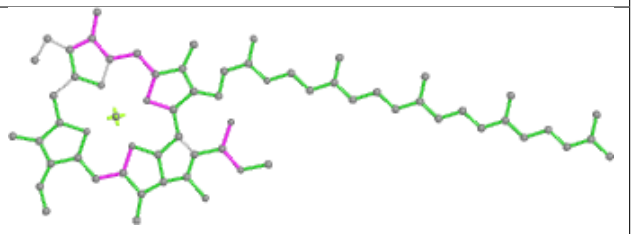
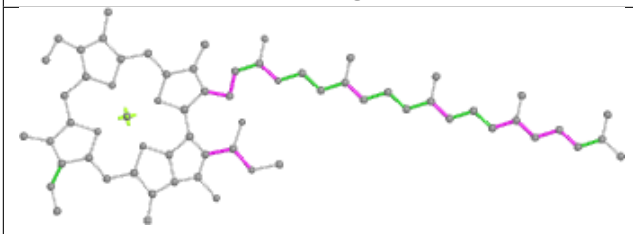
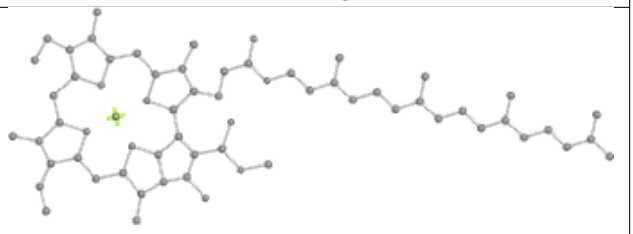


Bond angles

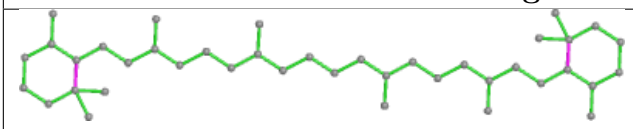


Torsions

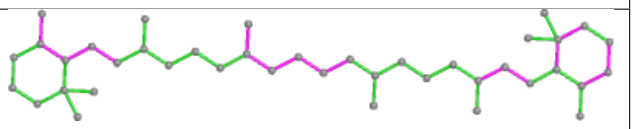


Rings

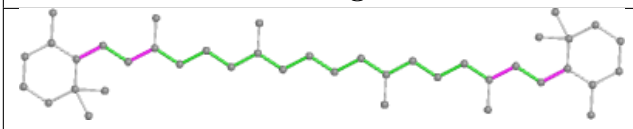
Ligand BCR B 617



Bond lengths



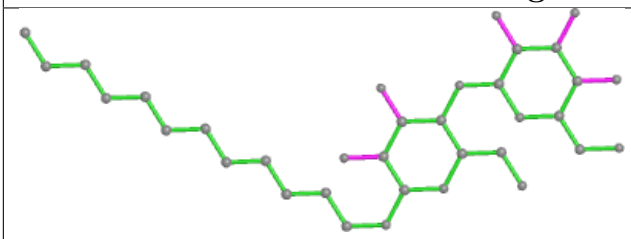
Bond angles



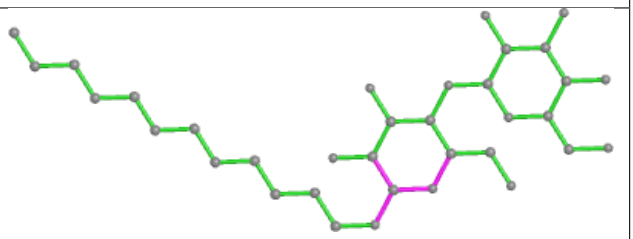
Torsions

Rings

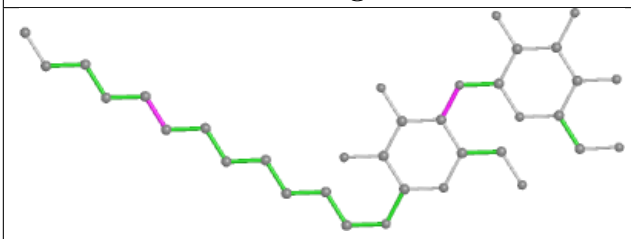
Ligand LMT I 102



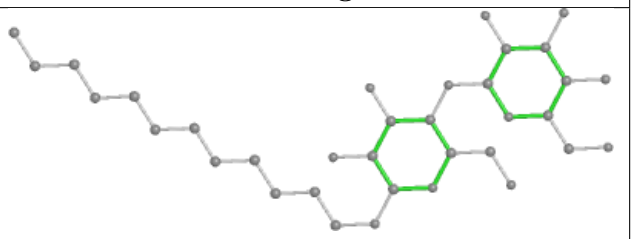
Bond lengths



Bond angles

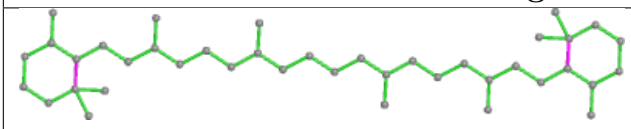


Torsions

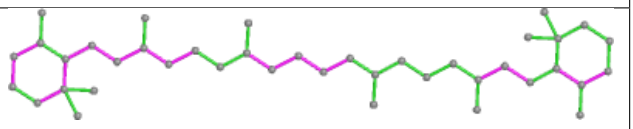


Rings

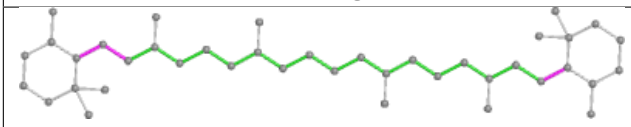
Ligand BCR c 513



Bond lengths



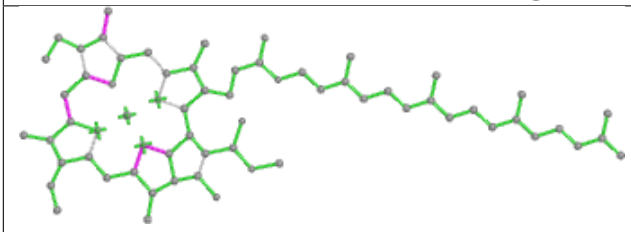
Bond angles



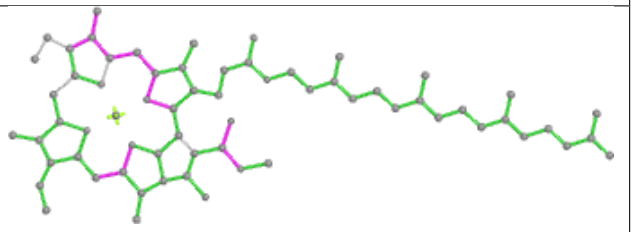
Torsions

Rings

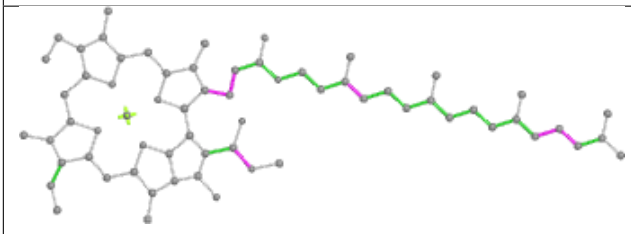
Ligand CLA b 611



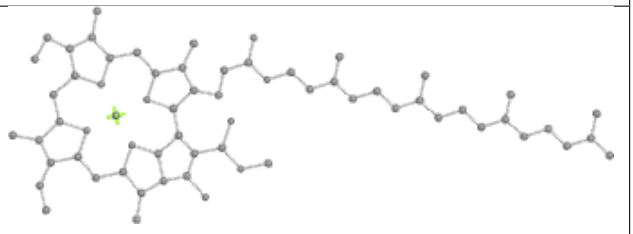
Bond lengths



Bond angles

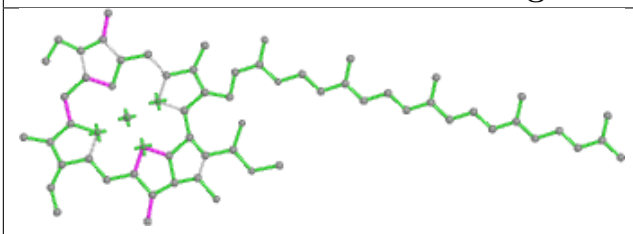


Torsions



Rings

Ligand CLA b 612



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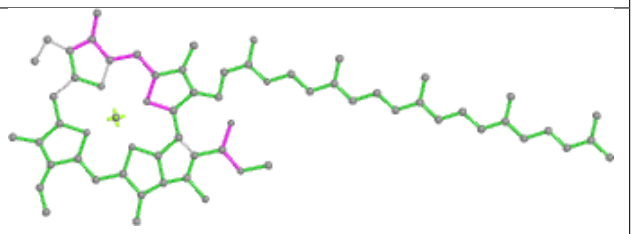

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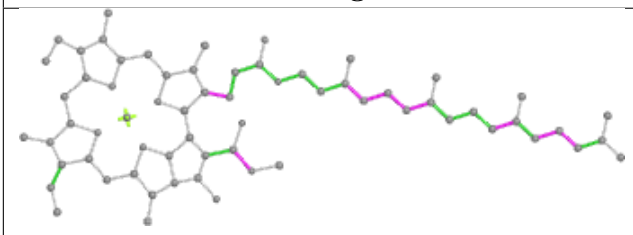

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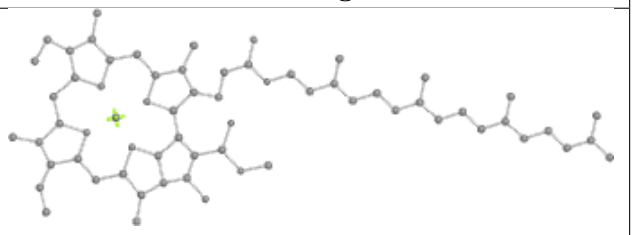
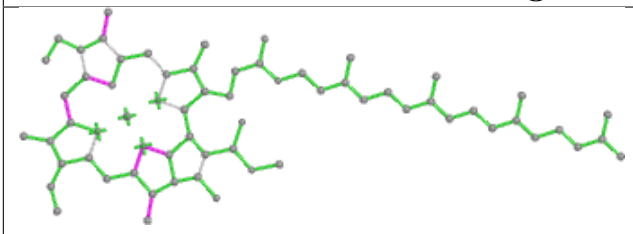


Rings

Ligand CLA b 616



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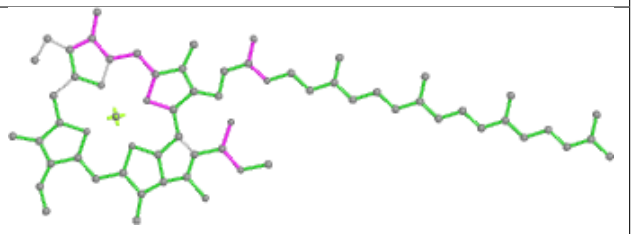
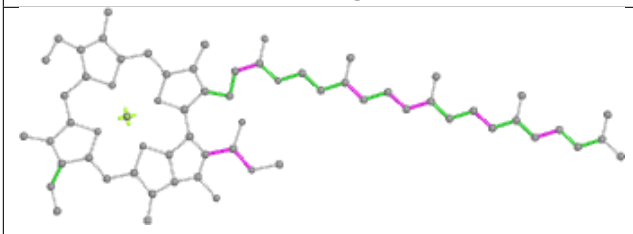
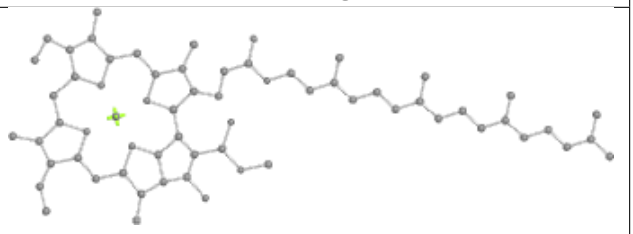


Bond angles

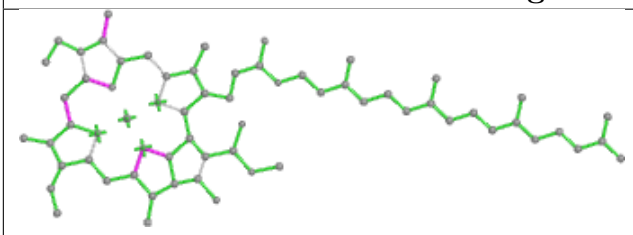


Torsions



Rings

Ligand CLA b 610



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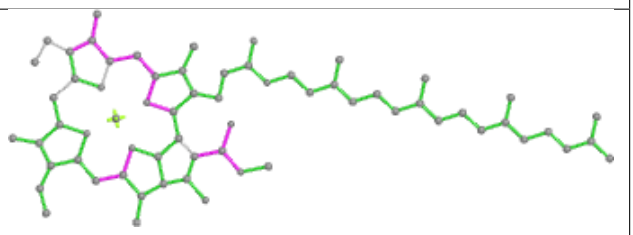
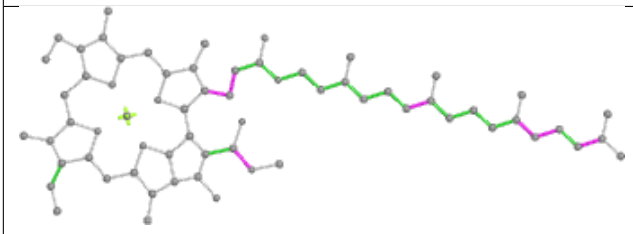


Bond angles



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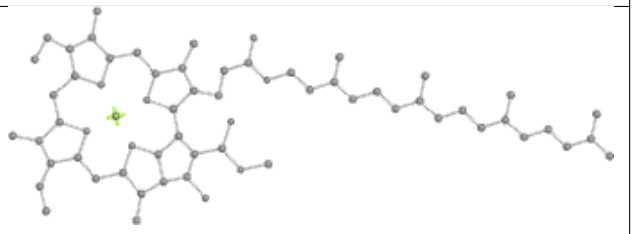
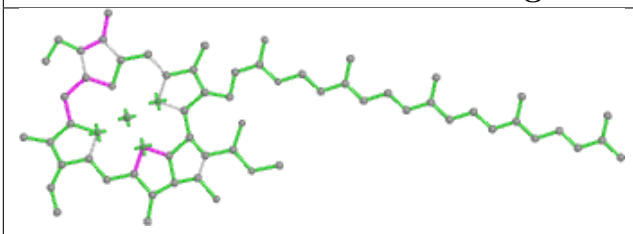


Rings

Ligand CLA B 610



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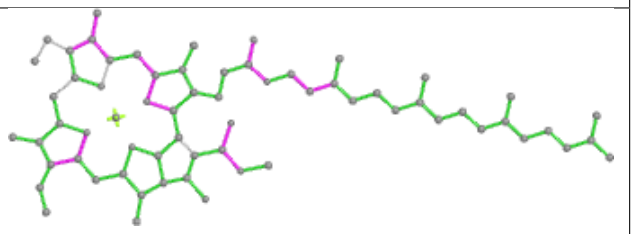
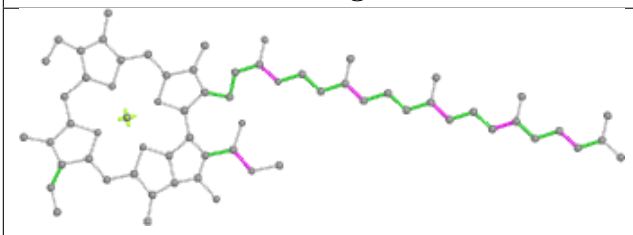


Bond angles



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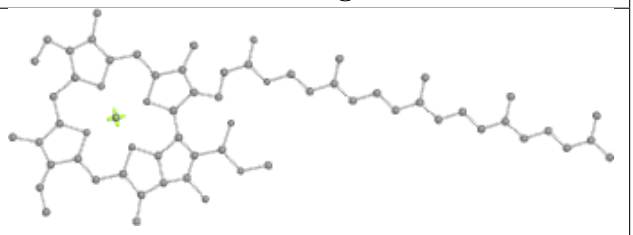
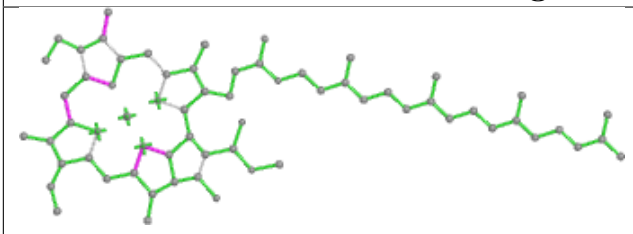


Rings

Ligand CLA c 511



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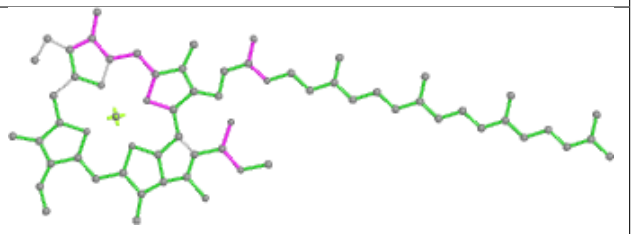
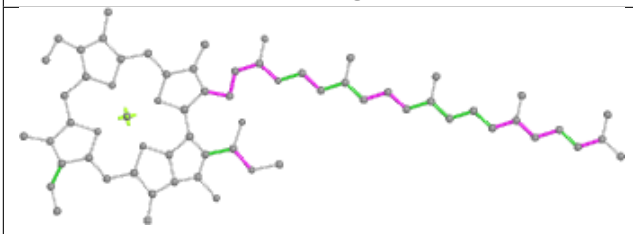


Bond angles



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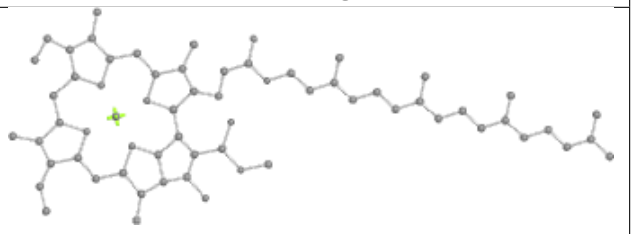
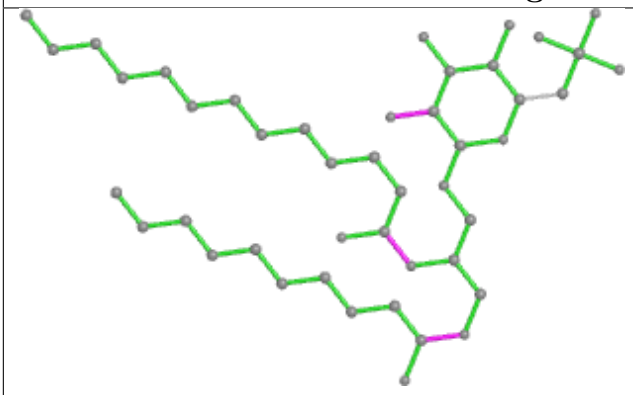


Rings

Ligand SQD F 103



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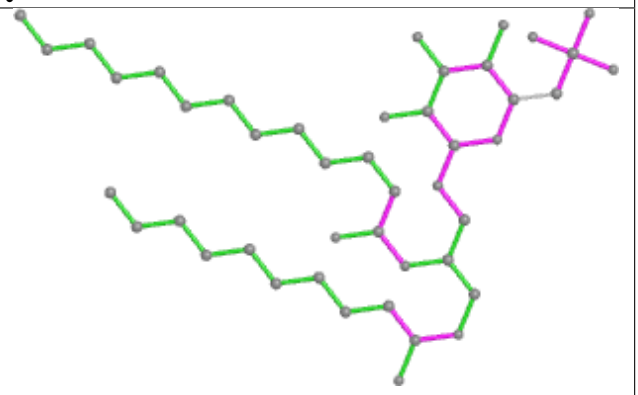
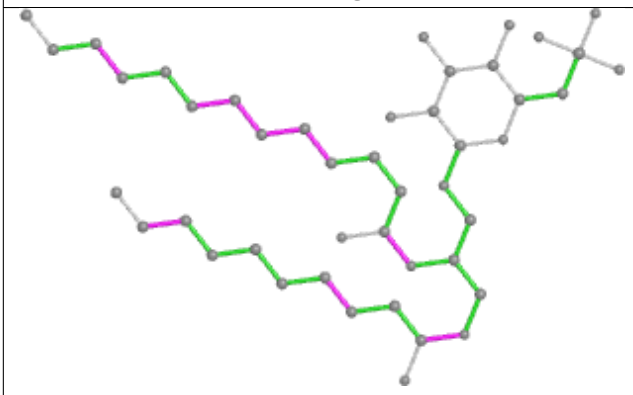


Bond angles



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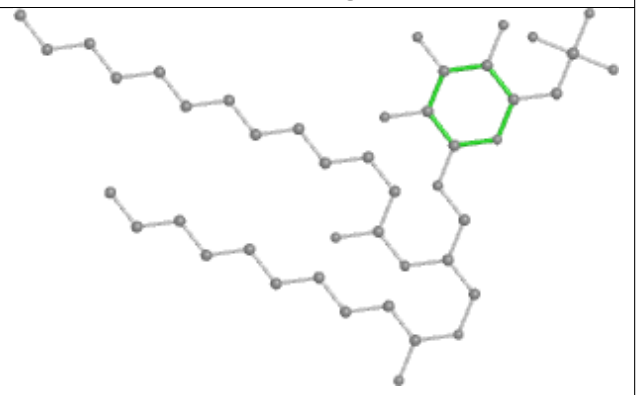
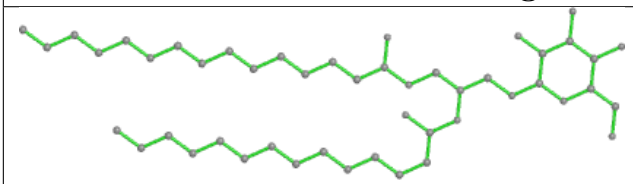
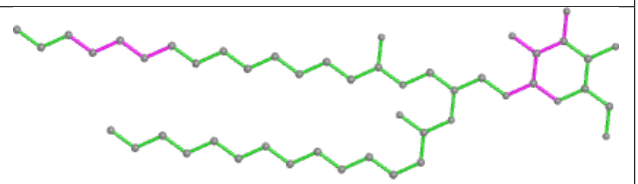


Rings

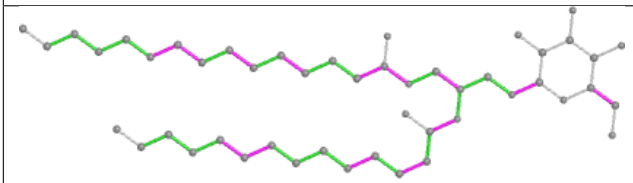
Ligand LMG C 521



Bond lengths



Bond angles



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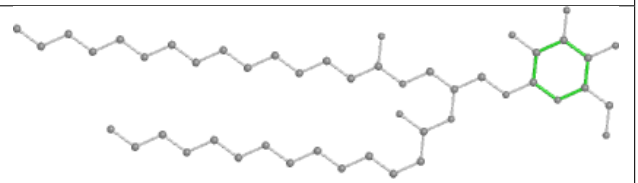
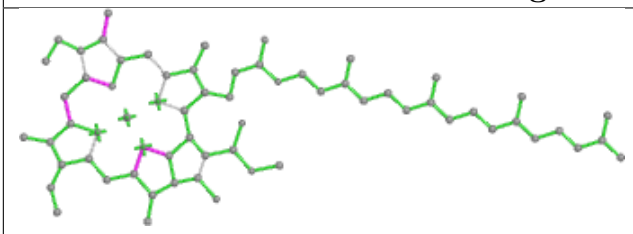


Rings

Ligand CLA c 502



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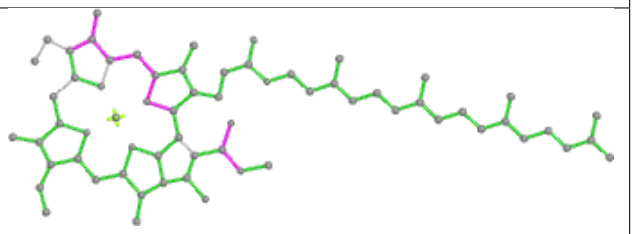
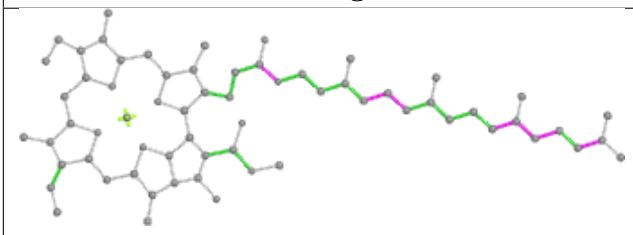
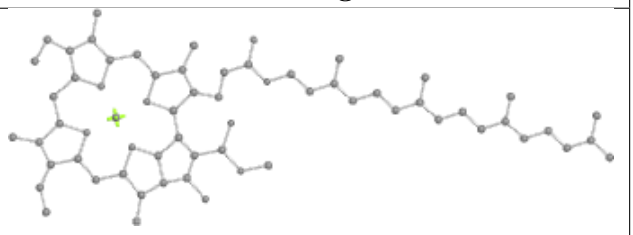


Bond angles

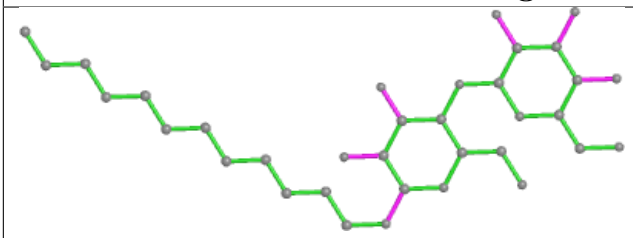


Torsions



Rings

Ligand LMT M 102



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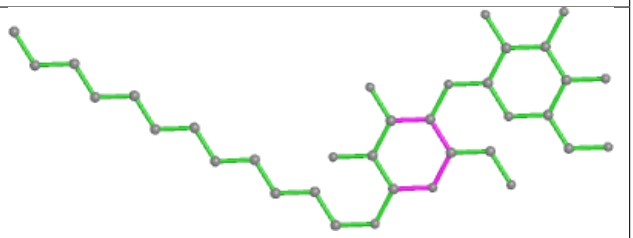
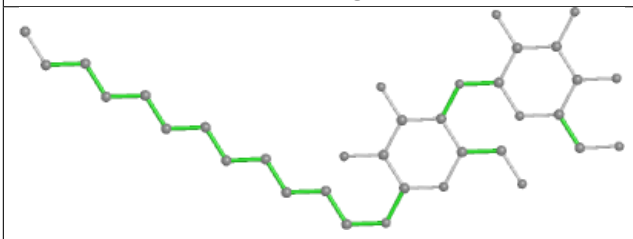


Bond angles



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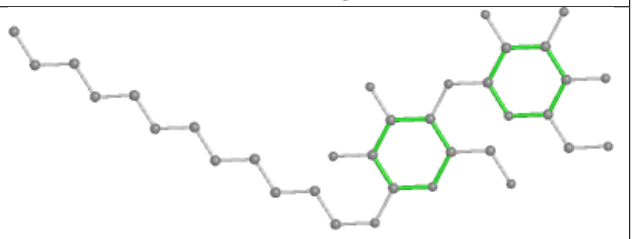
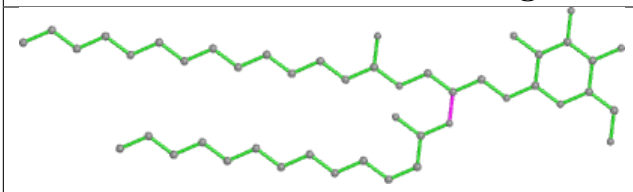


Rings

Ligand LMG D 409



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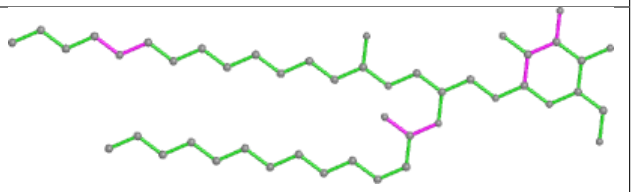
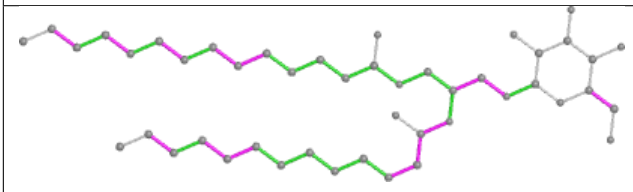
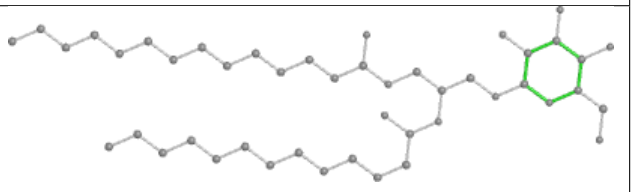


Bond angles

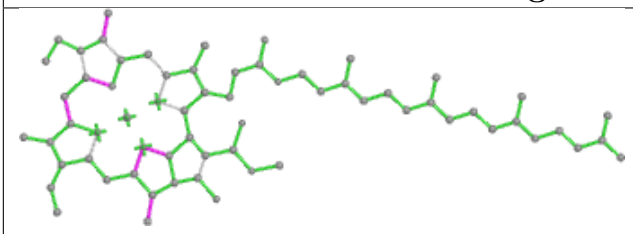


Torsions



Rings

Ligand CLA a 404



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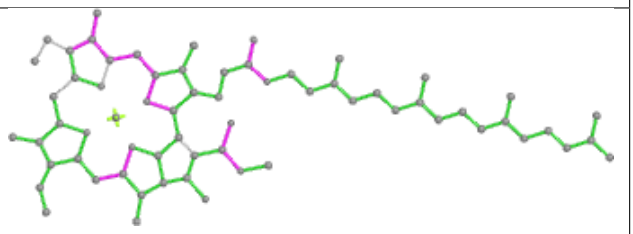
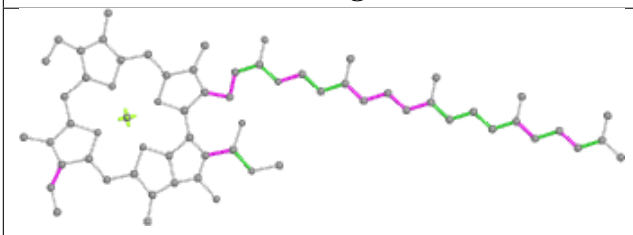
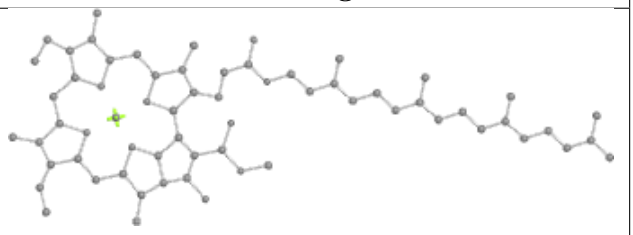


Bond angles

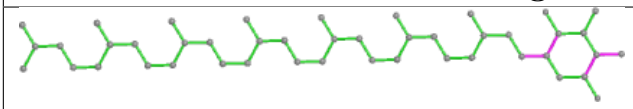


Torsions



Rings

Ligand PL9 A 407



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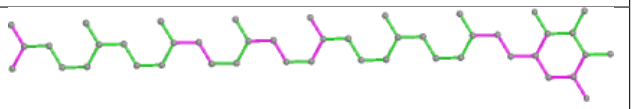
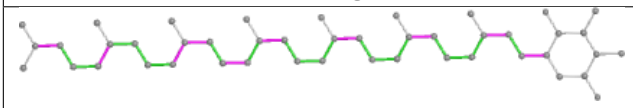
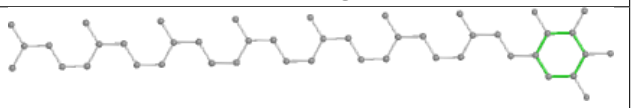


Bond angles

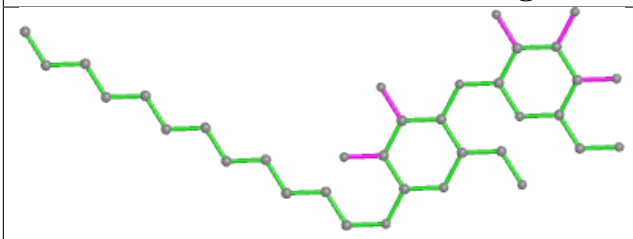


Torsions



Rings

Ligand LMT M 103



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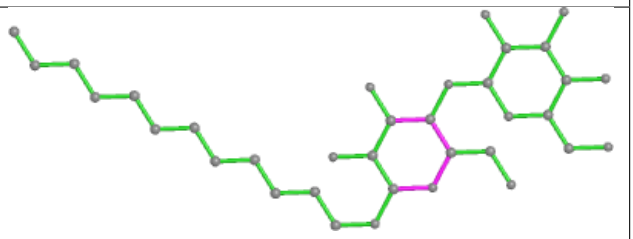
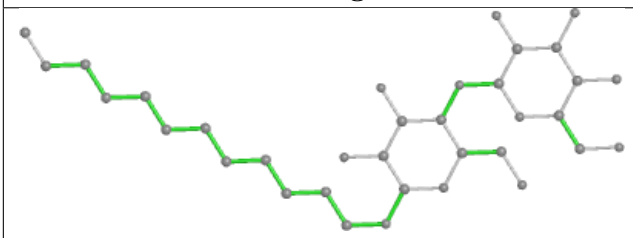
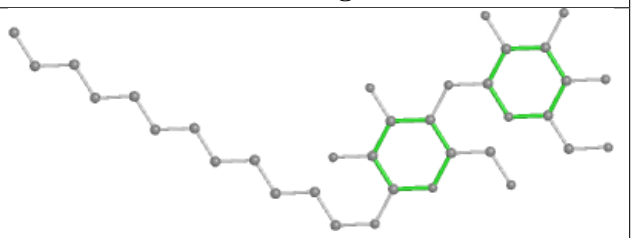


Bond angles

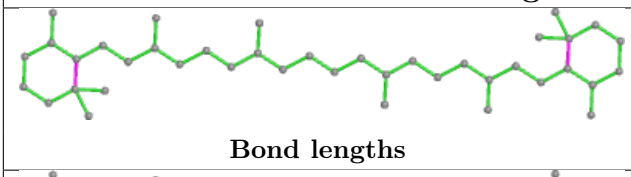


Torsions

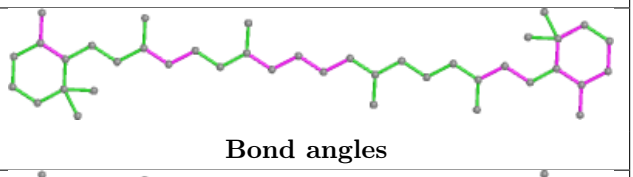


Rings

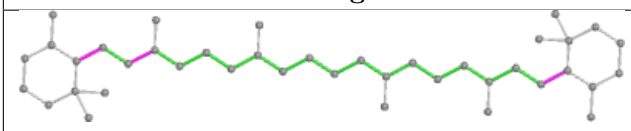
Ligand BCR C 513



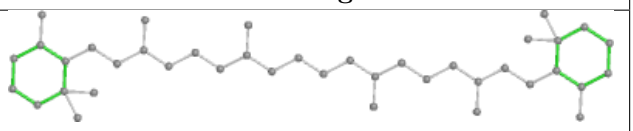
Bond lengths



Bond angles

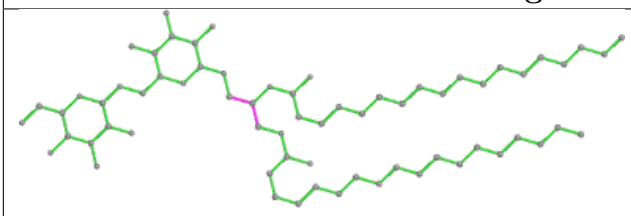


Torsions



Rings

Ligand DGD c 517



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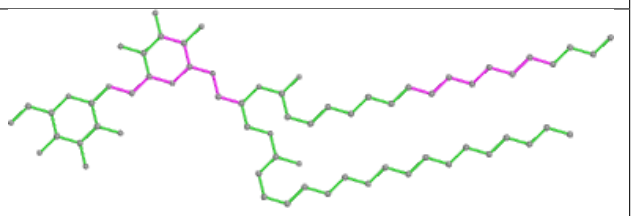
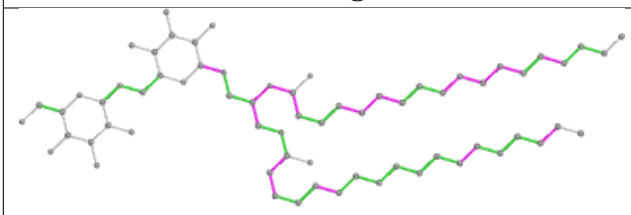
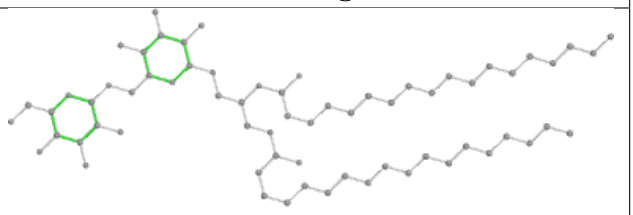


Bond angles

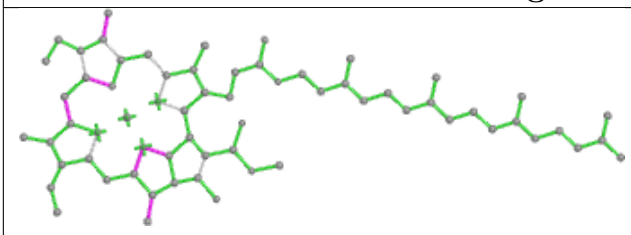


Torsions



Rings

Ligand CLA d 405



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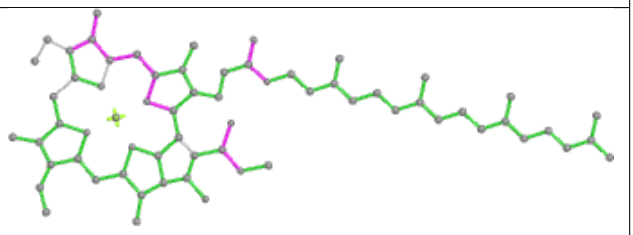
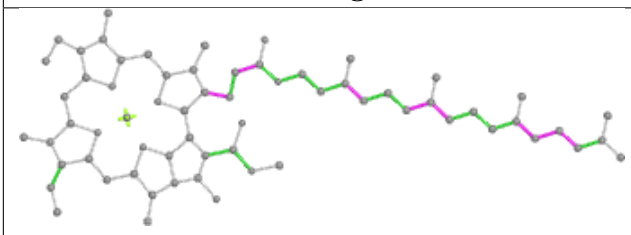


Bond angles



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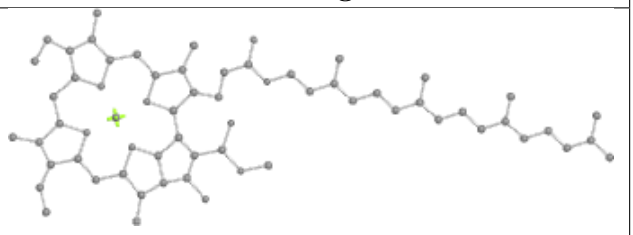
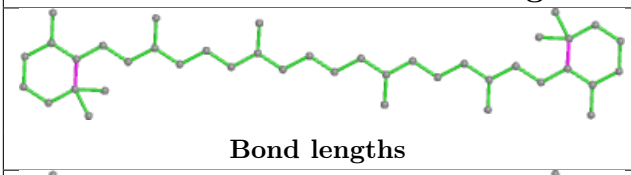
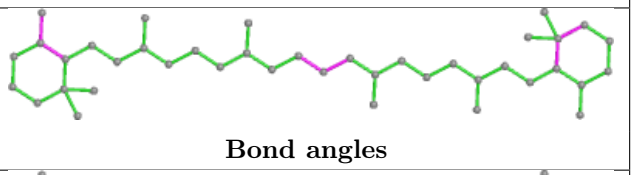


Rings

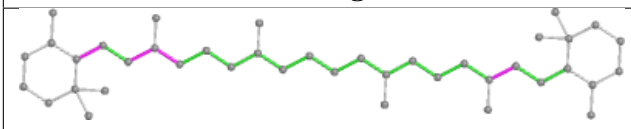
Ligand BCR x 101



Bond lengths



Bond angles



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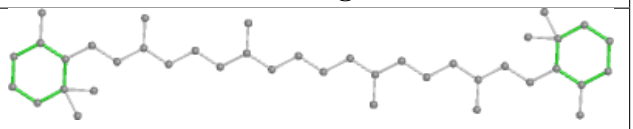
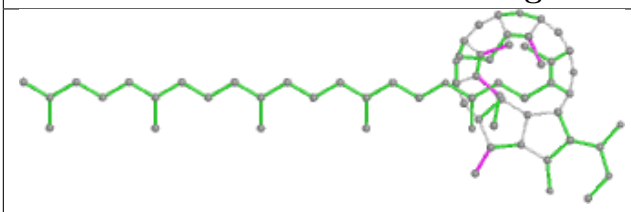


Rings

Ligand PHO d 401



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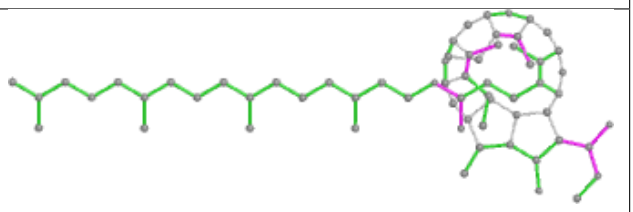
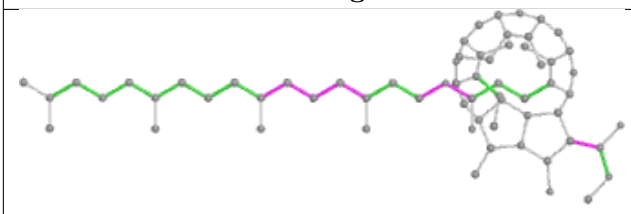


Bond angles



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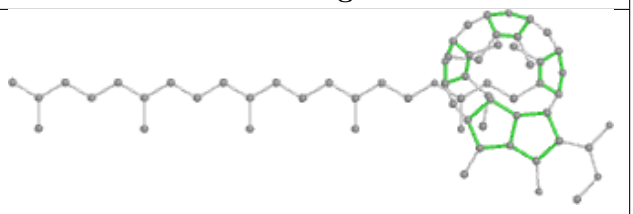
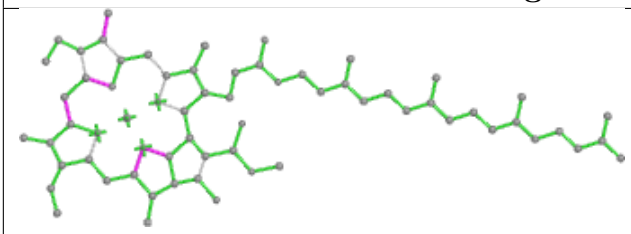


Rings

Ligand CLA C 501



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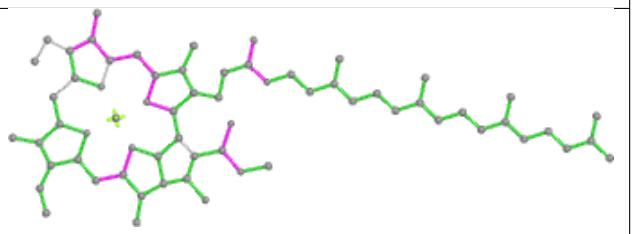
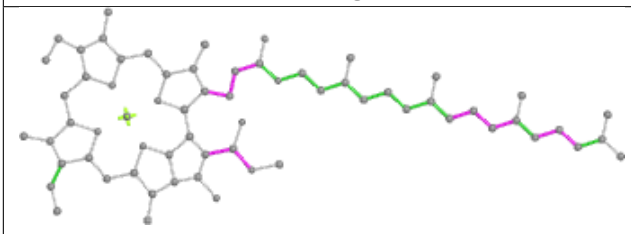


Bond angles



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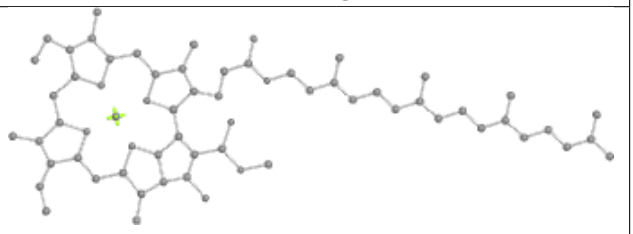
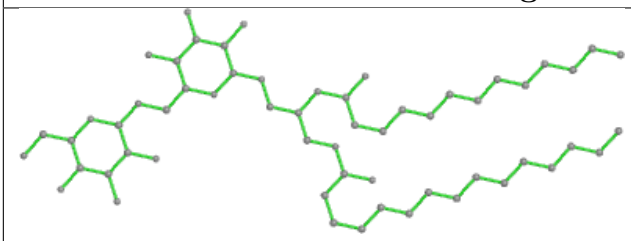


Rings

Ligand DGD B 620



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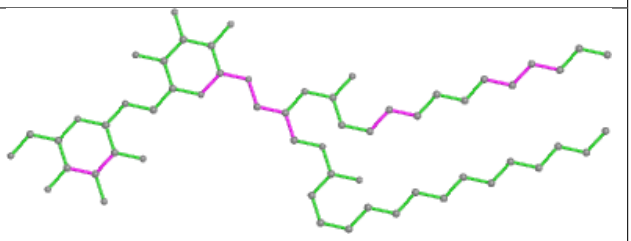
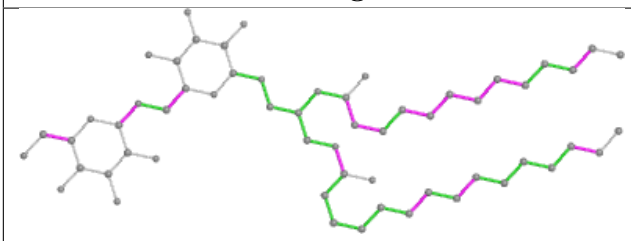


Bond angles



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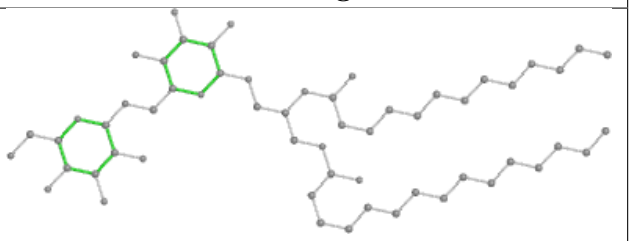
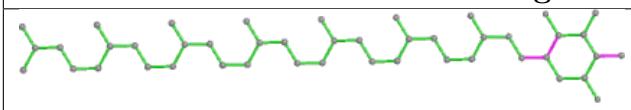


Rings

Ligand PL9 a 407



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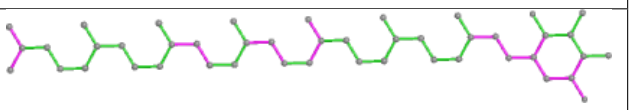
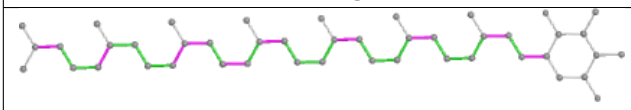


Bond angles



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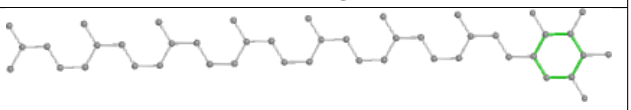
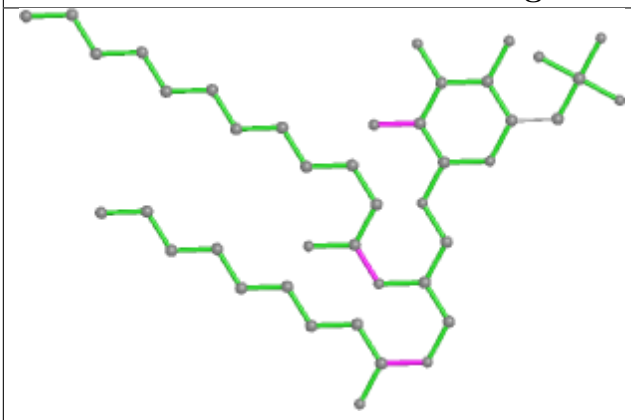


Rings

Ligand SQD B 622



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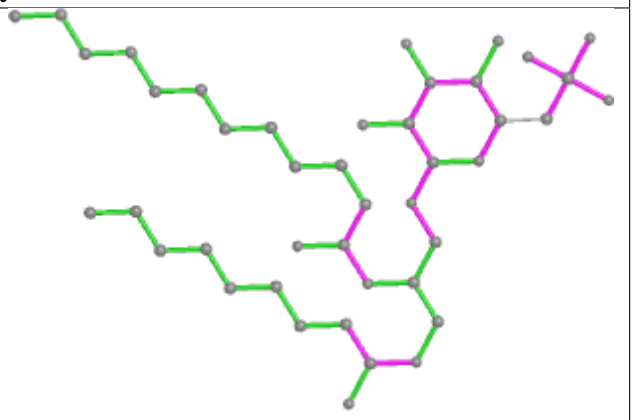
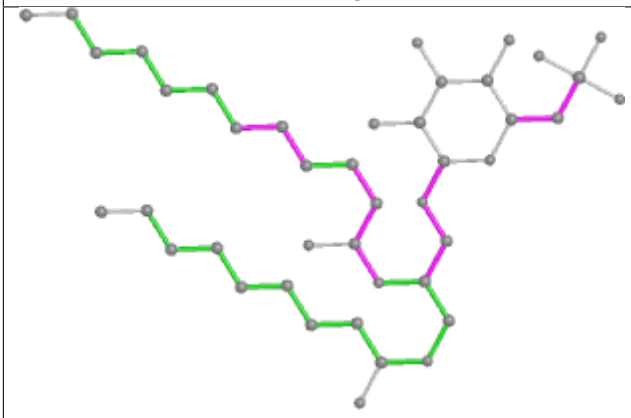
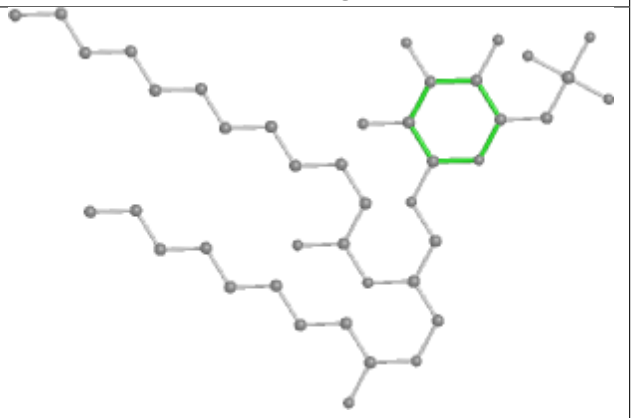


Bond angles

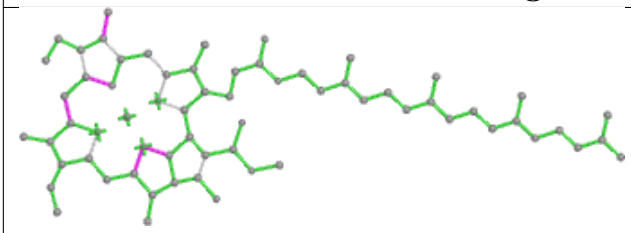


Torsions



Rings

Ligand CLA B 614



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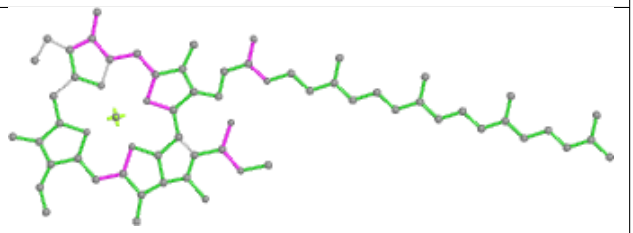
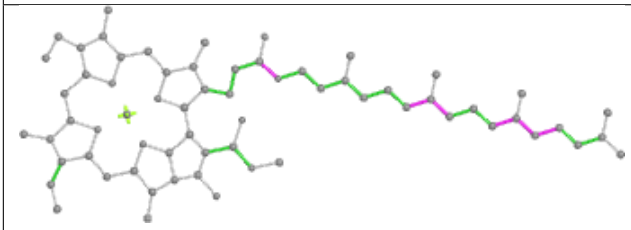


Bond angles



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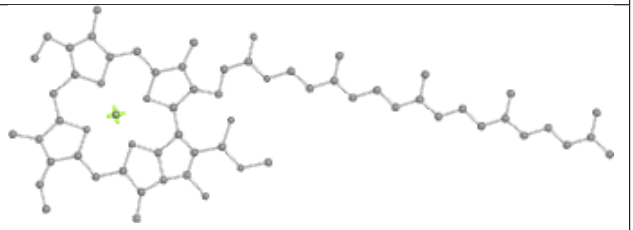
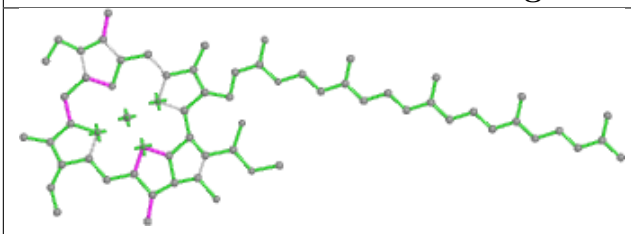


Rings

Ligand CLA B 606



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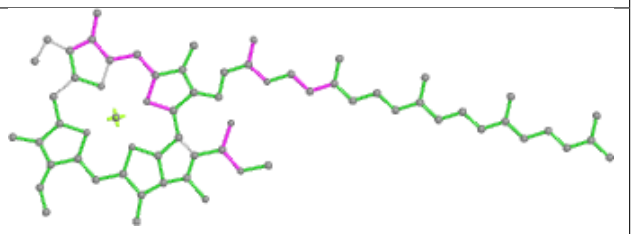
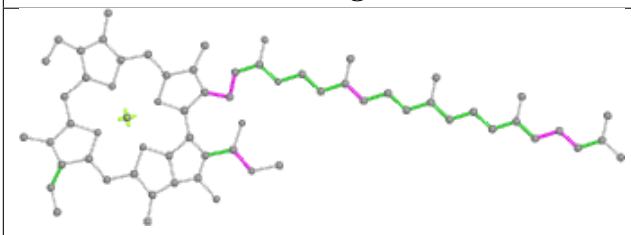
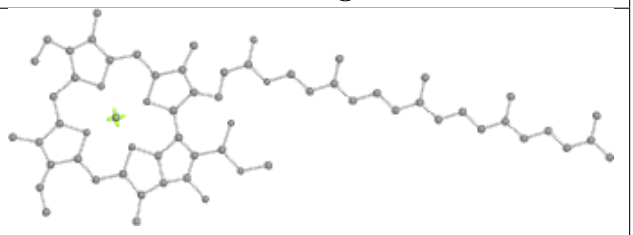


Bond angles

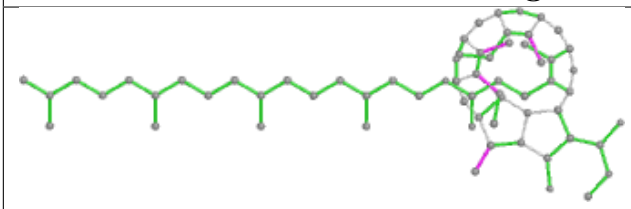


Torsions



Rings

Ligand PHO d 402



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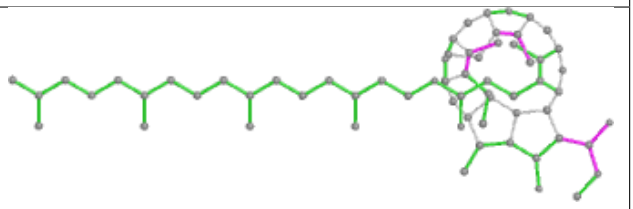
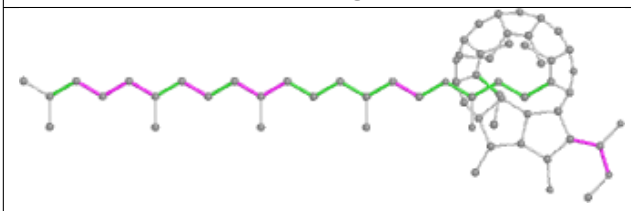


Bond angles



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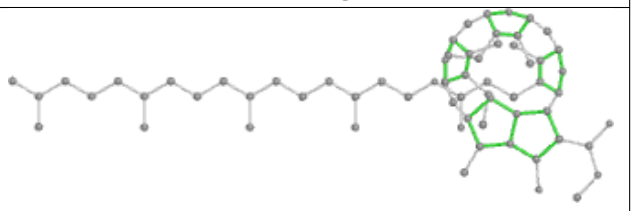
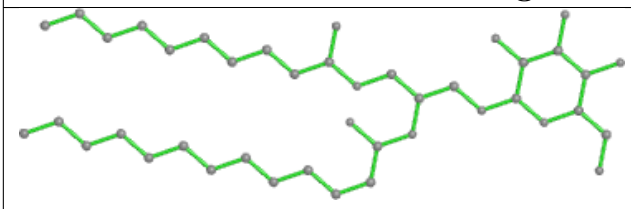


Rings

Ligand LMG M 101



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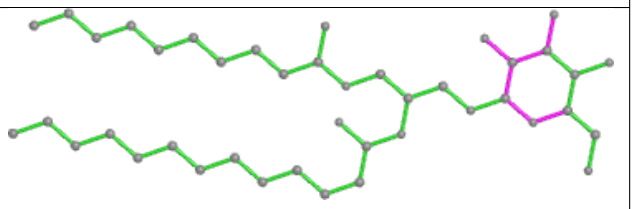
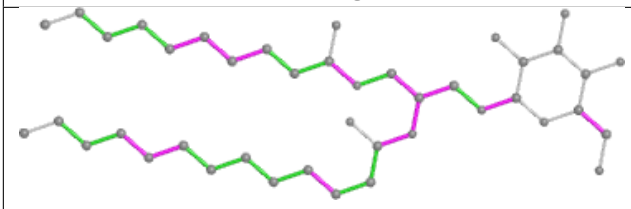
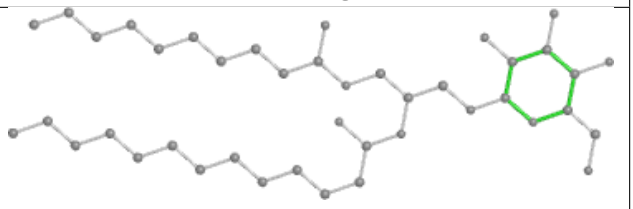


Bond angles

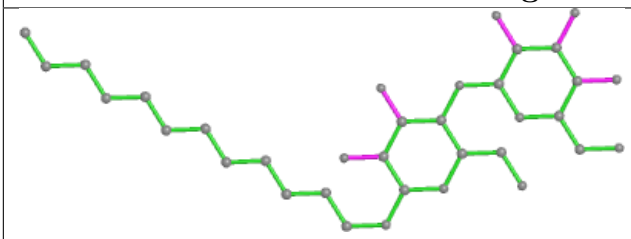


Torsions



Rings

Ligand LMT B 623



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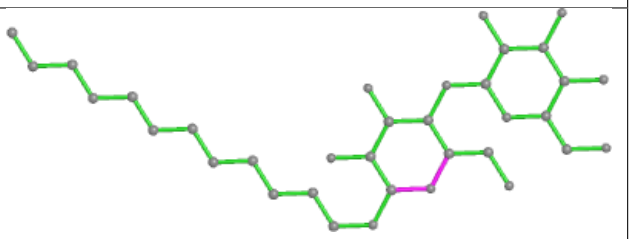
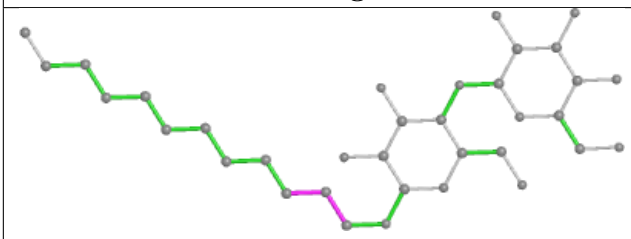
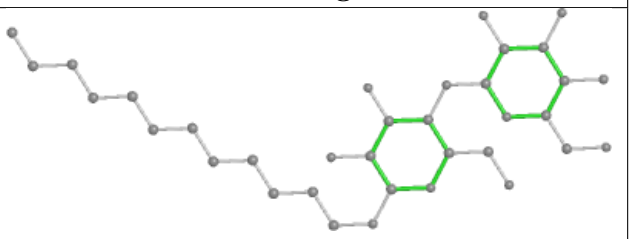


Bond angles

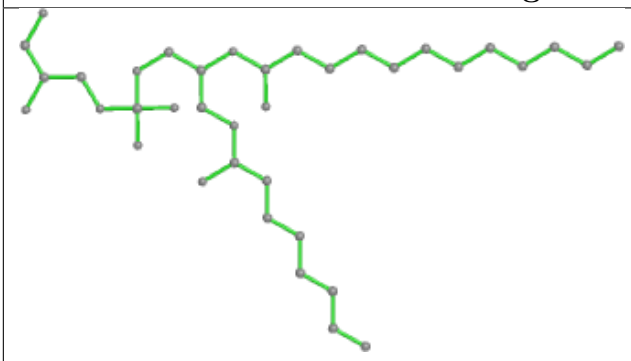


Torsions

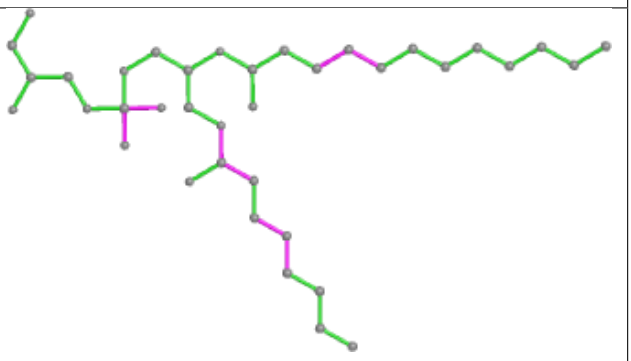


Rings

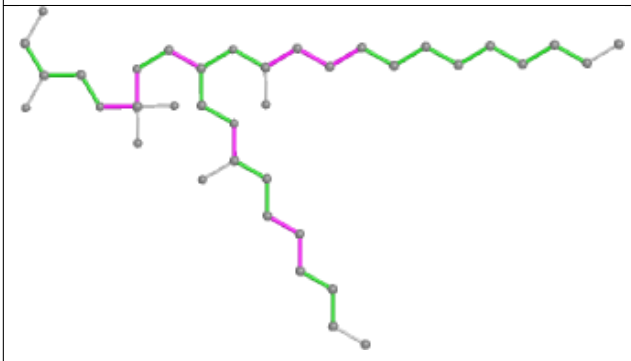
Ligand LHG C 518



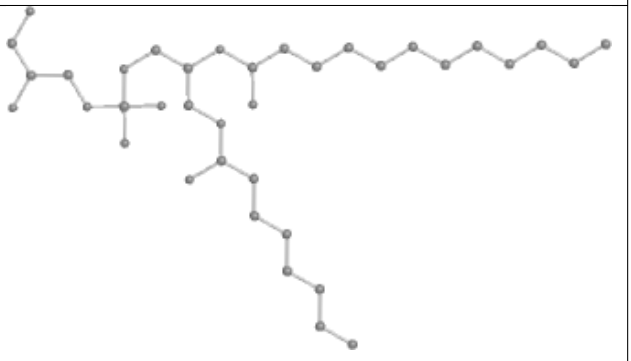
Bond lengths



Bond angles

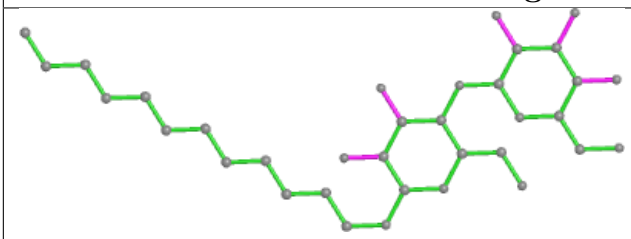


Torsions

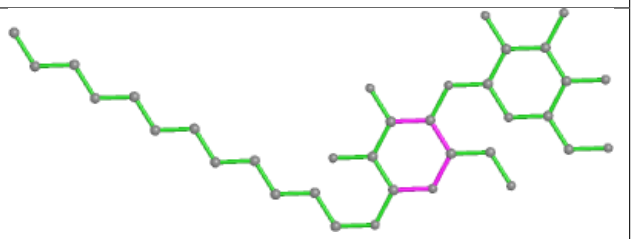


Rings

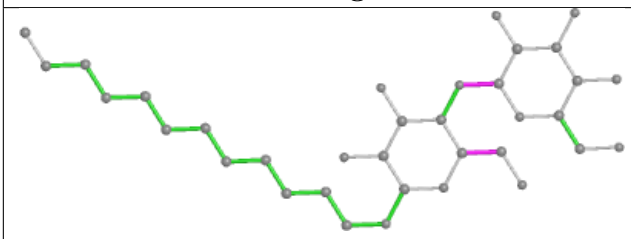
Ligand LMT b 629



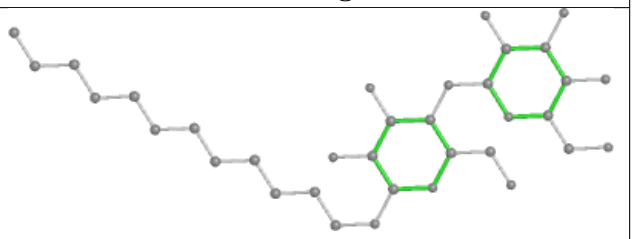
Bond lengths



Bond angles

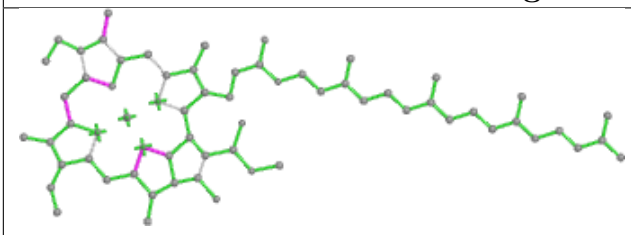


Torsions



Rings

Ligand CLA H 101



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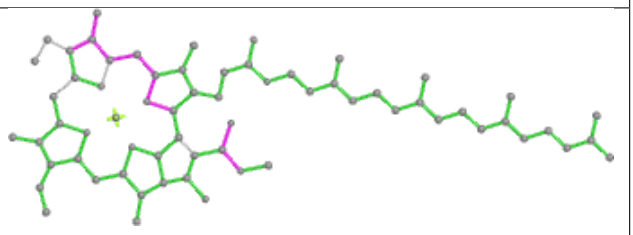

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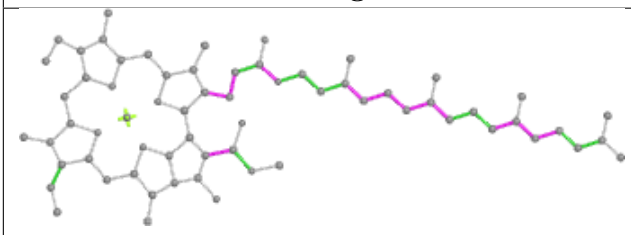
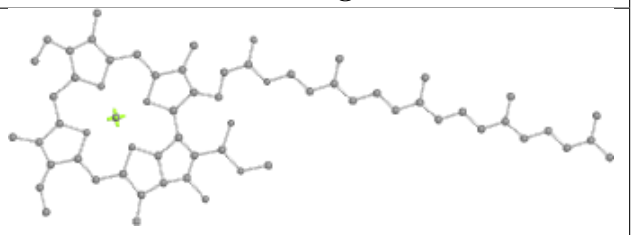
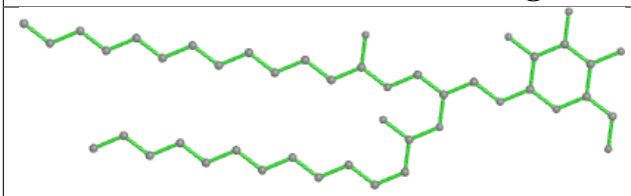


Torsions



Rings

Ligand LMG c 518



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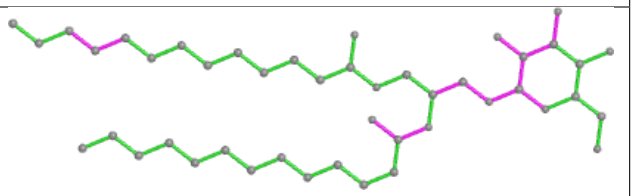
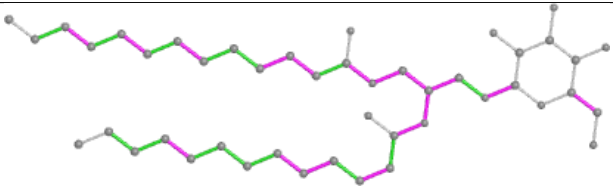


Bond angles



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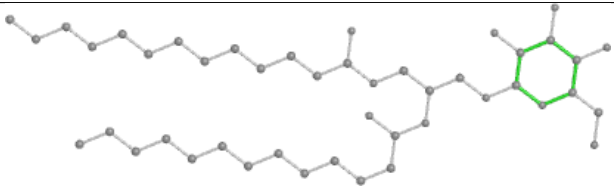
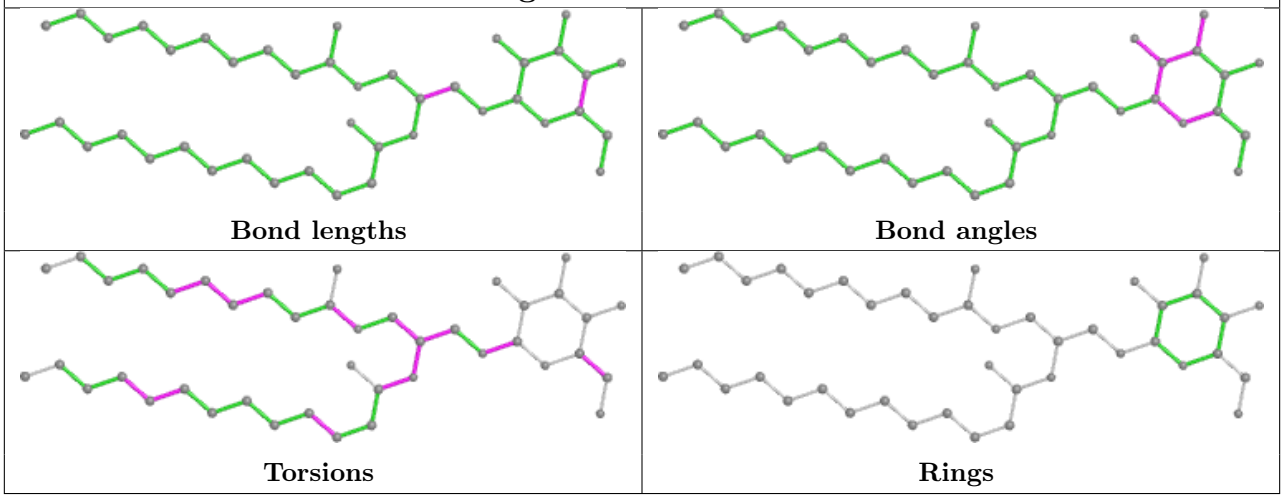
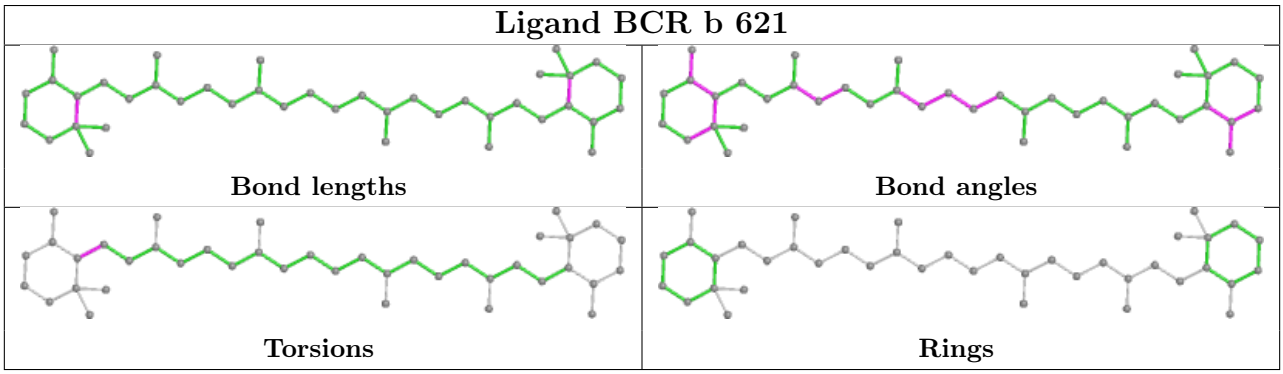


Rings

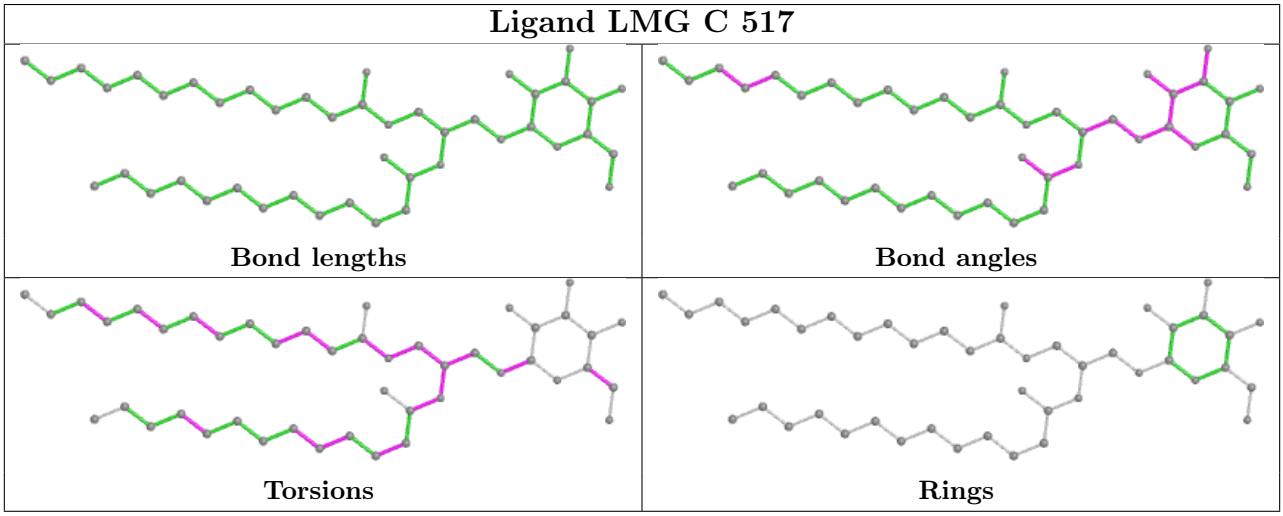
Ligand LMG m 101



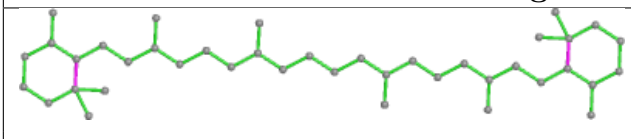
Ligand BCR b 621



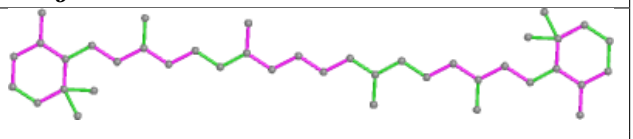
Ligand LMG C 517



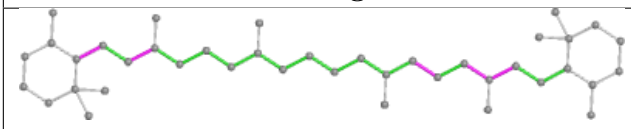
Ligand BCR j 102



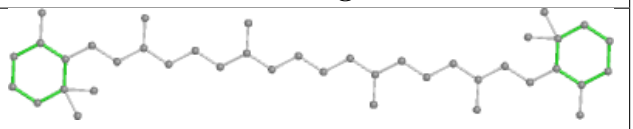
Bond lengths



Bond angles

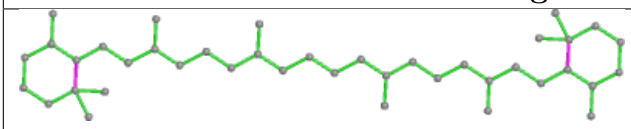


Torsions



Rings

Ligand BCR i 101



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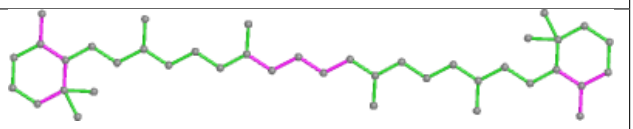
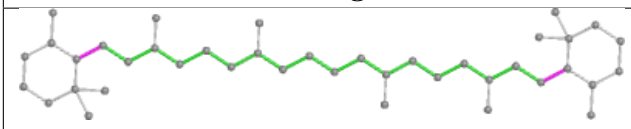


Bond angles



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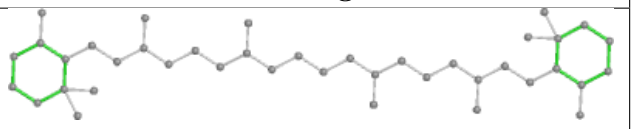
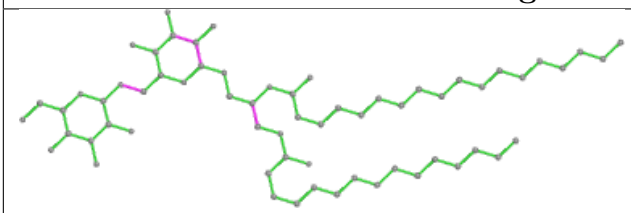


Rings

Ligand DGD D 407



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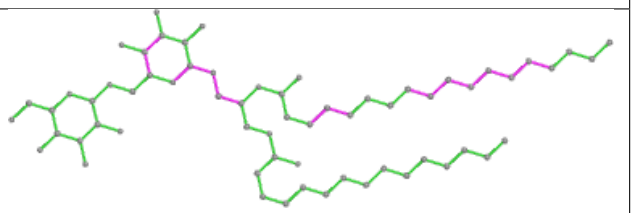
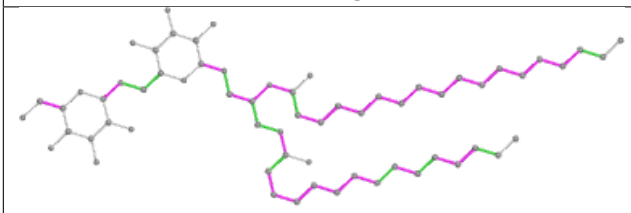


Bond angles



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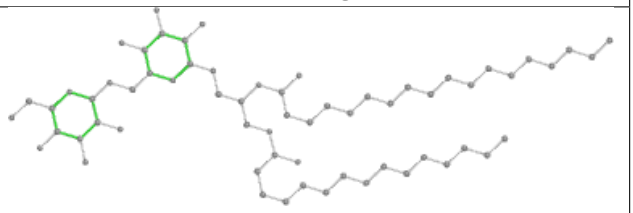
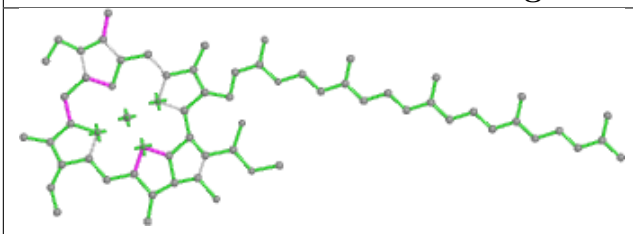


Rings

Ligand CLA C 510



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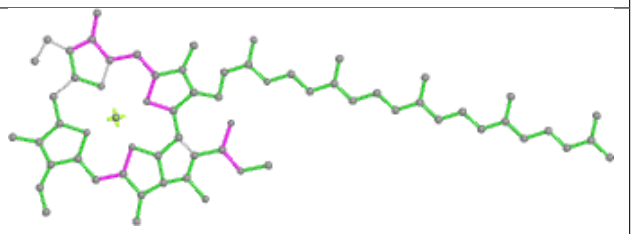
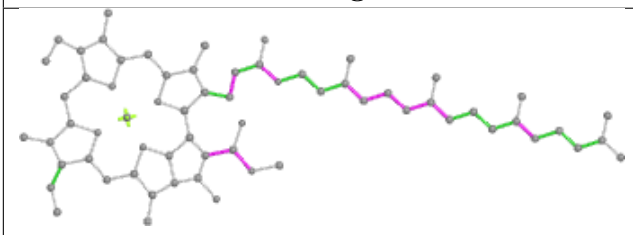
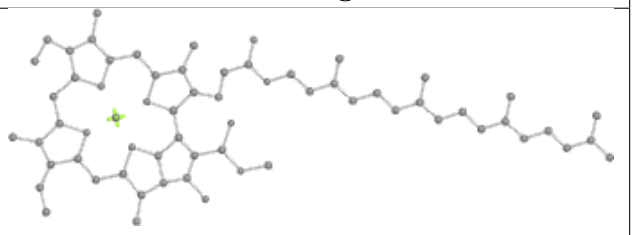


Bond angles

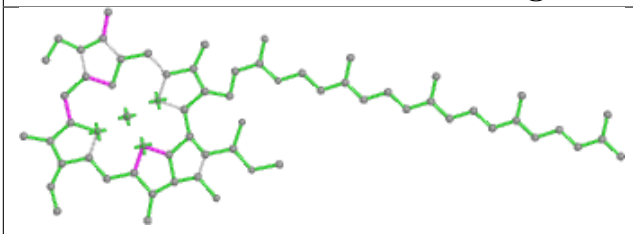


Torsions



Rings

Ligand CLA b 609



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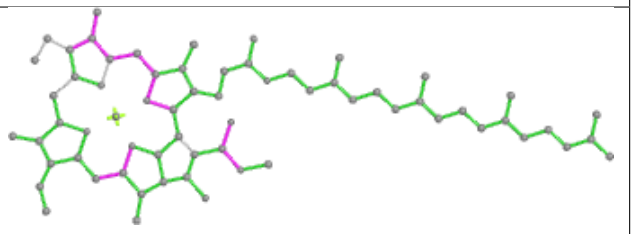
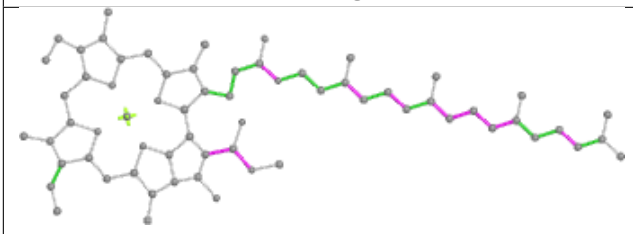
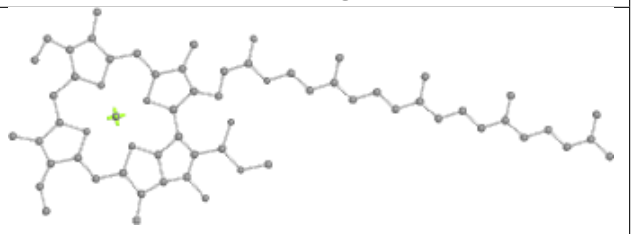


Bond angles

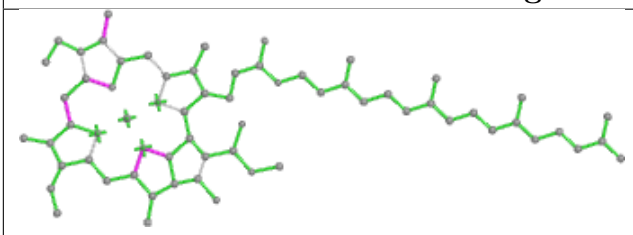


Torsions



Rings

Ligand CLA B 612



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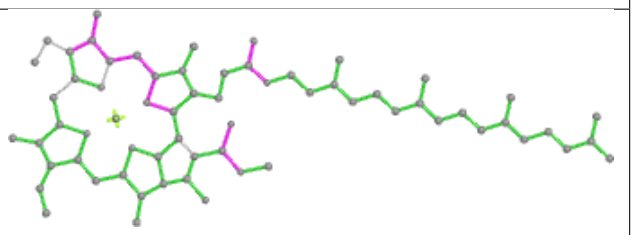
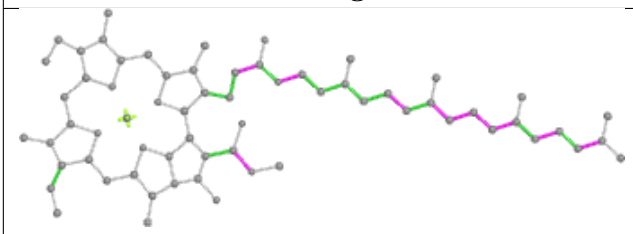


Bond angles



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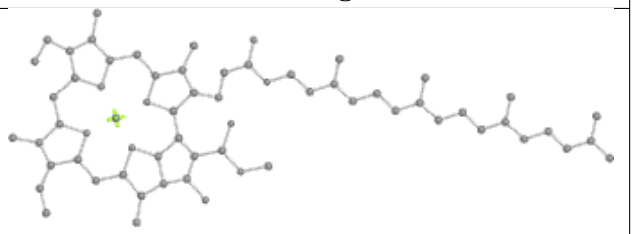
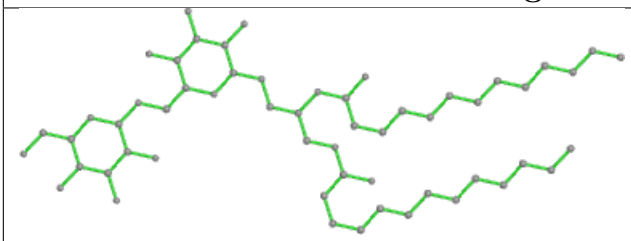


Rings

Ligand DGD a 408



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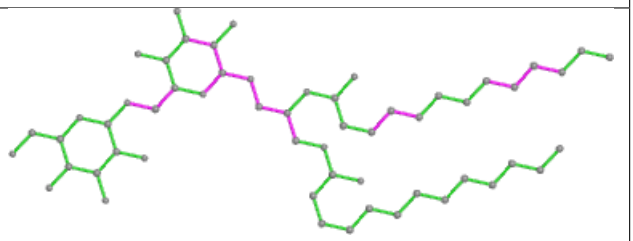
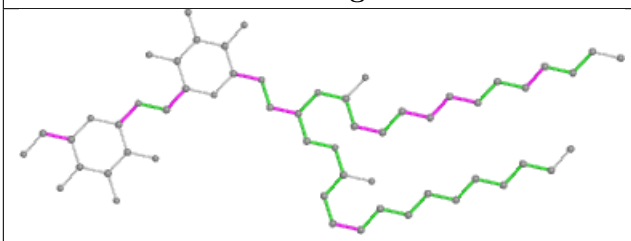
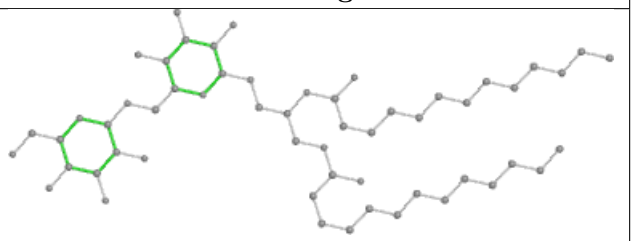


Bond angles

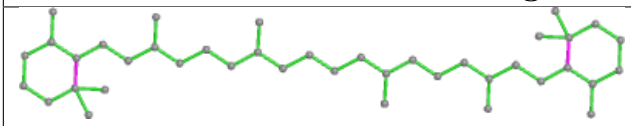


Torsions



Rings

Ligand BCR C 520



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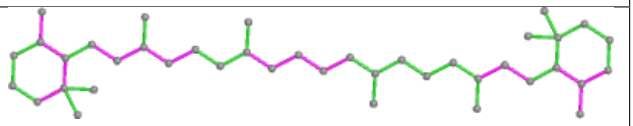
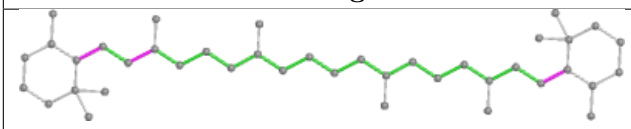
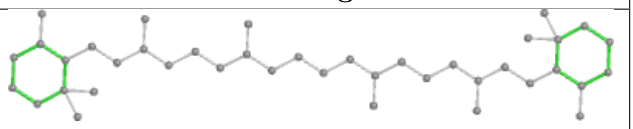


Bond angles

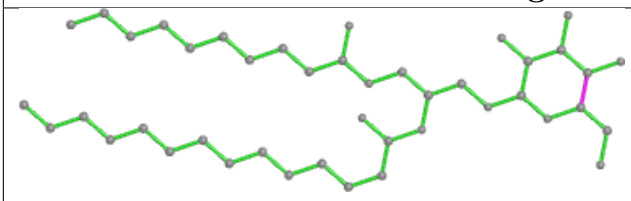


Torsions



Rings

Ligand LMG i 102



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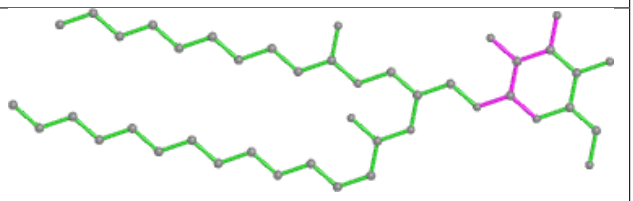
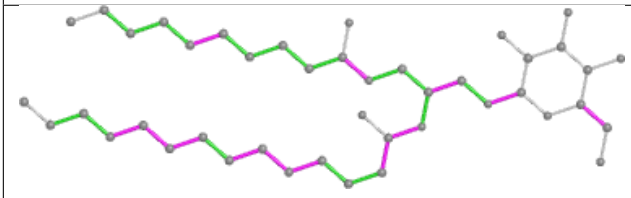
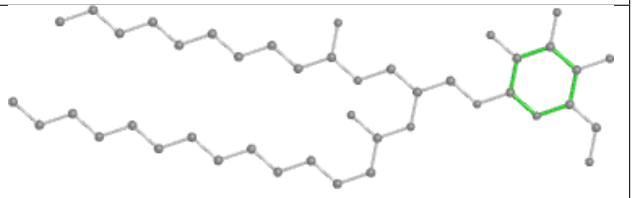


Bond angles

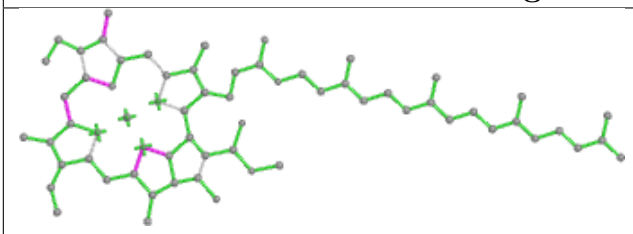


Torsions

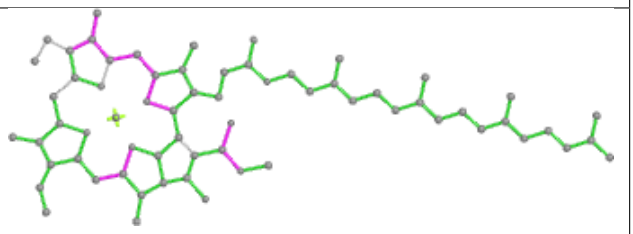


Rings

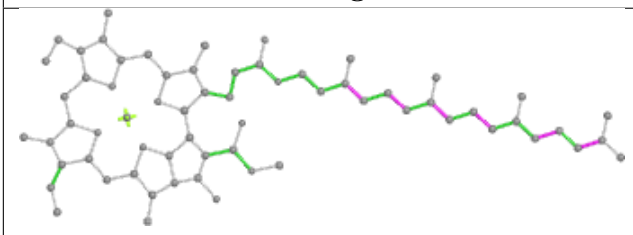
Ligand CLA A 406



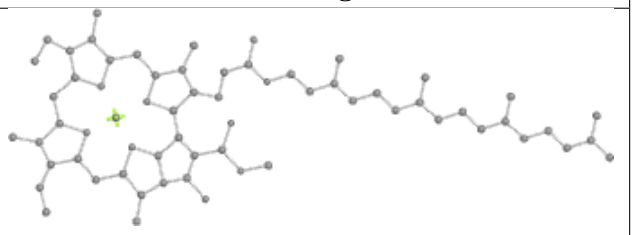
Bond lengths



Bond angles

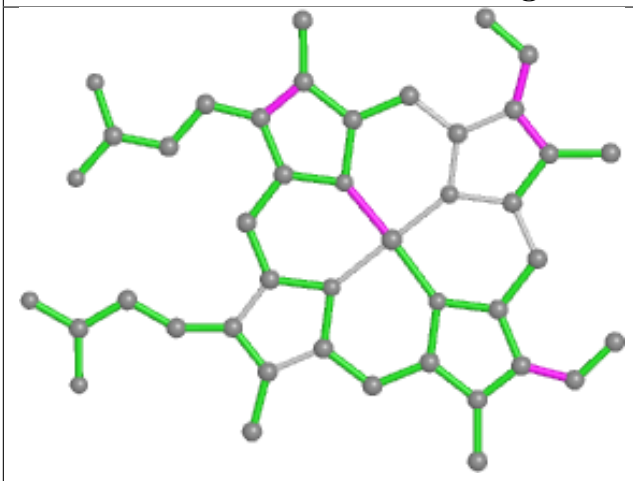


Torsions



Rings

Ligand HEM F 101



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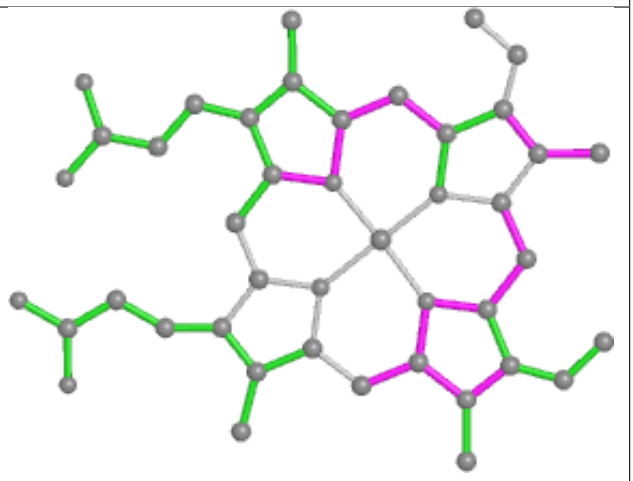
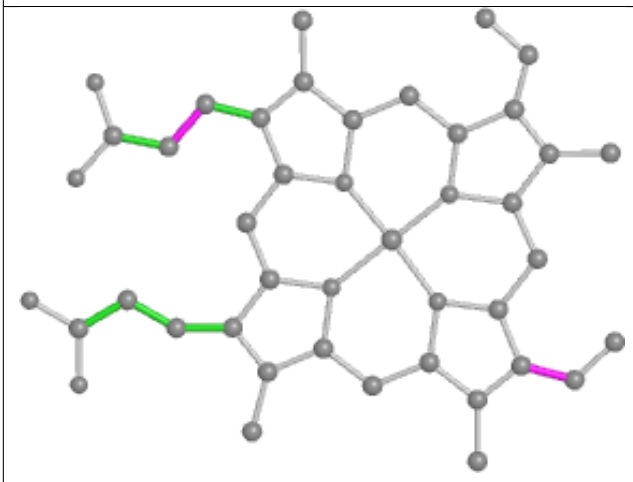
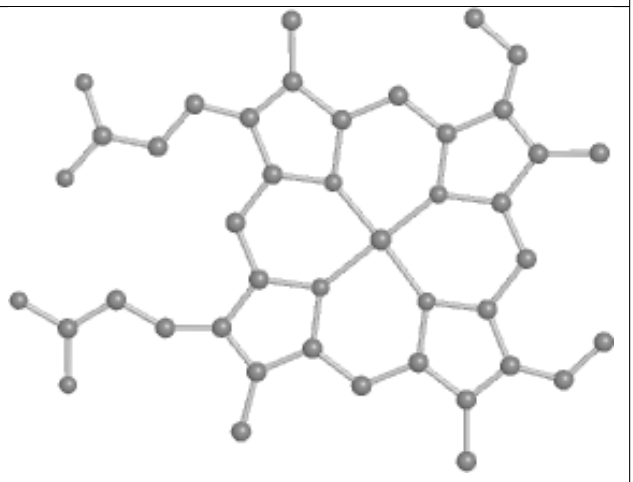


Bond angles

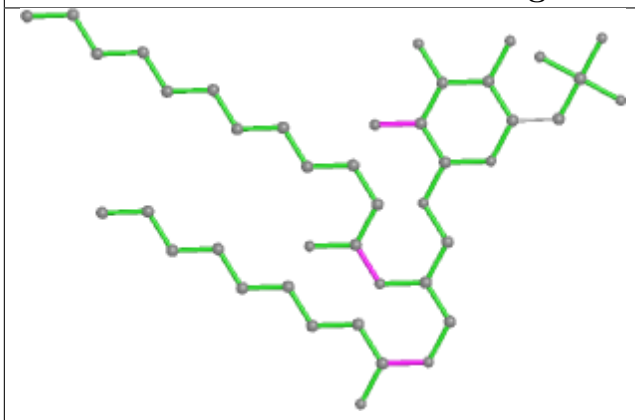


Torsions



Rings

Ligand SQD d 403



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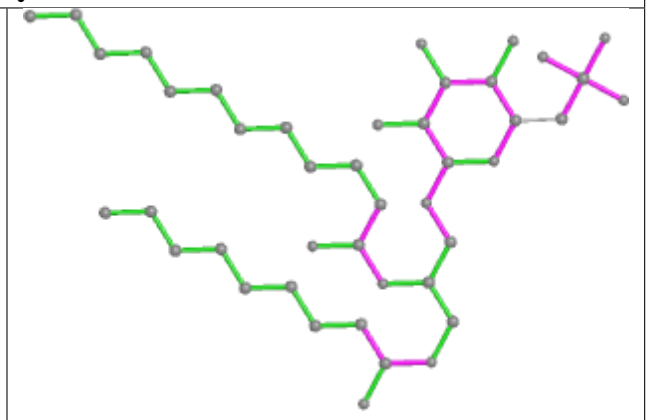
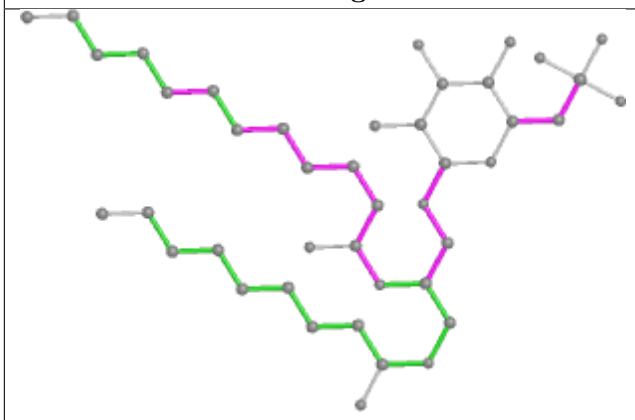


Bond angles



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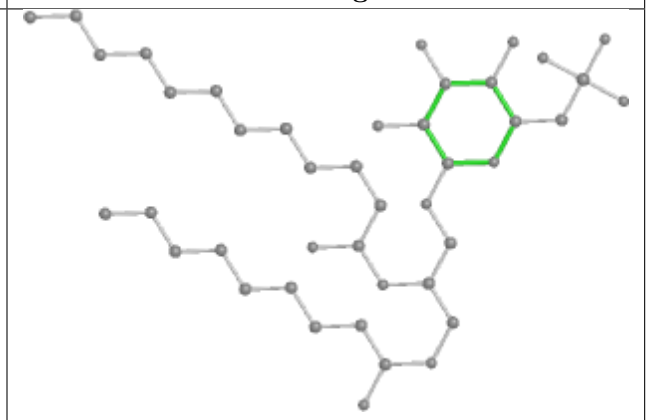
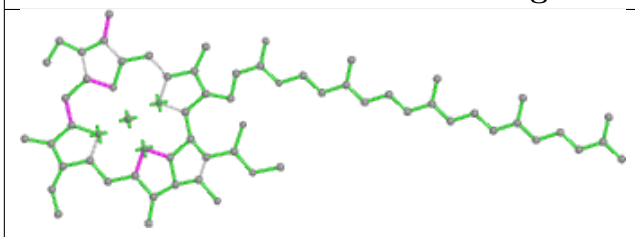


Rings

Ligand CLA c 505



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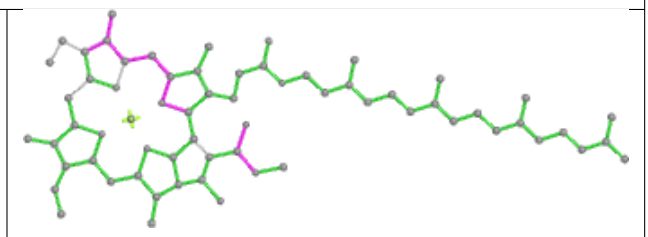
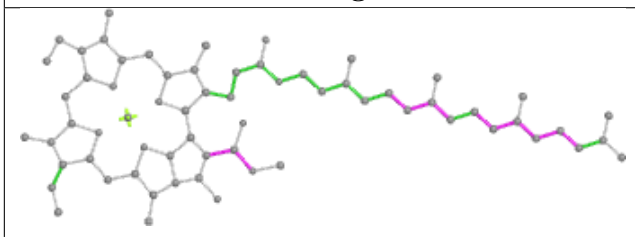
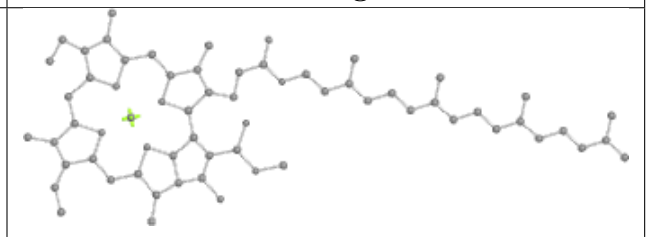


Bond angles

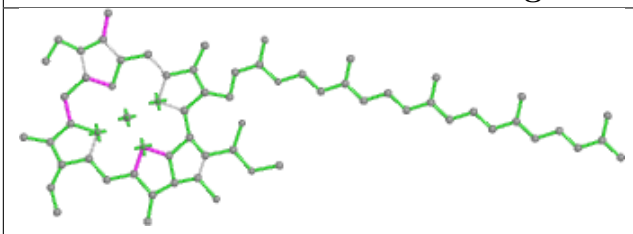


Torsions



Rings

Ligand CLA B 609



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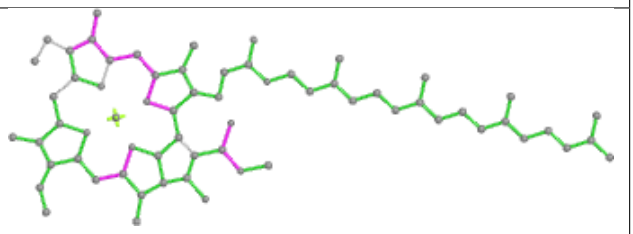
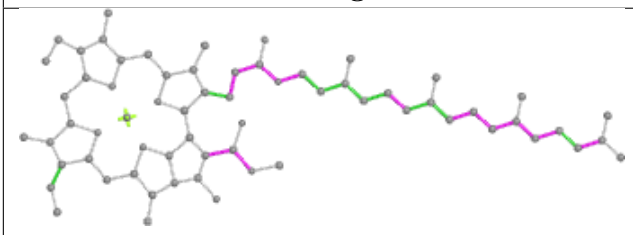


Bond angles



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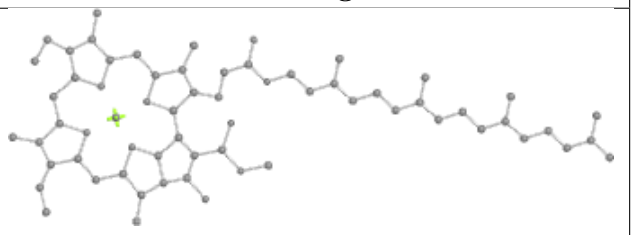
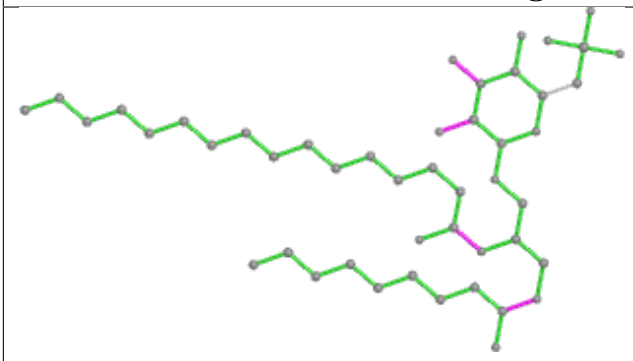


Rings

Ligand SQD b 602



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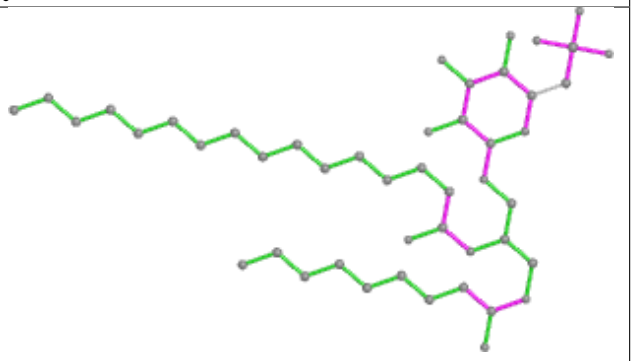
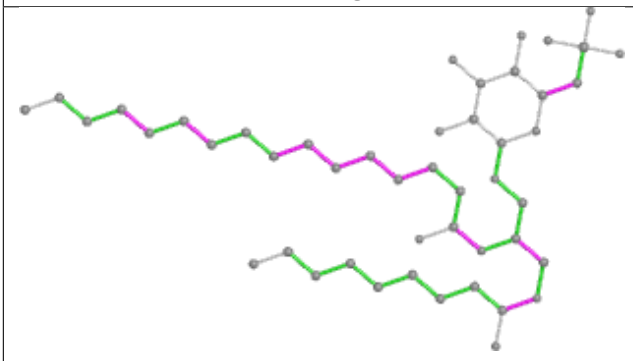
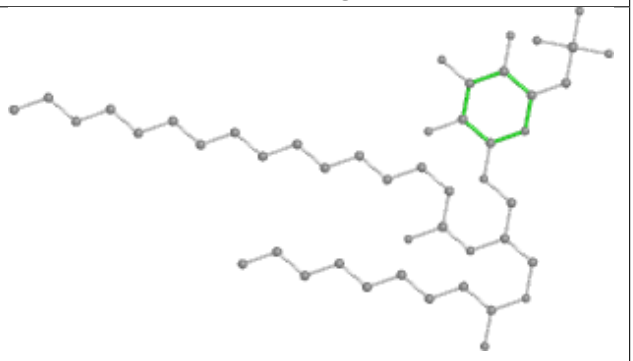


Bond angles

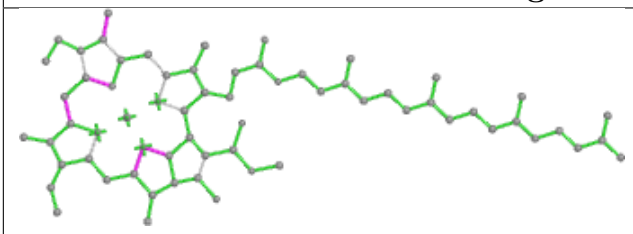


Torsions

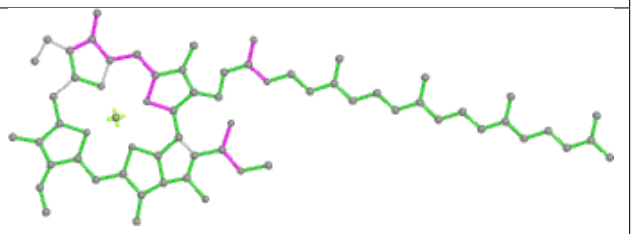


Rings

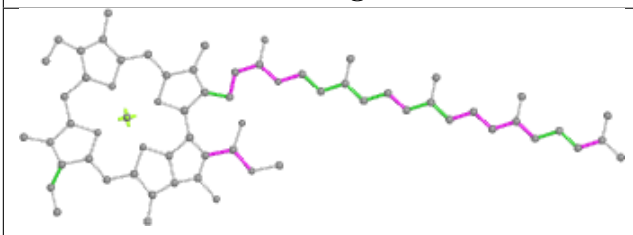
Ligand CLA b 614



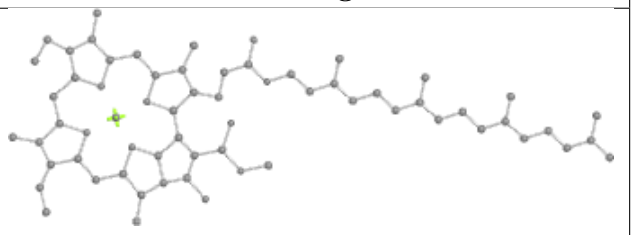
Bond lengths



Bond angles

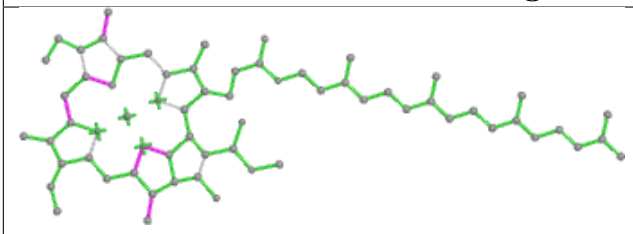


Torsions

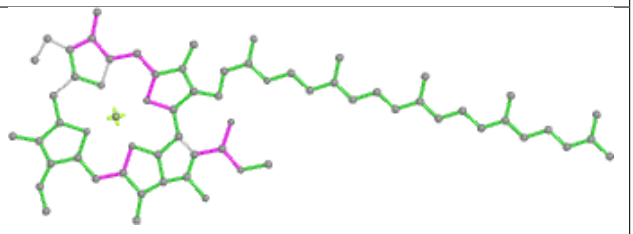


Rings

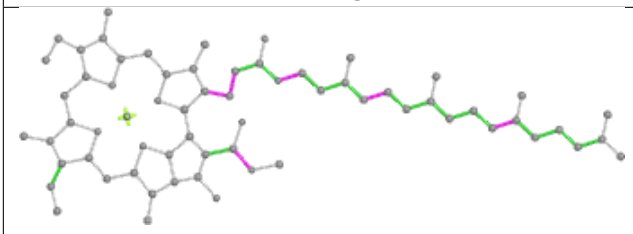
Ligand CLA A 402



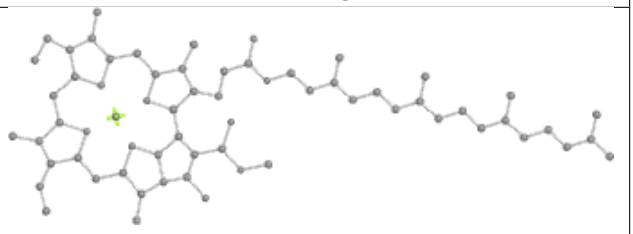
Bond lengths



Bond angles

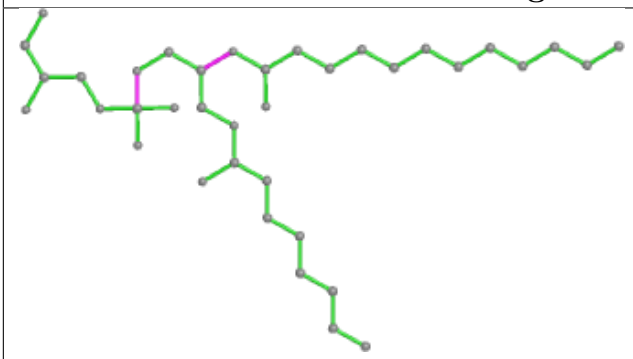


Torsions

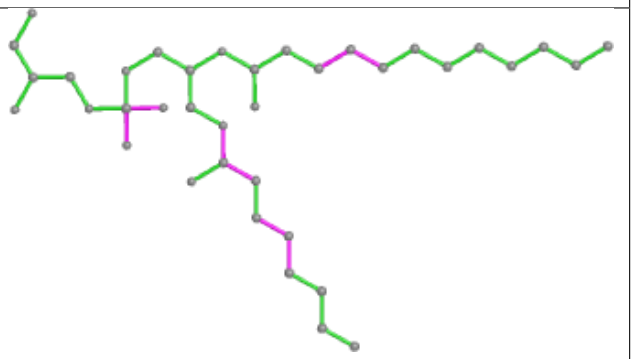


Rings

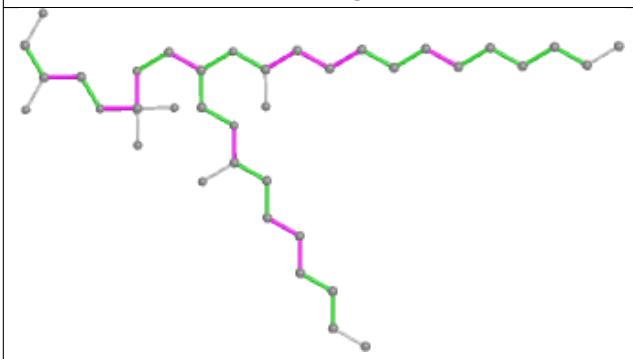
Ligand LHG c 519



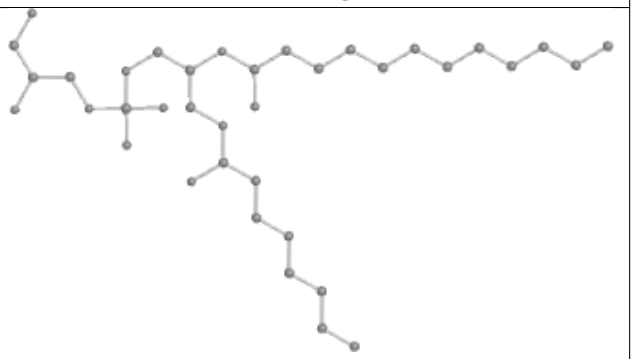
Bond lengths



Bond angles

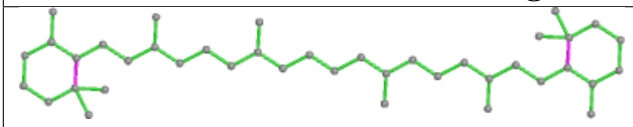


Torsions

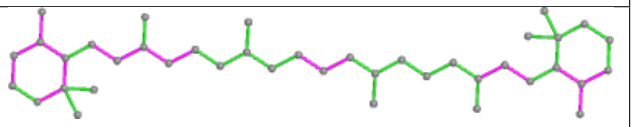


Rings

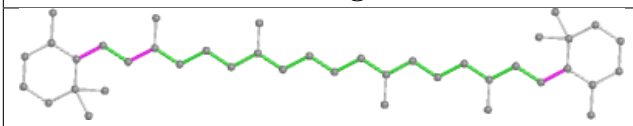
Ligand BCR b 624



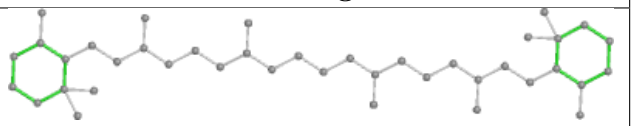
Bond lengths



Bond angles

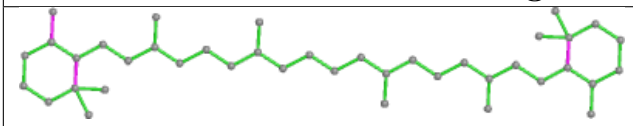


Torsions



Rings

Ligand BCR y 101



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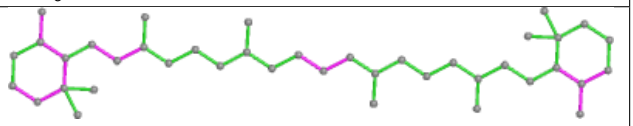
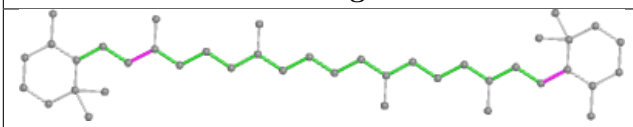
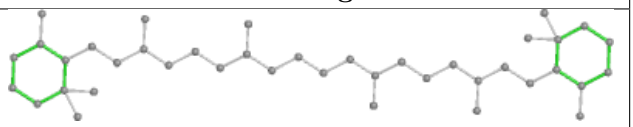


Bond angles

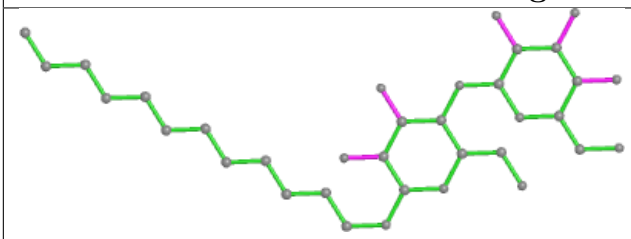


Torsions



Rings

Ligand LMT i 103



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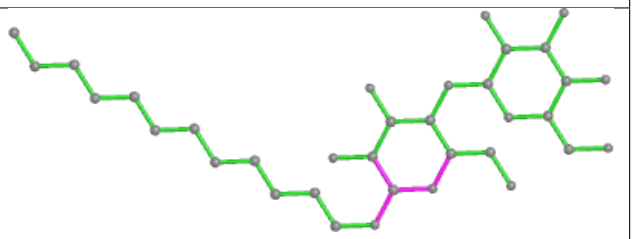
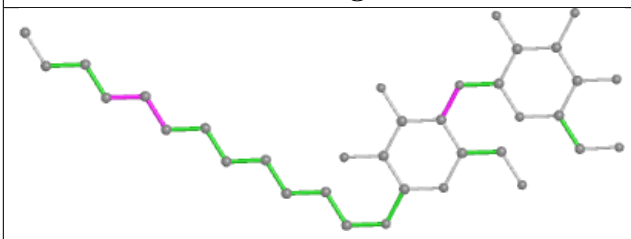
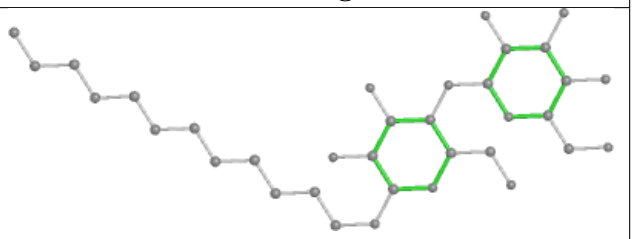


Bond angles

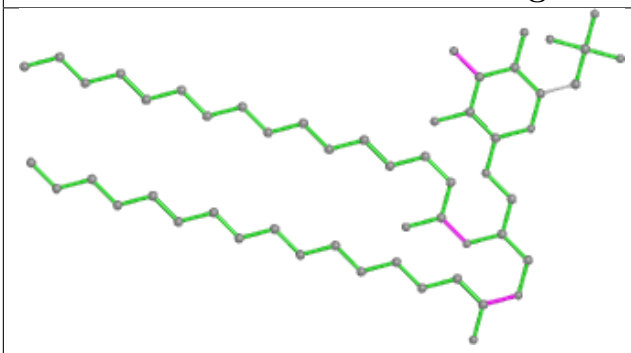


Torsions

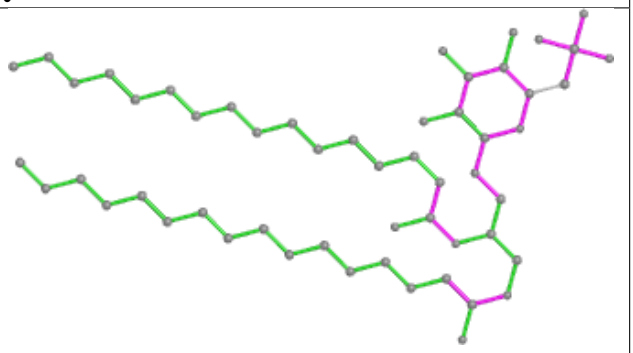


Rings

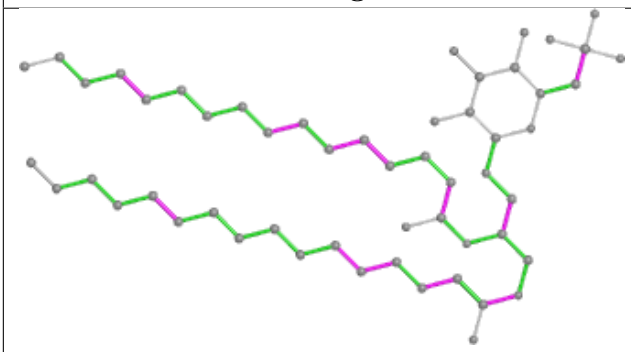
Ligand SQD a 401



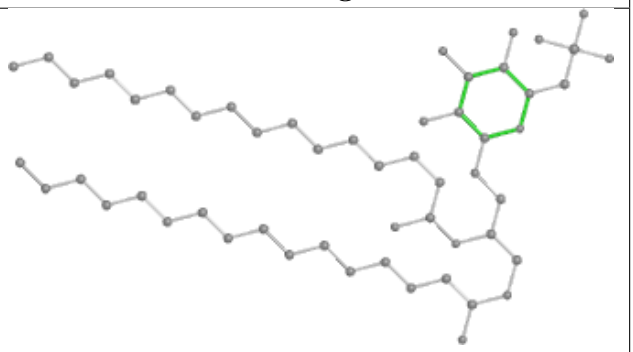
Bond lengths



Bond angles

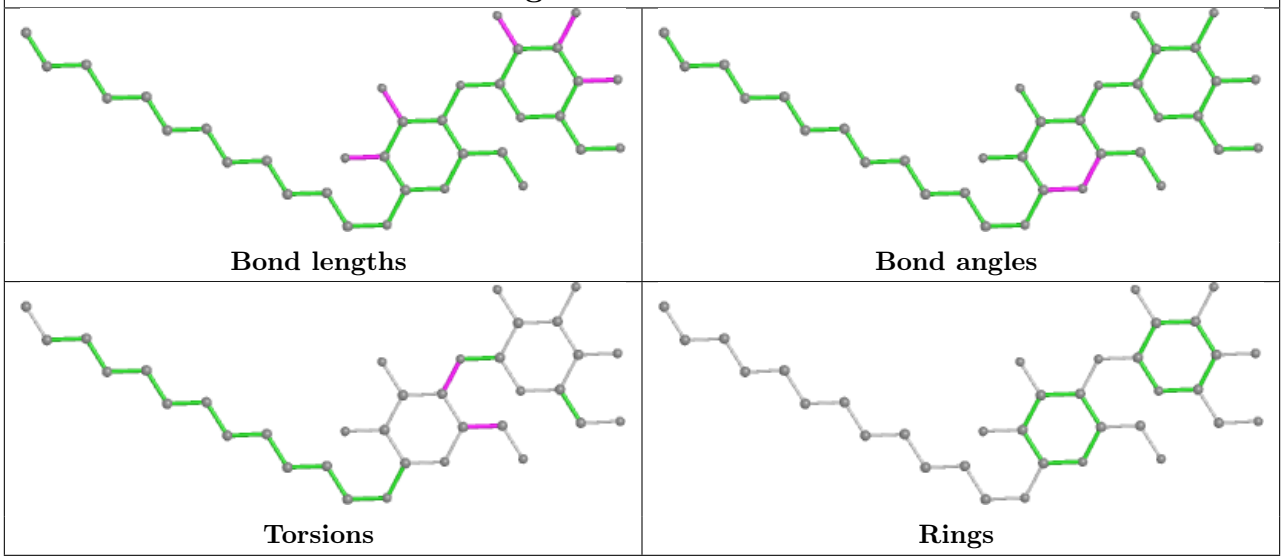


Torsions

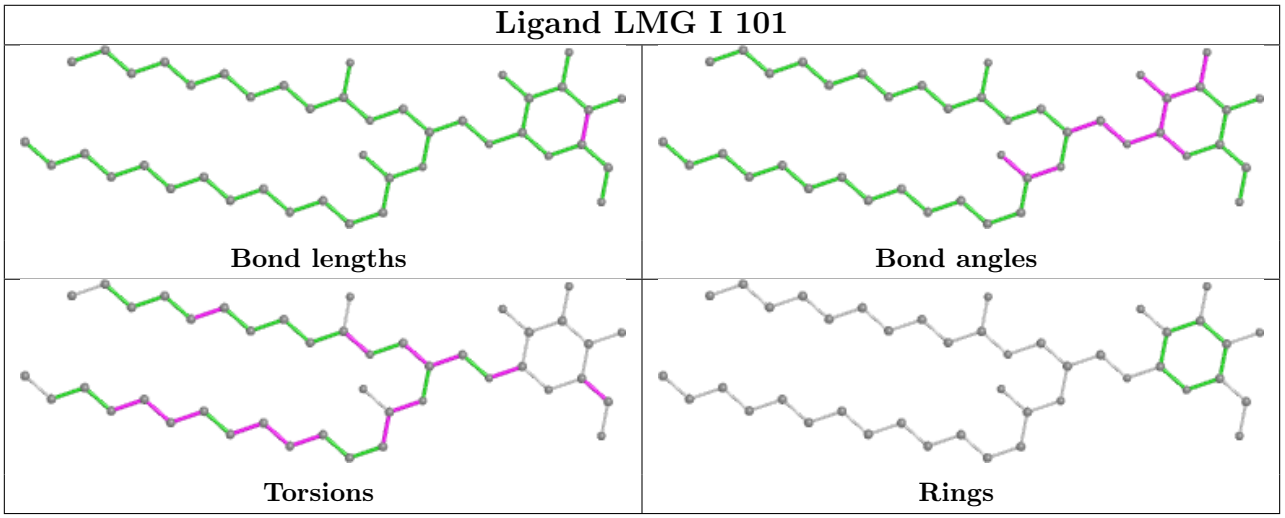


Rings

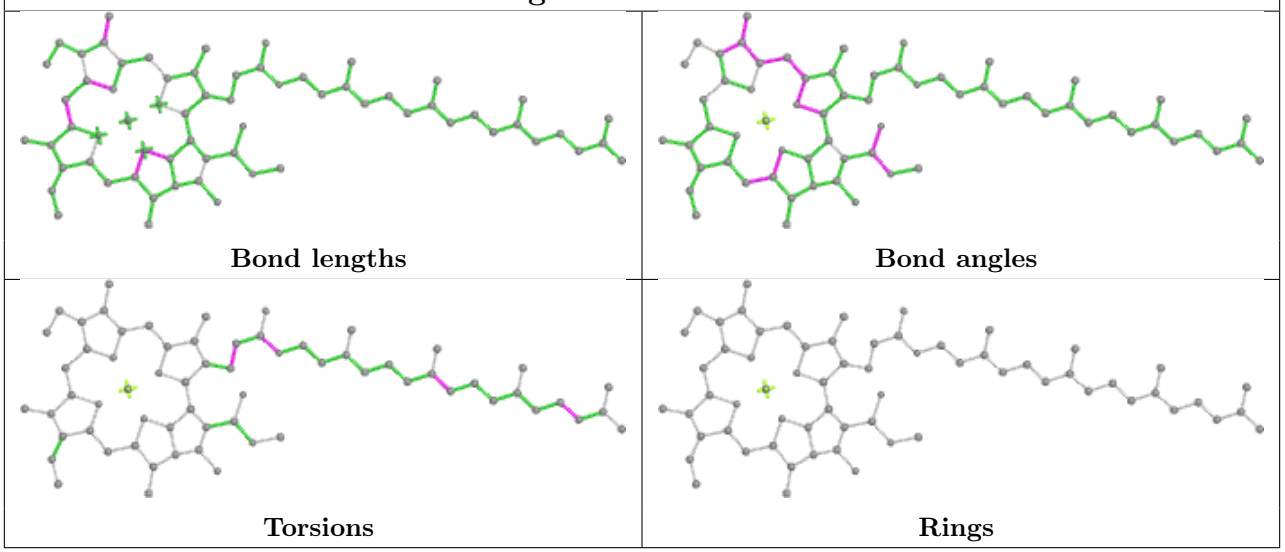
Ligand LMT b 603



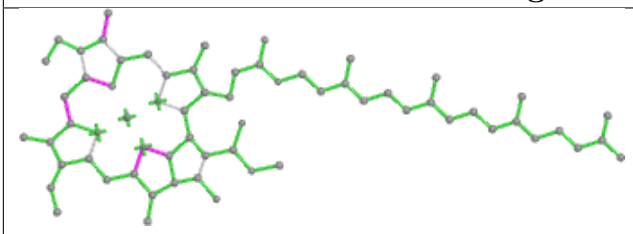
Ligand LMG I 101



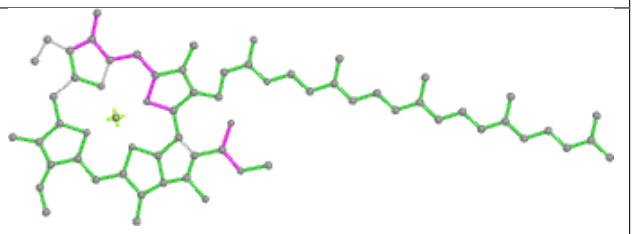
Ligand CLA d 406



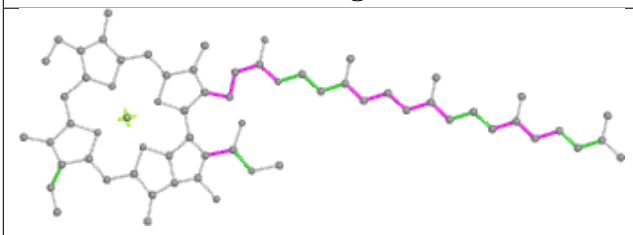
Ligand CLA b 606



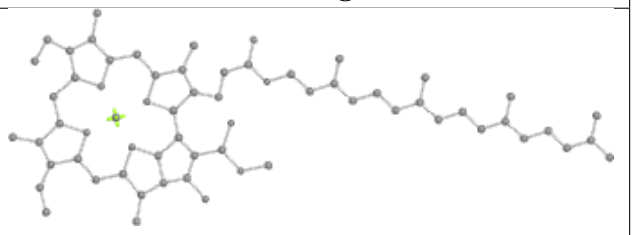
Bond lengths



Bond angles

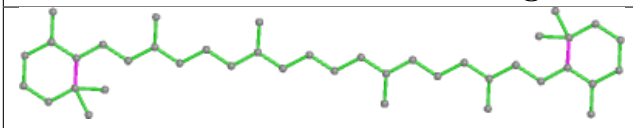


Torsions

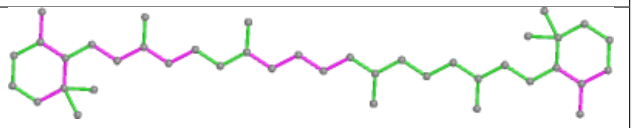


Rings

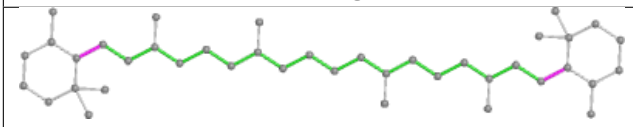
Ligand BCR B 616



Bond lengths



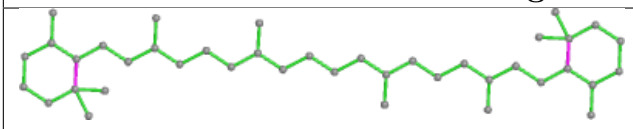
Bond angles



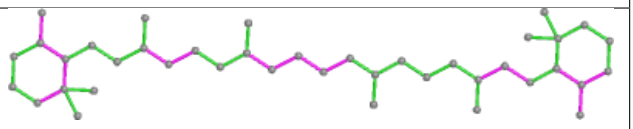
Torsions

Rings

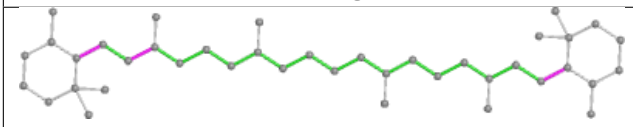
Ligand BCR c 521



Bond lengths



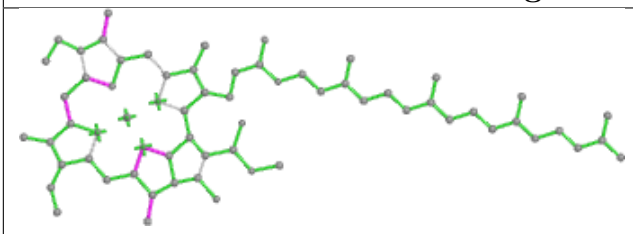
Bond angles



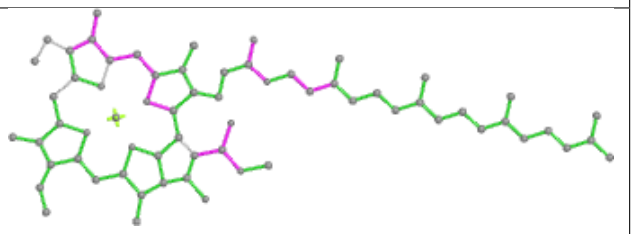
Torsions

Rings

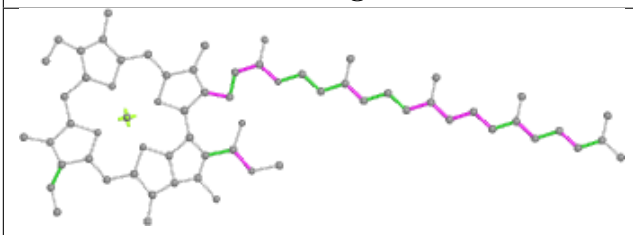
Ligand CLA C 504



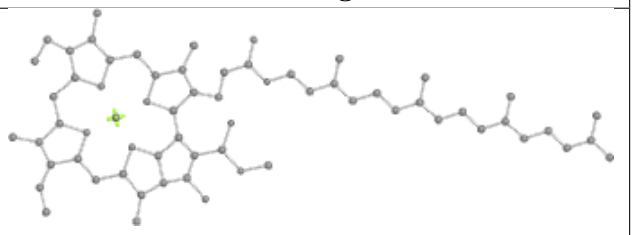
Bond lengths



Bond angles

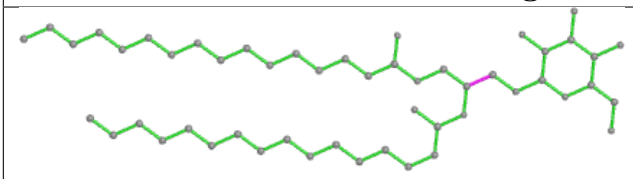


Torsions

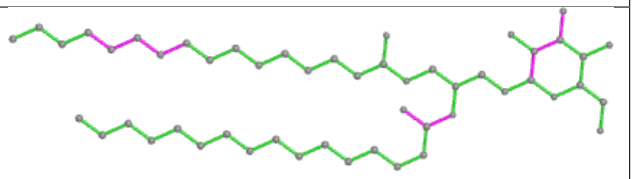


Rings

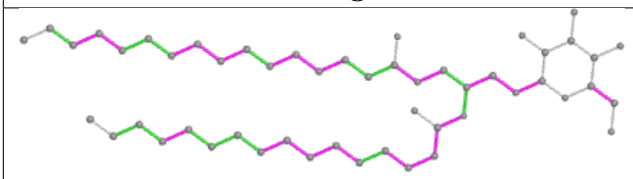
Ligand LMG L 101



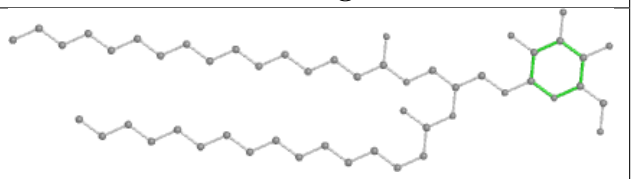
Bond lengths



Bond angles

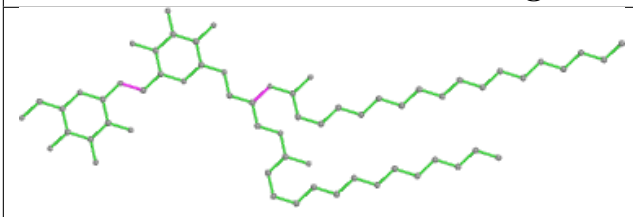


Torsions

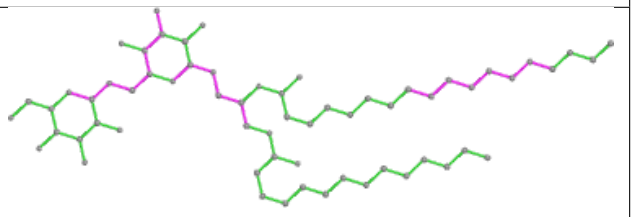


Rings

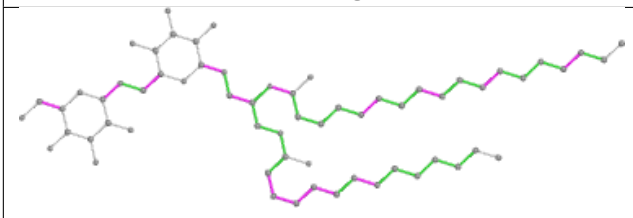
Ligand DGD c 516



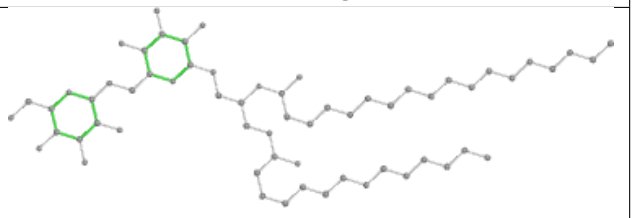
Bond lengths



Bond angles

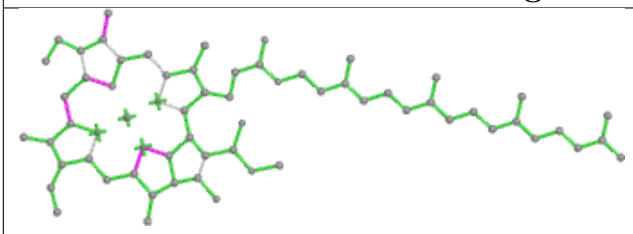


Torsions

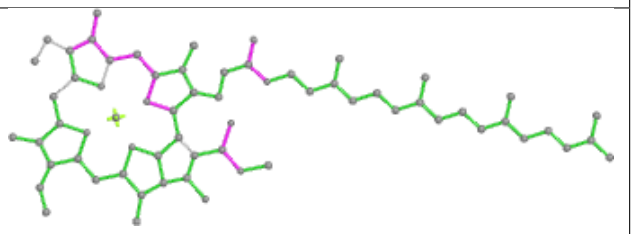


Rings

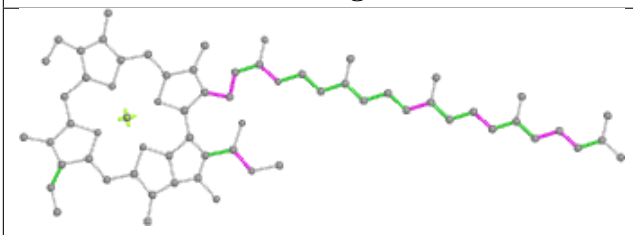
Ligand CLA C 519



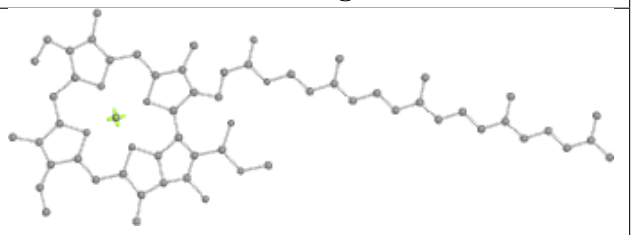
Bond lengths



Bond angles

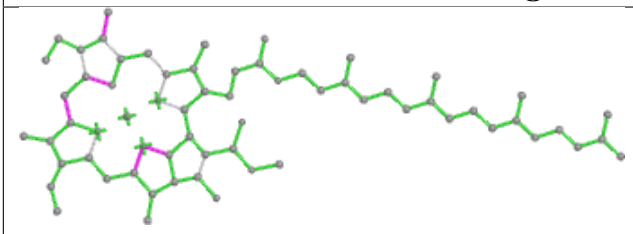


Torsions

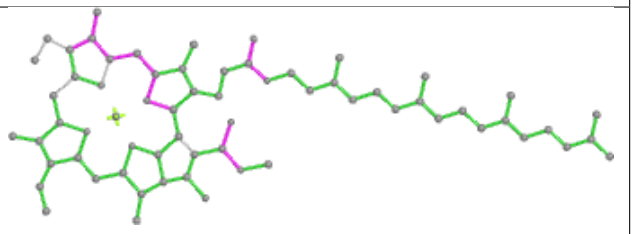


Rings

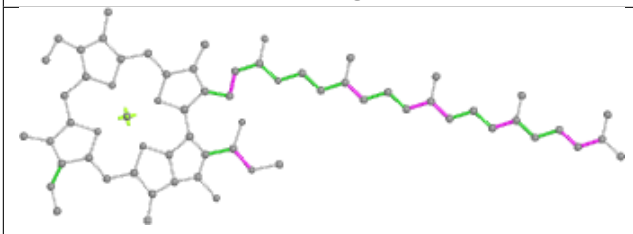
Ligand CLA B 602



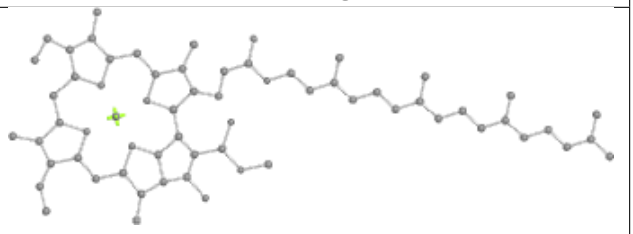
Bond lengths



Bond angles

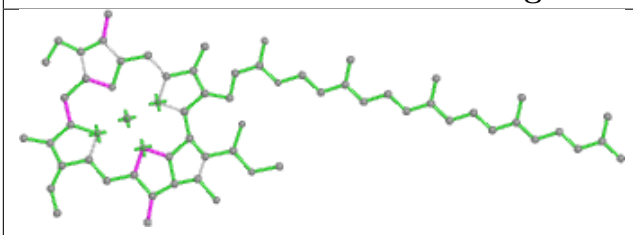


Torsions

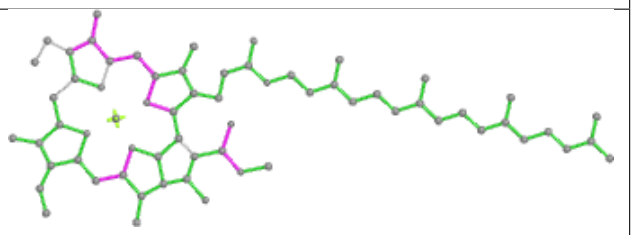


Rings

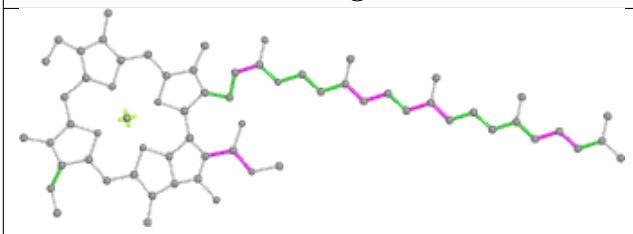
Ligand CLA C 509



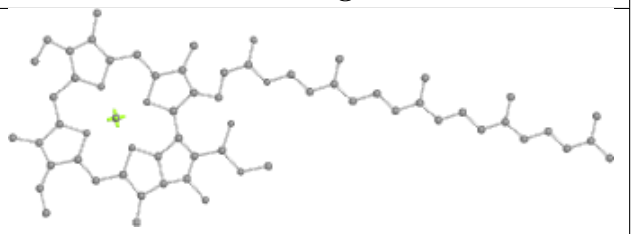
Bond lengths



Bond angles

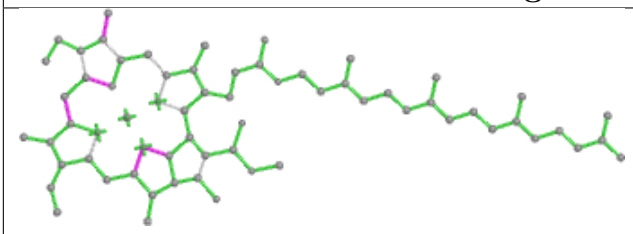


Torsions

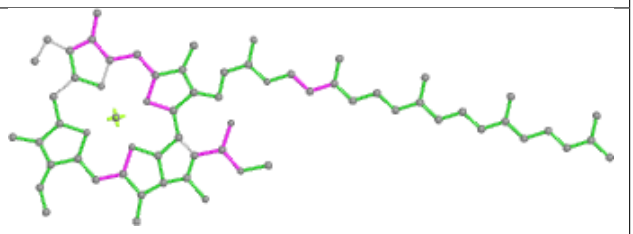


Rings

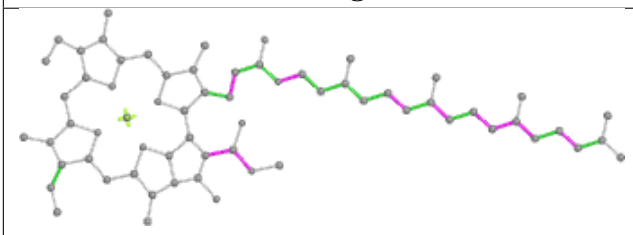
Ligand CLA C 507



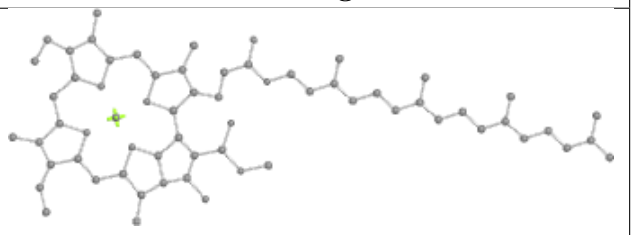
Bond lengths



Bond angles

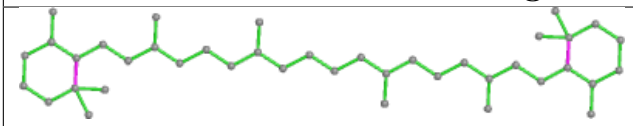


Torsions



Rings

Ligand BCR F 102



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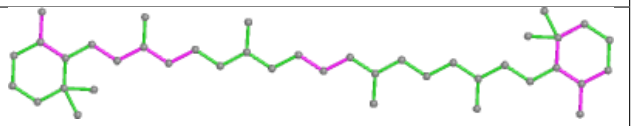
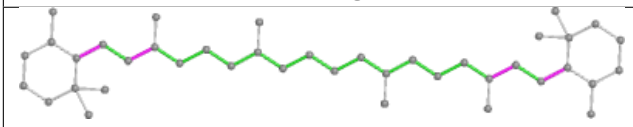


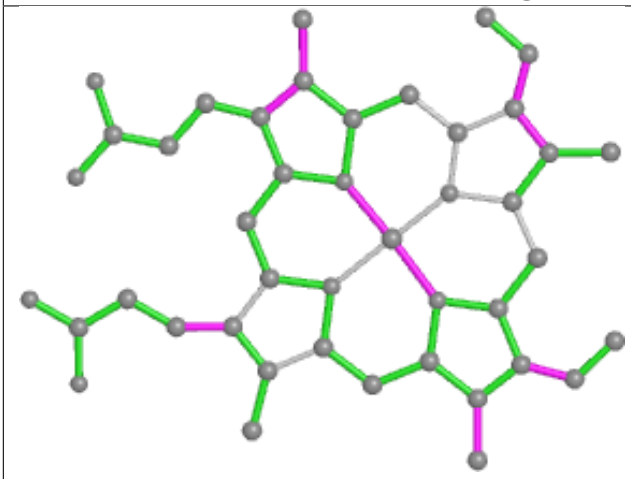
Bond angles



Torsions

Rings

Ligand HEM V 201



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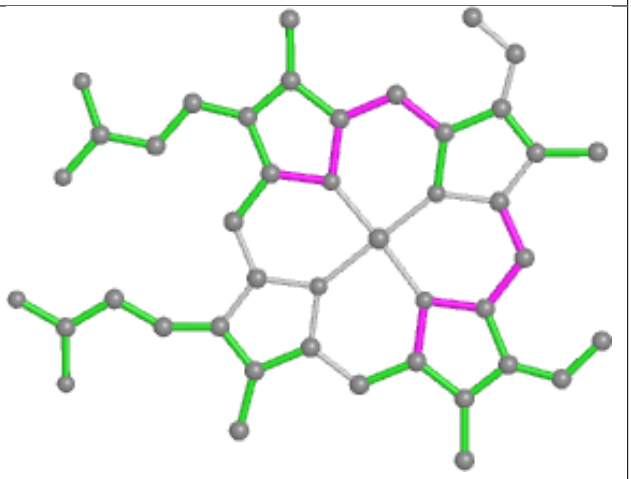
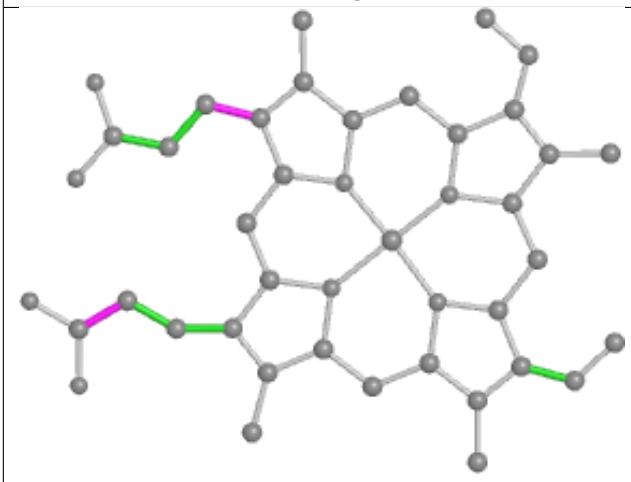
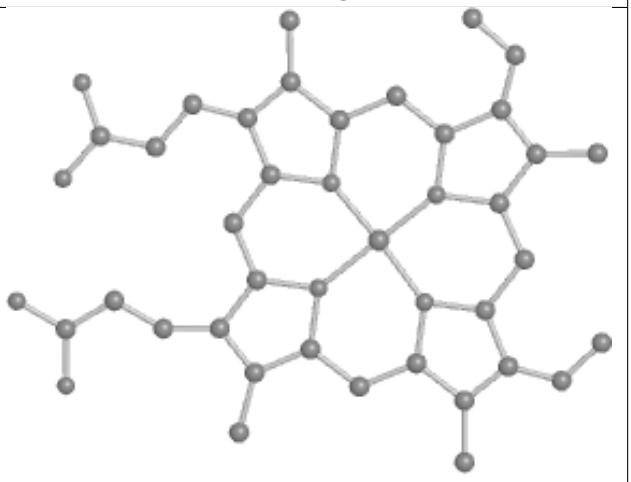


Bond angles

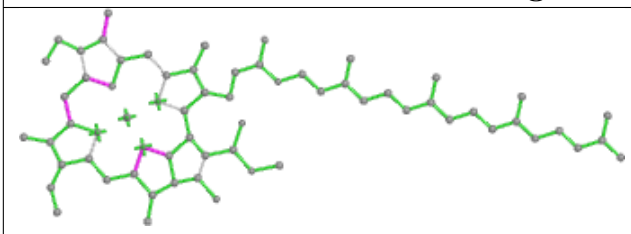


Torsions



Rings

Ligand CLA b 613



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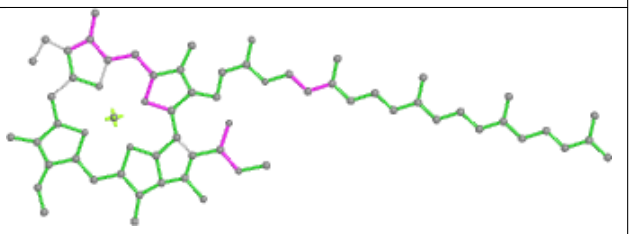
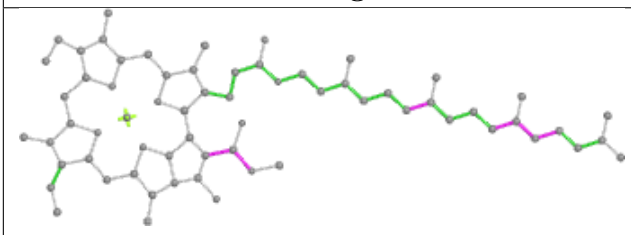
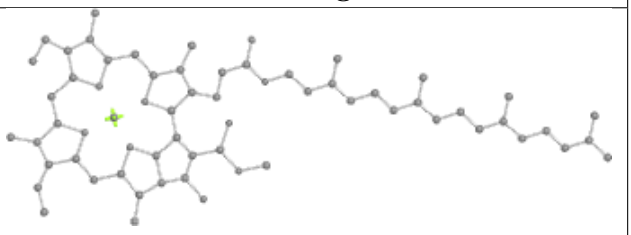


Bond angles

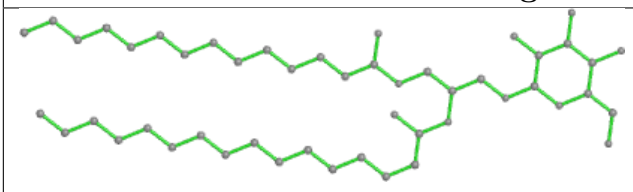


Torsions

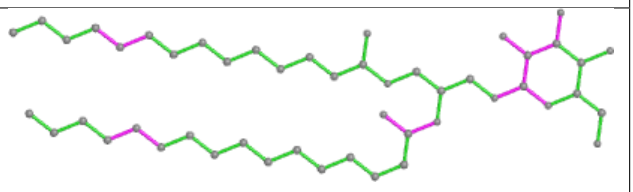


Rings

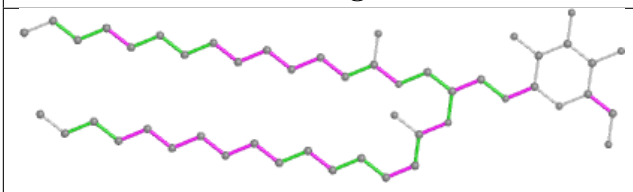
Ligand LMG B 625



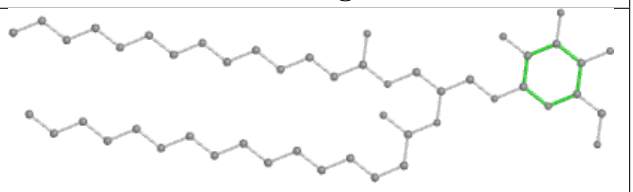
Bond lengths



Bond angles

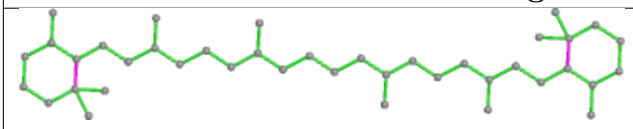


Torsions

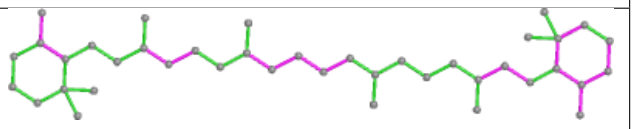


Rings

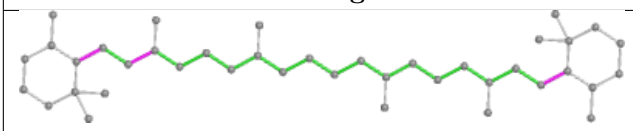
Ligand BCR c 514



Bond lengths



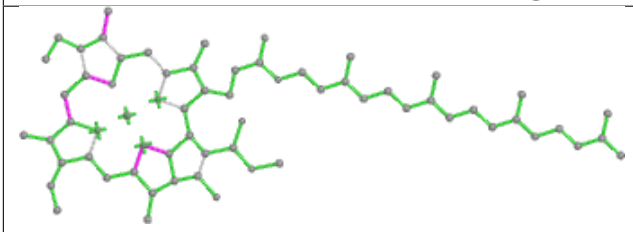
Bond angles



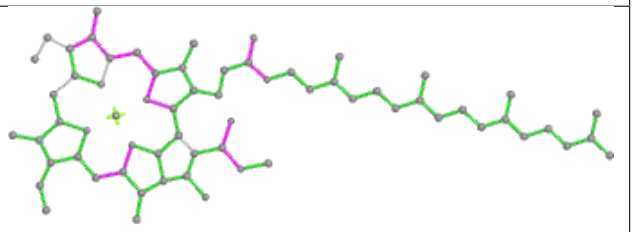
Torsions

Rings

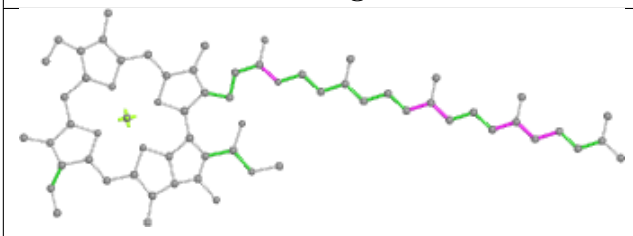
Ligand CLA b 619



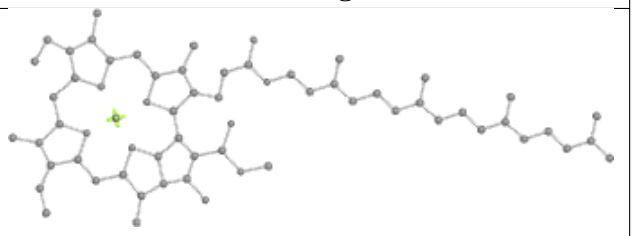
Bond lengths



Bond angles

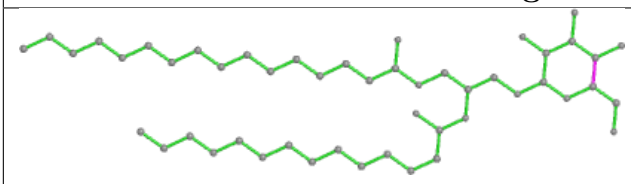


Torsions

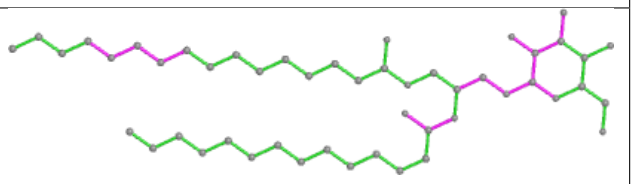


Rings

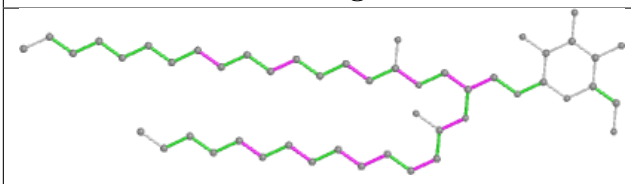
Ligand LMG b 626



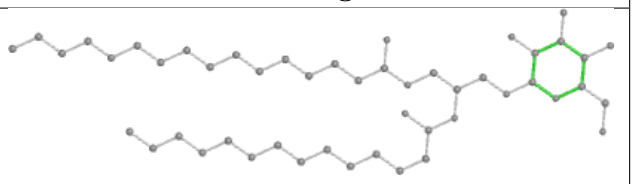
Bond lengths



Bond angles

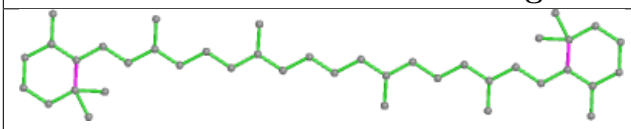


Torsions

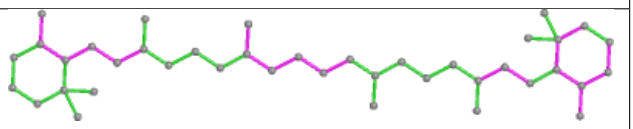


Rings

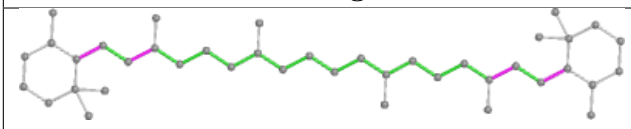
Ligand BCR b 622



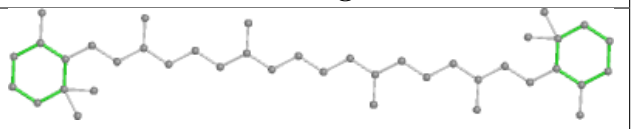
Bond lengths



Bond angles

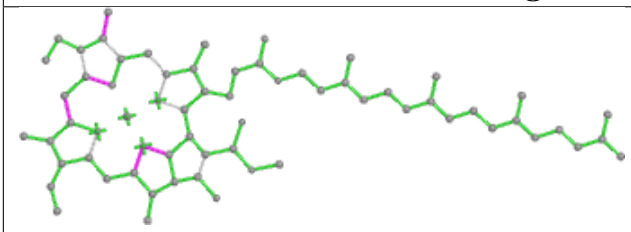


Torsions



Rings

Ligand CLA C 503



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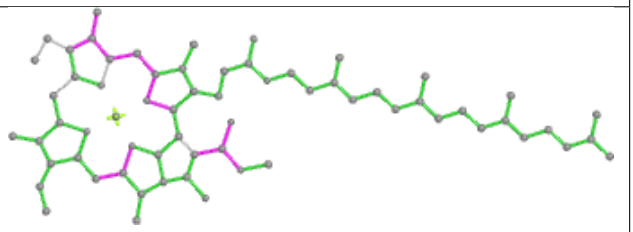
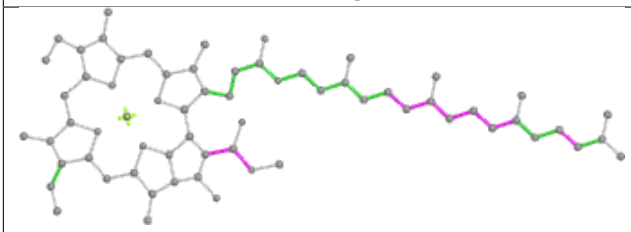
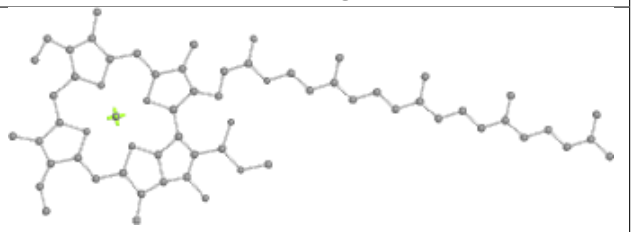


Bond angles

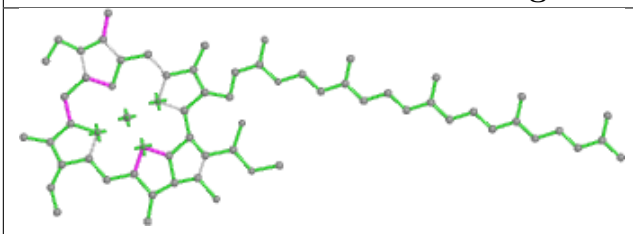


Torsions

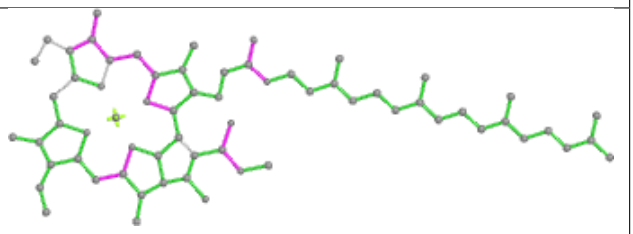


Rings

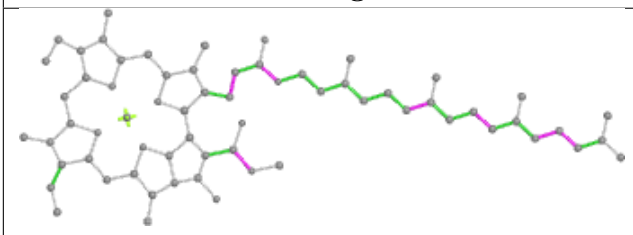
Ligand CLA c 520



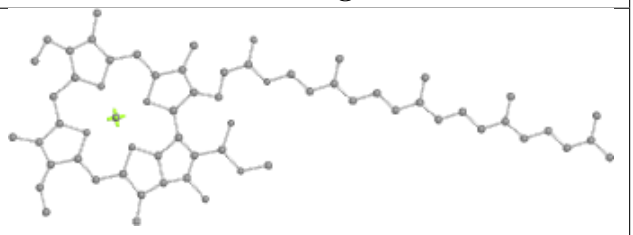
Bond lengths



Bond angles

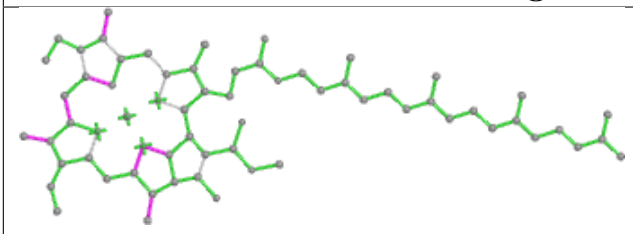


Torsions



Rings

Ligand CLA b 620



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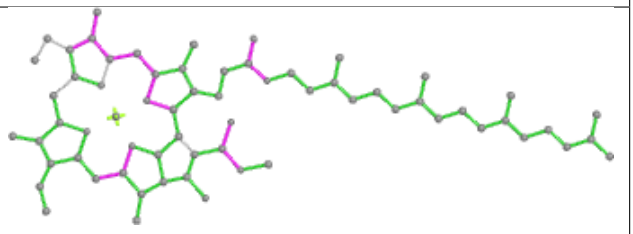
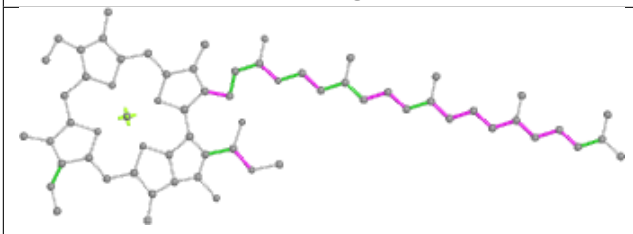
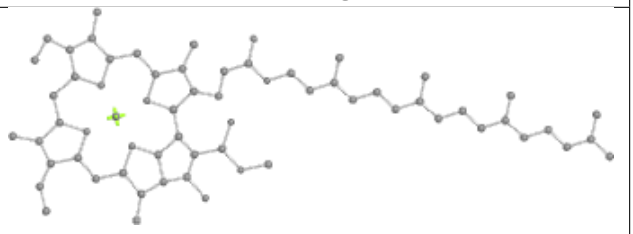


Bond angles

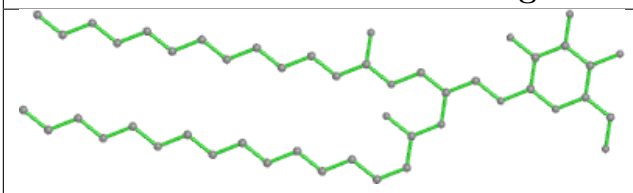


Torsions

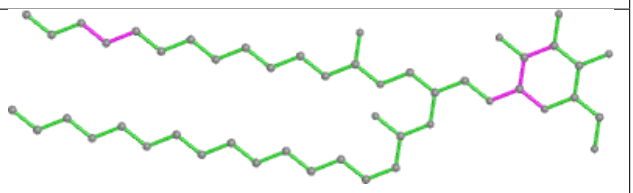


Rings

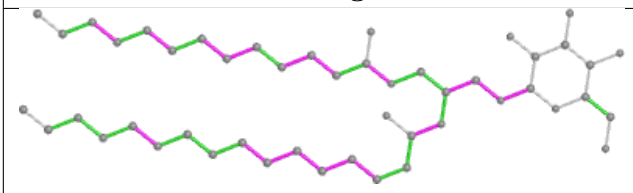
Ligand LMG D 406



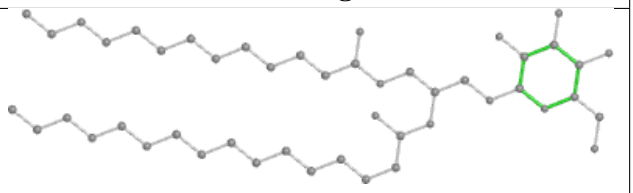
Bond lengths



Bond angles

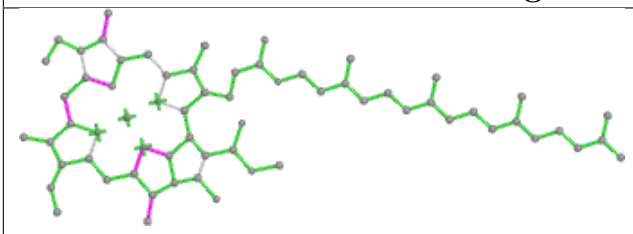


Torsions



Rings

Ligand CLA C 508



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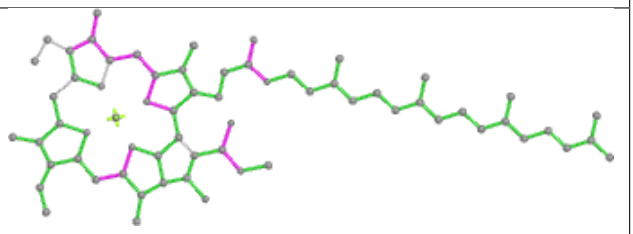
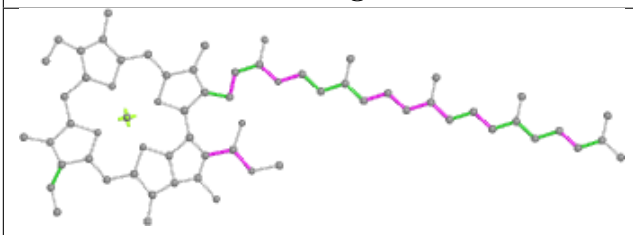
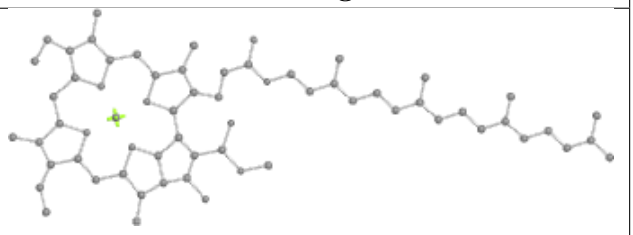


Bond angles

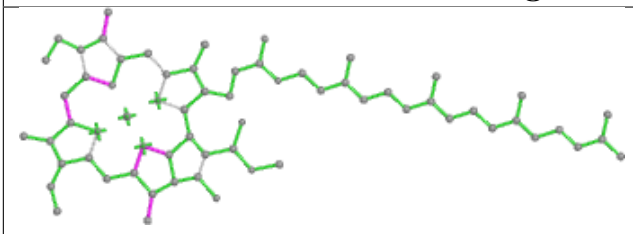


Torsions

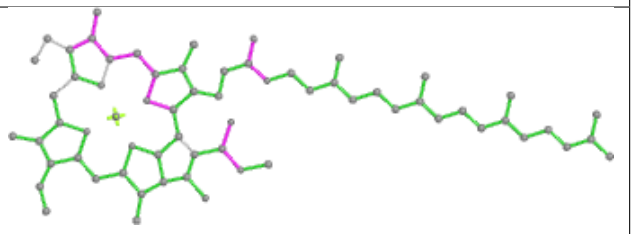


Rings

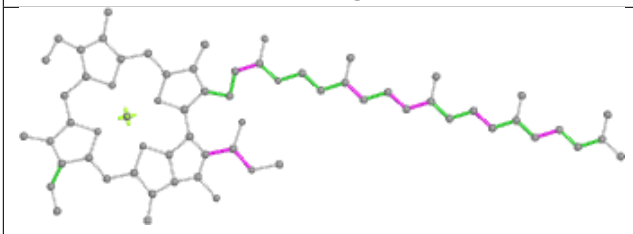
Ligand CLA B 611



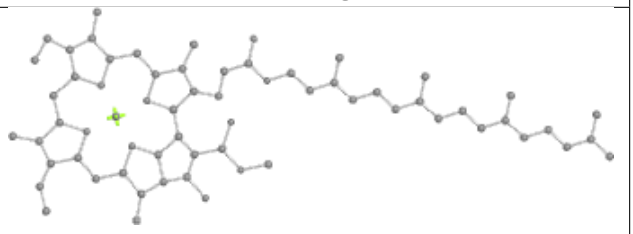
Bond lengths



Bond angles

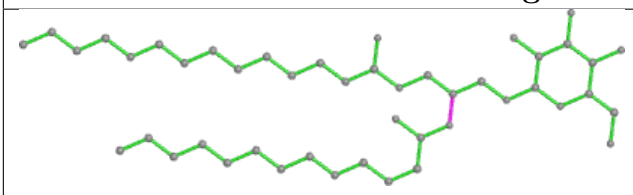


Torsions

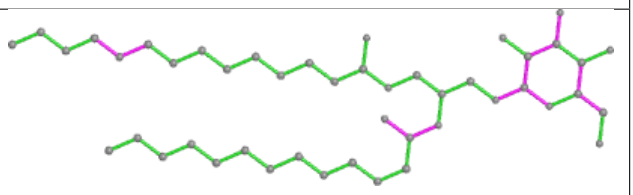


Rings

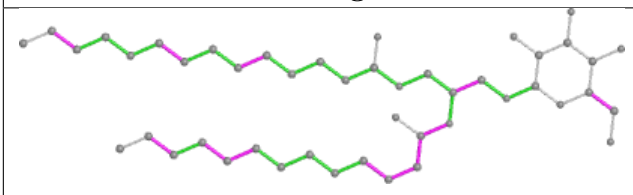
Ligand LMG d 412



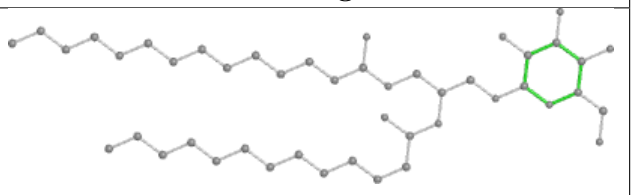
Bond lengths



Bond angles

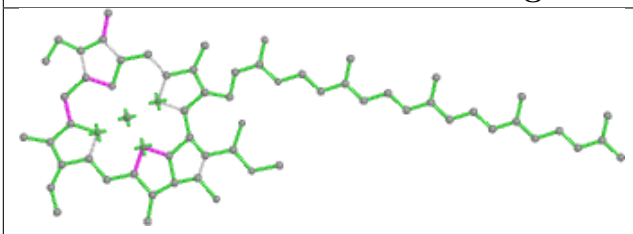


Torsions

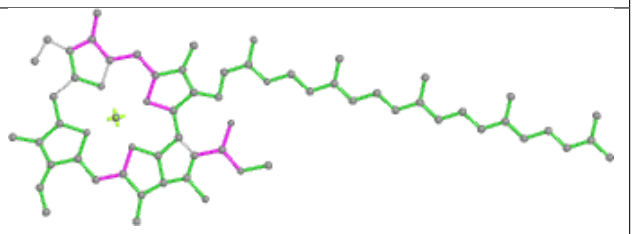


Rings

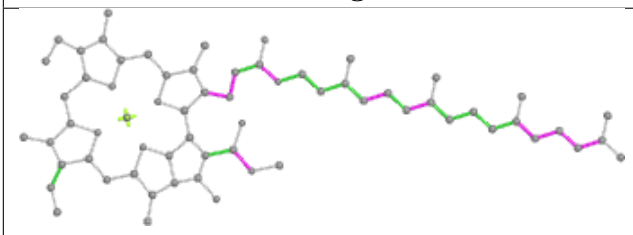
Ligand CLA B 605



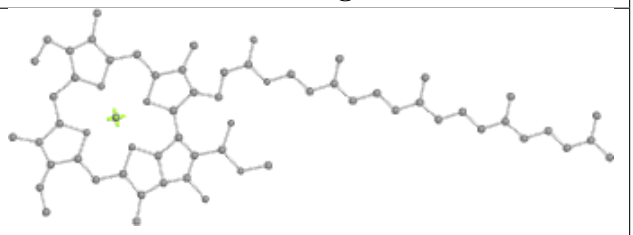
Bond lengths



Bond angles

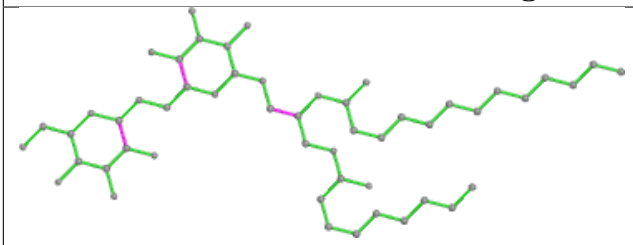


Torsions

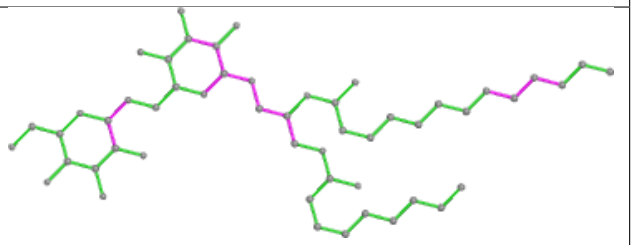


Rings

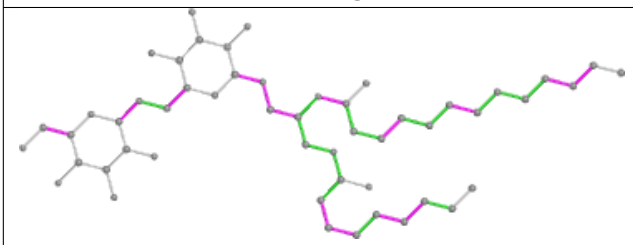
Ligand DGD B 626



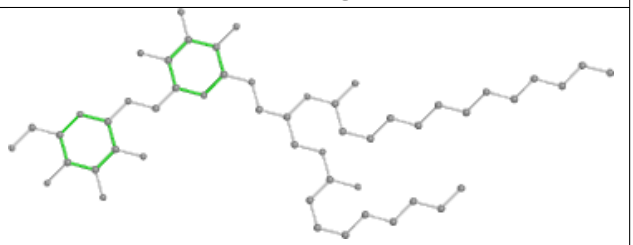
Bond lengths



Bond angles

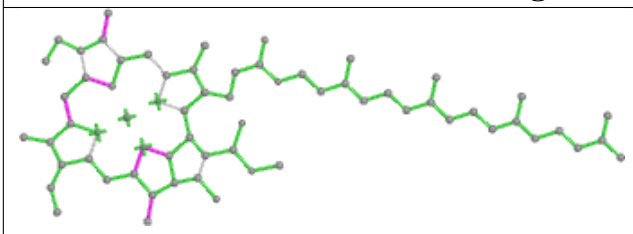


Torsions

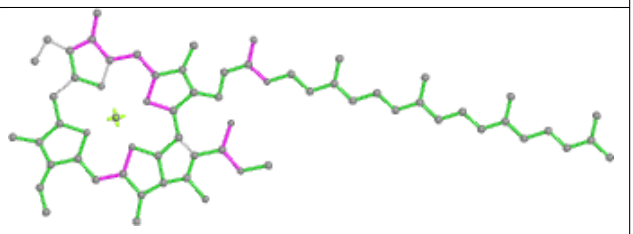


Rings

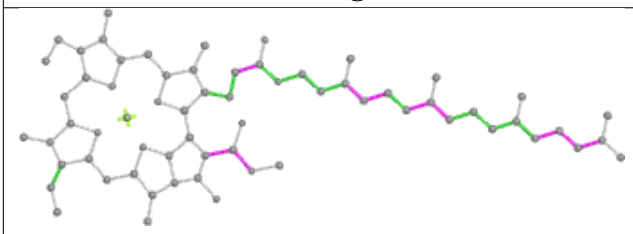
Ligand CLA c 509



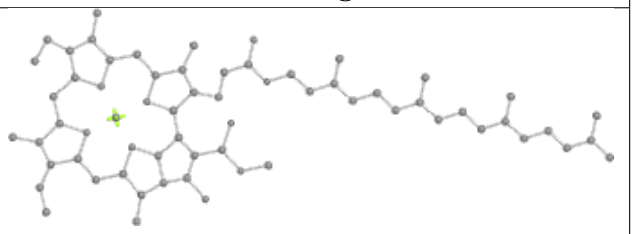
Bond lengths



Bond angles

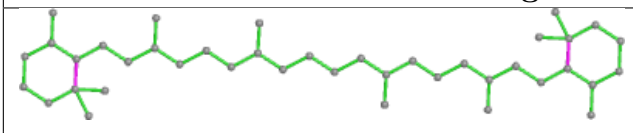


Torsions

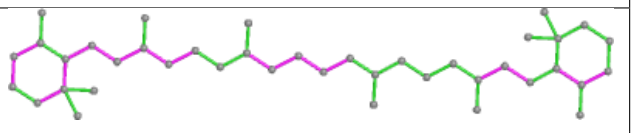


Rings

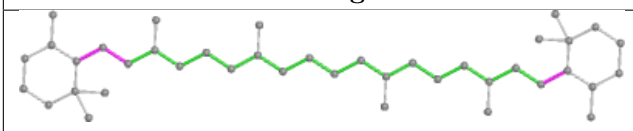
Ligand BCR K 101



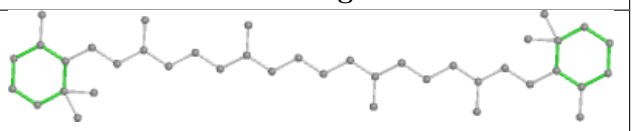
Bond lengths



Bond angles

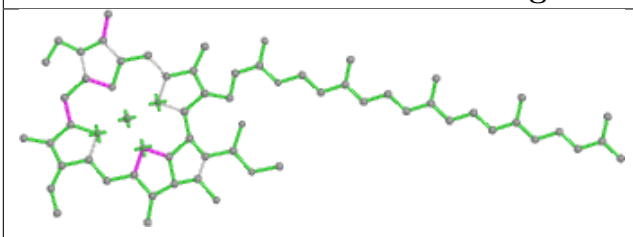


Torsions

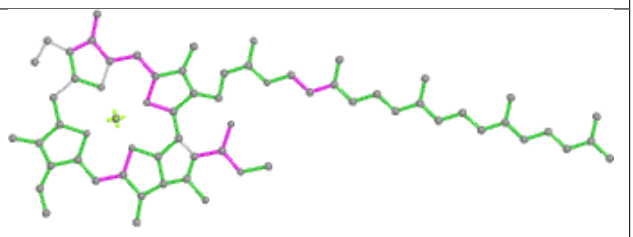


Rings

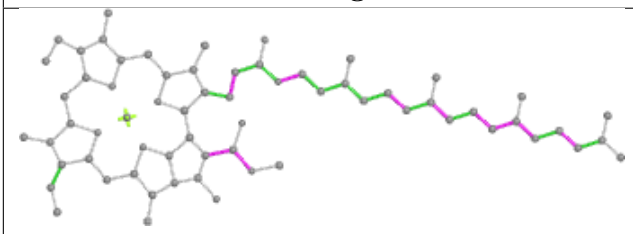
Ligand CLA c 507



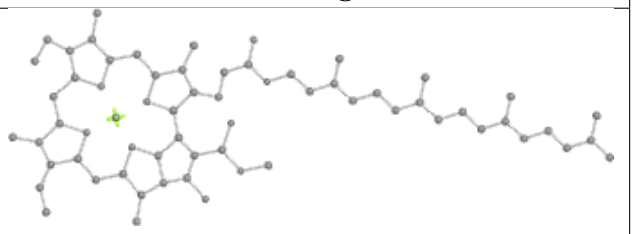
Bond lengths



Bond angles

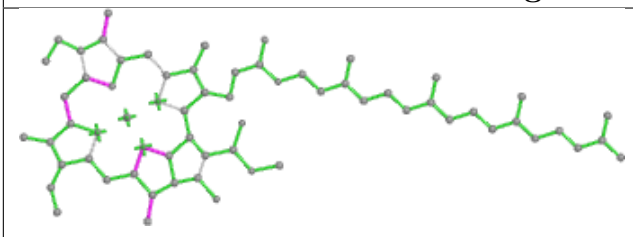


Torsions

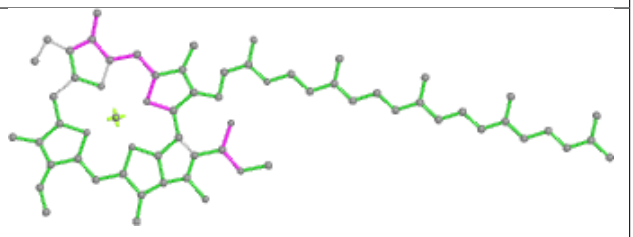


Rings

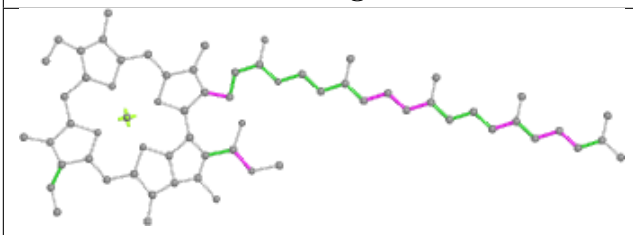
Ligand CLA B 607



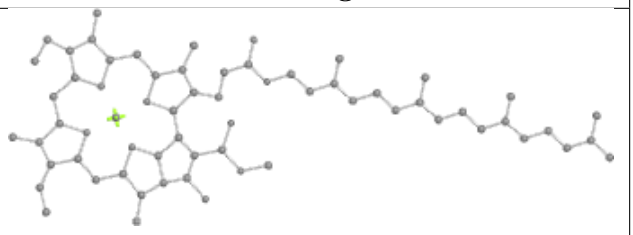
Bond lengths



Bond angles

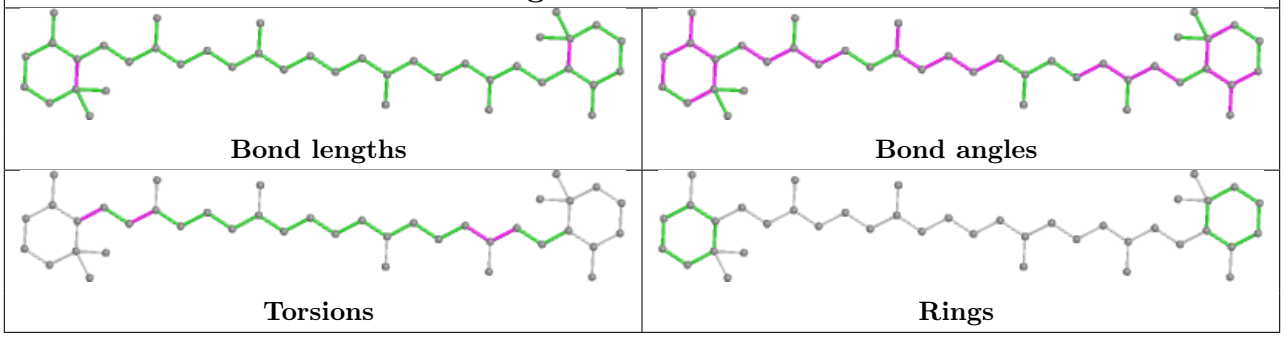


Torsions

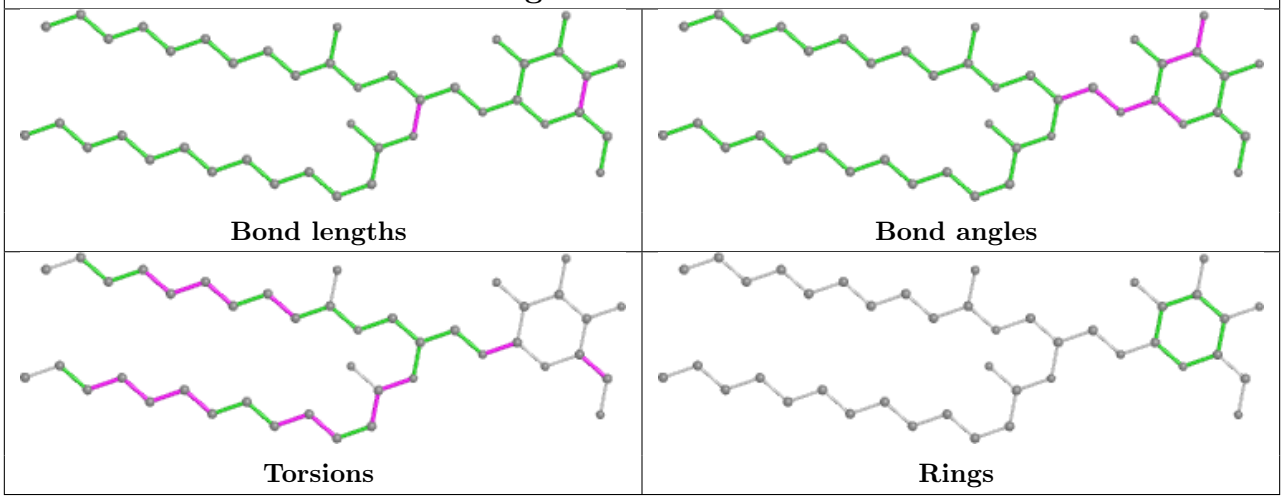


Rings

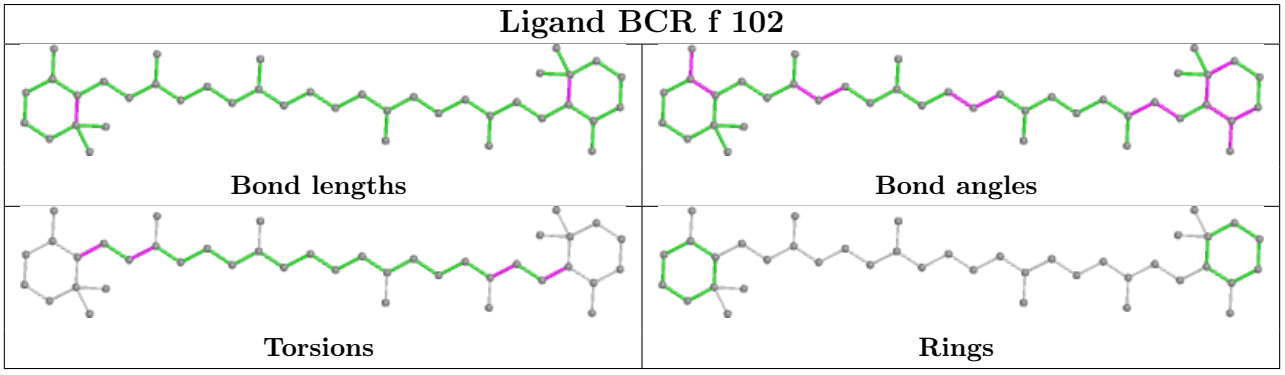
Ligand BCR J 102



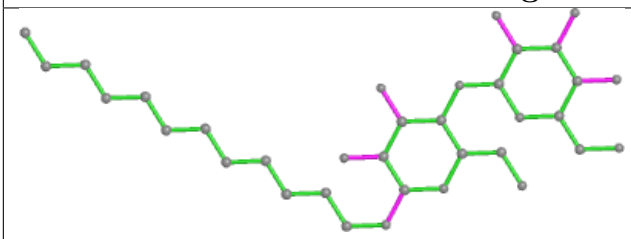
Ligand LMG a 402



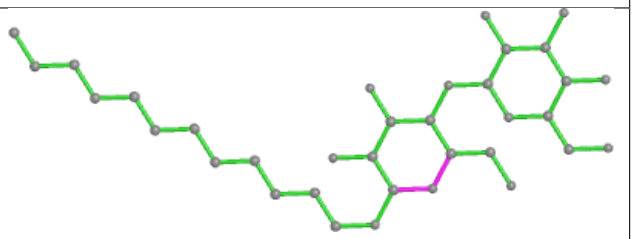
Ligand BCR f 102



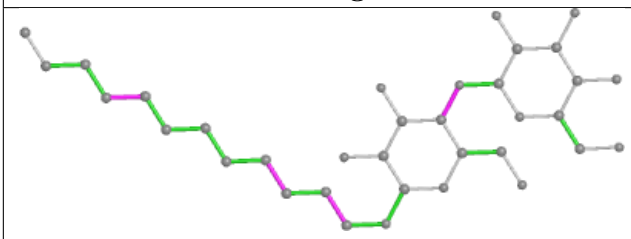
Ligand LMT B 629



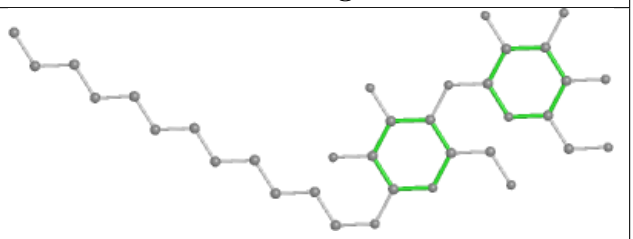
Bond lengths



Bond angles

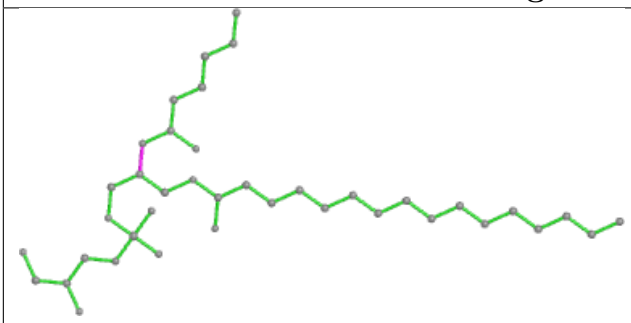


Torsions

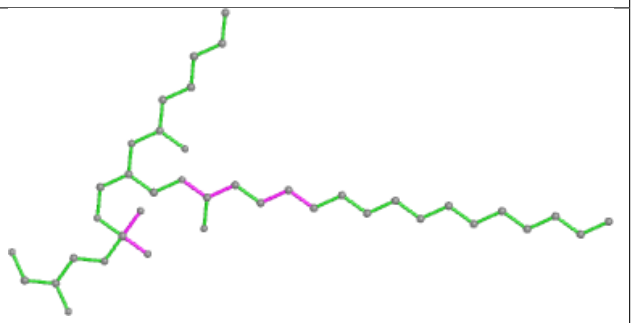


Rings

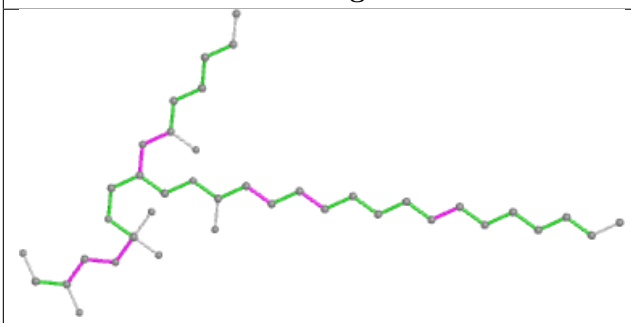
Ligand LHG a 409



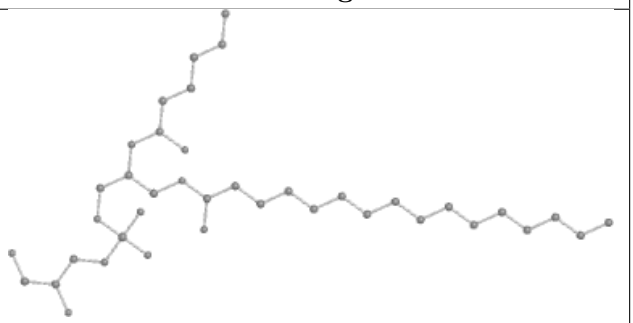
Bond lengths



Bond angles

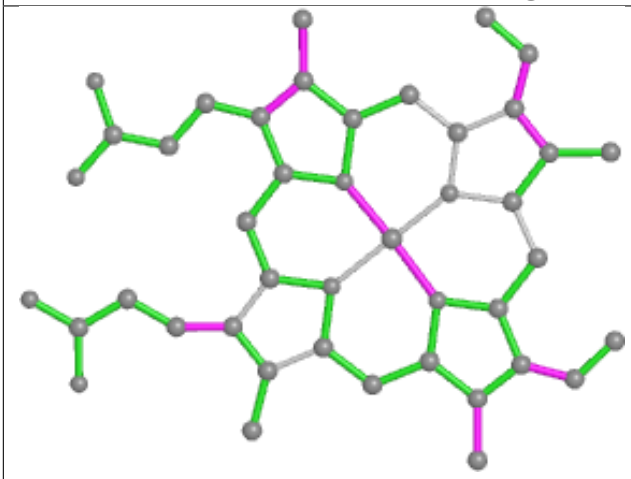


Torsions

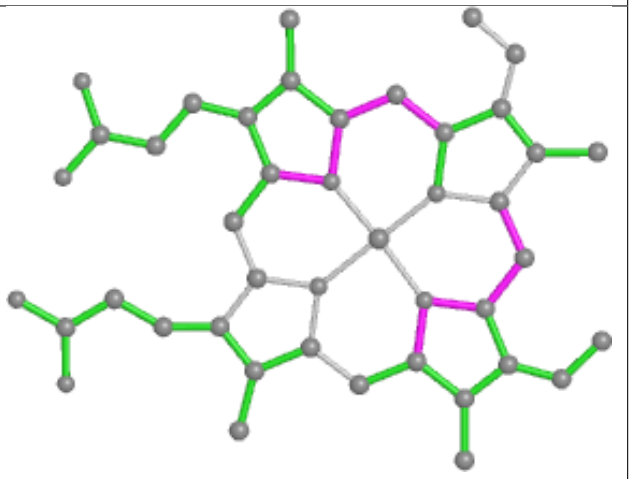


Rings

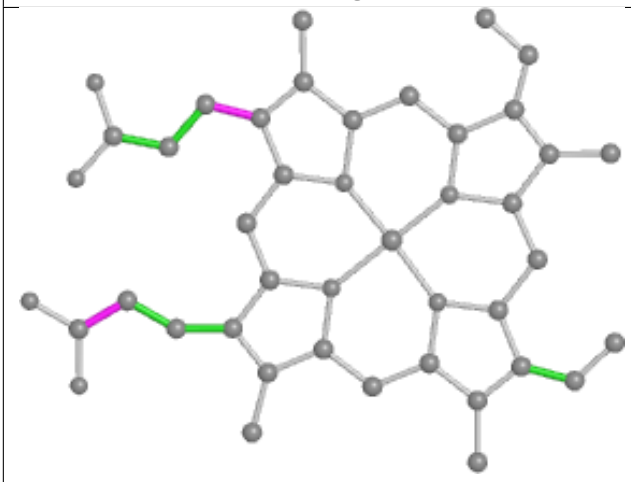
Ligand HEM v 201



Bond lengths



Bond angles



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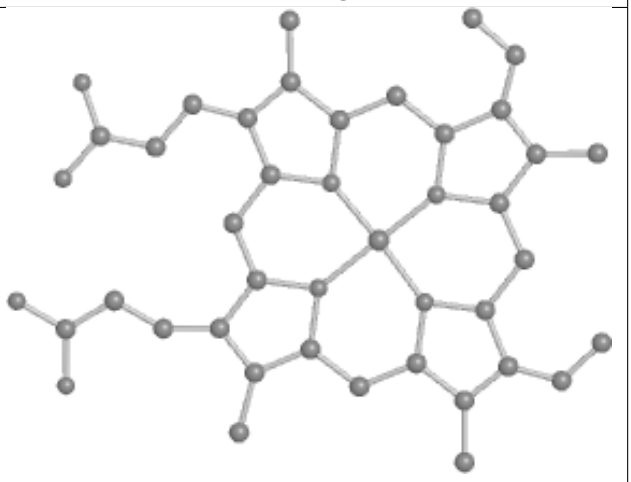
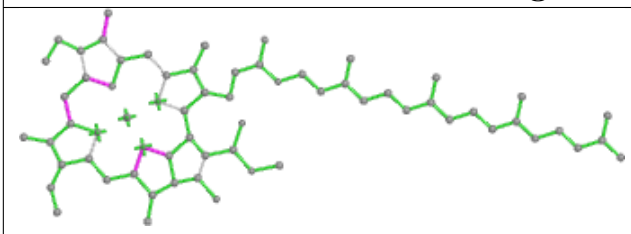


Rings

Ligand CLA c 508



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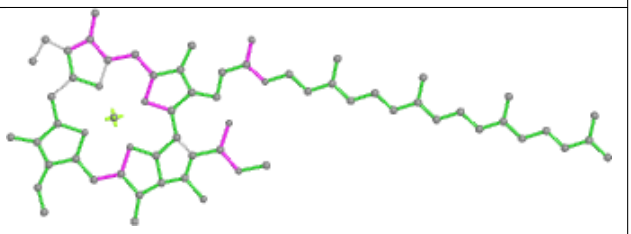
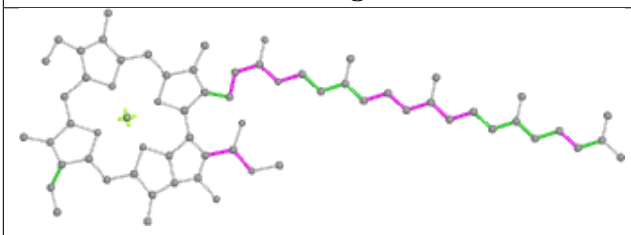


Bond angles



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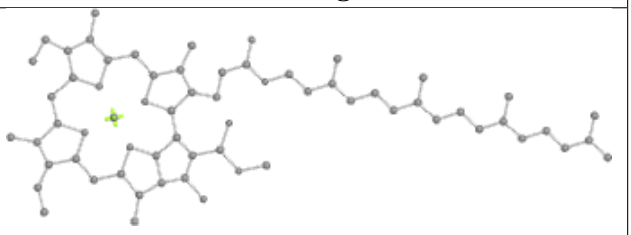
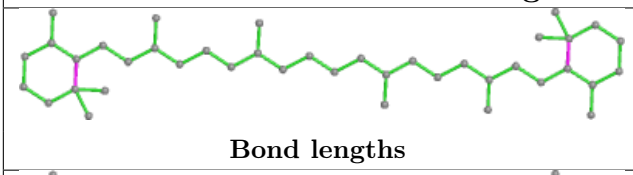


Rings

Ligand BCR B 618



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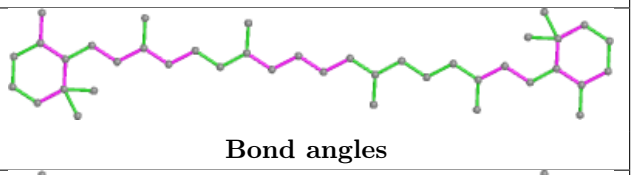
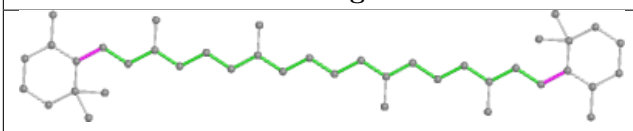
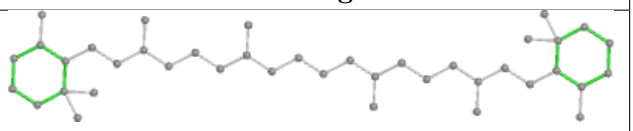


Bond angles

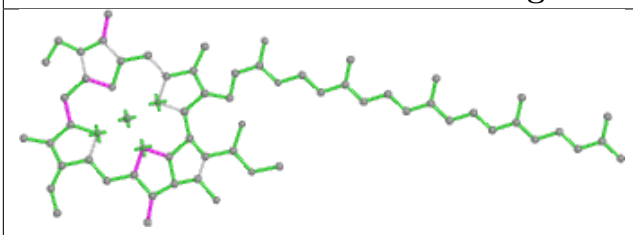


Torsions



Rings

Ligand CLA b 608



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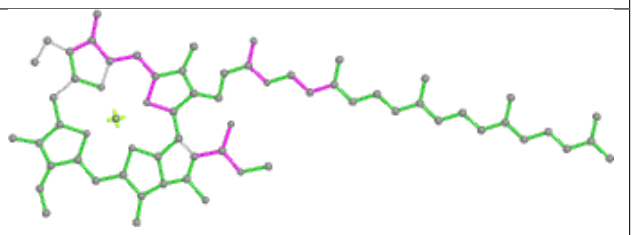
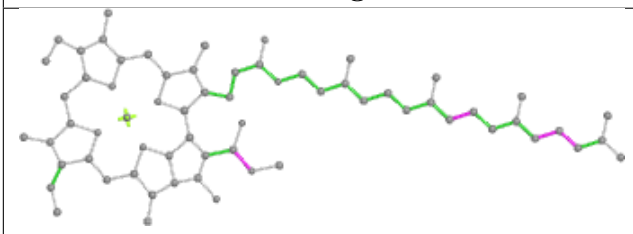


Bond angles



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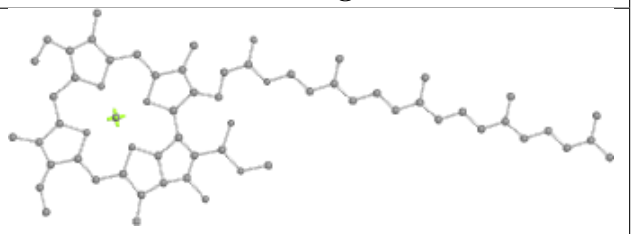
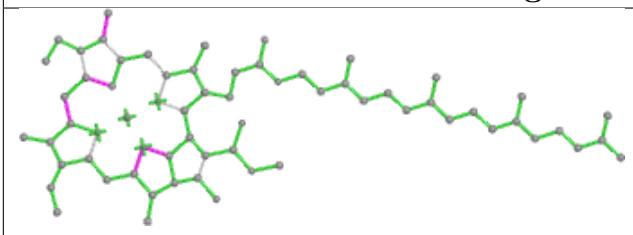


Rings

Ligand CLA B 608



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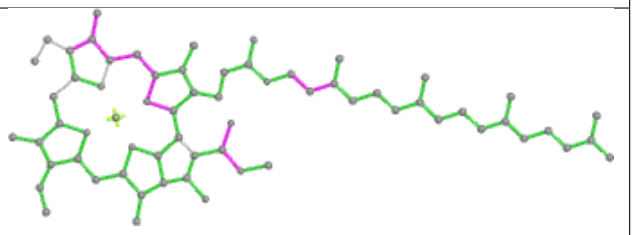
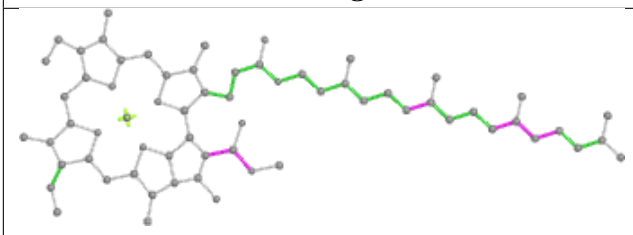
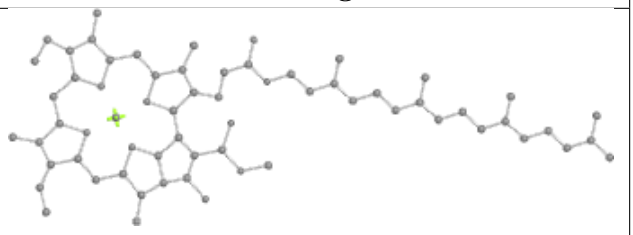


Bond angles

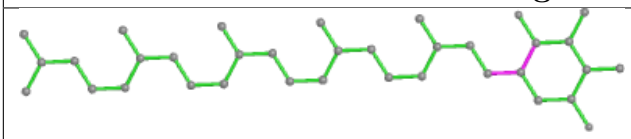


Torsions



Rings

Ligand PL9 J 101



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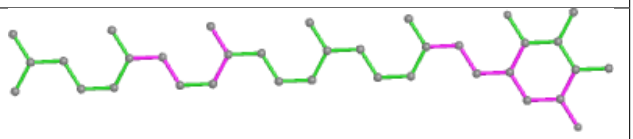
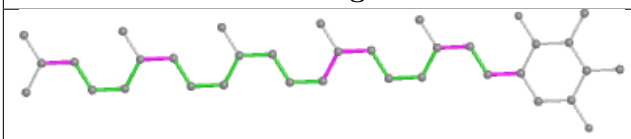
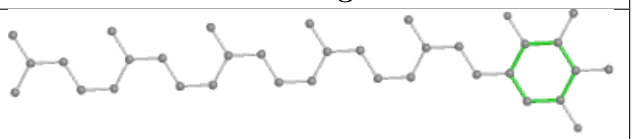


Bond angles

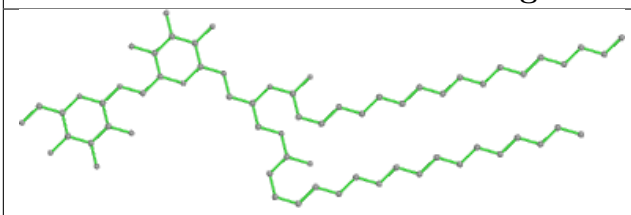


Torsions



Rings

Ligand DGD C 516



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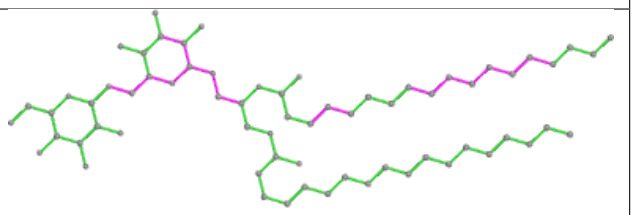
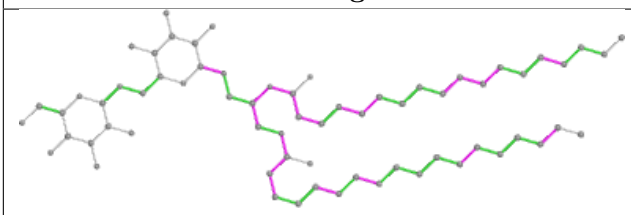
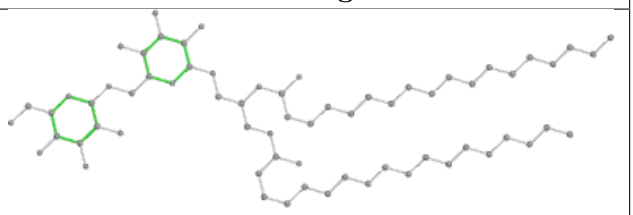


Bond angles

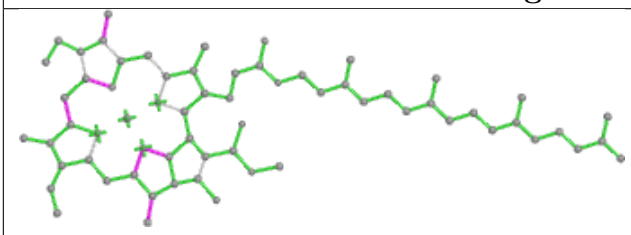


Torsions



Rings

Ligand CLA B 603



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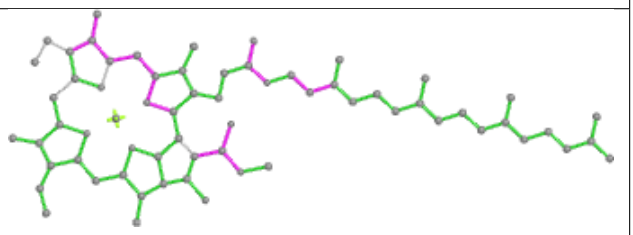
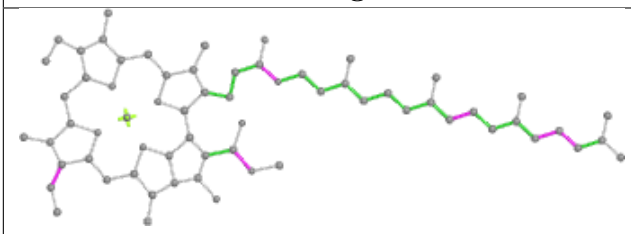
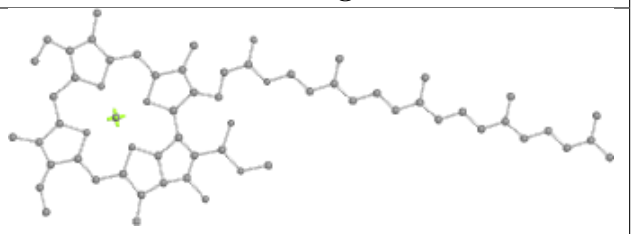


Bond angles

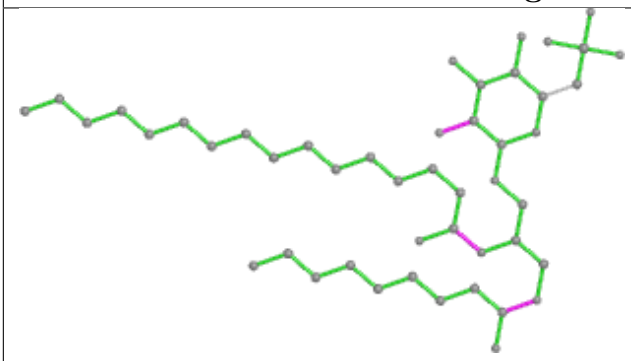


Torsions

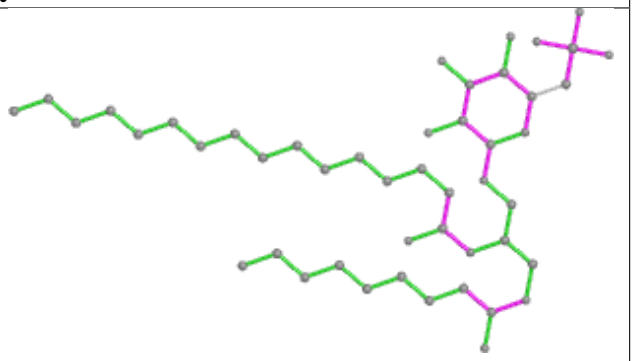


Rings

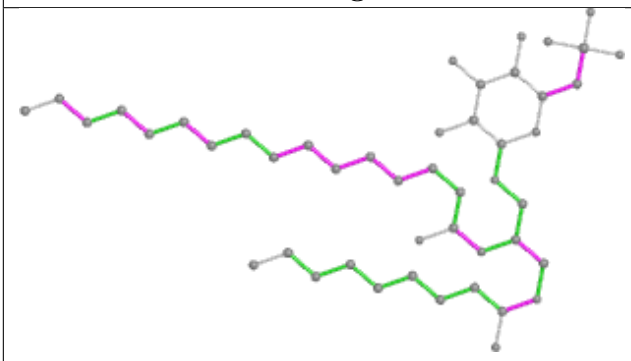
Ligand SQD B 627



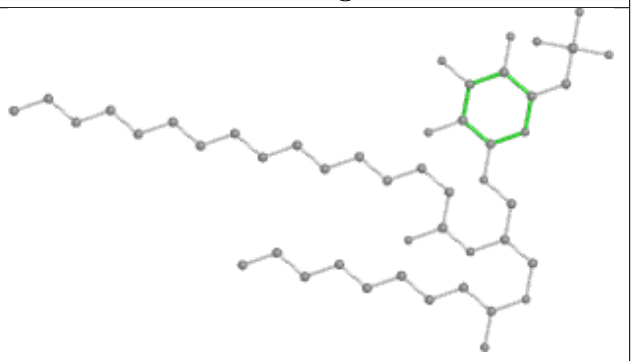
Bond lengths



Bond angles

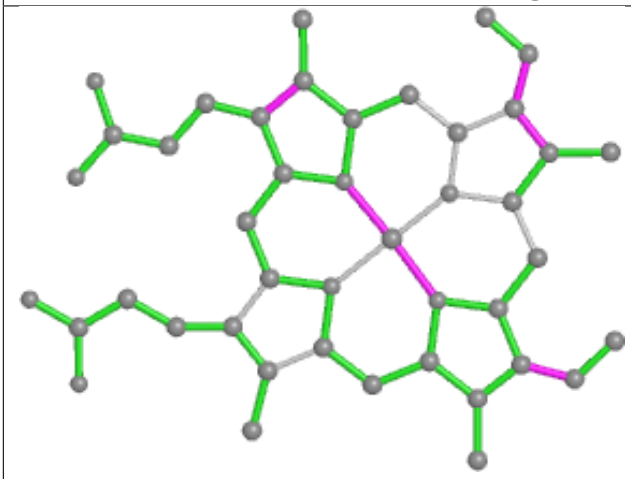


Torsions



Rings

Ligand HEM f 101



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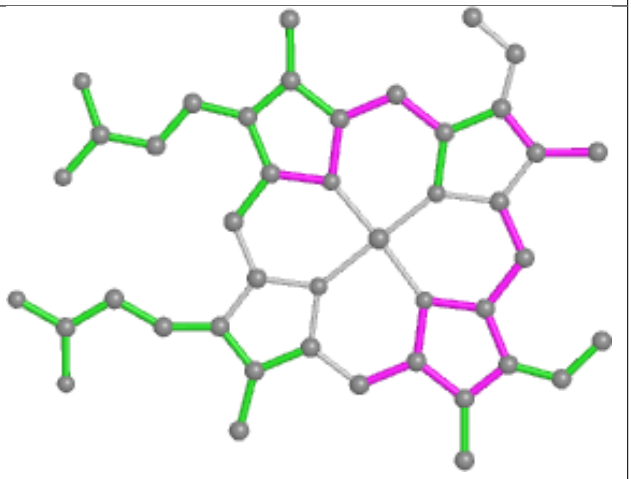
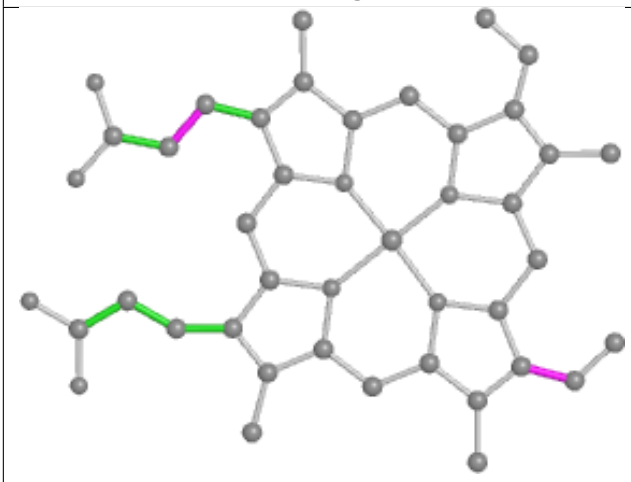
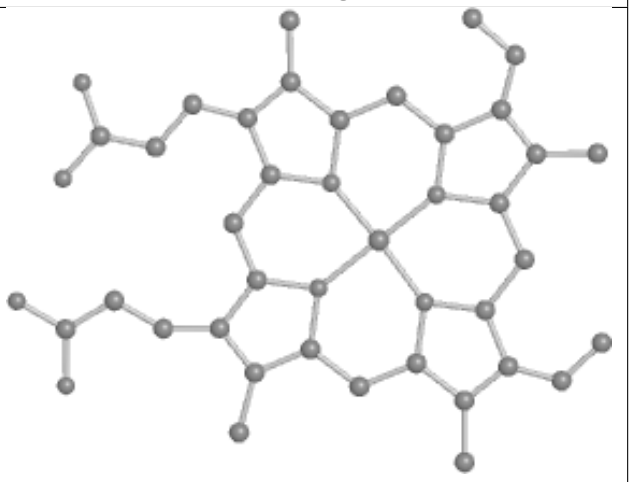


Bond angles

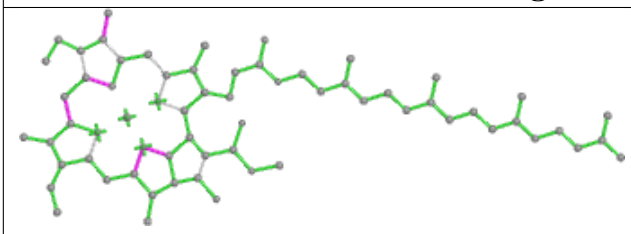


Torsions

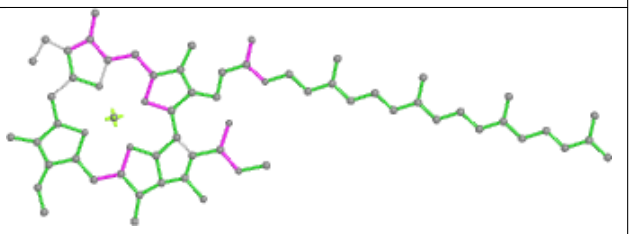


Rings

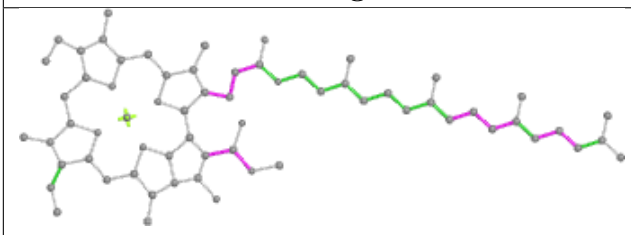
Ligand CLA c 501



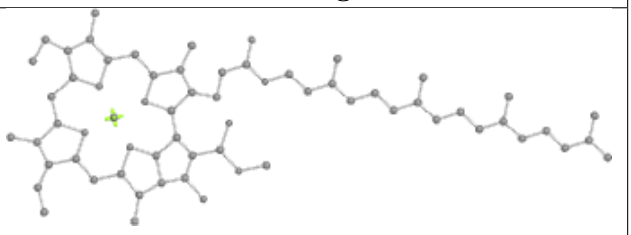
Bond lengths



Bond angles

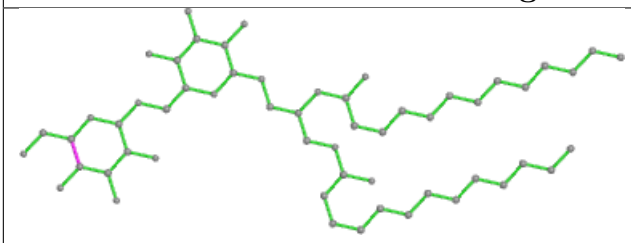


Torsions

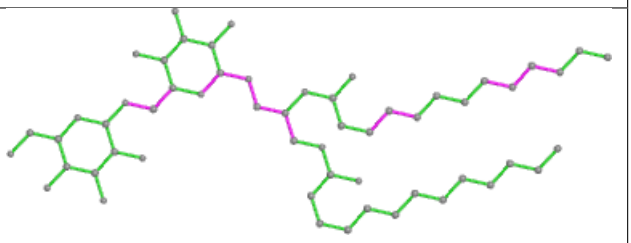


Rings

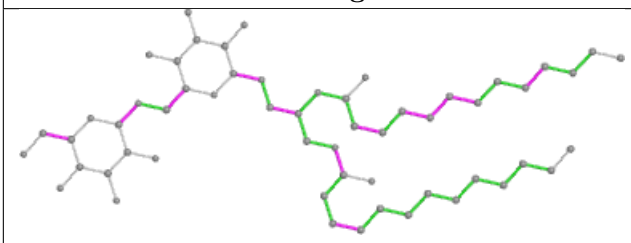
Ligand DGD A 409



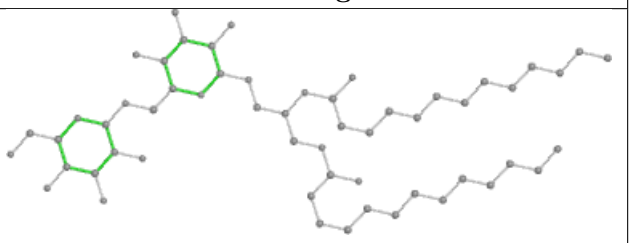
Bond lengths



Bond angles

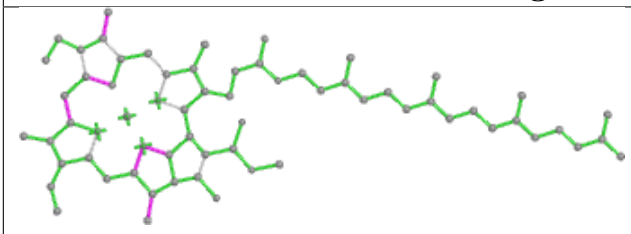


Torsions

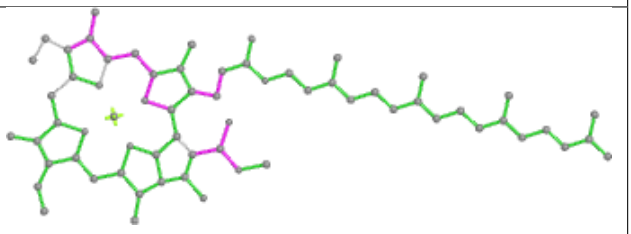


Rings

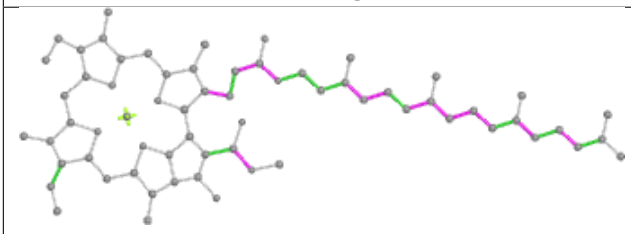
Ligand CLA c 504



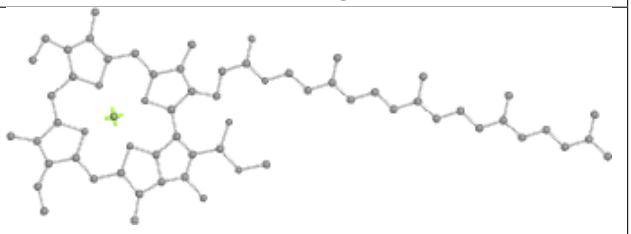
Bond lengths



Bond angles

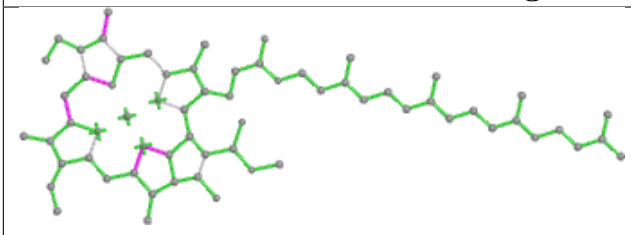


Torsions

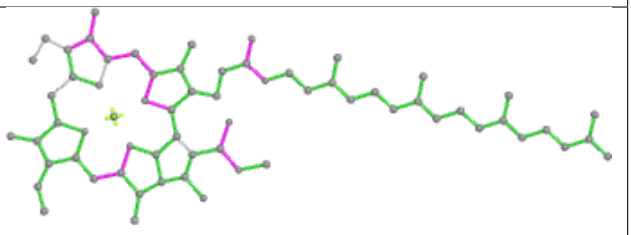


Rings

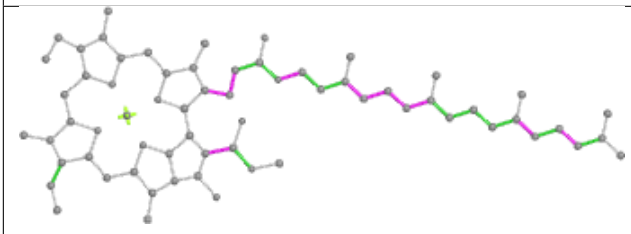
Ligand CLA A 403



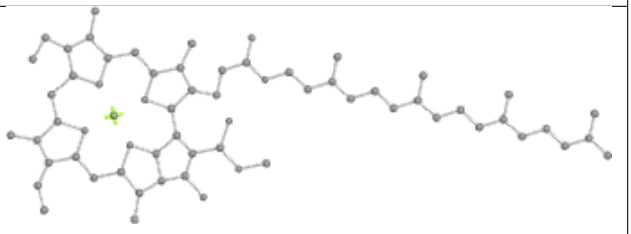
Bond lengths



Bond angles

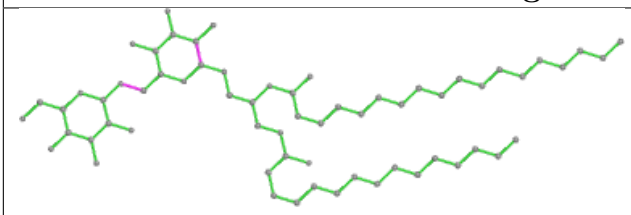


Torsions

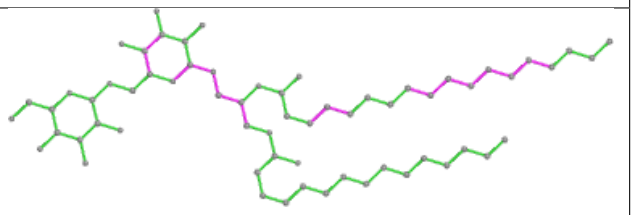


Rings

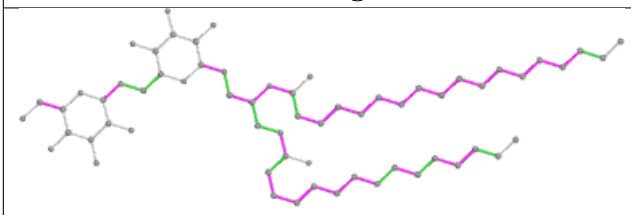
Ligand DGD d 410



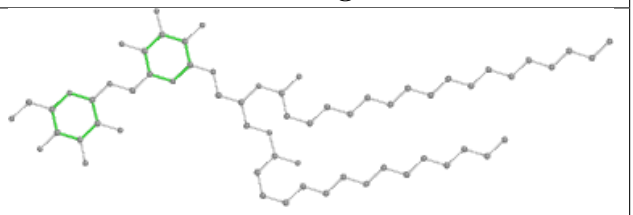
Bond lengths



Bond angles

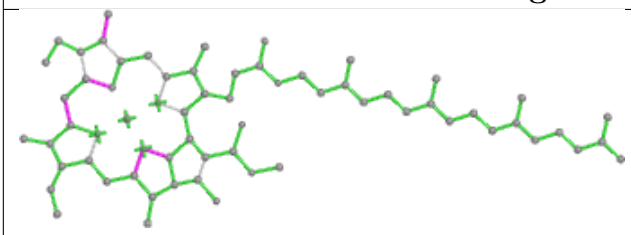


Torsions

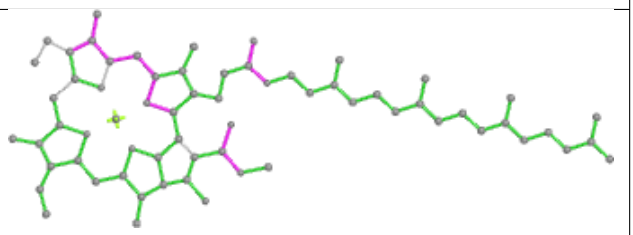


Rings

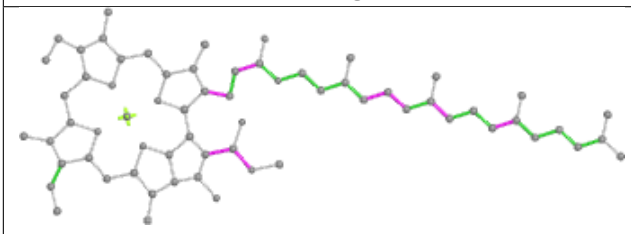
Ligand CLA c 506



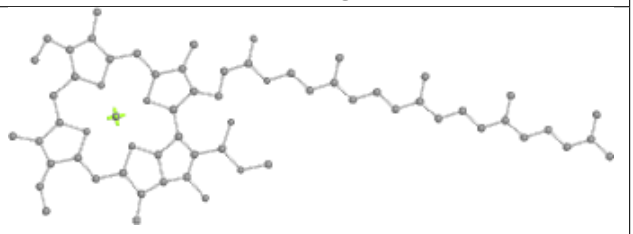
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/344 (97%)	0.68	41 (12%) 4 6	206, 208, 208, 209	0
1	a	335/344 (97%)	0.84	62 (18%) 1 2	206, 208, 209, 209	0
2	B	490/510 (96%)	0.43	41 (8%) 11 11	206, 207, 209, 210	0
2	b	490/510 (96%)	0.67	78 (15%) 1 3	206, 208, 209, 210	0
3	C	447/461 (96%)	0.54	48 (10%) 6 7	206, 208, 209, 209	0
3	c	447/461 (96%)	0.40	36 (8%) 12 11	205, 208, 209, 210	0
4	D	340/352 (96%)	0.34	21 (6%) 20 17	205, 207, 208, 210	0
4	d	340/352 (96%)	0.55	36 (10%) 6 7	206, 208, 209, 209	0
5	E	82/84 (97%)	0.65	7 (8%) 10 10	206, 208, 209, 209	0
5	e	82/84 (97%)	0.38	5 (6%) 21 18	207, 208, 209, 209	0
6	F	35/45 (77%)	0.08	2 (5%) 23 21	207, 207, 208, 209	0
6	f	35/45 (77%)	0.11	5 (14%) 2 4	207, 208, 209, 209	0
7	H	65/66 (98%)	0.74	11 (16%) 1 3	206, 208, 209, 209	0
7	h	65/66 (98%)	1.18	23 (35%) 0 1	206, 208, 209, 209	0
8	I	35/38 (92%)	1.08	9 (25%) 0 1	207, 208, 209, 209	0
8	i	35/38 (92%)	0.33	1 (2%) 51 41	206, 207, 209, 210	0
9	J	34/40 (85%)	0.46	3 (8%) 10 10	207, 208, 208, 209	0
9	j	34/40 (85%)	-0.36	0 100 100	206, 208, 209, 209	0
10	K	37/46 (80%)	0.12	2 (5%) 25 23	207, 208, 209, 209	0
10	k	37/46 (80%)	0.18	2 (5%) 25 23	207, 208, 209, 209	0
11	L	37/37 (100%)	0.68	3 (8%) 12 11	207, 208, 209, 209	0
11	l	37/37 (100%)	0.52	5 (13%) 3 4	206, 208, 209, 210	0
12	M	34/36 (94%)	0.56	3 (8%) 10 10	206, 207, 208, 209	0
12	m	34/36 (94%)	0.31	2 (5%) 22 19	207, 207, 208, 209	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.96	47 (19%) 1 2	205, 208, 209, 210	0
13	o	243/272 (89%)	0.91	32 (13%) 3 5	206, 208, 209, 210	0
14	T	32/32 (100%)	0.40	1 (3%) 49 39	206, 208, 208, 209	0
14	t	32/32 (100%)	0.67	3 (9%) 8 9	206, 207, 209, 209	0
15	U	97/134 (72%)	0.97	8 (8%) 11 11	206, 207, 208, 209	0
15	u	97/134 (72%)	1.15	19 (19%) 1 2	206, 207, 208, 209	0
16	V	137/163 (84%)	0.39	10 (7%) 15 13	206, 207, 208, 209	0
16	v	137/163 (84%)	0.76	19 (13%) 2 4	206, 208, 209, 209	0
17	g	28/46 (60%)	0.17	2 (7%) 16 14	207, 208, 209, 209	0
17	y	28/46 (60%)	0.40	2 (7%) 16 14	206, 208, 209, 209	0
18	X	37/41 (90%)	0.68	7 (18%) 1 2	206, 208, 209, 210	0
18	x	37/41 (90%)	0.87	6 (16%) 1 3	207, 208, 208, 209	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.24	1 (1%) 72 62	206, 207, 208, 209	0
20	z	62/62 (100%)	0.57	3 (4%) 30 26	207, 208, 209, 210	0
All	All	5214/5674 (91%)	0.60	606 (11%) 4 6	205, 208, 209, 210	0

All (606) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	9.2
1	A	190	HIS	6.9
3	c	202	PRO	6.7
2	B	84	THR	6.6
1	a	299	GLY	6.4
1	A	299	GLY	6.2
14	t	31	LYS	5.8
7	H	4	ARG	5.7
4	d	295	SER	5.7
1	a	190	HIS	5.6
2	b	431	GLU	5.6
13	o	54	GLY	5.6
13	O	90	GLU	5.5
1	A	11	ALA	5.5
13	o	55	ALA	5.4
1	A	10	SER	5.3

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Mol	Chain	Res	Type	RSRZ
13	o	51	THR	5.1
3	c	201	ASN	5.1
16	v	111	GLU	5.1
1	A	175	GLY	5.1
3	C	147	PHE	5.0
2	B	85	GLY	4.9
1	A	298	ASN	4.8
3	C	149	TYR	4.8
3	C	212	TYR	4.8
7	h	56	ASP	4.8
7	h	66	GLY	4.7
14	t	32	LYS	4.7
13	O	220	LYS	4.7
2	b	133	LEU	4.6
2	b	490	GLN	4.5
1	A	179	THR	4.5
13	O	91	PHE	4.4
7	h	3	ARG	4.4
18	X	47	GLN	4.4
13	O	175	PRO	4.4
1	a	179	THR	4.4
3	c	203	THR	4.4
3	C	148	GLY	4.4
2	B	83	GLU	4.4
1	a	236	GLY	4.3
2	B	378	LYS	4.3
6	f	11	VAL	4.3
3	c	372	PRO	4.3
13	o	84	ASN	4.3
4	d	197	HIS	4.2
3	C	266	TRP	4.2
7	h	26	GLY	4.2
5	e	82	GLN	4.2
16	v	35	THR	4.2
1	A	165	GLN	4.1
6	f	13	TYR	4.1
1	A	195	HIS	4.1
4	D	192	THR	4.1
3	C	209	ILE	4.1
2	b	482	ILE	4.1
1	a	175	GLY	4.0
13	o	53	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
2	b	127	ARG	4.0
3	c	199	ILE	4.0
3	c	178	LYS	4.0
1	a	198	HIS	4.0
14	t	30	THR	4.0
3	c	209	ILE	4.0
18	X	46	VAL	4.0
3	c	200	THR	4.0
15	u	107	GLU	4.0
1	A	177	SER	3.9
2	b	126	PRO	3.9
3	c	373	ASN	3.9
4	d	294	ARG	3.9
4	d	241	GLU	3.9
13	O	170	GLY	3.9
1	a	298	ASN	3.9
2	B	411	PHE	3.9
2	B	164	PRO	3.9
7	h	4	ARG	3.9
4	D	295	SER	3.9
13	O	244	GLU	3.9
16	v	34	LEU	3.8
3	C	325	GLY	3.8
3	c	260	ALA	3.8
18	x	13	THR	3.8
5	e	84	LYS	3.8
13	O	46	PRO	3.8
3	c	184	GLY	3.8
2	b	120	LEU	3.8
2	b	70	GLY	3.8
4	d	139	ARG	3.7
2	b	483	ASP	3.7
1	a	171	GLY	3.7
3	C	402	GLY	3.7
9	J	7	ARG	3.7
13	o	215	ARG	3.7
4	d	194	ASN	3.7
3	C	210	PHE	3.7
4	d	206	GLY	3.7
2	B	306	PRO	3.7
5	e	3	GLY	3.7
13	O	50	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
13	O	89	ALA	3.7
2	b	402	TYR	3.6
18	X	45	LYS	3.6
8	I	1	MET	3.6
13	O	79	LYS	3.6
13	o	220	LYS	3.6
2	b	491	VAL	3.6
6	f	12	SER	3.6
7	h	2	ALA	3.6
2	b	302	TRP	3.6
16	v	36	VAL	3.6
11	L	33	SER	3.6
3	c	256	PRO	3.6
2	b	296	ALA	3.6
3	C	155	ASN	3.6
15	U	39	LEU	3.6
15	u	74	THR	3.6
2	B	69	LEU	3.5
13	o	213	VAL	3.5
13	O	224	SER	3.5
20	z	1	MET	3.5
15	u	65	PHE	3.5
1	A	294	ALA	3.5
4	D	197	HIS	3.5
4	d	201	VAL	3.5
9	J	8	ILE	3.5
4	d	191	TRP	3.5
7	h	27	THR	3.5
2	b	485	GLU	3.5
4	D	198	MET	3.5
18	x	42	GLN	3.4
2	b	119	ASP	3.4
2	b	305	ILE	3.4
3	c	204	LEU	3.4
3	c	180	MET	3.4
2	b	304	ALA	3.4
7	H	63	LYS	3.4
15	U	38	GLU	3.4
1	a	199	GLN	3.4
13	o	52	ALA	3.4
4	d	239	GLN	3.4
13	O	258	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	150	ASP	3.4
3	c	264	PHE	3.4
1	A	266	ASN	3.4
7	H	64	ALA	3.3
3	C	201	ASN	3.3
1	a	178	GLY	3.3
2	b	298	LEU	3.3
1	A	80	GLY	3.3
1	A	178	GLY	3.3
3	C	154	LYS	3.3
15	U	40	VAL	3.3
13	O	76	PHE	3.3
16	v	46	THR	3.3
5	E	17	VAL	3.3
7	h	23	PRO	3.3
16	v	47	LEU	3.3
5	E	60	GLN	3.3
18	X	12	ILE	3.3
1	a	293	MET	3.3
13	O	242	GLU	3.3
15	u	70	GLY	3.3
4	d	199	MET	3.3
3	C	265	ILE	3.2
3	c	261	ARG	3.2
4	d	172	SER	3.2
18	x	11	THR	3.2
1	a	80	GLY	3.2
16	V	28	GLU	3.2
16	v	44	THR	3.2
1	A	191	ASN	3.2
2	b	397	VAL	3.2
13	o	171	GLU	3.2
20	Z	1	MET	3.2
2	b	178	VAL	3.2
8	I	32	PRO	3.2
7	H	6	TRP	3.2
7	H	3	ARG	3.2
13	o	190	LEU	3.2
7	h	14	LEU	3.2
1	A	293	MET	3.2
2	b	122	LEU	3.2
13	O	222	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	198	HIS	3.2
1	A	137	LEU	3.2
18	X	13	THR	3.2
13	O	84	ASN	3.2
3	c	179	ALA	3.2
13	O	171	GLU	3.1
13	O	219	THR	3.1
1	A	181	ASN	3.1
13	O	49	ASP	3.1
13	O	173	ASN	3.1
13	O	169	LYS	3.1
2	b	303	SER	3.1
3	C	203	THR	3.1
1	a	246	TYR	3.1
1	A	192	ILE	3.1
3	c	259	TRP	3.1
1	a	165	GLN	3.1
4	d	177	ALA	3.1
13	O	53	ARG	3.1
4	D	174	GLY	3.1
13	o	189	GLY	3.1
5	E	56	TYR	3.1
17	y	42	ARG	3.1
10	K	42	ALA	3.1
3	C	142	GLU	3.1
13	O	54	GLY	3.1
1	a	245	THR	3.1
1	a	303	ASN	3.1
1	A	138	GLY	3.1
2	b	395	GLN	3.1
1	a	286	THR	3.1
3	c	210	PHE	3.1
15	u	69	ARG	3.1
13	o	238	ALA	3.0
16	V	39	ASN	3.0
13	O	223	ILE	3.0
2	b	166	MET	3.0
13	o	173	ASN	3.0
7	h	5	THR	3.0
1	a	244	GLU	3.0
2	B	179	GLN	3.0
2	b	411	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	b	378	LYS	3.0
13	o	214	LYS	3.0
16	V	30	THR	3.0
1	A	15	GLU	3.0
16	V	43	LYS	3.0
1	a	282	GLY	3.0
3	C	204	LEU	3.0
2	b	398	THR	3.0
4	D	199	MET	3.0
1	A	301	ASN	3.0
4	d	240	ALA	3.0
1	a	170	ASP	3.0
7	h	15	ASN	3.0
12	M	1	MET	3.0
15	U	53	GLU	3.0
1	a	220	THR	3.0
3	C	403	SER	3.0
7	H	5	THR	3.0
3	c	149	TYR	3.0
3	c	365	TRP	3.0
4	d	195	PRO	2.9
2	b	299	GLU	2.9
15	u	39	LEU	2.9
10	k	11	LEU	2.9
3	C	143	TYR	2.9
16	v	146	LEU	2.9
3	C	256	PRO	2.9
7	H	62	TRP	2.9
1	A	286	THR	2.9
15	u	50	ALA	2.9
7	H	55	LEU	2.9
1	a	16	ARG	2.9
1	a	176	ILE	2.9
4	D	25	ASP	2.9
5	e	4	THR	2.9
4	d	265	ARG	2.9
2	B	180	PRO	2.9
7	h	16	SER	2.9
4	d	174	GLY	2.9
13	o	88	GLU	2.9
18	X	11	THR	2.9
4	d	227	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
15	u	57	LEU	2.9
1	a	319	ASP	2.9
3	C	263	ALA	2.9
7	h	6	TRP	2.9
2	B	165	GLY	2.9
2	b	179	GLN	2.9
7	h	11	LEU	2.9
7	h	25	TRP	2.9
17	y	46	LEU	2.9
3	C	144	SER	2.9
2	B	78	TRP	2.9
2	b	167	TRP	2.9
2	b	219	VAL	2.9
3	c	257	PHE	2.9
4	d	176	ALA	2.8
2	b	289	GLN	2.8
2	b	338	GLN	2.8
3	C	264	PHE	2.8
16	V	47	LEU	2.8
5	E	18	ARG	2.8
2	B	70	GLY	2.8
3	c	197	ARG	2.8
4	D	190	ASN	2.8
8	I	35	LYS	2.8
3	c	258	GLY	2.8
1	a	301	ASN	2.8
2	b	347	ARG	2.8
7	h	9	ASP	2.8
8	i	25	SER	2.8
2	b	339	ALA	2.8
13	O	48	LEU	2.8
13	o	240	THR	2.8
16	V	44	THR	2.8
4	d	192	THR	2.8
2	B	86	ILE	2.8
1	a	186	PHE	2.8
1	A	12	ASN	2.8
4	d	203	GLY	2.8
1	a	247	ASN	2.8
8	I	25	SER	2.8
1	a	240	GLY	2.7
2	b	288	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	409	GLY	2.7
2	b	349	LYS	2.7
4	d	202	ALA	2.7
14	T	27	PRO	2.7
2	B	347	ARG	2.7
2	B	121	GLU	2.7
2	B	490	GLN	2.7
1	A	199	GLN	2.7
2	B	127	ARG	2.7
2	b	69	LEU	2.7
4	D	26	ARG	2.7
1	a	224	ILE	2.7
2	b	350	GLU	2.7
15	U	70	GLY	2.7
15	u	45	GLU	2.7
3	C	152	LYS	2.7
13	O	174	VAL	2.7
1	a	325	ASN	2.7
4	D	227	GLU	2.7
2	b	341	LYS	2.7
12	M	4	ASN	2.7
16	V	29	LEU	2.7
2	b	117	TYR	2.7
8	I	34	ARG	2.7
3	C	411	ALA	2.7
6	f	14	PRO	2.7
1	a	139	MET	2.7
3	c	147	PHE	2.7
3	C	202	PRO	2.7
2	B	50	PRO	2.6
3	C	200	THR	2.6
13	O	168	PHE	2.6
3	C	255	THR	2.6
13	o	124	GLU	2.6
3	C	191	PRO	2.6
13	O	261	ILE	2.6
2	B	166	MET	2.6
6	f	15	ILE	2.6
13	o	239	GLY	2.6
1	a	328	MET	2.6
13	O	243	SER	2.6
16	v	45	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	a	195	HIS	2.6
2	b	121	GLU	2.6
4	D	194	ASN	2.6
4	d	190	ASN	2.6
7	H	54	ILE	2.6
8	I	3	THR	2.6
15	u	44	ASP	2.6
1	a	287	ALA	2.6
3	C	453	ALA	2.6
1	a	225	ARG	2.6
3	C	261	ARG	2.6
13	O	225	LEU	2.6
2	b	297	THR	2.6
11	l	33	SER	2.6
18	x	12	ILE	2.6
17	g	27	MET	2.6
16	v	31	PRO	2.6
15	u	40	VAL	2.6
2	B	356	VAL	2.6
3	C	332	GLN	2.6
15	U	69	ARG	2.6
3	C	141	GLU	2.6
4	d	200	GLY	2.6
1	A	289	GLY	2.5
2	b	123	PHE	2.5
2	b	388	SER	2.5
3	c	198	VAL	2.5
1	a	172	MET	2.5
6	F	15	ILE	2.5
2	b	132	ALA	2.5
15	u	71	LEU	2.5
1	A	78	ILE	2.5
16	v	29	LEU	2.5
4	d	155	SER	2.5
2	b	125	ASP	2.5
13	O	260	LYS	2.5
4	D	77	ALA	2.5
2	B	185	TRP	2.5
2	b	194	ASN	2.5
3	c	405	ASN	2.5
2	B	73	GLY	2.5
2	B	305	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	14	TRP	2.5
2	b	368	VAL	2.5
5	E	57	ALA	2.5
11	l	8	GLN	2.5
7	h	55	LEU	2.5
2	b	373	LYS	2.5
13	o	221	GLY	2.5
3	c	191	PRO	2.5
2	b	295	GLY	2.5
7	h	7	LEU	2.5
4	d	198	MET	2.5
16	v	49	GLU	2.5
3	C	326	ALA	2.5
1	a	153	SER	2.5
2	B	219	VAL	2.4
16	V	38	LEU	2.4
2	B	379	ALA	2.4
3	C	46	SER	2.4
2	b	177	SER	2.4
15	u	58	ASN	2.4
16	v	132	ASN	2.4
18	x	16	LEU	2.4
4	D	296	TYR	2.4
1	A	196	PRO	2.4
2	b	137	LYS	2.4
11	l	1	MET	2.4
3	C	213	LEU	2.4
3	C	140	LEU	2.4
4	d	95	PRO	2.4
13	O	47	THR	2.4
15	u	42	VAL	2.4
2	b	185	TRP	2.4
3	c	263	ALA	2.4
3	c	403	SER	2.4
16	v	142	ALA	2.4
1	A	201	GLY	2.4
13	o	169	LYS	2.4
7	h	13	PRO	2.4
3	c	146	PHE	2.4
1	a	166	GLY	2.4
3	C	181	PHE	2.4
9	J	11	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
13	o	258	GLU	2.4
2	b	403	GLY	2.4
2	B	370	LEU	2.4
13	o	210	ARG	2.4
1	a	223	LEU	2.4
15	u	75	LEU	2.4
3	C	157	MET	2.4
1	a	201	GLY	2.3
1	a	221	SER	2.3
2	b	195	PRO	2.3
17	g	23	THR	2.3
1	a	192	ILE	2.3
4	d	278	GLY	2.3
13	O	234	THR	2.3
7	H	53	LEU	2.3
13	o	228	ALA	2.3
4	D	195	PRO	2.3
3	C	151	TRP	2.3
7	h	18	TYR	2.3
2	b	300	GLU	2.3
1	A	81	ALA	2.3
1	A	16	ARG	2.3
1	a	169	SER	2.3
13	O	259	VAL	2.3
1	a	191	ASN	2.3
2	B	131	PRO	2.3
4	D	282	SER	2.3
13	o	237	ILE	2.3
12	M	2	GLU	2.3
13	o	168	PHE	2.3
2	b	489	GLU	2.3
15	u	115	THR	2.3
2	b	396	GLY	2.3
5	e	60	GLN	2.3
15	U	75	LEU	2.3
2	b	364	GLU	2.3
13	O	218	LEU	2.3
20	z	4	LEU	2.3
4	d	138	VAL	2.3
13	O	202	GLN	2.3
2	b	379	ALA	2.3
16	v	78	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	b	220	ARG	2.3
2	b	301	ALA	2.3
2	b	405	GLU	2.3
2	b	72	THR	2.3
13	O	206	GLU	2.3
13	O	262	GLN	2.3
13	o	89	ALA	2.2
2	b	408	GLY	2.2
2	b	385	ARG	2.2
2	b	484	PRO	2.2
13	O	94	THR	2.2
13	O	44	LYS	2.2
4	D	177	ALA	2.2
13	o	230	VAL	2.2
16	V	130	MET	2.2
1	A	161	TYR	2.2
16	V	37	PRO	2.2
1	a	167	SER	2.2
1	a	181	ASN	2.2
2	B	309	LEU	2.2
13	o	229	LYS	2.2
1	a	289	GLY	2.2
3	c	183	GLY	2.2
2	B	120	LEU	2.2
2	b	218	LEU	2.2
13	o	50	ASP	2.2
1	a	19	ASN	2.2
16	v	48	THR	2.2
2	B	420	TYR	2.2
3	C	340	TYR	2.2
3	c	364	PRO	2.2
4	D	171	PRO	2.2
6	F	11	VAL	2.2
7	h	12	ARG	2.2
1	a	137	LEU	2.2
2	B	124	ARG	2.2
3	C	145	SER	2.2
7	H	27	THR	2.2
7	h	8	GLY	2.2
12	m	4	ASN	2.2
1	a	310	LYS	2.2
2	B	181	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	291	SER	2.2
13	O	88	GLU	2.2
1	a	187	GLN	2.2
1	a	239	PHE	2.2
1	a	226	GLU	2.2
2	b	340	TRP	2.2
1	A	290	ILE	2.2
2	b	322	GLY	2.2
4	d	187	GLY	2.2
13	O	215	ARG	2.2
11	l	2	GLU	2.1
1	A	76	ASN	2.1
18	x	15	SER	2.1
2	b	134	ASP	2.1
3	C	199	ILE	2.1
3	c	196	VAL	2.1
1	a	149	ALA	2.1
11	L	30	LEU	2.1
1	a	327	GLY	2.1
10	K	46	ARG	2.1
8	I	2	GLU	2.1
2	B	183	PRO	2.1
2	b	351	GLY	2.1
13	O	245	GLN	2.1
13	O	55	ALA	2.1
4	d	83	ASN	2.1
4	d	179	PHE	2.1
4	D	200	GLY	2.1
1	A	268	SER	2.1
2	B	218	LEU	2.1
3	c	262	ARG	2.1
7	h	22	ALA	2.1
15	u	106	ARG	2.1
2	B	293	ALA	2.1
13	O	58	ILE	2.1
3	C	137	PRO	2.1
3	C	465	PRO	2.1
2	b	346	PHE	2.1
1	a	76	ASN	2.1
2	b	352	GLU	2.1
3	C	146	PHE	2.1
4	D	297	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	242	GLU	2.1
12	m	33	GLN	2.1
2	B	81	THR	2.1
20	z	2	THR	2.1
1	A	180	PHE	2.1
1	a	296	ASN	2.1
2	B	171	PRO	2.1
3	C	182	PHE	2.1
16	v	130	MET	2.1
1	a	202	VAL	2.1
4	D	278	GLY	2.1
13	O	93	PRO	2.1
16	v	113	GLU	2.1
1	A	170	ASP	2.1
1	a	18	CYS	2.1
8	I	26	GLY	2.1
10	k	12	PRO	2.1
15	u	41	ASN	2.1
11	l	34	TYR	2.1
13	o	91	PHE	2.1
13	O	51	THR	2.1
1	a	162	PRO	2.1
15	U	65	PHE	2.1
3	c	192	GLY	2.0
15	u	110	GLU	2.0
13	o	158	ASN	2.0
4	d	288	GLY	2.0
1	a	10	SER	2.0
4	d	165	SER	2.0
11	L	37	ASN	2.0
18	X	42	GLN	2.0
2	b	430	PHE	2.0
8	I	30	ARG	2.0
1	A	296	ASN	2.0
4	D	155	SER	2.0
2	b	234	ILE	2.0
4	d	136	VAL	2.0
5	E	21	VAL	2.0
2	B	259	GLY	2.0
2	B	410	THR	2.0
2	b	345	VAL	2.0
1	a	322	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
16	v	133	LEU	2.0
2	B	71	VAL	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
24	PL9	J	101	35/55	0.19	0.59	206,207,210,210	0
32	LMT	I	102	35/35	0.26	1.23	206,208,210,210	0
24	PL9	j	101	35/55	0.30	0.49	205,208,209,210	0
32	LMT	i	103	35/35	0.30	1.35	206,209,210,210	0
35	CA	O	301	1/1	0.31	0.46	208,208,208,208	0
35	CA	K	102	1/1	0.44	0.74	210,210,210,210	0
24	PL9	d	407	55/55	0.48	0.54	205,207,208,208	0
31	LMG	I	101	43/55	0.49	1.17	205,208,210,211	0
31	LMG	b	627	42/55	0.49	0.56	204,207,211,211	0
31	LMG	C	517	45/55	0.50	1.11	206,207,209,210	0
22	CLA	c	502	65/65	0.51	0.70	206,207,208,209	0
25	BCR	F	102	40/40	0.53	0.56	205,207,208,208	0
31	LMG	e	101	44/55	0.55	0.55	205,208,209,211	0
26	DGD	a	408	56/66	0.56	0.50	206,208,210,211	0
22	CLA	b	605	65/65	0.56	1.38	206,208,210,210	0
26	DGD	A	409	56/66	0.56	0.58	206,208,210,211	0
25	BCR	b	624	40/40	0.57	1.02	205,206,207,208	0
21	FE2	a	413	1/1	0.57	0.23	206,206,206,206	0
32	LMT	d	411	31/35	0.57	0.80	206,209,210,211	0
28	CL	A	411	1/1	0.60	0.80	204,204,204,204	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	J	102	40/40	0.60	0.36	205,207,209,209	0
25	BCR	H	102	40/40	0.61	1.22	206,207,209,210	0
35	CA	o	301	1/1	0.61	0.65	209,209,209,209	0
26	DGD	d	410	63/66	0.62	0.79	206,208,210,211	0
21	FE2	A	401	1/1	0.62	0.17	209,209,209,209	0
22	CLA	B	601	65/65	0.62	0.70	205,208,209,209	0
23	PHO	d	401	64/64	0.62	0.51	206,207,208,208	0
25	BCR	C	513	40/40	0.62	1.11	205,207,208,208	0
24	PL9	A	407	45/55	0.62	0.46	206,207,208,210	0
24	PL9	D	405	55/55	0.63	0.43	205,207,208,208	0
22	CLA	C	502	65/65	0.64	0.58	206,207,208,208	0
31	LMG	i	102	43/55	0.64	0.83	205,207,209,210	0
24	PL9	a	407	45/55	0.64	0.44	205,207,208,209	0
26	DGD	C	516	66/66	0.64	0.43	205,207,208,208	0
32	LMT	b	629	35/35	0.65	0.93	206,208,209,210	0
25	BCR	c	514	40/40	0.65	1.27	206,208,208,209	0
32	LMT	b	628	35/35	0.65	0.55	206,208,210,210	0
22	CLA	b	620	65/65	0.66	1.17	206,208,209,210	0
32	LMT	D	408	31/35	0.66	0.73	207,208,210,210	0
25	BCR	f	102	40/40	0.67	0.39	206,207,208,209	0
30	SQD	B	627	47/54	0.67	0.68	206,208,210,212	0
31	LMG	a	402	42/55	0.68	0.42	204,207,209,210	0
31	LMG	C	521	48/55	0.69	0.34	206,207,208,209	0
22	CLA	C	512	65/65	0.69	0.92	205,207,209,211	0
32	LMT	M	102	35/35	0.69	0.42	205,208,209,209	0
31	LMG	m	101	42/55	0.69	0.51	205,207,209,210	0
32	LMT	B	623	35/35	0.69	0.81	206,208,210,210	0
26	DGD	D	407	63/66	0.70	0.72	206,208,209,210	0
32	LMT	b	604	35/35	0.70	0.35	207,208,210,210	0
25	BCR	B	616	40/40	0.70	0.41	205,207,208,209	0
22	CLA	C	505	65/65	0.71	0.67	206,207,209,210	0
32	LMT	b	603	35/35	0.71	0.66	206,208,210,210	0
25	BCR	x	101	40/40	0.71	0.91	206,207,209,209	0
31	LMG	E	101	44/55	0.71	0.47	204,208,209,210	0
22	CLA	c	512	65/65	0.71	0.82	206,207,209,210	0
25	BCR	c	513	40/40	0.72	0.92	206,207,208,209	0
30	SQD	d	403	43/54	0.72	0.80	205,208,209,209	0
22	CLA	a	406	65/65	0.72	0.81	206,208,208,209	0
32	LMT	B	629	35/35	0.72	0.39	206,208,209,210	0
25	BCR	B	619	40/40	0.73	1.17	205,207,208,208	0
25	BCR	j	102	40/40	0.73	0.26	206,208,209,210	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LMG	c	518	45/55	0.73	0.88	206,208,209,210	0
30	SQD	b	602	47/54	0.73	0.44	205,208,209,212	0
25	BCR	g	101	40/40	0.73	0.82	205,207,208,209	0
32	LMT	B	624	35/35	0.74	0.53	206,207,211,212	0
32	LMT	B	628	35/35	0.74	0.61	206,208,210,211	0
30	SQD	B	622	43/54	0.74	0.60	205,208,209,212	0
22	CLA	C	508	65/65	0.74	0.87	205,207,208,209	0
25	BCR	B	617	40/40	0.74	0.34	205,207,208,209	0
22	CLA	a	405	65/65	0.75	0.41	205,207,209,209	0
31	LMG	c	522	48/55	0.75	0.33	205,207,209,210	0
22	CLA	b	619	65/65	0.75	0.96	206,208,209,209	0
26	DGD	B	626	52/66	0.75	0.55	206,208,210,211	0
22	CLA	B	613	65/65	0.75	0.46	206,207,208,209	0
25	BCR	b	622	40/40	0.75	0.32	205,207,208,208	0
25	BCR	A	408	40/40	0.75	0.55	206,207,208,208	0
22	CLA	c	510	65/65	0.76	0.46	206,208,209,211	0
25	BCR	C	520	40/40	0.76	1.09	206,207,209,210	0
25	BCR	b	623	40/40	0.76	0.31	205,206,207,207	0
32	LMT	M	103	35/35	0.77	0.35	206,208,209,209	0
22	CLA	C	506	65/65	0.77	0.94	206,207,208,209	0
22	CLA	d	405	65/65	0.77	0.46	205,207,208,208	0
22	CLA	C	511	65/65	0.77	1.22	206,207,208,209	0
25	BCR	i	101	40/40	0.77	0.70	206,207,208,208	0
22	CLA	a	404	65/65	0.78	0.80	204,207,208,208	0
26	DGD	b	625	58/66	0.78	0.37	206,207,208,209	0
22	CLA	A	406	65/65	0.78	0.78	206,208,209,209	0
22	CLA	b	618	65/65	0.78	0.38	206,207,209,210	0
31	LMG	d	409	48/55	0.79	0.34	206,207,209,210	0
27	LHG	c	519	37/49	0.79	0.28	204,207,210,213	0
22	CLA	c	505	65/65	0.79	0.81	205,207,208,209	0
22	CLA	b	612	65/65	0.80	0.49	205,207,209,209	0
30	SQD	A	414	54/54	0.80	0.45	205,207,209,210	0
22	CLA	b	616	65/65	0.80	0.45	206,207,208,209	0
23	PHO	A	405	64/64	0.80	0.40	205,207,208,209	0
30	SQD	a	401	54/54	0.80	0.60	205,208,210,213	0
26	DGD	b	601	52/66	0.80	0.47	204,208,209,210	0
22	CLA	B	603	65/65	0.80	0.60	205,207,208,208	0
25	BCR	c	521	40/40	0.80	1.53	206,208,209,209	0
22	CLA	a	403	65/65	0.80	0.58	205,207,208,210	0
22	CLA	A	404	65/65	0.81	0.44	204,207,208,209	0
22	CLA	b	613	65/65	0.81	0.65	205,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	606	65/65	0.81	0.51	205,207,209,210	0
22	CLA	b	608	65/65	0.81	0.44	205,207,208,209	0
31	LMG	M	101	42/55	0.81	0.36	205,208,209,210	0
30	SQD	F	103	45/54	0.81	0.63	205,208,209,210	0
27	LHG	C	518	37/49	0.81	0.29	205,208,210,211	0
27	LHG	a	409	39/49	0.81	0.32	206,207,209,209	0
22	CLA	c	508	65/65	0.81	0.56	205,208,209,209	0
30	SQD	f	103	45/54	0.81	0.72	205,208,210,210	0
22	CLA	C	504	65/65	0.82	0.42	205,207,208,209	0
23	PHO	d	402	64/64	0.82	0.26	206,207,209,209	0
25	BCR	y	101	40/40	0.82	0.81	206,207,208,208	0
22	CLA	C	507	65/65	0.82	0.36	206,207,208,208	0
33	BCT	d	404	4/4	0.82	0.85	206,207,208,208	0
22	CLA	c	506	65/65	0.82	0.92	206,208,209,209	0
22	CLA	B	615	65/65	0.82	0.99	206,207,209,209	0
31	LMG	D	409	46/55	0.82	0.35	205,207,208,209	0
22	CLA	c	511	65/65	0.83	0.97	206,208,209,209	0
22	CLA	C	509	65/65	0.83	0.37	205,207,208,208	0
22	CLA	B	614	65/65	0.83	0.91	205,207,208,209	0
22	CLA	d	406	65/65	0.83	0.66	206,207,209,209	0
31	LMG	l	101	51/55	0.83	0.29	206,207,209,209	0
34	HEM	v	201	43/43	0.83	0.72	206,207,208,209	0
22	CLA	b	614	65/65	0.83	0.71	206,207,209,210	0
23	PHO	D	401	64/64	0.83	0.36	205,207,208,209	0
35	CA	k	101	1/1	0.83	0.29	208,208,208,208	0
26	DGD	B	620	58/66	0.83	0.38	205,207,209,209	0
22	CLA	C	501	65/65	0.84	0.58	206,208,209,209	0
22	CLA	c	504	65/65	0.84	0.44	205,207,208,209	0
22	CLA	C	519	65/65	0.84	0.31	205,207,209,209	0
25	BCR	B	618	40/40	0.84	0.29	205,206,208,208	0
22	CLA	c	501	65/65	0.84	0.75	206,207,209,209	0
30	SQD	A	413	51/54	0.84	0.26	204,207,209,209	0
26	DGD	c	517	66/66	0.84	0.25	206,207,209,209	0
22	CLA	B	605	65/65	0.85	0.84	206,207,208,209	0
31	LMG	D	406	48/55	0.85	0.28	204,207,208,209	0
22	CLA	b	607	65/65	0.85	0.66	205,207,208,208	0
31	LMG	B	621	49/55	0.85	0.23	206,207,208,209	0
26	DGD	C	515	62/66	0.85	0.34	205,207,209,210	0
31	LMG	L	101	51/55	0.85	0.31	205,207,208,209	0
25	BCR	b	621	40/40	0.86	0.29	206,207,208,208	0
22	CLA	B	608	65/65	0.86	0.86	205,207,209,210	0
22	CLA	B	607	65/65	0.86	0.47	206,207,208,209	0

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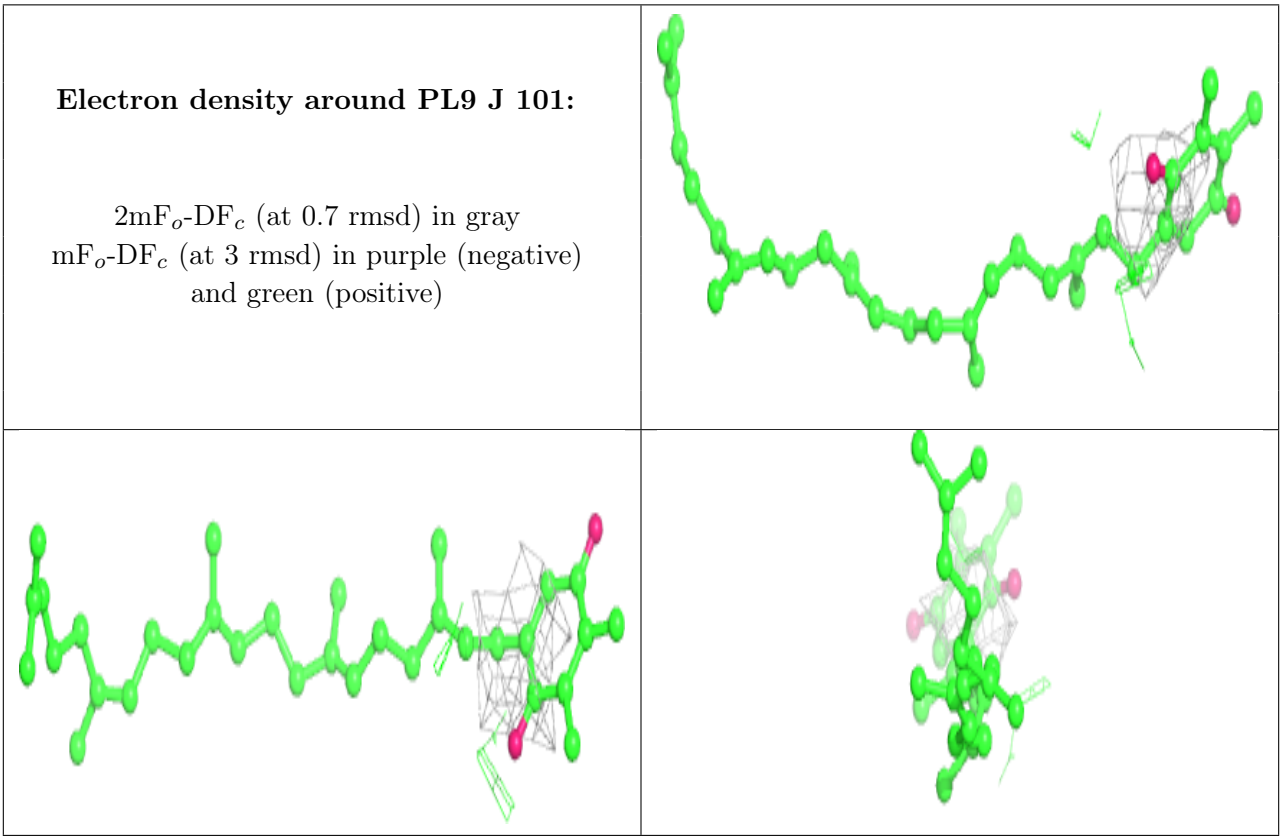
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	C	503	65/65	0.86	0.41	206,207,208,209	0
31	LMG	B	625	49/55	0.86	0.23	205,207,208,208	0
22	CLA	b	615	65/65	0.86	0.31	205,207,208,209	0
22	CLA	c	503	65/65	0.86	0.56	206,207,208,209	0
31	LMG	d	408	49/55	0.86	0.24	205,207,208,209	0
22	CLA	D	404	65/65	0.86	0.71	205,207,208,208	0
27	LHG	A	410	39/49	0.86	0.25	206,207,209,210	0
22	CLA	b	610	65/65	0.86	0.62	206,207,209,209	0
31	LMG	b	626	49/55	0.87	0.23	205,207,209,209	0
26	DGD	c	515	53/66	0.87	0.34	205,207,209,210	0
22	CLA	B	604	65/65	0.87	0.71	206,207,208,209	0
22	CLA	B	609	65/65	0.87	0.73	206,207,209,210	0
22	CLA	b	609	65/65	0.87	0.60	206,207,208,209	0
22	CLA	D	403	65/65	0.88	0.36	205,207,208,208	0
22	CLA	C	510	65/65	0.88	0.56	206,207,209,209	0
22	CLA	c	520	65/65	0.88	0.33	206,207,208,209	0
30	SQD	a	412	51/54	0.89	0.23	205,207,208,209	0
26	DGD	C	514	53/66	0.89	0.30	205,206,208,209	0
22	CLA	A	402	65/65	0.89	0.46	206,207,208,209	0
22	CLA	A	403	65/65	0.89	0.62	205,207,208,208	0
34	HEM	F	101	43/43	0.89	0.72	206,207,208,210	0
22	CLA	H	101	65/65	0.90	0.40	206,207,208,209	0
22	CLA	c	507	65/65	0.90	0.31	206,207,209,209	0
22	CLA	b	611	65/65	0.90	0.27	206,207,208,209	0
34	HEM	V	201	43/43	0.90	0.44	201,207,208,209	0
22	CLA	c	509	65/65	0.90	0.31	206,207,209,209	0
22	CLA	B	610	65/65	0.90	0.32	205,207,208,208	0
25	BCR	K	101	40/40	0.90	0.83	206,207,208,209	0
31	LMG	d	412	46/55	0.90	0.21	205,207,208,209	0
26	DGD	c	516	62/66	0.90	0.21	206,208,208,209	0
22	CLA	B	606	65/65	0.91	0.27	205,207,208,209	0
33	BCT	D	402	4/4	0.91	0.40	208,208,208,208	0
34	HEM	f	101	43/43	0.92	0.43	206,207,209,209	0
22	CLA	B	602	65/65	0.92	0.62	205,207,208,209	0
22	CLA	B	612	65/65	0.92	0.26	203,207,208,209	0
22	CLA	b	617	65/65	0.93	0.36	206,207,208,209	0
22	CLA	B	611	65/65	0.93	0.46	205,207,208,208	0
28	CL	a	410	1/1	0.94	0.40	205,205,205,205	0
29	OEX	A	412	10/10	0.94	0.50	197,202,205,206	0
29	OEX	a	411	10/10	0.97	0.54	200,204,205,206	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

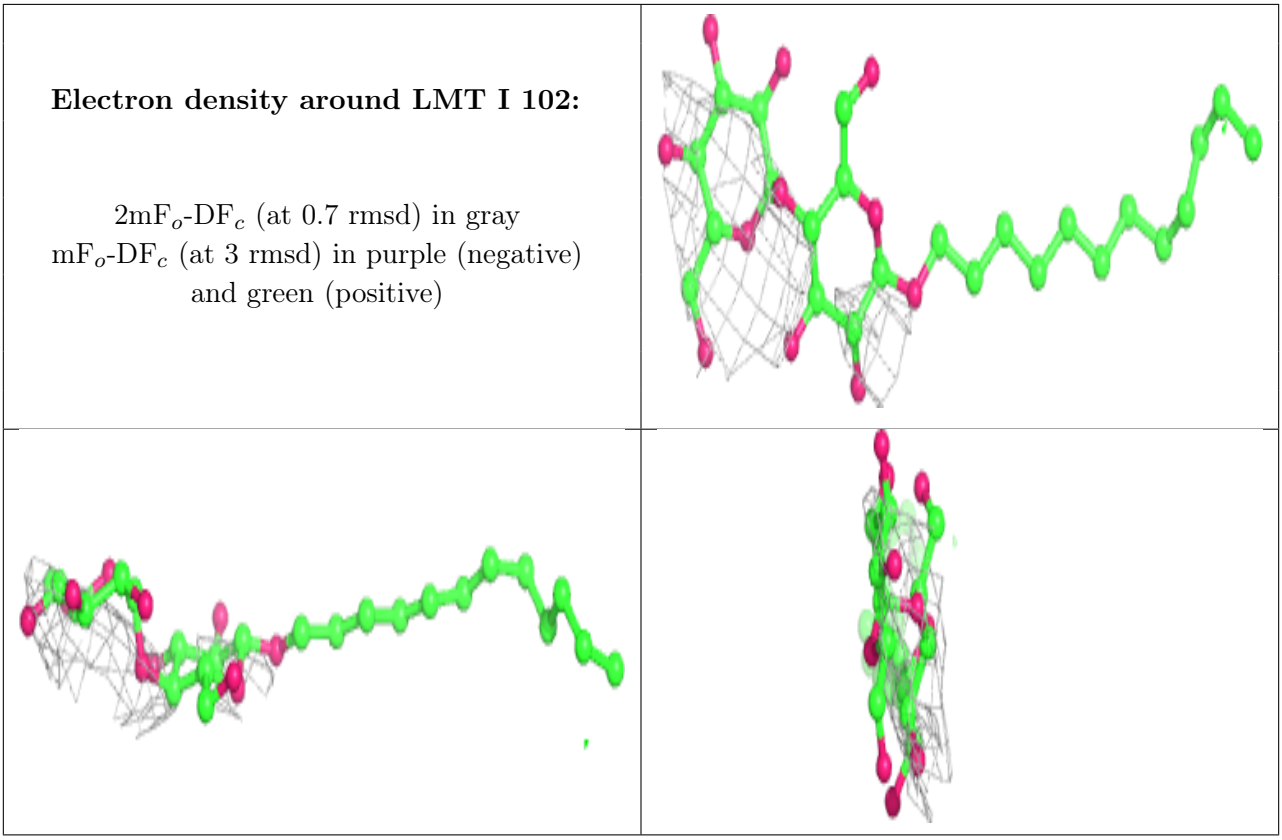
Electron density around PL9 J 101:

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



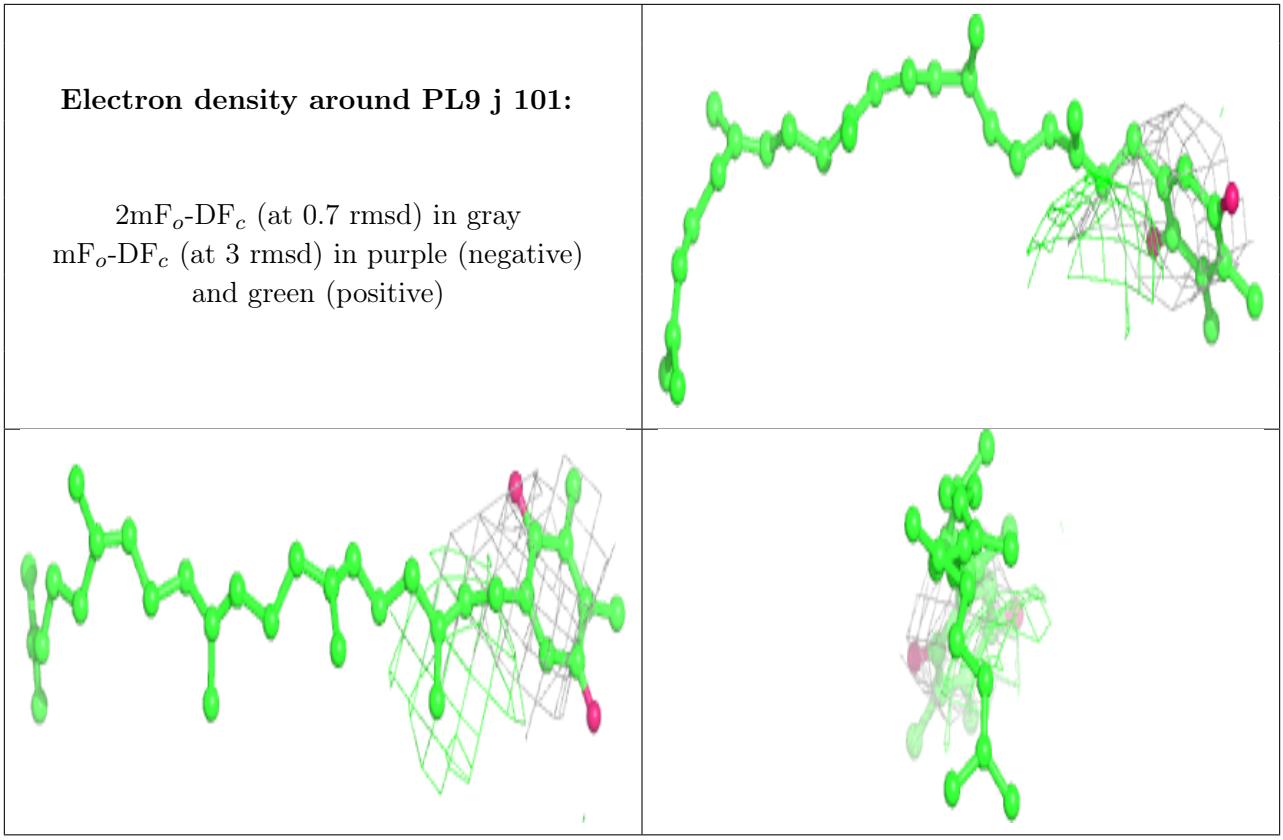
Electron density around LMT I 102:

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



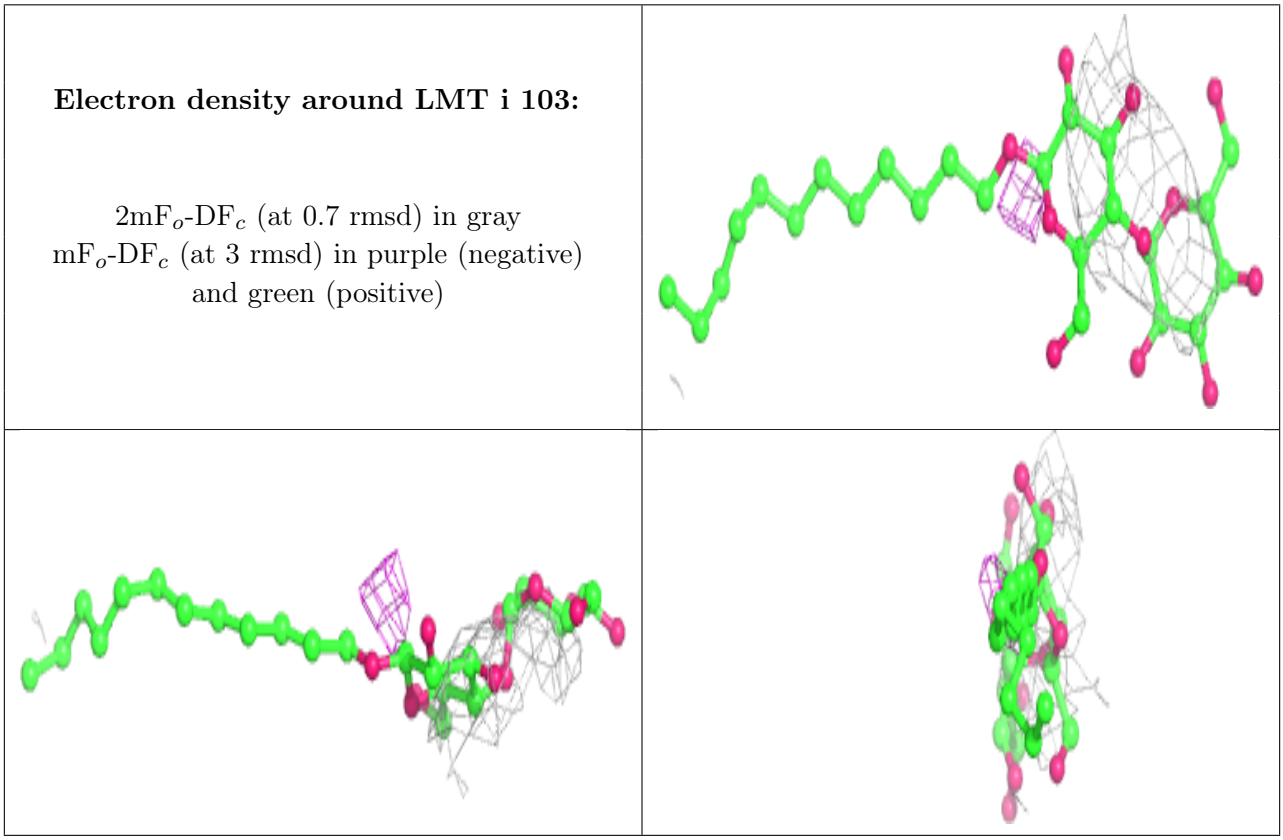
Electron density around PL9 j 101:

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



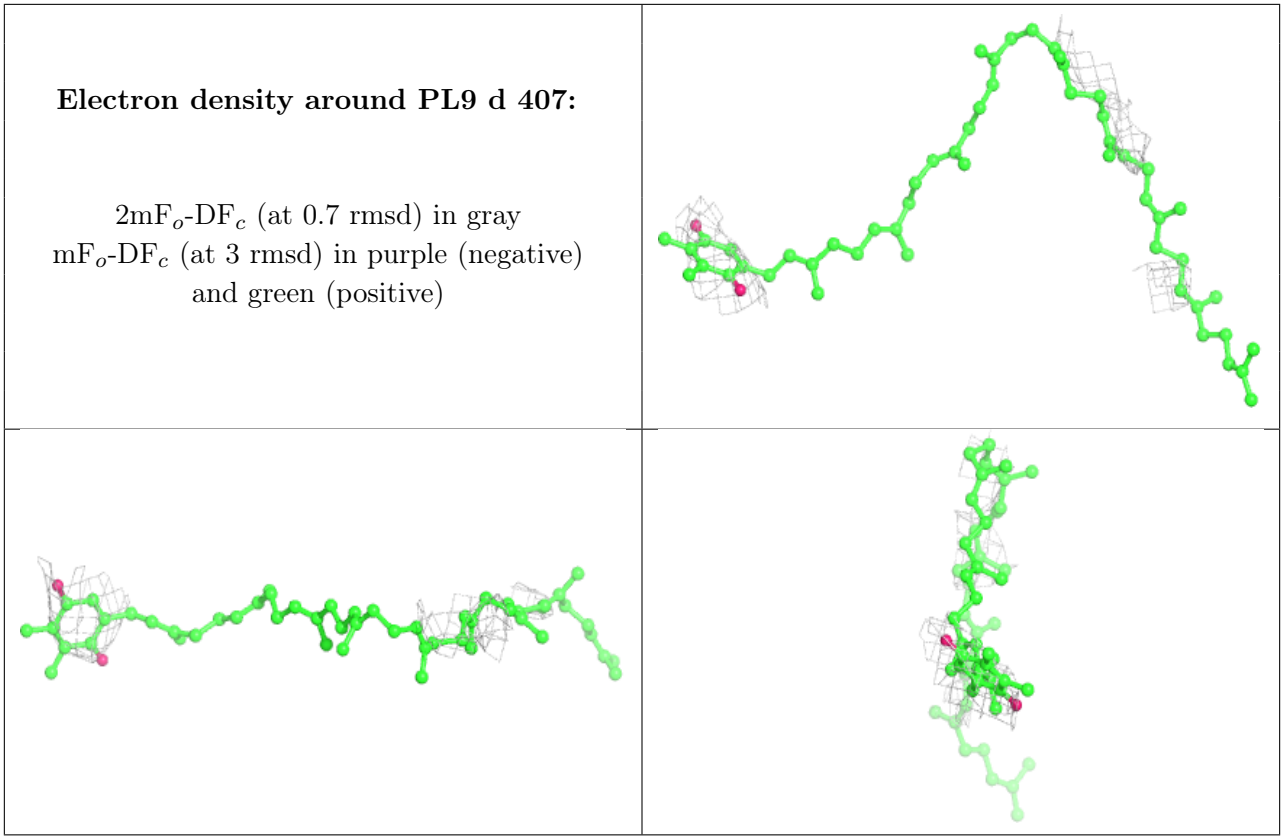
Electron density around LMT i 103:

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



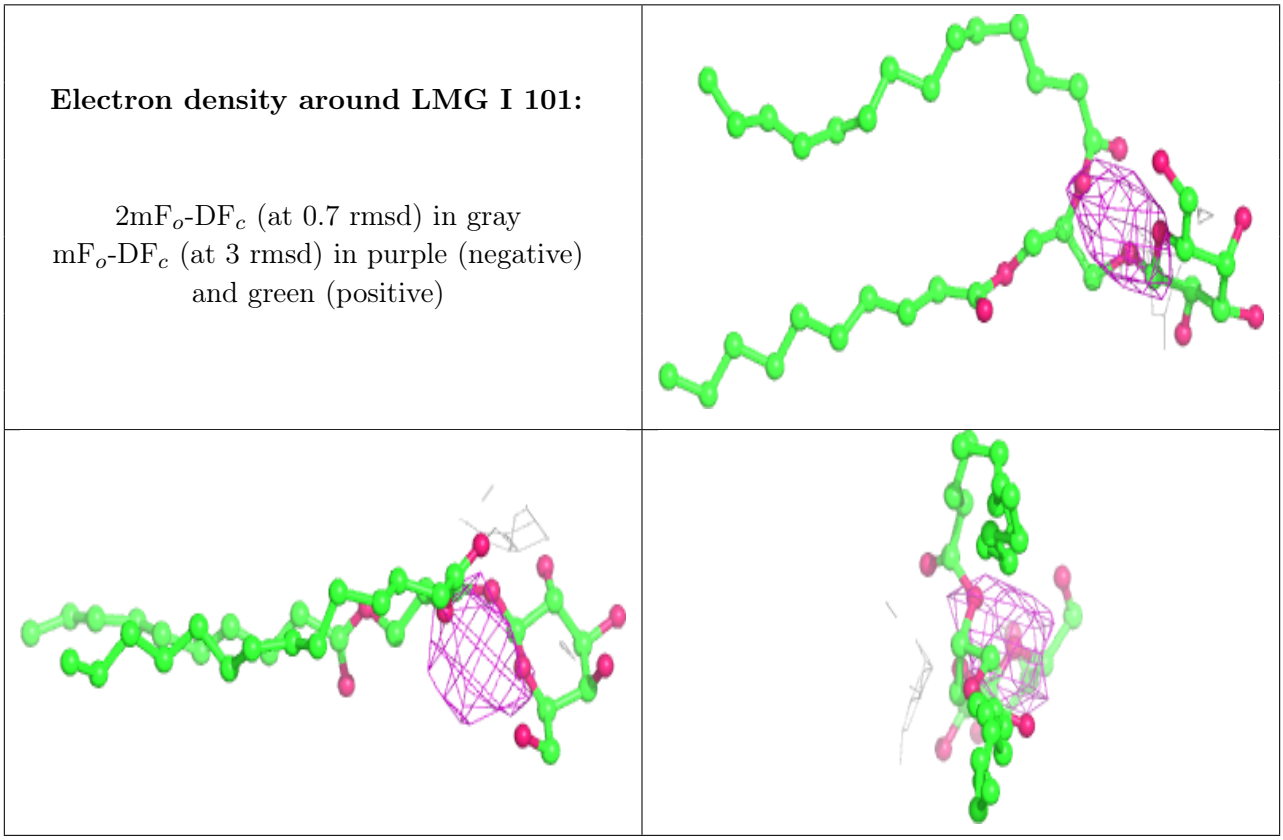
Electron density around PL9 d 407:

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



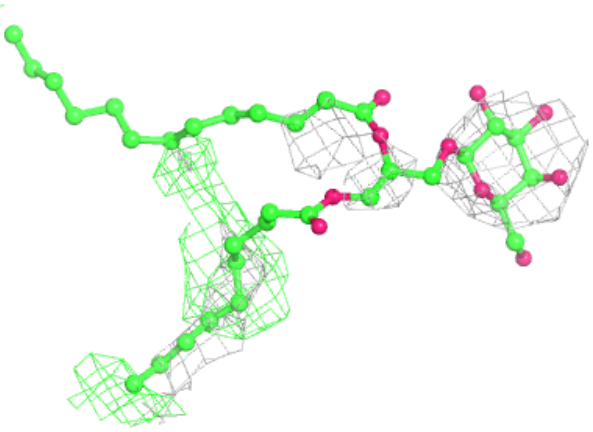
Electron density around LMG I 101:

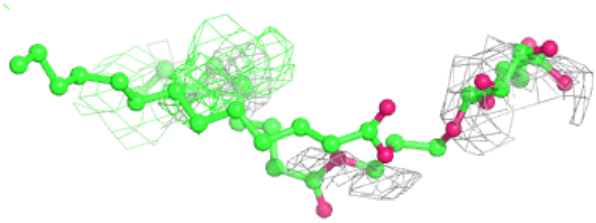
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

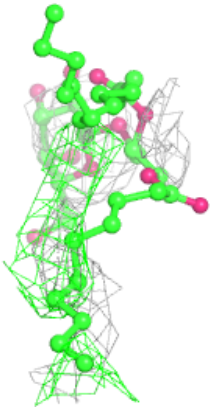


Electron density around LMG b 627:

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

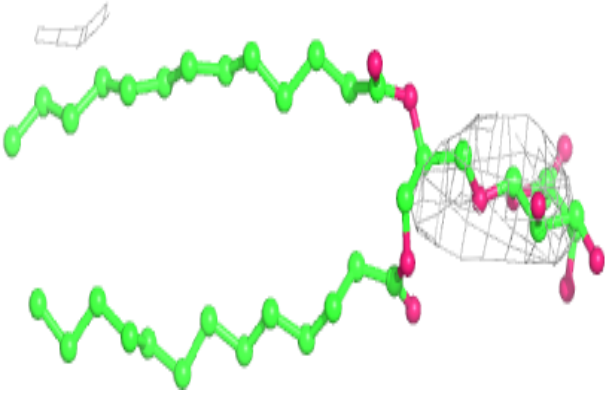


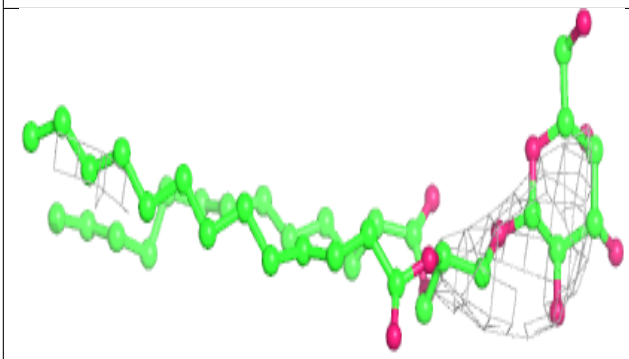


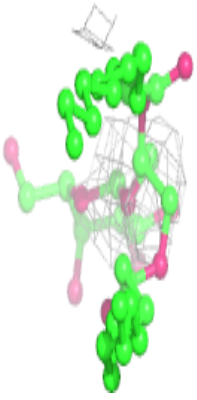


Electron density around LMG C 517:

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

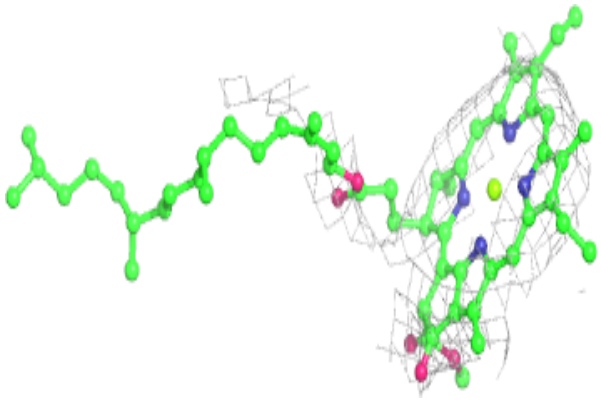


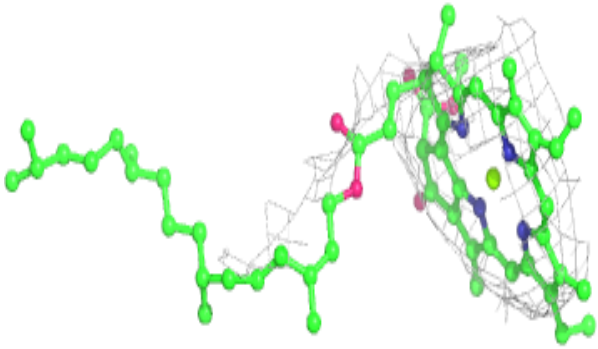


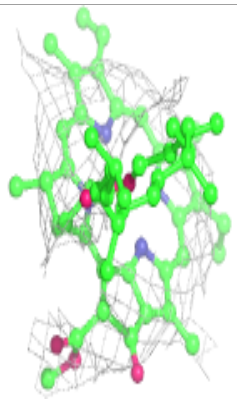


Electron density around CLA c 502:

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

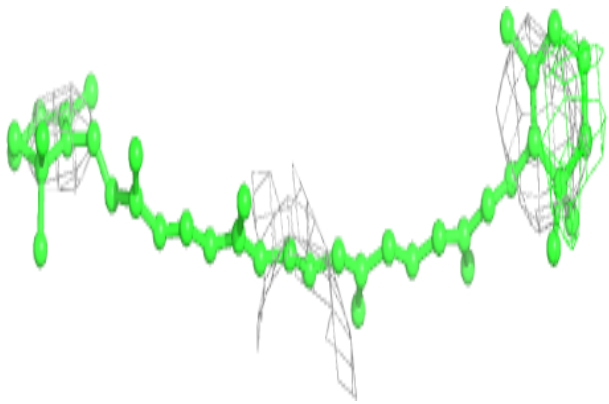


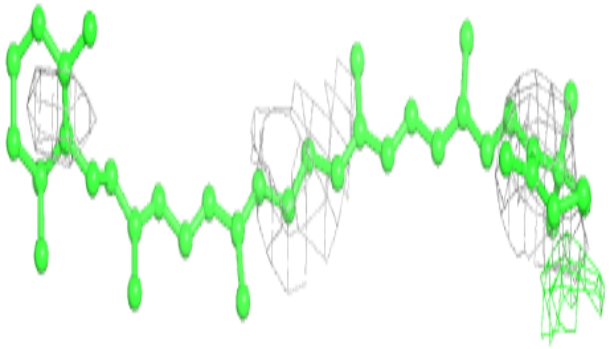


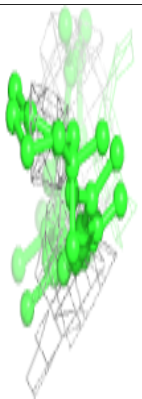


Electron density around BCR F 102:

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

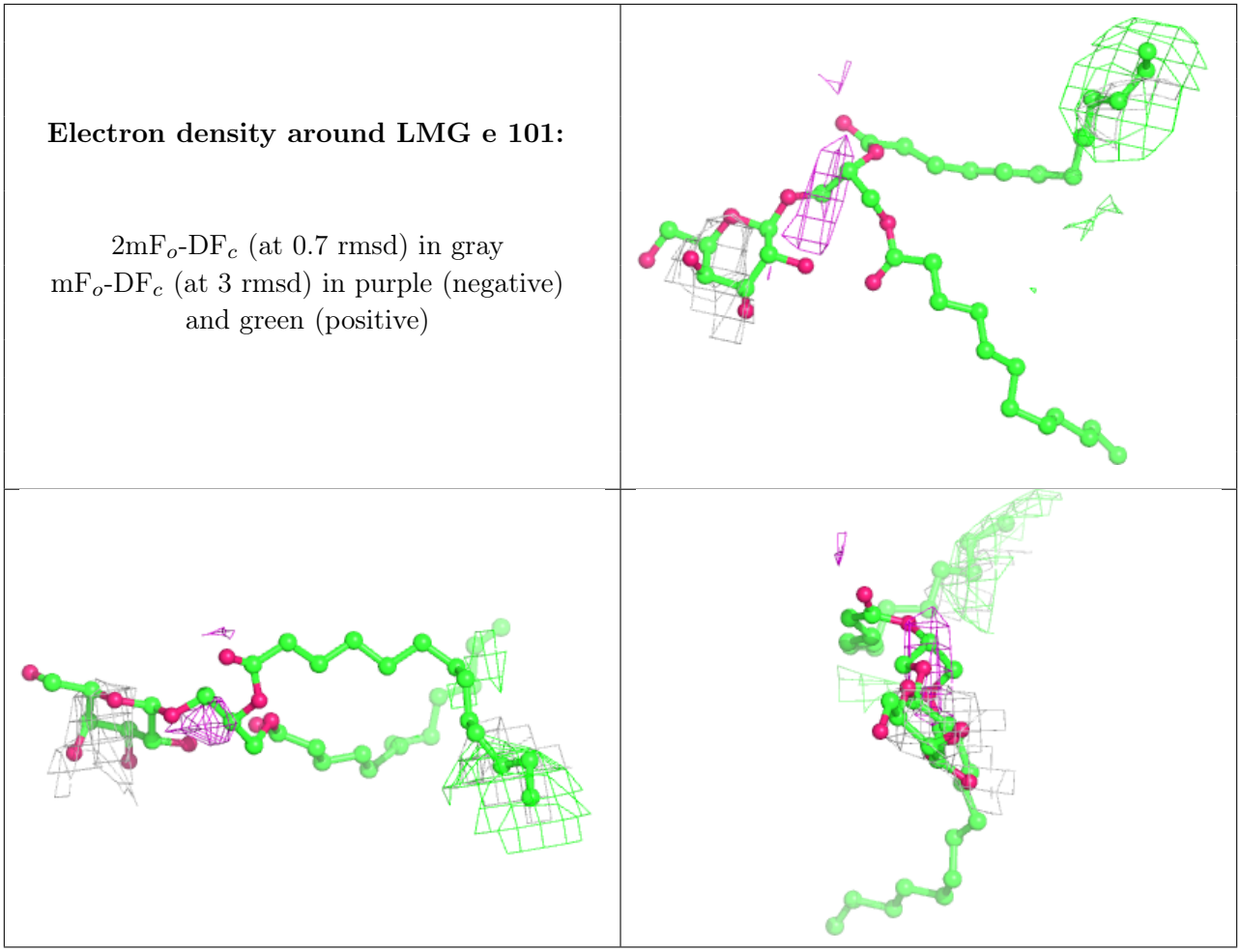






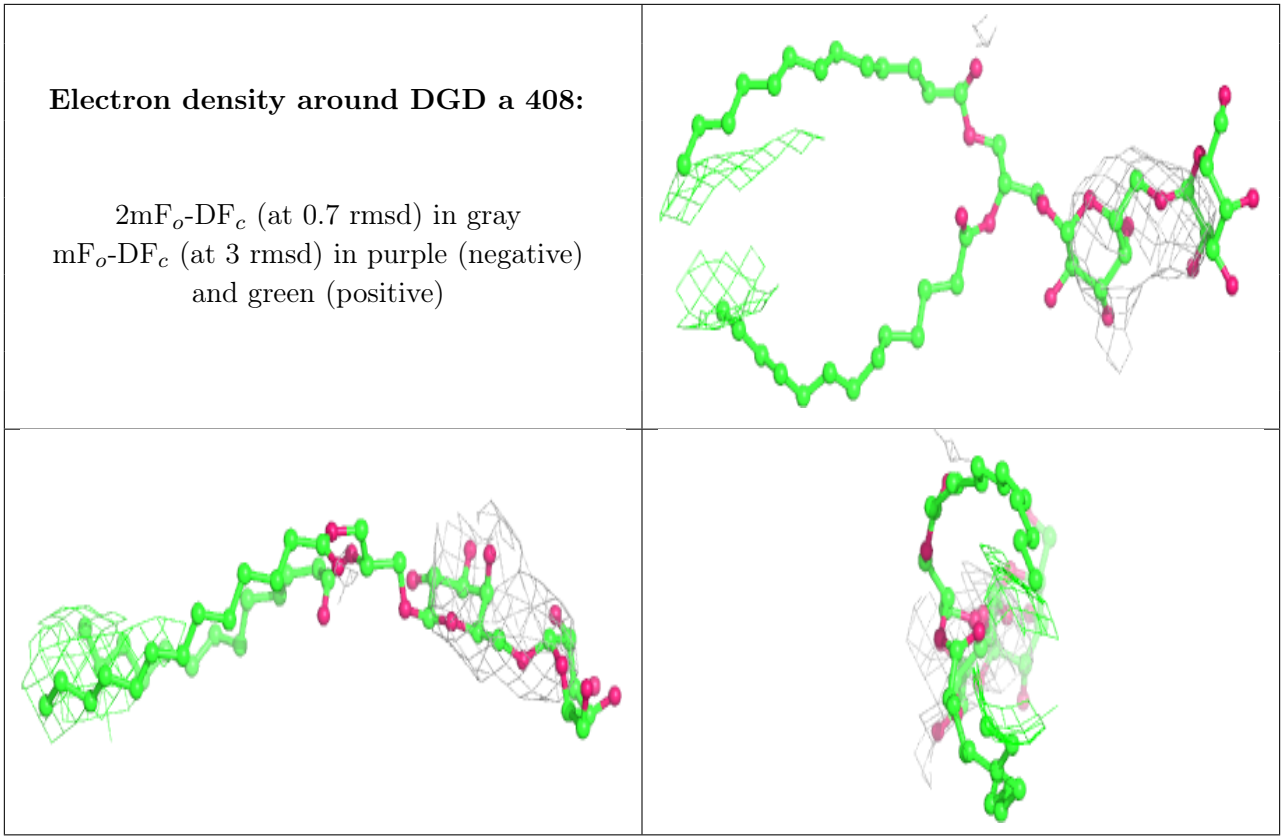
Electron density around LMG e 101:

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



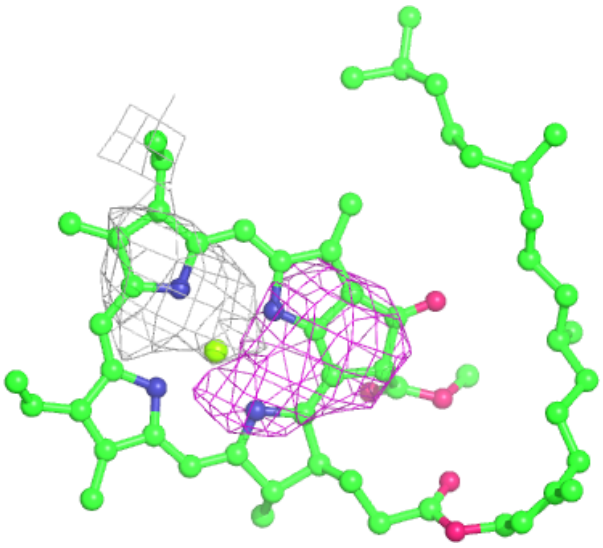
Electron density around DGD a 408:

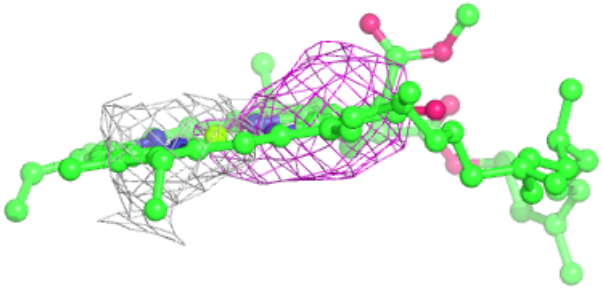
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

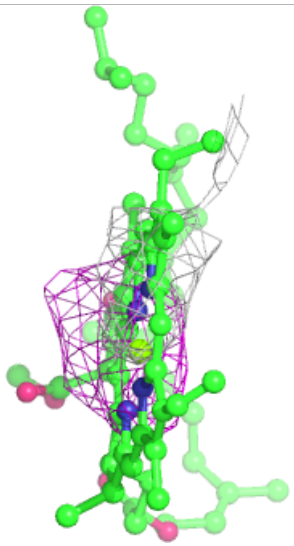


Electron density around CLA b 605:

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

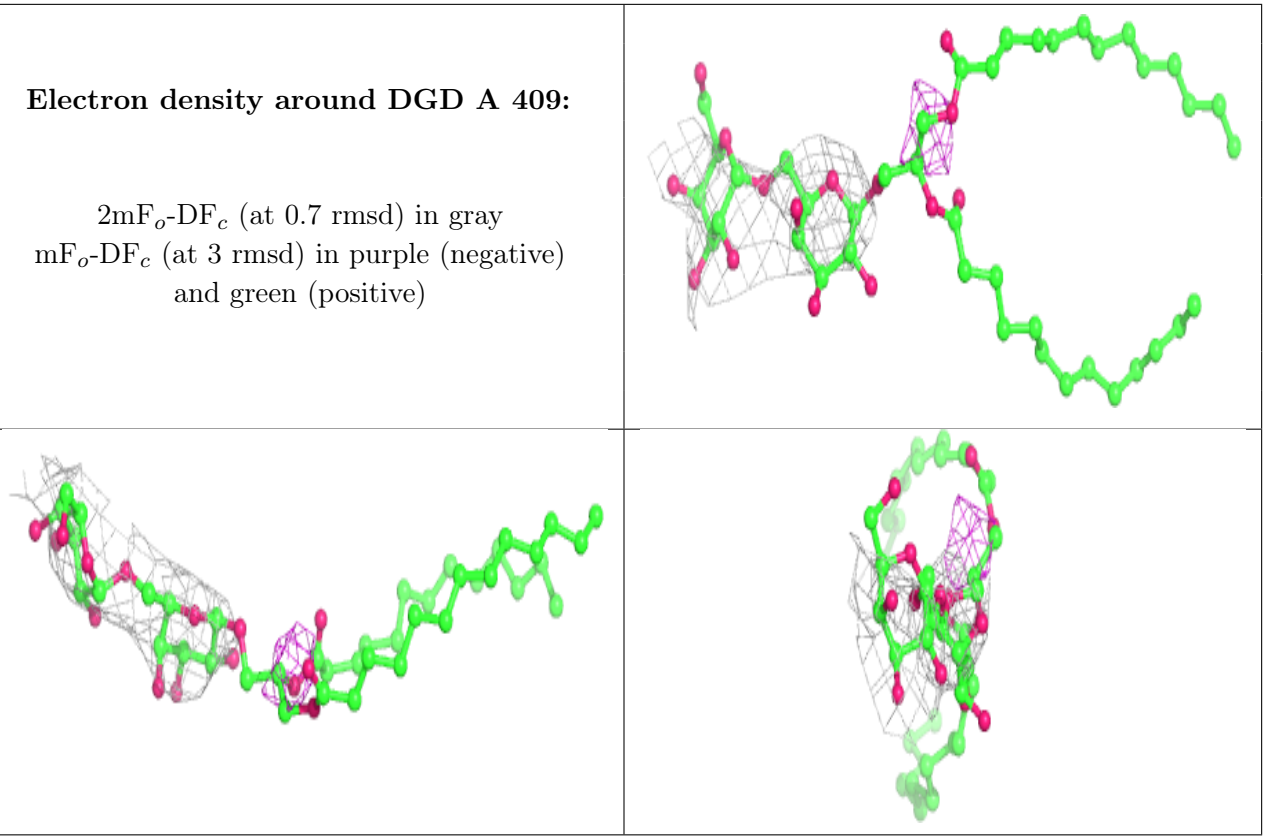






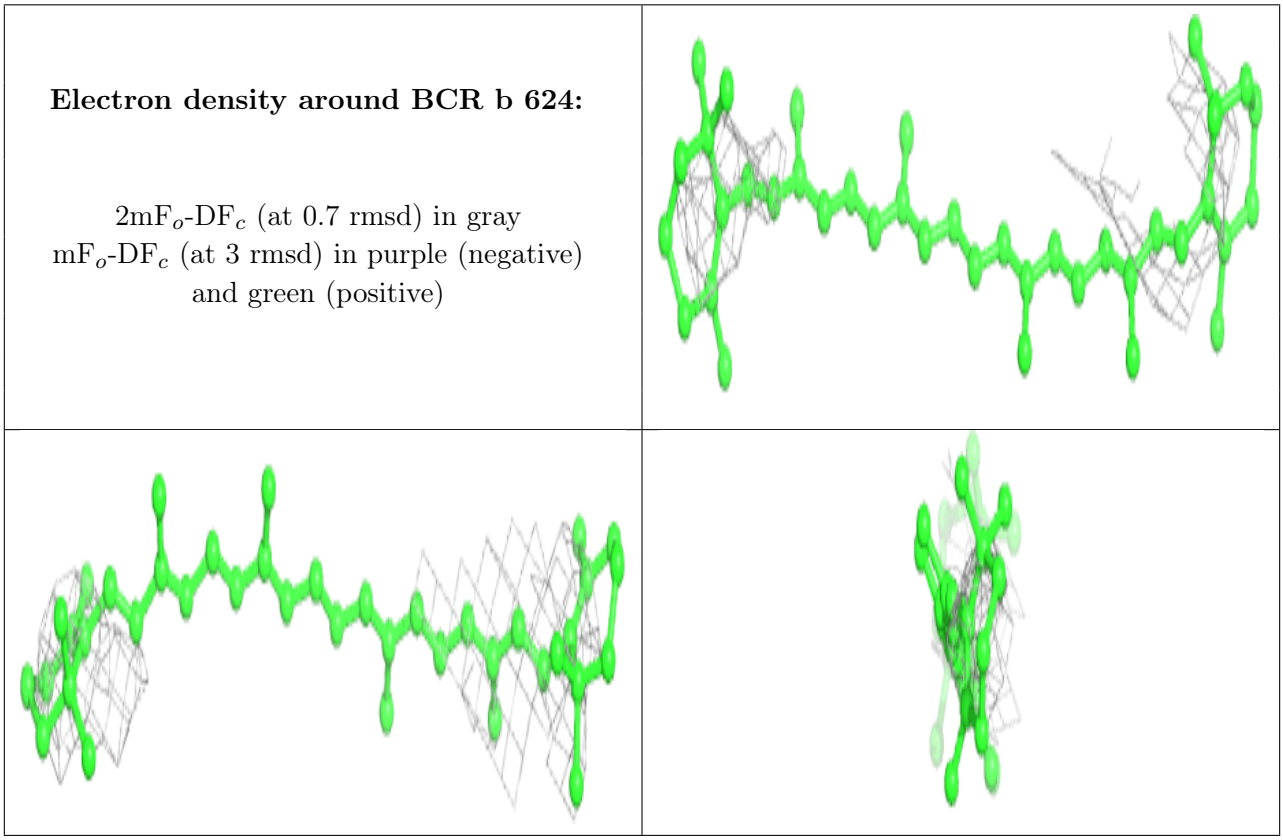
Electron density around DGD A 409:

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



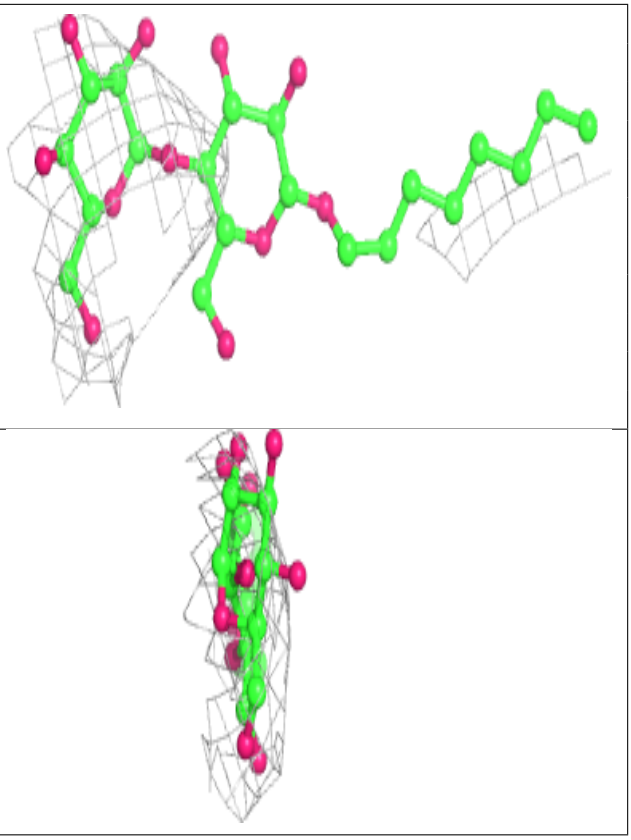
Electron density around BCR b 624:

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



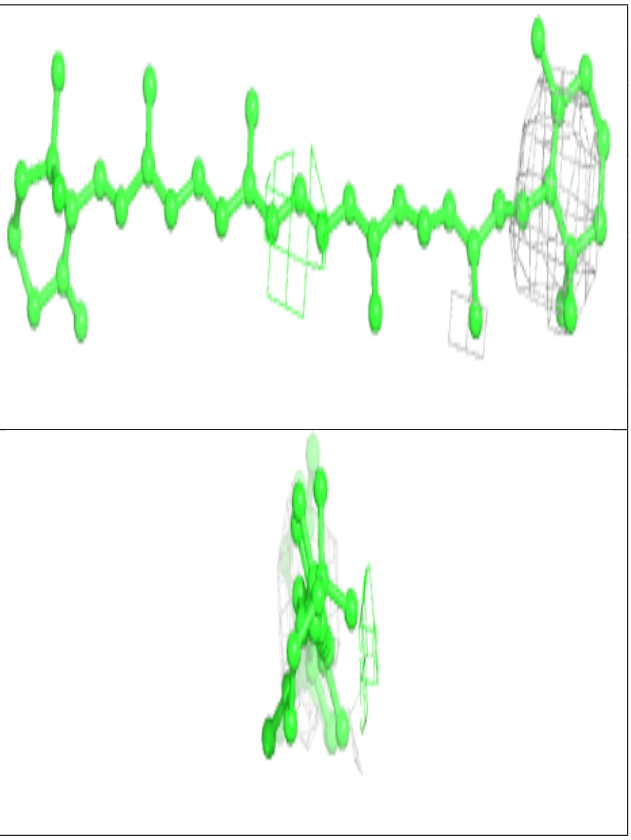
Electron density around LMT d 411:

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



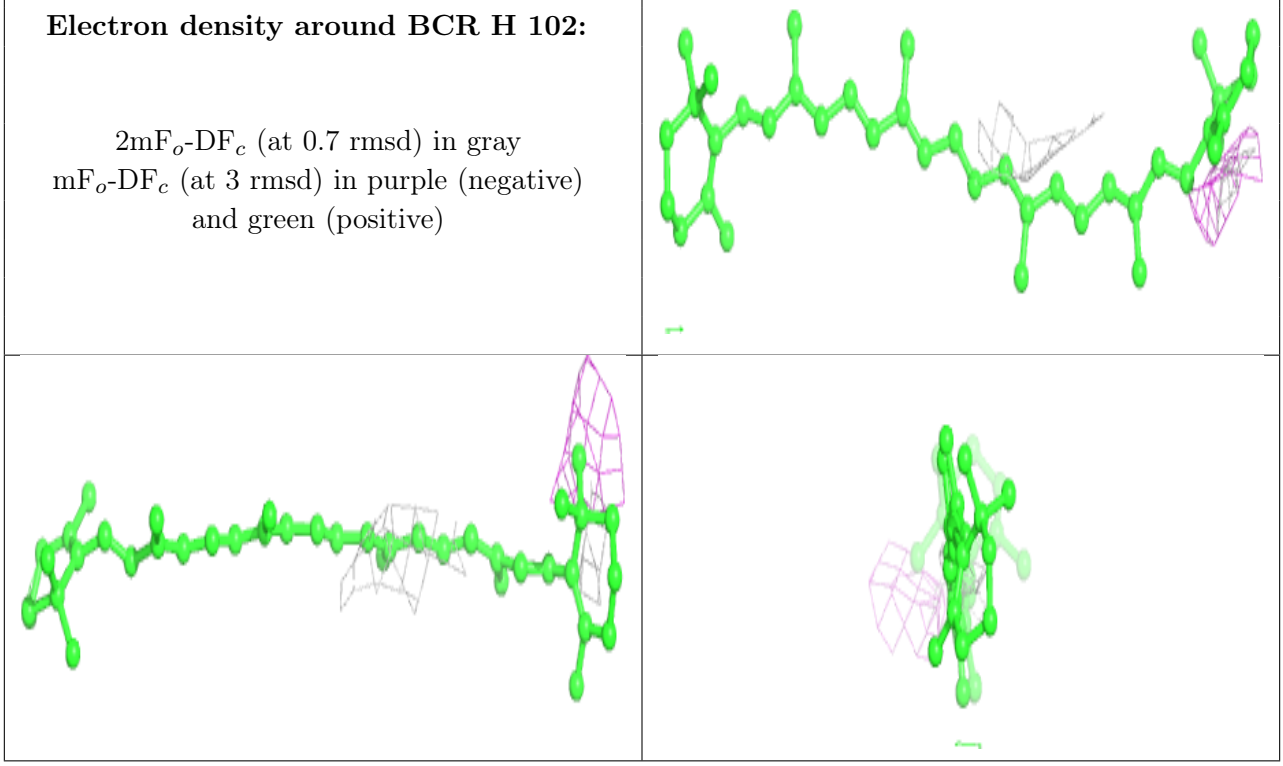
Electron density around BCR J 102:

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



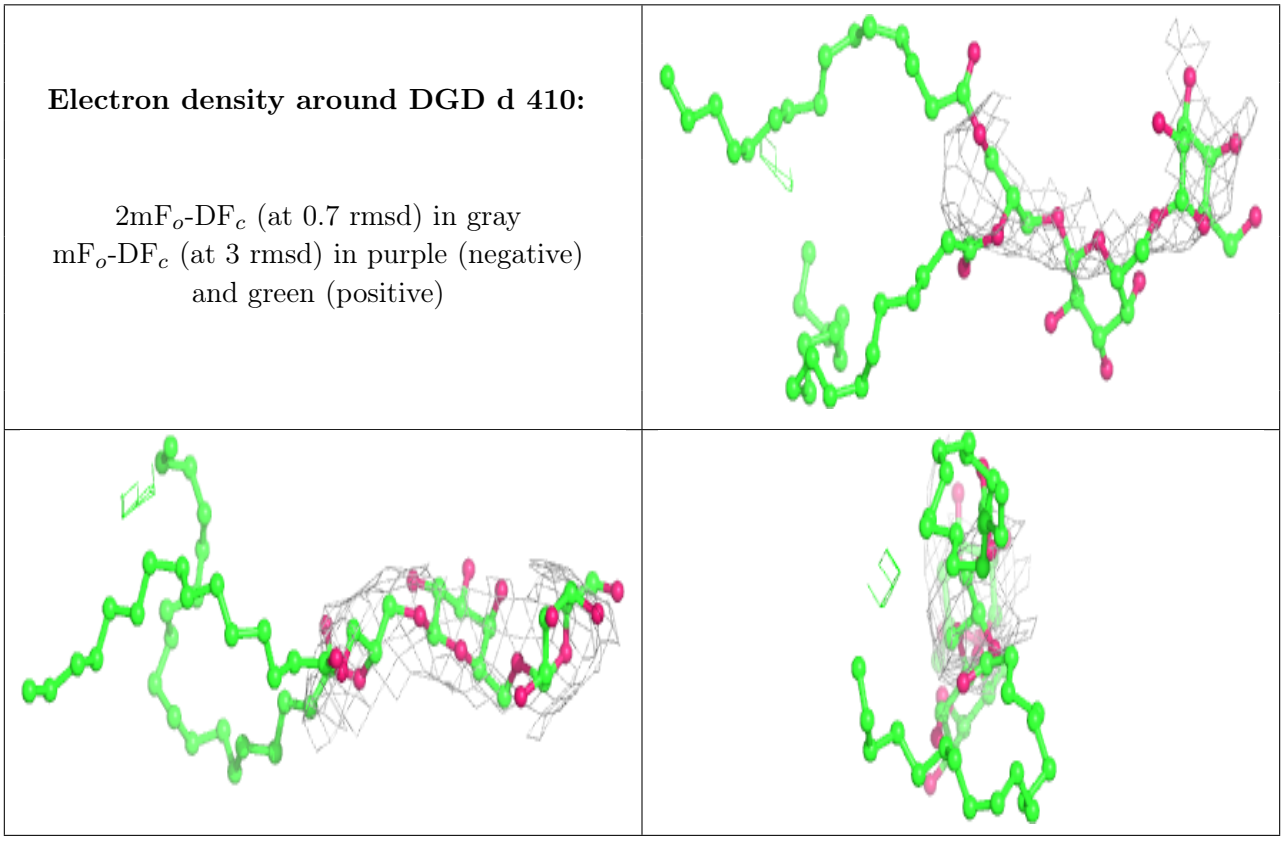
Electron density around BCR H 102:

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



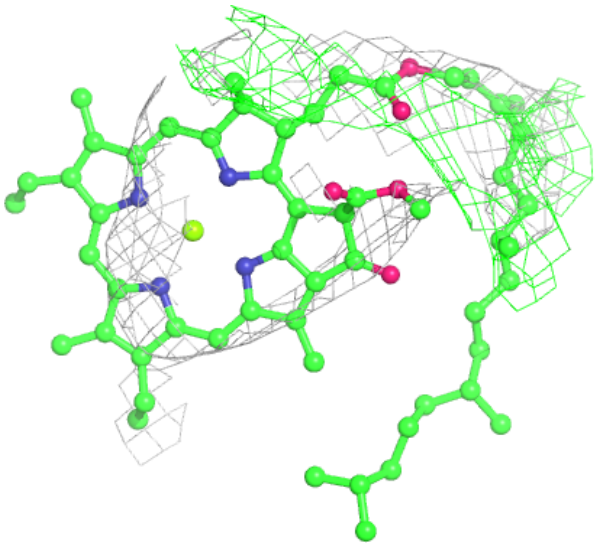
Electron density around DGD d 410:

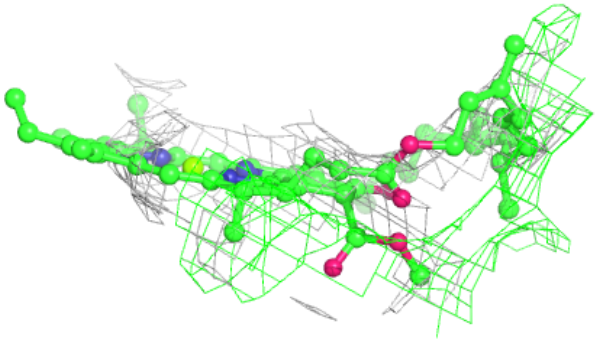
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

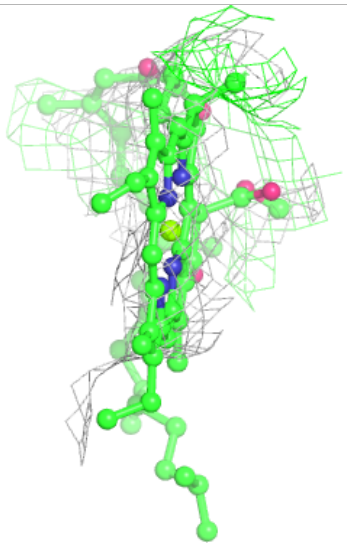


Electron density around CLA B 601:

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

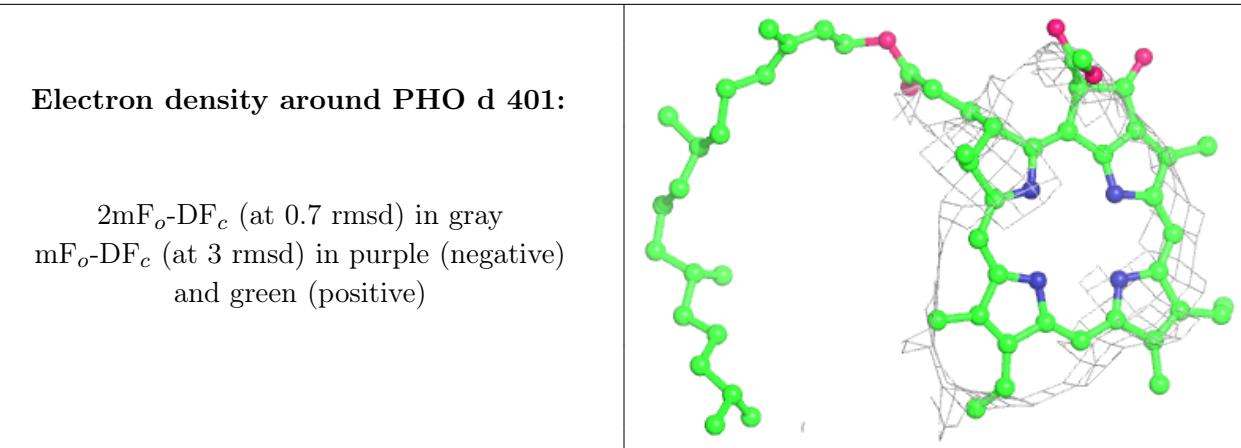






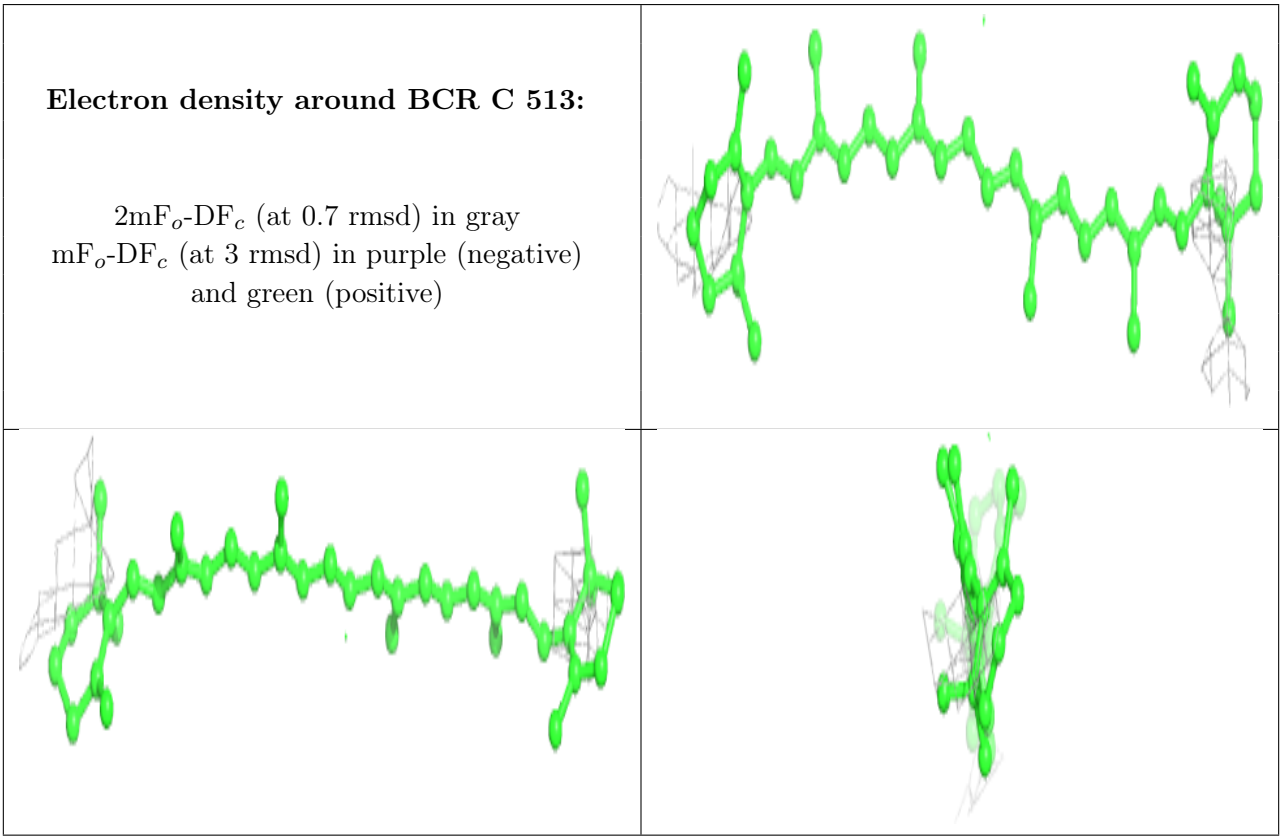
Electron density around PHO d 401:

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



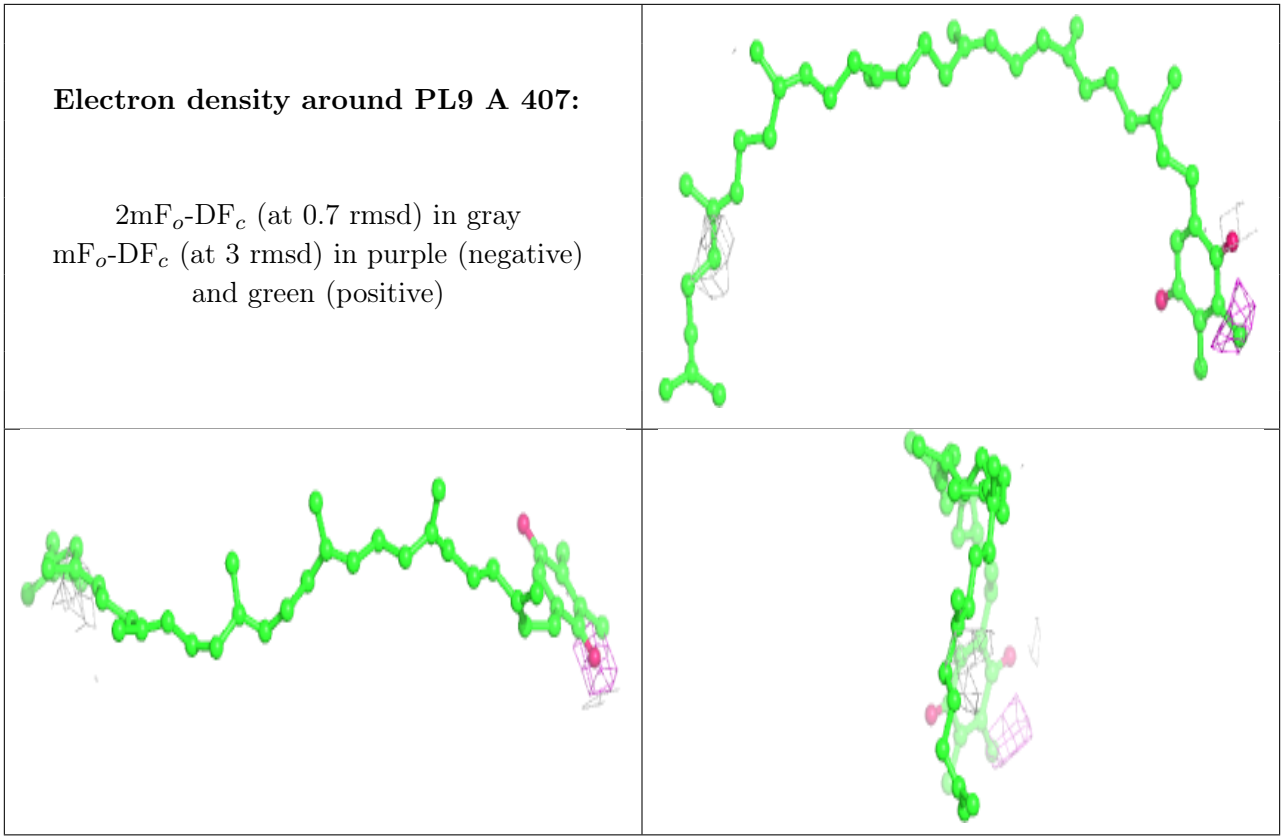
Electron density around BCR C 513:

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



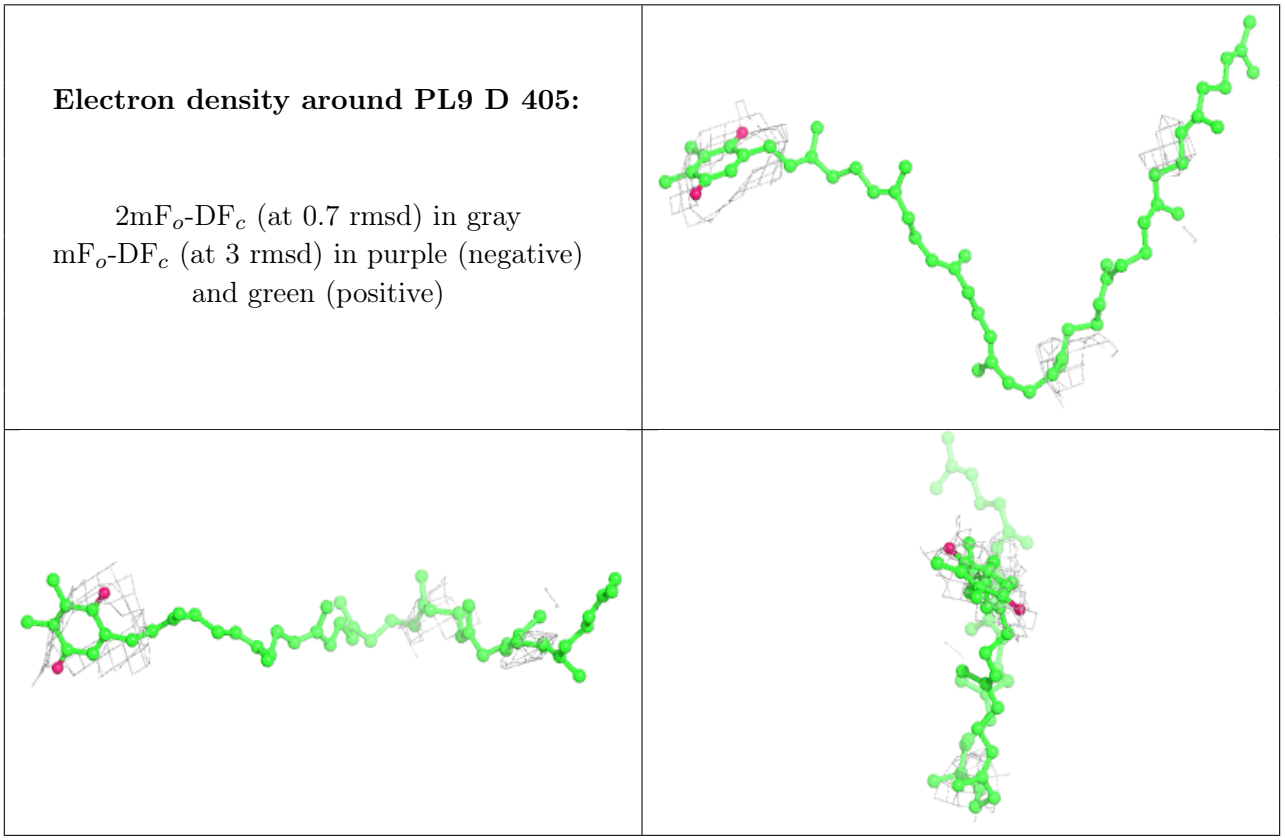
Electron density around PL9 A 407:

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



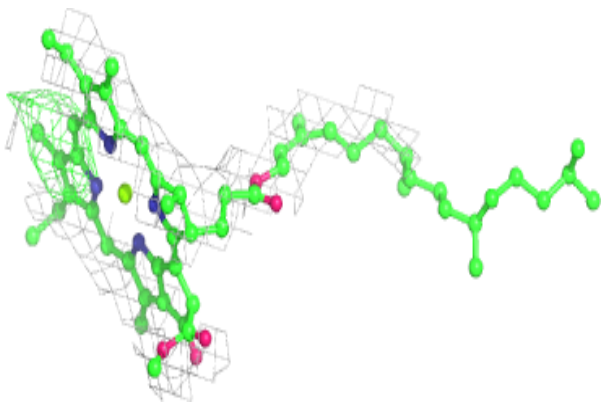
Electron density around PL9 D 405:

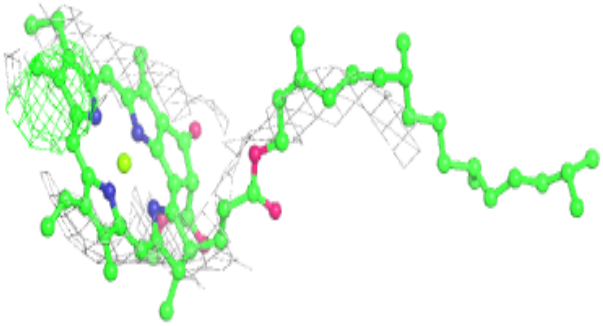
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

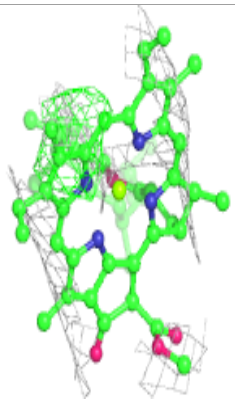


Electron density around CLA C 502:

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

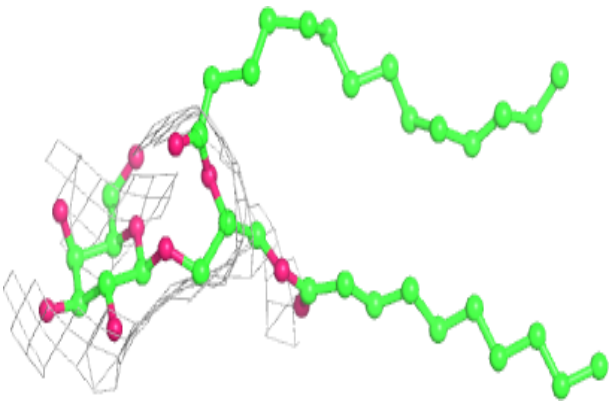


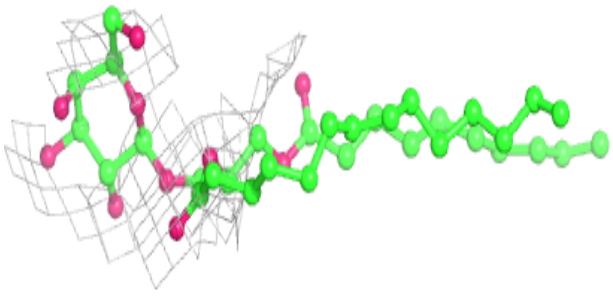


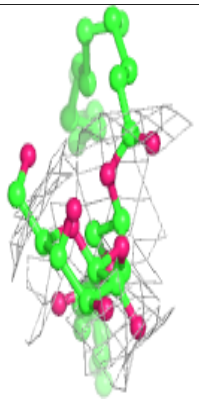


Electron density around LMG i 102:

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

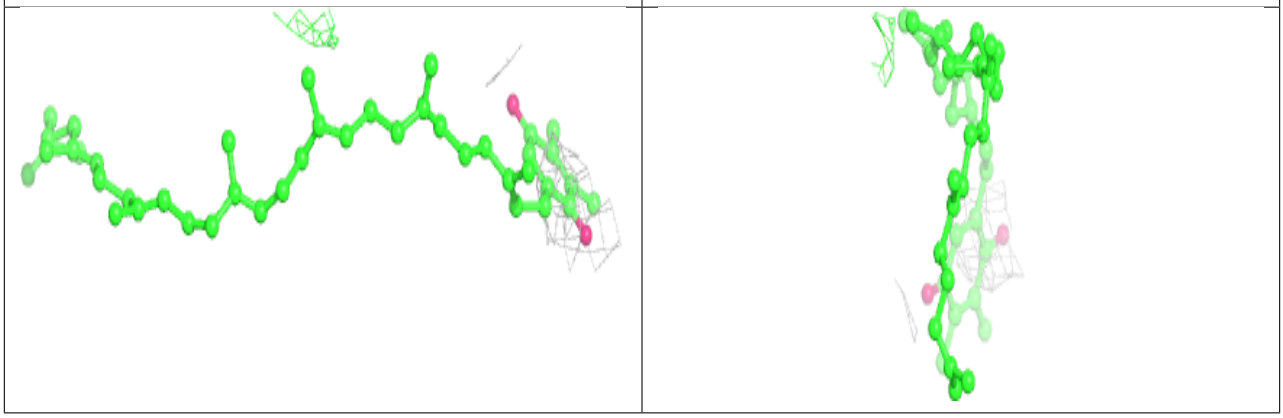






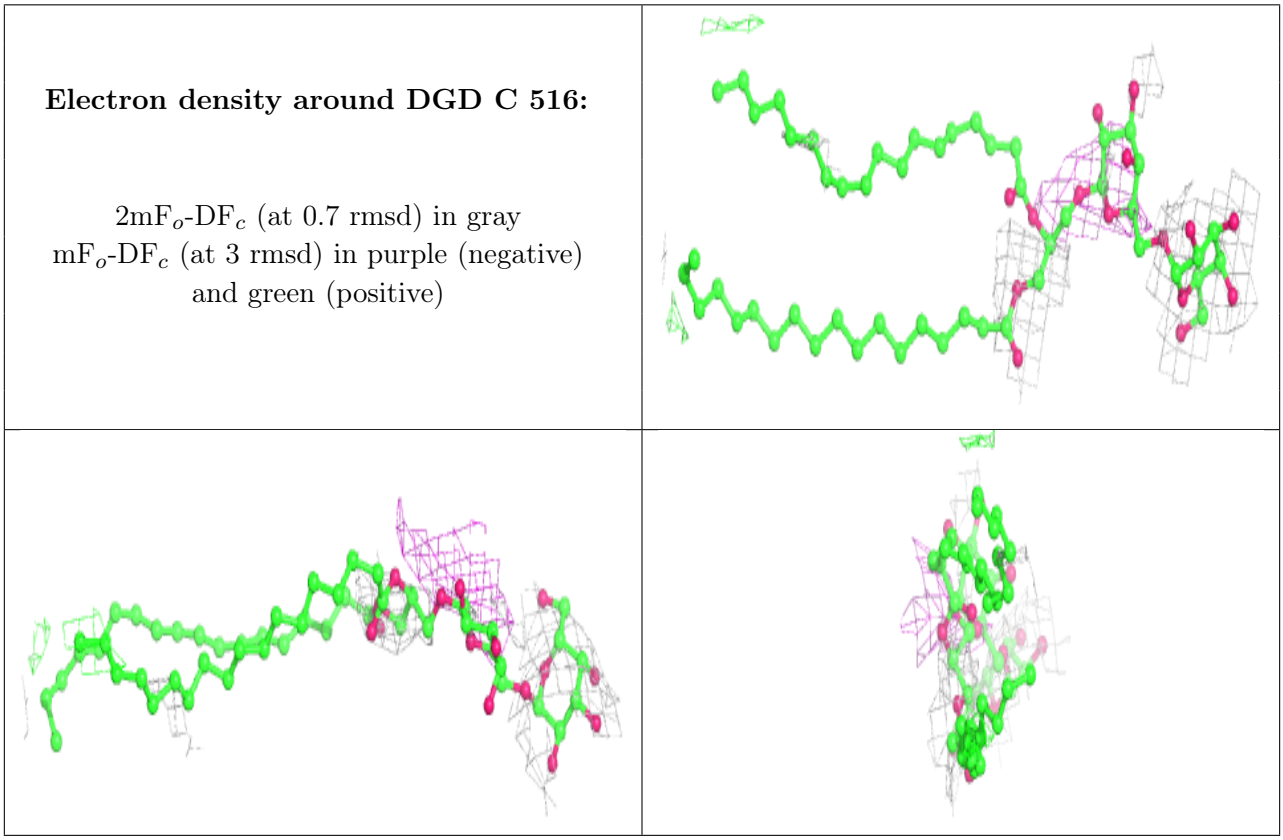
Electron density around PL9 a 407:

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



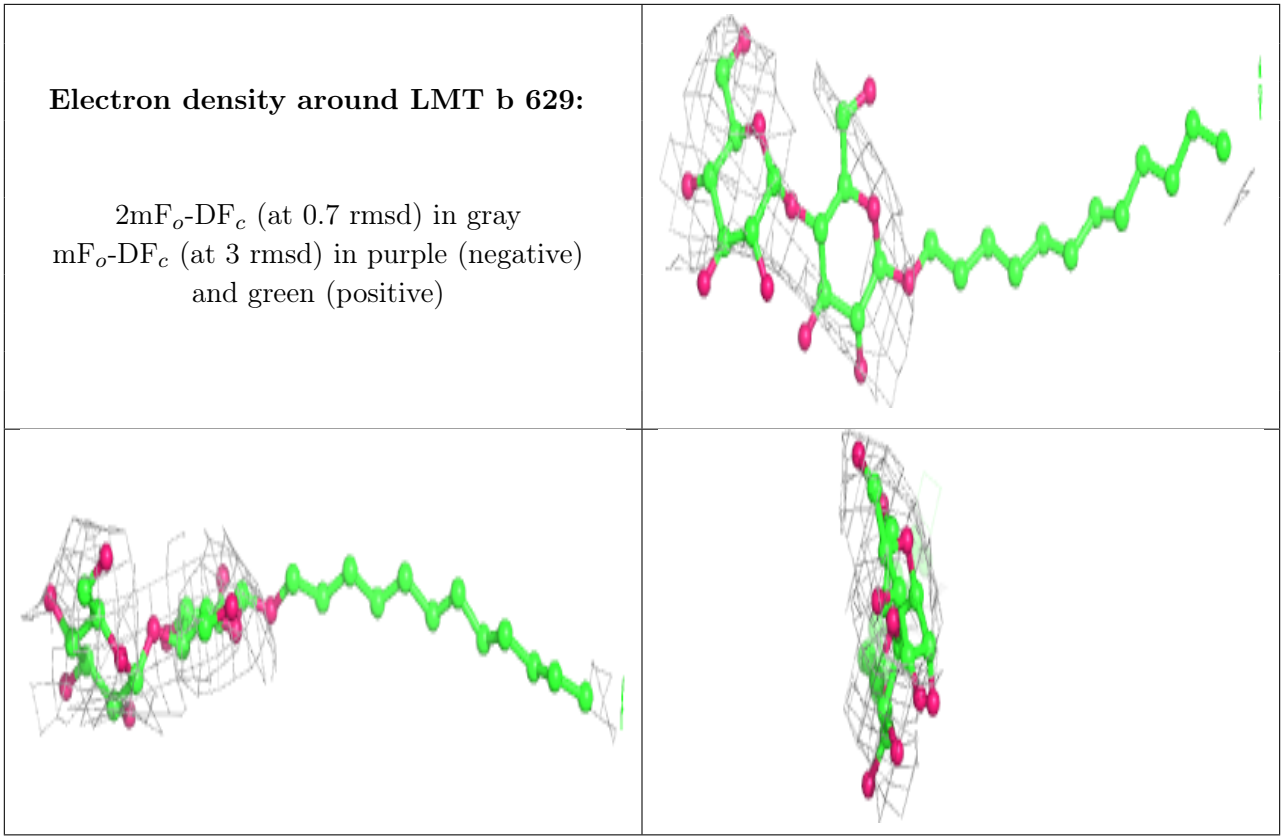
Electron density around DGD C 516:

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



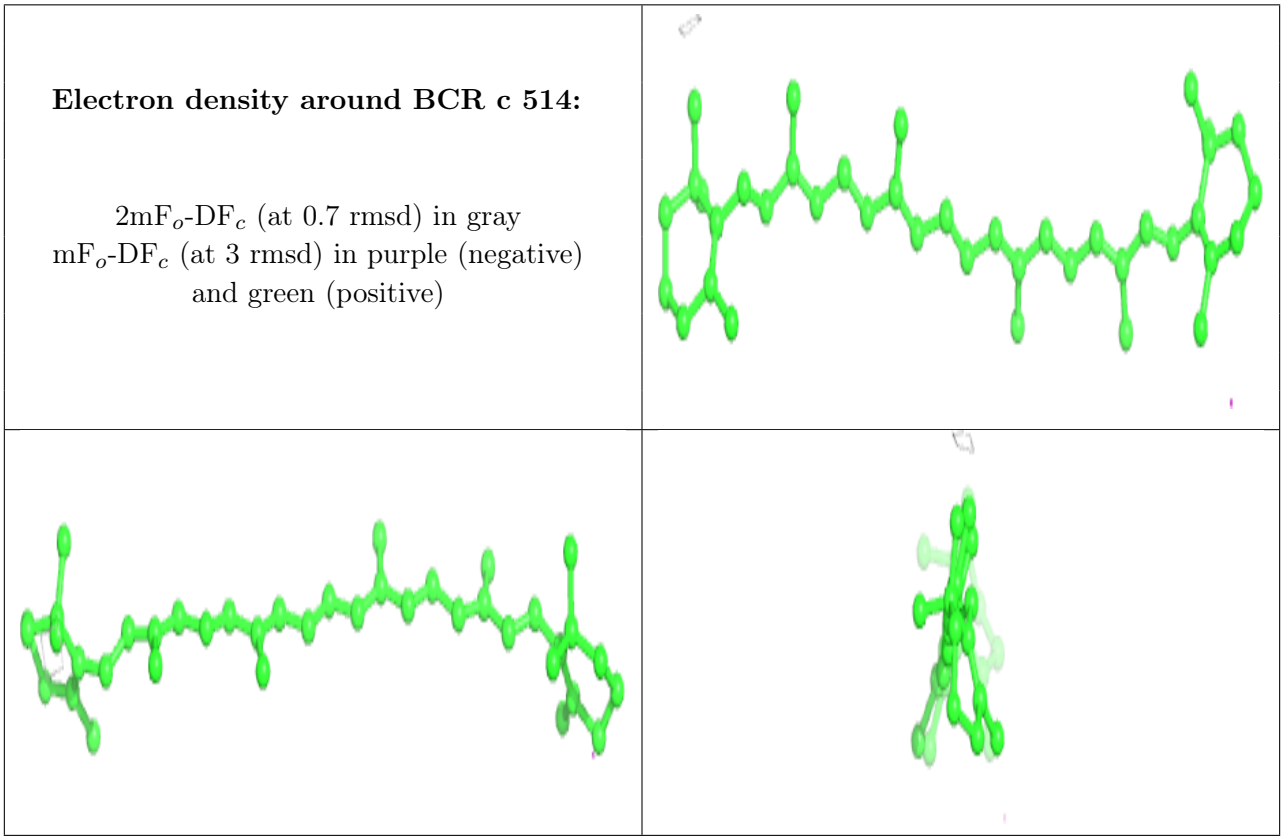
Electron density around LMT b 629:

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



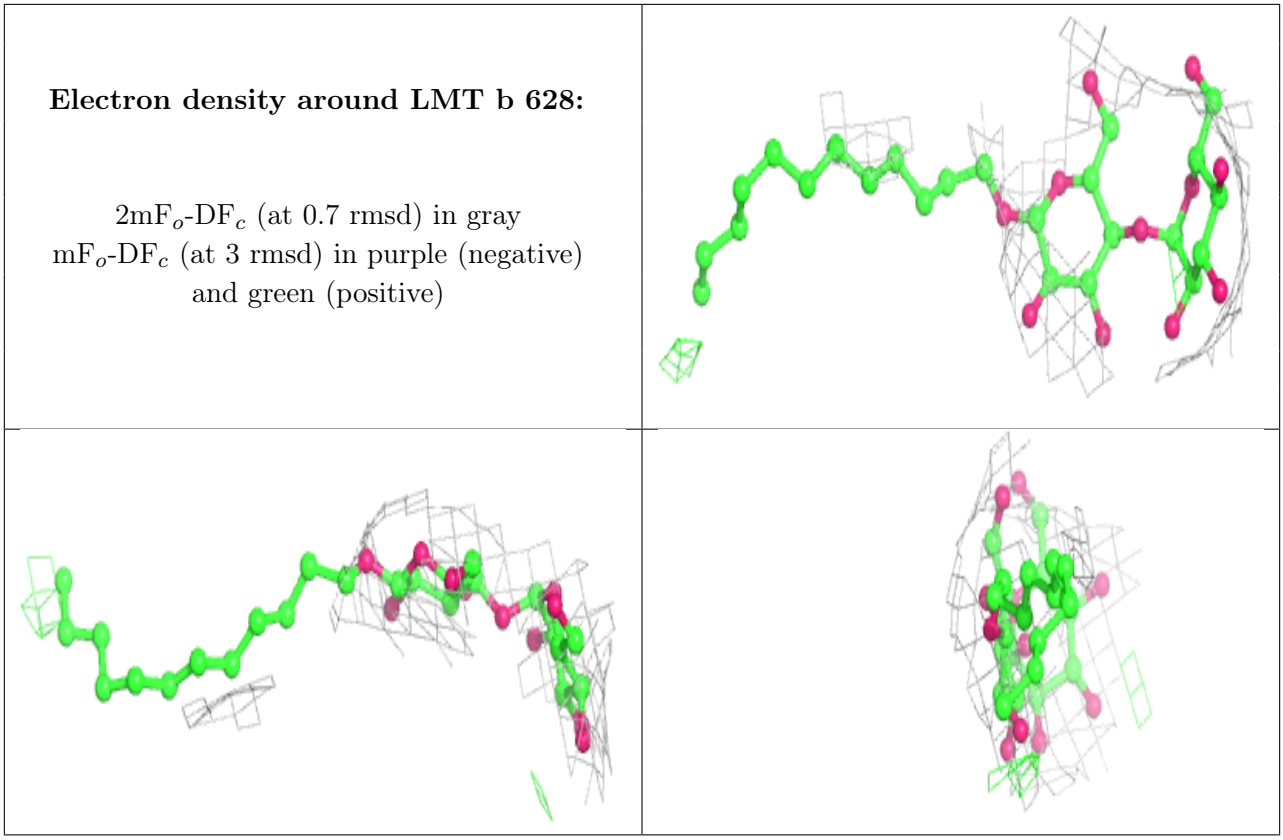
Electron density around BCR c 514:

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



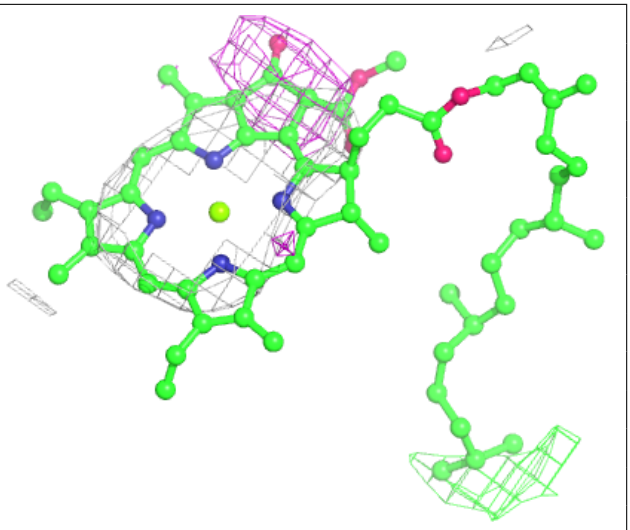
Electron density around LMT b 628:

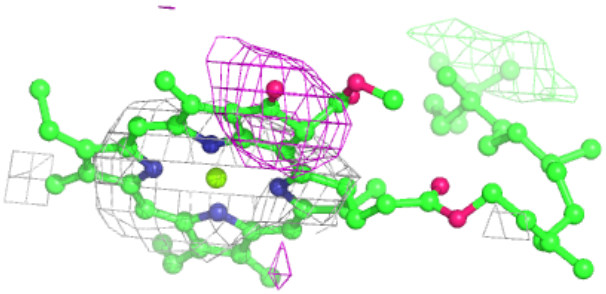
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

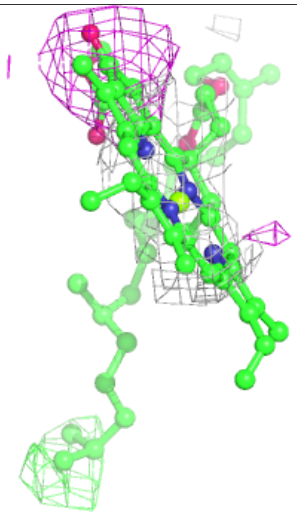


Electron density around CLA b 620:

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

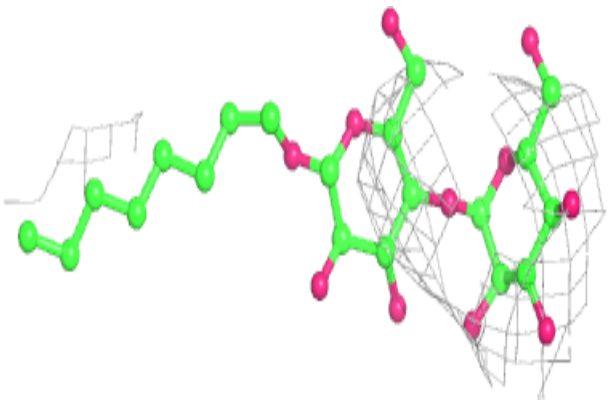


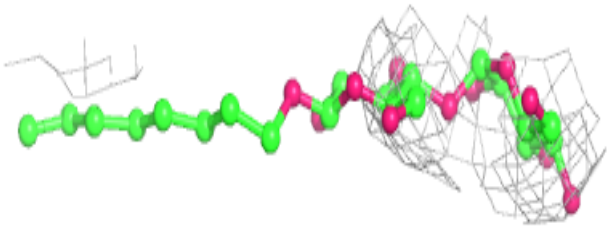


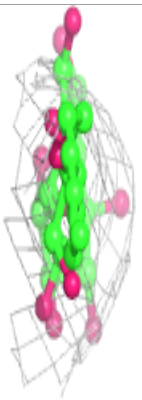


Electron density around LMT D 408:

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

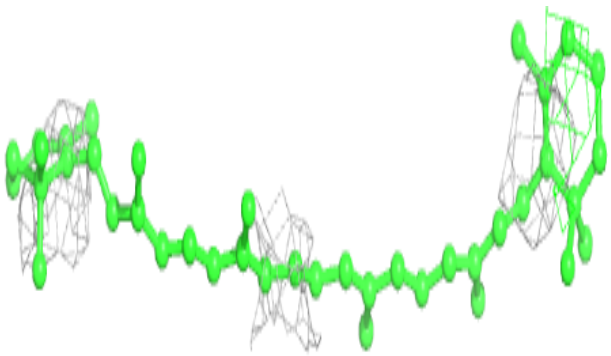


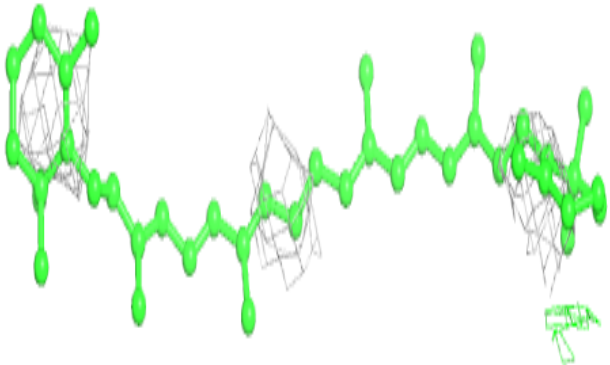


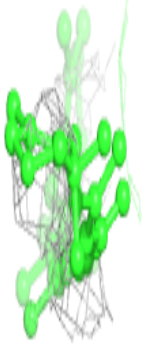


Electron density around BCR f 102:

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

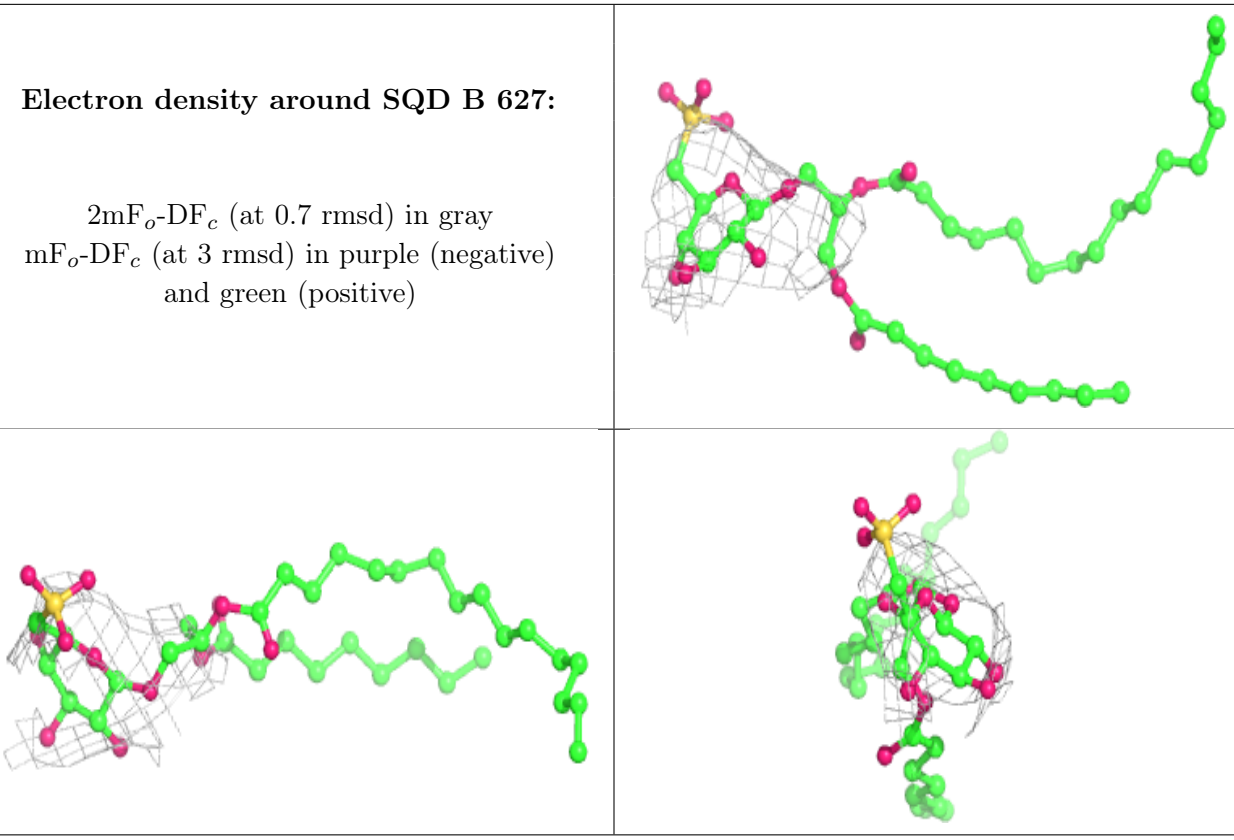






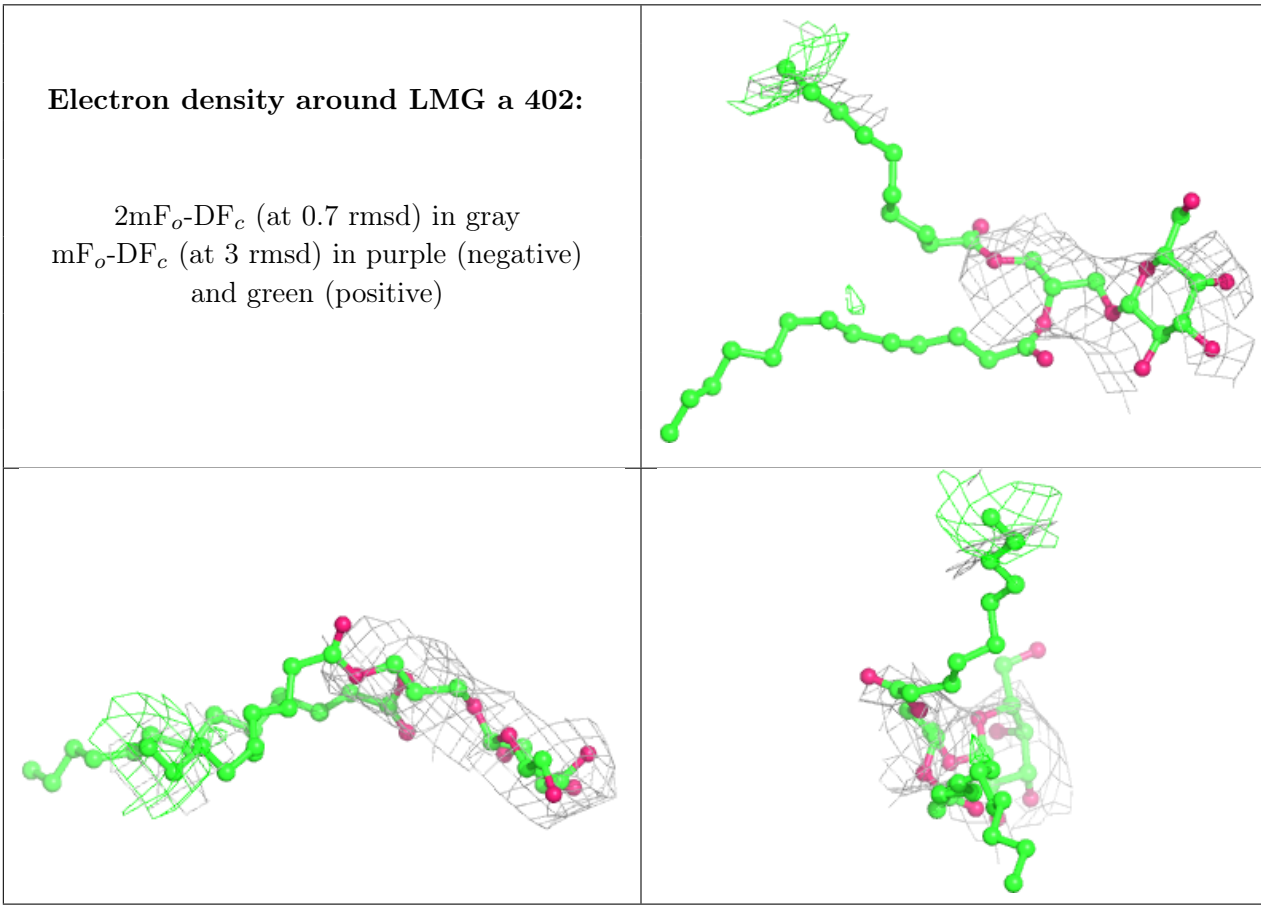
Electron density around SQD B 627:

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



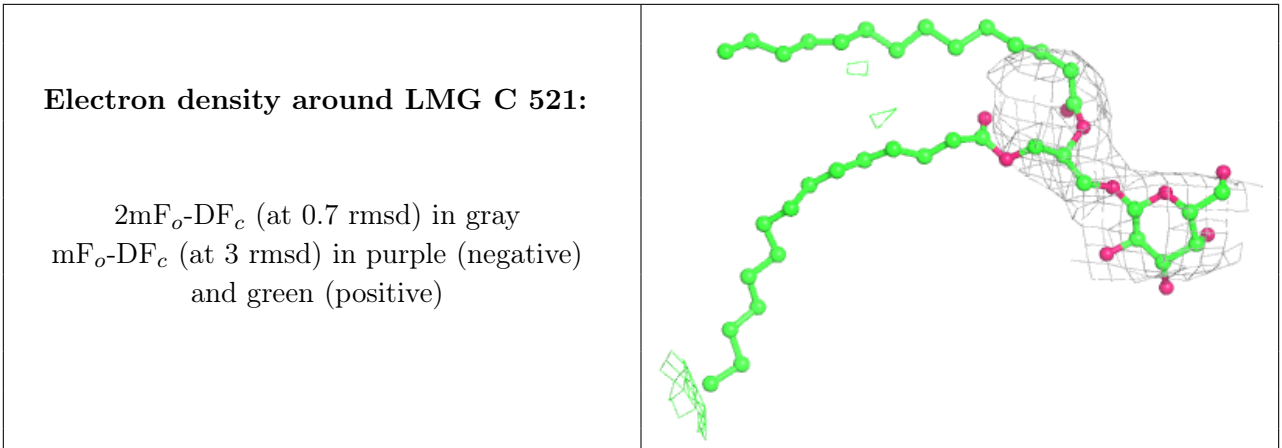
Electron density around LMG a 402:

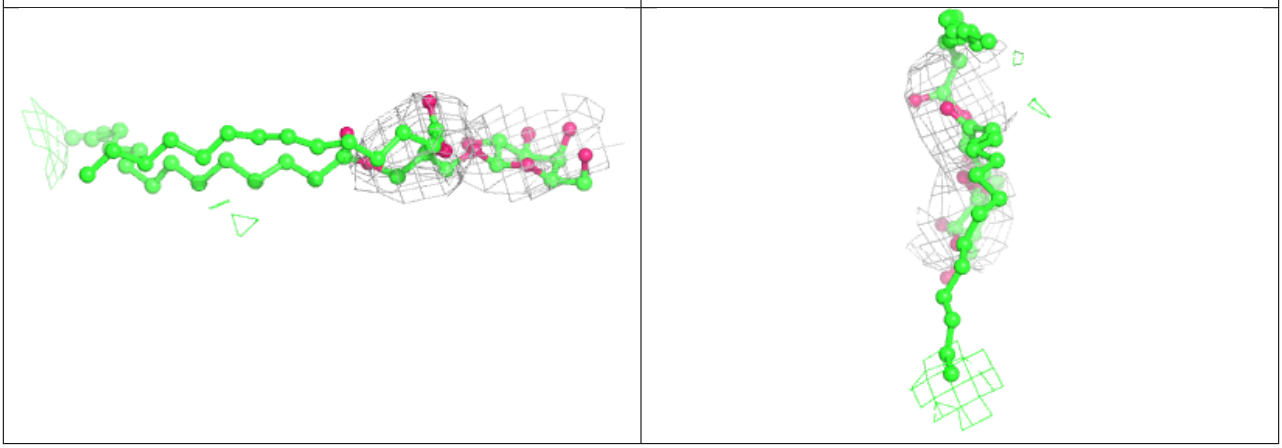
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG C 521:

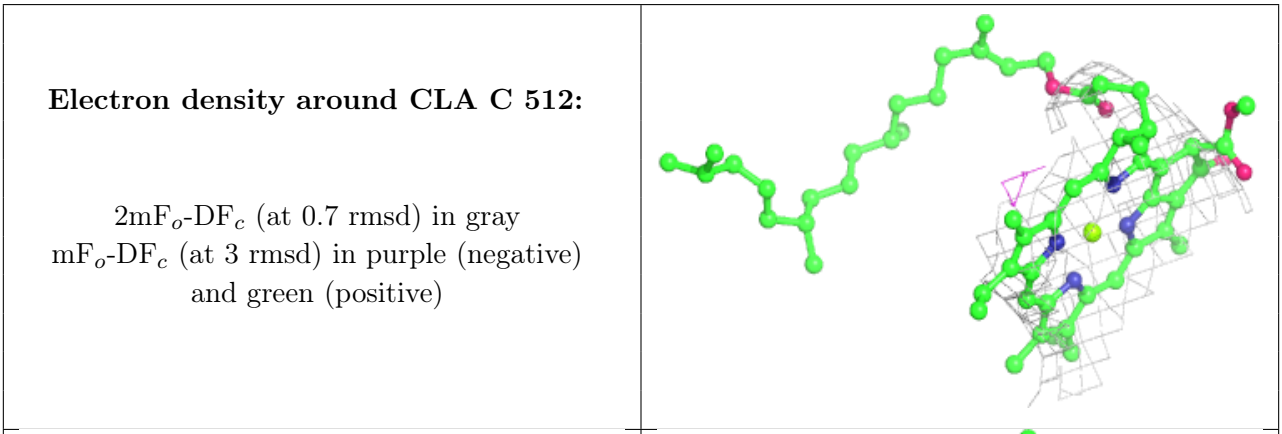
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

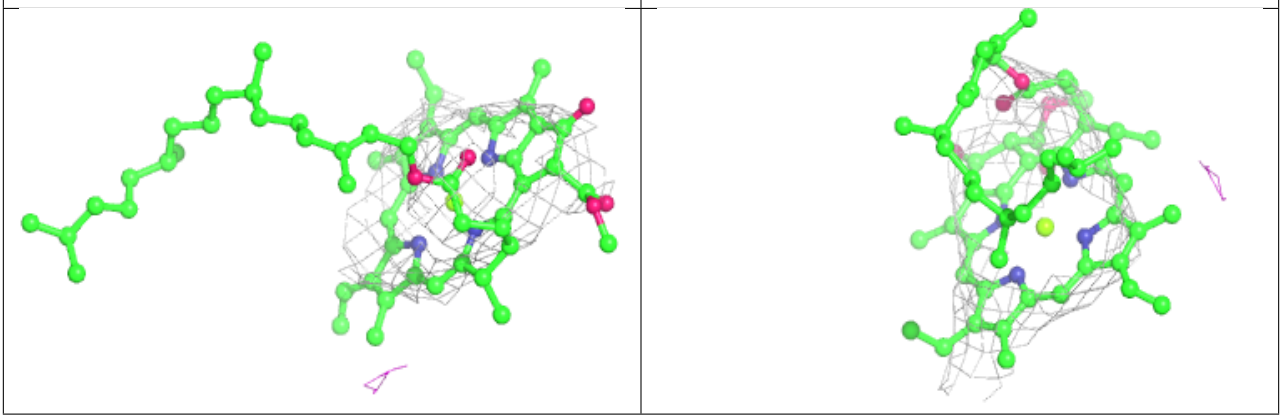




Electron density around CLA C 512:

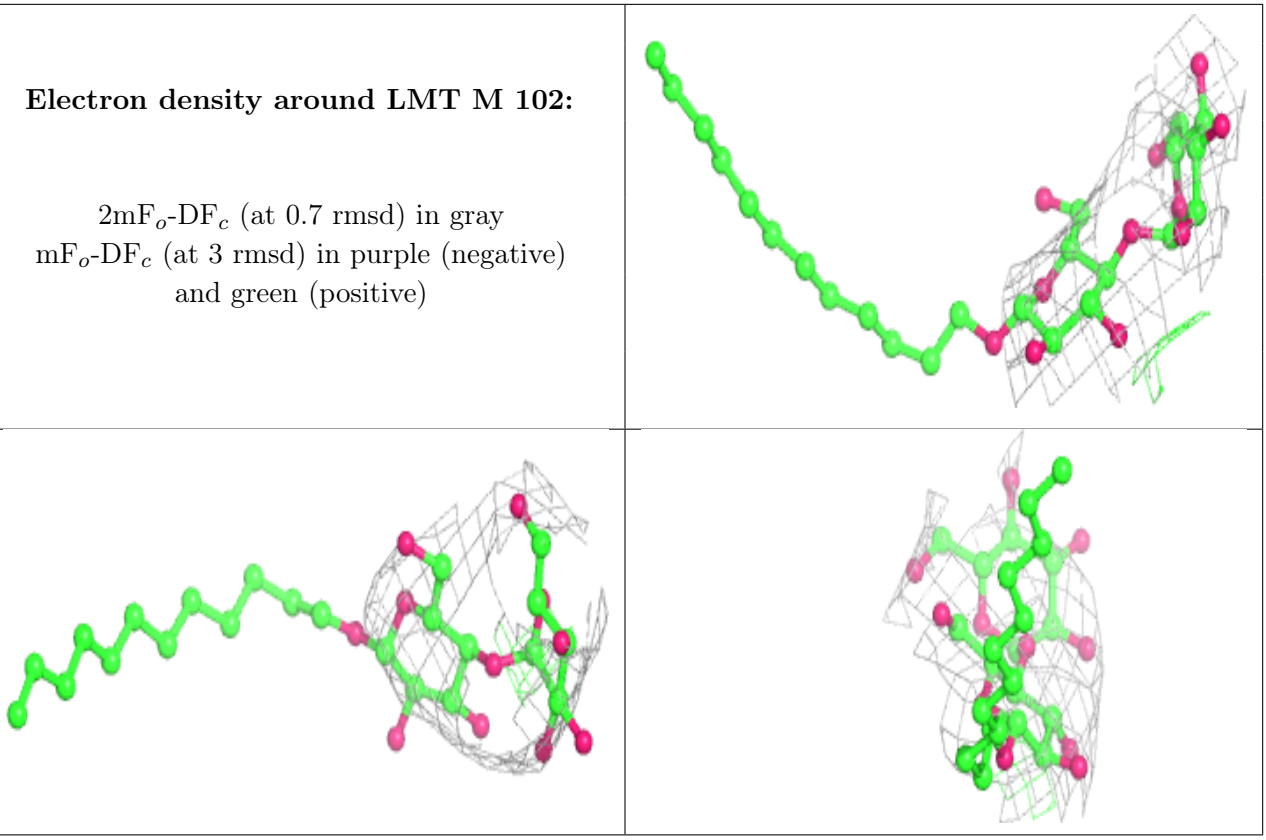
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





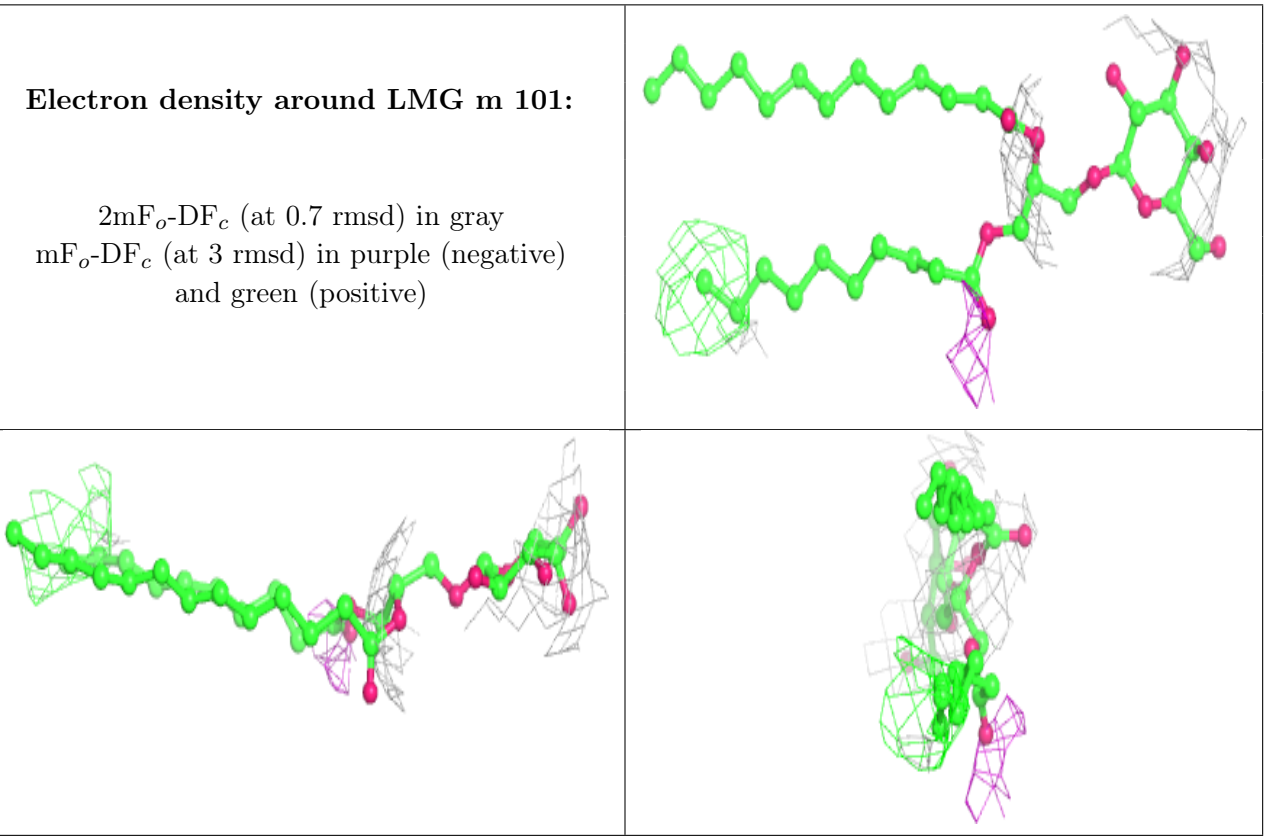
Electron density around LMT M 102:

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



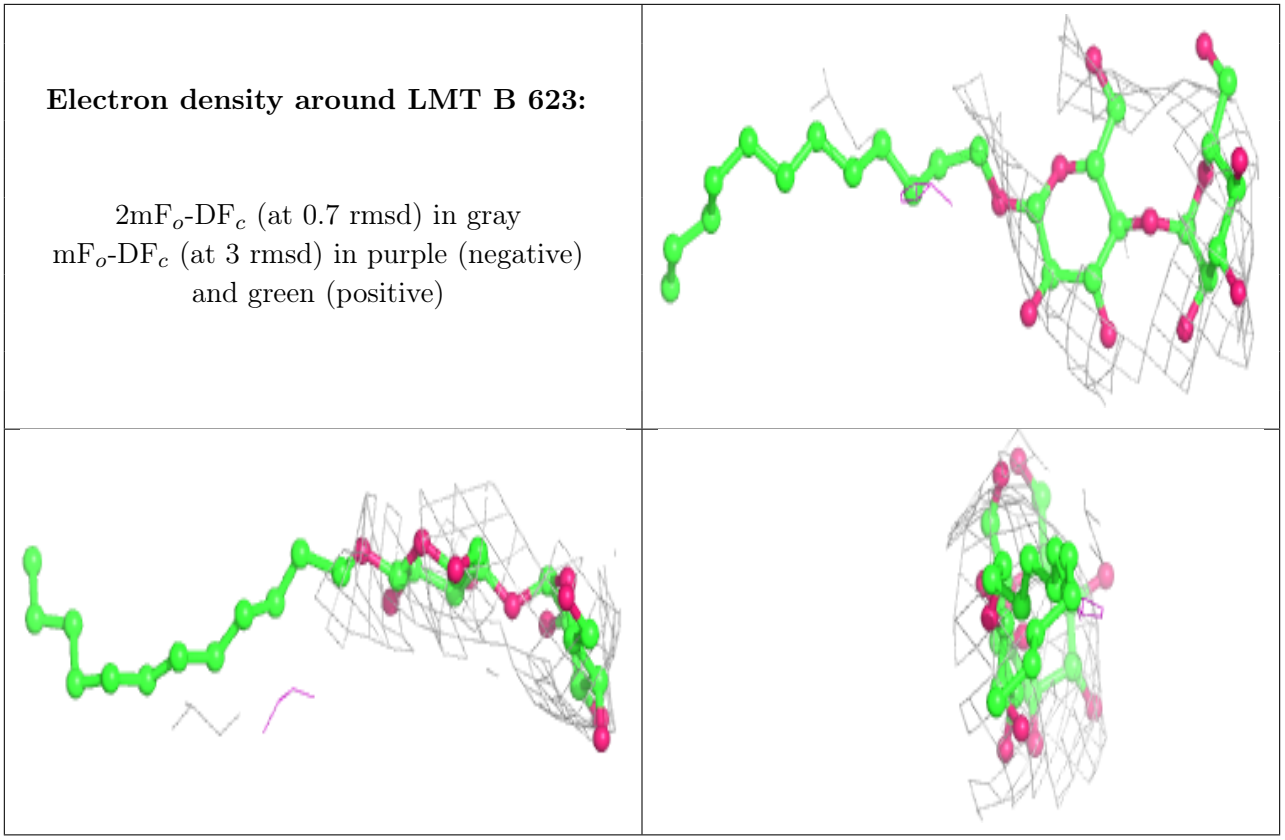
Electron density around LMG m 101:

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



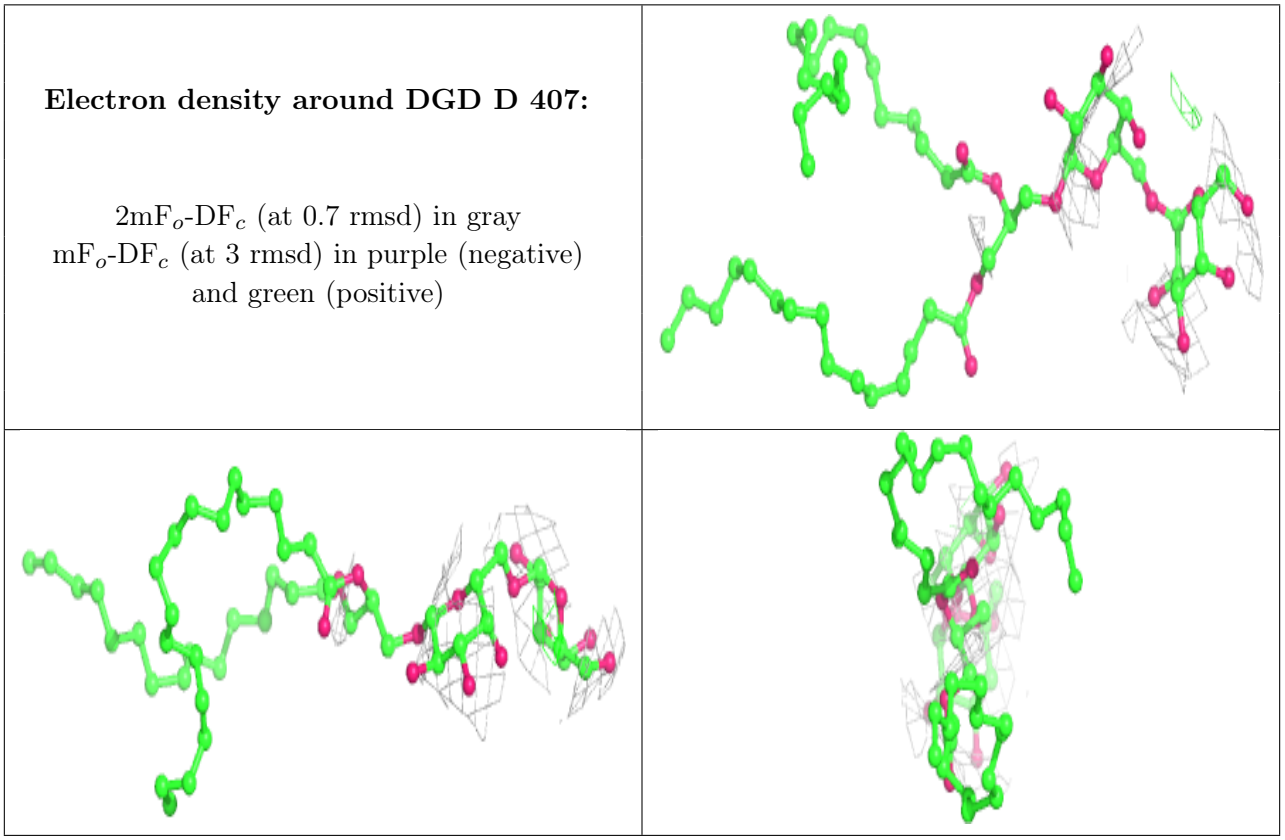
Electron density around LMT B 623:

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



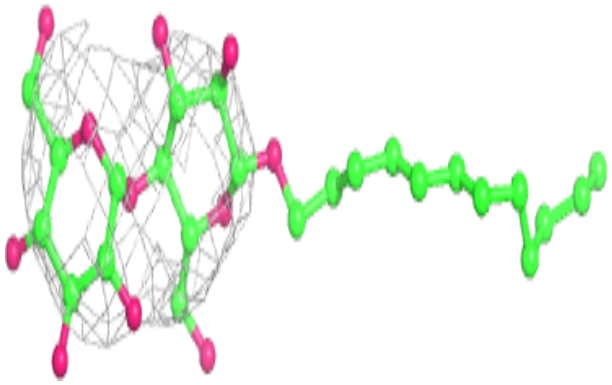
Electron density around DGD D 407:

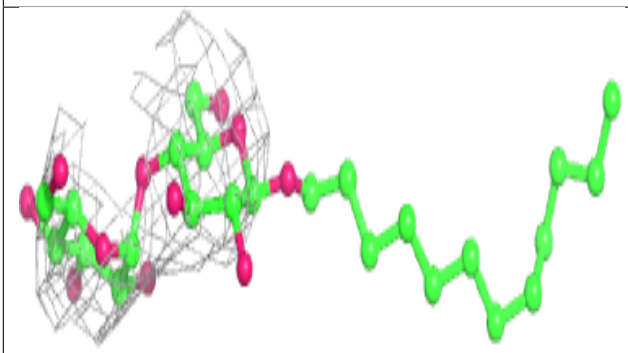
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

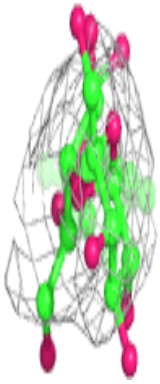


Electron density around LMT b 604:

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

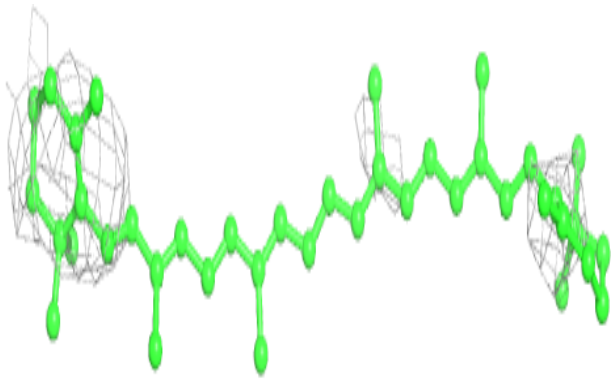


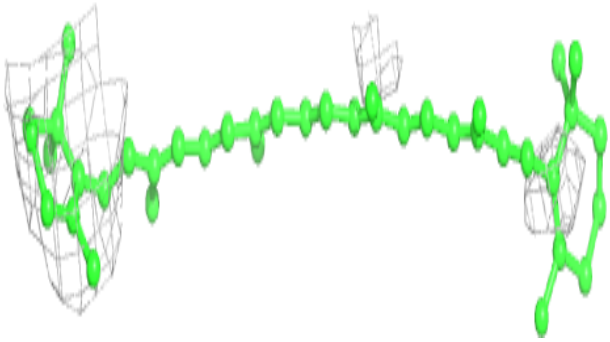


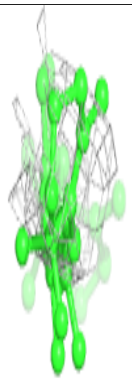


Electron density around BCR B 616:

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

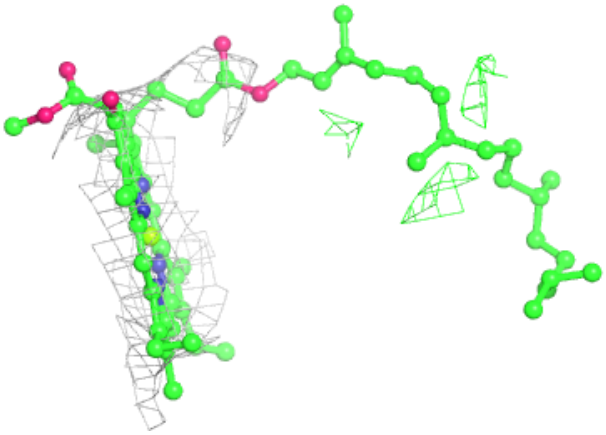


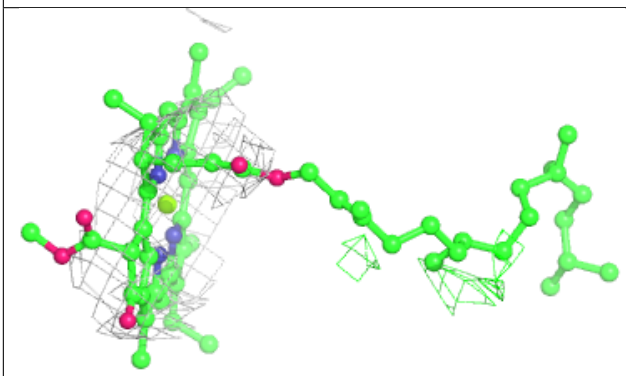


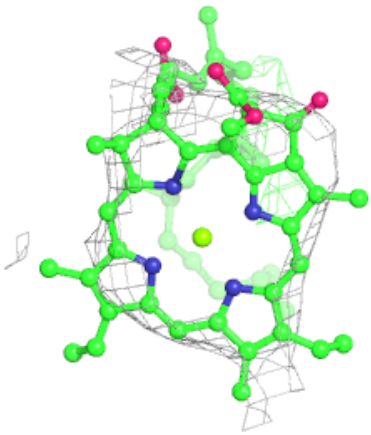


Electron density around CLA C 505:

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

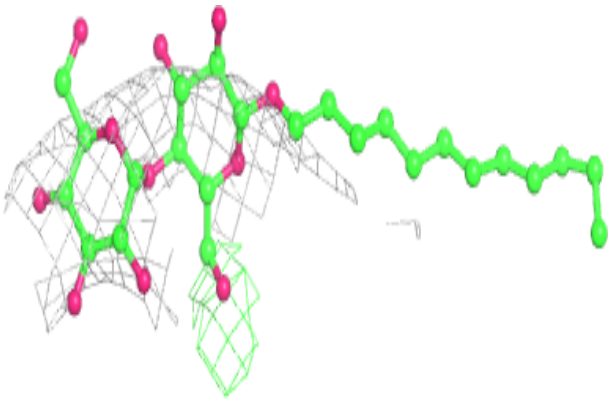


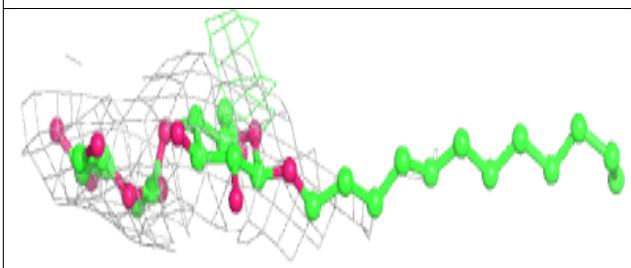


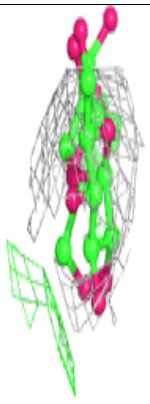


Electron density around LMT b 603:

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

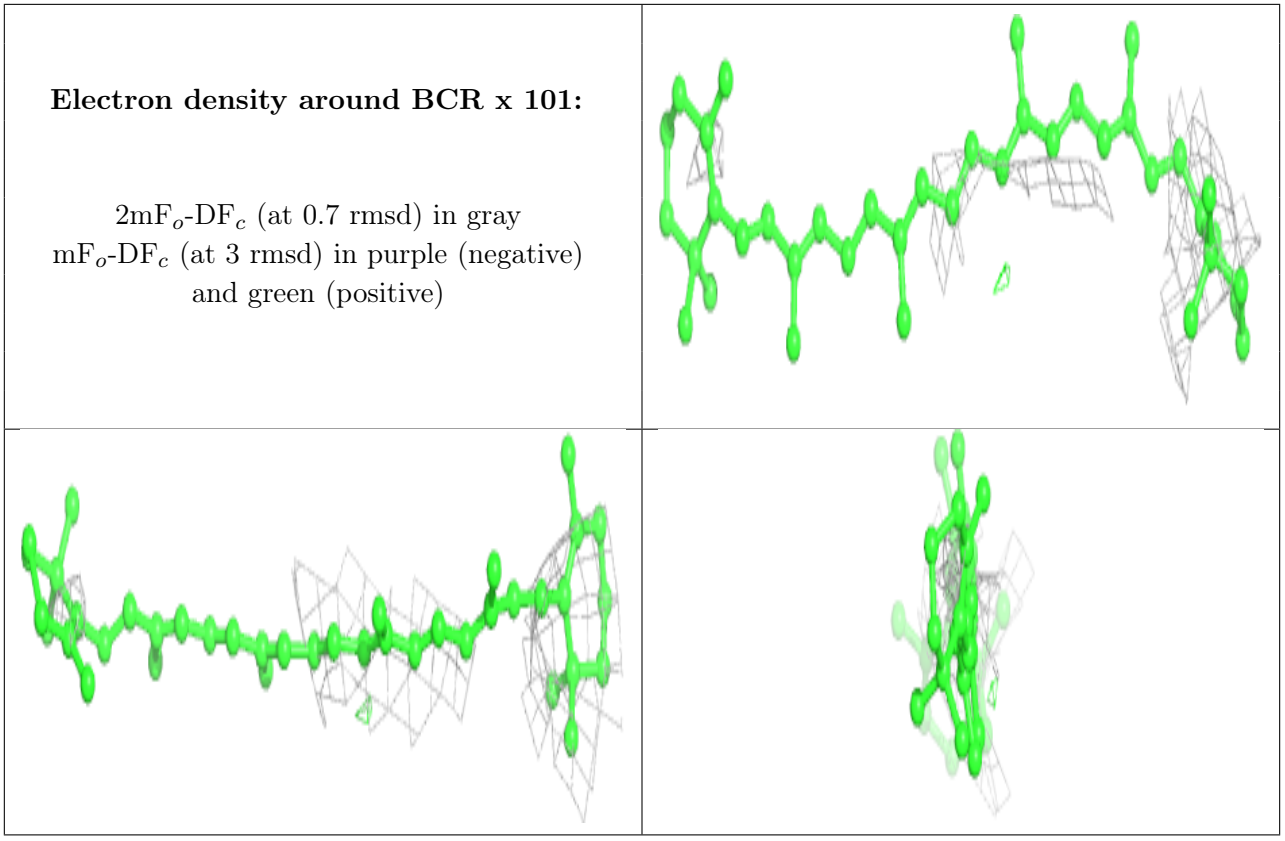






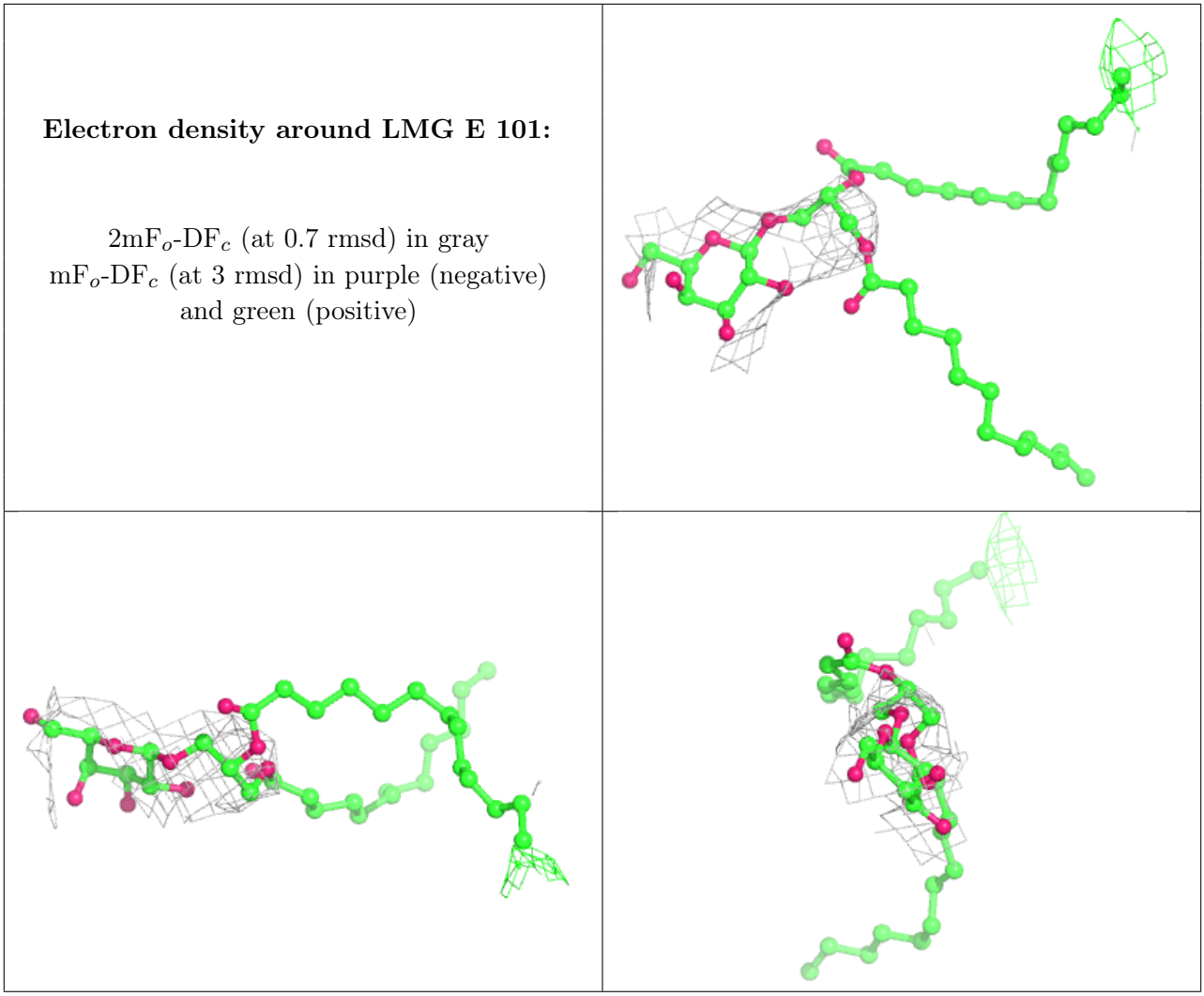
Electron density around BCR x 101:

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



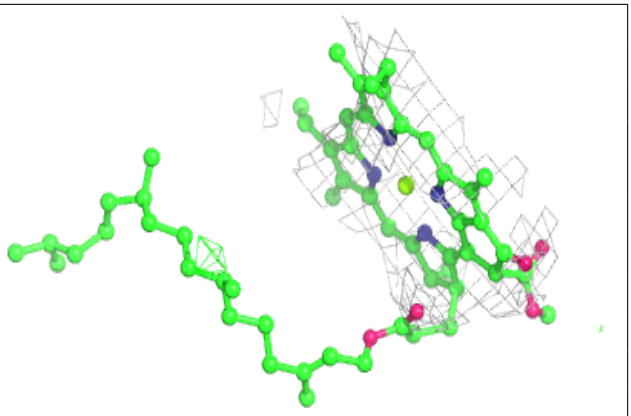
Electron density around LMG E 101:

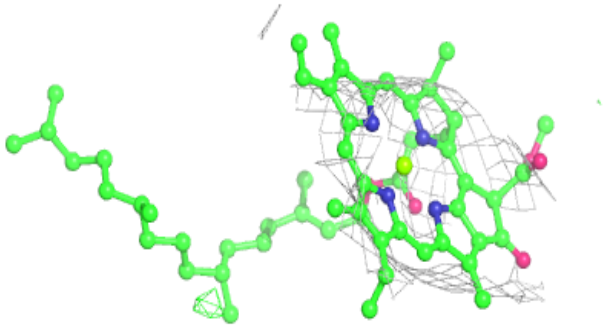
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

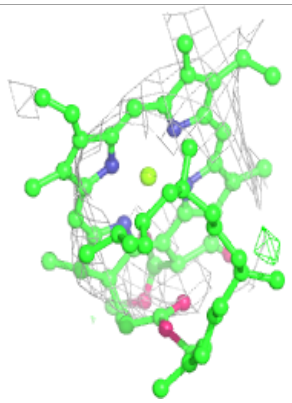


Electron density around CLA c 512:

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

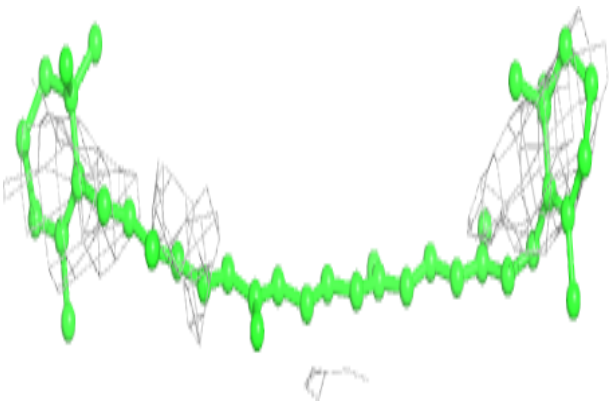


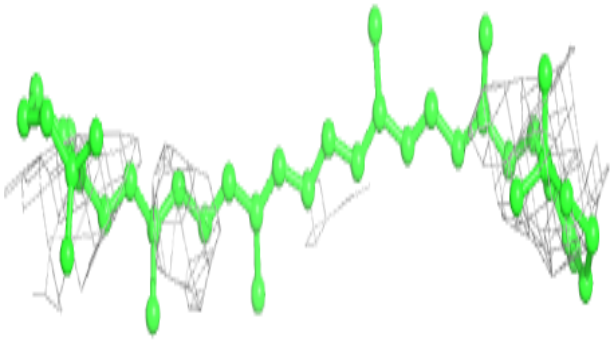




Electron density around BCR c 513:

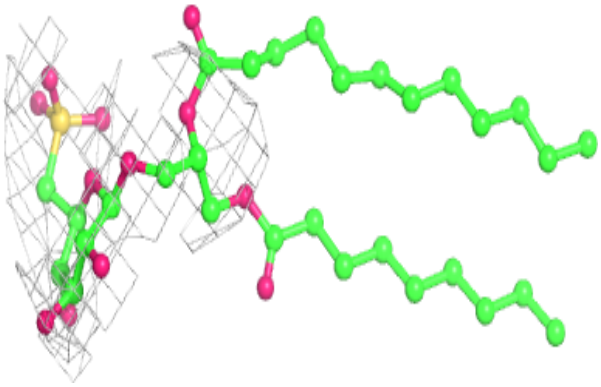
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

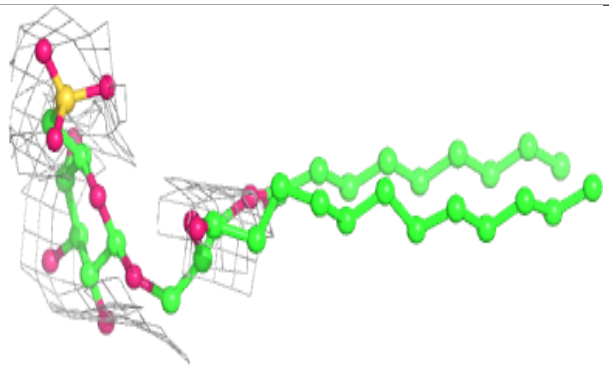


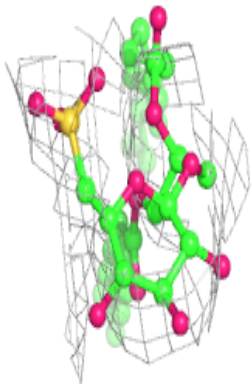


Electron density around SQD d 403:

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

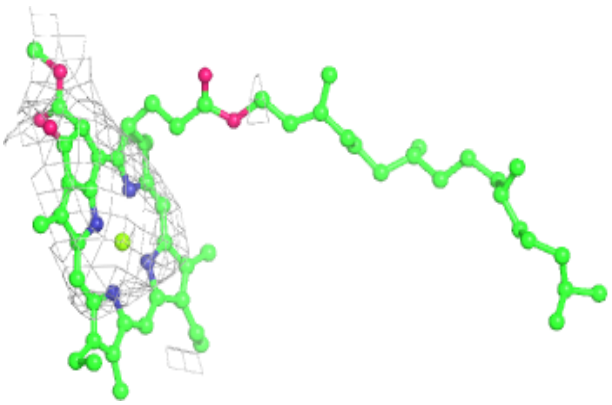


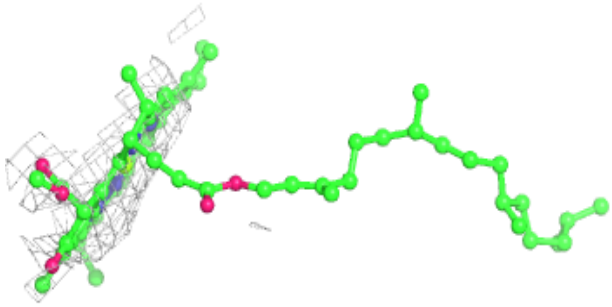


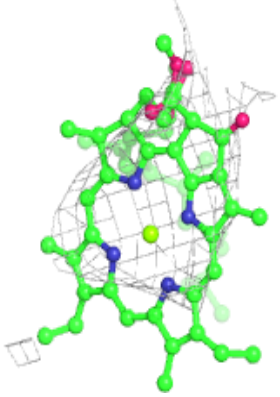


Electron density around CLA a 406:

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

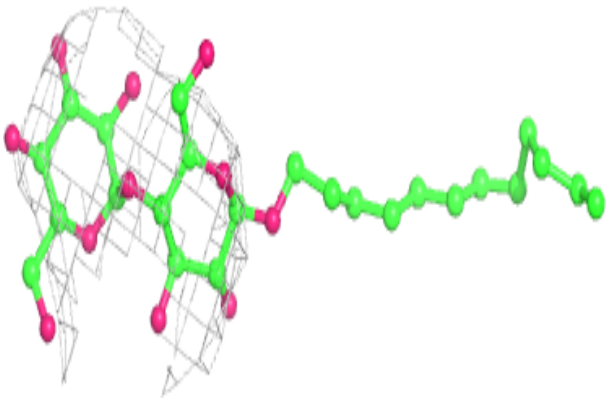


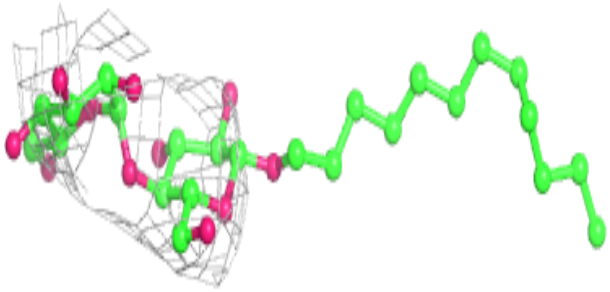


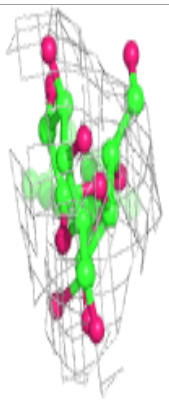


Electron density around LMT B 629:

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

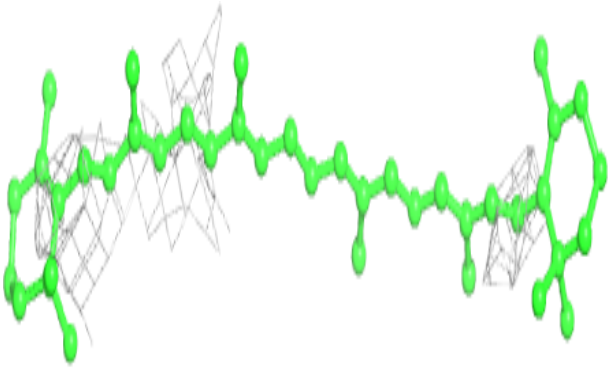


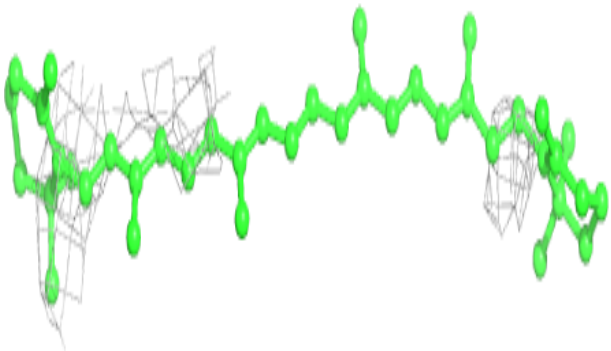


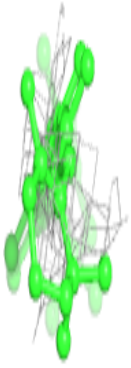


Electron density around BCR B 619:

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

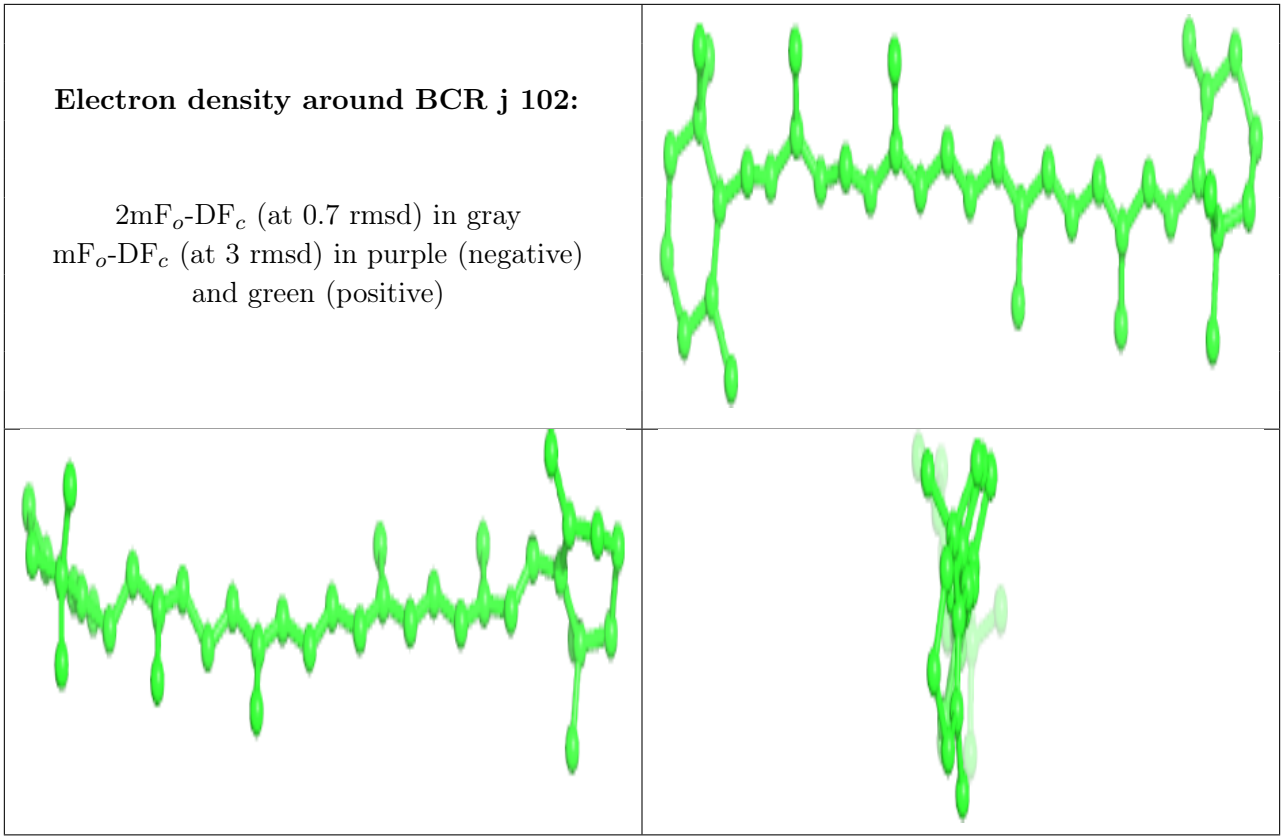






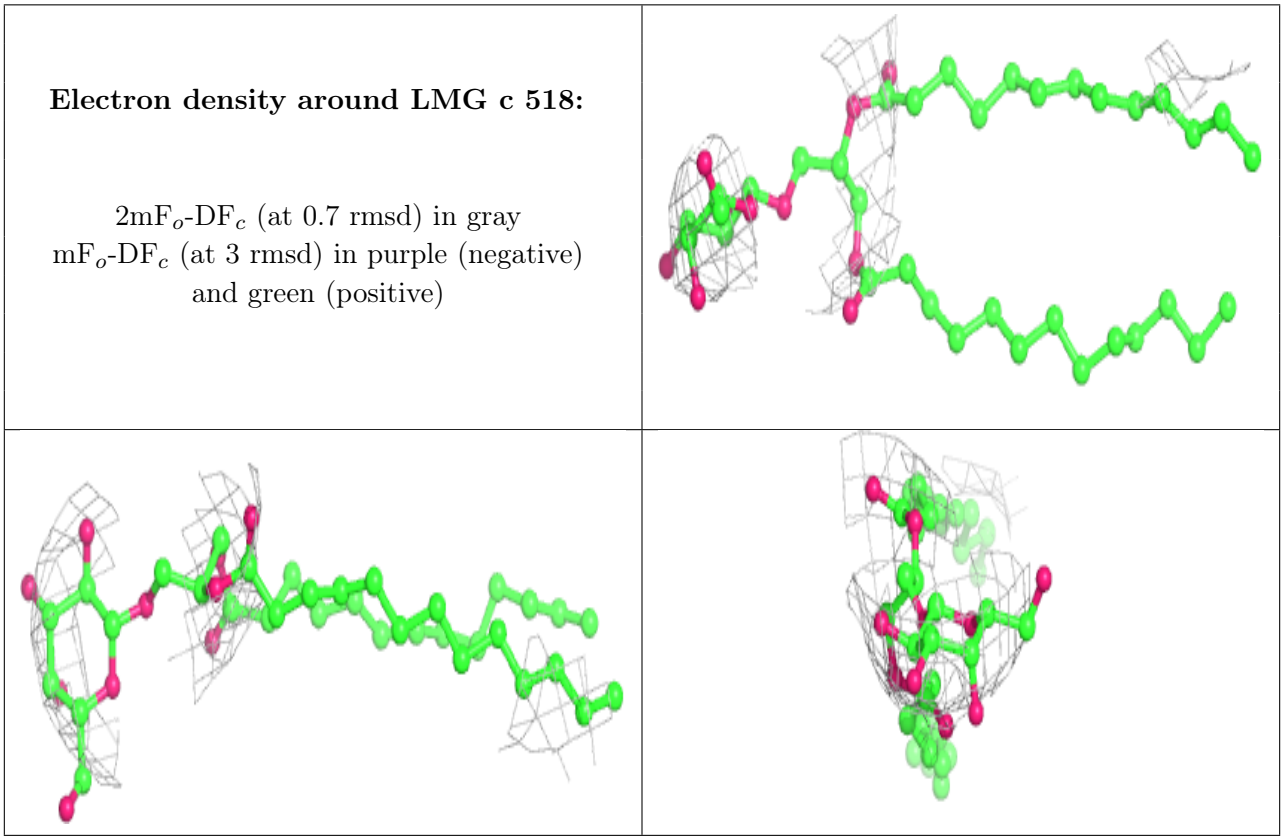
Electron density around BCR j 102:

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



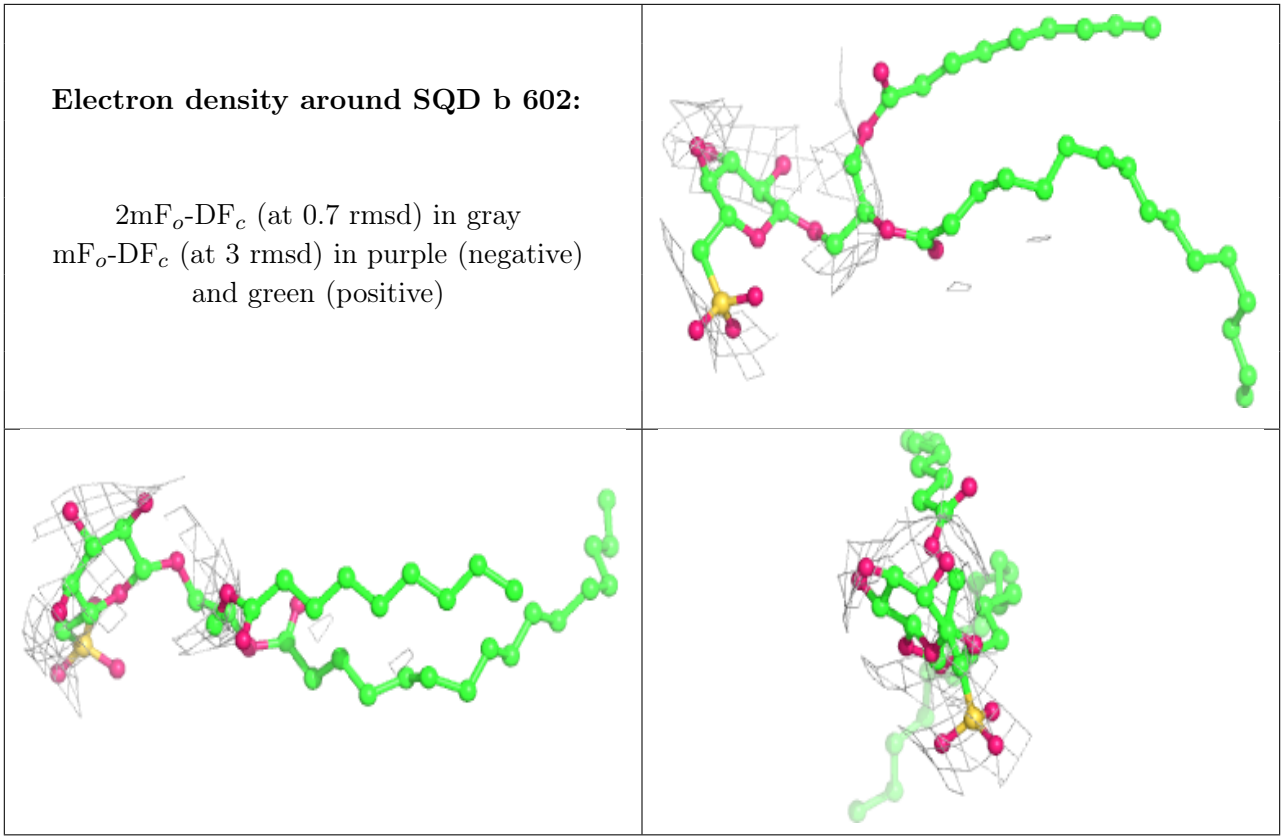
Electron density around LMG c 518:

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



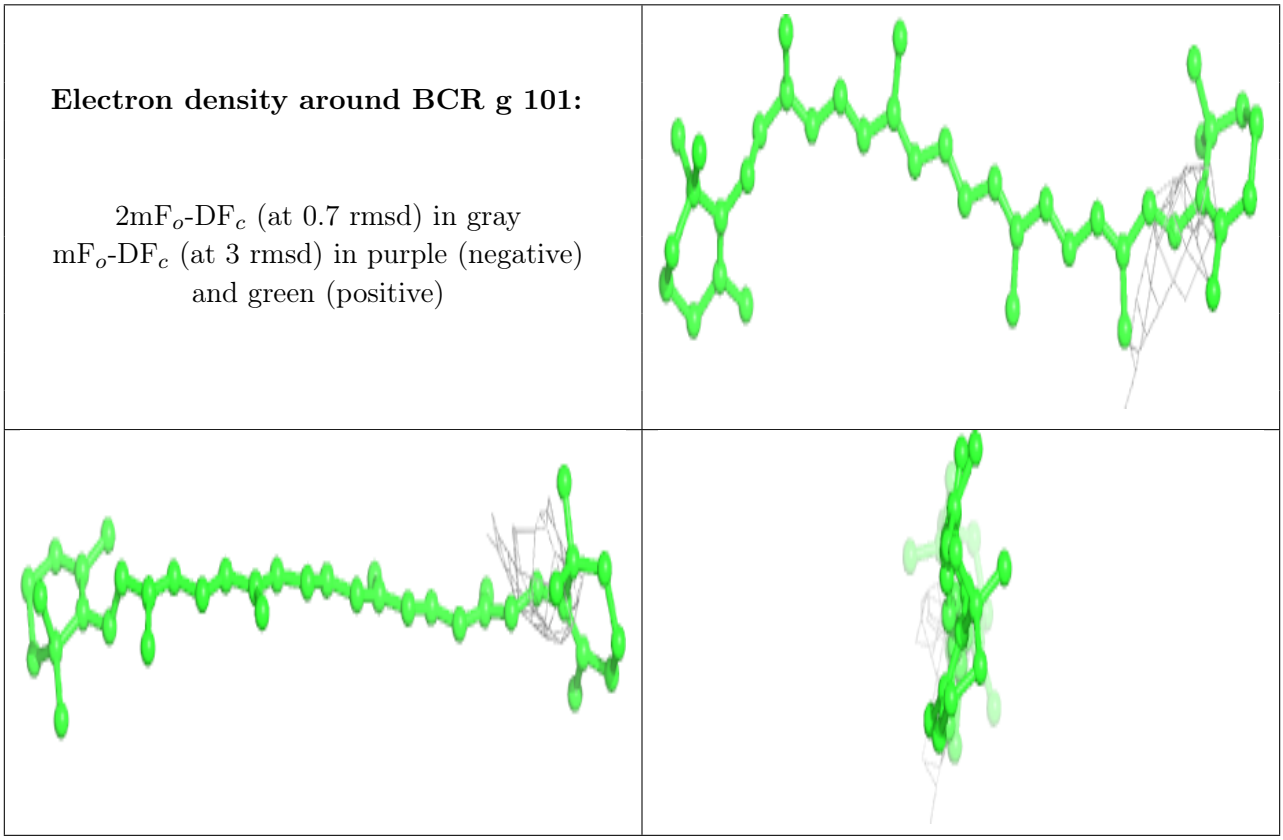
Electron density around SQD b 602:

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



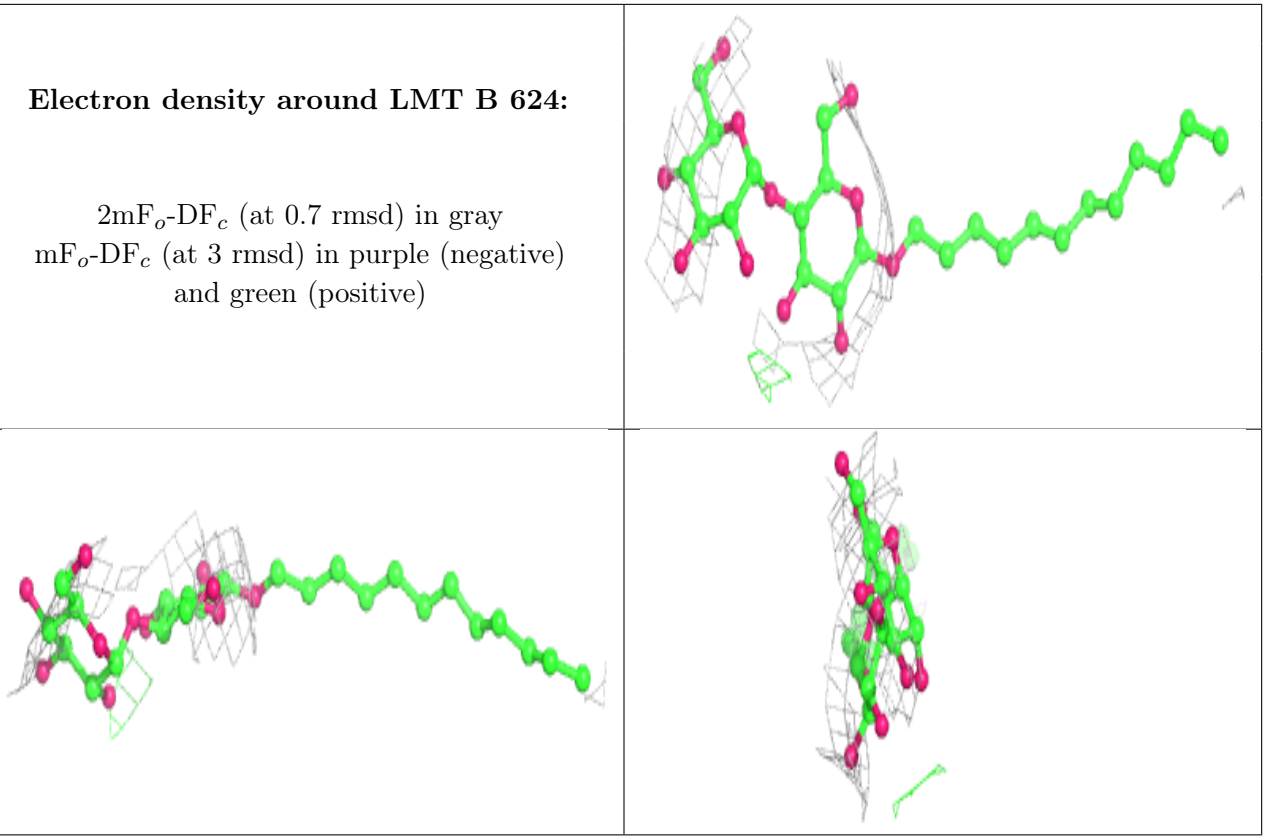
Electron density around BCR g 101:

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



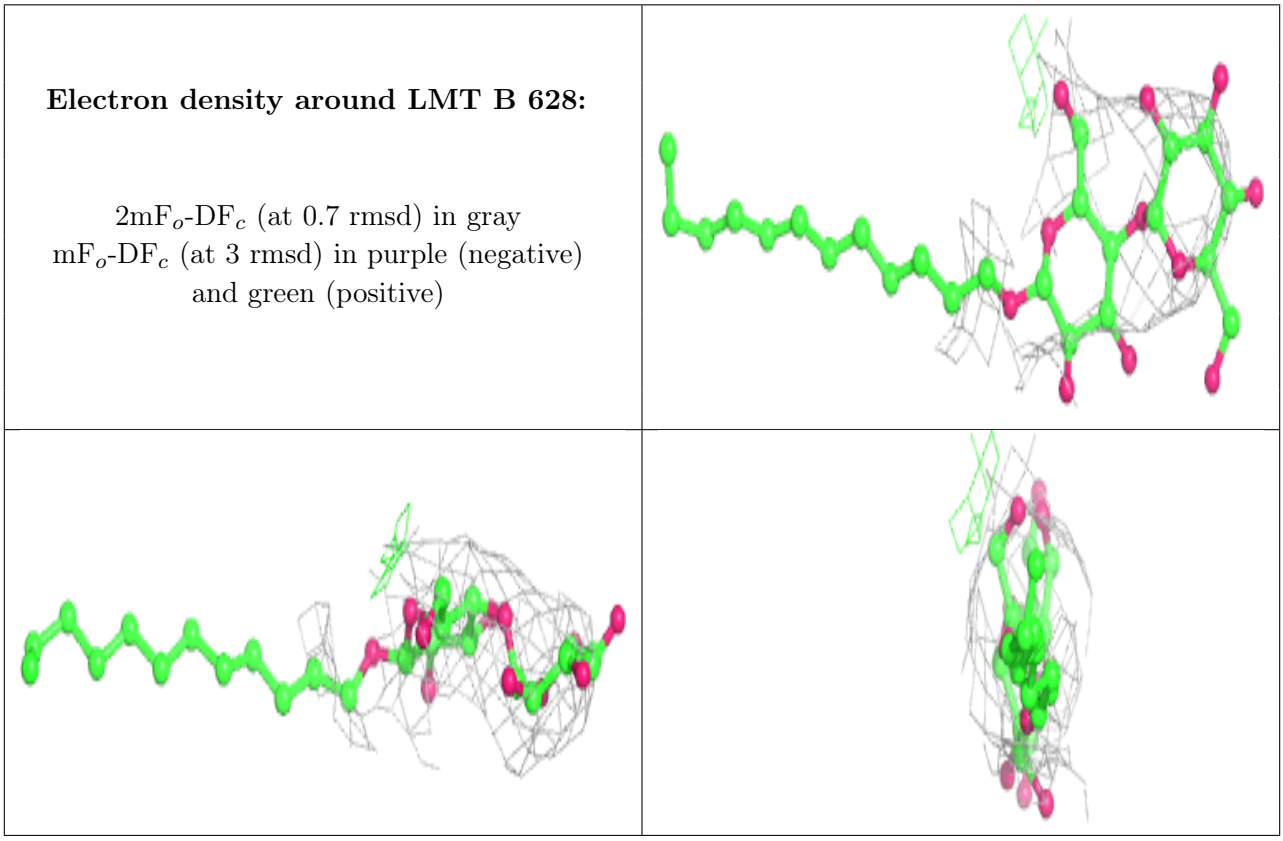
Electron density around LMT B 624:

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



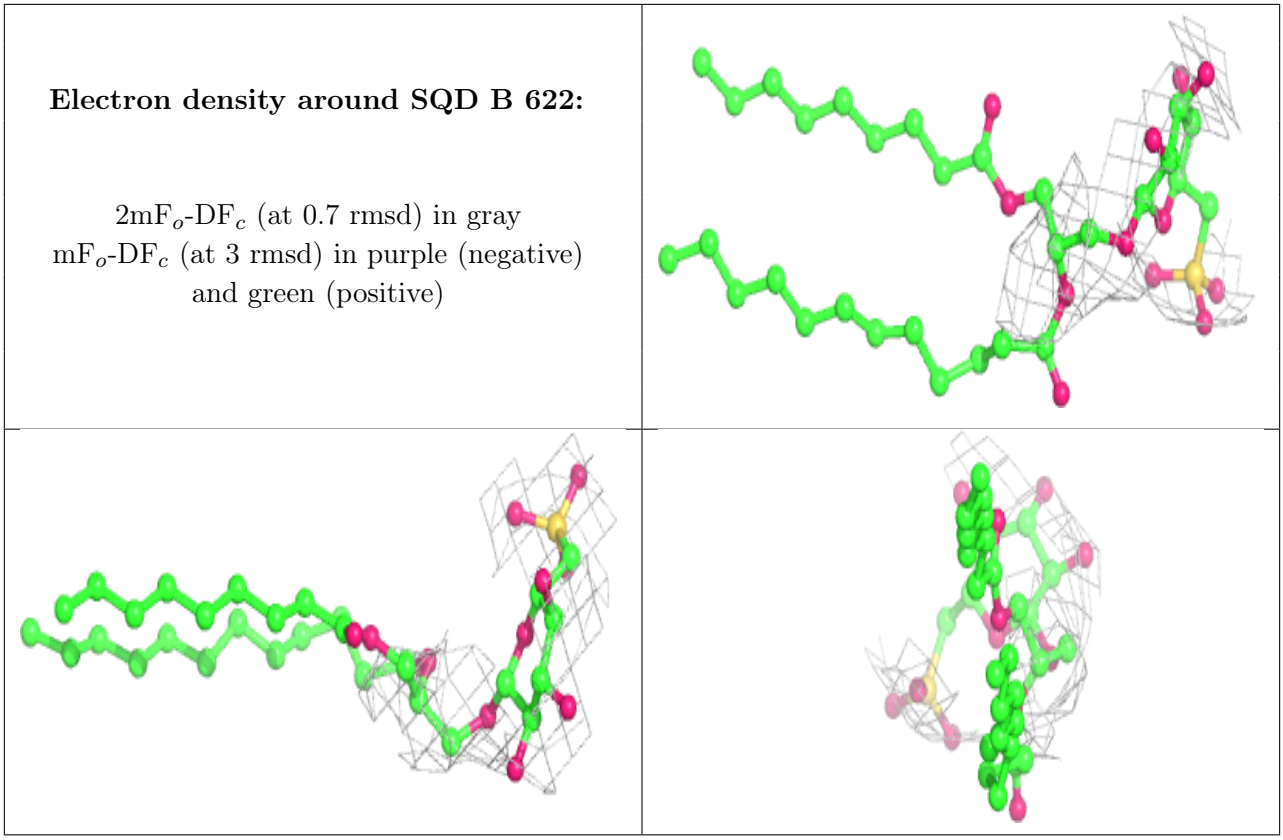
Electron density around LMT B 628:

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



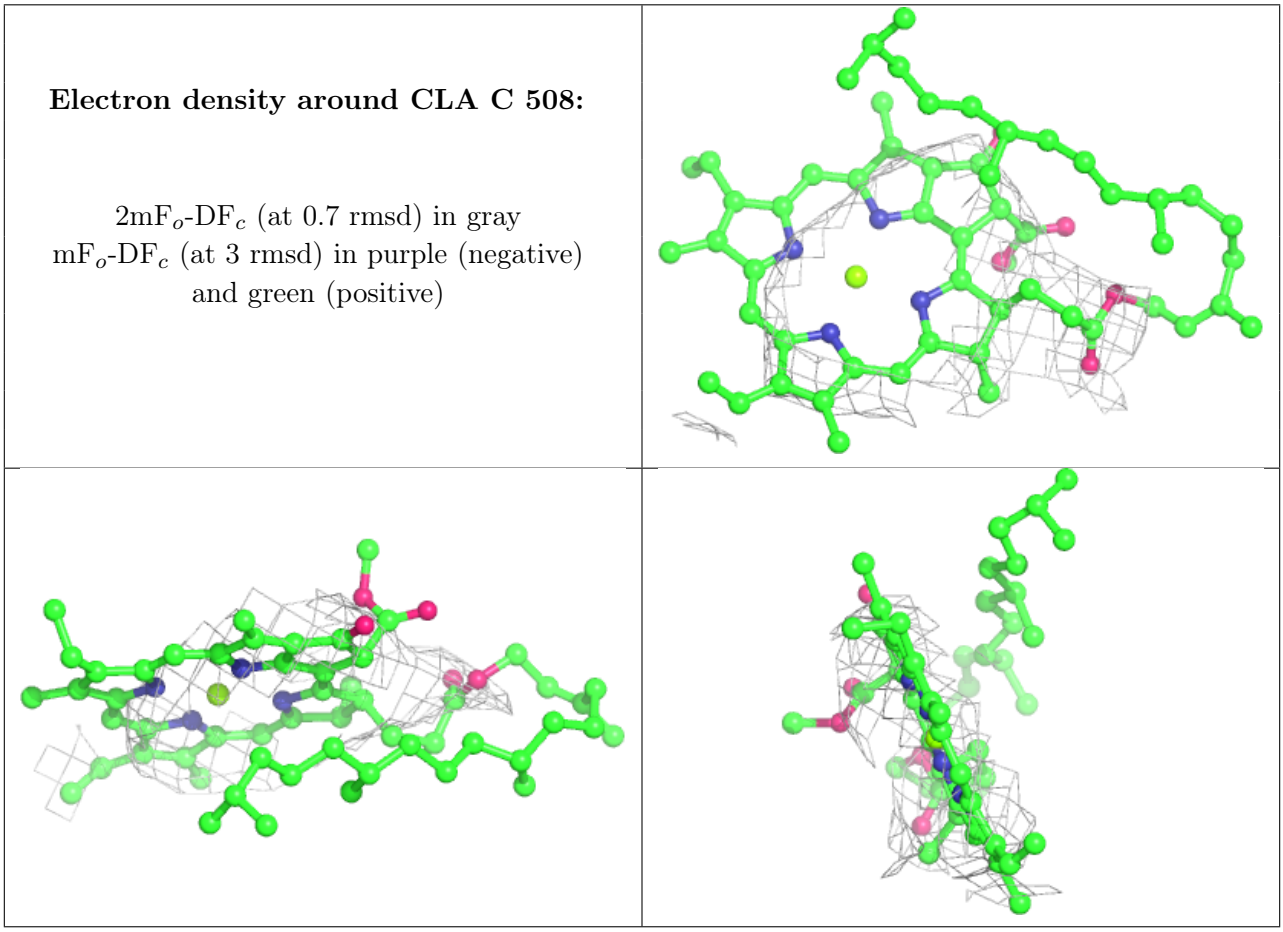
Electron density around SQD B 622:

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



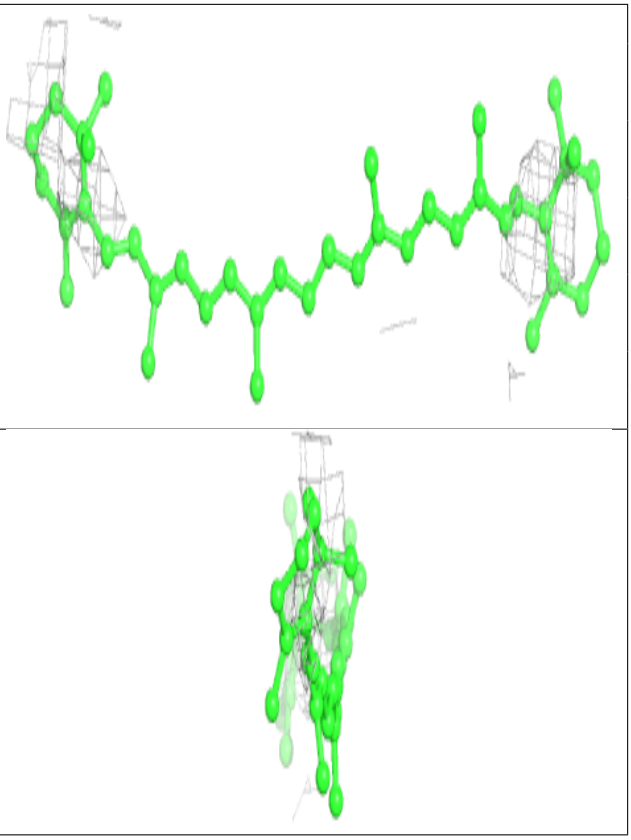
Electron density around CLA C 508:

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



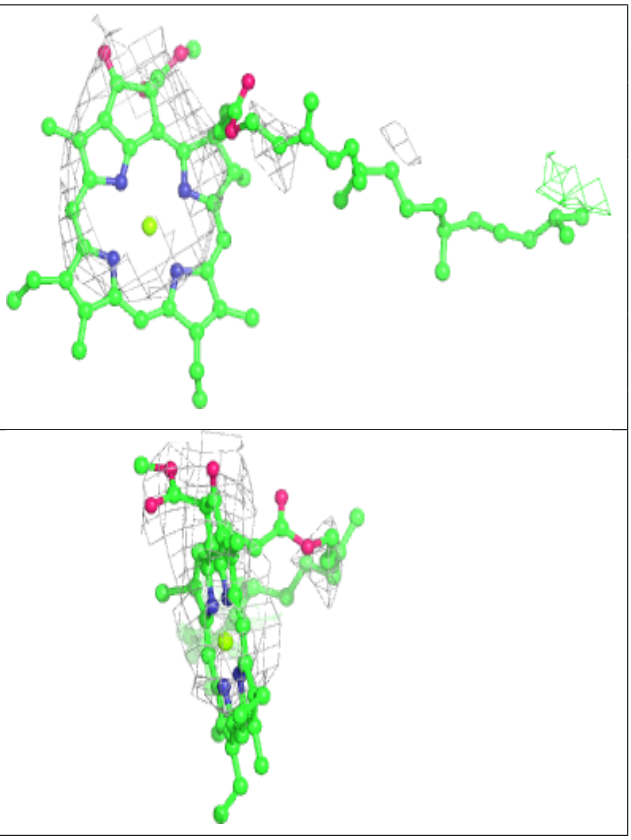
Electron density around BCR B 617:

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



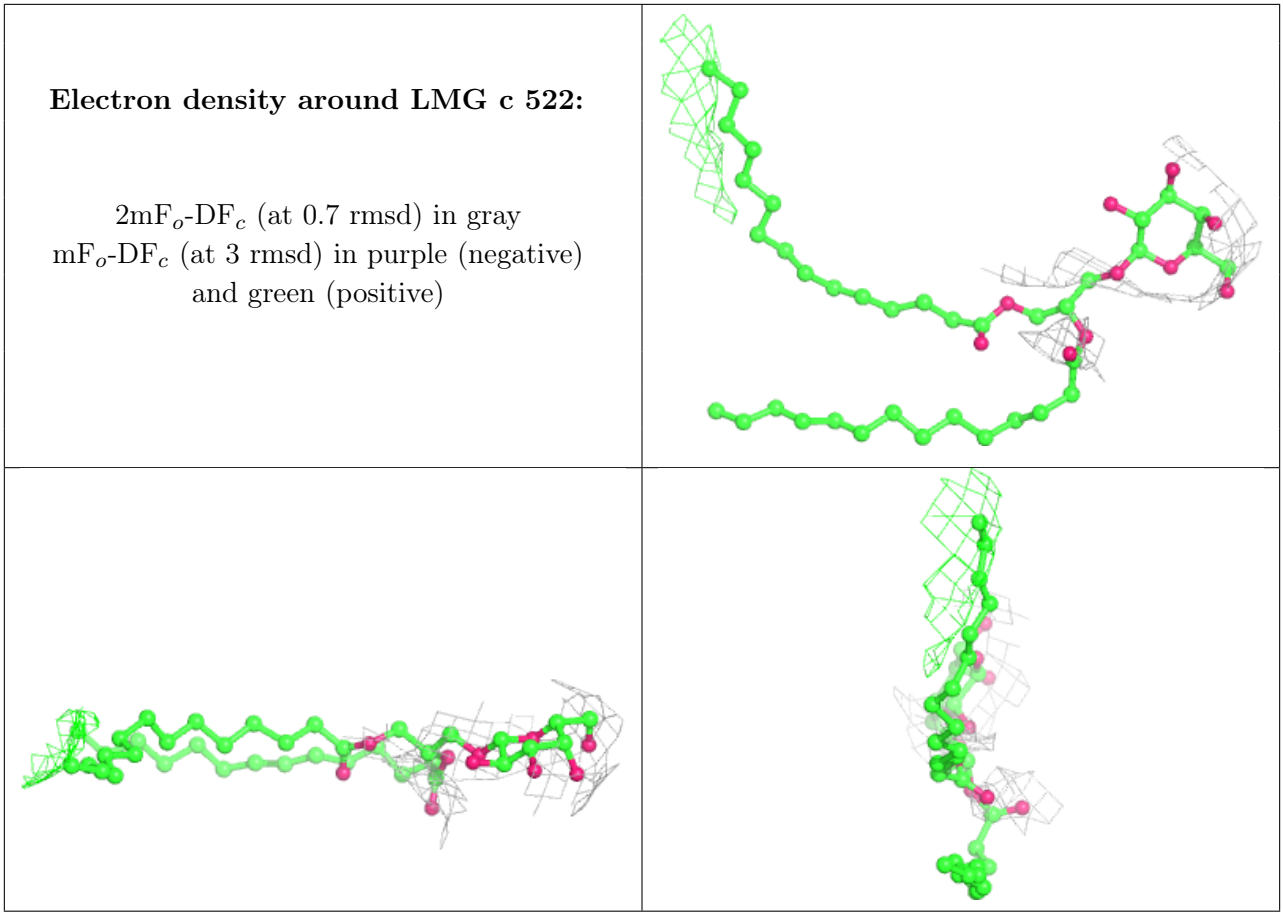
Electron density around CLA a 405:

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



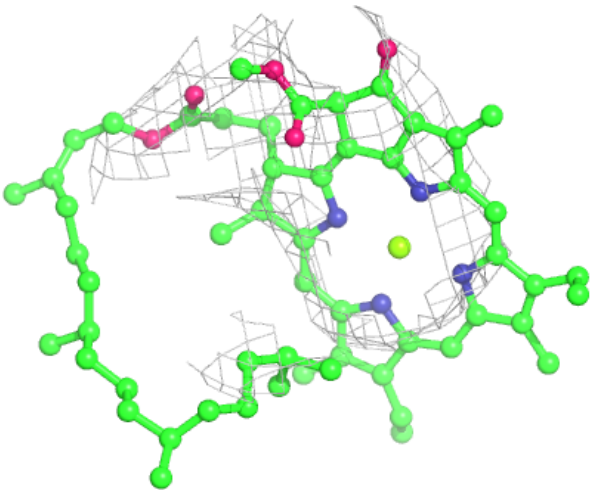
Electron density around LMG c 522:

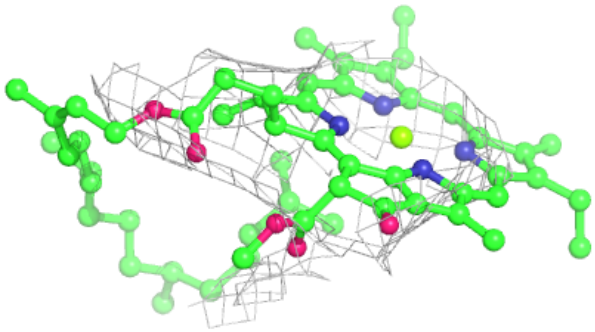
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

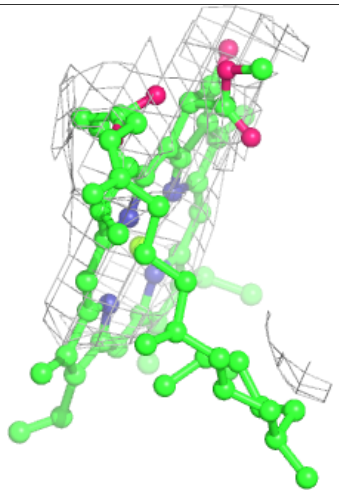


Electron density around CLA b 619:

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

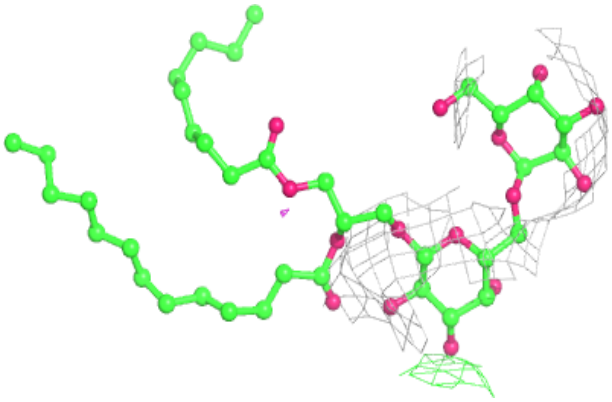


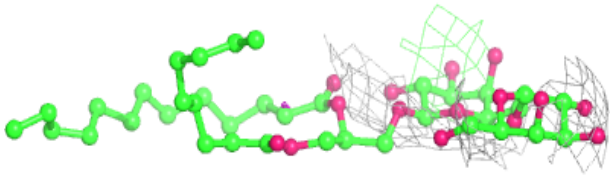


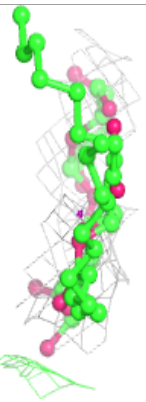


Electron density around DGD B 626:

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

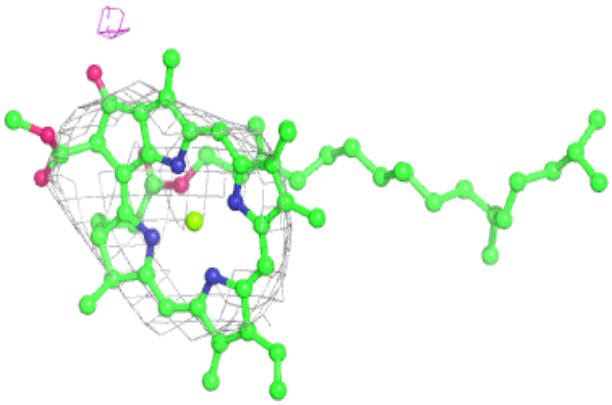


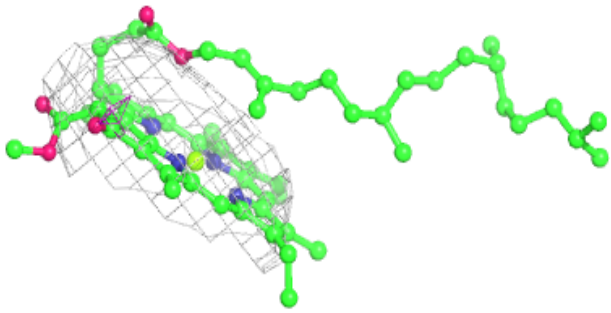


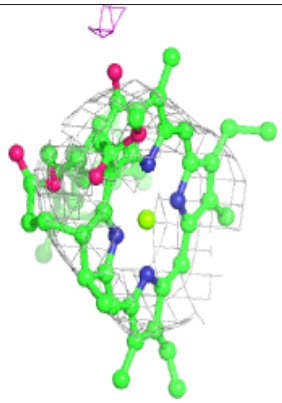


Electron density around CLA B 613:

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

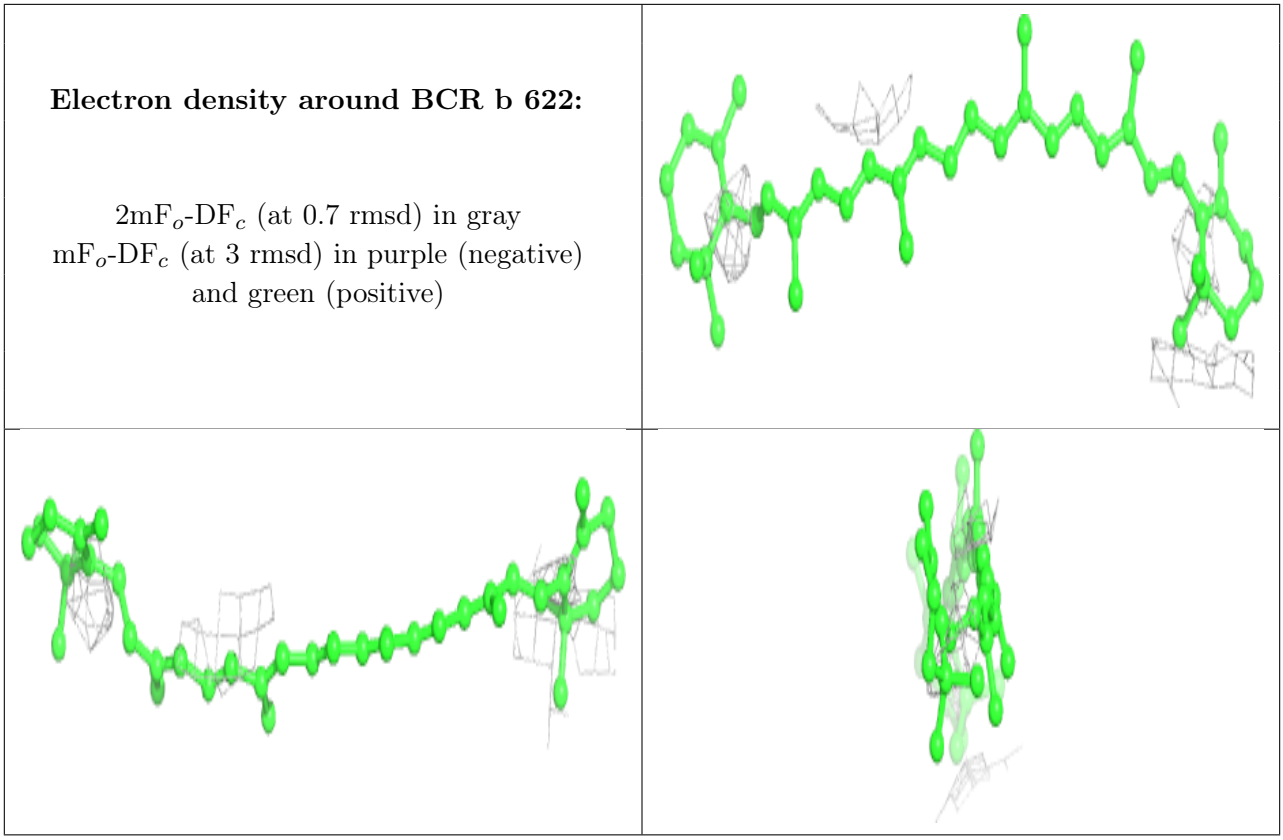






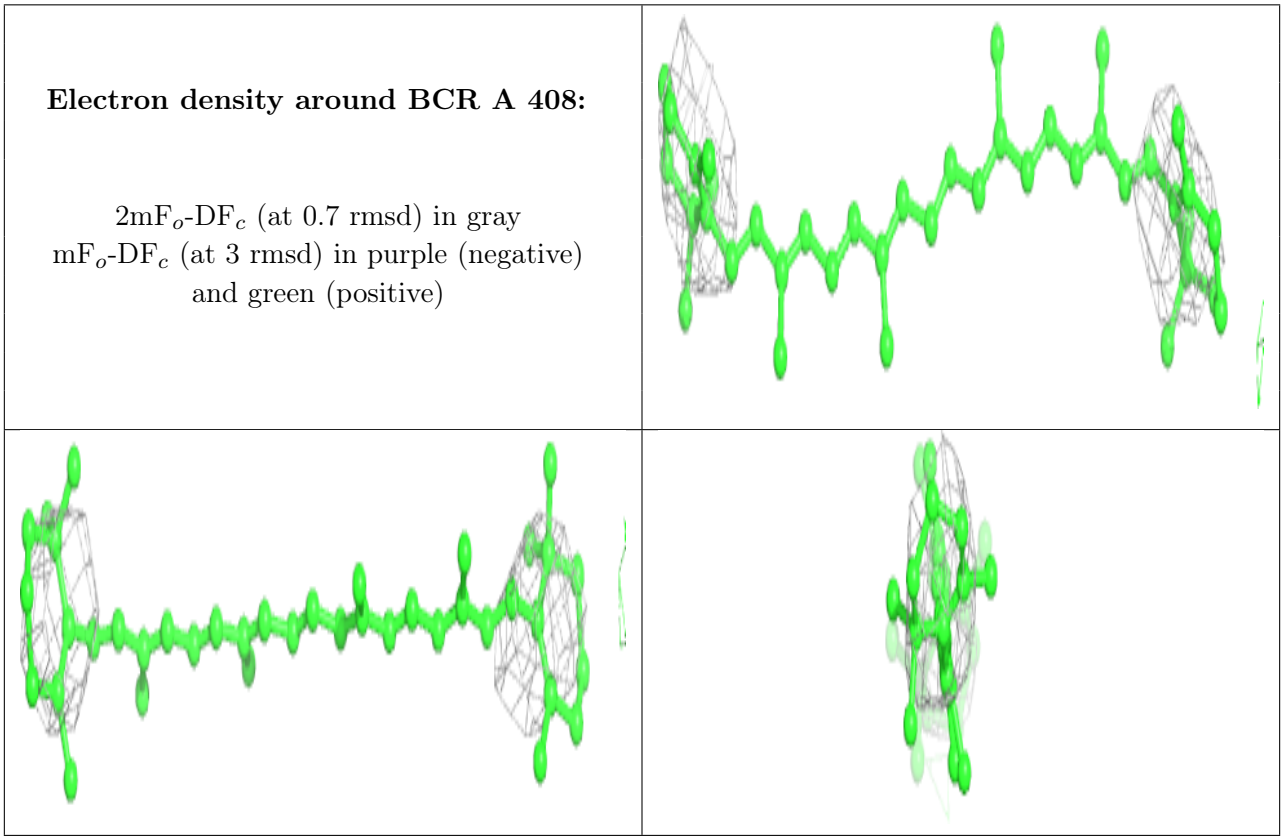
Electron density around BCR b 622:

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



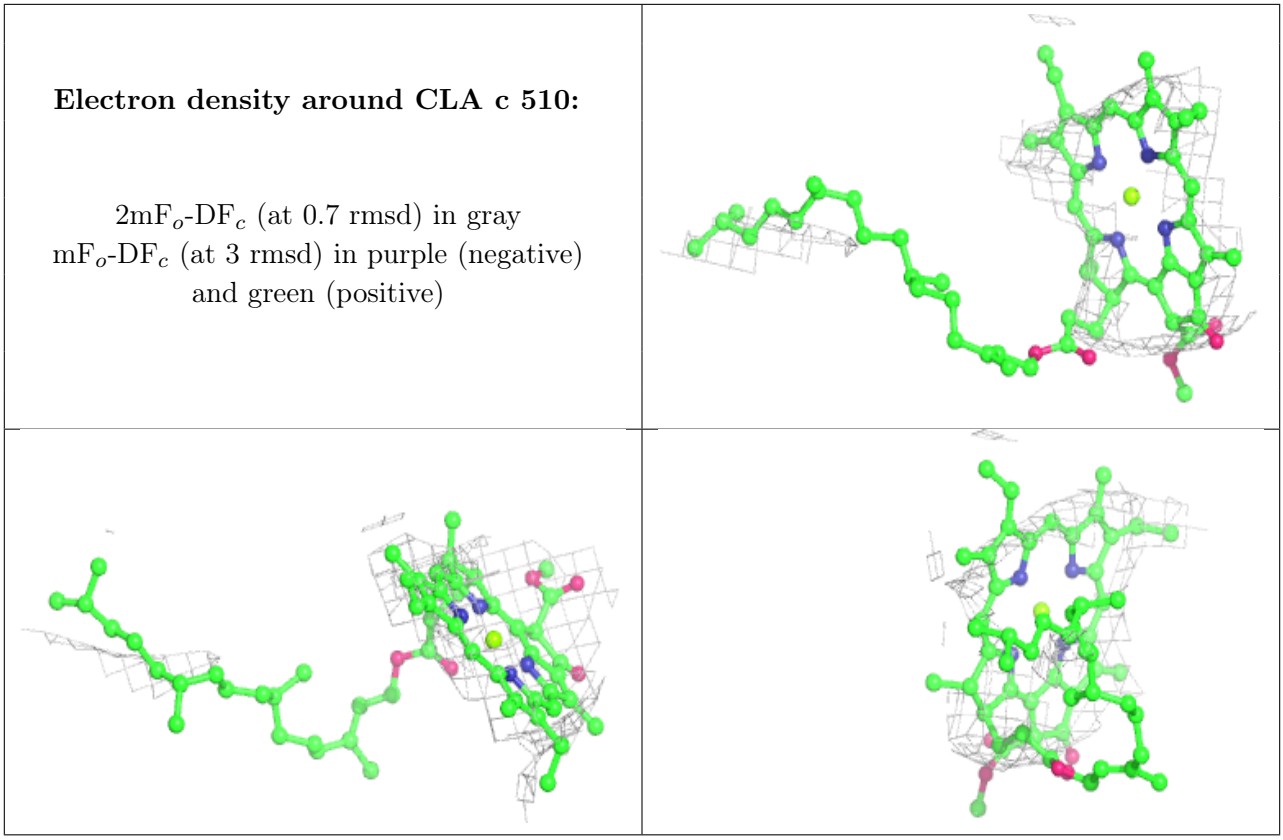
Electron density around BCR A 408:

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



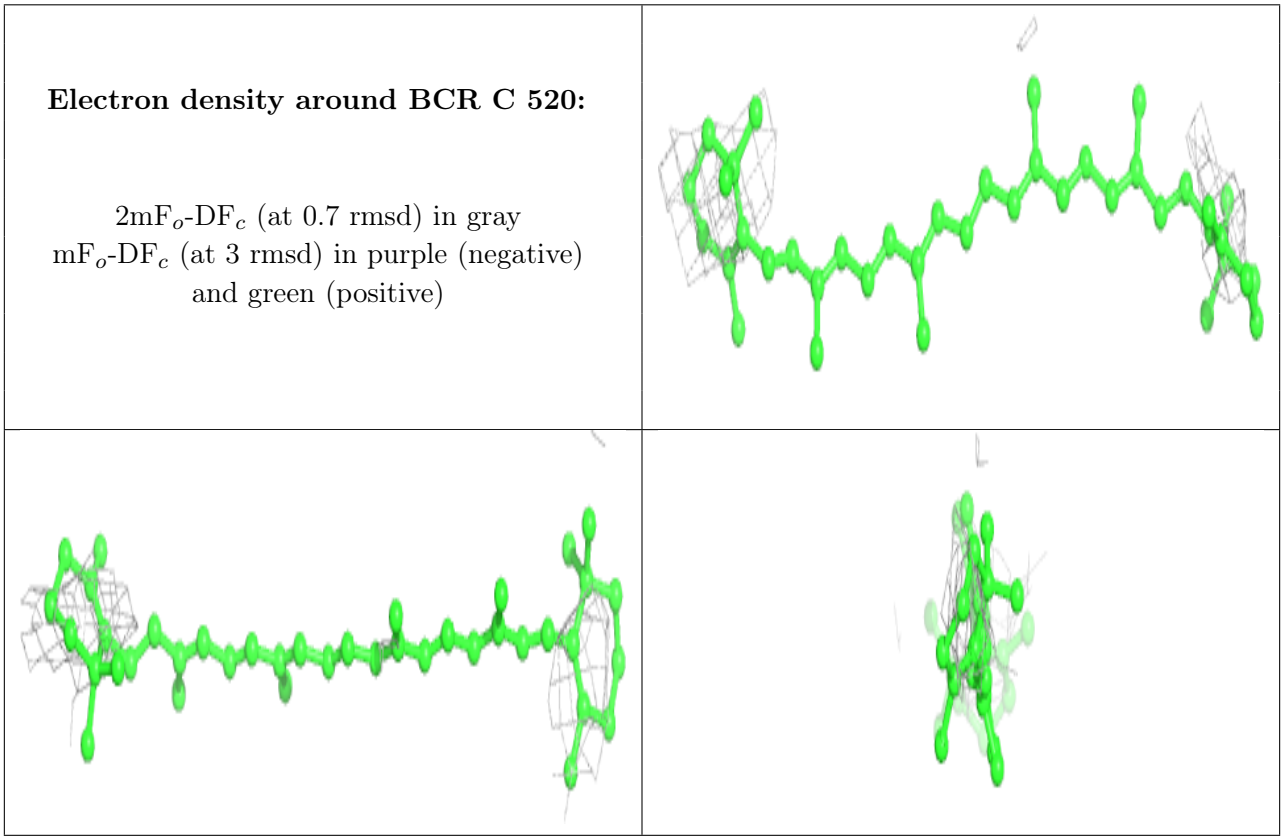
Electron density around CLA c 510:

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



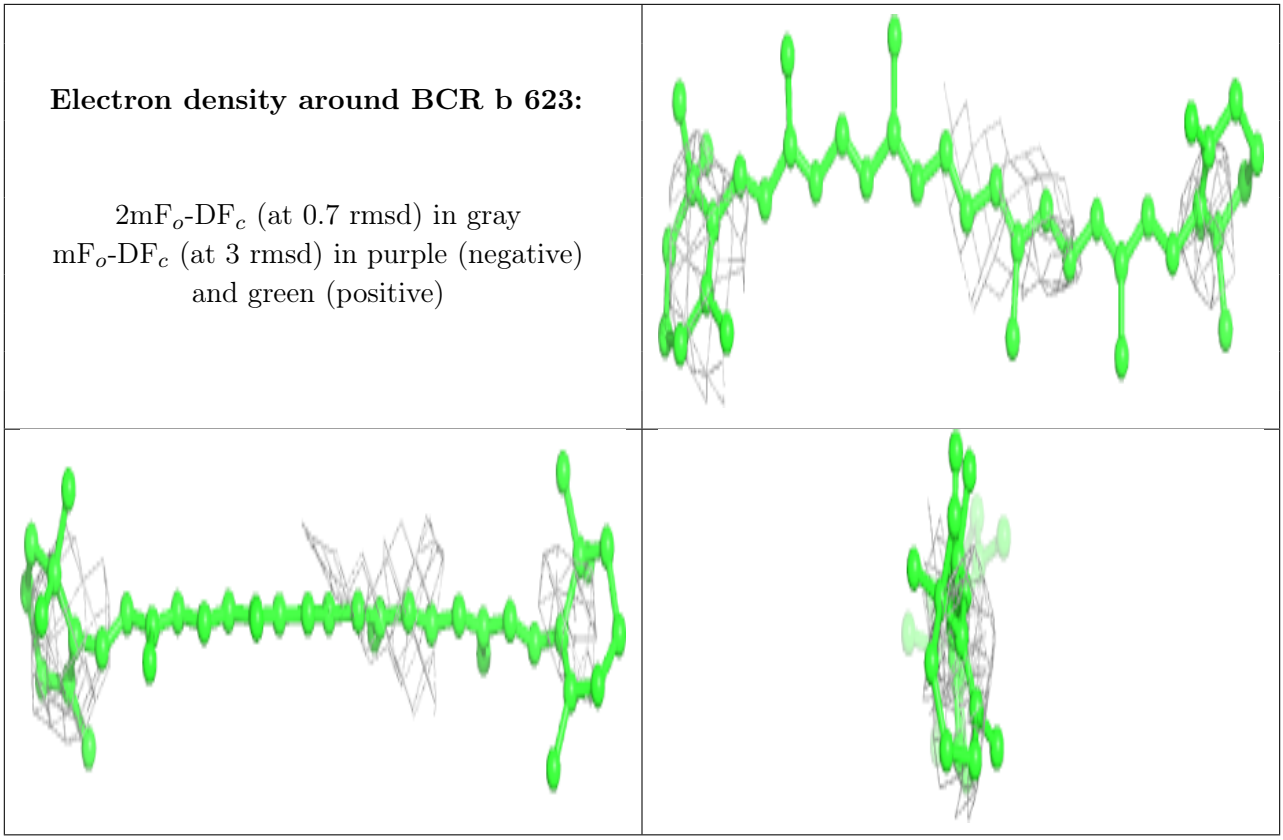
Electron density around BCR C 520:

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



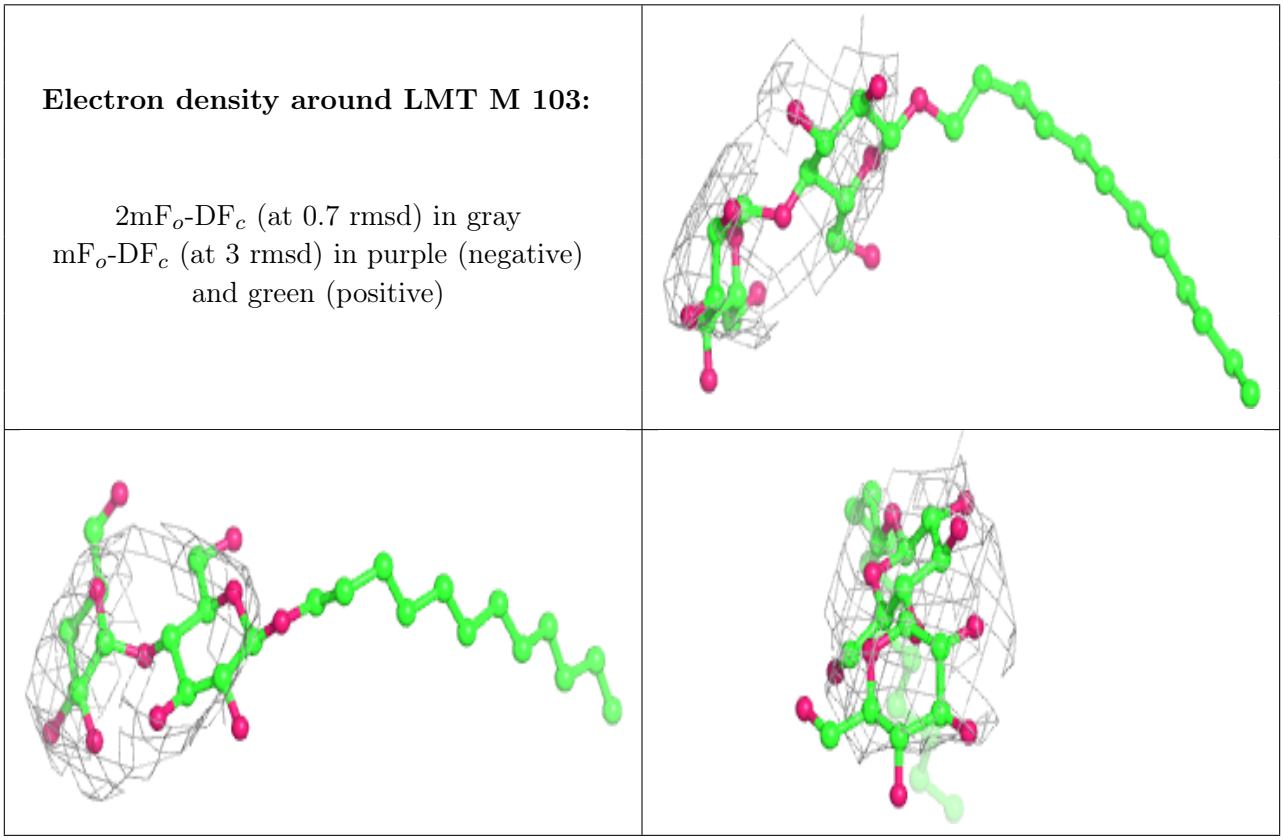
Electron density around BCR b 623:

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



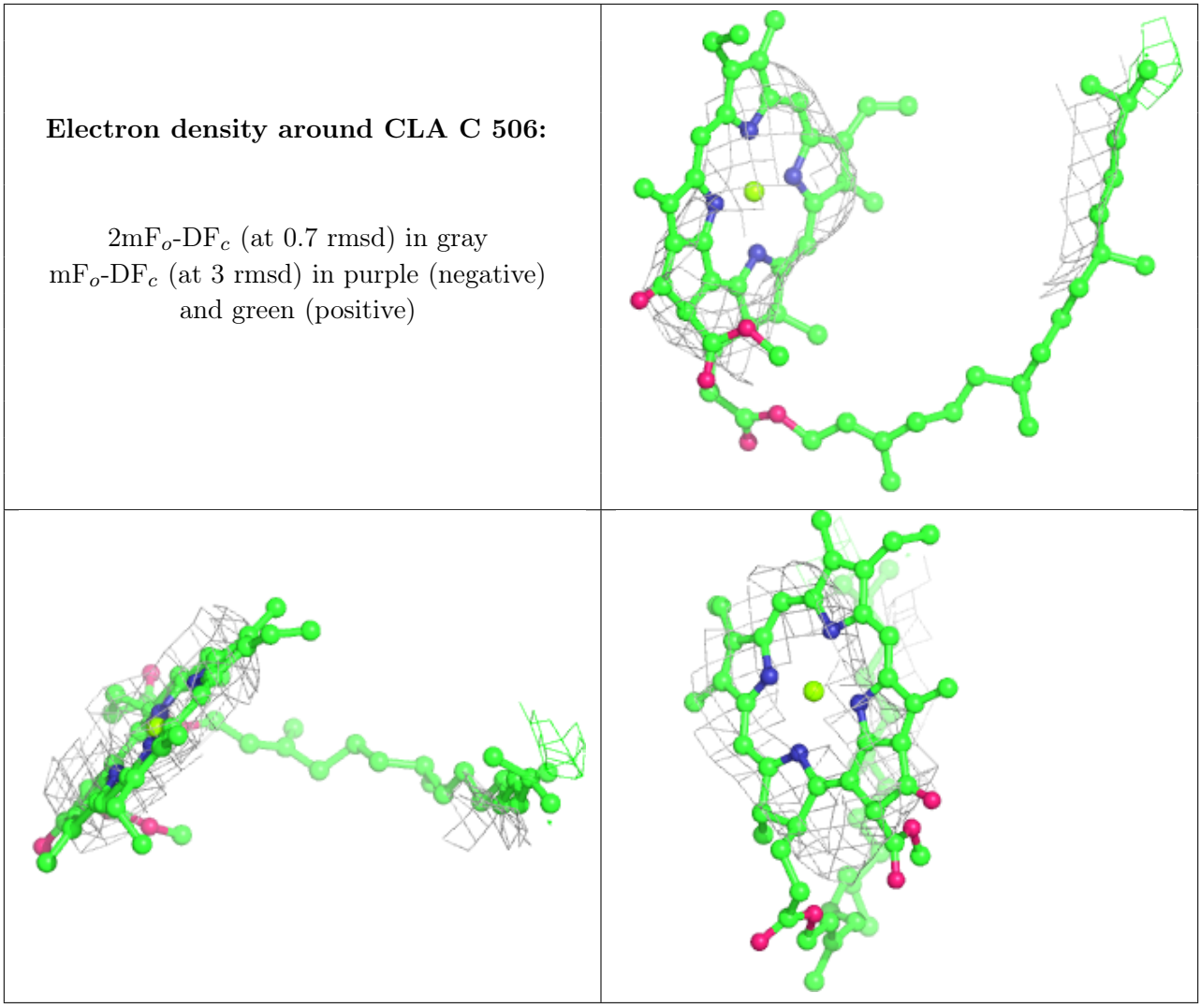
Electron density around LMT M 103:

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



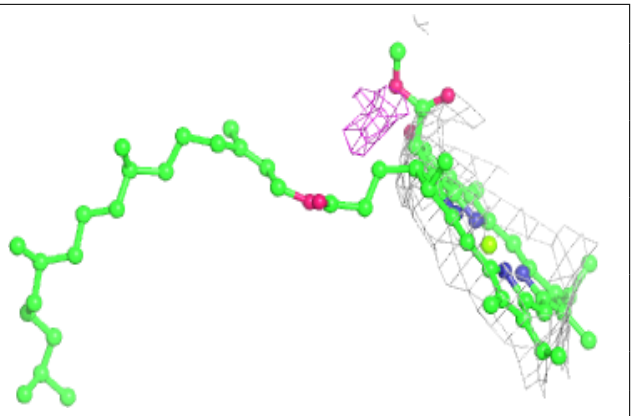
Electron density around CLA C 506:

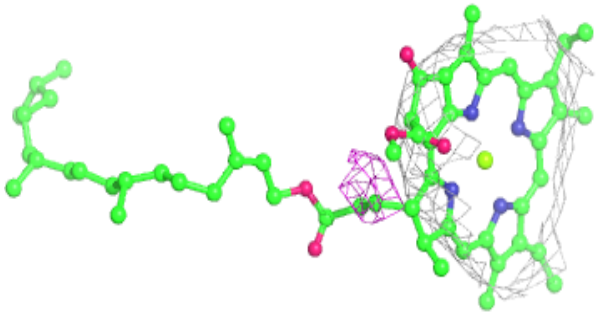
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

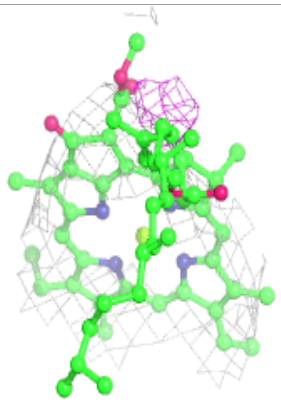


Electron density around CLA d 405:

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

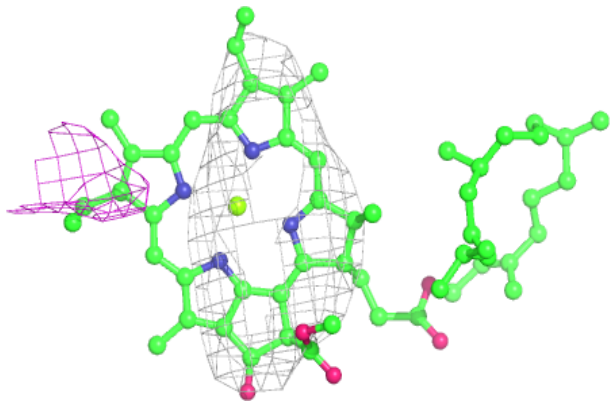


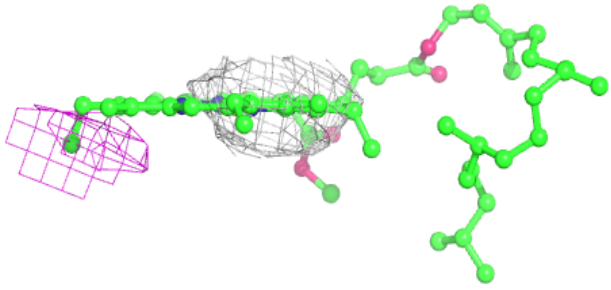


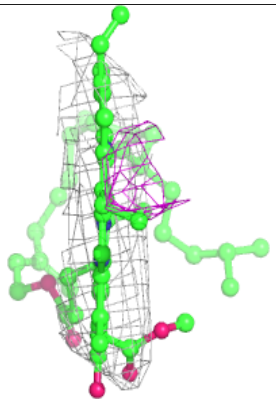


Electron density around CLA C 511:

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

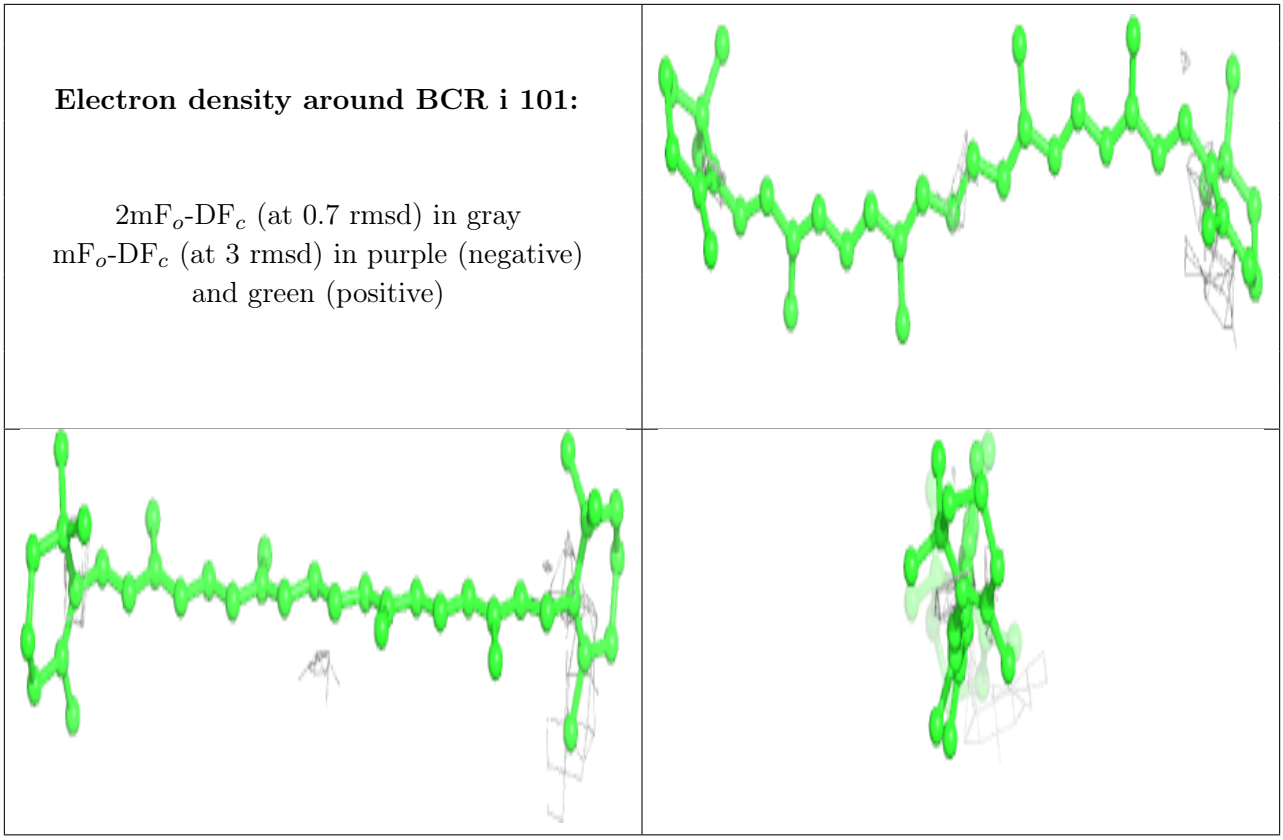






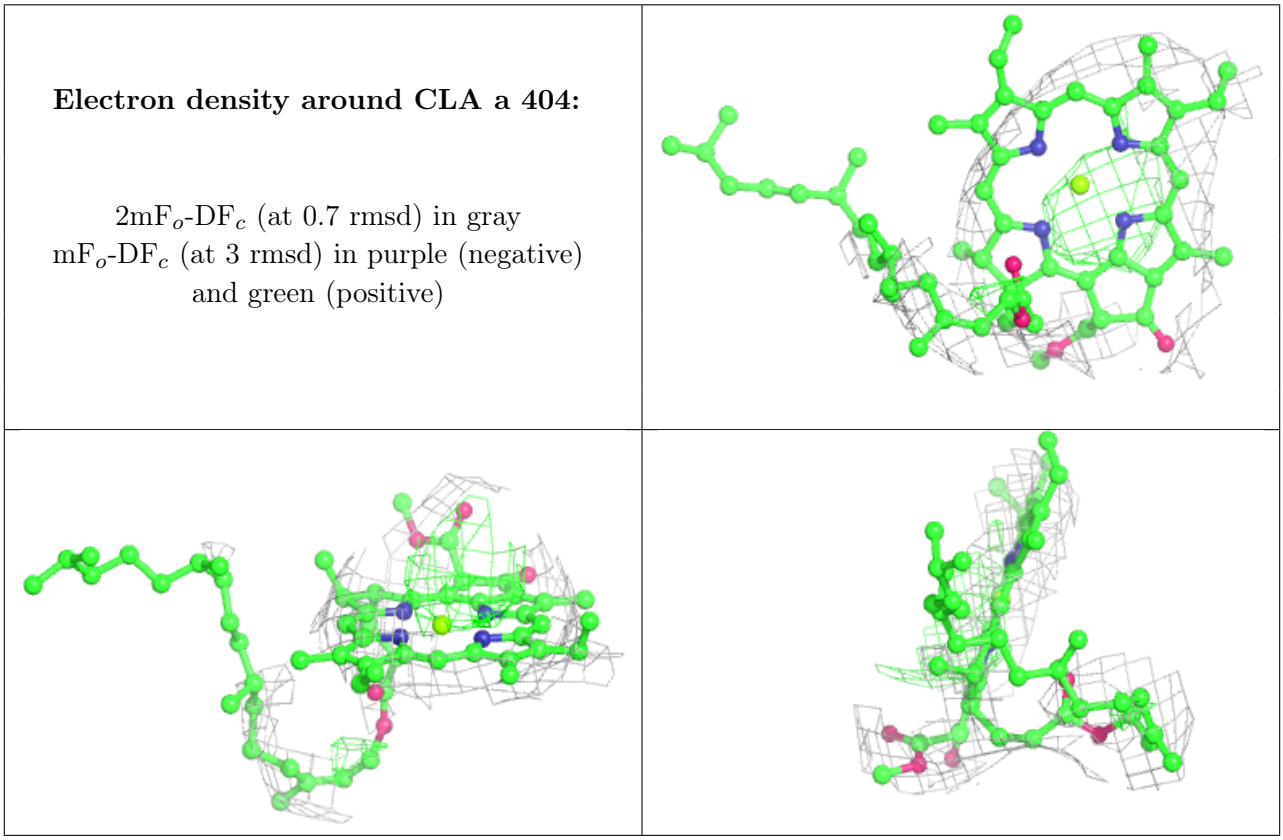
Electron density around BCR i 101:

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



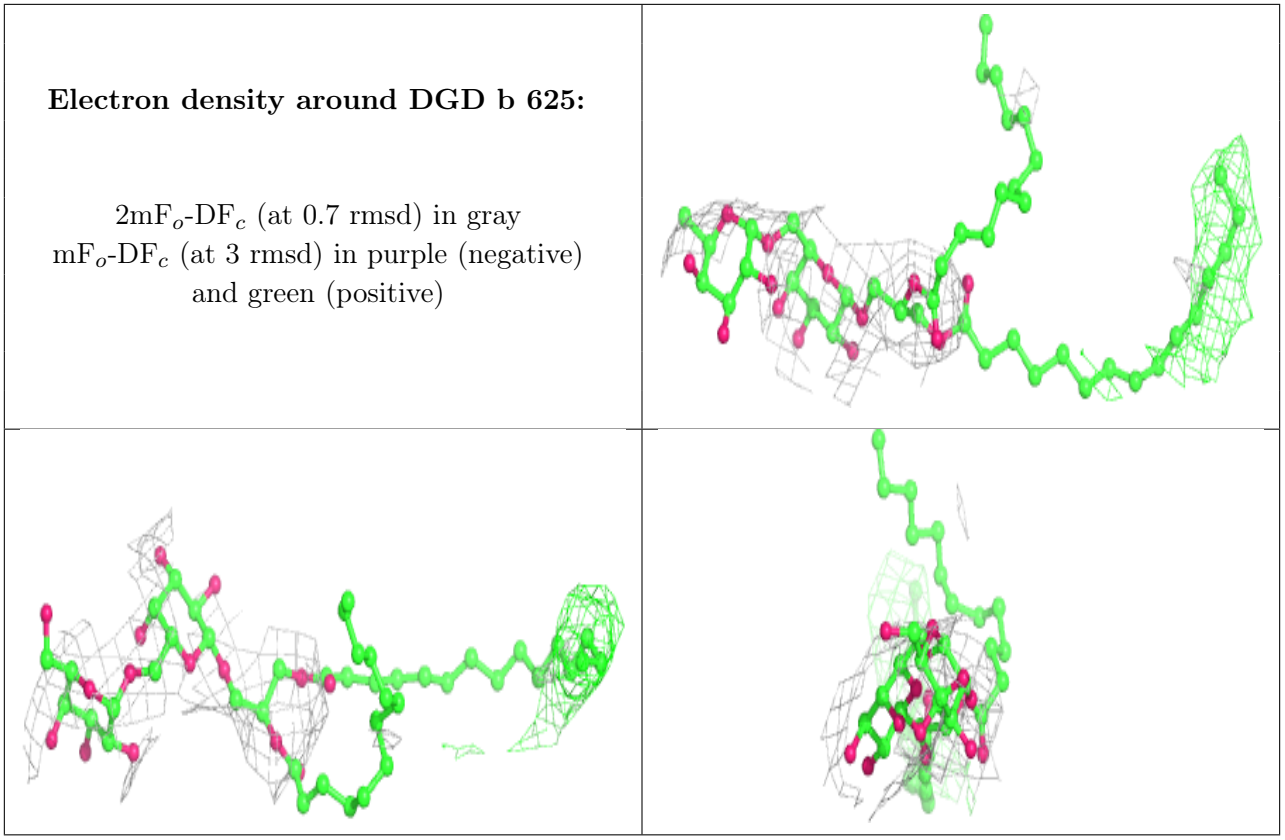
Electron density around CLA a 404:

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



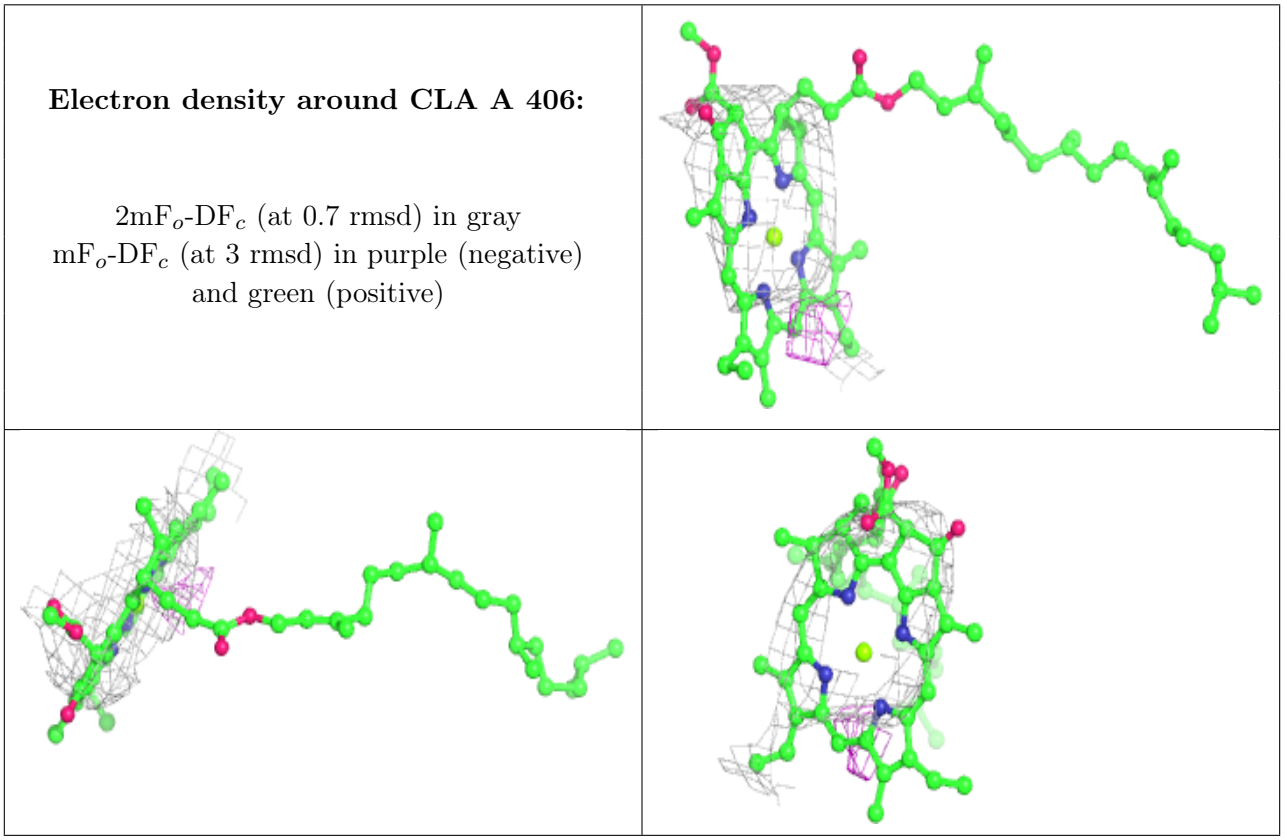
Electron density around DGD b 625:

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



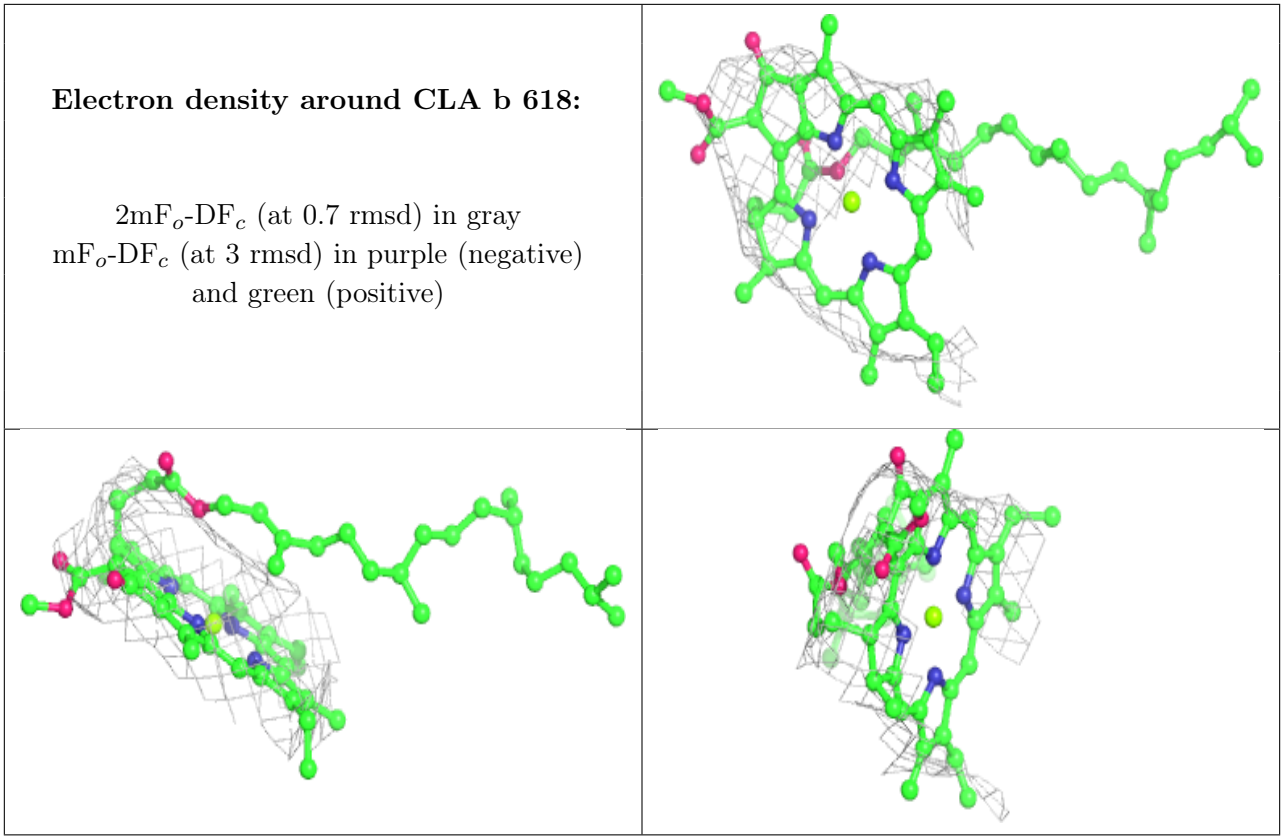
Electron density around CLA A 406:

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



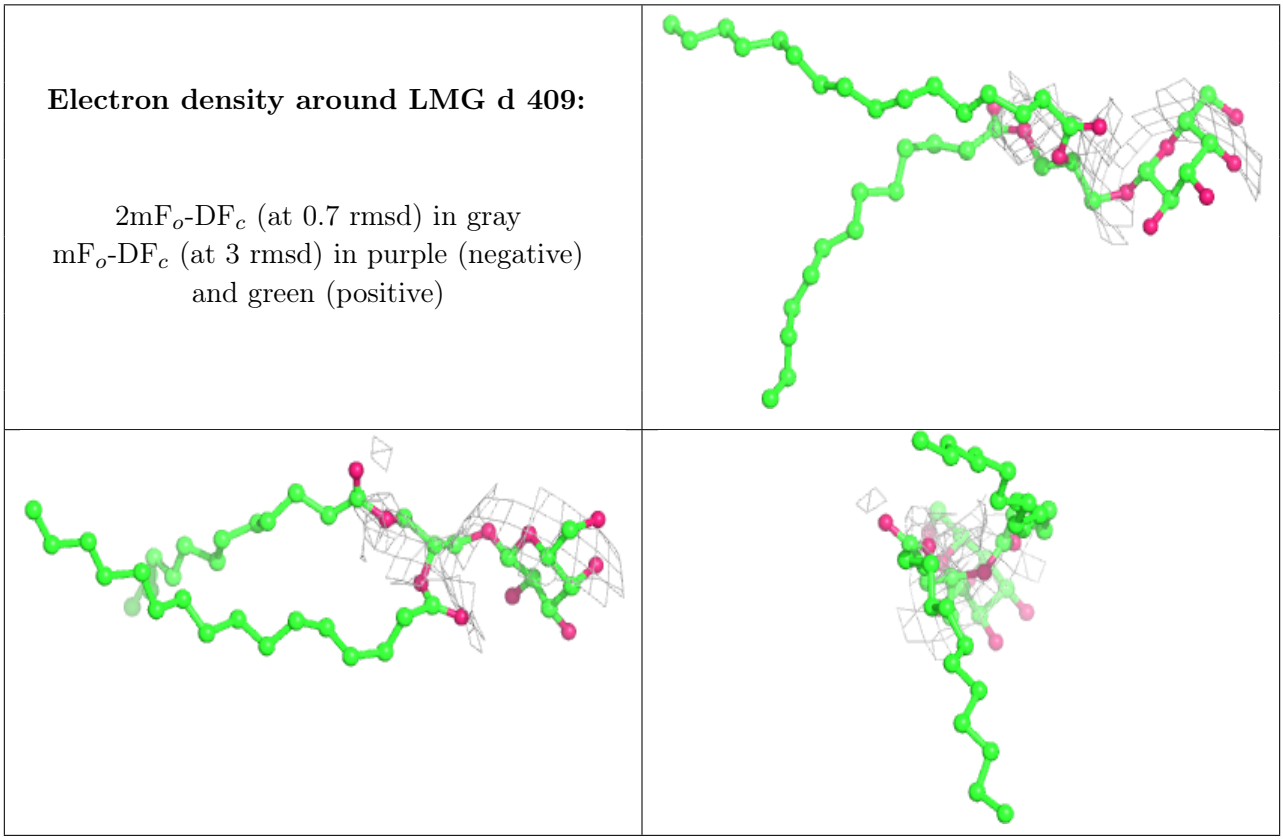
Electron density around CLA b 618:

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



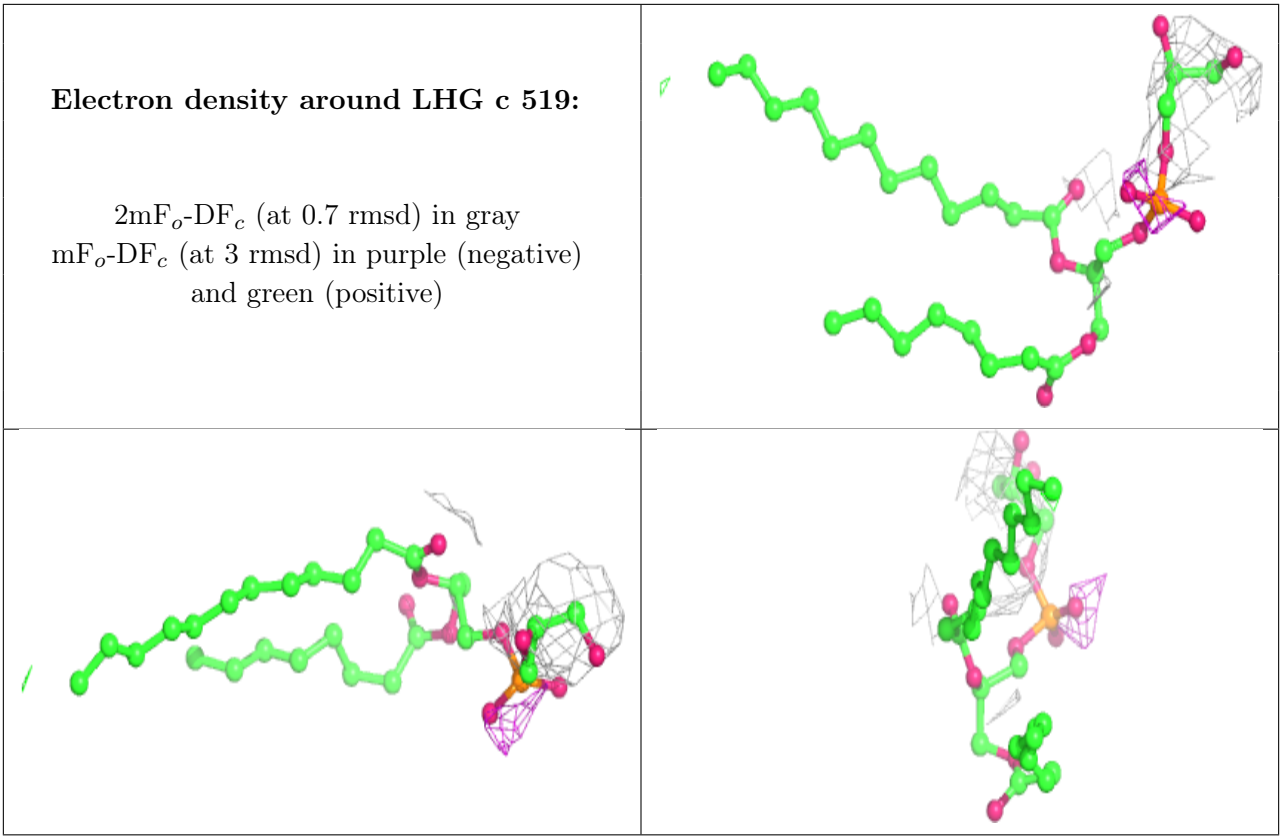
Electron density around LMG d 409:

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



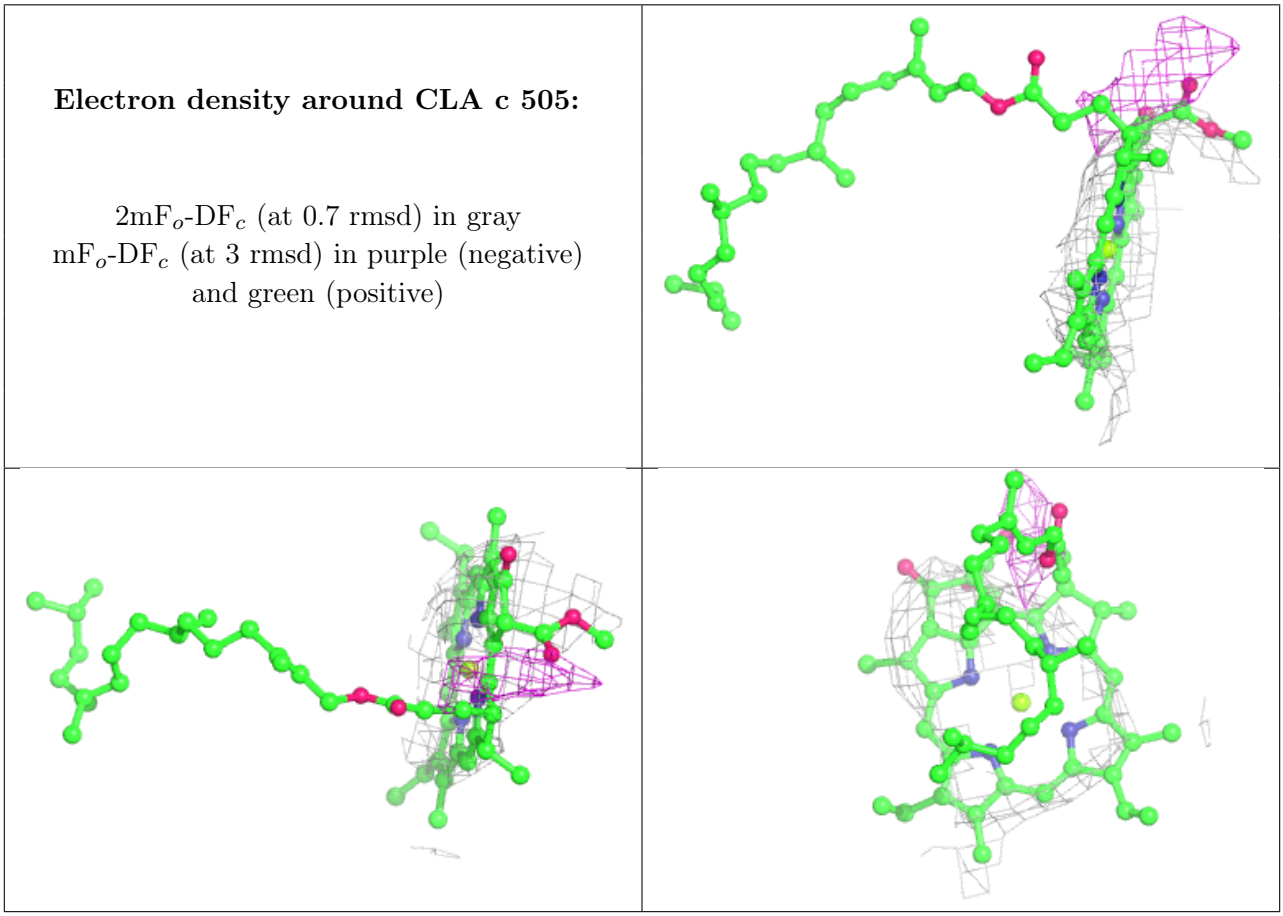
Electron density around LHG c 519:

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



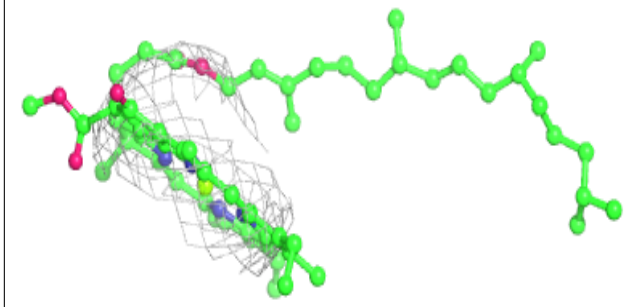
Electron density around CLA c 505:

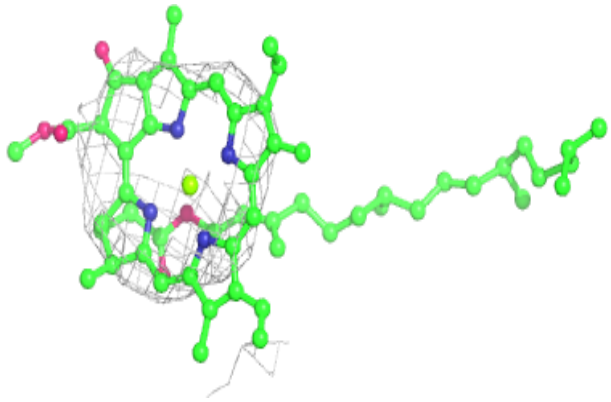
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

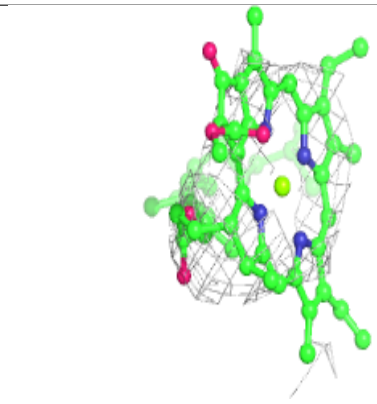


Electron density around CLA b 612:

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

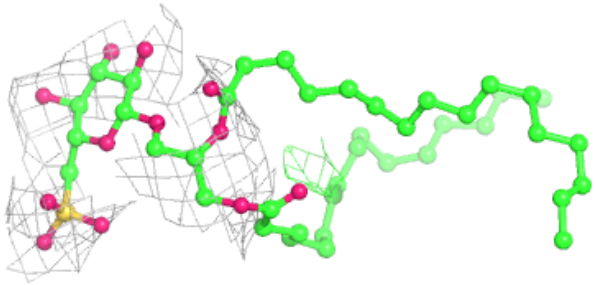


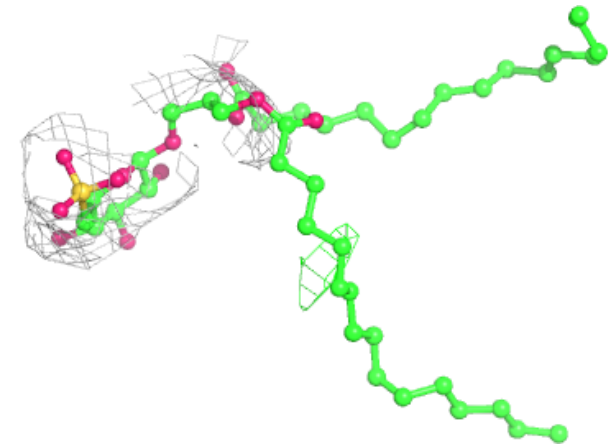


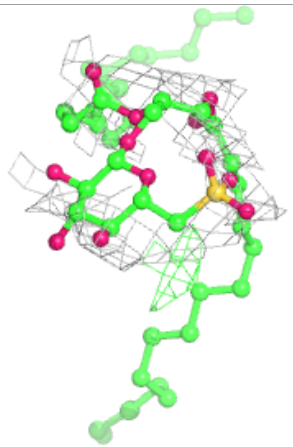


Electron density around SQD A 414:

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

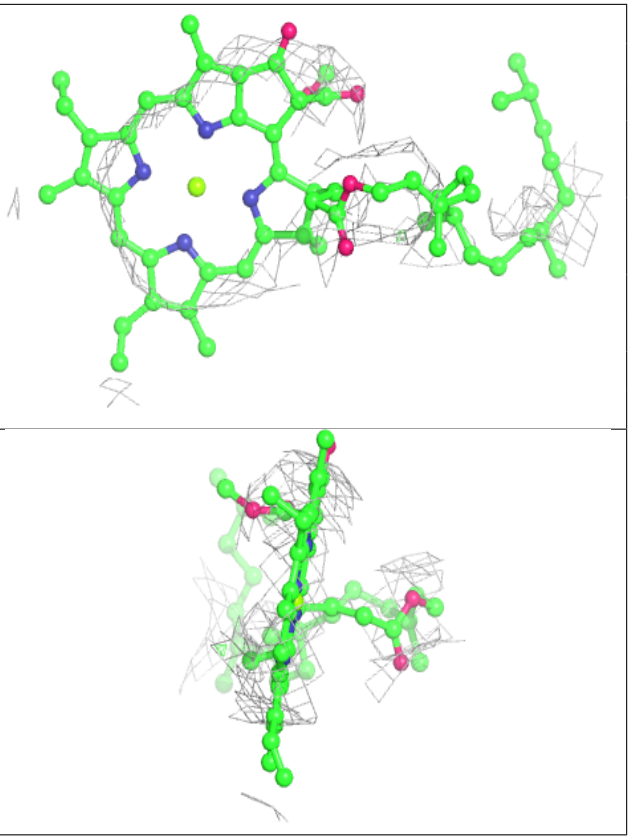






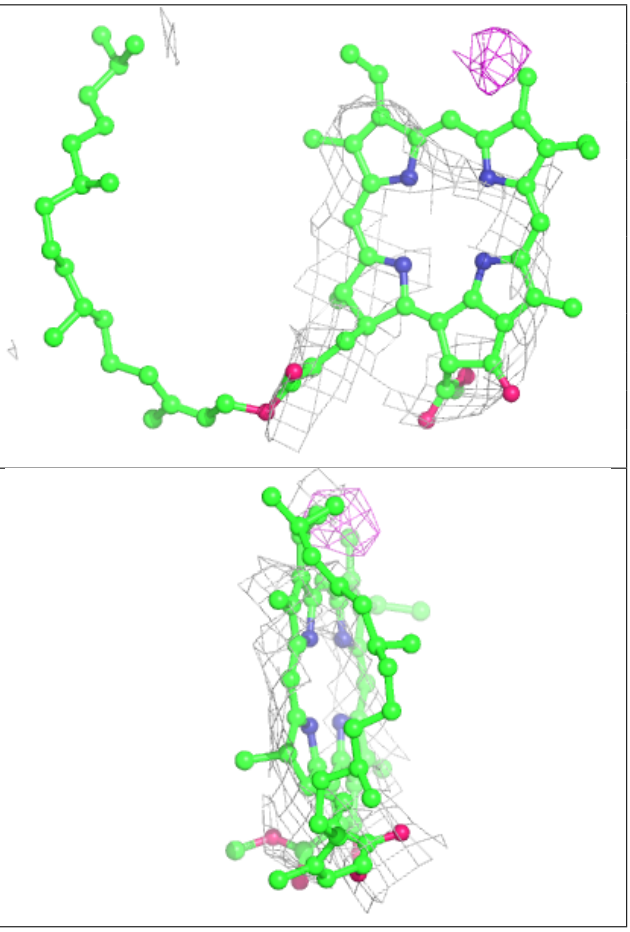
Electron density around CLA b 616:

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



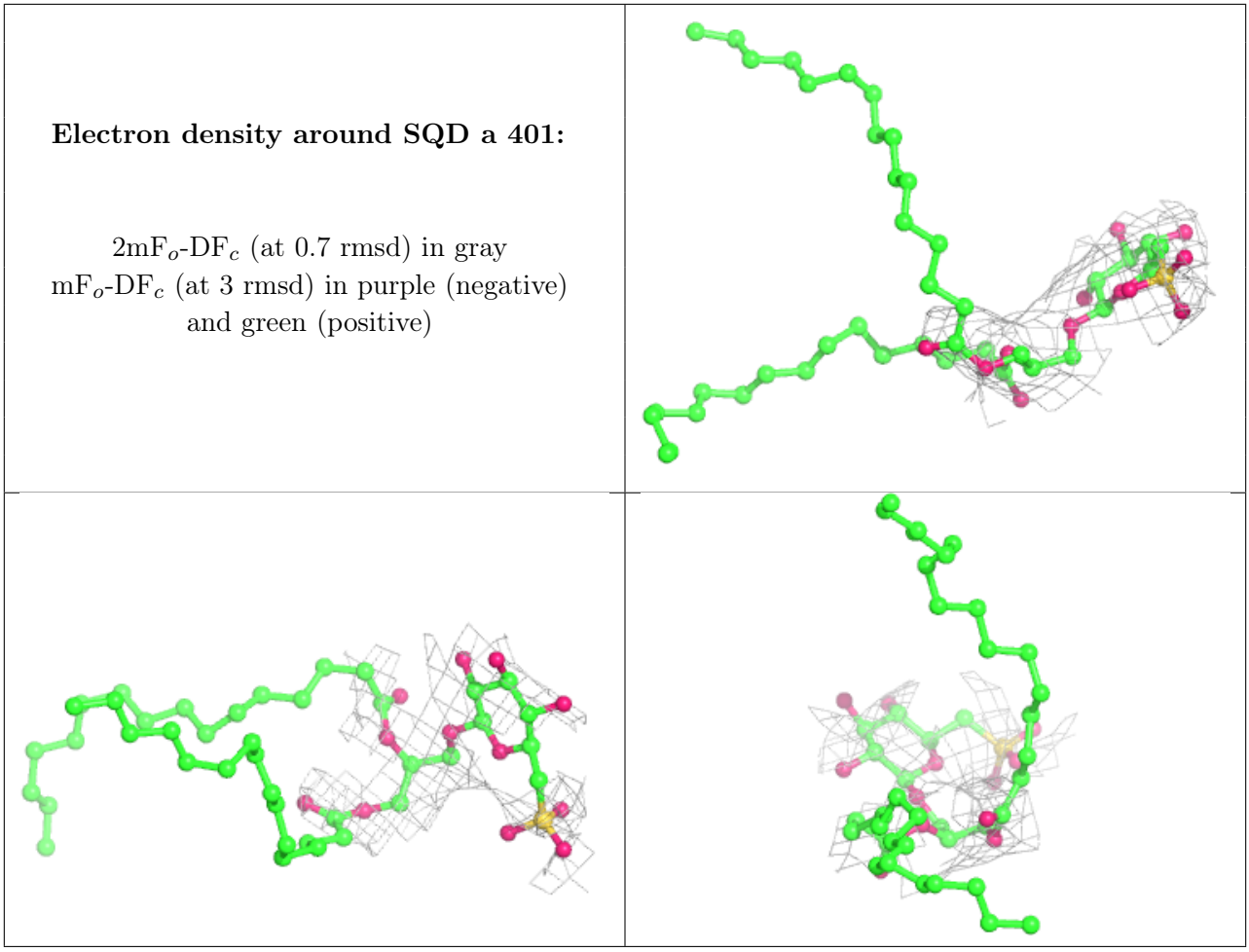
Electron density around PHO A 405:

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



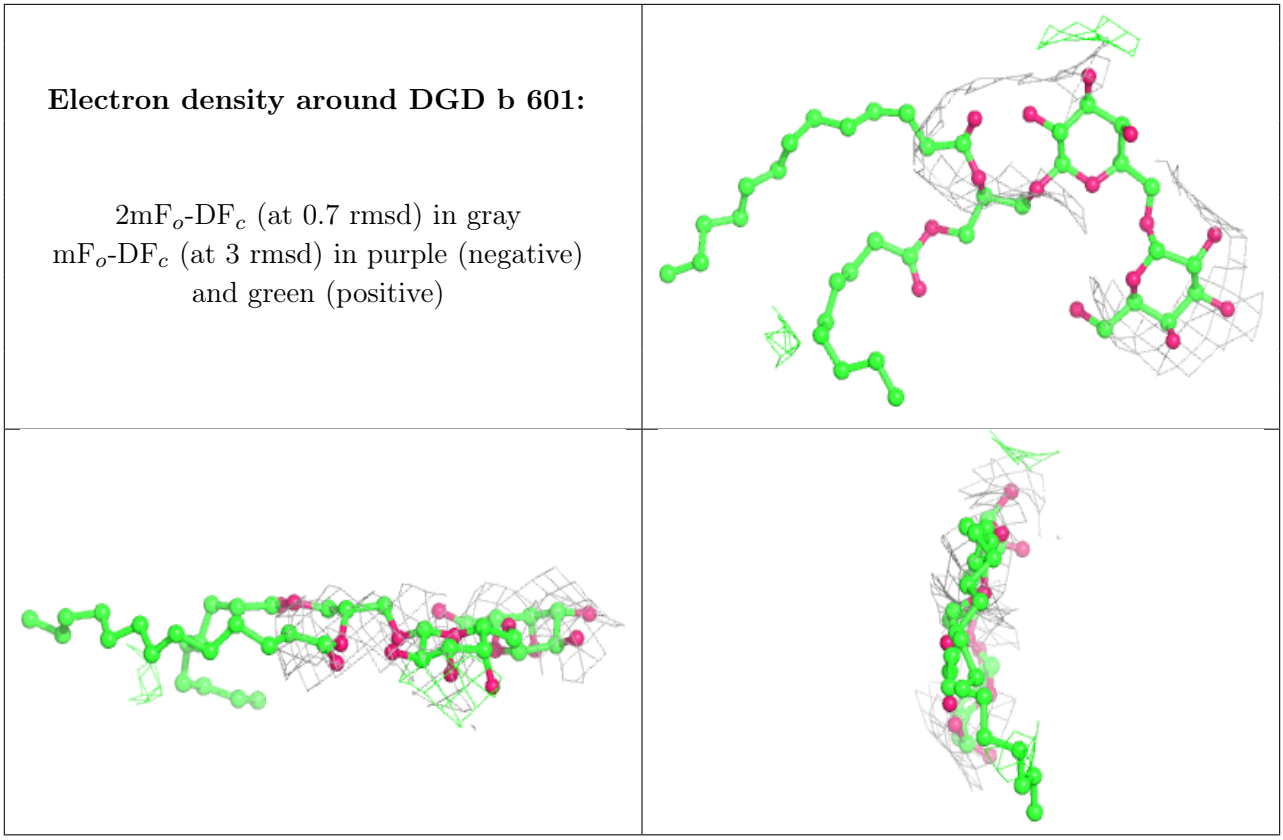
Electron density around SQD a 401:

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



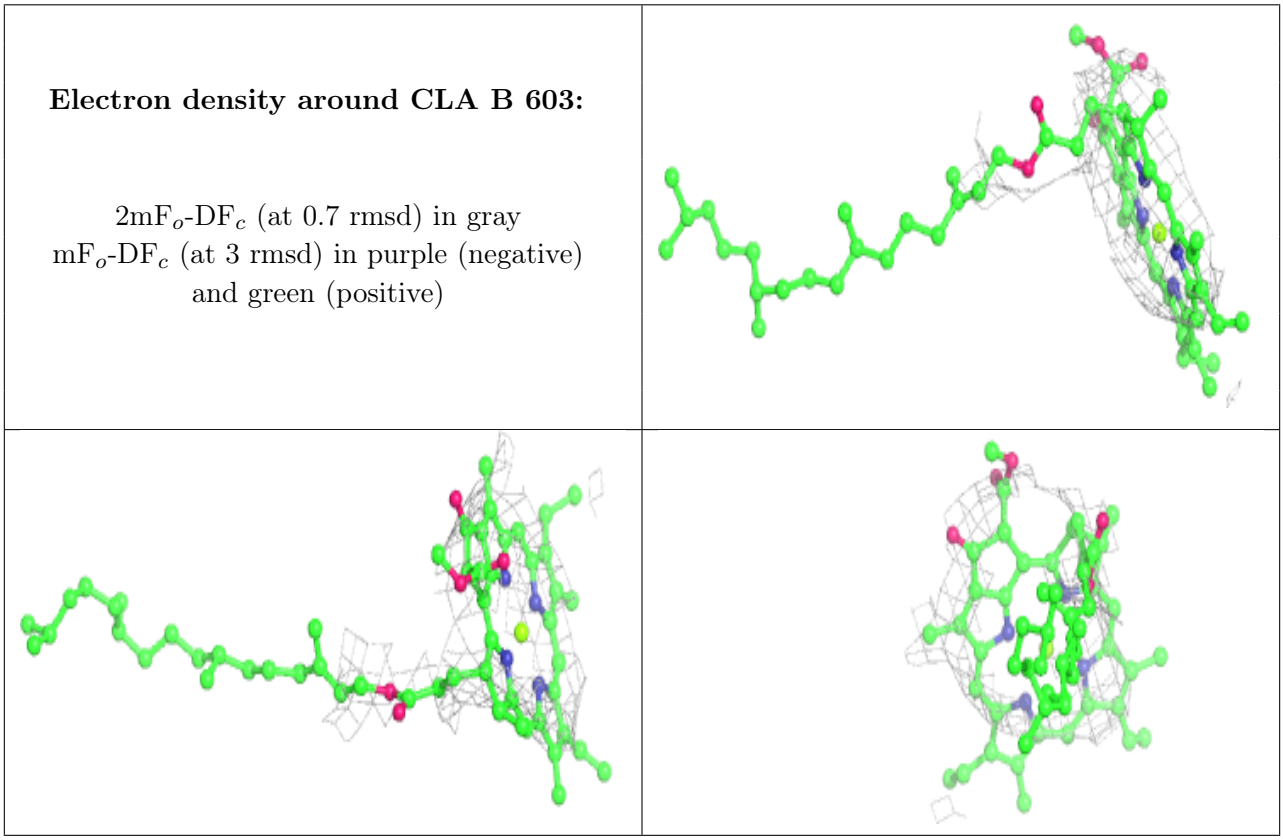
Electron density around DGD b 601:

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



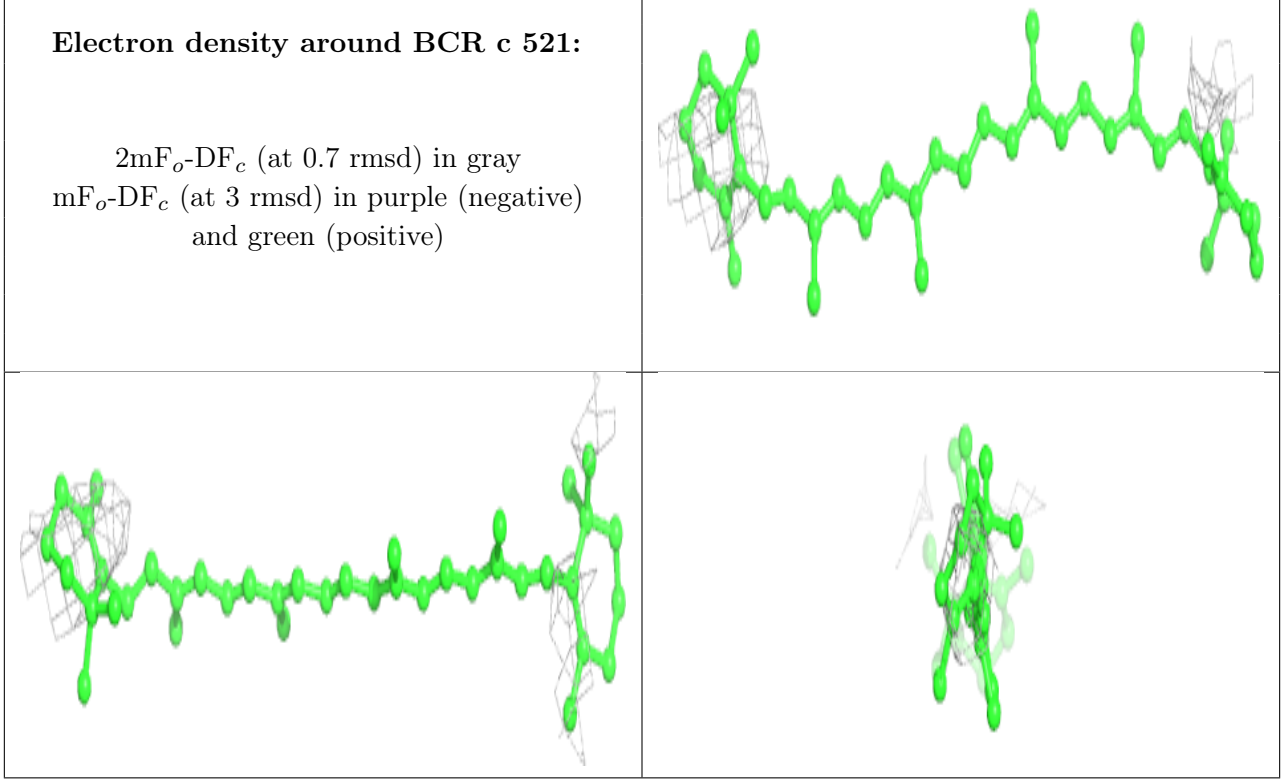
Electron density around CLA B 603:

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



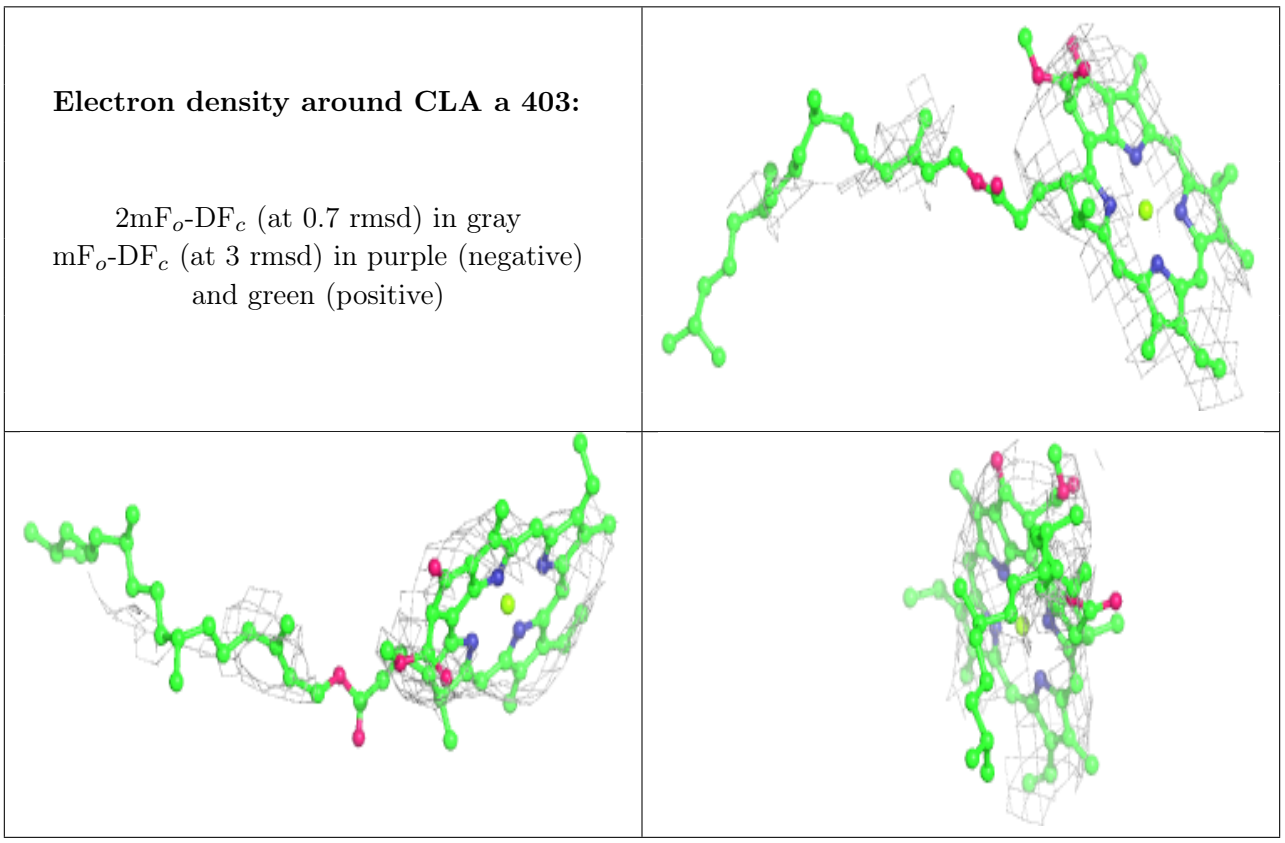
Electron density around BCR c 521:

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



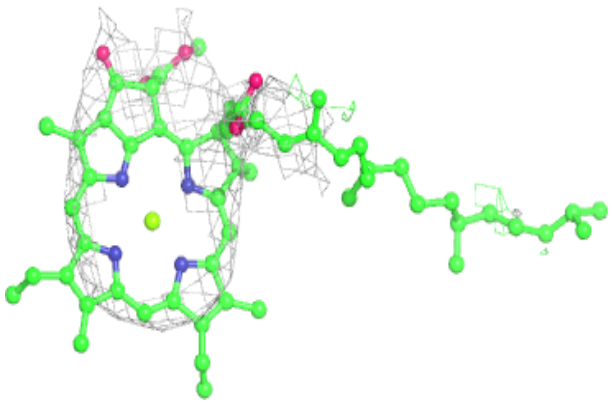
Electron density around CLA a 403:

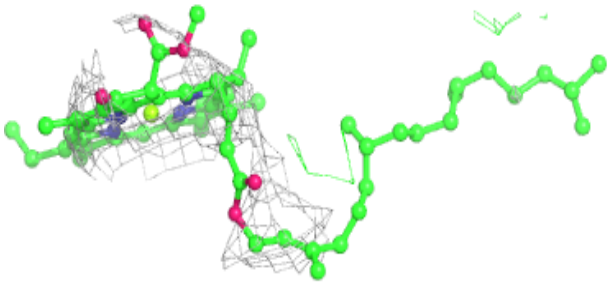
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

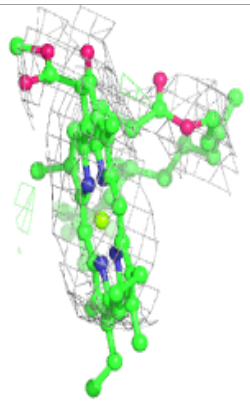


Electron density around CLA A 404:

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

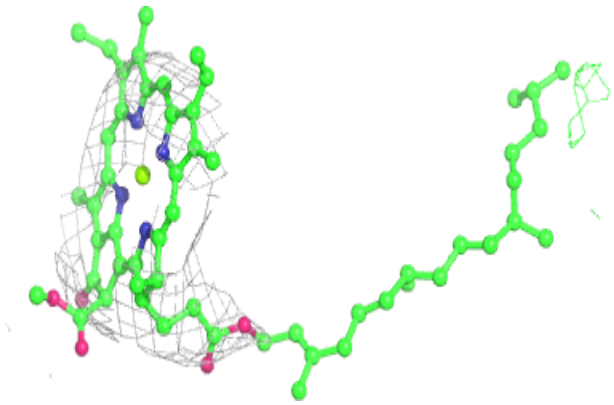


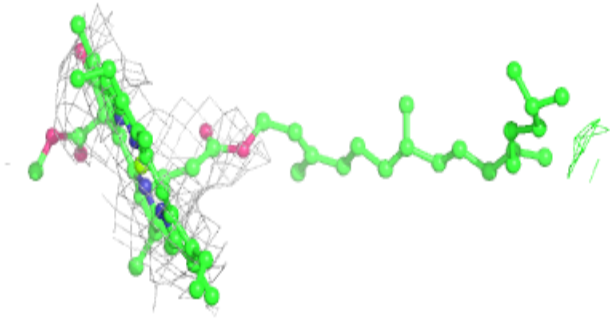


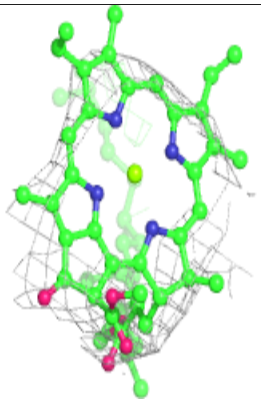


Electron density around CLA b 613:

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

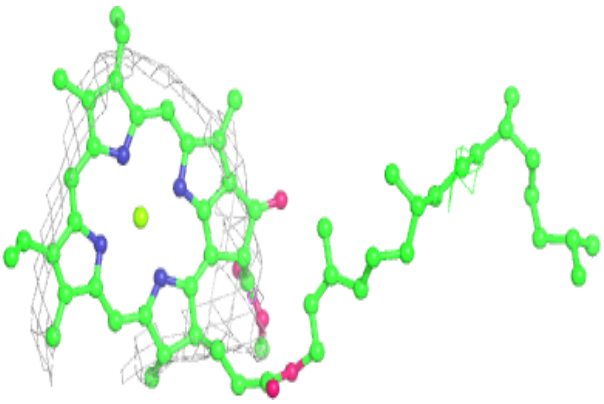


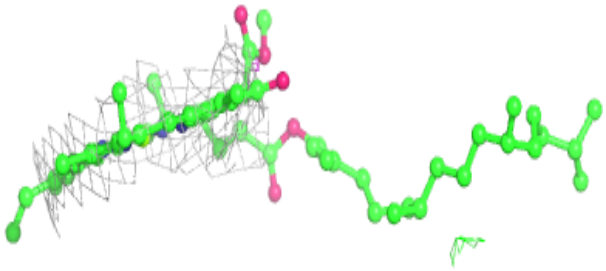


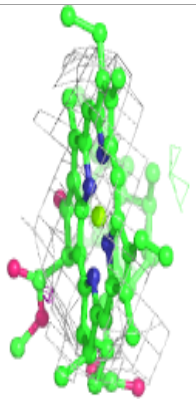


Electron density around CLA b 606:

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

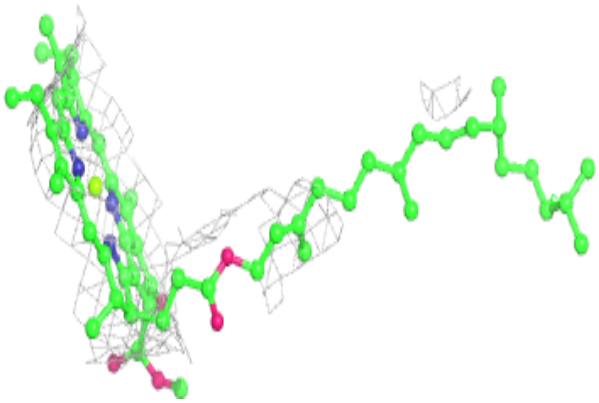


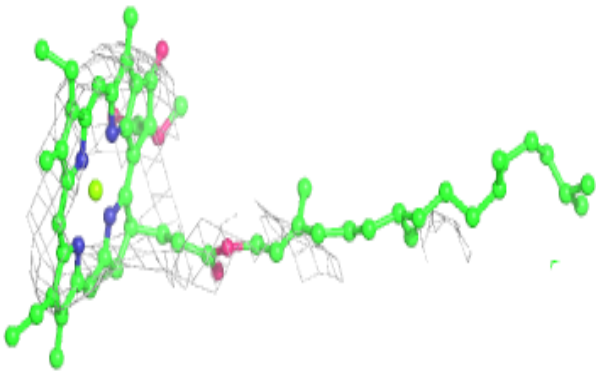


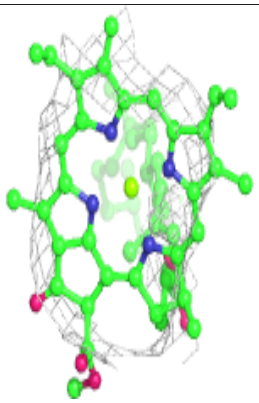


Electron density around CLA b 608:

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

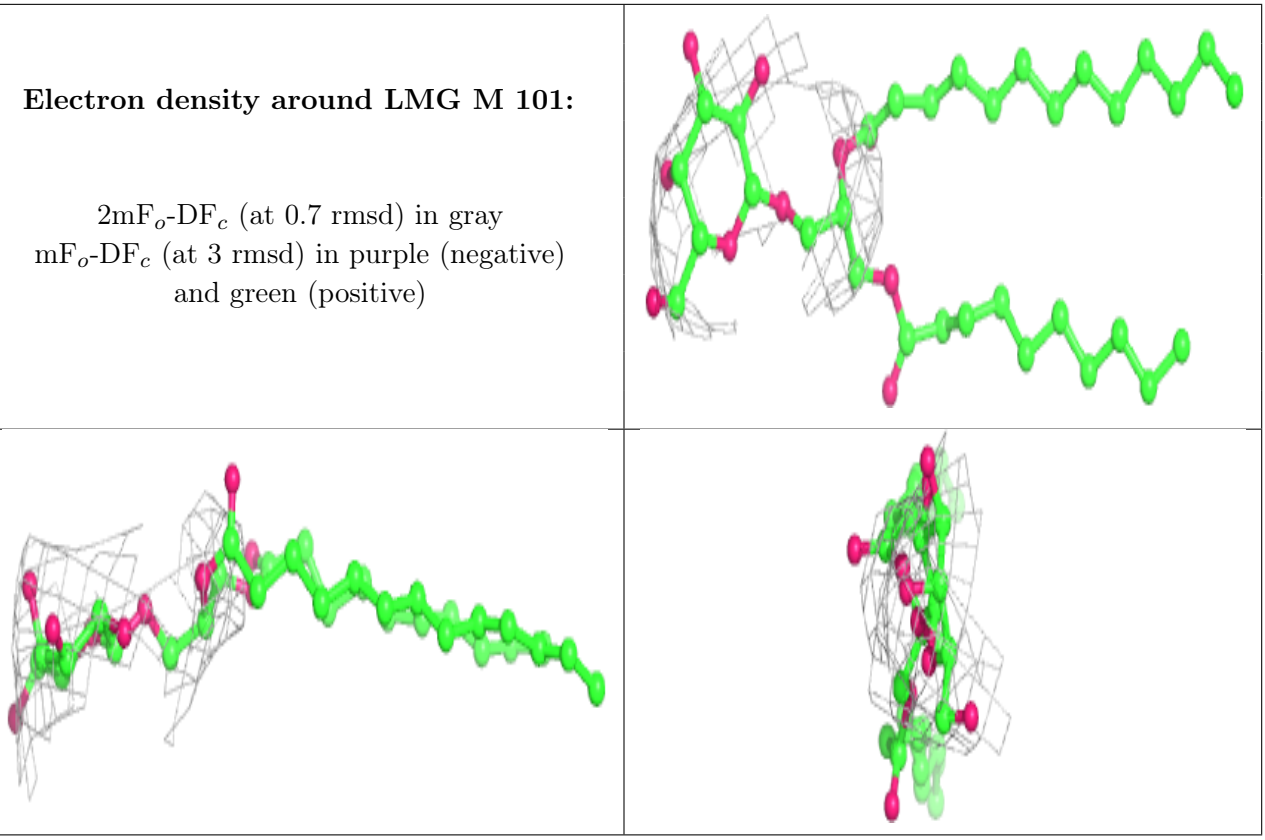






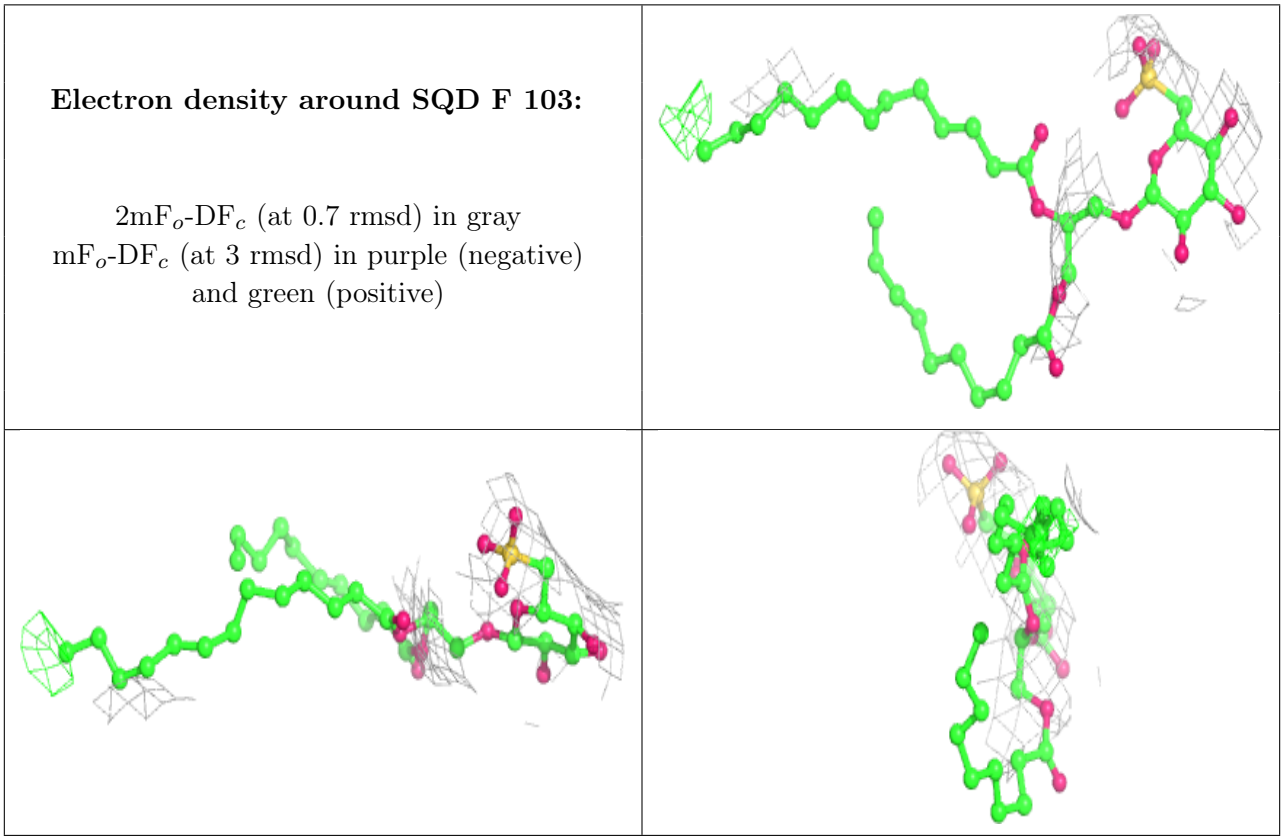
Electron density around LMG M 101:

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



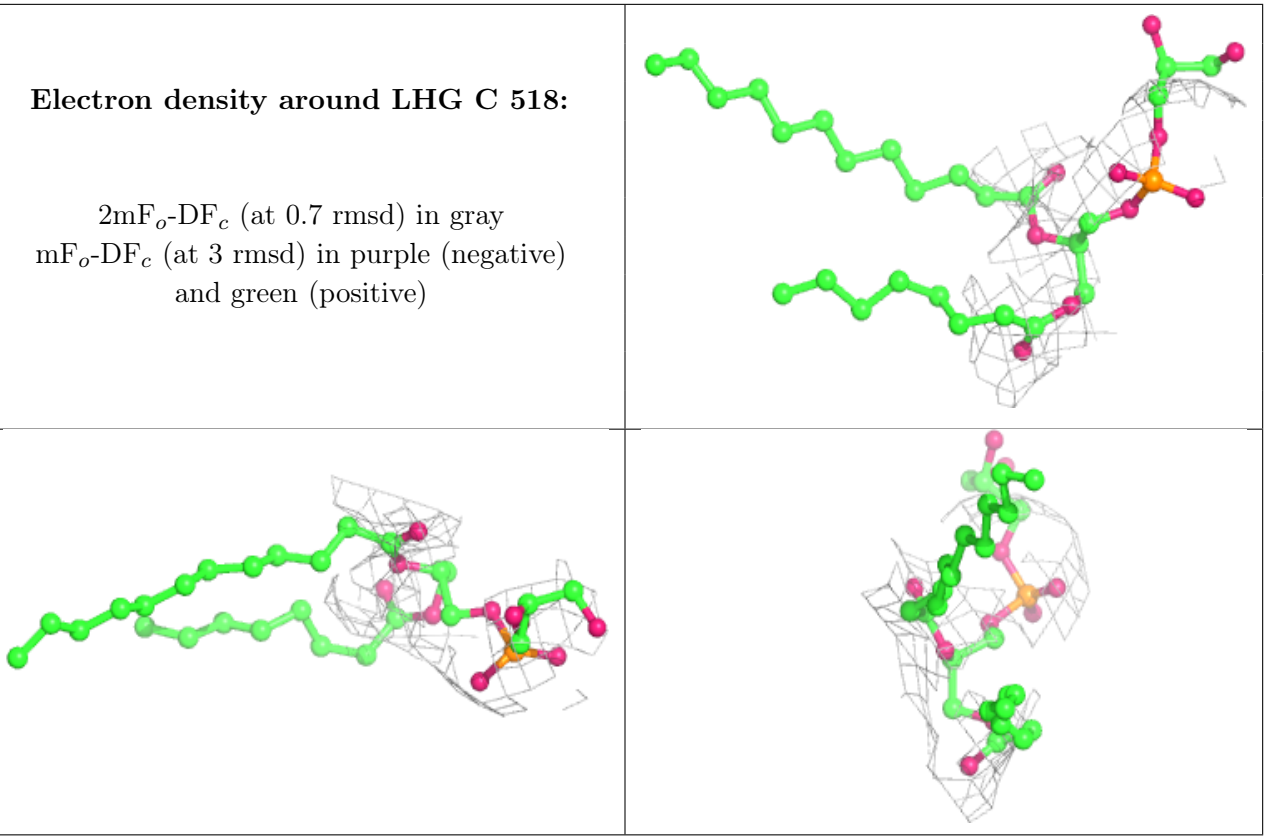
Electron density around SQD F 103:

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



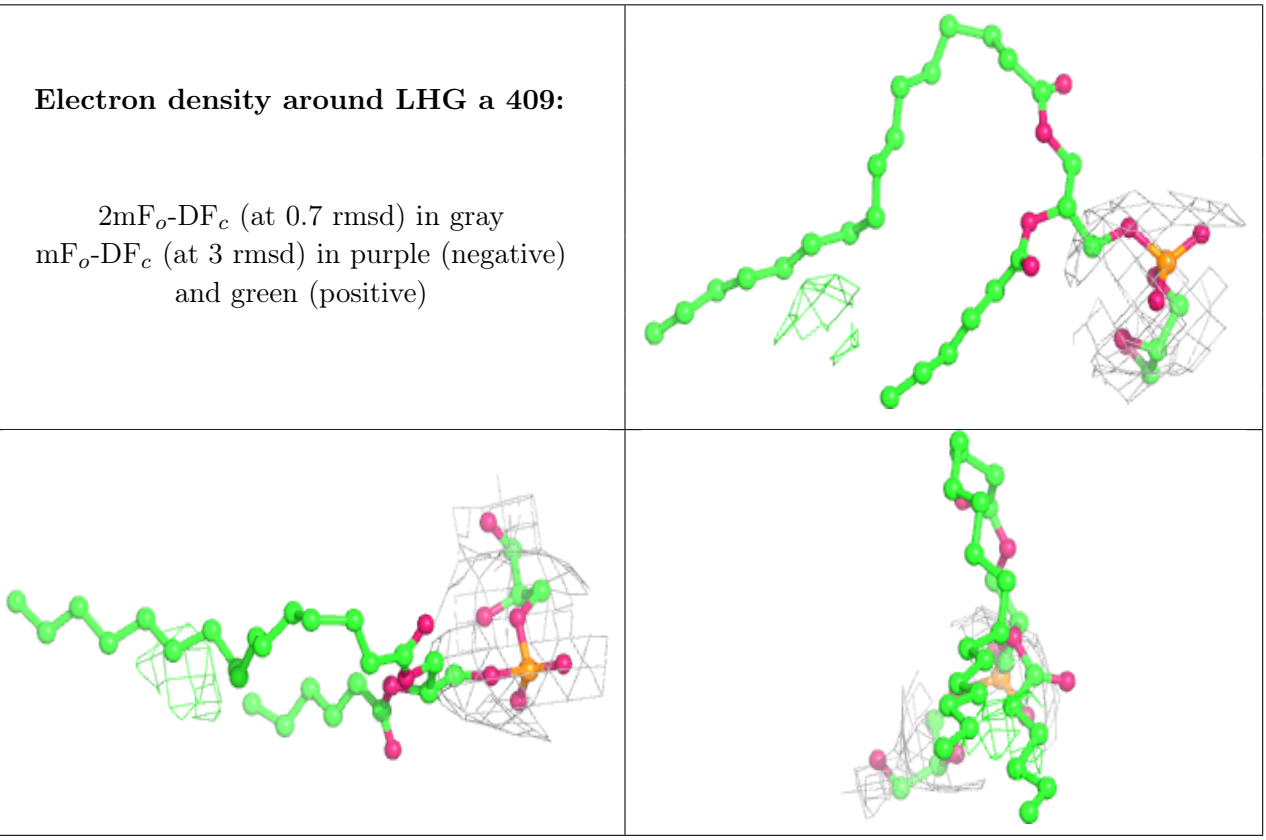
Electron density around LHG C 518:

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



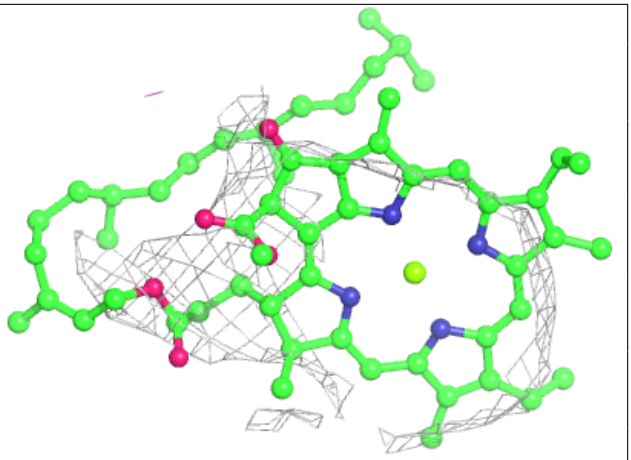
Electron density around LHG a 409:

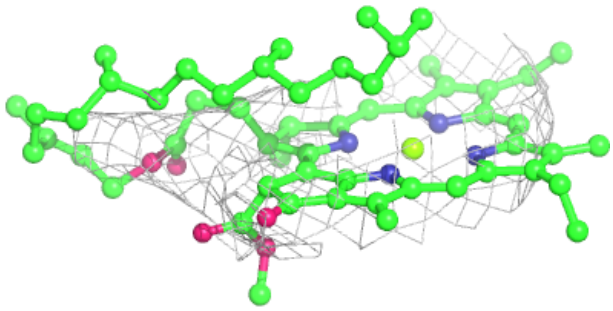
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

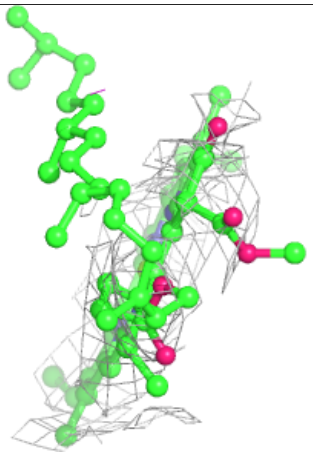


Electron density around CLA c 508:

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

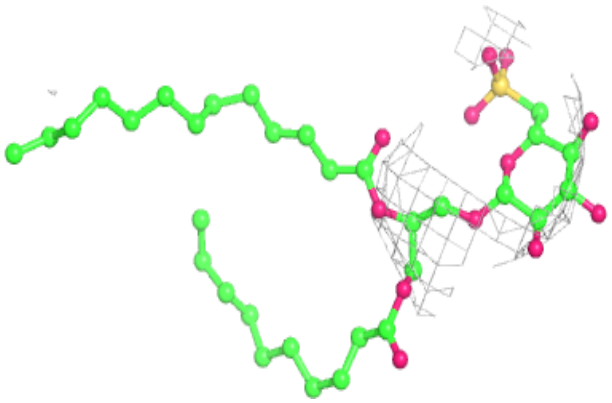


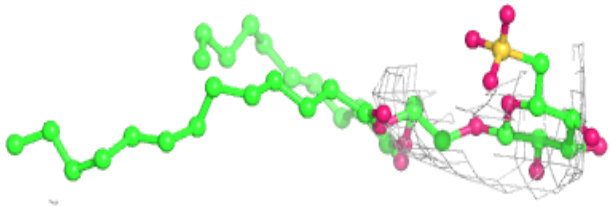


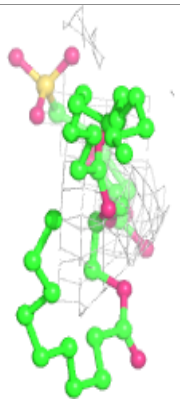


Electron density around SQD f 103:

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

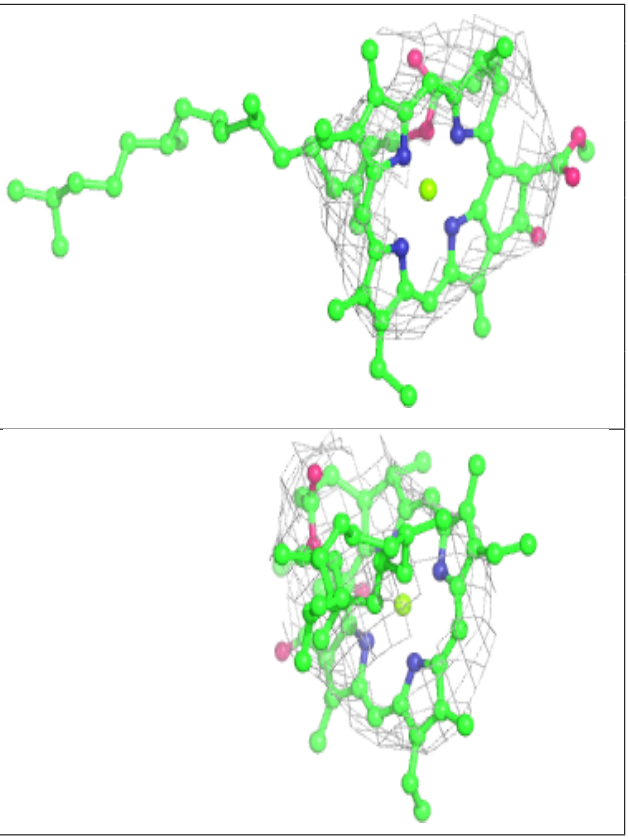


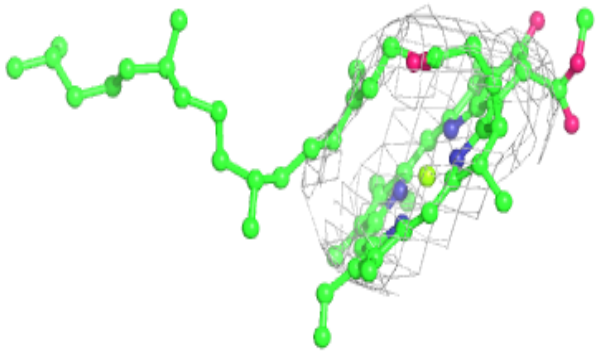




Electron density around CLA C 504:

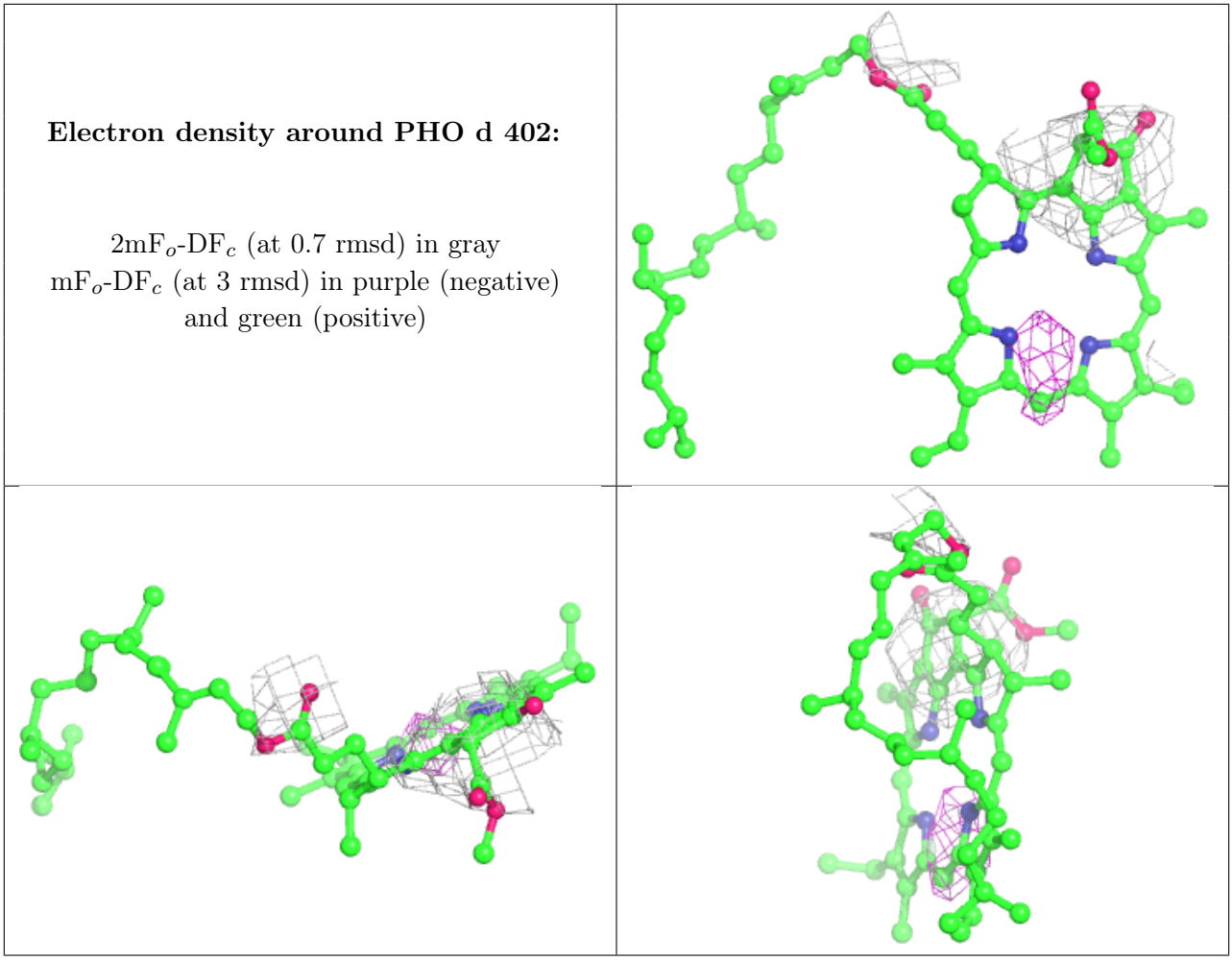
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





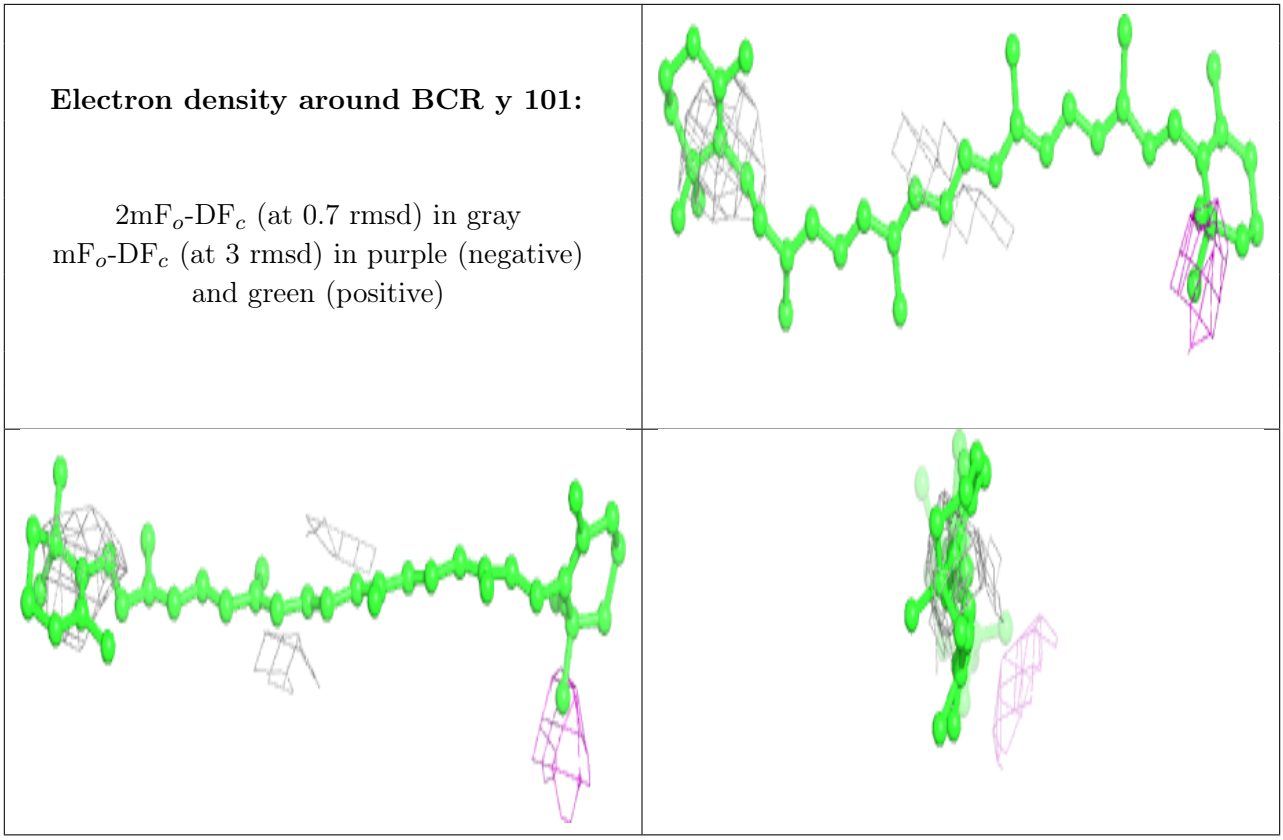
Electron density around PHO d 402:

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



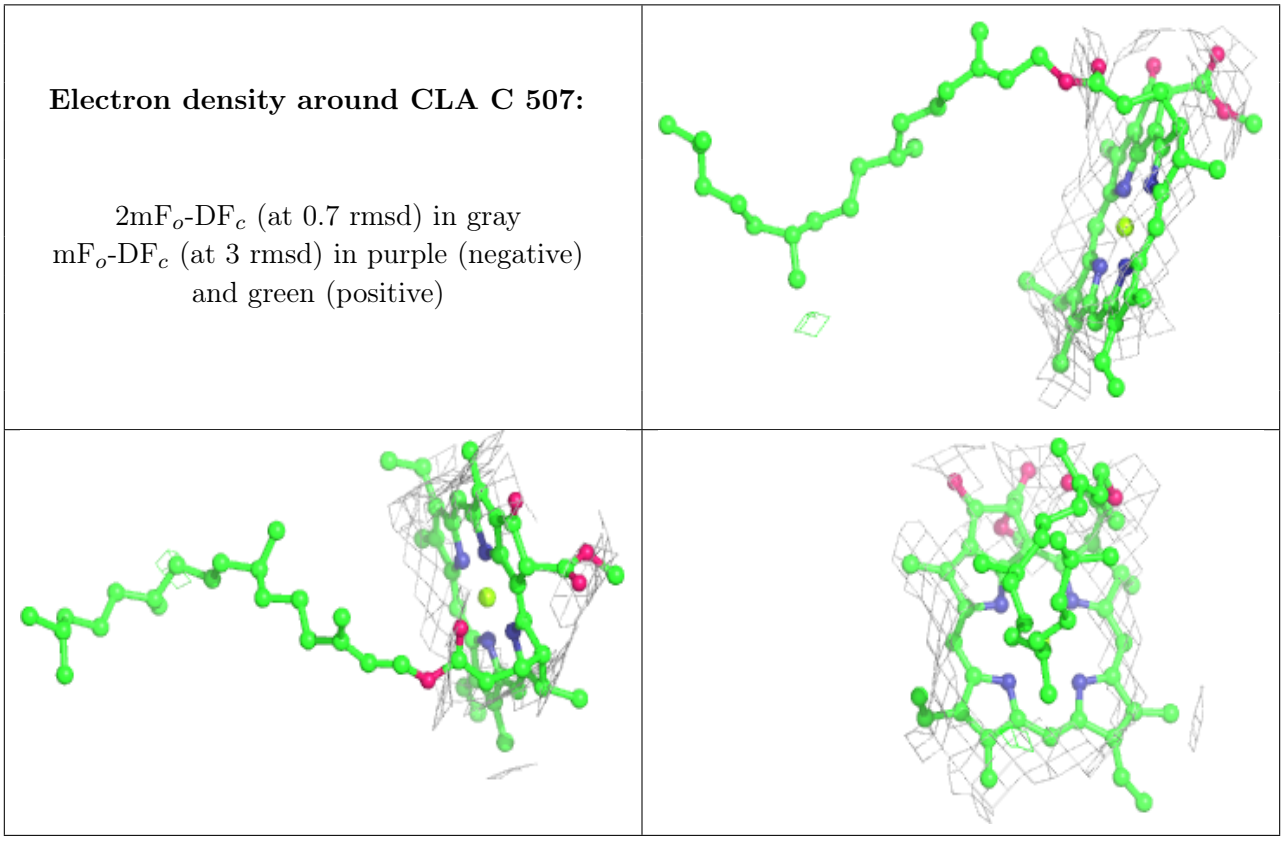
Electron density around BCR y 101:

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



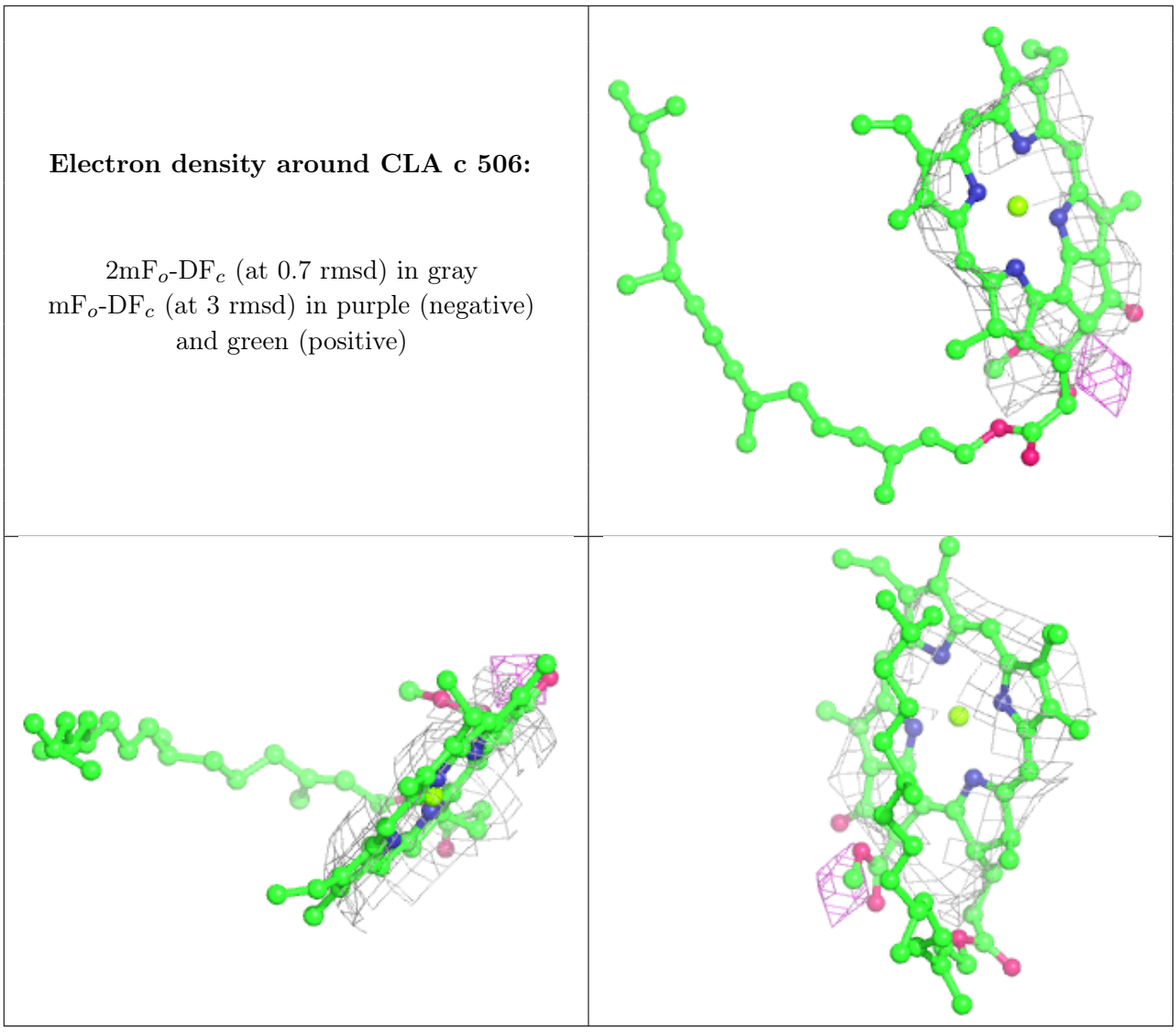
Electron density around CLA C 507:

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



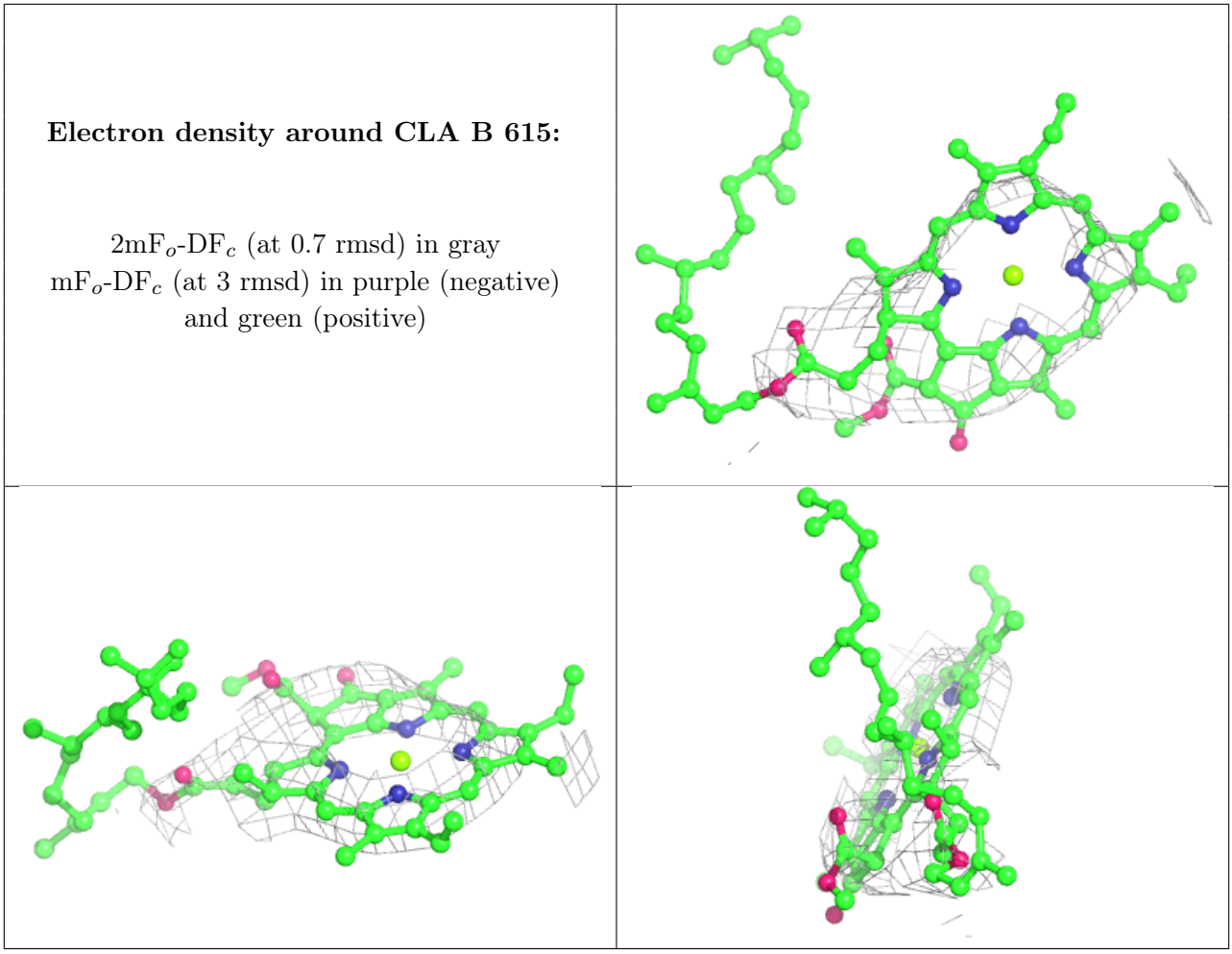
Electron density around CLA c 506:

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



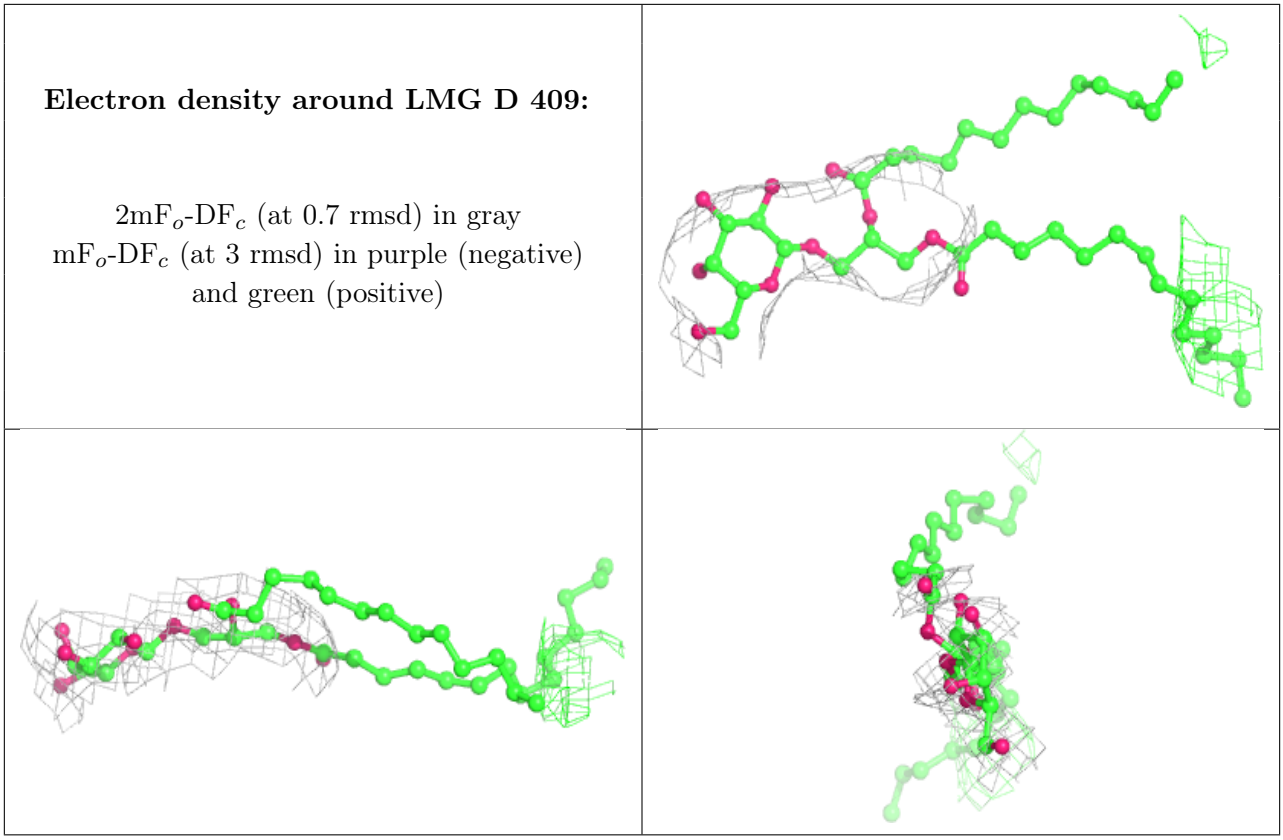
Electron density around CLA B 615:

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



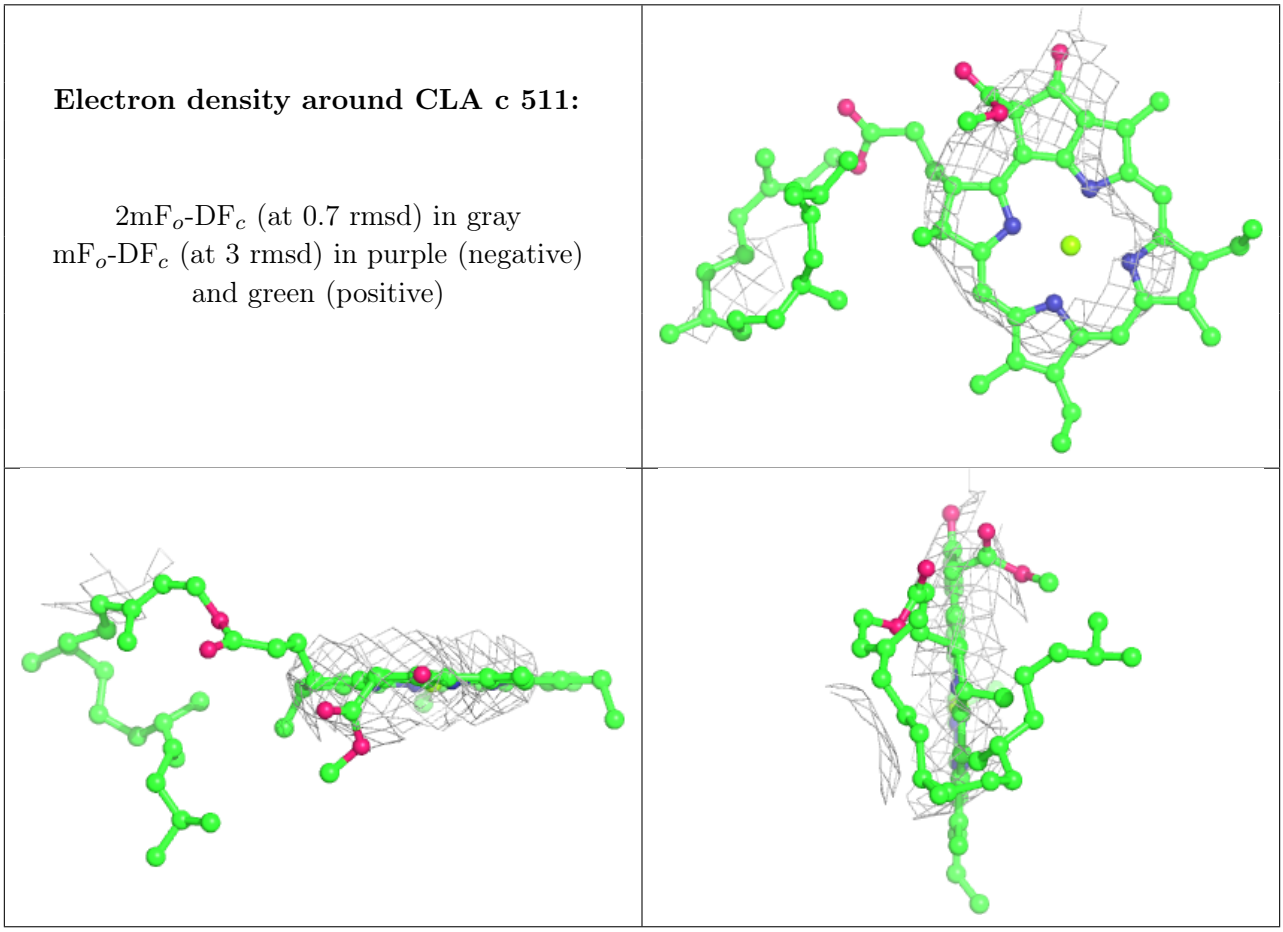
Electron density around LMG D 409:

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



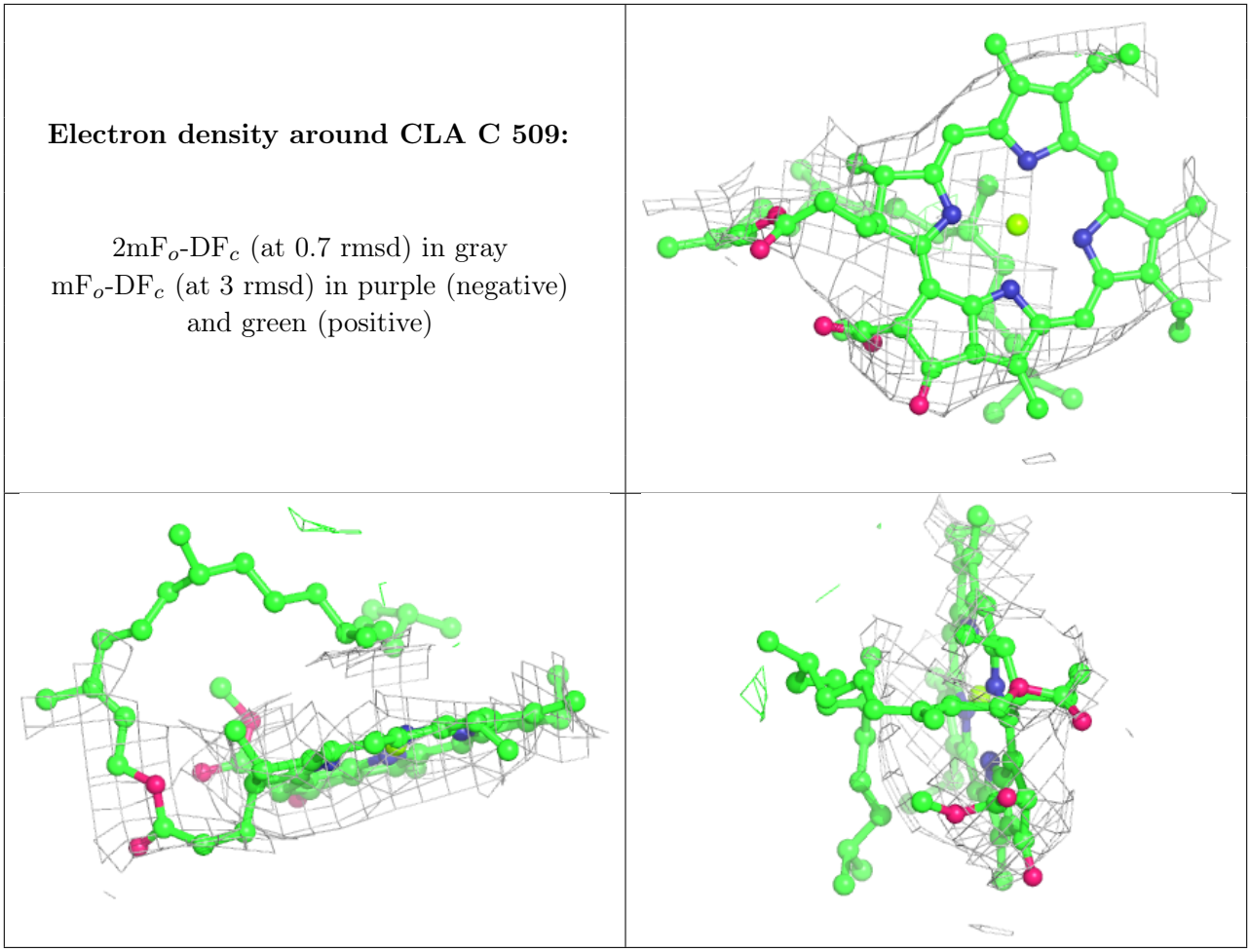
Electron density around CLA c 511:

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



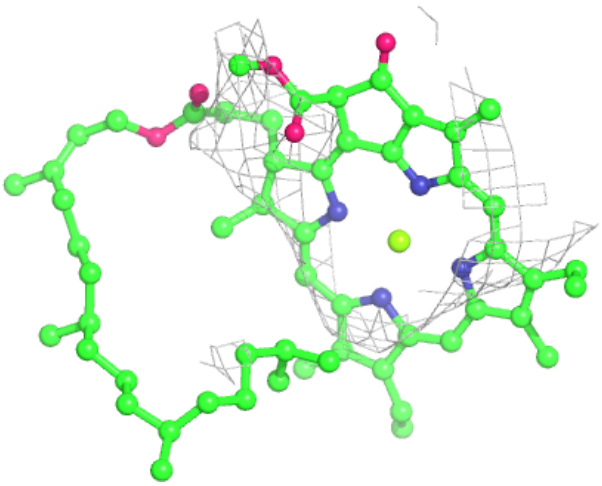
Electron density around CLA C 509:

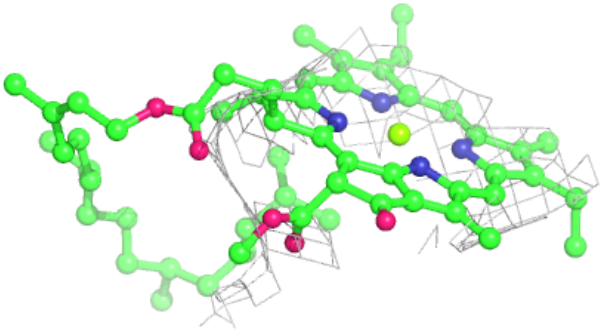
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

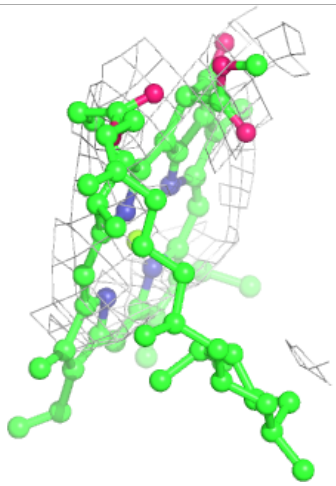


Electron density around CLA B 614:

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

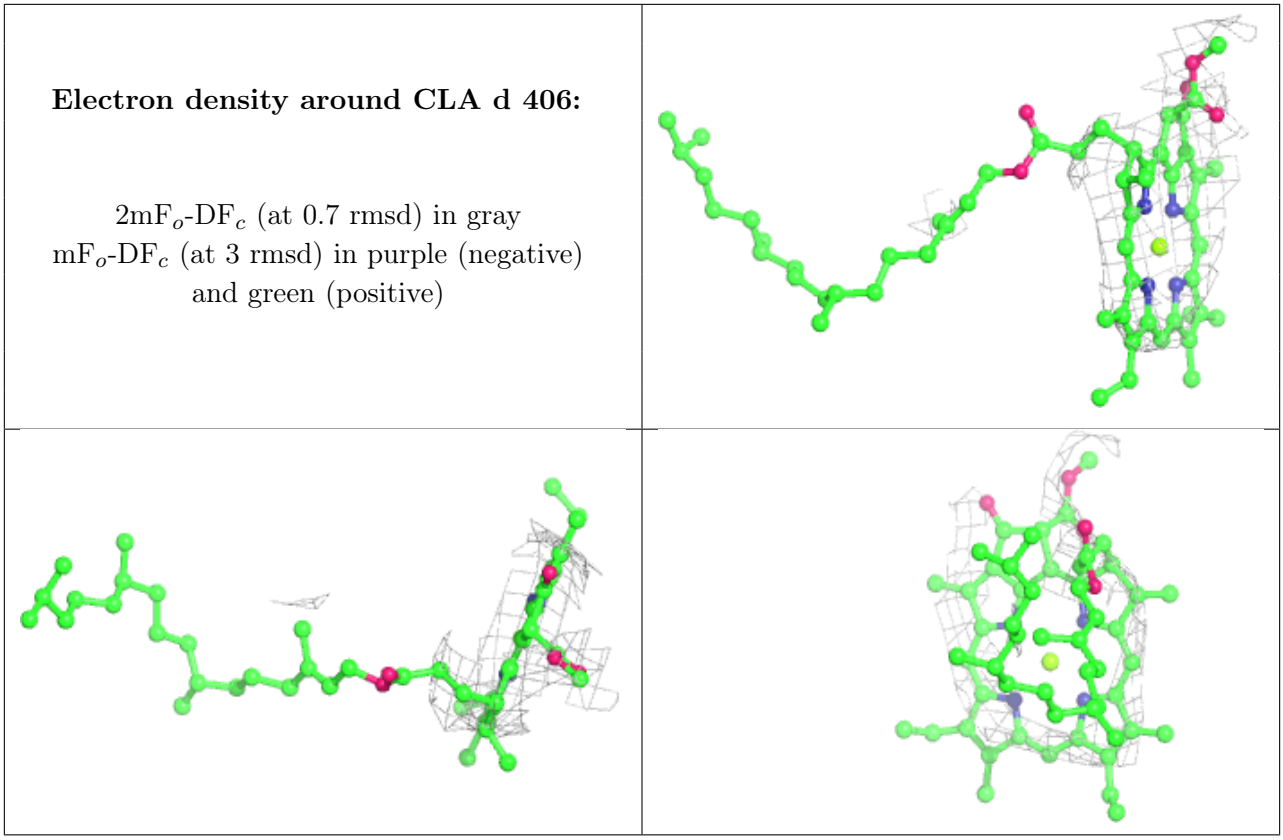






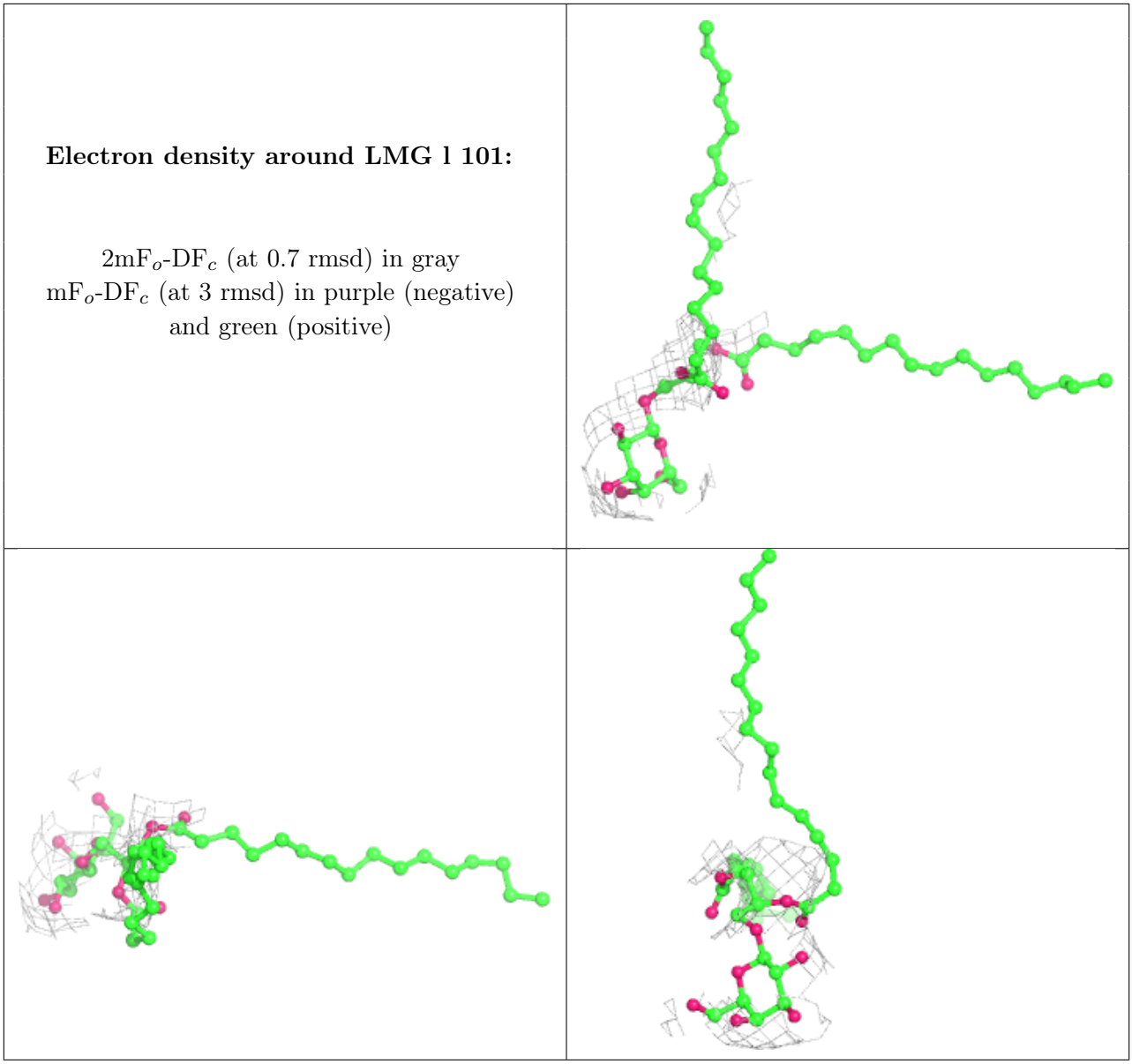
Electron density around CLA d 406:

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



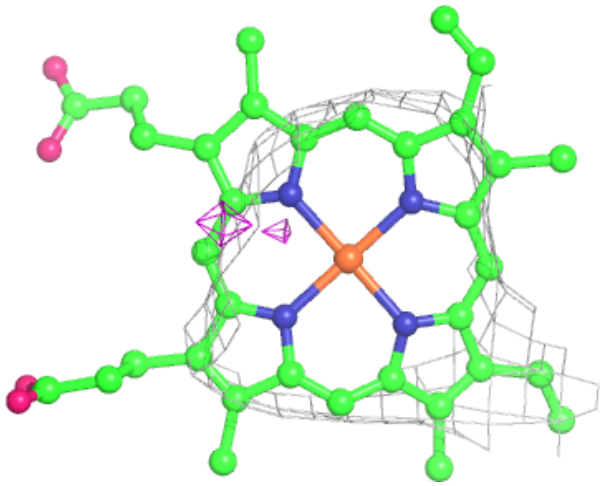
Electron density around LMG l 101:

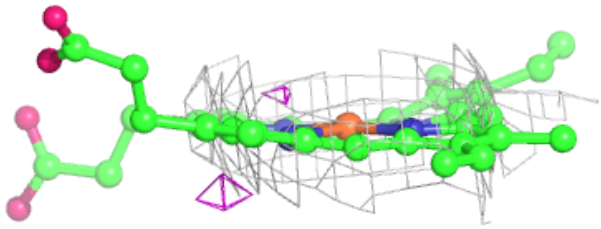
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

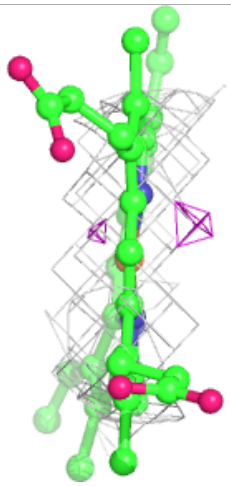


Electron density around HEM v 201:

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

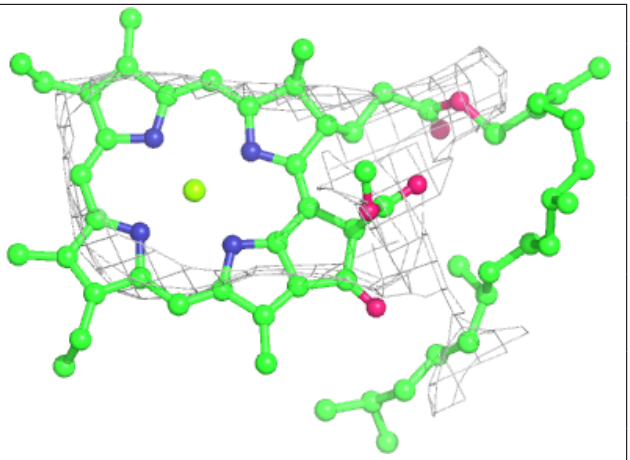


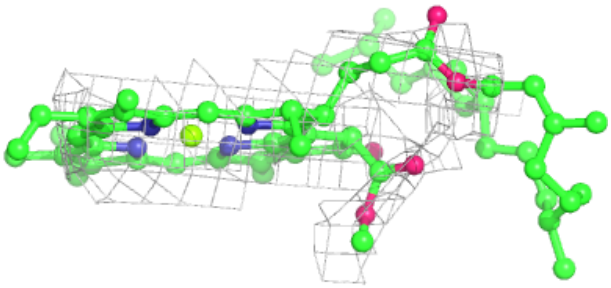


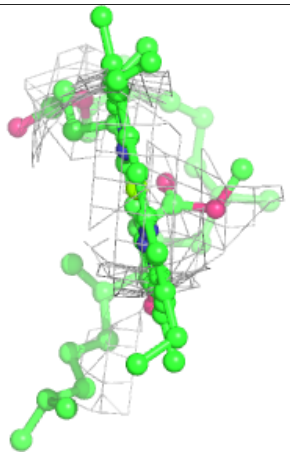


Electron density around CLA b 614:

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

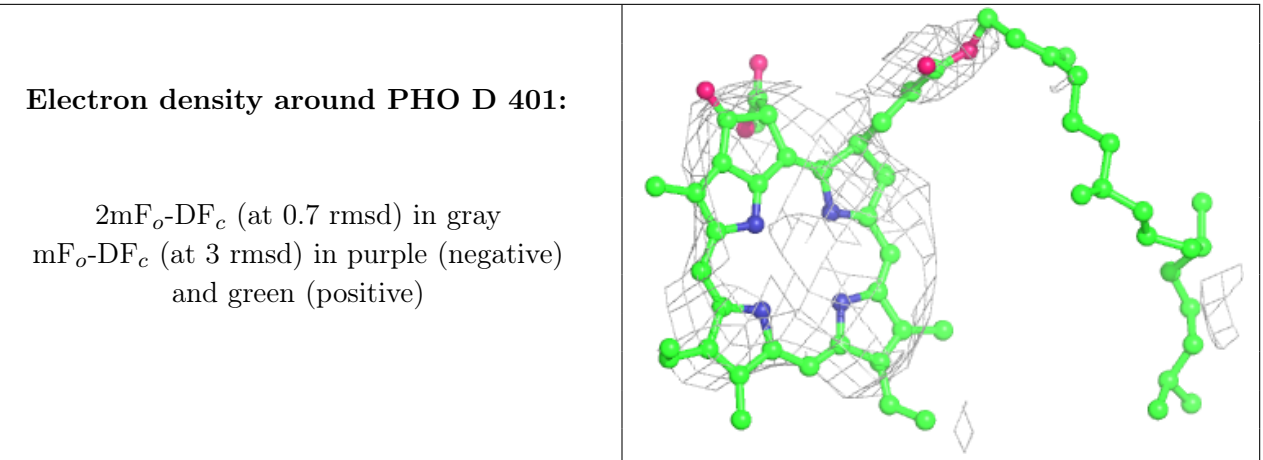


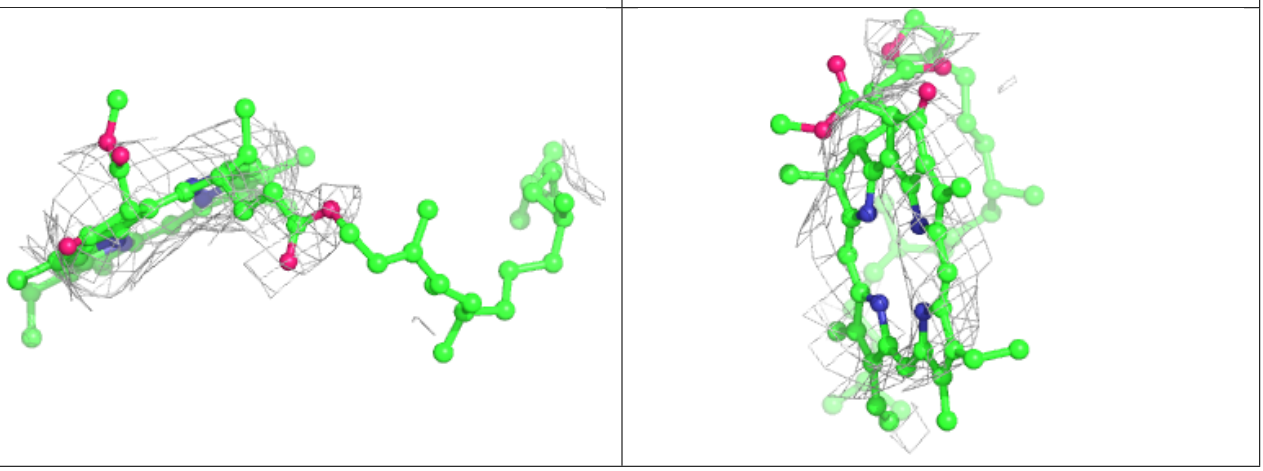




Electron density around PHO D 401:

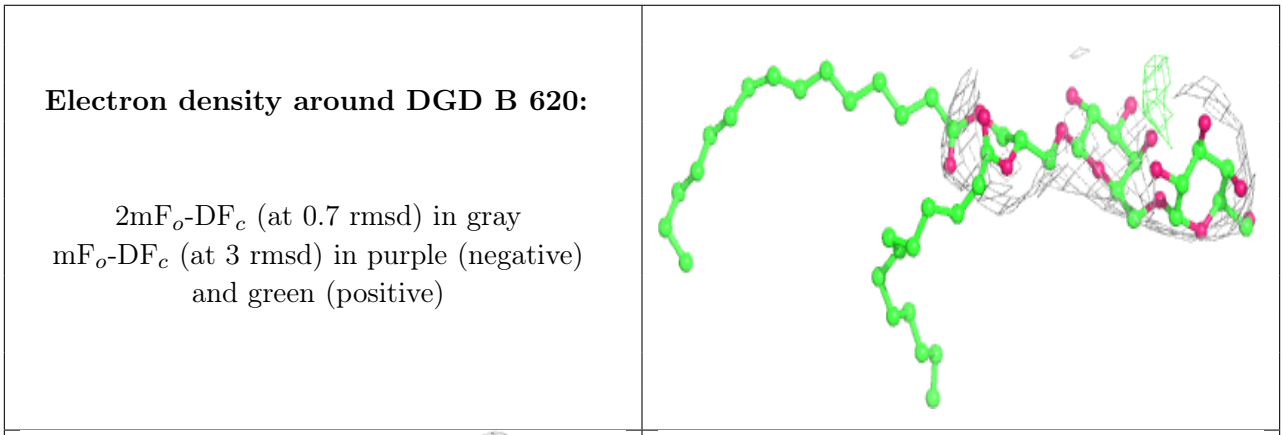
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

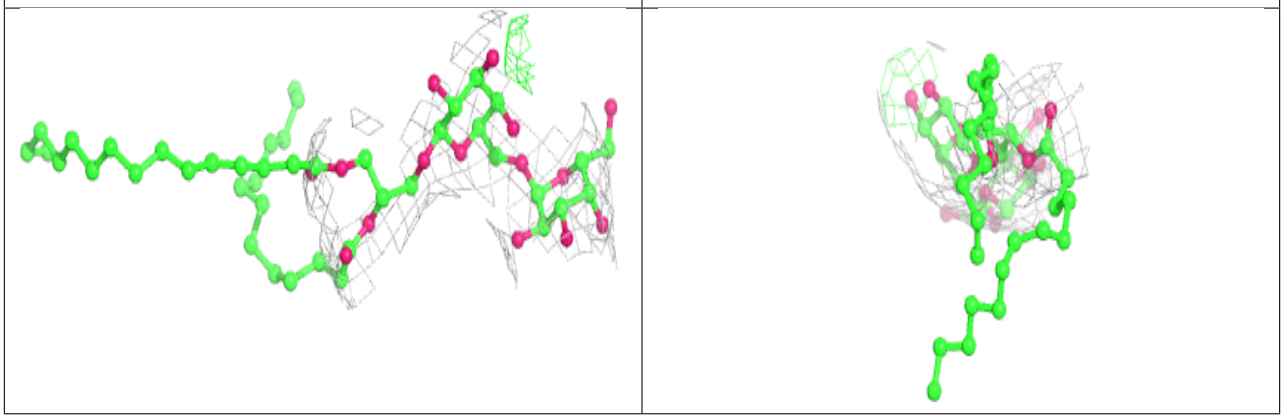




Electron density around DGD B 620:

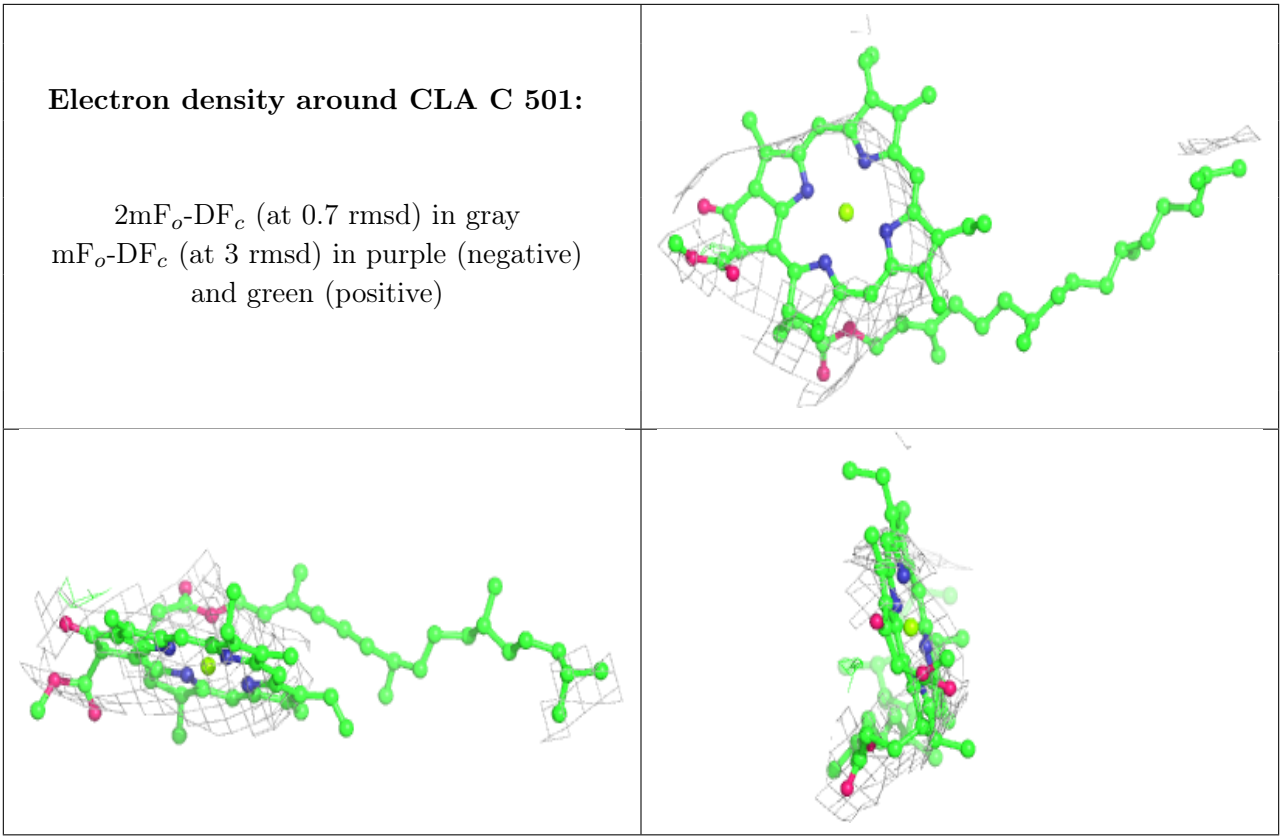
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





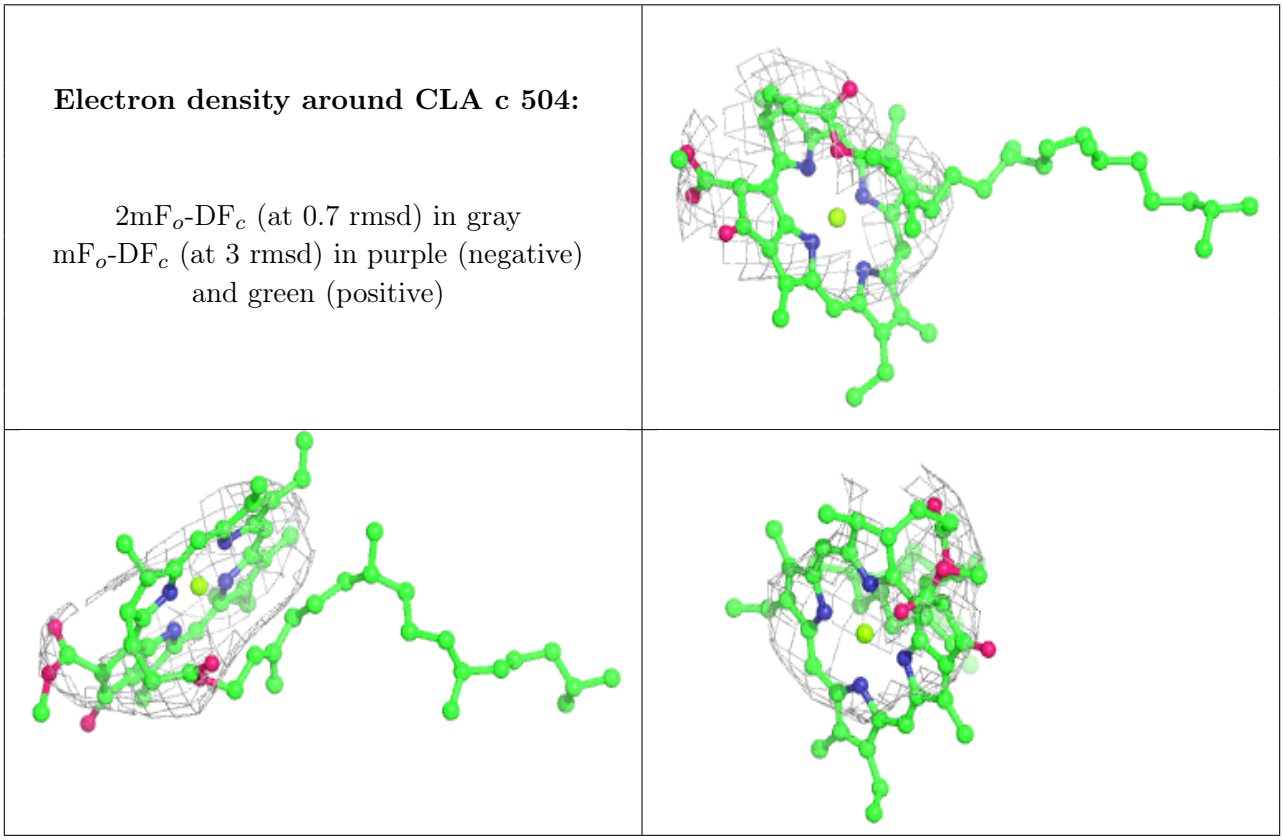
Electron density around CLA C 501:

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



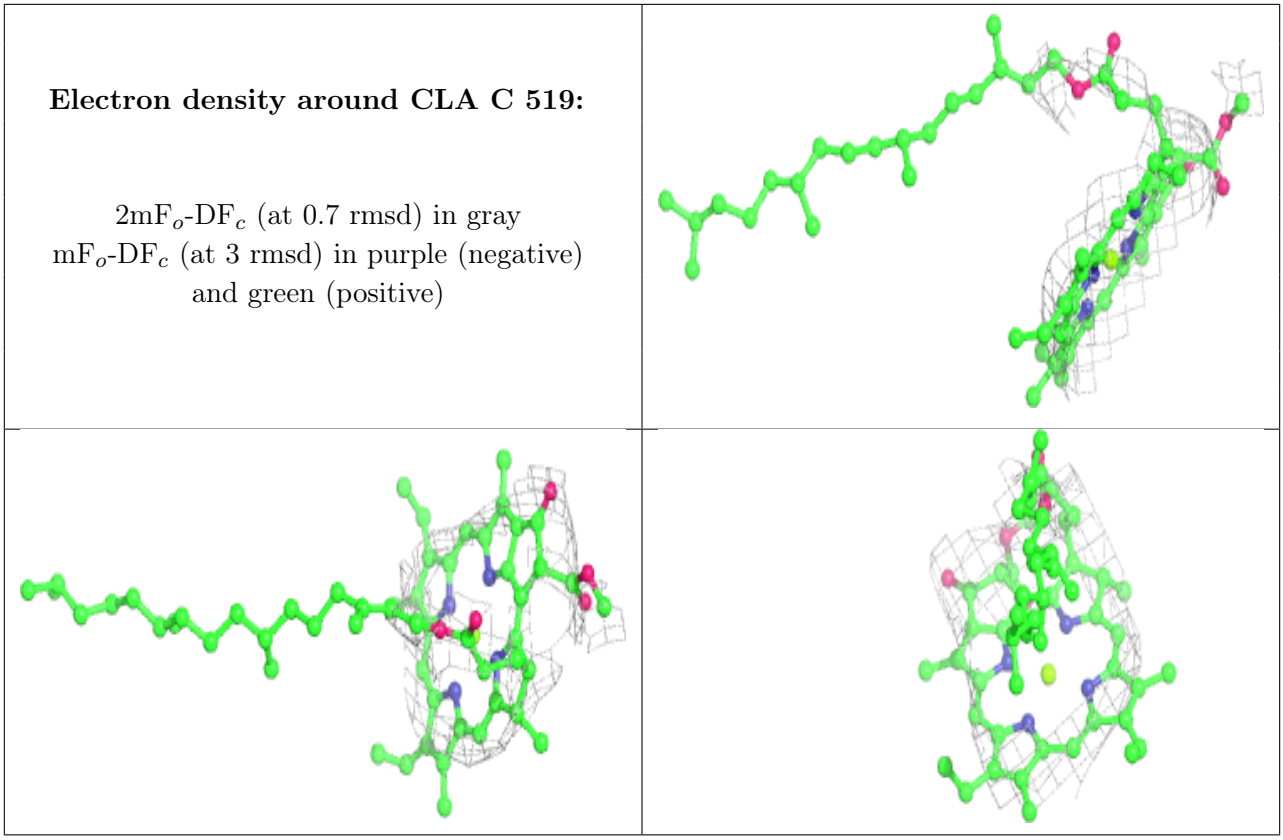
Electron density around CLA c 504:

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



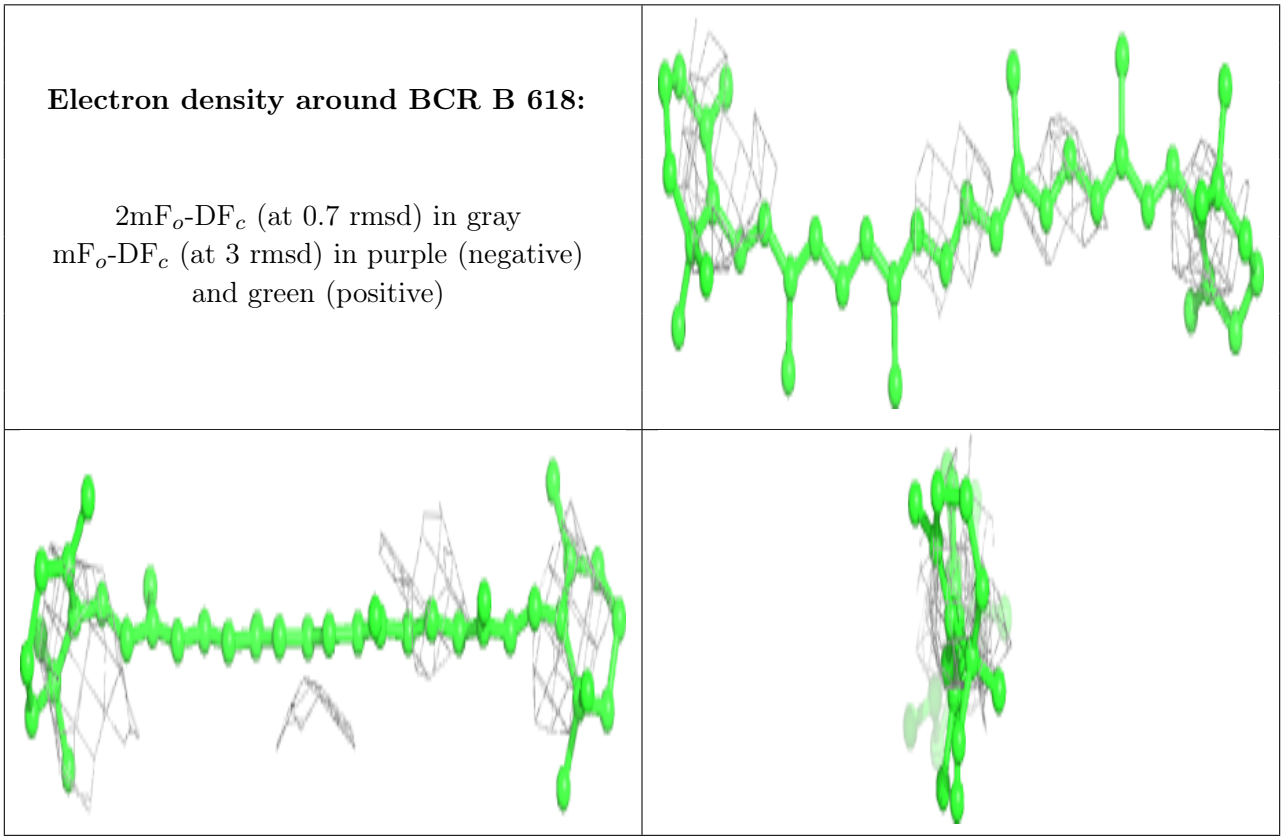
Electron density around CLA C 519:

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



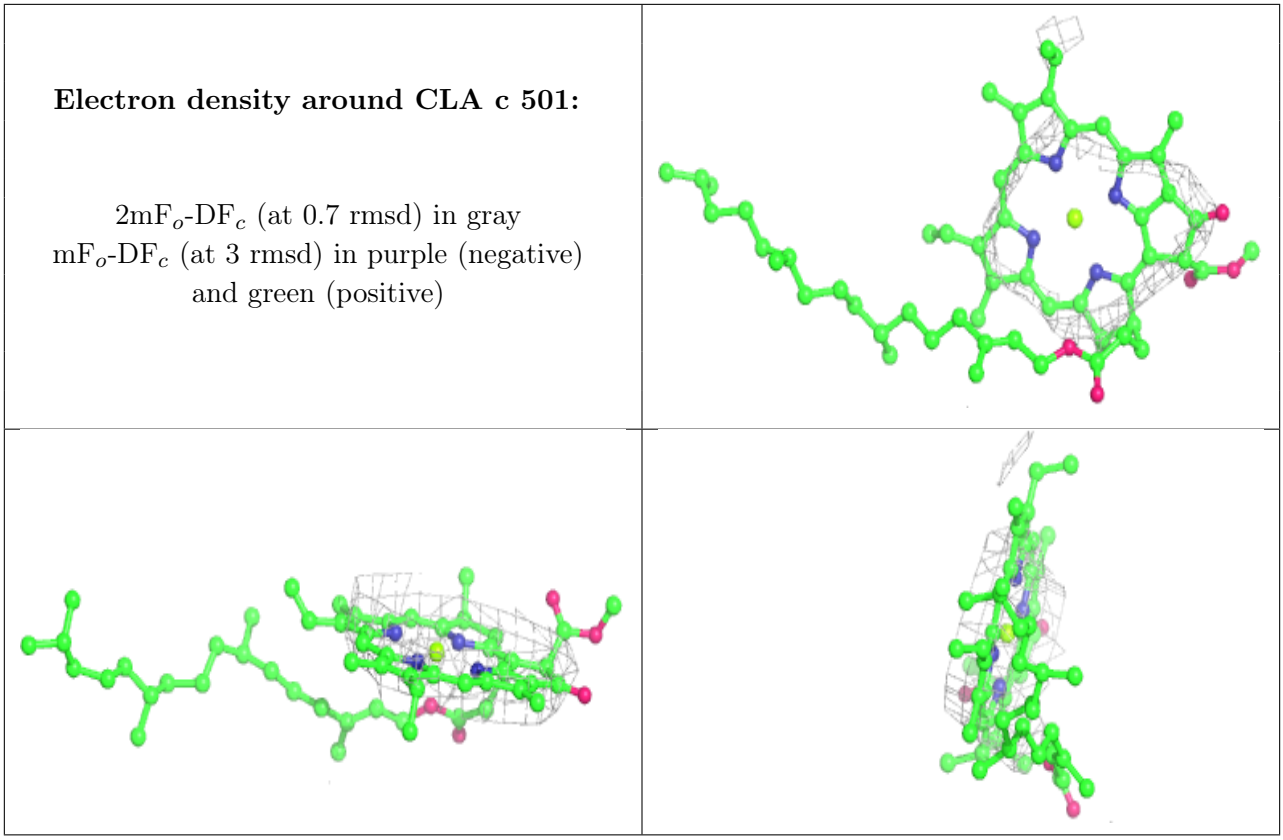
Electron density around BCR B 618:

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



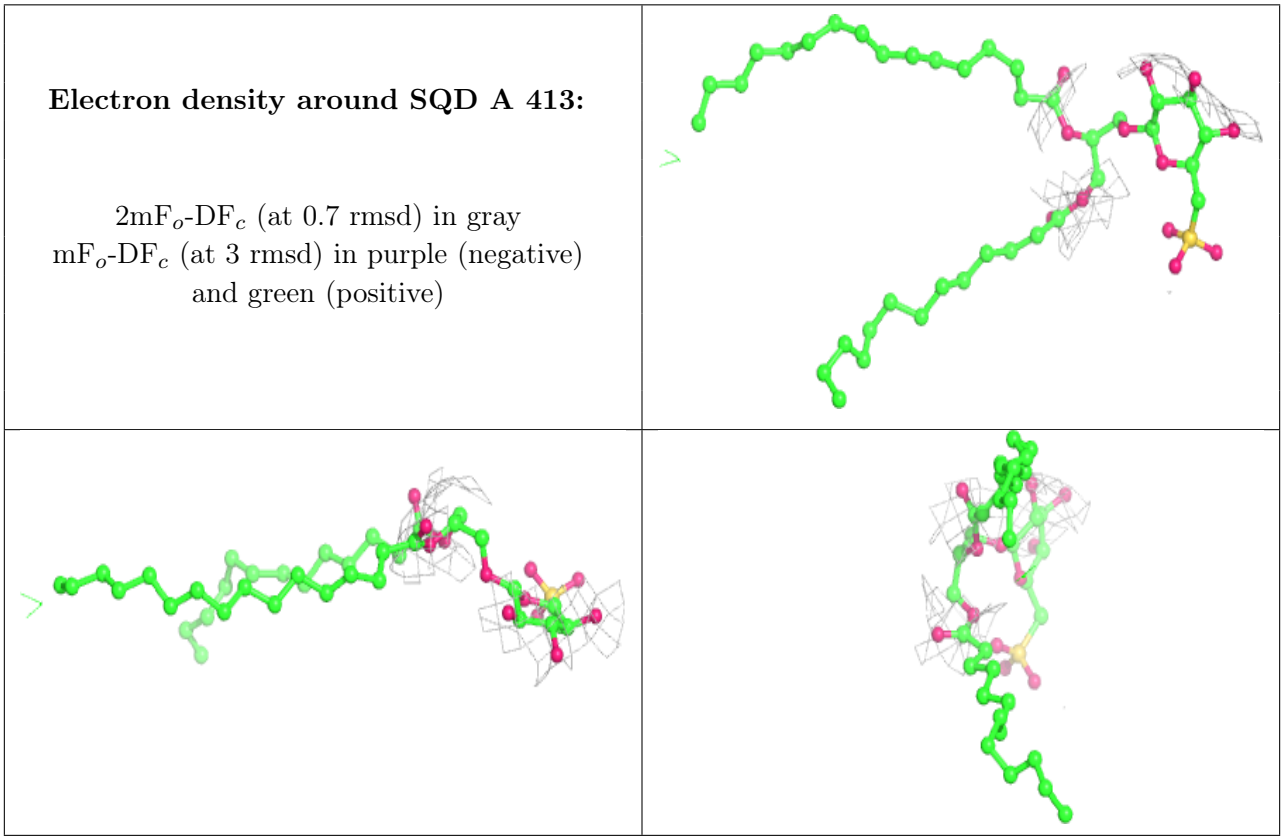
Electron density around CLA c 501:

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



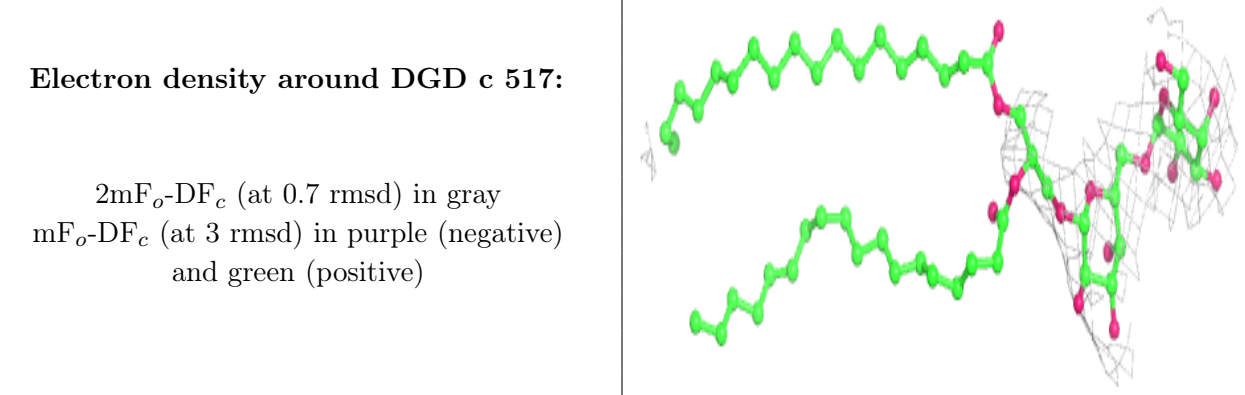
Electron density around SQD A 413:

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



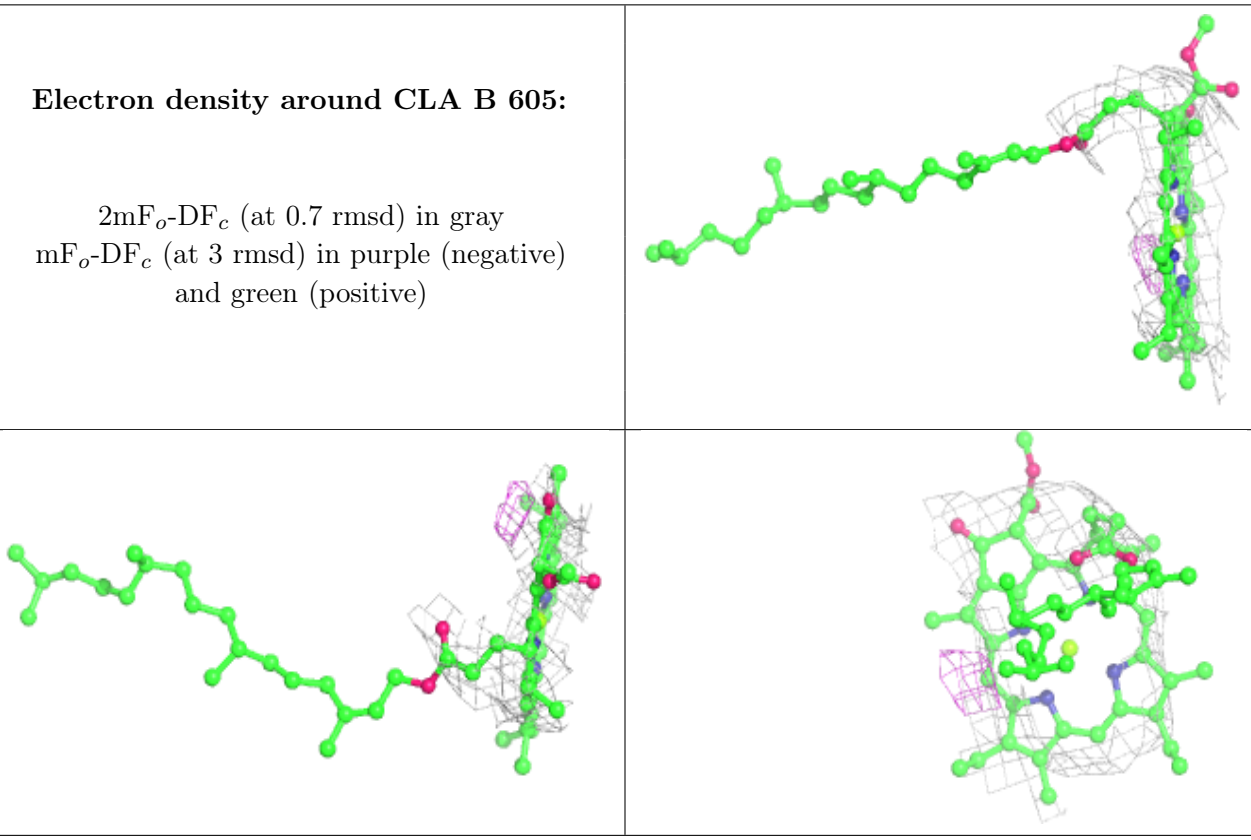
Electron density around DGD c 517:

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



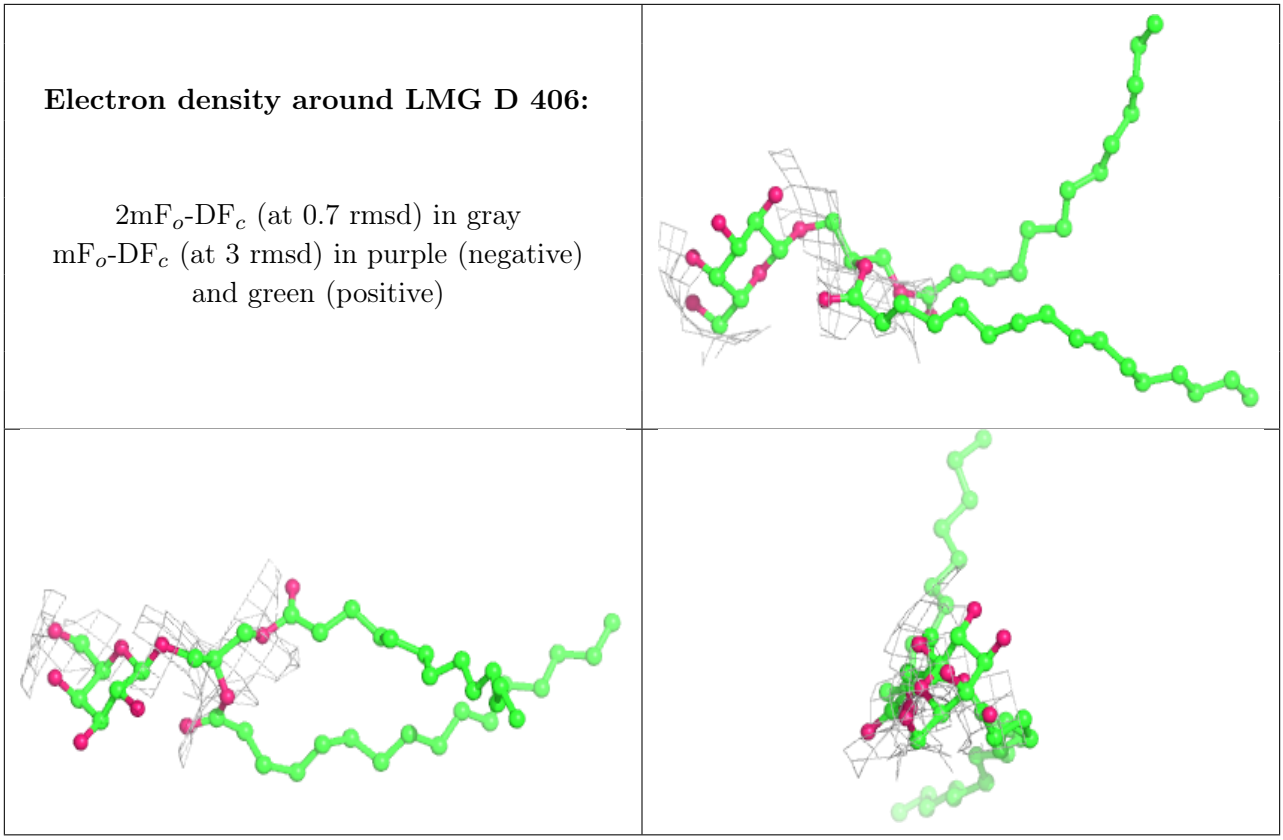
Electron density around CLA B 605:

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



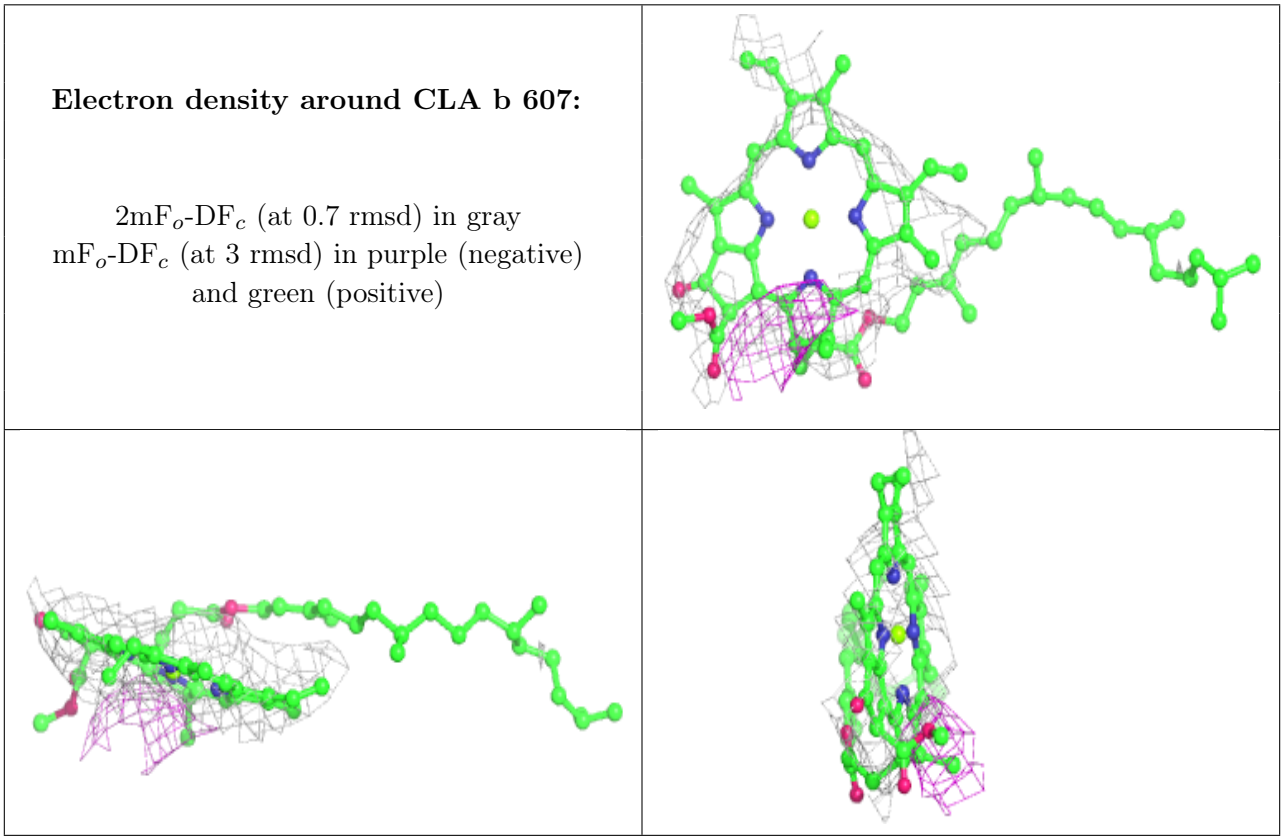
Electron density around LMG D 406:

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



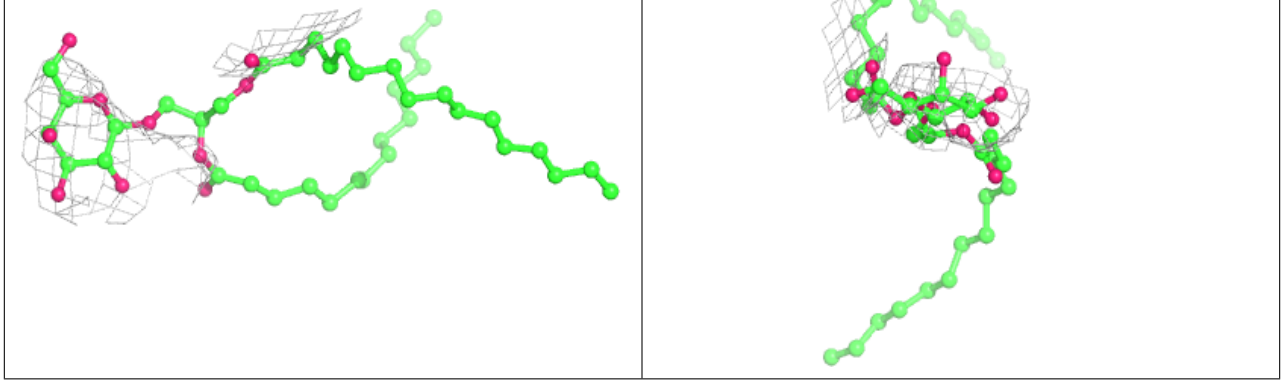
Electron density around CLA b 607:

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



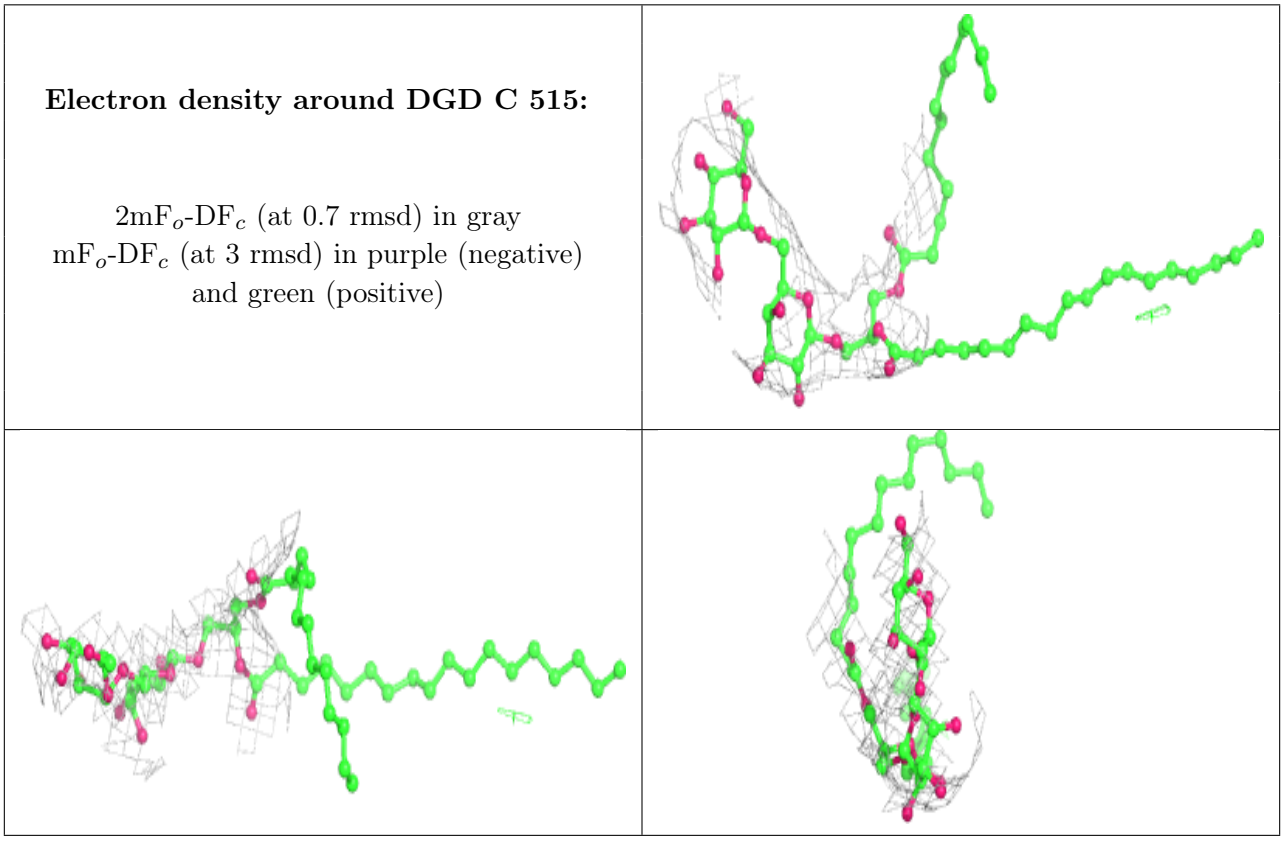
Electron density around LMG B 621:

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



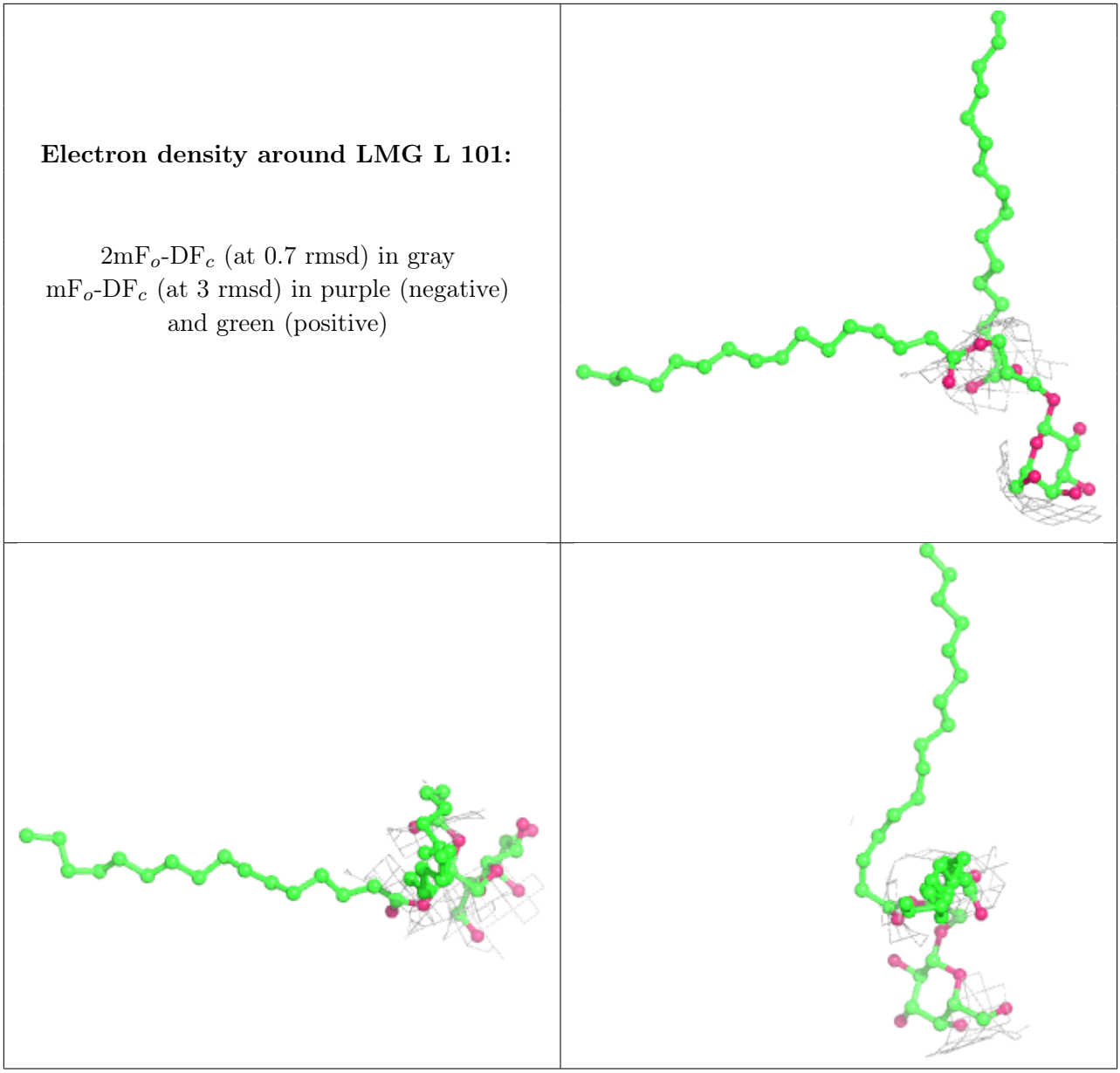
Electron density around DGD C 515:

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



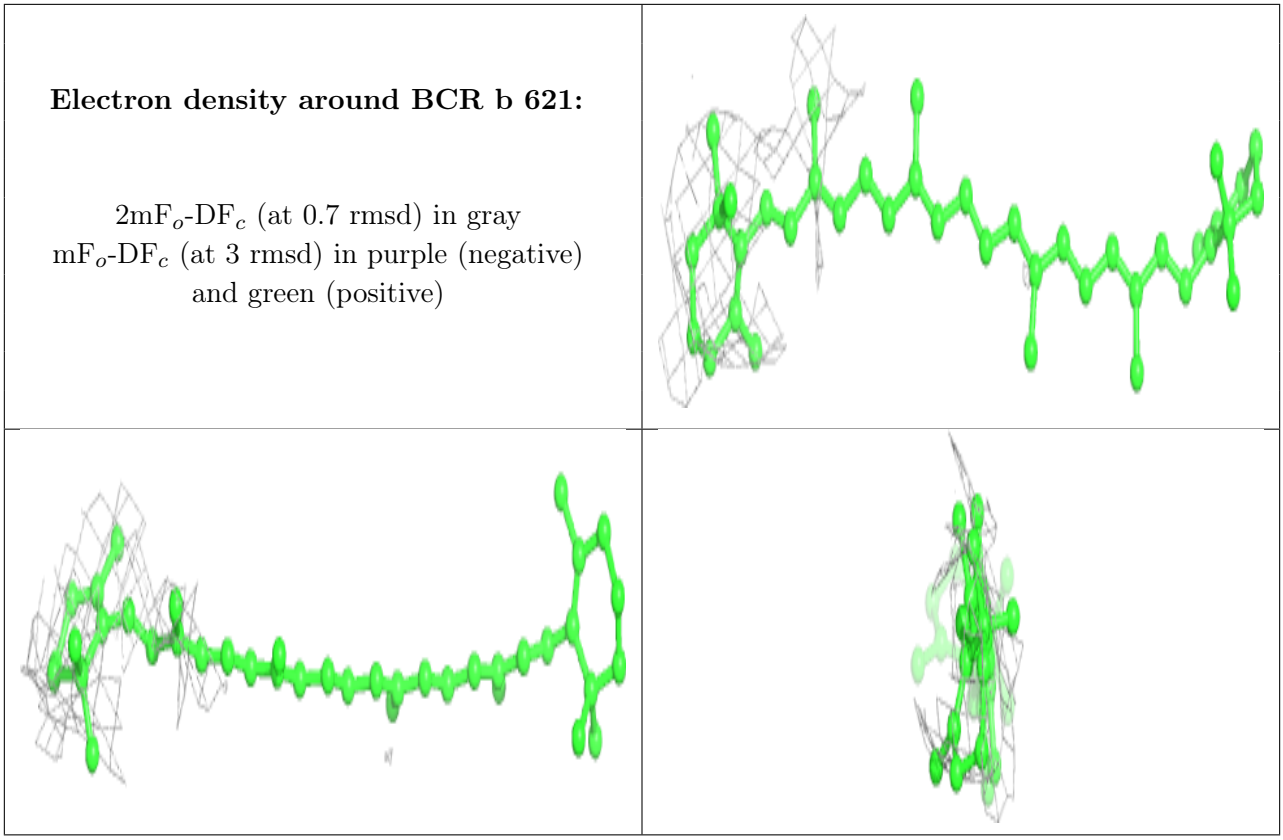
Electron density around LMG L 101:

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



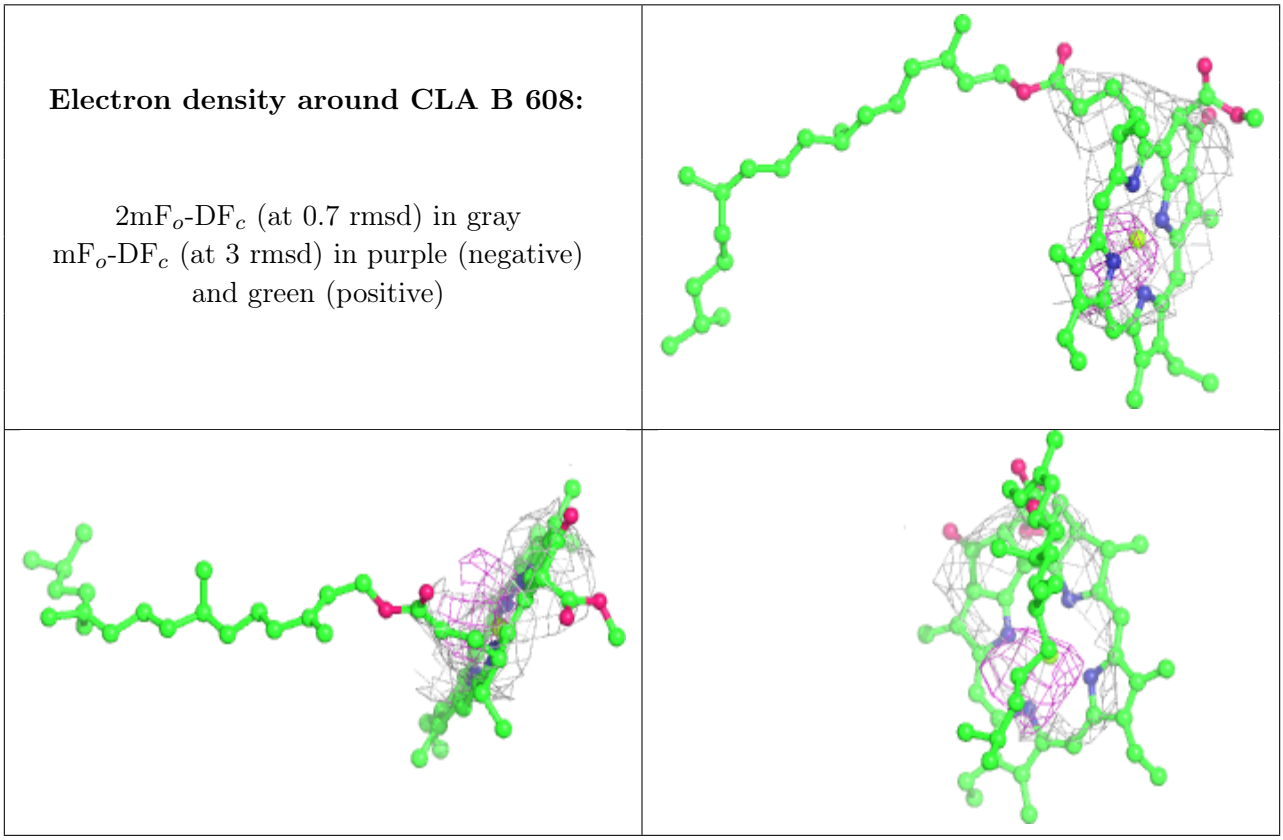
Electron density around BCR b 621:

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



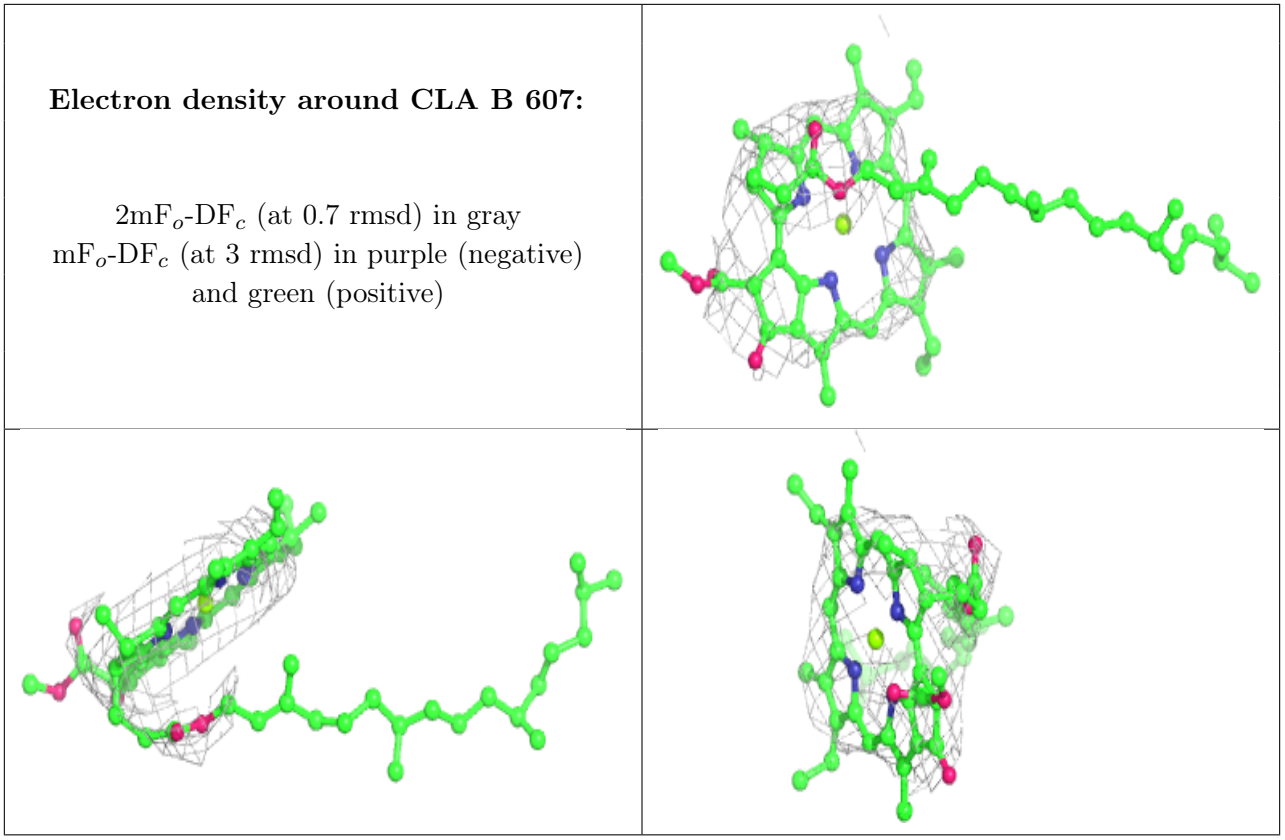
Electron density around CLA B 608:

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



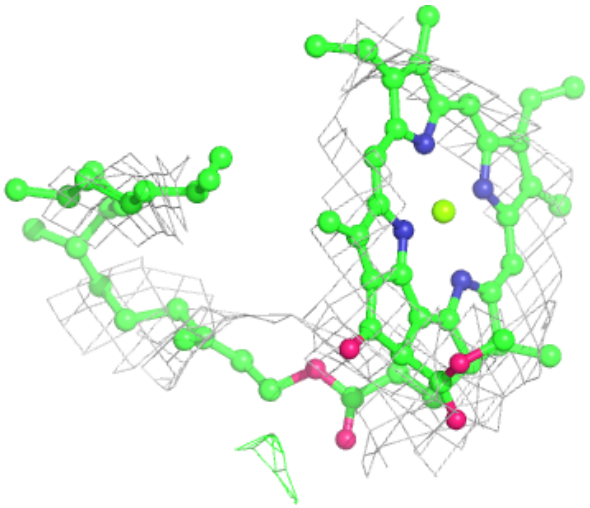
Electron density around CLA B 607:

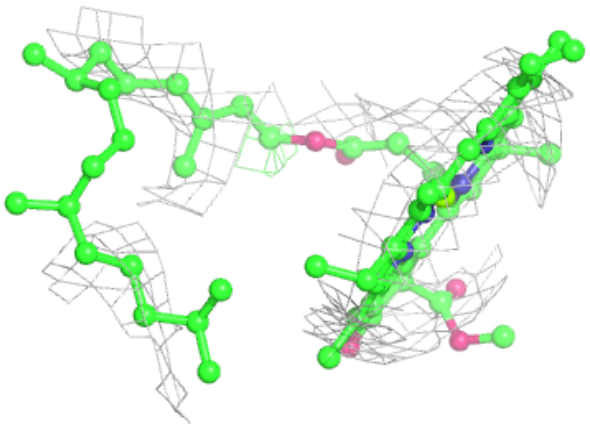
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

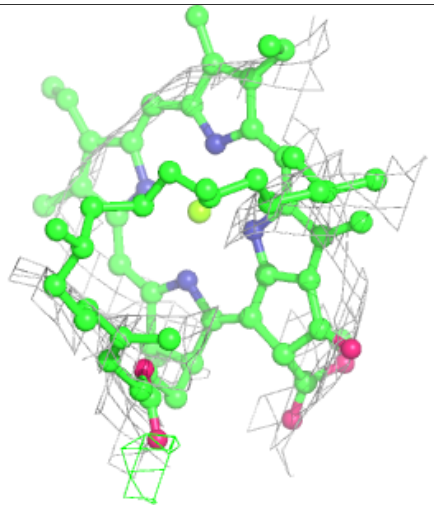


Electron density around CLA C 503:

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

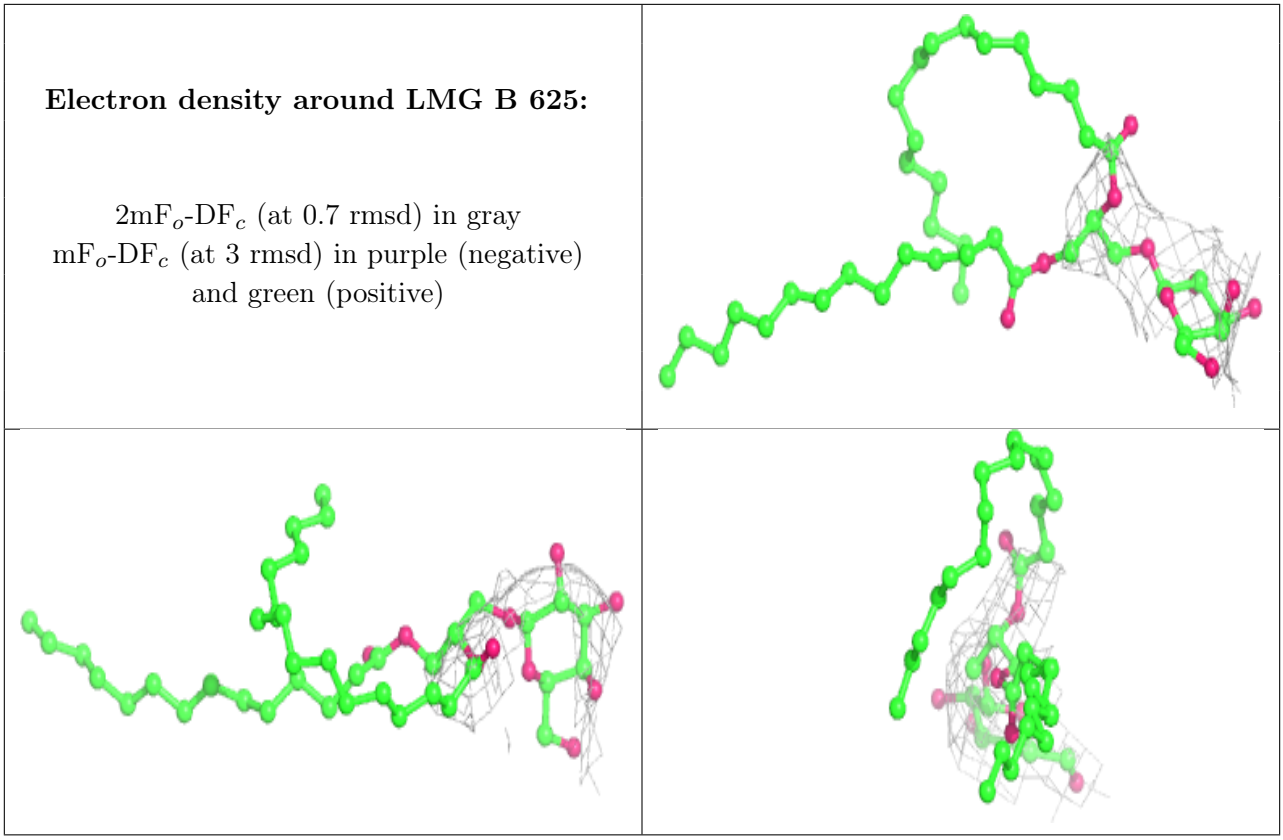






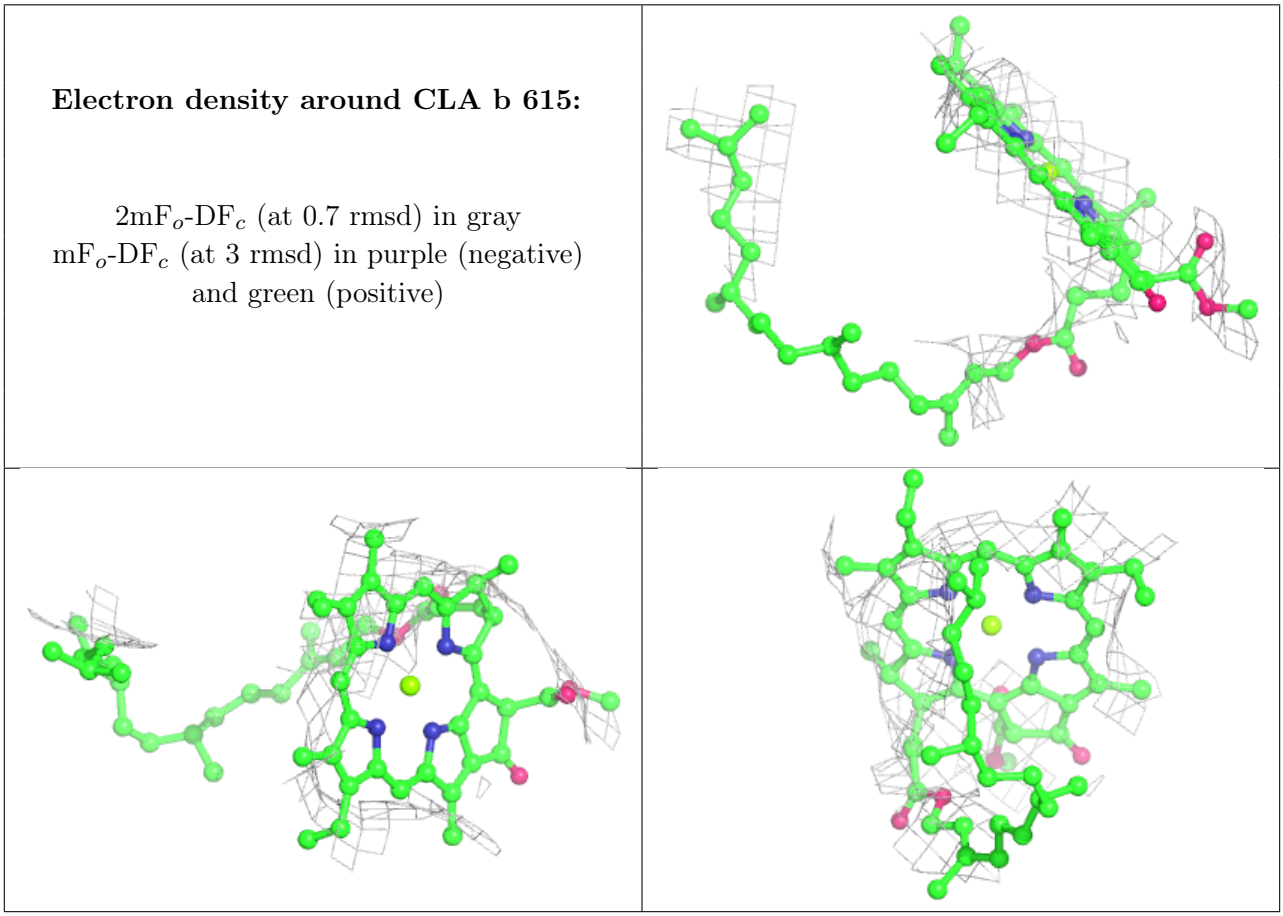
Electron density around LMG B 625:

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



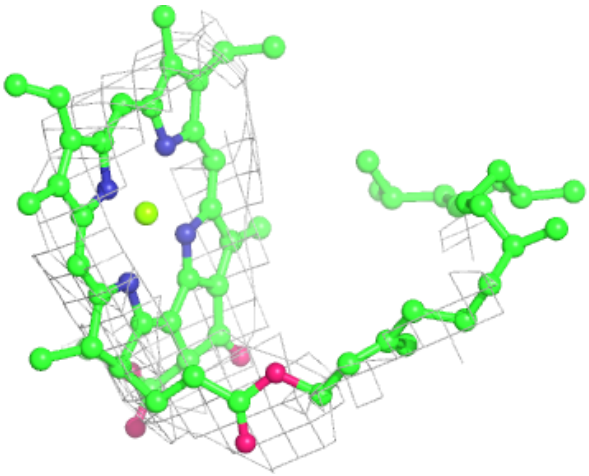
Electron density around CLA b 615:

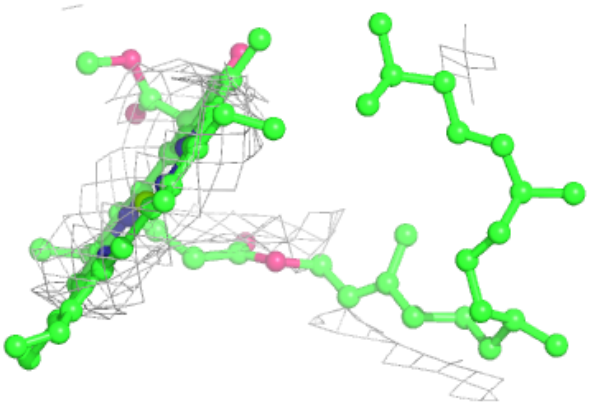
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

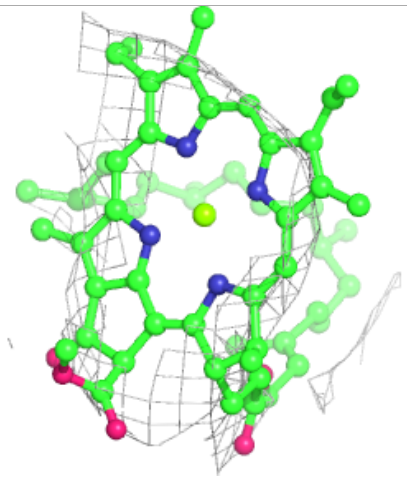


Electron density around CLA c 503:

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

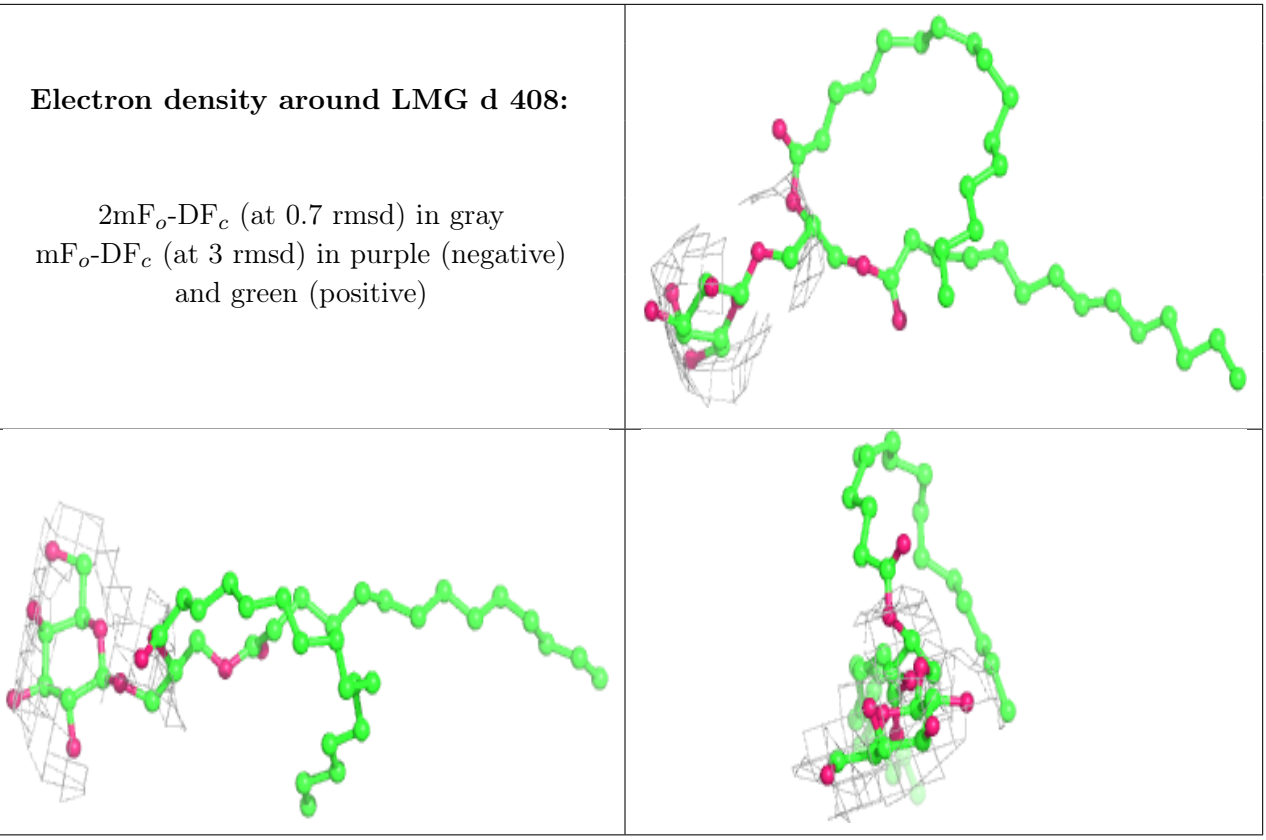






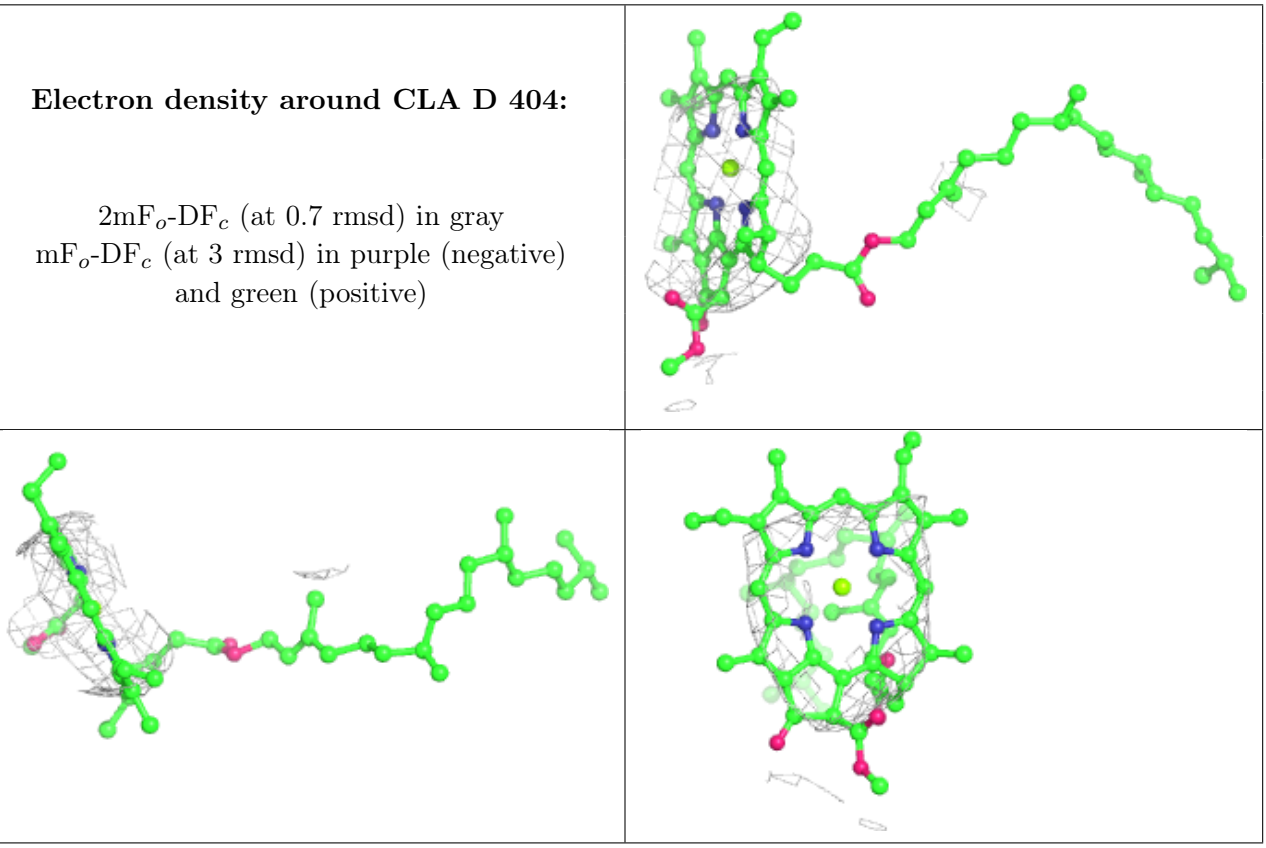
Electron density around LMG d 408:

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



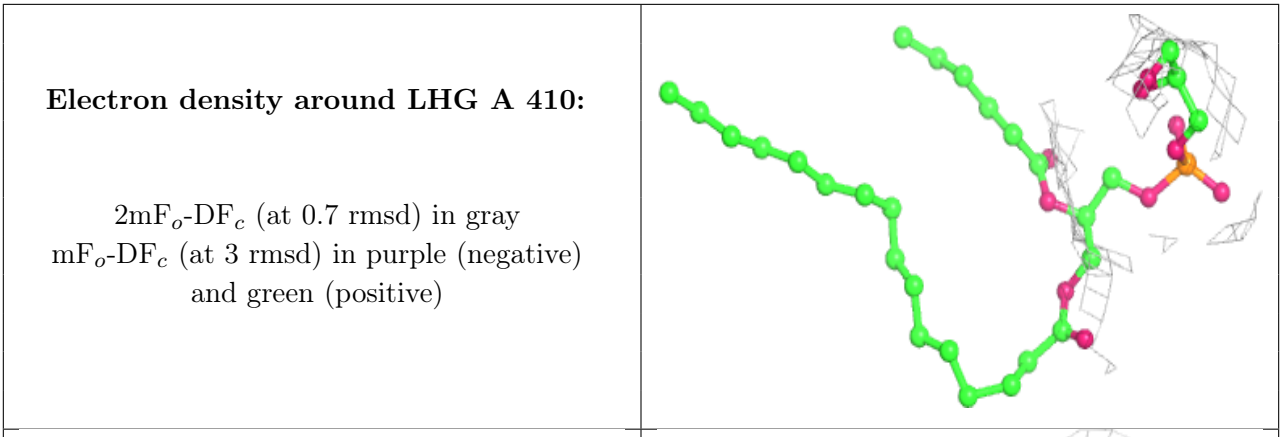
Electron density around CLA D 404:

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



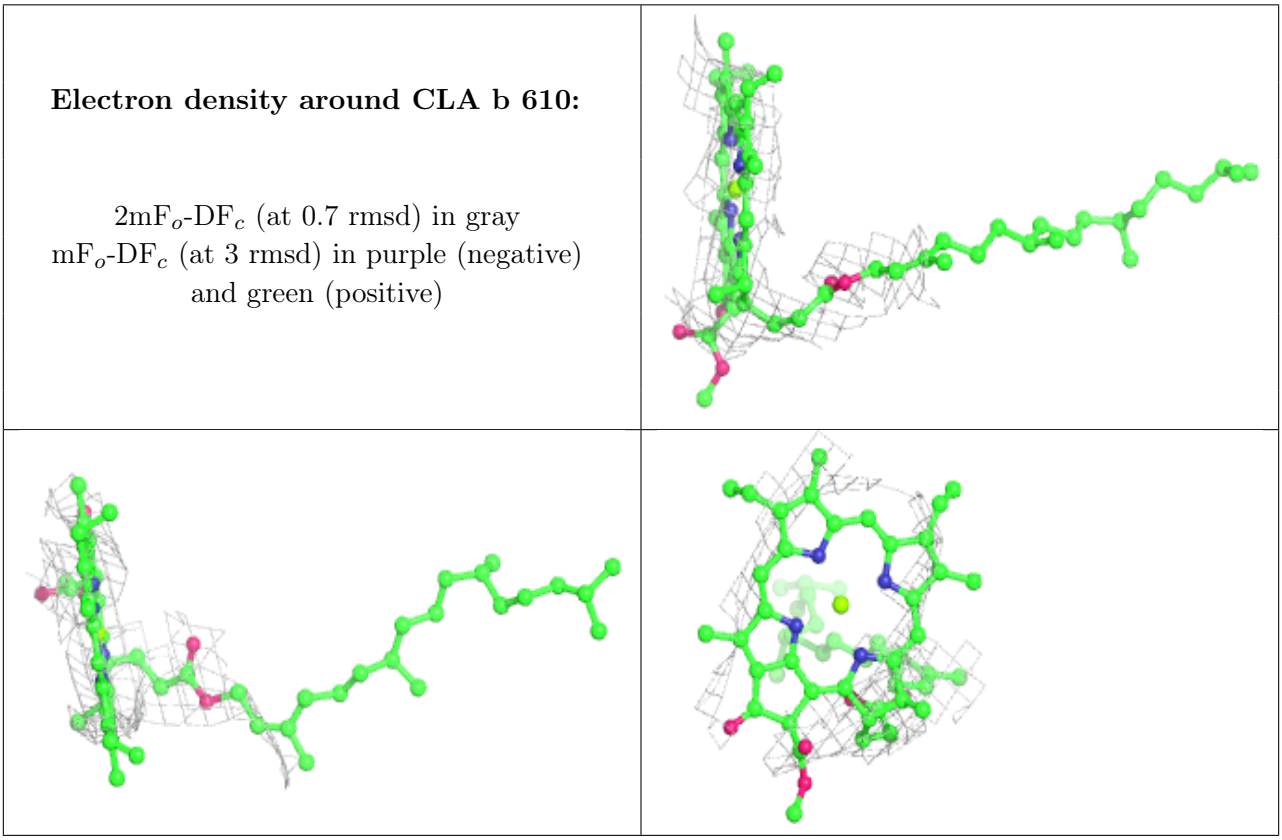
Electron density around LHG A 410:

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



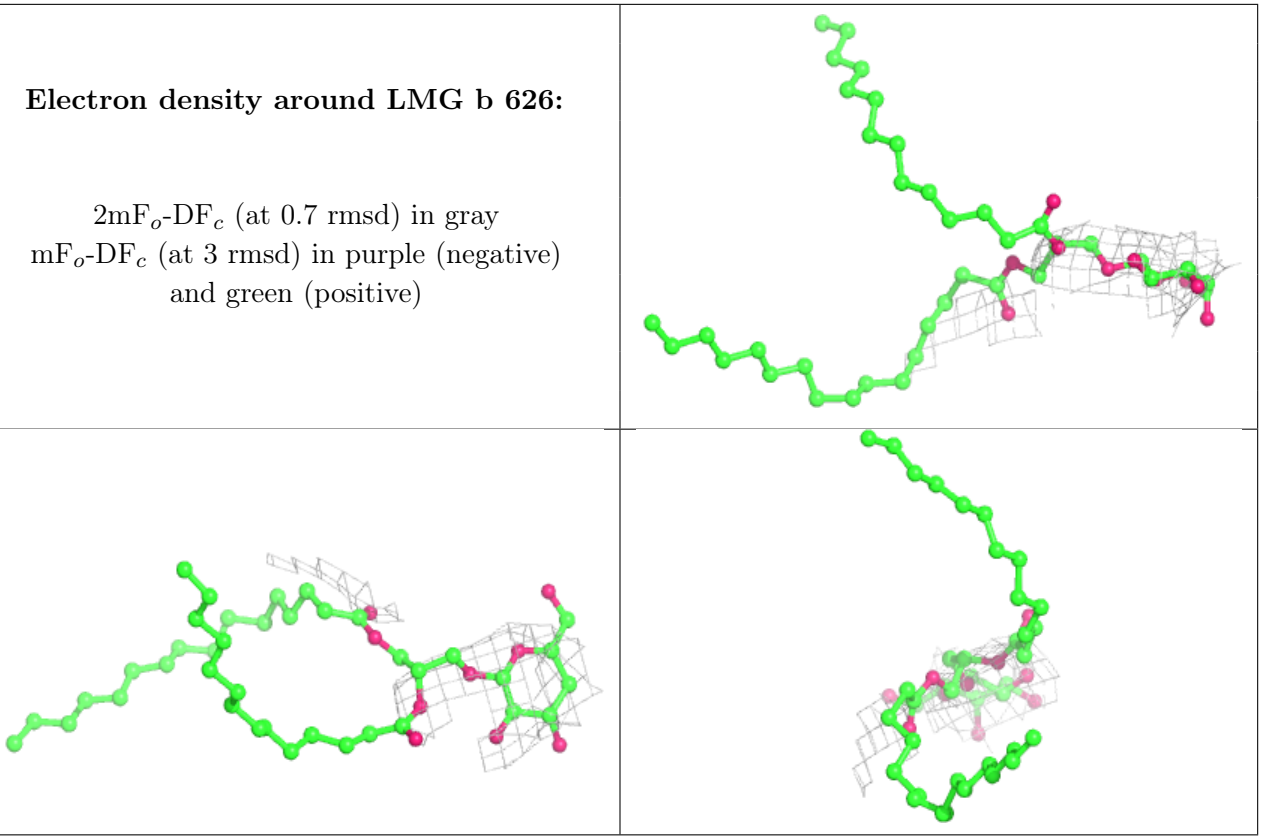
Electron density around CLA b 610:

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



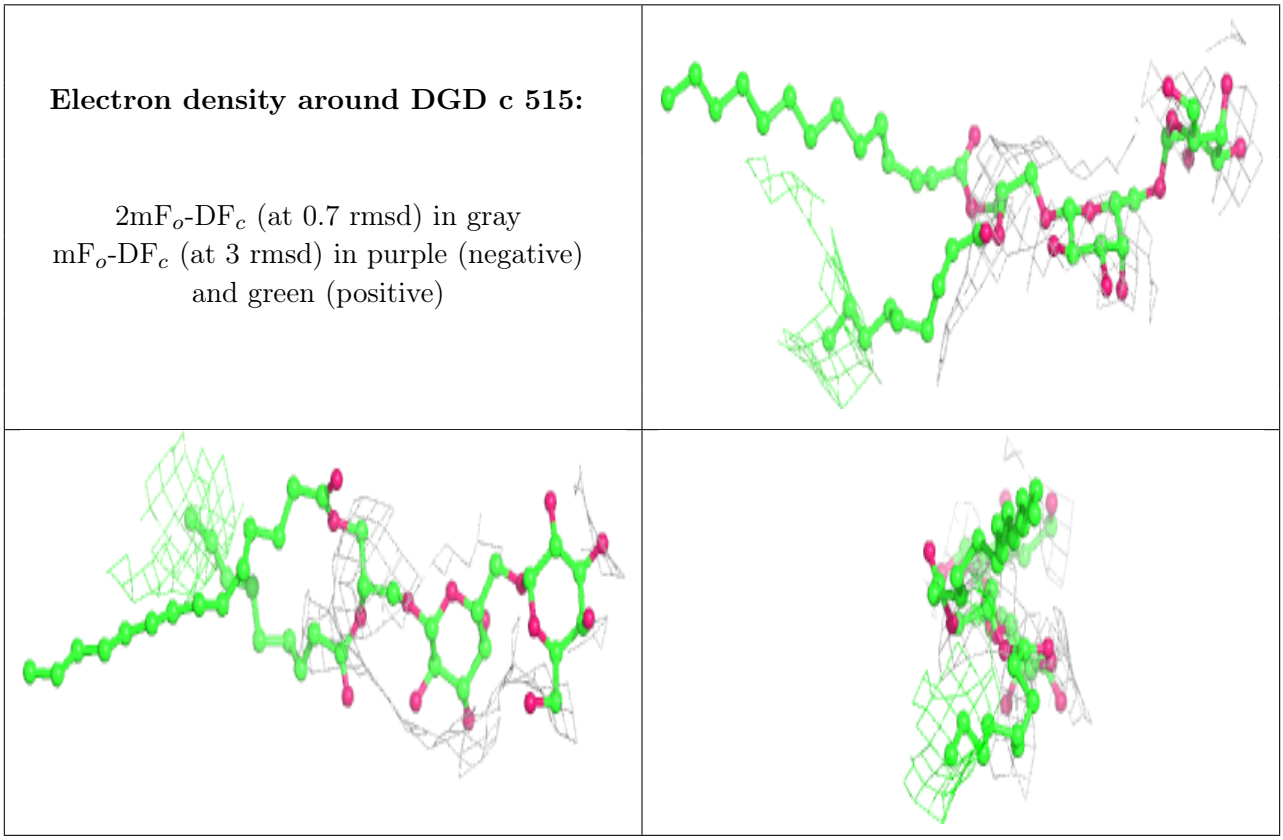
Electron density around LMG b 626:

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



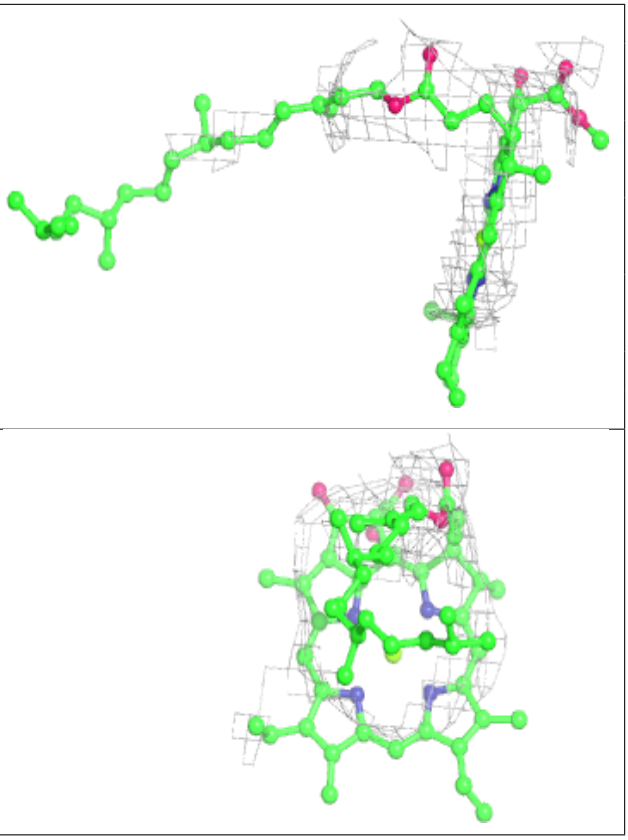
Electron density around DGD c 515:

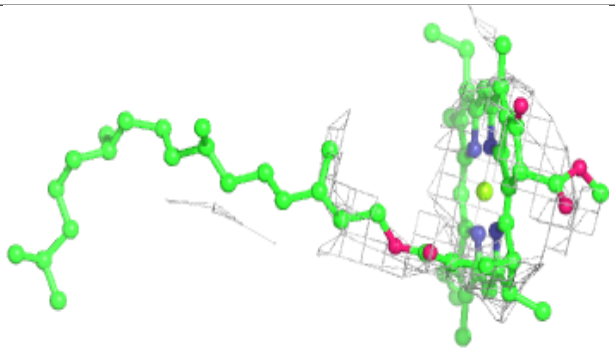
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 604:

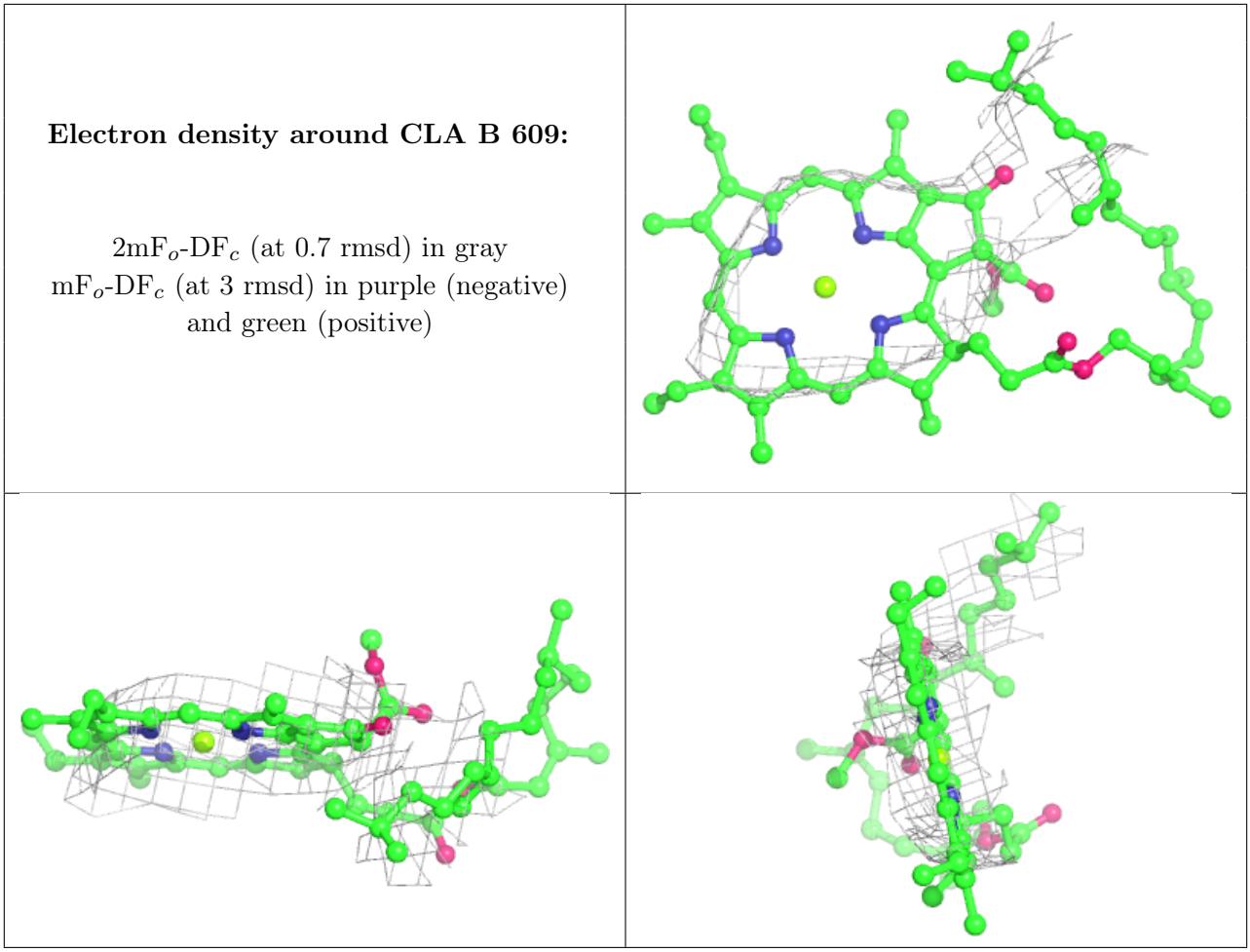
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





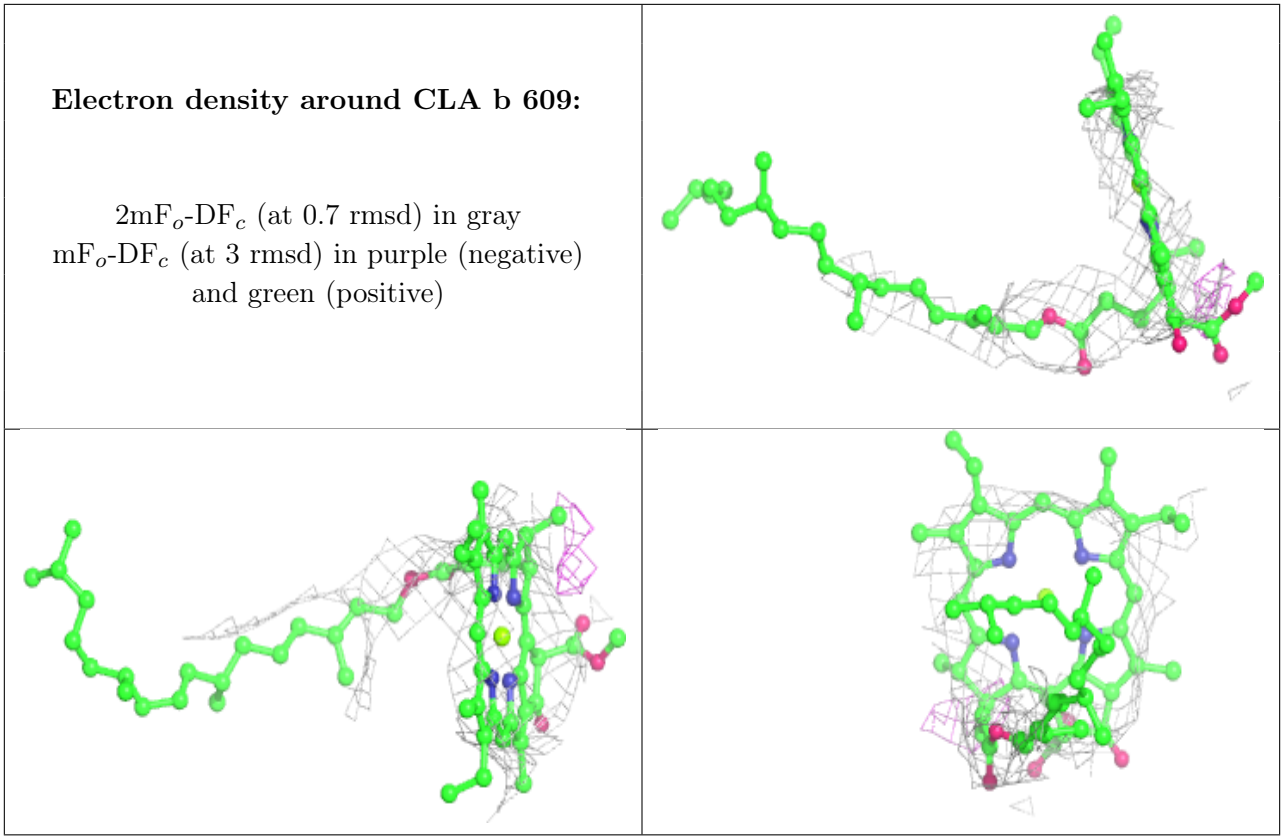
Electron density around CLA B 609:

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



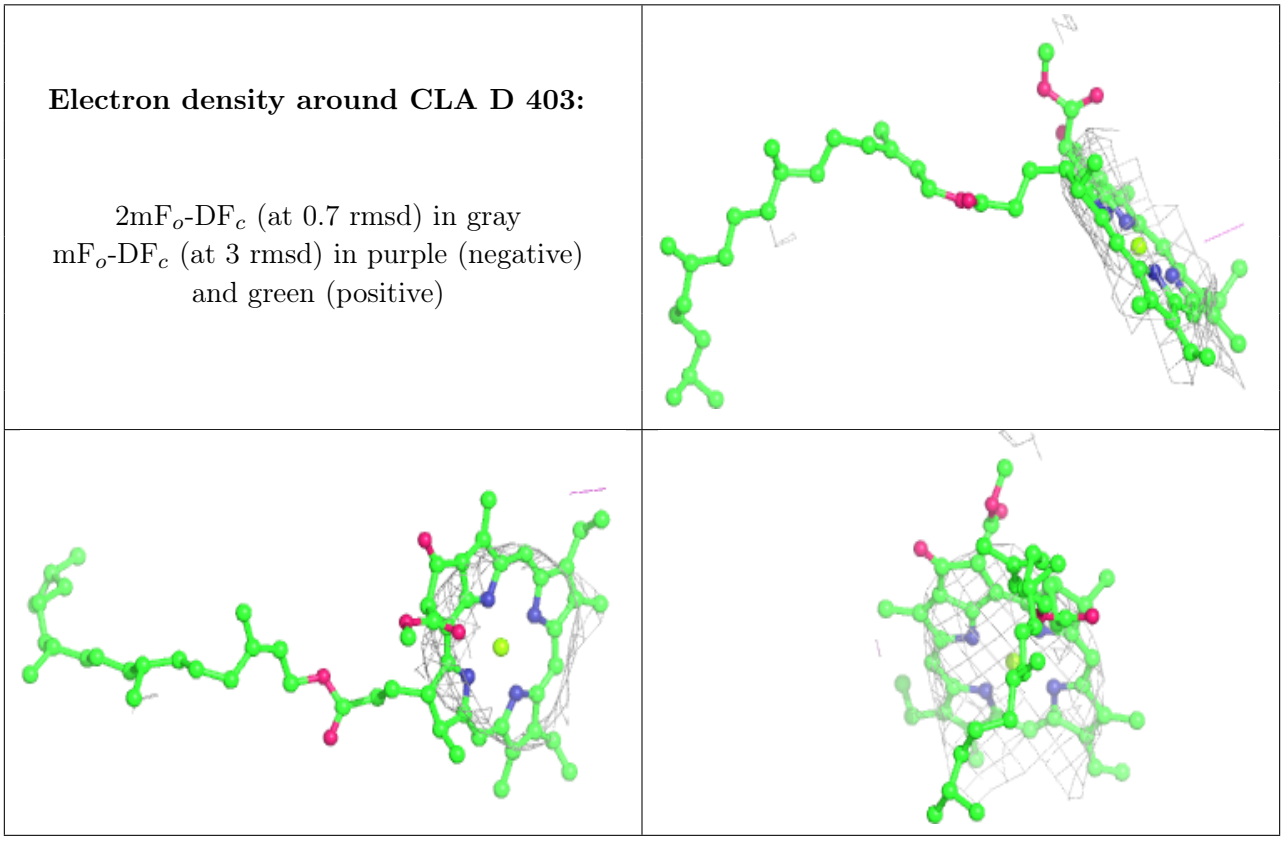
Electron density around CLA b 609:

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



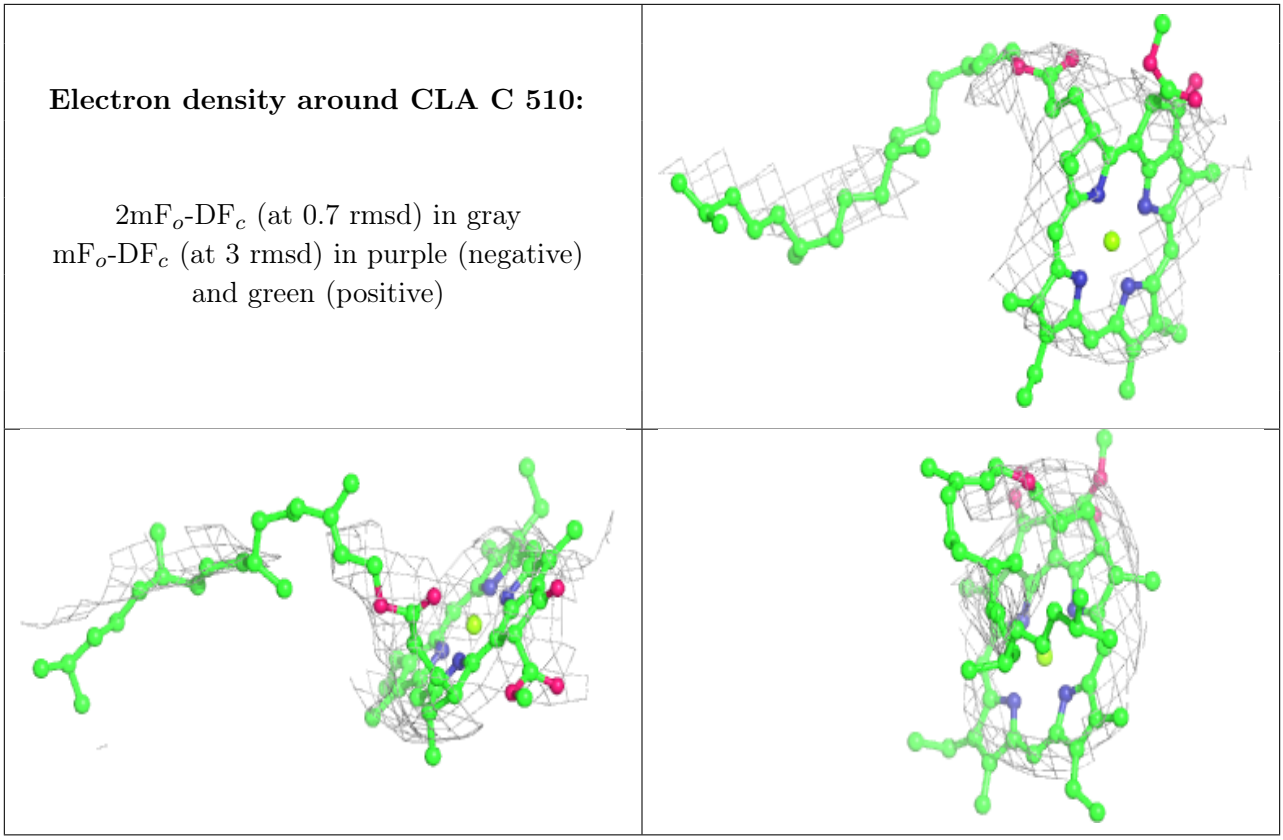
Electron density around CLA D 403:

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



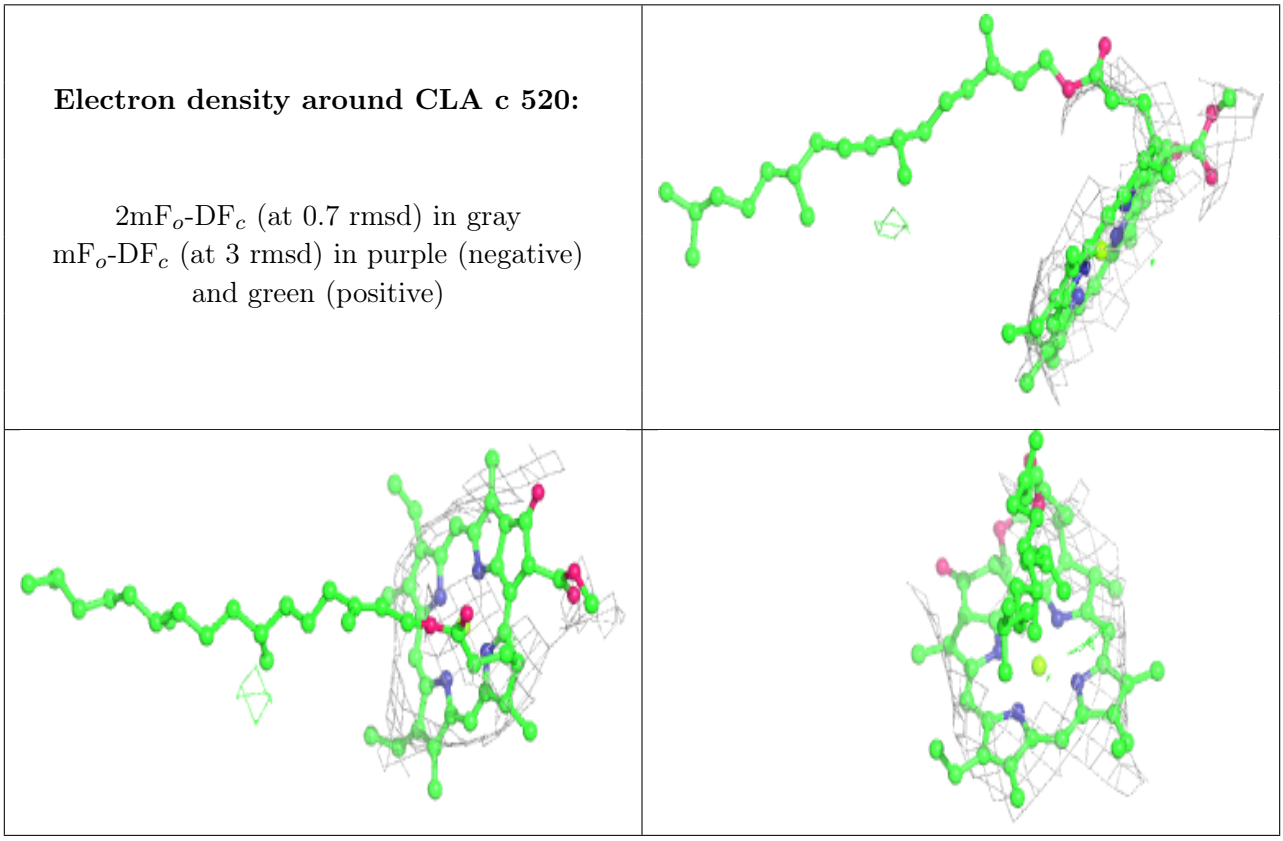
Electron density around CLA C 510:

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



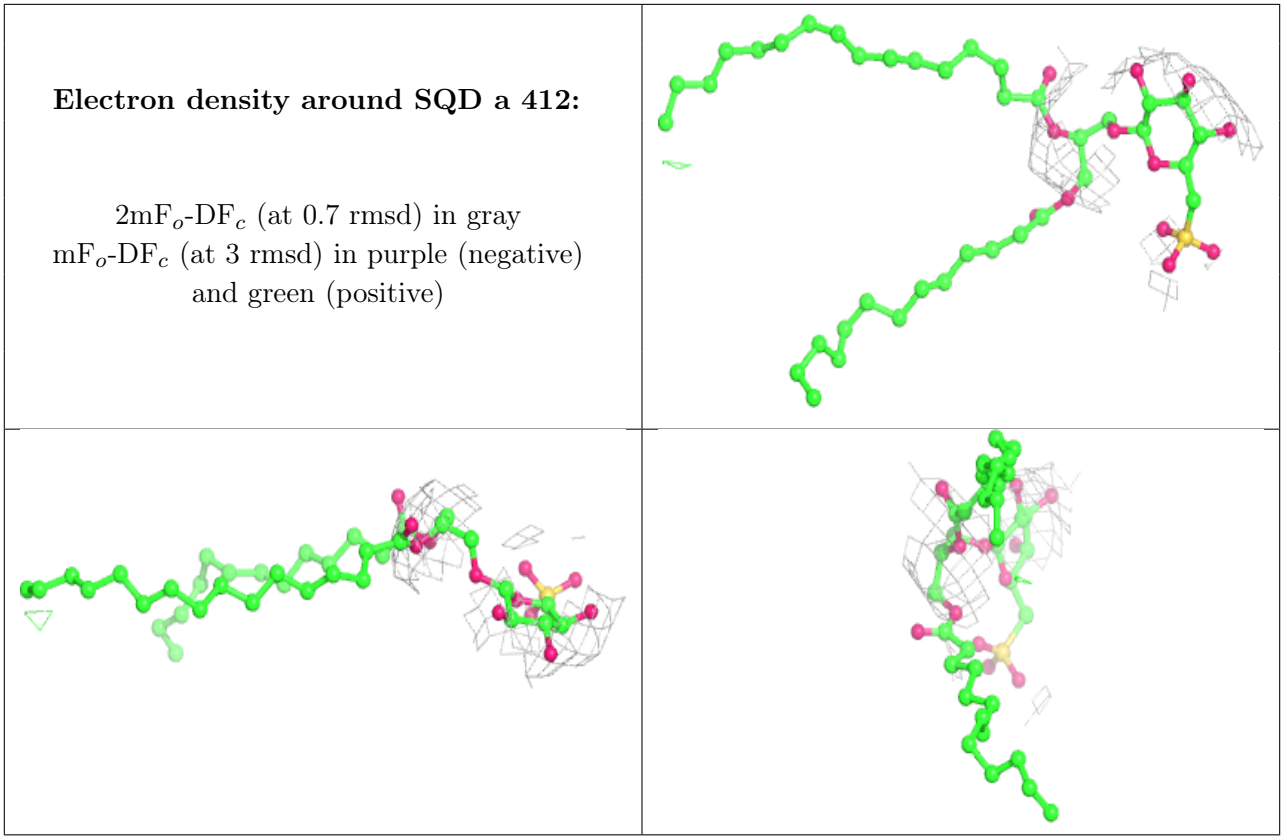
Electron density around CLA c 520:

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



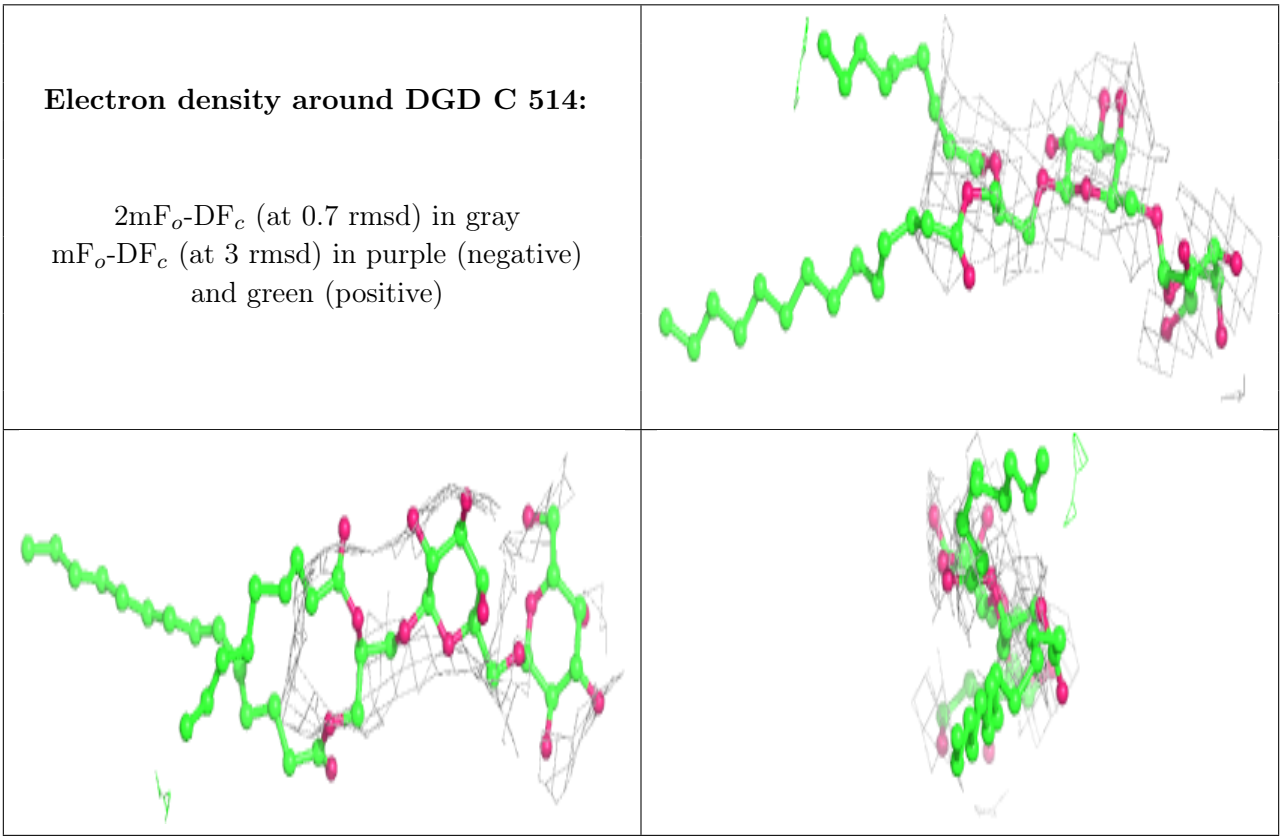
Electron density around SQD a 412:

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



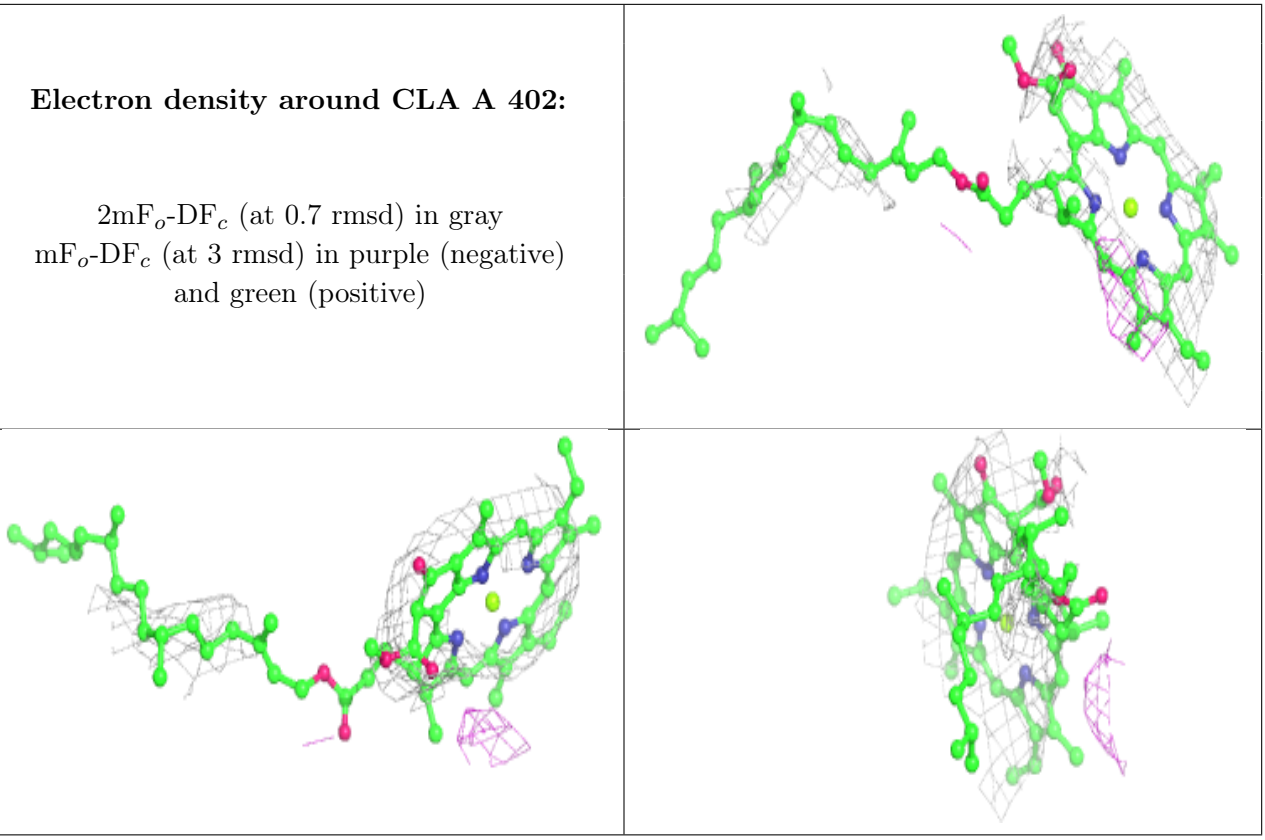
Electron density around DGD C 514:

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



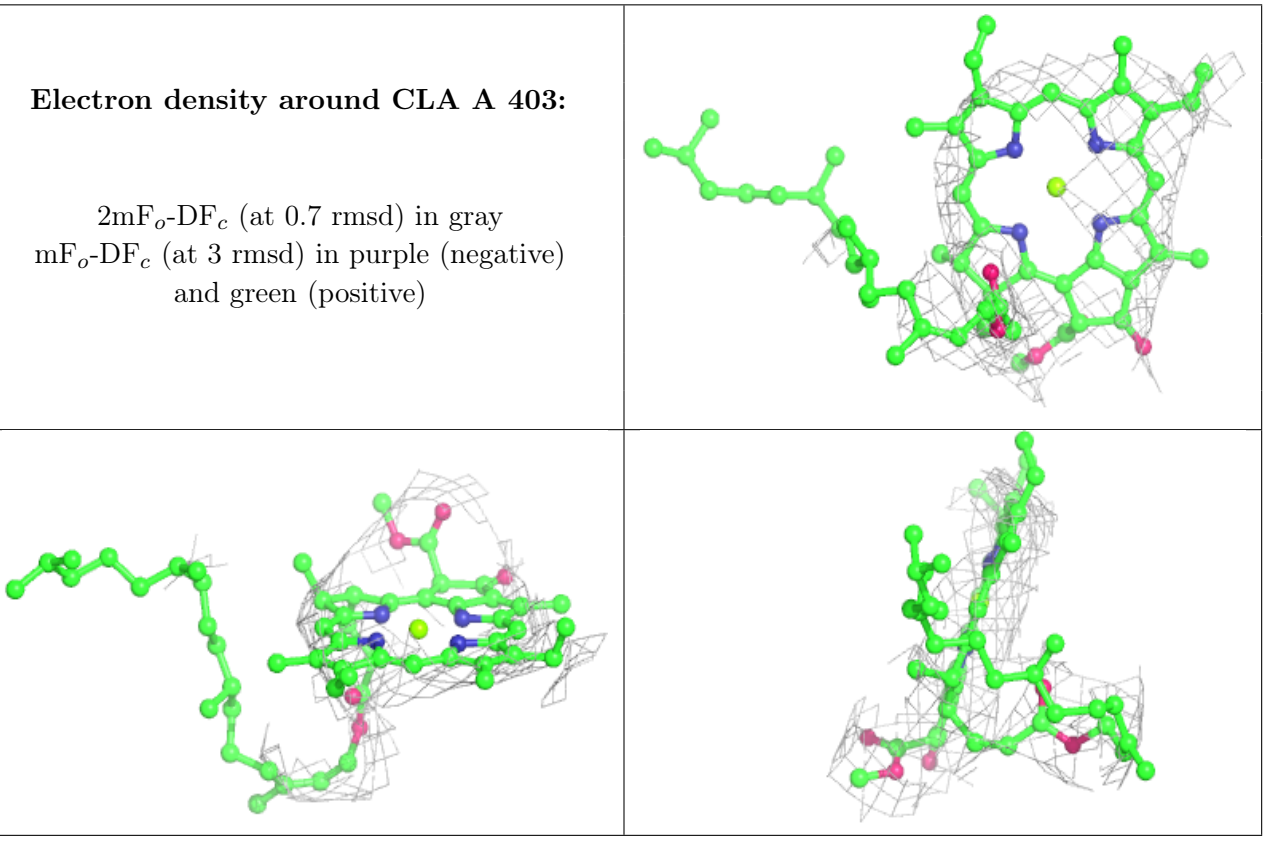
Electron density around CLA A 402:

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



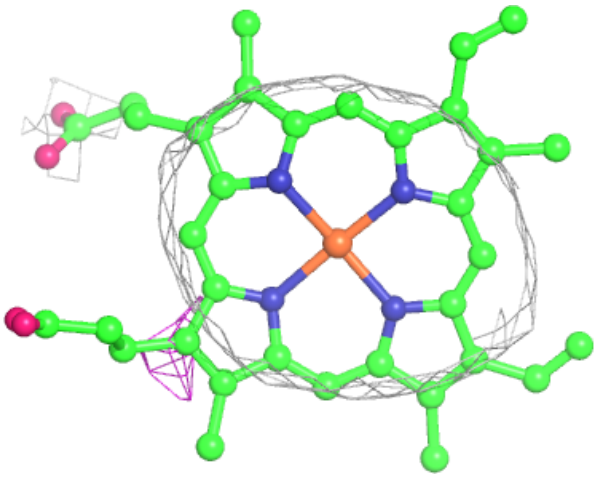
Electron density around CLA A 403:

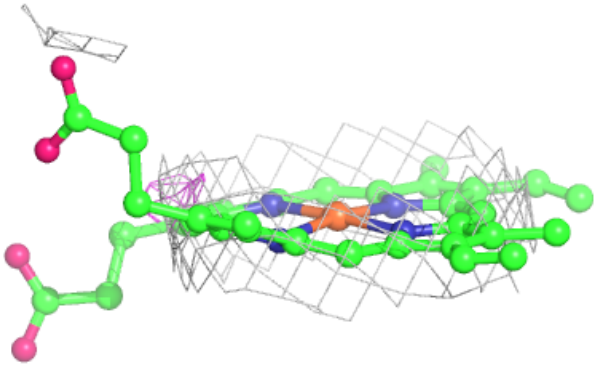
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

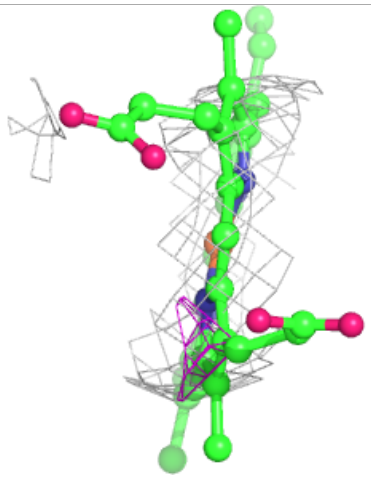


Electron density around HEM F 101:

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

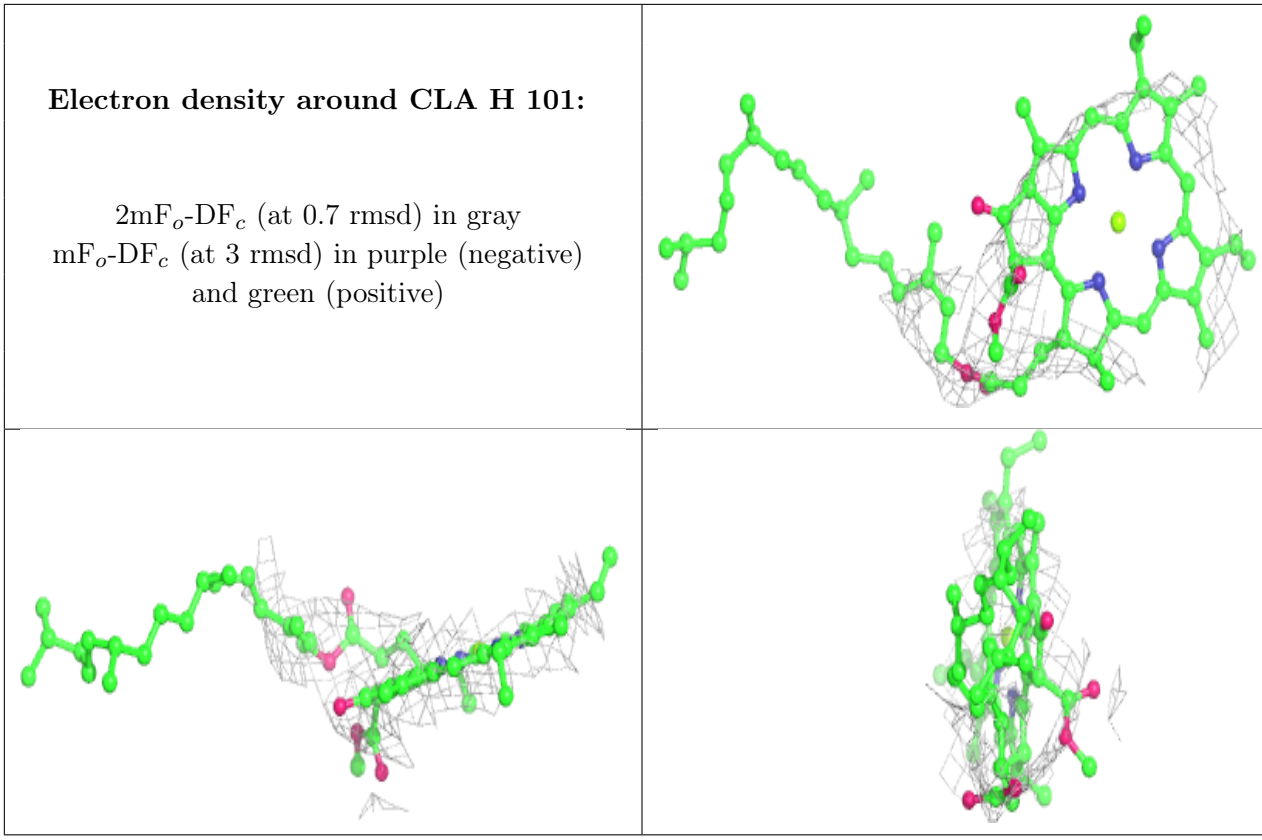






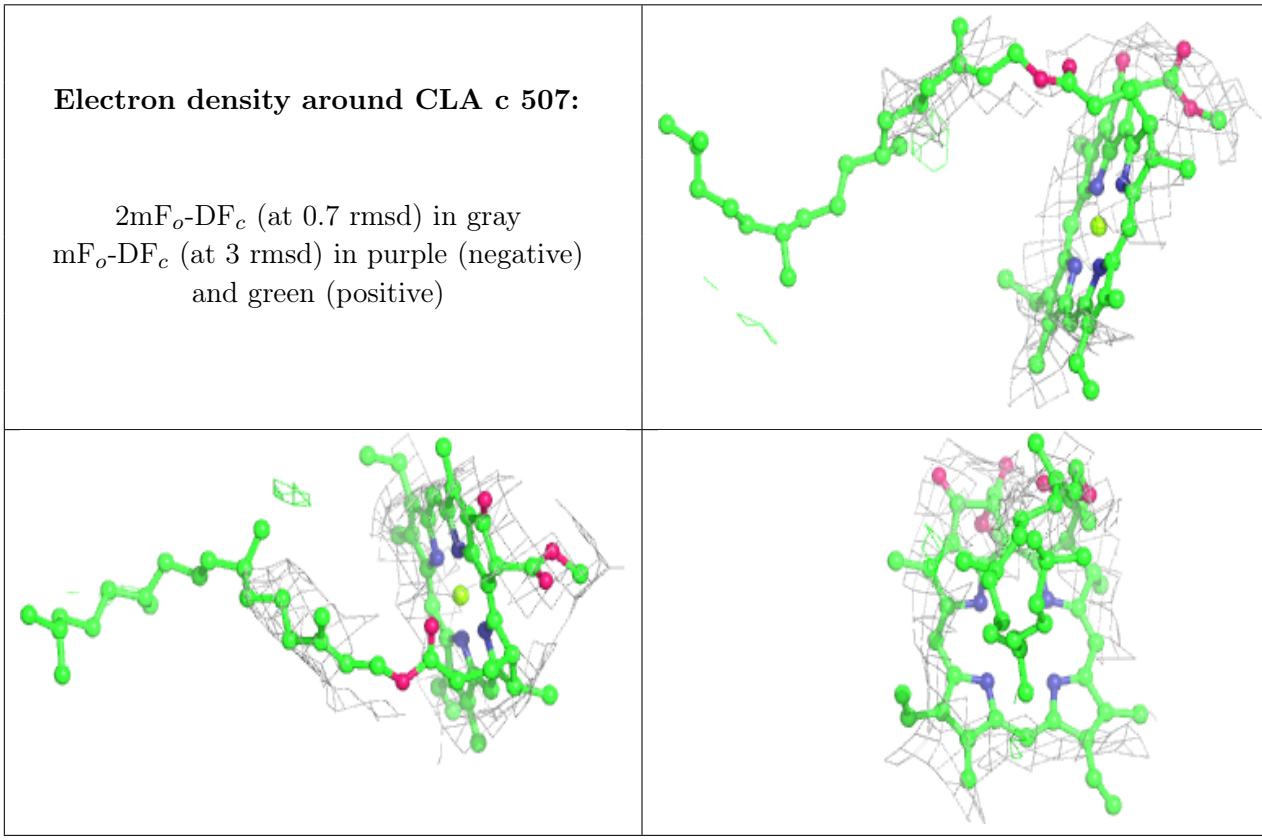
Electron density around CLA H 101:

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



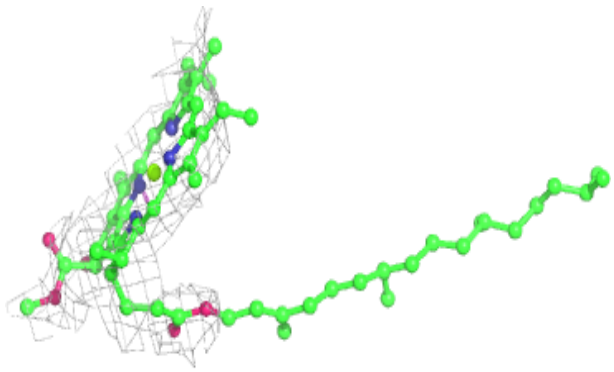
Electron density around CLA c 507:

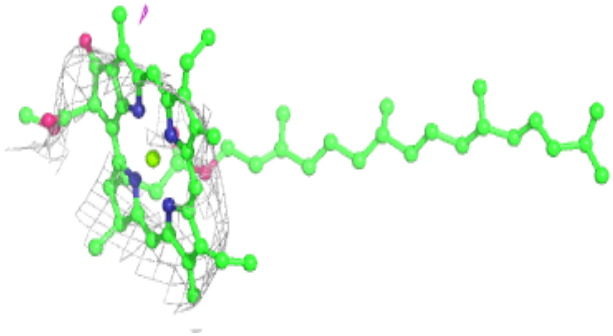
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

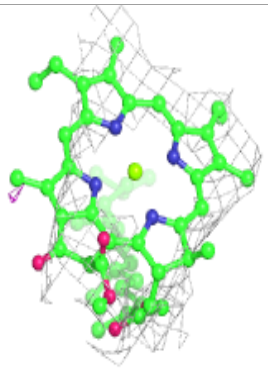


Electron density around CLA b 611:

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

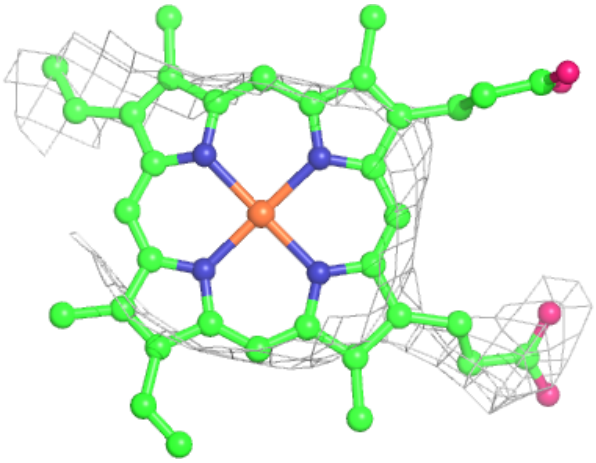


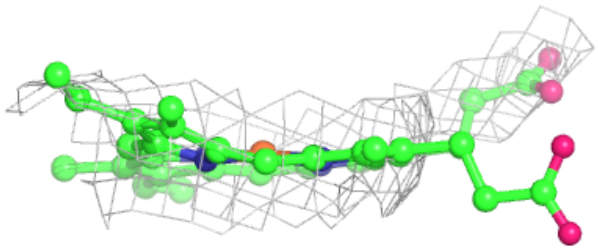


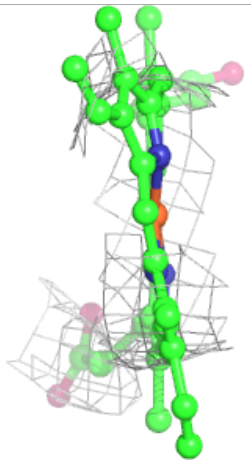


Electron density around HEM V 201:

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

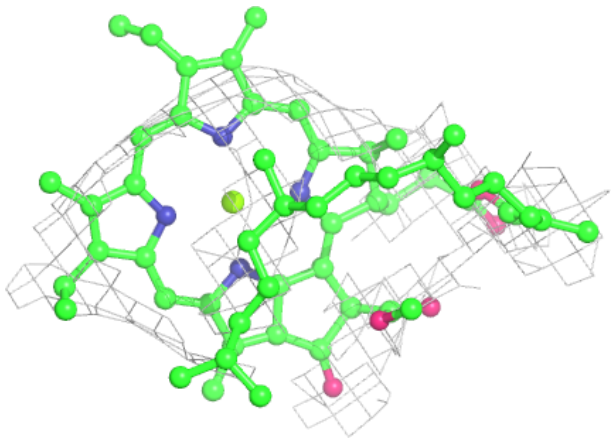


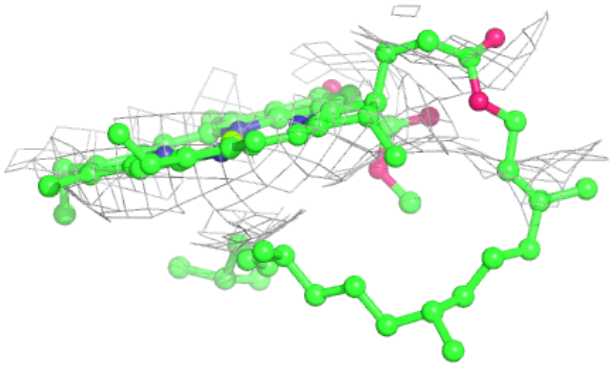


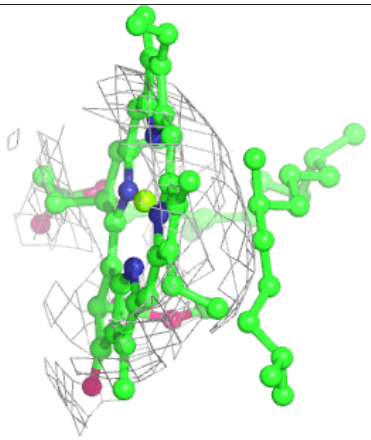


Electron density around CLA c 509:

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

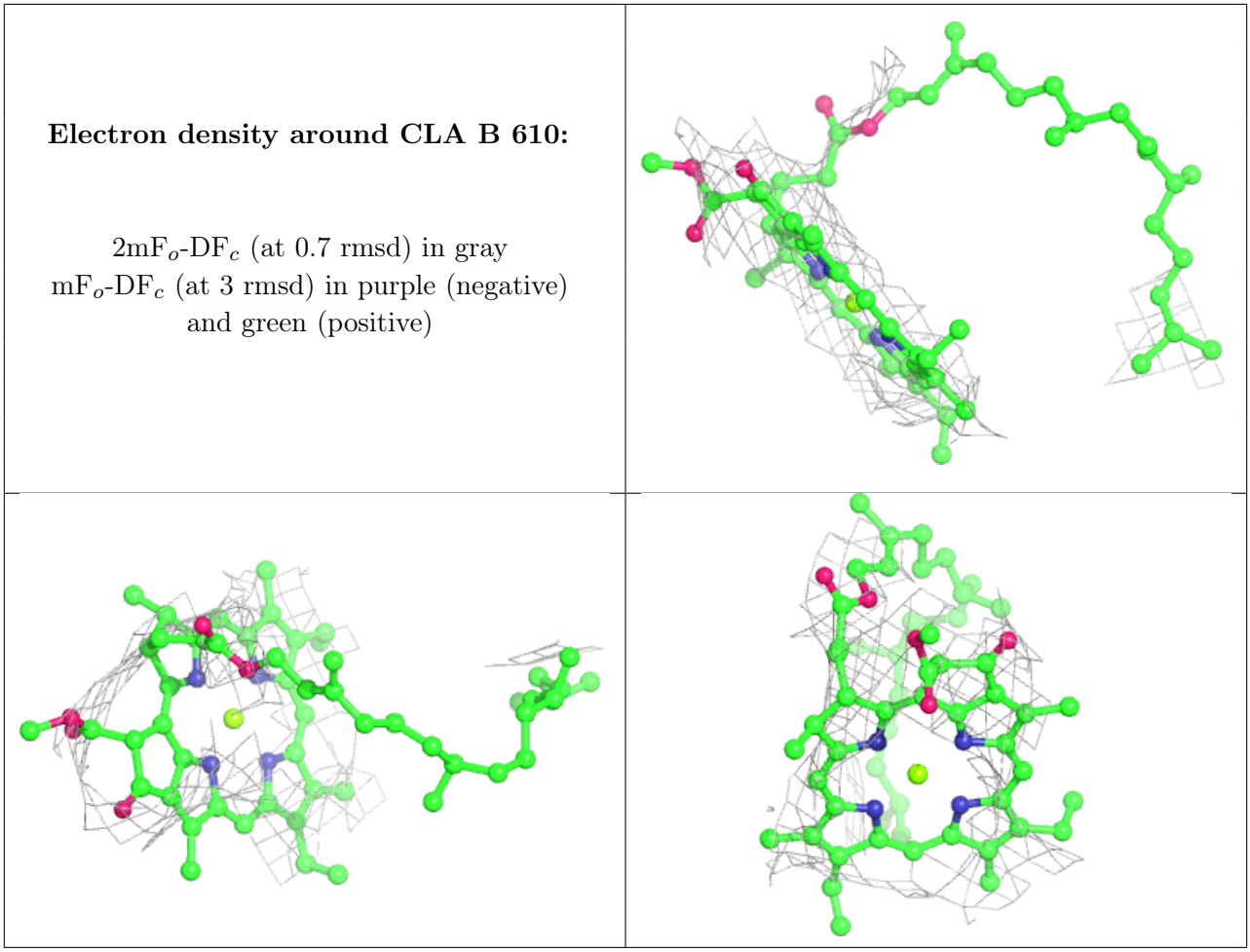






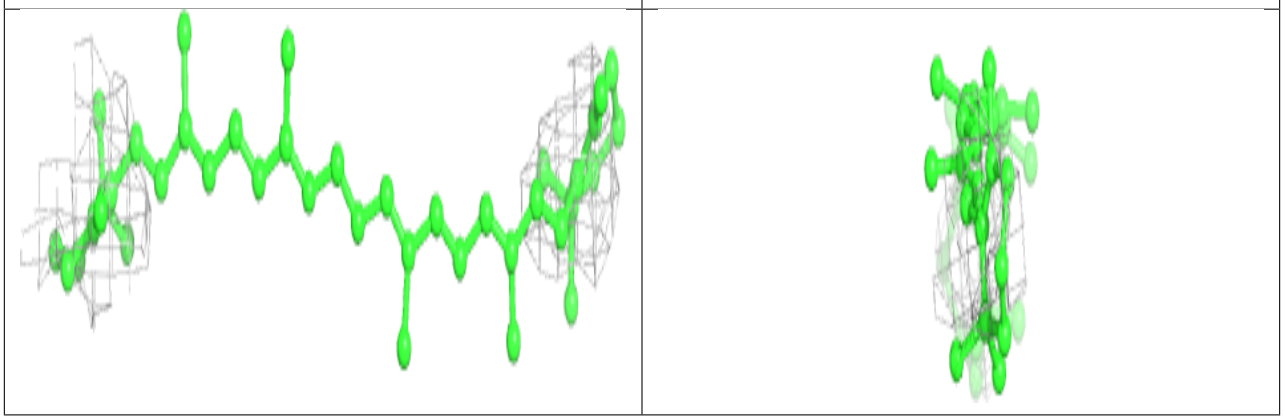
Electron density around CLA B 610:

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



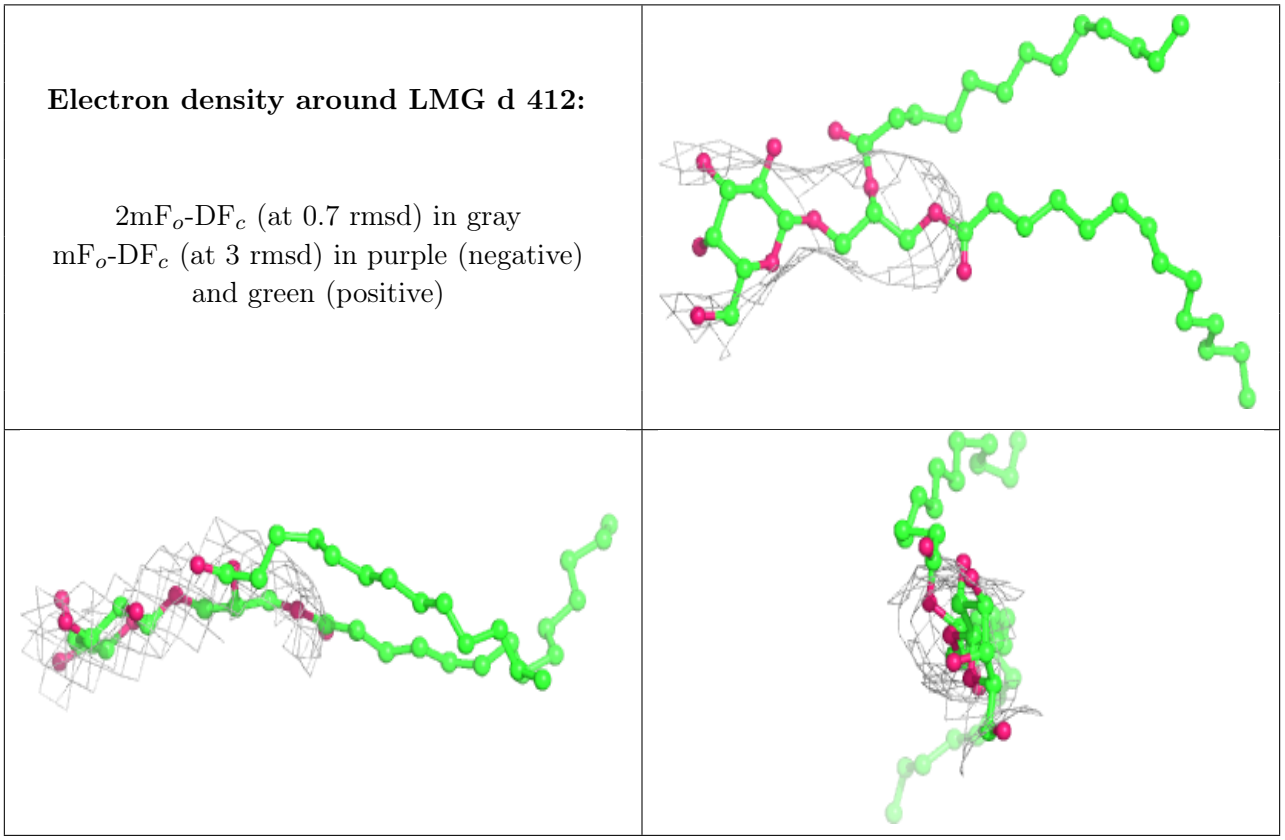
Electron density around BCR K 101:

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



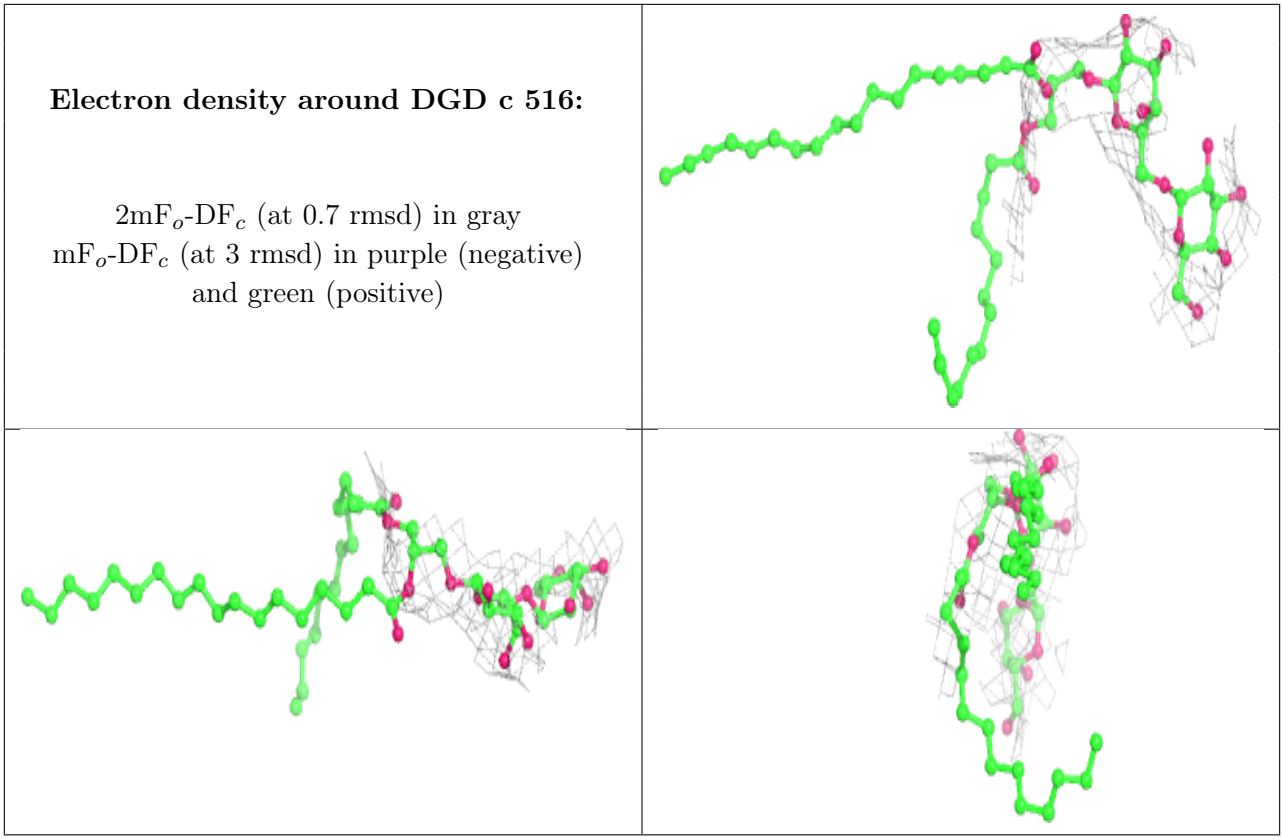
Electron density around LMG d 412:

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



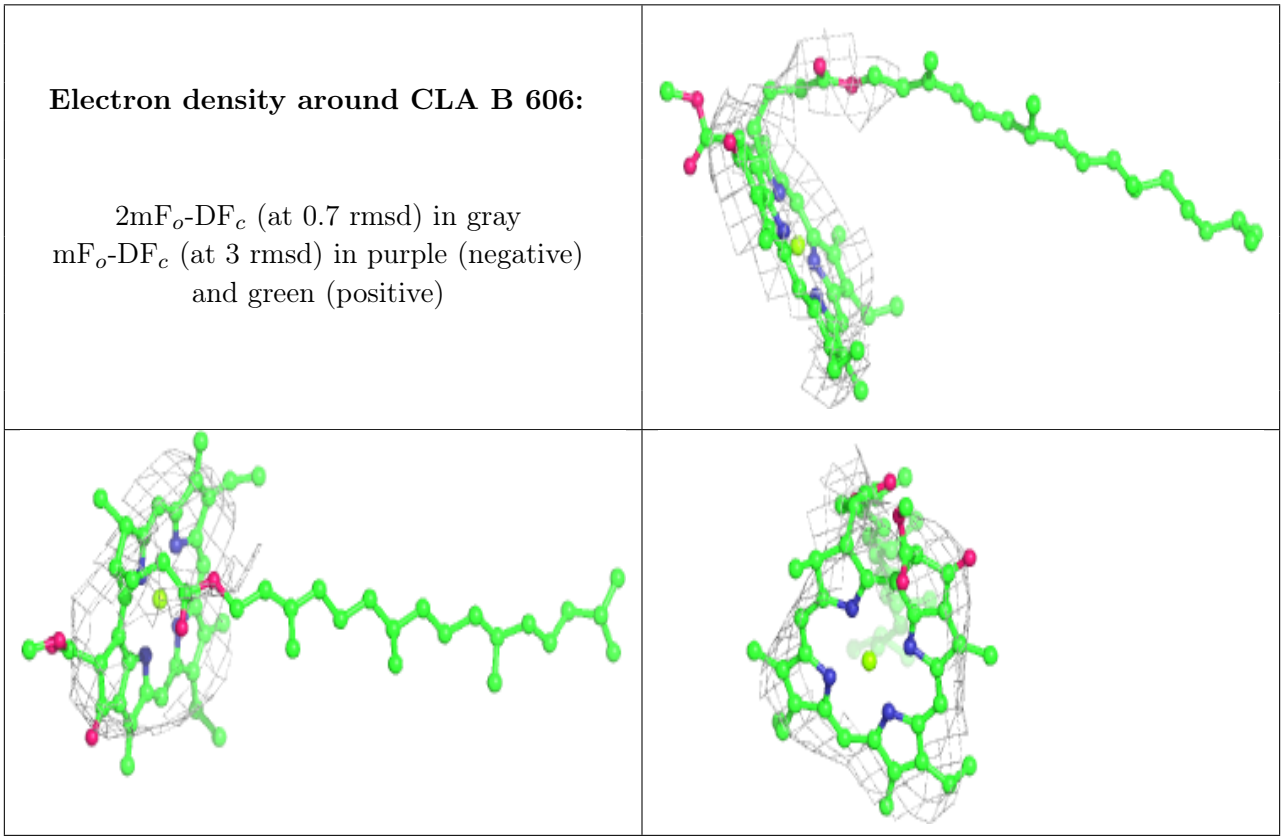
Electron density around DGD c 516:

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



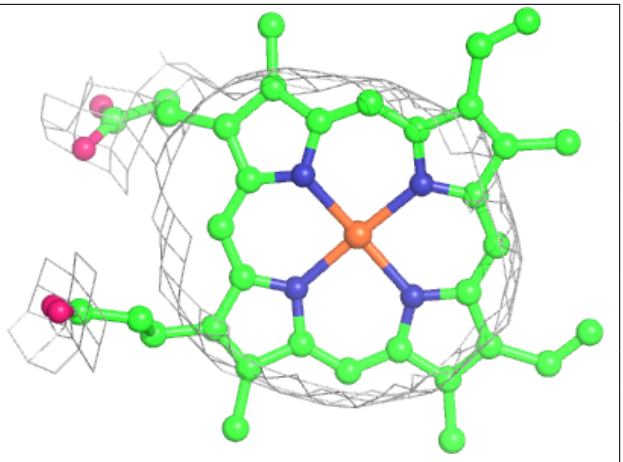
Electron density around CLA B 606:

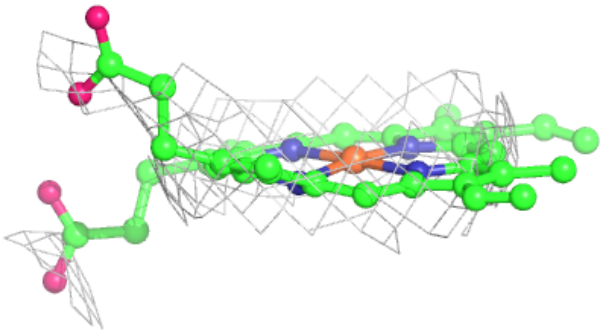
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

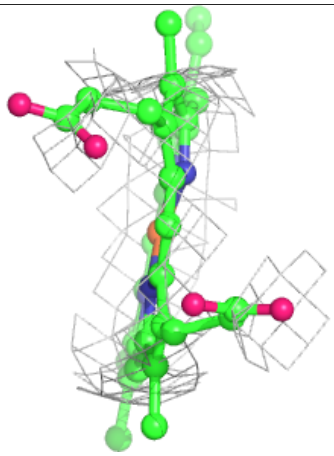


Electron density around HEM f 101:

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

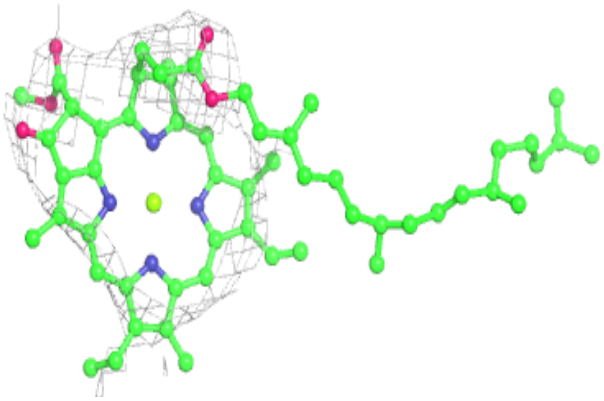


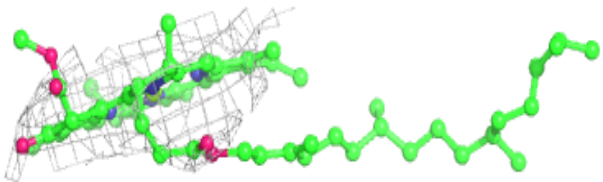


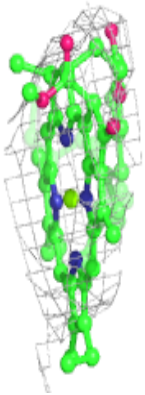


Electron density around CLA B 602:

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

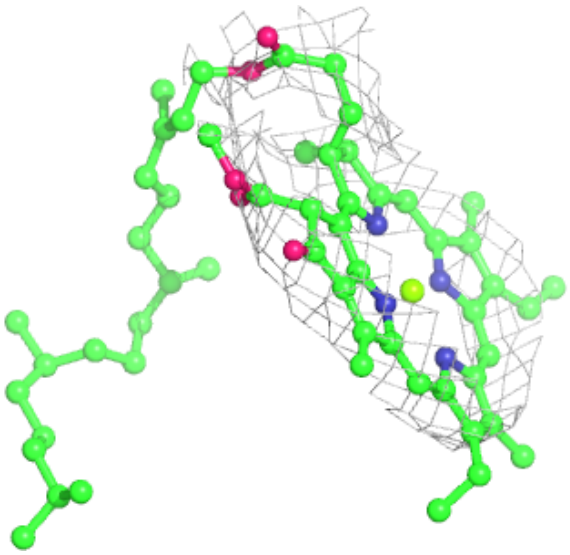


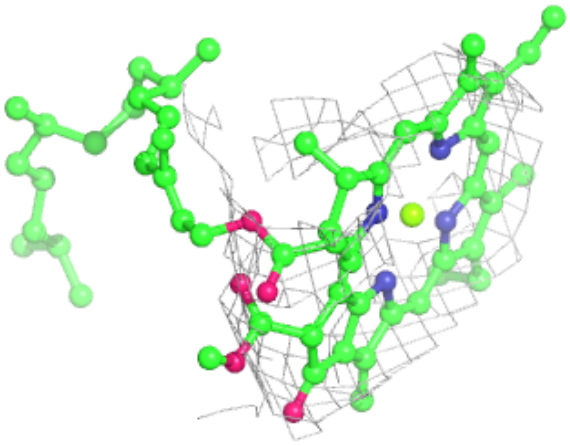


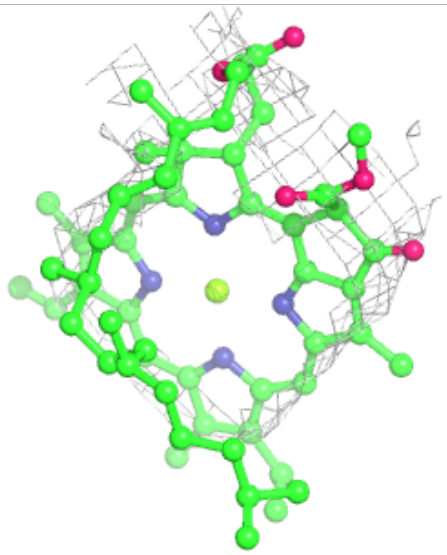


Electron density around CLA B 612:

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

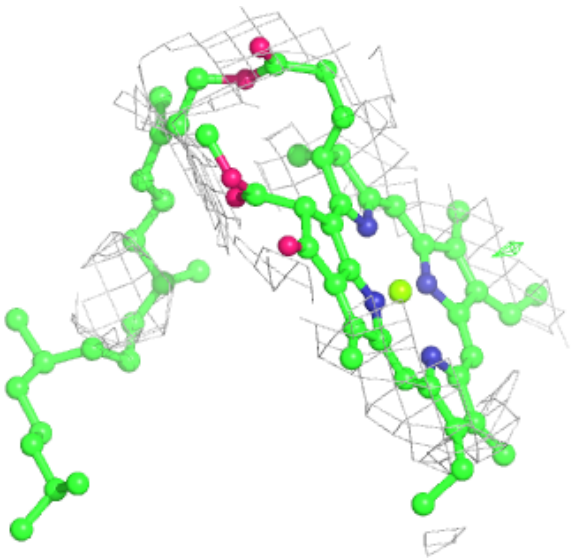


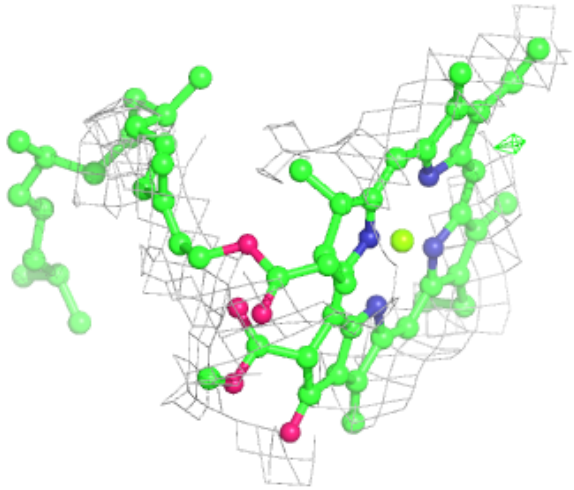


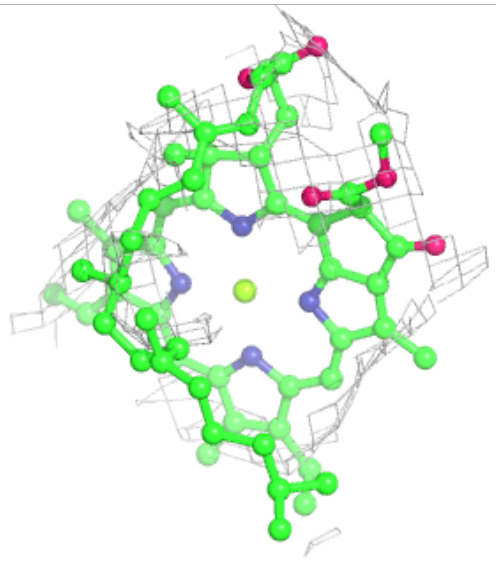


Electron density around CLA b 617:

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

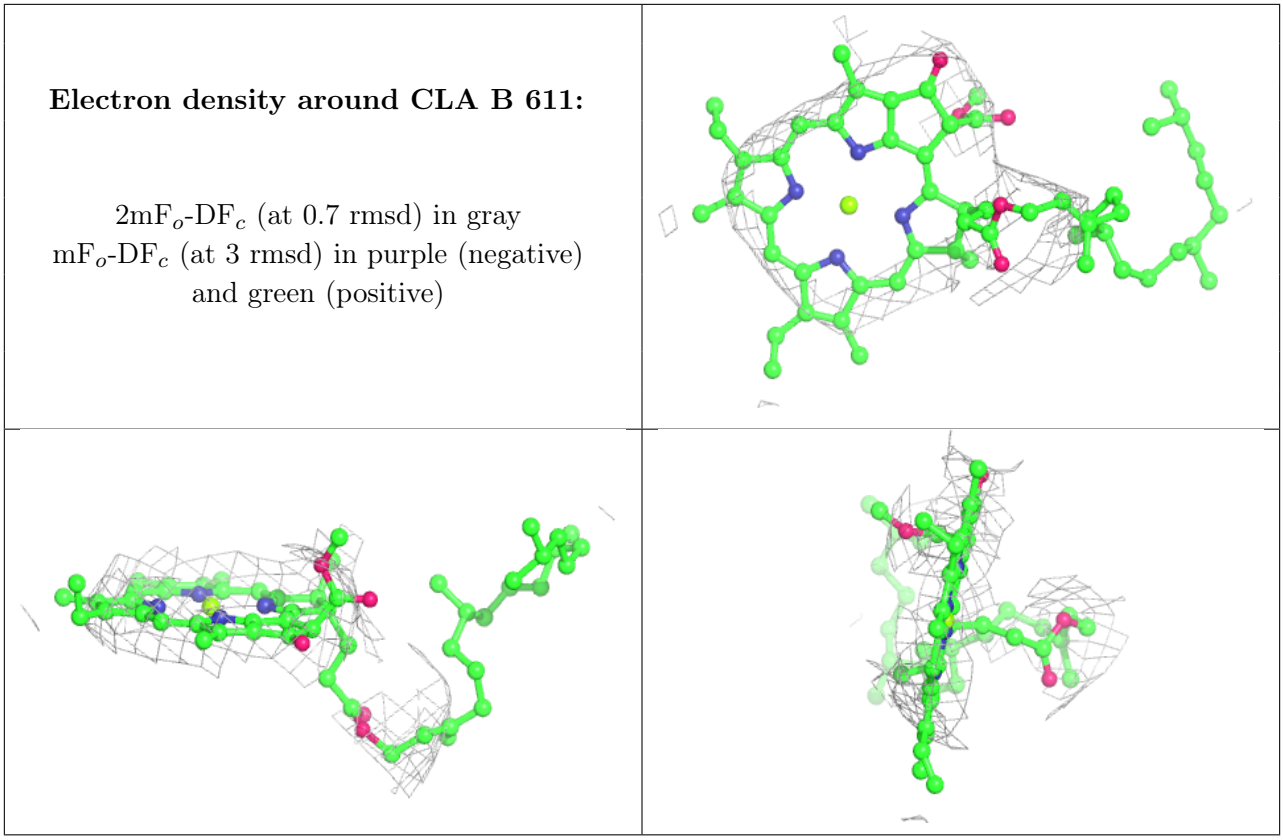






Electron density around CLA B 611:

$2mF_o$-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.