Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 08:52 PM EDT

PDB ID	:	4IXR
Title	:	RT fs X-ray diffraction of Photosystem II, first illuminated state
Authors	:	Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on	:	2013-01-27
Resolution	:	5.90 Å(reported)

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

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

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

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

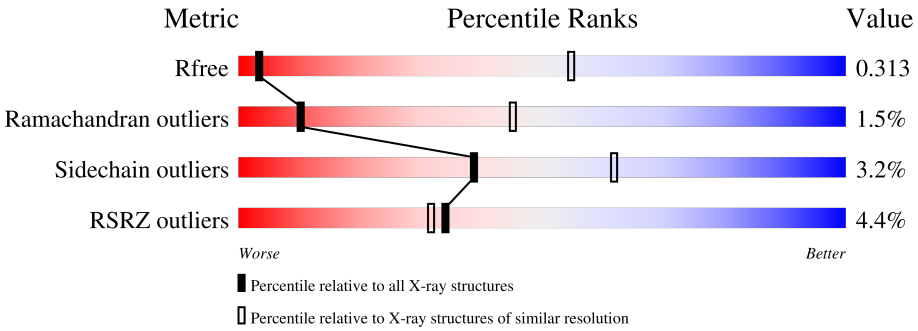
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.90 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	1016 (7.94-3.86)
Ramachandran outliers	138981	1011 (7.94-3.86)
Sidechain outliers	138945	1013 (7.94-3.82)
RSRZ outliers	127900	1014 (8.00-3.78)

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

Mol	Chain	Length	Quality of chain
1	A	360	2% 90% · 7%
1	a	360	% 91% · 7%
2	B	510	5% 93% · ·

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

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Mol	Chain	Length	Quality of chain
2	b	510	5% 93%
3	C	461	2% 93%
3	c	461	2% 92% 5%
4	D	352	% 92% 5%
4	d	352	% 92%
5	E	84	% 93%
5	e	84	4% 93%
6	F	45	4% 78% 22%
6	f	45	78% 22%
7	H	66	12% 88% 11%
7	h	66	5% 89% 9%
8	I	38	3% 84% 8% 8%
8	i	38	87% 5% 8%
9	J	40	2% 80% 5% 15%
9	j	40	2% 78% 8% 15%
10	K	46	76% 20%
10	k	46	7% 76% 20%
11	L	37	97%
11	l	37	97%
12	M	36	6% 94% 6%
12	m	36	8% 94% 6%
13	O	272	11% 87% 11%
13	o	272	7% 87% 11%
14	T	32	12% 94% 6%
14	t	32	94% 6%

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Mol	Chain	Length	Quality of chain
15	U	134	7% 69% 28%
15	u	134	4% 69% 28%
16	V	163	4% 83% 16%
16	v	163	6% 83% 16%
17	g	46	11% 54% 7% 39%
17	y	46	2% 54% 7% 39%
18	X	41	12% 83% 5% 10%
18	x	41	24% 83% 5% 10%
19	Z	62	11% 94% 6%
19	z	62	3% 92% 8%
20	G	28	100%
20	Y	28	100%

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	X
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	X
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	605	X	-	-	X
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	X
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	X
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	a	410	-	-	-	X
25	PL9	j	101	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	516	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	622	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	h	101	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	y	101	-	-	-	X
27	BCR	z	101	-	-	-	X
28	DGD	B	627	-	-	-	X
28	DGD	C	519	-	-	-	X
28	DGD	D	409	-	-	-	X
28	DGD	d	409	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	414	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	D	408	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	b	601	-	-	-	X
30	SQD	d	408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	f	102	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	521	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	519	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	101	-	-	-	X
31	LMG	k	103	-	-	-	X
32	CL	A	416	-	-	-	X
32	CL	a	418	-	-	-	X
33	LMT	B	624	-	-	-	X
33	LMT	B	625	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	B	629	-	-	-	X
33	LMT	D	410	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	604	-	-	-	X
33	LMT	b	626	-	-	-	X
33	LMT	b	627	-	-	-	X
33	LMT	d	410	-	-	-	X
33	LMT	i	102	-	-	-	X
35	CA	K	101	-	-	-	X
35	CA	O	301	-	-	-	X
35	CA	k	101	-	-	-	X
35	CA	o	301	-	-	-	X

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 50232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

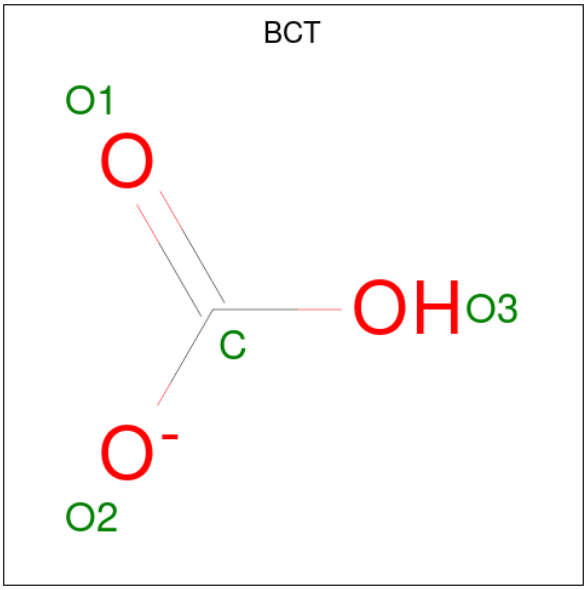
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

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

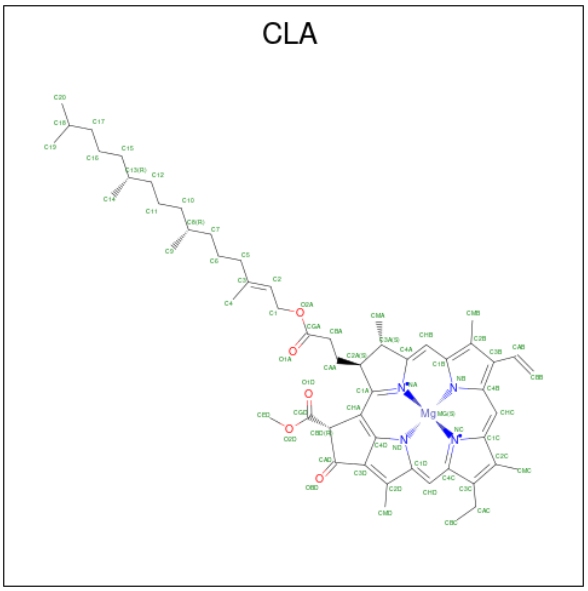
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total Fe 1 1	0	0
21	a	1	Total Fe 1 1	0	0

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



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

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



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

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

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

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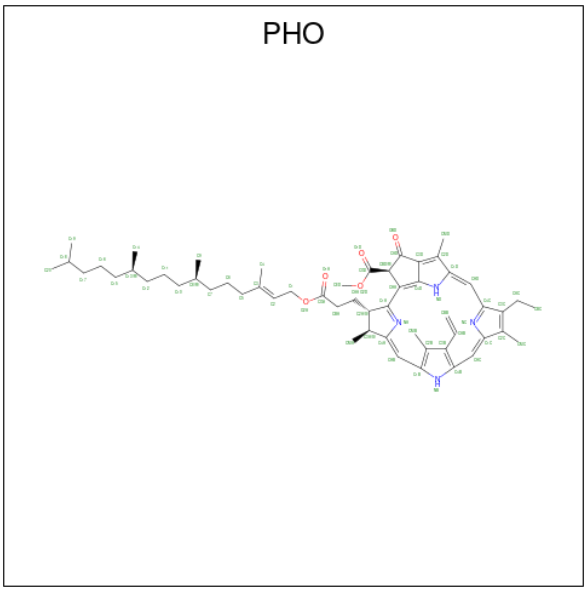
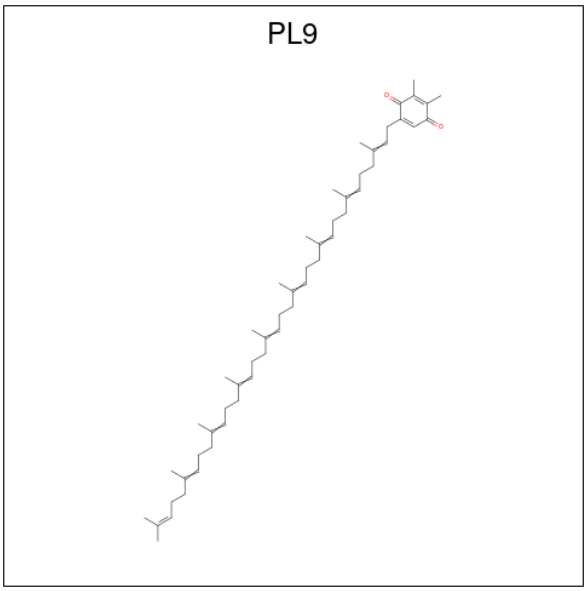
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



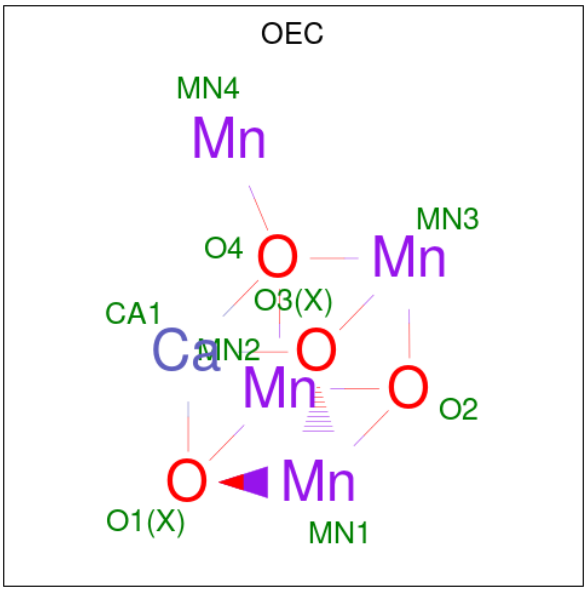
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



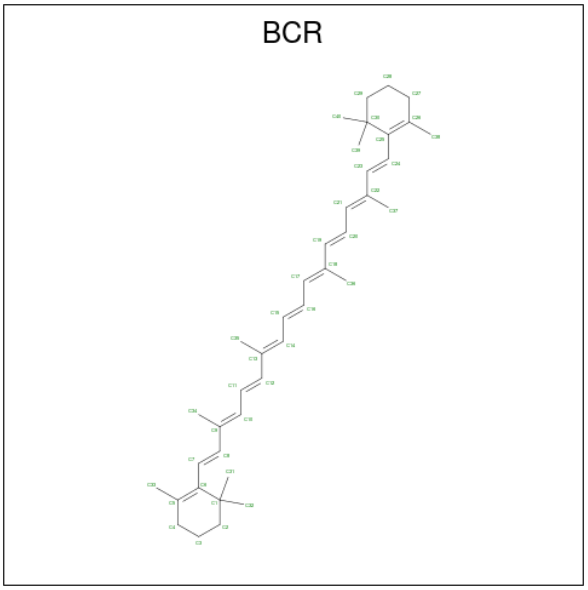
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 45 43 2	0	0
25	D	1	Total C O 55 53 2	0	0
25	J	1	Total C O 35 33 2	0	0
25	a	1	Total C O 45 43 2	0	0
25	d	1	Total C O 55 53 2	0	0
25	j	1	Total C O 35 33 2	0	0

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



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

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



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

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

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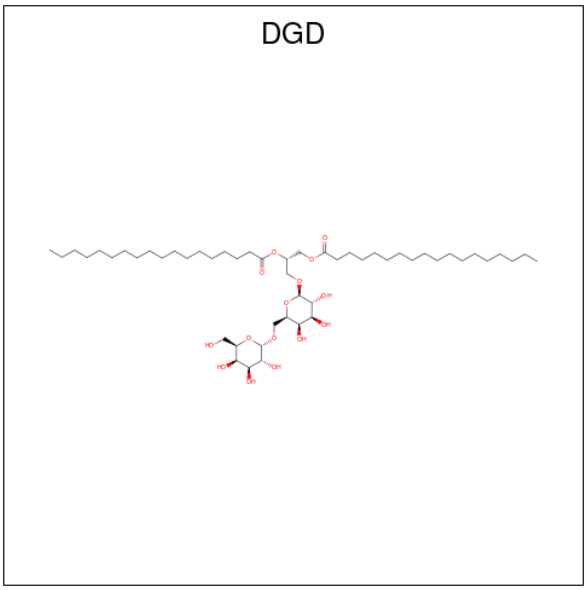
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	z	1	Total C 40 40	0	0

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



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

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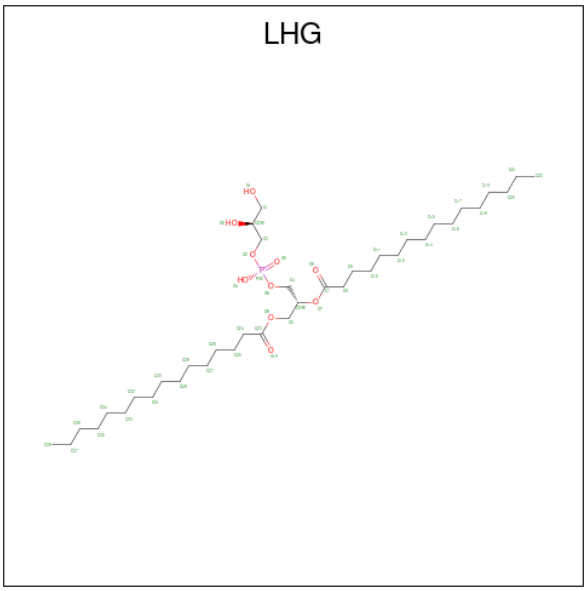
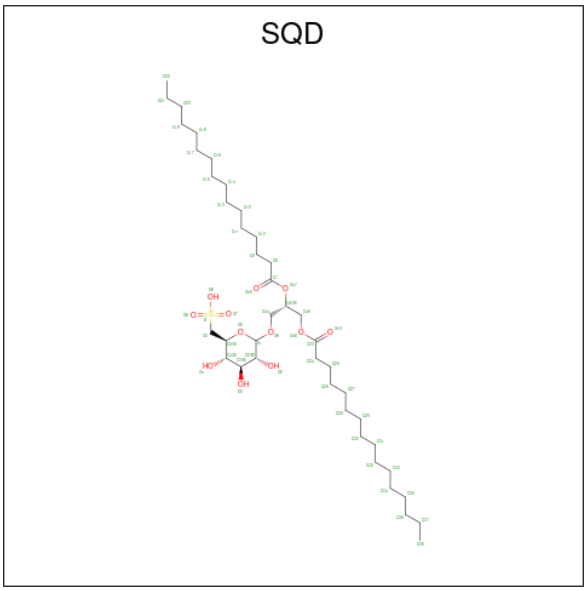
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	c	1	Total C O 53 38 15	0	0
28	c	1	Total C O 62 47 15	0	0
28	c	1	Total C O 66 51 15	0	0
28	d	1	Total C O 63 48 15	0	0

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



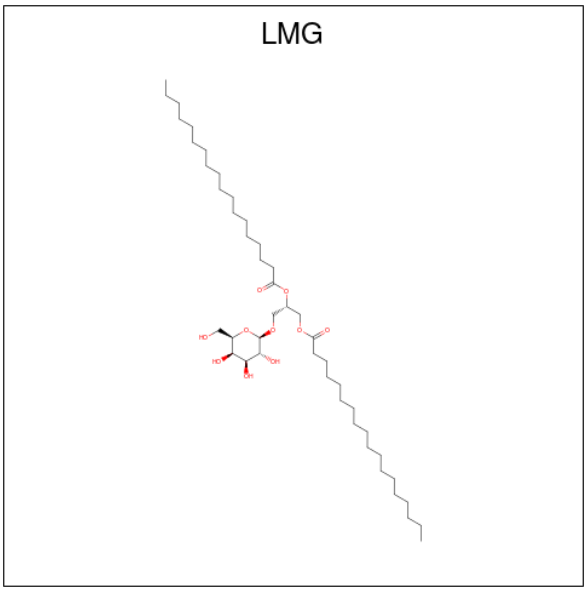
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O P 39 28 10 1	0	0
29	A	1	Total C O P 37 26 10 1	0	0
29	a	1	Total C O P 39 28 10 1	0	0
29	a	1	Total C O P 37 26 10 1	0	0

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



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

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



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

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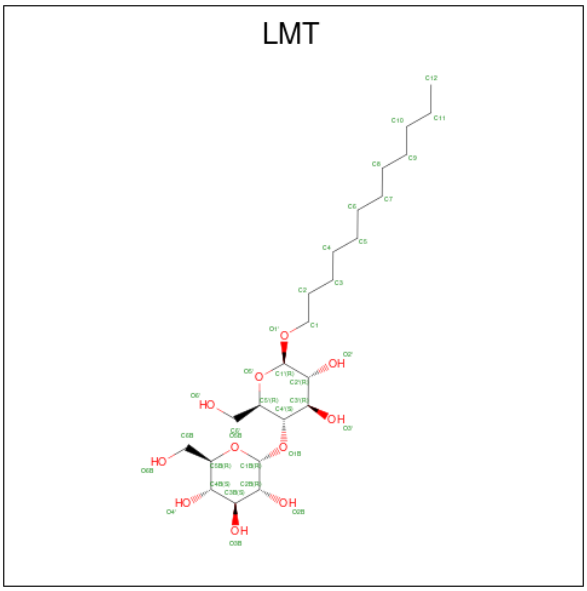
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C O 49 39 10	0	0
31	c	1	Total C O 45 35 10	0	0
31	d	1	Total C O 46 36 10	0	0
31	d	1	Total C O 48 38 10	0	0
31	e	1	Total C O 44 34 10	0	0
31	i	1	Total C O 43 33 10	0	0
31	k	1	Total C O 48 38 10	0	0
31	m	1	Total C O 42 32 10	0	0

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

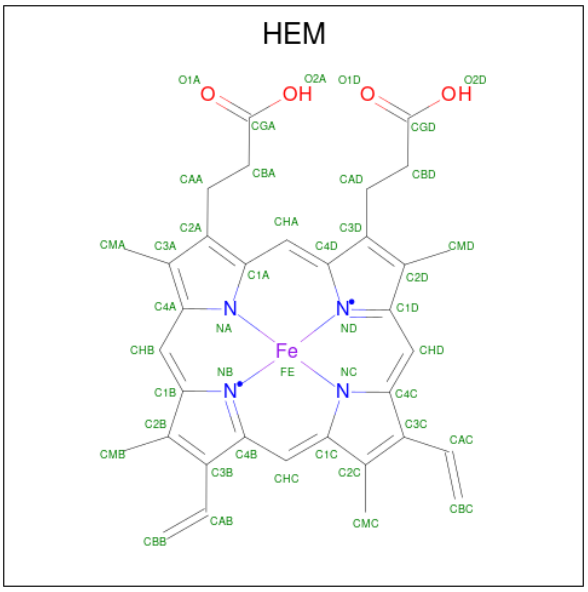
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total Cl 1 1	0	0
32	a	1	Total Cl 1 1	0	0

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



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

- 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).

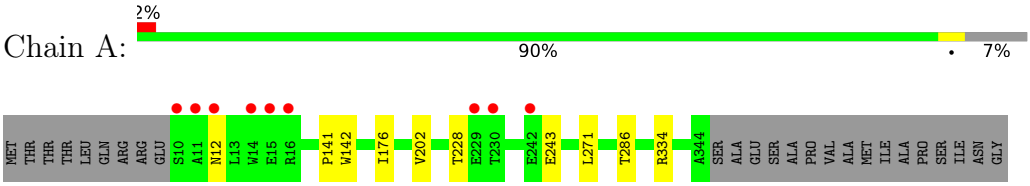
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	K	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		
35	o	1	Total	Ca	0	0
			1	1		

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.

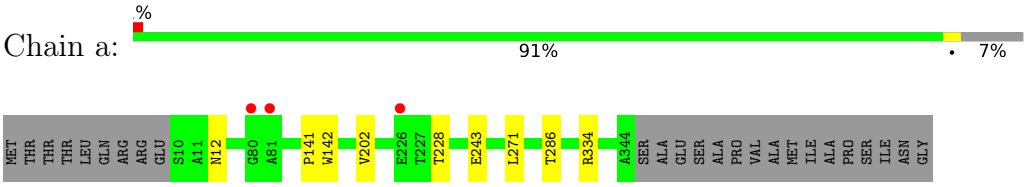
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



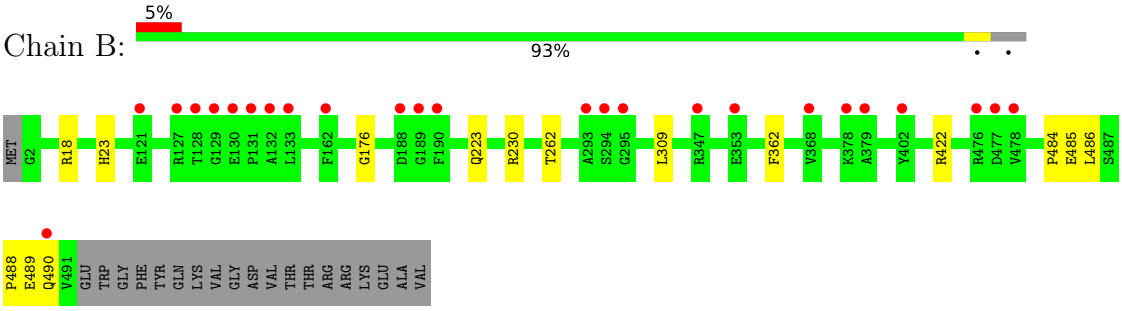
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



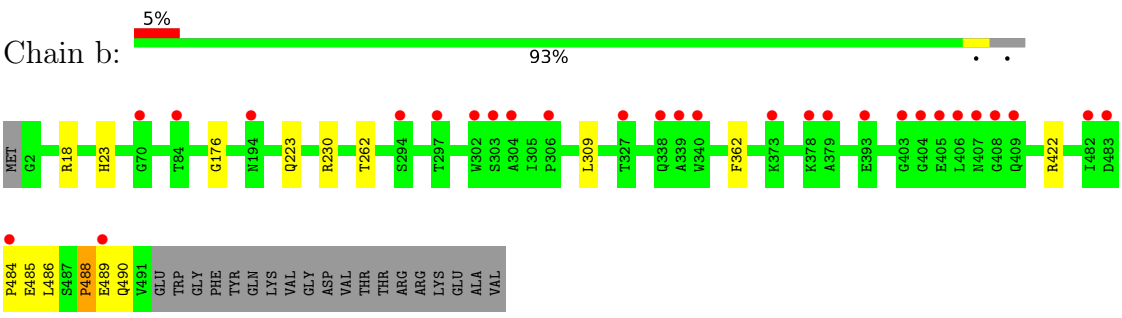
• Molecule 2: Photosystem II core light harvesting protein

Chain B:



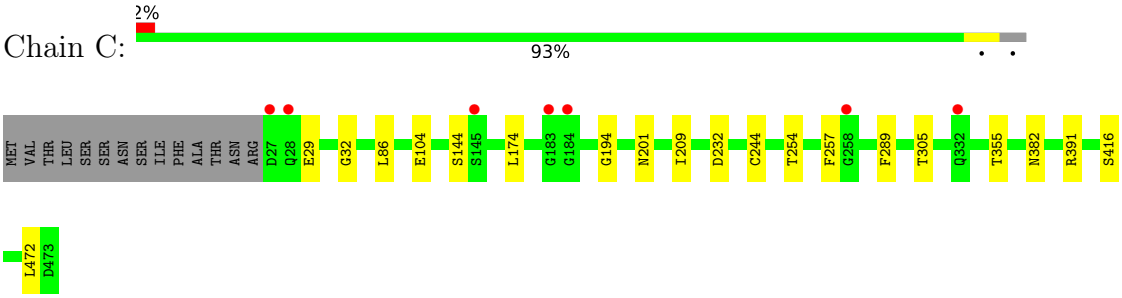
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



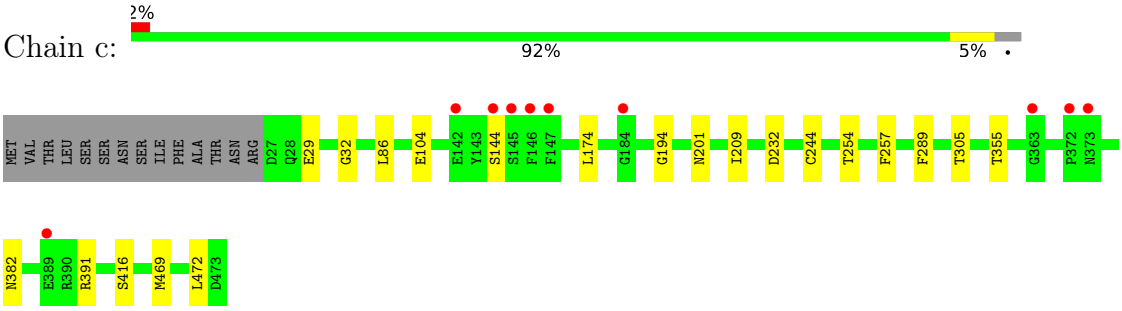
• Molecule 3: Photosystem II CP43 protein

Chain C:



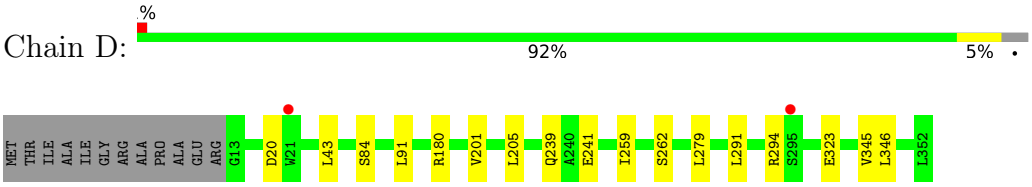
• Molecule 3: Photosystem II CP43 protein

Chain c:



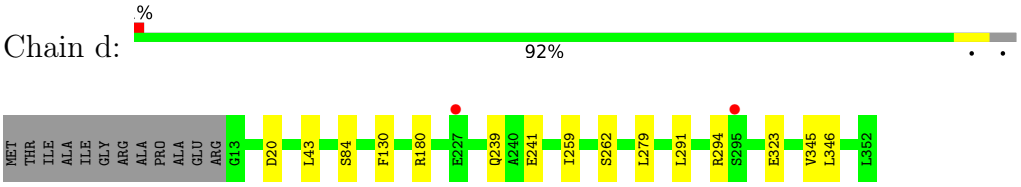
• Molecule 4: Photosystem II D2 protein

Chain D:



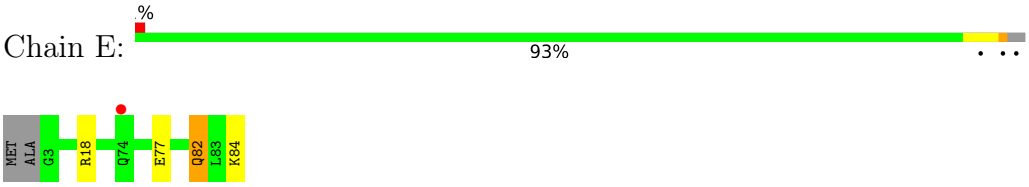
• Molecule 4: Photosystem II D2 protein

Chain d:



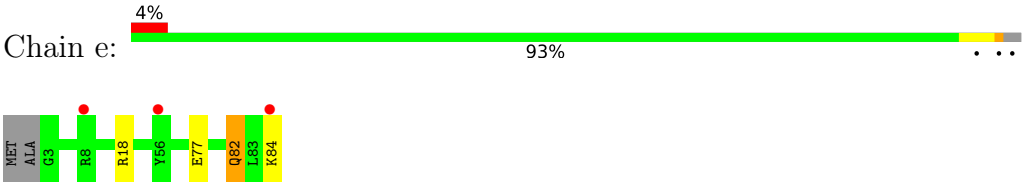
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



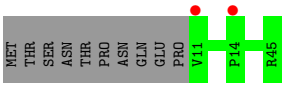
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



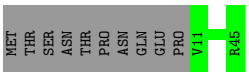
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



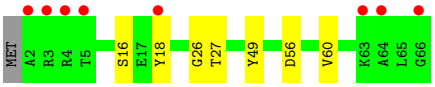
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



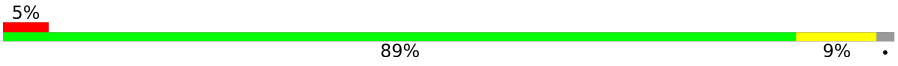
• Molecule 7: Photosystem II reaction center protein H

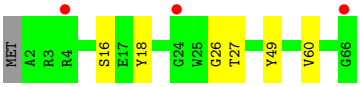
Chain H:



• Molecule 7: Photosystem II reaction center protein H

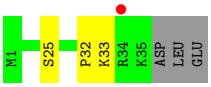
Chain h:





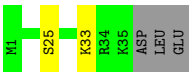
• Molecule 8: Photosystem II reaction center protein I

Chain I:



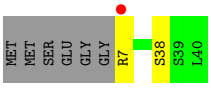
• Molecule 8: Photosystem II reaction center protein I

Chain i:



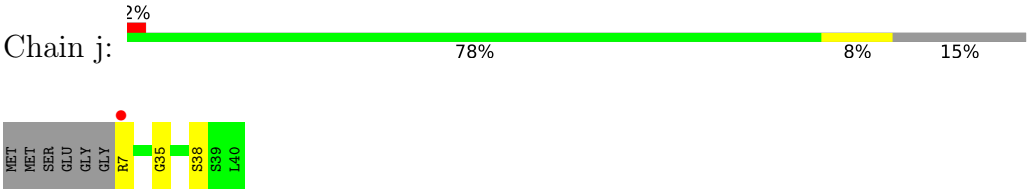
• Molecule 9: Photosystem II reaction center protein J

Chain J:



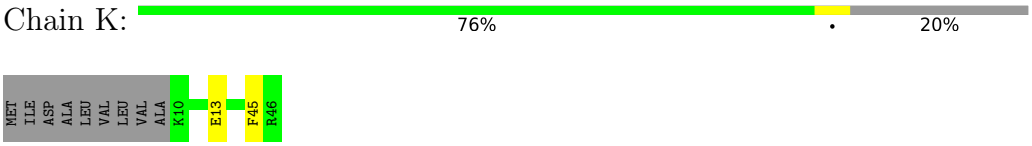
• Molecule 9: Photosystem II reaction center protein J

Chain j:



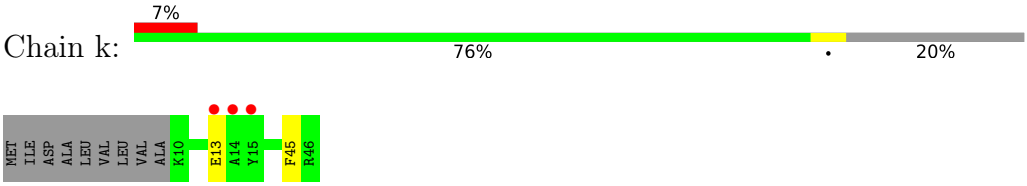
• Molecule 10: Photosystem II reaction center protein K

Chain K:



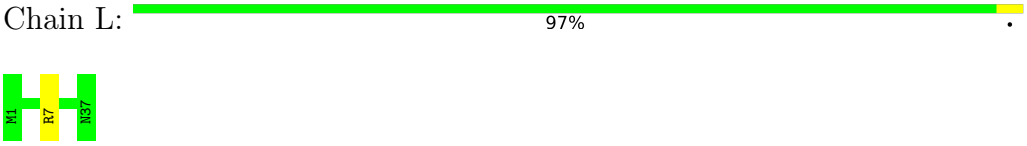
• Molecule 10: Photosystem II reaction center protein K

Chain k:



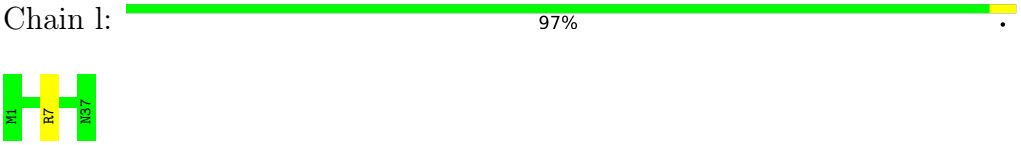
• Molecule 11: Photosystem II reaction center protein L

Chain L:



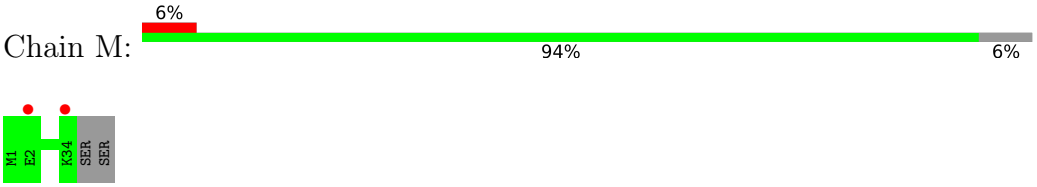
• Molecule 11: Photosystem II reaction center protein L

Chain l:



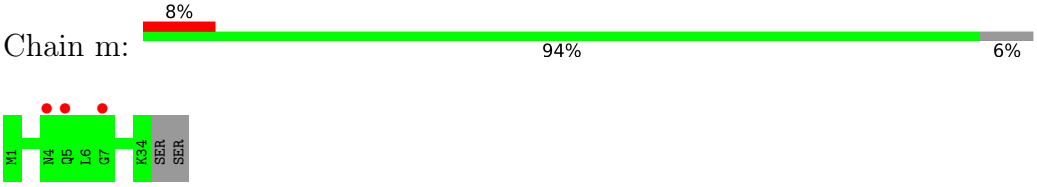
• Molecule 12: Photosystem II reaction center protein M

Chain M:



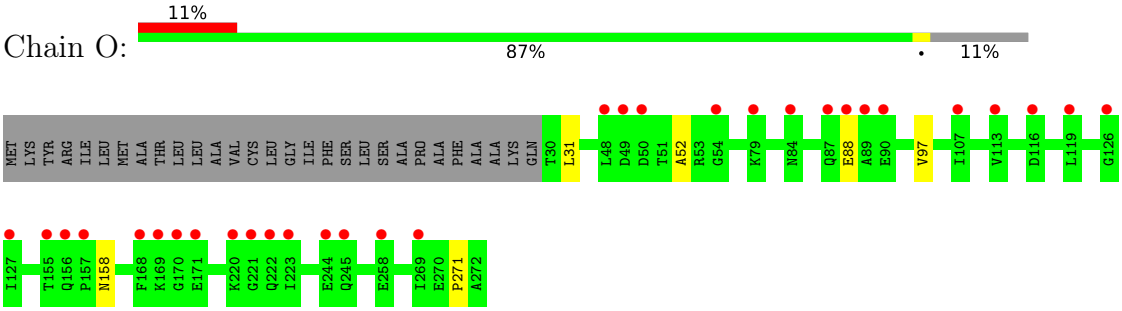
• Molecule 12: Photosystem II reaction center protein M

Chain m:



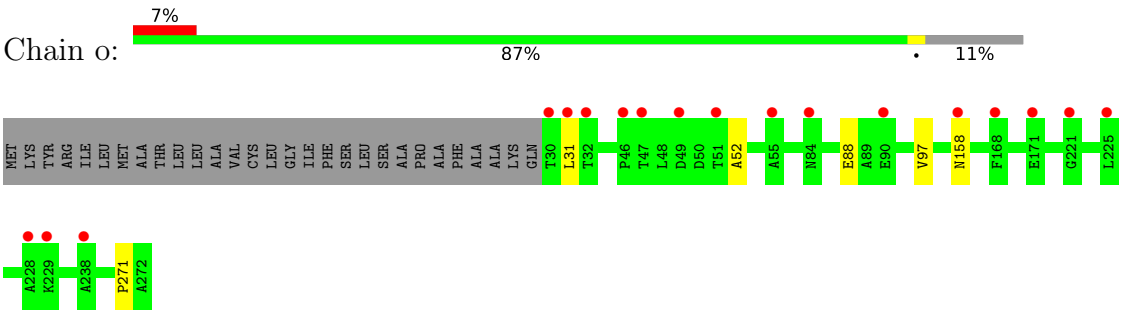
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



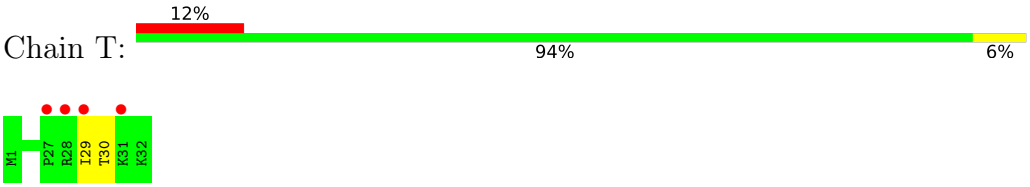
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



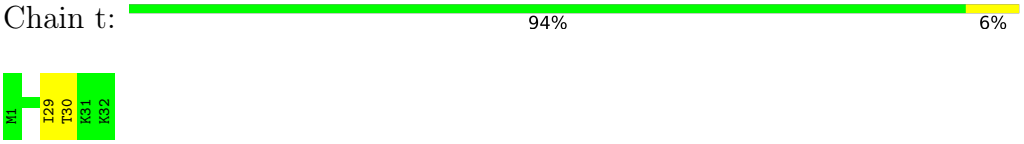
• Molecule 14: Photosystem II reaction center protein T

Chain T:



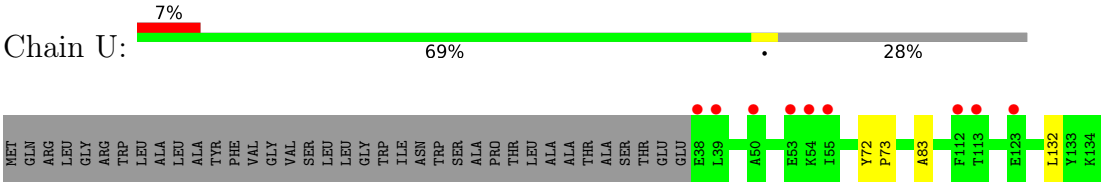
• Molecule 14: Photosystem II reaction center protein T

Chain t:



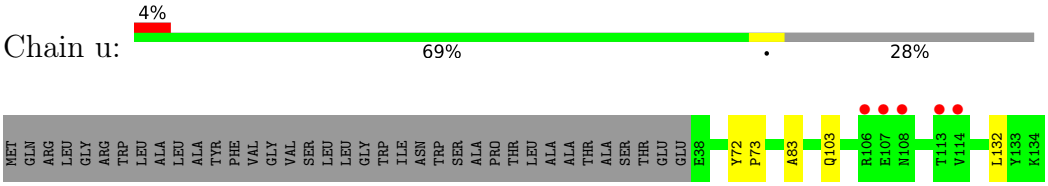
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



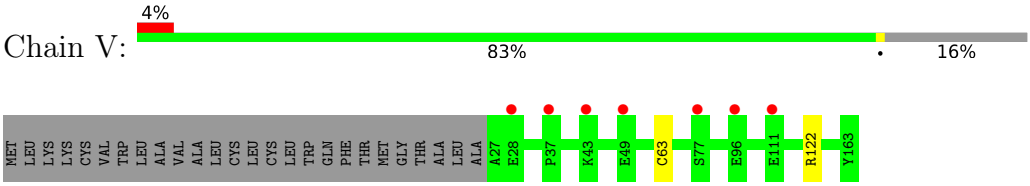
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



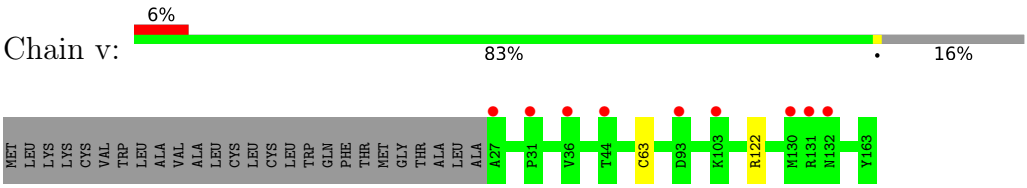
• Molecule 16: Cytochrome c-550

Chain V:



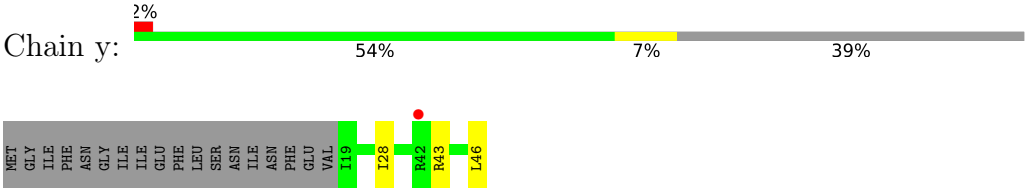
• Molecule 16: Cytochrome c-550

Chain v:



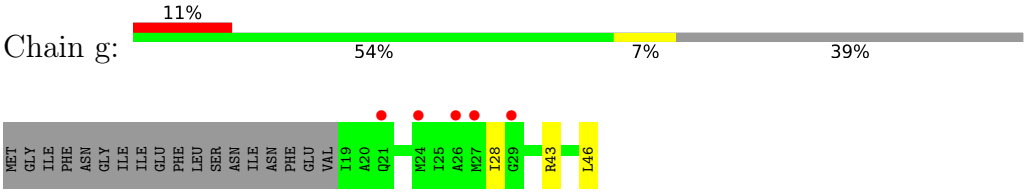
• Molecule 17: Photosystem II reaction center protein ycf12

Chain y:



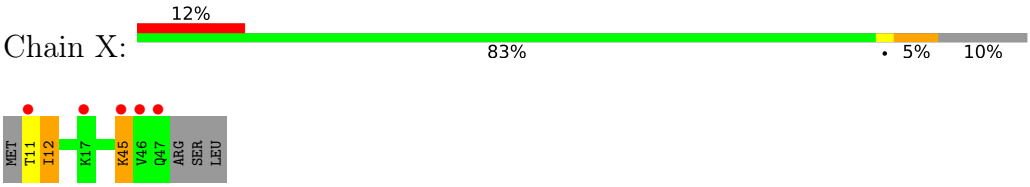
• Molecule 17: Photosystem II reaction center protein ycf12

Chain g:



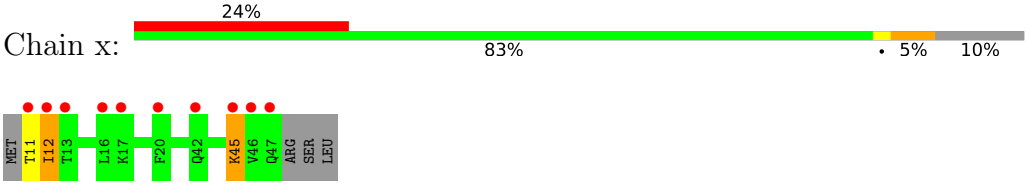
• Molecule 18: Photosystem II reaction center X protein

Chain X:



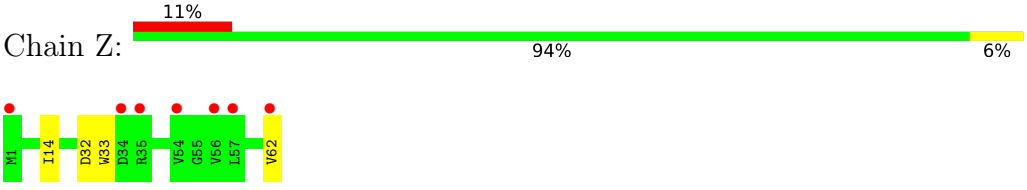
• Molecule 18: Photosystem II reaction center X protein

Chain x:



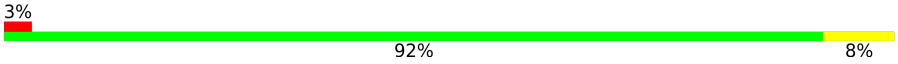
• Molecule 19: Photosystem II reaction center protein Z

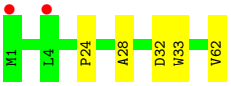
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

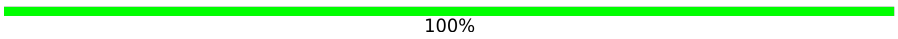
Chain z:





• Molecule 20: Photosystem II reaction center protein Y

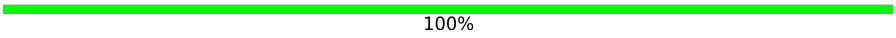
Chain G:



There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Y

Chain Y:



There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	131.98Å 227.57Å 306.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 5.90 82.97 – 5.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.97-5.90) 98.5 (82.97-5.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.285 , 0.313 0.285 , 0.313	Depositor DCC
R_{free} test set	1200 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	1.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.28	0/3986	0.46	0/5433
3	C	0.28	0/3556	0.46	0/4842
3	c	0.27	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.29	0/685	0.48	0/933
5	e	0.28	0/685	0.48	0/933
6	F	0.28	0/291	0.45	0/397
6	f	0.26	0/291	0.45	0/397
7	H	0.26	0/520	0.49	0/709
7	h	0.27	0/520	0.50	0/709
8	I	0.28	0/293	0.48	0/395
8	i	0.32	0/293	0.49	0/395
9	J	0.29	0/255	0.46	0/346
9	j	0.28	0/255	0.44	0/346
10	K	0.29	0/303	0.52	0/416
10	k	0.28	0/303	0.53	0/416
11	L	0.25	0/311	0.43	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.65	0/367
12	m	0.41	0/270	0.65	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.36	0/284	0.49	0/381
14	t	0.35	0/284	0.47	0/381
15	U	0.27	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.30	0/1081	0.52	0/1468
16	v	0.26	0/1081	0.46	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	g	0.24	0/202	0.51	0/272
17	y	0.25	0/202	0.52	0/272
18	X	0.30	0/273	0.52	0/370
18	x	0.32	0/273	0.50	0/370
19	Z	0.30	0/490	0.50	0/669
19	z	0.28	0/490	0.48	0/669
All	All	0.29	0/41948	0.48	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/360 (92%)	311 (93%)	17 (5%)	5 (2%)	10	45
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	13	50
2	B	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	15	54
2	b	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	15	54
3	C	445/461 (96%)	406 (91%)	33 (7%)	6 (1%)	12	48
3	c	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	12	48
4	D	338/352 (96%)	316 (94%)	20 (6%)	2 (1%)	25	65
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	20
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	20
8	I	33/38 (87%)	27 (82%)	4 (12%)	2 (6%)	1	16
8	i	33/38 (87%)	28 (85%)	4 (12%)	1 (3%)	4	28
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	27
9	j	32/40 (80%)	28 (88%)	2 (6%)	2 (6%)	1	16
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1	18
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	1	18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	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%)	206 (86%)	31 (13%)	4 (2%)	9	42
13	o	241/272 (89%)	208 (86%)	29 (12%)	4 (2%)	9	42
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	26
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	26
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4	26
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	4	26
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	24
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	24
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1	18
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	1	18
19	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	42
19	z	60/62 (97%)	54 (90%)	3 (5%)	3 (5%)	2	20
All	All	5138/5650 (91%)	4681 (91%)	378 (7%)	79 (2%)	10	45

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA
14	T	30	THR
18	X	45	LYS
1	a	12	ASN
1	a	142	TRP
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
14	t	30	THR
18	x	45	LYS
1	A	141	PRO
2	B	489	GLU
3	C	32	GLY
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
7	H	26	GLY
17	y	43	ARG
19	Z	32	ASP
1	a	141	PRO
2	b	489	GLU
3	c	32	GLY
3	c	144	SER
3	c	257	PHE
3	c	416	SER
4	d	239	GLN
5	e	82	GLN
7	h	26	GLY
9	j	38	SER
17	g	43	ARG
19	z	32	ASP
1	A	142	TRP
3	C	194	GLY
5	E	82	GLN
9	J	38	SER
13	O	88	GLU

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Mol	Chain	Res	Type
15	U	83	ALA
1	a	334	ARG
3	c	194	GLY
13	o	88	GLU
13	o	271	PRO
15	u	72	TYR
1	A	334	ARG
4	D	262	SER
13	O	271	PRO
15	U	72	TYR
4	d	262	SER
7	h	16	SER
8	i	25	SER
10	k	45	PHE
13	o	158	ASN
15	u	83	ALA
2	B	176	GLY
2	B	230	ARG
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
15	U	73	PRO
2	b	176	GLY
10	k	13	GLU
18	x	12	ILE
8	I	25	SER
13	O	158	ASN
18	X	12	ILE
2	b	230	ARG
19	z	28	ALA
15	u	73	PRO
8	I	32	PRO
3	C	209	ILE
1	A	176	ILE
3	c	209	ILE
19	z	24	PRO
9	j	35	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	271/291 (93%)	266 (98%)	5 (2%)	59	77
1	a	271/291 (93%)	266 (98%)	5 (2%)	59	77
2	B	390/407 (96%)	380 (97%)	10 (3%)	46	66
2	b	390/407 (96%)	379 (97%)	11 (3%)	43	65
3	C	347/362 (96%)	333 (96%)	14 (4%)	31	55
3	c	347/362 (96%)	332 (96%)	15 (4%)	29	54
4	D	275/283 (97%)	260 (94%)	15 (6%)	21	47
4	d	275/283 (97%)	262 (95%)	13 (5%)	26	51
5	E	72/73 (99%)	68 (94%)	4 (6%)	21	46
5	e	72/73 (99%)	68 (94%)	4 (6%)	21	46
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	13	38
7	h	53/55 (96%)	50 (94%)	3 (6%)	20	46
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	u	84/112 (75%)	82 (98%)	2 (2%)	49 69
16	V	116/138 (84%)	114 (98%)	2 (2%)	60 78
16	v	116/138 (84%)	114 (98%)	2 (2%)	60 78
17	g	20/37 (54%)	18 (90%)	2 (10%)	7 26
17	y	20/37 (54%)	18 (90%)	2 (10%)	7 26
18	X	30/34 (88%)	27 (90%)	3 (10%)	7 26
18	x	30/34 (88%)	27 (90%)	3 (10%)	7 26
19	Z	52/52 (100%)	49 (94%)	3 (6%)	20 45
19	z	52/52 (100%)	50 (96%)	2 (4%)	33 57
All	All	4244/4616 (92%)	4107 (97%)	137 (3%)	39 62

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	VAL
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	223	GLN
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	232	ASP
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR

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Mol	Chain	Res	Type
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	84	SER
4	D	91	LEU
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU
16	V	63	CYS
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	45	LYS
19	Z	14	ILE

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Mol	Chain	Res	Type
19	Z	33	TRP
19	Z	62	VAL
1	a	202	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	223	GLN
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	488	PRO
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	232	ASP
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	305	THR
3	c	355	THR
3	c	382	ASN
3	c	391	ARG
3	c	469	MET
3	c	472	LEU
4	d	20	ASP
4	d	43	LEU
4	d	84	SER
4	d	130	PHE
4	d	180	ARG
4	d	241	GLU
4	d	259	ILE
4	d	279	LEU
4	d	291	LEU

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Mol	Chain	Res	Type
4	d	294	ARG
4	d	323	GLU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	77	GLU
5	e	82	GLN
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	103	GLN
15	u	132	LEU
16	v	63	CYS
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	11	THR
18	x	12	ILE
18	x	45	LYS
19	z	33	TRP
19	z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	303	ASN
4	D	117	HIS
17	y	45	ASN
1	a	241	GLN
2	b	201	HIS
15	u	93	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
23	CLA	c	506	-	65,73,73	1.53	5 (7%)	76,113,113	1.45	8 (10%)
23	CLA	b	618	-	65,73,73	1.51	6 (9%)	76,113,113	1.39	6 (7%)
33	LMT	B	628	-	36,36,36	0.45	0	47,47,47	0.77	1 (2%)
33	LMT	i	102	-	36,36,36	0.48	1 (2%)	47,47,47	0.67	0
28	DGD	b	623	-	59,59,67	1.20	7 (11%)	73,73,81	1.14	5 (6%)
29	LHG	A	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.08	2 (5%)
23	CLA	c	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	9 (11%)
23	CLA	b	620	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	7 (9%)
23	CLA	c	511	-	65,73,73	1.56	5 (7%)	76,113,113	1.37	8 (10%)
28	DGD	B	627	-	53,53,67	1.22	6 (11%)	67,67,81	1.43	9 (13%)
27	BCR	j	102	-	41,41,41	0.71	0	56,56,56	3.35	25 (44%)
28	DGD	c	516	-	54,54,67	1.24	6 (11%)	68,68,81	1.25	7 (10%)
33	LMT	d	410	-	32,32,36	0.49	1 (3%)	43,43,47	0.69	1 (2%)
23	CLA	b	617	-	65,73,73	1.48	6 (9%)	76,113,113	1.49	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	PHO	D	402	-	51,69,69	1.04	5 (9%)	47,99,99	1.09	5 (10%)
31	LMG	A	414	-	51,51,55	1.15	6 (11%)	59,59,63	1.35	5 (8%)
34	HEM	f	101	6,5	41,50,50	1.97	6 (14%)	45,82,82	1.87	8 (17%)
23	CLA	c	510	-	65,73,73	1.49	6 (9%)	76,113,113	1.33	6 (7%)
31	LMG	I	101	-	43,43,55	1.25	8 (18%)	51,51,63	1.31	7 (13%)
30	SQD	a	401	-	53,54,54	0.99	4 (7%)	62,65,65	1.66	10 (16%)
23	CLA	B	615	-	65,73,73	1.50	5 (7%)	76,113,113	1.35	7 (9%)
31	LMG	m	102	-	42,42,55	1.33	7 (16%)	50,50,63	1.57	7 (14%)
23	CLA	C	503	-	65,73,73	1.47	5 (7%)	76,113,113	1.37	6 (7%)
27	BCR	T	102	-	41,41,41	0.70	0	56,56,56	2.24	16 (28%)
28	DGD	C	517	-	54,54,67	1.21	6 (11%)	68,68,81	1.25	6 (8%)
23	CLA	C	504	-	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	B	602	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	7 (9%)
28	DGD	c	517	-	63,63,67	1.21	10 (15%)	77,77,81	1.31	7 (9%)
28	DGD	A	411	-	57,57,67	1.23	7 (12%)	71,71,81	1.58	12 (16%)
31	LMG	a	416	-	51,51,55	1.11	6 (11%)	59,59,63	1.40	5 (8%)
29	LHG	a	417	-	36,36,48	1.09	2 (5%)	39,42,54	1.01	2 (5%)
23	CLA	C	511	3	65,73,73	1.50	6 (9%)	76,113,113	1.48	9 (11%)
25	PL9	a	410	-	45,45,55	1.25	7 (15%)	56,57,69	1.65	15 (26%)
27	BCR	C	515	-	41,41,41	0.67	0	56,56,56	1.91	16 (28%)
23	CLA	B	613	-	65,73,73	1.49	5 (7%)	76,113,113	1.31	7 (9%)
27	BCR	b	621	-	41,41,41	0.65	0	56,56,56	1.96	19 (33%)
23	CLA	C	501	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	9 (11%)
23	CLA	C	507	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	59,62,65	1.57	10 (16%)
28	DGD	C	518	-	63,63,67	1.22	10 (15%)	77,77,81	1.28	7 (9%)
23	CLA	b	611	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	7 (9%)
23	CLA	A	404	-	65,73,73	1.49	5 (7%)	76,113,113	1.42	9 (11%)
23	CLA	C	513	-	65,73,73	1.49	5 (7%)	76,113,113	1.39	9 (11%)
33	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
27	BCR	y	101	-	41,41,41	0.73	0	56,56,56	1.94	14 (25%)
23	CLA	b	619	-	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)
34	HEM	F	101	6,5	41,50,50	1.94	5 (12%)	45,82,82	1.82	7 (15%)
33	LMT	B	624	-	36,36,36	0.42	0	47,47,47	0.69	0
23	CLA	b	610	-	65,73,73	1.51	5 (7%)	76,113,113	1.37	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	a	406	-	65,73,73	1.52	6 (9%)	76,113,113	1.48	8 (10%)
23	CLA	c	512	-	65,73,73	1.51	6 (9%)	76,113,113	1.42	8 (10%)
31	LMG	E	101	-	44,44,55	1.19	7 (15%)	52,52,63	1.33	8 (15%)
33	LMT	I	102	-	36,36,36	0.42	0	47,47,47	0.67	0
23	CLA	B	616	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	6 (7%)
22	BCT	A	402	21	2,3,3	0.46	0	2,3,3	0.31	0
27	BCR	B	619	-	41,41,41	0.68	0	56,56,56	1.86	15 (26%)
33	LMT	M	102	-	36,36,36	0.44	0	47,47,47	0.67	0
31	LMG	c	519	-	45,45,55	1.21	7 (15%)	53,53,63	1.32	7 (13%)
23	CLA	c	507	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	9 (11%)
27	BCR	H	101	-	41,41,41	0.72	0	56,56,56	1.75	16 (28%)
25	PL9	j	101	-	35,35,55	1.19	5 (14%)	44,45,69	1.55	8 (18%)
33	LMT	b	627	-	36,36,36	0.43	0	47,47,47	0.65	0
31	LMG	a	402	-	42,42,55	1.23	6 (14%)	50,50,63	1.52	7 (14%)
23	CLA	b	609	-	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
23	CLA	B	601	-	65,73,73	1.54	5 (7%)	76,113,113	1.41	7 (9%)
28	DGD	b	602	-	53,53,67	1.23	6 (11%)	67,67,81	1.37	8 (11%)
31	LMG	b	624	-	49,49,55	1.17	7 (14%)	57,57,63	1.30	7 (12%)
27	BCR	B	620	-	41,41,41	0.73	0	56,56,56	2.14	15 (26%)
23	CLA	c	502	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	8 (10%)
31	LMG	B	623	-	49,49,55	1.19	8 (16%)	57,57,63	1.38	9 (15%)
23	CLA	B	607	-	65,73,73	1.49	5 (7%)	76,113,113	1.51	10 (13%)
31	LMG	d	407	-	48,48,55	1.17	8 (16%)	56,56,63	1.47	7 (12%)
33	LMT	b	626	-	36,36,36	0.39	0	47,47,47	0.74	1 (2%)
33	LMT	m	101	-	36,36,36	0.42	0	47,47,47	0.66	0
23	CLA	d	402	-	65,73,73	1.51	6 (9%)	76,113,113	1.48	8 (10%)
31	LMG	B	622	-	49,49,55	1.14	7 (14%)	57,57,63	1.30	6 (10%)
23	CLA	B	611	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	9 (11%)
34	HEM	V	201	16	41,50,50	2.03	8 (19%)	45,82,82	1.61	4 (8%)
33	LMT	b	604	-	36,36,36	0.40	0	47,47,47	0.63	0
33	LMT	b	603	-	36,36,36	0.44	0	47,47,47	0.75	1 (2%)
23	CLA	D	403	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	8 (10%)
31	LMG	D	406	-	46,46,55	1.17	6 (13%)	54,54,63	1.39	6 (11%)
24	PHO	a	407	-	51,69,69	1.03	5 (9%)	47,99,99	1.14	5 (10%)
27	BCR	a	412	-	41,41,41	0.74	0	56,56,56	1.90	12 (21%)
27	BCR	h	101	-	41,41,41	0.73	0	56,56,56	1.76	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	53,56,65	1.67	10 (18%)
31	LMG	d	406	-	46,46,55	1.18	7 (15%)	54,54,63	1.33	6 (11%)
28	DGD	C	519	-	67,67,67	1.12	7 (10%)	81,81,81	1.43	10 (12%)
27	BCR	B	618	-	41,41,41	0.67	0	56,56,56	2.26	20 (35%)
31	LMG	C	520	-	48,48,55	1.13	6 (12%)	56,56,63	1.31	6 (10%)
23	CLA	B	603	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
27	BCR	C	514	-	41,41,41	0.73	0	56,56,56	2.34	21 (37%)
31	LMG	M	101	-	42,42,55	1.28	7 (16%)	50,50,63	1.51	6 (12%)
27	BCR	d	405	-	41,41,41	0.67	0	56,56,56	2.15	16 (28%)
31	LMG	A	418	-	42,42,55	1.22	6 (14%)	50,50,63	1.51	9 (18%)
27	BCR	b	622	-	41,41,41	0.72	0	56,56,56	2.20	17 (30%)
28	DGD	d	409	-	64,64,67	1.14	5 (7%)	78,78,81	1.42	12 (15%)
23	CLA	b	605	-	65,73,73	1.50	6 (9%)	76,113,113	1.41	8 (10%)
28	DGD	a	413	-	57,57,67	1.19	7 (12%)	71,71,81	1.52	12 (16%)
23	CLA	B	609	-	65,73,73	1.51	5 (7%)	76,113,113	1.38	7 (9%)
33	LMT	D	410	-	32,32,36	0.50	1 (3%)	43,43,47	0.69	1 (2%)
25	PL9	D	404	-	55,55,55	1.25	8 (14%)	68,69,69	1.63	18 (26%)
28	DGD	B	621	-	59,59,67	1.22	8 (13%)	73,73,81	1.10	5 (6%)
31	LMG	b	625	-	49,49,55	1.18	8 (16%)	57,57,63	1.42	10 (17%)
23	CLA	C	505	-	65,73,73	1.51	6 (9%)	76,113,113	1.38	7 (9%)
27	BCR	C	516	-	41,41,41	0.70	0	56,56,56	1.95	16 (28%)
23	CLA	b	613	-	65,73,73	1.50	5 (7%)	76,113,113	1.31	8 (10%)
23	CLA	b	615	-	65,73,73	1.53	5 (7%)	76,113,113	1.39	7 (9%)
31	LMG	e	101	-	44,44,55	1.21	8 (18%)	52,52,63	1.35	9 (17%)
23	CLA	c	504	-	65,73,73	1.49	5 (7%)	76,113,113	1.44	7 (9%)
24	PHO	a	408	-	51,69,69	1.00	3 (5%)	47,99,99	1.13	3 (6%)
23	CLA	B	606	-	65,73,73	1.47	5 (7%)	76,113,113	1.33	7 (9%)
23	CLA	B	612	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	6 (7%)
27	BCR	J	102	-	41,41,41	0.73	0	56,56,56	3.36	26 (46%)
23	CLA	b	606	-	65,73,73	1.50	5 (7%)	76,113,113	1.41	7 (9%)
23	CLA	b	612	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	C	502	-	65,73,73	1.49	7 (10%)	76,113,113	1.37	6 (7%)
23	CLA	a	404	-	65,73,73	1.54	6 (9%)	76,113,113	1.45	9 (11%)
23	CLA	d	403	-	65,73,73	1.54	6 (9%)	76,113,113	1.36	8 (10%)
28	DGD	D	409	-	64,64,67	1.14	6 (9%)	78,78,81	1.41	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	614	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
31	LMG	i	101	-	43,43,55	1.26	8 (18%)	51,51,63	1.31	6 (11%)
31	LMG	k	103	-	48,48,55	1.13	6 (12%)	56,56,63	1.27	7 (12%)
24	PHO	A	406	-	51,69,69	1.02	4 (7%)	47,99,99	1.17	3 (6%)
25	PL9	A	408	-	45,45,55	1.28	7 (15%)	56,57,69	1.58	15 (26%)
23	CLA	C	509	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	8 (10%)
23	CLA	D	401	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
23	CLA	A	403	-	65,73,73	1.53	6 (9%)	76,113,113	1.34	8 (10%)
30	SQD	f	102	-	44,45,54	1.02	4 (9%)	53,56,65	1.68	11 (20%)
23	CLA	a	405	-	65,73,73	1.52	5 (7%)	76,113,113	1.46	11 (14%)
23	CLA	B	605	-	65,73,73	1.49	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	C	508	-	65,73,73	1.52	7 (10%)	76,113,113	1.40	8 (10%)
30	SQD	b	601	-	46,47,54	1.02	5 (10%)	55,58,65	1.62	9 (16%)
27	BCR	z	101	-	41,41,41	0.65	0	56,56,56	1.84	15 (26%)
27	BCR	k	102	-	41,41,41	0.74	0	56,56,56	1.96	16 (28%)
30	SQD	A	413	-	50,51,54	0.98	3 (6%)	59,62,65	1.54	10 (16%)
34	HEM	v	201	16	41,50,50	2.03	8 (19%)	45,82,82	1.76	6 (13%)
23	CLA	c	513	-	65,73,73	1.50	5 (7%)	76,113,113	1.40	8 (10%)
23	CLA	B	608	-	65,73,73	1.52	6 (9%)	76,113,113	1.40	8 (10%)
23	CLA	c	505	-	65,73,73	1.51	6 (9%)	76,113,113	1.46	9 (11%)
22	BCT	d	401	21	2,3,3	0.45	0	2,3,3	0.29	0
23	CLA	b	607	-	65,73,73	1.47	5 (7%)	76,113,113	1.38	9 (11%)
28	DGD	c	518	-	67,67,67	1.11	6 (8%)	81,81,81	1.47	13 (16%)
25	PL9	d	404	-	55,55,55	1.24	8 (14%)	68,69,69	1.72	19 (27%)
23	CLA	A	407	-	65,73,73	1.47	5 (7%)	76,113,113	1.36	6 (7%)
30	SQD	A	417	-	53,54,54	1.01	4 (7%)	62,65,65	1.63	12 (19%)
23	CLA	c	503	-	65,73,73	1.50	5 (7%)	76,113,113	1.31	7 (9%)
23	CLA	c	508	-	65,73,73	1.50	6 (9%)	76,113,113	1.43	9 (11%)
25	PL9	J	101	-	35,35,55	1.20	5 (14%)	44,45,69	1.56	8 (18%)
30	SQD	D	408	-	42,43,54	1.11	5 (11%)	51,54,65	1.99	10 (19%)
27	BCR	T	101	-	41,41,41	0.70	0	56,56,56	1.78	13 (23%)
23	CLA	B	614	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	6 (7%)
23	CLA	C	506	-	65,73,73	1.52	5 (7%)	76,113,113	1.42	7 (9%)
27	BCR	B	617	-	41,41,41	0.71	0	56,56,56	1.85	13 (23%)
27	BCR	c	515	-	41,41,41	0.70	0	56,56,56	1.99	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	616	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	6 (7%)
30	SQD	B	626	-	46,47,54	1.03	5 (10%)	55,58,65	1.57	10 (18%)
30	SQD	d	408	-	42,43,54	1.12	4 (9%)	51,54,65	1.98	10 (19%)
23	CLA	B	604	-	65,73,73	1.52	6 (9%)	76,113,113	1.36	8 (10%)
27	BCR	D	405	-	41,41,41	0.67	0	56,56,56	2.19	17 (30%)
33	LMT	B	629	-	36,36,36	0.46	0	47,47,47	0.65	0
23	CLA	C	510	-	65,73,73	1.52	6 (9%)	76,113,113	1.36	9 (11%)
23	CLA	C	512	-	65,73,73	1.50	5 (7%)	76,113,113	1.43	7 (9%)
23	CLA	A	405	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	9 (11%)
23	CLA	B	610	-	65,73,73	1.50	5 (7%)	76,113,113	1.39	9 (11%)
27	BCR	c	514	-	41,41,41	0.71	0	56,56,56	2.37	20 (35%)
29	LHG	A	412	-	38,38,48	1.05	2 (5%)	41,44,54	0.98	2 (4%)
23	CLA	b	608	-	65,73,73	1.50	6 (9%)	76,113,113	1.38	8 (10%)
23	CLA	a	409	-	65,73,73	1.52	6 (9%)	76,113,113	1.37	8 (10%)
23	CLA	c	509	-	65,73,73	1.55	5 (7%)	76,113,113	1.39	8 (10%)
31	LMG	D	407	-	48,48,55	1.18	8 (16%)	56,56,63	1.41	7 (12%)
27	BCR	A	410	-	41,41,41	0.74	0	56,56,56	1.89	11 (19%)
29	LHG	a	414	-	38,38,48	1.07	2 (5%)	41,44,54	1.00	2 (4%)
31	LMG	C	521	-	45,45,55	1.19	6 (13%)	53,53,63	1.36	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	-	1/1/15/20	17/37/115/115	-
23	CLA	b	618	-	1/1/15/20	16/37/115/115	-
33	LMT	B	628	-	-	3/21/61/61	0/2/2/2
33	LMT	i	102	-	-	3/21/61/61	0/2/2/2
28	DGD	b	623	-	-	19/47/87/95	0/2/2/2
29	LHG	A	415	-	-	13/41/41/53	-
23	CLA	c	501	-	1/1/15/20	13/37/115/115	-
23	CLA	b	620	-	1/1/15/20	18/37/115/115	-
23	CLA	c	511	-	1/1/15/20	16/37/115/115	-
28	DGD	B	627	-	-	16/41/81/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	j	102	-	-	6/29/63/63	0/2/2/2
28	DGD	c	516	-	-	20/42/82/95	0/2/2/2
33	LMT	d	410	-	-	0/17/57/61	0/2/2/2
23	CLA	b	617	-	1/1/15/20	16/37/115/115	-
24	PHO	D	402	-	-	9/37/103/103	0/5/6/6
31	LMG	A	414	-	-	21/46/66/70	0/1/1/1
34	HEM	f	101	6,5	-	3/12/54/54	-
23	CLA	c	510	-	1/1/15/20	16/37/115/115	-
31	LMG	I	101	-	-	19/38/58/70	0/1/1/1
30	SQD	a	401	-	-	18/49/69/69	0/1/1/1
23	CLA	B	615	-	1/1/15/20	10/37/115/115	-
31	LMG	m	102	-	-	15/37/57/70	0/1/1/1
23	CLA	C	503	-	1/1/15/20	15/37/115/115	-
27	BCR	T	102	-	-	7/29/63/63	0/2/2/2
28	DGD	C	517	-	-	19/42/82/95	0/2/2/2
23	CLA	C	504	-	1/1/15/20	10/37/115/115	-
23	CLA	B	602	-	1/1/15/20	19/37/115/115	-
28	DGD	c	517	-	-	23/51/91/95	0/2/2/2
28	DGD	A	411	-	-	10/45/85/95	0/2/2/2
31	LMG	a	416	-	-	19/46/66/70	0/1/1/1
29	LHG	a	417	-	-	13/41/41/53	-
23	CLA	C	511	3	1/1/15/20	15/37/115/115	-
25	PL9	a	410	-	-	22/41/61/73	0/1/1/1
27	BCR	C	515	-	-	2/29/63/63	0/2/2/2
23	CLA	B	613	-	1/1/15/20	15/37/115/115	-
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
23	CLA	C	501	-	1/1/15/20	13/37/115/115	-
23	CLA	C	507	-	1/1/15/20	11/37/115/115	-
30	SQD	a	415	-	-	20/46/66/69	0/1/1/1
28	DGD	C	518	-	-	21/51/91/95	0/2/2/2
23	CLA	b	611	-	1/1/15/20	9/37/115/115	-
23	CLA	A	404	-	1/1/15/20	17/37/115/115	-
23	CLA	C	513	-	1/1/15/20	18/37/115/115	-
33	LMT	B	625	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	y	101	-	-	8/29/63/63	0/2/2/2
23	CLA	b	619	-	1/1/15/20	8/37/115/115	-
34	HEM	F	101	6,5	-	3/12/54/54	-
33	LMT	B	624	-	-	2/21/61/61	0/2/2/2
23	CLA	b	610	-	1/1/15/20	12/37/115/115	-
23	CLA	a	406	-	1/1/15/20	11/37/115/115	-
23	CLA	c	512	-	1/1/15/20	19/37/115/115	-
31	LMG	E	101	-	-	18/39/59/70	0/1/1/1
33	LMT	I	102	-	-	3/21/61/61	0/2/2/2
23	CLA	B	616	-	1/1/15/20	18/37/115/115	-
27	BCR	B	619	-	-	1/29/63/63	0/2/2/2
33	LMT	M	102	-	-	0/21/61/61	0/2/2/2
31	LMG	c	519	-	-	21/40/60/70	0/1/1/1
23	CLA	c	507	-	1/1/15/20	13/37/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
25	PL9	j	101	-	-	13/29/49/73	0/1/1/1
33	LMT	b	627	-	-	2/21/61/61	0/2/2/2
31	LMG	a	402	-	-	18/37/57/70	0/1/1/1
23	CLA	b	609	-	1/1/15/20	15/37/115/115	-
23	CLA	B	601	-	1/1/15/20	16/37/115/115	-
28	DGD	b	602	-	-	19/41/81/95	0/2/2/2
31	LMG	b	624	-	-	23/44/64/70	0/1/1/1
27	BCR	B	620	-	-	2/29/63/63	0/2/2/2
23	CLA	c	502	-	1/1/15/20	10/37/115/115	-
31	LMG	B	623	-	-	15/44/64/70	0/1/1/1
23	CLA	B	607	-	1/1/15/20	9/37/115/115	-
31	LMG	d	407	-	-	19/43/63/70	0/1/1/1
33	LMT	b	626	-	-	2/21/61/61	0/2/2/2
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
23	CLA	d	402	-	1/1/15/20	12/37/115/115	-
31	LMG	B	622	-	-	23/44/64/70	0/1/1/1
23	CLA	B	611	-	1/1/15/20	9/37/115/115	-
34	HEM	V	201	16	-	3/12/54/54	-
33	LMT	b	604	-	-	3/21/61/61	0/2/2/2
33	LMT	b	603	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	403	-	1/1/15/20	7/37/115/115	-
31	LMG	D	406	-	-	12/41/61/70	0/1/1/1
24	PHO	a	407	-	-	13/37/103/103	0/5/6/6
27	BCR	a	412	-	-	2/29/63/63	0/2/2/2
27	BCR	h	101	-	-	2/29/63/63	0/2/2/2
30	SQD	F	102	-	-	16/40/60/69	0/1/1/1
31	LMG	d	406	-	-	11/41/61/70	0/1/1/1
28	DGD	C	519	-	-	23/55/95/95	0/2/2/2
27	BCR	B	618	-	-	9/29/63/63	0/2/2/2
31	LMG	C	520	-	-	18/43/63/70	0/1/1/1
23	CLA	B	603	-	1/1/15/20	14/37/115/115	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
31	LMG	M	101	-	-	15/37/57/70	0/1/1/1
27	BCR	d	405	-	-	6/29/63/63	0/2/2/2
31	LMG	A	418	-	-	16/37/57/70	0/1/1/1
27	BCR	b	622	-	-	3/29/63/63	0/2/2/2
28	DGD	d	409	-	-	31/52/92/95	0/2/2/2
23	CLA	b	605	-	1/1/15/20	14/37/115/115	-
28	DGD	a	413	-	-	12/45/85/95	0/2/2/2
23	CLA	B	609	-	1/1/15/20	11/37/115/115	-
33	LMT	D	410	-	-	0/17/57/61	0/2/2/2
25	PL9	D	404	-	-	13/53/73/73	0/1/1/1
28	DGD	B	621	-	-	19/47/87/95	0/2/2/2
31	LMG	b	625	-	-	16/44/64/70	0/1/1/1
23	CLA	C	505	-	1/1/15/20	18/37/115/115	-
27	BCR	C	516	-	-	8/29/63/63	0/2/2/2
23	CLA	b	613	-	1/1/15/20	11/37/115/115	-
23	CLA	b	615	-	1/1/15/20	11/37/115/115	-
31	LMG	e	101	-	-	18/39/59/70	0/1/1/1
23	CLA	c	504	-	1/1/15/20	10/37/115/115	-
24	PHO	a	408	-	-	14/37/103/103	0/5/6/6
23	CLA	B	606	-	1/1/15/20	10/37/115/115	-
23	CLA	B	612	-	1/1/15/20	10/37/115/115	-
27	BCR	J	102	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	-	1/1/15/20	19/37/115/115	-
23	CLA	b	612	-	1/1/15/20	15/37/115/115	-
23	CLA	C	502	-	1/1/15/20	11/37/115/115	-
23	CLA	a	404	-	1/1/15/20	8/37/115/115	-
23	CLA	d	403	-	1/1/15/20	8/37/115/115	-
28	DGD	D	409	-	-	30/52/92/95	0/2/2/2
23	CLA	b	614	-	1/1/15/20	18/37/115/115	-
31	LMG	i	101	-	-	19/38/58/70	0/1/1/1
31	LMG	k	103	-	-	18/43/63/70	0/1/1/1
24	PHO	A	406	-	-	13/37/103/103	0/5/6/6
25	PL9	A	408	-	-	23/41/61/73	0/1/1/1
23	CLA	C	509	-	1/1/15/20	16/37/115/115	-
23	CLA	D	401	-	1/1/15/20	12/37/115/115	-
23	CLA	A	403	-	1/1/15/20	8/37/115/115	-
30	SQD	f	102	-	-	15/40/60/69	0/1/1/1
23	CLA	a	405	-	1/1/15/20	17/37/115/115	-
23	CLA	B	605	-	1/1/15/20	15/37/115/115	-
23	CLA	C	508	-	1/1/15/20	15/37/115/115	-
30	SQD	b	601	-	-	13/42/62/69	0/1/1/1
27	BCR	z	101	-	-	4/29/63/63	0/2/2/2
27	BCR	k	102	-	-	8/29/63/63	0/2/2/2
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
34	HEM	v	201	16	-	3/12/54/54	-
23	CLA	c	513	-	1/1/15/20	18/37/115/115	-
23	CLA	B	608	-	1/1/15/20	15/37/115/115	-
23	CLA	c	505	-	1/1/15/20	18/37/115/115	-
23	CLA	b	607	-	1/1/15/20	15/37/115/115	-
28	DGD	c	518	-	-	21/55/95/95	0/2/2/2
25	PL9	d	404	-	-	13/53/73/73	0/1/1/1
23	CLA	A	407	-	1/1/15/20	7/37/115/115	-
30	SQD	A	417	-	-	16/49/69/69	0/1/1/1
23	CLA	c	503	-	1/1/15/20	15/37/115/115	-
23	CLA	c	508	-	1/1/15/20	14/37/115/115	-
25	PL9	J	101	-	-	11/29/49/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	D	408	-	-	12/38/58/69	0/1/1/1
27	BCR	T	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	614	-	1/1/15/20	16/37/115/115	-
23	CLA	C	506	-	1/1/15/20	17/37/115/115	-
27	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	BCR	c	515	-	-	8/29/63/63	0/2/2/2
23	CLA	b	616	-	1/1/15/20	14/37/115/115	-
30	SQD	B	626	-	-	14/42/62/69	0/1/1/1
30	SQD	d	408	-	-	12/38/58/69	0/1/1/1
23	CLA	B	604	-	1/1/15/20	9/37/115/115	-
27	BCR	D	405	-	-	6/29/63/63	0/2/2/2
33	LMT	B	629	-	-	3/21/61/61	0/2/2/2
23	CLA	C	510	-	1/1/15/20	16/37/115/115	-
23	CLA	C	512	-	1/1/15/20	19/37/115/115	-
23	CLA	A	405	-	1/1/15/20	12/37/115/115	-
23	CLA	B	610	-	1/1/15/20	17/37/115/115	-
27	BCR	c	514	-	-	6/29/63/63	0/2/2/2
29	LHG	A	412	-	-	17/43/43/53	-
23	CLA	b	608	-	1/1/15/20	7/37/115/115	-
23	CLA	a	409	-	1/1/15/20	7/37/115/115	-
23	CLA	c	509	-	1/1/15/20	16/37/115/115	-
31	LMG	D	407	-	-	20/43/63/70	0/1/1/1
27	BCR	A	410	-	-	2/29/63/63	0/2/2/2
29	LHG	a	414	-	-	18/43/43/53	-
31	LMG	C	521	-	-	20/40/60/70	0/1/1/1

All (779) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C3D-C2D	8.38	1.54	1.36
34	V	201	HEM	C3D-C2D	8.16	1.54	1.36
34	f	101	HEM	C3D-C2D	8.10	1.54	1.36
23	A	403	CLA	C4B-NB	8.10	1.42	1.35
34	F	101	HEM	C3D-C2D	8.07	1.53	1.36
23	a	404	CLA	C4B-NB	8.05	1.42	1.35
23	c	509	CLA	C4B-NB	7.94	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C4B-NB	7.89	1.42	1.35
23	b	615	CLA	C4B-NB	7.86	1.42	1.35
23	a	406	CLA	C4B-NB	7.86	1.42	1.35
23	d	403	CLA	C4B-NB	7.86	1.42	1.35
23	d	402	CLA	C4B-NB	7.81	1.42	1.35
23	c	511	CLA	C4B-NB	7.80	1.42	1.35
23	b	611	CLA	C4B-NB	7.74	1.42	1.35
23	c	506	CLA	C4B-NB	7.72	1.42	1.35
23	c	504	CLA	C4B-NB	7.69	1.42	1.35
23	a	409	CLA	C4B-NB	7.69	1.42	1.35
23	c	512	CLA	C4B-NB	7.66	1.42	1.35
23	a	405	CLA	C4B-NB	7.66	1.42	1.35
23	C	502	CLA	C4B-NB	7.63	1.42	1.35
23	c	501	CLA	C4B-NB	7.62	1.42	1.35
23	B	611	CLA	C4B-NB	7.59	1.42	1.35
23	B	607	CLA	C4B-NB	7.58	1.42	1.35
23	B	612	CLA	C4B-NB	7.57	1.42	1.35
23	B	604	CLA	C4B-NB	7.57	1.42	1.35
23	B	608	CLA	C4B-NB	7.57	1.42	1.35
23	c	503	CLA	C4B-NB	7.56	1.42	1.35
23	c	508	CLA	C4B-NB	7.56	1.42	1.35
23	c	505	CLA	C4B-NB	7.56	1.41	1.35
23	b	618	CLA	C4B-NB	7.55	1.41	1.35
23	B	605	CLA	C4B-NB	7.55	1.41	1.35
23	C	506	CLA	C4B-NB	7.54	1.41	1.35
23	b	609	CLA	C4B-NB	7.53	1.41	1.35
23	C	510	CLA	C4B-NB	7.52	1.41	1.35
23	C	512	CLA	C4B-NB	7.51	1.41	1.35
23	c	507	CLA	C4B-NB	7.51	1.41	1.35
23	D	401	CLA	C4B-NB	7.51	1.41	1.35
23	B	615	CLA	C4B-NB	7.50	1.41	1.35
23	B	603	CLA	C4B-NB	7.50	1.41	1.35
23	b	608	CLA	C4B-NB	7.49	1.41	1.35
23	b	620	CLA	C4B-NB	7.48	1.41	1.35
23	B	601	CLA	C4B-NB	7.47	1.41	1.35
23	b	610	CLA	C4B-NB	7.46	1.41	1.35
23	c	513	CLA	C4B-NB	7.45	1.41	1.35
23	C	505	CLA	C4B-NB	7.44	1.41	1.35
23	C	501	CLA	C4B-NB	7.43	1.41	1.35
23	b	613	CLA	C4B-NB	7.40	1.41	1.35
23	b	605	CLA	C4B-NB	7.39	1.41	1.35
23	C	509	CLA	C4B-NB	7.39	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C4B-NB	7.37	1.41	1.35
23	B	613	CLA	C4B-NB	7.32	1.41	1.35
23	D	403	CLA	C4B-NB	7.32	1.41	1.35
23	b	607	CLA	C4B-NB	7.31	1.41	1.35
23	B	610	CLA	C4B-NB	7.30	1.41	1.35
23	c	510	CLA	C4B-NB	7.30	1.41	1.35
23	B	616	CLA	C4B-NB	7.30	1.41	1.35
23	B	602	CLA	C4B-NB	7.29	1.41	1.35
23	B	609	CLA	C4B-NB	7.29	1.41	1.35
23	B	614	CLA	C4B-NB	7.28	1.41	1.35
23	C	511	CLA	C4B-NB	7.26	1.41	1.35
23	b	612	CLA	C4B-NB	7.25	1.41	1.35
23	A	404	CLA	C4B-NB	7.25	1.41	1.35
23	B	606	CLA	C4B-NB	7.24	1.41	1.35
23	b	617	CLA	C4B-NB	7.22	1.41	1.35
23	A	407	CLA	C4B-NB	7.19	1.41	1.35
23	b	606	CLA	C4B-NB	7.18	1.41	1.35
23	C	513	CLA	C4B-NB	7.16	1.41	1.35
23	A	405	CLA	C4B-NB	7.14	1.41	1.35
23	b	614	CLA	C4B-NB	7.14	1.41	1.35
23	b	619	CLA	C4B-NB	7.13	1.41	1.35
23	C	507	CLA	C4B-NB	7.07	1.41	1.35
23	b	616	CLA	C4B-NB	7.06	1.41	1.35
23	c	502	CLA	C4B-NB	7.04	1.41	1.35
23	C	504	CLA	C4B-NB	6.80	1.41	1.35
34	V	201	HEM	C3C-C2C	-4.92	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.72	1.33	1.40
23	B	601	CLA	C1D-ND	4.44	1.43	1.37
29	a	414	LHG	O8-C23	4.35	1.46	1.33
29	a	417	LHG	O8-C23	4.29	1.45	1.33
29	A	415	LHG	O8-C23	4.27	1.45	1.33
23	c	511	CLA	C1D-ND	4.26	1.43	1.37
29	A	412	LHG	O8-C23	4.24	1.45	1.33
29	a	417	LHG	O7-C7	4.21	1.46	1.34
23	c	509	CLA	C1D-ND	4.17	1.42	1.37
29	a	414	LHG	O7-C7	4.17	1.46	1.34
29	A	412	LHG	O7-C7	4.17	1.46	1.34
23	C	511	CLA	C1D-ND	4.15	1.42	1.37
29	A	415	LHG	O7-C7	4.15	1.46	1.34
23	B	608	CLA	C1D-ND	4.12	1.42	1.37
23	c	506	CLA	C1D-ND	4.12	1.42	1.37
23	C	506	CLA	C1D-ND	4.11	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C1D-ND	4.11	1.42	1.37
23	b	605	CLA	C1D-ND	4.09	1.42	1.37
23	b	614	CLA	C1D-ND	4.09	1.42	1.37
23	C	501	CLA	C1D-ND	4.08	1.42	1.37
23	B	613	CLA	C1D-ND	4.08	1.42	1.37
23	a	404	CLA	C1D-ND	4.07	1.42	1.37
23	b	606	CLA	C1D-ND	4.07	1.42	1.37
23	b	610	CLA	C1D-ND	4.06	1.42	1.37
23	c	502	CLA	C1D-ND	4.05	1.42	1.37
23	a	409	CLA	C1D-ND	4.04	1.42	1.37
23	b	619	CLA	C1D-ND	4.04	1.42	1.37
23	c	513	CLA	C1D-ND	4.03	1.42	1.37
23	a	405	CLA	C1D-ND	4.02	1.42	1.37
23	d	403	CLA	C1D-ND	4.01	1.42	1.37
23	c	505	CLA	C1D-ND	4.00	1.42	1.37
23	b	617	CLA	C1D-ND	3.98	1.42	1.37
23	C	507	CLA	C1D-ND	3.97	1.42	1.37
23	c	503	CLA	C1D-ND	3.97	1.42	1.37
23	C	513	CLA	C1D-ND	3.96	1.42	1.37
23	A	407	CLA	C1D-ND	3.94	1.42	1.37
23	B	602	CLA	C1D-ND	3.94	1.42	1.37
23	B	607	CLA	C1D-ND	3.94	1.42	1.37
23	c	512	CLA	C1D-ND	3.93	1.42	1.37
23	C	503	CLA	C1D-ND	3.93	1.42	1.37
23	C	504	CLA	C1D-ND	3.91	1.42	1.37
23	A	404	CLA	C1D-ND	3.91	1.42	1.37
23	b	611	CLA	C1D-ND	3.91	1.42	1.37
23	B	610	CLA	C1D-ND	3.88	1.42	1.37
23	C	509	CLA	C1D-ND	3.88	1.42	1.37
23	d	402	CLA	C1D-ND	3.87	1.42	1.37
23	b	613	CLA	C1D-ND	3.86	1.42	1.37
23	A	405	CLA	C1D-ND	3.86	1.42	1.37
23	C	505	CLA	C1D-ND	3.85	1.42	1.37
23	C	512	CLA	C1D-ND	3.84	1.42	1.37
23	B	616	CLA	C1D-ND	3.83	1.42	1.37
23	c	501	CLA	C1D-ND	3.83	1.42	1.37
23	a	406	CLA	C1D-ND	3.83	1.42	1.37
23	c	508	CLA	C1D-ND	3.83	1.42	1.37
34	F	101	HEM	C3C-C2C	-3.83	1.35	1.40
23	C	510	CLA	C1D-ND	3.82	1.42	1.37
23	b	607	CLA	C1D-ND	3.82	1.42	1.37
23	B	615	CLA	C1D-ND	3.81	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	101	HEM	C3C-CAC	3.81	1.55	1.47
23	c	504	CLA	C1D-ND	3.81	1.42	1.37
23	B	603	CLA	C1D-ND	3.81	1.42	1.37
23	B	604	CLA	C1D-ND	3.77	1.42	1.37
34	f	101	HEM	C3C-CAC	3.76	1.55	1.47
23	B	606	CLA	C1D-ND	3.75	1.42	1.37
23	b	609	CLA	C1D-ND	3.74	1.42	1.37
23	C	508	CLA	C1D-ND	3.73	1.42	1.37
23	D	401	CLA	C1D-ND	3.72	1.42	1.37
23	C	502	CLA	C1D-ND	3.72	1.42	1.37
23	D	403	CLA	C1D-ND	3.72	1.42	1.37
23	b	612	CLA	C1D-ND	3.72	1.42	1.37
23	b	608	CLA	C1D-ND	3.71	1.42	1.37
34	v	201	HEM	C3C-CAC	3.70	1.55	1.47
23	b	615	CLA	C1D-ND	3.69	1.42	1.37
23	B	605	CLA	C1D-ND	3.69	1.42	1.37
23	A	403	CLA	C1D-ND	3.69	1.42	1.37
23	c	507	CLA	C1D-ND	3.69	1.42	1.37
23	c	510	CLA	C1D-ND	3.68	1.42	1.37
34	V	201	HEM	C3C-CAC	3.64	1.55	1.47
34	f	101	HEM	C3C-C2C	-3.61	1.35	1.40
23	b	618	CLA	C1D-ND	3.61	1.42	1.37
23	b	620	CLA	C1D-ND	3.60	1.42	1.37
23	B	611	CLA	C1D-ND	3.59	1.42	1.37
23	B	614	CLA	C1D-ND	3.54	1.42	1.37
23	b	616	CLA	C1D-ND	3.47	1.42	1.37
25	A	408	PL9	C33-C34	3.46	1.41	1.33
23	b	606	CLA	CHC-C1C	3.39	1.43	1.35
25	D	404	PL9	C38-C39	3.38	1.41	1.33
23	a	409	CLA	CHC-C1C	3.35	1.43	1.35
23	B	612	CLA	C1D-ND	3.35	1.41	1.37
23	A	404	CLA	CHC-C1C	3.34	1.43	1.35
23	c	511	CLA	CHC-C1C	3.33	1.43	1.35
23	b	619	CLA	CHC-C1C	3.29	1.43	1.35
25	d	404	PL9	C38-C39	3.28	1.40	1.33
23	B	609	CLA	CHC-C1C	3.28	1.43	1.35
25	a	410	PL9	C33-C34	3.27	1.40	1.33
23	B	608	CLA	CHC-C1C	3.27	1.43	1.35
23	c	510	CLA	CHC-C1C	3.27	1.43	1.35
23	c	509	CLA	CHC-C1C	3.27	1.43	1.35
25	D	404	PL9	C33-C34	3.27	1.40	1.33
23	B	602	CLA	CHC-C1C	3.26	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	408	SQD	O48-C23	3.26	1.42	1.33
23	B	614	CLA	C4D-ND	-3.25	1.33	1.37
30	a	401	SQD	O48-C23	3.24	1.42	1.33
23	B	607	CLA	CHC-C1C	3.24	1.43	1.35
23	b	609	CLA	CHC-C1C	3.24	1.43	1.35
23	c	510	CLA	C4D-ND	-3.23	1.33	1.37
23	a	406	CLA	CHC-C1C	3.23	1.43	1.35
23	B	610	CLA	CHC-C1C	3.23	1.43	1.35
23	B	603	CLA	CHC-C1C	3.23	1.43	1.35
23	C	513	CLA	CHC-C1C	3.22	1.43	1.35
23	c	506	CLA	CHC-C1C	3.22	1.43	1.35
25	d	404	PL9	C33-C34	3.22	1.40	1.33
23	b	618	CLA	CHC-C1C	3.22	1.43	1.35
23	C	504	CLA	CHC-C1C	3.21	1.43	1.35
23	B	611	CLA	C4D-ND	-3.21	1.33	1.37
30	D	408	SQD	O48-C23	3.21	1.42	1.33
23	C	509	CLA	CHC-C1C	3.20	1.43	1.35
23	c	508	CLA	CHC-C1C	3.20	1.43	1.35
30	A	413	SQD	O48-C23	3.20	1.42	1.33
23	C	506	CLA	CHC-C1C	3.20	1.43	1.35
23	D	403	CLA	CHC-C1C	3.19	1.43	1.35
30	a	415	SQD	O48-C23	3.19	1.42	1.33
23	B	605	CLA	CHC-C1C	3.19	1.43	1.35
23	C	508	CLA	CHC-C1C	3.19	1.43	1.35
31	D	406	LMG	O7-C8	-3.19	1.38	1.46
25	D	404	PL9	C43-C44	3.19	1.40	1.33
23	D	403	CLA	C4D-ND	-3.18	1.33	1.37
28	C	517	DGD	O2G-C2G	-3.18	1.38	1.46
23	B	614	CLA	CHC-C1C	3.17	1.43	1.35
23	B	612	CLA	CHC-C1C	3.17	1.43	1.35
23	c	502	CLA	CHC-C1C	3.16	1.43	1.35
28	B	621	DGD	O2G-C2G	-3.16	1.38	1.46
25	a	410	PL9	C38-C39	3.16	1.41	1.32
23	b	614	CLA	CHC-C1C	3.16	1.43	1.35
28	b	602	DGD	O1G-C1A	3.16	1.42	1.33
23	C	512	CLA	CHC-C1C	3.14	1.43	1.35
30	b	601	SQD	O48-C23	3.14	1.42	1.33
28	C	519	DGD	O2G-C1B	3.14	1.43	1.34
23	B	601	CLA	CHC-C1C	3.14	1.43	1.35
23	A	403	CLA	CHC-C1C	3.14	1.43	1.35
23	B	604	CLA	C4D-ND	-3.13	1.33	1.37
23	d	403	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PL9	C38-C39	3.13	1.41	1.32
28	c	518	DGD	O2G-C1B	3.12	1.43	1.34
23	C	511	CLA	CHC-C1C	3.12	1.43	1.35
31	i	101	LMG	O7-C8	-3.12	1.38	1.46
23	b	613	CLA	CHC-C1C	3.11	1.42	1.35
23	B	604	CLA	CHC-C1C	3.11	1.42	1.35
23	B	613	CLA	CHC-C1C	3.11	1.42	1.35
31	d	406	LMG	O7-C8	-3.11	1.38	1.46
23	b	619	CLA	C4D-ND	-3.11	1.33	1.37
23	c	501	CLA	CHC-C1C	3.11	1.42	1.35
23	b	610	CLA	CHC-C1C	3.10	1.42	1.35
31	D	407	LMG	O7-C8	-3.10	1.38	1.46
23	c	512	CLA	CHC-C1C	3.10	1.42	1.35
23	c	503	CLA	CHC-C1C	3.10	1.42	1.35
23	D	401	CLA	CHC-C1C	3.10	1.42	1.35
30	A	417	SQD	O48-C23	3.10	1.42	1.33
23	B	611	CLA	CHC-C1C	3.10	1.42	1.35
23	d	402	CLA	C4D-ND	-3.09	1.33	1.37
23	C	507	CLA	CHC-C1C	3.09	1.42	1.35
23	a	405	CLA	CHC-C1C	3.09	1.42	1.35
23	b	611	CLA	CHC-C1C	3.09	1.42	1.35
23	C	503	CLA	CHC-C1C	3.09	1.42	1.35
23	C	501	CLA	CHC-C1C	3.09	1.42	1.35
30	B	626	SQD	O48-C23	3.09	1.42	1.33
28	c	516	DGD	O1G-C1A	3.08	1.42	1.33
23	c	505	CLA	CHC-C1C	3.08	1.42	1.35
23	a	409	CLA	C4D-ND	-3.08	1.33	1.37
23	b	607	CLA	CHC-C1C	3.07	1.42	1.35
34	f	101	HEM	FE-ND	3.07	2.12	1.96
23	C	505	CLA	CHC-C1C	3.07	1.42	1.35
23	a	405	CLA	C4D-ND	-3.07	1.33	1.37
23	a	406	CLA	C4D-ND	-3.07	1.33	1.37
31	B	622	LMG	O7-C8	-3.07	1.38	1.46
23	A	405	CLA	CHC-C1C	3.07	1.42	1.35
23	B	609	CLA	C4D-ND	-3.06	1.33	1.37
30	f	102	SQD	O48-C23	3.06	1.42	1.33
23	B	615	CLA	CHC-C1C	3.06	1.42	1.35
23	b	618	CLA	C4D-ND	-3.04	1.33	1.37
23	C	510	CLA	CHC-C1C	3.04	1.42	1.35
23	c	504	CLA	CHC-C1C	3.03	1.42	1.35
23	b	617	CLA	CHC-C1C	3.03	1.42	1.35
31	m	102	LMG	O1-C7	-3.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	102	SQD	O48-C23	3.02	1.42	1.33
28	b	623	DGD	O2G-C2G	-3.02	1.39	1.46
23	A	407	CLA	CHC-C1C	3.02	1.42	1.35
23	b	609	CLA	C4D-ND	-3.02	1.33	1.37
31	C	520	LMG	O7-C8	-3.01	1.39	1.46
23	c	505	CLA	C4D-ND	-3.01	1.33	1.37
30	d	408	SQD	O47-C7	3.01	1.42	1.34
23	a	404	CLA	CHC-C1C	3.01	1.42	1.35
23	b	608	CLA	C4D-ND	-3.00	1.33	1.37
23	B	612	CLA	C4D-ND	-3.00	1.33	1.37
31	C	521	LMG	O7-C10	3.00	1.42	1.34
23	b	612	CLA	CHC-C1C	3.00	1.42	1.35
23	B	616	CLA	CHC-C1C	2.99	1.42	1.35
31	I	101	LMG	O7-C8	-2.99	1.39	1.46
30	D	408	SQD	O47-C7	2.99	1.42	1.34
23	c	513	CLA	CHC-C1C	2.99	1.42	1.35
23	C	505	CLA	C4D-ND	-2.99	1.33	1.37
23	b	620	CLA	CHC-C1C	2.99	1.42	1.35
25	d	404	PL9	C43-C44	2.98	1.40	1.33
31	B	623	LMG	O7-C10	2.97	1.42	1.34
28	c	516	DGD	O2G-C2G	-2.97	1.39	1.46
23	B	605	CLA	C4D-ND	-2.97	1.33	1.37
31	k	103	LMG	O7-C8	-2.97	1.39	1.46
28	D	409	DGD	O1G-C1A	2.97	1.42	1.33
23	B	616	CLA	C4D-ND	-2.97	1.33	1.37
31	M	101	LMG	O7-C10	2.97	1.42	1.34
23	b	612	CLA	C4D-ND	-2.96	1.33	1.37
28	A	411	DGD	O2G-C1B	2.96	1.42	1.34
23	C	504	CLA	C4D-ND	-2.96	1.33	1.37
31	D	407	LMG	O3-C3	-2.96	1.36	1.43
25	J	101	PL9	C23-C24	2.96	1.40	1.33
23	C	509	CLA	C4D-ND	-2.95	1.33	1.37
30	F	102	SQD	O47-C7	2.95	1.42	1.34
23	b	606	CLA	C4D-ND	-2.95	1.33	1.37
23	b	615	CLA	CHC-C1C	2.95	1.42	1.35
28	B	627	DGD	O1G-C1A	2.95	1.42	1.33
31	c	519	LMG	O7-C10	2.95	1.42	1.34
23	B	606	CLA	CHC-C1C	2.94	1.42	1.35
31	A	414	LMG	O7-C10	2.94	1.42	1.34
31	m	102	LMG	O7-C8	-2.94	1.39	1.46
23	B	615	CLA	C4D-ND	-2.94	1.33	1.37
23	B	610	CLA	C4D-ND	-2.94	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	418	LMG	O7-C8	-2.93	1.39	1.46
28	B	627	DGD	O2G-C1B	2.93	1.42	1.34
28	C	517	DGD	O1G-C1A	2.93	1.41	1.33
31	b	625	LMG	O7-C8	-2.93	1.39	1.46
34	F	101	HEM	CAB-C3B	2.93	1.55	1.47
30	A	417	SQD	O47-C7	2.93	1.42	1.34
23	b	611	CLA	C4D-ND	-2.92	1.33	1.37
23	A	404	CLA	C4D-ND	-2.92	1.33	1.37
28	d	409	DGD	O1G-C1A	2.92	1.41	1.33
23	b	608	CLA	CHC-C1C	2.91	1.42	1.35
23	b	616	CLA	CHC-C1C	2.91	1.42	1.35
23	b	620	CLA	C4D-ND	-2.90	1.33	1.37
31	b	624	LMG	O7-C8	-2.90	1.39	1.46
31	a	416	LMG	O7-C10	2.90	1.42	1.34
23	b	616	CLA	C4D-ND	-2.90	1.33	1.37
28	a	413	DGD	O2G-C2G	-2.90	1.39	1.46
23	b	613	CLA	C4D-ND	-2.90	1.33	1.37
23	B	613	CLA	C4D-ND	-2.90	1.33	1.37
23	C	507	CLA	C4D-ND	-2.90	1.33	1.37
23	B	601	CLA	C4D-ND	-2.89	1.33	1.37
28	C	518	DGD	O1G-C1A	2.89	1.41	1.33
31	d	407	LMG	O7-C8	-2.89	1.39	1.46
28	b	602	DGD	O2G-C1B	2.89	1.42	1.34
31	a	416	LMG	O7-C8	-2.89	1.39	1.46
23	C	512	CLA	C4D-ND	-2.89	1.33	1.37
23	c	507	CLA	CHC-C1C	2.89	1.42	1.35
34	f	101	HEM	CAB-C3B	2.89	1.55	1.47
23	b	605	CLA	CHC-C1C	2.88	1.42	1.35
23	C	502	CLA	CHC-C1C	2.88	1.42	1.35
23	D	401	CLA	C4D-ND	-2.88	1.33	1.37
31	a	402	LMG	O7-C8	-2.87	1.39	1.46
23	A	407	CLA	C4D-ND	-2.87	1.33	1.37
28	c	517	DGD	O2G-C2G	-2.87	1.39	1.46
23	B	602	CLA	C4D-ND	-2.87	1.33	1.37
30	b	601	SQD	O47-C7	2.86	1.42	1.34
23	c	502	CLA	C4D-ND	-2.86	1.33	1.37
31	m	102	LMG	O7-C10	2.86	1.42	1.34
23	C	511	CLA	C4D-ND	-2.85	1.33	1.37
31	E	101	LMG	O7-C10	2.85	1.42	1.34
28	c	516	DGD	O2G-C1B	2.85	1.42	1.34
23	b	615	CLA	C4D-ND	-2.84	1.33	1.37
28	C	518	DGD	O2G-C2G	-2.84	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	623	LMG	O7-C8	-2.84	1.39	1.46
23	A	403	CLA	C4D-ND	-2.84	1.33	1.37
31	A	414	LMG	O3-C3	-2.84	1.36	1.43
30	a	401	SQD	O47-C7	2.83	1.42	1.34
28	D	409	DGD	O2G-C2G	-2.83	1.39	1.46
23	C	513	CLA	C4D-ND	-2.83	1.33	1.37
23	c	509	CLA	C4D-ND	-2.83	1.33	1.37
28	b	623	DGD	O1G-C1A	2.83	1.41	1.33
25	j	101	PL9	C13-C14	2.83	1.39	1.33
23	B	606	CLA	C4D-ND	-2.82	1.33	1.37
31	b	625	LMG	O3-C3	-2.82	1.36	1.43
23	c	501	CLA	C4D-ND	-2.82	1.33	1.37
28	c	518	DGD	O1G-C1A	2.81	1.41	1.33
23	A	405	CLA	C4D-ND	-2.81	1.33	1.37
23	B	607	CLA	C4D-ND	-2.81	1.33	1.37
23	C	510	CLA	C4D-ND	-2.80	1.33	1.37
23	C	503	CLA	C4D-ND	-2.80	1.33	1.37
23	b	610	CLA	C4D-ND	-2.80	1.33	1.37
31	B	623	LMG	O3-C3	-2.80	1.36	1.43
31	M	101	LMG	O7-C8	-2.79	1.39	1.46
23	b	615	CLA	CMB-C2B	-2.79	1.45	1.51
23	d	403	CLA	C4D-ND	-2.79	1.33	1.37
30	f	102	SQD	O47-C7	2.79	1.42	1.34
24	A	406	PHO	CAC-C3C	-2.79	1.47	1.52
31	b	625	LMG	O7-C10	2.79	1.42	1.34
31	A	414	LMG	O7-C8	-2.79	1.39	1.46
31	k	103	LMG	O8-C28	2.79	1.41	1.33
31	A	418	LMG	O7-C10	2.78	1.42	1.34
23	c	507	CLA	C4D-ND	-2.78	1.33	1.37
31	a	402	LMG	O7-C10	2.78	1.42	1.34
25	j	101	PL9	C18-C19	2.78	1.39	1.33
31	e	101	LMG	O7-C8	-2.77	1.39	1.46
31	C	521	LMG	O8-C28	2.77	1.41	1.33
23	d	402	CLA	CHC-C1C	2.77	1.42	1.35
31	M	101	LMG	O1-C7	-2.77	1.38	1.43
28	C	519	DGD	O1G-C1A	2.77	1.41	1.33
30	A	413	SQD	O47-C7	2.77	1.42	1.34
23	c	513	CLA	C4D-ND	-2.76	1.33	1.37
23	b	617	CLA	C4D-ND	-2.76	1.33	1.37
25	j	101	PL9	C23-C24	2.76	1.39	1.33
31	d	407	LMG	O3-C3	-2.76	1.36	1.43
25	J	101	PL9	C8-C9	2.76	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	CAB-C3B	2.76	1.55	1.47
23	C	508	CLA	C4D-ND	-2.76	1.33	1.37
31	e	101	LMG	O7-C10	2.76	1.42	1.34
31	I	101	LMG	O7-C10	2.76	1.42	1.34
23	C	506	CLA	C4D-ND	-2.75	1.33	1.37
25	A	408	PL9	C18-C19	2.75	1.39	1.33
31	b	624	LMG	O7-C10	2.75	1.42	1.34
31	m	102	LMG	O8-C28	2.75	1.41	1.33
30	B	626	SQD	O47-C7	2.75	1.42	1.34
23	B	603	CLA	C4D-ND	-2.75	1.33	1.37
31	a	416	LMG	O3-C3	-2.74	1.36	1.43
23	B	608	CLA	C4D-ND	-2.74	1.33	1.37
28	A	411	DGD	O1G-C1A	2.74	1.41	1.33
28	c	517	DGD	O2G-C1B	2.74	1.42	1.34
28	d	409	DGD	O2G-C2G	-2.74	1.39	1.46
24	a	408	PHO	CAC-C3C	-2.73	1.47	1.52
28	B	621	DGD	O1G-C1A	2.73	1.41	1.33
24	a	407	PHO	CAC-C3C	-2.73	1.47	1.52
30	a	415	SQD	O47-C7	2.73	1.42	1.34
28	B	627	DGD	O2G-C2G	-2.72	1.39	1.46
28	a	413	DGD	O1G-C1A	2.72	1.41	1.33
24	D	402	PHO	CAC-C3C	-2.72	1.47	1.52
25	j	101	PL9	C8-C9	2.72	1.39	1.33
23	c	503	CLA	C4D-ND	-2.72	1.33	1.37
23	b	614	CLA	C4D-ND	-2.72	1.34	1.37
25	J	101	PL9	C13-C14	2.72	1.39	1.33
25	d	404	PL9	C23-C24	2.71	1.39	1.33
25	J	101	PL9	C18-C19	2.71	1.39	1.33
25	D	404	PL9	C18-C19	2.71	1.39	1.33
31	c	519	LMG	O8-C28	2.71	1.41	1.33
31	c	519	LMG	O7-C8	-2.71	1.39	1.46
28	C	518	DGD	O2G-C1B	2.71	1.41	1.34
23	c	504	CLA	C4D-ND	-2.71	1.34	1.37
31	d	407	LMG	O7-C10	2.71	1.41	1.34
31	M	101	LMG	O8-C28	2.71	1.41	1.33
23	c	511	CLA	C4D-ND	-2.70	1.34	1.37
25	A	408	PL9	C13-C14	2.70	1.39	1.33
31	b	624	LMG	O8-C28	2.69	1.41	1.33
25	a	410	PL9	C13-C14	2.69	1.39	1.33
31	B	622	LMG	O7-C10	2.69	1.41	1.34
23	B	611	CLA	CMB-C2B	-2.68	1.46	1.51
31	E	101	LMG	O8-C28	2.68	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	CLA	C4D-ND	-2.68	1.34	1.37
25	A	408	PL9	C23-C24	2.68	1.39	1.33
31	a	402	LMG	O8-C28	2.67	1.41	1.33
28	c	517	DGD	O1G-C1A	2.67	1.41	1.33
34	V	201	HEM	FE-ND	2.67	2.10	1.96
31	m	102	LMG	O3-C3	-2.67	1.36	1.43
31	C	520	LMG	O8-C28	2.67	1.41	1.33
31	e	101	LMG	O8-C28	2.67	1.41	1.33
25	a	410	PL9	C23-C24	2.67	1.39	1.33
34	V	201	HEM	CAB-C3B	2.66	1.54	1.47
28	C	517	DGD	O2G-C1B	2.66	1.41	1.34
25	D	404	PL9	C23-C24	2.66	1.39	1.33
31	D	406	LMG	O3-C3	-2.66	1.36	1.43
25	A	408	PL9	C8-C9	2.66	1.39	1.33
31	d	407	LMG	O8-C28	2.66	1.41	1.33
31	A	418	LMG	O8-C9	-2.66	1.39	1.45
31	a	416	LMG	O8-C28	2.65	1.41	1.33
23	b	605	CLA	C4D-ND	-2.65	1.34	1.37
31	i	101	LMG	O3-C3	-2.65	1.36	1.43
28	a	413	DGD	O2G-C1B	2.65	1.41	1.34
28	B	621	DGD	O3G-C3G	-2.65	1.38	1.43
31	i	101	LMG	O7-C10	2.65	1.41	1.34
31	c	519	LMG	O3-C3	-2.65	1.36	1.43
28	b	602	DGD	O2G-C2G	-2.64	1.40	1.46
31	d	406	LMG	O7-C10	2.64	1.41	1.34
31	m	102	LMG	O8-C9	-2.64	1.39	1.45
31	d	406	LMG	O3-C3	-2.64	1.36	1.43
23	C	501	CLA	C4D-ND	-2.64	1.34	1.37
25	d	404	PL9	C13-C14	2.64	1.39	1.33
31	A	414	LMG	O8-C28	2.64	1.41	1.33
23	c	506	CLA	C4D-ND	-2.64	1.34	1.37
31	M	101	LMG	O3-C3	-2.63	1.36	1.43
31	a	402	LMG	O3-C3	-2.63	1.36	1.43
28	C	519	DGD	O2G-C2G	-2.63	1.40	1.46
31	I	101	LMG	O3-C3	-2.62	1.36	1.43
31	D	407	LMG	O8-C28	2.62	1.41	1.33
23	C	510	CLA	CMB-C2B	-2.62	1.46	1.51
31	C	520	LMG	O7-C10	2.62	1.41	1.34
31	B	622	LMG	O8-C28	2.62	1.41	1.33
28	A	411	DGD	O2G-C2G	-2.62	1.40	1.46
25	d	404	PL9	C18-C19	2.61	1.39	1.33
31	I	101	LMG	O8-C28	2.61	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	627	DGD	O6E-C5E	-2.61	1.38	1.44
28	c	518	DGD	O4D-C4D	-2.61	1.36	1.43
31	i	101	LMG	O8-C9	-2.60	1.39	1.45
31	C	521	LMG	O7-C8	-2.60	1.40	1.46
23	c	508	CLA	C4D-ND	-2.60	1.34	1.37
25	d	404	PL9	C8-C9	2.60	1.39	1.33
31	E	101	LMG	O7-C8	-2.59	1.40	1.46
31	k	103	LMG	O7-C10	2.59	1.41	1.34
28	C	519	DGD	O4D-C4D	-2.58	1.36	1.43
31	D	406	LMG	O7-C10	2.58	1.41	1.34
31	B	623	LMG	O8-C28	2.58	1.40	1.33
31	D	407	LMG	O7-C10	2.58	1.41	1.34
28	d	409	DGD	O2G-C1B	2.57	1.41	1.34
31	M	101	LMG	O8-C9	-2.57	1.39	1.45
31	C	520	LMG	O3-C3	-2.57	1.36	1.43
23	C	502	CLA	C4D-ND	-2.57	1.34	1.37
28	c	518	DGD	O2G-C2G	-2.56	1.40	1.46
31	b	624	LMG	O3-C3	-2.56	1.36	1.43
23	b	612	CLA	CMB-C2B	-2.56	1.46	1.51
31	e	101	LMG	O3-C3	-2.56	1.36	1.43
28	A	411	DGD	O4D-C4D	-2.56	1.36	1.43
23	c	512	CLA	C4D-ND	-2.56	1.34	1.37
31	b	625	LMG	O8-C28	2.55	1.40	1.33
23	b	605	CLA	CMB-C2B	-2.55	1.46	1.51
31	e	101	LMG	O8-C9	-2.55	1.39	1.45
31	C	521	LMG	O3-C3	-2.55	1.37	1.43
23	b	607	CLA	C4D-ND	-2.54	1.34	1.37
28	b	623	DGD	O2G-C1B	2.54	1.41	1.34
31	d	406	LMG	O8-C28	2.54	1.40	1.33
23	b	610	CLA	CMB-C2B	-2.54	1.46	1.51
28	b	602	DGD	O6E-C5E	-2.53	1.38	1.44
31	A	418	LMG	O3-C3	-2.53	1.37	1.43
31	b	624	LMG	O6-C5	-2.53	1.38	1.44
31	k	103	LMG	O3-C3	-2.53	1.37	1.43
23	B	601	CLA	CMB-C2B	-2.53	1.46	1.51
25	a	410	PL9	C8-C9	2.52	1.39	1.33
25	a	410	PL9	C18-C19	2.52	1.39	1.33
23	b	620	CLA	CMB-C2B	-2.52	1.46	1.51
31	E	101	LMG	O8-C9	-2.52	1.39	1.45
31	E	101	LMG	O3-C3	-2.51	1.37	1.43
25	D	404	PL9	C8-C9	2.51	1.39	1.33
31	D	406	LMG	O8-C28	2.51	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	CMB-C2B	-2.51	1.46	1.51
23	c	508	CLA	CMB-C2B	-2.51	1.46	1.51
31	B	622	LMG	O3-C3	-2.51	1.37	1.43
25	d	404	PL9	C28-C29	2.50	1.39	1.33
23	C	508	CLA	CMB-C2B	-2.50	1.46	1.51
25	D	404	PL9	C13-C14	2.50	1.39	1.33
23	B	610	CLA	CMB-C2B	-2.50	1.46	1.51
31	c	519	LMG	O8-C9	-2.49	1.39	1.45
23	b	617	CLA	CMB-C2B	-2.49	1.46	1.51
28	D	409	DGD	O2G-C1B	2.49	1.41	1.34
23	B	616	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	603	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	606	CLA	CMB-C2B	-2.48	1.46	1.51
23	c	507	CLA	CMB-C2B	-2.48	1.46	1.51
31	B	623	LMG	O8-C9	-2.48	1.39	1.45
31	I	101	LMG	O8-C9	-2.48	1.39	1.45
28	C	518	DGD	O4D-C4D	-2.48	1.37	1.43
28	b	623	DGD	O3G-C3G	-2.47	1.39	1.43
31	b	625	LMG	O8-C9	-2.47	1.39	1.45
23	C	507	CLA	CMB-C2B	-2.47	1.46	1.51
31	a	416	LMG	O8-C9	-2.47	1.39	1.45
23	A	404	CLA	CMB-C2B	-2.47	1.46	1.51
28	c	517	DGD	O5D-C6D	-2.47	1.39	1.43
23	b	618	CLA	CMB-C2B	-2.47	1.46	1.51
28	C	519	DGD	O3G-C3G	-2.47	1.39	1.43
28	c	517	DGD	O4D-C4D	-2.47	1.37	1.43
34	V	201	HEM	CAA-C2A	2.46	1.55	1.52
31	i	101	LMG	O8-C28	2.46	1.40	1.33
28	B	621	DGD	O2G-C1B	2.46	1.41	1.34
23	c	502	CLA	CMB-C2B	-2.46	1.46	1.51
23	B	608	CLA	CMB-C2B	-2.46	1.46	1.51
25	A	408	PL9	C28-C29	2.46	1.38	1.33
31	d	406	LMG	O8-C9	-2.45	1.39	1.45
23	b	606	CLA	CMB-C2B	-2.45	1.46	1.51
23	C	504	CLA	CMB-C2B	-2.45	1.46	1.51
23	a	405	CLA	CMB-C2B	-2.44	1.46	1.51
23	c	505	CLA	CMB-C2B	-2.44	1.46	1.51
23	C	505	CLA	CMB-C2B	-2.44	1.46	1.51
31	B	622	LMG	O8-C9	-2.43	1.39	1.45
23	b	614	CLA	CMB-C2B	-2.43	1.46	1.51
28	a	413	DGD	O4D-C4D	-2.43	1.37	1.43
31	A	418	LMG	O1-C7	-2.42	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	CMB-C2B	-2.42	1.46	1.51
23	B	615	CLA	CMB-C2B	-2.42	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.42	1.46	1.51
28	C	517	DGD	O6E-C5E	-2.42	1.38	1.44
28	c	516	DGD	O4D-C4D	-2.42	1.37	1.43
23	C	513	CLA	CMB-C2B	-2.41	1.46	1.51
31	A	418	LMG	O8-C28	2.41	1.40	1.33
23	b	607	CLA	CMB-C2B	-2.41	1.46	1.51
23	c	504	CLA	CMB-C2B	-2.41	1.46	1.51
23	B	613	CLA	CMB-C2B	-2.41	1.46	1.51
28	c	516	DGD	O6E-C5E	-2.41	1.38	1.44
30	A	417	SQD	O2-C2	-2.41	1.37	1.43
23	b	611	CLA	CMB-C2B	-2.41	1.46	1.51
23	C	501	CLA	CMB-C2B	-2.41	1.46	1.51
31	A	414	LMG	O8-C9	-2.41	1.39	1.45
23	A	405	CLA	CMB-C2B	-2.41	1.46	1.51
31	i	101	LMG	O1-C7	-2.41	1.39	1.43
23	B	607	CLA	CMB-C2B	-2.40	1.46	1.51
31	D	407	LMG	O8-C9	-2.40	1.39	1.45
23	A	407	CLA	CMB-C2B	-2.40	1.46	1.51
23	B	605	CLA	CMB-C2B	-2.40	1.46	1.51
23	C	511	CLA	CMB-C2B	-2.40	1.46	1.51
23	A	403	CLA	CMB-C2B	-2.40	1.46	1.51
23	c	513	CLA	CMB-C2B	-2.40	1.46	1.51
28	c	517	DGD	O6E-C5E	-2.40	1.38	1.44
23	C	509	CLA	CMB-C2B	-2.40	1.46	1.51
28	A	411	DGD	O3G-C3G	-2.40	1.39	1.43
23	a	404	CLA	CMB-C2B	-2.39	1.46	1.51
31	b	624	LMG	O8-C9	-2.39	1.39	1.45
23	C	502	CLA	CMB-C2B	-2.39	1.46	1.51
23	c	506	CLA	CMB-C2B	-2.38	1.46	1.51
23	C	512	CLA	CMB-C2B	-2.38	1.46	1.51
31	d	407	LMG	O8-C9	-2.38	1.39	1.45
28	b	602	DGD	O4D-C4D	-2.38	1.37	1.43
23	c	501	CLA	CMB-C2B	-2.38	1.46	1.51
31	B	622	LMG	O6-C5	-2.38	1.38	1.44
28	C	518	DGD	O6E-C5E	-2.38	1.38	1.44
23	C	506	CLA	CMB-C2B	-2.38	1.46	1.51
23	D	403	CLA	CMB-C2B	-2.38	1.46	1.51
31	D	406	LMG	O8-C9	-2.37	1.39	1.45
23	c	512	CLA	CMB-C2B	-2.37	1.46	1.51
23	B	614	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	CMB-C2B	-2.37	1.46	1.51
28	a	413	DGD	O3G-C3G	-2.37	1.39	1.43
25	a	410	PL9	C28-C29	2.37	1.38	1.33
23	B	602	CLA	CMB-C2B	-2.37	1.46	1.51
31	A	414	LMG	O1-C7	-2.36	1.39	1.43
31	C	521	LMG	O8-C9	-2.36	1.39	1.45
23	C	503	CLA	CMB-C2B	-2.36	1.46	1.51
28	C	518	DGD	O5D-C6D	-2.36	1.39	1.43
31	C	520	LMG	O8-C9	-2.35	1.39	1.45
23	B	609	CLA	CMB-C2B	-2.35	1.46	1.51
23	c	511	CLA	CMB-C2B	-2.35	1.46	1.51
23	b	619	CLA	CMB-C2B	-2.35	1.46	1.51
31	I	101	LMG	O1-C7	-2.35	1.39	1.43
28	B	621	DGD	O4D-C4D	-2.34	1.37	1.43
23	b	613	CLA	CMB-C2B	-2.34	1.46	1.51
31	b	624	LMG	O1-C7	-2.34	1.39	1.43
23	d	403	CLA	CMB-C2B	-2.34	1.46	1.51
23	d	402	CLA	CMB-C2B	-2.34	1.46	1.51
23	c	503	CLA	CMB-C2B	-2.34	1.46	1.51
23	a	406	CLA	CMB-C2B	-2.33	1.46	1.51
31	B	623	LMG	O1-C7	-2.33	1.39	1.43
28	B	627	DGD	O4D-C4D	-2.33	1.37	1.43
23	c	509	CLA	CMB-C2B	-2.33	1.46	1.51
25	D	404	PL9	C28-C29	2.32	1.38	1.33
31	d	406	LMG	O1-C7	-2.32	1.39	1.43
23	a	409	CLA	CMB-C2B	-2.32	1.46	1.51
25	J	101	PL9	C28-C29	2.30	1.39	1.32
23	B	612	CLA	CMB-C2B	-2.29	1.46	1.51
25	j	101	PL9	C28-C29	2.29	1.38	1.32
30	a	401	SQD	O2-C2	-2.28	1.37	1.43
30	A	417	SQD	C4-C5	-2.28	1.48	1.53
23	c	510	CLA	CMD-C2D	-2.28	1.46	1.50
23	D	401	CLA	CMB-C2B	-2.28	1.46	1.51
23	b	616	CLA	CMB-C2B	-2.28	1.46	1.51
31	a	402	LMG	O8-C9	-2.28	1.40	1.45
28	C	518	DGD	C4D-C5D	-2.27	1.48	1.53
31	i	101	LMG	O6-C5	-2.27	1.38	1.44
28	A	411	DGD	O1G-C1G	-2.27	1.40	1.45
28	C	518	DGD	O5D-C1E	-2.27	1.36	1.40
34	v	201	HEM	FE-ND	2.26	2.08	1.96
31	a	402	LMG	O1-C7	-2.26	1.39	1.43
31	k	103	LMG	O1-C7	-2.26	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I	101	LMG	O6-C5	-2.25	1.38	1.44
31	a	416	LMG	O1-C7	-2.25	1.39	1.43
30	B	626	SQD	O2-C2	-2.24	1.37	1.43
31	m	102	LMG	O6-C5	-2.24	1.38	1.44
31	D	407	LMG	O2-C2	-2.23	1.37	1.43
31	D	407	LMG	O6-C5	-2.23	1.38	1.44
28	C	517	DGD	O4D-C4D	-2.23	1.37	1.43
31	k	103	LMG	O8-C9	-2.23	1.40	1.45
28	B	621	DGD	O6D-C5D	-2.23	1.38	1.44
28	b	623	DGD	O6E-C5E	-2.22	1.39	1.44
28	c	518	DGD	O3G-C3G	-2.22	1.39	1.43
31	d	407	LMG	O2-C2	-2.21	1.37	1.43
31	B	623	LMG	O6-C5	-2.21	1.39	1.44
28	c	517	DGD	O6D-C5D	-2.21	1.39	1.44
31	c	519	LMG	O6-C5	-2.20	1.39	1.44
23	B	612	CLA	CMD-C2D	-2.20	1.46	1.50
28	c	517	DGD	O5D-C1E	-2.18	1.36	1.40
28	c	517	DGD	O1G-C1G	-2.18	1.40	1.45
34	v	201	HEM	CAA-C2A	2.18	1.55	1.52
31	d	407	LMG	O1-C7	-2.17	1.39	1.43
28	d	409	DGD	O4D-C4D	-2.17	1.37	1.43
31	E	101	LMG	O6-C5	-2.17	1.39	1.44
31	d	407	LMG	O6-C5	-2.17	1.39	1.44
30	b	601	SQD	O2-C2	-2.17	1.37	1.43
31	b	625	LMG	O6-C5	-2.17	1.39	1.44
23	A	403	CLA	CMD-C2D	-2.17	1.46	1.50
30	A	413	SQD	O2-C2	-2.16	1.37	1.43
31	e	101	LMG	O6-C5	-2.16	1.39	1.44
23	a	404	CLA	CMD-C2D	-2.15	1.46	1.50
28	D	409	DGD	O6E-C5E	-2.15	1.39	1.44
28	D	409	DGD	O4D-C4D	-2.15	1.37	1.43
24	a	407	PHO	CMB-C2B	-2.14	1.46	1.51
23	C	505	CLA	CMD-C2D	-2.14	1.46	1.50
28	b	623	DGD	O4D-C4D	-2.14	1.37	1.43
23	d	402	CLA	CMD-C2D	-2.13	1.46	1.50
24	D	402	PHO	CMD-C2D	-2.13	1.46	1.51
28	a	413	DGD	O1G-C1G	-2.13	1.40	1.45
23	B	608	CLA	CMD-C2D	-2.13	1.46	1.50
34	F	101	HEM	FE-ND	2.13	2.07	1.96
23	b	616	CLA	CMD-C2D	-2.13	1.46	1.50
31	C	521	LMG	O6-C5	-2.13	1.39	1.44
28	a	413	DGD	O6E-C5E	-2.12	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	FE-NB	2.12	2.07	1.96
24	a	407	PHO	CMD-C2D	-2.12	1.46	1.51
30	D	408	SQD	O3-C3	-2.12	1.38	1.43
28	B	621	DGD	O6E-C5E	-2.11	1.39	1.44
23	B	614	CLA	CMD-C2D	-2.11	1.46	1.50
30	d	408	SQD	O3-C3	-2.11	1.38	1.43
28	D	409	DGD	O5D-C6D	-2.11	1.39	1.43
30	F	102	SQD	O2-C2	-2.11	1.38	1.43
34	v	201	HEM	FE-NB	2.11	2.07	1.96
30	a	401	SQD	C4-C5	-2.11	1.48	1.53
28	C	518	DGD	O6D-C5D	-2.11	1.39	1.44
31	C	520	LMG	O1-C7	-2.11	1.39	1.43
23	B	604	CLA	CMD-C2D	-2.10	1.46	1.50
31	b	625	LMG	O2-C2	-2.10	1.38	1.43
34	v	201	HEM	CMB-C2B	2.10	1.55	1.50
23	c	505	CLA	CMD-C2D	-2.10	1.46	1.50
31	M	101	LMG	O6-C5	-2.10	1.39	1.44
28	d	409	DGD	O6E-C5E	-2.09	1.39	1.44
33	i	102	LMT	O1'-C1'	2.09	1.43	1.40
28	b	623	DGD	O6D-C5D	-2.09	1.39	1.44
23	C	510	CLA	CMD-C2D	-2.09	1.46	1.50
30	D	408	SQD	O4-C4	-2.09	1.38	1.43
23	b	618	CLA	CMD-C2D	-2.09	1.46	1.50
23	a	406	CLA	CMD-C2D	-2.09	1.46	1.50
28	c	518	DGD	O6E-C5E	-2.08	1.39	1.44
30	f	102	SQD	O2-C2	-2.08	1.38	1.43
30	B	626	SQD	O3-C3	-2.08	1.38	1.43
28	B	627	DGD	C4E-C5E	-2.08	1.48	1.53
23	b	608	CLA	CMD-C2D	-2.08	1.46	1.50
31	E	101	LMG	O2-C2	-2.08	1.38	1.43
28	C	517	DGD	C4E-C5E	-2.08	1.48	1.53
31	b	625	LMG	O1-C7	-2.08	1.40	1.43
28	A	411	DGD	O6E-C5E	-2.08	1.39	1.44
33	D	410	LMT	O1'-C1'	2.08	1.43	1.40
31	B	623	LMG	O2-C2	-2.08	1.38	1.43
24	D	402	PHO	CMC-C2C	-2.07	1.46	1.51
31	I	101	LMG	C4-C5	-2.07	1.48	1.53
31	D	407	LMG	O1-C7	-2.07	1.40	1.43
28	C	518	DGD	C4E-C5E	-2.07	1.48	1.53
31	d	406	LMG	O6-C5	-2.07	1.39	1.44
23	B	603	CLA	CMD-C2D	-2.07	1.46	1.50
24	A	406	PHO	CMC-C2C	-2.07	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	408	SQD	O4-C4	-2.07	1.38	1.43
23	c	502	CLA	CMD-C2D	-2.07	1.46	1.50
30	b	601	SQD	O3-C3	-2.06	1.38	1.43
28	c	517	DGD	C4D-C5D	-2.06	1.48	1.53
31	e	101	LMG	C4-C5	-2.06	1.48	1.53
30	F	102	SQD	O3-C3	-2.06	1.38	1.43
23	C	504	CLA	C3B-CAB	-2.06	1.43	1.47
24	A	406	PHO	CMD-C2D	-2.06	1.46	1.51
31	D	406	LMG	O6-C5	-2.06	1.39	1.44
31	e	101	LMG	O2-C2	-2.06	1.38	1.43
24	a	407	PHO	C3B-C2B	-2.06	1.37	1.40
23	b	612	CLA	CMD-C2D	-2.06	1.46	1.50
23	C	508	CLA	CMD-C2D	-2.05	1.46	1.50
28	C	519	DGD	O1G-C1G	-2.05	1.40	1.45
23	D	401	CLA	CMD-C2D	-2.05	1.46	1.50
28	B	621	DGD	O1G-C1G	-2.05	1.40	1.45
23	b	609	CLA	CMD-C2D	-2.05	1.46	1.50
23	d	403	CLA	CMD-C2D	-2.05	1.46	1.50
31	B	622	LMG	O1-C7	-2.05	1.40	1.43
24	A	406	PHO	CMB-C2B	-2.05	1.46	1.51
24	a	408	PHO	CMD-C2D	-2.05	1.46	1.51
30	a	415	SQD	O2-C2	-2.04	1.38	1.43
30	a	415	SQD	O3-C3	-2.04	1.38	1.43
23	b	616	CLA	CMC-C2C	-2.04	1.46	1.50
34	V	201	HEM	CMD-C2D	2.04	1.55	1.50
34	V	201	HEM	CMB-C2B	2.04	1.55	1.50
31	c	519	LMG	O1-C7	-2.04	1.40	1.43
24	a	408	PHO	CMC-C2C	-2.03	1.46	1.51
23	B	611	CLA	CMD-C2D	-2.03	1.46	1.50
23	B	616	CLA	CMC-C2C	-2.03	1.46	1.50
30	B	626	SQD	O4-C4	-2.03	1.38	1.43
23	C	502	CLA	CMD-C2D	-2.03	1.46	1.50
30	D	408	SQD	O2-C2	-2.03	1.38	1.43
24	D	402	PHO	CMB-C2B	-2.03	1.46	1.51
24	a	407	PHO	CMC-C2C	-2.03	1.46	1.51
33	d	410	LMT	O1'-C1'	2.03	1.43	1.40
23	C	502	CLA	CMC-C2C	-2.03	1.46	1.50
23	b	611	CLA	CMD-C2D	-2.02	1.46	1.50
28	b	602	DGD	O5D-C6D	-2.02	1.40	1.43
24	D	402	PHO	CBD-CGD	-2.02	1.49	1.52
23	b	605	CLA	CMC-C2C	-2.02	1.46	1.50
23	D	403	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	102	SQD	O4-C4	-2.02	1.38	1.43
23	b	617	CLA	CMD-C2D	-2.01	1.46	1.50
28	c	516	DGD	C4E-C5E	-2.01	1.48	1.53
23	c	508	CLA	C3D-C4D	2.01	1.48	1.44
23	a	409	CLA	CMC-C2C	-2.00	1.46	1.50
28	C	519	DGD	O6E-C5E	-2.00	1.39	1.44
23	C	511	CLA	C3B-C2B	-2.00	1.37	1.40
23	c	507	CLA	CMD-C2D	-2.00	1.46	1.50
30	f	102	SQD	O3-C3	-2.00	1.38	1.43
23	C	508	CLA	CMC-C2C	-2.00	1.46	1.50
23	c	502	CLA	C3D-C4D	2.00	1.48	1.44
23	c	512	CLA	C3D-C4D	2.00	1.48	1.44
31	i	101	LMG	C4-C5	-2.00	1.48	1.53
23	b	620	CLA	CMC-C2C	-2.00	1.46	1.50
30	b	601	SQD	O4-C4	-2.00	1.38	1.43
23	B	605	CLA	CMD-C2D	-2.00	1.46	1.50

All (1459) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	j	102	BCR	C32-C1-C6	-13.66	88.14	110.30
27	J	102	BCR	C32-C1-C6	-13.37	88.62	110.30
27	T	102	BCR	C7-C8-C9	-8.78	112.96	126.23
27	B	618	BCR	C7-C8-C9	-8.64	113.18	126.23
27	J	102	BCR	C32-C1-C31	-8.46	82.55	108.53
27	j	102	BCR	C32-C1-C31	-8.44	82.62	108.53
27	C	514	BCR	C7-C8-C9	8.31	138.79	126.23
27	c	514	BCR	C7-C8-C9	8.10	138.47	126.23
23	B	607	CLA	C4A-NA-C1A	7.89	110.25	106.71
23	d	402	CLA	C4A-NA-C1A	7.87	110.24	106.71
23	C	511	CLA	C4A-NA-C1A	7.84	110.23	106.71
23	c	505	CLA	C4A-NA-C1A	7.74	110.19	106.71
23	c	509	CLA	C4A-NA-C1A	7.52	110.09	106.71
23	b	618	CLA	C4A-NA-C1A	7.45	110.06	106.71
23	a	406	CLA	C4A-NA-C1A	7.44	110.05	106.71
23	b	617	CLA	C4A-NA-C1A	7.33	110.00	106.71
23	C	512	CLA	C4A-NA-C1A	7.20	109.94	106.71
23	c	504	CLA	C4A-NA-C1A	7.19	109.94	106.71
23	B	605	CLA	C4A-NA-C1A	7.15	109.92	106.71
23	a	404	CLA	C4A-NA-C1A	7.14	109.91	106.71
23	B	601	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	C	505	CLA	C4A-NA-C1A	7.03	109.87	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	v	201	HEM	C4D-ND-C1D	7.00	112.30	105.07
23	B	603	CLA	C4A-NA-C1A	6.98	109.84	106.71
23	c	512	CLA	C4A-NA-C1A	6.92	109.82	106.71
23	B	608	CLA	C4A-NA-C1A	6.91	109.81	106.71
23	b	611	CLA	C4A-NA-C1A	6.90	109.81	106.71
23	c	502	CLA	C4A-NA-C1A	6.86	109.79	106.71
23	b	619	CLA	C4A-NA-C1A	6.81	109.77	106.71
23	b	616	CLA	C4A-NA-C1A	6.80	109.76	106.71
23	c	511	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	b	610	CLA	C4A-NA-C1A	6.79	109.76	106.71
23	B	602	CLA	C4A-NA-C1A	6.78	109.76	106.71
23	B	604	CLA	C4A-NA-C1A	6.77	109.75	106.71
23	b	608	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	d	405	BCR	C7-C8-C9	-6.75	116.04	126.23
23	C	504	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	C	506	CLA	C4A-NA-C1A	6.74	109.74	106.71
23	B	609	CLA	C4A-NA-C1A	6.74	109.73	106.71
23	c	513	CLA	C4A-NA-C1A	6.73	109.73	106.71
23	C	509	CLA	C4A-NA-C1A	6.71	109.72	106.71
23	c	506	CLA	C4A-NA-C1A	6.70	109.72	106.71
23	a	409	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	c	501	CLA	C4A-NA-C1A	6.69	109.71	106.71
23	C	503	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	b	606	CLA	C4A-NA-C1A	6.68	109.71	106.71
23	C	513	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	d	403	CLA	C4A-NA-C1A	6.66	109.70	106.71
23	C	508	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	C	501	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	C	502	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	c	508	CLA	C4A-NA-C1A	6.61	109.68	106.71
23	b	609	CLA	C4A-NA-C1A	6.51	109.63	106.71
23	b	607	CLA	C4A-NA-C1A	6.49	109.62	106.71
23	b	620	CLA	C4A-NA-C1A	6.47	109.61	106.71
27	D	405	BCR	C7-C8-C9	-6.45	116.49	126.23
23	c	507	CLA	C4A-NA-C1A	6.43	109.59	106.71
23	b	615	CLA	C4A-NA-C1A	6.41	109.59	106.71
23	A	407	CLA	C4A-NA-C1A	6.39	109.58	106.71
27	j	102	BCR	C31-C1-C6	6.38	120.66	110.30
23	B	615	CLA	C4A-NA-C1A	6.37	109.57	106.71
23	B	612	CLA	C4A-NA-C1A	6.36	109.56	106.71
23	B	614	CLA	C4A-NA-C1A	6.33	109.55	106.71
27	J	102	BCR	C31-C1-C6	6.32	120.55	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	403	CLA	C4A-NA-C1A	6.32	109.55	106.71
34	f	101	HEM	C4D-ND-C1D	6.26	111.54	105.07
23	b	605	CLA	C4A-NA-C1A	6.25	109.52	106.71
23	C	507	CLA	C4A-NA-C1A	6.25	109.52	106.71
34	V	201	HEM	C4D-ND-C1D	6.24	111.51	105.07
23	B	613	CLA	C4A-NA-C1A	6.21	109.50	106.71
23	c	503	CLA	C4A-NA-C1A	6.21	109.50	106.71
23	B	611	CLA	C4A-NA-C1A	6.19	109.49	106.71
27	J	102	BCR	C15-C14-C13	-6.18	118.48	127.31
23	D	403	CLA	C4A-NA-C1A	6.18	109.48	106.71
23	A	404	CLA	C4A-NA-C1A	6.14	109.47	106.71
23	D	401	CLA	C4A-NA-C1A	6.11	109.45	106.71
28	c	518	DGD	C3G-O3G-C1D	6.11	125.67	113.74
30	D	408	SQD	O6-C1-C2	6.09	117.82	108.30
23	b	614	CLA	C4A-NA-C1A	6.06	109.43	106.71
27	b	622	BCR	C24-C23-C22	-6.04	117.11	126.23
34	F	101	HEM	C4D-ND-C1D	6.01	111.28	105.07
28	A	411	DGD	C3G-O3G-C1D	5.99	125.44	113.74
23	B	610	CLA	C4A-NA-C1A	5.93	109.37	106.71
23	B	616	CLA	C4A-NA-C1A	5.86	109.34	106.71
30	d	408	SQD	O6-C1-C2	5.85	117.43	108.30
23	b	613	CLA	C4A-NA-C1A	5.85	109.33	106.71
23	b	612	CLA	C4A-NA-C1A	5.83	109.33	106.71
28	a	413	DGD	C3G-O3G-C1D	5.81	125.08	113.74
23	B	606	CLA	C4A-NA-C1A	5.71	109.27	106.71
23	c	510	CLA	C4A-NA-C1A	5.67	109.25	106.71
30	D	408	SQD	C44-O6-C1	5.64	124.76	113.74
23	a	405	CLA	C4A-NA-C1A	5.64	109.24	106.71
27	B	618	BCR	C11-C10-C9	-5.60	119.32	127.31
27	c	514	BCR	C15-C14-C13	-5.54	119.40	127.31
28	C	519	DGD	C3G-O3G-C1D	5.54	124.56	113.74
27	J	102	BCR	C28-C27-C26	-5.51	104.23	114.08
27	j	102	BCR	C15-C14-C13	-5.45	119.54	127.31
27	J	102	BCR	C32-C1-C2	-5.42	87.22	108.91
23	A	405	CLA	C4A-NA-C1A	5.41	109.14	106.71
27	z	101	BCR	C15-C14-C13	-5.39	119.62	127.31
27	B	620	BCR	C24-C23-C22	-5.37	118.12	126.23
27	j	102	BCR	C32-C1-C2	-5.35	87.49	108.91
30	d	408	SQD	C44-O6-C1	5.34	124.17	113.74
27	b	622	BCR	C3-C4-C5	-5.34	104.54	114.08
28	D	409	DGD	O3G-C1D-C2D	5.29	116.57	108.30
27	j	102	BCR	C28-C27-C26	-5.24	104.72	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	C4A-NA-C1A	5.10	109.00	106.71
27	D	405	BCR	C11-C10-C9	-5.09	120.04	127.31
28	d	409	DGD	O3G-C1D-C2D	5.09	116.26	108.30
27	D	405	BCR	C28-C27-C26	-5.09	105.00	114.08
27	j	102	BCR	C20-C21-C22	-5.07	120.07	127.31
30	b	601	SQD	O7-S-C6	5.05	112.94	106.94
27	a	412	BCR	C33-C5-C6	-5.03	118.88	124.53
27	j	102	BCR	C11-C10-C9	-4.97	120.22	127.31
27	J	102	BCR	C20-C21-C22	-4.96	120.23	127.31
27	d	405	BCR	C28-C27-C26	-4.95	105.24	114.08
27	C	516	BCR	C7-C8-C9	-4.94	118.76	126.23
27	j	102	BCR	C24-C23-C22	-4.93	118.79	126.23
27	y	101	BCR	C15-C14-C13	-4.90	120.32	127.31
27	c	514	BCR	C33-C5-C6	-4.86	119.07	124.53
30	f	102	SQD	O7-S-C6	4.86	112.71	106.94
25	J	101	PL9	C7-C3-C4	4.82	120.80	116.88
27	B	618	BCR	C3-C4-C5	-4.82	105.46	114.08
27	B	620	BCR	C3-C4-C5	-4.80	105.51	114.08
27	C	515	BCR	C15-C14-C13	-4.79	120.47	127.31
27	T	102	BCR	C28-C27-C26	-4.76	105.58	114.08
27	C	514	BCR	C33-C5-C6	-4.73	119.21	124.53
27	B	620	BCR	C16-C17-C18	-4.71	120.59	127.31
27	T	102	BCR	C3-C4-C5	-4.69	105.70	114.08
30	B	626	SQD	O7-S-C6	4.68	112.50	106.94
30	d	408	SQD	O9-S-C6	4.67	112.49	106.94
27	T	102	BCR	C11-C10-C9	-4.64	120.68	127.31
27	J	102	BCR	C24-C23-C22	-4.64	119.23	126.23
27	c	515	BCR	C7-C8-C9	-4.63	119.24	126.23
27	k	102	BCR	C15-C14-C13	-4.63	120.70	127.31
27	A	410	BCR	C33-C5-C6	-4.63	119.33	124.53
31	a	416	LMG	C7-O1-C1	4.62	122.77	113.74
27	b	622	BCR	C16-C17-C18	-4.56	120.80	127.31
25	j	101	PL9	C7-C3-C4	4.55	120.58	116.88
27	J	102	BCR	C11-C10-C9	-4.55	120.82	127.31
27	C	514	BCR	C8-C7-C6	4.51	139.88	127.20
27	C	514	BCR	C15-C14-C13	-4.47	120.93	127.31
27	b	621	BCR	C15-C14-C13	-4.45	120.96	127.31
27	k	102	BCR	C24-C23-C22	-4.43	119.54	126.23
27	c	515	BCR	C15-C14-C13	-4.43	120.99	127.31
28	c	517	DGD	O5D-C6D-C5D	-4.42	100.87	109.05
27	y	101	BCR	C16-C17-C18	-4.41	121.01	127.31
27	J	102	BCR	C16-C17-C18	-4.41	121.02	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	619	BCR	C20-C21-C22	-4.40	121.03	127.31
27	y	101	BCR	C7-C8-C9	-4.40	119.59	126.23
27	B	617	BCR	C16-C17-C18	-4.40	121.03	127.31
27	B	620	BCR	C15-C14-C13	-4.38	121.06	127.31
27	B	619	BCR	C28-C27-C26	-4.36	106.29	114.08
30	d	408	SQD	O47-C7-C8	4.33	120.83	111.50
31	d	407	LMG	O1-C1-C2	4.31	115.04	108.30
27	C	516	BCR	C15-C14-C13	-4.29	121.19	127.31
27	b	621	BCR	C28-C27-C26	-4.28	106.44	114.08
27	c	514	BCR	C8-C7-C6	4.26	139.18	127.20
27	B	618	BCR	C28-C27-C26	-4.25	106.48	114.08
27	j	102	BCR	C7-C8-C9	-4.25	119.81	126.23
27	k	102	BCR	C38-C26-C25	-4.24	119.77	124.53
34	V	201	HEM	C4C-CHD-C1D	4.23	128.15	122.56
27	H	101	BCR	C33-C5-C6	-4.23	119.78	124.53
27	b	621	BCR	C7-C8-C9	-4.21	119.87	126.23
27	B	620	BCR	C38-C26-C25	-4.21	119.80	124.53
27	a	412	BCR	C16-C17-C18	-4.20	121.31	127.31
23	b	614	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
23	B	610	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
27	C	515	BCR	C16-C17-C18	-4.18	121.34	127.31
27	D	405	BCR	C16-C17-C18	-4.18	121.34	127.31
28	C	519	DGD	C1D-O6D-C5D	-4.18	105.49	113.69
30	D	408	SQD	O9-S-C6	4.18	111.90	106.94
28	c	518	DGD	C1D-O6D-C5D	-4.17	105.50	113.69
27	d	405	BCR	C33-C5-C6	-4.17	119.85	124.53
27	b	622	BCR	C7-C8-C9	-4.17	119.94	126.23
27	d	405	BCR	C15-C14-C13	-4.16	121.37	127.31
27	D	405	BCR	C33-C5-C6	-4.16	119.86	124.53
27	d	405	BCR	C11-C10-C9	-4.16	121.37	127.31
25	d	404	PL9	C7-C3-C4	4.14	120.24	116.88
27	c	515	BCR	C16-C17-C18	-4.13	121.41	127.31
27	C	514	BCR	C3-C4-C5	-4.13	106.70	114.08
27	A	410	BCR	C15-C14-C13	-4.12	121.42	127.31
30	F	102	SQD	O7-S-C6	4.12	111.83	106.94
30	A	413	SQD	O9-S-C6	4.11	111.83	106.94
28	C	518	DGD	O5D-C6D-C5D	-4.09	101.47	109.05
27	z	101	BCR	C16-C17-C18	-4.09	121.47	127.31
27	b	621	BCR	C20-C21-C22	-4.08	121.48	127.31
27	c	515	BCR	C28-C27-C26	-4.08	106.80	114.08
28	A	411	DGD	O2G-C1B-C2B	4.08	120.29	111.50
30	F	102	SQD	O9-S-C6	4.07	111.77	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	101	BCR	C24-C23-C22	-4.06	120.10	126.23
31	B	623	LMG	O7-C10-C11	4.04	120.22	111.50
27	B	617	BCR	C15-C14-C13	-4.04	121.55	127.31
27	a	412	BCR	C24-C23-C22	-4.04	120.14	126.23
27	B	617	BCR	C7-C8-C9	-4.04	120.14	126.23
30	D	408	SQD	O47-C7-C8	4.03	120.18	111.50
27	b	622	BCR	C15-C14-C13	-4.02	121.58	127.31
27	D	405	BCR	C15-C14-C13	-4.01	121.59	127.31
27	a	412	BCR	C38-C26-C25	-4.01	120.03	124.53
28	a	413	DGD	O2G-C1B-C2B	4.00	120.13	111.50
30	F	102	SQD	O47-C7-C8	4.00	120.12	111.50
31	b	624	LMG	O7-C10-C11	4.00	120.12	111.50
34	v	201	HEM	C4C-CHD-C1D	4.00	127.83	122.56
27	a	412	BCR	C15-C14-C13	-4.00	121.61	127.31
27	b	622	BCR	C38-C26-C25	-4.00	120.04	124.53
27	k	102	BCR	C7-C8-C9	-3.99	120.20	126.23
31	m	102	LMG	O7-C10-C11	3.99	120.10	111.50
28	B	627	DGD	O5D-C1E-C2E	3.99	114.53	108.30
30	a	415	SQD	O7-S-C6	3.99	111.68	106.94
31	M	101	LMG	O7-C10-C11	3.99	120.09	111.50
27	B	617	BCR	C24-C23-C22	-3.98	120.22	126.23
27	T	101	BCR	C15-C14-C13	-3.98	121.64	127.31
27	y	101	BCR	C3-C4-C5	-3.97	106.99	114.08
31	D	407	LMG	O1-C1-C2	3.96	114.49	108.30
27	c	514	BCR	C11-C10-C9	-3.96	121.66	127.31
31	B	622	LMG	O7-C10-C11	3.96	120.03	111.50
23	b	616	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
27	B	620	BCR	C20-C21-C22	-3.95	121.67	127.31
27	T	101	BCR	C33-C5-C6	-3.94	120.10	124.53
25	A	408	PL9	C7-C3-C4	3.94	120.08	116.88
30	b	601	SQD	O9-S-C6	3.94	111.62	106.94
27	T	101	BCR	C20-C21-C22	-3.94	121.69	127.31
27	h	101	BCR	C33-C5-C6	-3.93	120.11	124.53
27	k	102	BCR	C16-C17-C18	-3.93	121.70	127.31
30	a	415	SQD	O9-S-C6	3.93	111.61	106.94
27	B	619	BCR	C15-C14-C13	-3.93	121.70	127.31
23	b	617	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
25	a	410	PL9	C7-C3-C4	3.92	120.06	116.88
27	h	101	BCR	C16-C17-C18	-3.90	121.75	127.31
27	C	515	BCR	C24-C23-C22	-3.89	120.35	126.23
23	c	504	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
31	m	102	LMG	C3-C4-C5	3.88	117.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	414	LMG	O7-C10-C11	3.88	119.86	111.50
30	f	102	SQD	O47-C7-C8	3.87	119.85	111.50
27	b	622	BCR	C11-C10-C9	-3.87	121.79	127.31
27	d	405	BCR	C16-C17-C18	-3.87	121.79	127.31
23	B	613	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
31	a	416	LMG	O7-C10-C11	3.86	119.82	111.50
27	C	516	BCR	C28-C27-C26	-3.84	107.21	114.08
30	f	102	SQD	O9-S-O7	-3.84	100.65	113.95
28	A	411	DGD	C1D-O6D-C5D	-3.84	106.15	113.69
27	J	102	BCR	C7-C8-C9	-3.84	120.44	126.23
27	b	621	BCR	C24-C23-C22	-3.83	120.45	126.23
31	d	406	LMG	O7-C10-C11	3.82	119.74	111.50
30	a	415	SQD	O9-S-O7	-3.82	100.72	113.95
23	C	507	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
23	B	603	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
23	d	402	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
27	j	102	BCR	C16-C17-C18	-3.82	121.86	127.31
30	A	417	SQD	O7-S-C6	3.82	111.47	106.94
30	A	413	SQD	O9-S-O7	-3.82	100.74	113.95
29	A	415	LHG	O7-C7-C8	3.81	119.72	111.50
30	F	102	SQD	O9-S-O7	-3.81	100.75	113.95
30	a	401	SQD	C44-O6-C1	3.81	121.19	113.74
30	a	401	SQD	O7-S-C6	3.81	111.47	106.94
28	d	409	DGD	O2D-C2D-C1D	3.81	119.30	110.05
31	C	521	LMG	O7-C10-C11	3.81	119.70	111.50
28	D	409	DGD	C3G-O3G-C1D	3.81	121.17	113.74
30	F	102	SQD	C1-O5-C5	3.80	121.16	113.69
27	D	405	BCR	C24-C23-C22	-3.80	120.49	126.23
27	a	412	BCR	C3-C4-C5	-3.80	107.30	114.08
27	y	101	BCR	C38-C26-C25	-3.79	120.27	124.53
30	A	417	SQD	O47-C7-C8	3.79	119.67	111.50
27	B	617	BCR	C33-C5-C6	-3.78	120.28	124.53
30	D	408	SQD	O9-S-O7	-3.78	100.87	113.95
23	D	401	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
23	B	612	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
23	C	508	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
34	f	101	HEM	C4B-CHC-C1C	3.74	127.50	122.56
30	d	408	SQD	O9-S-O7	-3.74	100.99	113.95
27	C	515	BCR	C33-C5-C6	-3.74	120.33	124.53
23	B	614	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
30	A	417	SQD	O5-C5-C4	3.73	116.47	109.69
31	D	406	LMG	O7-C10-C11	3.73	119.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	407	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
27	A	410	BCR	C3-C4-C5	-3.72	107.44	114.08
23	c	506	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
31	b	625	LMG	O7-C10-C11	3.72	119.51	111.50
27	c	514	BCR	C3-C4-C5	-3.71	107.44	114.08
27	A	410	BCR	C16-C17-C18	-3.71	122.01	127.31
30	A	413	SQD	C1-O5-C5	3.71	120.98	113.69
25	a	410	PL9	C35-C34-C36	3.71	121.52	115.27
30	d	408	SQD	C1-O5-C5	3.71	120.97	113.69
30	a	401	SQD	O5-C5-C4	3.71	116.43	109.69
30	D	408	SQD	C1-O5-C5	3.71	120.97	113.69
27	h	101	BCR	C15-C14-C13	-3.71	122.02	127.31
23	c	508	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
28	B	627	DGD	O2G-C1B-C2B	3.71	119.49	111.50
31	a	402	LMG	O7-C10-C11	3.71	119.49	111.50
27	c	515	BCR	C11-C10-C9	-3.70	122.03	127.31
27	z	101	BCR	C24-C23-C22	-3.70	120.65	126.23
28	C	519	DGD	C2G-O2G-C1B	3.70	126.89	117.79
29	a	417	LHG	O7-C7-C8	3.69	119.46	111.50
31	A	418	LMG	O7-C10-C11	3.69	119.45	111.50
23	B	611	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
30	a	401	SQD	O47-C7-C8	3.68	119.44	111.50
27	b	621	BCR	C3-C4-C5	-3.68	107.50	114.08
27	C	516	BCR	C38-C26-C25	-3.67	120.40	124.53
23	A	404	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
28	c	517	DGD	O2G-C1B-C2B	3.67	119.41	111.50
23	b	612	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
27	H	101	BCR	C24-C23-C22	-3.65	120.72	126.23
23	B	606	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
23	B	608	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
31	c	519	LMG	O7-C10-C11	3.64	119.35	111.50
31	d	407	LMG	C1-O6-C5	-3.63	106.56	113.69
23	b	614	CLA	CMB-C2B-C3B	3.63	131.46	124.68
30	B	626	SQD	C44-O6-C1	3.62	120.81	113.74
30	b	601	SQD	O9-S-O7	-3.62	101.43	113.95
23	a	405	CLA	C1-C2-C3	-3.62	119.79	126.04
30	a	401	SQD	C1-O5-C5	3.62	120.79	113.69
23	a	405	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
25	a	410	PL9	C25-C24-C26	3.61	121.35	115.27
23	C	503	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
30	A	413	SQD	O7-S-C6	3.61	111.23	106.94
27	d	405	BCR	C24-C23-C22	-3.61	120.79	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
27	C	516	BCR	C16-C17-C18	-3.60	122.17	127.31
23	B	616	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
23	b	619	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
25	d	404	PL9	C25-C24-C26	3.59	121.31	115.27
27	J	102	BCR	C2-C1-C6	3.59	116.01	110.48
30	f	102	SQD	C1-O5-C5	3.59	120.73	113.69
30	a	415	SQD	O47-C7-C8	3.58	119.22	111.50
27	b	622	BCR	C4-C5-C6	-3.58	117.53	122.73
28	D	409	DGD	O2D-C2D-C1D	3.57	118.71	110.05
28	c	518	DGD	C2G-O2G-C1B	3.57	126.57	117.79
27	k	102	BCR	C3-C4-C5	-3.56	107.72	114.08
28	C	518	DGD	O2G-C1B-C2B	3.56	119.17	111.50
27	z	101	BCR	C3-C4-C5	-3.55	107.73	114.08
30	A	417	SQD	C44-O6-C1	3.55	120.68	113.74
27	A	410	BCR	C38-C26-C25	-3.55	120.54	124.53
28	B	627	DGD	C3D-C4D-C5D	3.55	116.57	110.24
31	C	520	LMG	O7-C10-C11	3.55	119.14	111.50
27	c	514	BCR	C35-C13-C14	-3.55	117.96	122.92
23	a	404	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
27	B	620	BCR	C11-C10-C9	-3.54	122.25	127.31
30	A	417	SQD	C1-O5-C5	3.54	120.64	113.69
23	A	405	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
34	F	101	HEM	CBA-CAA-C2A	-3.54	106.58	112.62
23	b	607	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
23	B	607	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
31	m	102	LMG	C1-O6-C5	-3.54	106.75	113.69
27	C	515	BCR	C3-C4-C5	-3.54	107.76	114.08
27	j	102	BCR	C2-C1-C6	3.53	115.92	110.48
30	B	626	SQD	O9-S-O7	-3.53	101.72	113.95
23	C	504	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
23	b	606	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
31	D	407	LMG	C7-O1-C1	3.52	120.62	113.74
28	B	627	DGD	C3G-O3G-C1D	3.50	120.58	113.74
27	C	514	BCR	C11-C10-C9	-3.50	122.32	127.31
34	f	101	HEM	C4C-CHD-C1D	3.50	127.17	122.56
27	k	102	BCR	C20-C21-C22	-3.49	122.33	127.31
23	b	616	CLA	CMB-C2B-C3B	3.49	131.20	124.68
30	b	601	SQD	C44-O6-C1	3.48	120.55	113.74
23	C	506	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	D	403	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
23	c	510	CLA	CMB-C2B-C1B	-3.47	123.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c	514	BCR	C16-C17-C18	-3.47	122.35	127.31
23	B	610	CLA	CMB-C2B-C3B	3.47	131.17	124.68
27	h	101	BCR	C24-C23-C22	-3.46	121.00	126.23
23	b	615	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
25	A	408	PL9	C25-C24-C26	3.46	121.09	115.27
34	f	101	HEM	CBA-CAA-C2A	-3.46	106.72	112.62
31	A	414	LMG	C7-O1-C1	3.46	120.50	113.74
23	b	618	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
27	C	516	BCR	C33-C5-C6	-3.45	120.65	124.53
30	a	401	SQD	O9-S-O7	-3.45	102.02	113.95
27	z	101	BCR	C33-C5-C6	-3.44	120.67	124.53
30	D	408	SQD	O7-S-C6	3.43	111.02	106.94
23	b	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
34	F	101	HEM	C4B-CHC-C1C	3.43	127.08	122.56
23	c	513	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
30	a	401	SQD	O6-C1-C2	3.42	113.64	108.30
27	c	515	BCR	C33-C5-C6	-3.42	120.69	124.53
34	f	101	HEM	C1B-NB-C4B	3.42	108.60	105.07
30	a	415	SQD	C1-O5-C5	3.41	120.39	113.69
27	B	617	BCR	C11-C10-C9	-3.41	122.44	127.31
27	C	515	BCR	C11-C10-C9	-3.41	122.44	127.31
27	H	101	BCR	C16-C17-C18	-3.41	122.44	127.31
27	A	410	BCR	C20-C21-C22	-3.41	122.44	127.31
24	A	406	PHO	O2D-CGD-O1D	-3.41	117.17	123.84
23	B	606	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
30	B	626	SQD	O9-S-C6	3.40	110.98	106.94
23	A	403	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
31	M	101	LMG	C3-C4-C5	3.40	116.30	110.24
28	b	602	DGD	C3D-C4D-C5D	3.40	116.30	110.24
31	m	102	LMG	C6-C5-C4	-3.39	105.07	113.00
27	B	620	BCR	C4-C5-C6	-3.39	117.81	122.73
27	B	618	BCR	C38-C26-C25	-3.38	120.73	124.53
29	a	414	LHG	O7-C7-C8	3.38	118.79	111.50
28	b	623	DGD	C1D-O6D-C5D	-3.38	107.05	113.69
23	C	507	CLA	CMB-C2B-C3B	3.38	131.00	124.68
27	c	515	BCR	C38-C26-C25	-3.38	120.73	124.53
31	k	103	LMG	O7-C10-C11	3.37	118.77	111.50
27	b	622	BCR	C20-C21-C22	-3.37	122.50	127.31
25	D	404	PL9	C35-C34-C36	3.37	120.94	115.27
23	b	612	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
23	C	502	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
30	f	102	SQD	O8-S-C6	3.37	111.11	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
30	A	413	SQD	O8-S-C6	3.37	111.11	105.74
23	a	406	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
31	E	101	LMG	C7-O1-C1	3.36	120.30	113.74
29	A	412	LHG	O7-C7-C8	3.36	118.73	111.50
23	C	510	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
23	B	607	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
25	D	404	PL9	C7-C3-C4	3.35	119.60	116.88
25	j	101	PL9	C25-C24-C26	3.35	120.90	115.27
27	b	621	BCR	C16-C17-C18	-3.34	122.55	127.31
27	T	102	BCR	C38-C26-C25	-3.33	120.79	124.53
23	b	617	CLA	CMB-C2B-C3B	3.33	130.91	124.68
23	B	615	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
23	D	401	CLA	CMB-C2B-C3B	3.33	130.90	124.68
27	A	410	BCR	C11-C10-C9	-3.32	122.57	127.31
30	A	417	SQD	O9-S-O7	-3.32	102.45	113.95
23	A	405	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
27	B	619	BCR	C3-C4-C5	-3.32	108.15	114.08
27	C	514	BCR	C20-C21-C22	-3.32	122.57	127.31
23	B	609	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
31	M	101	LMG	C6-C5-C4	-3.31	105.25	113.00
28	d	409	DGD	C3G-O3G-C1D	3.30	120.19	113.74
23	A	404	CLA	C1-C2-C3	-3.30	120.34	126.04
31	D	406	LMG	C7-O1-C1	3.29	120.17	113.74
28	B	621	DGD	C1D-O6D-C5D	-3.29	107.23	113.69
27	c	514	BCR	C20-C21-C22	-3.29	122.62	127.31
27	T	101	BCR	C7-C8-C9	-3.28	121.27	126.23
28	a	413	DGD	O6D-C5D-C6D	3.28	113.29	106.67
23	b	611	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
27	J	102	BCR	C31-C1-C2	3.28	122.03	108.91
31	A	414	LMG	C1-O6-C5	-3.28	107.25	113.69
27	k	102	BCR	C33-C5-C6	-3.28	120.84	124.53
30	A	417	SQD	O5-C1-C2	3.28	117.29	110.35
31	a	402	LMG	C3-C4-C5	3.28	116.09	110.24
23	c	503	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
23	B	605	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
27	j	102	BCR	C31-C1-C2	3.27	121.99	108.91
31	e	101	LMG	C7-O1-C1	3.27	120.13	113.74
31	D	406	LMG	O8-C28-C29	3.27	122.16	111.91
31	a	402	LMG	C7-O1-C1	3.26	120.11	113.74
27	c	515	BCR	C3-C4-C5	-3.26	108.26	114.08
31	M	101	LMG	C1-O6-C5	-3.26	107.30	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	502	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
28	b	602	DGD	O5D-C1E-C2E	3.26	113.39	108.30
23	b	605	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
27	c	514	BCR	C7-C6-C5	-3.25	113.58	121.46
27	j	102	BCR	C29-C30-C25	3.24	115.47	110.48
23	B	613	CLA	CMB-C2B-C3B	3.24	130.74	124.68
27	T	101	BCR	C11-C10-C9	-3.24	122.69	127.31
28	c	516	DGD	O2G-C1B-C2B	3.24	118.48	111.50
23	d	403	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
23	B	601	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
23	B	603	CLA	CMB-C2B-C3B	3.24	130.73	124.68
25	d	404	PL9	C35-C34-C36	3.24	120.71	115.27
25	A	408	PL9	C35-C34-C36	3.23	120.71	115.27
23	B	614	CLA	CMB-C2B-C3B	3.23	130.72	124.68
23	B	602	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
34	F	101	HEM	C4C-CHD-C1D	3.22	126.81	122.56
23	b	607	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
31	b	625	LMG	O1-C1-C2	3.22	113.33	108.30
31	A	418	LMG	C7-O1-C1	3.22	120.02	113.74
27	T	101	BCR	C16-C17-C18	-3.21	122.72	127.31
34	v	201	HEM	C4B-CHC-C1C	3.21	126.80	122.56
30	f	102	SQD	C44-O6-C1	3.21	120.01	113.74
27	y	101	BCR	C24-C23-C22	-3.21	121.39	126.23
30	A	413	SQD	O47-C7-C8	3.21	118.42	111.50
28	A	411	DGD	C3G-C2G-C1G	-3.20	104.21	111.79
23	D	401	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
31	d	406	LMG	C7-O1-C1	3.20	119.99	113.74
23	a	409	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
34	F	101	HEM	C3B-C2B-C1B	3.20	108.86	106.49
27	J	102	BCR	C29-C30-C25	3.20	115.40	110.48
28	C	517	DGD	O5D-C1E-C2E	3.20	113.29	108.30
27	C	516	BCR	C3-C4-C5	-3.20	108.37	114.08
25	D	404	PL9	C22-C23-C24	-3.20	119.96	127.66
27	A	410	BCR	C24-C23-C22	-3.19	121.41	126.23
27	B	619	BCR	C16-C17-C18	-3.19	122.75	127.31
23	c	512	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
25	d	404	PL9	C7-C8-C9	-3.18	121.49	126.79
27	C	516	BCR	C20-C21-C22	-3.18	122.77	127.31
27	C	514	BCR	C28-C27-C26	-3.18	108.40	114.08
23	c	512	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
30	a	401	SQD	O5-C1-C2	3.18	117.07	110.35
27	C	514	BCR	C1-C6-C7	3.18	124.76	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	CMB-C2B-C3B	3.17	130.62	124.68
23	b	619	CLA	CMB-C2B-C3B	3.17	130.62	124.68
27	H	101	BCR	C15-C14-C13	-3.17	122.78	127.31
23	b	607	CLA	CMB-C2B-C3B	3.17	130.61	124.68
27	z	101	BCR	C20-C21-C22	-3.17	122.79	127.31
23	C	513	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
28	C	517	DGD	O2G-C1B-C2B	3.16	118.31	111.50
31	k	103	LMG	O8-C28-C29	3.16	121.82	111.91
23	c	502	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
28	d	409	DGD	O5D-C1E-C2E	3.15	113.22	108.30
30	a	401	SQD	C1-C2-C3	3.14	116.54	110.00
23	B	612	CLA	CMB-C2B-C3B	3.14	130.56	124.68
27	j	102	BCR	C27-C26-C25	-3.14	118.17	122.73
23	A	404	CLA	CMB-C2B-C3B	3.14	130.55	124.68
23	C	507	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
23	A	407	CLA	CMB-C2B-C3B	3.13	130.53	124.68
27	b	622	BCR	C33-C5-C4	3.13	119.63	113.62
23	c	506	CLA	CMB-C2B-C3B	3.13	130.53	124.68
23	B	607	CLA	CMB-C2B-C3B	3.12	130.52	124.68
31	C	521	LMG	O8-C28-C29	3.12	121.71	111.91
27	C	514	BCR	C7-C6-C5	-3.12	113.90	121.46
23	c	505	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
28	C	519	DGD	O5D-C1E-C2E	3.12	113.17	108.30
27	c	514	BCR	C1-C6-C7	3.11	124.58	115.78
23	c	503	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
31	a	402	LMG	C6-C5-C4	-3.11	105.72	113.00
34	F	101	HEM	C1B-NB-C4B	3.11	108.28	105.07
31	d	407	LMG	O7-C10-C11	3.11	118.19	111.50
23	a	406	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
30	d	408	SQD	O5-C5-C4	3.10	115.33	109.69
23	C	511	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
23	b	606	CLA	CMB-C2B-C3B	3.10	130.48	124.68
25	J	101	PL9	C25-C24-C26	3.10	120.48	115.27
28	B	621	DGD	O3D-C3D-C4D	3.09	117.50	110.35
30	D	408	SQD	O5-C5-C4	3.09	115.31	109.69
23	B	607	CLA	CHB-C4A-NA	3.09	128.78	124.51
27	y	101	BCR	C33-C5-C6	-3.09	121.06	124.53
31	B	623	LMG	O1-C1-C2	3.08	113.12	108.30
25	D	404	PL9	C25-C24-C26	3.08	120.45	115.27
23	b	612	CLA	CMB-C2B-C3B	3.08	130.43	124.68
27	H	101	BCR	C20-C21-C22	-3.08	122.92	127.31
28	b	602	DGD	C3G-O3G-C1D	3.07	119.74	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	519	LMG	C1-O6-C5	-3.07	107.66	113.69
23	c	504	CLA	CMB-C2B-C3B	3.07	130.42	124.68
25	d	404	PL9	C7-C3-C2	-3.07	119.26	123.30
23	d	402	CLA	CMB-C2B-C3B	3.07	130.42	124.68
23	C	510	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	c	504	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
27	b	621	BCR	C11-C10-C9	-3.05	122.95	127.31
28	a	413	DGD	C1D-O6D-C5D	-3.05	107.70	113.69
23	c	501	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	b	605	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	d	404	PL9	C37-C38-C39	-3.04	120.35	127.66
30	a	415	SQD	O8-S-C6	3.04	110.58	105.74
31	A	414	LMG	O8-C28-C29	3.04	121.43	111.91
23	b	608	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
31	B	622	LMG	C7-O1-C1	3.03	119.67	113.74
27	B	619	BCR	C33-C5-C6	-3.03	121.12	124.53
23	C	511	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
24	a	408	PHO	CMB-C2B-C3B	3.03	130.35	124.68
23	c	510	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
27	B	620	BCR	C7-C8-C9	-3.03	121.66	126.23
31	A	418	LMG	C3-C4-C5	3.02	115.63	110.24
25	D	404	PL9	C12-C13-C14	-3.02	120.38	127.66
23	C	506	CLA	CMB-C2B-C3B	3.02	130.33	124.68
31	i	101	LMG	O7-C10-C11	3.02	118.00	111.50
31	D	407	LMG	C1-O6-C5	-3.02	107.77	113.69
31	D	407	LMG	O7-C10-C11	3.02	118.00	111.50
23	C	509	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
28	A	411	DGD	O6D-C5D-C6D	3.01	112.75	106.67
27	J	102	BCR	C27-C26-C25	-3.01	118.36	122.73
23	B	604	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
28	c	517	DGD	O3G-C1D-C2D	3.01	113.01	108.30
23	c	506	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	A	406	PHO	CMB-C2B-C3B	3.01	130.31	124.68
27	B	617	BCR	C38-C26-C25	-3.01	121.15	124.53
27	C	514	BCR	C38-C26-C25	-3.01	121.15	124.53
27	B	620	BCR	C33-C5-C4	3.01	119.40	113.62
34	f	101	HEM	C3B-C2B-C1B	3.01	108.72	106.49
23	C	505	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	a	410	PL9	C22-C23-C24	-3.01	120.42	127.66
23	C	503	CLA	CMB-C2B-C3B	3.00	130.30	124.68
31	C	520	LMG	O8-C28-C29	3.00	121.33	111.91
23	B	606	CLA	CMB-C2B-C3B	3.00	130.30	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	101	BCR	C8-C7-C6	-3.00	118.77	127.20
23	B	608	CLA	CMB-C2B-C3B	3.00	130.29	124.68
23	c	501	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
23	B	609	CLA	CMB-C2B-C3B	2.99	130.26	124.68
23	c	508	CLA	CMB-C2B-C3B	2.99	130.26	124.68
27	B	618	BCR	C4-C5-C6	-2.99	118.40	122.73
25	d	404	PL9	C22-C23-C24	-2.98	120.47	127.66
23	C	508	CLA	CMB-C2B-C3B	2.98	130.26	124.68
31	C	520	LMG	C1-O6-C5	-2.98	107.83	113.69
31	B	623	LMG	O8-C28-C29	2.98	121.26	111.91
23	d	403	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
27	B	619	BCR	C11-C10-C9	-2.97	123.07	127.31
27	c	514	BCR	C28-C27-C26	-2.97	108.78	114.08
23	c	511	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
27	C	515	BCR	C20-C21-C22	-2.96	123.08	127.31
30	a	415	SQD	C44-O6-C1	2.96	119.52	113.74
23	c	510	CLA	CMB-C2B-C3B	2.96	130.22	124.68
24	a	407	PHO	O2D-CGD-O1D	-2.96	118.05	123.84
27	c	514	BCR	C34-C9-C10	-2.96	118.78	122.92
31	b	625	LMG	C7-O1-C1	2.96	119.52	113.74
31	c	519	LMG	O8-C28-C29	2.95	121.18	111.91
23	c	511	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
25	D	404	PL9	C37-C38-C39	-2.95	120.55	127.66
30	F	102	SQD	C44-O6-C1	2.95	119.50	113.74
23	D	403	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	b	610	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
27	B	618	BCR	C2-C1-C6	2.95	115.02	110.48
31	I	101	LMG	O7-C10-C11	2.94	117.84	111.50
27	T	102	BCR	C38-C26-C27	2.94	119.26	113.62
27	B	620	BCR	C2-C1-C6	2.94	115.01	110.48
30	A	417	SQD	C1-C2-C3	2.94	116.12	110.00
23	b	613	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
27	T	102	BCR	C2-C1-C6	2.94	115.00	110.48
31	d	406	LMG	O8-C28-C29	2.94	121.12	111.91
31	A	418	LMG	C6-C5-C4	-2.93	106.14	113.00
24	A	406	PHO	O1D-CGD-CBD	2.93	129.62	124.74
23	c	507	CLA	CMB-C2B-C3B	2.93	130.15	124.68
27	C	515	BCR	C15-C16-C17	-2.92	117.49	123.47
23	b	606	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
31	b	625	LMG	O8-C28-C29	2.92	121.07	111.91
23	B	616	CLA	CMB-C2B-C3B	2.92	130.14	124.68
28	c	518	DGD	O1G-C1A-C2A	2.91	121.05	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	411	DGD	C4D-C3D-C2D	-2.91	105.74	110.82
23	a	405	CLA	CMB-C2B-C3B	2.91	130.12	124.68
23	b	618	CLA	CMB-C2B-C3B	2.91	130.12	124.68
28	C	519	DGD	O6D-C5D-C6D	2.90	112.53	106.67
27	h	101	BCR	C20-C21-C22	-2.90	123.17	127.31
23	c	513	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	b	613	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
24	a	408	PHO	O2D-CGD-O1D	-2.89	118.18	123.84
24	a	408	PHO	O1D-CGD-CBD	2.89	129.56	124.74
23	c	502	CLA	CMB-C2B-C3B	2.89	130.08	124.68
23	b	615	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	A	405	CLA	C1-C2-C3	-2.88	121.06	126.04
27	h	101	BCR	C10-C11-C12	-2.88	114.22	123.22
24	a	407	PHO	O1D-CGD-CBD	2.88	129.54	124.74
27	b	621	BCR	C33-C5-C6	-2.88	121.29	124.53
23	B	604	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
30	d	408	SQD	O7-S-C6	2.87	110.36	106.94
25	A	408	PL9	C22-C23-C24	-2.87	120.74	127.66
25	J	101	PL9	C7-C3-C2	-2.87	119.52	123.30
23	b	617	CLA	CHB-C4A-NA	2.87	128.48	124.51
31	a	416	LMG	O8-C28-C29	2.87	120.90	111.91
23	C	512	CLA	CMB-C2B-C3B	2.87	130.04	124.68
23	b	614	CLA	O2D-CGD-O1D	-2.87	118.24	123.84
27	c	515	BCR	C20-C21-C22	-2.87	123.22	127.31
30	d	408	SQD	O8-S-C6	2.86	110.30	105.74
23	b	617	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	C	513	CLA	CMB-C2B-C3B	2.86	130.03	124.68
27	D	405	BCR	C3-C4-C5	-2.86	108.97	114.08
27	j	102	BCR	C33-C5-C6	-2.86	121.32	124.53
27	J	102	BCR	C35-C13-C14	-2.86	118.92	122.92
27	B	619	BCR	C24-C23-C22	-2.86	121.92	126.23
31	d	407	LMG	O8-C28-C29	2.86	120.87	111.91
31	d	407	LMG	C1-C2-C3	-2.86	104.05	110.00
34	v	201	HEM	C1B-NB-C4B	2.85	108.02	105.07
27	d	405	BCR	C38-C26-C27	2.85	119.10	113.62
31	b	624	LMG	C7-O1-C1	2.85	119.31	113.74
23	c	508	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	b	611	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	A	405	CLA	CMB-C2B-C3B	2.85	130.00	124.68
31	a	416	LMG	C1-O6-C5	-2.85	108.10	113.69
23	a	406	CLA	C1-C2-C3	-2.84	121.12	126.04
30	f	102	SQD	O9-S-C6	2.84	110.32	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	402	PHO	O1D-CGD-CBD	2.84	129.47	124.74
23	B	614	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
27	B	617	BCR	C20-C21-C22	-2.84	123.25	127.31
23	B	611	CLA	CMB-C2B-C3B	2.84	129.99	124.68
23	C	509	CLA	CHB-C4A-NA	2.84	128.44	124.51
27	C	514	BCR	C34-C9-C10	-2.84	118.95	122.92
23	b	609	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
23	C	503	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
28	C	519	DGD	O1G-C1A-C2A	2.83	120.80	111.91
23	a	409	CLA	CMB-C2B-C3B	2.83	129.97	124.68
28	b	602	DGD	O2G-C1B-C2B	2.83	117.60	111.50
27	J	102	BCR	C33-C5-C6	-2.83	121.35	124.53
23	a	406	CLA	CHB-C4A-NA	2.83	128.42	124.51
28	A	411	DGD	O4D-C4D-C5D	-2.82	102.31	109.30
23	C	505	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
23	c	513	CLA	CMB-C2B-C3B	2.82	129.94	124.68
31	A	418	LMG	O8-C28-C29	2.81	120.74	111.91
27	B	618	BCR	C38-C26-C27	2.81	119.02	113.62
31	e	101	LMG	O8-C28-C29	2.81	120.72	111.91
27	b	622	BCR	C2-C1-C6	2.81	114.80	110.48
23	c	512	CLA	CHB-C4A-NA	2.81	128.39	124.51
30	F	102	SQD	O5-C5-C4	2.81	114.79	109.69
27	d	405	BCR	C29-C30-C25	2.81	114.80	110.48
23	C	502	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	b	618	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	b	606	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	B	611	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
27	c	515	BCR	C29-C30-C25	2.79	114.78	110.48
27	C	515	BCR	C7-C8-C9	-2.79	122.02	126.23
27	J	102	BCR	C38-C26-C27	2.79	118.98	113.62
31	b	624	LMG	O8-C28-C29	2.79	120.66	111.91
28	c	516	DGD	O5D-C1E-C2E	2.79	112.66	108.30
23	c	512	CLA	CMB-C2B-C3B	2.79	129.89	124.68
28	b	602	DGD	C6D-C5D-C4D	-2.79	106.28	112.09
31	E	101	LMG	O8-C28-C29	2.79	120.65	111.91
30	F	102	SQD	O8-S-C6	2.79	110.18	105.74
30	D	408	SQD	O8-S-C6	2.78	110.18	105.74
23	A	403	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
28	d	409	DGD	O1G-C1A-C2A	2.78	120.63	111.91
30	a	415	SQD	O5-C5-C4	2.78	114.74	109.69
23	B	609	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	B	607	CLA	C1B-CHB-C4A	-2.77	124.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	j	101	PL9	C7-C3-C2	-2.77	119.66	123.30
23	C	501	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	C	512	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
28	b	623	DGD	O3D-C3D-C4D	2.77	116.75	110.35
27	T	102	BCR	C29-C30-C25	2.77	114.74	110.48
31	B	622	LMG	O8-C28-C29	2.77	120.59	111.91
23	A	404	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	c	504	CLA	CHB-C4A-NA	2.76	128.34	124.51
23	b	611	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	b	610	CLA	CMB-C2B-C3B	2.76	129.85	124.68
23	B	605	CLA	CMB-C2B-C3B	2.76	129.84	124.68
31	I	101	LMG	O8-C28-C29	2.76	120.57	111.91
23	C	506	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	b	606	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
27	j	102	BCR	C38-C26-C27	2.75	118.90	113.62
23	c	508	CLA	CHB-C4A-NA	2.75	128.32	124.51
30	A	417	SQD	O6-C1-C2	2.75	112.59	108.30
23	B	605	CLA	CHB-C4A-NA	2.75	128.31	124.51
31	D	406	LMG	O8-C28-O10	-2.74	116.67	123.59
31	C	521	LMG	C1-O6-C5	-2.74	108.30	113.69
30	A	413	SQD	O5-C5-C4	2.74	114.68	109.69
30	f	102	SQD	O5-C5-C4	2.74	114.68	109.69
33	D	410	LMT	C1B-O1B-C4'	-2.74	111.17	117.96
23	B	609	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
27	D	405	BCR	C38-C26-C27	2.74	118.88	113.62
28	c	518	DGD	C4D-C3D-C2D	-2.74	106.04	110.82
23	C	501	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
27	C	514	BCR	C16-C17-C18	-2.74	123.40	127.31
23	B	605	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
23	b	619	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	c	503	CLA	CMB-C2B-C3B	2.73	129.79	124.68
23	b	609	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
27	C	516	BCR	C29-C30-C25	2.73	114.69	110.48
27	a	412	BCR	C34-C9-C10	-2.73	119.10	122.92
31	k	103	LMG	C1-O6-C5	-2.73	108.33	113.69
23	C	508	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	C	506	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	a	406	CLA	CMB-C2B-C3B	2.72	129.76	124.68
23	c	509	CLA	CHB-C4A-NA	2.71	128.27	124.51
23	b	616	CLA	CHB-C4A-NA	2.71	128.26	124.51
28	b	623	DGD	O2G-C1B-C2B	2.71	117.35	111.50
31	a	402	LMG	O8-C28-C29	2.71	120.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	CMB-C2B-C3B	2.71	129.75	124.68
31	B	622	LMG	O1-C1-C2	2.71	112.53	108.30
23	b	620	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	b	620	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
28	c	518	DGD	O6D-C5D-C6D	2.71	112.13	106.67
31	B	623	LMG	C1-O6-C5	-2.71	108.38	113.69
30	B	626	SQD	O5-C5-C4	2.71	114.61	109.69
23	C	504	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
28	C	518	DGD	O4D-C4D-C5D	-2.70	102.58	109.30
23	a	405	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
27	T	102	BCR	C4-C5-C6	-2.70	118.81	122.73
31	I	101	LMG	C7-O1-C1	2.70	119.02	113.74
23	b	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
23	B	616	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
27	y	101	BCR	C33-C5-C4	2.70	118.80	113.62
25	J	101	PL9	C20-C19-C21	2.70	119.81	115.27
31	d	406	LMG	O8-C28-O10	-2.70	116.78	123.59
23	B	603	CLA	CHB-C4A-NA	2.70	128.24	124.51
27	H	101	BCR	C10-C11-C12	-2.70	114.80	123.22
23	B	608	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
31	C	521	LMG	C7-O1-C1	2.69	119.00	113.74
23	B	610	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
30	b	601	SQD	O5-C5-C4	2.69	114.58	109.69
28	C	518	DGD	O3G-C1D-C2D	2.69	112.50	108.30
23	c	509	CLA	CMB-C2B-C1B	-2.69	124.34	128.46
27	B	618	BCR	C21-C20-C19	-2.69	114.84	123.22
23	b	619	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	C	513	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	B	609	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
27	k	102	BCR	C35-C13-C14	-2.68	119.17	122.92
31	D	406	LMG	C3-C4-C5	2.68	115.02	110.24
28	D	409	DGD	O1G-C1A-C2A	2.68	120.32	111.91
28	C	518	DGD	O6E-C1E-C2E	2.68	116.02	110.35
31	c	519	LMG	O1-C1-C2	2.68	112.48	108.30
23	B	608	CLA	CHB-C4A-NA	2.67	128.21	124.51
27	B	618	BCR	C33-C5-C4	2.67	118.75	113.62
23	B	615	CLA	CMB-C2B-C3B	2.67	129.68	124.68
23	C	506	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
23	C	504	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
27	C	516	BCR	C11-C10-C9	-2.67	123.50	127.31
25	D	404	PL9	C7-C8-C9	-2.67	122.35	126.79
23	b	607	CLA	CHB-C4A-NA	2.66	128.20	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	502	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	b	608	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
27	y	101	BCR	C20-C21-C22	-2.66	123.51	127.31
27	d	405	BCR	C38-C26-C25	-2.66	121.54	124.53
31	m	102	LMG	O8-C28-C29	2.66	120.26	111.91
23	C	510	CLA	C1-C2-C3	-2.66	121.44	126.04
27	B	618	BCR	C29-C30-C25	2.66	114.58	110.48
31	D	407	LMG	C1-C2-C3	-2.65	104.47	110.00
31	d	406	LMG	C3-C4-C5	2.65	114.97	110.24
27	T	102	BCR	C33-C5-C4	2.65	118.71	113.62
23	B	610	CLA	C1-C2-C3	-2.65	121.46	126.04
31	D	407	LMG	O8-C28-C29	2.65	120.22	111.91
28	C	518	DGD	O1G-C1A-C2A	2.65	120.22	111.91
23	B	615	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
27	C	515	BCR	C28-C27-C26	-2.64	109.36	114.08
23	C	507	CLA	CHB-C4A-NA	2.64	128.16	124.51
27	c	514	BCR	C38-C26-C25	-2.64	121.56	124.53
23	c	510	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
31	C	520	LMG	C7-O1-C1	2.64	118.89	113.74
27	A	410	BCR	C34-C9-C10	-2.64	119.23	122.92
23	C	507	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
31	C	521	LMG	O1-C1-C2	2.63	112.42	108.30
23	B	601	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
27	H	101	BCR	C38-C26-C25	-2.63	121.57	124.53
23	C	509	CLA	CMB-C2B-C3B	2.63	129.60	124.68
27	D	405	BCR	C23-C24-C25	-2.63	119.82	127.20
23	a	409	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
27	h	101	BCR	C38-C26-C25	-2.63	121.58	124.53
27	C	515	BCR	C8-C7-C6	-2.63	119.82	127.20
23	C	504	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	a	404	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
23	b	613	CLA	CMB-C2B-C3B	2.62	129.59	124.68
23	c	506	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
27	H	101	BCR	C33-C5-C4	2.62	118.65	113.62
31	E	101	LMG	O7-C10-C11	2.62	117.14	111.50
28	D	409	DGD	O5D-C1E-C2E	2.62	112.39	108.30
23	c	505	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
27	B	619	BCR	C29-C30-C25	2.62	114.51	110.48
31	I	101	LMG	C1-O6-C5	-2.62	108.55	113.69
27	T	102	BCR	C21-C20-C19	-2.62	115.06	123.22
31	i	101	LMG	C1-O6-C5	-2.61	108.56	113.69
23	b	614	CLA	CHB-C4A-NA	2.61	128.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	CMB-C2B-C3B	2.61	129.57	124.68
25	d	404	PL9	C32-C33-C34	-2.61	121.37	127.66
31	E	101	LMG	C8-O7-C10	2.61	124.22	117.79
23	a	409	CLA	CHB-C4A-NA	2.61	128.12	124.51
28	c	516	DGD	C1D-O6D-C5D	-2.61	108.56	113.69
27	T	101	BCR	C38-C26-C25	-2.61	121.60	124.53
27	C	514	BCR	C35-C13-C14	-2.61	119.27	122.92
23	c	513	CLA	CHD-C1D-ND	-2.61	122.06	124.45
23	b	605	CLA	CMB-C2B-C3B	2.61	129.56	124.68
23	c	505	CLA	CMB-C2B-C3B	2.61	129.56	124.68
27	a	412	BCR	C11-C10-C9	-2.60	123.59	127.31
23	B	601	CLA	CMB-C2B-C3B	2.60	129.55	124.68
27	b	621	BCR	C29-C30-C25	2.60	114.48	110.48
25	D	404	PL9	C40-C39-C41	2.60	119.64	115.27
27	J	102	BCR	C36-C18-C17	-2.60	119.28	122.92
28	b	602	DGD	O1G-C1A-C2A	2.60	120.06	111.91
23	c	507	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	A	404	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
23	a	404	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	C	511	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	B	604	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	C	512	CLA	CHB-C4A-NA	2.59	128.09	124.51
28	a	413	DGD	C3G-C2G-C1G	-2.59	105.67	111.79
23	A	405	CLA	O2D-CGD-CBD	2.58	115.86	111.27
23	c	506	CLA	CHB-C4A-NA	2.58	128.09	124.51
31	i	101	LMG	C7-O1-C1	2.58	118.79	113.74
23	a	405	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
23	A	404	CLA	CHB-C4A-NA	2.58	128.08	124.51
31	i	101	LMG	O8-C28-C29	2.58	120.00	111.91
28	C	519	DGD	C4D-C3D-C2D	-2.58	106.32	110.82
27	J	102	BCR	C1-C6-C5	-2.58	118.98	122.61
33	B	628	LMT	O1B-C4'-C3'	2.57	114.12	107.28
27	d	405	BCR	C16-C15-C14	-2.57	118.21	123.47
23	B	601	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	b	608	CLA	C1-C2-C3	-2.57	121.60	126.04
23	C	513	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
23	c	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	b	619	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
27	y	101	BCR	C35-C13-C14	-2.57	119.33	122.92
23	d	402	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	a	404	CLA	C1-C2-C3	-2.56	121.61	126.04
23	a	404	CLA	CMB-C2B-C3B	2.56	129.47	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	CMB-C2B-C3B	2.56	129.47	124.68
23	B	601	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
23	b	609	CLA	CMB-C2B-C3B	2.56	129.46	124.68
23	B	602	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	d	404	PL9	C12-C13-C14	-2.56	121.50	127.66
23	C	503	CLA	CHB-C4A-NA	2.55	128.04	124.51
31	d	407	LMG	C7-O1-C1	2.55	118.73	113.74
27	C	514	BCR	C24-C23-C22	-2.55	122.38	126.23
25	a	410	PL9	C7-C3-C2	-2.55	119.94	123.30
27	z	101	BCR	C8-C7-C6	-2.55	120.04	127.20
30	b	601	SQD	O47-C7-C8	2.55	117.00	111.50
23	c	513	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	b	611	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
27	b	621	BCR	C8-C7-C6	-2.55	120.05	127.20
30	b	601	SQD	O48-C23-C24	2.55	119.90	111.91
23	c	502	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
29	A	415	LHG	O8-C23-C24	2.54	119.89	111.91
28	B	627	DGD	O6D-C1D-O3G	2.54	116.00	109.97
23	b	614	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
30	B	626	SQD	O48-C23-C24	2.54	119.88	111.91
28	c	518	DGD	O5D-C1E-C2E	2.54	112.27	108.30
27	T	102	BCR	C23-C24-C25	-2.54	120.08	127.20
27	d	405	BCR	C3-C4-C5	-2.54	109.55	114.08
23	A	403	CLA	CMB-C2B-C3B	2.53	129.42	124.68
23	C	508	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	B	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	c	509	CLA	C1-C2-C3	-2.53	121.67	126.04
27	h	101	BCR	C15-C16-C17	-2.53	118.29	123.47
23	D	401	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
27	J	102	BCR	C37-C22-C21	-2.53	119.38	122.92
23	b	609	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
27	d	405	BCR	C23-C24-C25	-2.53	120.10	127.20
28	c	517	DGD	O1G-C1A-C2A	2.53	119.84	111.91
33	b	626	LMT	C1B-O1B-C4'	-2.53	111.71	117.96
27	B	617	BCR	C3-C4-C5	-2.53	109.57	114.08
23	B	611	CLA	CHB-C4A-NA	2.53	128.00	124.51
23	C	510	CLA	CHD-C1D-ND	-2.52	122.14	124.45
23	D	403	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
23	B	614	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
28	A	411	DGD	C3D-C4D-C5D	2.52	114.73	110.24
23	C	511	CLA	CMB-C2B-C3B	2.52	129.39	124.68
31	a	402	LMG	C1-O6-C5	-2.52	108.75	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	CHB-C4A-NA	2.52	127.99	124.51
31	e	101	LMG	O7-C10-C11	2.52	116.92	111.50
28	c	518	DGD	O3D-C3D-C4D	2.52	116.16	110.35
27	D	405	BCR	C21-C20-C19	-2.51	115.37	123.22
28	a	413	DGD	C3D-C4D-C5D	2.51	114.72	110.24
23	c	501	CLA	CHB-C4A-NA	2.51	127.99	124.51
28	C	517	DGD	O3D-C3D-C4D	2.51	116.16	110.35
27	h	101	BCR	C8-C7-C6	-2.51	120.15	127.20
23	B	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	b	612	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	B	611	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	a	409	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
27	D	405	BCR	C29-C30-C25	2.51	114.34	110.48
23	c	501	CLA	CMB-C2B-C3B	2.51	129.37	124.68
23	C	501	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	b	618	CLA	CHB-C4A-NA	2.51	127.98	124.51
28	a	413	DGD	O1G-C1A-C2A	2.50	119.76	111.91
31	M	101	LMG	O8-C28-C29	2.49	119.73	111.91
25	a	410	PL9	C12-C13-C14	-2.49	121.66	127.66
23	b	615	CLA	CMB-C2B-C3B	2.49	129.34	124.68
27	j	102	BCR	C35-C13-C14	-2.49	119.43	122.92
23	a	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
27	T	102	BCR	C15-C14-C13	-2.49	123.75	127.31
28	b	602	DGD	O4D-C4D-C5D	-2.49	103.11	109.30
28	b	602	DGD	O6D-C1D-O3G	2.49	115.87	109.97
28	B	621	DGD	O2G-C1B-C2B	2.49	116.86	111.50
23	b	608	CLA	CMB-C2B-C3B	2.49	129.33	124.68
28	b	623	DGD	C3G-O3G-C1D	2.48	118.59	113.74
23	A	407	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	a	412	BCR	C34-C9-C8	2.48	121.99	118.08
28	B	621	DGD	O1G-C1A-C2A	2.48	119.69	111.91
23	C	513	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
25	A	408	PL9	C7-C3-C2	-2.48	120.04	123.30
27	C	516	BCR	C38-C26-C27	2.47	118.36	113.62
23	B	611	CLA	C1-C2-C3	-2.47	121.77	126.04
27	D	405	BCR	C27-C26-C25	-2.47	119.15	122.73
23	a	404	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	A	405	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
23	B	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	h	101	BCR	C34-C9-C8	2.46	121.95	118.08
31	b	625	LMG	C6-C5-C4	-2.46	107.25	113.00
23	b	605	CLA	C1-C2-C3	-2.45	121.80	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	C	516	BCR	C15-C16-C17	-2.45	118.45	123.47
27	H	101	BCR	C3-C4-C5	-2.45	109.70	114.08
27	T	102	BCR	C15-C16-C17	-2.45	118.46	123.47
28	a	413	DGD	O4D-C4D-C5D	-2.45	103.22	109.30
23	c	505	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
27	H	101	BCR	C35-C13-C12	2.45	121.93	118.08
23	c	502	CLA	C1-C2-C3	-2.45	121.81	126.04
23	D	401	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
27	a	412	BCR	C20-C21-C22	-2.44	123.82	127.31
23	c	510	CLA	CHB-C4A-NA	2.44	127.89	124.51
31	k	103	LMG	C7-O1-C1	2.44	118.51	113.74
25	d	404	PL9	C40-C39-C41	2.44	119.38	115.27
28	a	413	DGD	C6E-C5E-C4E	-2.44	107.29	113.00
23	D	403	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
28	C	519	DGD	O2G-C1B-C2B	2.44	116.76	111.50
23	c	506	CLA	C1-C2-C3	-2.44	121.83	126.04
28	B	627	DGD	O1G-C1A-C2A	2.44	119.55	111.91
23	B	605	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	B	607	CLA	CHD-C1D-ND	-2.44	122.22	124.45
25	A	408	PL9	C20-C19-C21	2.43	119.37	115.27
25	j	101	PL9	C22-C23-C24	-2.43	121.80	127.66
23	c	509	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	B	613	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	B	608	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	A	407	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	c	504	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
27	B	619	BCR	C37-C22-C21	-2.43	119.52	122.92
33	d	410	LMT	C1B-O1B-C4'	-2.42	111.96	117.96
23	b	613	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	c	511	CLA	CMB-C2B-C3B	2.42	129.21	124.68
27	c	515	BCR	C38-C26-C27	2.42	118.27	113.62
27	B	619	BCR	C15-C16-C17	-2.42	118.52	123.47
25	d	404	PL9	C20-C19-C21	2.42	119.34	115.27
30	a	401	SQD	O48-C23-C24	2.42	119.50	111.91
30	a	415	SQD	O48-C23-C24	2.42	119.50	111.91
27	j	102	BCR	C1-C6-C5	-2.42	119.21	122.61
27	j	102	BCR	C39-C30-C25	-2.42	106.38	110.30
29	a	417	LHG	O8-C23-C24	2.42	119.49	111.91
23	C	512	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
27	c	514	BCR	C24-C23-C22	-2.41	122.59	126.23
25	D	404	PL9	C15-C14-C16	2.41	119.32	115.27
27	B	618	BCR	C23-C24-C25	-2.41	120.44	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
27	a	412	BCR	C23-C24-C25	-2.41	120.44	127.20
23	C	502	CLA	C1-C2-C3	-2.40	121.88	126.04
23	d	403	CLA	CHB-C4A-NA	2.40	127.84	124.51
27	h	101	BCR	C3-C4-C5	-2.40	109.79	114.08
27	z	101	BCR	C11-C10-C9	-2.40	123.88	127.31
30	A	413	SQD	C44-O6-C1	2.40	118.43	113.74
27	b	622	BCR	C38-C26-C27	2.40	118.22	113.62
23	c	509	CLA	CHD-C1D-ND	-2.40	122.25	124.45
23	a	406	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	c	507	CLA	C1-C2-C3	-2.40	121.90	126.04
27	z	101	BCR	C23-C24-C25	-2.40	120.47	127.20
23	c	511	CLA	CHD-C1D-ND	-2.40	122.25	124.45
31	D	407	LMG	O8-C28-O10	-2.40	117.55	123.59
23	d	403	CLA	CMB-C2B-C3B	2.40	129.16	124.68
28	d	409	DGD	O3D-C3D-C4D	2.39	115.88	110.35
31	e	101	LMG	O1-C1-C2	2.39	112.04	108.30
23	C	509	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	b	617	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	a	405	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
23	b	615	CLA	C1-C2-C3	-2.39	121.91	126.04
23	d	403	CLA	O2D-CGD-CBD	2.39	115.52	111.27
28	C	517	DGD	O1G-C1A-C2A	2.39	119.41	111.91
23	b	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	c	503	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	d	404	PL9	C51-C49-C50	2.39	119.88	114.60
27	z	101	BCR	C28-C27-C26	-2.39	109.81	114.08
27	T	101	BCR	C3-C4-C5	-2.39	109.81	114.08
23	a	404	CLA	CHD-C1D-ND	-2.39	122.26	124.45
23	C	513	CLA	C1-C2-C3	-2.39	121.91	126.04
23	a	405	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
27	B	617	BCR	C36-C18-C17	-2.39	119.58	122.92
23	d	402	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
23	b	618	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
23	a	409	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
33	b	603	LMT	O1B-C4'-C3'	2.38	113.62	107.28
31	b	625	LMG	C1-O6-C5	-2.38	109.02	113.69
23	B	606	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	b	607	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
27	B	617	BCR	C23-C24-C25	-2.38	120.53	127.20
24	D	402	PHO	CMB-C2B-C3B	2.38	129.12	124.68
27	j	102	BCR	C37-C22-C21	-2.38	119.60	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	j	101	PL9	C12-C13-C14	-2.37	121.94	127.66
23	b	606	CLA	C1-C2-C3	-2.37	121.94	126.04
27	d	405	BCR	C33-C5-C4	2.37	118.18	113.62
31	m	102	LMG	O4-C4-C3	-2.37	104.86	110.35
28	A	411	DGD	O1G-C1A-C2A	2.37	119.36	111.91
30	F	102	SQD	O5-C1-C2	2.37	115.37	110.35
23	b	605	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	D	408	SQD	O48-C23-C24	2.37	119.35	111.91
23	C	513	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
30	B	626	SQD	O47-C7-C8	2.37	116.60	111.50
23	b	613	CLA	C1-C2-C3	-2.36	121.95	126.04
28	d	409	DGD	O2G-C1B-C2B	2.36	116.60	111.50
23	b	615	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	C	505	CLA	CMB-C2B-C3B	2.36	129.09	124.68
27	D	405	BCR	C34-C9-C10	-2.36	119.62	122.92
27	d	405	BCR	C21-C20-C19	-2.36	115.86	123.22
23	D	403	CLA	CHB-C4A-NA	2.36	127.77	124.51
23	A	405	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	B	619	BCR	C2-C1-C6	2.36	114.11	110.48
23	C	501	CLA	CHD-C1D-ND	-2.35	122.29	124.45
28	d	409	DGD	O5D-C6D-C5D	2.35	113.40	109.05
23	B	604	CLA	CMB-C2B-C3B	2.35	129.08	124.68
23	B	603	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
25	J	101	PL9	C12-C13-C14	-2.35	122.00	127.66
23	B	604	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	C	518	DGD	C1D-O6D-C5D	-2.35	109.07	113.69
27	B	618	BCR	C15-C14-C13	-2.35	123.96	127.31
23	C	505	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
25	a	410	PL9	C20-C19-C21	2.35	119.22	115.27
23	C	509	CLA	C1-C2-C3	-2.35	121.98	126.04
23	C	505	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	B	602	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
28	c	517	DGD	C1D-O6D-C5D	-2.35	109.08	113.69
23	b	616	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
23	b	617	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
27	B	620	BCR	C38-C26-C27	2.35	118.12	113.62
28	a	413	DGD	C4D-C3D-C2D	-2.35	106.73	110.82
27	T	102	BCR	C16-C17-C18	-2.34	123.96	127.31
27	h	101	BCR	C35-C13-C12	2.34	121.77	118.08
31	A	418	LMG	O8-C28-O10	-2.34	117.69	123.59
23	c	508	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	c	512	CLA	O2A-CGA-O1A	-2.34	117.69	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	c	513	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
27	d	405	BCR	C27-C26-C25	-2.33	119.34	122.73
23	c	501	CLA	C1-C2-C3	-2.33	122.01	126.04
27	y	101	BCR	C11-C10-C9	-2.33	123.98	127.31
27	k	102	BCR	C33-C5-C4	2.33	118.10	113.62
28	c	517	DGD	O6E-C1E-C2E	2.33	115.28	110.35
31	i	101	LMG	C3-C4-C5	2.33	114.40	110.24
23	C	510	CLA	C2D-C1D-ND	-2.33	108.39	110.10
25	j	101	PL9	C15-C14-C16	2.33	119.19	115.27
23	B	610	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
27	J	102	BCR	C11-C12-C13	-2.33	119.87	126.42
25	J	101	PL9	C15-C14-C16	2.33	119.19	115.27
31	b	624	LMG	C4-C3-C2	2.33	114.89	110.82
27	c	515	BCR	C23-C24-C25	-2.33	120.66	127.20
23	A	407	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
31	e	101	LMG	C1-O6-C5	-2.33	109.12	113.69
25	a	410	PL9	C7-C8-C9	-2.32	122.92	126.79
23	a	405	CLA	CHD-C1D-ND	-2.32	122.32	124.45
31	e	101	LMG	C6-C5-C4	-2.32	107.56	113.00
27	j	102	BCR	C34-C9-C10	-2.32	119.67	122.92
30	d	408	SQD	O48-C23-C24	2.32	119.19	111.91
24	a	407	PHO	CMC-C2C-C3C	2.32	129.32	124.94
31	B	622	LMG	C4-C3-C2	2.32	114.87	110.82
25	a	410	PL9	C32-C33-C34	-2.32	122.08	127.66
23	b	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
28	b	623	DGD	O1G-C1A-C2A	2.31	119.17	111.91
23	A	405	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
24	D	402	PHO	CMC-C2C-C3C	2.31	129.30	124.94
31	A	418	LMG	C1-O6-C5	-2.31	109.15	113.69
25	A	408	PL9	C12-C13-C14	-2.31	122.09	127.66
31	e	101	LMG	O7-C10-O9	-2.31	118.12	123.70
27	T	102	BCR	C24-C23-C22	-2.31	122.75	126.23
25	a	410	PL9	C17-C18-C19	-2.31	122.10	127.66
27	B	618	BCR	C35-C13-C12	2.31	121.71	118.08
27	B	618	BCR	C34-C9-C10	-2.31	119.69	122.92
25	D	404	PL9	C32-C33-C34	-2.30	122.11	127.66
23	C	513	CLA	CHD-C1D-ND	-2.30	122.34	124.45
27	D	405	BCR	C38-C26-C25	-2.30	121.94	124.53
34	V	201	HEM	C1B-NB-C4B	2.30	107.45	105.07
25	d	404	PL9	C36-C34-C33	-2.30	116.47	121.12
23	B	615	CLA	CHD-C1D-ND	-2.30	122.34	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	O2D-CGD-CBD	2.29	115.35	111.27
23	B	603	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
25	D	404	PL9	C7-C3-C2	-2.29	120.28	123.30
24	D	402	PHO	O2D-CGD-O1D	-2.29	119.35	123.84
23	b	605	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	D	402	PHO	O2A-CGA-O1A	-2.29	117.81	123.59
27	B	618	BCR	C16-C17-C18	-2.29	124.04	127.31
23	C	510	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
28	c	518	DGD	O2G-C1B-C2B	2.29	116.44	111.50
31	k	103	LMG	O8-C28-O10	-2.29	117.81	123.59
23	b	612	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	C	508	CLA	CHD-C1D-ND	-2.29	122.35	124.45
31	e	101	LMG	C8-O7-C10	2.29	123.43	117.79
28	a	413	DGD	O3D-C3D-C4D	2.29	115.65	110.35
23	B	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
27	C	515	BCR	C23-C24-C25	-2.29	120.77	127.20
25	d	404	PL9	C53-C6-C1	2.29	119.67	114.99
31	a	416	LMG	O6-C5-C6	2.29	112.12	106.44
23	C	509	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
27	c	514	BCR	C33-C5-C4	2.28	118.00	113.62
28	A	411	DGD	O3D-C3D-C4D	2.28	115.63	110.35
28	c	516	DGD	C6E-C5E-C4E	-2.28	107.66	113.00
23	C	503	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
31	E	101	LMG	O9-C10-C11	-2.28	114.83	123.73
25	A	408	PL9	C26-C24-C23	-2.28	116.50	121.12
23	C	508	CLA	C1-C2-C3	-2.28	122.10	126.04
28	c	517	DGD	O4D-C4D-C5D	-2.28	103.64	109.30
28	c	516	DGD	O1G-C1A-C2A	2.28	119.06	111.91
28	d	409	DGD	C2G-O2G-C1B	2.28	123.40	117.79
23	B	605	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
31	c	519	LMG	C3-C4-C5	2.28	114.30	110.24
23	b	614	CLA	CHD-C1D-ND	-2.28	122.36	124.45
30	A	413	SQD	O48-C23-C24	2.28	119.05	111.91
31	c	519	LMG	C6-C5-C4	-2.28	107.67	113.00
23	A	404	CLA	CHD-C1D-ND	-2.28	122.36	124.45
23	B	601	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
23	b	620	CLA	CHD-C1D-ND	-2.27	122.36	124.45
31	I	101	LMG	C6-C5-C4	-2.27	107.68	113.00
30	B	626	SQD	C10-C9-C8	-2.27	105.02	113.19
31	b	624	LMG	C1-O6-C5	-2.27	109.23	113.69
27	b	621	BCR	C27-C26-C25	-2.27	119.43	122.73
31	i	101	LMG	O8-C28-O10	-2.27	117.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C	519	DGD	O1G-C1A-O1A	-2.27	117.87	123.59
23	c	507	CLA	CHB-C4A-NA	2.27	127.65	124.51
34	F	101	HEM	CHB-C1B-NB	2.27	127.18	124.38
23	C	502	CLA	CHB-C4A-NA	2.27	127.64	124.51
23	b	612	CLA	C1-C2-C3	-2.27	122.12	126.04
25	D	404	PL9	C51-C49-C50	2.26	119.60	114.60
31	C	521	LMG	C3-C4-C5	2.26	114.28	110.24
25	A	408	PL9	C30-C29-C31	2.26	119.08	115.27
23	C	501	CLA	CMB-C2B-C3B	2.26	128.91	124.68
23	C	511	CLA	C1-C2-C3	-2.26	122.13	126.04
30	b	601	SQD	C10-C9-C8	-2.26	105.06	113.19
23	B	606	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	d	402	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
27	T	101	BCR	C23-C24-C25	-2.26	120.86	127.20
23	b	607	CLA	O2D-CGD-CBD	2.26	115.28	111.27
25	d	404	PL9	C15-C14-C16	2.26	119.07	115.27
28	d	409	DGD	O2G-C1B-O1B	-2.26	118.25	123.70
31	A	418	LMG	O1-C1-C2	2.26	111.83	108.30
23	B	608	CLA	CHD-C1D-ND	-2.26	122.38	124.45
27	C	514	BCR	C33-C5-C4	2.26	117.95	113.62
28	B	627	DGD	C1E-C2E-C3E	2.25	114.69	110.00
27	C	515	BCR	C38-C26-C25	-2.25	122.00	124.53
23	C	511	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
28	B	627	DGD	C4D-C3D-C2D	-2.25	106.89	110.82
31	a	402	LMG	O3-C3-C4	-2.25	105.14	110.35
23	c	511	CLA	CHB-C4A-NA	2.25	127.62	124.51
28	A	411	DGD	C6E-C5E-C4E	-2.25	107.73	113.00
27	k	102	BCR	C38-C26-C27	2.25	117.94	113.62
23	B	615	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	B	612	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
34	v	201	HEM	CHC-C4B-NB	2.24	126.87	124.43
28	A	411	DGD	C6D-C5D-C4D	-2.24	107.41	112.09
30	f	102	SQD	O48-C23-C24	2.24	118.95	111.91
31	B	623	LMG	C3-C4-C5	2.24	114.24	110.24
23	b	610	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
27	j	102	BCR	C15-C16-C17	-2.24	118.89	123.47
28	B	627	DGD	C6D-C5D-C4D	-2.24	107.42	112.09
23	A	403	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
27	z	101	BCR	C38-C26-C25	-2.24	122.02	124.53
27	C	515	BCR	C33-C5-C4	2.24	117.92	113.62
27	H	101	BCR	C7-C8-C9	-2.24	122.86	126.23
31	E	101	LMG	O1-C1-C2	2.23	111.79	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	j	101	PL9	C20-C19-C21	2.23	119.03	115.27
23	b	605	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	B	613	CLA	CHD-C1D-ND	-2.23	122.41	124.45
23	c	508	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
23	b	613	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
25	A	408	PL9	C11-C9-C8	-2.22	116.62	121.12
23	c	512	CLA	CHD-C1D-ND	-2.22	122.41	124.45
30	a	415	SQD	O6-C1-C2	2.22	111.77	108.30
23	d	403	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	c	507	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
30	A	417	SQD	O48-C23-C24	2.22	118.87	111.91
34	f	101	HEM	CHC-C4B-C3B	2.22	127.97	124.57
23	A	403	CLA	CHB-C4A-NA	2.22	127.58	124.51
27	b	621	BCR	C38-C26-C27	2.22	117.87	113.62
27	D	405	BCR	C33-C5-C4	2.21	117.87	113.62
23	b	610	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
31	C	520	LMG	O8-C28-O10	-2.21	118.01	123.59
28	c	516	DGD	O3D-C3D-C4D	2.21	115.46	110.35
27	c	515	BCR	C15-C16-C17	-2.21	118.94	123.47
31	B	623	LMG	O8-C28-O10	-2.21	118.02	123.59
23	b	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
23	B	604	CLA	C1-C2-C3	-2.21	122.22	126.04
23	b	619	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
27	C	516	BCR	C21-C20-C19	-2.21	116.33	123.22
25	d	404	PL9	C42-C43-C44	-2.21	122.35	127.66
23	c	501	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
31	b	624	LMG	O4-C4-C3	-2.21	105.25	110.35
27	k	102	BCR	C35-C13-C12	2.21	121.55	118.08
23	C	504	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
27	C	515	BCR	C10-C11-C12	-2.20	116.34	123.22
31	d	406	LMG	C6-C5-C4	-2.20	107.84	113.00
27	y	101	BCR	C35-C13-C12	2.20	121.55	118.08
23	C	508	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
27	C	516	BCR	C23-C24-C25	-2.20	121.02	127.20
23	C	511	CLA	CHD-C1D-ND	-2.20	122.43	124.45
28	C	517	DGD	C3G-O3G-C1D	2.20	118.04	113.74
27	h	101	BCR	C36-C18-C19	2.20	121.54	118.08
31	I	101	LMG	C3-C4-C5	2.20	114.16	110.24
23	B	614	CLA	CHB-C4A-NA	2.20	127.55	124.51
31	E	101	LMG	O7-C10-O9	-2.20	118.39	123.70
23	b	613	CLA	CHB-C4A-NA	2.20	127.55	124.51
25	j	101	PL9	C10-C9-C11	2.20	118.97	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
23	C	501	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
30	F	102	SQD	O48-C23-C24	2.19	118.79	111.91
23	c	503	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
23	c	509	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
27	B	618	BCR	C15-C16-C17	-2.19	118.98	123.47
23	B	604	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	B	603	CLA	CHD-C1D-ND	-2.19	122.44	124.45
23	c	501	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
27	B	618	BCR	C31-C1-C6	-2.19	106.75	110.30
28	c	518	DGD	O3G-C1D-C2D	2.18	111.71	108.30
23	c	509	CLA	CMB-C2B-C3B	2.18	128.76	124.68
27	b	621	BCR	C35-C13-C14	-2.18	119.86	122.92
27	b	622	BCR	C28-C27-C26	-2.18	110.18	114.08
23	d	402	CLA	O1D-CGD-CBD	2.18	128.94	124.48
27	b	621	BCR	C33-C5-C4	2.18	117.80	113.62
23	D	401	CLA	O1D-CGD-CBD	2.18	128.94	124.48
23	C	501	CLA	C1-C2-C3	-2.18	122.28	126.04
23	B	605	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	B	613	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
25	A	408	PL9	C32-C33-C34	-2.17	122.43	127.66
27	c	514	BCR	C12-C13-C14	2.17	122.28	118.94
23	b	616	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
27	B	619	BCR	C7-C8-C9	-2.17	122.95	126.23
31	b	625	LMG	O3-C3-C4	-2.17	105.33	110.35
23	c	508	CLA	C1-C2-C3	-2.17	122.29	126.04
27	H	101	BCR	C16-C15-C14	-2.17	119.03	123.47
28	c	516	DGD	C1G-O1G-C1A	2.17	125.15	117.12
23	b	620	CLA	CHB-C4A-NA	2.17	127.51	124.51
27	j	102	BCR	C11-C12-C13	-2.17	120.33	126.42
30	A	417	SQD	O8-S-C6	2.16	109.19	105.74
28	c	518	DGD	C6E-C5E-C4E	-2.16	107.94	113.00
27	C	516	BCR	C33-C5-C4	2.16	117.77	113.62
27	h	101	BCR	C33-C5-C4	2.16	117.77	113.62
27	D	405	BCR	C16-C15-C14	-2.16	119.05	123.47
23	c	512	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
30	B	626	SQD	C1-O5-C5	2.16	117.92	113.69
23	b	611	CLA	CHD-C1D-ND	-2.16	122.47	124.45
25	D	404	PL9	C53-C6-C1	2.16	119.40	114.99
30	B	626	SQD	O8-S-C6	2.16	109.17	105.74
23	C	509	CLA	O2D-CGD-O1D	-2.15	119.62	123.84
27	c	514	BCR	C29-C30-C25	2.15	113.80	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	f	102	SQD	O5-C1-C2	2.15	114.90	110.35
28	D	409	DGD	C6D-O5D-C1E	-2.15	109.54	113.74
25	a	410	PL9	C53-C6-C1	2.15	119.39	114.99
31	b	624	LMG	C3-C4-C5	2.15	114.08	110.24
23	B	609	CLA	C1-C2-C3	-2.15	122.32	126.04
23	B	610	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
27	C	514	BCR	C29-C30-C25	2.15	113.79	110.48
27	A	410	BCR	C23-C24-C25	-2.15	121.17	127.20
23	B	616	CLA	CHB-C4A-NA	2.15	127.48	124.51
23	D	403	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
31	e	101	LMG	O9-C10-C11	-2.14	115.37	123.73
30	A	417	SQD	O2-C2-C3	-2.14	105.39	110.35
25	A	408	PL9	C53-C6-C1	2.14	119.37	114.99
27	H	101	BCR	C36-C18-C19	2.14	121.45	118.08
31	b	625	LMG	O8-C28-O10	-2.14	118.19	123.59
23	b	620	CLA	CMB-C2B-C3B	2.14	128.68	124.68
28	D	409	DGD	O2G-C1B-O1B	-2.14	118.54	123.70
23	A	403	CLA	C1-C2-C3	-2.14	122.35	126.04
23	B	612	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
27	y	101	BCR	C32-C1-C6	-2.13	106.85	110.30
27	b	621	BCR	C37-C22-C21	-2.13	119.94	122.92
27	k	102	BCR	C23-C24-C25	-2.13	121.23	127.20
27	B	617	BCR	C36-C18-C19	2.13	121.43	118.08
23	d	402	CLA	CHB-C4A-NA	2.12	127.45	124.51
25	d	404	PL9	C10-C9-C11	2.12	118.84	115.27
23	c	511	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	b	617	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	A	404	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	c	507	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
23	b	609	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	A	403	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
27	c	515	BCR	C21-C20-C19	-2.12	116.61	123.22
23	C	501	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	B	615	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
23	c	505	CLA	CBA-CAA-C2A	2.11	120.10	113.86
28	c	518	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
23	B	608	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
31	B	622	LMG	O4-C4-C3	-2.11	105.47	110.35
25	J	101	PL9	C22-C23-C24	-2.11	122.57	127.66
31	k	103	LMG	C3-C4-C5	2.11	114.00	110.24
28	C	517	DGD	O2G-C1B-O1B	-2.11	118.60	123.70
23	C	505	CLA	CBA-CAA-C2A	2.11	120.09	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	O1D-CGD-CBD	2.11	128.80	124.48
25	A	408	PL9	C15-C14-C16	2.11	118.82	115.27
25	A	408	PL9	C10-C9-C11	2.11	118.81	115.27
25	D	404	PL9	C20-C19-C21	2.11	118.81	115.27
31	C	521	LMG	C6-C5-C4	-2.11	108.07	113.00
23	c	507	CLA	CHD-C1D-ND	-2.11	122.52	124.45
27	H	101	BCR	C15-C16-C17	-2.10	119.16	123.47
30	b	601	SQD	C1-O5-C5	2.10	117.82	113.69
31	E	101	LMG	C1-O6-C5	-2.10	109.56	113.69
24	a	407	PHO	O2A-CGA-O1A	-2.10	118.28	123.59
27	C	514	BCR	C34-C9-C8	2.10	121.39	118.08
27	b	621	BCR	C15-C16-C17	-2.10	119.17	123.47
28	D	409	DGD	O2G-C1B-C2B	2.10	116.03	111.50
31	b	625	LMG	O6-C5-C4	2.10	113.51	109.69
27	B	619	BCR	C27-C26-C25	-2.10	119.68	122.73
23	a	404	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
23	c	505	CLA	CHD-C1D-ND	-2.10	122.52	124.45
29	a	414	LHG	O8-C23-C24	2.10	118.49	111.91
31	I	101	LMG	C8-O7-C10	2.10	122.95	117.79
27	j	102	BCR	C36-C18-C17	-2.10	119.99	122.92
27	B	620	BCR	C35-C13-C14	-2.09	119.99	122.92
27	c	514	BCR	C23-C24-C25	-2.09	121.32	127.20
23	B	607	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
28	a	413	DGD	O6D-C1D-O3G	2.09	114.93	109.97
23	c	501	CLA	CHD-C1D-ND	-2.09	122.53	124.45
25	a	410	PL9	C15-C14-C16	2.09	118.78	115.27
25	D	404	PL9	C27-C28-C29	-2.09	122.64	127.66
23	C	511	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
23	c	505	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
23	b	617	CLA	C1-C2-C3	-2.08	122.44	126.04
23	b	608	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	C	510	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	b	612	CLA	C2D-C1D-ND	-2.08	108.57	110.10
30	A	413	SQD	O5-C1-C2	2.08	114.76	110.35
31	B	623	LMG	O3-C3-C4	-2.08	105.53	110.35
28	B	621	DGD	C4D-C3D-C2D	-2.08	107.19	110.82
27	J	102	BCR	C34-C9-C10	-2.08	120.01	122.92
31	B	623	LMG	O6-C5-C4	2.08	113.47	109.69
27	J	102	BCR	C30-C25-C26	-2.08	119.69	122.61
27	B	618	BCR	C24-C23-C22	-2.07	123.10	126.23
27	b	621	BCR	C2-C1-C6	2.07	113.67	110.48
27	k	102	BCR	C32-C1-C6	-2.07	106.94	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	z	101	BCR	C15-C16-C17	-2.07	119.23	123.47
23	d	403	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	a	410	PL9	C10-C9-C11	2.07	118.75	115.27
27	C	514	BCR	C2-C3-C4	-2.06	106.76	111.38
25	d	404	PL9	C17-C18-C19	-2.06	122.69	127.66
23	a	406	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
28	D	409	DGD	C1D-O6D-C5D	-2.06	109.64	113.69
27	C	516	BCR	C2-C1-C6	2.06	113.65	110.48
23	c	502	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	b	608	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
31	k	103	LMG	C6-C5-C4	-2.06	108.18	113.00
31	m	102	LMG	O8-C9-C8	-2.06	102.44	108.43
27	z	101	BCR	C33-C5-C4	2.06	117.57	113.62
29	A	412	LHG	O8-C23-C24	2.06	118.36	111.91
31	c	519	LMG	C7-O1-C1	2.06	117.75	113.74
25	D	404	PL9	C30-C29-C31	2.05	118.73	115.27
27	B	617	BCR	C8-C7-C6	-2.05	121.44	127.20
31	D	406	LMG	C1-O6-C5	-2.05	109.66	113.69
31	d	407	LMG	O8-C28-O10	-2.05	118.41	123.59
23	a	405	CLA	C16-C15-C13	-2.05	109.28	115.92
31	A	414	LMG	O8-C28-O10	-2.05	118.42	123.59
27	b	622	BCR	C23-C24-C25	-2.05	121.44	127.20
23	c	511	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
27	B	620	BCR	C32-C1-C6	-2.05	106.97	110.30
27	C	515	BCR	C36-C18-C19	2.05	121.31	118.08
27	k	102	BCR	C11-C10-C9	-2.05	124.39	127.31
23	c	508	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	d	404	PL9	C47-C48-C49	-2.05	120.75	127.75
27	c	515	BCR	C35-C13-C14	-2.05	120.06	122.92
27	a	412	BCR	C38-C26-C27	2.05	117.55	113.62
27	b	622	BCR	C20-C19-C18	-2.05	120.67	126.42
25	A	408	PL9	C41-C39-C40	2.04	119.12	114.60
27	C	514	BCR	C23-C24-C25	-2.04	121.47	127.20
27	J	102	BCR	C15-C16-C17	-2.04	119.30	123.47
23	D	401	CLA	CHB-C4A-NA	2.04	127.33	124.51
31	A	418	LMG	O3-C3-C4	-2.04	105.64	110.35
23	B	611	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	D	404	PL9	C10-C9-C11	2.03	118.69	115.27
25	D	404	PL9	C36-C34-C33	-2.03	117.00	121.12
27	H	101	BCR	C21-C20-C19	-2.03	116.87	123.22
23	c	503	CLA	O2D-CGD-CBD	2.03	114.88	111.27
27	k	102	BCR	C28-C27-C26	-2.03	110.45	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	T	101	BCR	C36-C18-C17	-2.03	120.08	122.92
27	b	622	BCR	C21-C20-C19	-2.03	116.87	123.22
27	c	515	BCR	C33-C5-C4	2.03	117.52	113.62
25	J	101	PL9	C10-C9-C11	2.03	118.69	115.27
31	C	521	LMG	O8-C28-O10	-2.03	118.46	123.59
27	y	101	BCR	C36-C18-C17	-2.03	120.08	122.92
30	f	102	SQD	O6-C1-C2	2.03	111.47	108.30
23	B	607	CLA	O2D-CGD-CBD	2.03	114.88	111.27
31	M	101	LMG	O3-C3-C4	-2.03	105.66	110.35
28	d	409	DGD	O1G-C1A-O1A	-2.03	118.47	123.59
27	c	515	BCR	C2-C1-C6	2.03	113.60	110.48
28	c	518	DGD	O6D-C1D-O3G	2.03	114.77	109.97
23	C	506	CLA	CAA-CBA-CGA	-2.03	107.33	113.25
34	V	201	HEM	C4B-CHC-C1C	2.02	125.23	122.56
31	b	625	LMG	C3-C4-C5	2.02	113.85	110.24
27	z	101	BCR	C35-C13-C14	-2.02	120.09	122.92
28	C	519	DGD	O3D-C3D-C4D	2.02	115.03	110.35
27	B	619	BCR	C33-C5-C4	2.02	117.50	113.62
25	a	410	PL9	C27-C28-C29	-2.02	122.79	127.66
27	C	514	BCR	C39-C30-C25	-2.02	107.02	110.30
27	z	101	BCR	C36-C18-C17	-2.02	120.09	122.92
27	J	102	BCR	C39-C30-C25	-2.02	107.02	110.30
23	C	504	CLA	C3A-C2A-C1A	2.02	104.36	101.34
27	T	101	BCR	C8-C7-C6	-2.02	121.53	127.20
23	B	602	CLA	C1-C2-C3	-2.02	122.55	126.04
23	b	607	CLA	C1-C2-C3	-2.02	122.55	126.04
27	B	620	BCR	C28-C27-C26	-2.02	110.48	114.08
23	B	610	CLA	C2D-C1D-ND	-2.02	108.62	110.10
23	D	403	CLA	C1-C2-C3	-2.02	122.56	126.04
27	B	618	BCR	C35-C13-C14	-2.02	120.10	122.92
27	b	622	BCR	C31-C1-C6	-2.01	107.03	110.30
27	T	101	BCR	C28-C27-C26	-2.01	110.48	114.08
27	c	514	BCR	C34-C9-C8	2.01	121.25	118.08
34	v	201	HEM	C3B-C2B-C1B	2.01	107.98	106.49
28	d	409	DGD	C6D-O5D-C1E	-2.01	109.81	113.74
23	b	620	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
23	b	607	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	c	504	CLA	CHD-C1D-ND	-2.01	122.61	124.45
23	B	607	CLA	C1-C2-C3	-2.01	122.57	126.04
23	c	506	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
31	C	521	LMG	O3-C3-C4	-2.01	105.70	110.35
25	a	410	PL9	C26-C24-C23	-2.01	117.05	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	409	CLA	C1-C2-C3	-2.01	122.57	126.04
23	B	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
27	b	621	BCR	C31-C1-C6	-2.01	107.05	110.30
33	B	625	LMT	C1B-O1B-C4'	-2.01	113.00	117.96
31	B	623	LMG	C7-O1-C1	2.00	117.65	113.74
24	a	407	PHO	CMB-C2B-C3B	2.00	128.43	124.68
34	f	101	HEM	CHB-C1B-NB	2.00	126.86	124.38
27	A	410	BCR	C33-C5-C4	2.00	117.46	113.62
31	C	520	LMG	C3-C4-C5	2.00	113.81	110.24

All (70) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	ND
23	A	404	CLA	ND
23	A	405	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	608	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	501	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	D	401	CLA	ND
23	D	403	CLA	ND
23	a	404	CLA	ND
23	a	405	CLA	ND
23	a	406	CLA	ND
23	a	409	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	608	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	b	617	CLA	ND
23	b	618	CLA	ND
23	b	619	CLA	ND
23	b	620	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402	CLA	ND
23	d	403	CLA	ND

All (2130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404	CLA	C1A-C2A-CAA-CBA
23	A	404	CLA	CHA-CBD-CGD-O1D
23	A	404	CLA	CHA-CBD-CGD-O2D
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C1A-C2A-CAA-CBA
23	B	602	CLA	C3A-C2A-CAA-CBA
23	B	602	CLA	C2-C3-C5-C6
23	B	602	CLA	C4-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	B	603	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
23	B	604	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C1A-C2A-CAA-CBA
23	B	606	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C1A-C2A-CAA-CBA
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	C3A-C2A-CAA-CBA
23	B	616	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	C	505	CLA	C1A-C2A-CAA-CBA
23	C	505	CLA	C3A-C2A-CAA-CBA
23	C	505	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	C6-C7-C8-C9
23	C	512	CLA	C1A-C2A-CAA-CBA
23	D	401	CLA	C2-C3-C5-C6
23	D	401	CLA	C4-C3-C5-C6
23	a	405	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	CHA-CBD-CGD-O1D
23	a	405	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	CBD-CGD-O2D-CED
23	b	606	CLA	C1A-C2A-CAA-CBA
23	b	606	CLA	C3A-C2A-CAA-CBA
23	b	606	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C4-C3-C5-C6
23	b	606	CLA	C6-C7-C8-C9
23	b	607	CLA	C2-C3-C5-C6
23	b	607	CLA	C4-C3-C5-C6
23	b	608	CLA	CBD-CGD-O2D-CED
23	b	609	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C1A-C2A-CAA-CBA
23	b	610	CLA	C3A-C2A-CAA-CBA
23	b	611	CLA	C1A-C2A-CAA-CBA
23	b	611	CLA	C3A-C2A-CAA-CBA
23	b	611	CLA	CBD-CGD-O2D-CED
23	b	612	CLA	C1A-C2A-CAA-CBA
23	b	614	CLA	CBD-CGD-O2D-CED
23	b	618	CLA	CHA-CBD-CGD-O1D
23	b	618	CLA	CAD-CBD-CGD-O1D
23	b	618	CLA	CAD-CBD-CGD-O2D
23	b	620	CLA	C3A-C2A-CAA-CBA
23	b	620	CLA	CBD-CGD-O2D-CED
23	c	504	CLA	CBD-CGD-O2D-CED
23	c	505	CLA	C1A-C2A-CAA-CBA
23	c	505	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CHA-CBD-CGD-O1D
23	c	511	CLA	CHA-CBD-CGD-O2D
23	c	512	CLA	C1A-C2A-CAA-CBA
23	d	402	CLA	C2-C3-C5-C6
23	d	402	CLA	C4-C3-C5-C6
25	A	408	PL9	C7-C8-C9-C11
25	A	408	PL9	C12-C13-C14-C16
25	A	408	PL9	C17-C18-C19-C20
25	A	408	PL9	C17-C18-C19-C21
25	A	408	PL9	C22-C23-C24-C25
25	A	408	PL9	C24-C26-C27-C28
25	A	408	PL9	C27-C28-C29-C30
25	A	408	PL9	C27-C28-C29-C31
25	A	408	PL9	C30-C29-C31-C32
25	A	408	PL9	C33-C34-C36-C37
25	D	404	PL9	C27-C28-C29-C30
25	D	404	PL9	C27-C28-C29-C31
25	D	404	PL9	C34-C36-C37-C38
25	J	101	PL9	C7-C8-C9-C10
25	J	101	PL9	C7-C8-C9-C11
25	J	101	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	J	101	PL9	C22-C23-C24-C26
25	a	410	PL9	C7-C8-C9-C11
25	a	410	PL9	C12-C13-C14-C16
25	a	410	PL9	C17-C18-C19-C20
25	a	410	PL9	C17-C18-C19-C21
25	a	410	PL9	C24-C26-C27-C28
25	a	410	PL9	C27-C28-C29-C30
25	a	410	PL9	C27-C28-C29-C31
25	a	410	PL9	C28-C29-C31-C32
25	a	410	PL9	C30-C29-C31-C32
25	a	410	PL9	C33-C34-C36-C37
25	d	404	PL9	C27-C28-C29-C30
25	d	404	PL9	C27-C28-C29-C31
25	d	404	PL9	C34-C36-C37-C38
25	j	101	PL9	C7-C8-C9-C10
25	j	101	PL9	C7-C8-C9-C11
25	j	101	PL9	C22-C23-C24-C25
25	j	101	PL9	C22-C23-C24-C26
27	B	618	BCR	C21-C22-C23-C24
27	B	618	BCR	C37-C22-C23-C24
27	B	618	BCR	C23-C24-C25-C26
27	B	618	BCR	C23-C24-C25-C30
27	C	514	BCR	C11-C12-C13-C14
27	C	514	BCR	C11-C12-C13-C35
27	C	516	BCR	C1-C6-C7-C8
27	C	516	BCR	C7-C8-C9-C10
27	C	516	BCR	C7-C8-C9-C34
27	D	405	BCR	C5-C6-C7-C8
27	D	405	BCR	C7-C8-C9-C10
27	D	405	BCR	C7-C8-C9-C34
27	T	101	BCR	C1-C6-C7-C8
27	T	102	BCR	C21-C22-C23-C24
27	T	102	BCR	C37-C22-C23-C24
27	T	102	BCR	C23-C24-C25-C26
27	T	102	BCR	C23-C24-C25-C30
27	y	101	BCR	C1-C6-C7-C8
27	y	101	BCR	C7-C8-C9-C10
27	y	101	BCR	C7-C8-C9-C34
27	y	101	BCR	C21-C22-C23-C24
27	y	101	BCR	C37-C22-C23-C24
27	y	101	BCR	C23-C24-C25-C30
27	c	514	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	c	514	BCR	C11-C12-C13-C35
27	c	515	BCR	C1-C6-C7-C8
27	c	515	BCR	C7-C8-C9-C10
27	c	515	BCR	C7-C8-C9-C34
27	c	515	BCR	C37-C22-C23-C24
27	c	515	BCR	C23-C24-C25-C30
27	d	405	BCR	C7-C8-C9-C10
27	d	405	BCR	C7-C8-C9-C34
27	k	102	BCR	C7-C8-C9-C10
27	k	102	BCR	C7-C8-C9-C34
27	k	102	BCR	C21-C22-C23-C24
27	k	102	BCR	C37-C22-C23-C24
27	z	101	BCR	C1-C6-C7-C8
28	A	411	DGD	C2D-C1D-O3G-C3G
28	A	411	DGD	O6D-C1D-O3G-C3G
28	B	621	DGD	C2E-C1E-O5D-C6D
28	B	621	DGD	O6E-C1E-O5D-C6D
28	B	627	DGD	C2B-C1B-O2G-C2G
28	B	627	DGD	O1B-C1B-O2G-C2G
28	B	627	DGD	C2E-C1E-O5D-C6D
28	C	517	DGD	C2D-C1D-O3G-C3G
28	C	518	DGD	C2B-C1B-O2G-C2G
28	C	518	DGD	O1B-C1B-O2G-C2G
28	C	518	DGD	O2G-C2G-C3G-O3G
28	C	519	DGD	C2D-C1D-O3G-C3G
28	C	519	DGD	O6D-C1D-O3G-C3G
28	D	409	DGD	C2B-C1B-O2G-C2G
28	D	409	DGD	O6D-C1D-O3G-C3G
28	a	413	DGD	C2D-C1D-O3G-C3G
28	a	413	DGD	O6D-C1D-O3G-C3G
28	b	602	DGD	C2B-C1B-O2G-C2G
28	b	602	DGD	O1B-C1B-O2G-C2G
28	b	602	DGD	O2G-C2G-C3G-O3G
28	b	602	DGD	C2E-C1E-O5D-C6D
28	b	623	DGD	C2E-C1E-O5D-C6D
28	b	623	DGD	O6E-C1E-O5D-C6D
28	c	516	DGD	C2D-C1D-O3G-C3G
28	c	516	DGD	C2E-C1E-O5D-C6D
28	c	517	DGD	C2B-C1B-O2G-C2G
28	c	517	DGD	O1B-C1B-O2G-C2G
28	c	517	DGD	O2G-C2G-C3G-O3G
28	c	518	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
28	c	518	DGD	O6D-C1D-O3G-C3G
28	d	409	DGD	C2B-C1B-O2G-C2G
28	d	409	DGD	O6D-C1D-O3G-C3G
29	A	412	LHG	C3-O3-P-O5
29	A	412	LHG	C4-O6-P-O4
29	A	415	LHG	C4-O6-P-O4
29	A	415	LHG	C4-O6-P-O5
29	a	414	LHG	C3-O3-P-O5
29	a	414	LHG	C4-O6-P-O4
29	a	414	LHG	C4-O6-P-O5
29	a	417	LHG	C4-O6-P-O4
29	a	417	LHG	C4-O6-P-O5
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	O5-C1-O6-C44
30	A	417	SQD	O6-C44-C45-O47
30	A	417	SQD	C24-C23-O48-C46
30	B	626	SQD	O5-C5-C6-S
30	D	408	SQD	C2-C1-O6-C44
30	D	408	SQD	O6-C44-C45-O47
30	D	408	SQD	O49-C7-O47-C45
30	D	408	SQD	C8-C7-O47-C45
30	F	102	SQD	O5-C1-O6-C44
30	a	401	SQD	O6-C44-C45-O47
30	a	401	SQD	C24-C23-O48-C46
30	a	415	SQD	C2-C1-O6-C44
30	a	415	SQD	O5-C1-O6-C44
30	b	601	SQD	O5-C5-C6-S
30	d	408	SQD	C2-C1-O6-C44
30	d	408	SQD	O6-C44-C45-O47
30	d	408	SQD	O49-C7-O47-C45
30	d	408	SQD	C8-C7-O47-C45
30	f	102	SQD	O5-C1-O6-C44
31	B	622	LMG	O1-C7-C8-O7
31	B	622	LMG	O9-C10-O7-C8
31	B	622	LMG	C11-C10-O7-C8
31	B	623	LMG	O9-C10-O7-C8
31	B	623	LMG	C11-C10-O7-C8
31	C	520	LMG	C2-C1-O1-C7
31	C	520	LMG	O6-C1-O1-C7
31	C	520	LMG	C11-C10-O7-C8
31	C	521	LMG	C2-C1-O1-C7
31	C	521	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
31	C	521	LMG	O9-C10-O7-C8
31	C	521	LMG	C11-C10-O7-C8
31	D	406	LMG	C11-C10-O7-C8
31	D	407	LMG	C2-C1-O1-C7
31	D	407	LMG	O6-C1-O1-C7
31	E	101	LMG	C2-C1-O1-C7
31	E	101	LMG	O6-C1-O1-C7
31	M	101	LMG	C2-C1-O1-C7
31	M	101	LMG	O6-C1-O1-C7
31	M	101	LMG	O9-C10-O7-C8
31	b	624	LMG	O1-C7-C8-O7
31	b	624	LMG	O9-C10-O7-C8
31	b	624	LMG	C11-C10-O7-C8
31	b	625	LMG	O9-C10-O7-C8
31	b	625	LMG	C11-C10-O7-C8
31	c	519	LMG	C2-C1-O1-C7
31	c	519	LMG	O6-C1-O1-C7
31	c	519	LMG	C8-C9-O8-C28
31	c	519	LMG	O9-C10-O7-C8
31	c	519	LMG	C11-C10-O7-C8
31	d	406	LMG	O9-C10-O7-C8
31	d	406	LMG	C11-C10-O7-C8
31	d	407	LMG	C2-C1-O1-C7
31	d	407	LMG	O6-C1-O1-C7
31	e	101	LMG	C2-C1-O1-C7
31	e	101	LMG	O6-C1-O1-C7
31	k	103	LMG	C2-C1-O1-C7
31	k	103	LMG	O6-C1-O1-C7
31	k	103	LMG	C11-C10-O7-C8
31	m	102	LMG	C2-C1-O1-C7
31	m	102	LMG	O9-C10-O7-C8
23	A	403	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	C	505	CLA	O1D-CGD-O2D-CED
23	a	404	CLA	O1D-CGD-O2D-CED
23	b	608	CLA	O1D-CGD-O2D-CED
23	c	505	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	O1D-CGD-O2D-CED
23	B	616	CLA	O1D-CGD-O2D-CED
23	b	620	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
23	A	403	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	607	CLA	CBD-CGD-O2D-CED
23	B	611	CLA	CBD-CGD-O2D-CED
23	B	613	CLA	CBD-CGD-O2D-CED
23	B	614	CLA	CBD-CGD-O2D-CED
23	C	501	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	506	CLA	CBD-CGD-O2D-CED
23	C	508	CLA	CBD-CGD-O2D-CED
23	C	509	CLA	CBD-CGD-O2D-CED
23	a	404	CLA	CBD-CGD-O2D-CED
23	b	607	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	503	CLA	CBD-CGD-O2D-CED
23	c	506	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CBD-CGD-O2D-CED
23	c	509	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
30	A	417	SQD	O10-C23-O48-C46
30	a	401	SQD	O10-C23-O48-C46
30	f	102	SQD	O10-C23-O48-C46
31	B	622	LMG	O10-C28-O8-C9
31	D	407	LMG	O10-C28-O8-C9
31	E	101	LMG	O10-C28-O8-C9
31	a	416	LMG	O10-C28-O8-C9
31	b	624	LMG	O10-C28-O8-C9
31	d	407	LMG	O10-C28-O8-C9
33	B	628	LMT	C3'-C4'-O1B-C1B
33	b	603	LMT	C3'-C4'-O1B-C1B
23	c	511	CLA	O1D-CGD-O2D-CED
28	B	621	DGD	C4D-C5D-C6D-O5D
31	C	521	LMG	C8-C9-O8-C28
23	B	601	CLA	O1D-CGD-O2D-CED
23	C	504	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	O1D-CGD-O2D-CED
23	b	605	CLA	O1D-CGD-O2D-CED
23	b	614	CLA	O1D-CGD-O2D-CED
23	c	504	CLA	O1D-CGD-O2D-CED
31	d	407	LMG	C29-C28-O8-C9
31	e	101	LMG	C29-C28-O8-C9
28	c	517	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C37-C38-C39-C41
25	a	410	PL9	C37-C38-C39-C40
25	a	410	PL9	C37-C38-C39-C41
23	B	606	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	CBD-CGD-O2D-CED
23	b	618	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
24	A	406	PHO	CBD-CGD-O2D-CED
24	a	408	PHO	CBD-CGD-O2D-CED
28	D	409	DGD	O1A-C1A-O1G-C1G
28	d	409	DGD	O1A-C1A-O1G-C1G
30	F	102	SQD	O10-C23-O48-C46
31	A	414	LMG	O10-C28-O8-C9
31	C	521	LMG	O10-C28-O8-C9
31	c	519	LMG	O10-C28-O8-C9
31	e	101	LMG	O10-C28-O8-C9
23	B	605	CLA	O1D-CGD-O2D-CED
23	b	609	CLA	O1D-CGD-O2D-CED
28	D	409	DGD	O6D-C5D-C6D-O5D
28	d	409	DGD	O6D-C5D-C6D-O5D
23	C	512	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	O1D-CGD-O2D-CED
23	B	610	CLA	O1D-CGD-O2D-CED
23	b	611	CLA	O1D-CGD-O2D-CED
23	c	508	CLA	O1D-CGD-O2D-CED
23	c	509	CLA	O1D-CGD-O2D-CED
28	C	517	DGD	O1B-C1B-O2G-C2G
28	D	409	DGD	O1B-C1B-O2G-C2G
28	c	516	DGD	O1B-C1B-O2G-C2G
28	d	409	DGD	O1B-C1B-O2G-C2G
31	A	418	LMG	O9-C10-O7-C8
31	D	406	LMG	O9-C10-O7-C8
31	E	101	LMG	O9-C10-O7-C8
31	e	101	LMG	O9-C10-O7-C8
31	i	101	LMG	O9-C10-O7-C8
28	C	518	DGD	C4E-C5E-C6E-O5E
23	A	405	CLA	C3-C5-C6-C7
23	a	406	CLA	C3-C5-C6-C7
24	D	402	PHO	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	a	407	PHO	C3-C5-C6-C7
28	D	409	DGD	C2A-C1A-O1G-C1G
28	d	409	DGD	C2A-C1A-O1G-C1G
30	f	102	SQD	C24-C23-O48-C46
31	A	414	LMG	C29-C28-O8-C9
31	C	521	LMG	C29-C28-O8-C9
31	D	407	LMG	C29-C28-O8-C9
31	E	101	LMG	C29-C28-O8-C9
31	a	416	LMG	C29-C28-O8-C9
31	c	519	LMG	C29-C28-O8-C9
28	a	413	DGD	O6E-C5E-C6E-O5E
28	C	517	DGD	C2B-C1B-O2G-C2G
28	c	516	DGD	C2B-C1B-O2G-C2G
30	F	102	SQD	C8-C7-O47-C45
30	f	102	SQD	C8-C7-O47-C45
31	M	101	LMG	C11-C10-O7-C8
31	m	102	LMG	C11-C10-O7-C8
23	B	611	CLA	O1D-CGD-O2D-CED
23	b	607	CLA	O1D-CGD-O2D-CED
23	c	506	CLA	O1D-CGD-O2D-CED
23	b	613	CLA	CBD-CGD-O2D-CED
28	A	411	DGD	O6E-C5E-C6E-O5E
31	k	103	LMG	O6-C5-C6-O5
33	b	604	LMT	C3'-C4'-O1B-C1B
23	B	605	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
25	A	408	PL9	C35-C34-C36-C37
25	a	410	PL9	C35-C34-C36-C37
25	d	404	PL9	C35-C34-C36-C37
25	A	408	PL9	C28-C29-C31-C32
23	B	601	CLA	C2A-CAA-CBA-CGA
23	B	607	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C2A-CAA-CBA-CGA
23	C	512	CLA	C2A-CAA-CBA-CGA
23	b	605	CLA	C2A-CAA-CBA-CGA
23	b	611	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	O1D-CGD-O2D-CED
33	B	629	LMT	C3'-C4'-O1B-C1B
23	B	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C3-C5-C6-C7
23	b	612	CLA	C3-C5-C6-C7
23	b	618	CLA	C3-C5-C6-C7
30	F	102	SQD	C24-C23-O48-C46
31	B	622	LMG	C29-C28-O8-C9
31	C	520	LMG	C29-C28-O8-C9
31	b	624	LMG	C29-C28-O8-C9
31	k	103	LMG	C29-C28-O8-C9
28	c	517	DGD	O6E-C5E-C6E-O5E
31	C	520	LMG	O6-C5-C6-O5
23	C	506	CLA	O1D-CGD-O2D-CED
28	b	623	DGD	C4D-C5D-C6D-O5D
25	A	408	PL9	C12-C13-C14-C15
25	a	410	PL9	C12-C13-C14-C15
25	a	410	PL9	C22-C23-C24-C25
23	C	508	CLA	O1D-CGD-O2D-CED
31	I	101	LMG	O9-C10-O7-C8
31	a	402	LMG	O9-C10-O7-C8
25	A	408	PL9	C22-C23-C24-C26
25	a	410	PL9	C22-C23-C24-C26
31	A	418	LMG	O6-C5-C6-O5
28	A	411	DGD	C4E-C5E-C6E-O5E
23	B	608	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	612	CLA	CBD-CGD-O2D-CED
23	b	617	CLA	O1D-CGD-O2D-CED
29	A	412	LHG	O2-C2-C3-O3
29	a	414	LHG	O2-C2-C3-O3
23	B	602	CLA	C3-C5-C6-C7
23	C	509	CLA	C3-C5-C6-C7
23	b	606	CLA	C3-C5-C6-C7
28	D	409	DGD	C4D-C5D-C6D-O5D
28	d	409	DGD	C4D-C5D-C6D-O5D
31	I	101	LMG	C29-C28-O8-C9
31	i	101	LMG	C29-C28-O8-C9
31	k	103	LMG	O10-C28-O8-C9
31	b	624	LMG	O6-C5-C6-O5
23	B	614	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
31	A	418	LMG	C11-C10-O7-C8
31	I	101	LMG	C11-C10-O7-C8
31	a	402	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
31	i	101	LMG	C11-C10-O7-C8
33	i	102	LMT	C3'-C4'-O1B-C1B
23	b	612	CLA	CBD-CGD-O2D-CED
31	a	402	LMG	O6-C5-C6-O5
28	C	518	DGD	O6E-C5E-C6E-O5E
31	M	101	LMG	O6-C5-C6-O5
28	a	413	DGD	C4E-C5E-C6E-O5E
23	C	501	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	O1D-CGD-O2D-CED
33	I	102	LMT	C3'-C4'-O1B-C1B
23	c	509	CLA	C3-C5-C6-C7
23	b	615	CLA	O1D-CGD-O2D-CED
31	A	414	LMG	O6-C5-C6-O5
31	B	622	LMG	O6-C5-C6-O5
31	C	521	LMG	O6-C5-C6-O5
31	c	519	LMG	O6-C5-C6-O5
28	B	621	DGD	C4E-C5E-C6E-O5E
31	C	520	LMG	O10-C28-O8-C9
34	V	201	HEM	C3D-CAD-CBD-CGD
34	v	201	HEM	C3D-CAD-CBD-CGD
24	D	402	PHO	C4-C3-C5-C6
24	a	407	PHO	C4-C3-C5-C6
31	B	622	LMG	C4-C5-C6-O5
31	k	103	LMG	C4-C5-C6-O5
24	D	402	PHO	C2-C3-C5-C6
24	a	407	PHO	C2-C3-C5-C6
23	B	610	CLA	C2A-CAA-CBA-CGA
28	c	516	DGD	O6E-C5E-C6E-O5E
28	b	623	DGD	C4E-C5E-C6E-O5E
28	B	621	DGD	O6D-C1D-O3G-C3G
28	B	627	DGD	O6E-C1E-O5D-C6D
28	b	602	DGD	O6E-C1E-O5D-C6D
28	b	623	DGD	O6D-C1D-O3G-C3G
28	c	516	DGD	O6D-C1D-O3G-C3G
31	A	418	LMG	O6-C1-O1-C7
31	a	402	LMG	O6-C1-O1-C7
31	m	102	LMG	O6-C1-O1-C7
25	A	408	PL9	C29-C31-C32-C33
25	a	410	PL9	C29-C31-C32-C33
23	b	616	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	O1D-CGD-O2D-CED
28	B	621	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
28	C	517	DGD	O6E-C5E-C6E-O5E
31	a	416	LMG	O6-C5-C6-O5
28	c	516	DGD	C4E-C5E-C6E-O5E
31	d	407	LMG	C11-C10-O7-C8
31	a	416	LMG	C4-C5-C6-O5
25	D	404	PL9	C22-C23-C24-C25
25	d	404	PL9	C22-C23-C24-C25
23	C	513	CLA	O1D-CGD-O2D-CED
31	C	520	LMG	O9-C10-O7-C8
31	A	414	LMG	C4-C5-C6-O5
31	C	520	LMG	C4-C5-C6-O5
31	b	624	LMG	C4-C5-C6-O5
23	B	605	CLA	CBA-CGA-O2A-C1
23	B	616	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
23	b	620	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
24	D	402	PHO	CBA-CGA-O2A-C1
24	a	407	PHO	CBA-CGA-O2A-C1
23	B	607	CLA	C15-C16-C17-C18
23	B	609	CLA	C13-C15-C16-C17
23	B	612	CLA	C5-C6-C7-C8
23	c	509	CLA	C5-C6-C7-C8
23	d	402	CLA	C15-C16-C17-C18
31	E	101	LMG	C28-C29-C30-C31
31	d	406	LMG	C10-C11-C12-C13
28	C	517	DGD	C2E-C1E-O5D-C6D
28	B	627	DGD	O2G-C2G-C3G-O3G
31	C	521	LMG	C4-C5-C6-O5
23	B	605	CLA	C2-C3-C5-C6
23	b	609	CLA	C2-C3-C5-C6
23	B	608	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	C	509	CLA	C6-C7-C8-C9
23	a	405	CLA	C6-C7-C8-C9
23	b	612	CLA	C6-C7-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	c	501	CLA	O1D-CGD-O2D-CED
24	a	408	PHO	O1D-CGD-O2D-CED
27	B	618	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
27	C	516	BCR	C37-C22-C23-C24
27	D	405	BCR	C37-C22-C23-C24
27	J	102	BCR	C37-C22-C23-C24
27	T	102	BCR	C7-C8-C9-C34
27	d	405	BCR	C37-C22-C23-C24
27	B	618	BCR	C7-C8-C9-C10
27	C	514	BCR	C7-C8-C9-C10
27	T	102	BCR	C7-C8-C9-C10
23	b	610	CLA	O1D-CGD-O2D-CED
28	b	623	DGD	O6E-C5E-C6E-O5E
30	B	626	SQD	C8-C7-O47-C45
28	C	517	DGD	C4E-C5E-C6E-O5E
31	D	406	LMG	C10-C11-C12-C13
31	e	101	LMG	C28-C29-C30-C31
23	B	616	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
24	D	402	PHO	O1A-CGA-O2A-C1
24	a	407	PHO	O1A-CGA-O2A-C1
31	I	101	LMG	O10-C28-O8-C9
23	A	405	CLA	C10-C11-C12-C13
23	B	601	CLA	C13-C15-C16-C17
23	C	501	CLA	C15-C16-C17-C18
23	C	503	CLA	C10-C11-C12-C13
23	C	509	CLA	C5-C6-C7-C8
23	D	401	CLA	C13-C15-C16-C17
23	a	406	CLA	C10-C11-C12-C13
23	b	615	CLA	C15-C16-C17-C18
23	b	620	CLA	C10-C11-C12-C13
23	c	503	CLA	C10-C11-C12-C13
23	c	504	CLA	C13-C15-C16-C17
31	c	519	LMG	C4-C5-C6-O5
31	m	102	LMG	C29-C28-O8-C9
23	B	604	CLA	C13-C15-C16-C17
23	D	401	CLA	C15-C16-C17-C18
23	b	611	CLA	C15-C16-C17-C18
23	b	612	CLA	C15-C16-C17-C18
23	b	614	CLA	C8-C10-C11-C12
23	b	616	CLA	C5-C6-C7-C8
23	b	620	CLA	C5-C6-C7-C8
23	c	501	CLA	C15-C16-C17-C18
24	a	408	PHO	C15-C16-C17-C18
28	C	517	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
28	a	413	DGD	C1B-C2B-C3B-C4B
28	c	516	DGD	C1B-C2B-C3B-C4B
28	d	409	DGD	C1B-C2B-C3B-C4B
31	C	521	LMG	C28-C29-C30-C31
31	I	101	LMG	O6-C5-C6-O5
23	B	611	CLA	C15-C16-C17-C18
23	B	612	CLA	C13-C15-C16-C17
23	B	616	CLA	C5-C6-C7-C8
23	B	616	CLA	C10-C11-C12-C13
23	C	506	CLA	C15-C16-C17-C18
23	C	513	CLA	C15-C16-C17-C18
23	b	608	CLA	C13-C15-C16-C17
23	b	611	CLA	C13-C15-C16-C17
23	b	613	CLA	C13-C15-C16-C17
23	b	616	CLA	C13-C15-C16-C17
23	c	506	CLA	C15-C16-C17-C18
23	c	513	CLA	C15-C16-C17-C18
23	d	402	CLA	C13-C15-C16-C17
24	A	406	PHO	C15-C16-C17-C18
23	B	606	CLA	O1D-CGD-O2D-CED
25	A	408	PL9	C7-C8-C9-C10
28	B	627	DGD	C1A-C2A-C3A-C4A
28	D	409	DGD	C1B-C2B-C3B-C4B
28	b	602	DGD	C1A-C2A-C3A-C4A
30	a	415	SQD	C7-C8-C9-C10
31	B	623	LMG	C10-C11-C12-C13
31	b	625	LMG	C10-C11-C12-C13
31	c	519	LMG	C28-C29-C30-C31
23	B	607	CLA	C13-C15-C16-C17
23	B	608	CLA	C15-C16-C17-C18
23	B	610	CLA	C8-C10-C11-C12
23	C	504	CLA	C13-C15-C16-C17
23	b	605	CLA	C13-C15-C16-C17
23	c	501	CLA	C8-C10-C11-C12
23	c	504	CLA	C15-C16-C17-C18
23	c	508	CLA	C10-C11-C12-C13
23	c	508	CLA	C15-C16-C17-C18
23	c	512	CLA	CBA-CGA-O2A-C1
30	b	601	SQD	C24-C23-O48-C46
23	b	618	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
31	i	101	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
31	m	102	LMG	O6-C5-C6-O5
23	A	404	CLA	C15-C16-C17-C18
23	C	501	CLA	C8-C10-C11-C12
23	C	504	CLA	C15-C16-C17-C18
23	a	405	CLA	C15-C16-C17-C18
23	c	507	CLA	C5-C6-C7-C8
28	A	411	DGD	C1B-C2B-C3B-C4B
28	c	516	DGD	C1A-C2A-C3A-C4A
31	C	521	LMG	C10-C11-C12-C13
31	c	519	LMG	C10-C11-C12-C13
30	b	601	SQD	C8-C7-O47-C45
23	C	506	CLA	C13-C15-C16-C17
23	C	508	CLA	C10-C11-C12-C13
23	C	508	CLA	C15-C16-C17-C18
23	C	507	CLA	C11-C10-C8-C7
23	C	511	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
23	a	404	CLA	C3-C5-C6-C7
23	B	605	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	O1A-CGA-O2A-C1
23	b	620	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	O1D-CGD-O2D-CED
24	A	406	PHO	O1D-CGD-O2D-CED
23	C	506	CLA	C5-C6-C7-C8
23	a	406	CLA	C15-C16-C17-C18
23	c	504	CLA	C10-C11-C12-C13
23	c	506	CLA	C13-C15-C16-C17
23	c	510	CLA	C15-C16-C17-C18
28	C	517	DGD	O6E-C1E-O5D-C6D
28	c	516	DGD	O6E-C1E-O5D-C6D
23	C	504	CLA	C10-C11-C12-C13
23	C	505	CLA	C10-C11-C12-C13
23	c	505	CLA	C10-C11-C12-C13
25	D	404	PL9	C29-C31-C32-C33
25	d	404	PL9	C29-C31-C32-C33
28	b	623	DGD	C1B-C2B-C3B-C4B
28	C	519	DGD	O1B-C1B-O2G-C2G
30	F	102	SQD	O49-C7-O47-C45
23	A	403	CLA	C3-C5-C6-C7
23	B	613	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C5-C6-C7-C8
23	C	510	CLA	C15-C16-C17-C18
23	c	501	CLA	C10-C11-C12-C13
23	c	506	CLA	C5-C6-C7-C8
30	b	601	SQD	O10-C23-O48-C46
31	i	101	LMG	O10-C28-O8-C9
28	B	621	DGD	C1B-C2B-C3B-C4B
31	A	418	LMG	C4-C5-C6-O5
23	b	619	CLA	C13-C15-C16-C17
23	c	511	CLA	C5-C6-C7-C8
31	D	407	LMG	C11-C10-O7-C8
23	b	613	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	C15-C16-C17-C18
23	B	615	CLA	C13-C15-C16-C17
23	B	616	CLA	C13-C15-C16-C17
29	A	412	LHG	C4-O6-P-O3
29	A	415	LHG	C3-O3-P-O6
29	A	415	LHG	C4-O6-P-O3
29	a	414	LHG	C4-O6-P-O3
29	a	417	LHG	C3-O3-P-O6
29	a	417	LHG	C4-O6-P-O3
28	C	517	DGD	C1A-C2A-C3A-C4A
30	A	413	SQD	C7-C8-C9-C10
23	A	404	CLA	C3-C5-C6-C7
23	C	511	CLA	C5-C6-C7-C8
28	B	621	DGD	O6D-C5D-C6D-O5D
31	C	520	LMG	C10-C11-C12-C13
28	C	518	DGD	C4D-C5D-C6D-O5D
29	A	412	LHG	C1-C2-C3-O3
29	a	414	LHG	C1-C2-C3-O3
28	c	518	DGD	O1B-C1B-O2G-C2G
30	f	102	SQD	O49-C7-O47-C45
31	k	103	LMG	O9-C10-O7-C8
25	D	404	PL9	C35-C34-C36-C37
23	B	608	CLA	C5-C6-C7-C8
23	b	612	CLA	C5-C6-C7-C8
23	b	617	CLA	C5-C6-C7-C8
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
30	B	626	SQD	C24-C23-O48-C46
31	M	101	LMG	C29-C28-O8-C9
28	C	518	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	O6D-C5D-C6D-O5D
28	c	517	DGD	C4D-C5D-C6D-O5D
31	B	623	LMG	C31-C32-C33-C34
31	b	624	LMG	C31-C32-C33-C34
31	b	625	LMG	C31-C32-C33-C34
23	b	620	CLA	C13-C15-C16-C17
23	B	616	CLA	C3-C5-C6-C7
23	b	620	CLA	C3-C5-C6-C7
28	C	517	DGD	C3A-C4A-C5A-C6A
28	b	623	DGD	C6B-C7B-C8B-C9B
28	d	409	DGD	C3A-C4A-C5A-C6A
29	a	417	LHG	C11-C10-C9-C8
30	b	601	SQD	C11-C10-C9-C8
31	A	414	LMG	C14-C15-C16-C17
31	A	414	LMG	C29-C30-C31-C32
31	M	101	LMG	C29-C30-C31-C32
31	a	416	LMG	C14-C15-C16-C17
31	a	416	LMG	C34-C35-C36-C37
23	C	512	CLA	CBA-CGA-O2A-C1
28	c	516	DGD	C3A-C4A-C5A-C6A
28	c	518	DGD	C9B-CAB-CBB-CCB
28	d	409	DGD	C7B-C8B-C9B-CAB
30	A	413	SQD	C14-C15-C16-C17
31	A	414	LMG	C34-C35-C36-C37
31	A	418	LMG	C11-C12-C13-C14
31	m	102	LMG	C29-C30-C31-C32
28	D	409	DGD	C1G-C2G-O2G-C1B
28	d	409	DGD	C1G-C2G-O2G-C1B
31	E	101	LMG	C7-C8-O7-C10
31	e	101	LMG	C7-C8-O7-C10
23	a	409	CLA	C10-C11-C12-C13
28	D	409	DGD	C7B-C8B-C9B-CAB
30	B	626	SQD	C11-C10-C9-C8
30	a	415	SQD	C14-C15-C16-C17
31	a	402	LMG	C11-C12-C13-C14
28	C	519	DGD	C9B-CAB-CBB-CCB
29	A	412	LHG	C25-C26-C27-C28
30	F	102	SQD	C12-C13-C14-C15
30	f	102	SQD	C12-C13-C14-C15
31	B	622	LMG	C31-C32-C33-C34
31	a	416	LMG	C29-C30-C31-C32
31	b	624	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
28	B	627	DGD	C2A-C3A-C4A-C5A
28	D	409	DGD	C3A-C4A-C5A-C6A
31	d	407	LMG	C36-C37-C38-C39
28	C	518	DGD	C2D-C1D-O3G-C3G
28	C	518	DGD	C2E-C1E-O5D-C6D
28	c	517	DGD	C2D-C1D-O3G-C3G
28	c	517	DGD	C2E-C1E-O5D-C6D
31	B	623	LMG	C2-C1-O1-C7
31	I	101	LMG	C2-C1-O1-C7
31	i	101	LMG	C2-C1-O1-C7
31	M	101	LMG	C4-C5-C6-O5
28	C	519	DGD	C3B-C4B-C5B-C6B
28	b	602	DGD	C2A-C3A-C4A-C5A
29	A	415	LHG	C11-C10-C9-C8
29	a	417	LHG	C24-C25-C26-C27
31	D	407	LMG	C36-C37-C38-C39
31	b	625	LMG	C34-C35-C36-C37
23	B	609	CLA	O1D-CGD-O2D-CED
23	C	510	CLA	C4-C3-C5-C6
25	J	101	PL9	C12-C13-C14-C15
25	j	101	PL9	C12-C13-C14-C15
28	A	411	DGD	C5B-C6B-C7B-C8B
28	B	621	DGD	C6B-C7B-C8B-C9B
28	d	409	DGD	CAB-CBB-CCB-CDB
29	a	414	LHG	C25-C26-C27-C28
31	B	622	LMG	C30-C31-C32-C33
31	B	623	LMG	C34-C35-C36-C37
31	c	519	LMG	C12-C13-C14-C15
31	d	407	LMG	C19-C20-C21-C22
23	A	403	CLA	C11-C12-C13-C14
23	B	601	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C10-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	C	513	CLA	C14-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C14
23	c	505	CLA	C11-C10-C8-C9
23	c	507	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C10-C8-C9
24	A	406	PHO	C11-C10-C8-C9
24	a	408	PHO	C11-C10-C8-C9
28	b	623	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
28	c	518	DGD	C3B-C4B-C5B-C6B
29	A	415	LHG	C24-C25-C26-C27
30	A	413	SQD	C27-C28-C29-C30
31	A	418	LMG	C18-C19-C20-C21
31	D	407	LMG	C15-C16-C17-C18
31	d	407	LMG	C15-C16-C17-C18
23	b	605	CLA	C10-C11-C12-C13
23	c	512	CLA	O1A-CGA-O2A-C1
27	C	514	BCR	C7-C8-C9-C34
27	c	514	BCR	C7-C8-C9-C34
28	a	413	DGD	C5B-C6B-C7B-C8B
28	d	409	DGD	CDB-CEB-CFB-CGB
30	F	102	SQD	C11-C12-C13-C14
31	I	101	LMG	C16-C17-C18-C19
31	i	101	LMG	C16-C17-C18-C19
27	c	514	BCR	C7-C8-C9-C10
23	a	405	CLA	C3-C5-C6-C7
23	a	409	CLA	C5-C6-C7-C8
28	D	409	DGD	C2A-C3A-C4A-C5A
31	i	101	LMG	C14-C15-C16-C17
33	b	603	LMT	C2-C3-C4-C5
28	c	517	DGD	C1A-C2A-C3A-C4A
31	B	622	LMG	C28-C29-C30-C31
23	B	608	CLA	O1D-CGD-O2D-CED
25	d	404	PL9	C47-C48-C49-C51
28	C	518	DGD	C2A-C3A-C4A-C5A
28	D	409	DGD	CAB-CBB-CCB-CDB
28	D	409	DGD	CDB-CEB-CFB-CGB
28	D	409	DGD	CEB-CFB-CGB-CHB
28	d	409	DGD	C2A-C3A-C4A-C5A
28	d	409	DGD	CCB-CDB-CEB-CFB
30	f	102	SQD	C11-C12-C13-C14
31	D	407	LMG	C14-C15-C16-C17
31	E	101	LMG	C15-C16-C17-C18
31	a	402	LMG	C18-C19-C20-C21
31	d	407	LMG	C14-C15-C16-C17
33	B	628	LMT	C2-C3-C4-C5
33	i	102	LMT	C6-C7-C8-C9
28	C	517	DGD	O6D-C1D-O3G-C3G
23	A	407	CLA	C10-C11-C12-C13
23	C	501	CLA	C10-C11-C12-C13
23	c	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	C	517	DGD	C3B-C4B-C5B-C6B
28	D	409	DGD	C4B-C5B-C6B-C7B
28	d	409	DGD	C4B-C5B-C6B-C7B
30	a	415	SQD	C27-C28-C29-C30
31	C	521	LMG	C12-C13-C14-C15
31	D	407	LMG	C19-C20-C21-C22
31	I	101	LMG	C14-C15-C16-C17
33	B	628	LMT	C7-C8-C9-C10
28	D	409	DGD	CCB-CDB-CEB-CFB
31	i	101	LMG	C13-C14-C15-C16
33	b	603	LMT	C7-C8-C9-C10
28	C	518	DGD	C1A-C2A-C3A-C4A
31	b	624	LMG	C28-C29-C30-C31
23	d	403	CLA	C15-C16-C17-C18
30	B	626	SQD	O10-C23-O48-C46
28	c	516	DGD	C3B-C4B-C5B-C6B
28	d	409	DGD	CEB-CFB-CGB-CHB
31	a	402	LMG	C31-C32-C33-C34
31	b	625	LMG	C13-C14-C15-C16
31	c	519	LMG	C29-C30-C31-C32
31	d	407	LMG	C13-C14-C15-C16
31	e	101	LMG	C15-C16-C17-C18
23	B	612	CLA	O1D-CGD-O2D-CED
23	A	404	CLA	C3A-C2A-CAA-CBA
23	B	607	CLA	C3A-C2A-CAA-CBA
23	B	608	CLA	C3A-C2A-CAA-CBA
23	C	507	CLA	C3A-C2A-CAA-CBA
23	C	512	CLA	C3A-C2A-CAA-CBA
23	a	405	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	c	505	CLA	C3A-C2A-CAA-CBA
23	c	507	CLA	C3A-C2A-CAA-CBA
23	c	512	CLA	C3A-C2A-CAA-CBA
28	B	627	DGD	C5B-C6B-C7B-C8B
28	b	623	DGD	C5B-C6B-C7B-C8B
28	c	516	DGD	C4A-C5A-C6A-C7A
31	C	521	LMG	C29-C30-C31-C32
31	D	407	LMG	C13-C14-C15-C16
31	I	101	LMG	C13-C14-C15-C16
33	I	102	LMT	C6-C7-C8-C9
28	c	517	DGD	C2A-C3A-C4A-C5A
31	B	622	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	b	624	LMG	C18-C19-C20-C21
28	c	518	DGD	O1G-C1G-C2G-C3G
23	C	510	CLA	CBD-CGD-O2D-CED
28	D	409	DGD	C3B-C4B-C5B-C6B
30	B	626	SQD	C9-C10-C11-C12
23	C	506	CLA	C10-C11-C12-C13
23	c	510	CLA	C4-C3-C5-C6
23	b	609	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	C2-C3-C5-C6
28	C	519	DGD	C2B-C1B-O2G-C2G
28	c	518	DGD	C2B-C1B-O2G-C2G
25	j	101	PL9	C27-C28-C29-C31
23	c	503	CLA	C5-C6-C7-C8
28	D	409	DGD	C6B-C7B-C8B-C9B
28	c	516	DGD	C4B-C5B-C6B-C7B
28	c	517	DGD	CCB-CDB-CEB-CFB
31	A	418	LMG	C31-C32-C33-C34
31	k	103	LMG	C10-C11-C12-C13
23	B	613	CLA	C16-C17-C18-C19
31	A	414	LMG	C30-C31-C32-C33
28	C	519	DGD	CAB-CBB-CCB-CDB
28	b	602	DGD	C9B-CAB-CBB-CCB
31	b	624	LMG	C19-C20-C21-C22
28	C	517	DGD	C4A-C5A-C6A-C7A
28	d	409	DGD	C3B-C4B-C5B-C6B
31	I	101	LMG	C12-C13-C14-C15
31	i	101	LMG	C12-C13-C14-C15
34	V	201	HEM	C2D-C3D-CAD-CBD
28	C	517	DGD	C4B-C5B-C6B-C7B
33	b	626	LMT	C1-C2-C3-C4
23	C	509	CLA	C2-C1-O2A-CGA
28	d	409	DGD	C5A-C6A-C7A-C8A
23	C	512	CLA	O1A-CGA-O2A-C1
28	C	518	DGD	CCB-CDB-CEB-CFB
28	c	518	DGD	CAB-CBB-CCB-CDB
28	d	409	DGD	C6B-C7B-C8B-C9B
30	B	626	SQD	C11-C12-C13-C14
27	C	514	BCR	C1-C6-C7-C8
27	C	515	BCR	C1-C6-C7-C8
27	C	515	BCR	C5-C6-C7-C8
27	C	516	BCR	C5-C6-C7-C8
27	C	516	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	C	516	BCR	C23-C24-C25-C30
27	D	405	BCR	C1-C6-C7-C8
27	H	101	BCR	C1-C6-C7-C8
27	H	101	BCR	C5-C6-C7-C8
27	y	101	BCR	C5-C6-C7-C8
27	y	101	BCR	C23-C24-C25-C26
27	c	514	BCR	C1-C6-C7-C8
27	c	515	BCR	C5-C6-C7-C8
27	c	515	BCR	C23-C24-C25-C26
27	d	405	BCR	C1-C6-C7-C8
27	d	405	BCR	C5-C6-C7-C8
27	h	101	BCR	C1-C6-C7-C8
27	h	101	BCR	C5-C6-C7-C8
27	k	102	BCR	C1-C6-C7-C8
27	k	102	BCR	C5-C6-C7-C8
27	k	102	BCR	C23-C24-C25-C26
27	k	102	BCR	C23-C24-C25-C30
27	z	101	BCR	C5-C6-C7-C8
31	d	406	LMG	O6-C5-C6-O5
23	c	504	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	C13-C15-C16-C17
23	D	403	CLA	C15-C16-C17-C18
23	c	506	CLA	C10-C11-C12-C13
23	c	513	CLA	C13-C15-C16-C17
33	B	624	LMT	C1-C2-C3-C4
34	F	101	HEM	C3D-CAD-CBD-CGD
34	f	101	HEM	C3D-CAD-CBD-CGD
30	b	601	SQD	C9-C10-C11-C12
31	b	624	LMG	C13-C14-C15-C16
31	D	407	LMG	C28-C29-C30-C31
30	D	408	SQD	C9-C10-C11-C12
31	D	407	LMG	C32-C33-C34-C35
25	J	101	PL9	C27-C28-C29-C31
23	B	601	CLA	C10-C11-C12-C13
23	C	503	CLA	C5-C6-C7-C8
23	A	405	CLA	C6-C7-C8-C10
23	B	601	CLA	C6-C7-C8-C10
23	B	603	CLA	C11-C12-C13-C15
23	C	506	CLA	C11-C10-C8-C7
23	C	510	CLA	C2-C3-C5-C6
23	C	513	CLA	C11-C10-C8-C7
23	C	513	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	a	406	CLA	C6-C7-C8-C10
23	b	605	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	513	CLA	C11-C10-C8-C7
24	A	406	PHO	C11-C10-C8-C7
24	a	408	PHO	C11-C10-C8-C7
23	b	609	CLA	O1A-CGA-O2A-C1
23	B	602	CLA	C5-C6-C7-C8
23	b	605	CLA	C16-C17-C18-C20
31	d	407	LMG	O9-C10-O7-C8
31	d	407	LMG	C28-C29-C30-C31
23	b	615	CLA	CBA-CGA-O2A-C1
31	b	625	LMG	C29-C28-O8-C9
28	b	602	DGD	C3A-C4A-C5A-C6A
31	a	416	LMG	C30-C31-C32-C33
23	A	403	CLA	C2A-CAA-CBA-CGA
23	C	501	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
23	C	513	CLA	C13-C15-C16-C17
30	F	102	SQD	C10-C11-C12-C13
30	f	102	SQD	C10-C11-C12-C13
31	B	623	LMG	C13-C14-C15-C16
23	b	606	CLA	C5-C6-C7-C8
28	d	409	DGD	C5B-C6B-C7B-C8B
25	a	410	PL9	C7-C8-C9-C10
30	a	415	SQD	C17-C18-C19-C20
31	b	624	LMG	C36-C37-C38-C39
31	B	623	LMG	O6-C1-O1-C7
31	I	101	LMG	O6-C1-O1-C7
23	B	614	CLA	C15-C16-C17-C18
23	b	606	CLA	C13-C15-C16-C17
23	b	612	CLA	O1D-CGD-O2D-CED
28	B	627	DGD	C3A-C4A-C5A-C6A
28	D	409	DGD	C5B-C6B-C7B-C8B
31	A	414	LMG	C11-C10-O7-C8
31	E	101	LMG	C11-C10-O7-C8
31	e	101	LMG	C11-C10-O7-C8
31	E	101	LMG	C17-C18-C19-C20
31	I	101	LMG	C4-C5-C6-O5
23	C	512	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
28	C	517	DGD	C5A-C6A-C7A-C8A
30	b	601	SQD	C11-C12-C13-C14
30	d	408	SQD	C9-C10-C11-C12
31	B	622	LMG	C36-C37-C38-C39
31	D	407	LMG	O9-C10-O7-C8
30	A	417	SQD	C18-C19-C20-C21
28	C	519	DGD	O1G-C1G-C2G-O2G
28	c	518	DGD	O1G-C1G-C2G-O2G
31	B	623	LMG	C29-C28-O8-C9
28	b	602	DGD	C5B-C6B-C7B-C8B
30	A	413	SQD	C17-C18-C19-C20
23	b	618	CLA	C15-C16-C17-C18
23	A	404	CLA	C4-C3-C5-C6
28	D	409	DGD	C5A-C6A-C7A-C8A
31	B	622	LMG	C19-C20-C21-C22
23	A	405	CLA	C6-C7-C8-C9
23	B	601	CLA	C6-C7-C8-C9
23	B	603	CLA	C11-C12-C13-C14
23	C	503	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C10-C8-C9
23	a	404	CLA	C11-C12-C13-C14
23	a	406	CLA	C6-C7-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	b	607	CLA	C11-C12-C13-C14
23	b	613	CLA	C6-C7-C8-C9
23	b	617	CLA	C11-C10-C8-C9
23	c	503	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C10-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	c	513	CLA	C11-C10-C8-C9
23	c	513	CLA	C14-C13-C15-C16
31	D	406	LMG	O6-C5-C6-O5
28	B	627	DGD	C9B-CAB-CBB-CCB
30	a	401	SQD	C18-C19-C20-C21
23	c	504	CLA	C2A-CAA-CBA-CGA
29	A	412	LHG	C30-C31-C32-C33
31	a	402	LMG	C32-C33-C34-C35
34	V	201	HEM	C4D-C3D-CAD-CBD
27	j	102	BCR	C7-C8-C9-C34
33	b	627	LMT	C2B-C1B-O1B-C4'
23	c	504	CLA	O1A-CGA-O2A-C1
23	B	616	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	C	501	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	b	620	CLA	C1A-C2A-CAA-CBA
23	c	501	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
23	B	613	CLA	C16-C17-C18-C20
23	b	605	CLA	C16-C17-C18-C19
28	B	621	DGD	C5B-C6B-C7B-C8B
23	A	407	CLA	C5-C6-C7-C8
23	B	602	CLA	C13-C15-C16-C17
23	C	503	CLA	C8-C10-C11-C12
23	C	505	CLA	C15-C16-C17-C18
31	E	101	LMG	O6-C5-C6-O5
23	C	502	CLA	C3-C5-C6-C7
29	a	414	LHG	O6-C4-C5-C6
28	c	516	DGD	C5A-C6A-C7A-C8A
31	a	402	LMG	C4-C5-C6-O5
28	c	518	DGD	C1A-C2A-C3A-C4A
31	A	414	LMG	C20-C21-C22-C23
31	D	406	LMG	C31-C32-C33-C34
31	a	416	LMG	C15-C16-C17-C18
30	a	415	SQD	C11-C10-C9-C8
23	b	616	CLA	O1D-CGD-O2D-CED
28	B	627	DGD	C2B-C3B-C4B-C5B
28	b	602	DGD	C2B-C3B-C4B-C5B
23	c	502	CLA	C3-C5-C6-C7
33	B	625	LMT	C2B-C1B-O1B-C4'
31	e	101	LMG	C17-C18-C19-C20
23	C	505	CLA	C4-C3-C5-C6
25	j	101	PL9	C15-C14-C16-C17
30	A	417	SQD	C10-C11-C12-C13
31	A	414	LMG	C15-C16-C17-C18
31	B	622	LMG	C20-C21-C22-C23
31	a	416	LMG	C20-C21-C22-C23
23	b	617	CLA	C16-C17-C18-C19
28	B	621	DGD	O1G-C1G-C2G-C3G
28	C	519	DGD	O1G-C1G-C2G-C3G
28	D	409	DGD	C1G-C2G-C3G-O3G
28	b	602	DGD	C1G-C2G-C3G-O3G
28	b	623	DGD	O1G-C1G-C2G-C3G
28	d	409	DGD	C8B-C9B-CAB-CBB
28	d	409	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
30	A	417	SQD	O6-C44-C45-C46
30	B	626	SQD	C44-C45-C46-O48
30	a	401	SQD	O6-C44-C45-C46
30	b	601	SQD	C44-C45-C46-O48
31	A	414	LMG	O1-C7-C8-C9
31	C	520	LMG	C7-C8-C9-O8
31	D	407	LMG	O1-C7-C8-C9
31	I	101	LMG	O1-C7-C8-C9
31	d	407	LMG	O1-C7-C8-C9
31	i	101	LMG	O1-C7-C8-C9
31	k	103	LMG	C7-C8-C9-O8
28	B	621	DGD	CAB-CBB-CCB-CDB
31	i	101	LMG	C4-C5-C6-O5
31	D	407	LMG	C8-C7-O1-C1
31	a	416	LMG	C8-C7-O1-C1
28	b	623	DGD	C3B-C4B-C5B-C6B
31	d	406	LMG	C31-C32-C33-C34
23	B	604	CLA	C8-C10-C11-C12
23	b	608	CLA	C8-C10-C11-C12
28	B	621	DGD	C3B-C4B-C5B-C6B
30	A	413	SQD	C11-C10-C9-C8
31	B	622	LMG	C10-C11-C12-C13
23	b	615	CLA	O1A-CGA-O2A-C1
29	a	414	LHG	C30-C31-C32-C33
31	i	101	LMG	O6-C1-O1-C7
30	A	417	SQD	C12-C13-C14-C15
30	a	401	SQD	C12-C13-C14-C15
30	a	401	SQD	C32-C33-C34-C35
23	c	503	CLA	C8-C10-C11-C12
31	A	418	LMG	C28-C29-C30-C31
31	a	416	LMG	C11-C10-O7-C8
31	D	406	LMG	C38-C39-C40-C41
23	C	502	CLA	C13-C15-C16-C17
31	e	101	LMG	O6-C5-C6-O5
31	d	406	LMG	C38-C39-C40-C41
23	C	504	CLA	CBA-CGA-O2A-C1
23	D	403	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
30	A	413	SQD	C10-C11-C12-C13
31	E	101	LMG	C19-C20-C21-C22
31	d	407	LMG	C32-C33-C34-C35
23	c	507	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	C15-C16-C17-C18
23	c	502	CLA	C13-C15-C16-C17
30	A	417	SQD	C32-C33-C34-C35
31	e	101	LMG	C19-C20-C21-C22
23	A	403	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
23	b	617	CLA	C2-C1-O2A-CGA
23	c	509	CLA	C2-C1-O2A-CGA
31	B	622	LMG	C15-C16-C17-C18
31	k	103	LMG	C16-C17-C18-C19
31	d	407	LMG	C10-C11-C12-C13
28	C	518	DGD	CAB-CBB-CCB-CDB
23	c	505	CLA	C15-C16-C17-C18
31	B	623	LMG	C15-C16-C17-C18
23	C	505	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
29	a	417	LHG	O6-C4-C5-O7
31	b	624	LMG	C20-C21-C22-C23
23	b	608	CLA	C15-C16-C17-C18
31	A	418	LMG	C15-C16-C17-C18
23	B	616	CLA	C15-C16-C17-C18
23	b	609	CLA	C15-C16-C17-C18
28	D	409	DGD	C2D-C1D-O3G-C3G
28	d	409	DGD	C2D-C1D-O3G-C3G
30	A	413	SQD	O6-C44-C45-O47
30	a	415	SQD	O6-C44-C45-O47
31	A	414	LMG	O1-C7-C8-O7
31	E	101	LMG	O1-C7-C8-O7
31	d	407	LMG	C11-C12-C13-C14
31	b	625	LMG	O10-C28-O8-C9
31	m	102	LMG	O10-C28-O8-C9
31	i	101	LMG	C18-C19-C20-C21
33	B	625	LMT	O5B-C1B-O1B-C4'
23	c	505	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6
23	B	603	CLA	C6-C7-C8-C10
23	B	605	CLA	C11-C10-C8-C7
23	B	610	CLA	C11-C12-C13-C15
23	B	610	CLA	C12-C13-C15-C16
23	B	611	CLA	C11-C10-C8-C7
23	B	613	CLA	C11-C10-C8-C7
23	B	615	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C12-C13-C15-C16
23	B	616	CLA	C11-C10-C8-C7
23	C	502	CLA	C11-C12-C13-C15
23	C	503	CLA	C11-C10-C8-C7
23	C	503	CLA	C11-C12-C13-C15
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C6-C7-C8-C10
23	C	506	CLA	C11-C12-C13-C15
23	C	510	CLA	C11-C10-C8-C7
23	C	511	CLA	C12-C13-C15-C16
23	D	401	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C7
23	b	619	CLA	C12-C13-C15-C16
23	b	620	CLA	C11-C10-C8-C7
23	c	502	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C10-C8-C7
23	c	503	CLA	C11-C12-C13-C15
23	c	505	CLA	C2-C3-C5-C6
23	c	505	CLA	C6-C7-C8-C10
23	c	510	CLA	C6-C7-C8-C10
23	c	511	CLA	C12-C13-C15-C16
23	d	402	CLA	C12-C13-C15-C16
24	A	406	PHO	C12-C13-C15-C16
24	a	408	PHO	C12-C13-C15-C16
23	c	510	CLA	C3-C5-C6-C7
31	B	623	LMG	O10-C28-O8-C9
28	D	409	DGD	CBA-CCA-CDA-CEA
28	c	517	DGD	CAB-CBB-CCB-CDB
23	A	404	CLA	C6-C7-C8-C9
23	B	603	CLA	C6-C7-C8-C9
23	B	606	CLA	C14-C13-C15-C16
23	B	609	CLA	C6-C7-C8-C9
23	B	613	CLA	C11-C10-C8-C9
23	B	615	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C14
23	C	502	CLA	C14-C13-C15-C16
23	C	503	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C6-C7-C8-C9
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C10-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	D	401	CLA	C14-C13-C15-C16
23	b	607	CLA	C6-C7-C8-C9
23	b	610	CLA	C14-C13-C15-C16
23	b	619	CLA	C14-C13-C15-C16
23	c	502	CLA	C11-C12-C13-C14
23	c	502	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C14
23	c	505	CLA	C6-C7-C8-C9
23	c	505	CLA	C14-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C9
23	c	511	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C12-C13-C14
23	d	402	CLA	C14-C13-C15-C16
24	A	406	PHO	C14-C13-C15-C16
24	a	407	PHO	C6-C7-C8-C9
24	a	408	PHO	C14-C13-C15-C16
23	A	407	CLA	C13-C15-C16-C17
33	b	627	LMT	O5B-C1B-O1B-C4'
23	c	513	CLA	C2A-CAA-CBA-CGA
28	b	623	DGD	CAB-CBB-CCB-CDB
23	B	610	CLA	C16-C17-C18-C20
23	a	409	CLA	C13-C15-C16-C17
23	b	620	CLA	C15-C16-C17-C18
23	c	509	CLA	C15-C16-C17-C18
31	E	101	LMG	C18-C19-C20-C21
23	B	611	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	CBA-CGA-O2A-C1
29	A	415	LHG	C24-C23-O8-C6
31	D	407	LMG	C10-C11-C12-C13
23	B	616	CLA	C8-C10-C11-C12
23	b	620	CLA	C8-C10-C11-C12
30	a	401	SQD	C10-C11-C12-C13
31	B	622	LMG	C17-C18-C19-C20
33	I	102	LMT	C5'-C4'-O1B-C1B
23	c	512	CLA	C16-C17-C18-C20
28	C	518	DGD	O6E-C1E-O5D-C6D
28	c	517	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
29	A	412	LHG	O6-C4-C5-C6
23	C	510	CLA	C3-C5-C6-C7
25	j	101	PL9	C19-C21-C22-C23
28	d	409	DGD	CBA-CCA-CDA-CEA
31	I	101	LMG	C18-C19-C20-C21
23	C	509	CLA	CBA-CGA-O2A-C1
28	C	517	DGD	C2A-C3A-C4A-C5A
31	C	520	LMG	C16-C17-C18-C19
23	C	513	CLA	C4-C3-C5-C6
23	a	405	CLA	C4-C3-C5-C6
25	J	101	PL9	C15-C14-C16-C17
23	C	513	CLA	C2-C3-C5-C6
23	c	513	CLA	C2-C3-C5-C6
30	D	408	SQD	C7-C8-C9-C10
31	A	418	LMG	C12-C13-C14-C15
23	d	403	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
31	B	622	LMG	C13-C14-C15-C16
23	B	610	CLA	CBA-CGA-O2A-C1
29	a	417	LHG	C24-C23-O8-C6
31	a	402	LMG	C28-C29-C30-C31
23	A	403	CLA	C3A-C2A-CAA-CBA
30	A	413	SQD	C15-C16-C17-C18
31	b	625	LMG	C15-C16-C17-C18
31	e	101	LMG	C18-C19-C20-C21
23	b	617	CLA	C16-C17-C18-C20
28	D	409	DGD	C8B-C9B-CAB-CBB
31	m	102	LMG	C11-C12-C13-C14
33	i	102	LMT	C5'-C4'-O1B-C1B
28	B	627	DGD	C1G-C2G-C3G-O3G
28	c	517	DGD	C1G-C2G-C3G-O3G
30	A	413	SQD	O6-C44-C45-C46
30	a	415	SQD	O6-C44-C45-C46
30	d	408	SQD	O6-C44-C45-C46
31	B	623	LMG	C7-C8-C9-O8
31	M	101	LMG	C7-C8-C9-O8
31	b	625	LMG	C7-C8-C9-O8
31	m	102	LMG	C7-C8-C9-O8
28	A	411	DGD	C3B-C4B-C5B-C6B
28	c	518	DGD	CFA-CGA-CHA-CIA
30	A	413	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	a	402	LMG	C12-C13-C14-C15
28	D	409	DGD	C1A-C2A-C3A-C4A
23	C	504	CLA	O1A-CGA-O2A-C1
23	C	512	CLA	C3-C5-C6-C7
31	D	407	LMG	C11-C12-C13-C14
23	D	403	CLA	O1A-CGA-O2A-C1
24	a	407	PHO	C5-C6-C7-C8
28	C	519	DGD	CDB-CEB-CFB-CGB
31	c	519	LMG	C13-C14-C15-C16
31	C	521	LMG	C13-C14-C15-C16
28	d	409	DGD	C1A-C2A-C3A-C4A
30	d	408	SQD	C7-C8-C9-C10
23	c	512	CLA	C3-C5-C6-C7
28	c	516	DGD	C2A-C3A-C4A-C5A
30	a	415	SQD	C10-C11-C12-C13
29	a	414	LHG	O6-C4-C5-O7
23	C	505	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	O1A-CGA-O2A-C1
23	b	614	CLA	C16-C17-C18-C19
23	c	508	CLA	C5-C6-C7-C8
30	B	626	SQD	C12-C13-C14-C15
31	b	624	LMG	C17-C18-C19-C20
28	b	602	DGD	O1G-C1G-C2G-O2G
30	B	626	SQD	O47-C45-C46-O48
30	a	415	SQD	O47-C45-C46-O48
30	b	601	SQD	O47-C45-C46-O48
30	f	102	SQD	O47-C45-C46-O48
31	B	623	LMG	O7-C8-C9-O8
31	I	101	LMG	O1-C7-C8-O7
31	b	625	LMG	O7-C8-C9-O8
31	i	101	LMG	O1-C7-C8-O7
30	A	417	SQD	C30-C31-C32-C33
30	b	601	SQD	C15-C16-C17-C18
31	A	414	LMG	C31-C32-C33-C34
29	A	412	LHG	C8-C7-O7-C5
23	B	601	CLA	C16-C17-C18-C20
28	a	413	DGD	C8B-C9B-CAB-CBB
23	a	405	CLA	C5-C6-C7-C8
25	J	101	PL9	C19-C21-C22-C23
25	J	101	PL9	C24-C26-C27-C28
25	a	410	PL9	C14-C16-C17-C18
25	a	410	PL9	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
31	A	418	LMG	C32-C33-C34-C35
31	M	101	LMG	C11-C12-C13-C14
23	B	610	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
23	B	615	CLA	C6-C7-C8-C9
23	C	505	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C12-C13-C14
23	b	613	CLA	C14-C13-C15-C16
23	b	619	CLA	C6-C7-C8-C9
23	b	619	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
24	D	402	PHO	C6-C7-C8-C9
23	c	511	CLA	CBA-CGA-O2A-C1
30	a	415	SQD	C31-C32-C33-C34
28	C	519	DGD	CDA-CEA-CFA-CGA
23	b	617	CLA	C13-C15-C16-C17
23	c	505	CLA	C8-C10-C11-C12
24	D	402	PHO	C5-C6-C7-C8
31	C	520	LMG	C30-C31-C32-C33
23	C	512	CLA	C16-C17-C18-C20
30	a	401	SQD	C23-C24-C25-C26
27	B	617	BCR	C1-C6-C7-C8
27	B	617	BCR	C5-C6-C7-C8
27	C	514	BCR	C5-C6-C7-C8
27	J	102	BCR	C1-C6-C7-C8
27	J	102	BCR	C5-C6-C7-C8
27	T	101	BCR	C5-C6-C7-C8
27	c	514	BCR	C5-C6-C7-C8
27	j	102	BCR	C1-C6-C7-C8
27	j	102	BCR	C5-C6-C7-C8
23	C	508	CLA	C5-C6-C7-C8
28	B	627	DGD	CAB-CBB-CCB-CDB
27	b	622	BCR	C37-C22-C23-C24
25	D	404	PL9	C47-C48-C49-C51
28	c	518	DGD	CDB-CEB-CFB-CGB
30	a	415	SQD	C15-C16-C17-C18
27	D	405	BCR	C21-C22-C23-C24
27	c	515	BCR	C21-C22-C23-C24
27	d	405	BCR	C21-C22-C23-C24
31	m	102	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
29	A	412	LHG	O9-C7-O7-C5
31	b	624	LMG	C15-C16-C17-C18
28	C	519	DGD	C1A-C2A-C3A-C4A
29	A	412	LHG	C23-C24-C25-C26
23	b	607	CLA	C8-C10-C11-C12
23	c	512	CLA	C5-C6-C7-C8
23	B	611	CLA	O1A-CGA-O2A-C1
23	c	507	CLA	O1D-CGD-O2D-CED
31	a	402	LMG	C15-C16-C17-C18
23	c	501	CLA	C13-C15-C16-C17
29	a	417	LHG	O6-C4-C5-C6
33	B	624	LMT	C4-C5-C6-C7
23	A	404	CLA	C12-C13-C15-C16
23	B	601	CLA	C11-C12-C13-C15
23	B	602	CLA	C6-C7-C8-C10
23	B	602	CLA	C11-C10-C8-C7
23	B	606	CLA	C12-C13-C15-C16
23	B	608	CLA	C6-C7-C8-C10
23	B	609	CLA	C12-C13-C15-C16
23	B	612	CLA	C6-C7-C8-C10
23	B	613	CLA	C11-C12-C13-C15
23	C	501	CLA	C11-C12-C13-C15
23	C	502	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C10-C8-C7
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	508	CLA	C12-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C7
23	C	510	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10
23	C	512	CLA	C11-C12-C13-C15
23	C	512	CLA	C12-C13-C15-C16
23	b	605	CLA	C11-C12-C13-C15
23	b	606	CLA	C6-C7-C8-C10
23	b	607	CLA	C6-C7-C8-C10
23	b	609	CLA	C11-C10-C8-C7
23	b	610	CLA	C12-C13-C15-C16
23	b	612	CLA	C6-C7-C8-C10
23	b	613	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C10-C8-C7
23	b	617	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	b	619	CLA	C11-C10-C8-C7
23	b	620	CLA	C12-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C15
23	c	502	CLA	C12-C13-C15-C16
23	c	505	CLA	C11-C10-C8-C7
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
23	c	508	CLA	C11-C10-C8-C7
23	c	508	CLA	C12-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C7
23	c	511	CLA	C6-C7-C8-C10
23	c	512	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
23	b	614	CLA	O1A-CGA-O2A-C1
31	A	418	LMG	C17-C18-C19-C20
23	B	610	CLA	C10-C11-C12-C13
27	B	618	BCR	C13-C14-C15-C16
23	b	608	CLA	CBA-CGA-O2A-C1
30	A	417	SQD	C33-C34-C35-C36
23	C	504	CLA	C2A-CAA-CBA-CGA
28	B	621	DGD	C7A-C8A-C9A-CAA
28	c	518	DGD	C8B-C9B-CAB-CBB
23	B	601	CLA	C16-C17-C18-C19
23	c	512	CLA	C16-C17-C18-C19
23	A	404	CLA	C5-C6-C7-C8
23	B	605	CLA	C5-C6-C7-C8
23	B	612	CLA	C10-C11-C12-C13
23	b	616	CLA	C10-C11-C12-C13
23	c	505	CLA	CBA-CGA-O2A-C1
28	b	623	DGD	C4B-C5B-C6B-C7B
29	a	417	LHG	C25-C26-C27-C28
34	v	201	HEM	C2D-C3D-CAD-CBD
31	I	101	LMG	C29-C30-C31-C32
23	B	605	CLA	C15-C16-C17-C18
23	C	509	CLA	C15-C16-C17-C18
23	b	609	CLA	C5-C6-C7-C8
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	a	408	PHO	CAD-CBD-CGD-O2D
28	C	519	DGD	C3G-C2G-O2G-C1B
31	C	521	LMG	C9-C8-O7-C10
31	c	519	LMG	C9-C8-O7-C10
23	C	507	CLA	C3-C5-C6-C7
28	C	518	DGD	C7B-C8B-C9B-CAB
31	M	101	LMG	C30-C31-C32-C33
23	b	609	CLA	C10-C11-C12-C13
23	c	509	CLA	C10-C11-C12-C13
28	C	517	DGD	C2B-C3B-C4B-C5B
23	C	511	CLA	CBA-CGA-O2A-C1
30	D	408	SQD	O5-C1-O6-C44
31	b	625	LMG	O6-C1-O1-C7
28	C	518	DGD	C1G-C2G-C3G-O3G
31	B	622	LMG	O1-C7-C8-C9
31	b	624	LMG	O1-C7-C8-C9
23	C	509	CLA	O1A-CGA-O2A-C1
31	M	101	LMG	O10-C28-O8-C9
28	C	519	DGD	CFA-CGA-CHA-CIA
29	A	412	LHG	O6-C4-C5-O7
28	a	413	DGD	C3B-C4B-C5B-C6B
31	d	406	LMG	C11-C12-C13-C14
34	v	201	HEM	C4D-C3D-CAD-CBD
34	F	101	HEM	C4B-C3B-CAB-CBB
34	f	101	HEM	C4B-C3B-CAB-CBB
23	a	404	CLA	C2A-CAA-CBA-CGA
23	C	505	CLA	C8-C10-C11-C12
23	a	406	CLA	C2C-C3C-CAC-CBC
30	b	601	SQD	C12-C13-C14-C15
23	b	607	CLA	C16-C17-C18-C19
28	b	602	DGD	CAB-CBB-CCB-CDB
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	CHA-CBD-CGD-O2D
23	b	611	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	CHA-CBD-CGD-O2D
23	b	613	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	O1A-CGA-O2A-C1
29	A	415	LHG	O10-C23-O8-C6
31	k	103	LMG	C30-C31-C32-C33
30	F	102	SQD	C2-C1-O6-C44
31	b	625	LMG	C2-C1-O1-C7
30	B	626	SQD	C15-C16-C17-C18
28	D	409	DGD	O2G-C2G-C3G-O3G
28	b	623	DGD	O1G-C1G-C2G-O2G
28	d	409	DGD	O2G-C2G-C3G-O3G
30	A	413	SQD	O47-C45-C46-O48
31	a	416	LMG	O1-C7-C8-O7
31	e	101	LMG	O1-C7-C8-O7
31	m	102	LMG	O7-C8-C9-O8
23	B	608	CLA	C13-C15-C16-C17
30	f	102	SQD	C29-C30-C31-C32
31	b	625	LMG	C35-C36-C37-C38
30	a	415	SQD	C16-C17-C18-C19
30	A	413	SQD	C8-C7-O47-C45
25	D	404	PL9	C15-C14-C16-C17
25	d	404	PL9	C15-C14-C16-C17
31	a	416	LMG	C31-C32-C33-C34
30	b	601	SQD	O49-C7-O47-C45
23	A	404	CLA	C14-C13-C15-C16
23	B	609	CLA	C14-C13-C15-C16
23	B	612	CLA	C6-C7-C8-C9
23	b	608	CLA	O1A-CGA-O2A-C1
23	c	511	CLA	O1A-CGA-O2A-C1
31	a	402	LMG	O10-C28-O8-C9
28	C	518	DGD	C4B-C5B-C6B-C7B
23	C	510	CLA	C16-C17-C18-C19
23	C	510	CLA	O1D-CGD-O2D-CED
24	a	407	PHO	CBD-CGD-O2D-CED
30	a	401	SQD	C30-C31-C32-C33
23	c	505	CLA	O1A-CGA-O2A-C1
29	a	417	LHG	O10-C23-O8-C6
27	A	410	BCR	C7-C8-C9-C34
27	B	618	BCR	C11-C12-C13-C35
27	J	102	BCR	C7-C8-C9-C34
27	j	102	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	z	101	BCR	C7-C8-C9-C34
28	C	519	DGD	C8B-C9B-CAB-CBB
30	a	401	SQD	C33-C34-C35-C36
27	b	622	BCR	C21-C22-C23-C24
29	A	415	LHG	C25-C26-C27-C28
23	B	603	CLA	C16-C17-C18-C19
23	B	614	CLA	C5-C6-C7-C8
29	A	412	LHG	C3-O3-P-O6
28	b	623	DGD	C7A-C8A-C9A-CAA
29	A	412	LHG	C2-C3-O3-P
29	a	414	LHG	C2-C3-O3-P
23	A	404	CLA	C2-C3-C5-C6
28	B	621	DGD	C4B-C5B-C6B-C7B
28	B	621	DGD	C7B-C8B-C9B-CAB
29	A	412	LHG	C4-O6-P-O5
29	A	415	LHG	C3-O3-P-O5
29	a	417	LHG	C3-O3-P-O5
23	B	614	CLA	C16-C17-C18-C20
23	C	512	CLA	C16-C17-C18-C19
31	B	623	LMG	C35-C36-C37-C38
23	b	610	CLA	C13-C15-C16-C17
23	b	614	CLA	C10-C11-C12-C13
24	A	406	PHO	C10-C11-C12-C13
23	B	604	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	CBA-CGA-O2A-C1
28	c	518	DGD	O6E-C5E-C6E-O5E
29	A	415	LHG	O6-C4-C5-C6
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
28	c	517	DGD	C4B-C5B-C6B-C7B
28	c	516	DGD	C2B-C3B-C4B-C5B
30	A	413	SQD	C16-C17-C18-C19
33	B	629	LMT	C5'-C4'-O1B-C1B
23	B	603	CLA	C11-C10-C8-C7
23	B	608	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C10
23	a	405	CLA	C12-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	c	506	CLA	C11-C12-C13-C15
23	d	403	CLA	C11-C10-C8-C7
29	A	415	LHG	O6-C4-C5-O7
31	i	101	LMG	C29-C30-C31-C32
28	D	409	DGD	CBB-CCB-CDB-CEB
30	a	401	SQD	C26-C27-C28-C29
31	a	402	LMG	C17-C18-C19-C20
23	B	610	CLA	C5-C6-C7-C8
31	b	624	LMG	C10-C11-C12-C13
23	C	511	CLA	O1A-CGA-O2A-C1
31	a	402	LMG	C30-C31-C32-C33
23	a	406	CLA	C5-C6-C7-C8
23	A	407	CLA	C16-C17-C18-C19
23	b	607	CLA	C16-C17-C18-C20
29	a	414	LHG	C23-C24-C25-C26
31	b	625	LMG	C28-C29-C30-C31
30	D	408	SQD	O6-C44-C45-C46
30	a	415	SQD	C44-C45-C46-O48
30	f	102	SQD	C44-C45-C46-O48
31	E	101	LMG	O1-C7-C8-C9
31	e	101	LMG	O1-C7-C8-C9
29	a	414	LHG	O9-C7-O7-C5
28	B	621	DGD	O1G-C1G-C2G-O2G
31	C	520	LMG	O7-C8-C9-O8
31	D	407	LMG	O1-C7-C8-O7
31	M	101	LMG	O7-C8-C9-O8
31	d	407	LMG	O1-C7-C8-O7
31	k	103	LMG	O7-C8-C9-O8
31	B	622	LMG	C29-C30-C31-C32
28	c	518	DGD	CDA-CEA-CFA-CGA
30	F	102	SQD	C29-C30-C31-C32
30	a	401	SQD	C45-C44-O6-C1
31	A	414	LMG	C8-C7-O1-C1
31	d	407	LMG	C8-C7-O1-C1
23	a	409	CLA	C16-C17-C18-C19
23	B	603	CLA	C15-C16-C17-C18
23	c	507	CLA	C3-C5-C6-C7
31	b	624	LMG	C29-C30-C31-C32
30	a	401	SQD	C17-C18-C19-C20
31	D	406	LMG	C11-C12-C13-C14
30	a	415	SQD	C8-C7-O47-C45
30	A	417	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	B	610	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C10-C8-C9
23	B	613	CLA	C11-C12-C13-C14
23	B	616	CLA	C11-C10-C8-C9
23	C	501	CLA	C11-C12-C13-C14
23	C	503	CLA	C6-C7-C8-C9
23	C	506	CLA	C11-C12-C13-C14
23	C	508	CLA	C14-C13-C15-C16
23	C	509	CLA	C11-C10-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	C	512	CLA	C14-C13-C15-C16
23	D	401	CLA	C6-C7-C8-C9
23	a	405	CLA	C14-C13-C15-C16
23	b	609	CLA	C11-C10-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	b	615	CLA	C11-C10-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	b	617	CLA	C11-C12-C13-C14
23	b	620	CLA	C11-C10-C8-C9
23	c	501	CLA	C11-C12-C13-C14
23	c	508	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C9
23	c	510	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16
23	d	402	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C10-C8-C9
23	B	604	CLA	O1A-CGA-O2A-C1
31	B	622	LMG	C16-C17-C18-C19
31	a	402	LMG	C13-C14-C15-C16
28	A	411	DGD	C8B-C9B-CAB-CBB
30	d	408	SQD	O5-C1-O6-C44
25	A	408	PL9	C14-C16-C17-C18
25	A	408	PL9	C19-C21-C22-C23
25	D	404	PL9	C9-C11-C12-C13
31	i	101	LMG	C17-C18-C19-C20
23	B	615	CLA	O1A-CGA-O2A-C1
33	b	604	LMT	C5'-C4'-O1B-C1B
27	T	102	BCR	C13-C14-C15-C16
31	A	418	LMG	C13-C14-C15-C16
23	b	614	CLA	C5-C6-C7-C8
23	b	617	CLA	C10-C11-C12-C13
23	b	618	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	a	408	PHO	C13-C15-C16-C17
28	D	409	DGD	CAA-CBA-CCA-CDA
27	j	102	BCR	C7-C8-C9-C10
28	C	518	DGD	C7A-C8A-C9A-CAA
28	c	517	DGD	C3A-C4A-C5A-C6A
23	B	612	CLA	C4-C3-C5-C6
23	b	616	CLA	C4-C3-C5-C6
31	A	414	LMG	C35-C36-C37-C38
25	J	101	PL9	C13-C14-C16-C17
24	A	406	PHO	C13-C15-C16-C17
23	B	614	CLA	C16-C17-C18-C19
28	c	517	DGD	C7A-C8A-C9A-CAA
31	C	520	LMG	C12-C13-C14-C15
23	A	405	CLA	C5-C6-C7-C8
28	c	518	DGD	C3G-C2G-O2G-C1B
23	B	614	CLA	C2A-CAA-CBA-CGA
30	B	626	SQD	O49-C7-O47-C45
23	b	606	CLA	O1A-CGA-O2A-C1
23	B	606	CLA	C13-C15-C16-C17
23	C	508	CLA	C2-C1-O2A-CGA
23	b	605	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
28	c	517	DGD	C7B-C8B-C9B-CAB
23	C	512	CLA	CAA-CBA-CGA-O2A
29	a	414	LHG	C8-C7-O7-C5
31	A	414	LMG	C38-C39-C40-C41
31	A	418	LMG	C30-C31-C32-C33
28	C	519	DGD	CEA-CFA-CGA-CHA
27	a	412	BCR	C23-C24-C25-C26
27	a	412	BCR	C23-C24-C25-C30
23	c	512	CLA	CAA-CBA-CGA-O2A
23	B	613	CLA	C10-C11-C12-C13
23	B	613	CLA	C13-C15-C16-C17
30	f	102	SQD	C24-C25-C26-C27
23	B	603	CLA	C16-C17-C18-C20
23	C	510	CLA	C16-C17-C18-C20
28	C	518	DGD	O6D-C1D-O3G-C3G
23	b	612	CLA	C13-C15-C16-C17
28	B	627	DGD	O1G-C1G-C2G-O2G
30	F	102	SQD	O47-C45-C46-O48
31	C	521	LMG	O1-C7-C8-O7
28	B	627	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
28	a	413	DGD	C2A-C3A-C4A-C5A
29	a	414	LHG	C3-O3-P-O6
30	A	417	SQD	C23-C24-C25-C26
28	c	518	DGD	CEA-CFA-CGA-CHA
23	b	606	CLA	CBA-CGA-O2A-C1
28	b	602	DGD	O1G-C1G-C2G-C3G
30	A	413	SQD	C44-C45-C46-O48
23	B	611	CLA	C4-C3-C5-C6
28	A	411	DGD	C2A-C3A-C4A-C5A
30	D	408	SQD	C10-C11-C12-C13
23	C	503	CLA	C6-C7-C8-C10
23	b	612	CLA	C11-C12-C13-C15
23	c	503	CLA	C6-C7-C8-C10
23	c	504	CLA	C6-C7-C8-C10
23	B	605	CLA	C11-C10-C8-C9
23	B	609	CLA	C11-C12-C13-C14
23	D	403	CLA	C11-C10-C8-C9
23	a	409	CLA	C11-C10-C8-C9
23	b	620	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
33	B	629	LMT	C1-C2-C3-C4
23	B	604	CLA	C2C-C3C-CAC-CBC
33	b	626	LMT	C4-C5-C6-C7
23	A	407	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
23	b	618	CLA	C16-C17-C18-C20
28	C	519	DGD	O1A-C1A-O1G-C1G
23	C	510	CLA	C13-C15-C16-C17
27	C	516	BCR	C21-C22-C23-C24
27	J	102	BCR	C21-C22-C23-C24
28	b	602	DGD	C8B-C9B-CAB-CBB
31	I	101	LMG	C17-C18-C19-C20
25	j	101	PL9	C12-C13-C14-C16
23	a	405	CLA	C2-C3-C5-C6
25	j	101	PL9	C13-C14-C16-C17
23	b	610	CLA	C16-C17-C18-C20
31	d	406	LMG	O10-C28-O8-C9
31	k	103	LMG	C12-C13-C14-C15
23	B	605	CLA	C10-C11-C12-C13
23	b	618	CLA	C16-C17-C18-C19
28	c	517	DGD	O6D-C1D-O3G-C3G
25	d	404	PL9	C39-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
30	b	601	SQD	C19-C20-C21-C22
23	C	509	CLA	C10-C11-C12-C13
31	I	101	LMG	C19-C20-C21-C22
23	B	608	CLA	O1A-CGA-O2A-C1
29	A	412	LHG	C24-C25-C26-C27
31	E	101	LMG	C31-C32-C33-C34
23	c	503	CLA	C15-C16-C17-C18
23	A	405	CLA	C2C-C3C-CAC-CBC
23	A	404	CLA	C2-C1-O2A-CGA
23	B	601	CLA	C2-C1-O2A-CGA
23	B	614	CLA	C2-C1-O2A-CGA
23	a	405	CLA	C2-C1-O2A-CGA
23	b	618	CLA	C2-C1-O2A-CGA
23	b	618	CLA	C4C-C3C-CAC-CBC
23	b	607	CLA	C15-C16-C17-C18
28	a	413	DGD	C2E-C1E-O5D-C6D
23	D	403	CLA	C2A-CAA-CBA-CGA
23	a	405	CLA	C2A-CAA-CBA-CGA
23	b	607	CLA	C2A-CAA-CBA-CGA
23	b	618	CLA	C2A-CAA-CBA-CGA
31	c	519	LMG	O1-C7-C8-O7
31	a	416	LMG	C38-C39-C40-C41
23	C	513	CLA	C3A-C2A-CAA-CBA
23	a	404	CLA	C3A-C2A-CAA-CBA
23	c	513	CLA	C3A-C2A-CAA-CBA
23	a	406	CLA	C4C-C3C-CAC-CBC
30	A	413	SQD	O49-C7-O47-C45
25	A	408	PL9	C4-C3-C7-C8
25	a	410	PL9	C4-C3-C7-C8
23	B	615	CLA	C11-C12-C13-C14
23	a	405	CLA	C11-C10-C8-C9
23	b	620	CLA	C11-C12-C13-C14
23	c	503	CLA	C6-C7-C8-C9
23	B	604	CLA	C4C-C3C-CAC-CBC
31	a	416	LMG	C35-C36-C37-C38
30	B	626	SQD	C19-C20-C21-C22
28	D	409	DGD	O1G-C1G-C2G-C3G
28	d	409	DGD	O1G-C1G-C2G-C3G
31	a	402	LMG	C7-C8-C9-O8
31	a	416	LMG	O1-C7-C8-C9
25	d	404	PL9	C32-C33-C34-C36
24	a	407	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	c	518	DGD	C7A-C8A-C9A-CAA
27	B	620	BCR	C37-C22-C23-C24
28	d	409	DGD	CBB-CCB-CDB-CEB
31	D	406	LMG	C17-C18-C19-C20
33	b	604	LMT	C1-C2-C3-C4
29	a	414	LHG	C4-C5-O7-C7
31	m	102	LMG	C9-C8-O7-C10
23	B	603	CLA	C8-C10-C11-C12
23	b	610	CLA	C4-C3-C5-C6
23	b	615	CLA	C4-C3-C5-C6
23	A	403	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C1A-C2A-CAA-CBA
23	a	404	CLA	C1A-C2A-CAA-CBA
23	A	407	CLA	C11-C10-C8-C7
23	B	605	CLA	C11-C12-C13-C15
23	C	504	CLA	C6-C7-C8-C10
23	C	508	CLA	C11-C12-C13-C15
23	C	509	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	b	609	CLA	C11-C12-C13-C15
23	b	616	CLA	C6-C7-C8-C10
23	c	508	CLA	C11-C12-C13-C15
23	c	509	CLA	C6-C7-C8-C10
30	f	102	SQD	C26-C27-C28-C29
23	B	602	CLA	O1A-CGA-O2A-C1
31	d	407	LMG	C34-C35-C36-C37
23	B	602	CLA	CBA-CGA-O2A-C1
28	C	519	DGD	O6E-C5E-C6E-O5E
23	b	617	CLA	C8-C10-C11-C12
25	D	404	PL9	C47-C48-C49-C50
23	A	404	CLA	C2A-CAA-CBA-CGA
23	C	509	CLA	C2A-CAA-CBA-CGA
23	C	511	CLA	C2A-CAA-CBA-CGA
23	c	511	CLA	C2A-CAA-CBA-CGA
23	d	403	CLA	C2A-CAA-CBA-CGA
23	C	501	CLA	C13-C15-C16-C17
23	c	510	CLA	C13-C15-C16-C17
23	B	613	CLA	C8-C10-C11-C12
28	b	623	DGD	C7B-C8B-C9B-CAB
23	c	510	CLA	C16-C17-C18-C19
28	c	517	DGD	C4A-C5A-C6A-C7A
29	a	417	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
29	a	414	LHG	C24-C25-C26-C27
31	m	102	LMG	C4-C5-C6-O5
31	b	625	LMG	C12-C13-C14-C15
31	C	521	LMG	O7-C8-C9-O8
23	B	608	CLA	CBA-CGA-O2A-C1
31	c	519	LMG	C34-C35-C36-C37
24	a	408	PHO	C10-C11-C12-C13
25	j	101	PL9	C24-C26-C27-C28
31	C	520	LMG	C29-C30-C31-C32
24	a	407	PHO	C2-C1-O2A-CGA
23	B	612	CLA	C2-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
25	d	404	PL9	C13-C14-C16-C17
23	B	616	CLA	C11-C12-C13-C14
23	b	613	CLA	C11-C12-C13-C14
23	b	619	CLA	C11-C12-C13-C14
31	A	414	LMG	C12-C13-C14-C15
28	C	518	DGD	C3A-C4A-C5A-C6A
28	d	409	DGD	CAA-CBA-CCA-CDA
27	B	619	BCR	C1-C6-C7-C8
27	b	622	BCR	C23-C24-C25-C30
30	F	102	SQD	C26-C27-C28-C29
23	b	609	CLA	C8-C10-C11-C12
28	b	602	DGD	C5A-C6A-C7A-C8A
23	B	611	CLA	C2-C3-C5-C6
28	b	602	DGD	C2G-C3G-O3G-C1D
28	c	517	DGD	C5D-C6D-O5D-C1E
25	d	404	PL9	C47-C48-C49-C50
30	F	102	SQD	C24-C25-C26-C27
23	b	610	CLA	C16-C17-C18-C19
30	a	401	SQD	C25-C26-C27-C28
28	C	519	DGD	CBB-CCB-CDB-CEB
30	a	415	SQD	C29-C30-C31-C32
23	b	612	CLA	C4-C3-C5-C6
30	F	102	SQD	C15-C16-C17-C18
31	i	101	LMG	C19-C20-C21-C22
23	B	601	CLA	C12-C13-C15-C16
23	B	609	CLA	C11-C12-C13-C15
23	B	615	CLA	C11-C12-C13-C15
23	b	615	CLA	C2-C3-C5-C6
23	c	506	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	D	406	LMG	C19-C20-C21-C22
31	B	622	LMG	C2-C1-O1-C7
31	c	519	LMG	O7-C8-C9-O8
23	b	618	CLA	C2C-C3C-CAC-CBC
30	d	408	SQD	C10-C11-C12-C13
23	D	403	CLA	C8-C10-C11-C12
23	D	401	CLA	C3-C5-C6-C7
31	I	101	LMG	C15-C16-C17-C18
28	A	411	DGD	C4B-C5B-C6B-C7B
28	a	413	DGD	C4B-C5B-C6B-C7B
31	k	103	LMG	O8-C28-C29-C30
23	C	511	CLA	C4-C3-C5-C6
23	C	503	CLA	C15-C16-C17-C18
30	A	417	SQD	C26-C27-C28-C29
23	B	606	CLA	C16-C17-C18-C20
23	A	404	CLA	C11-C10-C8-C9
23	A	407	CLA	C11-C10-C8-C9
23	B	603	CLA	C11-C10-C8-C9
23	B	605	CLA	C11-C12-C13-C14
23	B	608	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C9
23	C	506	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C12-C13-C14
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D
31	M	101	LMG	C9-C8-O7-C10
24	D	402	PHO	C15-C16-C17-C18
23	c	512	CLA	C2-C1-O2A-CGA
31	C	521	LMG	C34-C35-C36-C37
31	D	407	LMG	C31-C32-C33-C34
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	507	CLA	CAA-CBA-CGA-O2A
28	C	518	DGD	CBB-CCB-CDB-CEB
30	f	102	SQD	C15-C16-C17-C18
31	d	406	LMG	C17-C18-C19-C20
23	c	511	CLA	C4-C3-C5-C6
31	e	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C15-C16-C17-C18
25	D	404	PL9	C13-C14-C16-C17
23	b	617	CLA	CAA-CBA-CGA-O2A
27	B	618	BCR	C11-C12-C13-C14
27	B	620	BCR	C21-C22-C23-C24
27	J	102	BCR	C7-C8-C9-C10
27	j	102	BCR	C21-C22-C23-C24
30	F	102	SQD	C44-C45-C46-O48
31	C	521	LMG	O1-C7-C8-C9
31	C	521	LMG	C7-C8-C9-O8
31	c	519	LMG	O1-C7-C8-C9
31	D	406	LMG	O10-C28-O8-C9
31	B	623	LMG	C12-C13-C14-C15
23	D	401	CLA	CAA-CBA-CGA-O2A
23	d	402	CLA	CAA-CBA-CGA-O2A
31	A	414	LMG	O7-C10-C11-C12
31	D	407	LMG	C29-C30-C31-C32
23	B	616	CLA	O2A-C1-C2-C3
23	C	512	CLA	O2A-C1-C2-C3
23	C	513	CLA	O2A-C1-C2-C3
23	b	620	CLA	O2A-C1-C2-C3
23	c	512	CLA	O2A-C1-C2-C3
24	A	406	PHO	O2A-C1-C2-C3
24	a	408	PHO	O2A-C1-C2-C3
28	c	517	DGD	CBB-CCB-CDB-CEB
31	a	416	LMG	O7-C10-C11-C12
23	c	510	CLA	C16-C17-C18-C20
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	CHA-CBD-CGD-O1D
23	B	609	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	513	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	613	CLA	CHA-CBD-CGD-O2D
23	b	616	CLA	CHA-CBD-CGD-O2D
23	b	618	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	513	CLA	CHA-CBD-CGD-O2D
23	c	501	CLA	CAA-CBA-CGA-O2A
30	A	413	SQD	C19-C20-C21-C22
23	B	614	CLA	CAA-CBA-CGA-O2A
30	a	401	SQD	O47-C7-C8-C9
28	a	413	DGD	O2G-C2G-C3G-O3G
31	D	406	LMG	O1-C7-C8-O7
31	d	406	LMG	O1-C7-C8-O7
31	e	101	LMG	O9-C10-C11-C12
31	k	103	LMG	C29-C30-C31-C32
23	A	405	CLA	C4C-C3C-CAC-CBC
23	B	614	CLA	C4C-C3C-CAC-CBC
31	C	520	LMG	C35-C36-C37-C38
23	d	403	CLA	C8-C10-C11-C12
23	b	612	CLA	O1A-CGA-O2A-C1
28	B	621	DGD	O2G-C1B-C2B-C3B
30	D	408	SQD	O47-C7-C8-C9
30	d	408	SQD	O47-C7-C8-C9
31	m	102	LMG	O8-C28-C29-C30
24	a	408	PHO	CHA-CBD-CGD-O1D
23	b	614	CLA	C13-C15-C16-C17
28	C	519	DGD	C7A-C8A-C9A-CAA
31	b	624	LMG	C16-C17-C18-C19
28	b	623	DGD	O2G-C1B-C2B-C3B
31	E	101	LMG	O7-C10-C11-C12
31	M	101	LMG	O8-C28-C29-C30
31	e	101	LMG	O7-C10-C11-C12
23	d	403	CLA	C4-C3-C5-C6
28	C	519	DGD	CCB-CDB-CEB-CFB
23	D	401	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	619	CLA	C11-C12-C13-C15
23	C	502	CLA	C16-C17-C18-C20
23	c	502	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	A	415	LHG	C9-C10-C11-C12
31	B	622	LMG	O6-C1-O1-C7
23	C	501	CLA	CAA-CBA-CGA-O2A
28	C	517	DGD	O1G-C1A-C2A-C3A
28	c	516	DGD	O1G-C1A-C2A-C3A
23	B	601	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C10-C8-C9
23	B	602	CLA	C11-C12-C13-C14
23	b	609	CLA	C11-C12-C13-C14
23	b	612	CLA	C11-C12-C13-C14
23	c	504	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	c	507	CLA	C11-C12-C13-C14
23	c	508	CLA	C11-C12-C13-C14
23	c	513	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C10-C8-C9
24	a	408	PHO	C6-C7-C8-C9
23	C	502	CLA	CBA-CGA-O2A-C1
24	A	406	PHO	CBA-CGA-O2A-C1
28	B	621	DGD	O1B-C1B-C2B-C3B
31	E	101	LMG	O9-C10-C11-C12
24	A	406	PHO	O1A-CGA-O2A-C1
25	D	404	PL9	C21-C22-C23-C24
25	d	404	PL9	C21-C22-C23-C24
25	j	101	PL9	C21-C22-C23-C24
23	d	402	CLA	CAA-CBA-CGA-O1A
23	c	507	CLA	CAA-CBA-CGA-O2A
31	C	520	LMG	O8-C28-C29-C30
23	A	404	CLA	C2C-C3C-CAC-CBC
28	c	518	DGD	CBB-CCB-CDB-CEB
31	a	416	LMG	C12-C13-C14-C15
25	A	408	PL9	C15-C14-C16-C17
30	B	626	SQD	C10-C11-C12-C13
23	c	510	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CBD-CGD-O2D-CED
28	c	518	DGD	CBA-CCA-CDA-CEA
23	a	406	CLA	O1D-CGD-O2D-CED
23	b	617	CLA	CAA-CBA-CGA-O1A
27	z	101	BCR	C7-C8-C9-C10
23	a	405	CLA	C2C-C3C-CAC-CBC
23	B	601	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	C	520	LMG	C34-C35-C36-C37
31	A	414	LMG	C16-C17-C18-C19
25	D	404	PL9	C46-C47-C48-C49
23	C	512	CLA	C2-C1-O2A-CGA
24	D	402	PHO	C2-C1-O2A-CGA
30	F	102	SQD	C9-C10-C11-C12
23	D	401	CLA	CAA-CBA-CGA-O1A
28	b	623	DGD	O1B-C1B-C2B-C3B
28	d	409	DGD	C8A-C9A-CAA-CBA
31	c	519	LMG	C7-C8-C9-O8
23	c	509	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	CAA-CBA-CGA-O1A
23	A	405	CLA	O1A-CGA-O2A-C1
23	b	618	CLA	CAA-CBA-CGA-O2A
23	B	605	CLA	C8-C10-C11-C12
24	a	407	PHO	C15-C16-C17-C18
23	C	507	CLA	CAA-CBA-CGA-O1A
23	C	502	CLA	O1A-CGA-O2A-C1
28	b	602	DGD	C2D-C1D-O3G-C3G
31	b	624	LMG	C2-C1-O1-C7
30	a	415	SQD	C19-C20-C21-C22
31	k	103	LMG	C34-C35-C36-C37
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	501	CLA	CAA-CBA-CGA-O1A
28	C	517	DGD	O1A-C1A-C2A-C3A
23	C	510	CLA	CAA-CBA-CGA-O2A
23	b	616	CLA	CAA-CBA-CGA-O2A
34	F	101	HEM	CAA-CBA-CGA-O2A
23	b	616	CLA	C3-C5-C6-C7
23	d	402	CLA	C5-C6-C7-C8
23	c	507	CLA	CAA-CBA-CGA-O1A
23	C	505	CLA	CAA-CBA-CGA-O2A
31	c	519	LMG	C36-C37-C38-C39
28	c	516	DGD	O1A-C1A-C2A-C3A
25	j	101	PL9	C17-C18-C19-C21
23	A	404	CLA	C4C-C3C-CAC-CBC
30	f	102	SQD	C27-C28-C29-C30
25	a	410	PL9	C15-C14-C16-C17
23	a	405	CLA	C16-C17-C18-C20
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	501	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	510	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	b	613	CLA	CAD-CBD-CGD-O1D
23	c	510	CLA	CAD-CBD-CGD-O1D
29	A	412	LHG	C4-C5-O7-C7
29	a	414	LHG	C6-C5-O7-C7
30	D	408	SQD	O5-C5-C6-S
30	d	408	SQD	O5-C5-C6-S
28	c	518	DGD	O1A-C1A-O1G-C1G
23	B	614	CLA	CAA-CBA-CGA-O1A
31	D	406	LMG	O9-C10-C11-C12
23	C	507	CLA	C6-C7-C8-C9
23	D	401	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14
23	b	607	CLA	C11-C10-C8-C9
23	b	615	CLA	C6-C7-C8-C9
34	f	101	HEM	CAA-CBA-CGA-O2A
30	a	401	SQD	O49-C7-C8-C9
28	C	519	DGD	CBA-CCA-CDA-CEA
31	a	402	LMG	C16-C17-C18-C19
23	A	405	CLA	CBA-CGA-O2A-C1
30	A	417	SQD	O47-C7-C8-C9
30	a	401	SQD	C9-C10-C11-C12
31	A	418	LMG	O10-C28-O8-C9
23	B	602	CLA	CAA-CBA-CGA-O2A
30	d	408	SQD	O49-C7-C8-C9
23	B	608	CLA	C4-C3-C5-C6
31	i	101	LMG	C15-C16-C17-C18
25	J	101	PL9	C12-C13-C14-C16
23	B	602	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C12-C13-C15
23	b	605	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	b	606	CLA	C12-C13-C15-C16
23	b	613	CLA	C11-C12-C13-C15
23	b	615	CLA	C6-C7-C8-C10
23	c	513	CLA	C11-C12-C13-C15
23	d	402	CLA	C11-C10-C8-C7
24	a	407	PHO	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	a	408	PHO	C6-C7-C8-C10
23	c	510	CLA	CAA-CBA-CGA-O1A
23	b	614	CLA	CAA-CBA-CGA-O2A
30	A	413	SQD	O47-C7-C8-C9
30	a	415	SQD	O47-C7-C8-C9
27	A	410	BCR	C7-C8-C9-C10
30	A	417	SQD	O49-C7-C8-C9
31	A	414	LMG	O9-C10-C11-C12
23	B	610	CLA	CAA-CBA-CGA-O2A
23	B	612	CLA	CAA-CBA-CGA-O2A
23	c	505	CLA	CAA-CBA-CGA-O2A
31	b	624	LMG	O6-C1-O1-C7
31	d	406	LMG	O9-C10-C11-C12
31	k	103	LMG	O10-C28-C29-C30
28	c	516	DGD	C2A-C1A-O1G-C1G
28	B	627	DGD	C5A-C6A-C7A-C8A
25	A	408	PL9	C16-C17-C18-C19
23	b	605	CLA	CAA-CBA-CGA-O2A
23	C	510	CLA	CAA-CBA-CGA-O1A
23	b	616	CLA	CAA-CBA-CGA-O1A
30	D	408	SQD	O49-C7-C8-C9
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	612	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	C3-C5-C6-C7
30	A	413	SQD	O49-C7-C8-C9
30	a	415	SQD	O49-C7-C8-C9
28	C	519	DGD	C2B-C3B-C4B-C5B
30	A	417	SQD	C25-C26-C27-C28
23	B	601	CLA	CAA-CBA-CGA-O2A

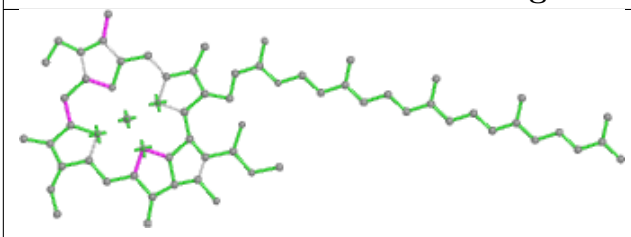
There are no ring outliers.

No monomer is involved in short contacts.

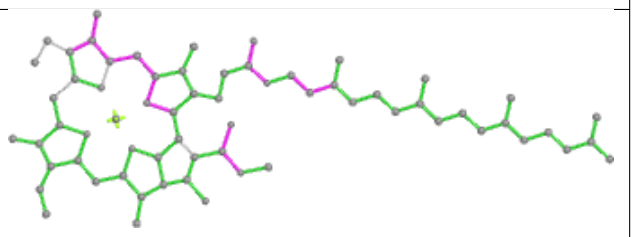
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

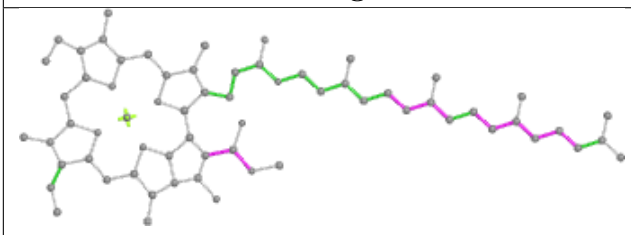
Ligand CLA c 506



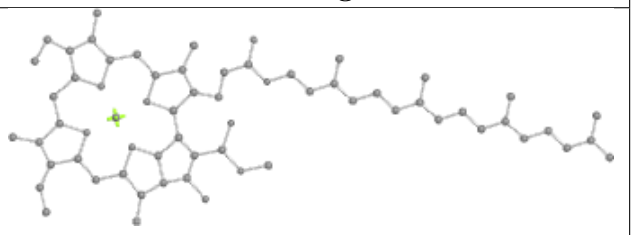
Bond lengths



Bond angles

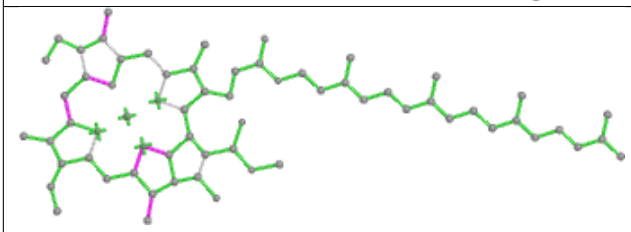


Torsions

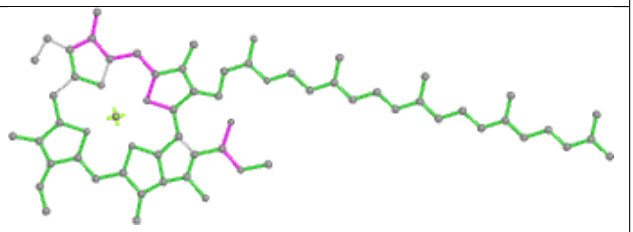


Rings

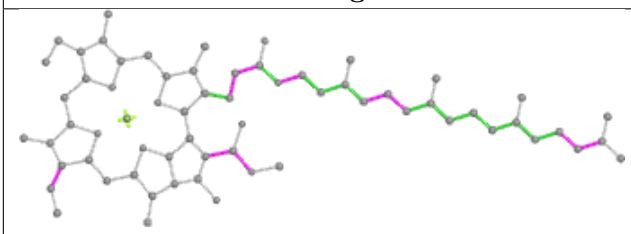
Ligand CLA b 618



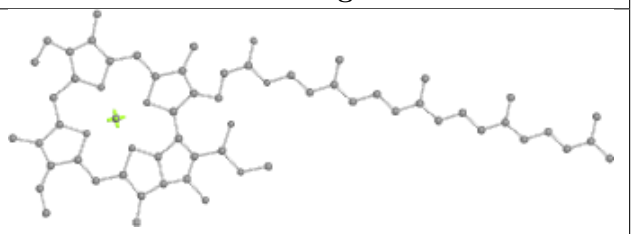
Bond lengths



Bond angles

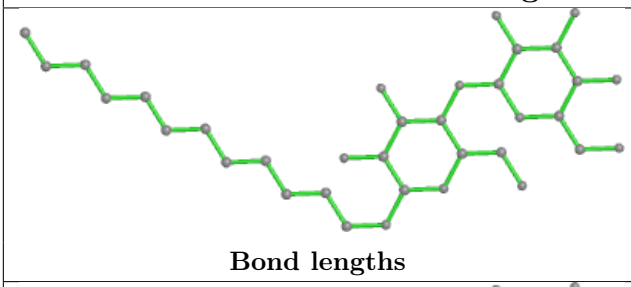


Torsions



Rings

Ligand LMT B 628



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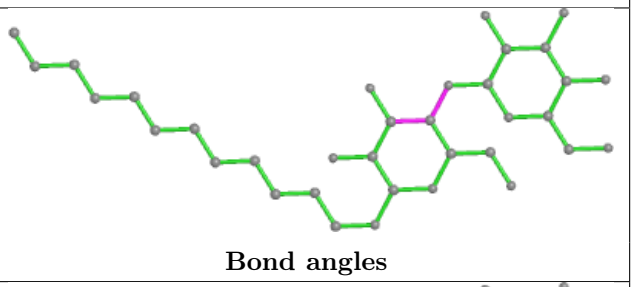
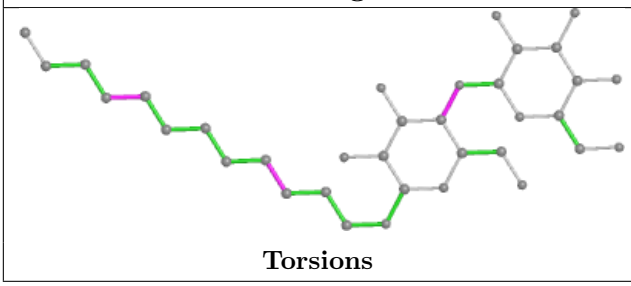
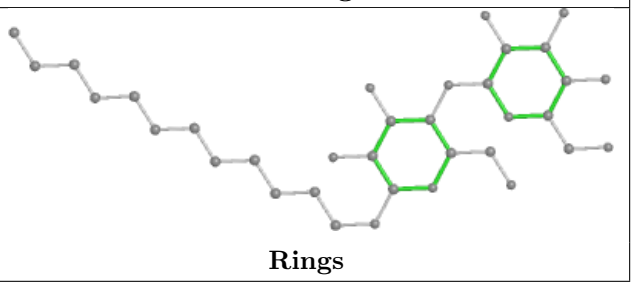


Bond angles

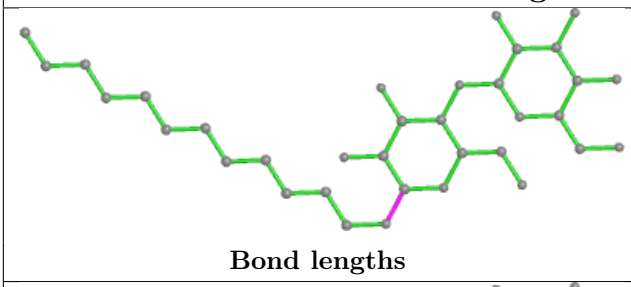


Torsions

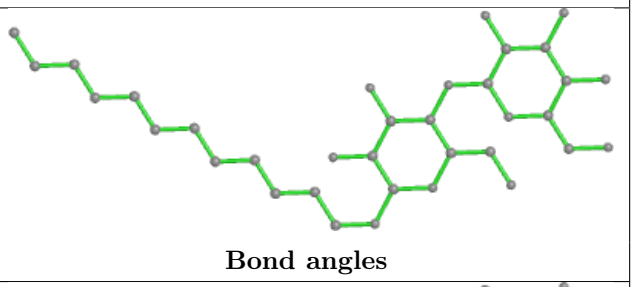


Rings

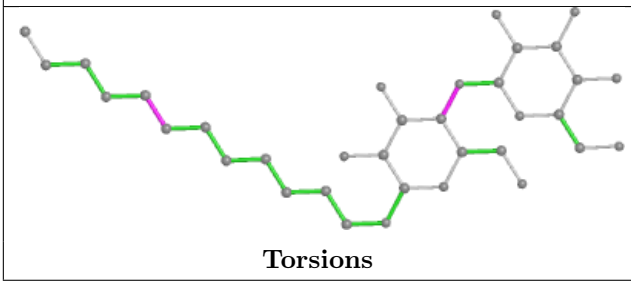
Ligand LMT i 102



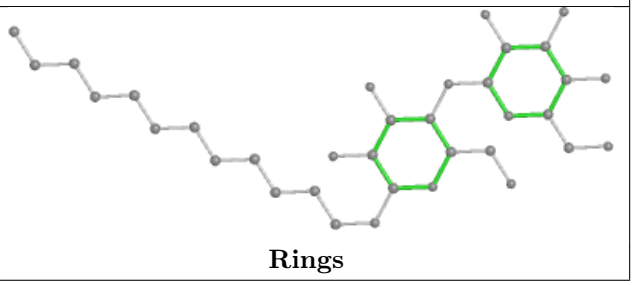
Bond lengths



Bond angles

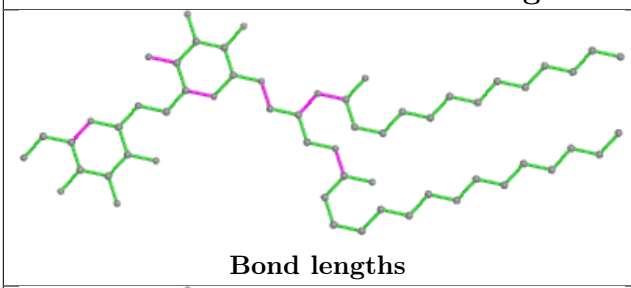


Torsions



Rings

Ligand DGD b 623



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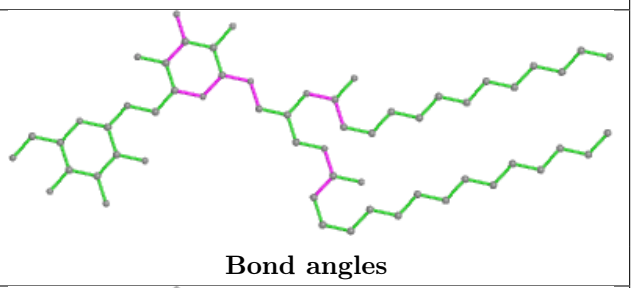
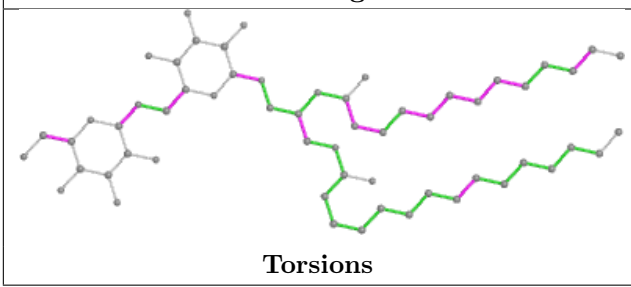
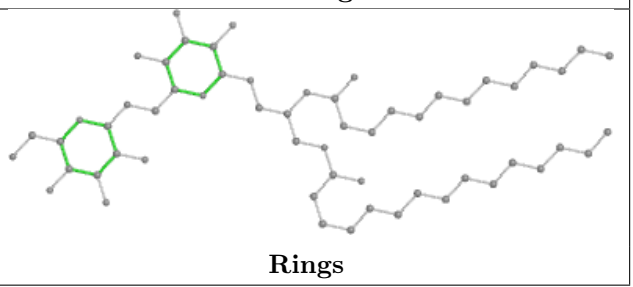


Bond angles

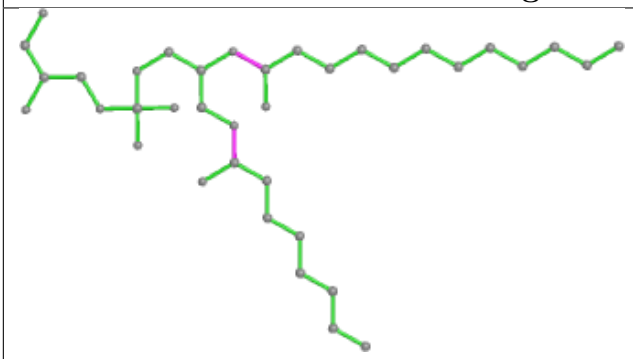


Torsions



Rings

Ligand LHG A 415



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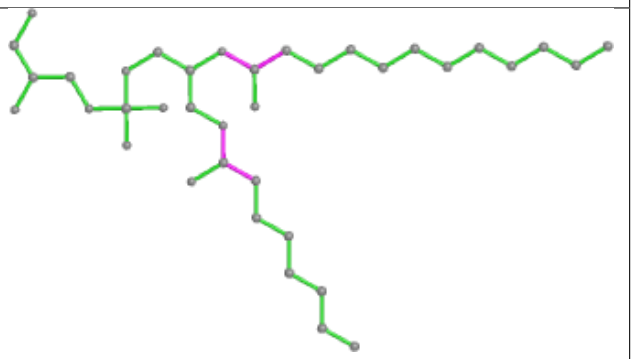
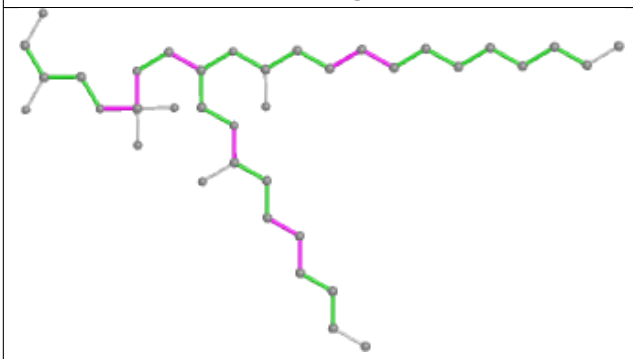
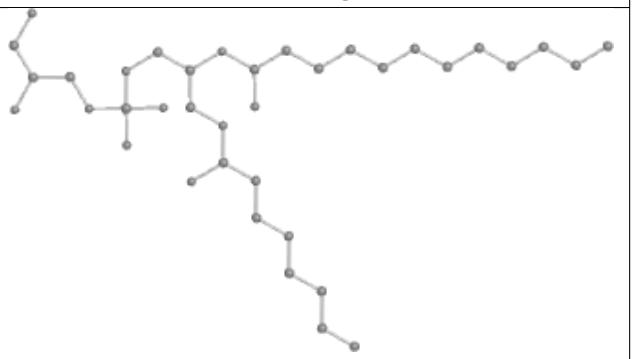


Bond angles

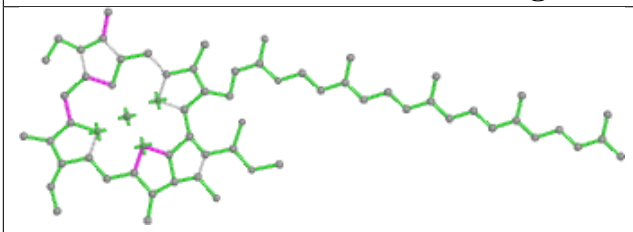


Torsions



Rings

Ligand CLA c 501



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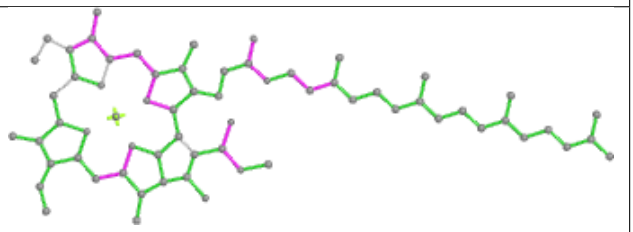
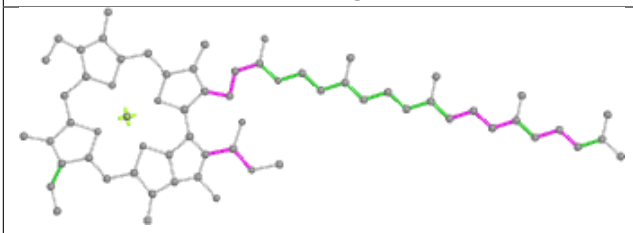
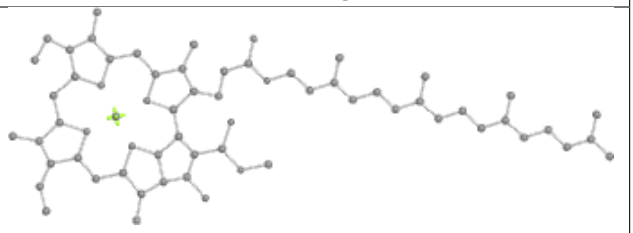


Bond angles

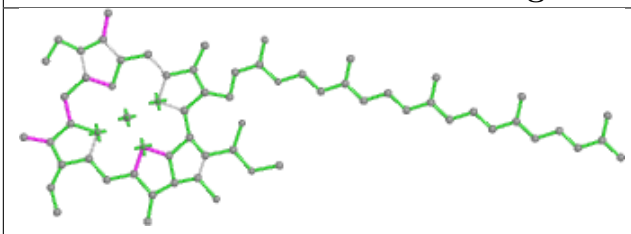


Torsions

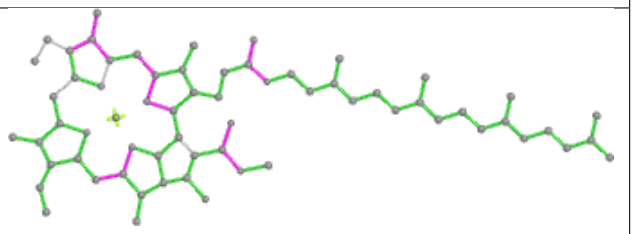


Rings

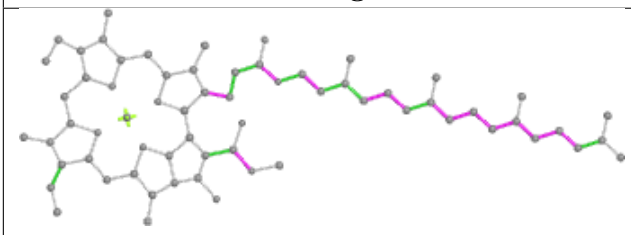
Ligand CLA b 620



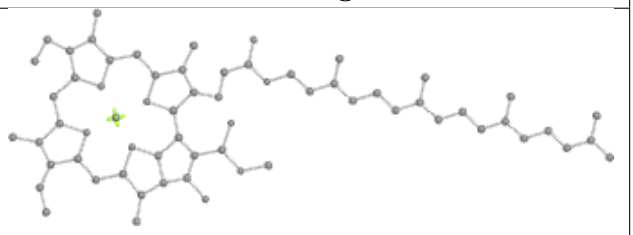
Bond lengths



Bond angles

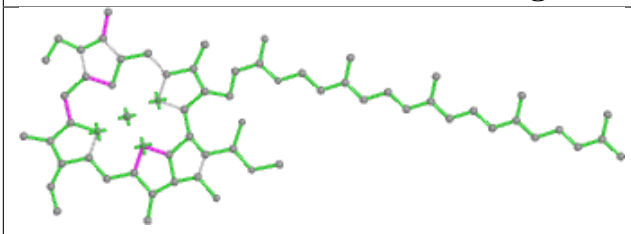


Torsions



Rings

Ligand CLA c 511



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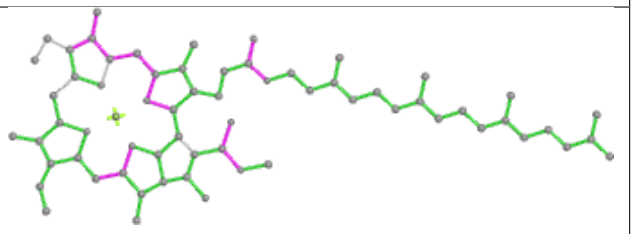
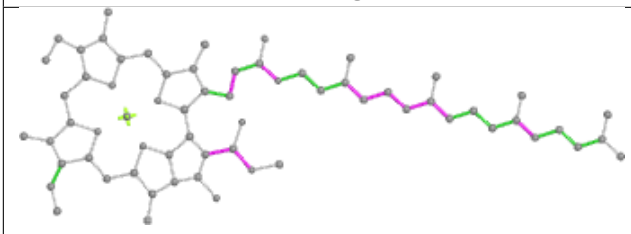
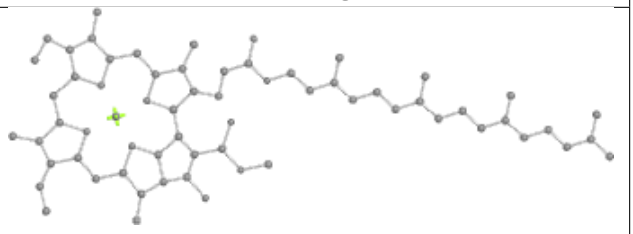


Bond angles

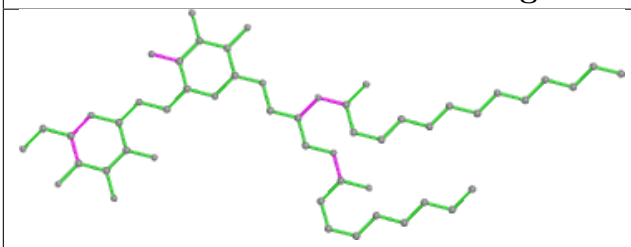


Torsions

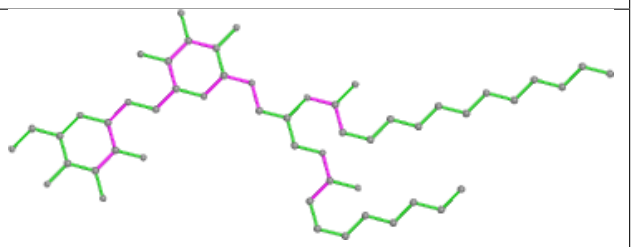


Rings

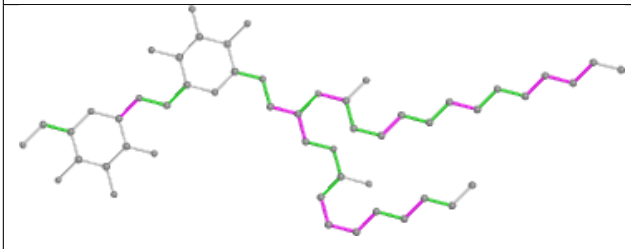
Ligand DGD B 627



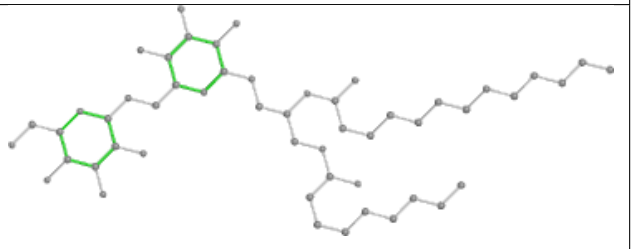
Bond lengths



Bond angles

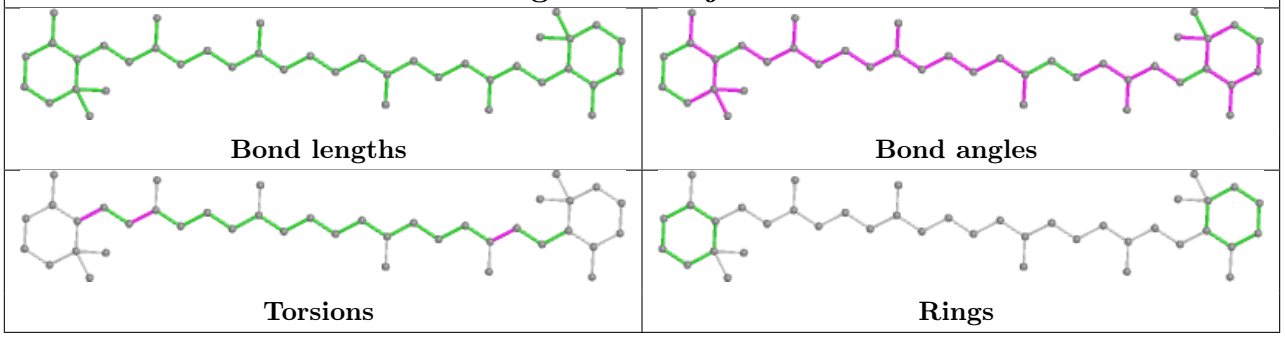


Torsions

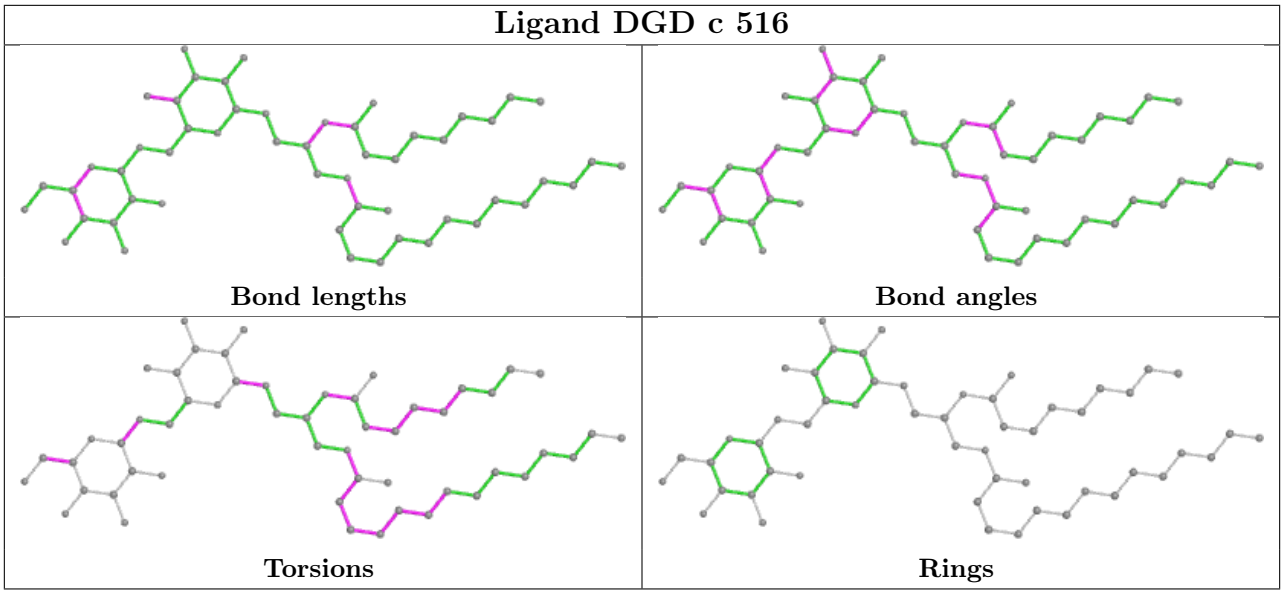


Rings

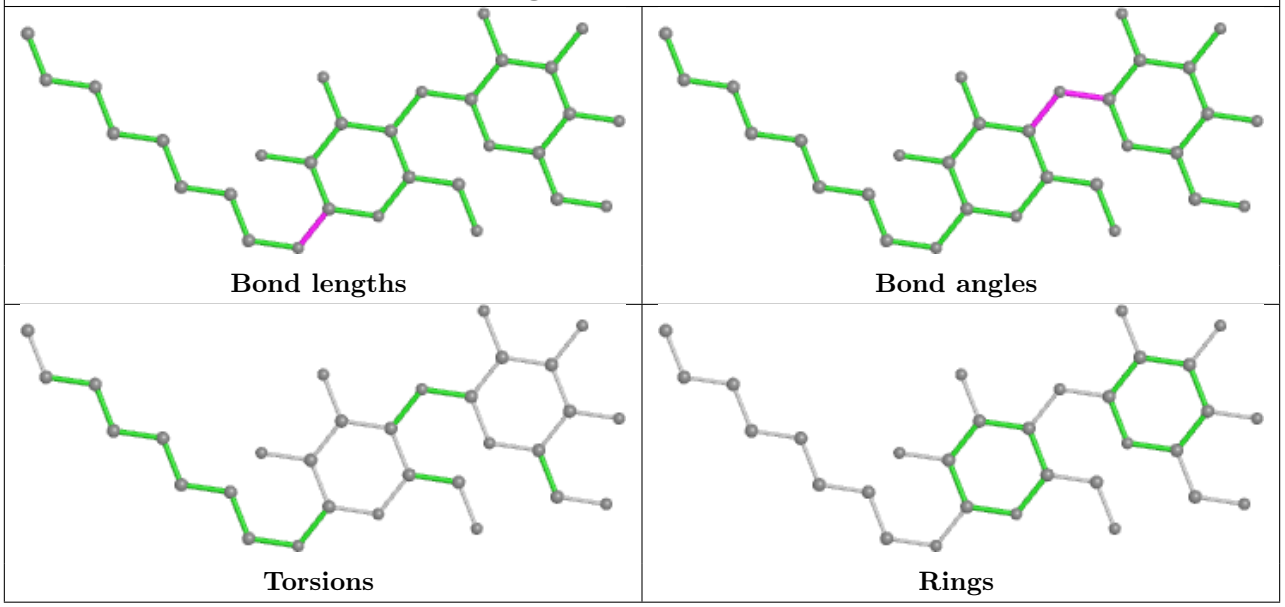
Ligand BCR j 102



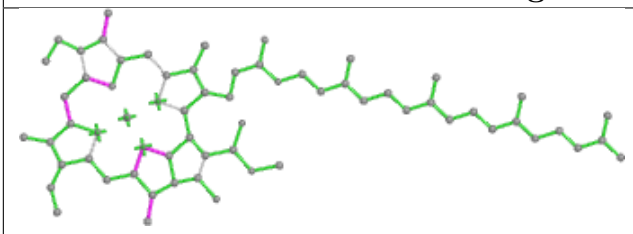
Ligand DGD c 516



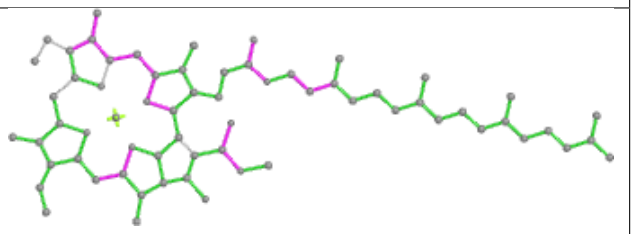
Ligand LMT d 410



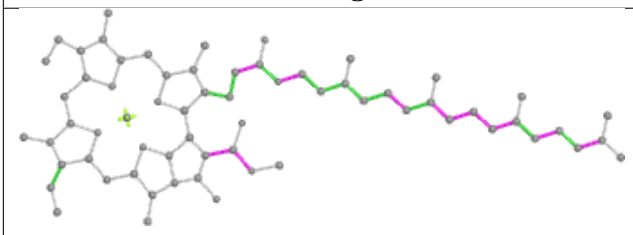
Ligand CLA b 617



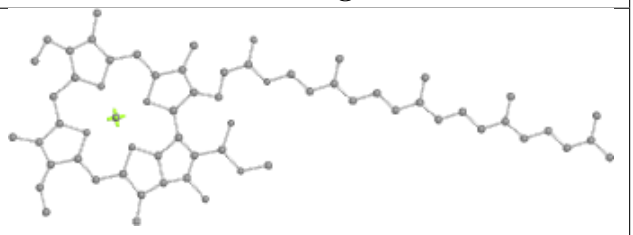
Bond lengths



Bond angles

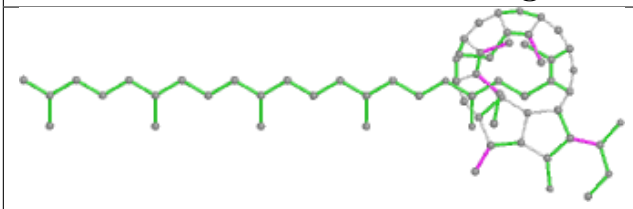


Torsions



Rings

Ligand PHO D 402



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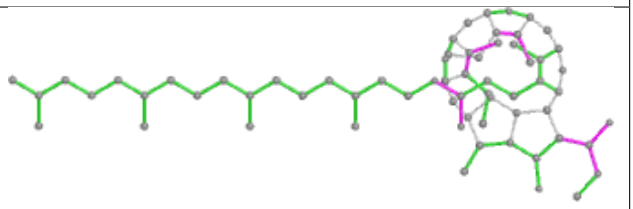
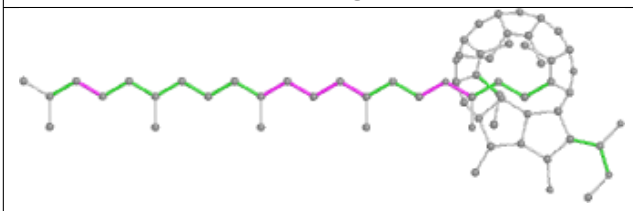


Bond angles



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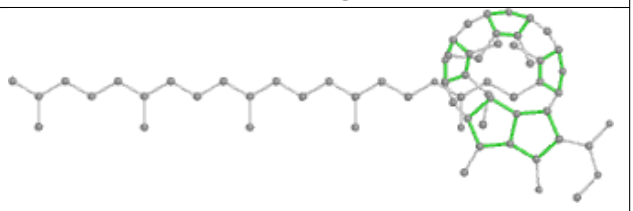
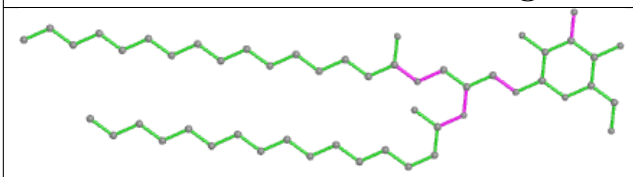
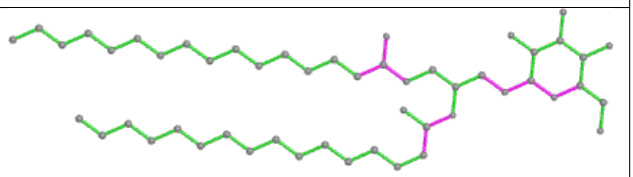


Rings

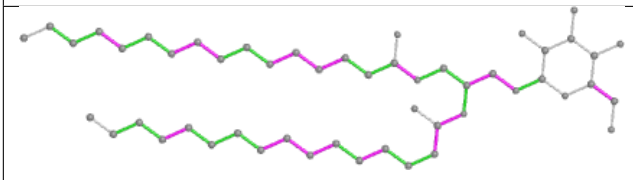
Ligand LMG A 414



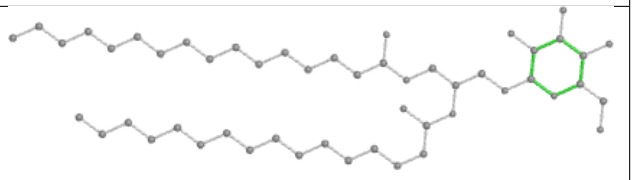
Bond lengths



Bond angles

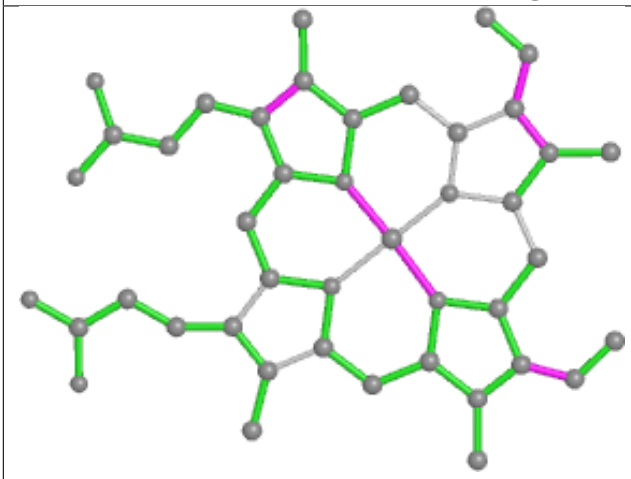


Torsions

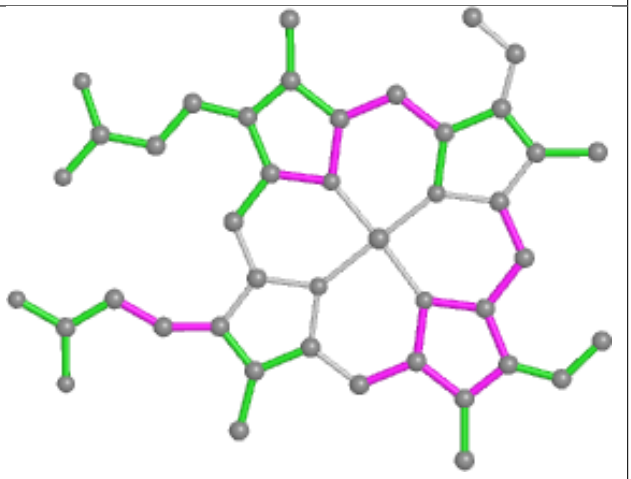


Rings

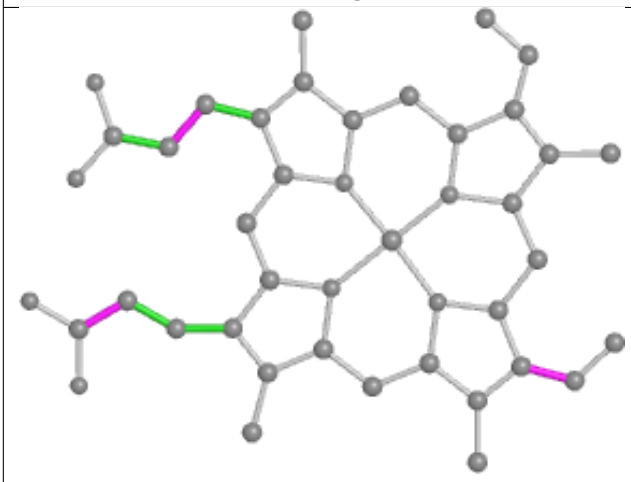
Ligand HEM f 101



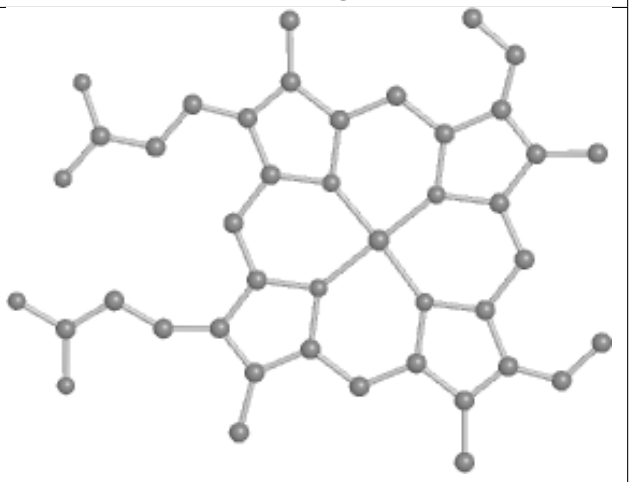
Bond lengths



Bond angles

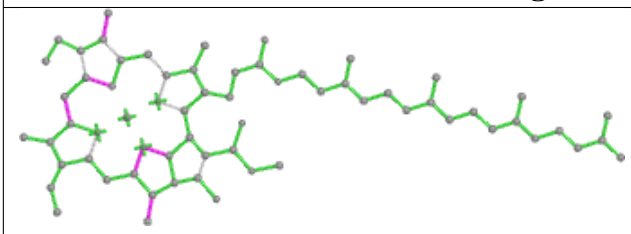


Torsions

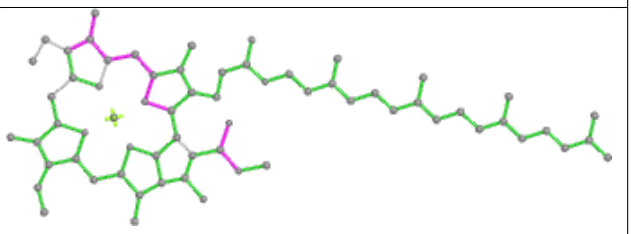


Rings

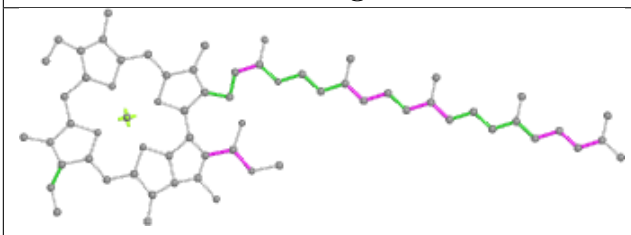
Ligand CLA c 510



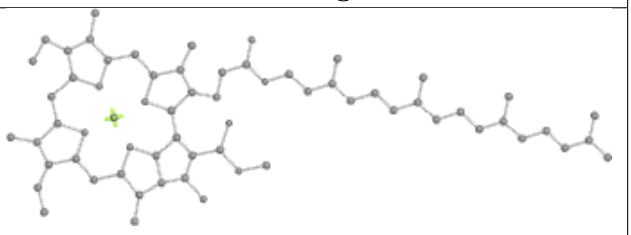
Bond lengths



Bond angles

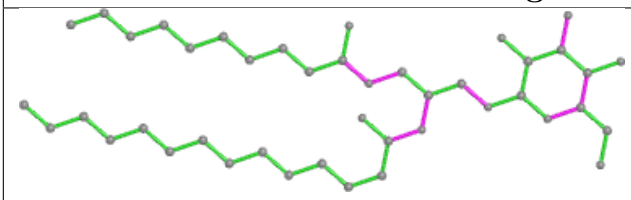


Torsions



Rings

Ligand LMG I 101



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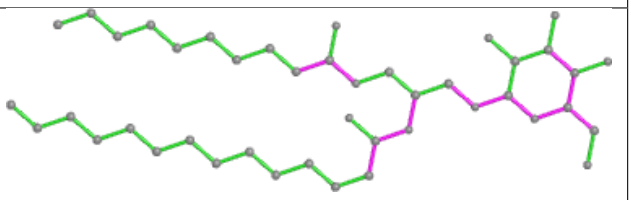
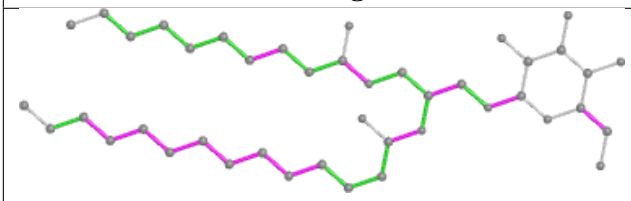


Bond angles



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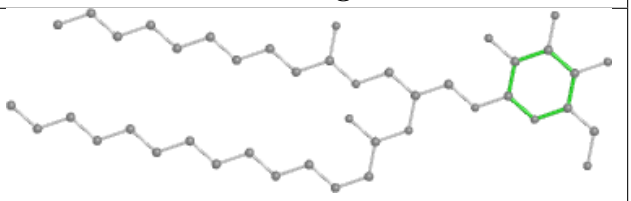
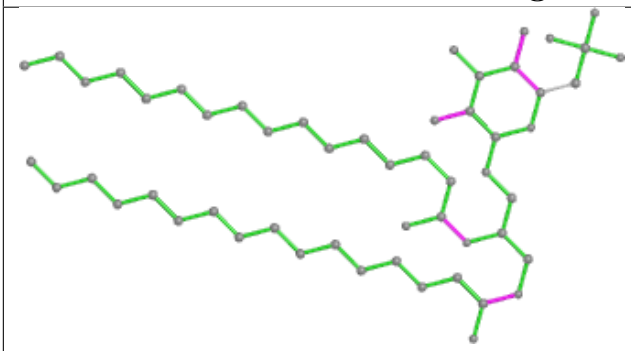


Rings

Ligand SQD a 401



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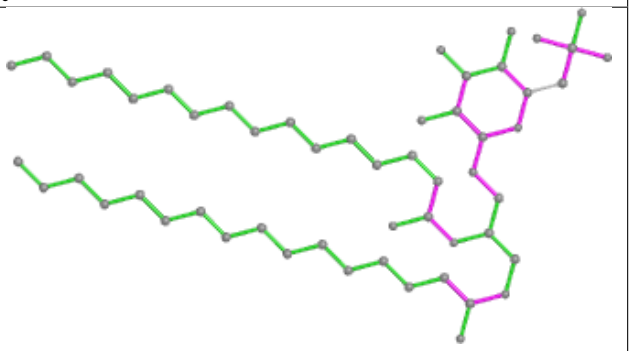
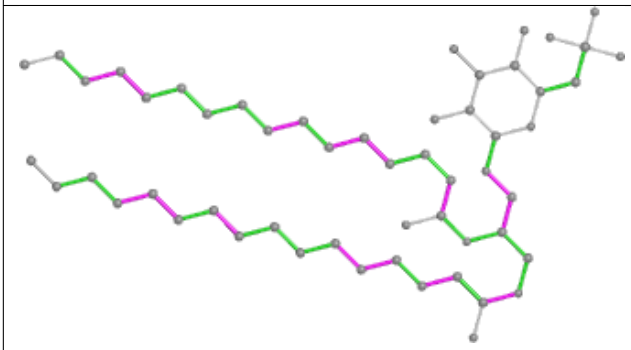


Bond angles



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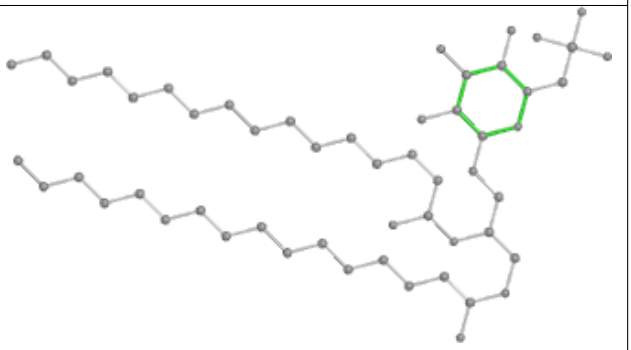
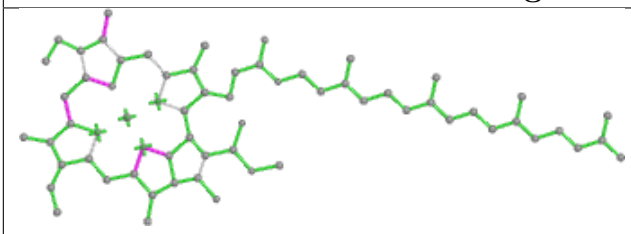


Rings

Ligand CLA B 615



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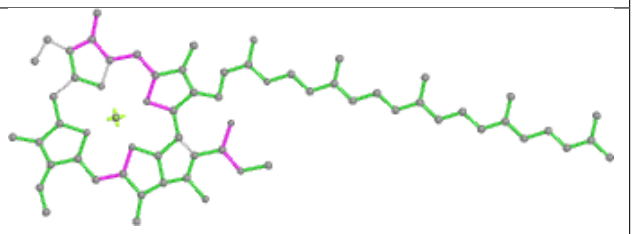
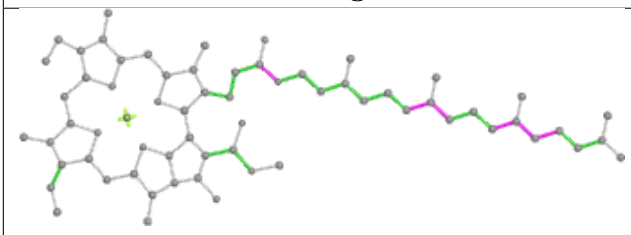


Bond angles



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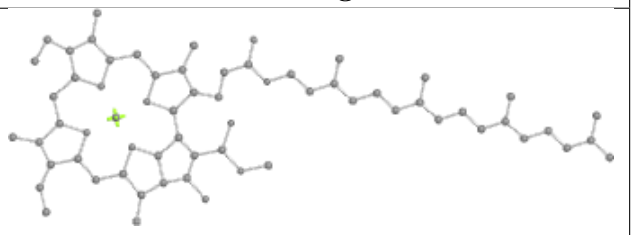
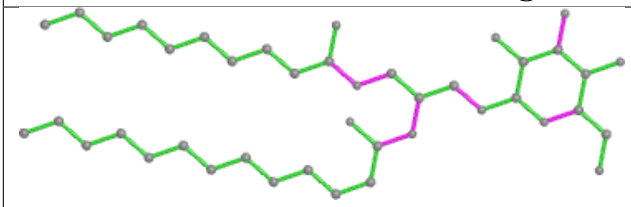


Rings

Ligand LMG m 102



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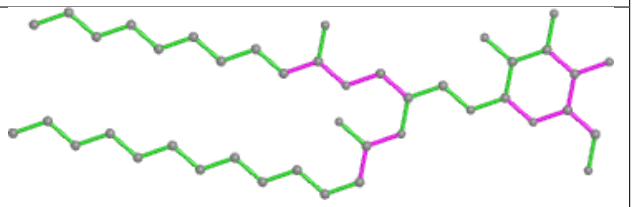

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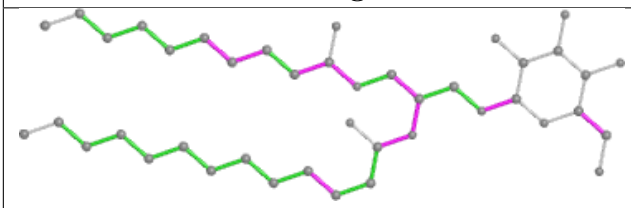

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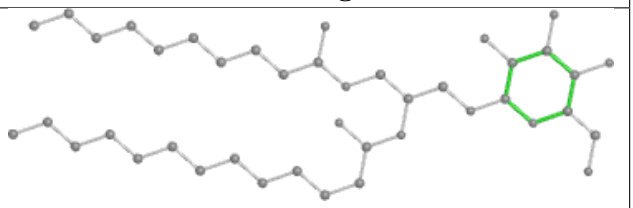
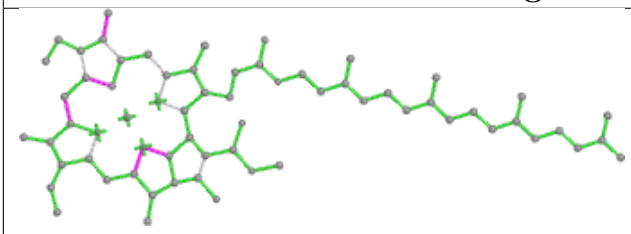


Rings

Ligand CLA C 503



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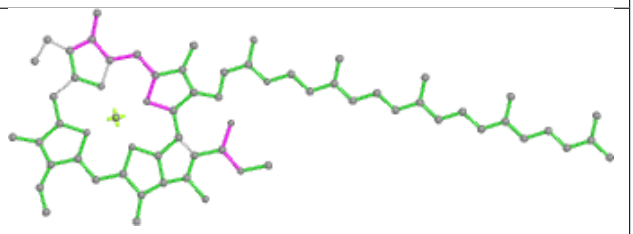
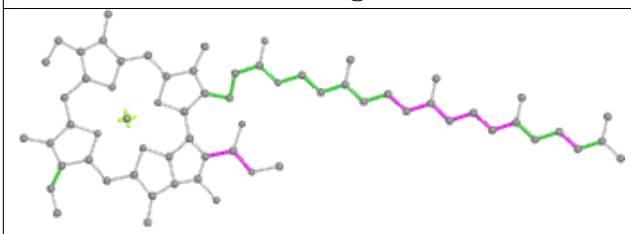


Bond angles



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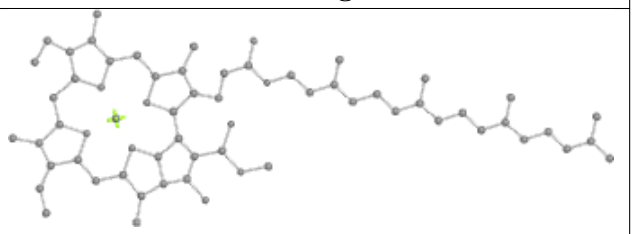
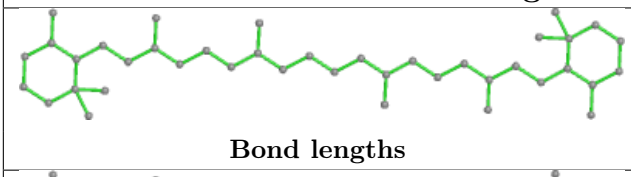


Rings

Ligand BCR T 102



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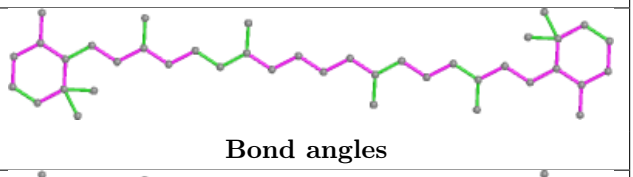
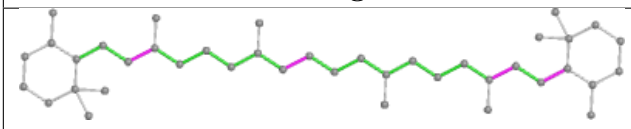


Bond angles



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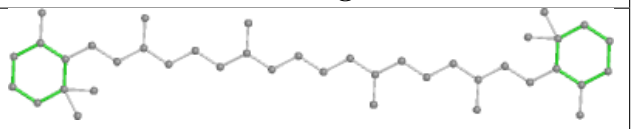
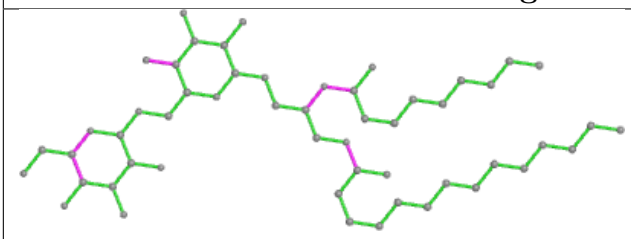


Rings

Ligand DGD C 517



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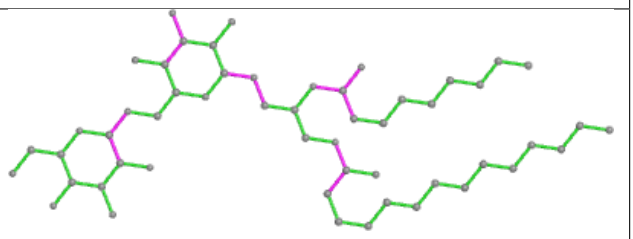
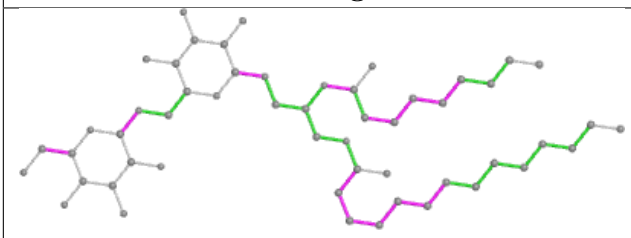


Bond angles



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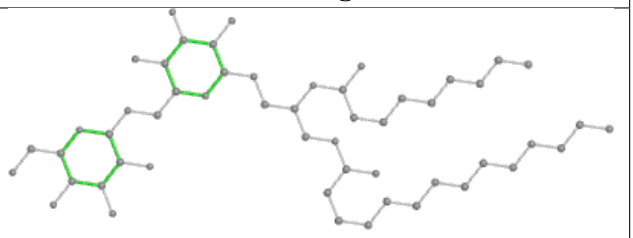
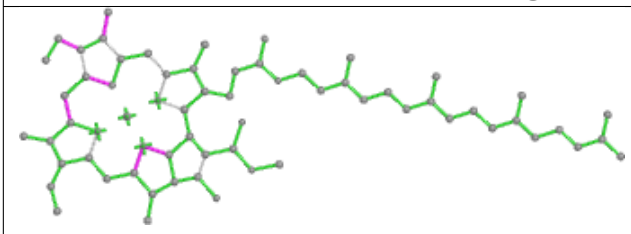


Rings

Ligand CLA C 504



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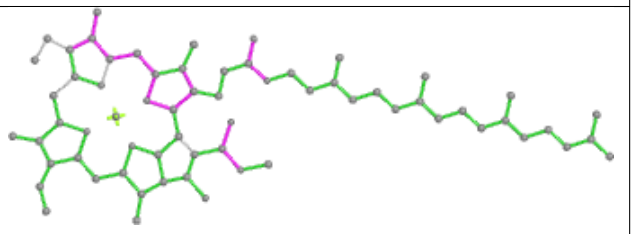
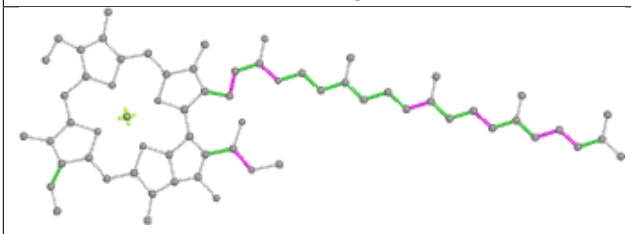
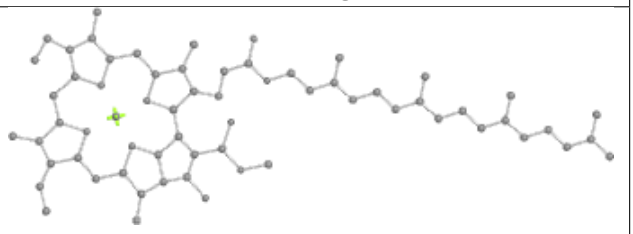


Bond angles

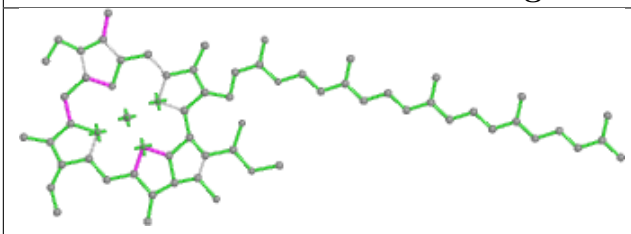


Torsions

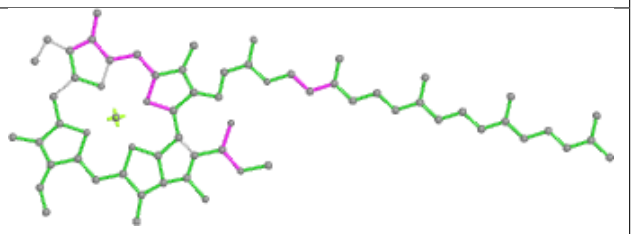


Rings

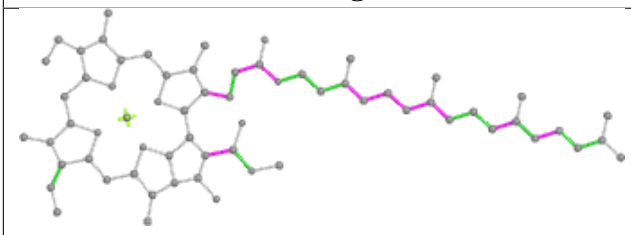
Ligand CLA B 602



Bond lengths



Bond angles



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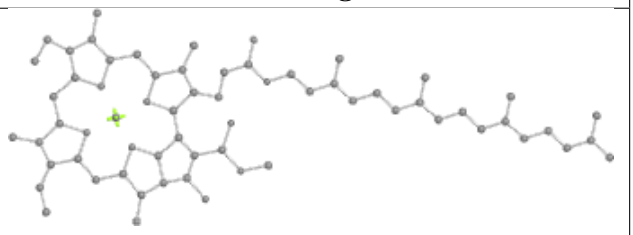
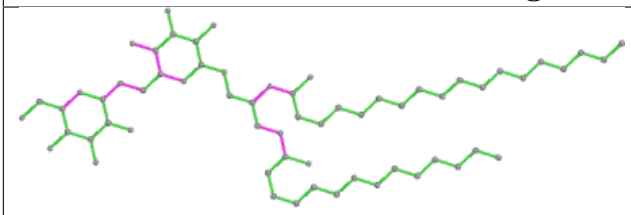


Rings

Ligand DGD c 517



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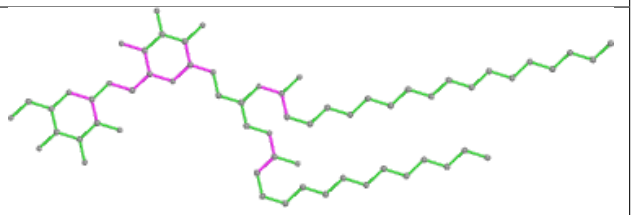
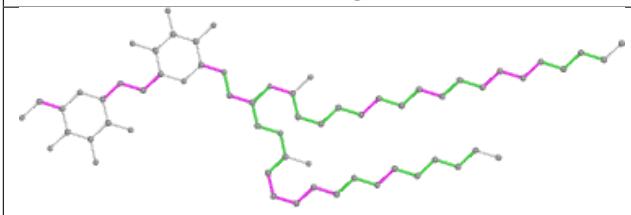


Bond angles



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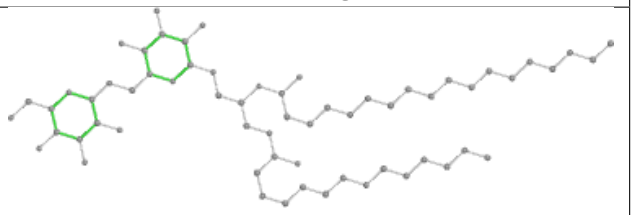
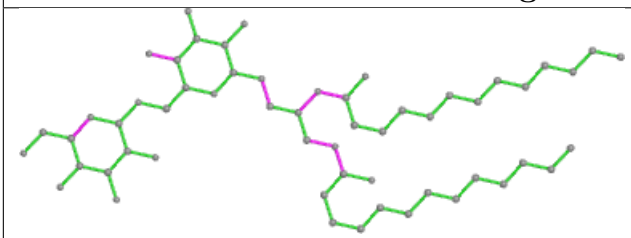


Rings

Ligand DGD A 411



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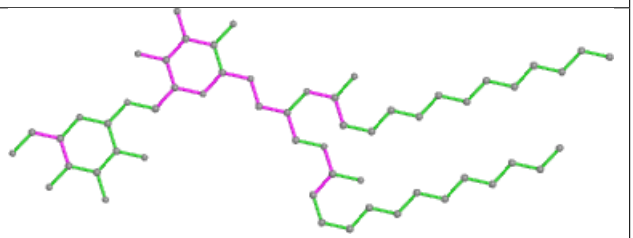
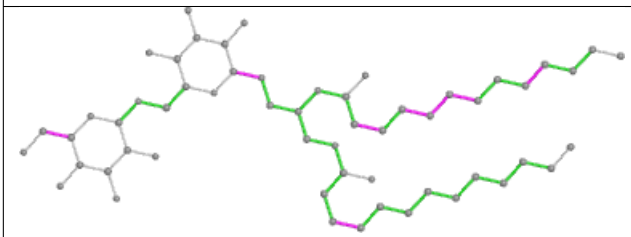


Bond angles



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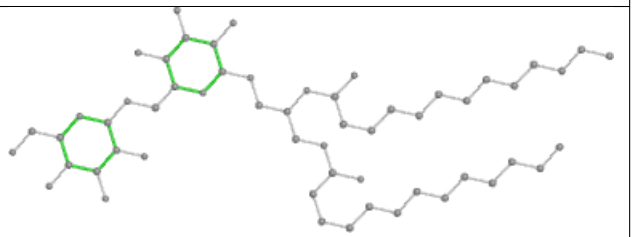
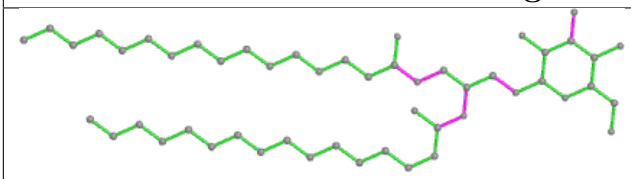


Rings

Ligand LMG a 416



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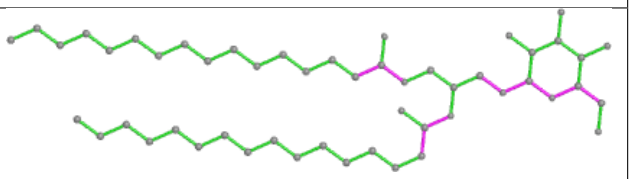
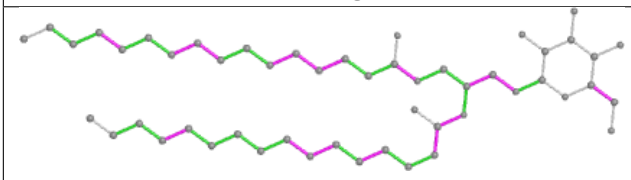
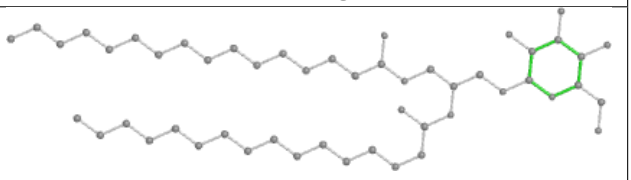


Bond angles

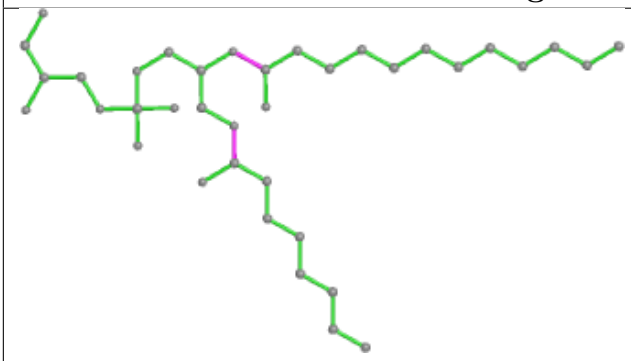


Torsions



Rings

Ligand LHG a 417



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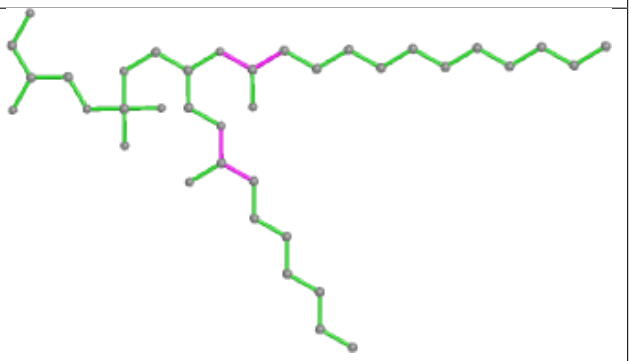
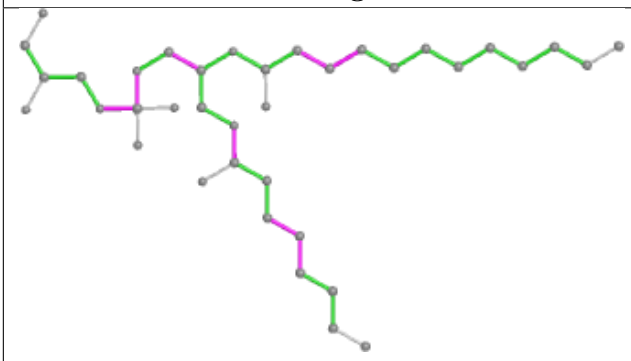
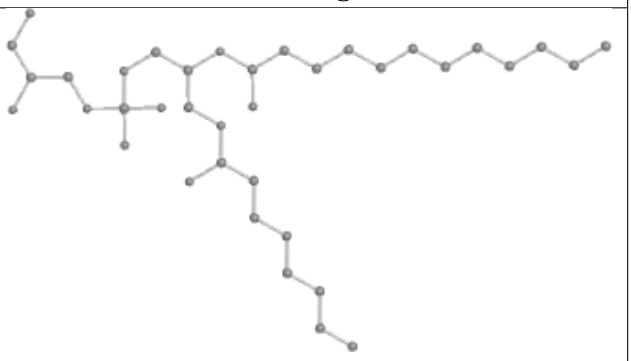


Bond angles

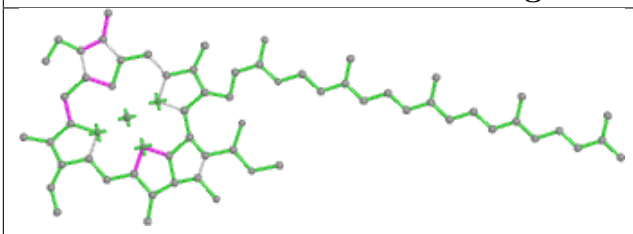


Torsions

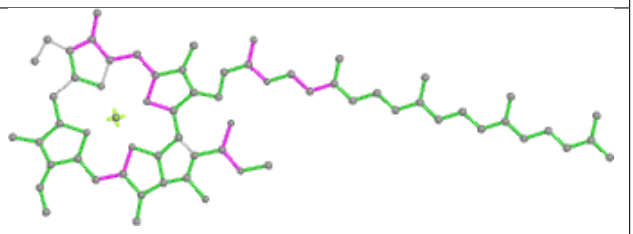


Rings

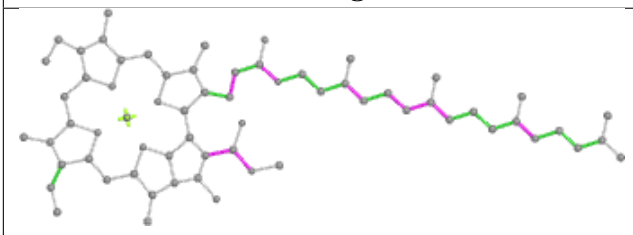
Ligand CLA C 511



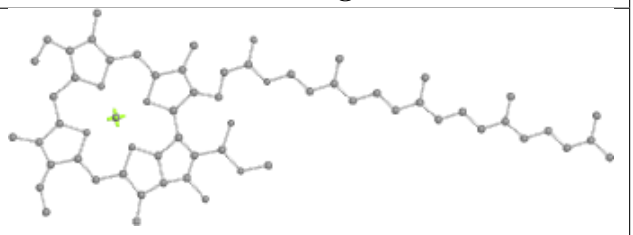
Bond lengths



Bond angles

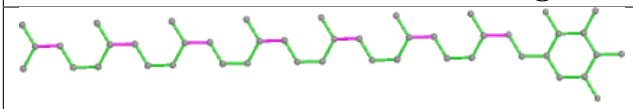


Torsions



Rings

Ligand PL9 a 410



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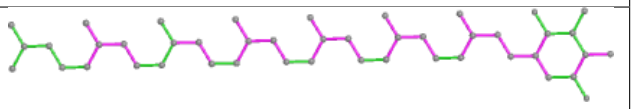
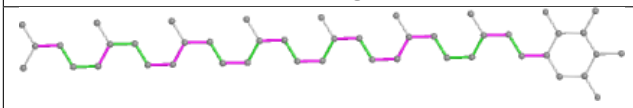
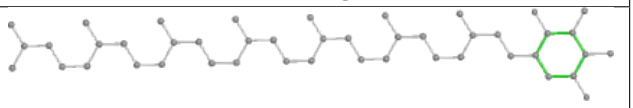


Bond angles

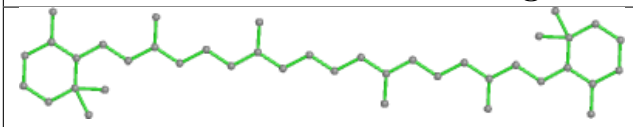


Torsions



Rings

Ligand BCR C 515



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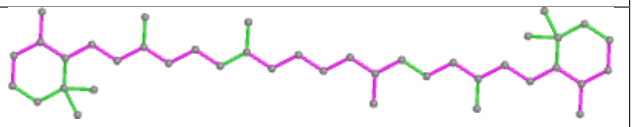
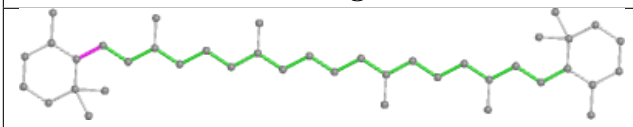


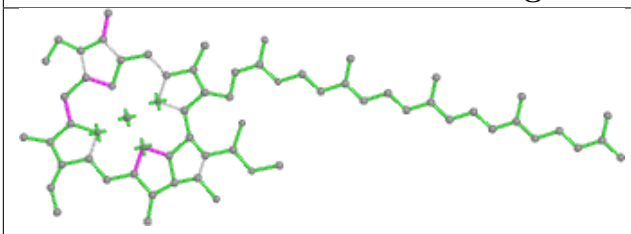
Bond angles



Torsions

Rings

Ligand CLA B 613



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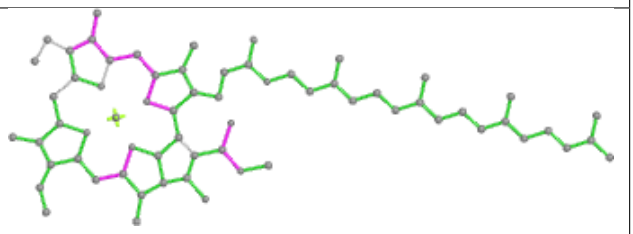
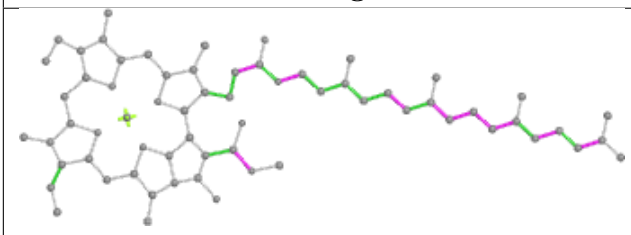
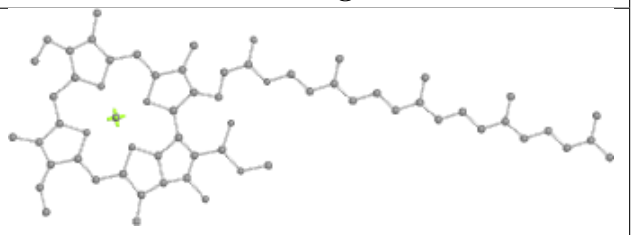


Bond angles

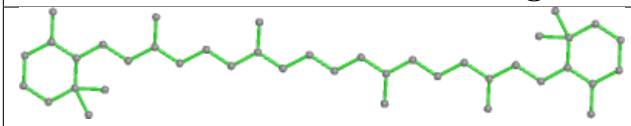


Torsions

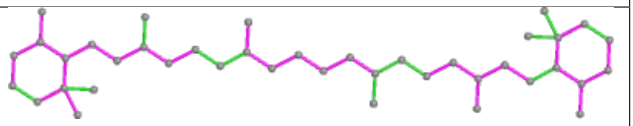


Rings

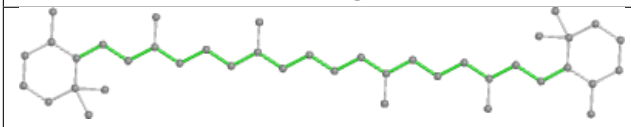
Ligand BCR b 621



Bond lengths



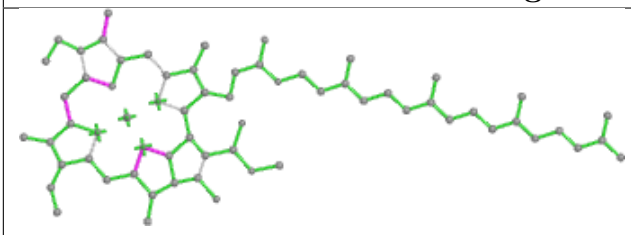
Bond angles



Torsions

Rings

Ligand CLA C 501



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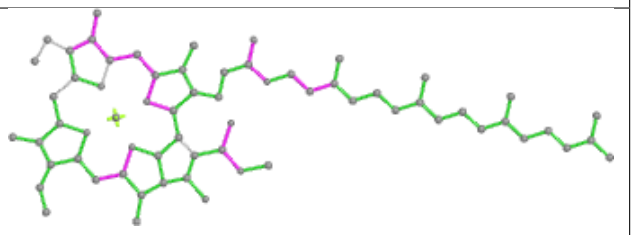
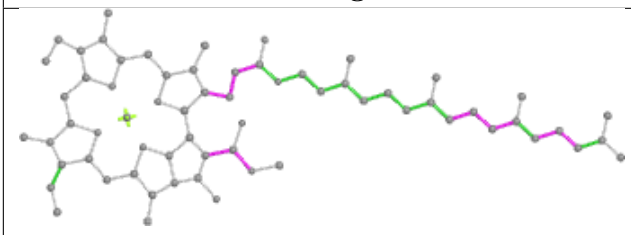
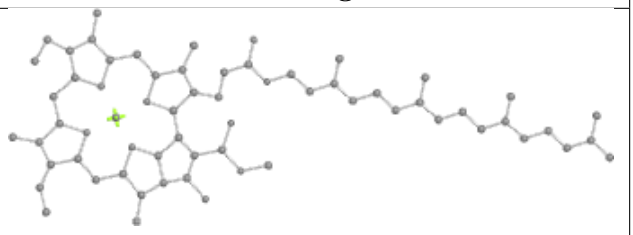


Bond angles

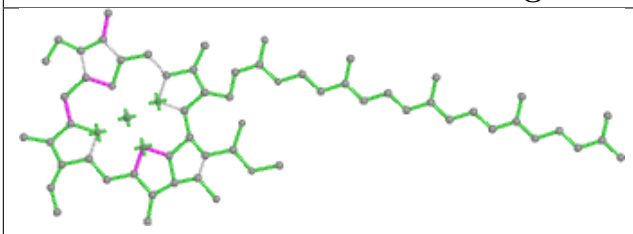


Torsions

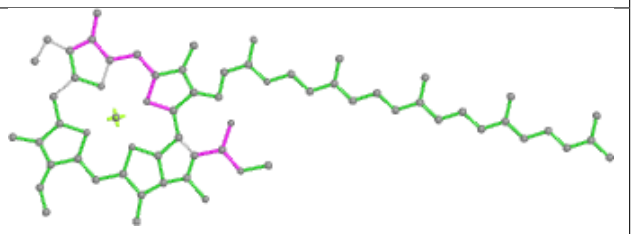


Rings

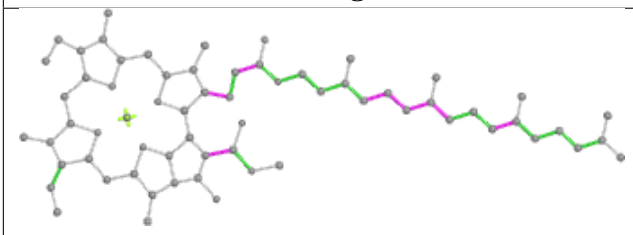
Ligand CLA C 507



Bond lengths



Bond angles



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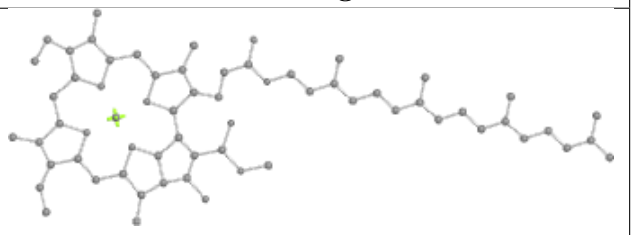
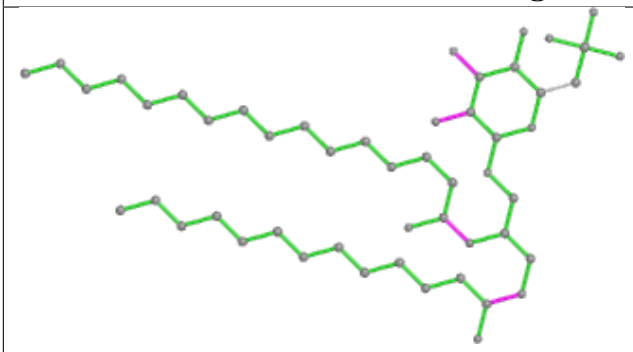


Rings

Ligand SQD a 415



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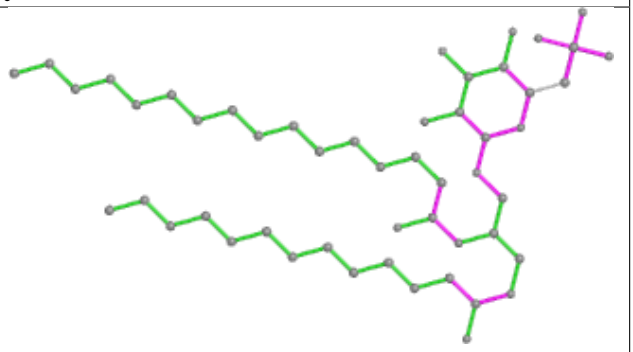
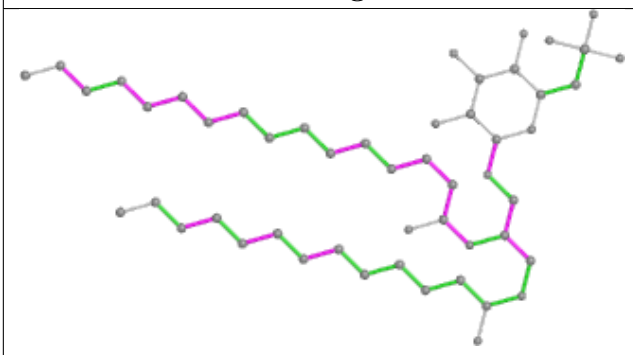
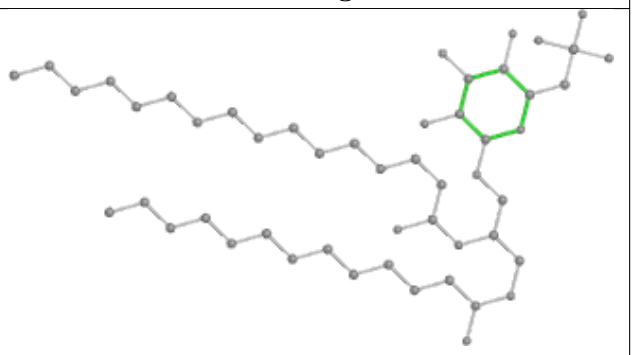


Bond angles

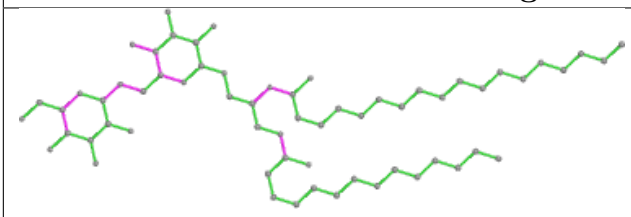


Torsions

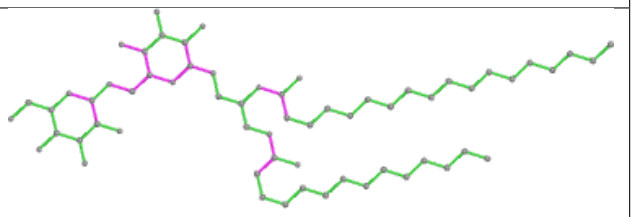


Rings

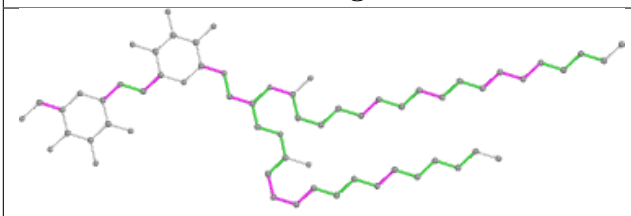
Ligand DGD C 518



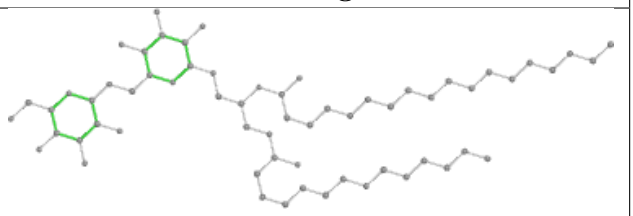
Bond lengths



Bond angles

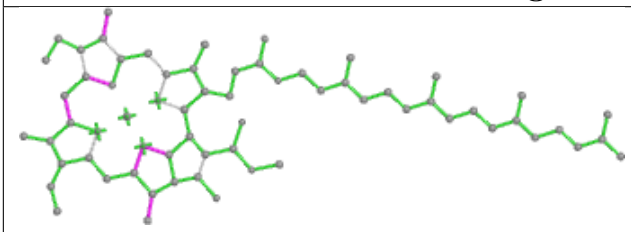


Torsions



Rings

Ligand CLA b 611



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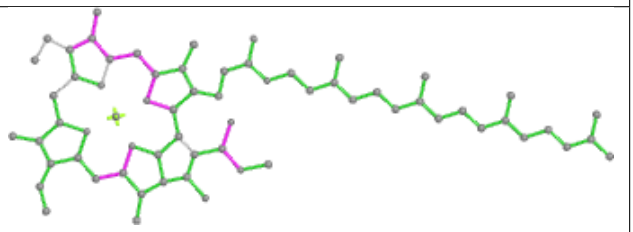
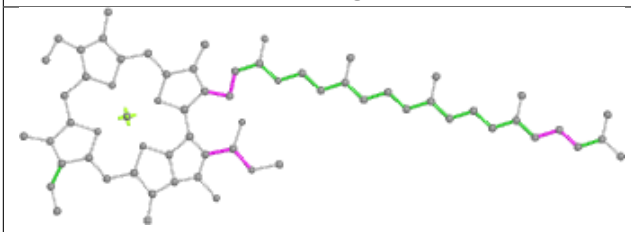
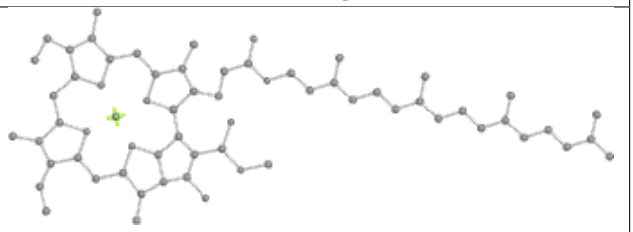


Bond angles

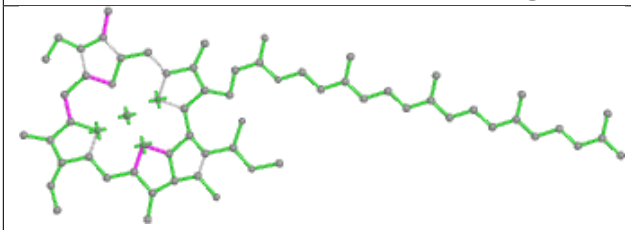


Torsions



Rings

Ligand CLA A 404



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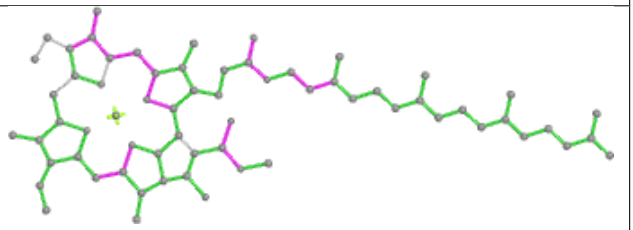
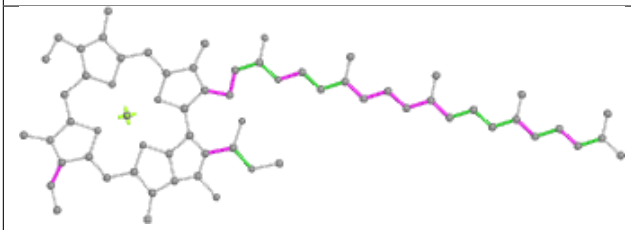


Bond angles



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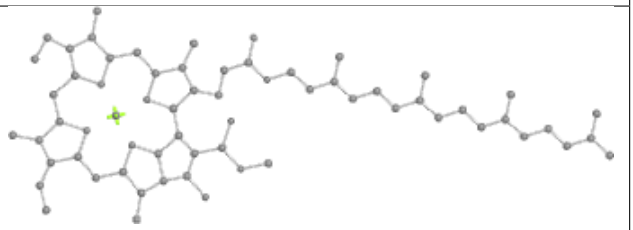
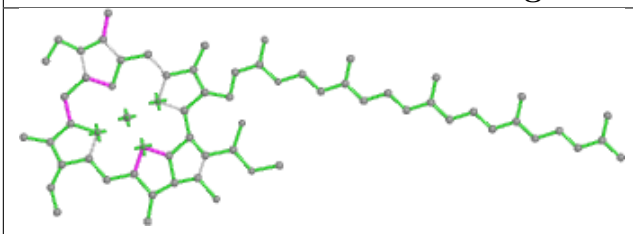


Rings

Ligand CLA C 513



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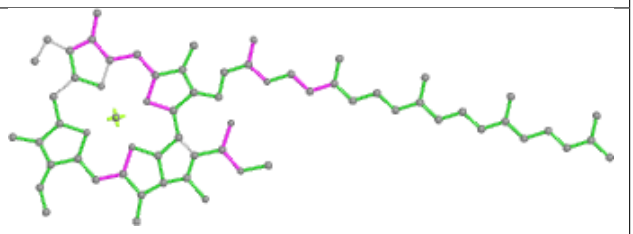
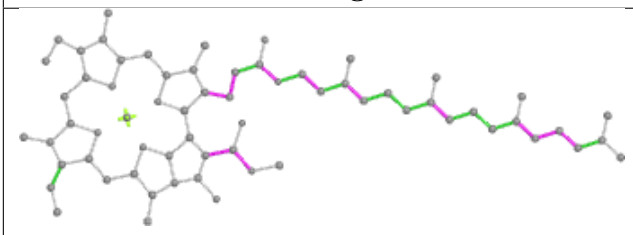
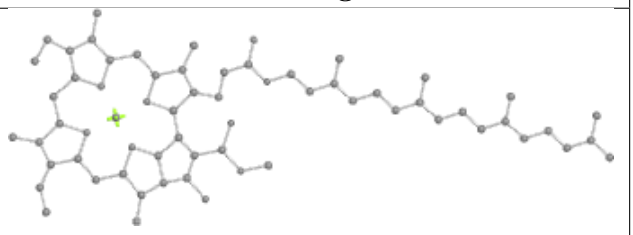


Bond angles

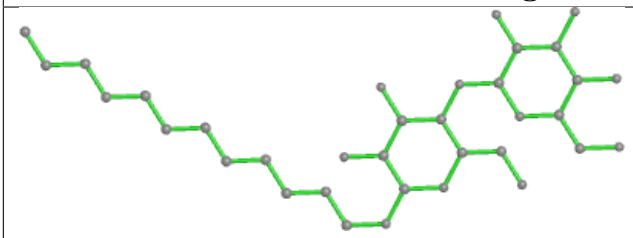


Torsions

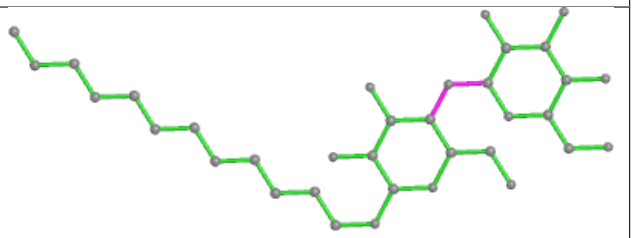


Rings

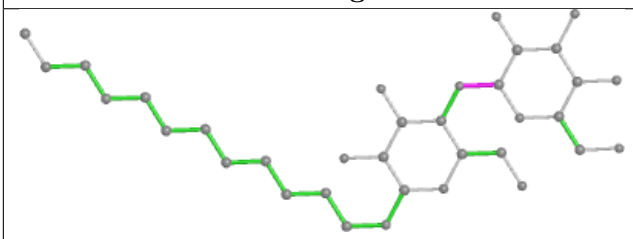
Ligand LMT B 625



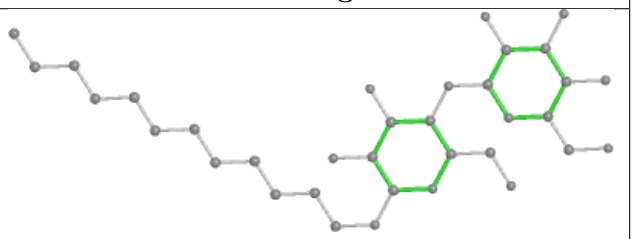
Bond lengths



Bond angles

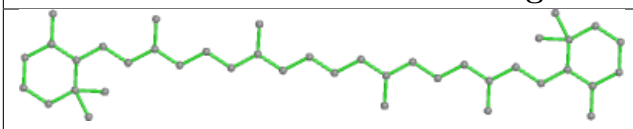


Torsions

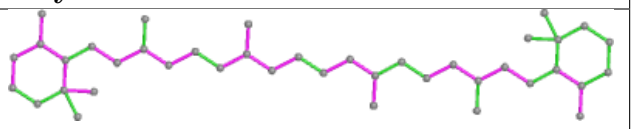


Rings

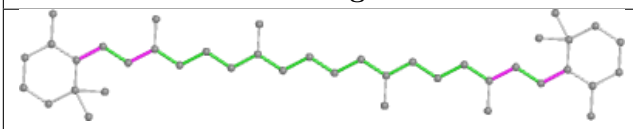
Ligand BCR y 101



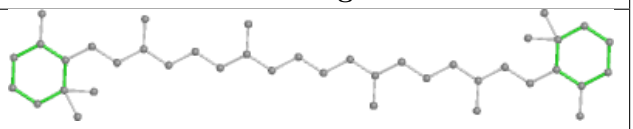
Bond lengths



Bond angles

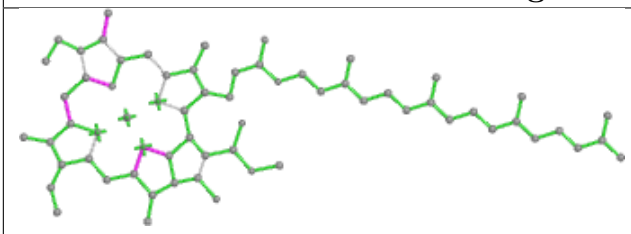


Torsions

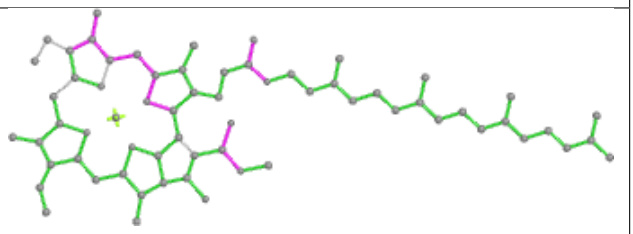


Rings

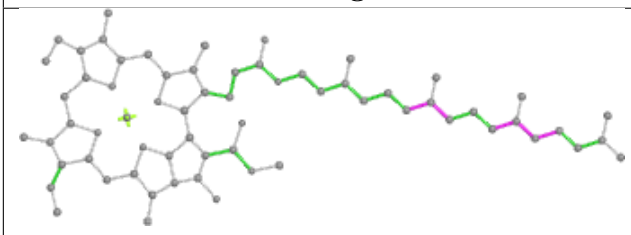
Ligand CLA b 619



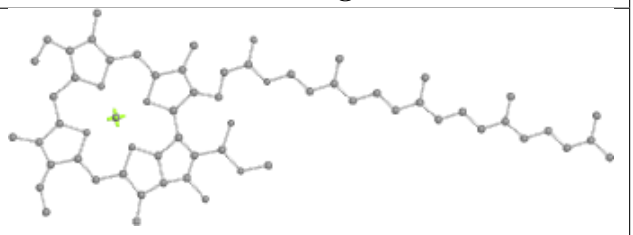
Bond lengths



Bond angles

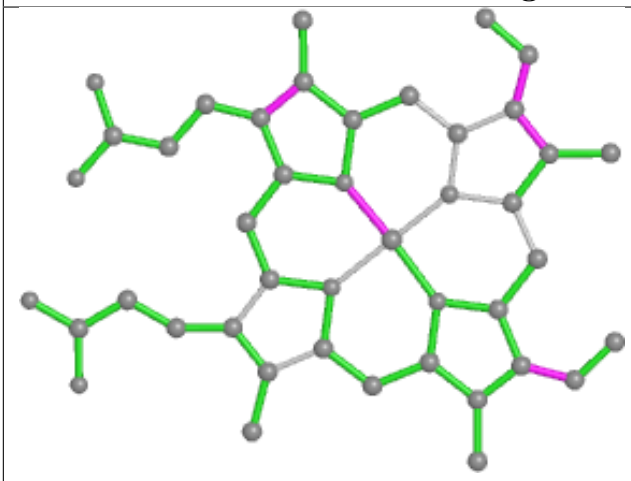


Torsions

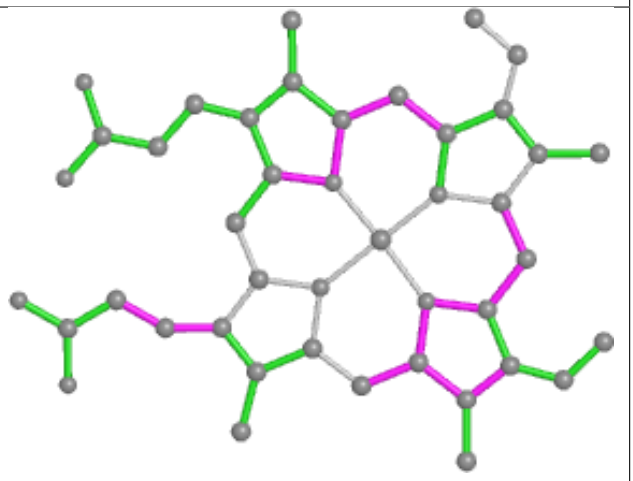


Rings

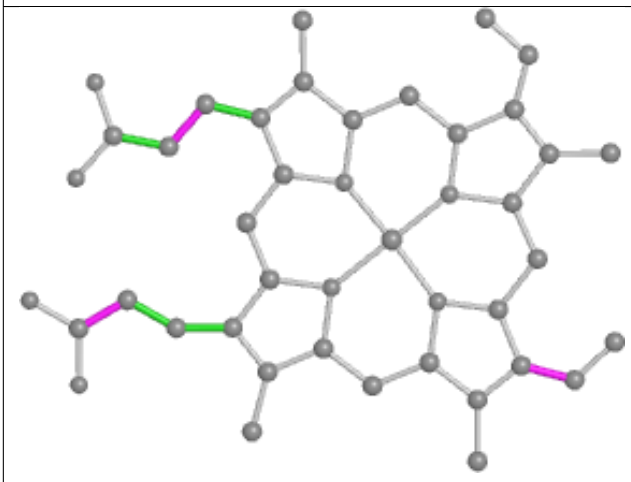
Ligand HEM F 101



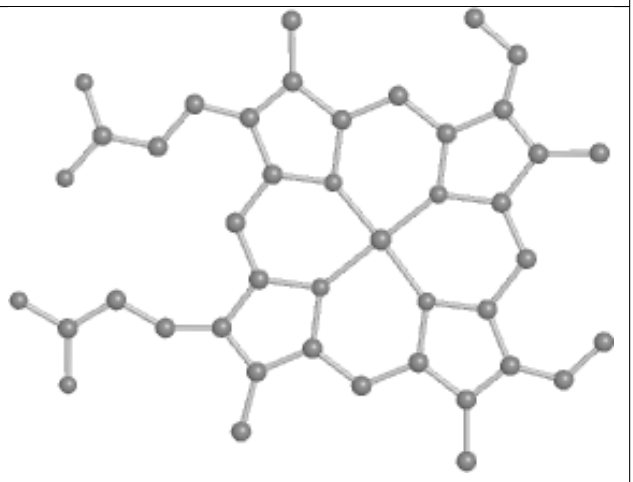
Bond lengths



Bond angles

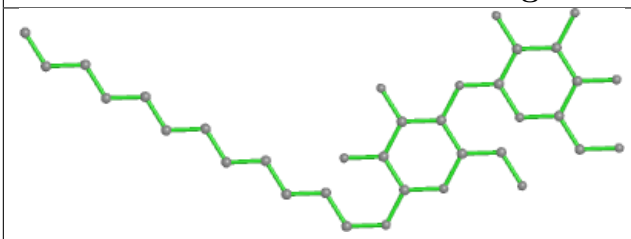


Torsions



Rings

Ligand LMT B 624



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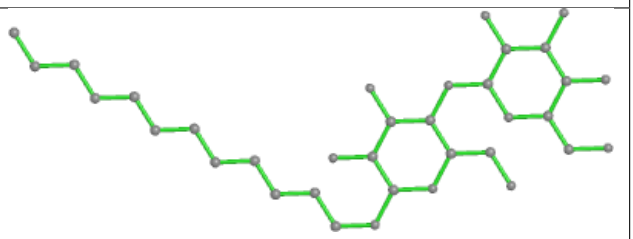
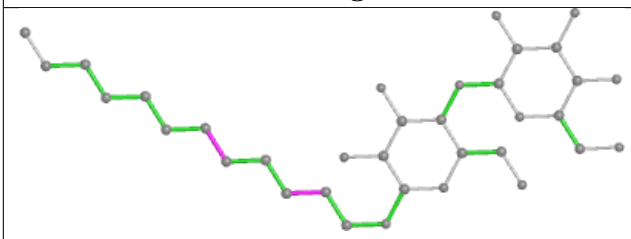
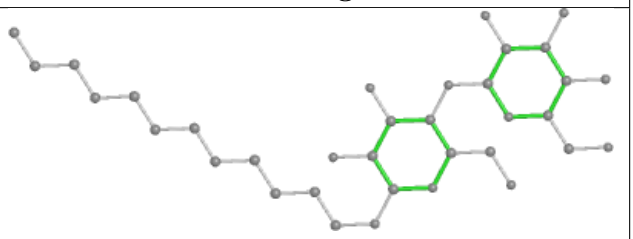


Bond angles

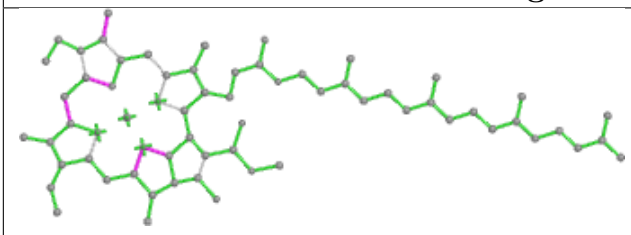


Torsions



Rings

Ligand CLA b 610



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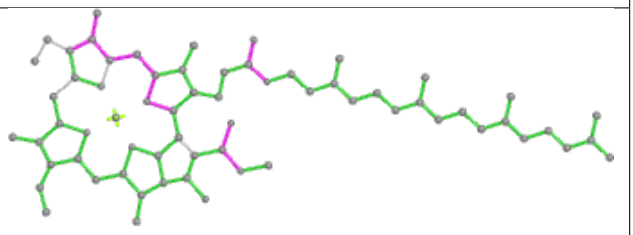
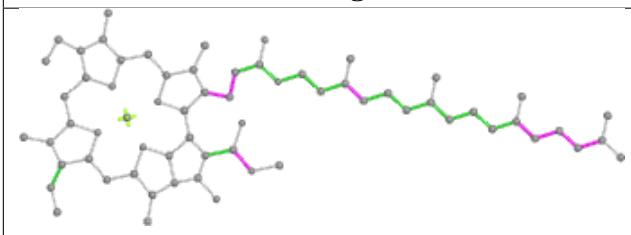
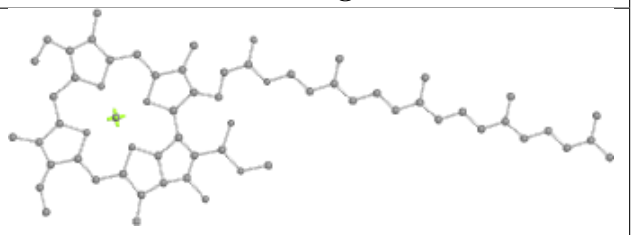


Bond angles

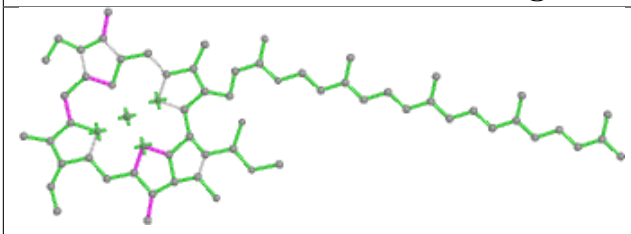


Torsions



Rings

Ligand CLA a 406



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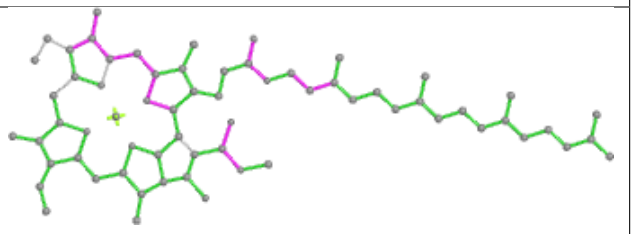
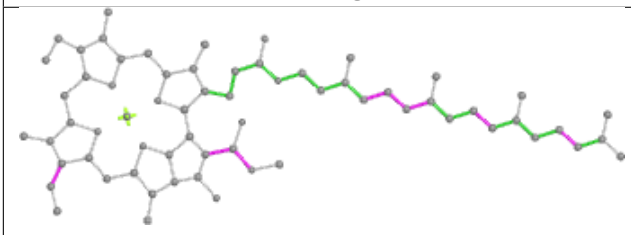
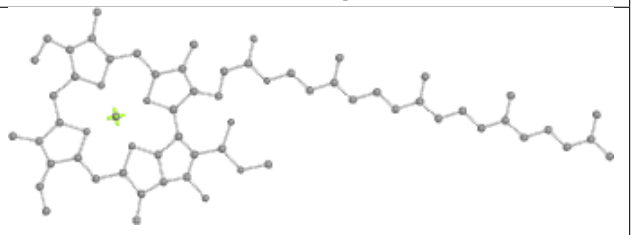


Bond angles

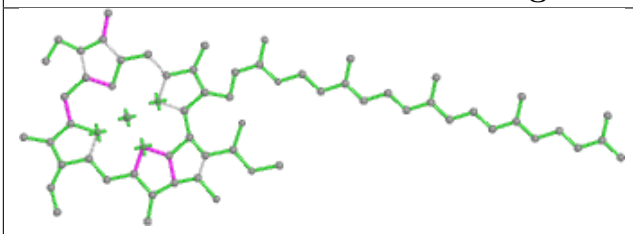


Torsions



Rings

Ligand CLA c 512



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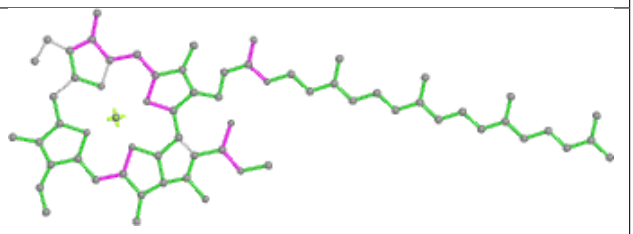
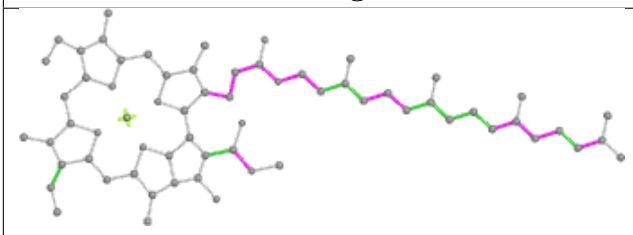


Bond angles



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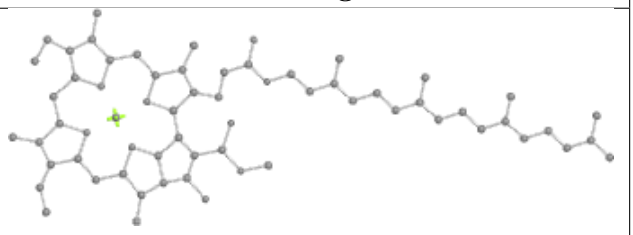
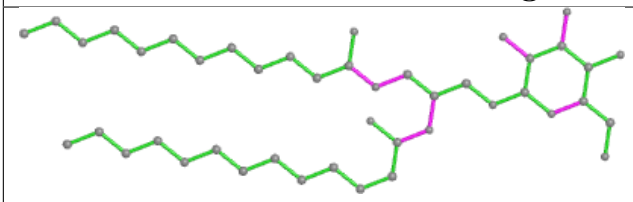


Rings

Ligand LMG E 101



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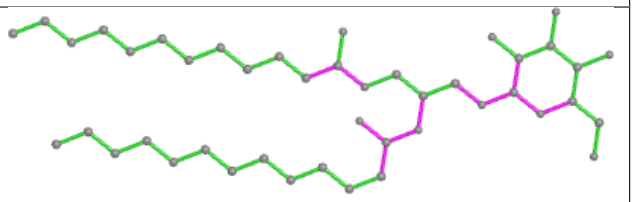
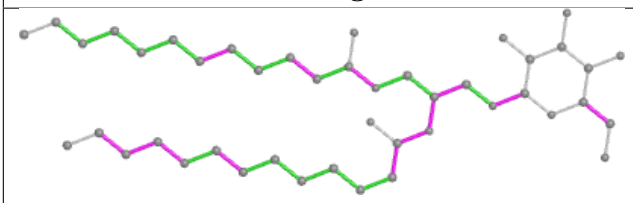
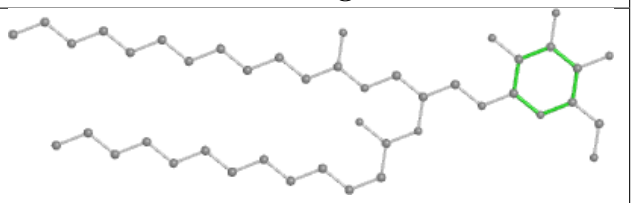


Bond angles

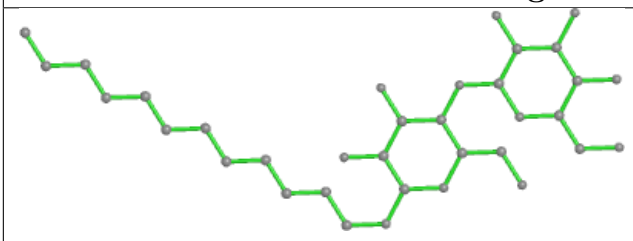


Torsions



Rings

Ligand LMT I 102



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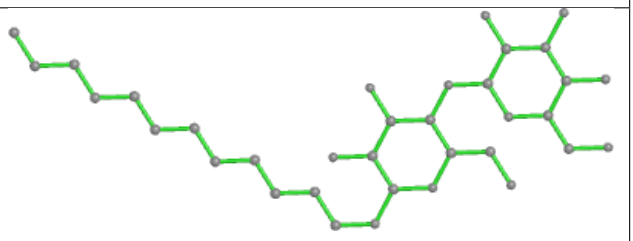
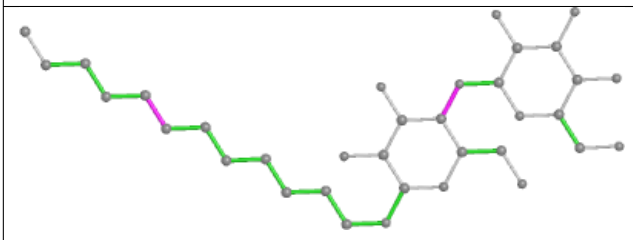


Bond angles



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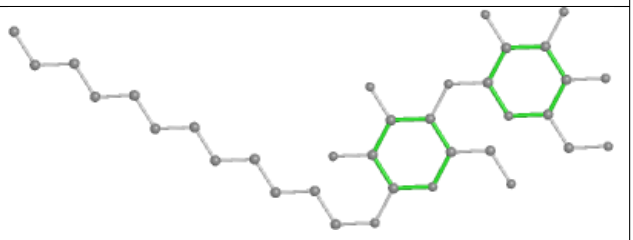
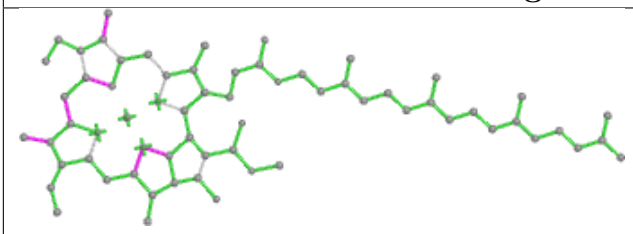
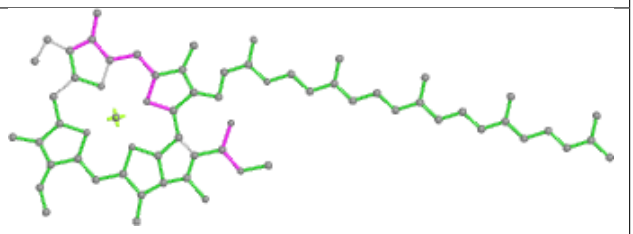


Rings

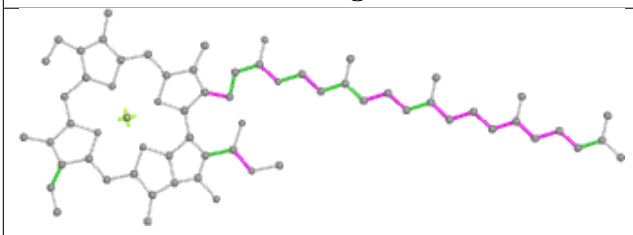
Ligand CLA B 616



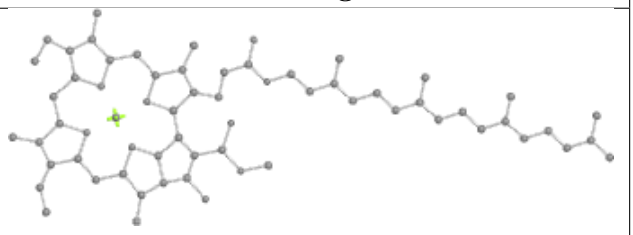
Bond lengths



Bond angles

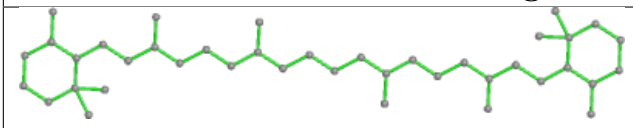


Torsions

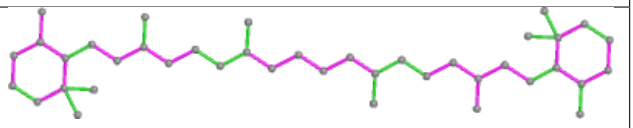


Rings

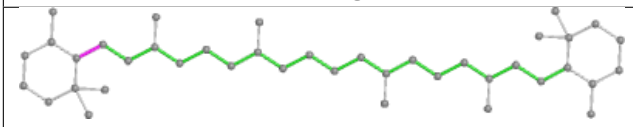
Ligand BCR B 619



Bond lengths



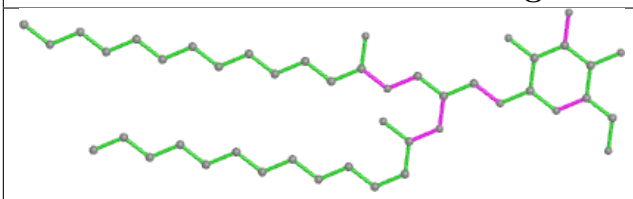
Bond angles



Torsions

Rings

Ligand LMG c 519



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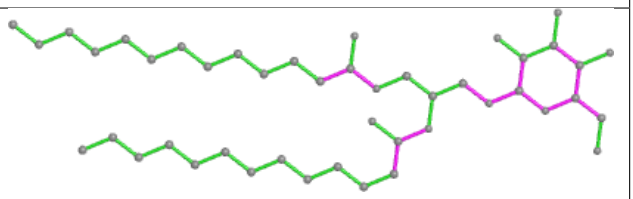
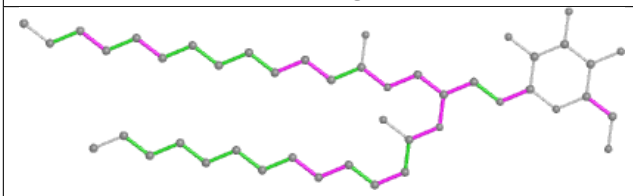
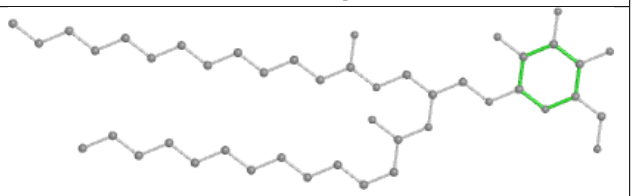


Bond angles

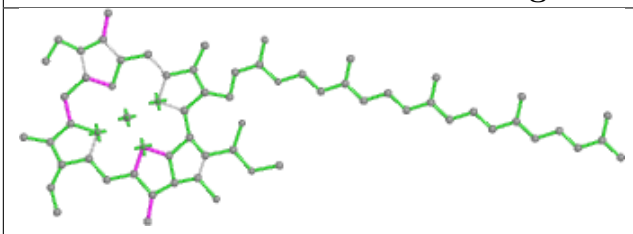


Torsions



Rings

Ligand CLA c 507



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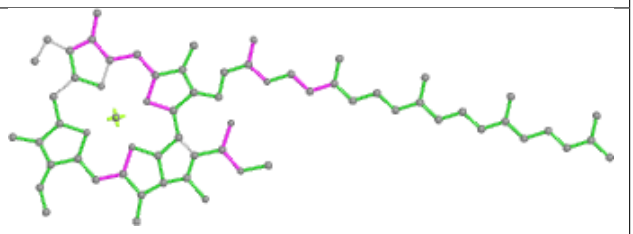
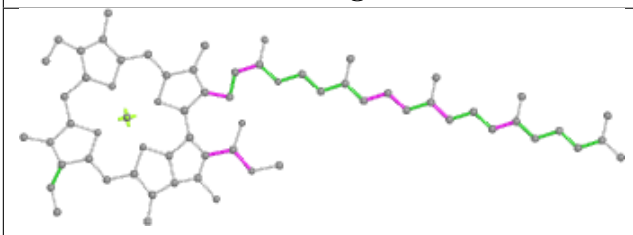
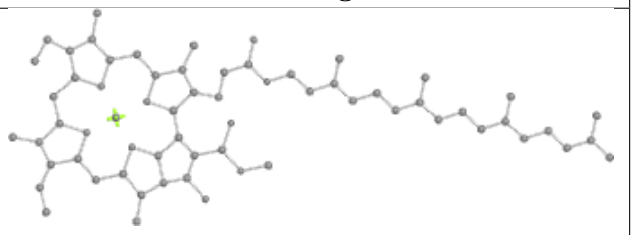


Bond angles

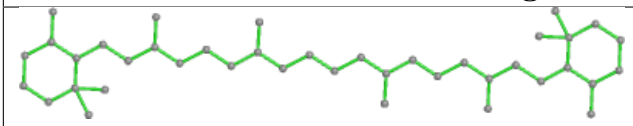


Torsions

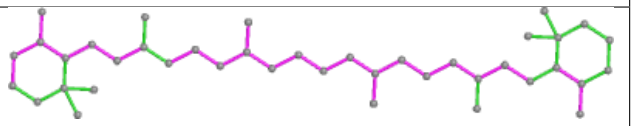


Rings

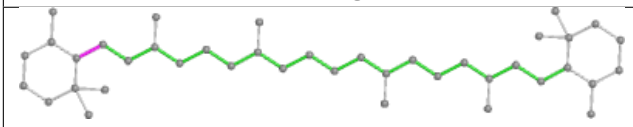
Ligand BCR H 101



Bond lengths



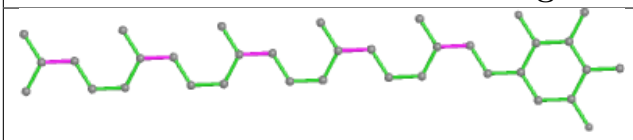
Bond angles



Torsions

Rings

Ligand PL9 j 101



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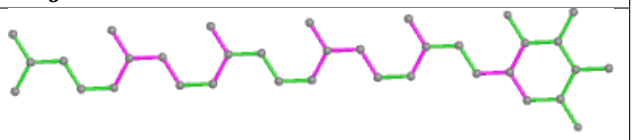
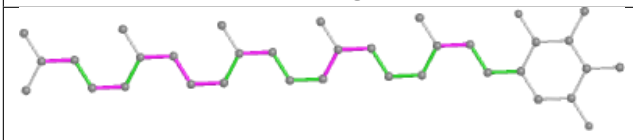
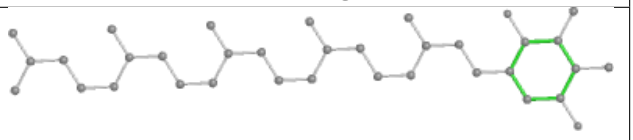


Bond angles

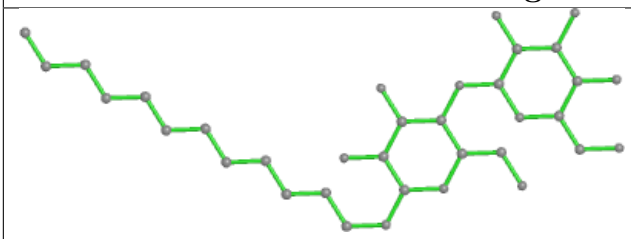


Torsions

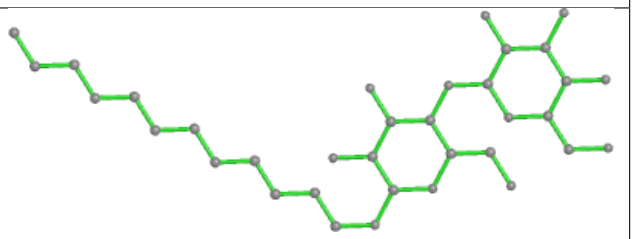


Rings

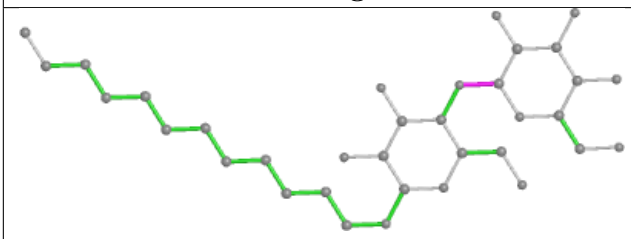
Ligand LMT b 627



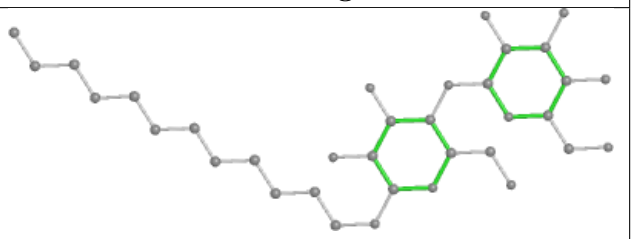
Bond lengths



Bond angles

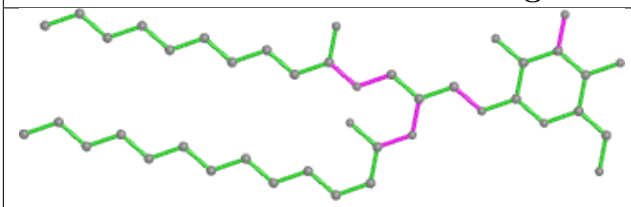


Torsions

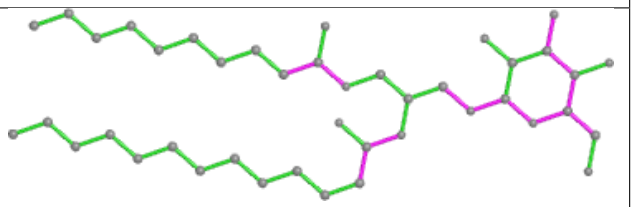


Rings

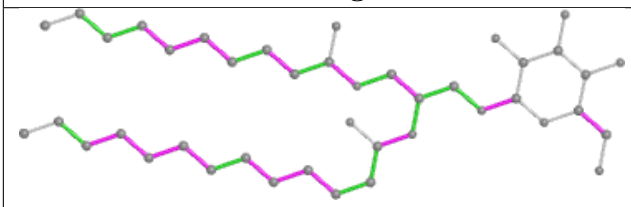
Ligand LMG a 402



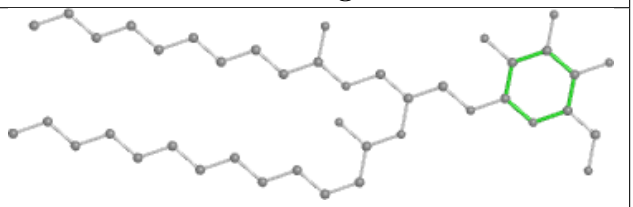
Bond lengths



Bond angles

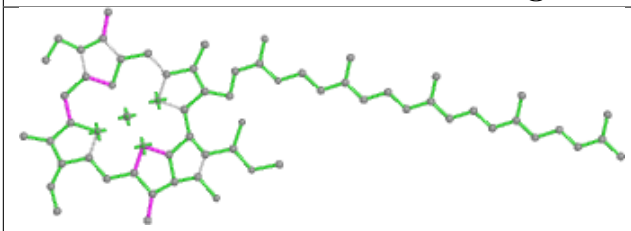


Torsions



Rings

Ligand CLA b 609



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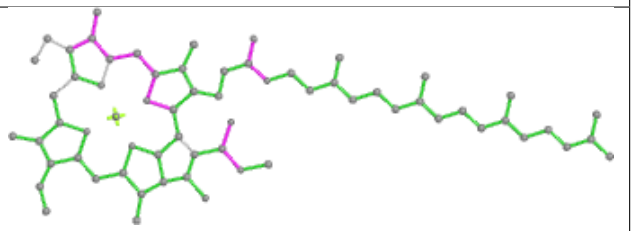
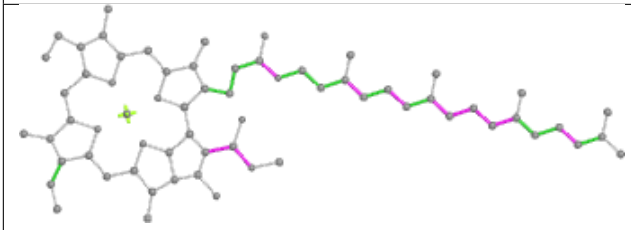
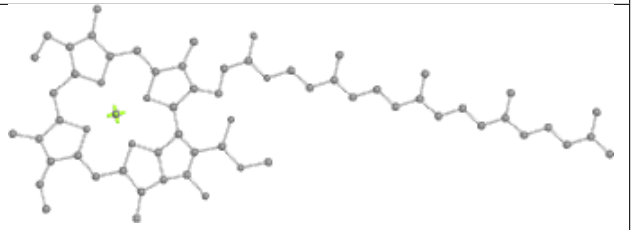


Bond angles

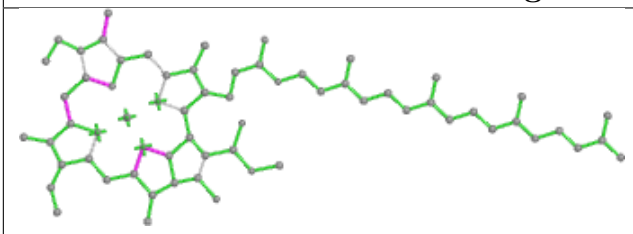


Torsions



Rings

Ligand CLA B 601



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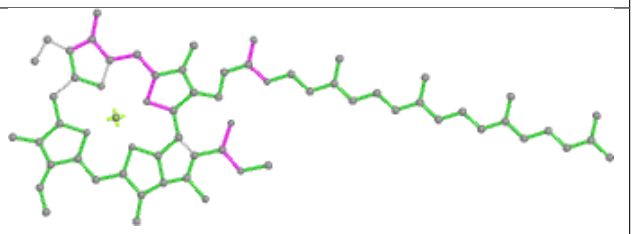
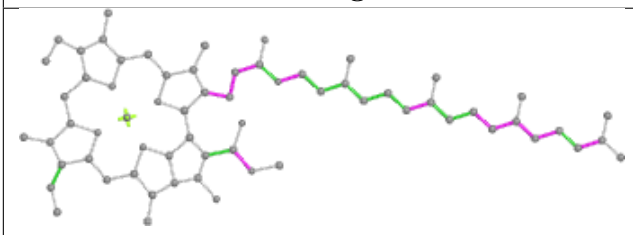
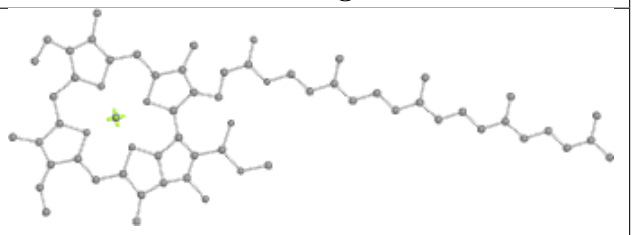


Bond angles

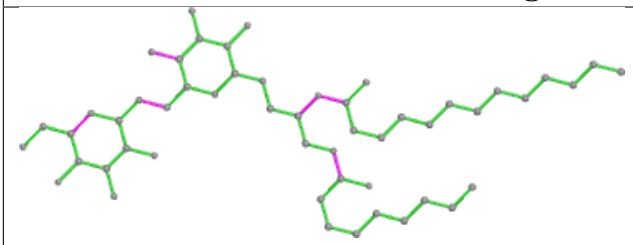


Torsions

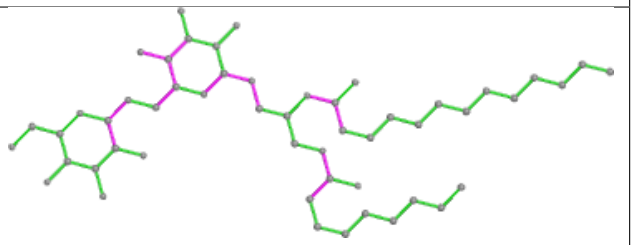


Rings

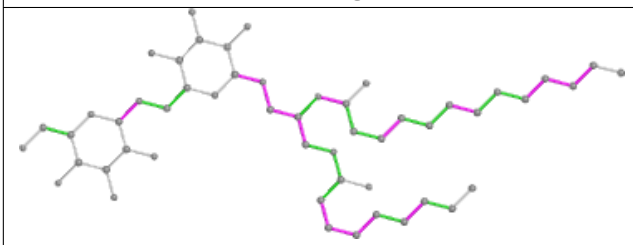
Ligand DGD b 602



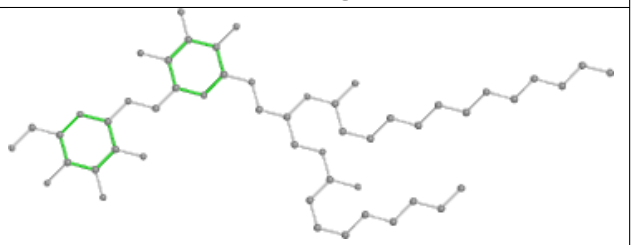
Bond lengths



Bond angles

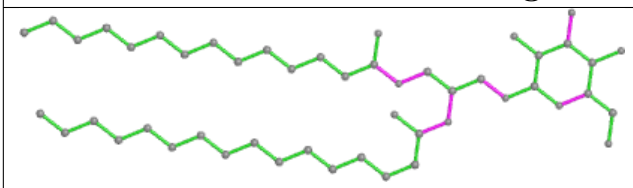


Torsions

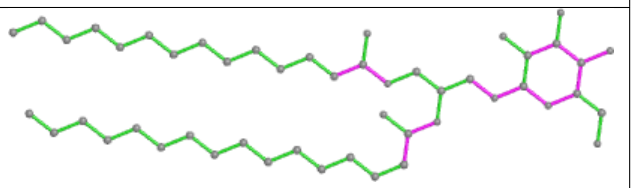


Rings

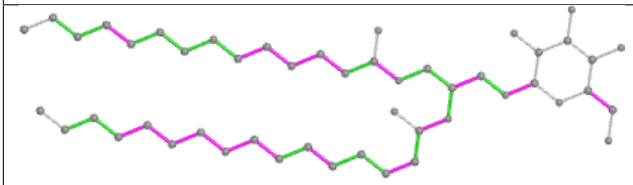
Ligand LMG b 624



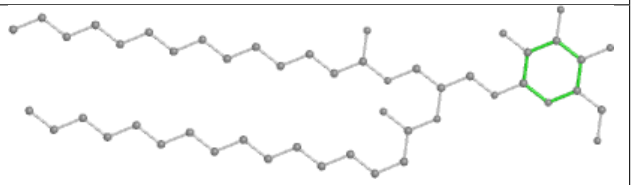
Bond lengths



Bond angles

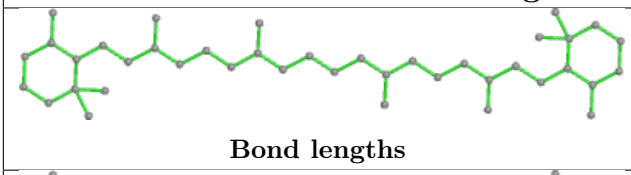


Torsions



Rings

Ligand BCR B 620



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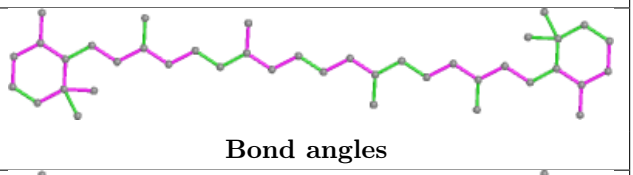
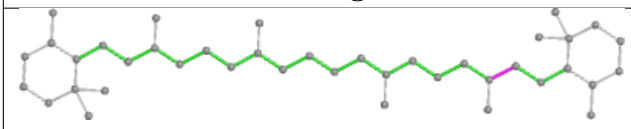
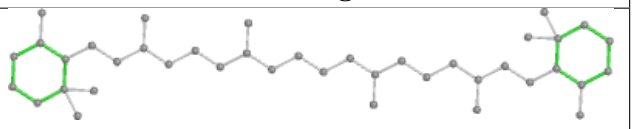


Bond angles

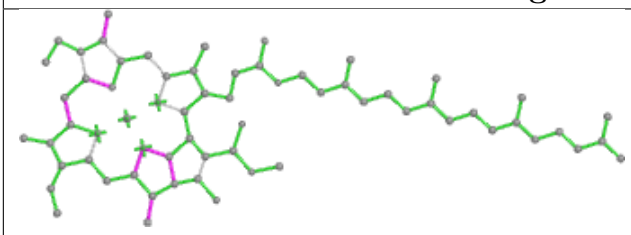


Torsions

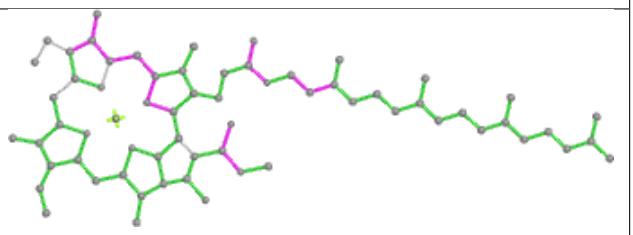


Rings

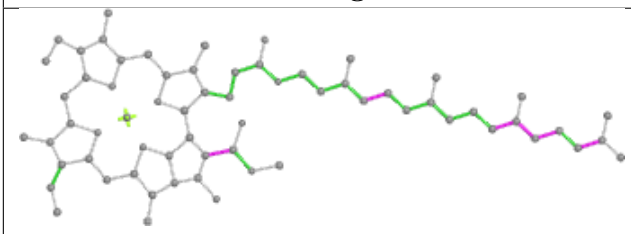
Ligand CLA c 502



Bond lengths



Bond angles



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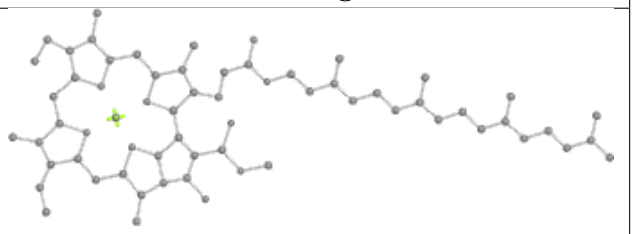
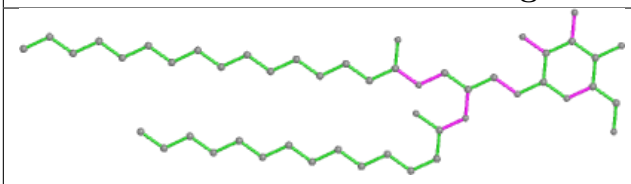
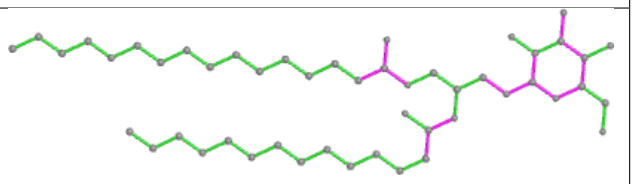


Rings

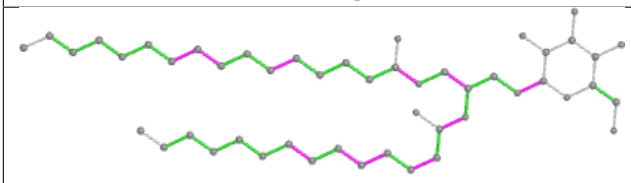
Ligand LMG B 623



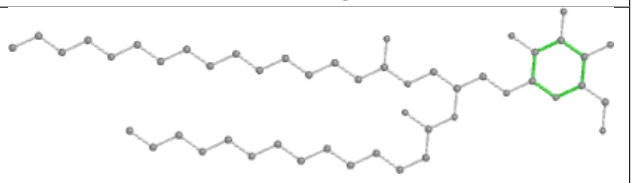
Bond lengths



Bond angles

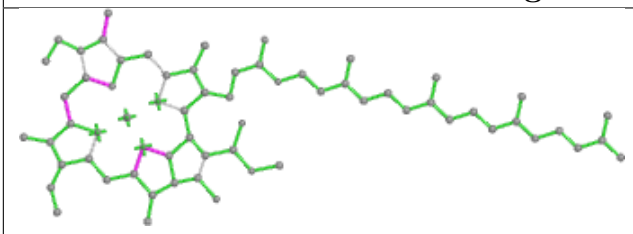


Torsions

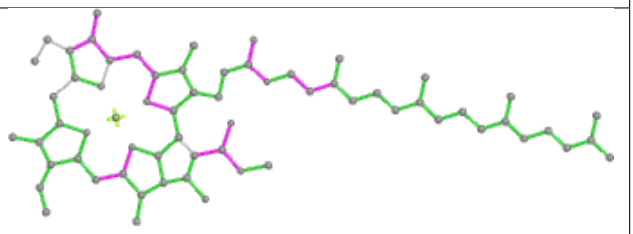


Rings

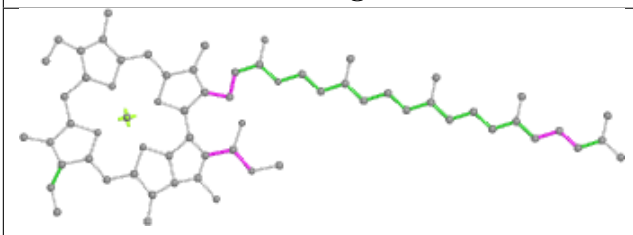
Ligand CLA B 607



Bond lengths



Bond angles



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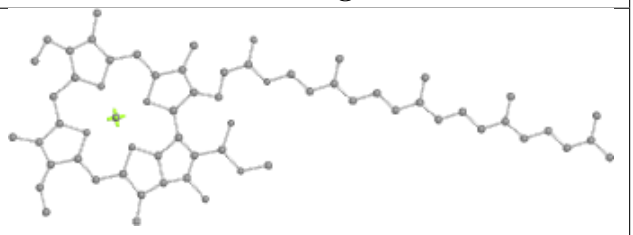
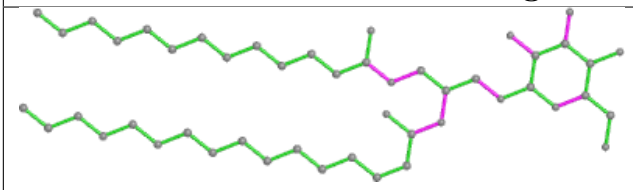


Rings

Ligand LMG d 407



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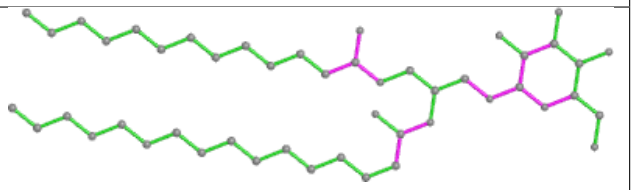
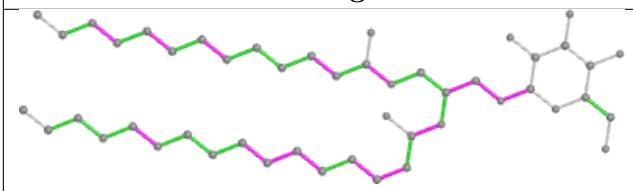
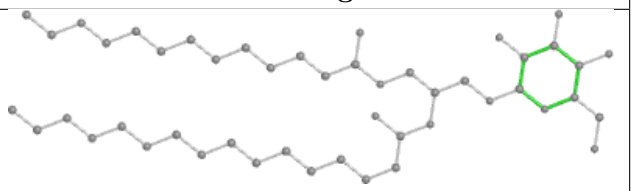


Bond angles

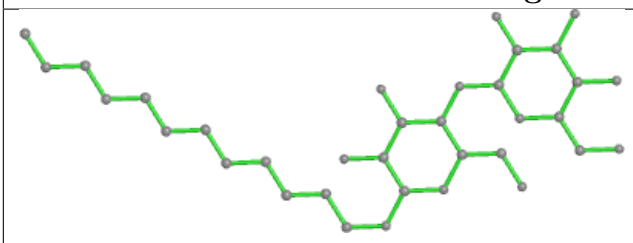


Torsions



Rings

Ligand LMT b 626



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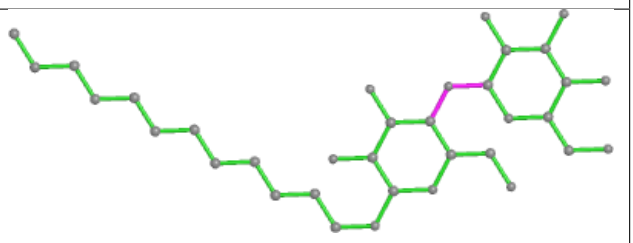
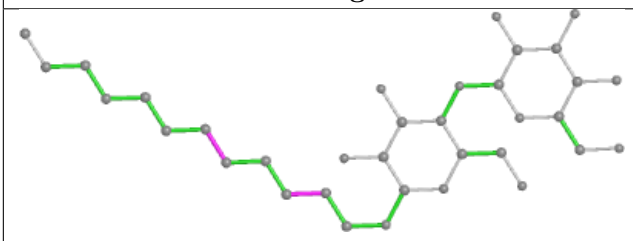
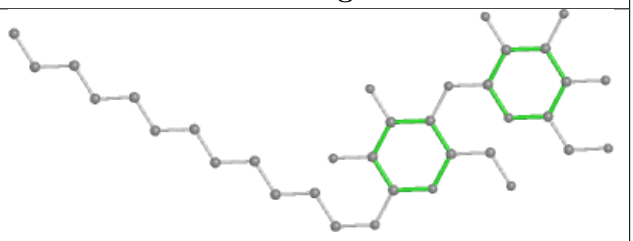


Bond angles

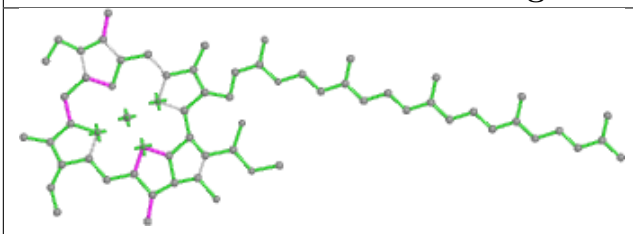


Torsions

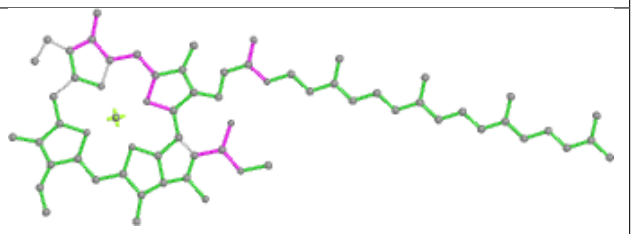


Rings

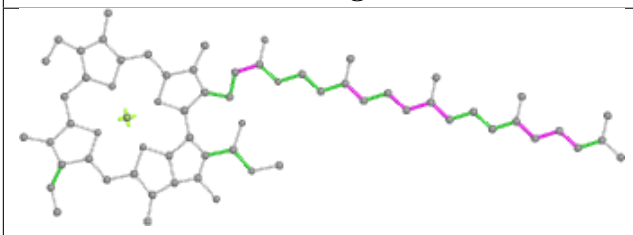
Ligand CLA d 402



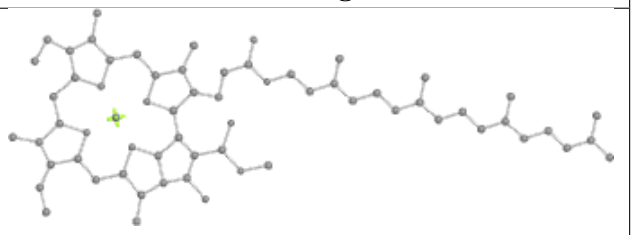
Bond lengths



Bond angles

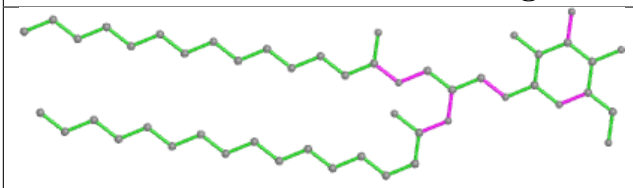


Torsions

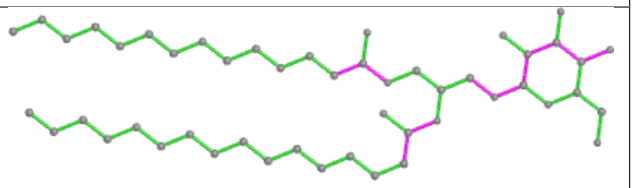


Rings

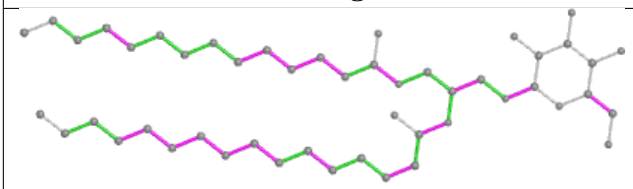
Ligand LMG B 622



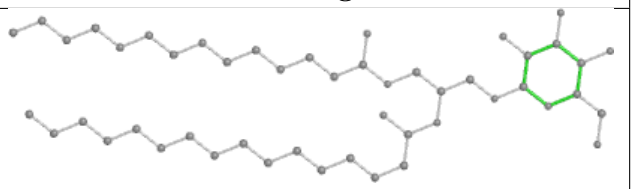
Bond lengths



Bond angles

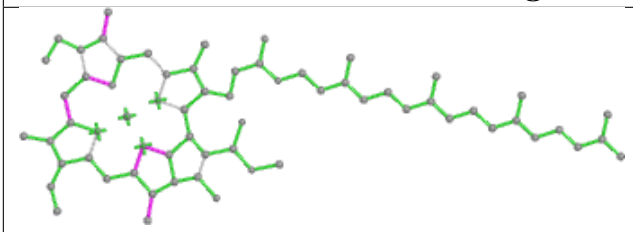


Torsions

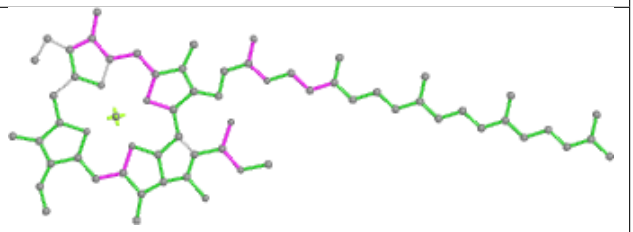


Rings

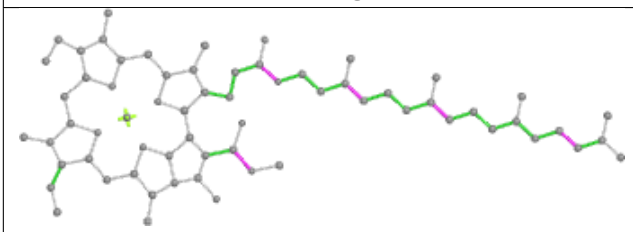
Ligand CLA B 611



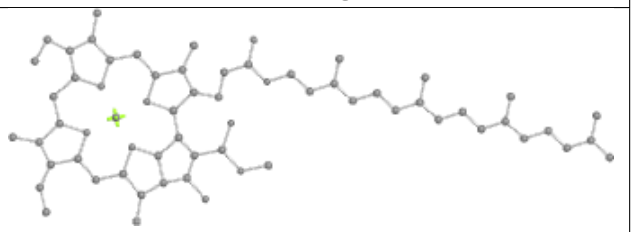
Bond lengths



Bond angles

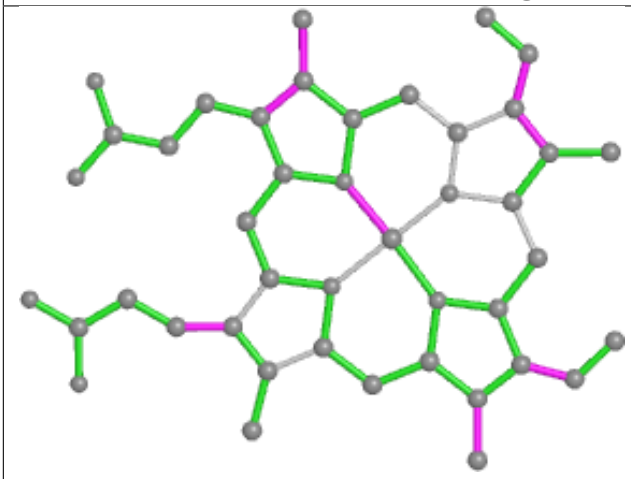


Torsions



Rings

Ligand HEM V 201



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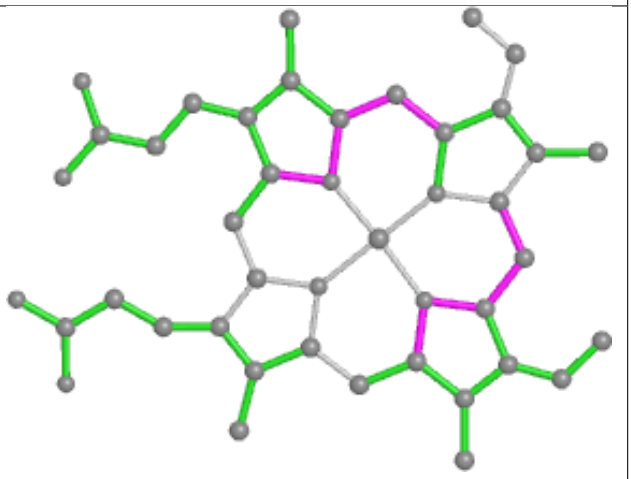

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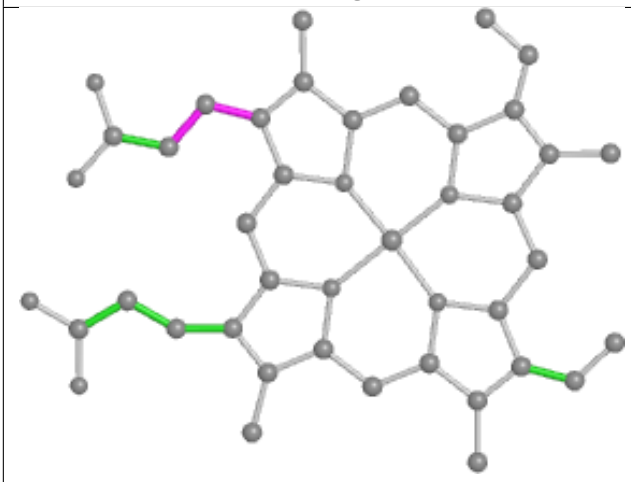
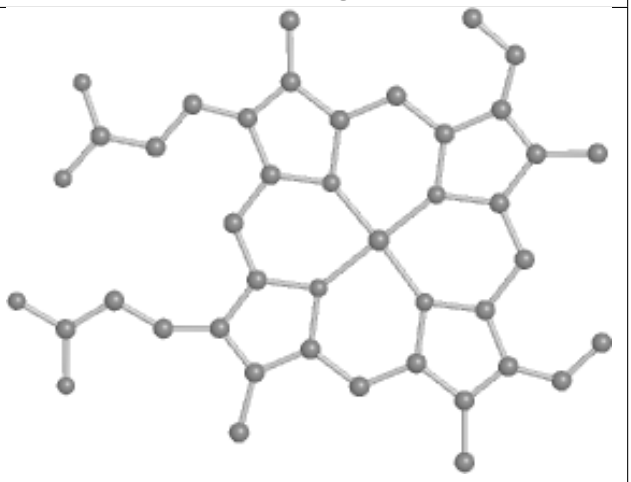
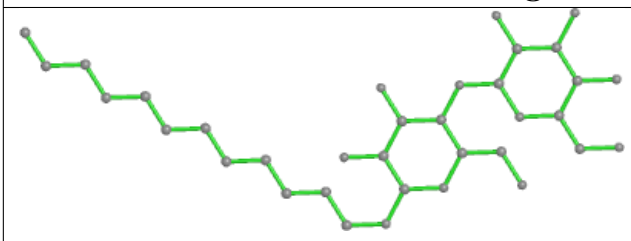


Torsions



Rings

Ligand LMT b 604



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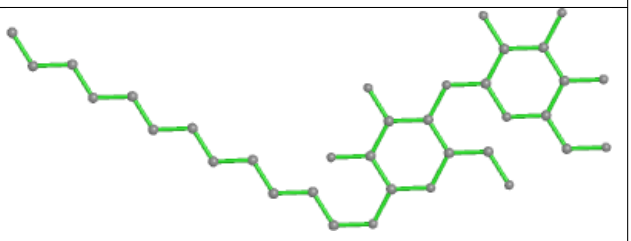

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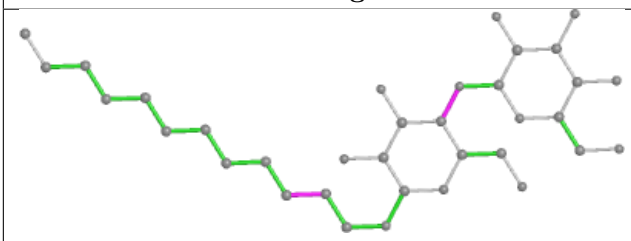

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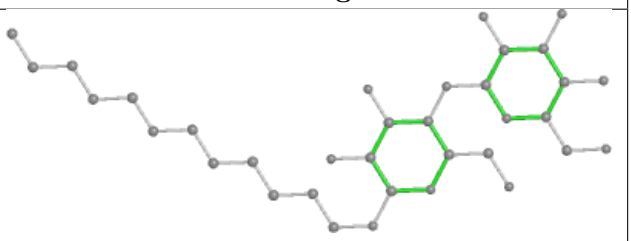
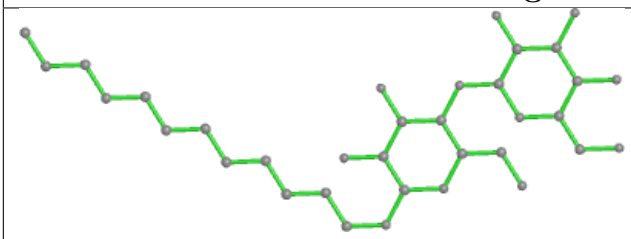


Rings

Ligand LMT b 603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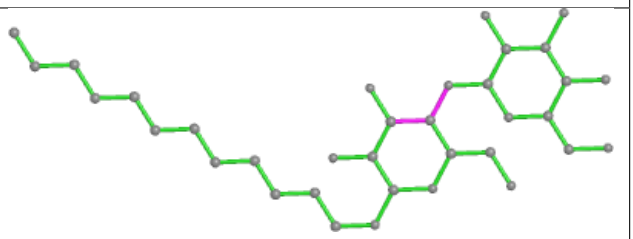
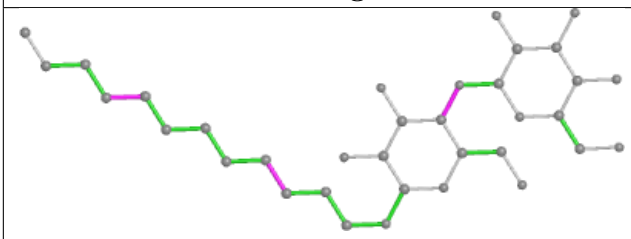
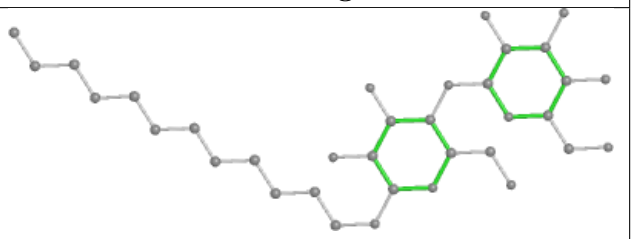
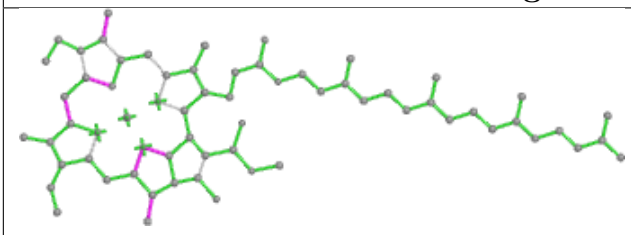

Bond angles


Torsions


Rings

Ligand CLA D 403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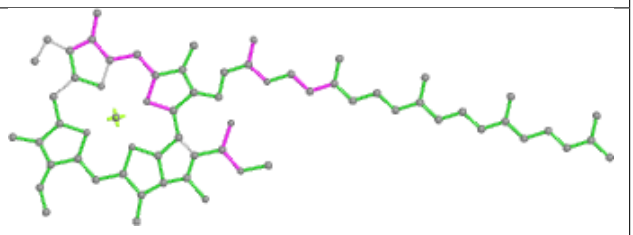
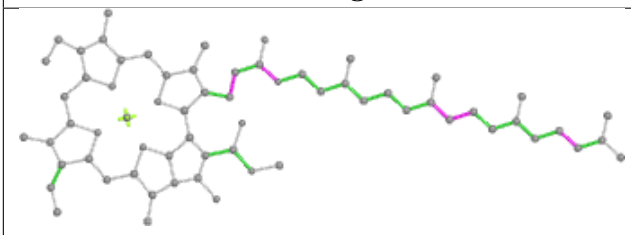
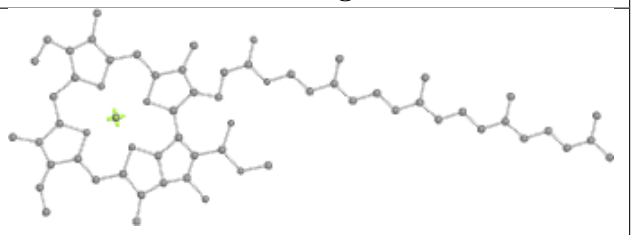
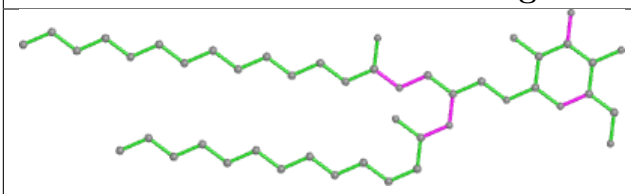

Bond angles


Torsions


Rings

Ligand LMG D 406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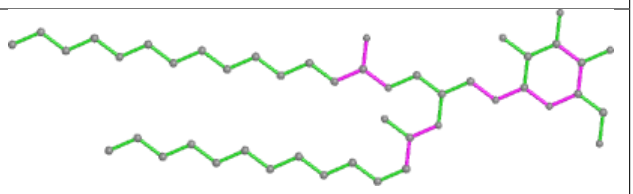
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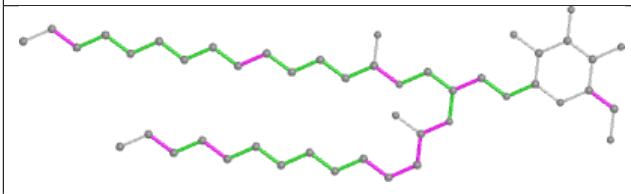
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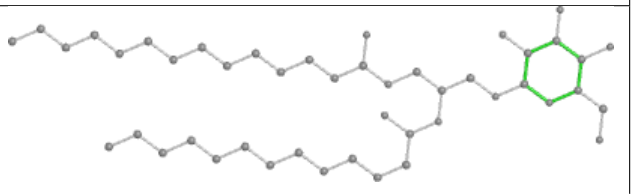
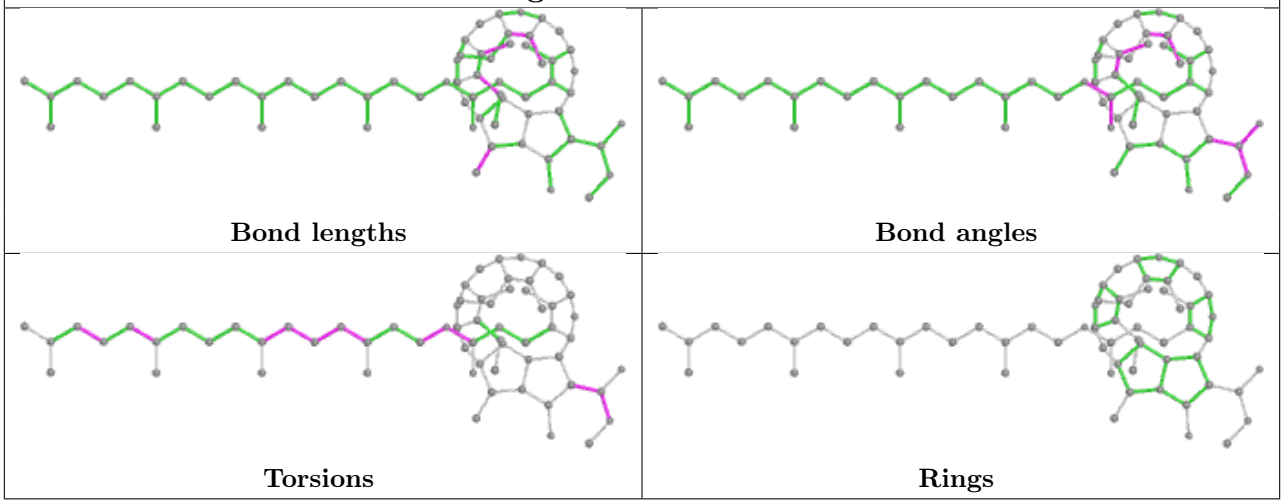

Rings

Ligand PHO a 407



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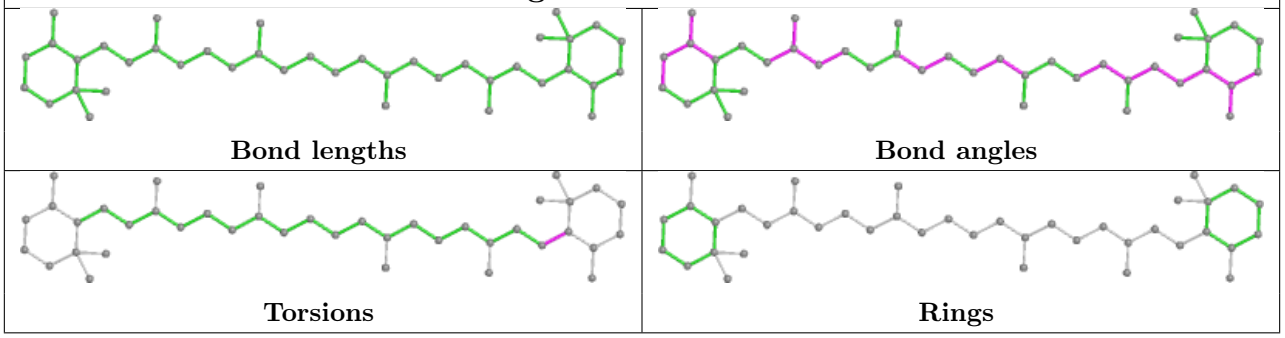

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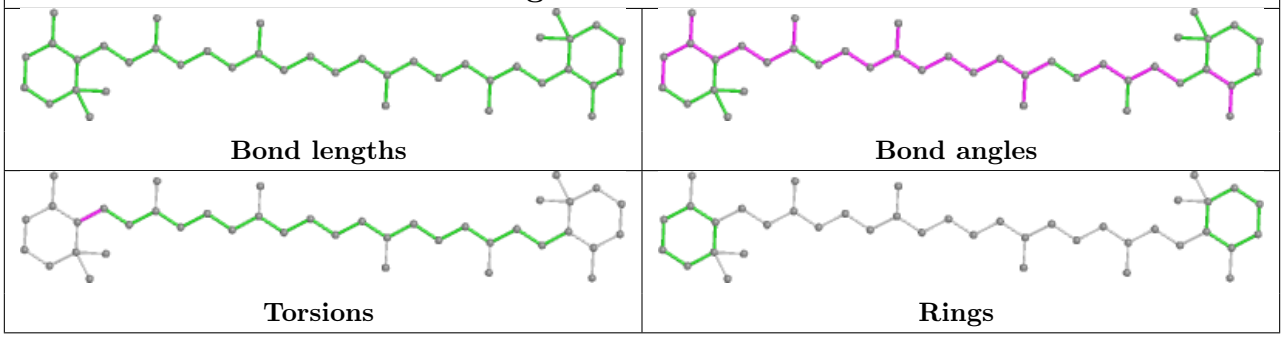
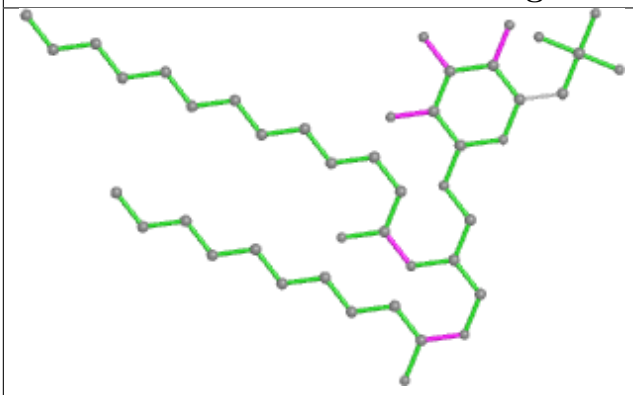
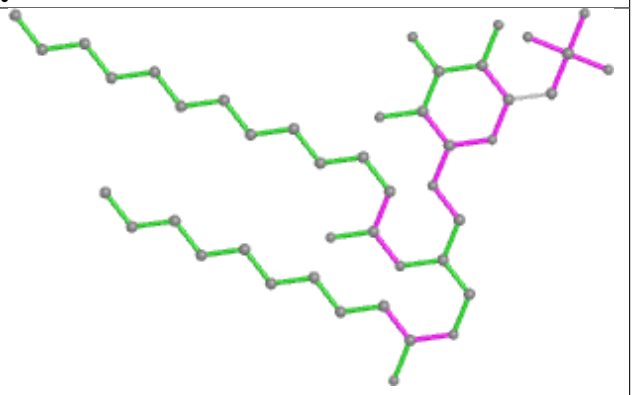


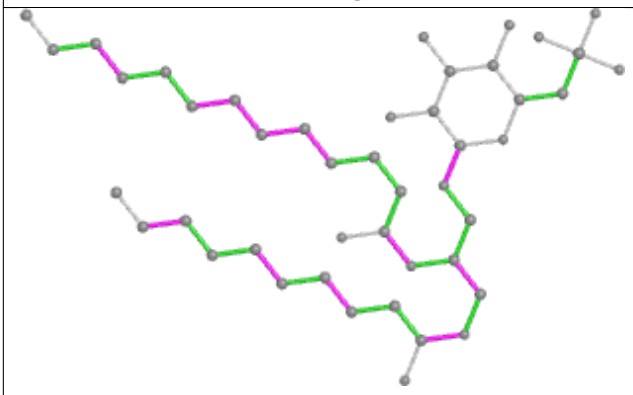
Ligand SQD F 102



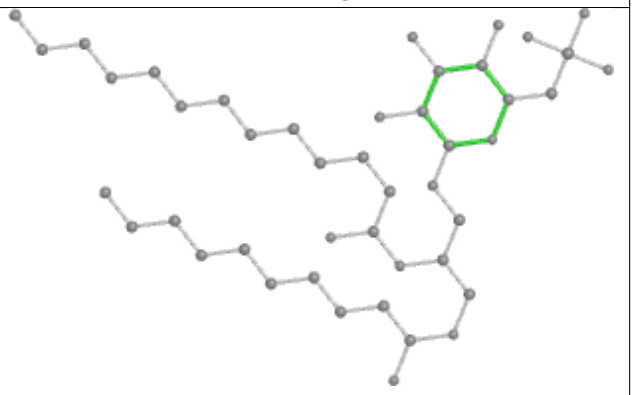
Bond lengths



Bond angles

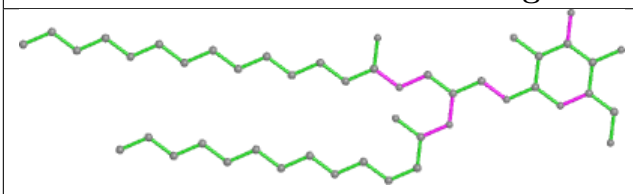


Torsions



Rings

Ligand LMG d 406



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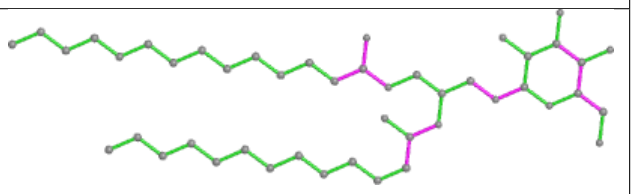
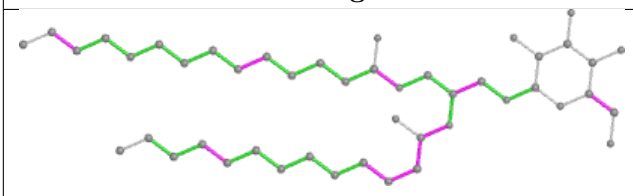


Bond angles



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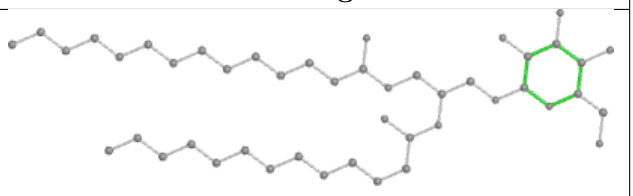
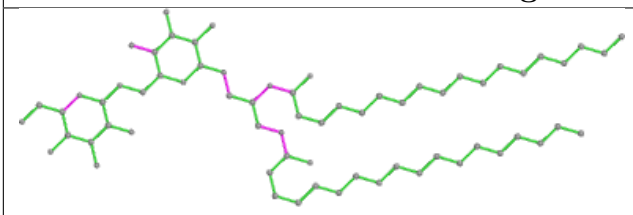


Rings

Ligand DGD C 519



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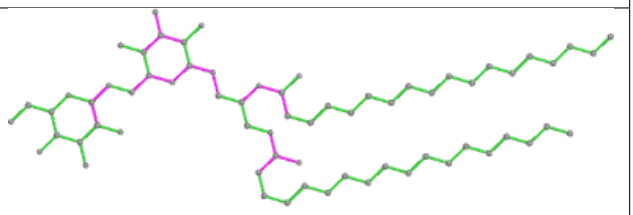
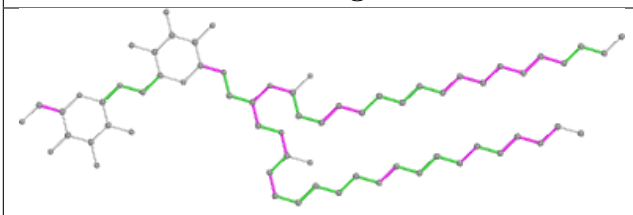


Bond angles



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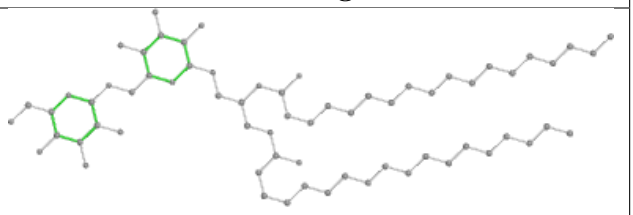
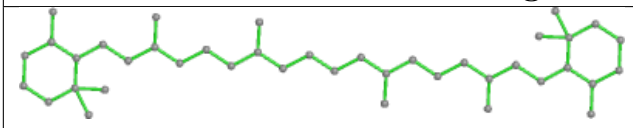


Rings

Ligand BCR B 618



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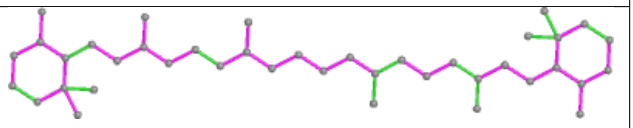
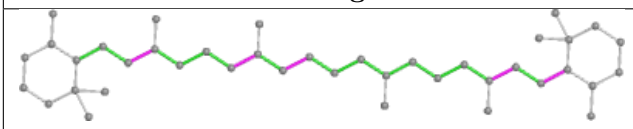
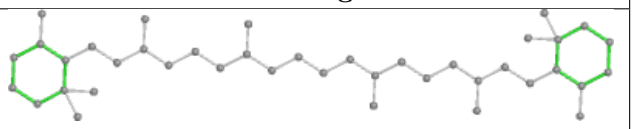


Bond angles

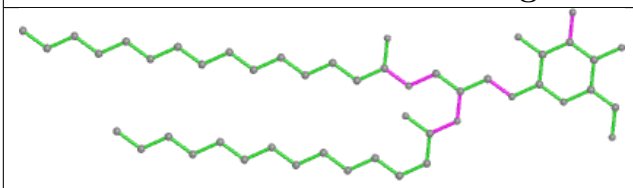


Torsions



Rings

Ligand LMG C 520



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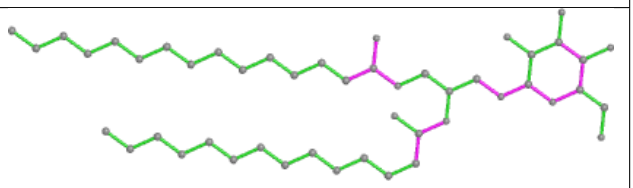
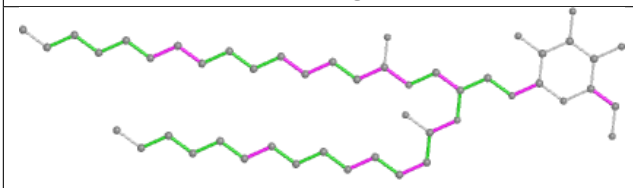
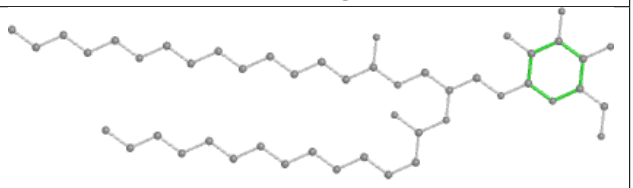


Bond angles

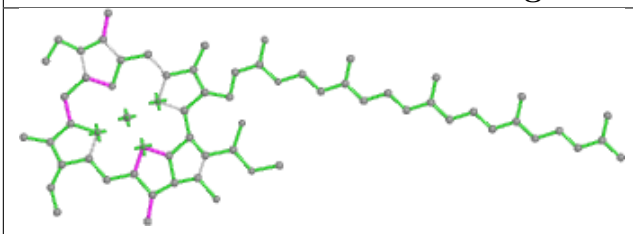


Torsions



Rings

Ligand CLA B 603



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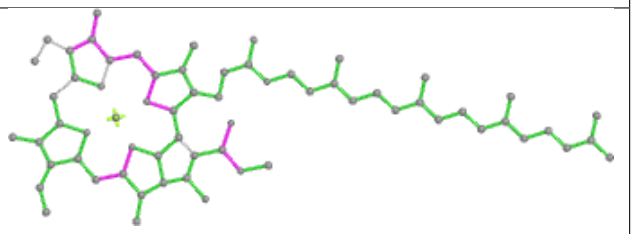
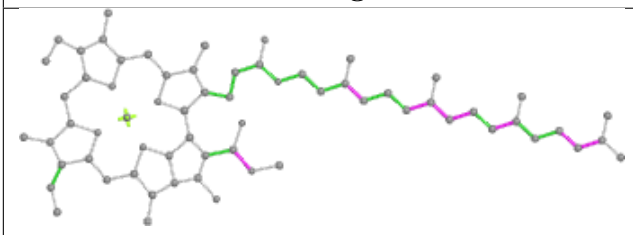
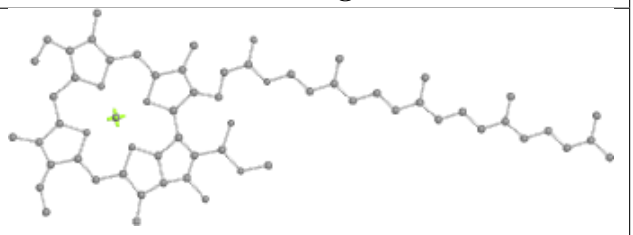


Bond angles

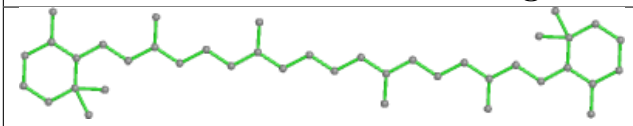


Torsions

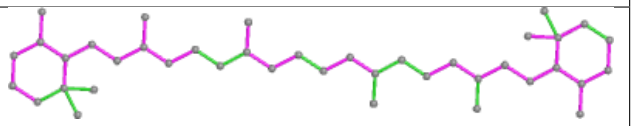


Rings

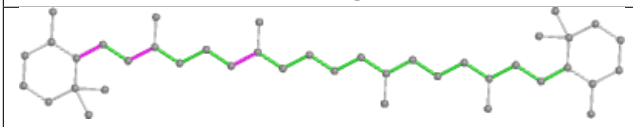
Ligand BCR C 514



Bond lengths



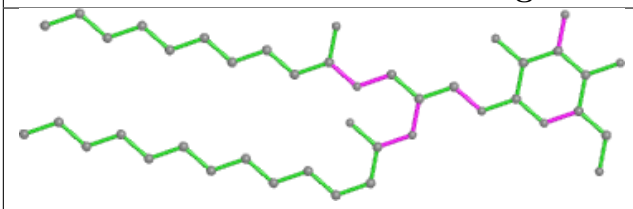
Bond angles



Torsions

Rings

Ligand LMG M 101



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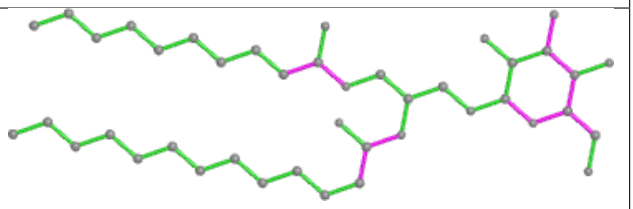
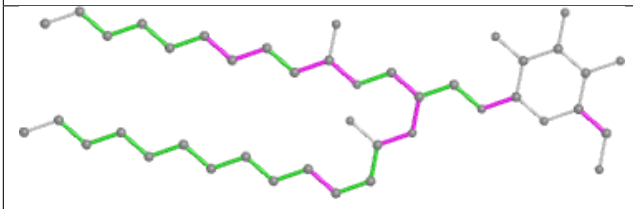
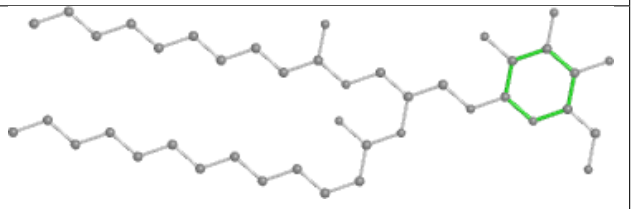


Bond angles

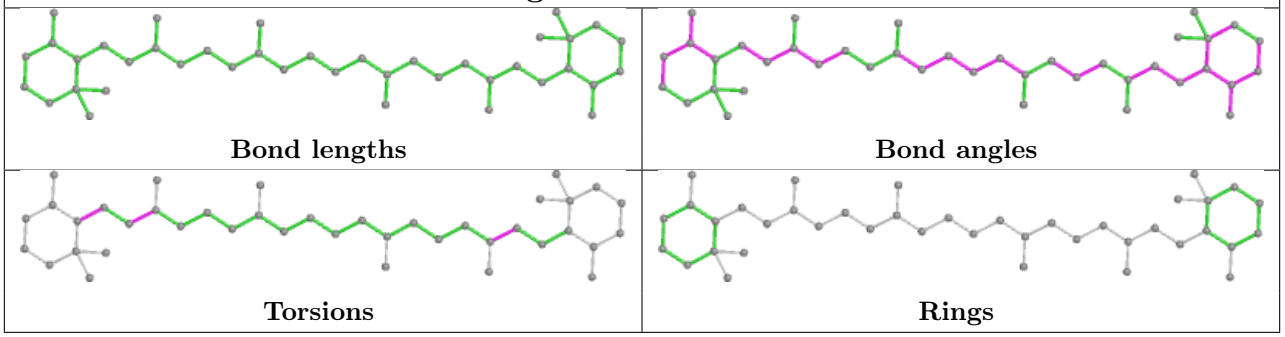


Torsions

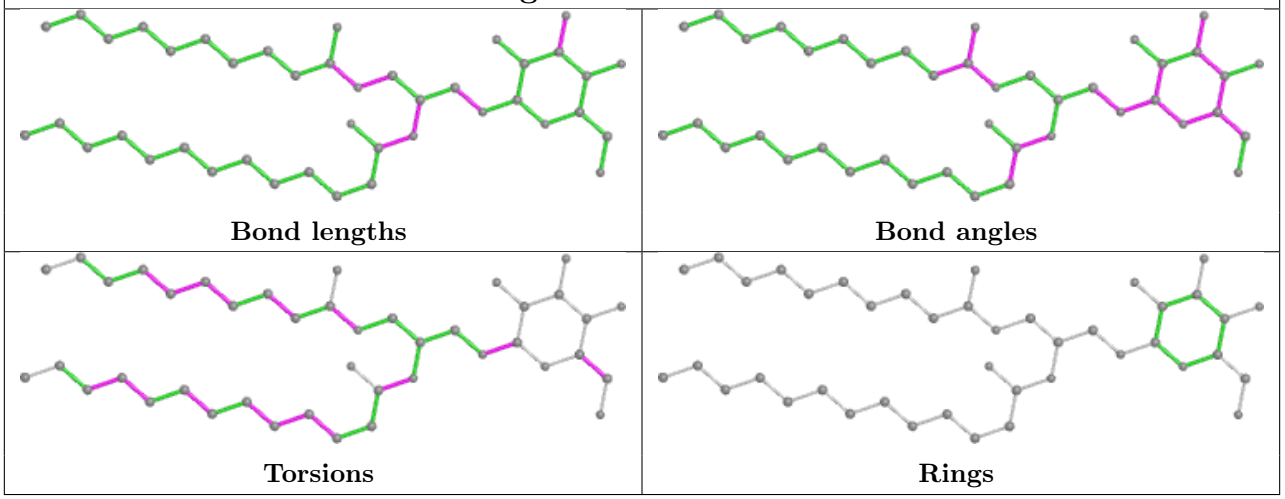


Rings

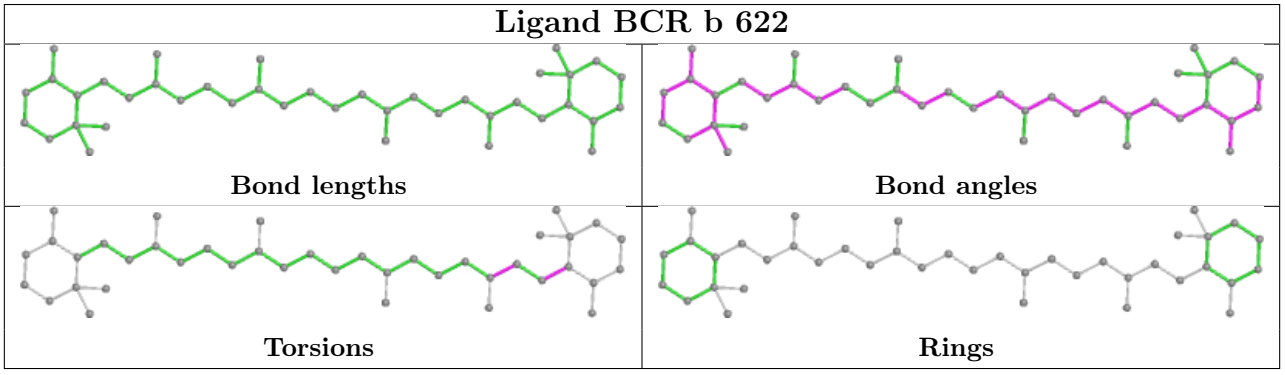
Ligand BCR d 405



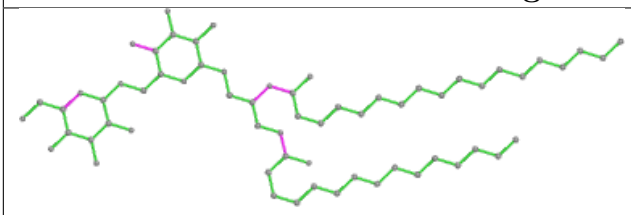
Ligand LMG A 418



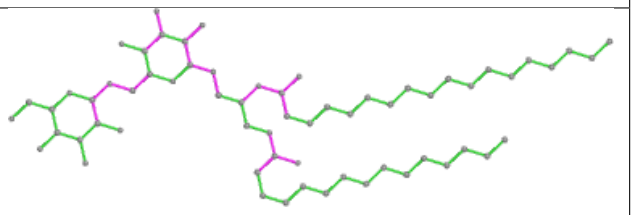
Ligand BCR b 622



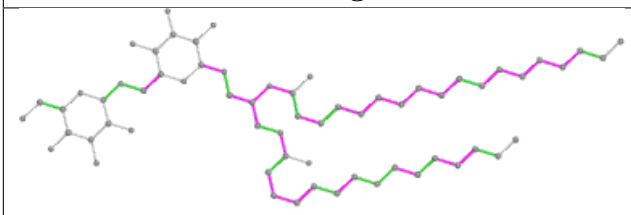
Ligand DGD d 409



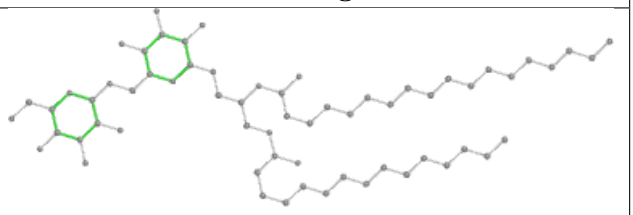
Bond lengths



Bond angles

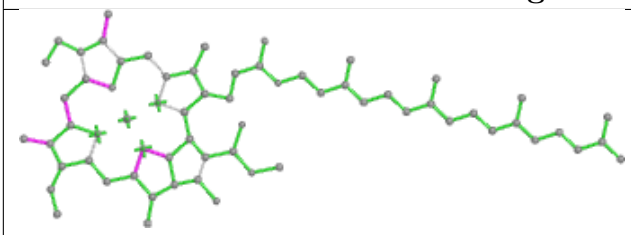


Torsions



Rings

Ligand CLA b 605



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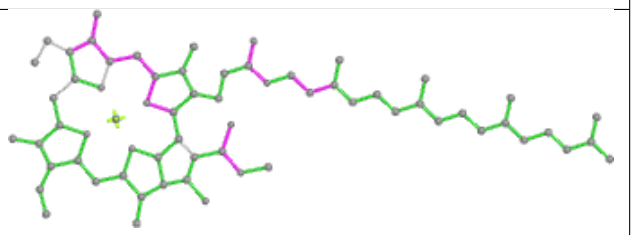
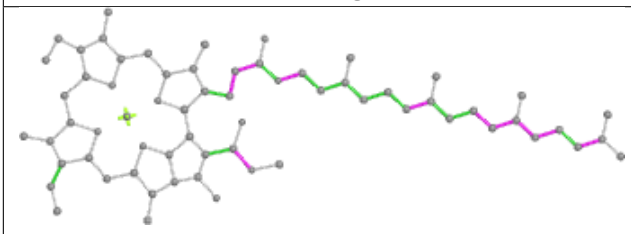


Bond angles



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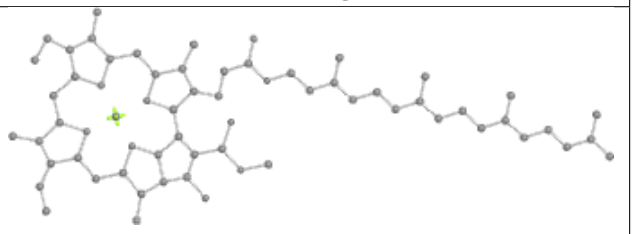
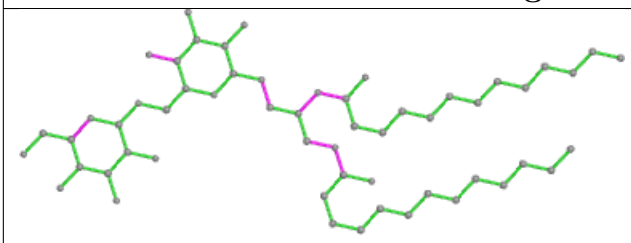


Rings

Ligand DGD a 413



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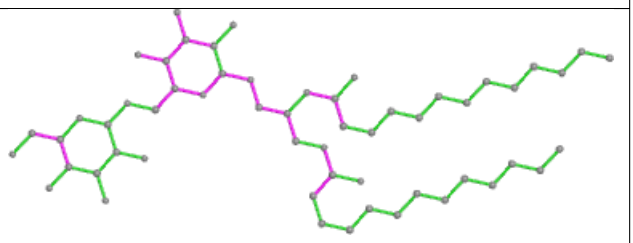
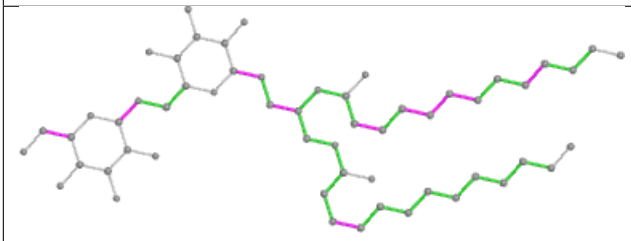


Bond angles



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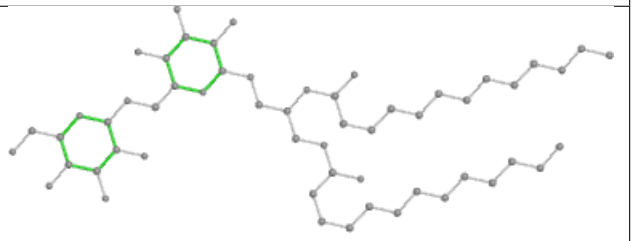
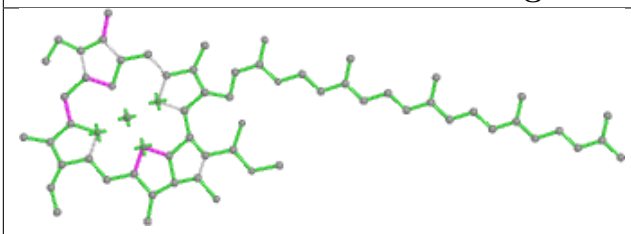


Rings

Ligand CLA B 609



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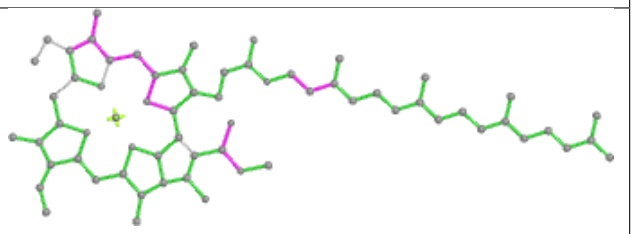
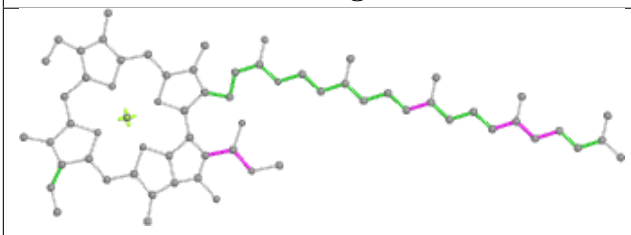


Bond angles



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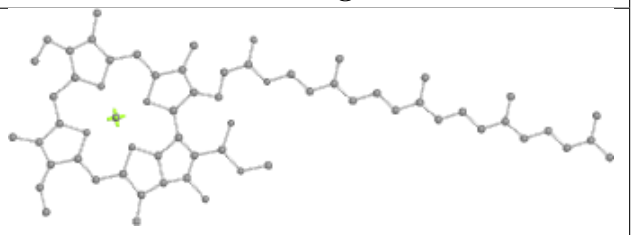
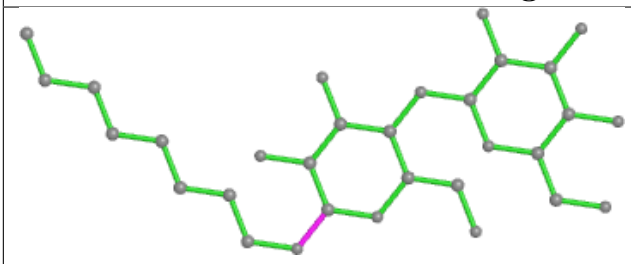


Rings

Ligand LMT D 410



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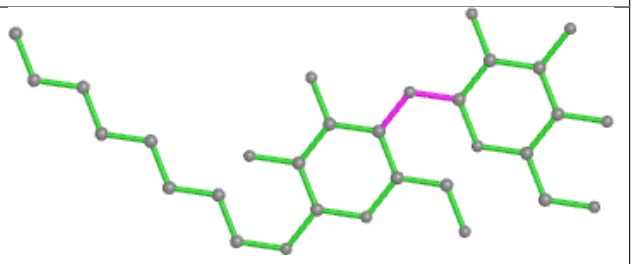
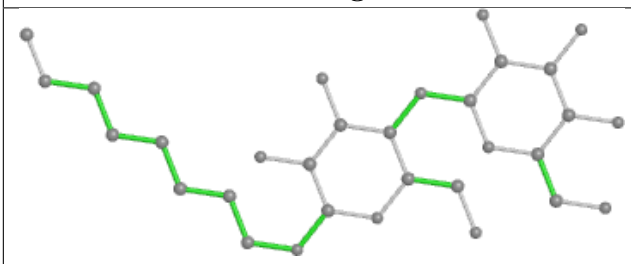


Bond angles



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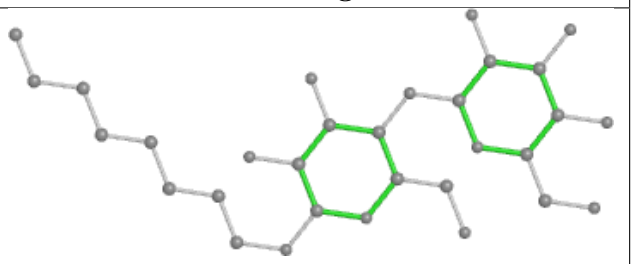
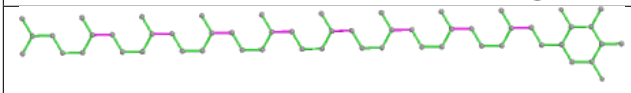


Rings

Ligand PL9 D 404



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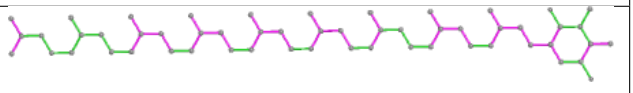
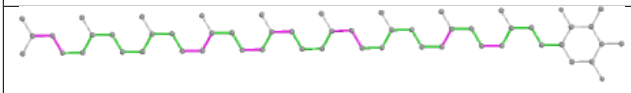
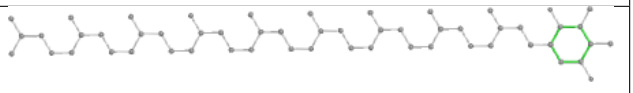


Bond angles

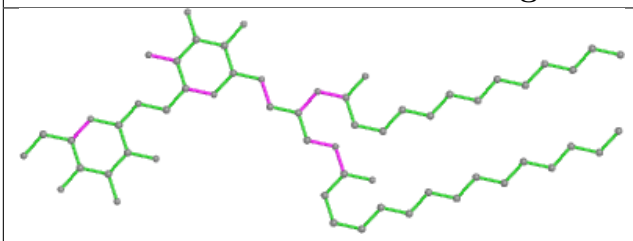


Torsions



Rings

Ligand DGD B 621



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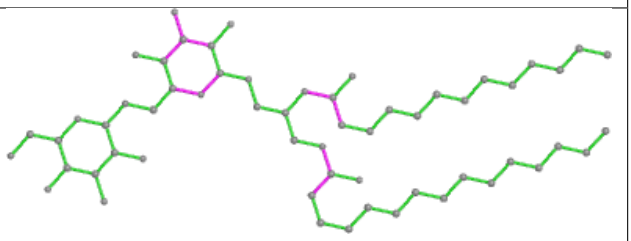
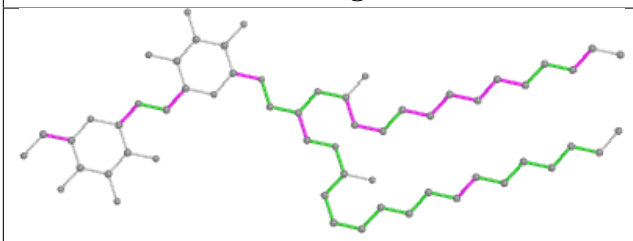


Bond angles



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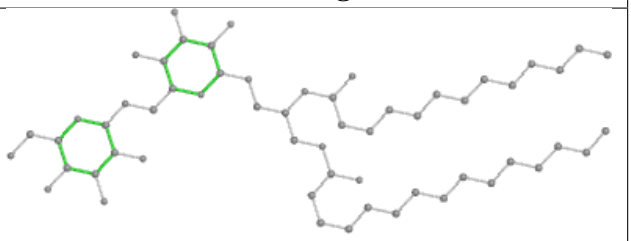
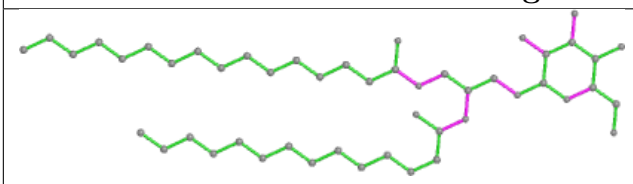


Rings

Ligand LMG b 625



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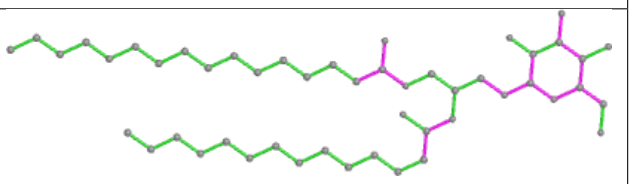

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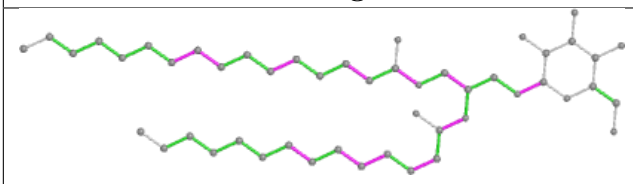

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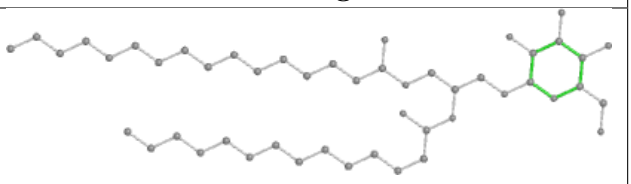

Rings

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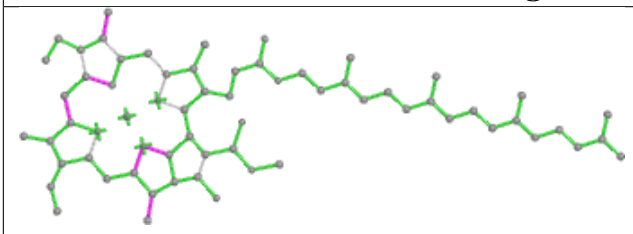

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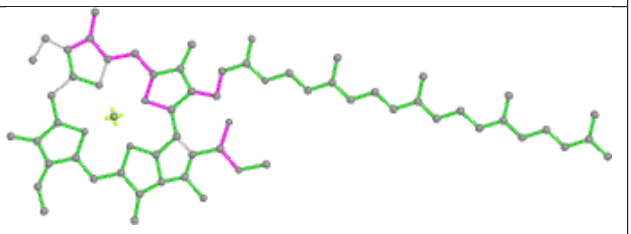

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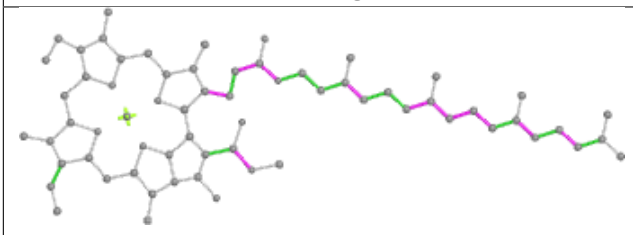
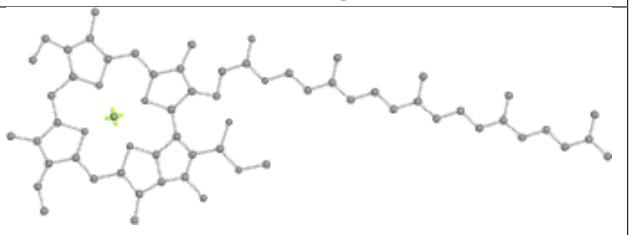
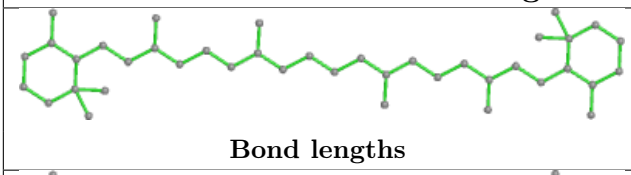


Torsions



Rings

Ligand BCR C 516



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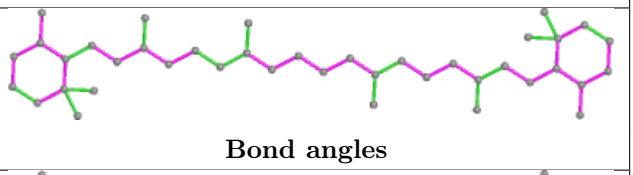
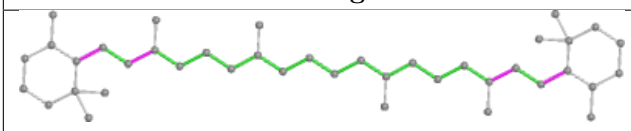


Bond angles



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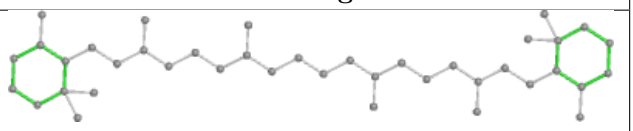
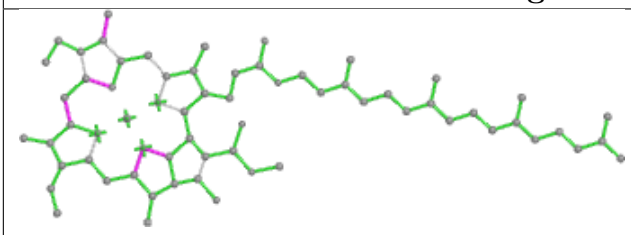


Rings

Ligand CLA b 613



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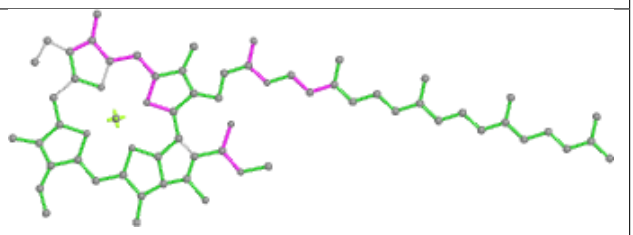
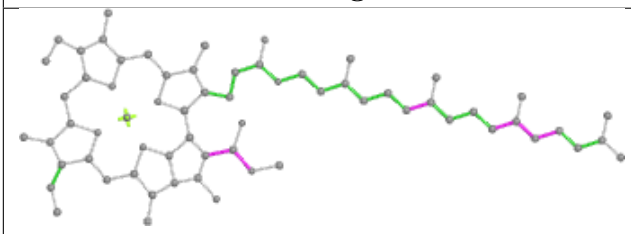
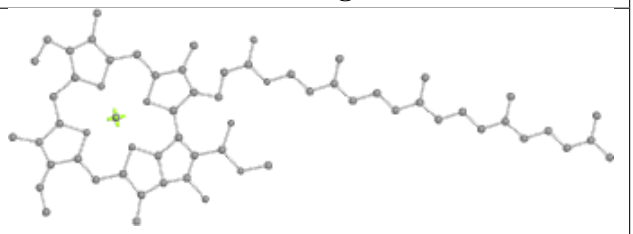


Bond angles

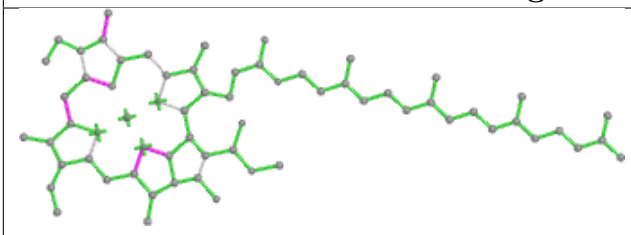


Torsions

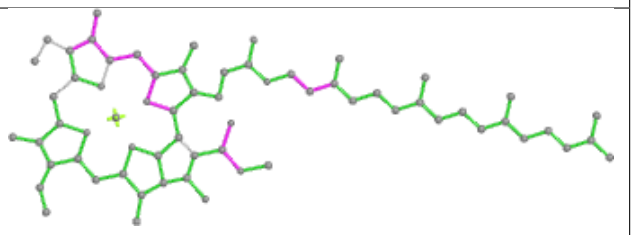


Rings

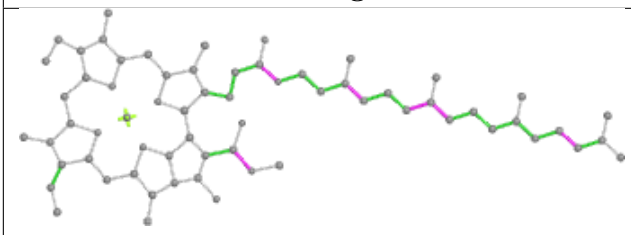
Ligand CLA b 615



Bond lengths



Bond angles



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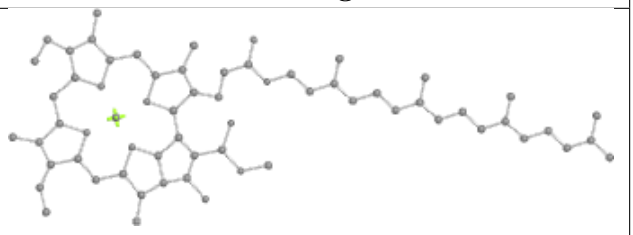
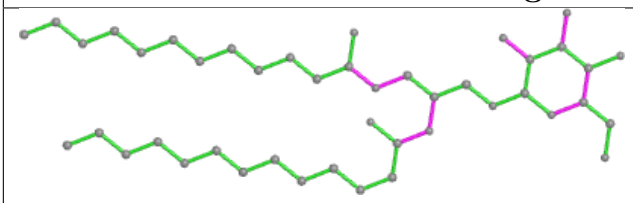


Rings

Ligand LMG e 101



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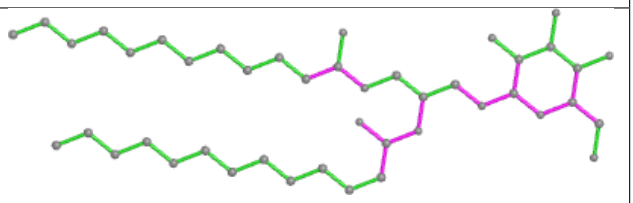
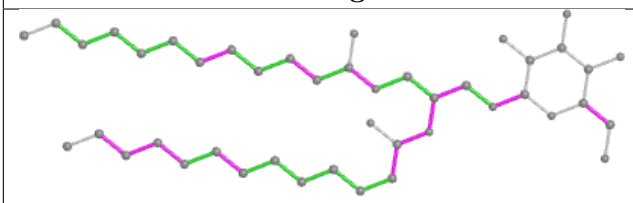
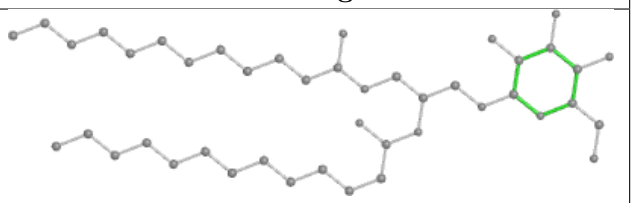


Bond angles

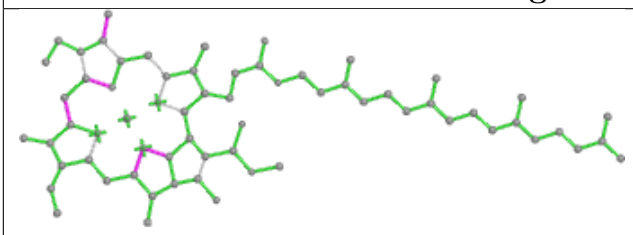


Torsions



Rings

Ligand CLA c 504



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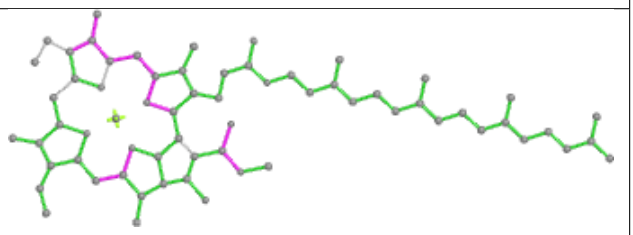
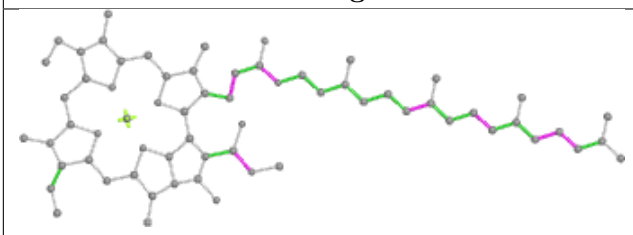


Bond angles



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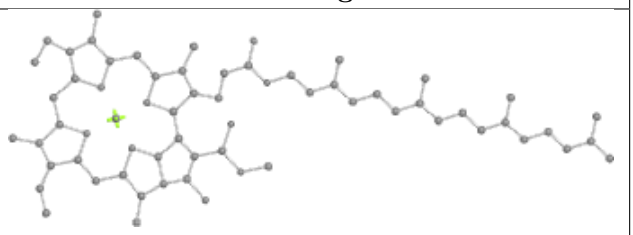
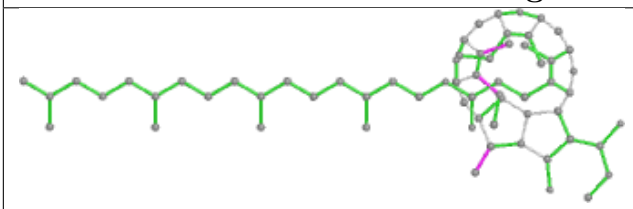


Rings

Ligand PHO a 408



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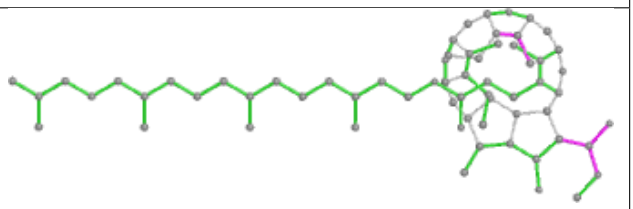

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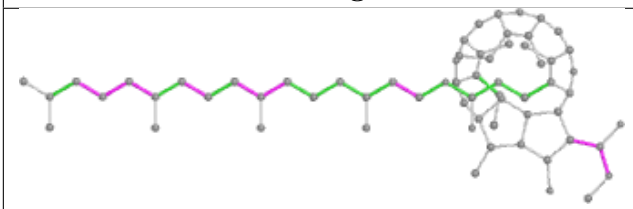
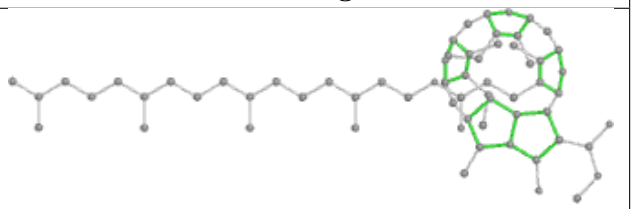
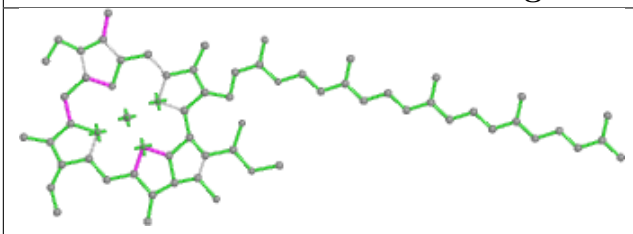


Torsions



Rings

Ligand CLA B 606



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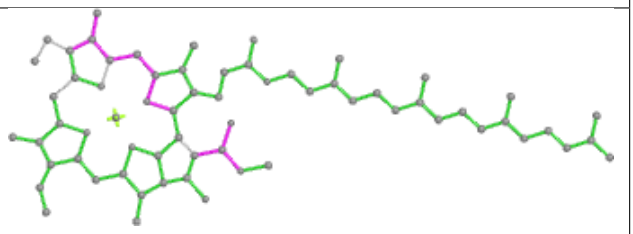
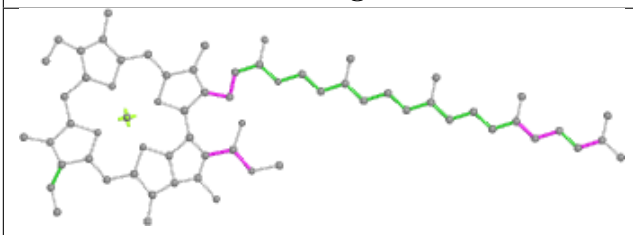


Bond angles



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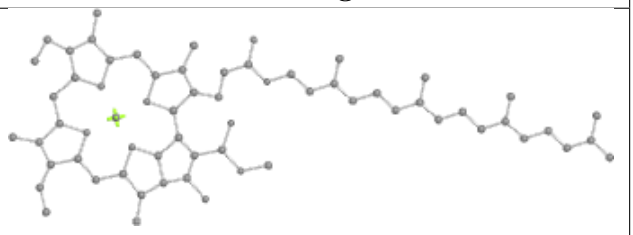
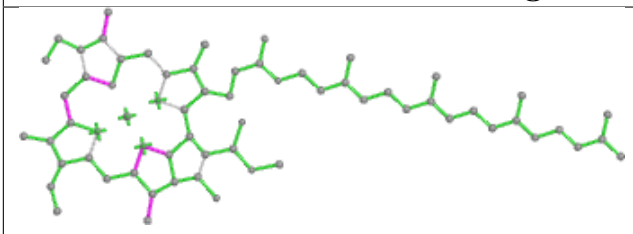


Rings

Ligand CLA B 612



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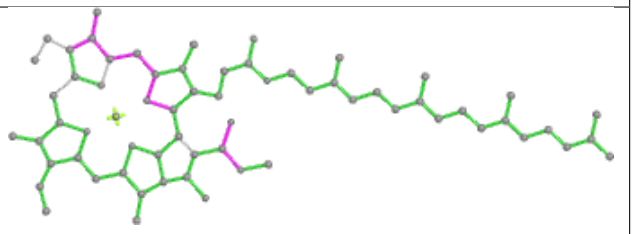
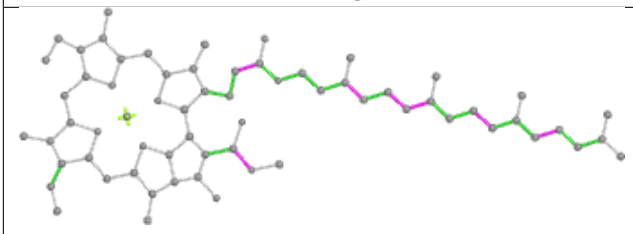


Bond angles



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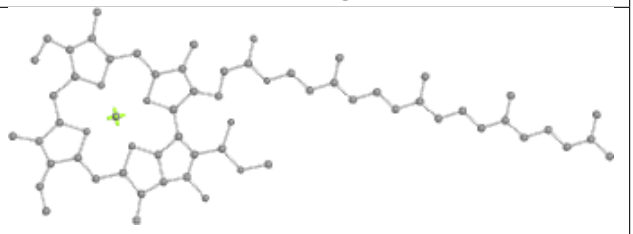
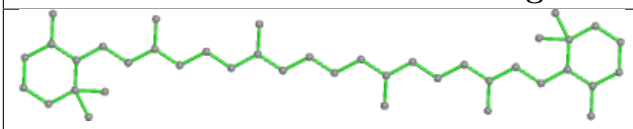


Rings

Ligand BCR J 102



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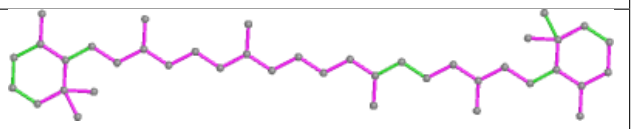
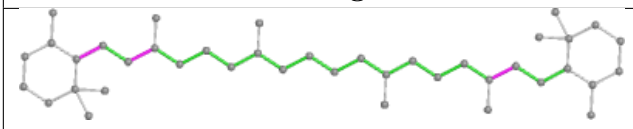


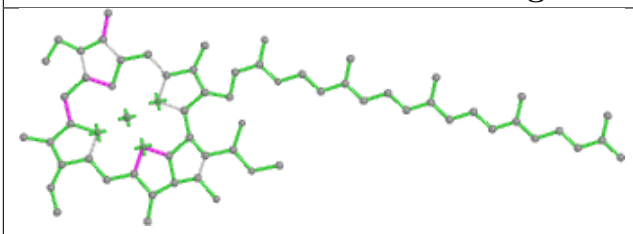
Bond angles



Torsions

Rings

Ligand CLA b 606



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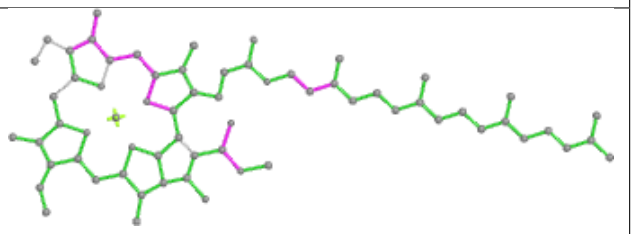

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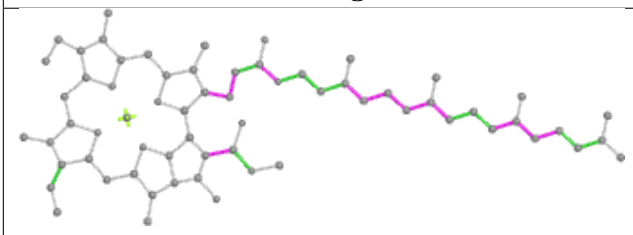

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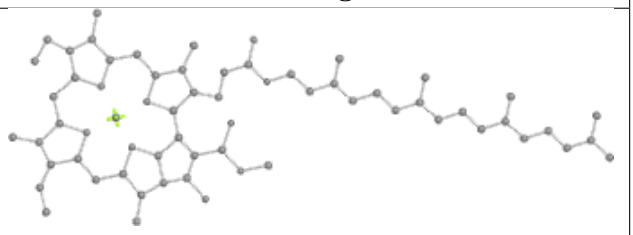
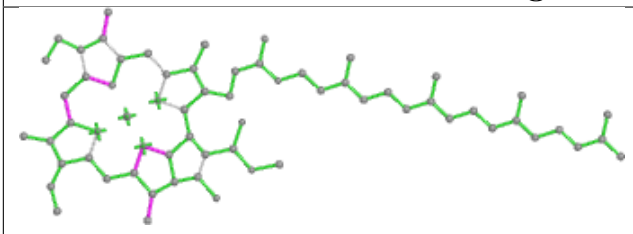


Rings

Ligand CLA b 612



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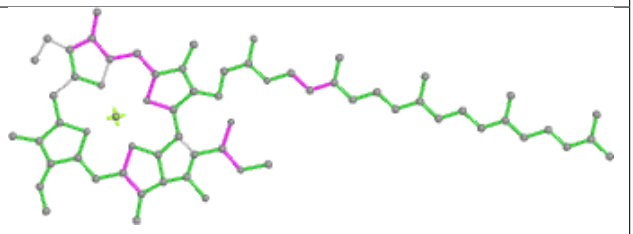
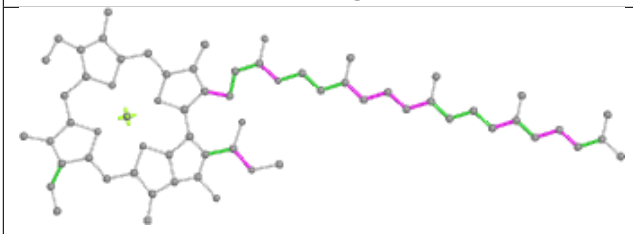


Bond angles



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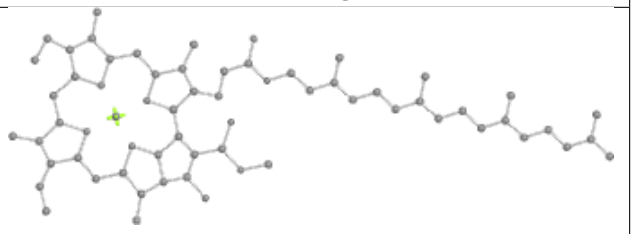
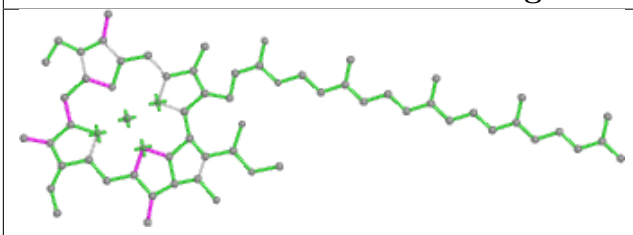


Rings

Ligand CLA C 502



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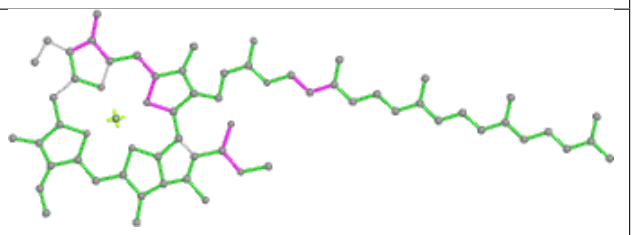

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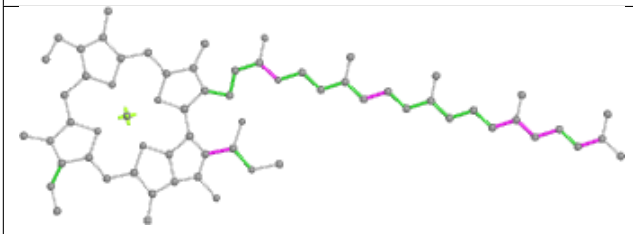

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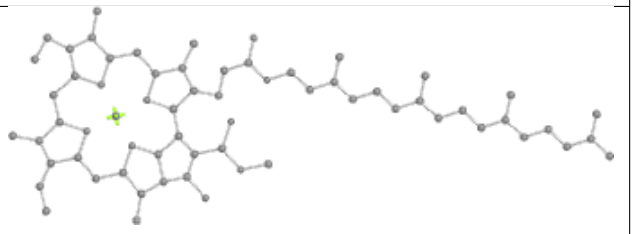
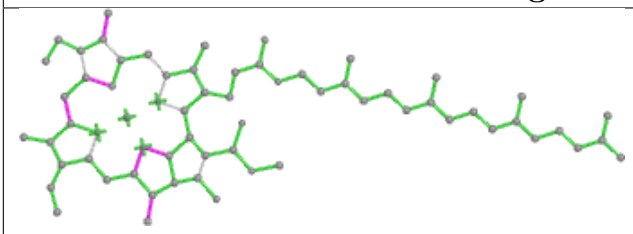


Rings

Ligand CLA a 404



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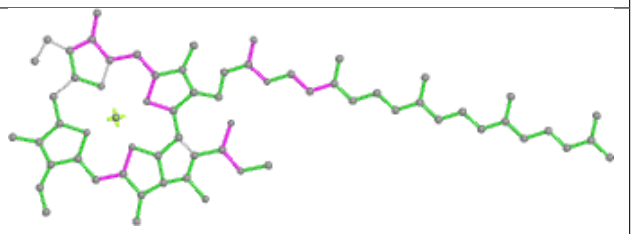

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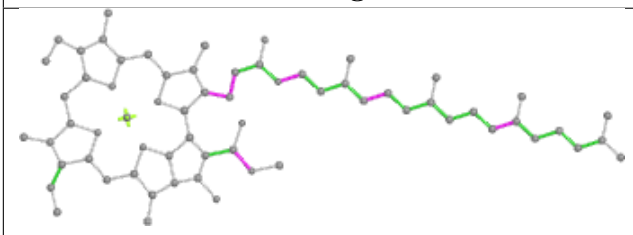

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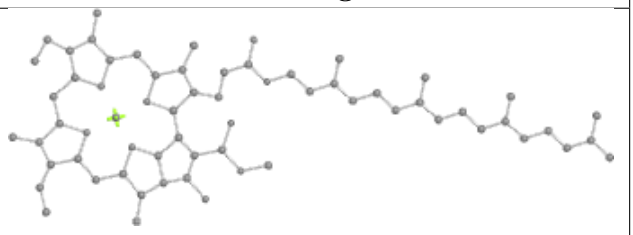
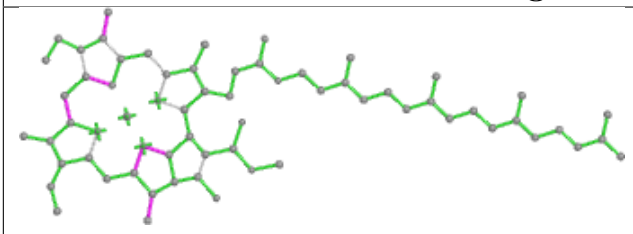


Rings

Ligand CLA d 403



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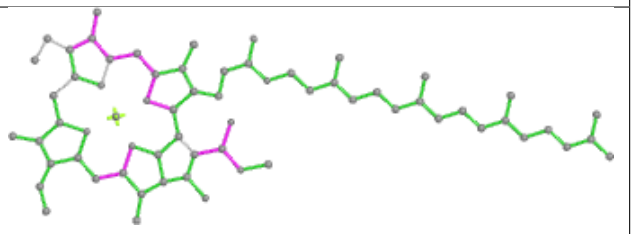

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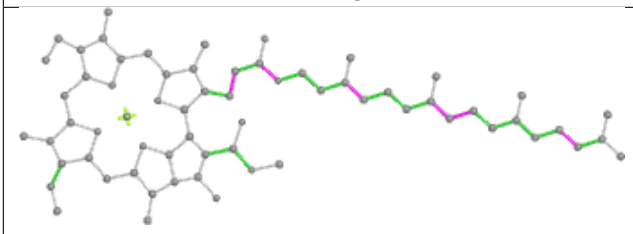

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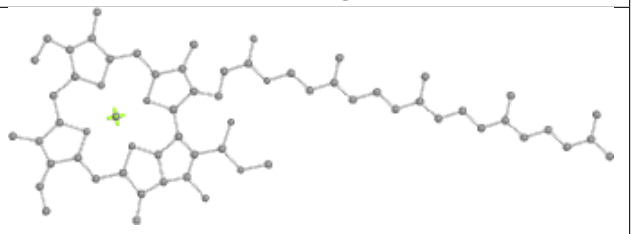
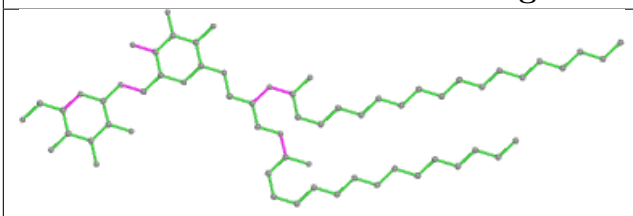


Rings

Ligand DGD D 409



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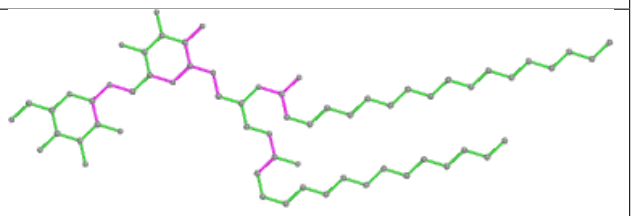

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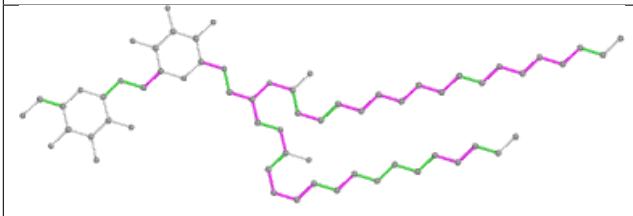

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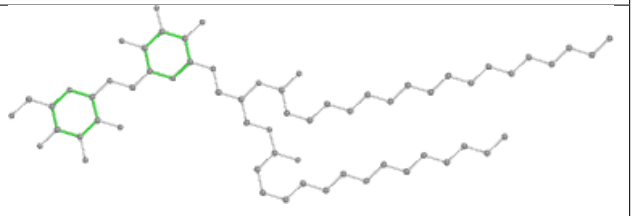
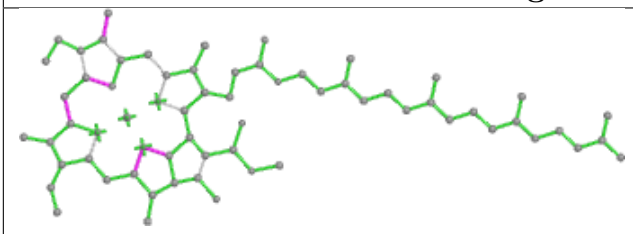


Rings

Ligand CLA b 614



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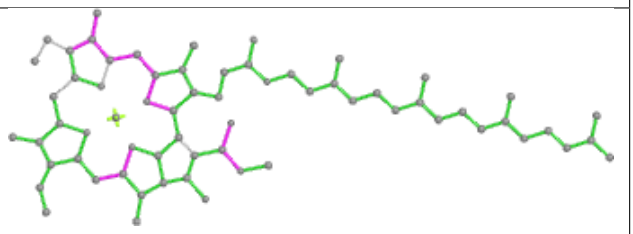
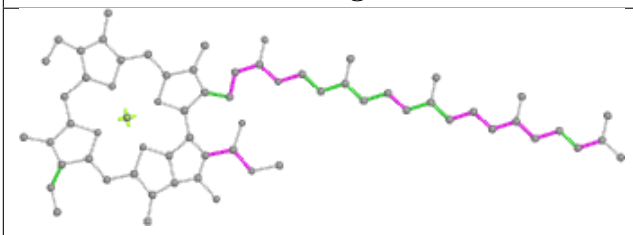


Bond angles



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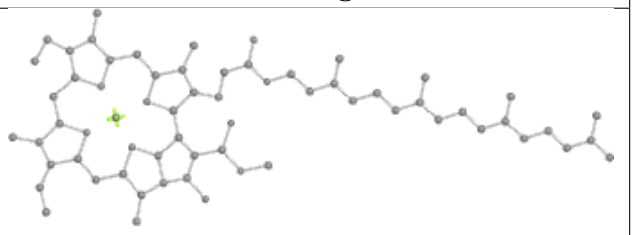
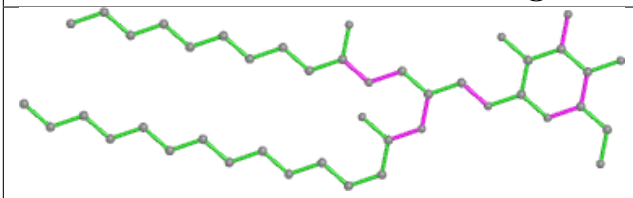


Rings

Ligand LMG i 101



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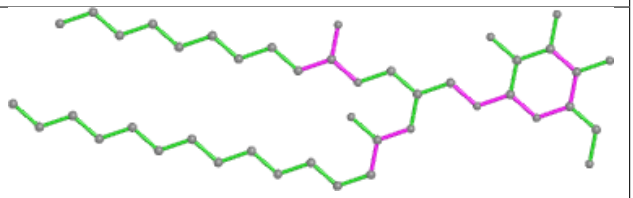
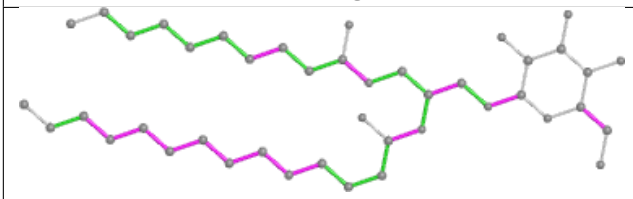


Bond angles



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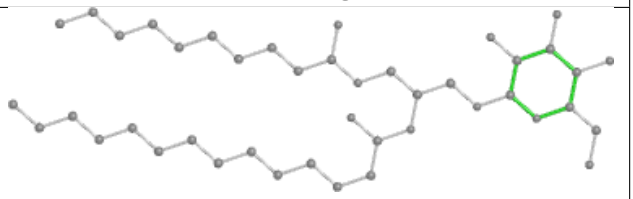
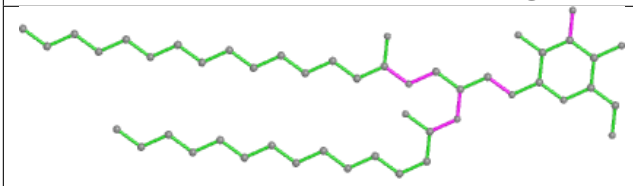


Rings

Ligand LMG k 103



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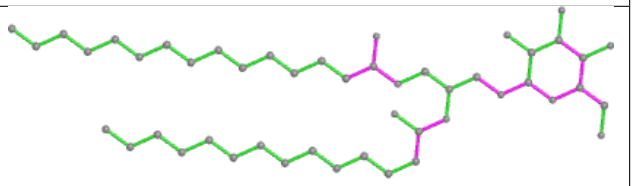
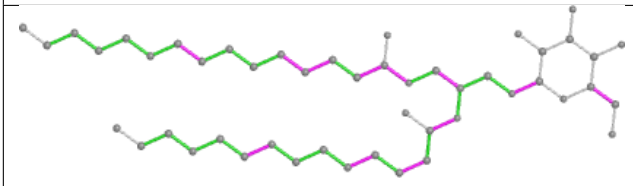
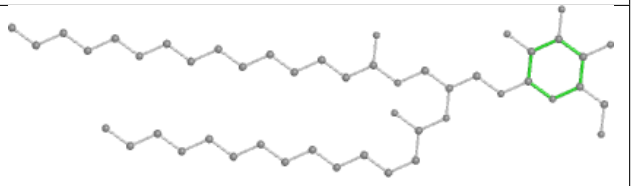


Bond angles

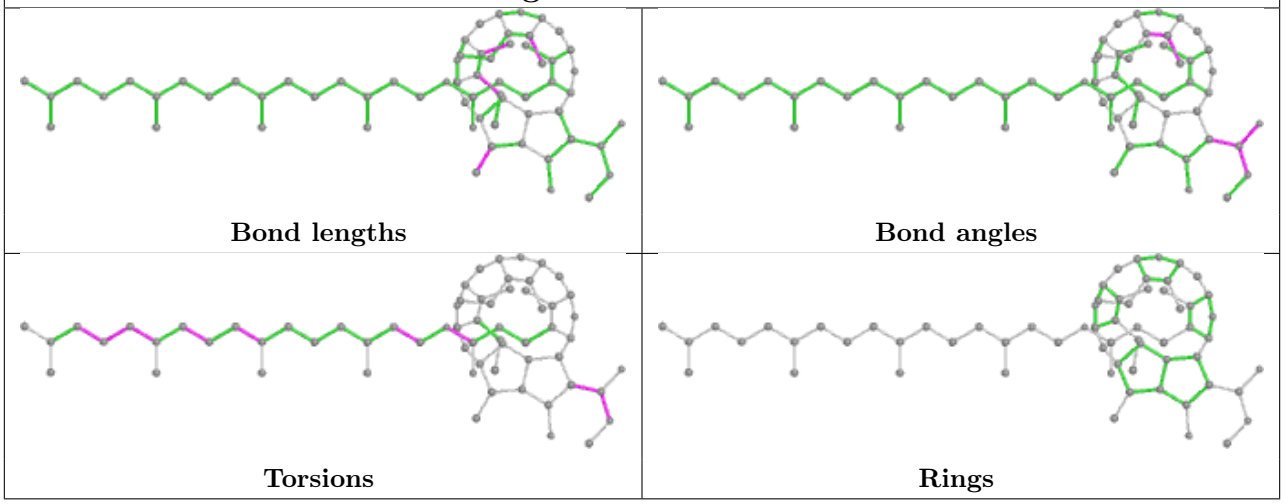


Torsions

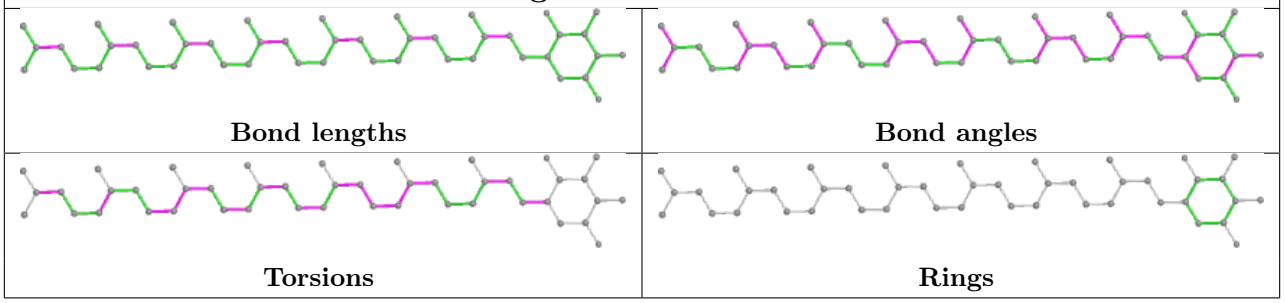


Rings

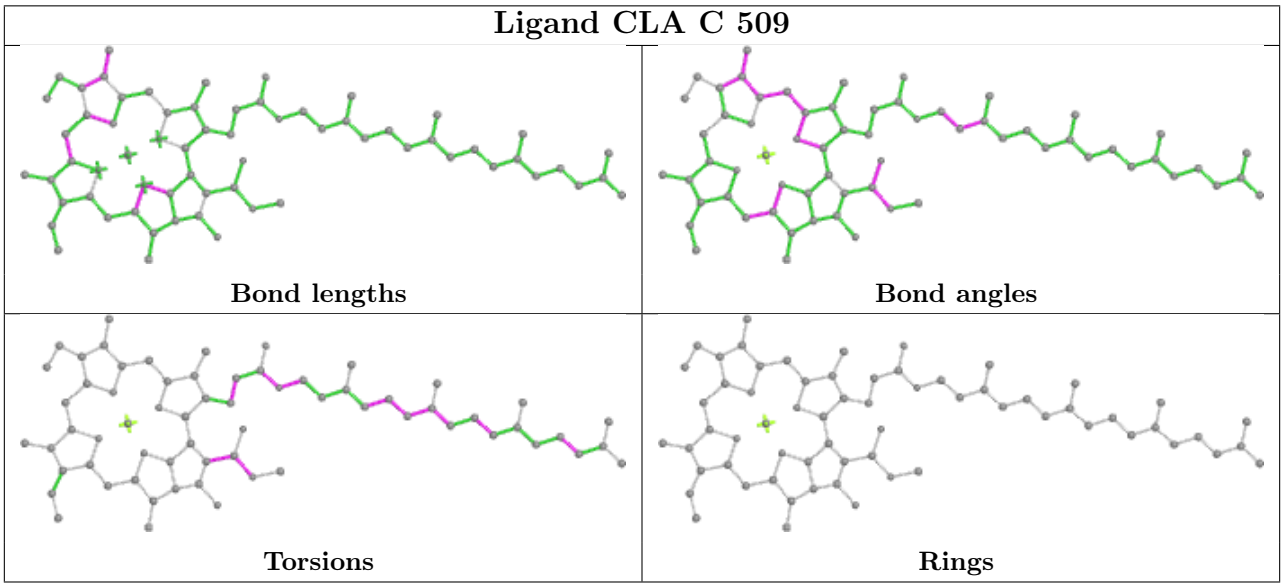
Ligand PHO A 406



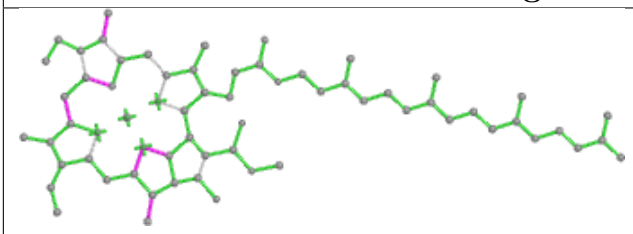
Ligand PL9 A 408



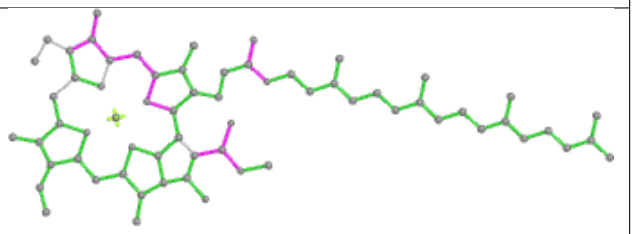
Ligand CLA C 509



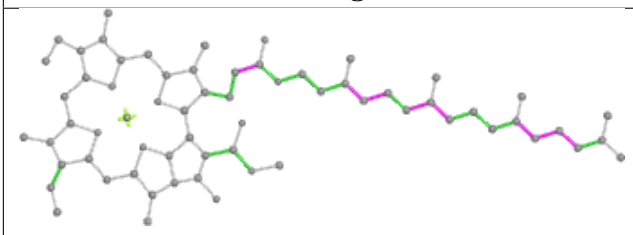
Ligand CLA D 401



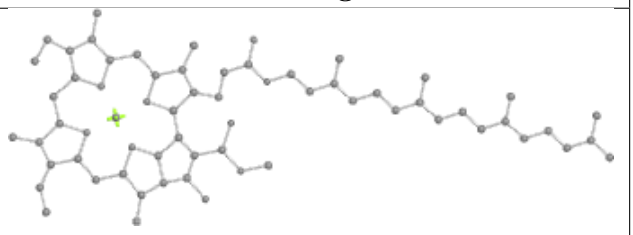
Bond lengths



Bond angles

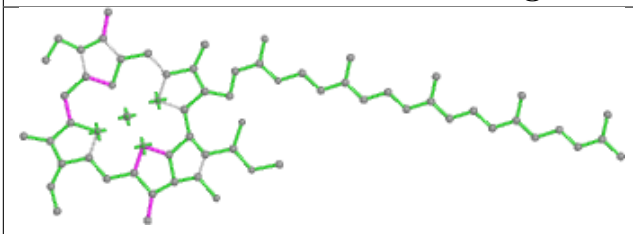


Torsions



Rings

Ligand CLA A 403



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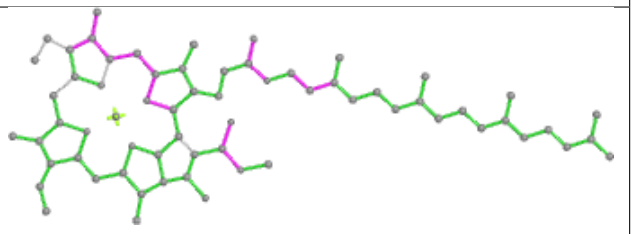
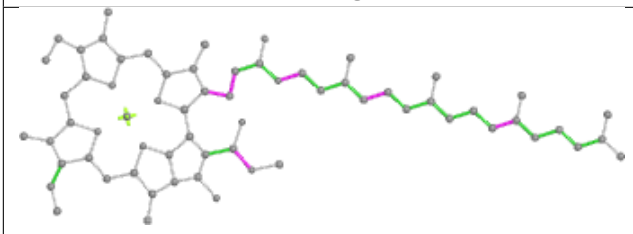
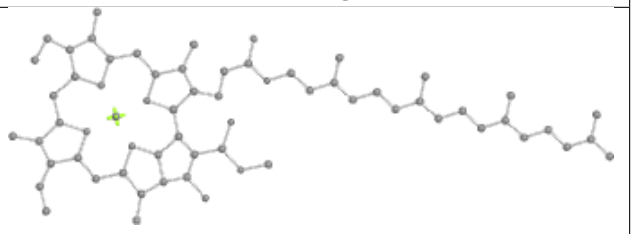


Bond angles

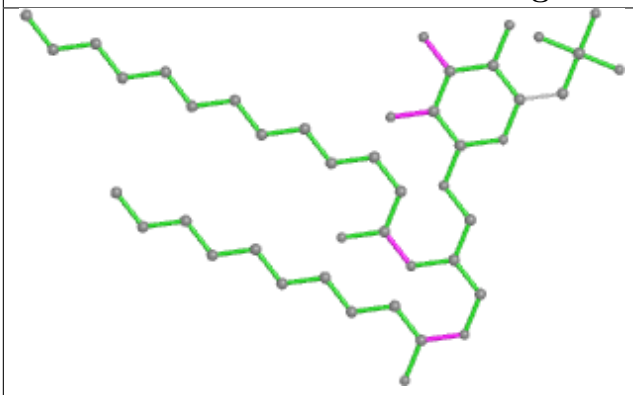


Torsions



Rings

Ligand SQD f 102



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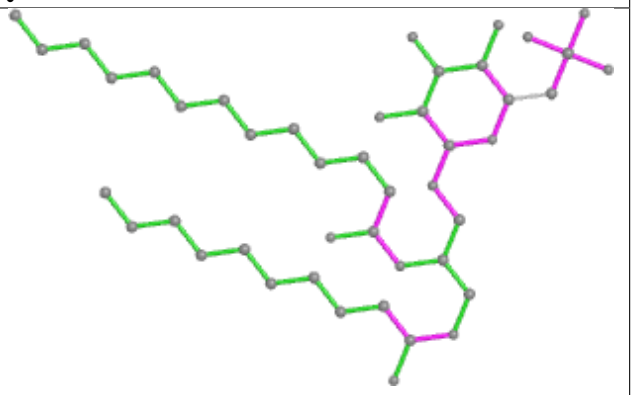
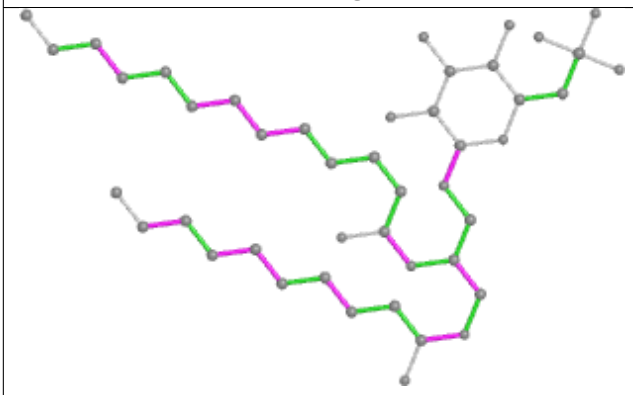
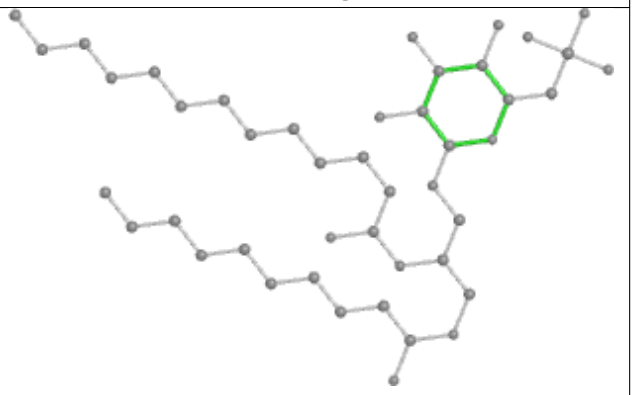


Bond angles

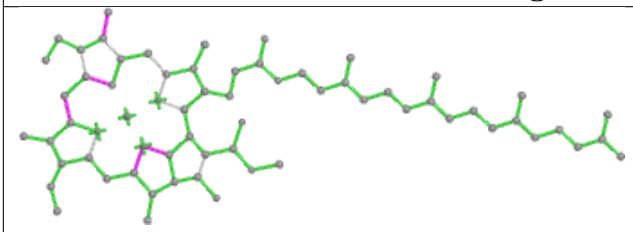


Torsions



Rings

Ligand CLA a 405



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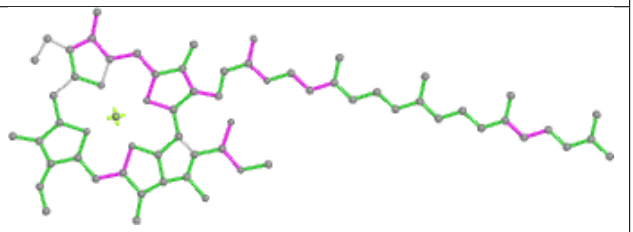
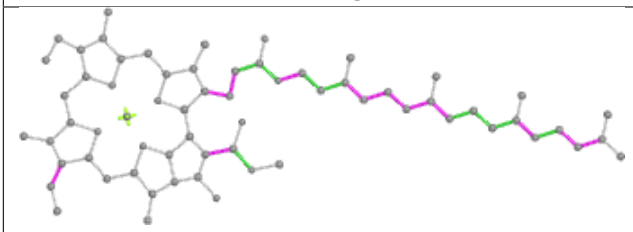
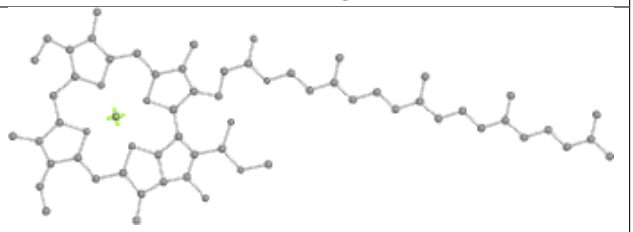


Bond angles

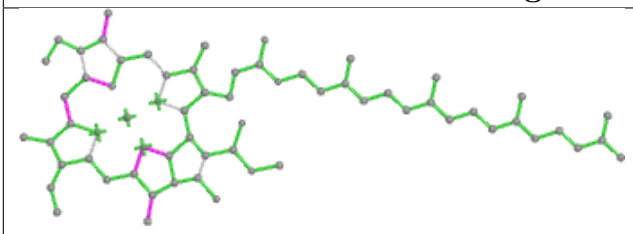


Torsions

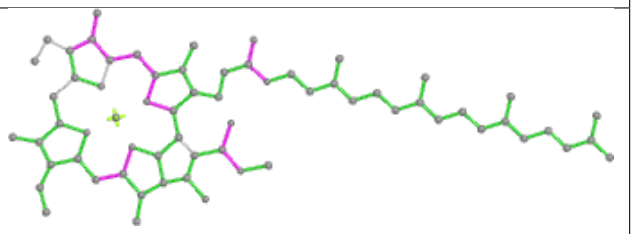


Rings

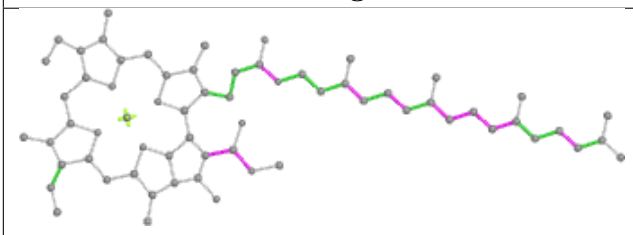
Ligand CLA B 605



Bond lengths



Bond angles



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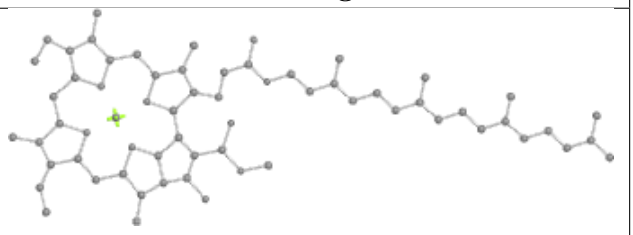
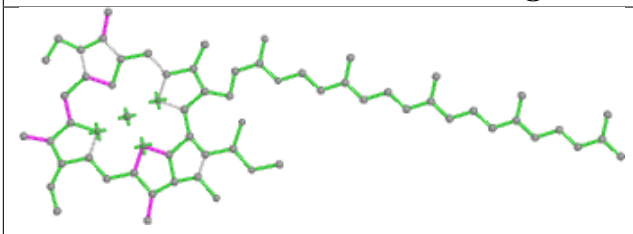


Rings

Ligand CLA C 508



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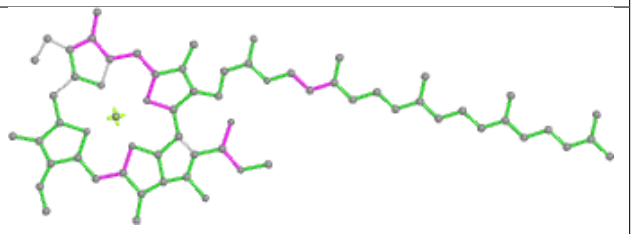
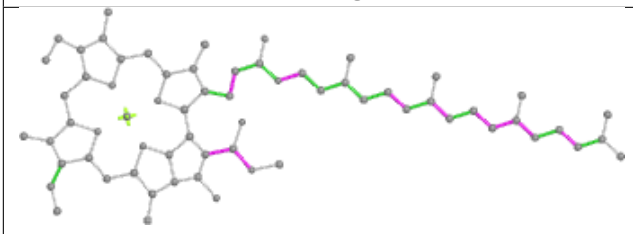


Bond angles



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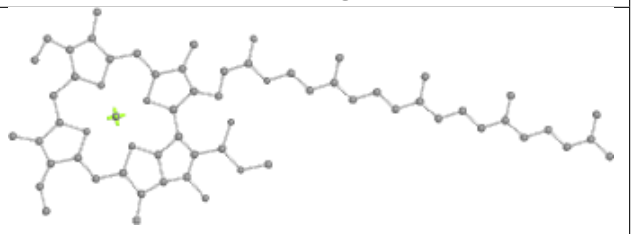
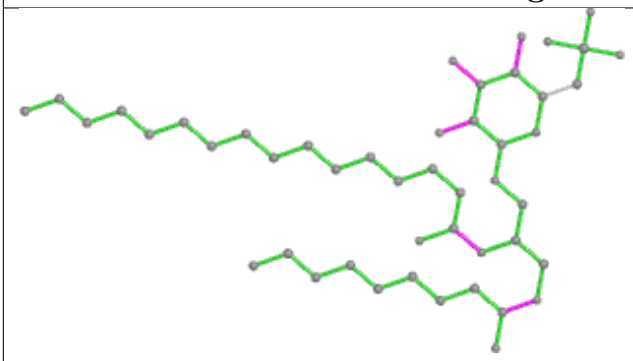


Rings

Ligand SQD b 601



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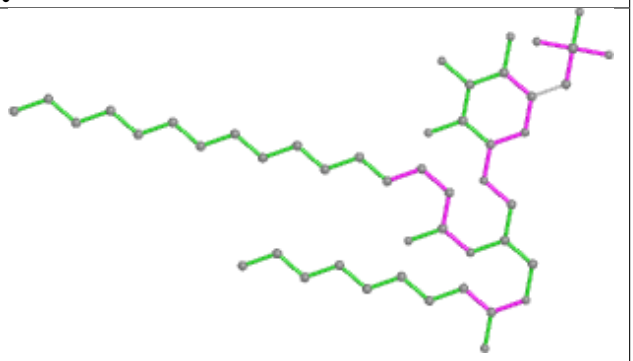
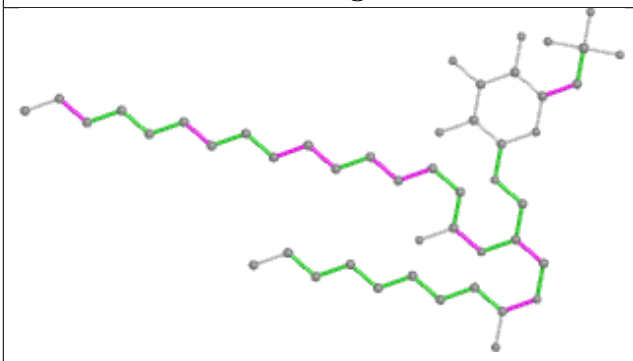


Bond angles



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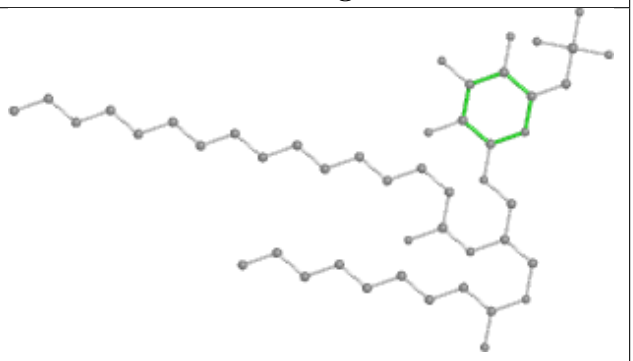
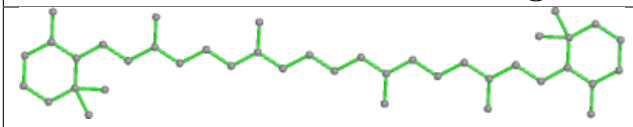


Rings

Ligand BCR z 101



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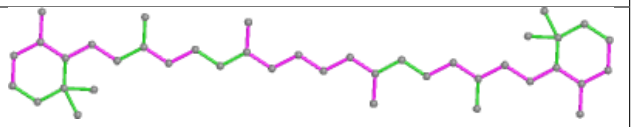
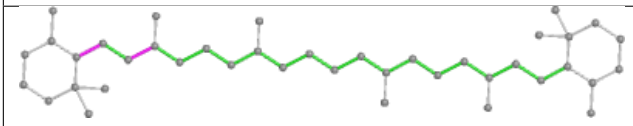
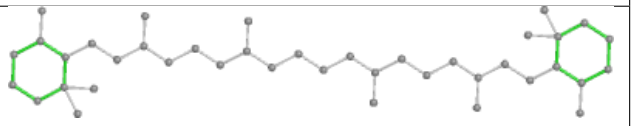


Bond angles

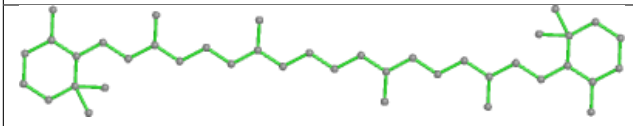


Torsions



Rings

Ligand BCR k 102



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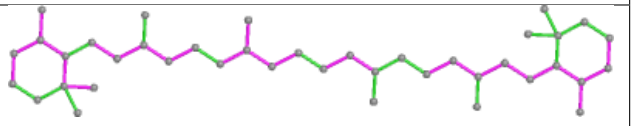
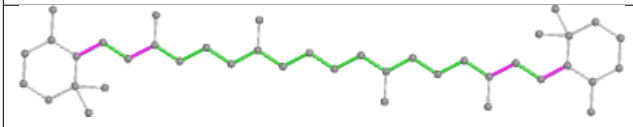
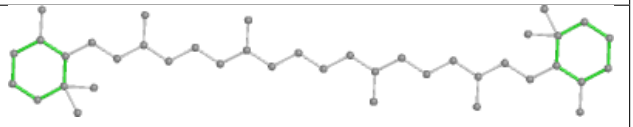


Bond angles

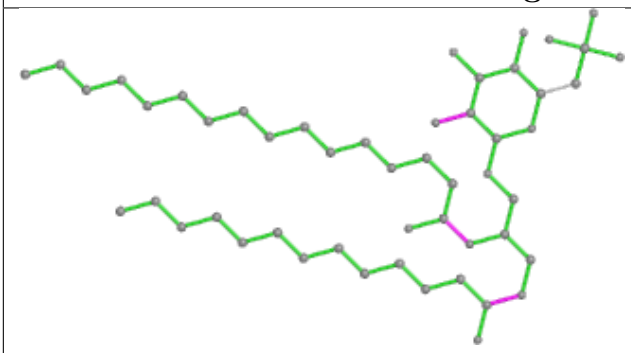


Torsions



Rings

Ligand SQD A 413



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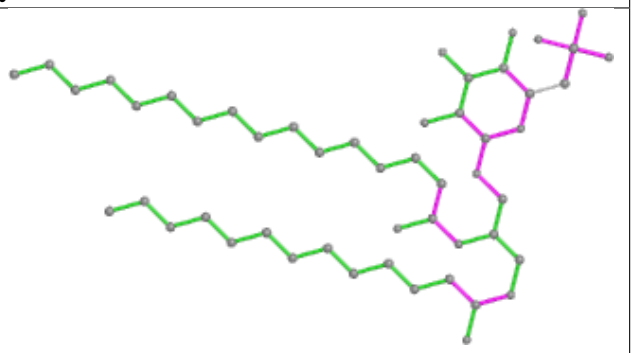
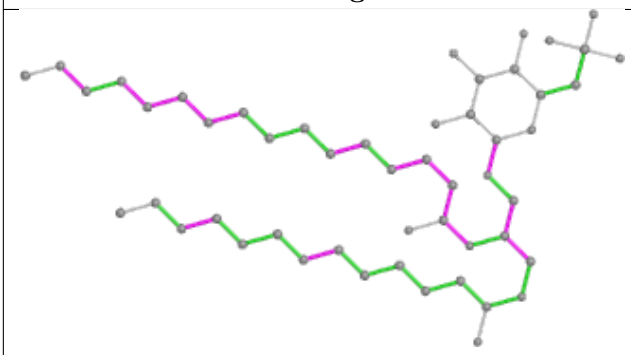


Bond angles



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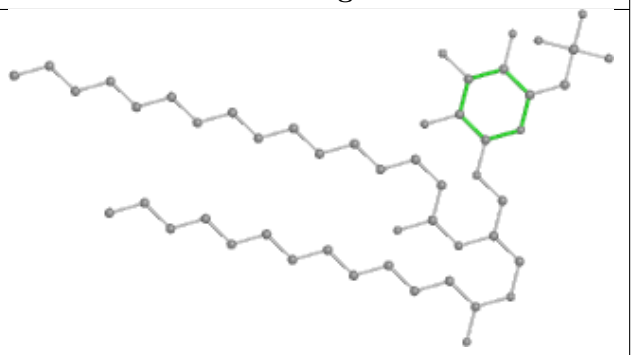
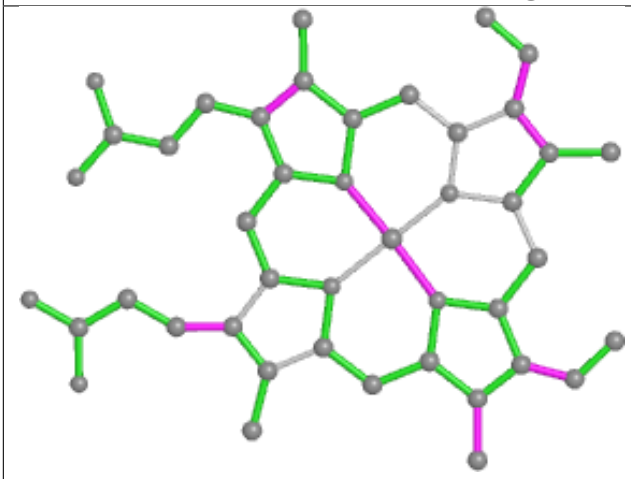


Rings

Ligand HEM v 201



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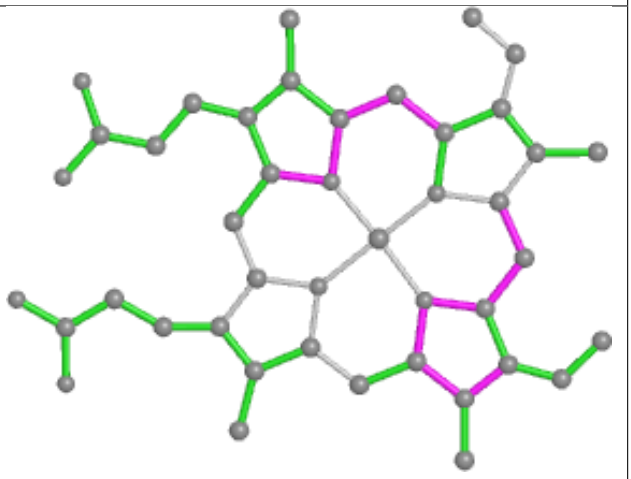
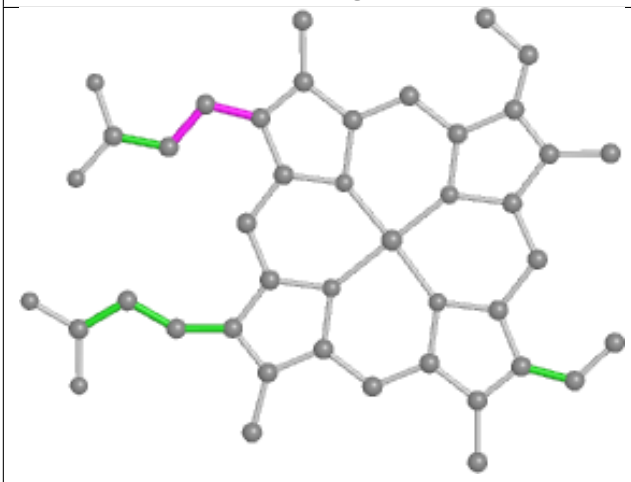
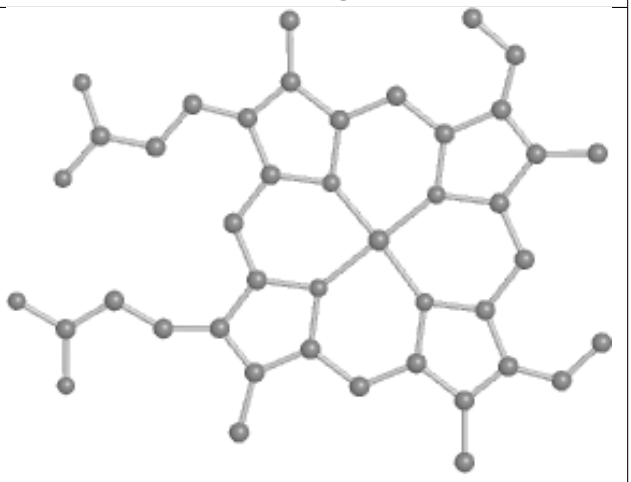


Bond angles

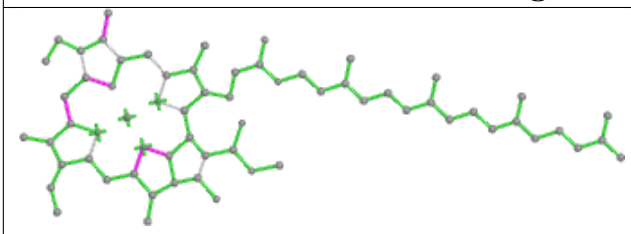


Torsions



Rings

Ligand CLA c 513



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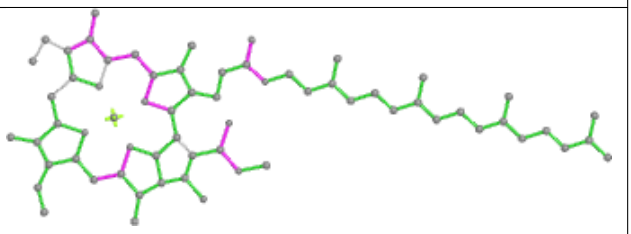
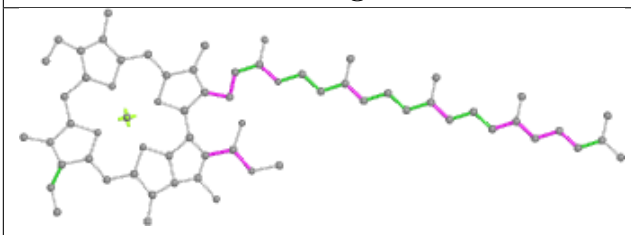
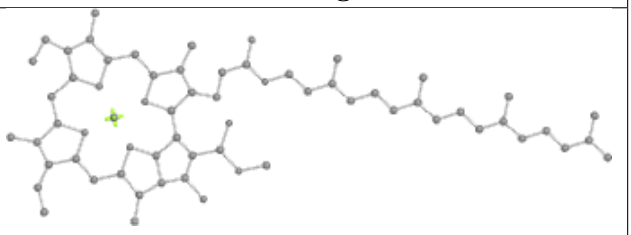


Bond angles

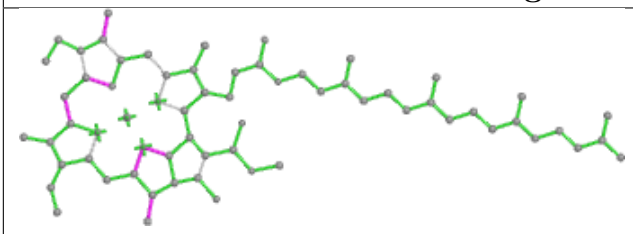


Torsions

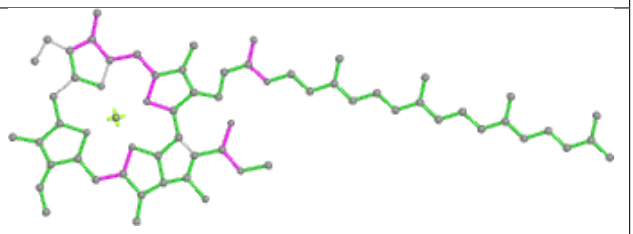


Rings

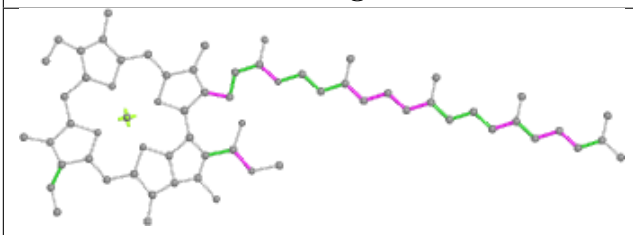
Ligand CLA B 608



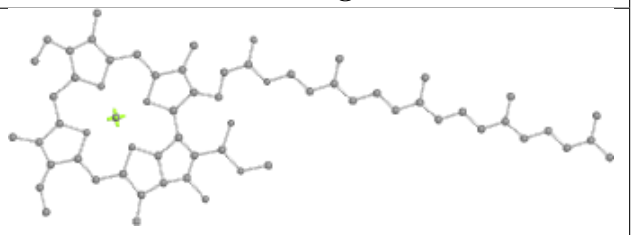
Bond lengths



Bond angles

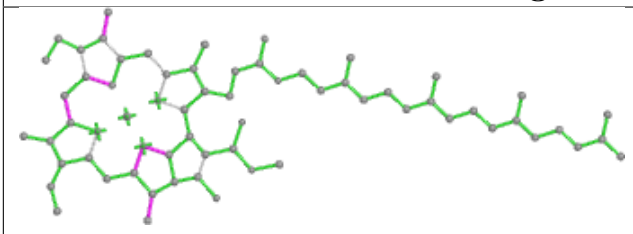


Torsions

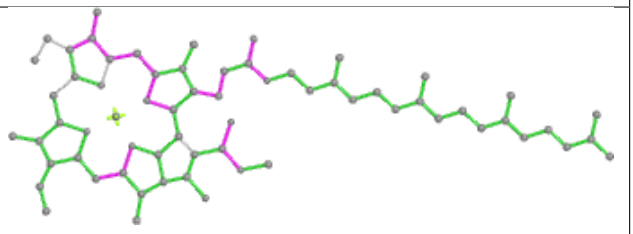


Rings

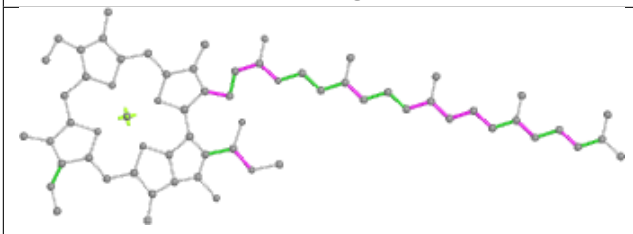
Ligand CLA c 505



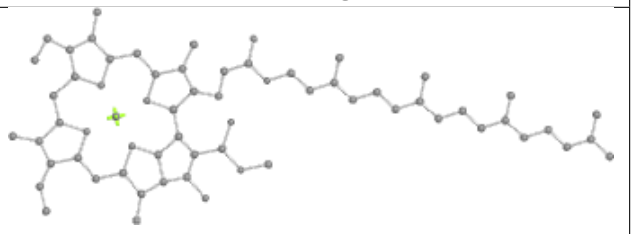
Bond lengths



Bond angles

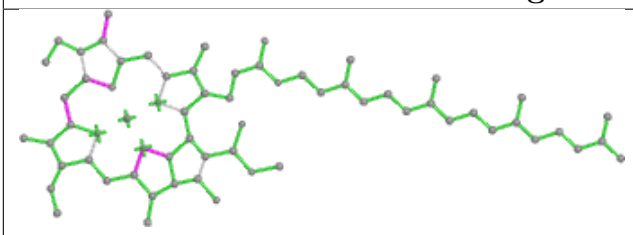


Torsions

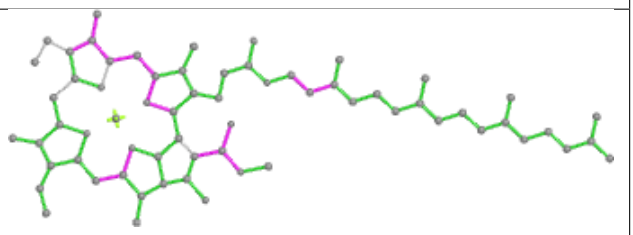


Rings

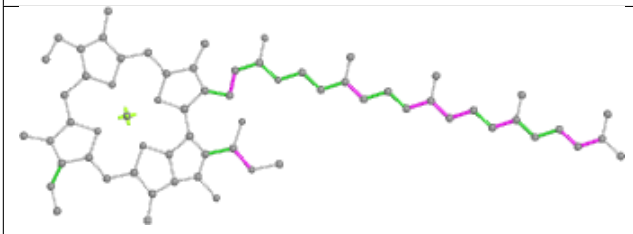
Ligand CLA b 607



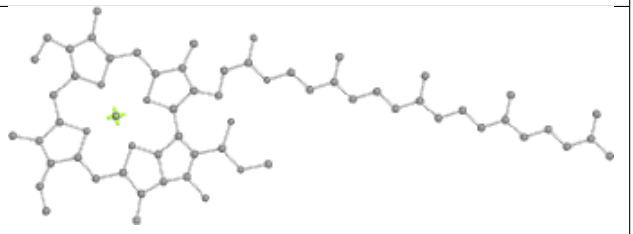
Bond lengths



Bond angles

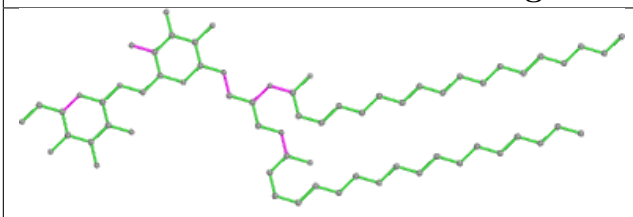


Torsions



Rings

Ligand DGD c 518



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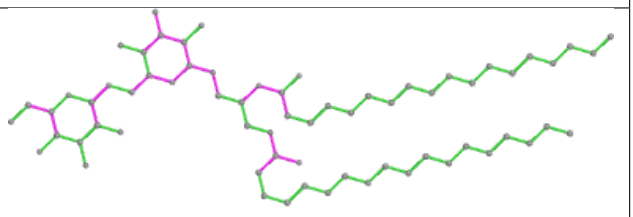
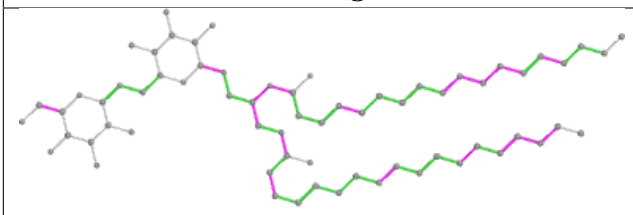
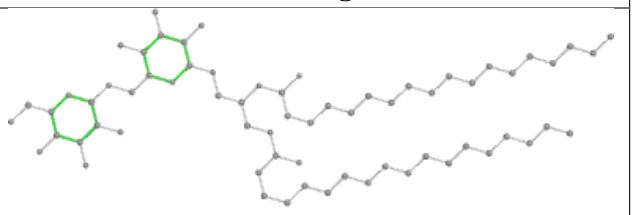


Bond angles

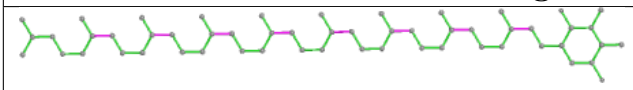


Torsions

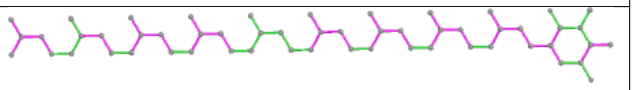


Rings

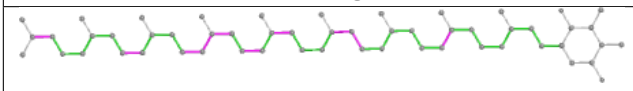
Ligand PL9 d 404



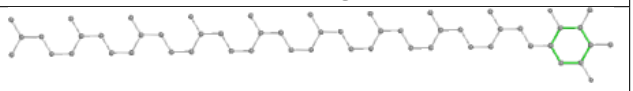
Bond lengths



Bond angles

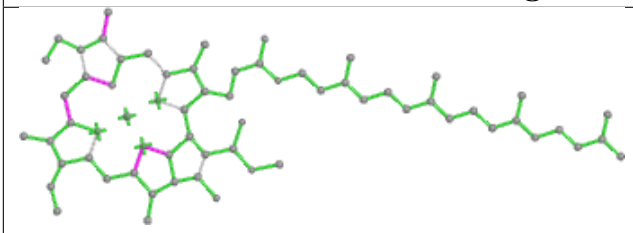


Torsions



Rings

Ligand CLA A 407



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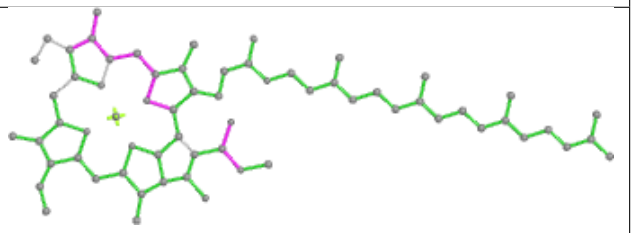
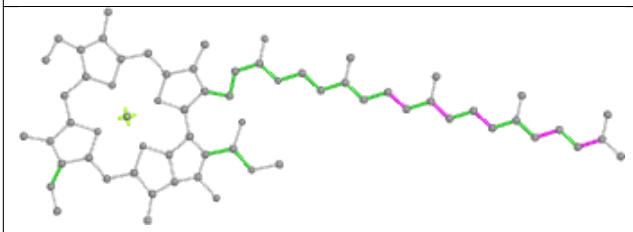


Bond angles



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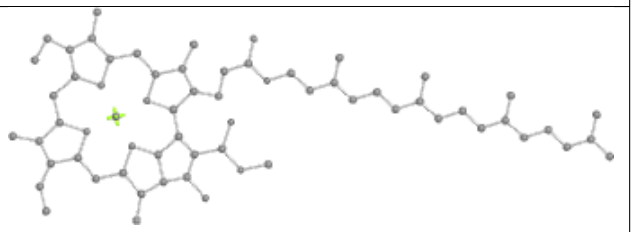
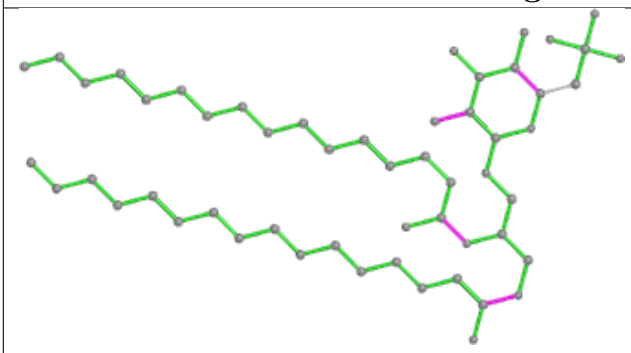


Rings

Ligand SQD A 417



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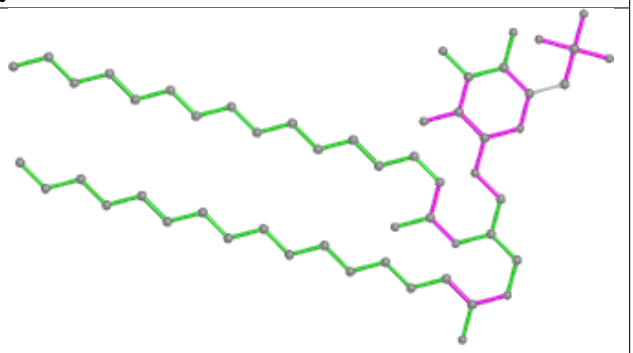
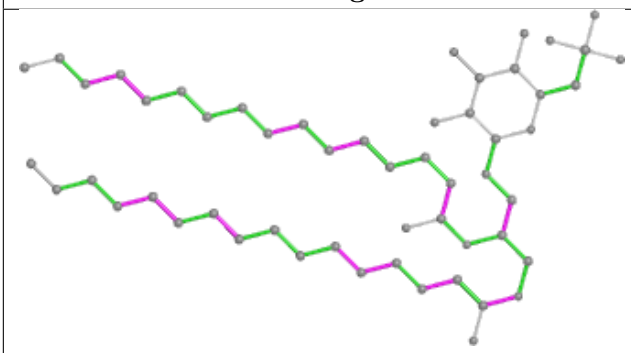
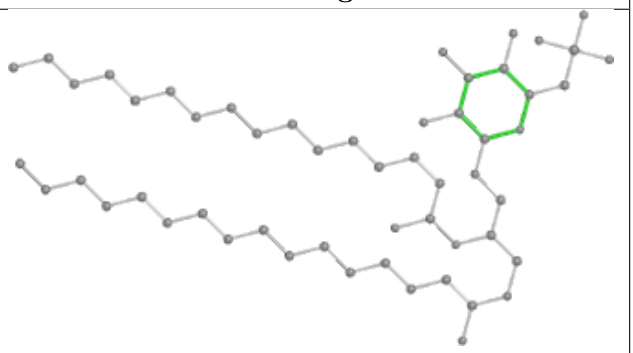


Bond angles

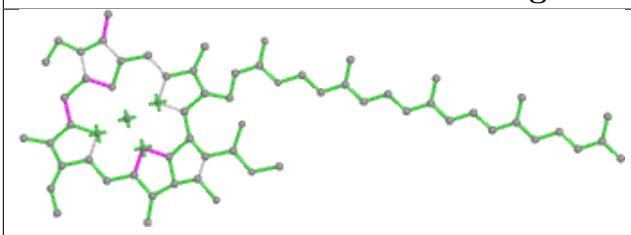


Torsions



Rings

Ligand CLA c 503



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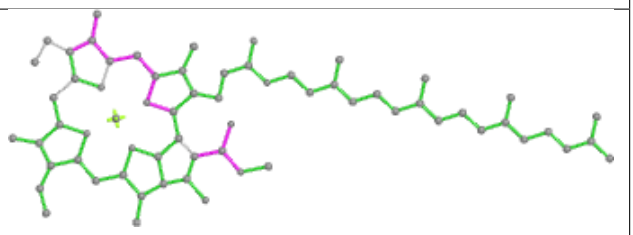
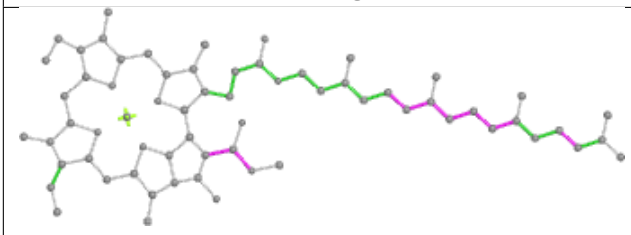


Bond angles



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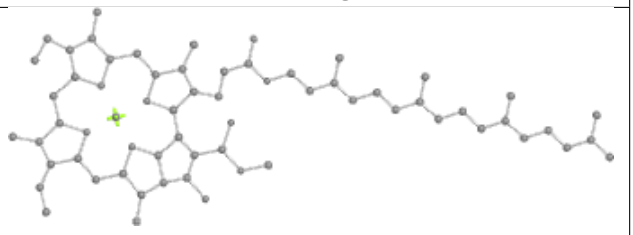
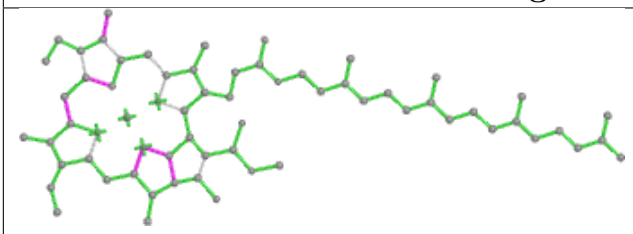
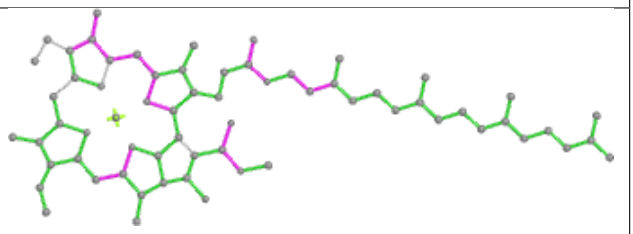


Rings

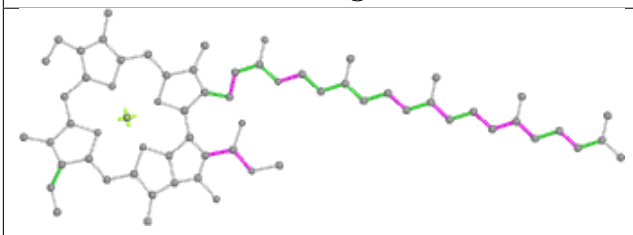
Ligand CLA c 508



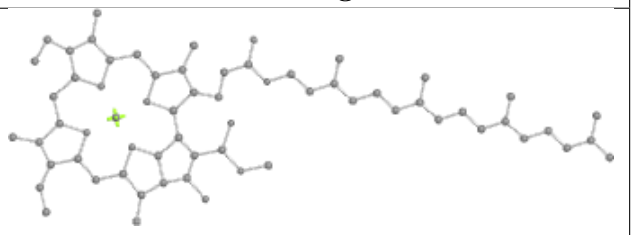
Bond lengths



Bond angles

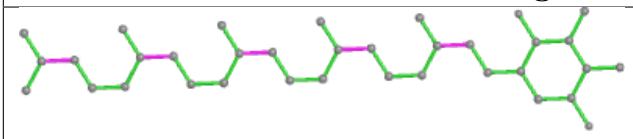


Torsions

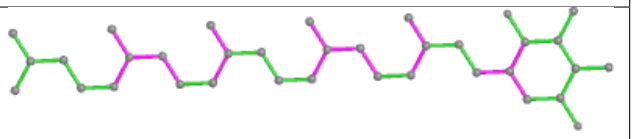


Rings

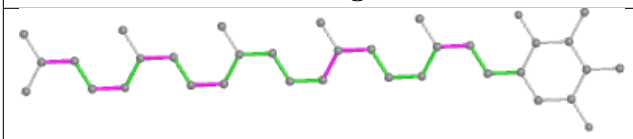
Ligand PL9 J 101



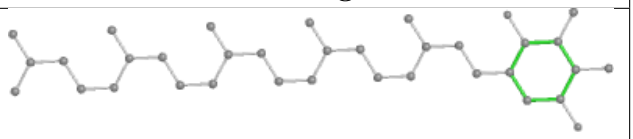
Bond lengths



Bond angles

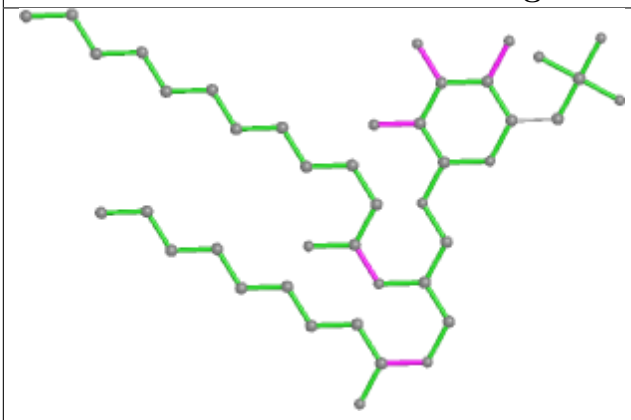


Torsions



Rings

Ligand SQD D 408



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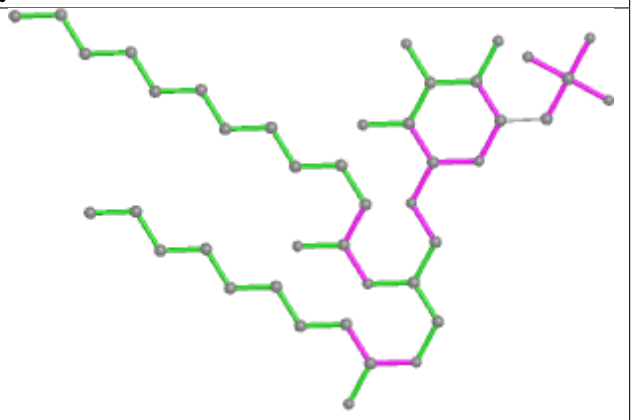
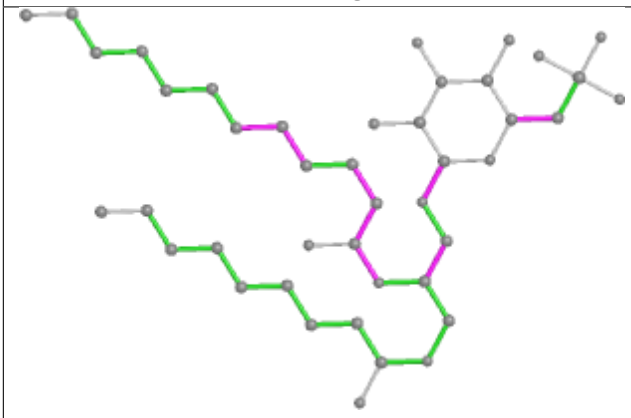


Bond angles



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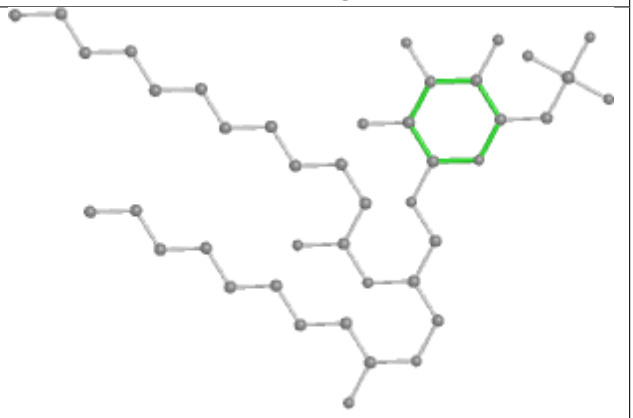
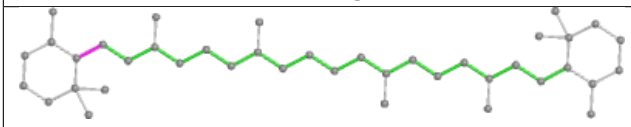


Rings

Ligand BCR T 101

Bond lengths

Bond angles



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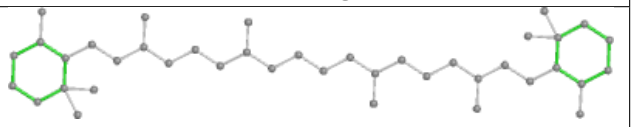
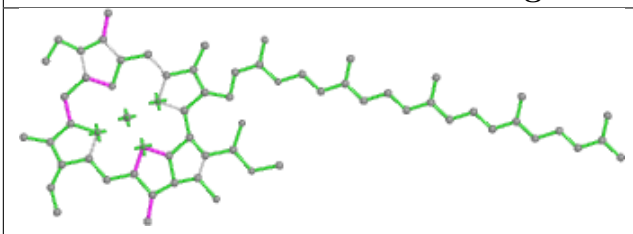
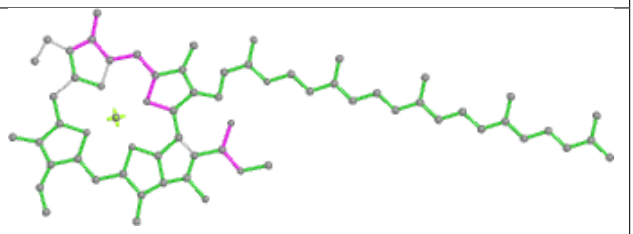


Rings

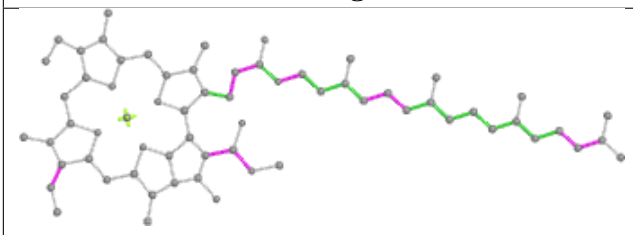
Ligand CLA B 614



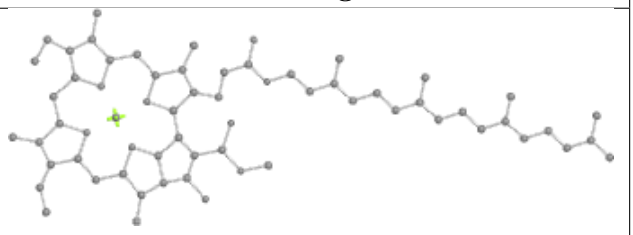
Bond lengths



Bond angles

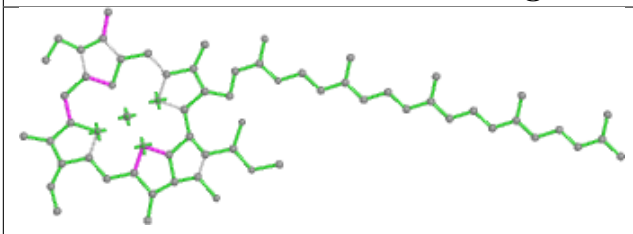


Torsions

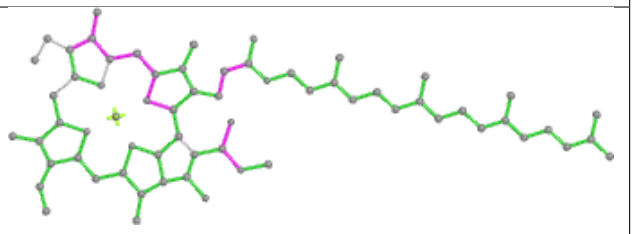


Rings

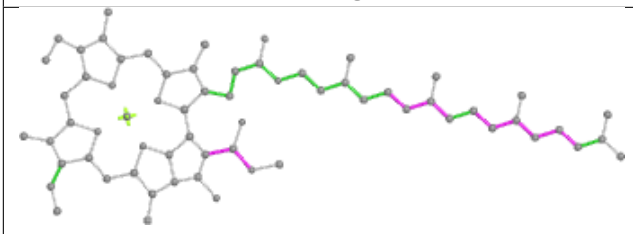
Ligand CLA C 506



Bond lengths



Bond angles



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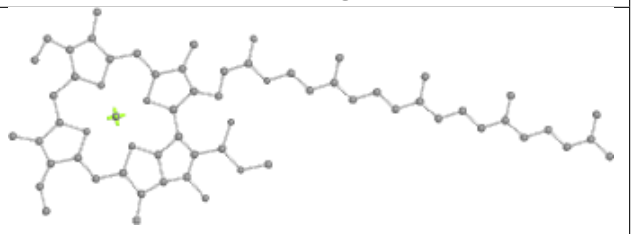
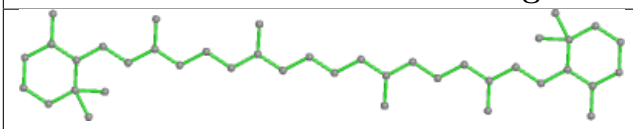
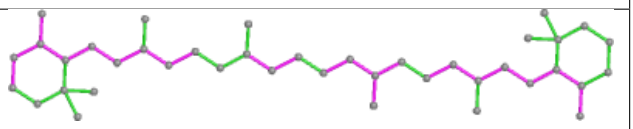


Rings

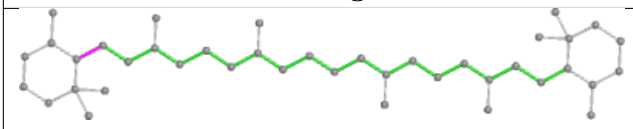
Ligand BCR B 617



Bond lengths



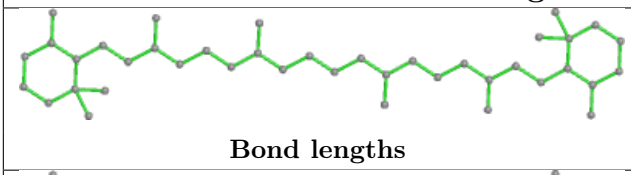
Bond angles



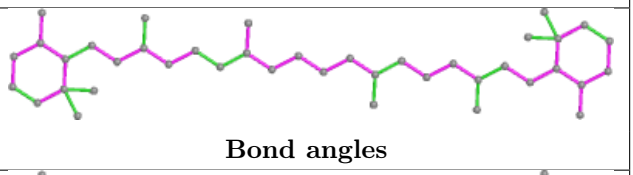
Torsions

Rings

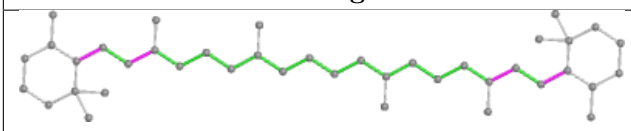
Ligand BCR c 515



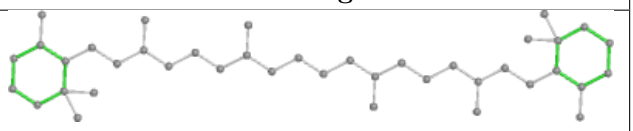
Bond lengths



Bond angles

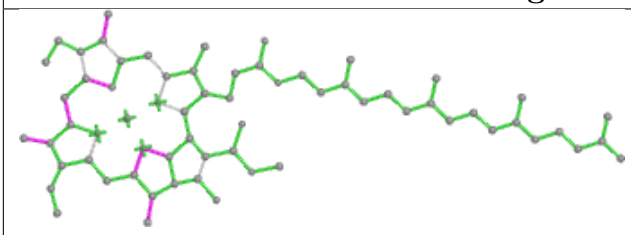


Torsions



Rings

Ligand CLA b 616



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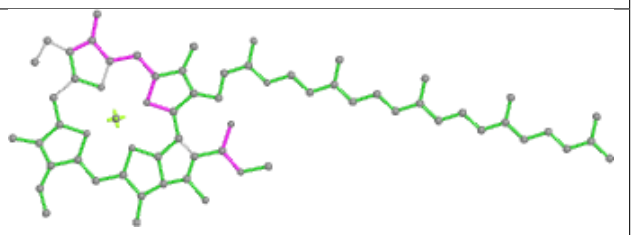
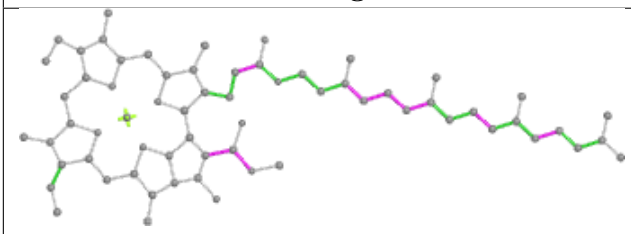


Bond angles



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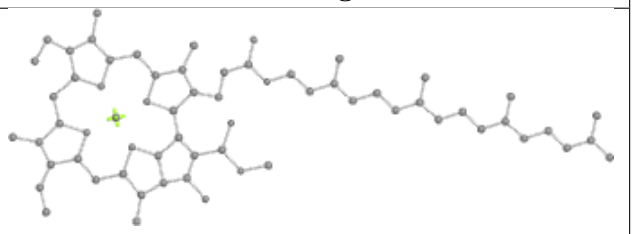
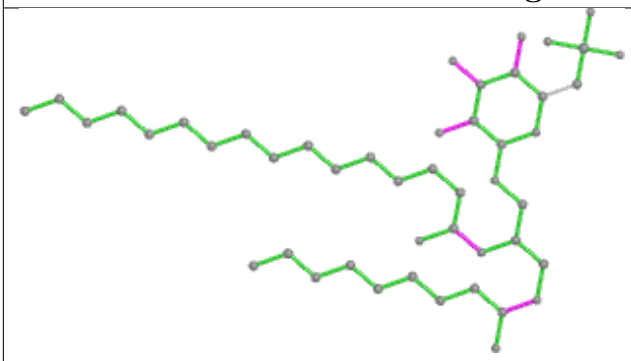


Rings

Ligand SQD B 626



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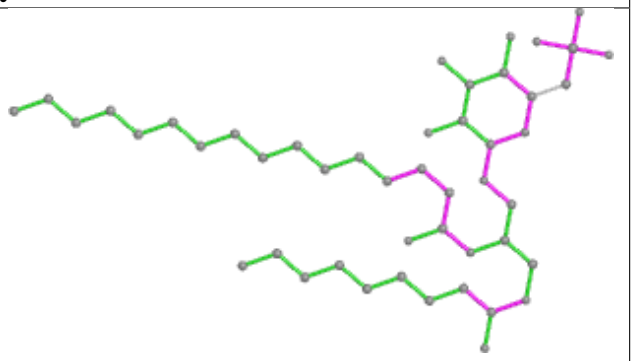
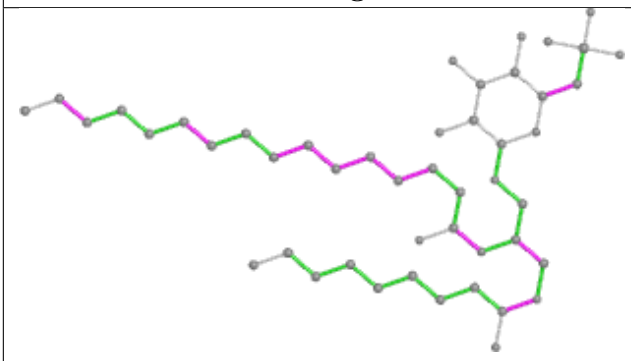
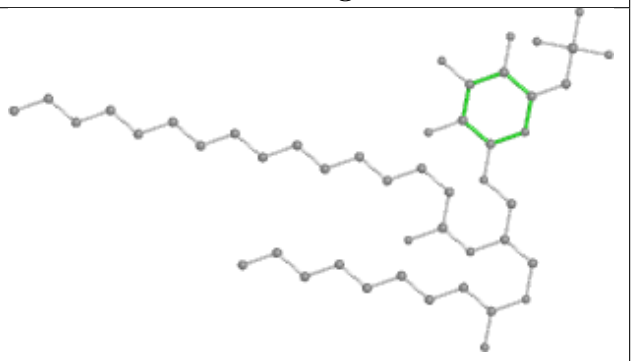


Bond angles

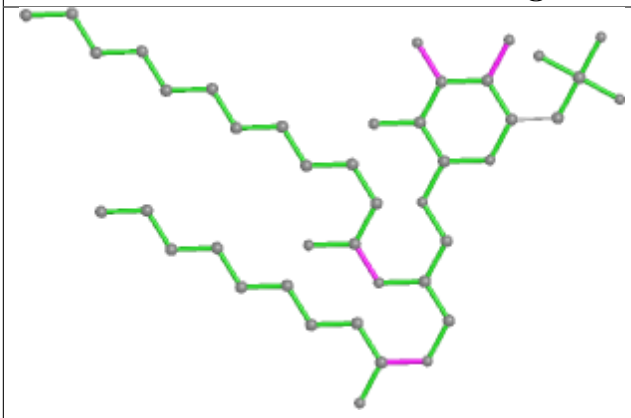


Torsions



Rings

Ligand SQD d 408



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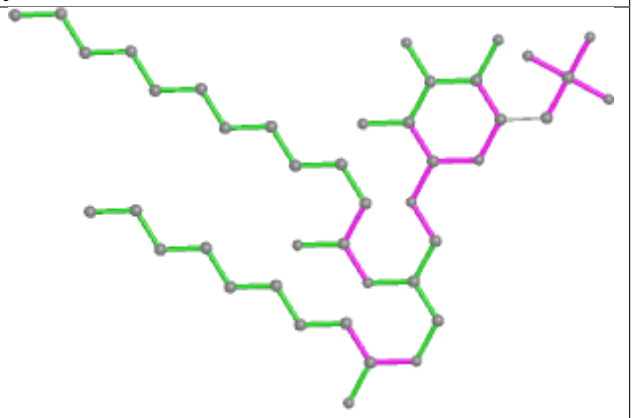
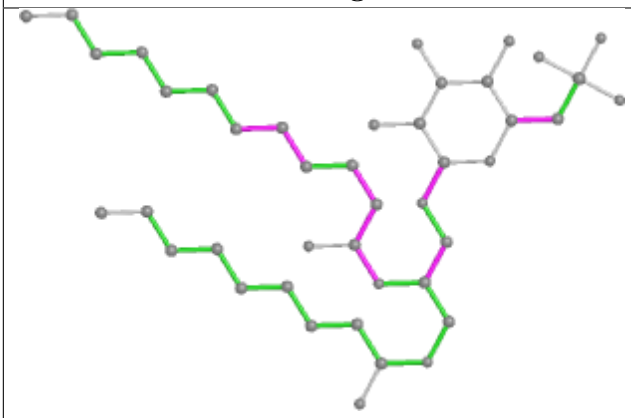
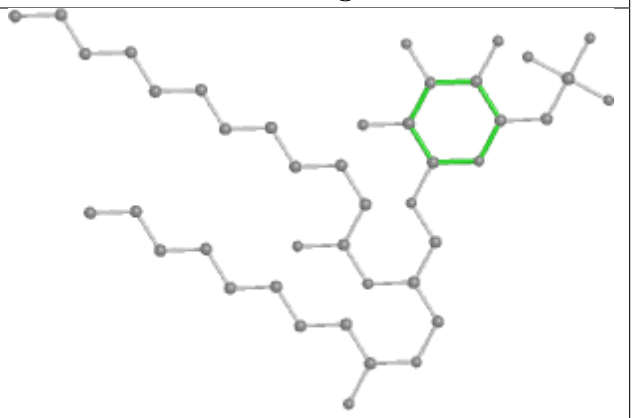


Bond angles

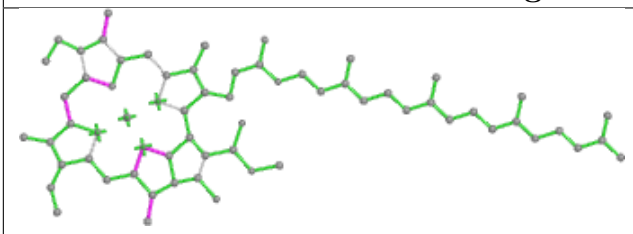


Torsions

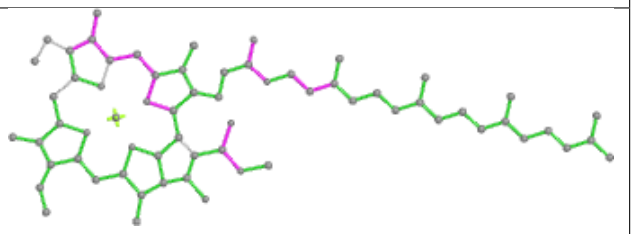


Rings

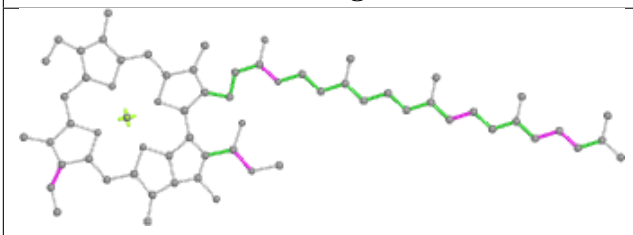
Ligand CLA B 604



Bond lengths



Bond angles



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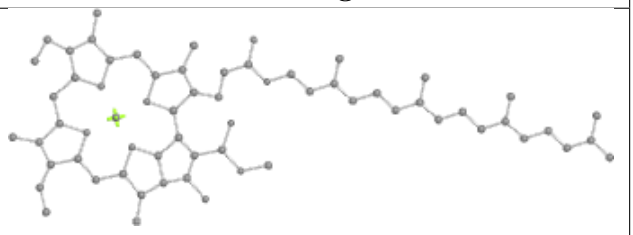
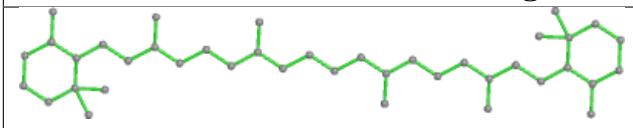


Rings

Ligand BCR D 405



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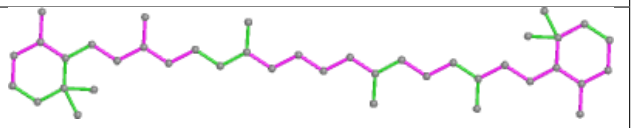
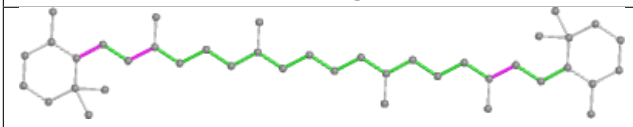


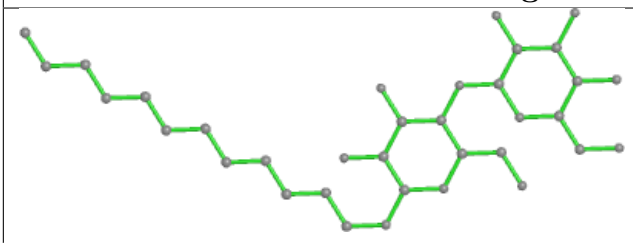
Bond angles



Torsions

Rings

Ligand LMT B 629



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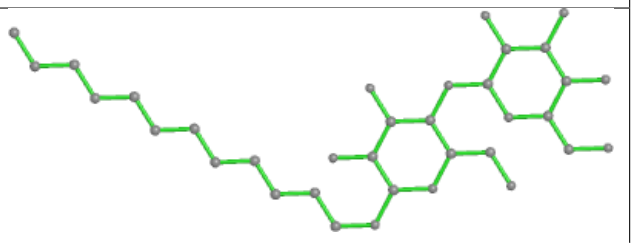
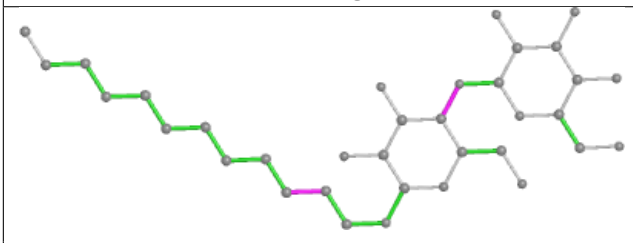
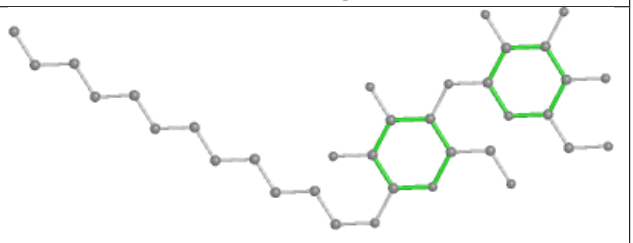


Bond angles

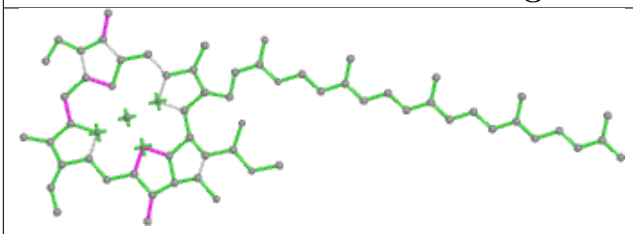


Torsions



Rings

Ligand CLA C 510



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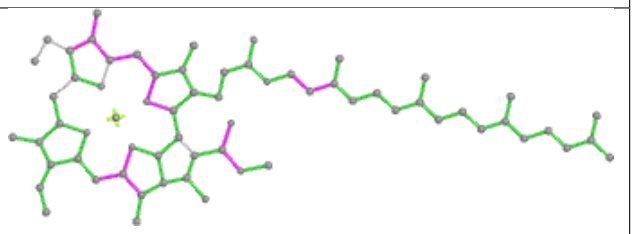
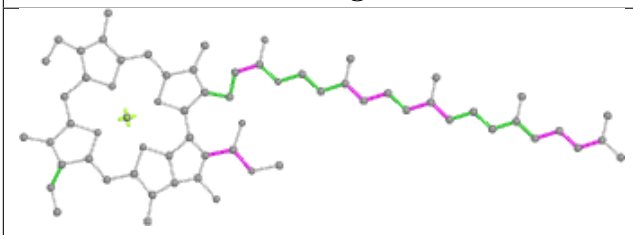


Bond angles



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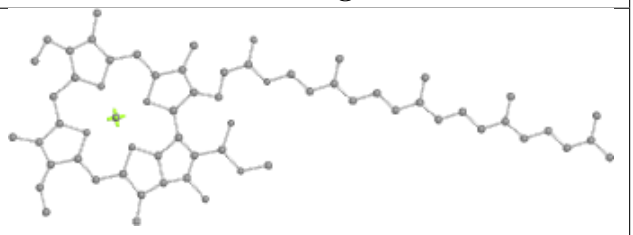
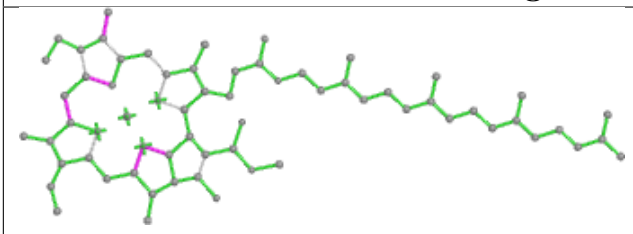


Rings

Ligand CLA C 512



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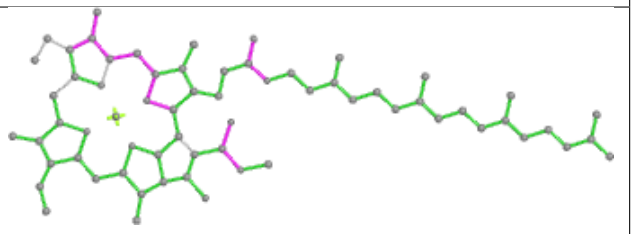
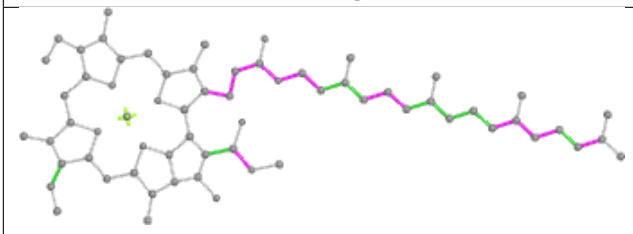
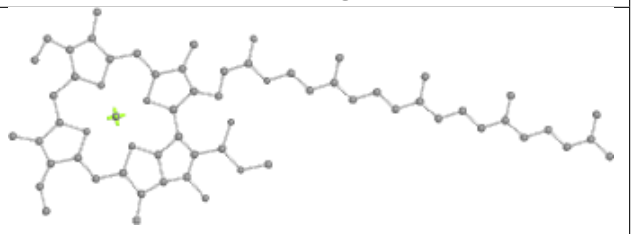


Bond angles

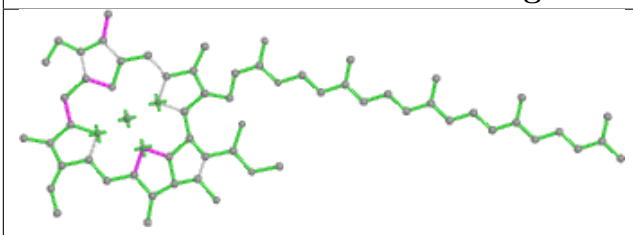


Torsions



Rings

Ligand CLA A 405



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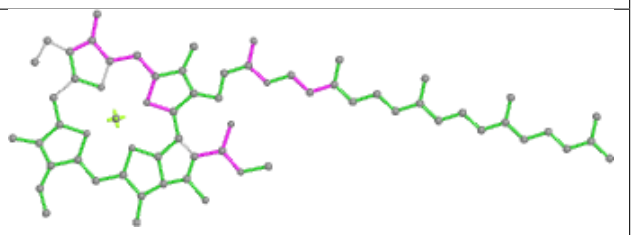
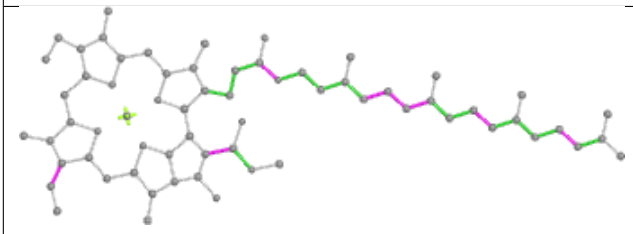


Bond angles



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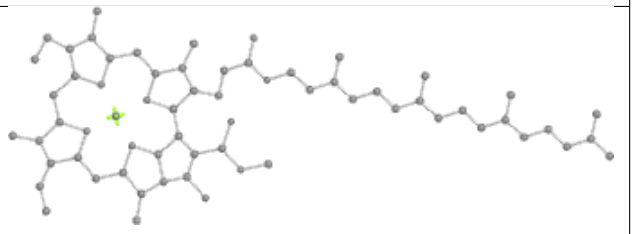
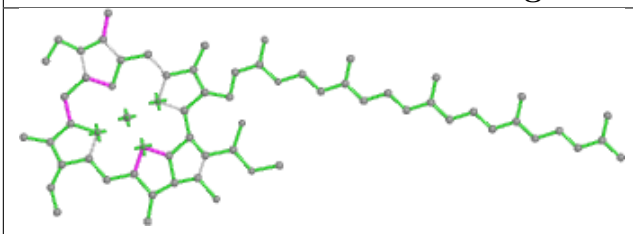
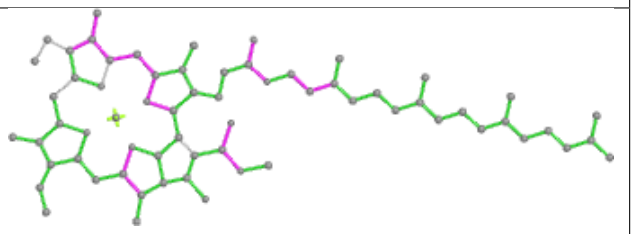


Rings

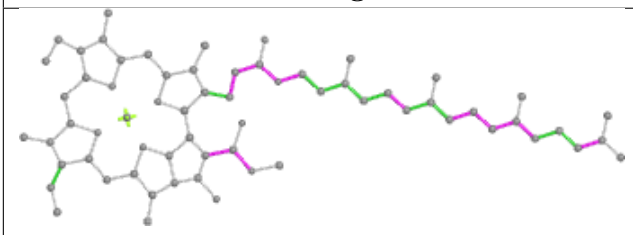
Ligand CLA B 610



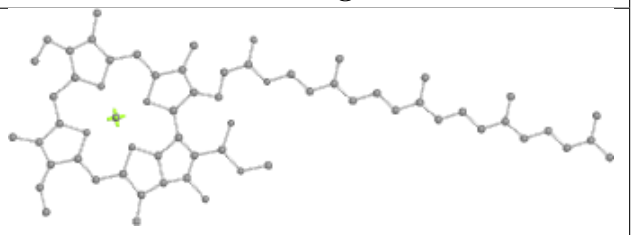
Bond lengths



Bond angles

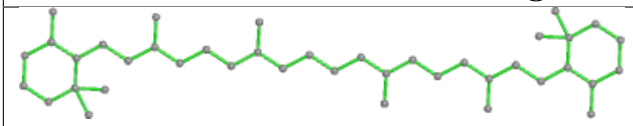


Torsions



Rings

Ligand BCR c 514



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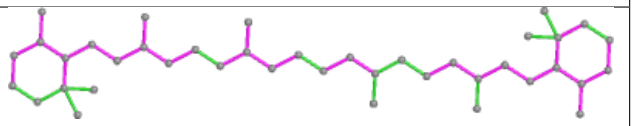
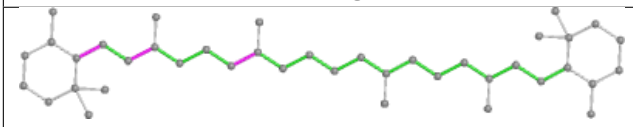


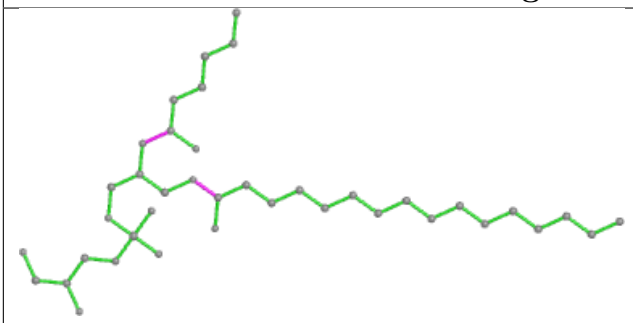
Bond angles



Torsions

Rings

Ligand LHG A 412



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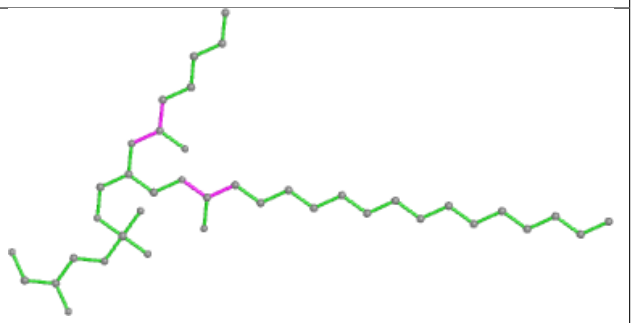
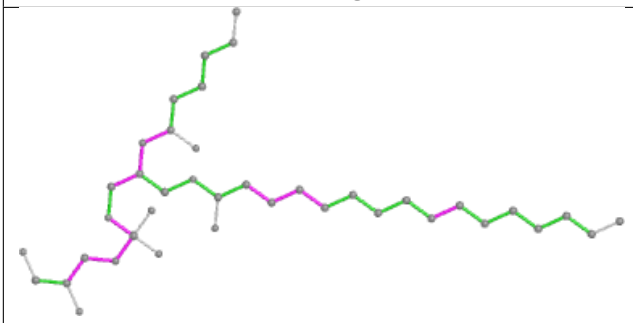
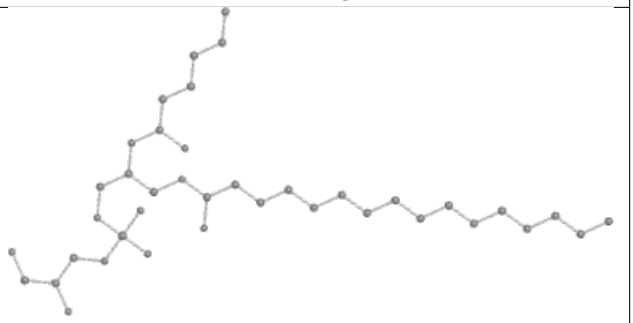


Bond angles

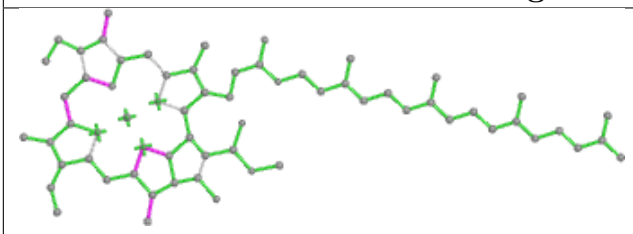


Torsions



Rings

Ligand CLA b 608



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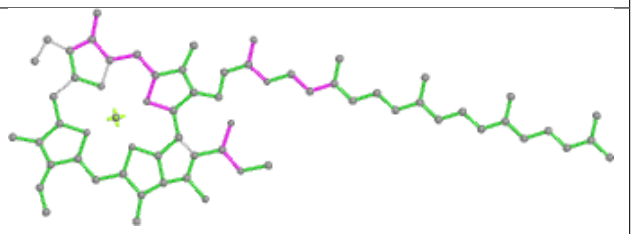
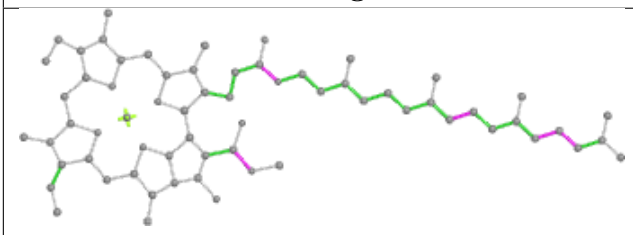
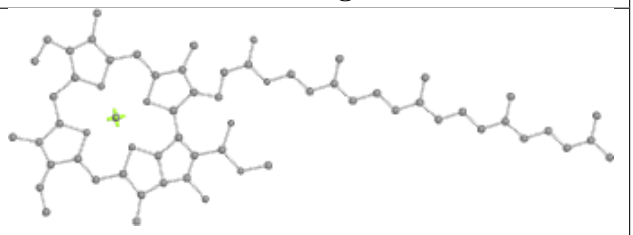


Bond angles

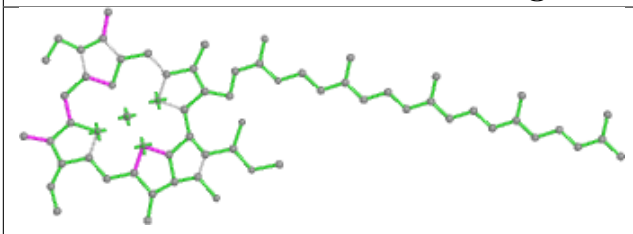


Torsions

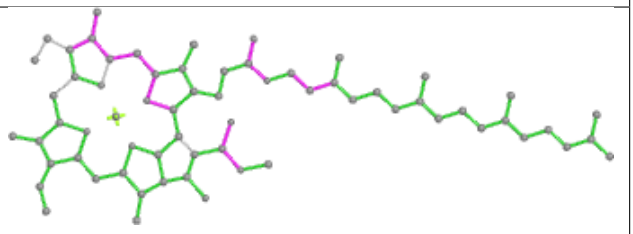


Rings

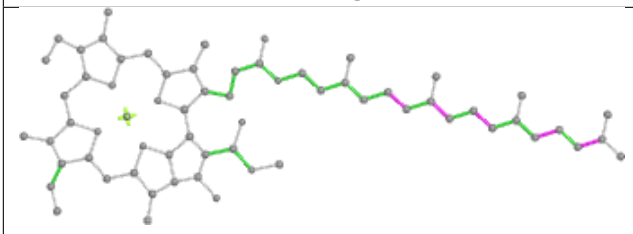
Ligand CLA a 409



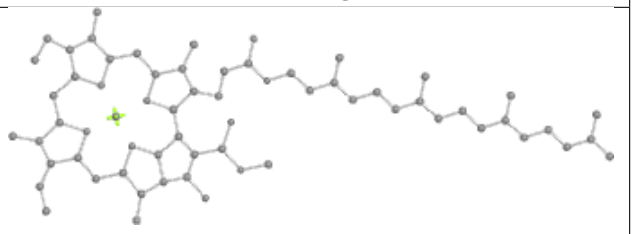
Bond lengths



Bond angles

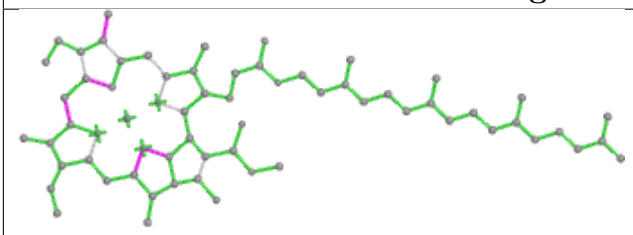


Torsions

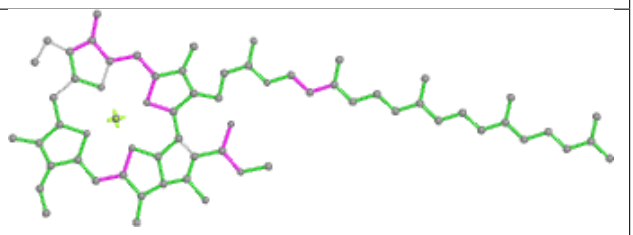


Rings

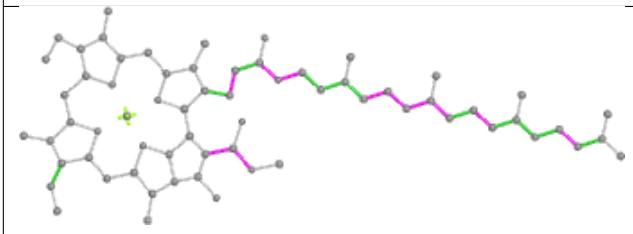
Ligand CLA c 509



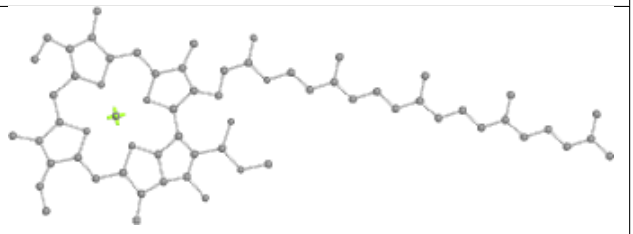
Bond lengths



Bond angles

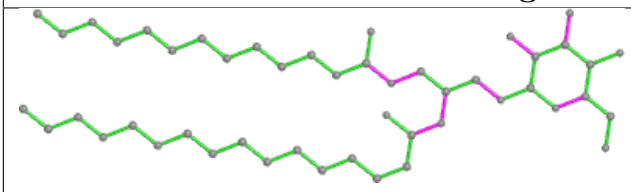


Torsions

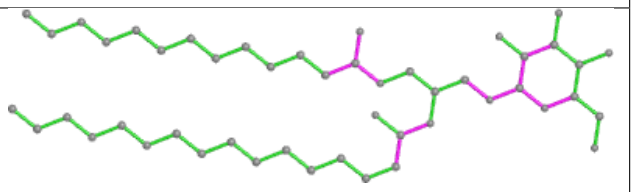


Rings

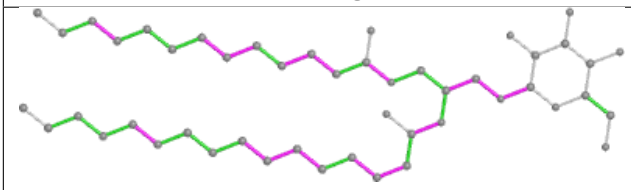
Ligand LMG D 407



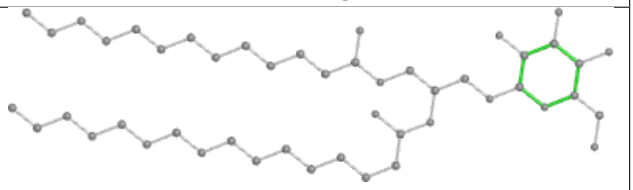
Bond lengths



Bond angles

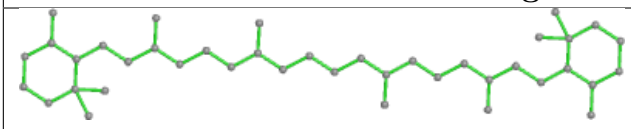


Torsions

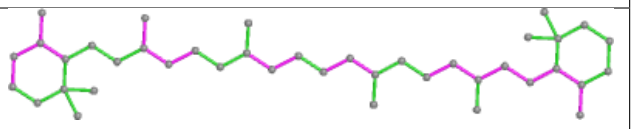


Rings

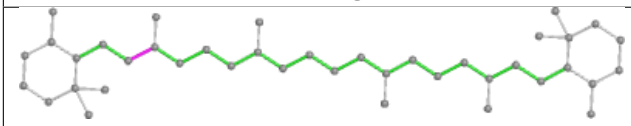
Ligand BCR A 410



Bond lengths



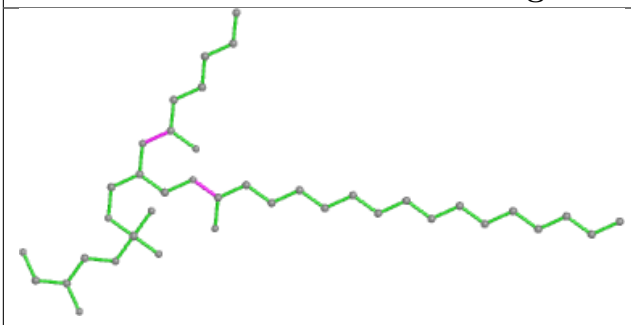
Bond angles



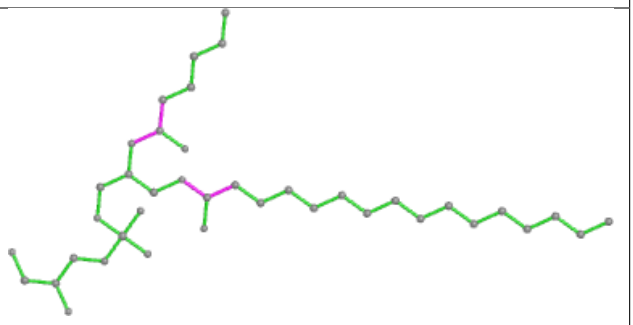
Torsions

Rings

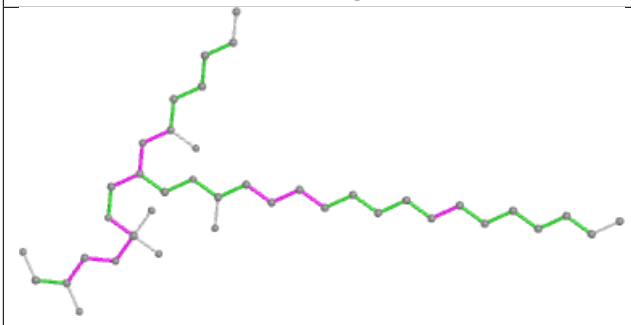
Ligand LHG a 414



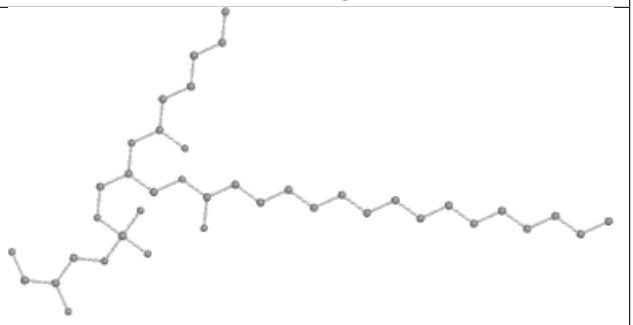
Bond lengths



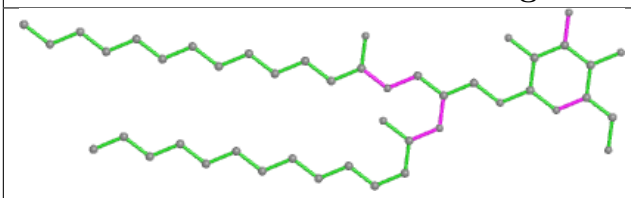
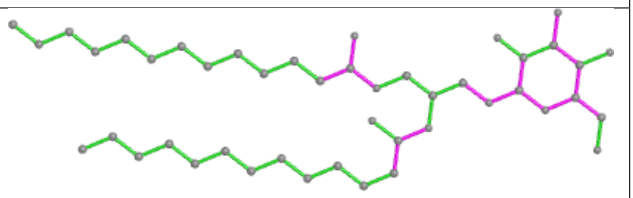
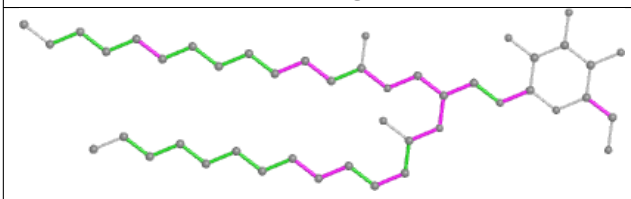
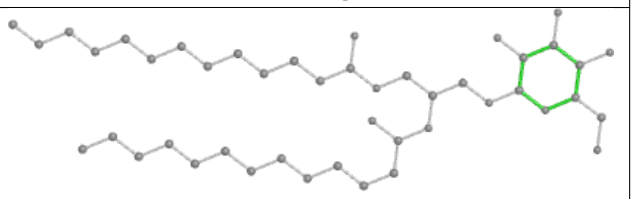
Bond angles



Torsions



Rings

Ligand LMG C 521	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/360 (93%)	0.09	9 (2%) 54 47	43, 64, 104, 149	0
1	a	335/360 (93%)	-0.12	3 (0%) 84 77	44, 65, 106, 149	0
2	B	490/510 (96%)	0.32	25 (5%) 28 27	46, 69, 103, 159	0
2	b	490/510 (96%)	0.30	28 (5%) 23 23	47, 71, 104, 159	0
3	C	447/461 (96%)	0.05	7 (1%) 72 64	54, 79, 106, 132	0
3	c	447/461 (96%)	0.19	10 (2%) 62 54	56, 81, 105, 135	0
4	D	340/352 (96%)	-0.04	2 (0%) 89 84	44, 66, 103, 137	0
4	d	340/352 (96%)	-0.08	2 (0%) 89 84	45, 66, 102, 134	0
5	E	82/84 (97%)	0.06	1 (1%) 79 71	68, 92, 125, 130	0
5	e	82/84 (97%)	0.36	3 (3%) 41 37	70, 92, 125, 129	0
6	F	35/45 (77%)	0.03	2 (5%) 23 23	68, 84, 119, 139	0
6	f	35/45 (77%)	0.31	0 100 100	73, 85, 120, 141	0
7	H	65/66 (98%)	0.76	8 (12%) 4 8	77, 94, 122, 138	0
7	h	65/66 (98%)	0.58	3 (4%) 32 30	73, 93, 120, 144	0
8	I	35/38 (92%)	0.16	1 (2%) 51 44	65, 79, 107, 118	0
8	i	35/38 (92%)	0.01	0 100 100	66, 81, 106, 120	0
9	J	34/40 (85%)	0.01	1 (2%) 51 44	69, 85, 95, 112	0
9	j	34/40 (85%)	-0.25	1 (2%) 51 44	74, 88, 95, 116	0
10	K	37/46 (80%)	0.10	0 100 100	77, 87, 101, 122	0
10	k	37/46 (80%)	0.25	3 (8%) 12 13	73, 88, 108, 123	0
11	L	37/37 (100%)	-0.02	0 100 100	48, 62, 128, 156	0
11	l	37/37 (100%)	-0.13	0 100 100	52, 60, 126, 158	0
12	M	34/36 (94%)	0.08	2 (5%) 22 22	56, 71, 110, 164	0
12	m	34/36 (94%)	0.24	3 (8%) 10 12	55, 69, 108, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	0.82	31 (12%) 3 7	50, 78, 122, 169	0
13	o	243/272 (89%)	0.59	18 (7%) 14 15	52, 78, 121, 167	0
14	T	32/32 (100%)	0.27	4 (12%) 3 7	55, 67, 158, 174	0
14	t	32/32 (100%)	-0.09	0 100 100	54, 69, 159, 168	0
15	U	97/134 (72%)	0.90	9 (9%) 8 11	56, 71, 92, 108	0
15	u	97/134 (72%)	0.74	5 (5%) 27 27	55, 71, 90, 111	0
16	V	137/163 (84%)	0.31	7 (5%) 28 27	53, 71, 86, 101	0
16	v	137/163 (84%)	0.72	9 (6%) 18 17	59, 72, 88, 95	0
17	g	28/46 (60%)	0.78	5 (17%) 1 4	95, 108, 126, 132	0
17	y	28/46 (60%)	0.29	1 (3%) 42 38	89, 107, 126, 131	0
18	X	37/41 (90%)	0.93	5 (13%) 3 6	76, 93, 124, 140	0
18	x	37/41 (90%)	0.90	10 (27%) 0 2	75, 90, 126, 141	0
19	Z	62/62 (100%)	1.06	7 (11%) 5 8	86, 104, 168, 185	0
19	z	62/62 (100%)	0.68	2 (3%) 47 41	88, 105, 172, 187	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.26	227 (4%) 34 32	43, 75, 115, 187	0

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	170	GLY	5.8
2	B	129	GLY	5.3
13	o	84	ASN	4.2
2	b	483	ASP	4.1
15	U	54	LYS	4.1
10	k	14	ALA	4.0
4	d	295	SER	3.8
15	u	107	GLU	3.7
7	H	2	ALA	3.6
2	B	378	LYS	3.6
15	U	113	THR	3.6
7	H	4	ARG	3.5
13	O	90	GLU	3.5
14	T	28	ARG	3.4
13	o	46	PRO	3.4
18	X	47	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	130	GLU	3.4
2	B	128	THR	3.4
14	T	31	LYS	3.4
2	b	482	ILE	3.3
18	x	47	GLN	3.3
5	e	84	LYS	3.3
2	B	379	ALA	3.3
13	o	30	THR	3.3
13	O	157	PRO	3.3
2	b	302	TRP	3.2
19	Z	62	VAL	3.2
16	v	131	ARG	3.2
2	b	407	ASN	3.2
7	H	64	ALA	3.2
3	C	183	GLY	3.1
2	B	294	SER	3.1
3	C	184	GLY	3.1
13	o	171	GLU	3.1
2	b	70	GLY	3.1
2	b	405	GLU	3.1
1	A	11	ALA	3.1
3	C	27	ASP	3.1
19	z	1	MET	3.1
13	O	169	LYS	3.1
2	B	127	ARG	3.0
2	b	484	PRO	3.0
1	A	16	ARG	3.0
13	O	223	ILE	3.0
13	o	221	GLY	3.0
18	X	46	VAL	3.0
13	O	269	ILE	3.0
13	O	84	ASN	2.9
10	k	13	GLU	2.9
3	c	372	PRO	2.9
1	A	12	ASN	2.9
1	A	15	GLU	2.9
13	O	222	GLN	2.9
2	B	132	ALA	2.8
2	B	477	ASP	2.8
2	b	409	GLN	2.8
1	A	229	GLU	2.8
1	A	10	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	b	393	GLU	2.8
9	j	7	ARG	2.8
13	O	79	LYS	2.8
15	U	38	GLU	2.8
15	U	53	GLU	2.8
2	B	133	LEU	2.8
2	b	294	SER	2.8
2	B	402	TYR	2.7
13	o	47	THR	2.7
19	Z	34	ASP	2.7
7	H	5	THR	2.7
17	y	42	ARG	2.7
7	h	24	GLY	2.7
19	Z	1	MET	2.7
2	b	304	ALA	2.7
13	O	220	LYS	2.7
15	U	55	ILE	2.7
15	u	113	THR	2.7
13	O	119	LEU	2.7
18	X	17	LYS	2.6
18	x	13	THR	2.6
13	O	245	GLN	2.6
13	o	55	ALA	2.6
1	a	80	GLY	2.6
2	B	476	ARG	2.6
4	d	227	GLU	2.6
4	D	295	SER	2.6
1	A	230	THR	2.6
17	g	27	MET	2.6
13	O	49	ASP	2.6
3	C	332	GLN	2.6
13	O	126	GLY	2.5
13	o	158	ASN	2.5
19	Z	54	VAL	2.5
13	O	155	THR	2.5
7	H	66	GLY	2.5
2	B	490	GLN	2.5
12	m	5	GLN	2.5
16	v	103	LYS	2.5
18	x	11	THR	2.5
7	H	18	TYR	2.5
2	b	194	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
7	H	63	LYS	2.4
13	O	87	GLN	2.4
2	B	190	PHE	2.4
2	b	408	GLY	2.4
3	c	142	GLU	2.4
13	O	244	GLU	2.4
2	B	293	ALA	2.4
13	O	258	GLU	2.4
3	c	147	PHE	2.4
2	b	403	GLY	2.4
18	x	46	VAL	2.4
2	b	489	GLU	2.4
13	O	107	ILE	2.4
17	g	21	GLN	2.4
13	O	171	GLU	2.4
13	O	54	GLY	2.4
13	o	31	LEU	2.4
16	V	28	GLU	2.4
3	c	184	GLY	2.4
2	B	131	PRO	2.4
13	O	50	ASP	2.4
13	O	168	PHE	2.4
15	u	114	VAL	2.4
3	c	144	SER	2.3
13	o	32	THR	2.3
16	v	44	THR	2.3
17	g	29	GLY	2.3
2	B	189	GLY	2.3
2	b	339	ALA	2.3
2	B	295	GLY	2.3
15	U	112	PHE	2.3
19	Z	56	VAL	2.3
2	b	404	GLY	2.3
13	o	229	LYS	2.3
3	c	146	PHE	2.3
13	o	225	LEU	2.3
19	z	4	LEU	2.3
2	B	347	ARG	2.3
19	Z	57	LEU	2.3
13	O	221	GLY	2.3
3	C	145	SER	2.3
16	V	96	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	28	GLN	2.3
2	B	188	ASP	2.3
13	o	51	THR	2.3
18	x	16	LEU	2.2
15	U	123	GLU	2.2
18	x	42	GLN	2.2
16	v	130	MET	2.2
2	B	162	PHE	2.2
6	F	14	PRO	2.2
2	B	478	VAL	2.2
13	O	48	LEU	2.2
5	e	56	TYR	2.2
2	b	327	THR	2.2
3	C	258	GLY	2.2
2	b	340	TRP	2.2
17	g	24	MET	2.2
1	A	242	GLU	2.2
12	M	2	GLU	2.2
16	v	93	ASP	2.2
16	V	49	GLU	2.2
15	u	106	ARG	2.2
5	e	8	ARG	2.2
18	x	20	PHE	2.2
2	B	368	VAL	2.2
18	x	17	LYS	2.2
16	v	36	VAL	2.2
3	c	145	SER	2.2
4	D	21	TRP	2.2
2	b	338	GLN	2.2
12	m	4	ASN	2.2
16	v	132	ASN	2.2
7	h	4	ARG	2.2
2	b	84	THR	2.2
13	o	49	ASP	2.2
16	V	77	SER	2.2
17	g	26	ALA	2.1
3	c	373	ASN	2.1
1	a	81	ALA	2.1
13	O	156	GLN	2.1
15	u	108	ASN	2.1
2	B	353	GLU	2.1
2	b	379	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	b	303	SER	2.1
12	m	7	GLY	2.1
18	x	12	ILE	2.1
13	o	168	PHE	2.1
7	H	3	ARG	2.1
16	v	27	ALA	2.1
16	v	31	PRO	2.1
3	c	363	GLY	2.1
18	X	11	THR	2.1
8	I	34	ARG	2.1
13	O	89	ALA	2.1
15	U	39	LEU	2.1
5	E	74	GLN	2.1
18	X	45	LYS	2.1
2	B	121	GLU	2.1
2	b	373	LYS	2.1
7	h	66	GLY	2.1
3	c	389	GLU	2.1
2	b	306	PRO	2.1
1	A	14	TRP	2.1
1	a	226	GLU	2.1
12	M	34	LYS	2.0
13	o	238	ALA	2.0
14	T	29	ILE	2.0
16	V	37	PRO	2.0
16	V	111	GLU	2.0
14	T	27	PRO	2.0
13	O	127	ILE	2.0
6	F	11	VAL	2.0
13	o	90	GLU	2.0
18	x	45	LYS	2.0
2	b	297	THR	2.0
2	b	378	LYS	2.0
9	J	7	ARG	2.0
13	o	228	ALA	2.0
19	Z	35	ARG	2.0
10	k	15	TYR	2.0
15	U	50	ALA	2.0
13	O	113	VAL	2.0
16	V	43	LYS	2.0
2	b	406	LEU	2.0
13	O	88	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
13	O	116	ASP	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
25	PL9	J	101	35/55	0.30	0.53	119,157,178,182	0
31	LMG	C	521	45/55	0.32	1.13	84,119,143,175	0
25	PL9	j	101	35/55	0.33	0.42	120,160,178,182	0
35	CA	k	101	1/1	0.33	0.52	103,103,103,103	0
35	CA	O	301	1/1	0.35	0.47	112,112,112,112	0
33	LMT	d	410	31/35	0.38	0.88	83,134,157,157	0
33	LMT	B	628	35/35	0.39	0.61	72,126,141,144	0
33	LMT	i	102	35/35	0.39	1.06	99,137,146,152	0
32	CL	A	416	1/1	0.45	1.00	49,49,49,49	0
31	LMG	E	101	44/55	0.47	0.64	87,123,132,139	0
33	LMT	B	629	35/35	0.49	0.67	70,137,165,168	0
27	BCR	j	102	40/40	0.50	0.50	110,128,180,184	0
23	CLA	b	605	65/65	0.50	0.91	88,108,124,137	0
33	LMT	B	624	35/35	0.50	0.82	80,142,170,171	0
23	CLA	B	601	65/65	0.53	0.99	92,108,131,137	0
31	LMG	c	519	45/55	0.55	0.97	86,119,142,171	0
28	DGD	D	409	63/66	0.56	0.74	104,127,181,188	0
27	BCR	B	620	40/40	0.57	0.94	75,86,98,103	0
33	LMT	b	627	35/35	0.57	0.88	100,140,152,154	0
27	BCR	J	102	40/40	0.58	0.45	108,125,177,180	0
33	LMT	b	603	35/35	0.60	0.48	73,119,136,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DGD	d	409	63/66	0.60	0.61	106,128,181,190	0
33	LMT	D	410	31/35	0.60	0.94	83,133,154,159	0
33	LMT	b	626	35/35	0.62	0.66	76,139,174,176	0
29	LHG	A	415	37/49	0.62	0.57	104,133,190,202	0
27	BCR	B	618	40/40	0.62	0.36	75,82,94,95	0
31	LMG	A	418	42/55	0.63	0.44	81,105,123,147	0
35	CA	K	101	1/1	0.63	0.53	86,86,86,86	0
30	SQD	d	408	43/54	0.64	0.74	67,109,152,157	0
27	BCR	k	102	40/40	0.64	0.77	72,80,109,111	0
25	PL9	a	410	45/55	0.64	0.46	82,103,121,125	0
27	BCR	D	405	40/40	0.65	0.52	68,81,105,110	0
33	LMT	I	102	35/35	0.65	0.69	99,135,144,145	0
35	CA	o	301	1/1	0.65	0.47	98,98,98,98	0
27	BCR	b	622	40/40	0.66	0.64	72,83,94,96	0
28	DGD	C	519	66/66	0.66	0.43	55,72,100,114	0
23	CLA	c	513	65/65	0.66	1.07	93,109,142,148	0
31	LMG	a	402	42/55	0.66	0.52	72,100,119,143	0
27	BCR	z	101	40/40	0.67	1.32	86,96,112,115	0
23	CLA	C	506	65/65	0.67	0.60	79,91,125,133	0
30	SQD	B	626	47/54	0.68	0.42	75,100,144,148	0
30	SQD	b	601	47/54	0.68	0.41	81,103,147,151	0
27	BCR	y	101	40/40	0.68	0.79	79,86,106,109	0
31	LMG	e	101	44/55	0.68	0.43	91,122,132,136	0
25	PL9	A	408	45/55	0.68	0.48	89,101,119,127	0
33	LMT	b	604	35/35	0.68	0.49	69,133,158,160	0
23	CLA	c	502	65/65	0.68	0.61	63,75,100,106	0
30	SQD	F	102	45/54	0.69	0.76	87,127,149,152	0
29	LHG	a	417	37/49	0.70	0.37	110,135,197,206	0
27	BCR	A	410	40/40	0.70	0.47	52,68,85,90	0
23	CLA	B	616	65/65	0.70	0.71	79,93,147,152	0
27	BCR	T	102	40/40	0.71	0.33	71,79,86,86	0
27	BCR	B	619	40/40	0.71	0.34	62,75,83,86	0
28	DGD	B	627	52/66	0.71	0.50	75,105,178,180	0
27	BCR	H	101	40/40	0.71	1.03	83,96,130,131	0
23	CLA	b	620	65/65	0.71	0.58	75,98,145,147	0
30	SQD	a	415	51/54	0.71	0.39	88,101,128,129	0
30	SQD	D	408	43/54	0.72	0.66	71,103,148,152	0
33	LMT	B	625	35/35	0.72	0.74	95,139,149,152	0
28	DGD	A	411	56/66	0.72	0.38	77,102,146,153	0
27	BCR	b	621	40/40	0.72	0.28	63,73,84,87	0
27	BCR	a	412	40/40	0.73	0.42	54,71,84,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	SQD	A	413	51/54	0.73	0.39	81,99,128,131	0
31	LMG	i	101	43/55	0.73	0.66	84,120,162,177	0
23	CLA	B	614	65/65	0.73	0.41	63,83,125,129	0
27	BCR	h	101	40/40	0.74	0.94	85,94,124,127	0
31	LMG	I	101	43/55	0.74	0.56	73,118,166,178	0
31	LMG	M	101	42/55	0.74	0.35	83,111,135,144	0
23	CLA	C	507	65/65	0.74	0.67	79,93,100,104	0
31	LMG	B	622	49/55	0.75	0.33	61,79,105,117	0
28	DGD	a	413	56/66	0.75	0.38	76,100,145,148	0
23	CLA	C	513	65/65	0.75	0.94	95,109,142,149	0
31	LMG	k	103	48/55	0.75	0.43	79,100,112,115	0
27	BCR	C	516	40/40	0.75	0.57	74,86,95,100	0
30	SQD	f	102	45/54	0.75	0.60	88,133,148,152	0
25	PL9	d	404	55/55	0.75	0.32	45,65,78,85	0
30	SQD	a	401	54/54	0.76	0.43	76,114,149,152	0
23	CLA	c	512	65/65	0.77	1.06	83,104,146,152	0
25	PL9	D	404	55/55	0.77	0.32	42,61,71,77	0
31	LMG	m	102	42/55	0.77	0.38	73,111,128,138	0
28	DGD	c	518	66/66	0.77	0.33	54,73,105,118	0
30	SQD	A	417	54/54	0.78	0.37	77,113,147,154	0
27	BCR	c	515	40/40	0.78	0.80	75,86,95,101	0
23	CLA	C	504	65/65	0.78	0.36	62,83,138,145	0
21	FE2	A	401	1/1	0.78	0.17	64,64,64,64	0
32	CL	a	418	1/1	0.78	0.49	49,49,49,49	0
23	CLA	a	406	65/65	0.78	0.36	55,71,140,147	0
27	BCR	B	617	40/40	0.78	0.33	67,74,81,84	0
23	CLA	B	602	65/65	0.79	0.63	68,87,95,96	0
23	CLA	B	606	65/65	0.79	0.72	67,81,110,121	0
27	BCR	d	405	40/40	0.79	0.37	69,82,102,106	0
27	BCR	T	101	40/40	0.79	0.31	68,75,82,83	0
23	CLA	c	506	65/65	0.79	0.49	78,92,122,128	0
23	CLA	C	502	65/65	0.79	0.50	59,75,108,111	0
23	CLA	B	608	65/65	0.79	0.64	64,75,93,97	0
23	CLA	C	505	65/65	0.79	0.41	69,77,86,91	0
23	CLA	C	510	65/65	0.80	0.38	67,74,83,93	0
31	LMG	D	406	46/55	0.80	0.33	58,73,116,129	0
23	CLA	b	612	65/65	0.80	0.51	63,75,95,98	0
29	LHG	a	414	39/49	0.80	0.41	60,78,94,102	0
27	BCR	c	514	40/40	0.80	1.10	76,82,88,89	0
23	CLA	C	511	65/65	0.80	0.55	74,88,102,109	0
31	LMG	a	416	51/55	0.80	0.33	62,80,93,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DGD	b	602	52/66	0.80	0.41	79,107,180,186	0
28	DGD	b	623	58/66	0.80	0.36	57,74,99,107	0
27	BCR	C	515	40/40	0.80	1.05	85,92,115,116	0
23	CLA	a	409	65/65	0.81	0.46	55,67,129,133	0
33	LMT	m	101	35/35	0.81	0.41	68,93,112,114	0
31	LMG	b	625	49/55	0.81	0.31	51,75,86,89	0
31	LMG	C	520	48/55	0.81	0.29	89,100,109,112	0
23	CLA	b	613	65/65	0.81	0.73	65,93,104,114	0
23	CLA	b	619	65/65	0.81	0.59	85,97,108,116	0
23	CLA	b	618	65/65	0.82	0.32	60,82,123,130	0
31	LMG	d	407	48/55	0.82	0.36	58,70,85,120	0
28	DGD	c	516	53/66	0.82	0.31	63,77,96,103	0
28	DGD	C	518	62/66	0.82	0.34	58,81,134,144	0
23	CLA	c	507	65/65	0.82	0.67	83,93,105,111	0
23	CLA	c	511	65/65	0.82	0.68	75,91,102,108	0
33	LMT	M	102	35/35	0.82	0.52	69,96,112,115	0
23	CLA	B	615	65/65	0.82	0.83	83,96,106,116	0
23	CLA	c	505	65/65	0.82	0.35	70,77,83,85	0
23	CLA	B	604	65/65	0.83	0.58	59,67,104,124	0
23	CLA	C	512	65/65	0.83	0.84	89,101,144,149	0
29	LHG	A	412	39/49	0.83	0.29	59,79,89,93	0
23	CLA	d	402	65/65	0.83	0.37	49,57,81,95	0
31	LMG	B	623	49/55	0.83	0.31	58,76,84,87	0
23	CLA	d	403	65/65	0.83	0.67	72,88,121,128	0
23	CLA	c	503	65/65	0.83	0.81	77,89,97,103	0
23	CLA	c	504	65/65	0.83	0.34	75,83,133,138	0
23	CLA	A	407	65/65	0.84	0.49	56,66,127,129	0
27	BCR	C	514	40/40	0.84	1.00	73,80,87,94	0
23	CLA	b	614	65/65	0.84	0.60	66,82,88,91	0
34	HEM	v	201	43/43	0.84	0.51	57,68,75,76	0
31	LMG	A	414	51/55	0.84	0.26	63,77,92,95	0
23	CLA	b	607	65/65	0.84	0.77	68,82,92,103	0
23	CLA	B	610	65/65	0.84	0.67	69,81,88,92	0
24	PHO	A	406	64/64	0.84	0.36	50,69,77,81	0
23	CLA	C	501	65/65	0.85	0.48	69,82,90,95	0
23	CLA	c	501	65/65	0.85	0.82	67,82,92,94	0
23	CLA	A	405	65/65	0.85	0.30	44,69,140,145	0
34	HEM	V	201	43/43	0.85	0.47	58,69,74,76	0
23	CLA	c	509	65/65	0.85	0.51	67,85,91,97	0
23	CLA	b	608	65/65	0.85	0.40	61,68,107,117	0
28	DGD	B	621	58/66	0.85	0.38	46,71,101,105	0
23	CLA	C	509	65/65	0.85	0.62	62,81,95,98	0

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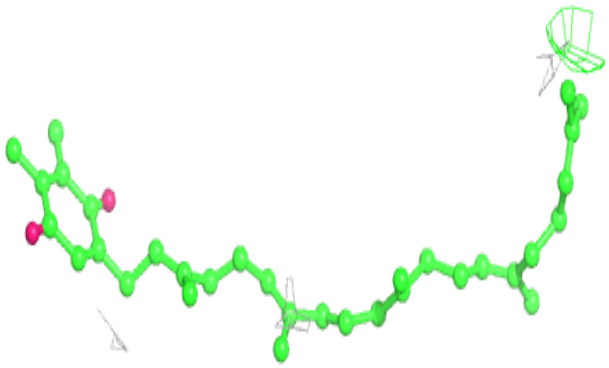
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	DGD	c	517	62/66	0.85	0.30	64,84,132,141	0
24	PHO	a	408	64/64	0.86	0.33	58,68,79,86	0
23	CLA	D	403	65/65	0.86	0.88	74,87,123,124	0
23	CLA	b	606	65/65	0.86	0.47	70,87,96,97	0
22	BCT	d	401	4/4	0.86	0.49	87,91,92,94	0
23	CLA	B	607	65/65	0.86	0.28	52,66,82,85	0
31	LMG	b	624	49/55	0.86	0.27	59,82,102,113	0
31	LMG	D	407	48/55	0.86	0.26	54,72,81,120	0
23	CLA	B	605	65/65	0.87	0.66	58,78,86,92	0
21	FE2	a	403	1/1	0.87	0.16	72,72,72,72	0
23	CLA	b	609	65/65	0.87	0.51	61,76,84,88	0
23	CLA	b	610	65/65	0.87	0.52	70,83,112,126	0
28	DGD	C	517	53/66	0.87	0.29	61,79,96,101	0
23	CLA	b	611	65/65	0.87	0.32	54,64,89,92	0
23	CLA	B	611	65/65	0.87	0.31	63,72,80,87	0
23	CLA	a	405	65/65	0.87	0.31	44,53,69,73	0
23	CLA	C	508	65/65	0.87	0.32	71,86,117,132	0
23	CLA	B	613	65/65	0.87	0.30	46,64,88,93	0
23	CLA	C	503	65/65	0.87	0.49	71,88,99,105	0
22	BCT	A	402	4/4	0.87	0.32	85,90,90,94	0
24	PHO	a	407	64/64	0.88	0.28	53,63,70,73	0
34	HEM	F	101	43/43	0.88	0.45	89,105,127,130	0
23	CLA	D	401	65/65	0.88	0.28	49,59,87,97	0
24	PHO	D	402	64/64	0.88	0.29	51,62,72,74	0
23	CLA	B	603	65/65	0.89	0.66	65,81,94,109	0
23	CLA	B	612	65/65	0.89	0.50	61,72,82,86	0
34	HEM	f	101	43/43	0.89	0.50	89,105,124,126	0
31	LMG	d	406	46/55	0.89	0.24	63,73,116,130	0
23	CLA	a	404	65/65	0.90	0.33	53,60,67,74	0
23	CLA	c	510	65/65	0.90	0.42	67,75,84,89	0
23	CLA	A	404	65/65	0.90	0.29	44,54,67,74	0
23	CLA	B	609	65/65	0.90	0.74	74,89,104,106	0
23	CLA	c	508	65/65	0.90	0.36	70,85,118,134	0
23	CLA	A	403	65/65	0.91	0.29	52,58,66,70	0
23	CLA	b	615	65/65	0.91	0.28	54,72,80,87	0
23	CLA	b	616	65/65	0.91	0.34	61,73,83,86	0
23	CLA	b	617	65/65	0.92	0.27	57,67,91,93	0
26	OEC	a	411	5/9	0.92	0.35	35,44,62,68	0
26	OEC	A	409	5/9	0.94	0.43	35,44,57,62	0

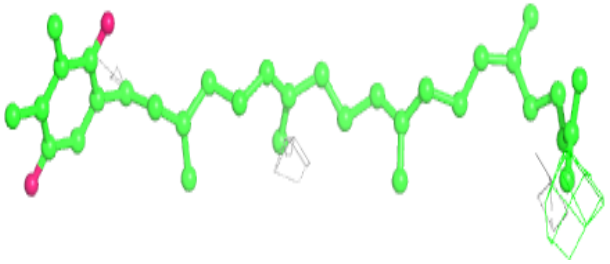
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

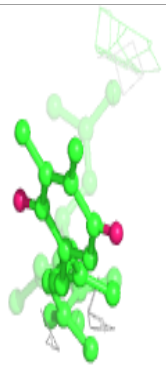
orientation to approximate a three-dimensional view.

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)

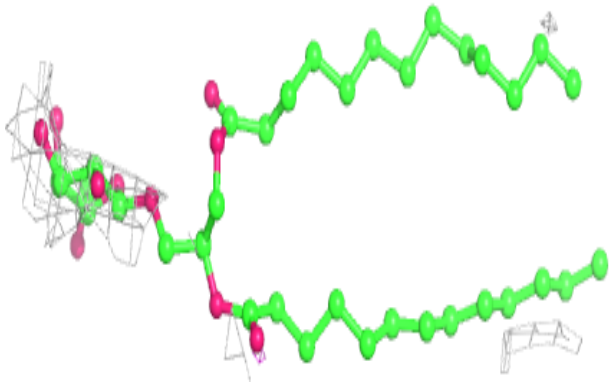


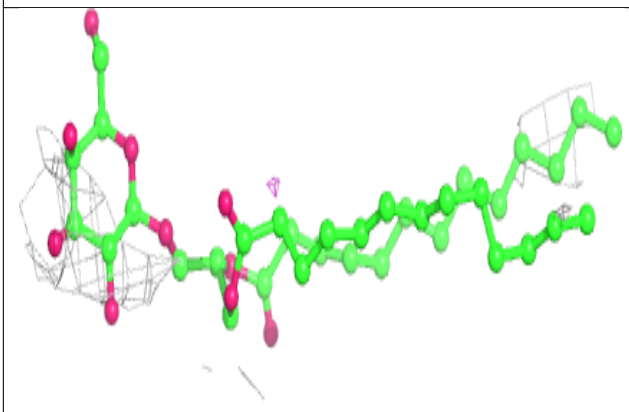


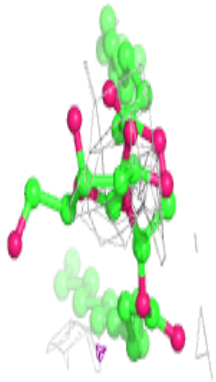


Electron density around LMG C 521:

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

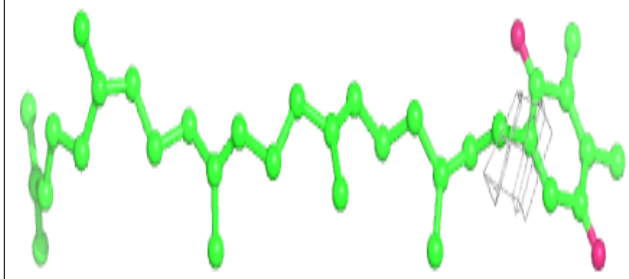


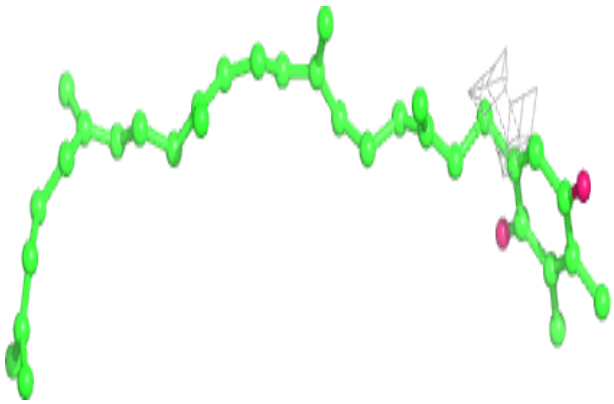




Electron density around PL9 j 101:

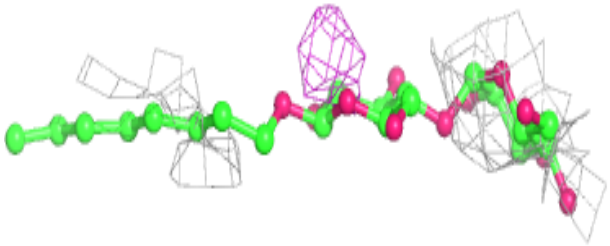
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

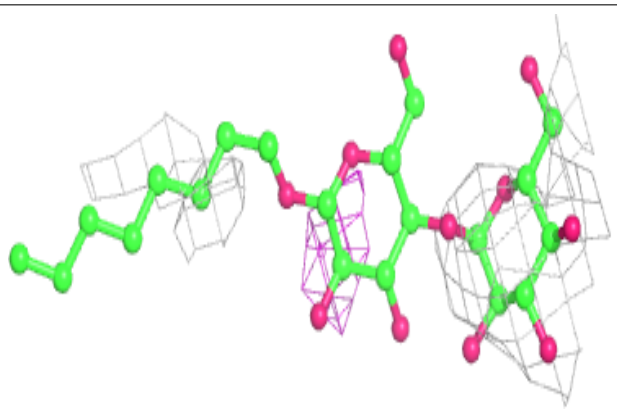


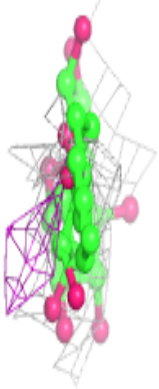


Electron density around LMT d 410:

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

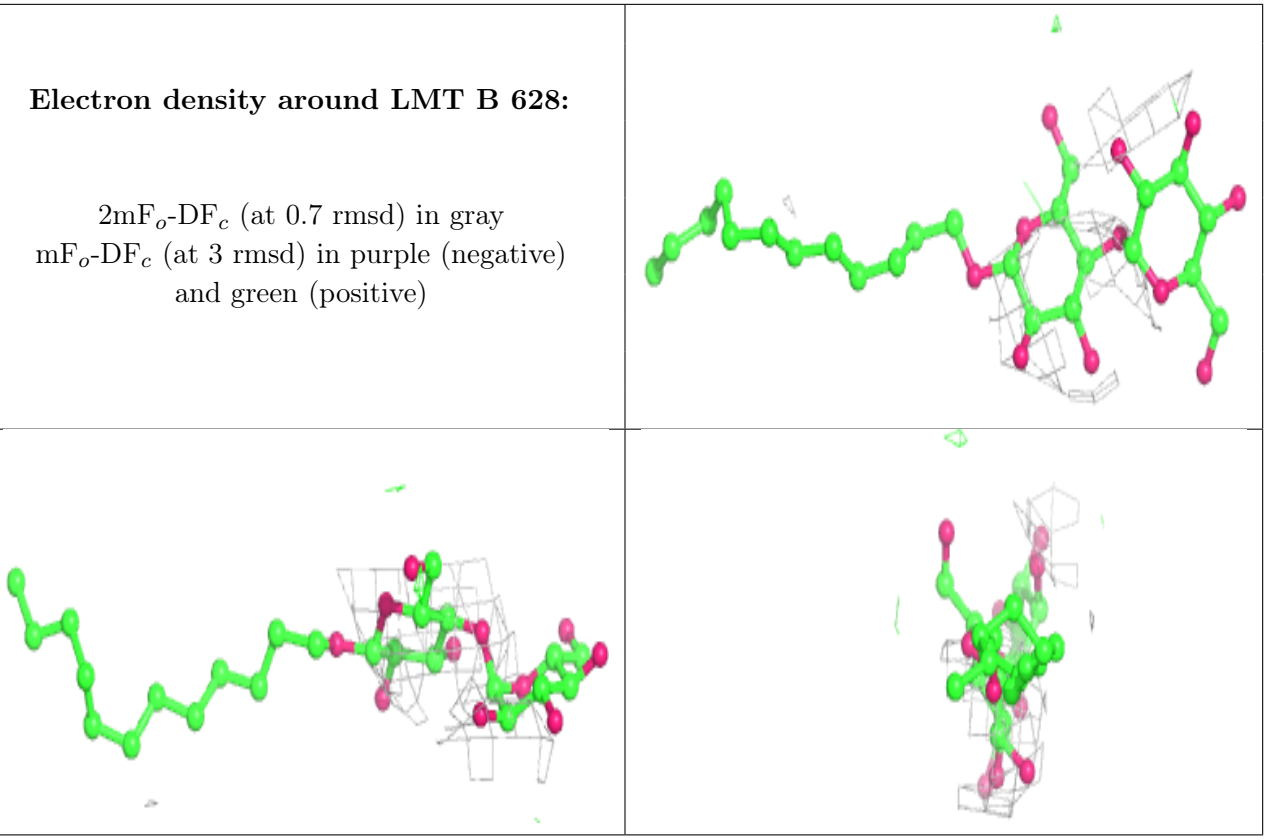






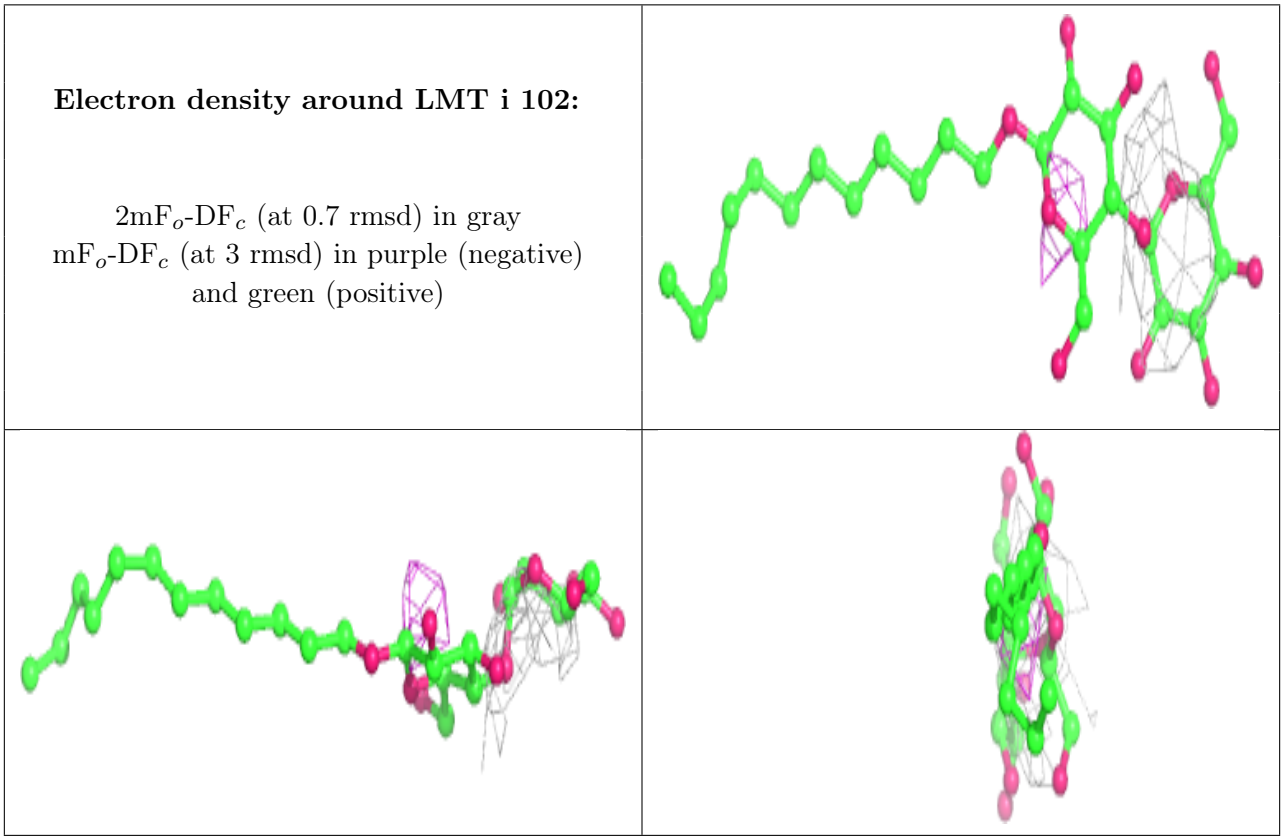
Electron density around LMT B 628:

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



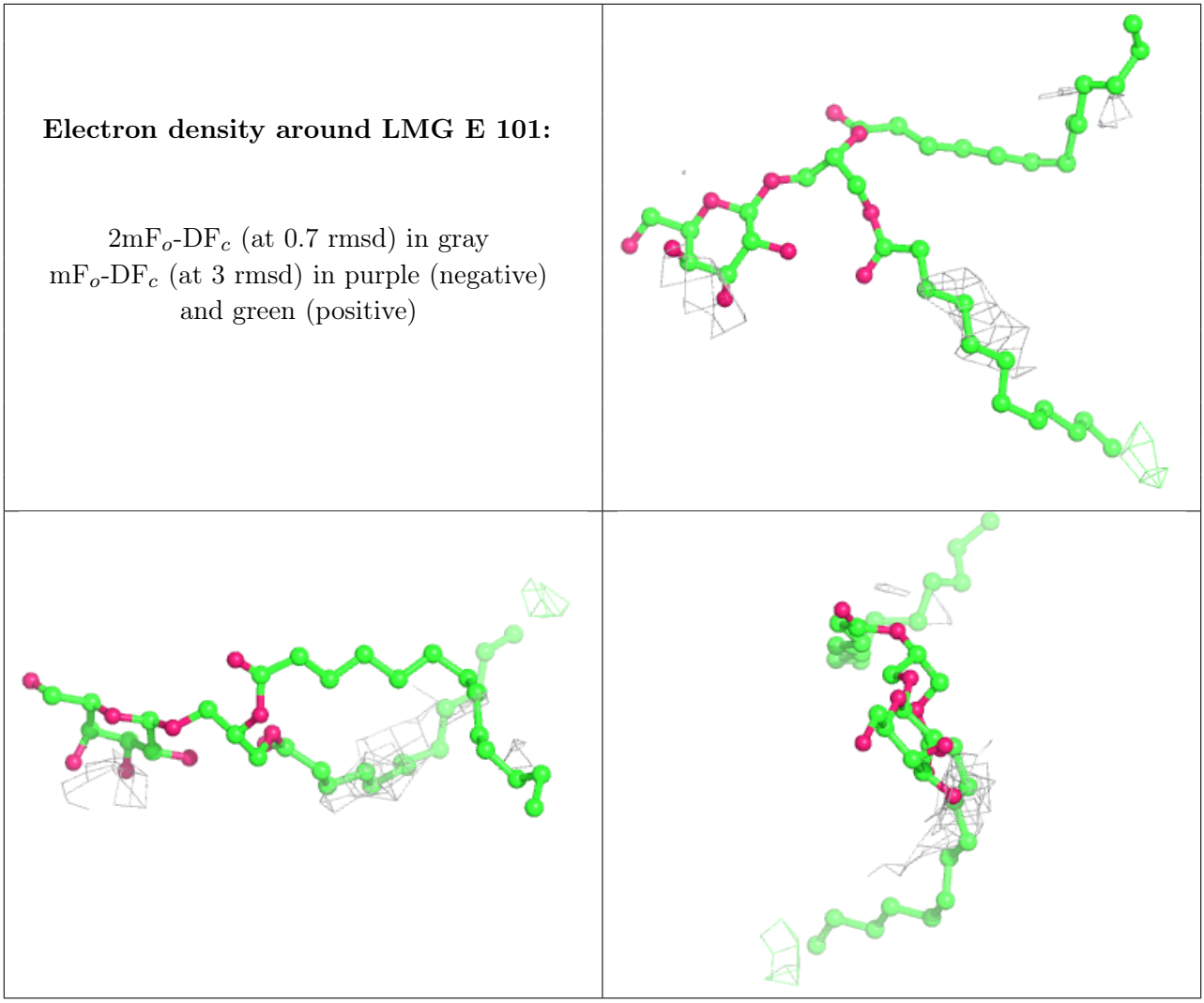
Electron density around LMT i 102:

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



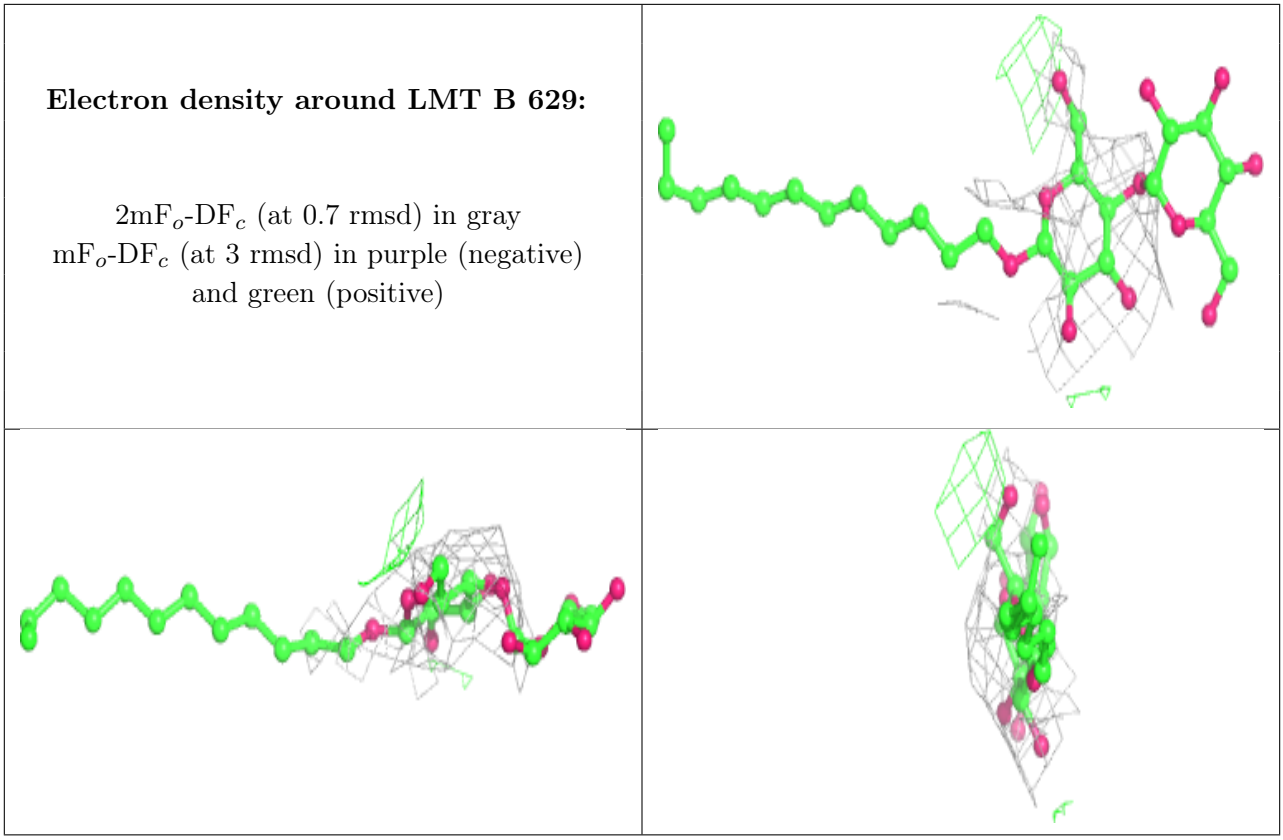
Electron density around LMG E 101:

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



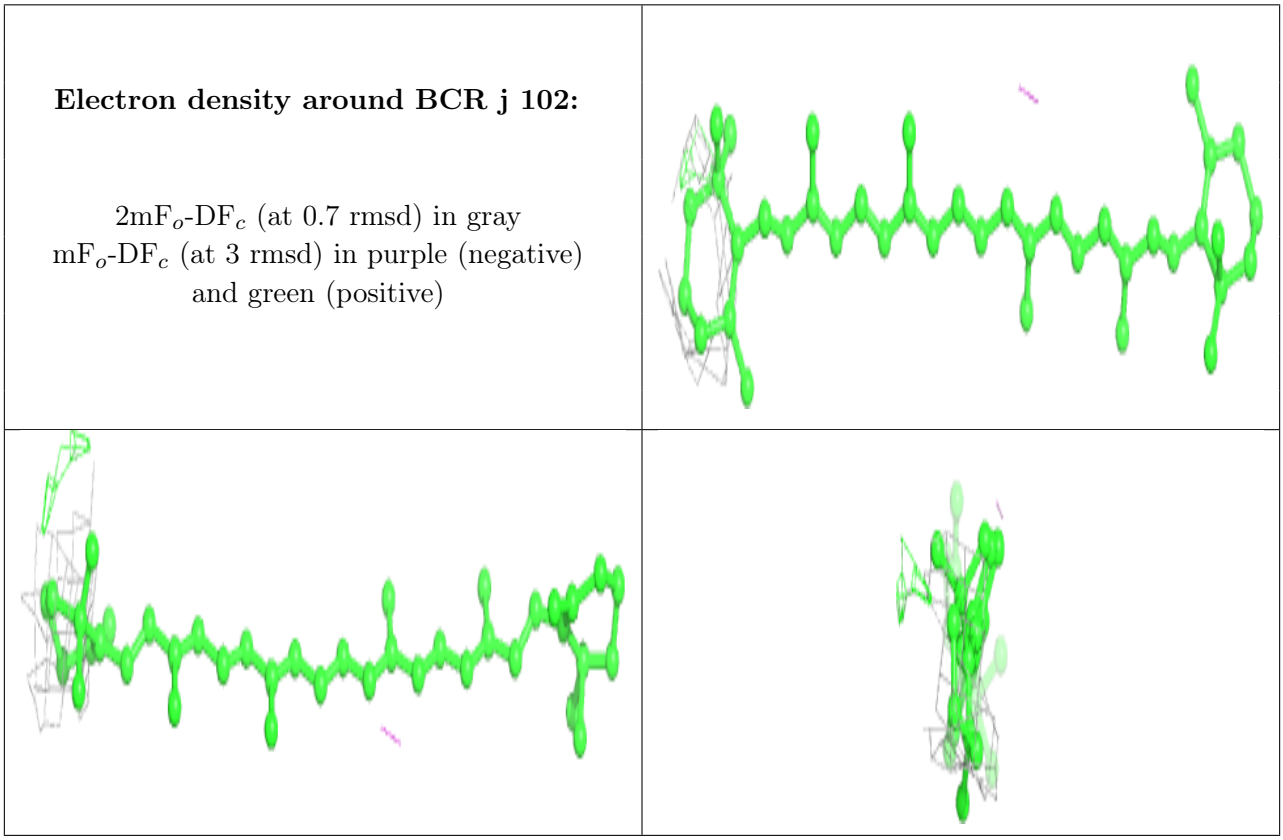
Electron density around LMT B 629:

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



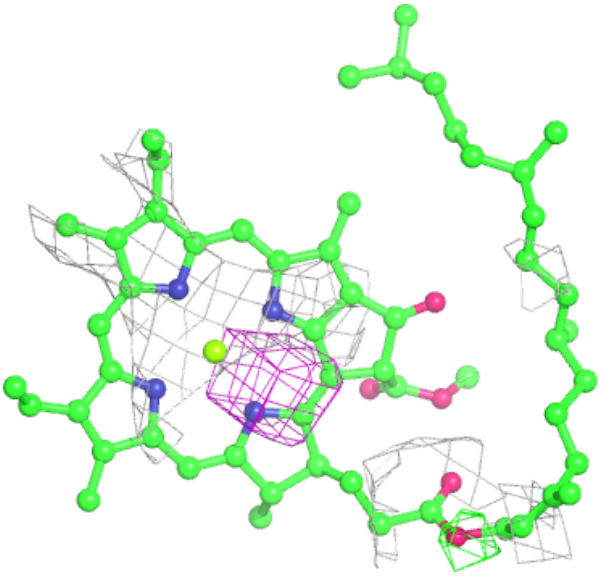
Electron density around BCR j 102:

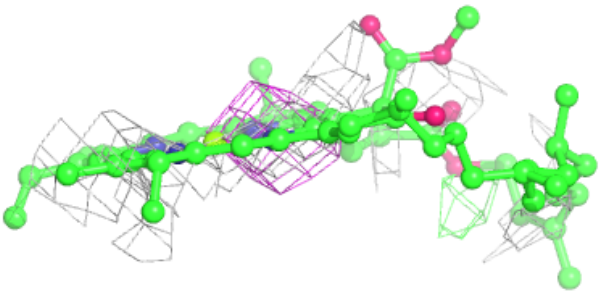
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

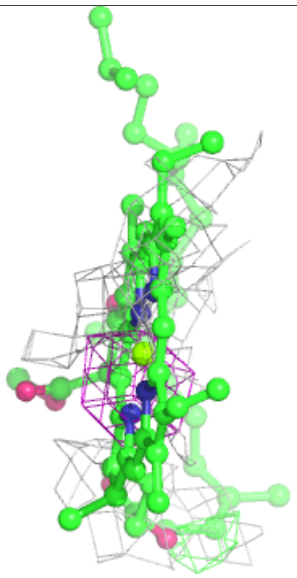


Electron density around CLA b 605:

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

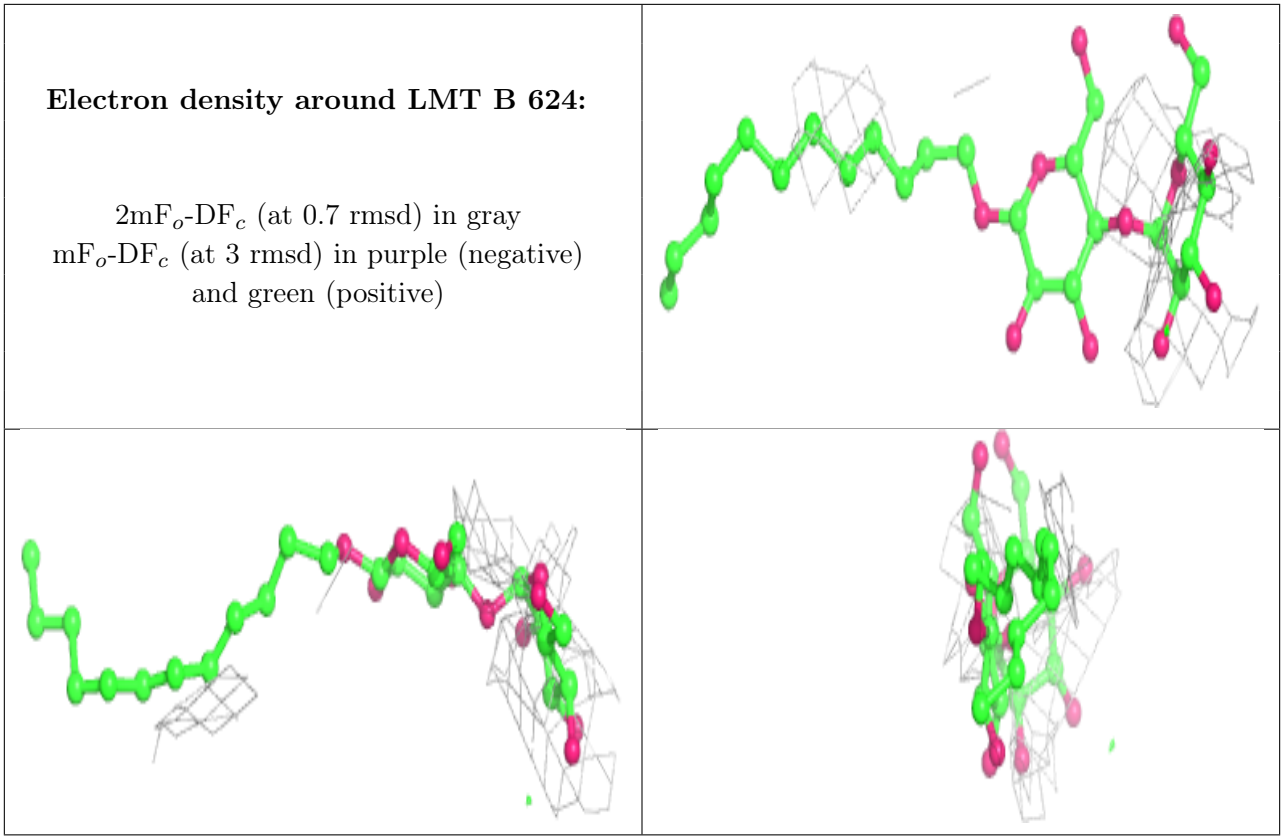






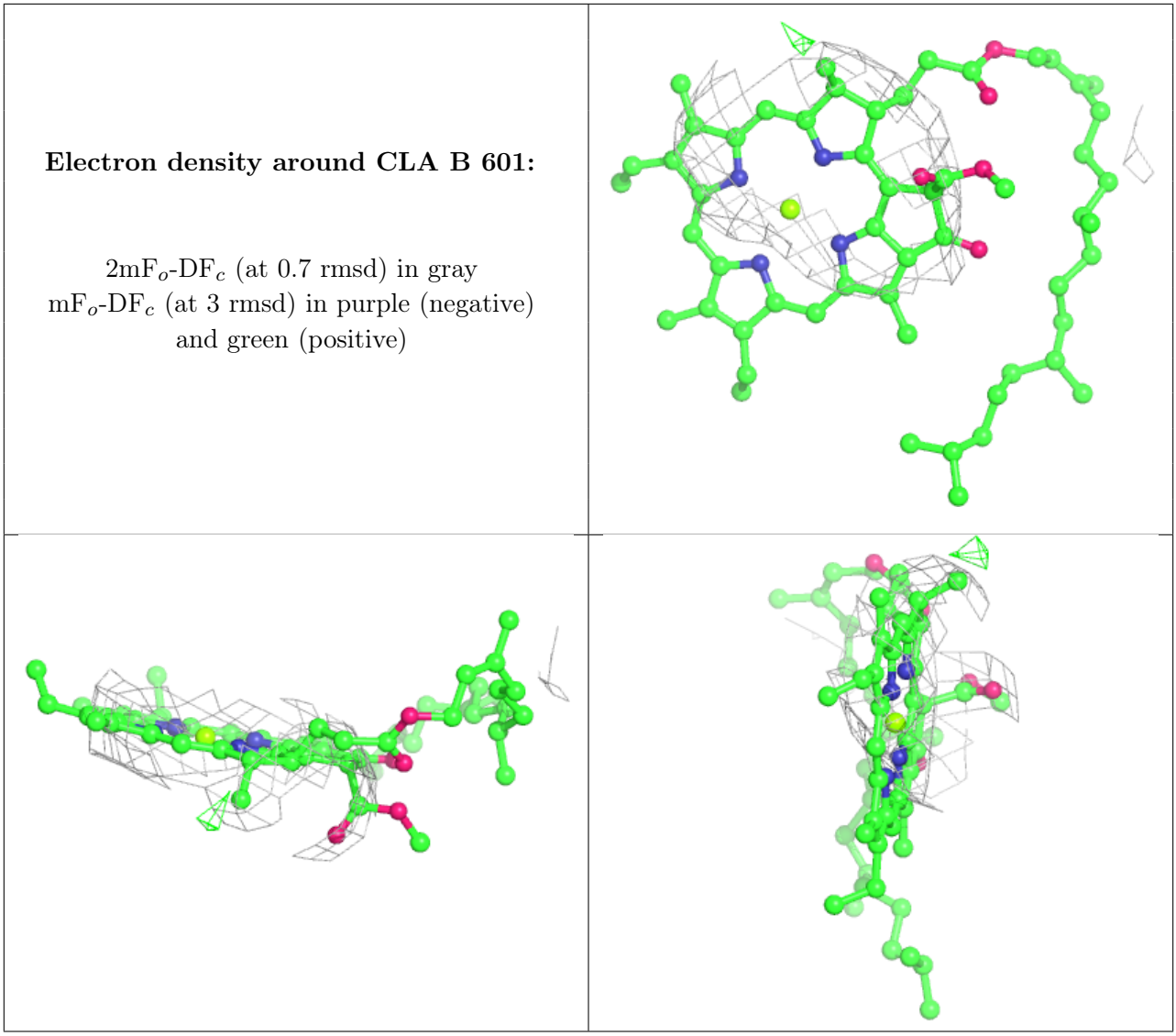
Electron density around LMT B 624:

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



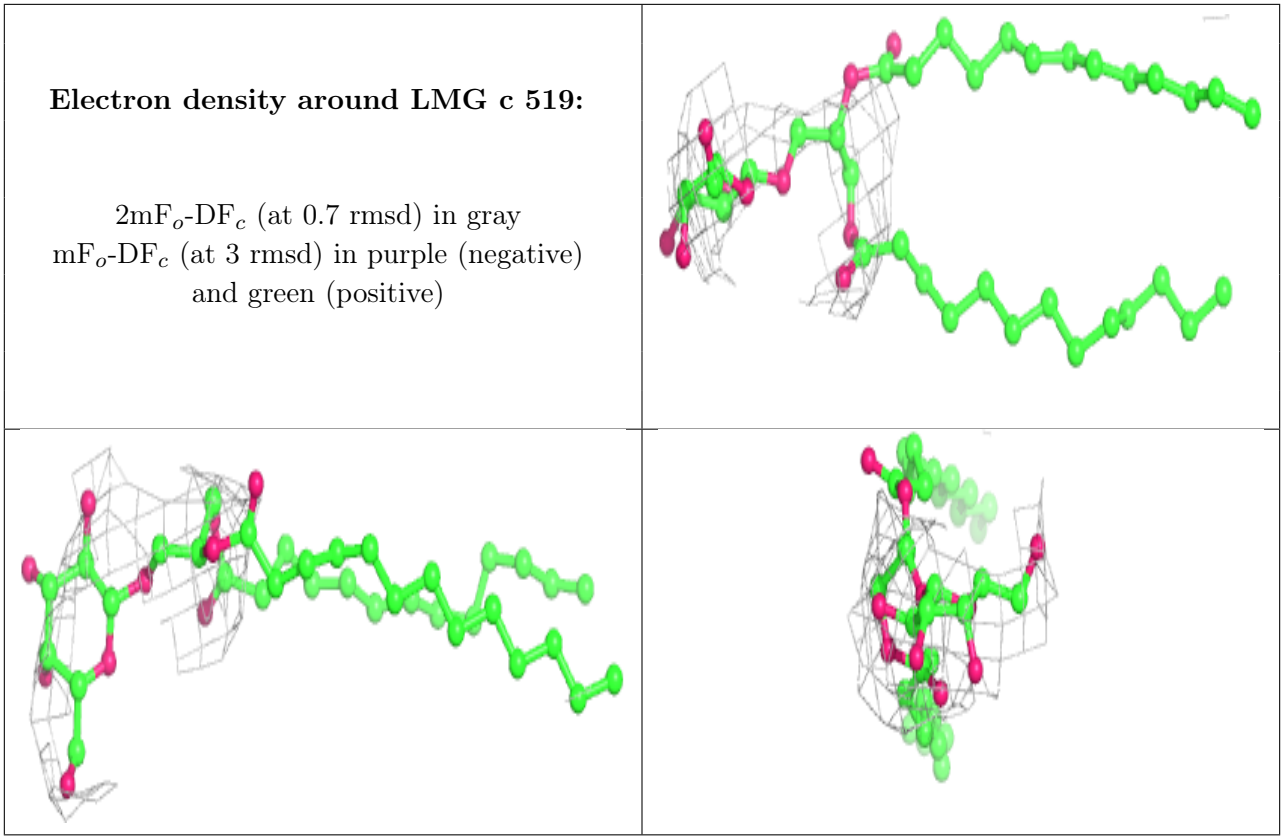
Electron density around CLA B 601:

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



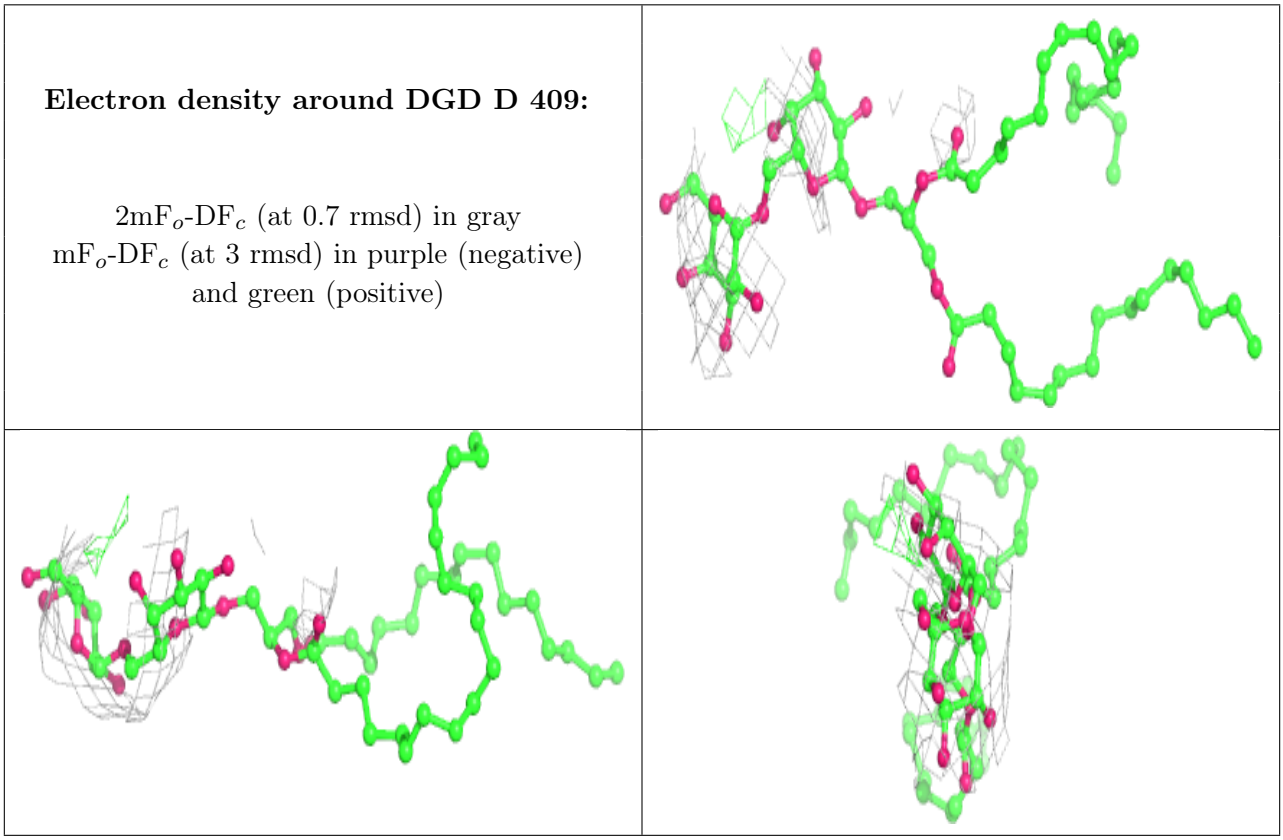
Electron density around LMG c 519:

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



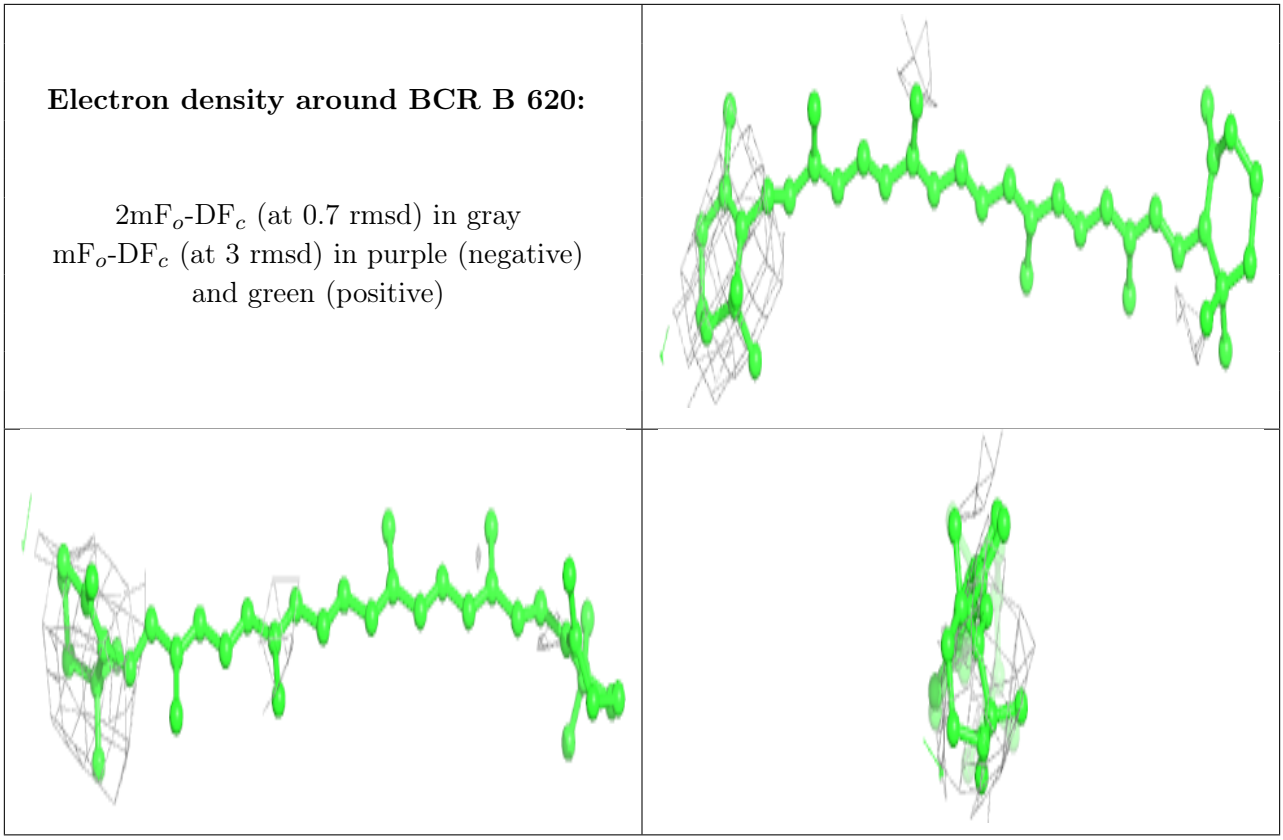
Electron density around DGD D 409:

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



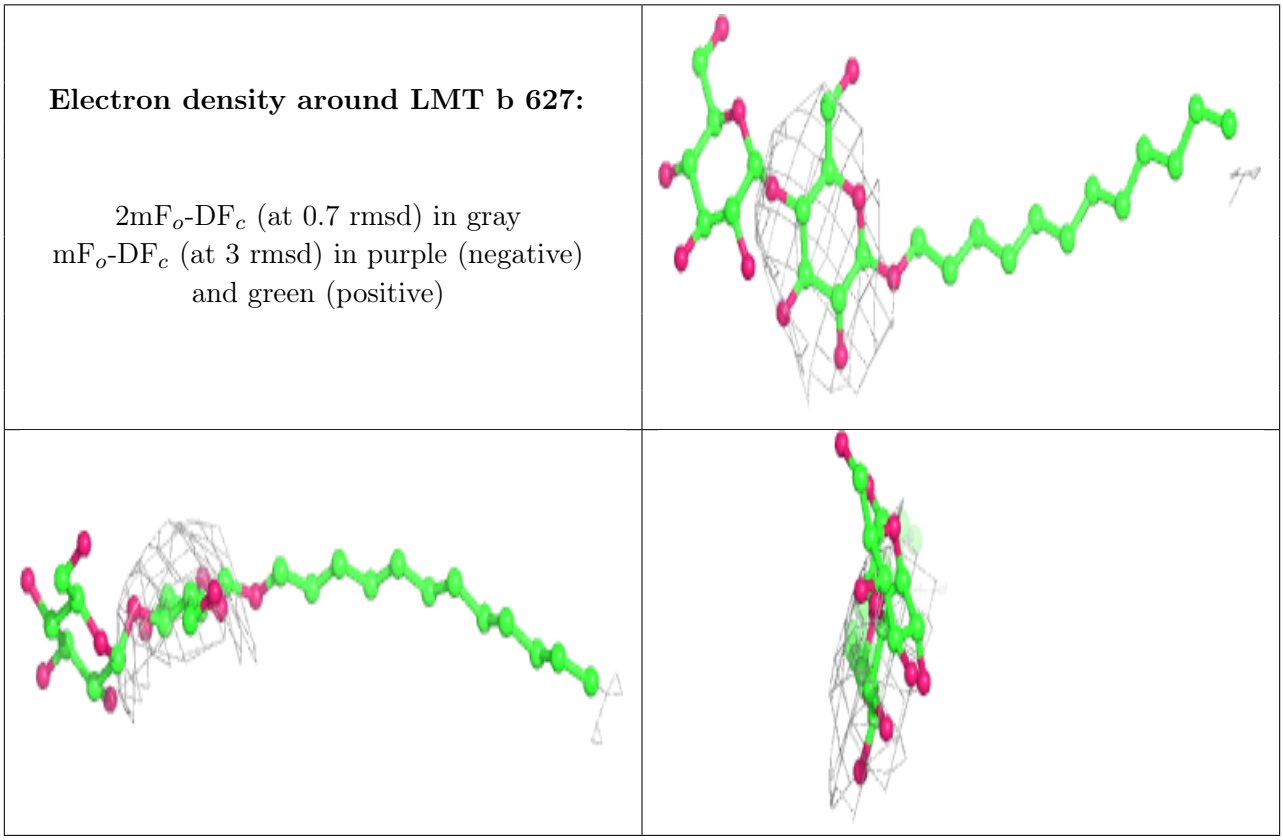
Electron density around BCR B 620:

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



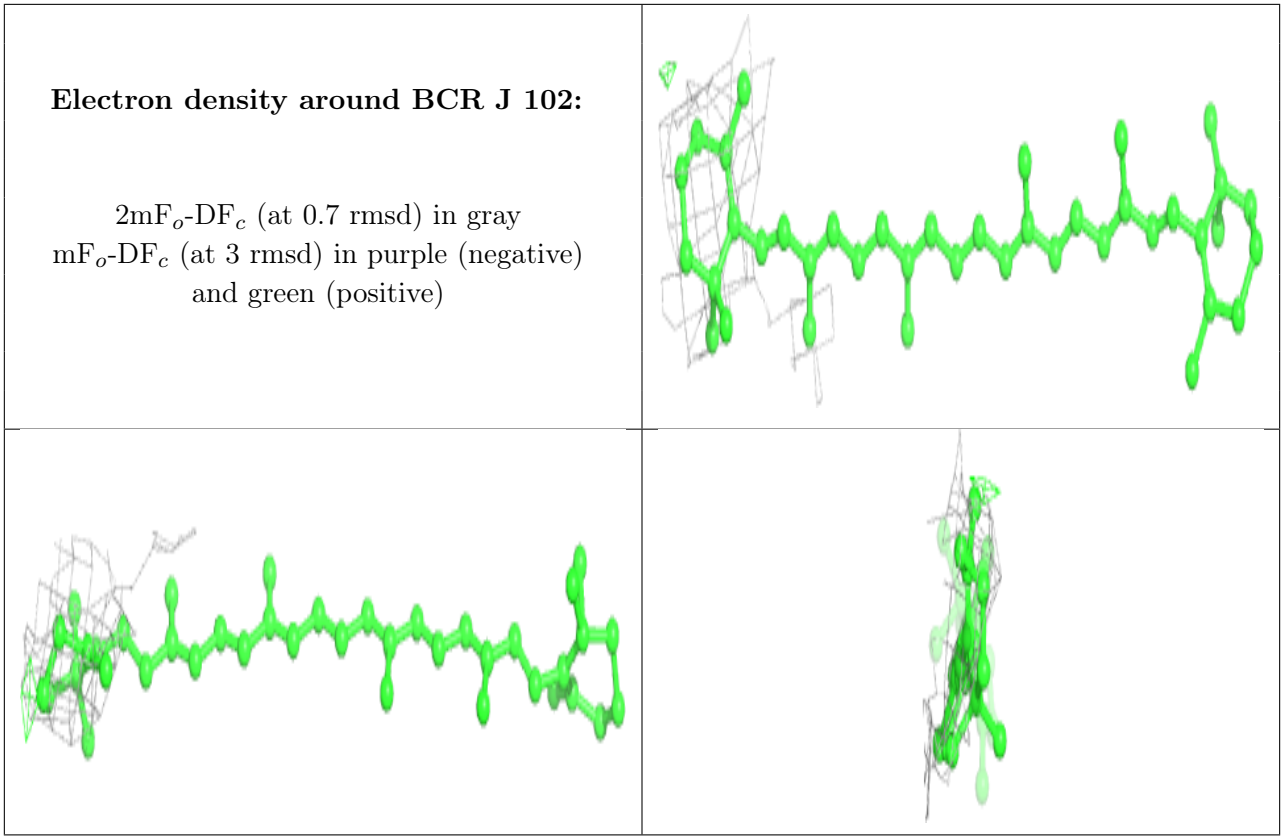
Electron density around LMT b 627:

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



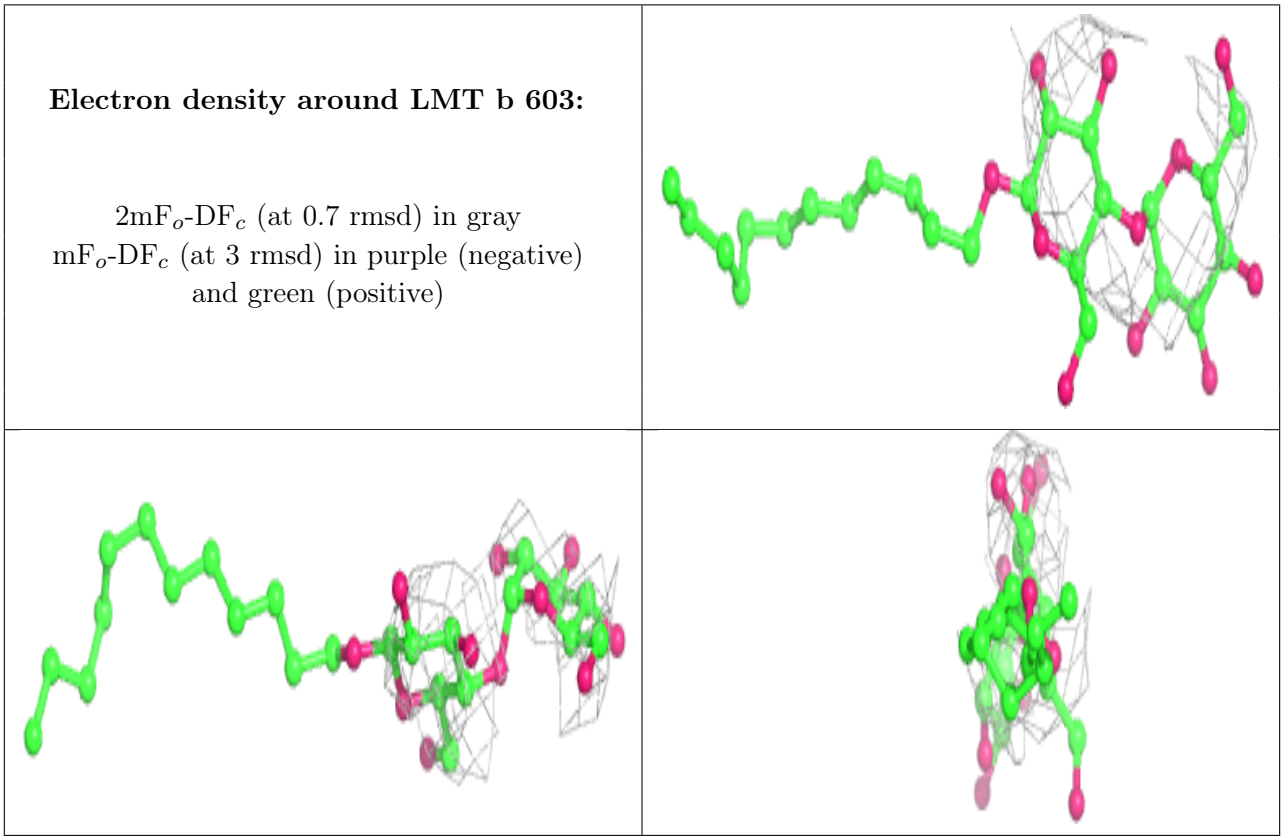
Electron density around BCR J 102:

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



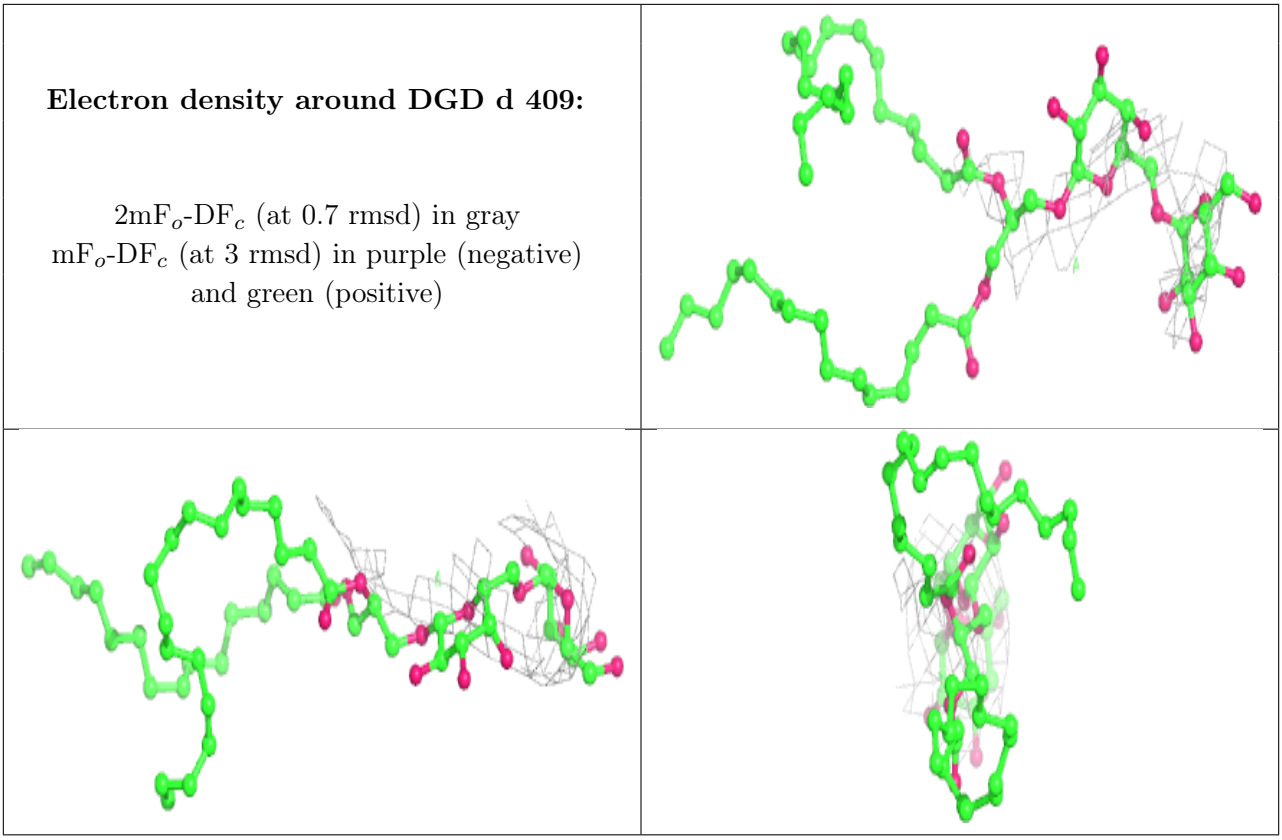
Electron density around LMT b 603:

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



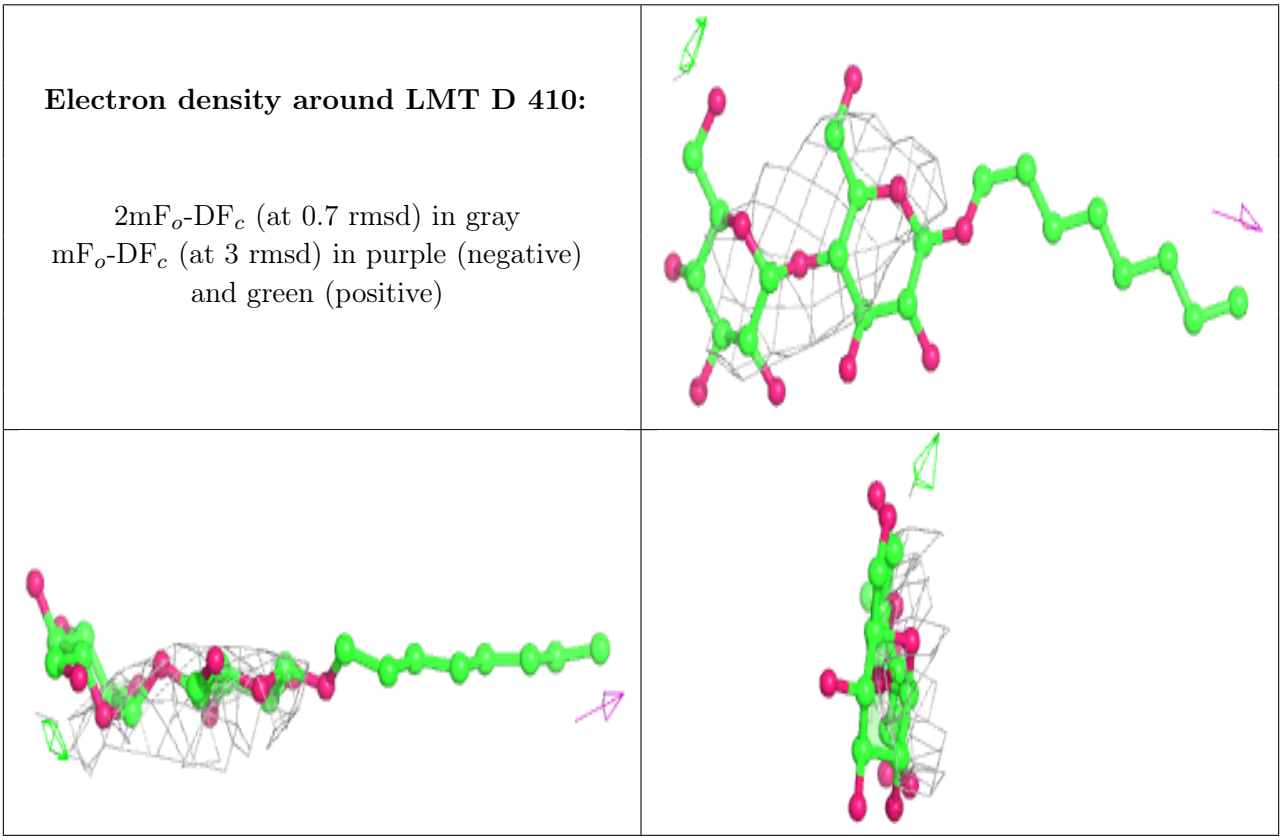
Electron density around DGD d 409:

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



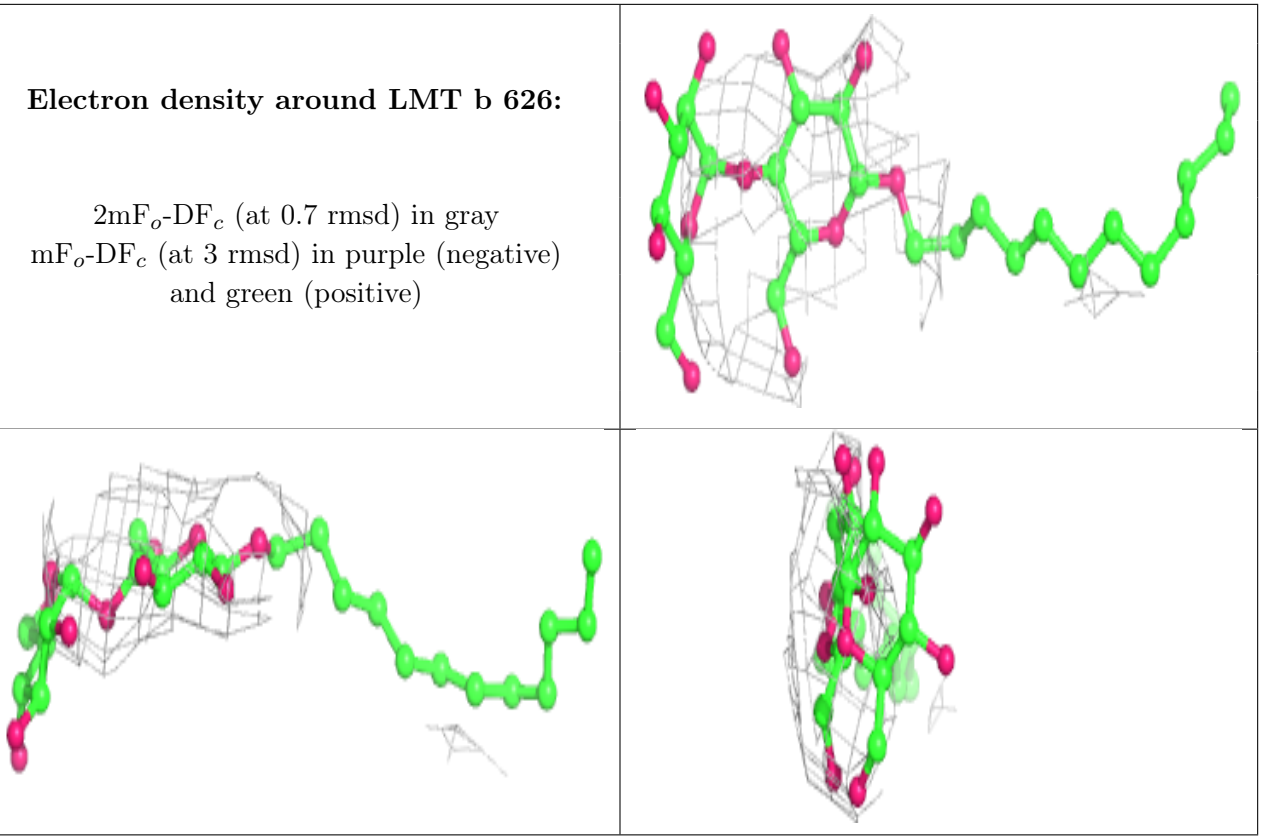
Electron density around LMT D 410:

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



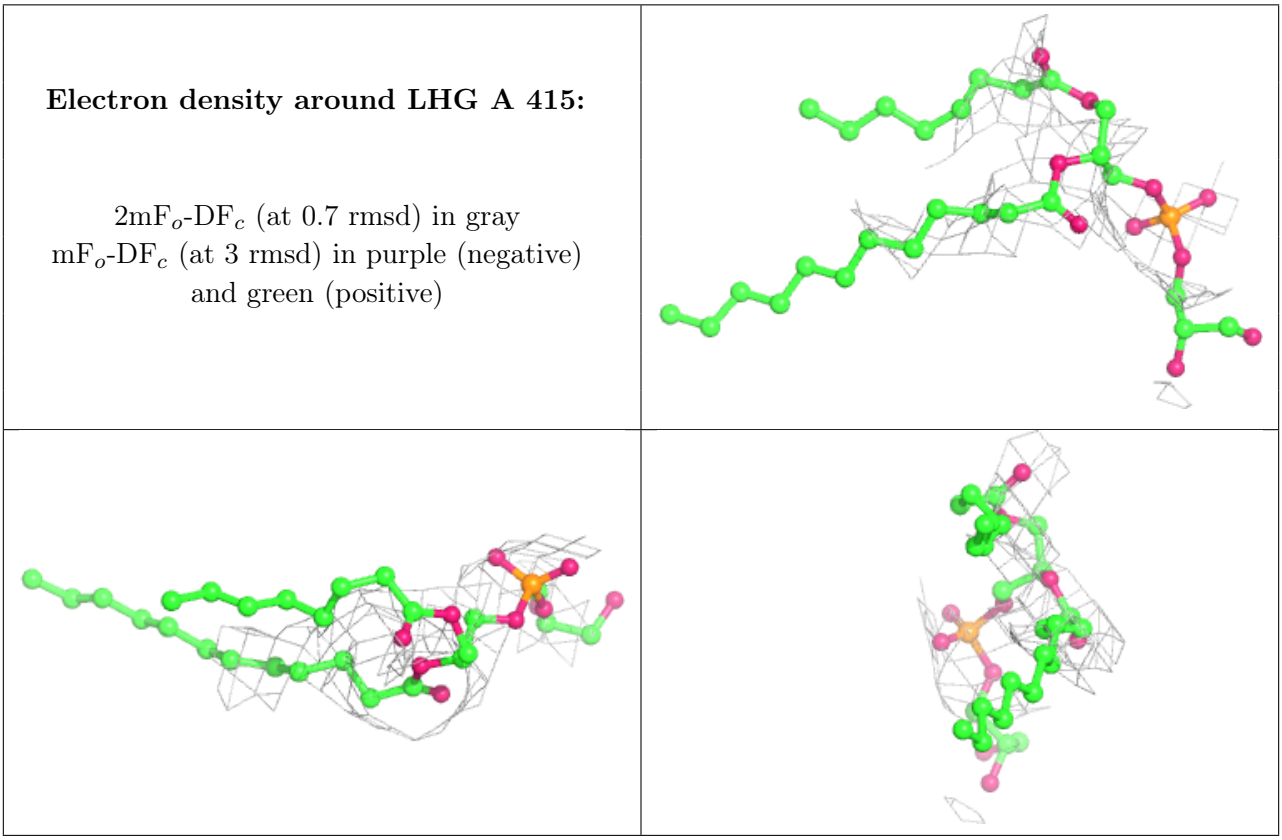
Electron density around LMT b 626:

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



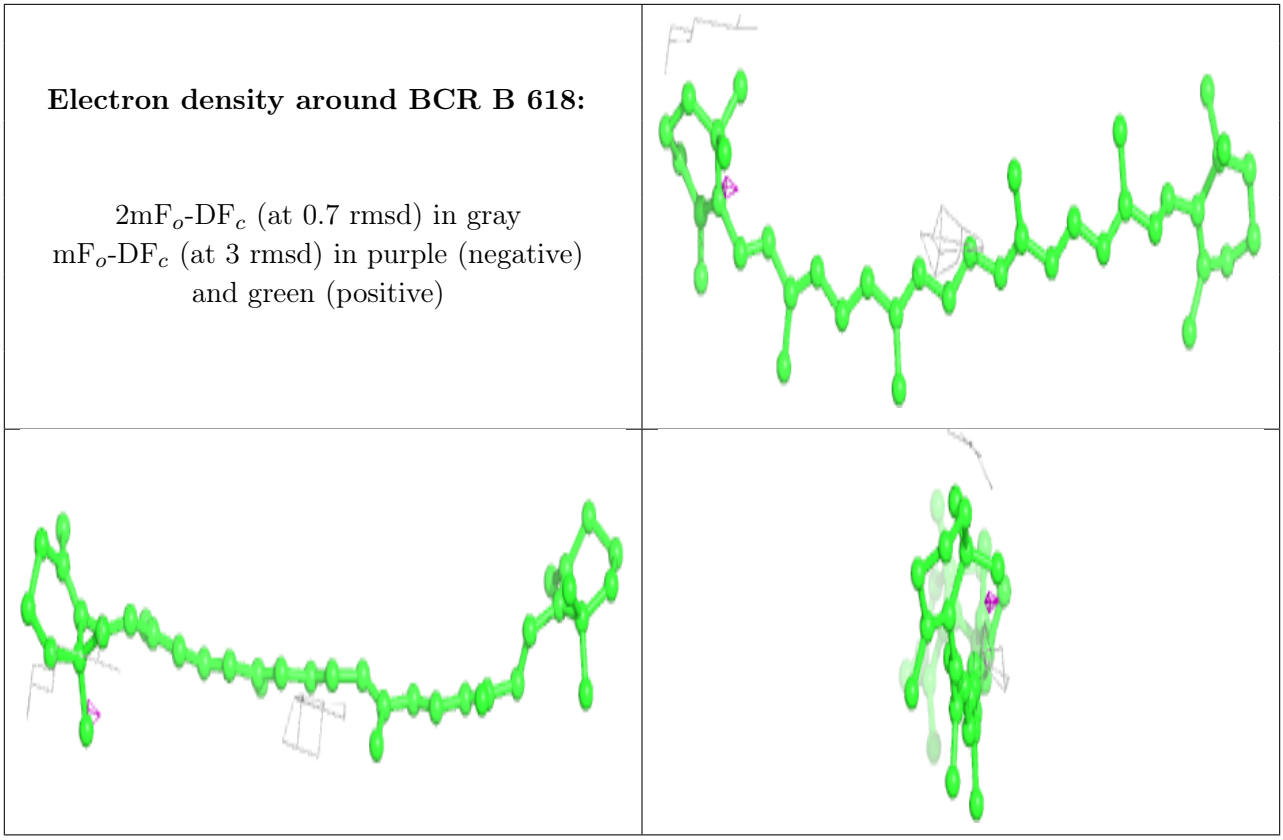
Electron density around LHG A 415:

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



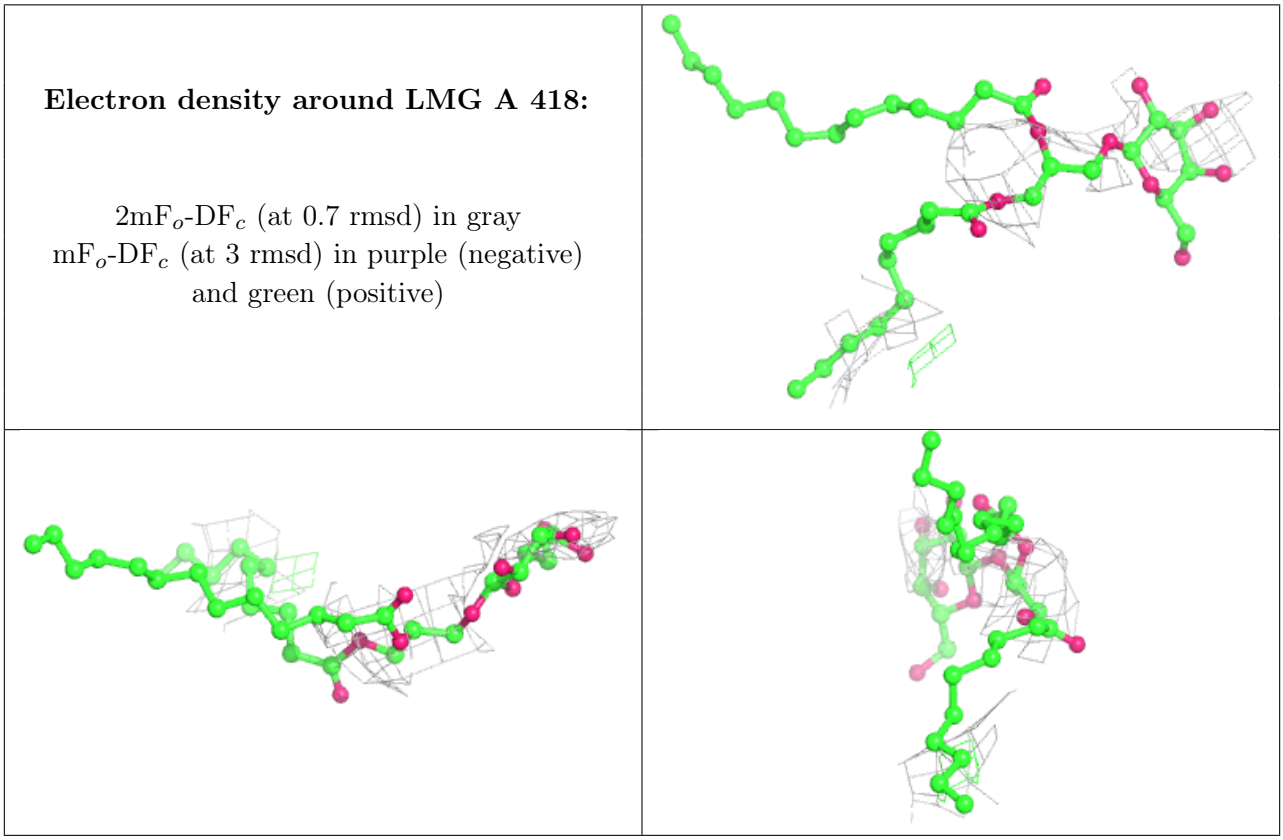
Electron density around BCR B 618:

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



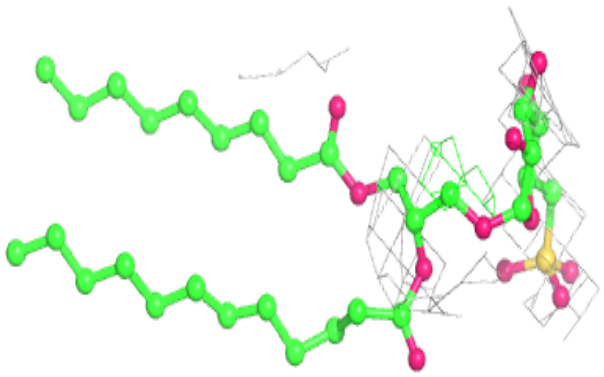
Electron density around LMG A 418:

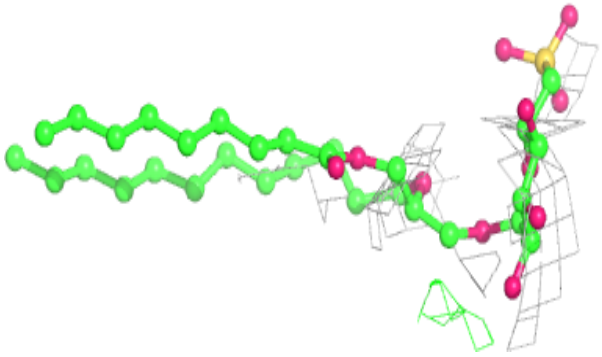
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

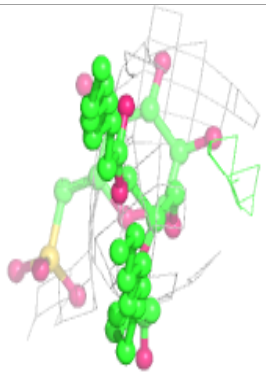


Electron density around SQD d 408:

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

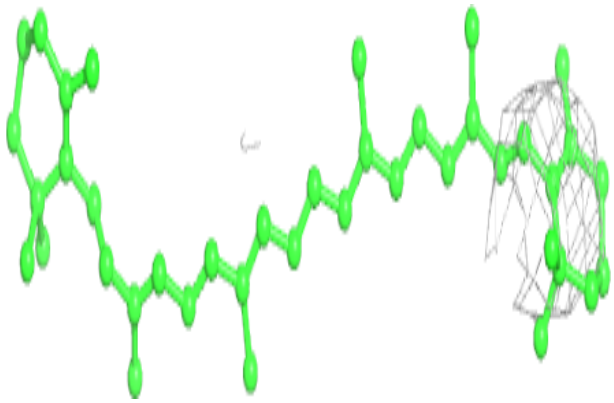


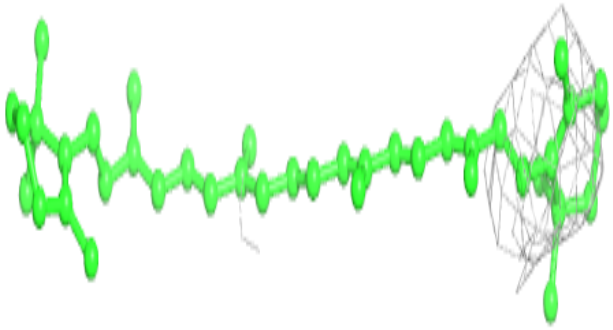




Electron density around BCR k 102:

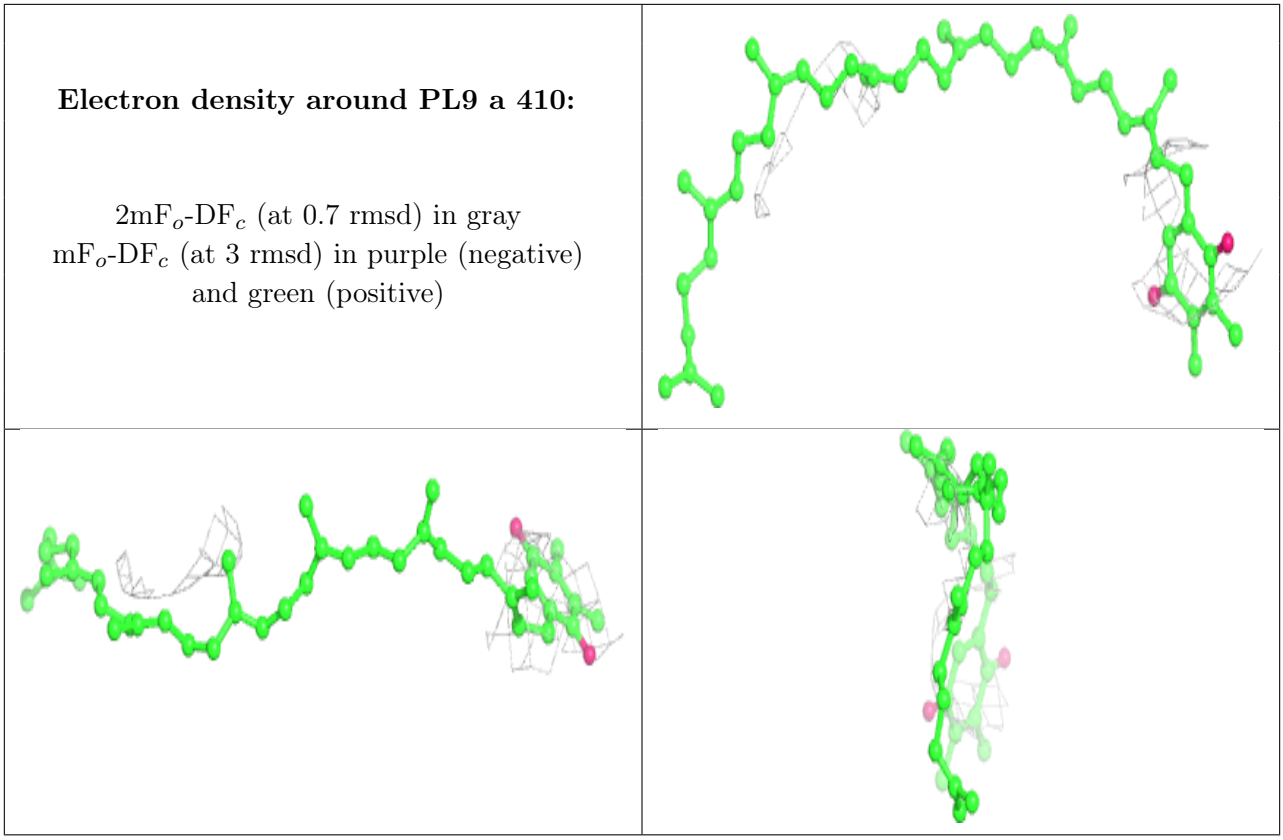
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





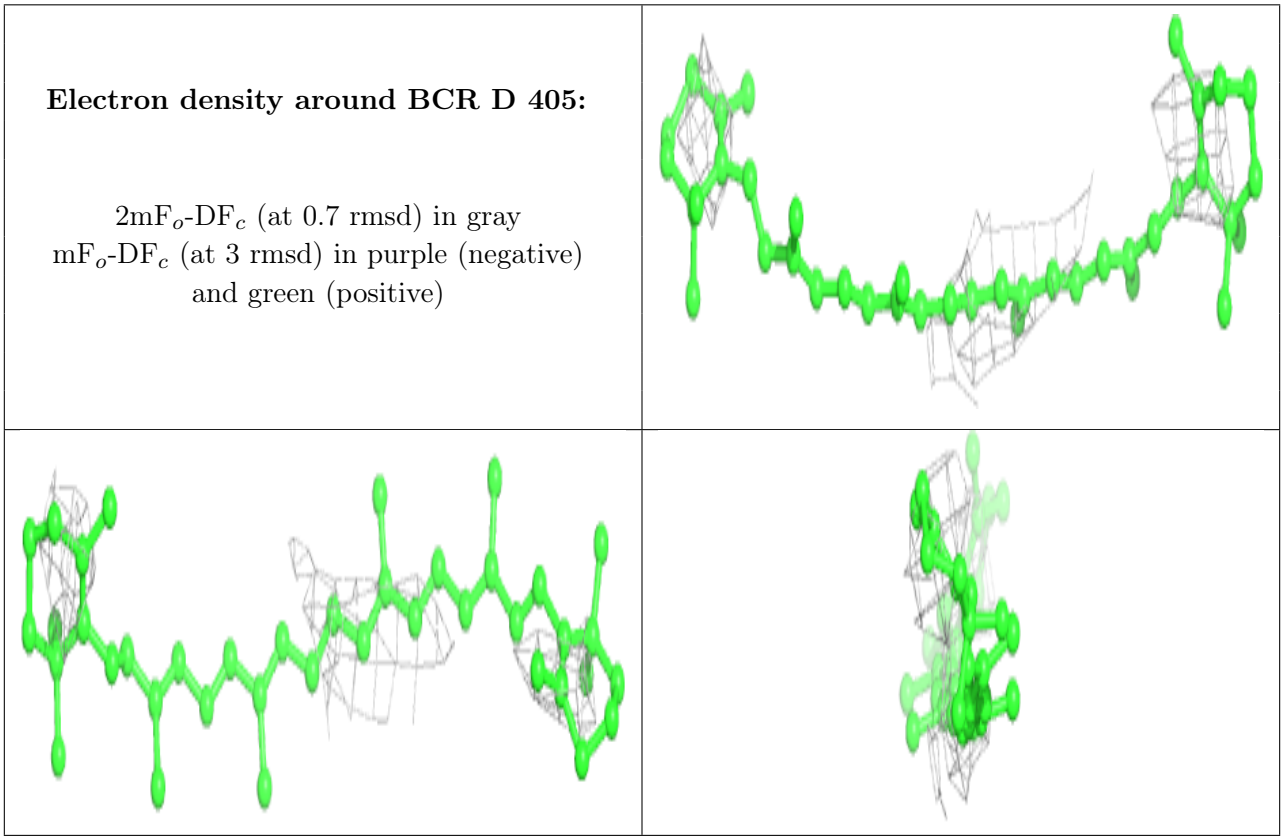
Electron density around PL9 a 410:

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



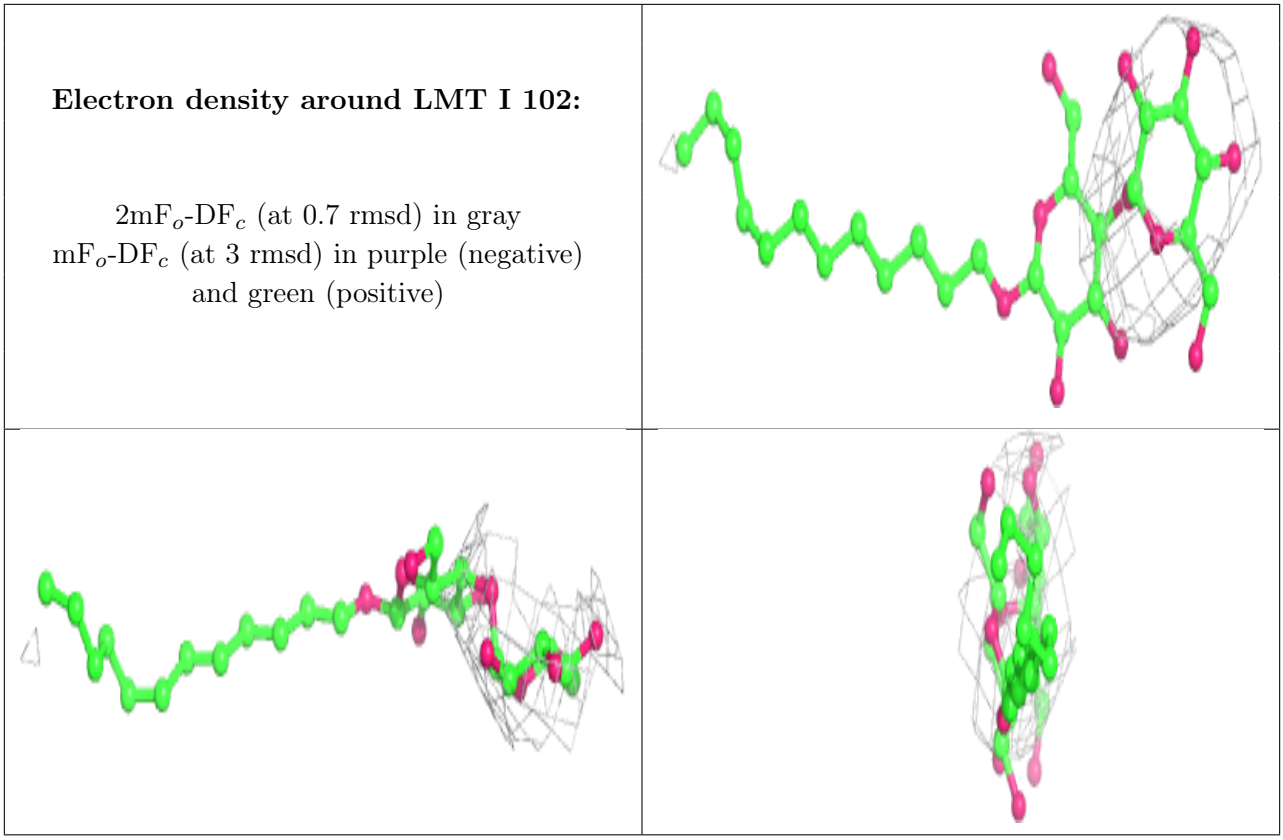
Electron density around BCR D 405:

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



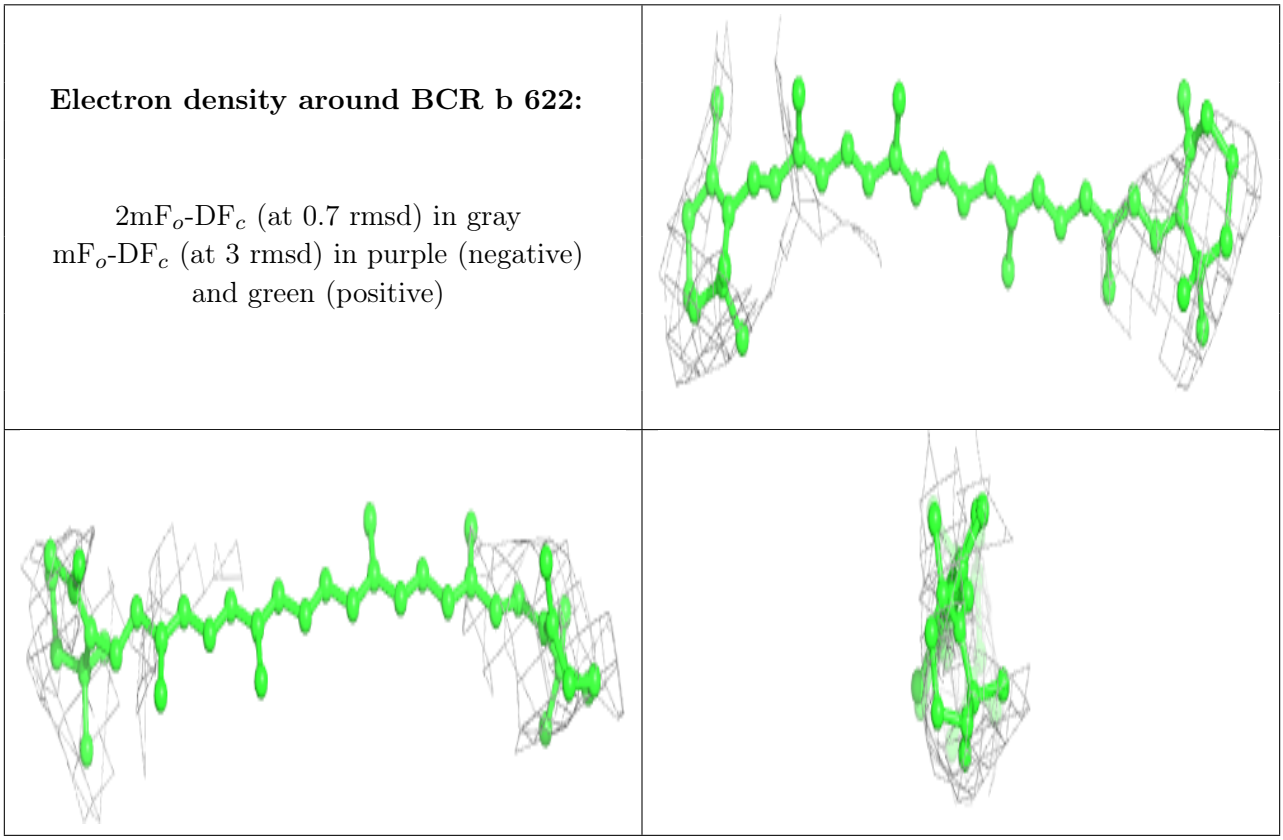
Electron density around LMT I 102:

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



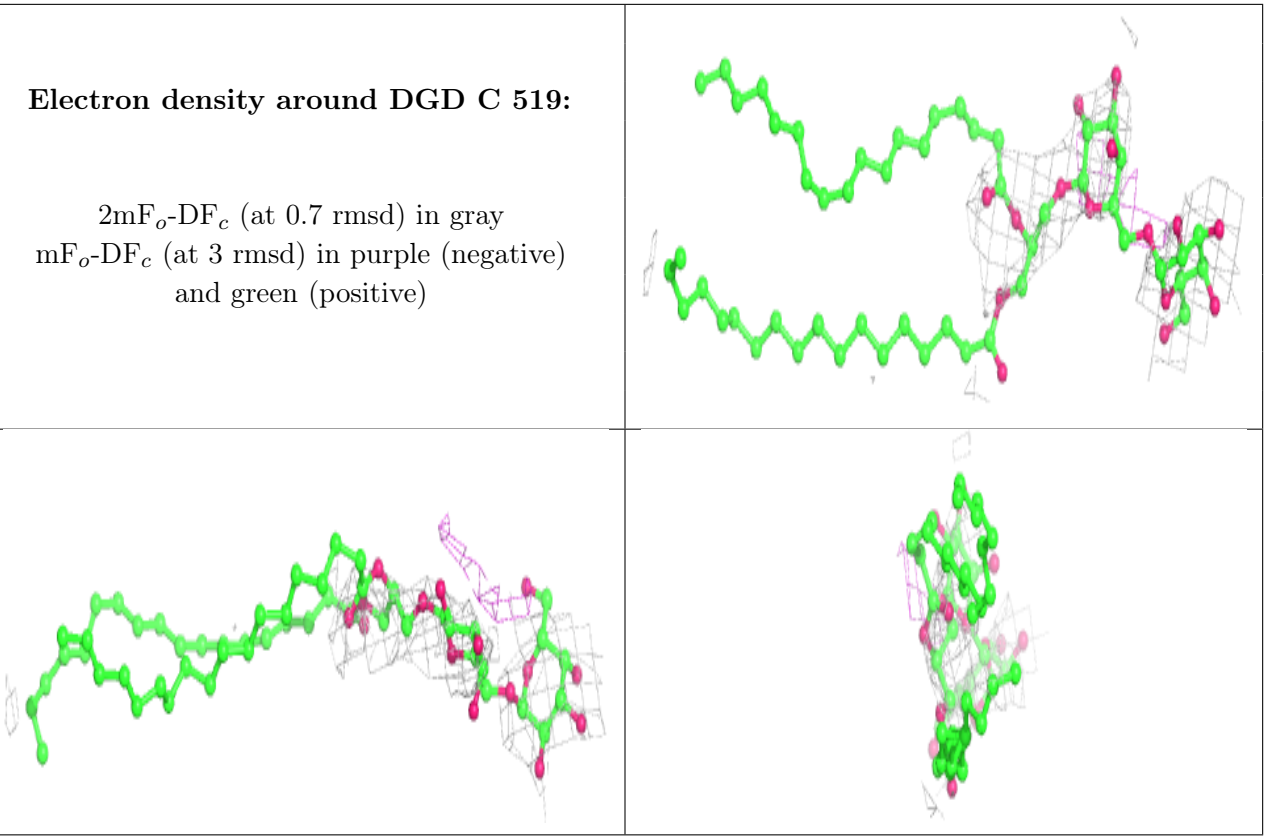
Electron density around BCR b 622:

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



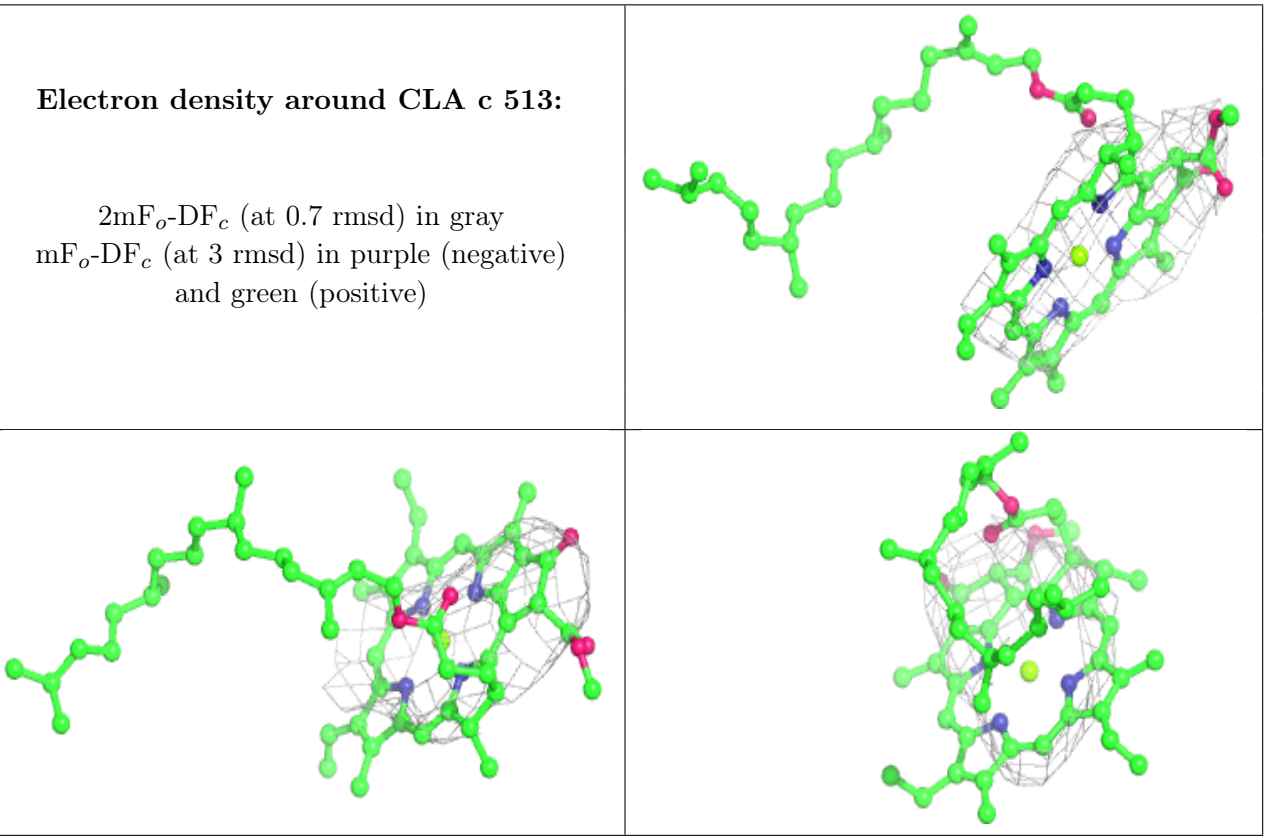
Electron density around DGD C 519:

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



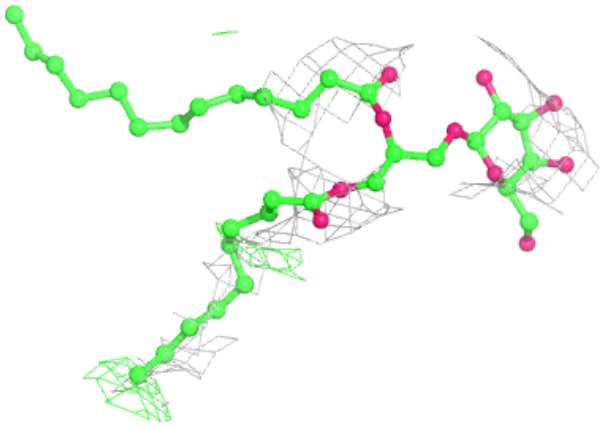
Electron density around CLA c 513:

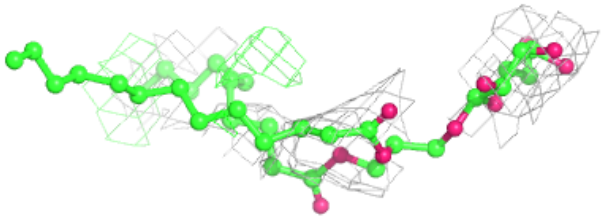
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

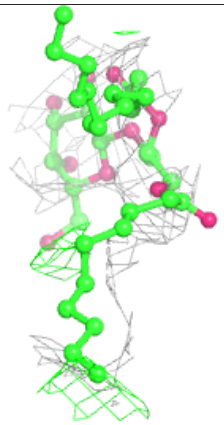


Electron density around LMG a 402:

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

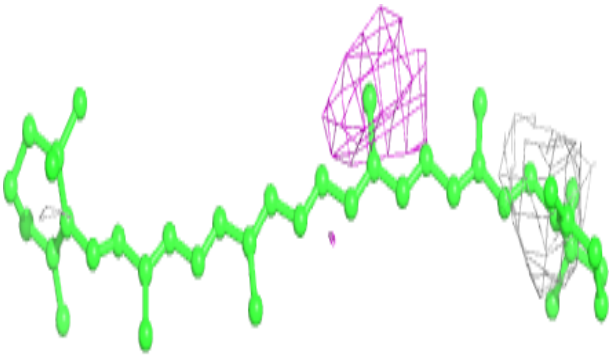


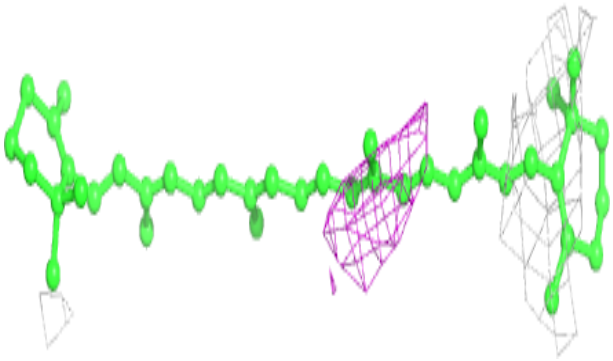




Electron density around BCR z 101:

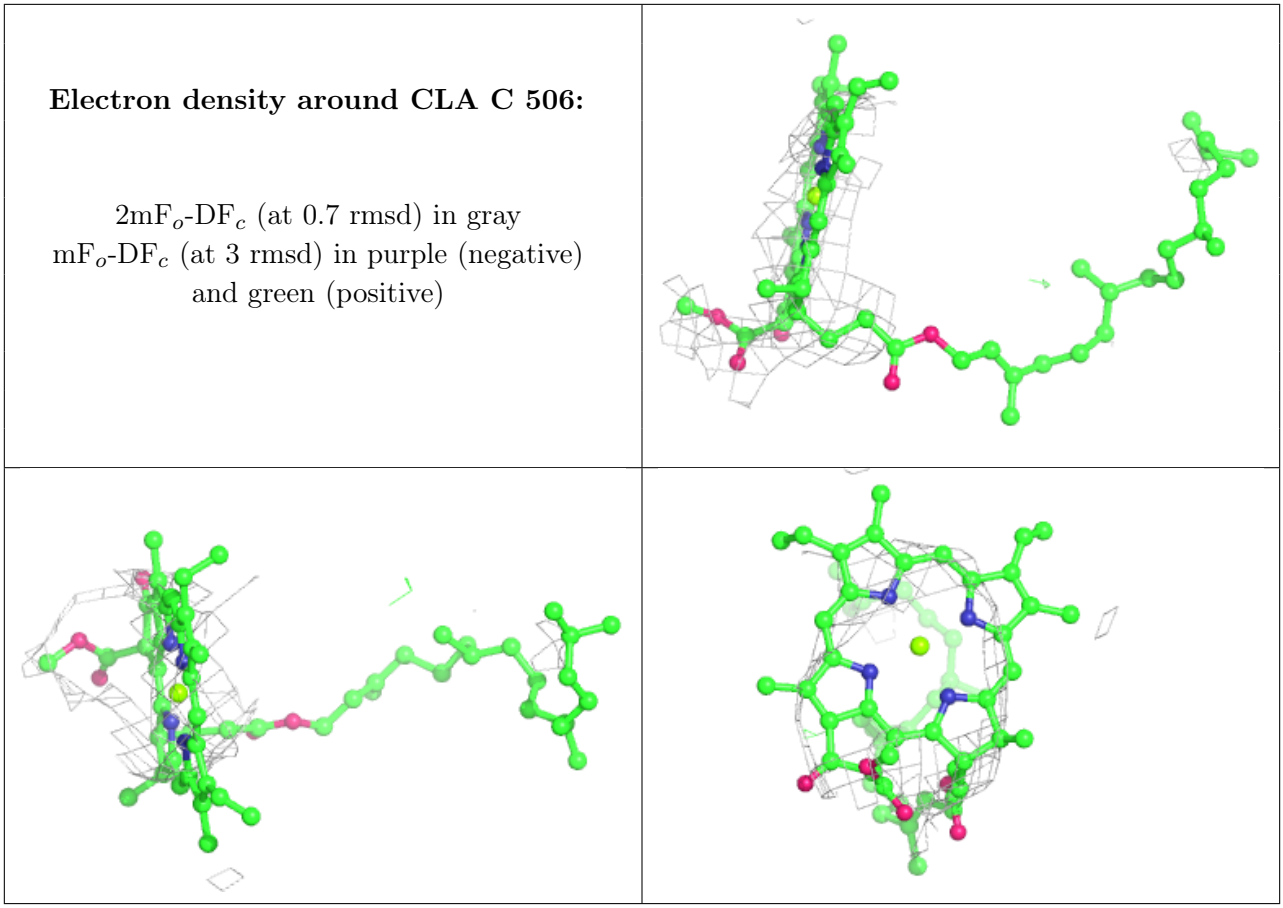
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





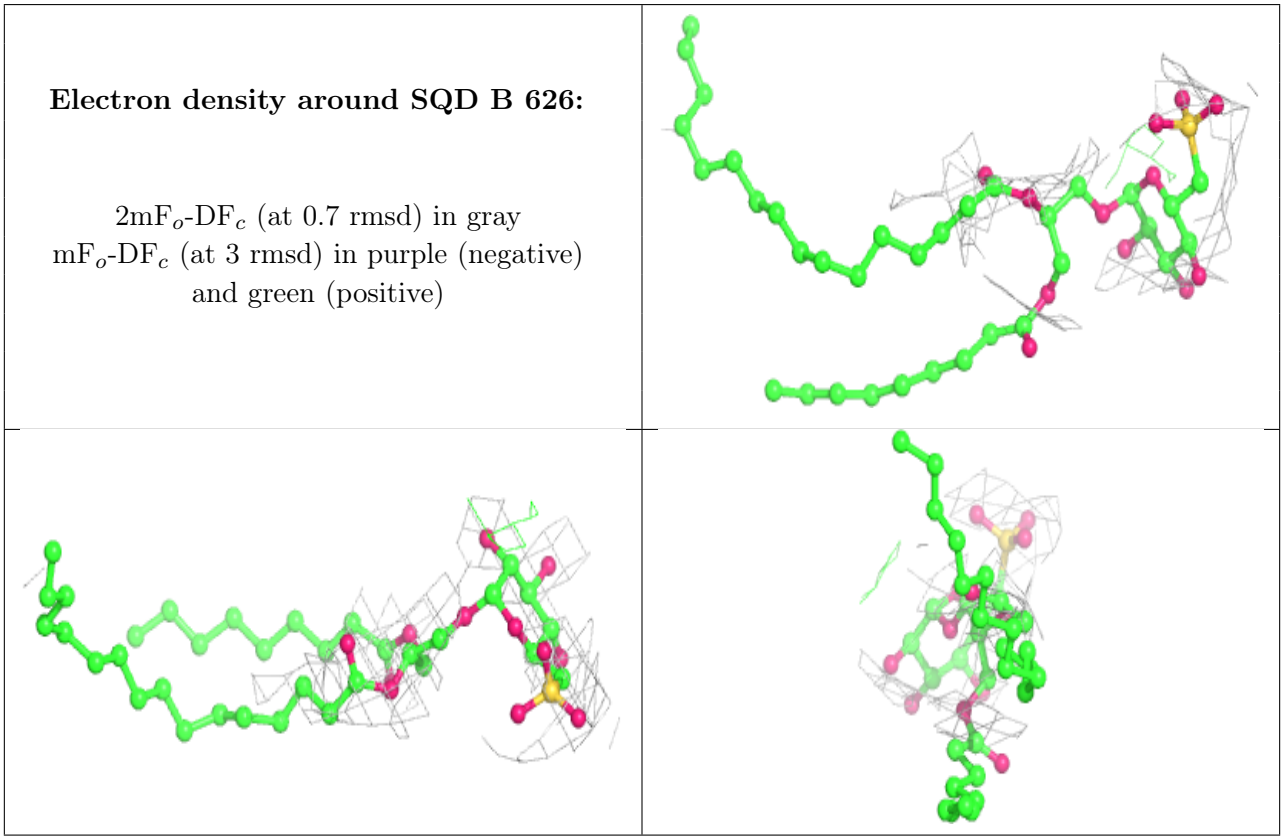
Electron density around CLA C 506:

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



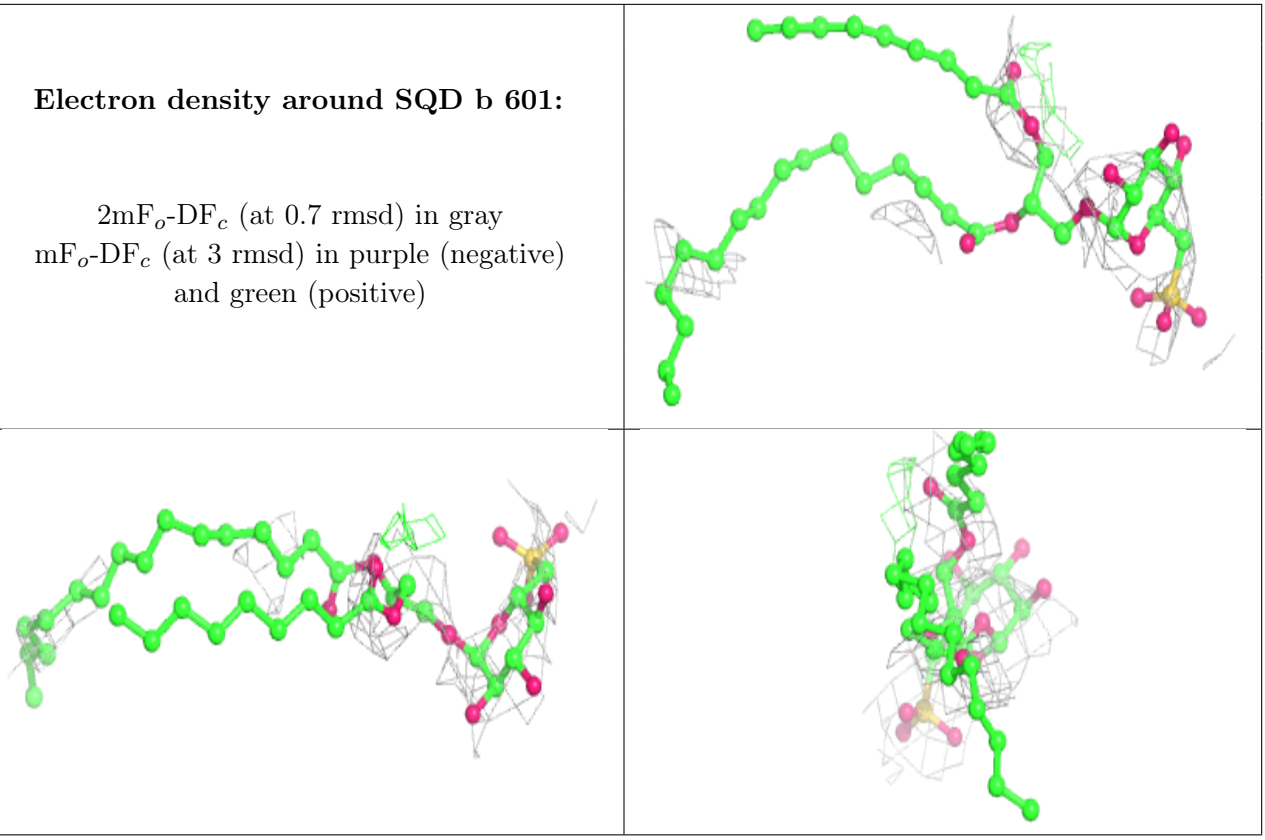
Electron density around SQD B 626:

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



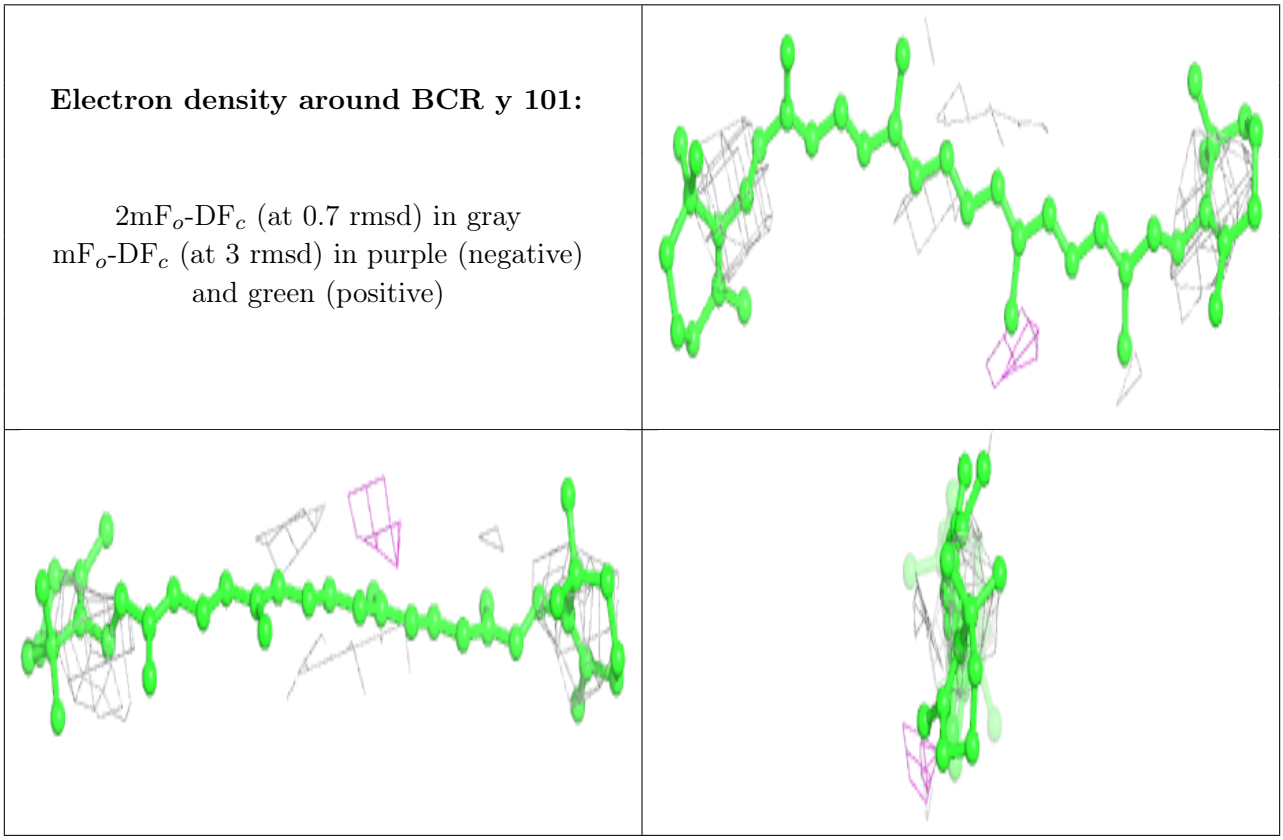
Electron density around SQD b 601:

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



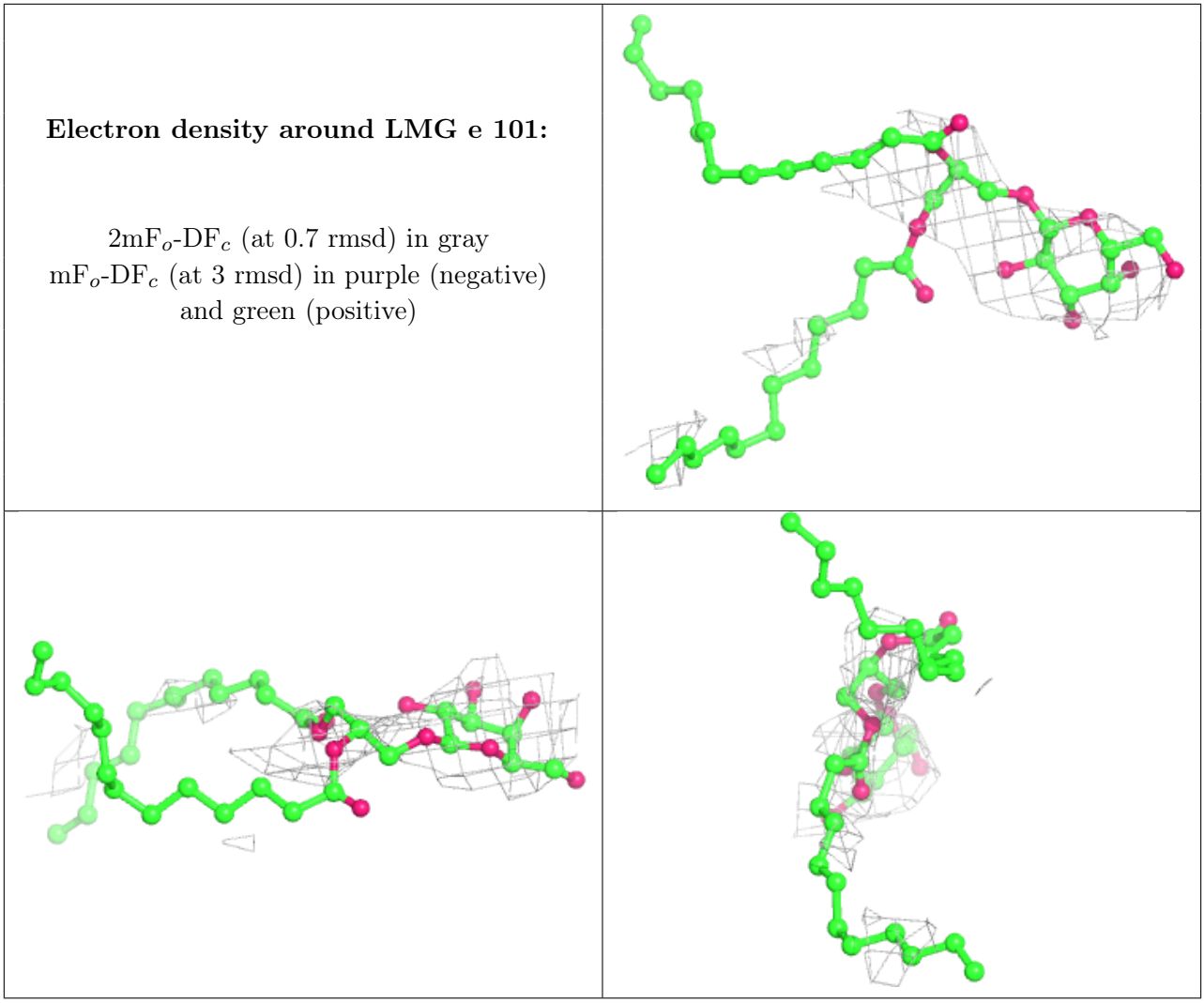
Electron density around BCR y 101:

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



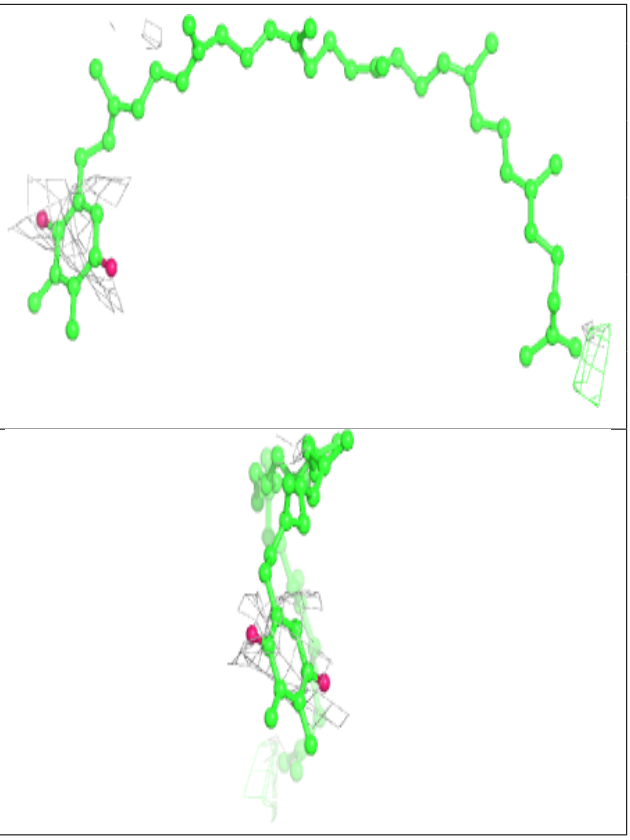
Electron density around LMG e 101:

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



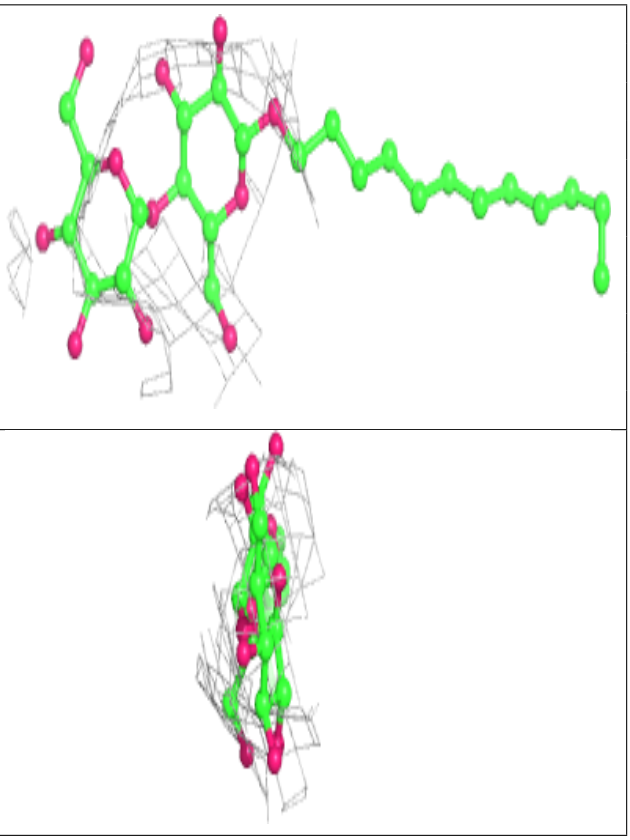
Electron density around PL9 A 408:

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



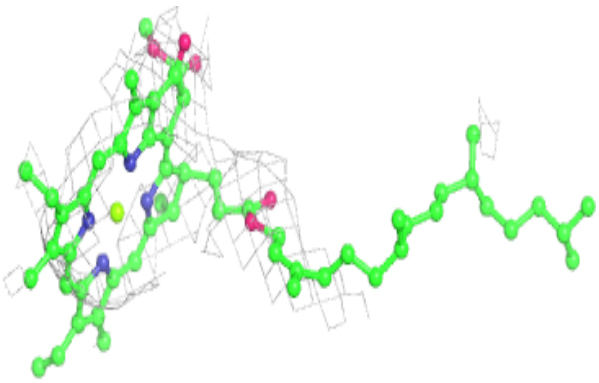
Electron density around LMT b 604:

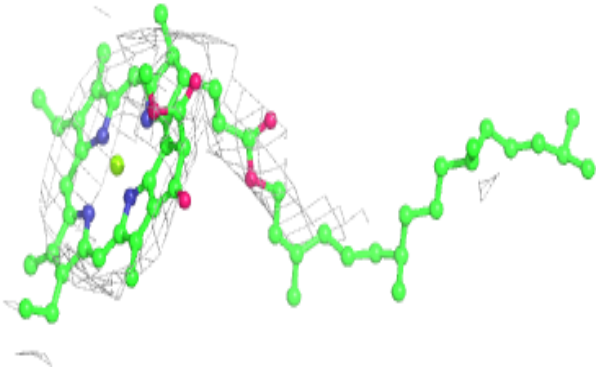
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

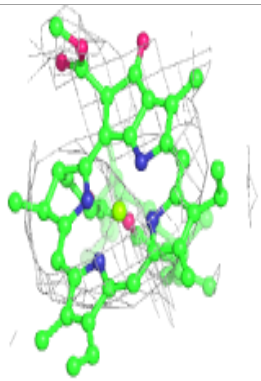


Electron density around CLA c 502:

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

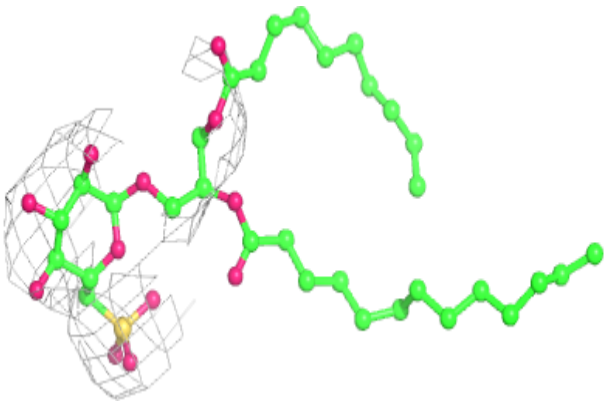


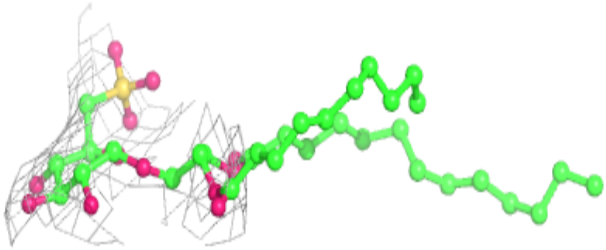


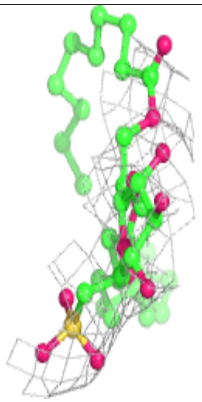


Electron density around SQD F 102:

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

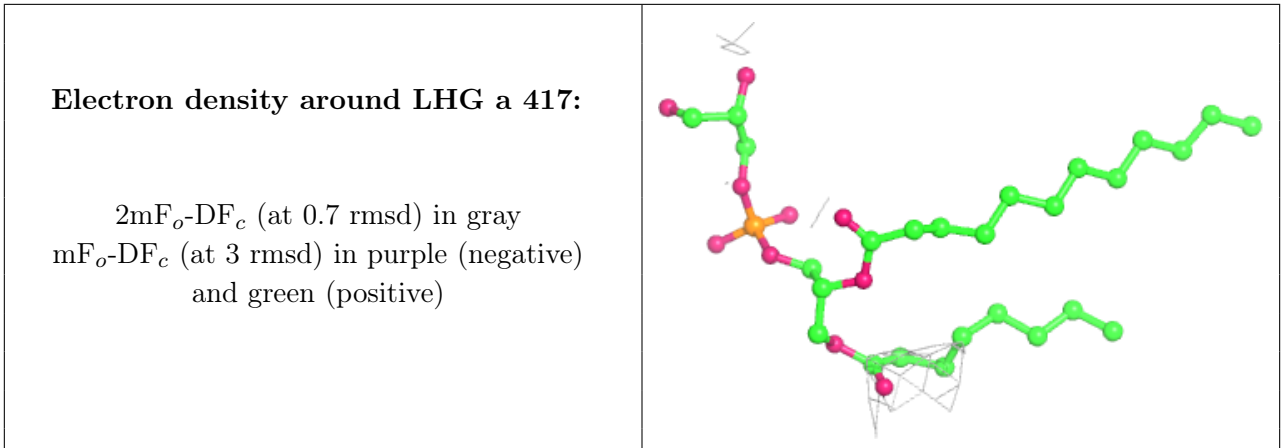






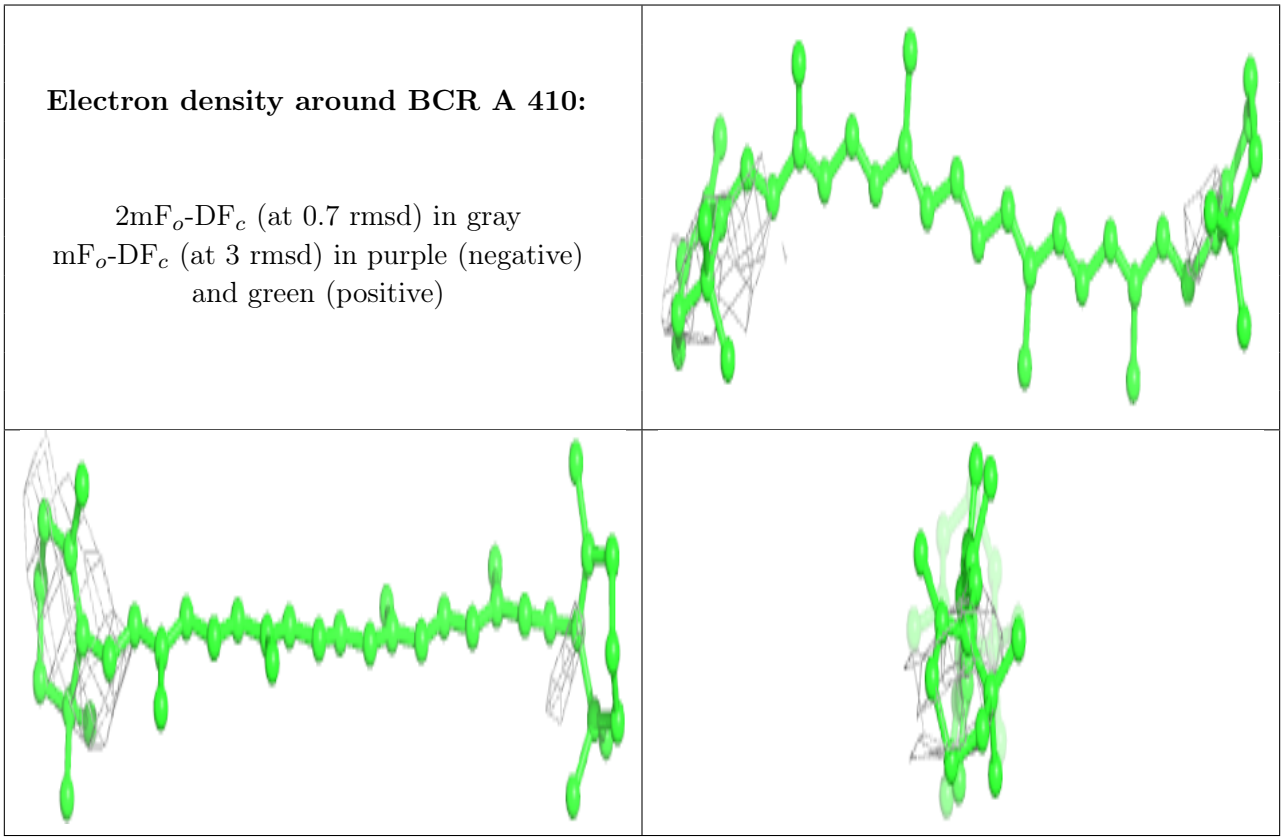
Electron density around LHG a 417:

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



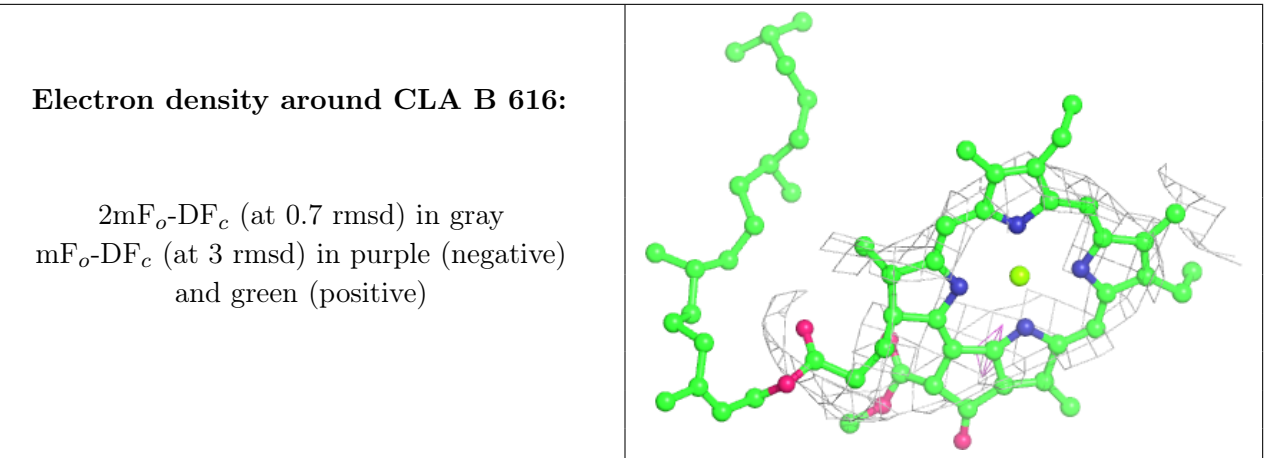
Electron density around BCR A 410:

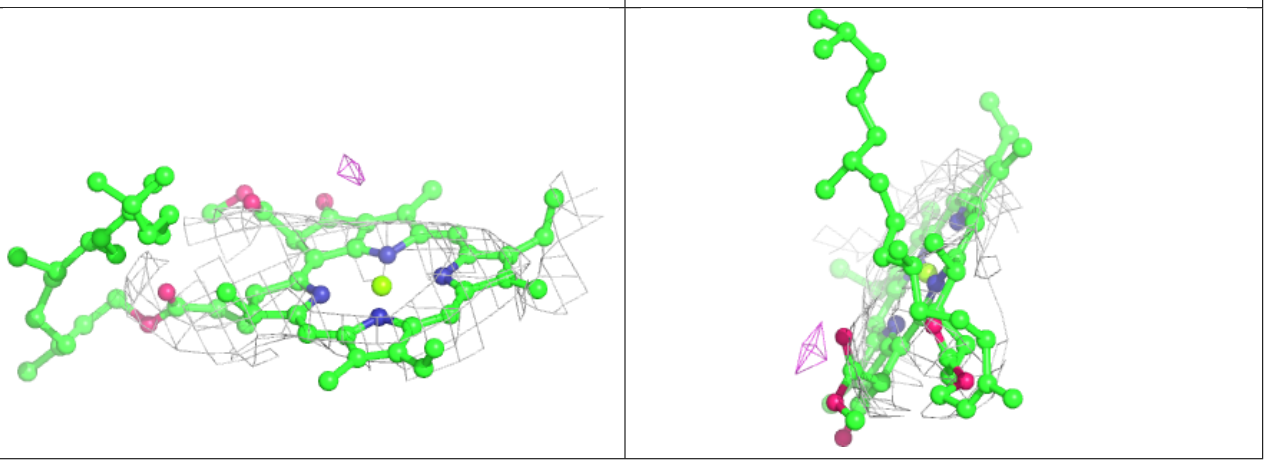
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 616:

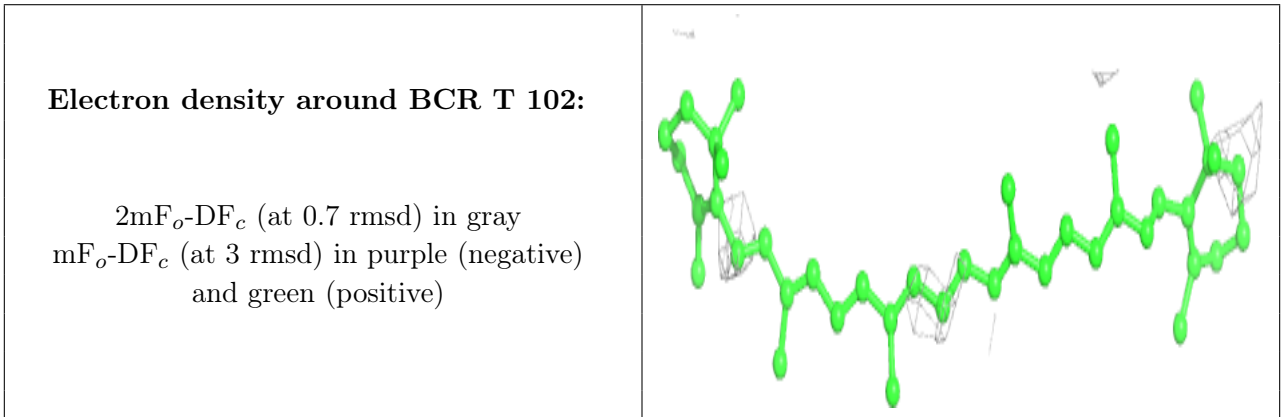
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

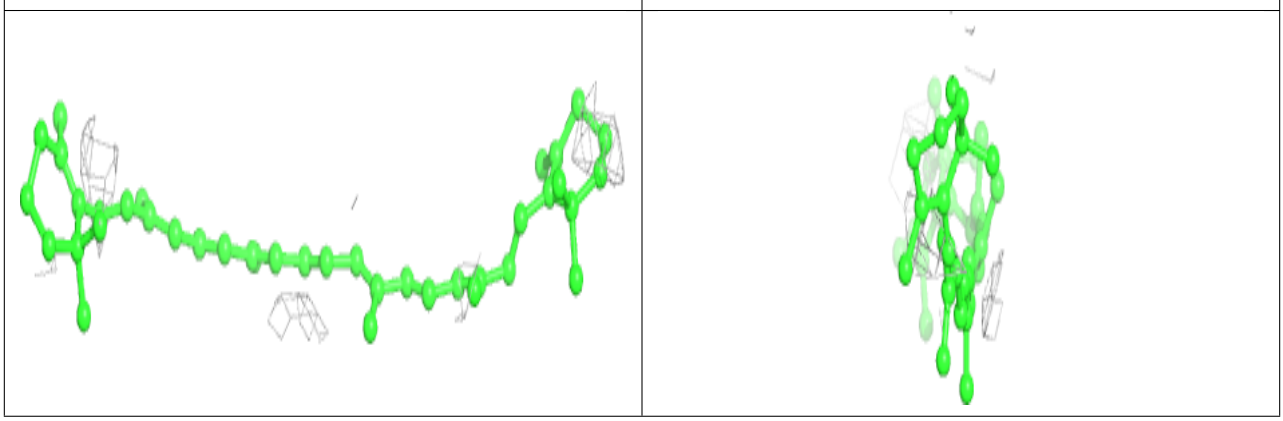




Electron density around BCR T 102:

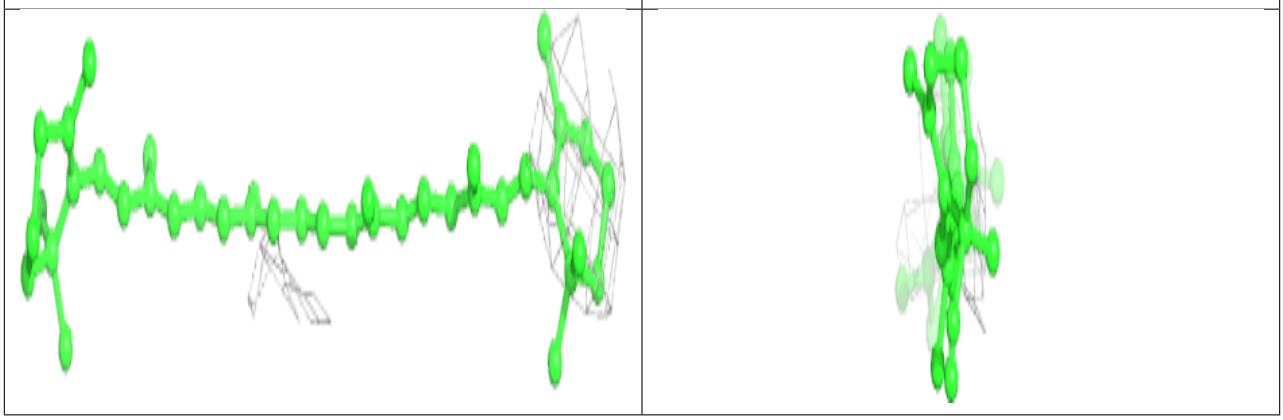
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





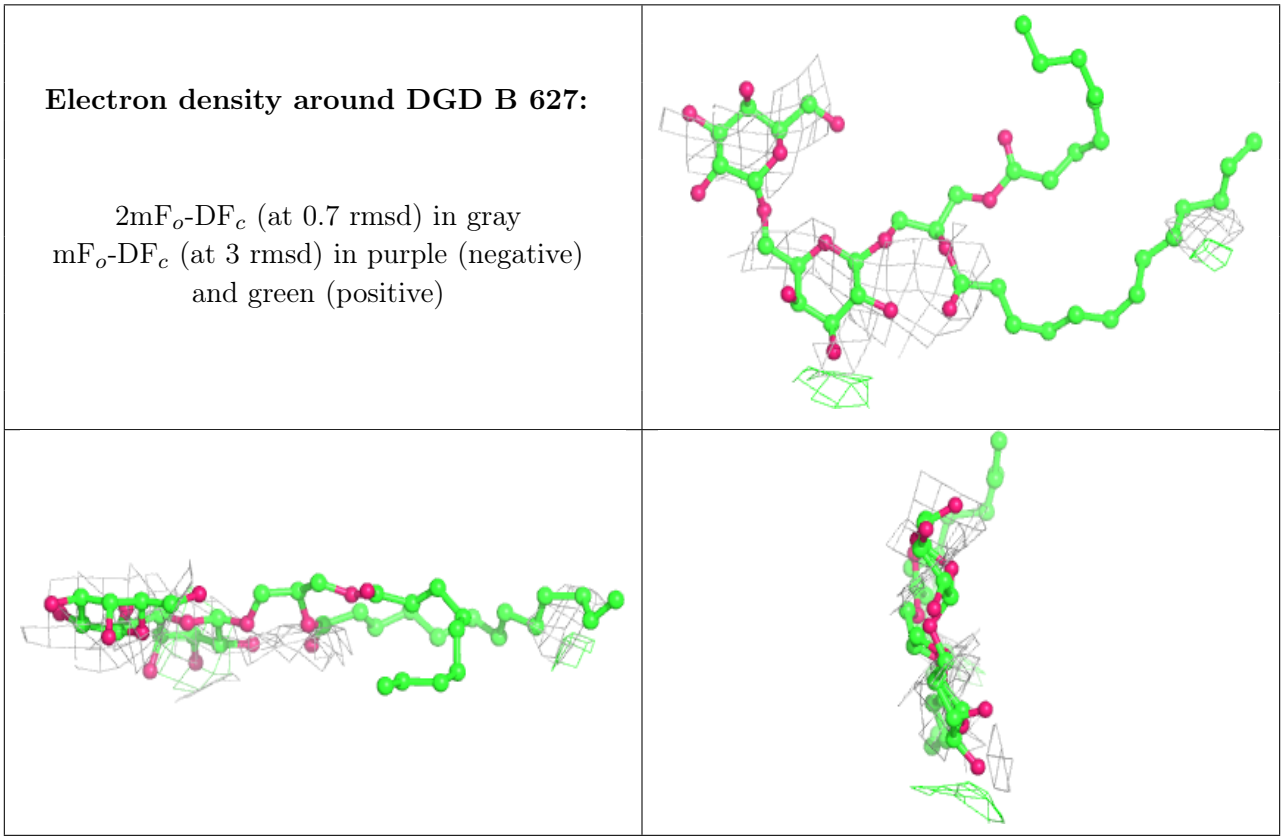
Electron density around BCR B 619:

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



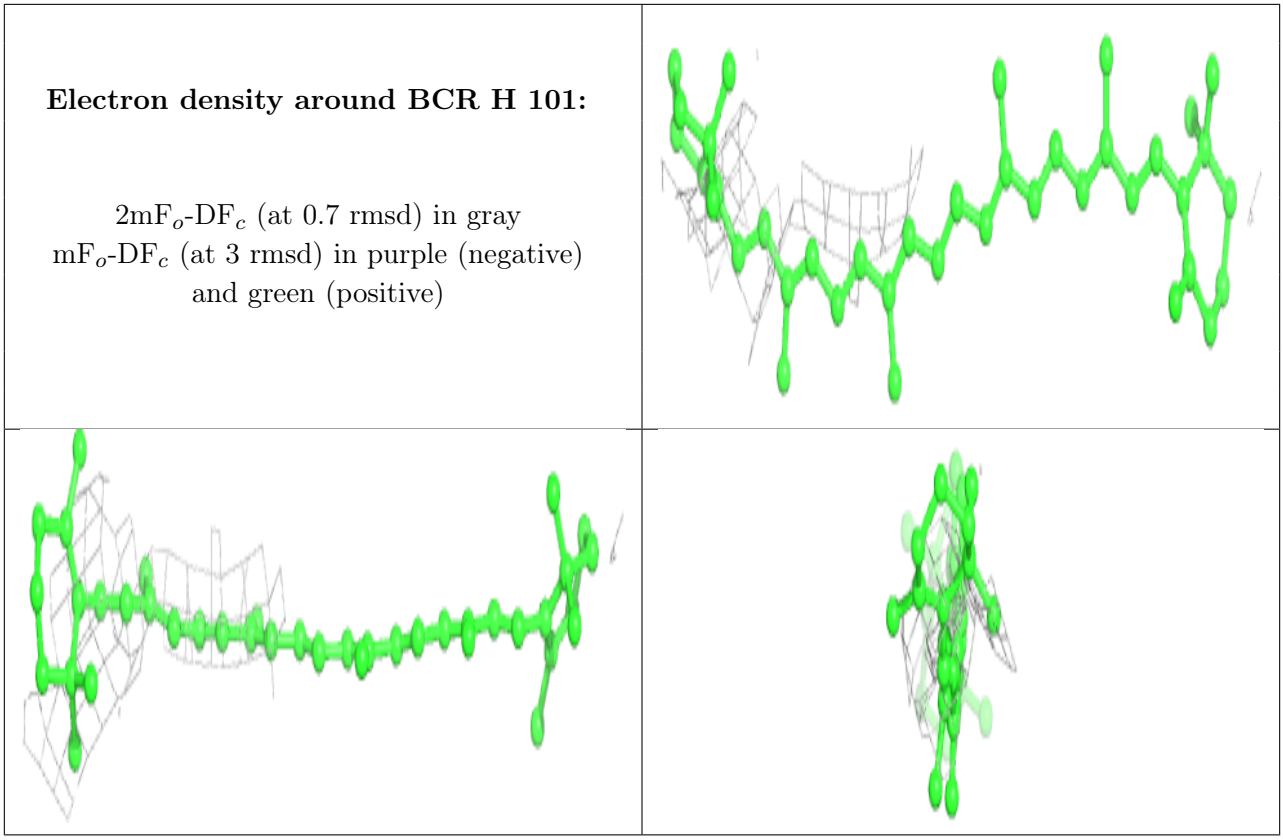
Electron density around DGD B 627:

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



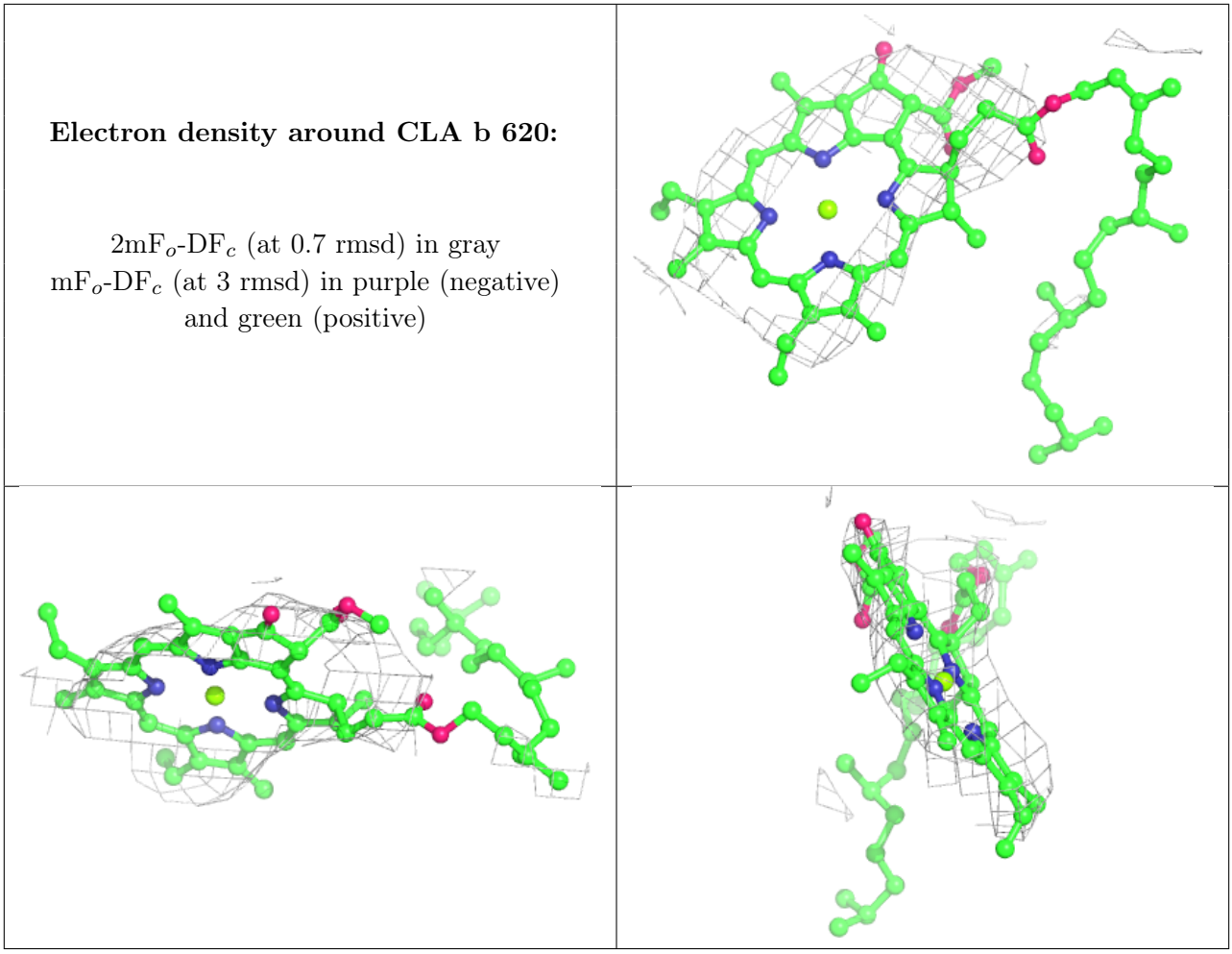
Electron density around BCR H 101:

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



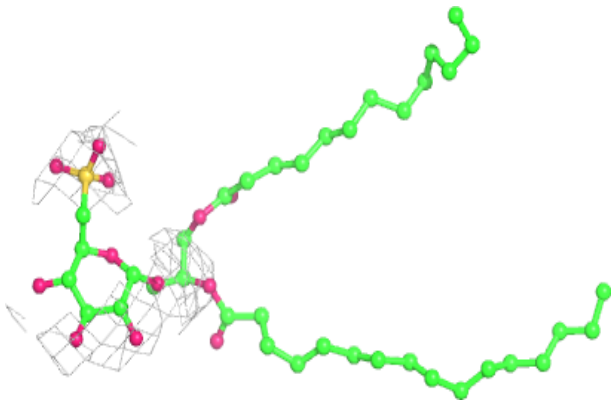
Electron density around CLA b 620:

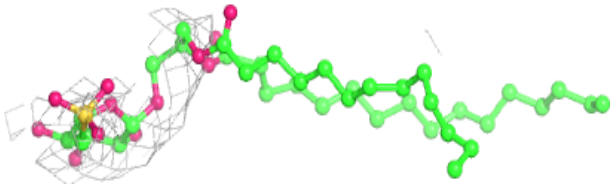
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

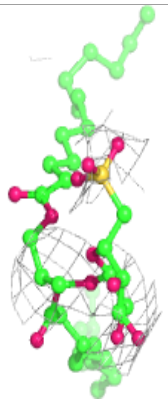


Electron density around SQD a 415:

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

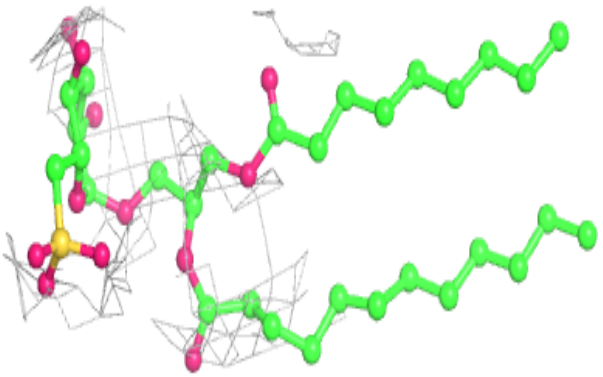


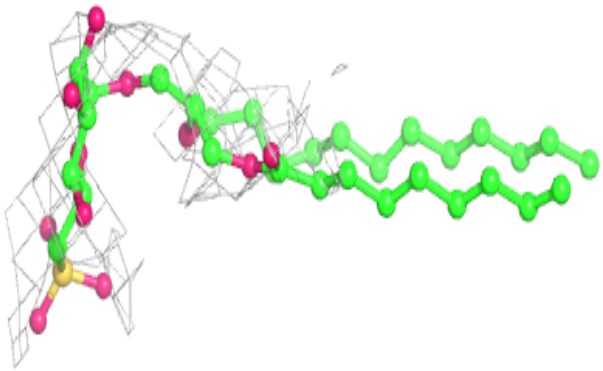


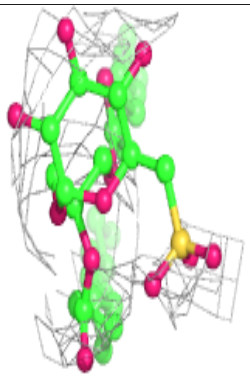


Electron density around SQD D 408:

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

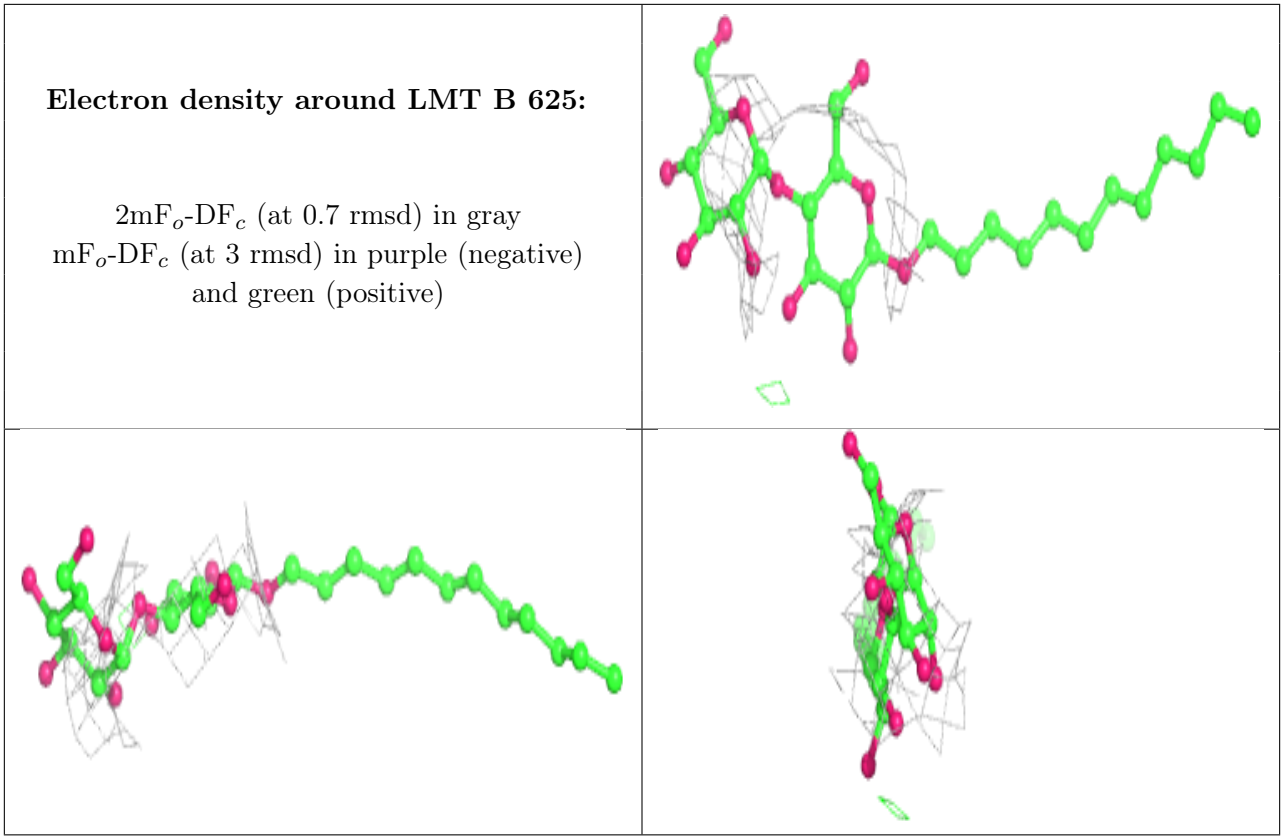






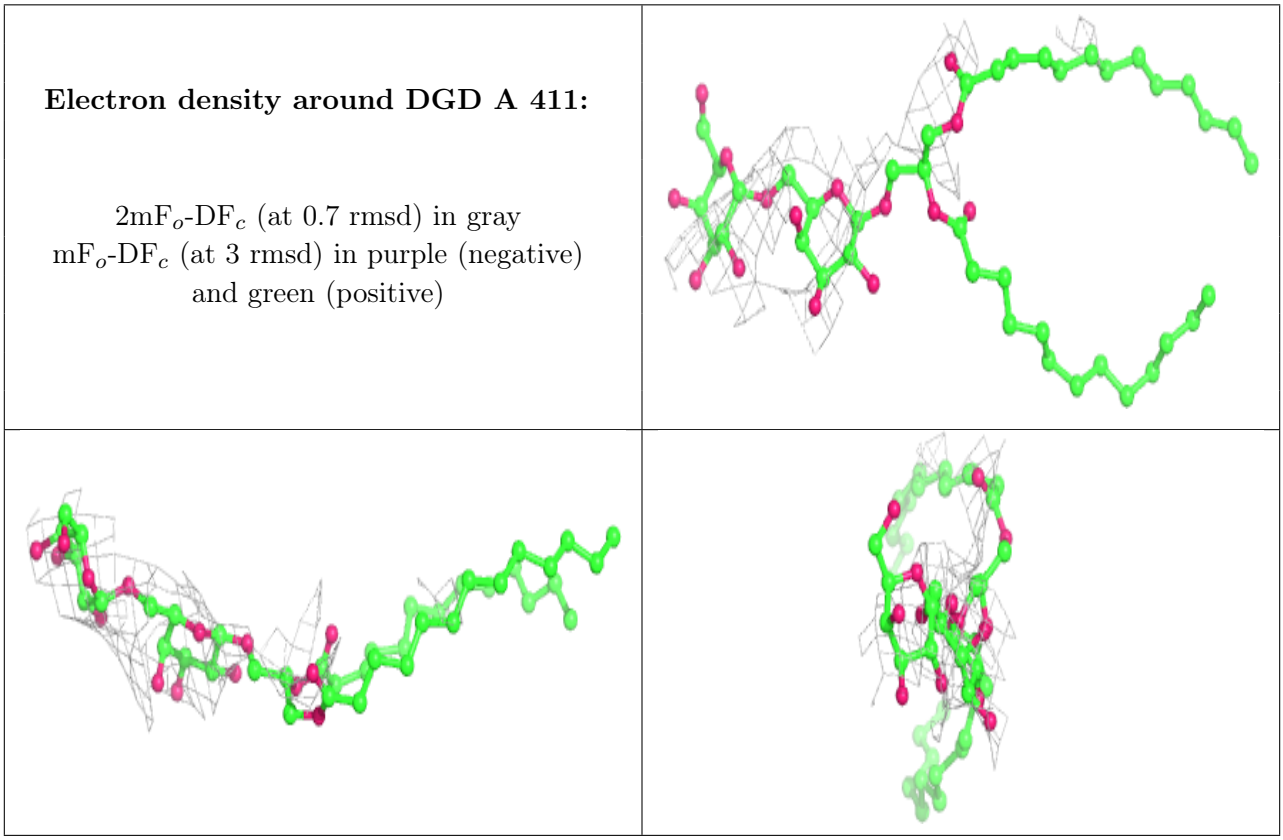
Electron density around LMT B 625:

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



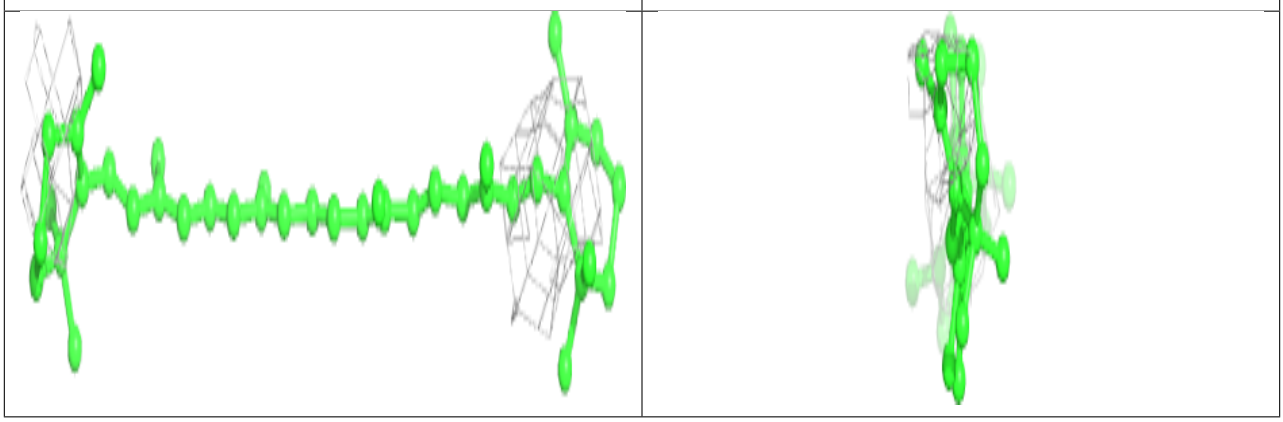
Electron density around DGD A 411:

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



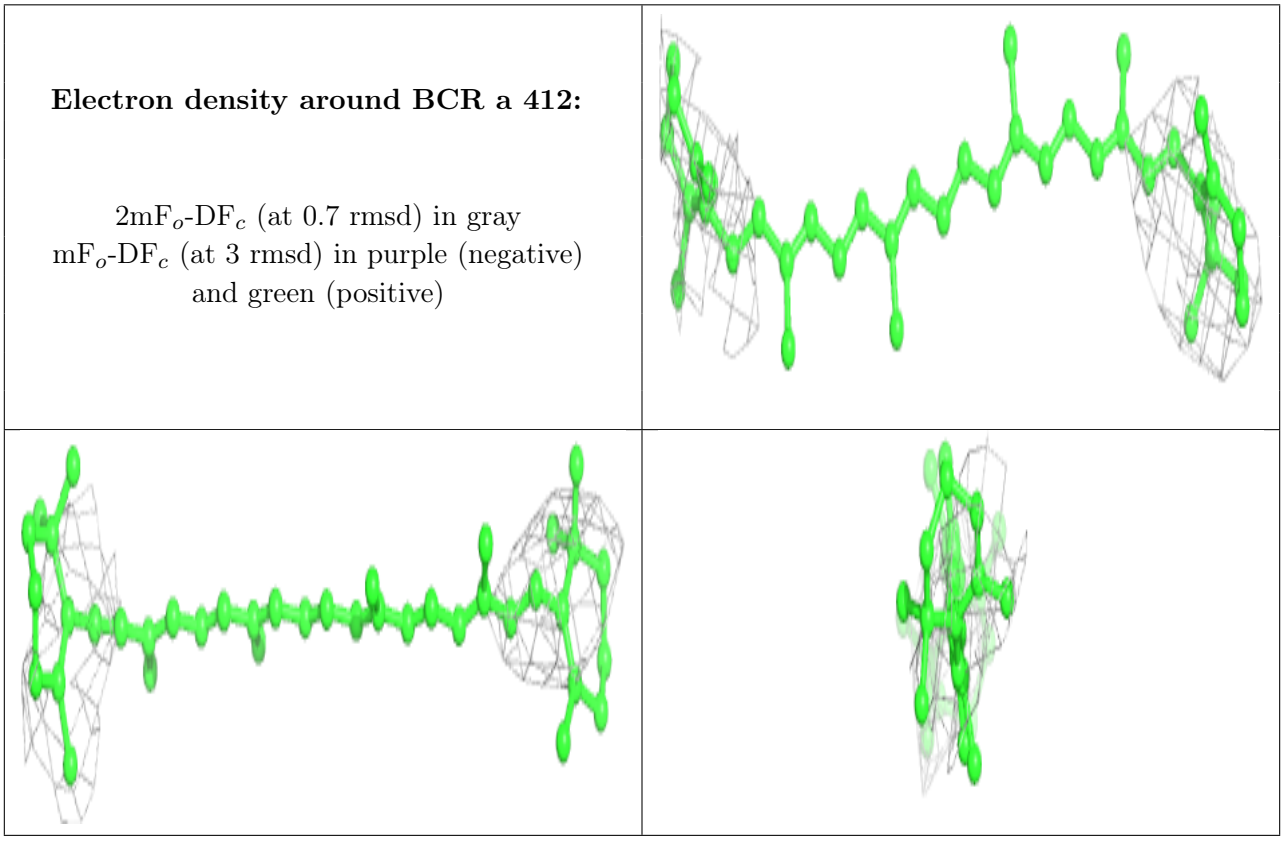
Electron density around BCR b 621:

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



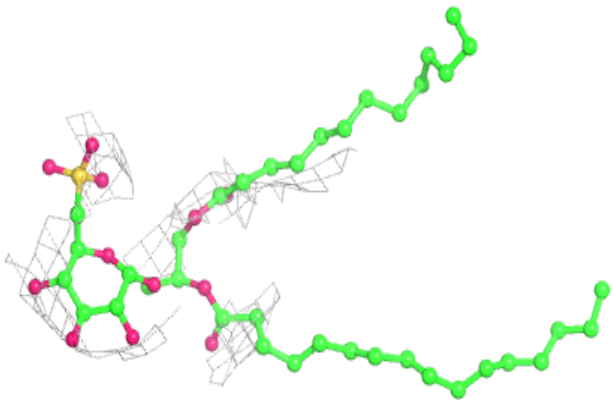
Electron density around BCR a 412:

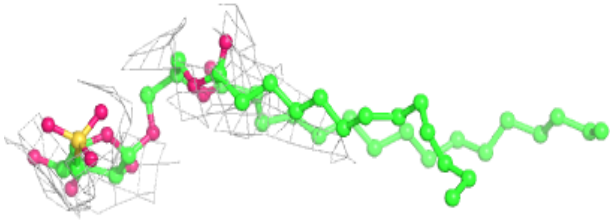
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

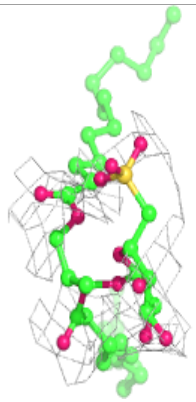


Electron density around SQD A 413:

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

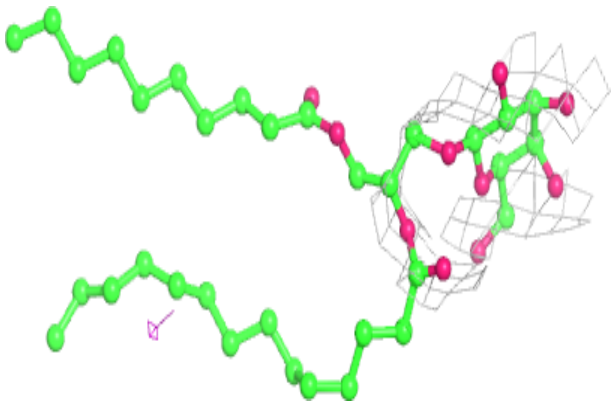


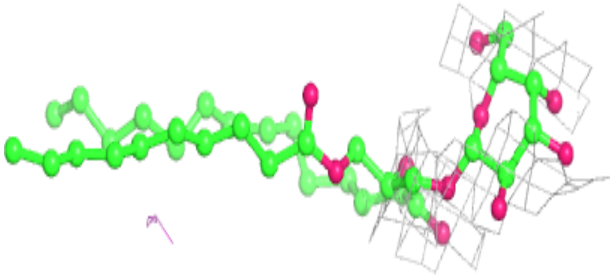


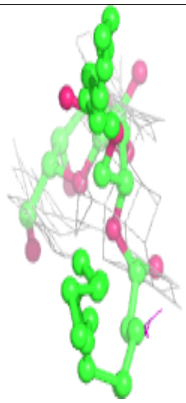


Electron density around LMG i 101:

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

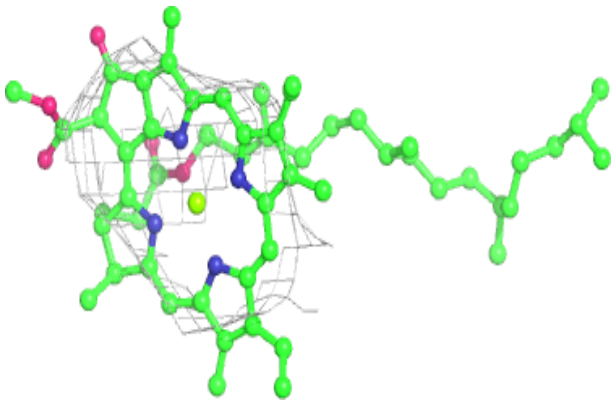


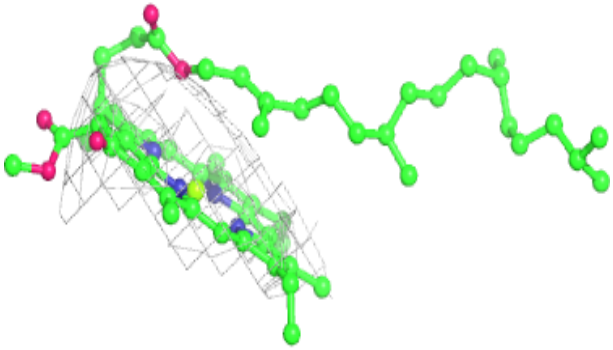


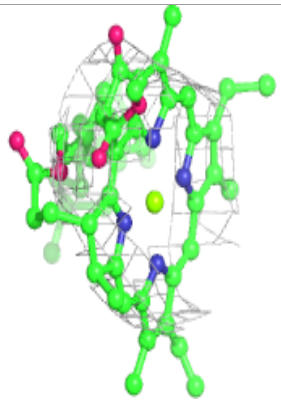


Electron density around CLA B 614:

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

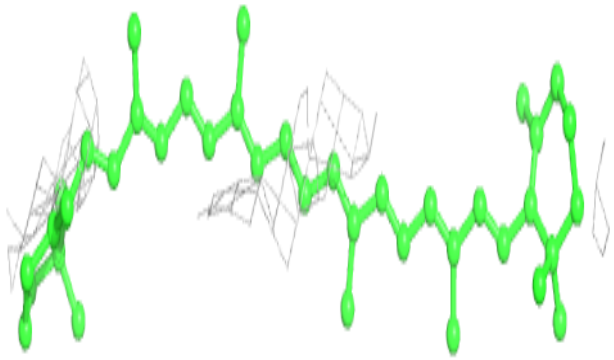


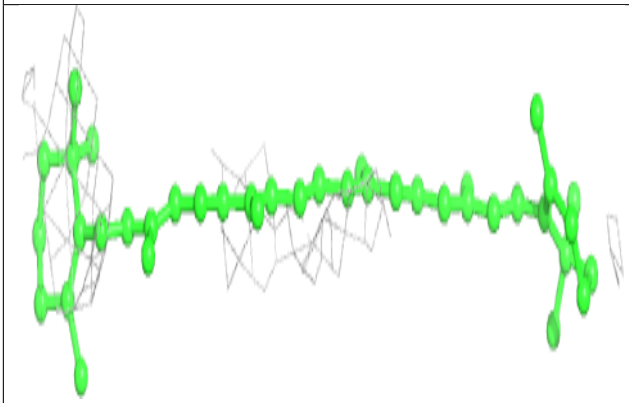


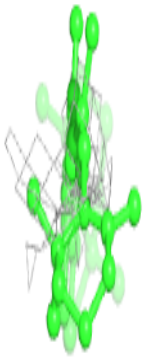


Electron density around BCR h 101:

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

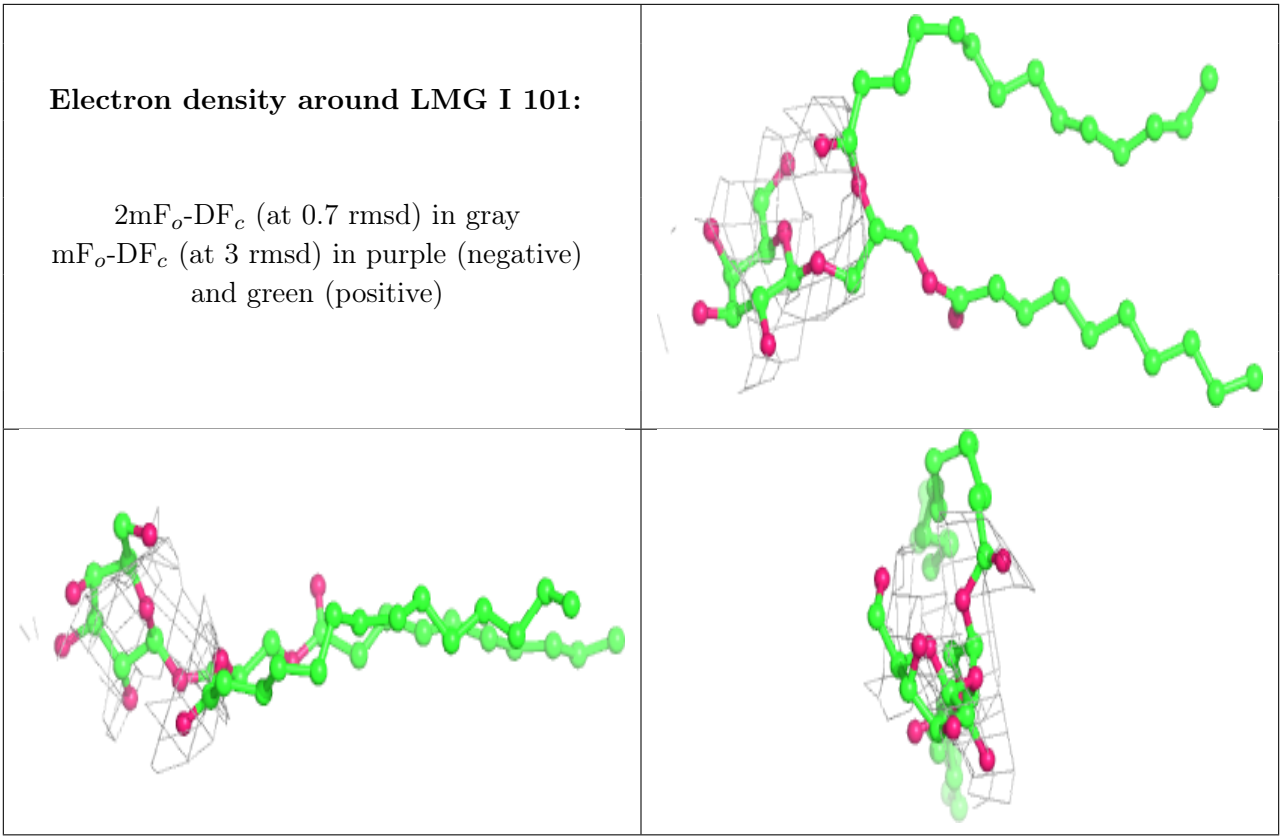






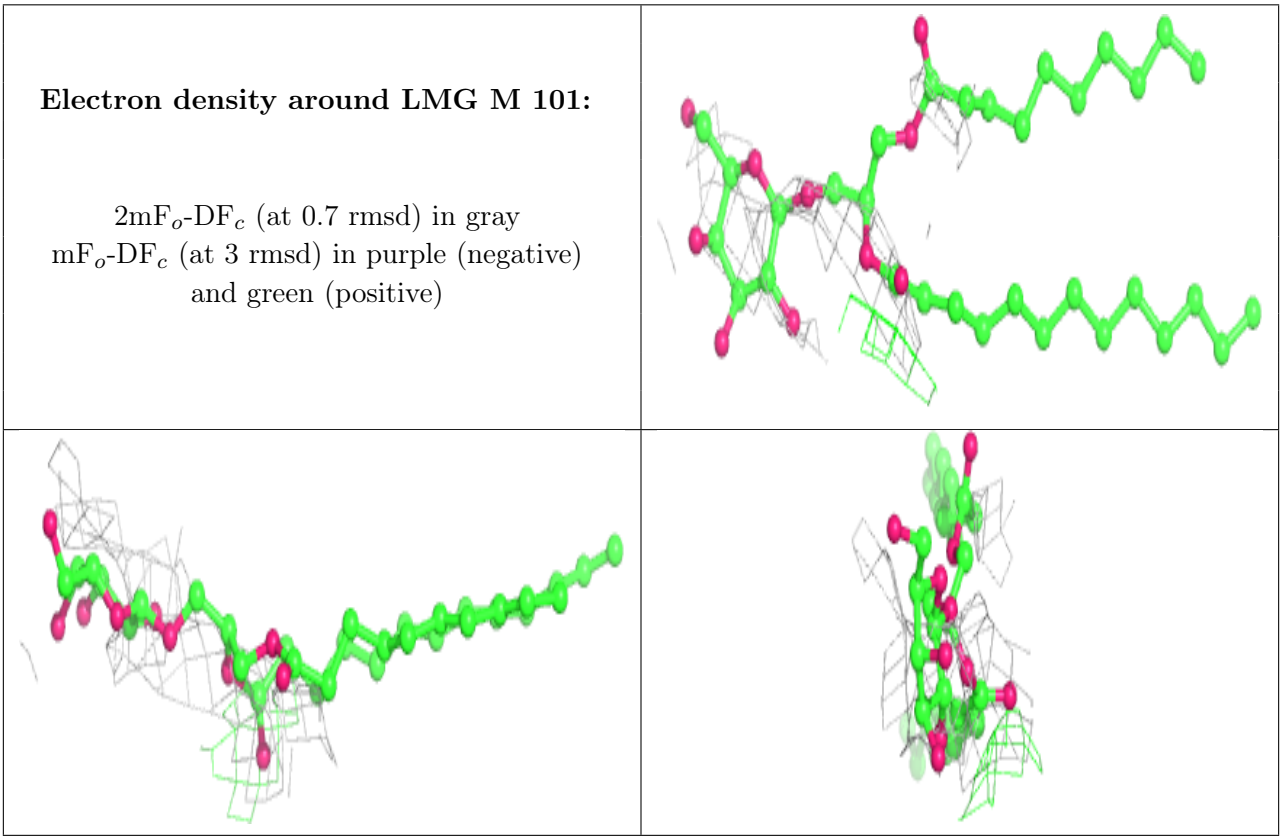
Electron density around LMG I 101:

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



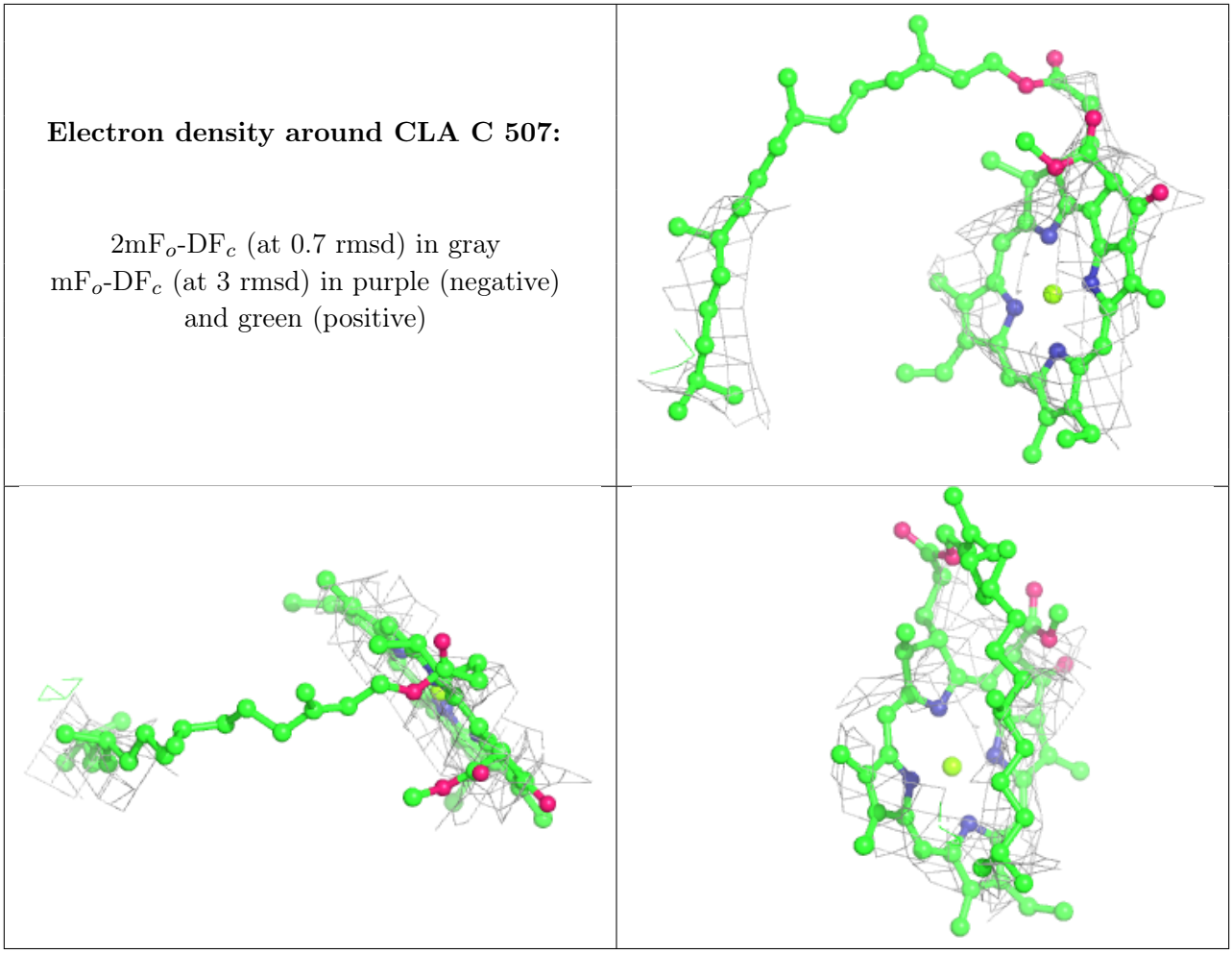
Electron density around LMG M 101:

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



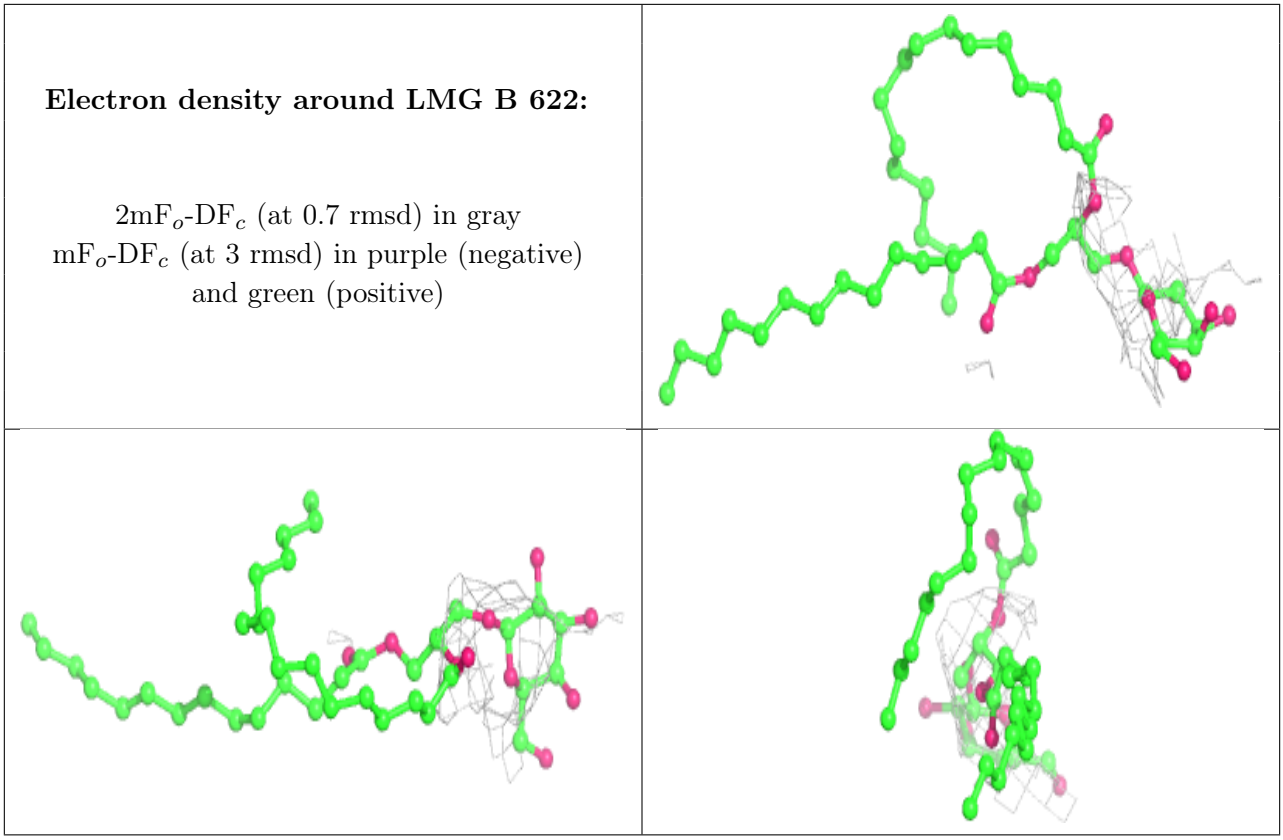
Electron density around CLA C 507:

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



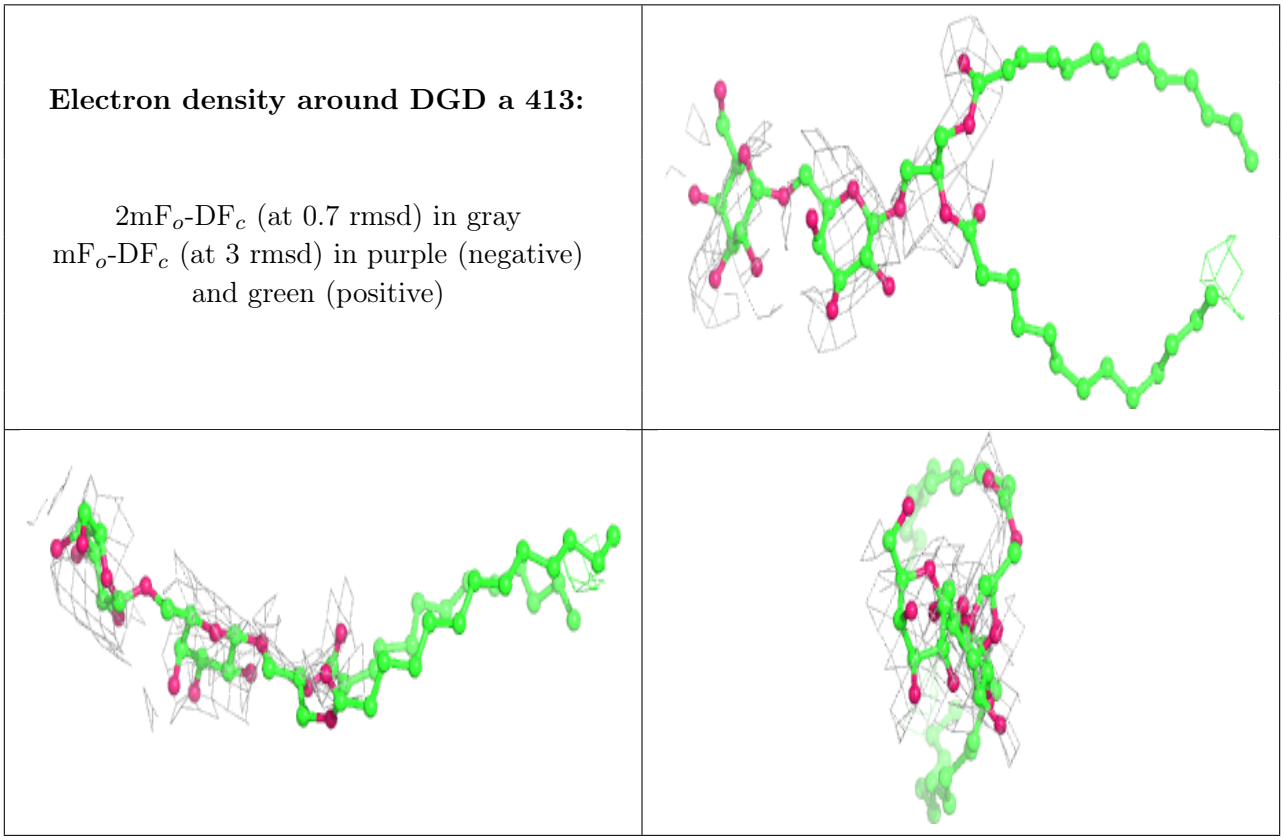
Electron density around LMG B 622:

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



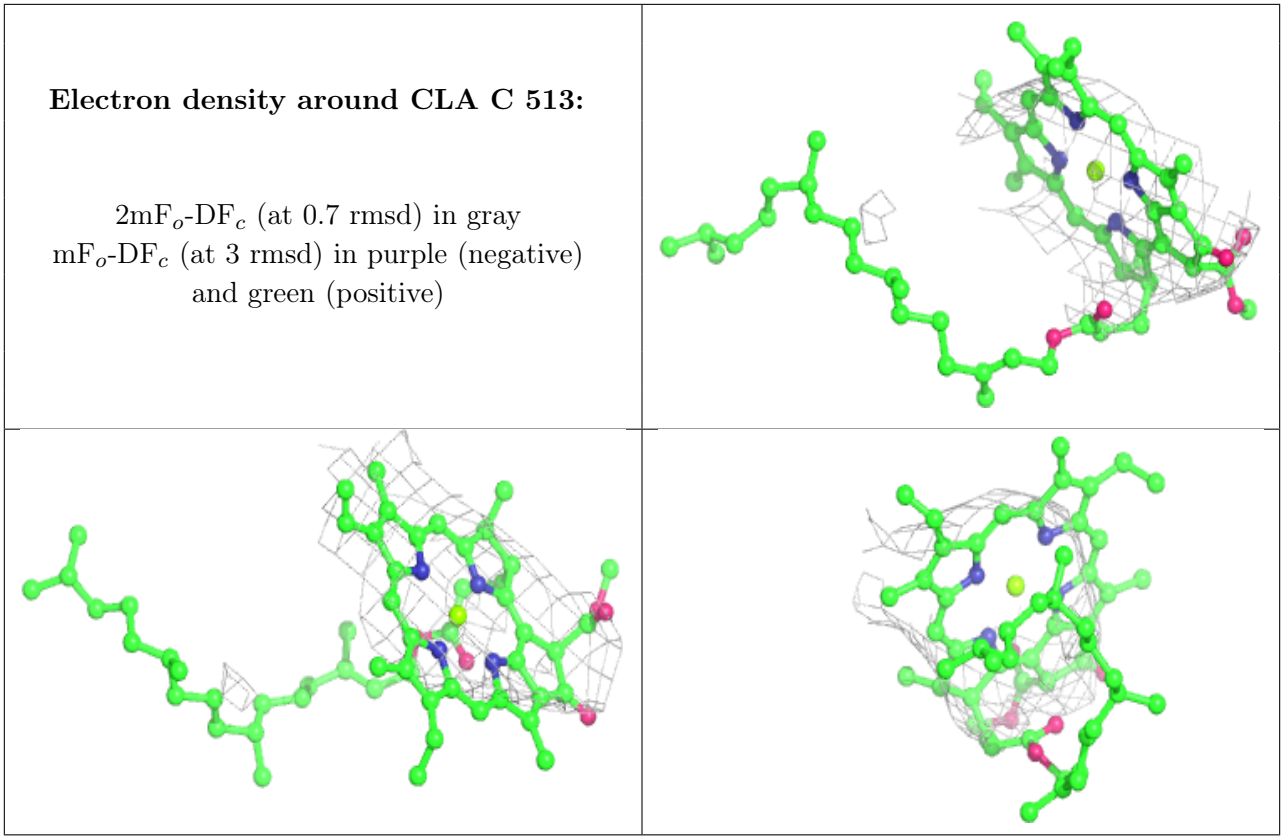
Electron density around DGD a 413:

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



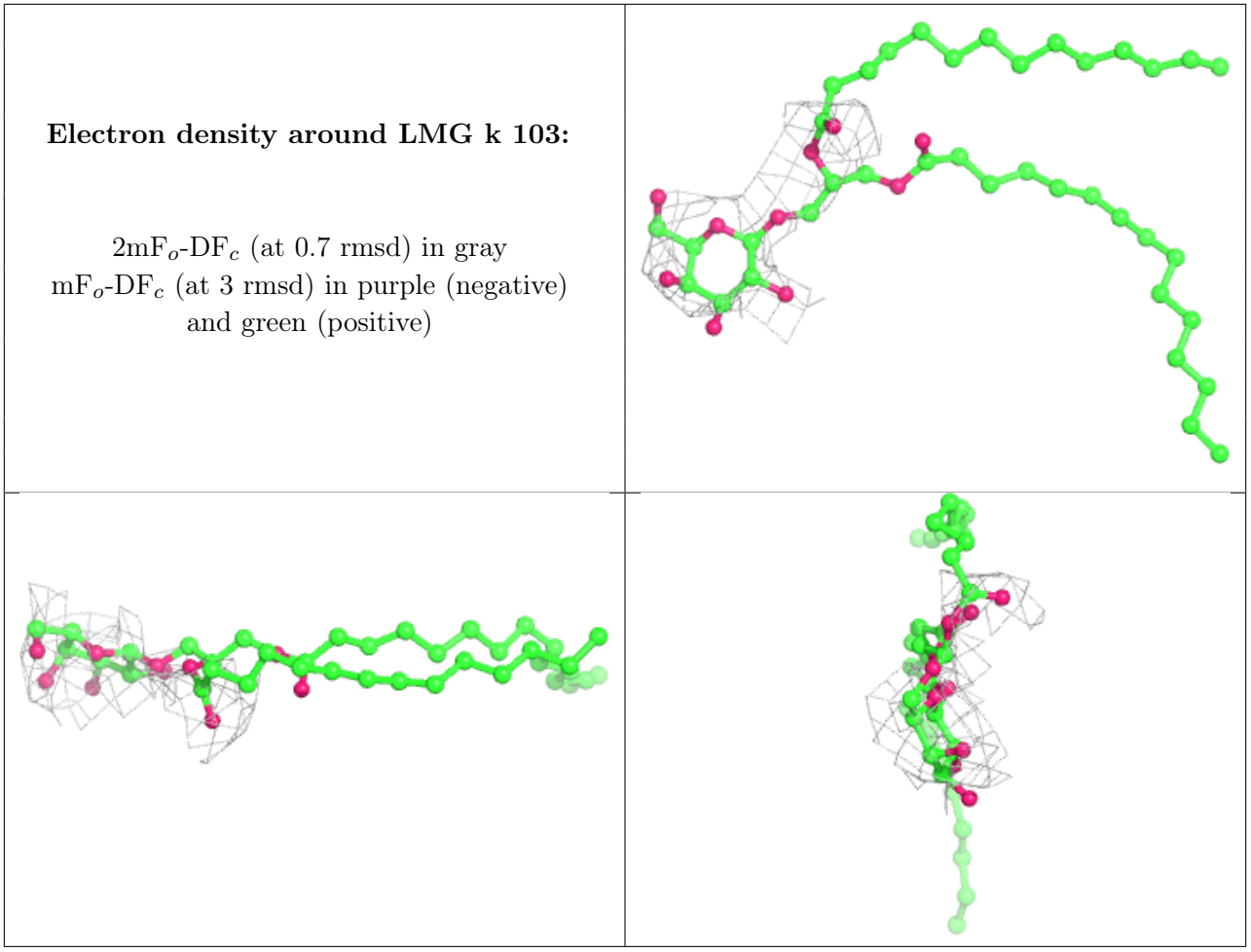
Electron density around CLA C 513:

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



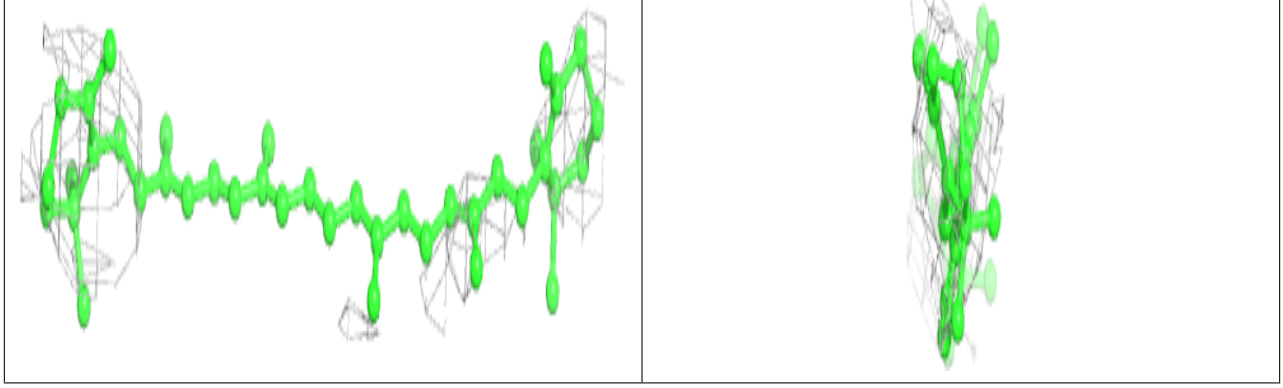
Electron density around LMG k 103:

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



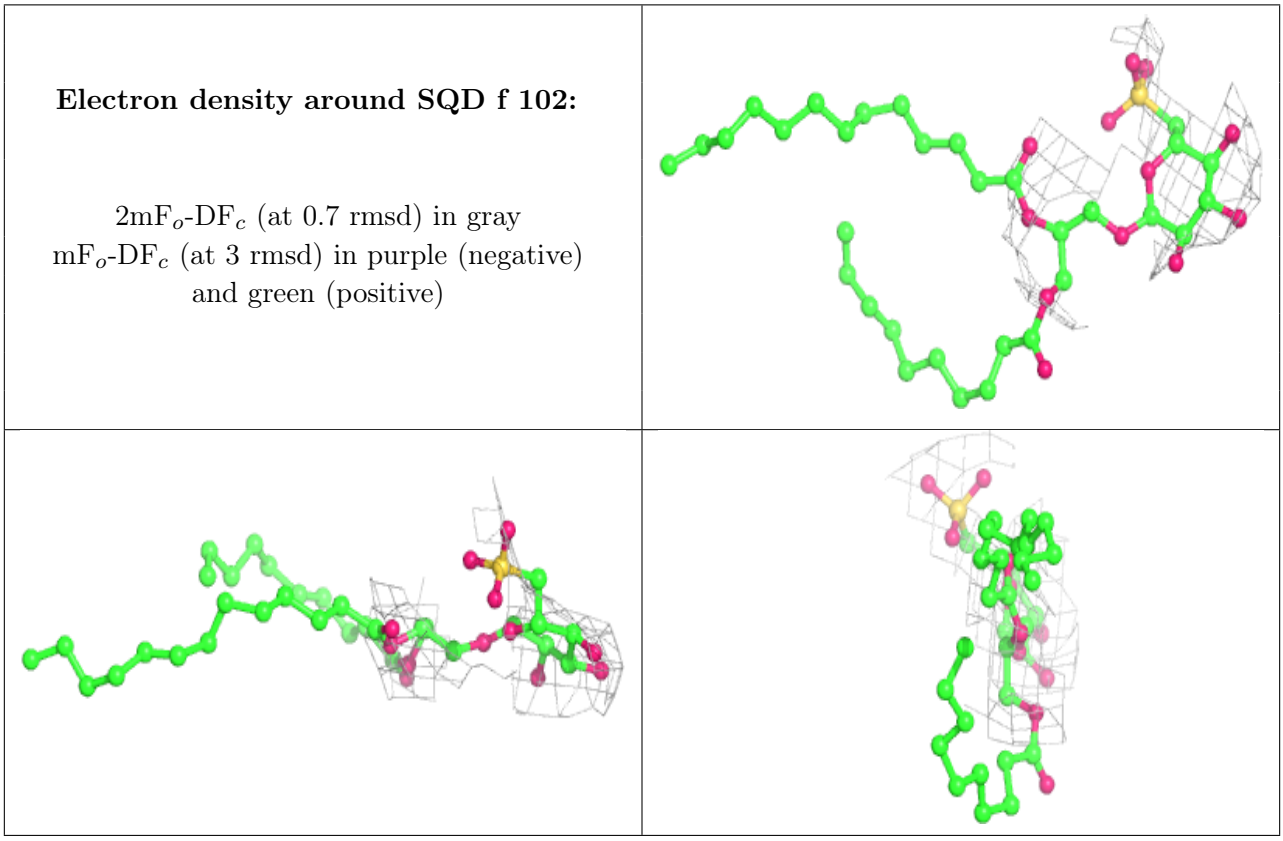
Electron density around BCR C 516:

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



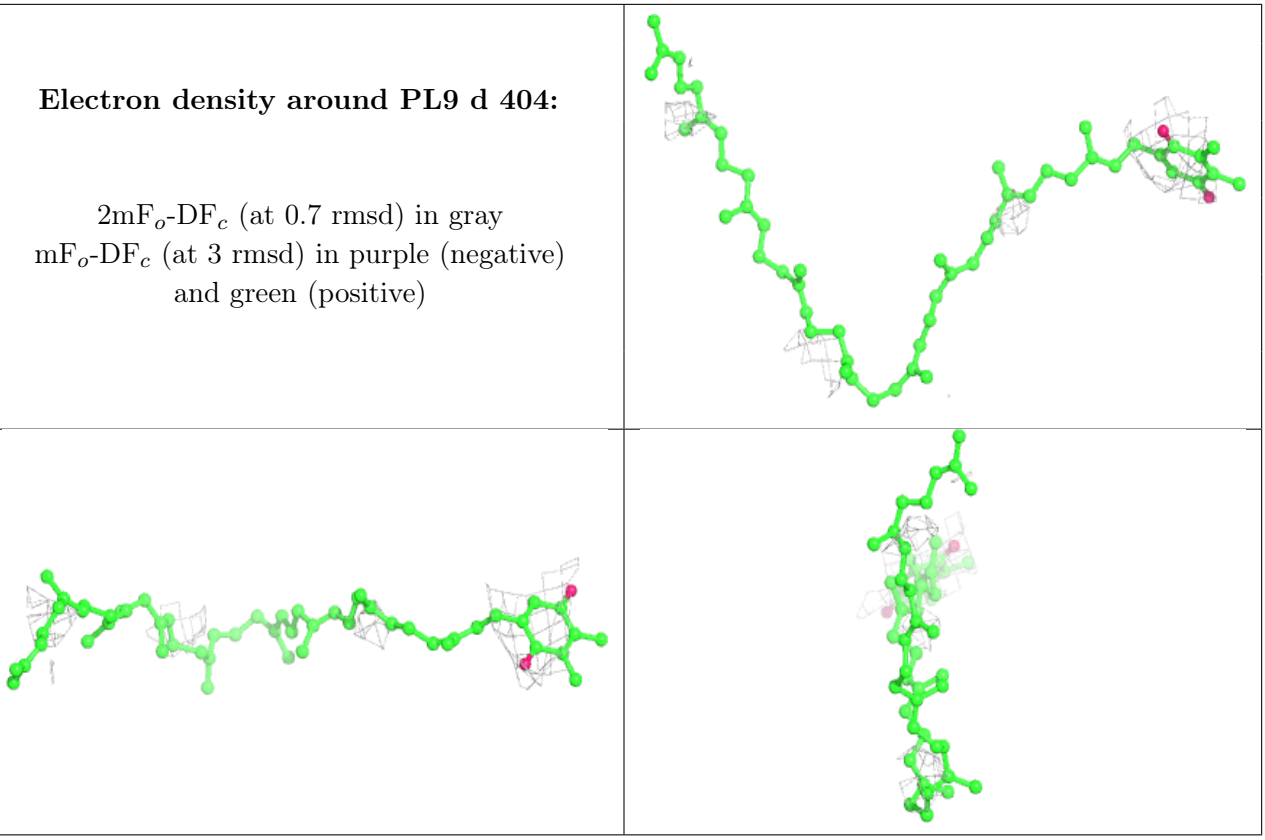
Electron density around SQD f 102:

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



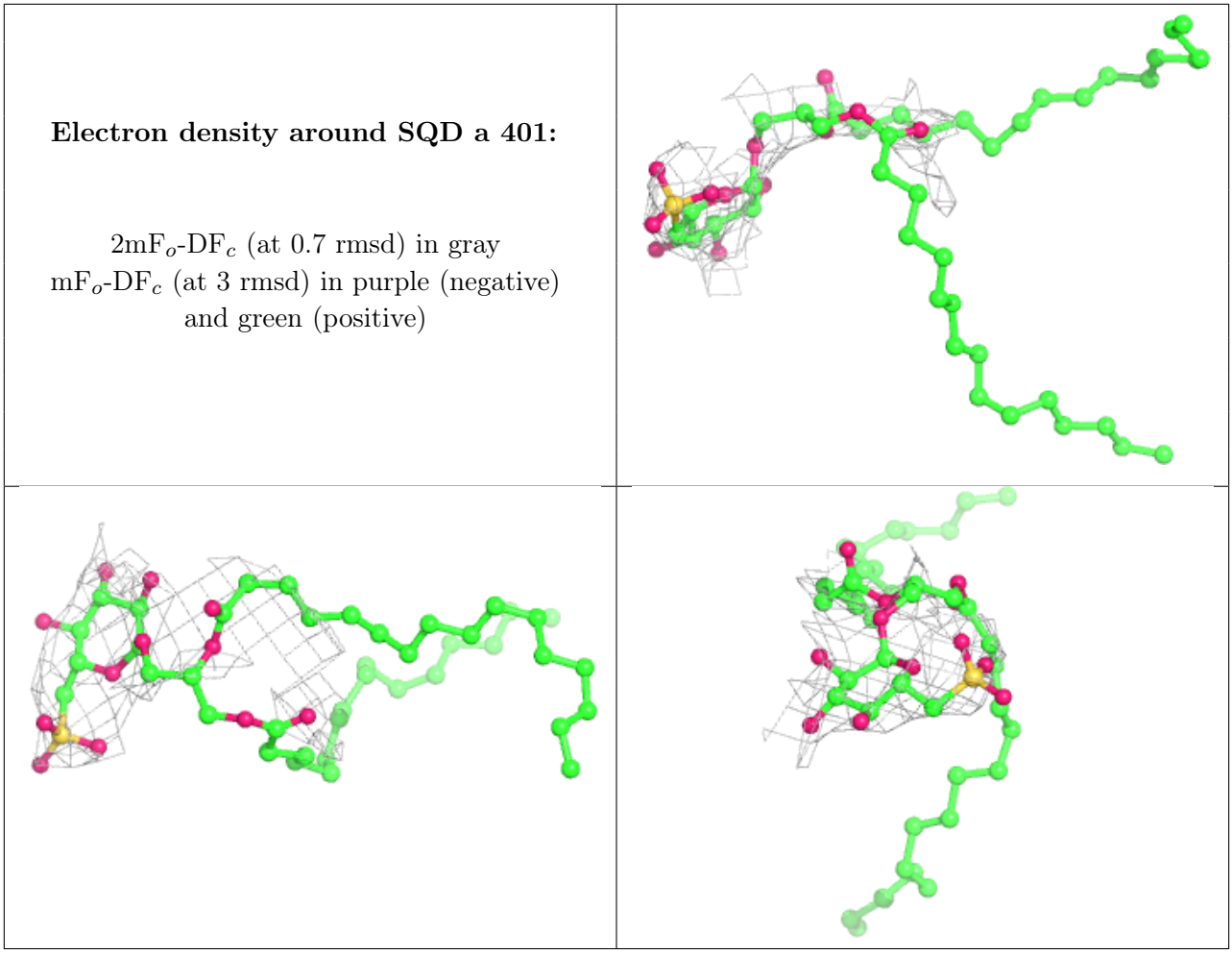
Electron density around PL9 d 404:

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



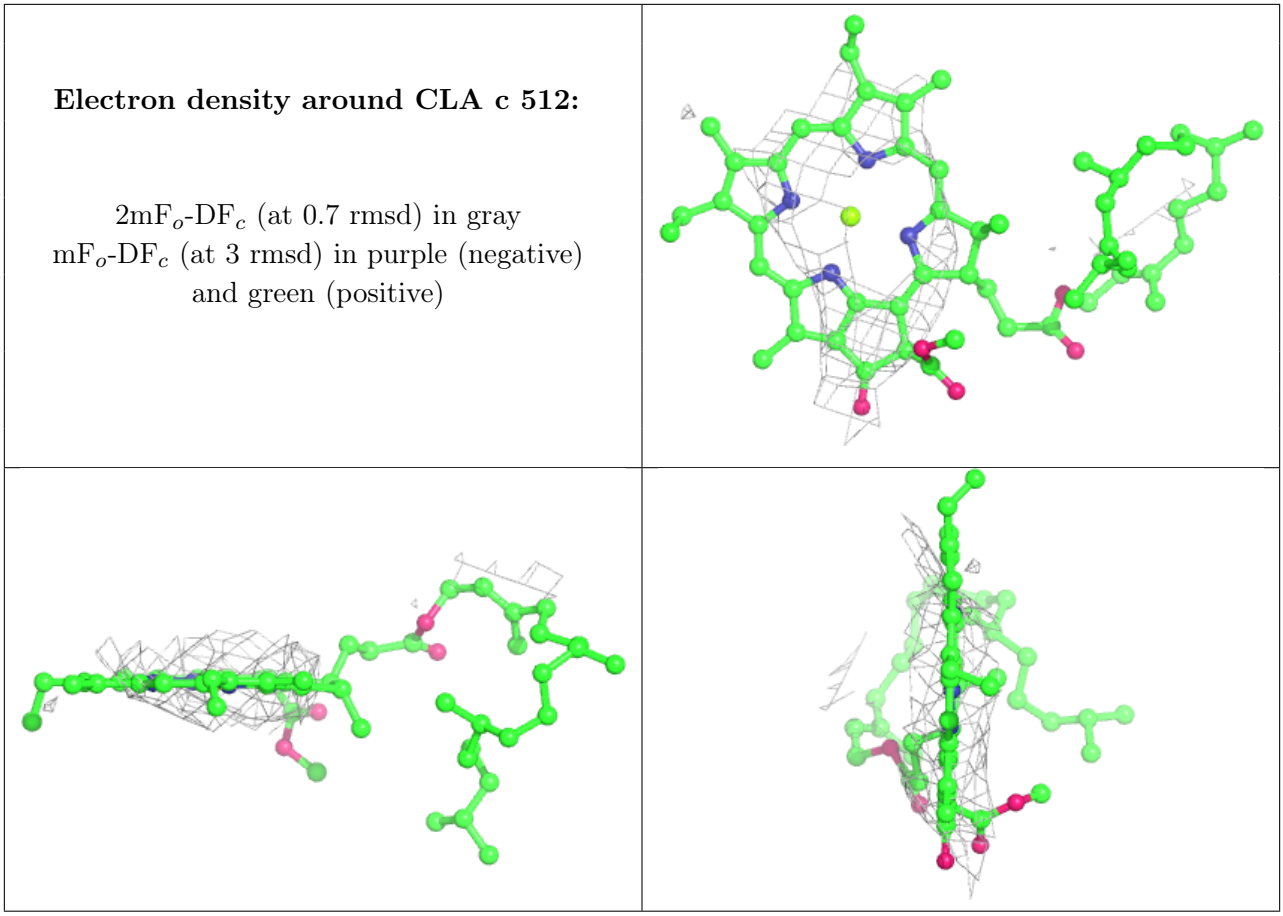
Electron density around SQD a 401:

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



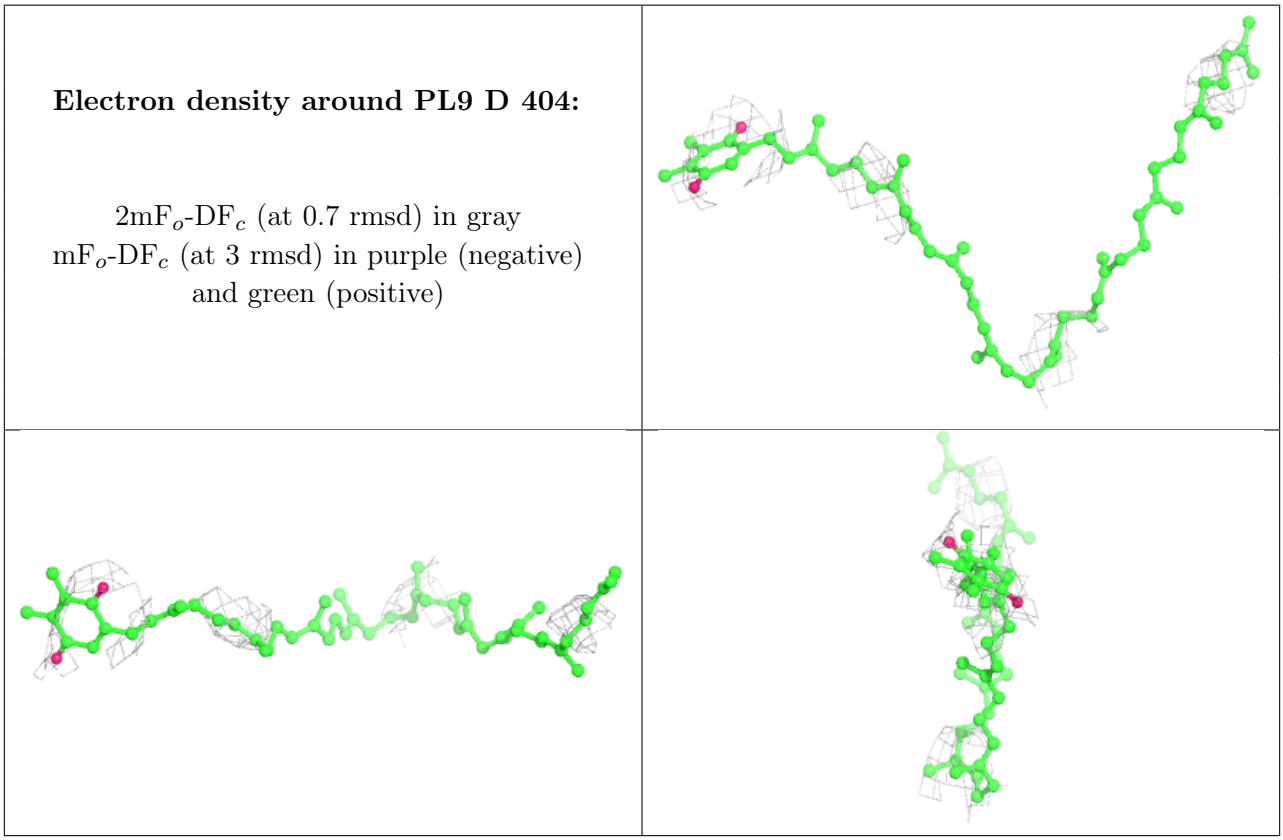
Electron density around CLA c 512:

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



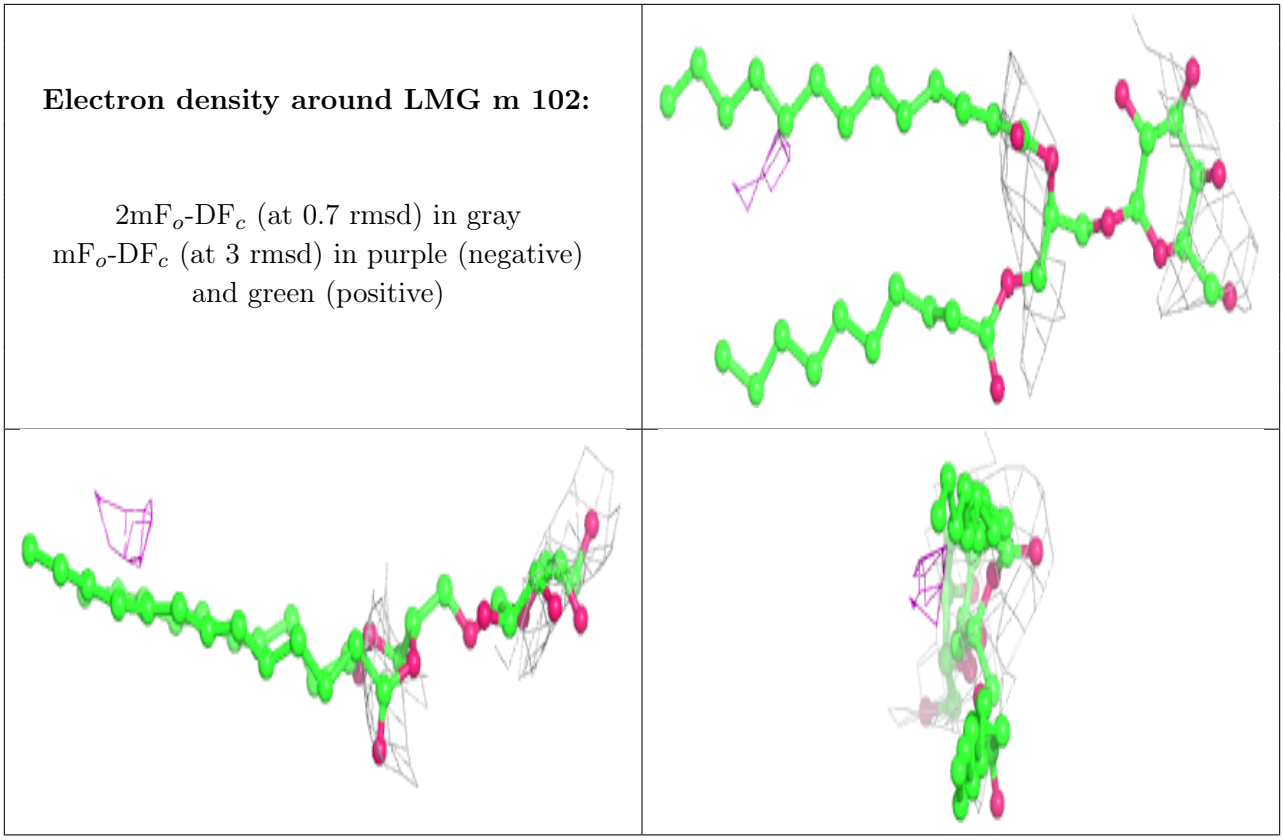
Electron density around PL9 D 404:

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



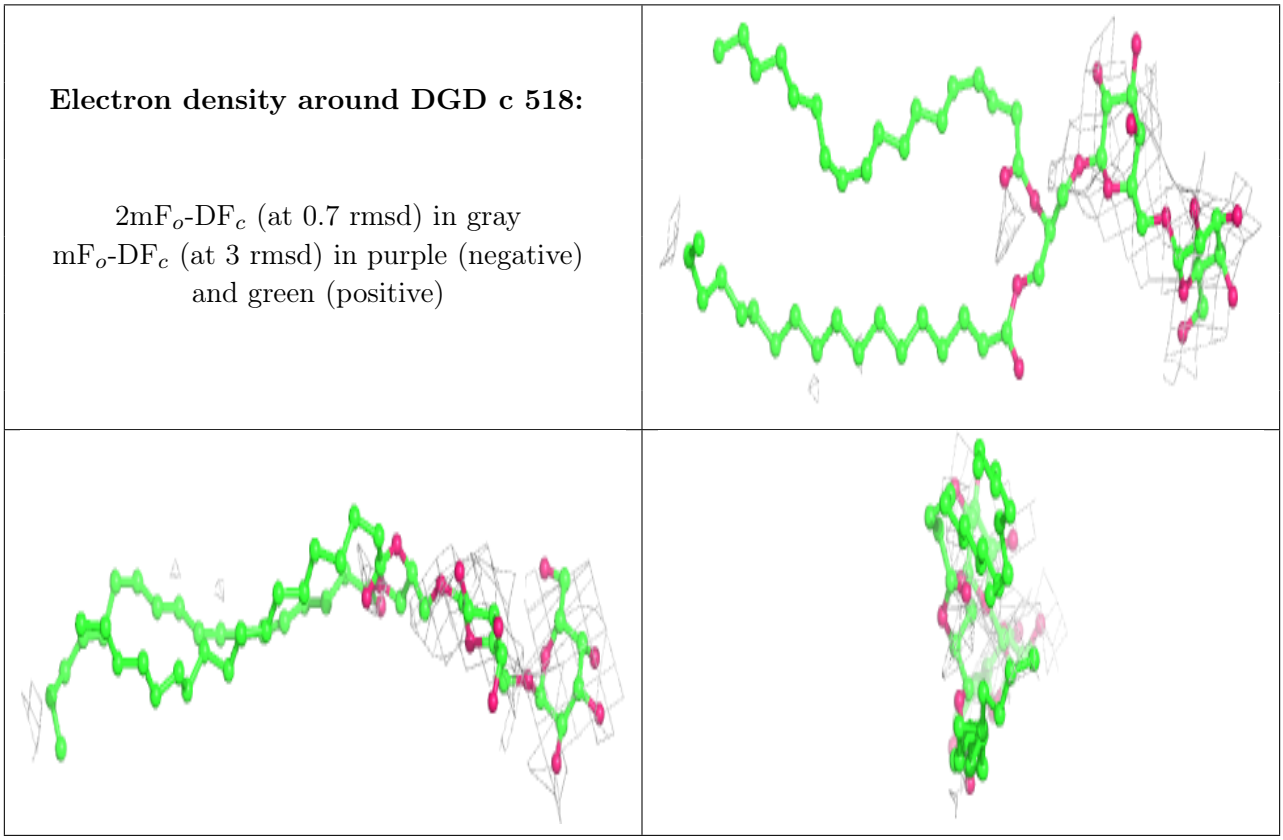
Electron density around LMG m 102:

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



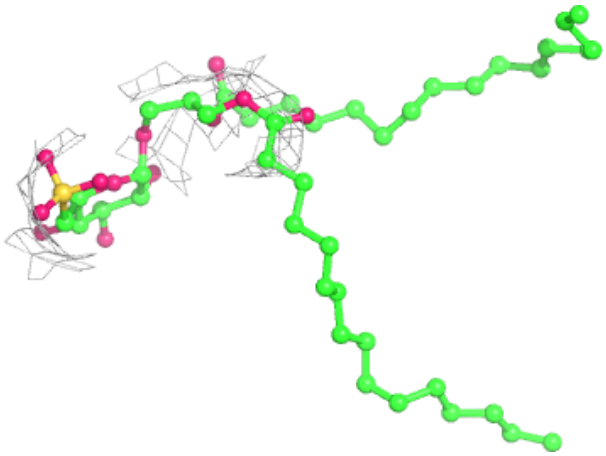
Electron density around DGD c 518:

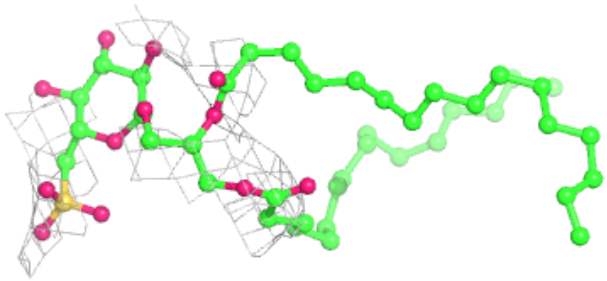
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

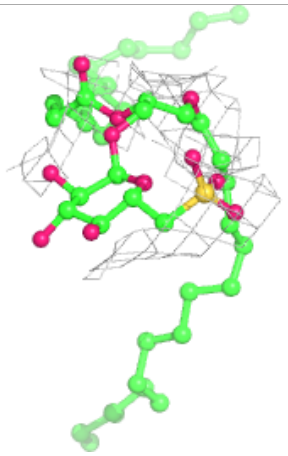


Electron density around SQD A 417:

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

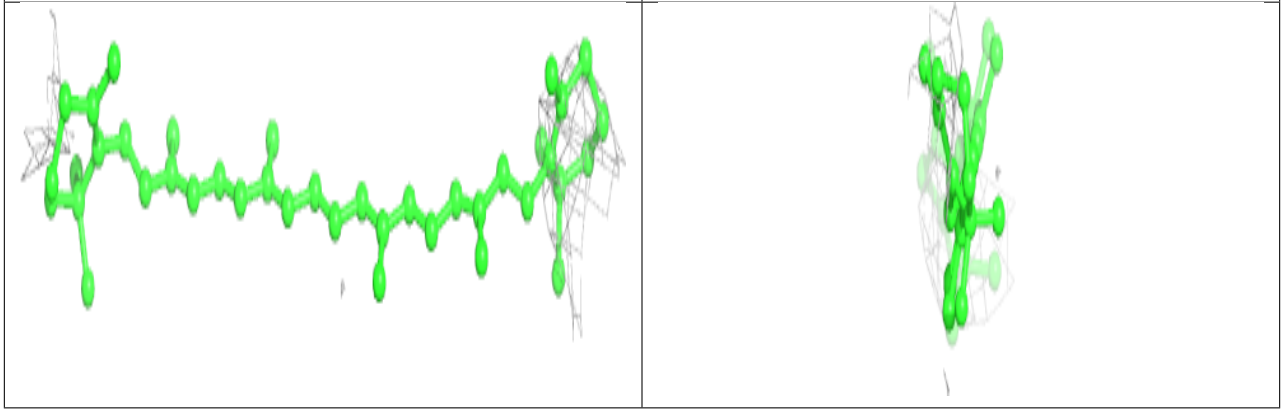






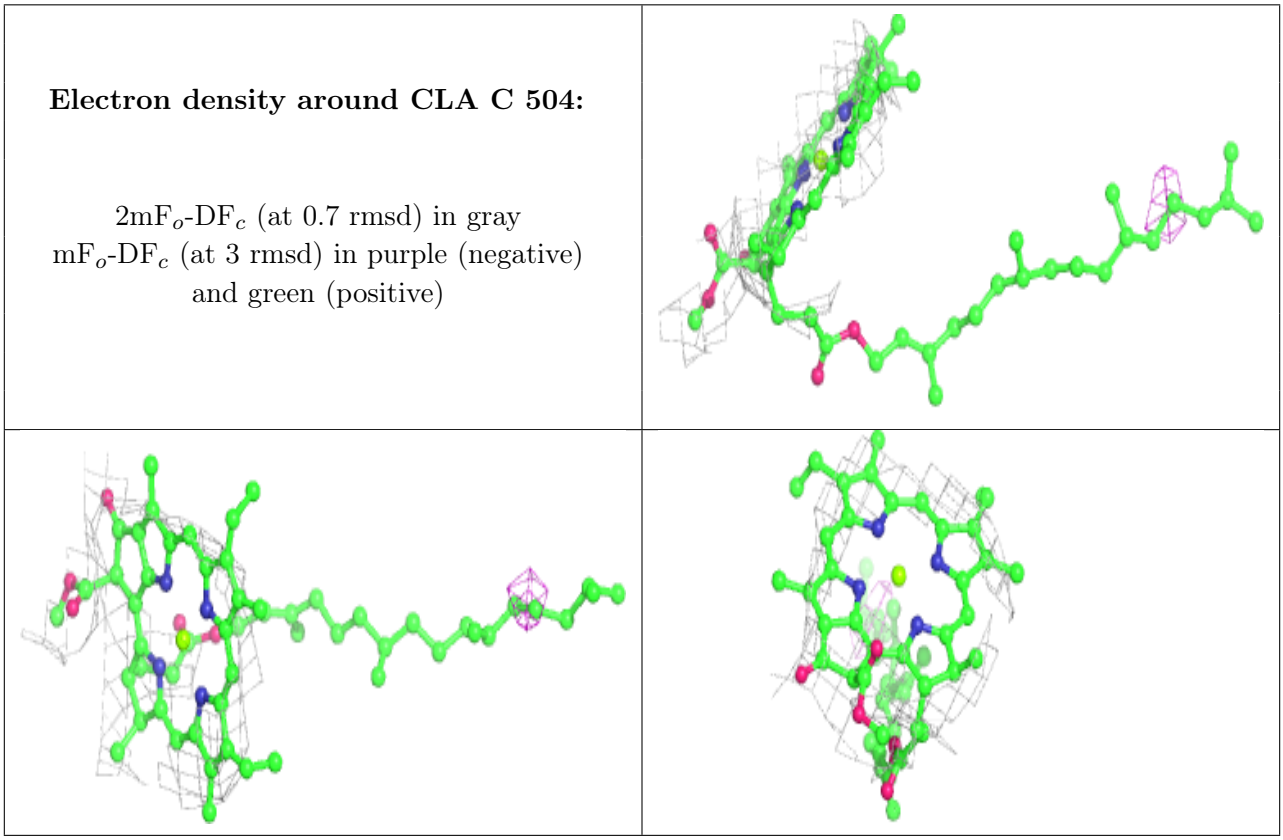
Electron density around BCR c 515:

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



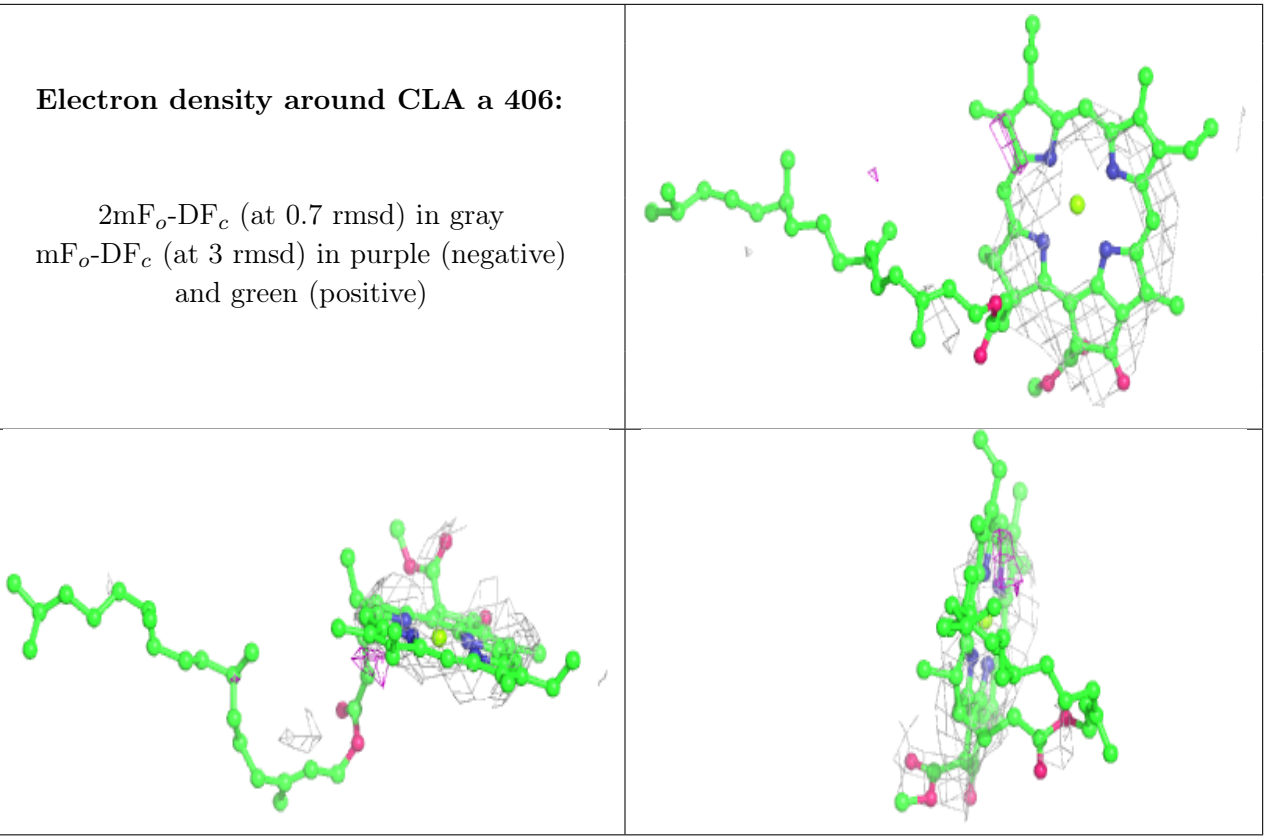
Electron density around CLA C 504:

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



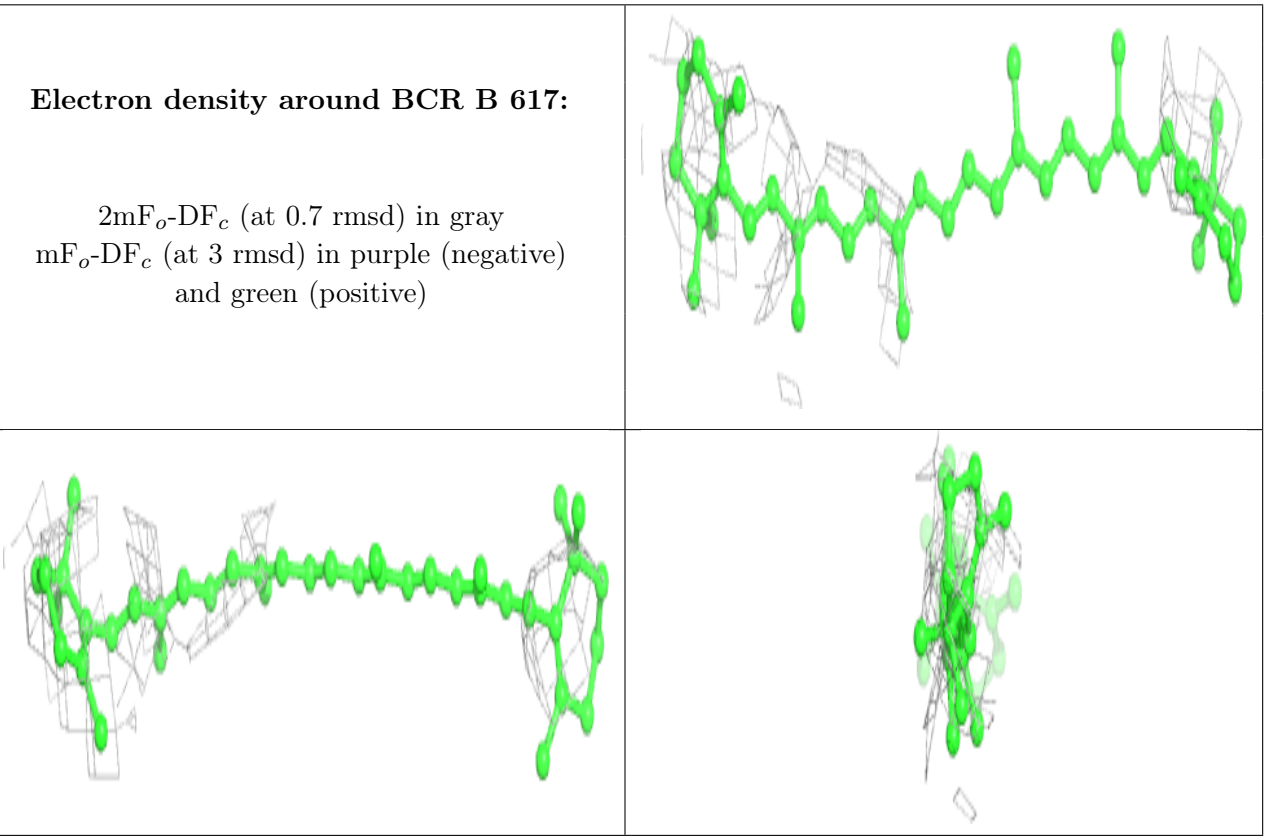
Electron density around CLA a 406:

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



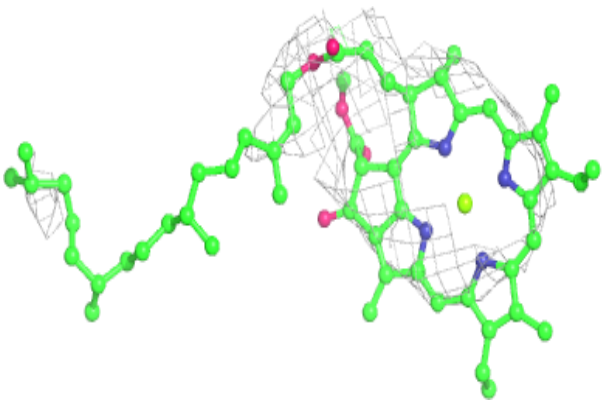
Electron density around BCR B 617:

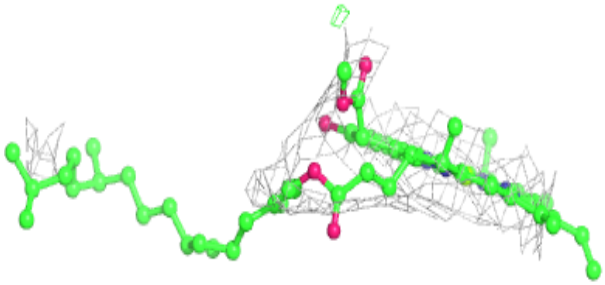
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

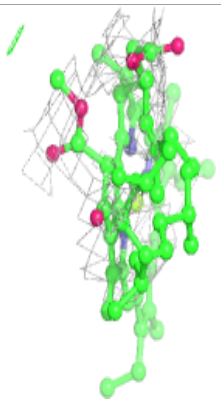


Electron density around CLA B 602:

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

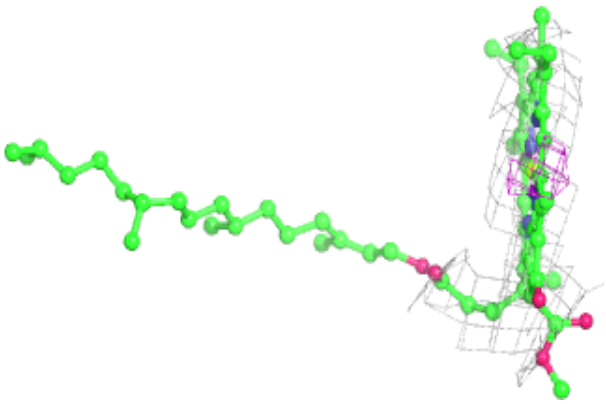


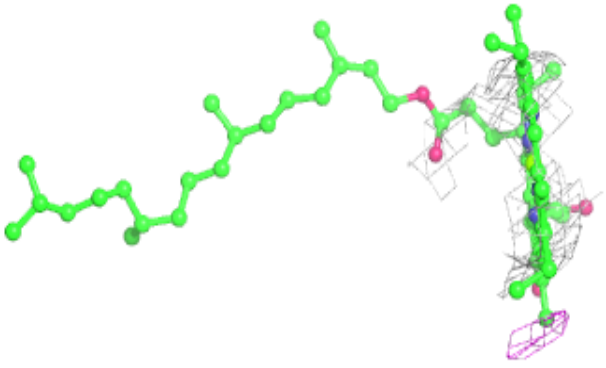


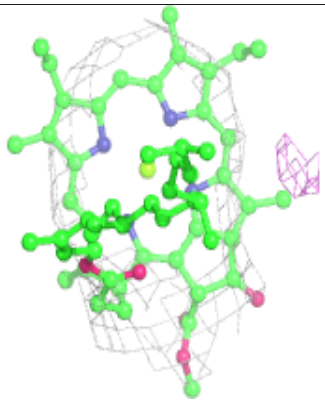


Electron density around CLA B 606:

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

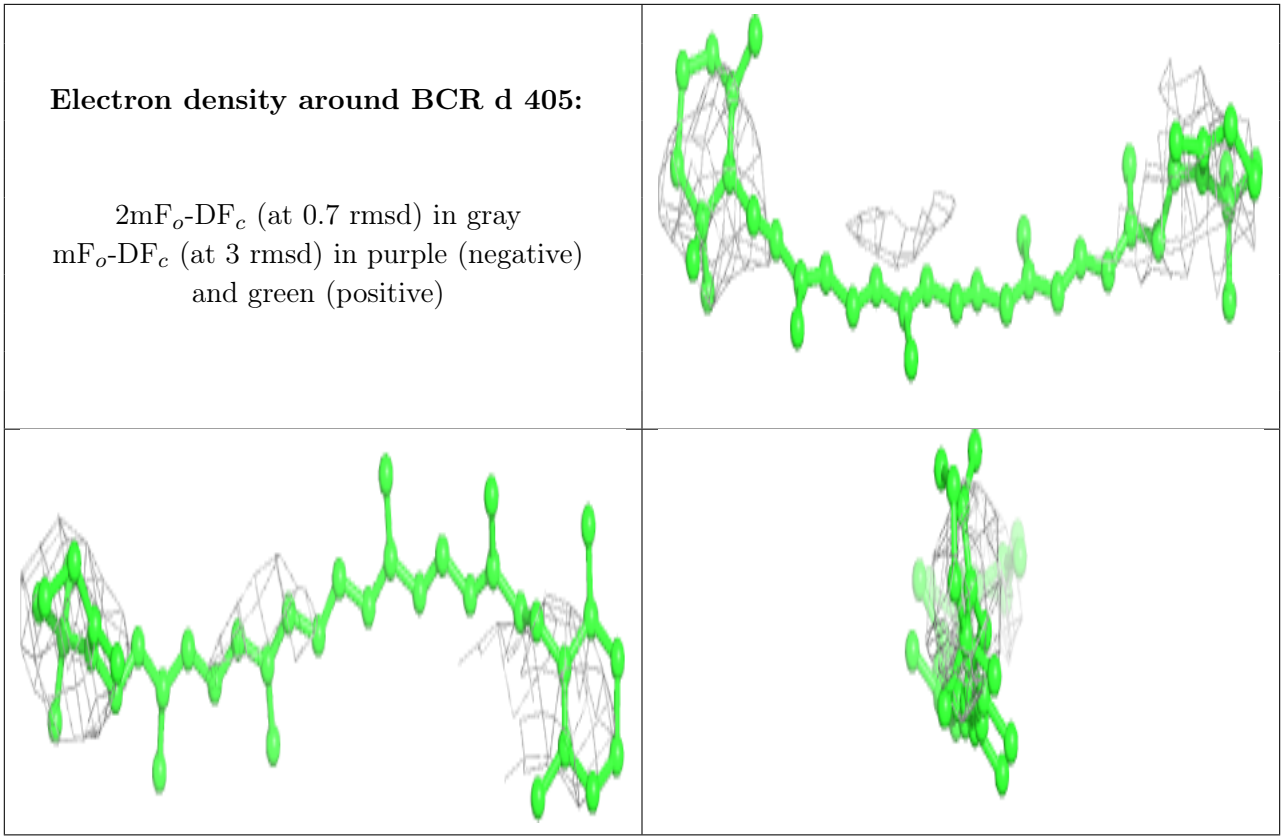






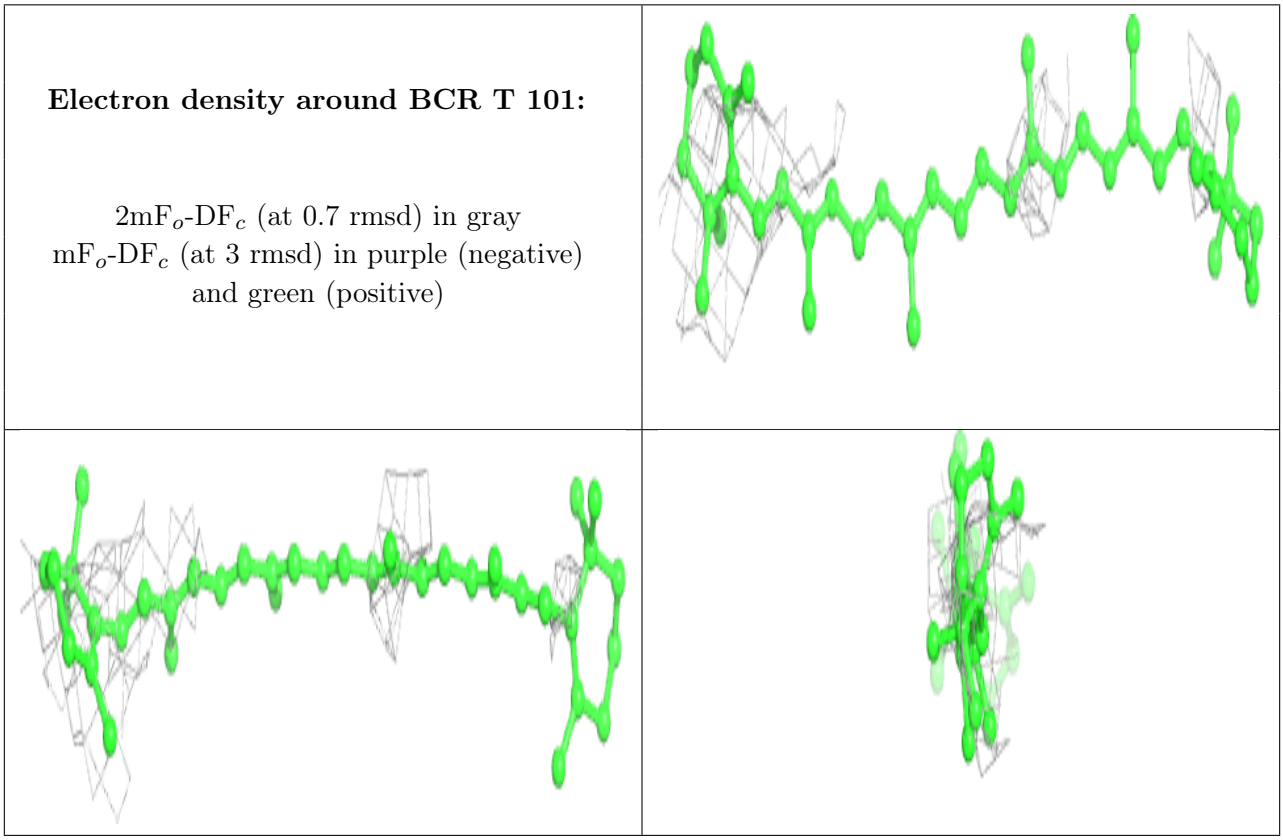
Electron density around BCR d 405:

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



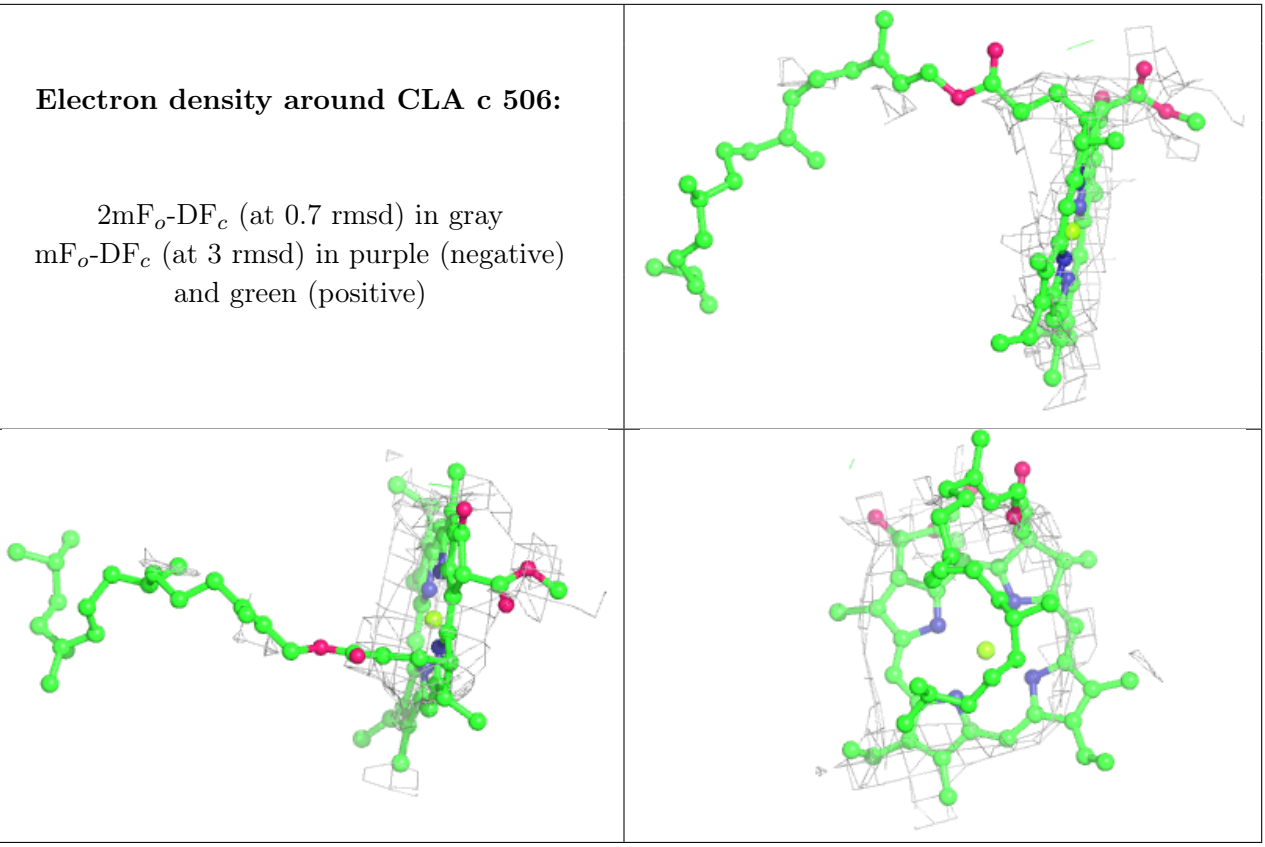
Electron density around BCR T 101:

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



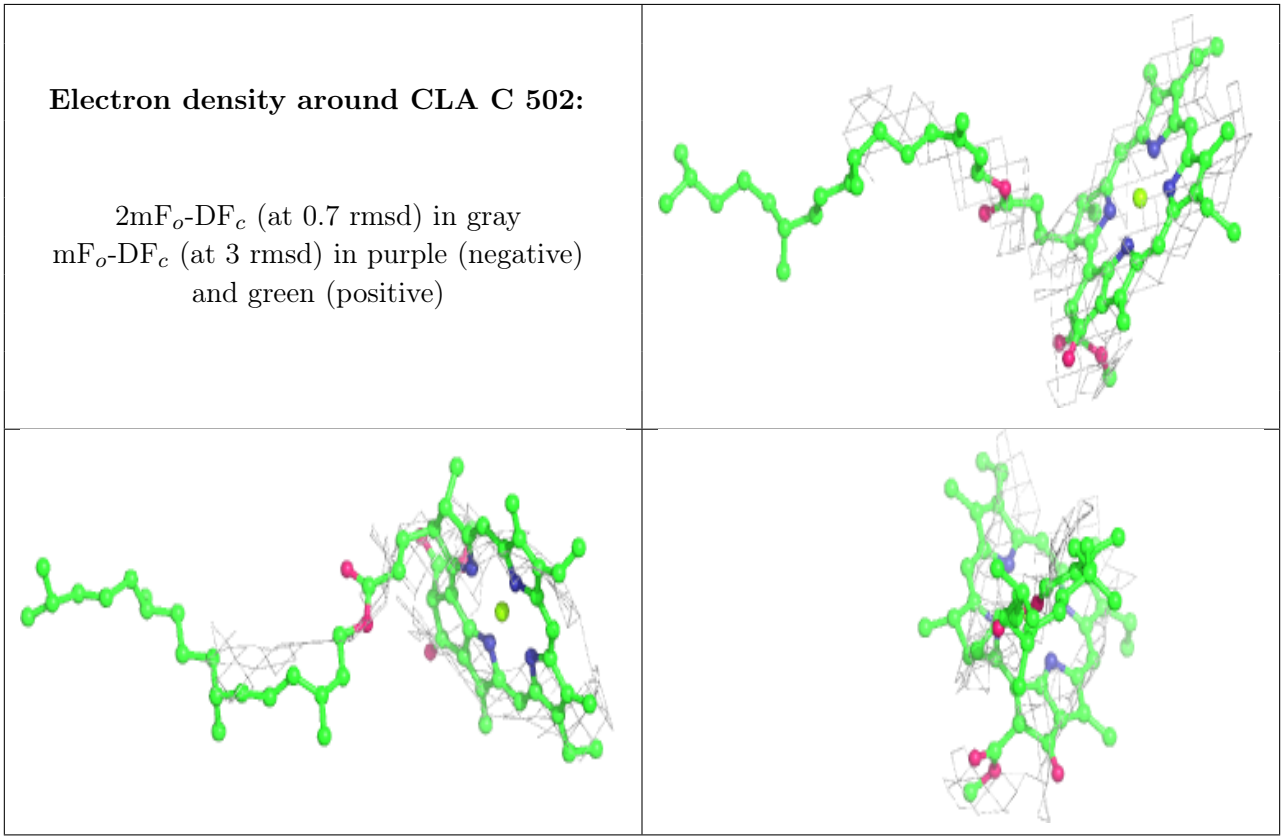
Electron density around CLA c 506:

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



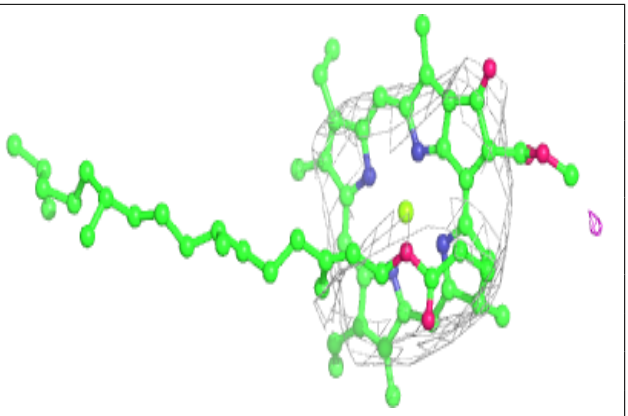
Electron density around CLA C 502:

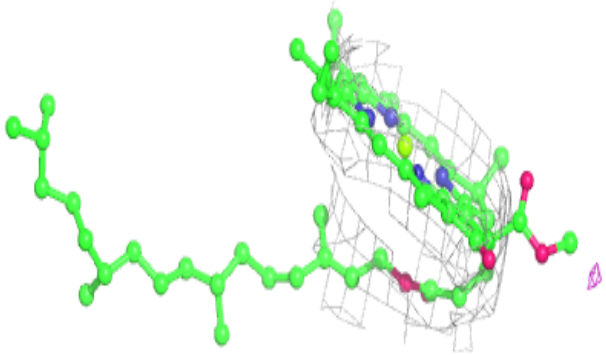
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

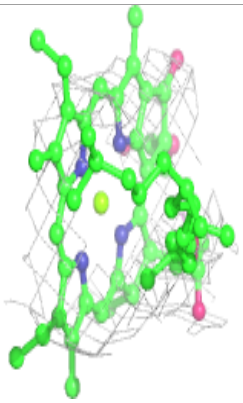


Electron density around CLA B 608:

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

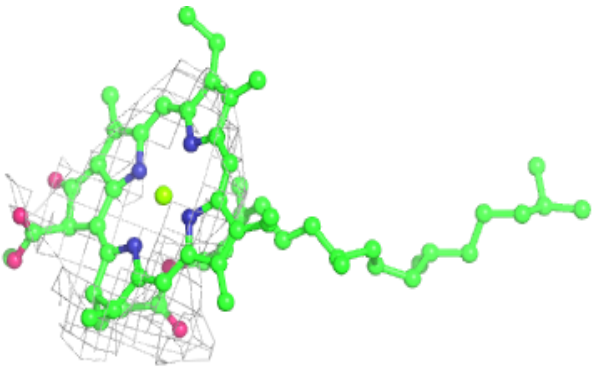


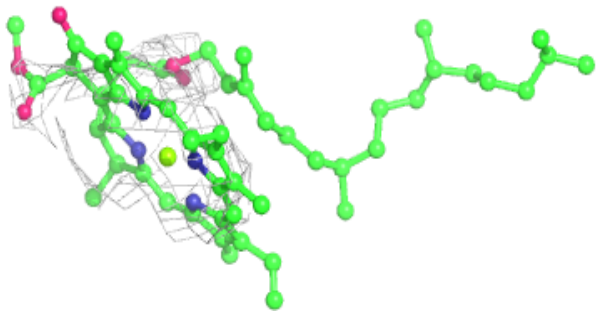


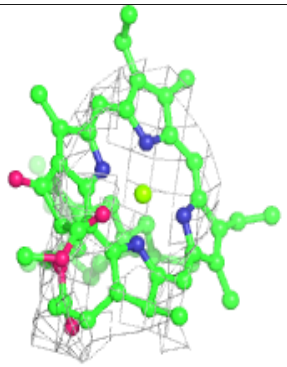


Electron density around CLA C 505:

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

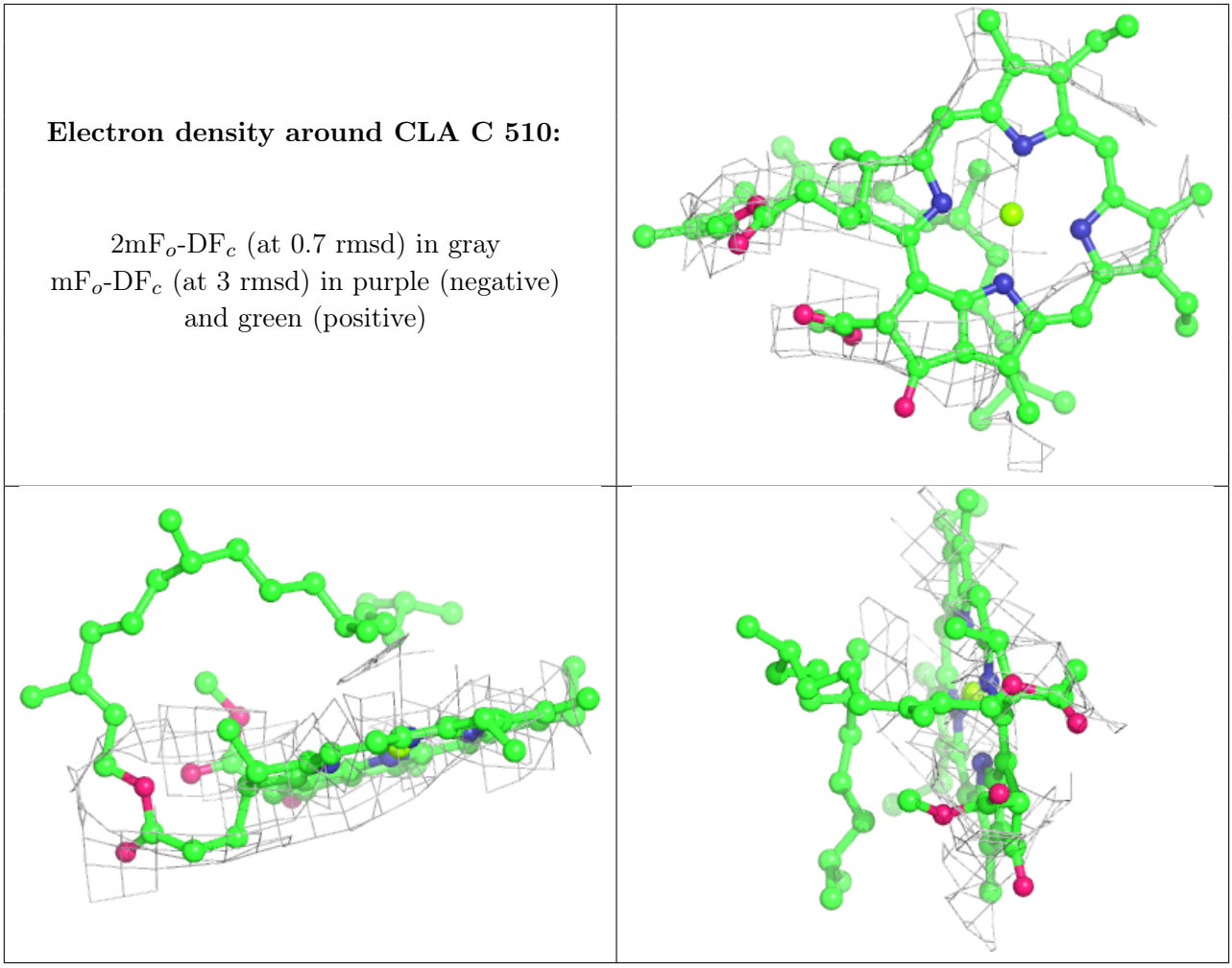






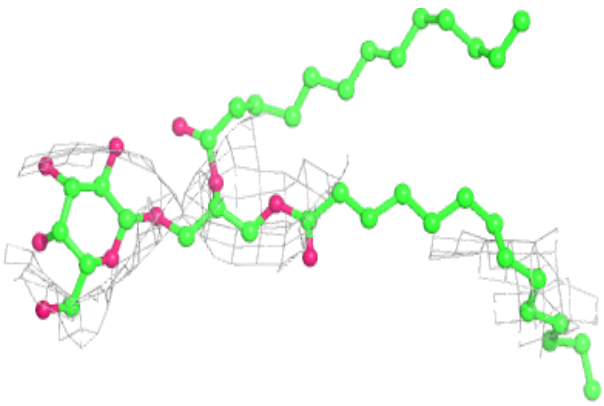
Electron density around CLA C 510:

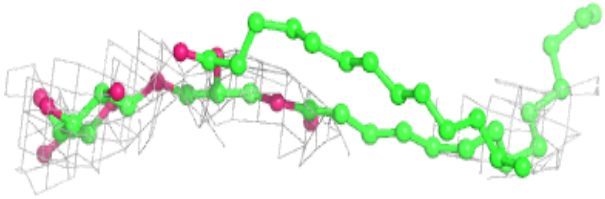
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

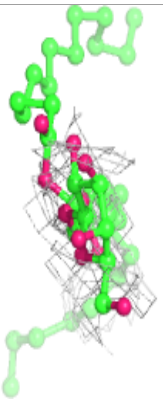


Electron density around LMG D 406:

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

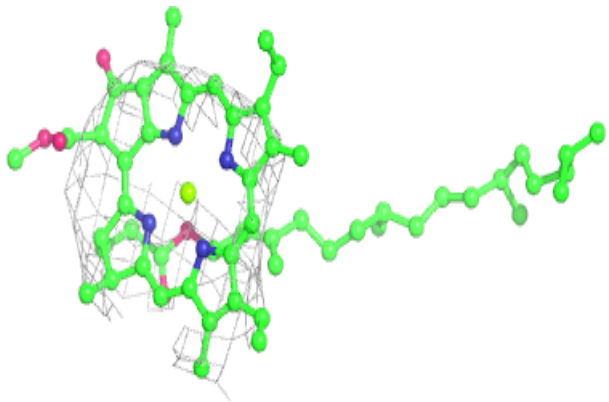


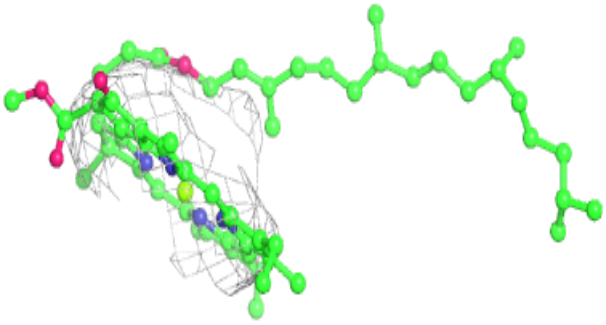


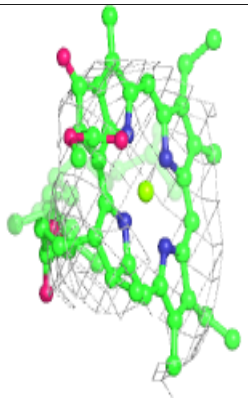


Electron density around CLA b 612:

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

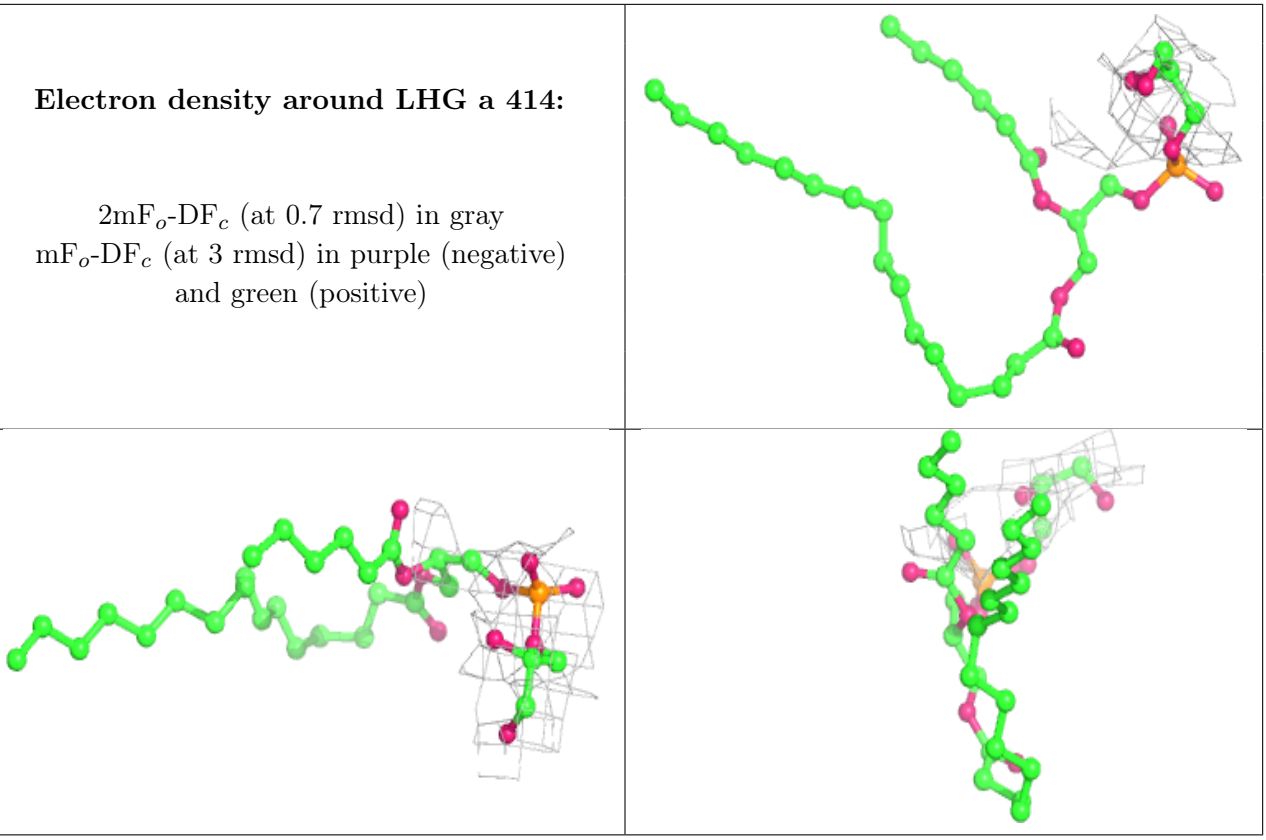






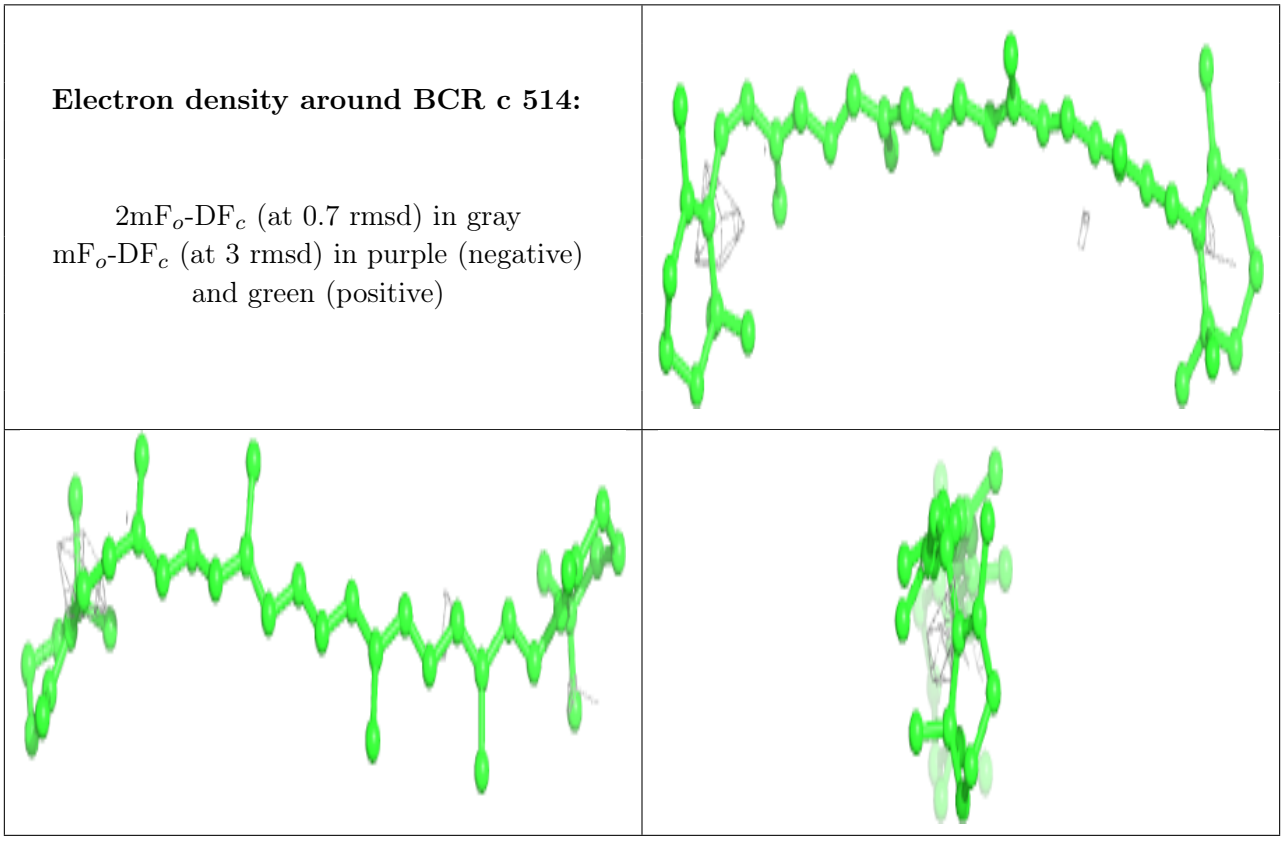
Electron density around LHG a 414:

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



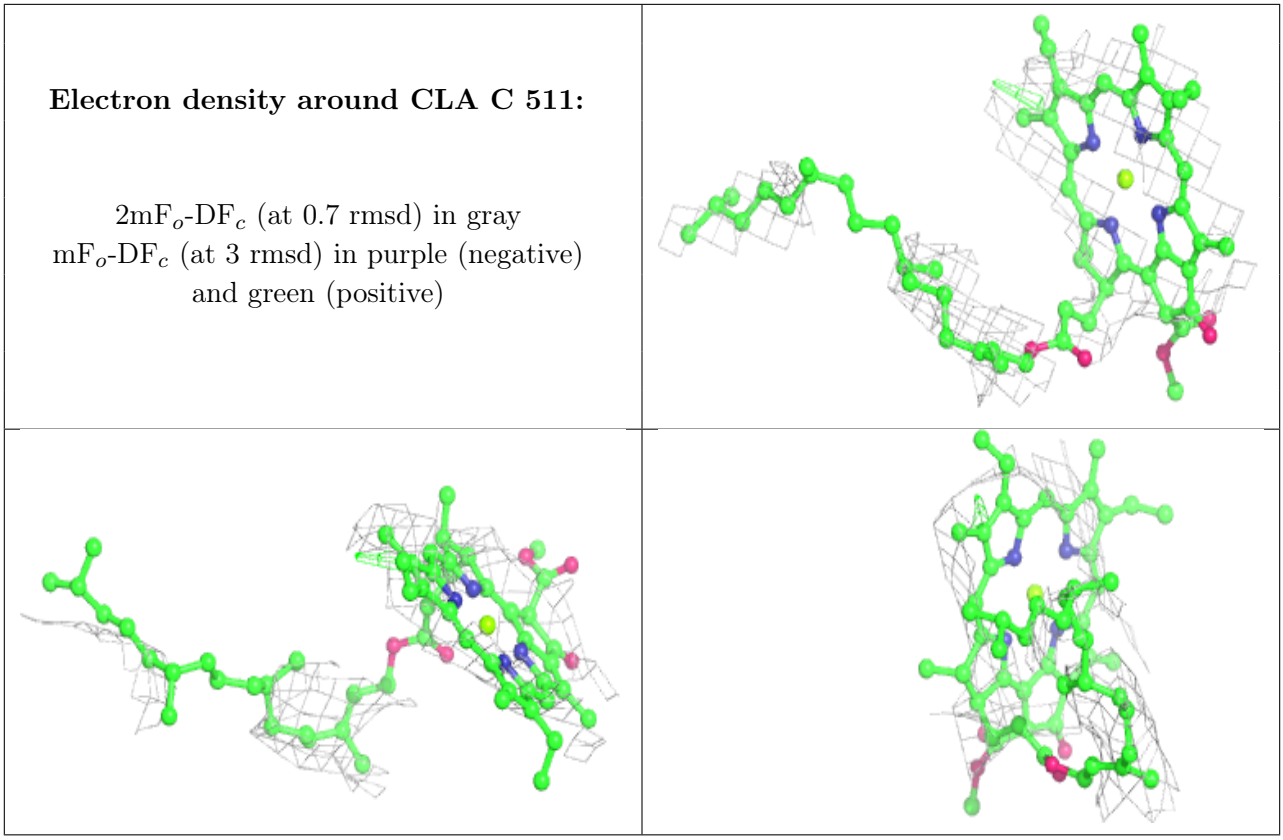
Electron density around BCR c 514:

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



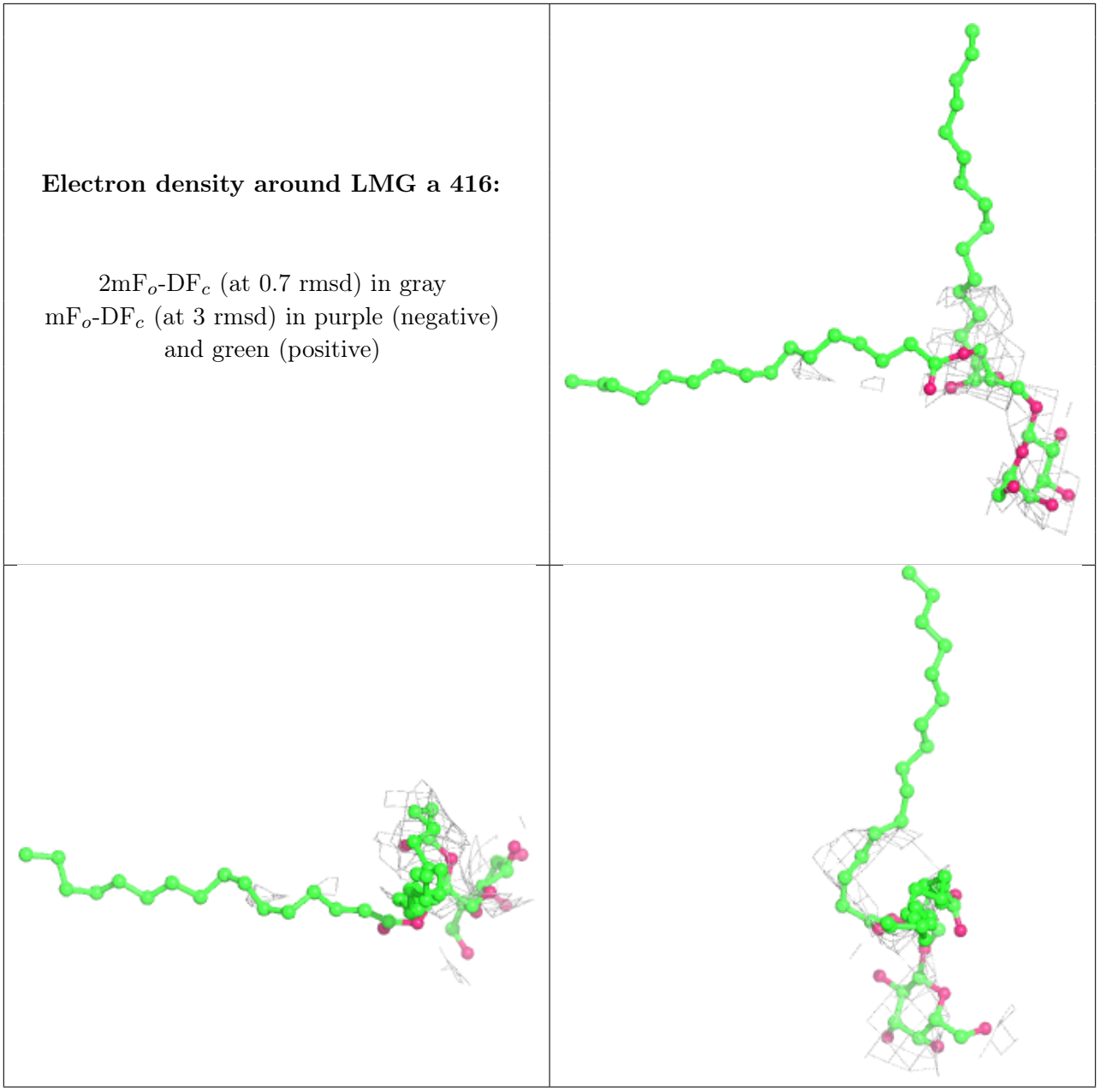
Electron density around CLA C 511:

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



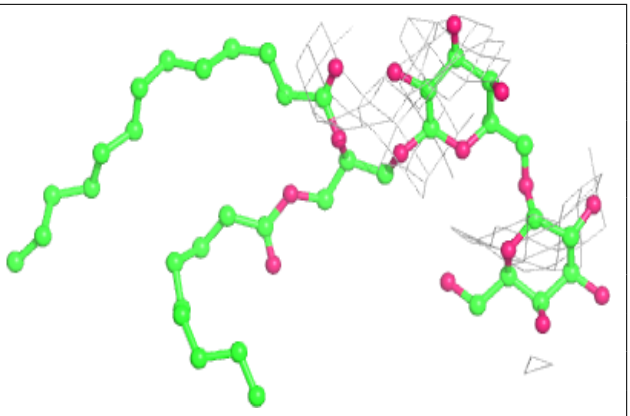
Electron density around LMG a 416:

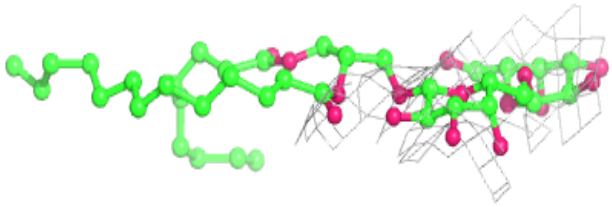
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD b 602:

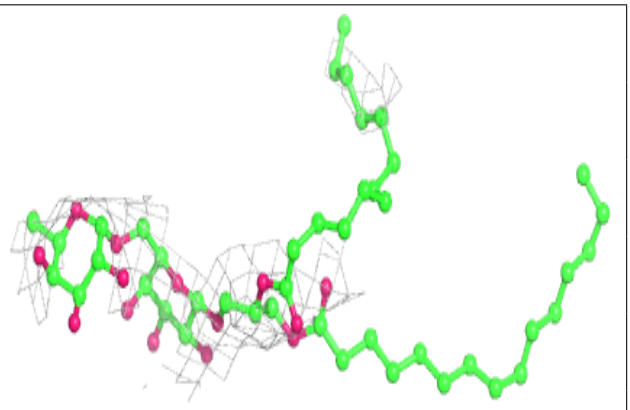
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

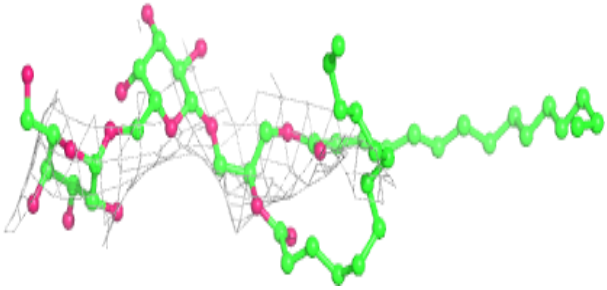


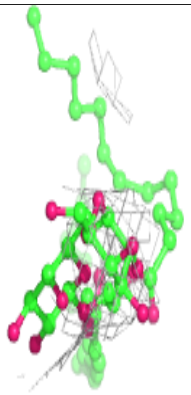


Electron density around DGD b 623:

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

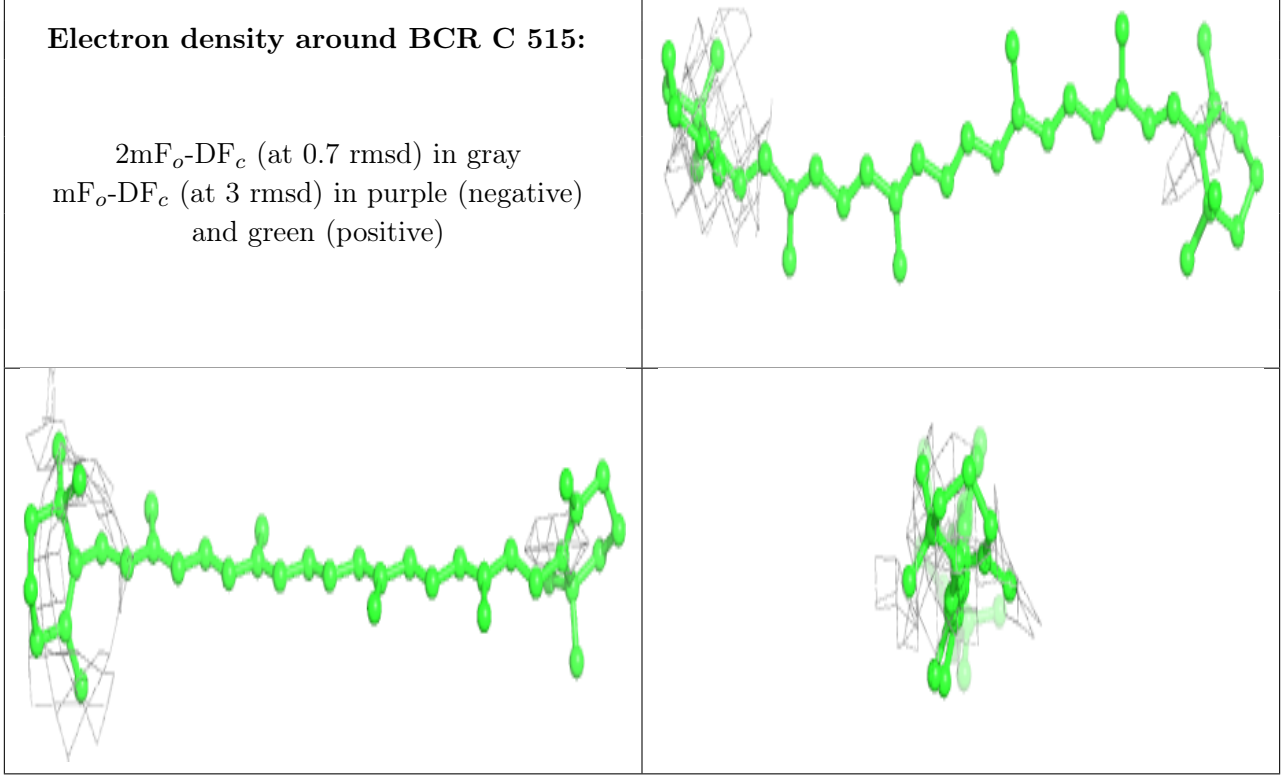






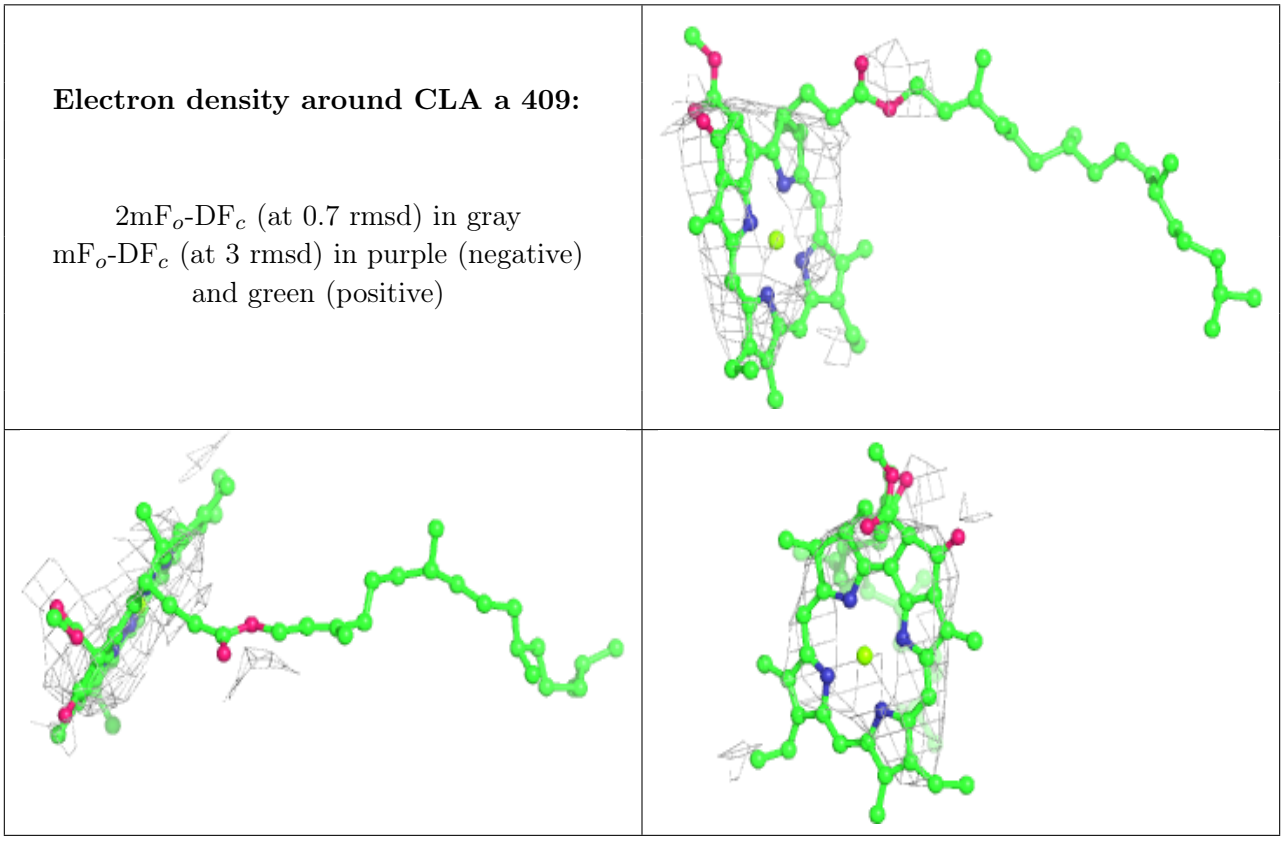
Electron density around BCR C 515:

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



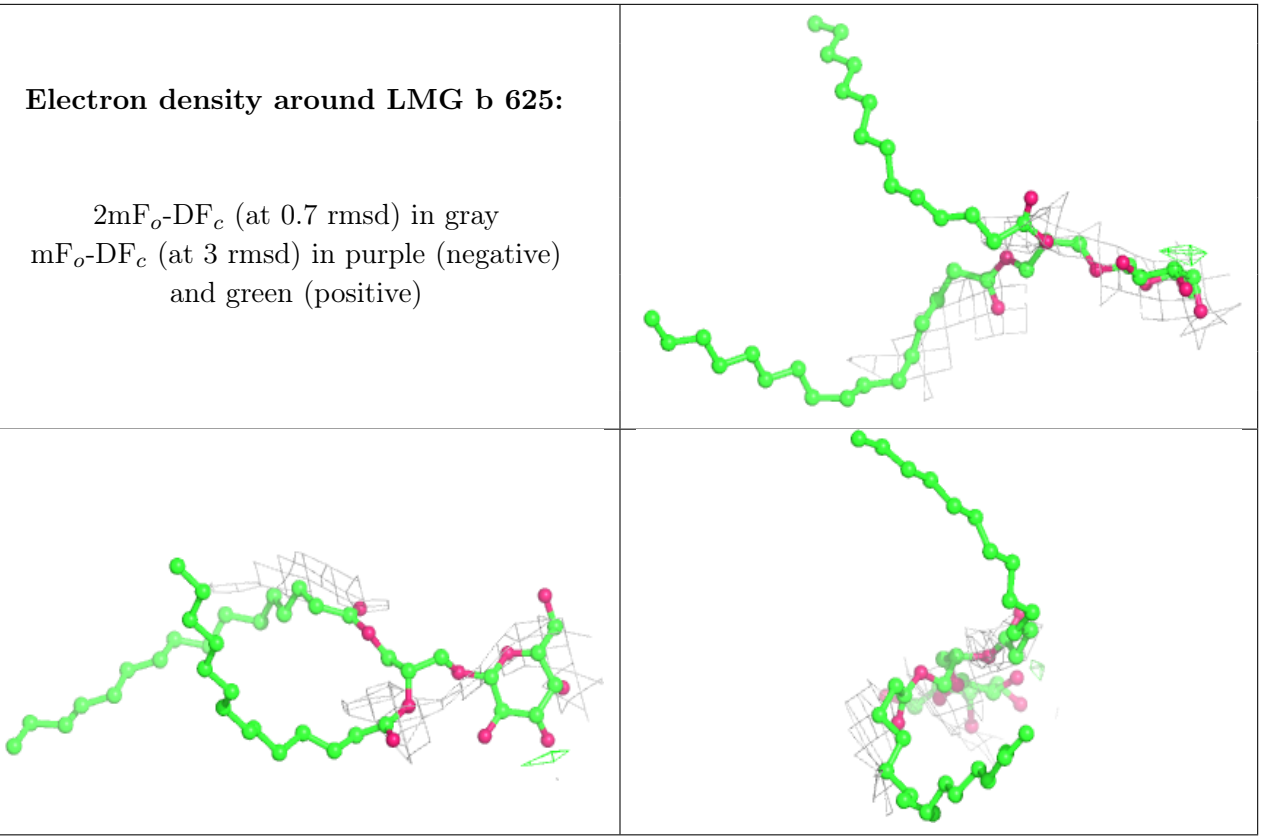
Electron density around CLA a 409:

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



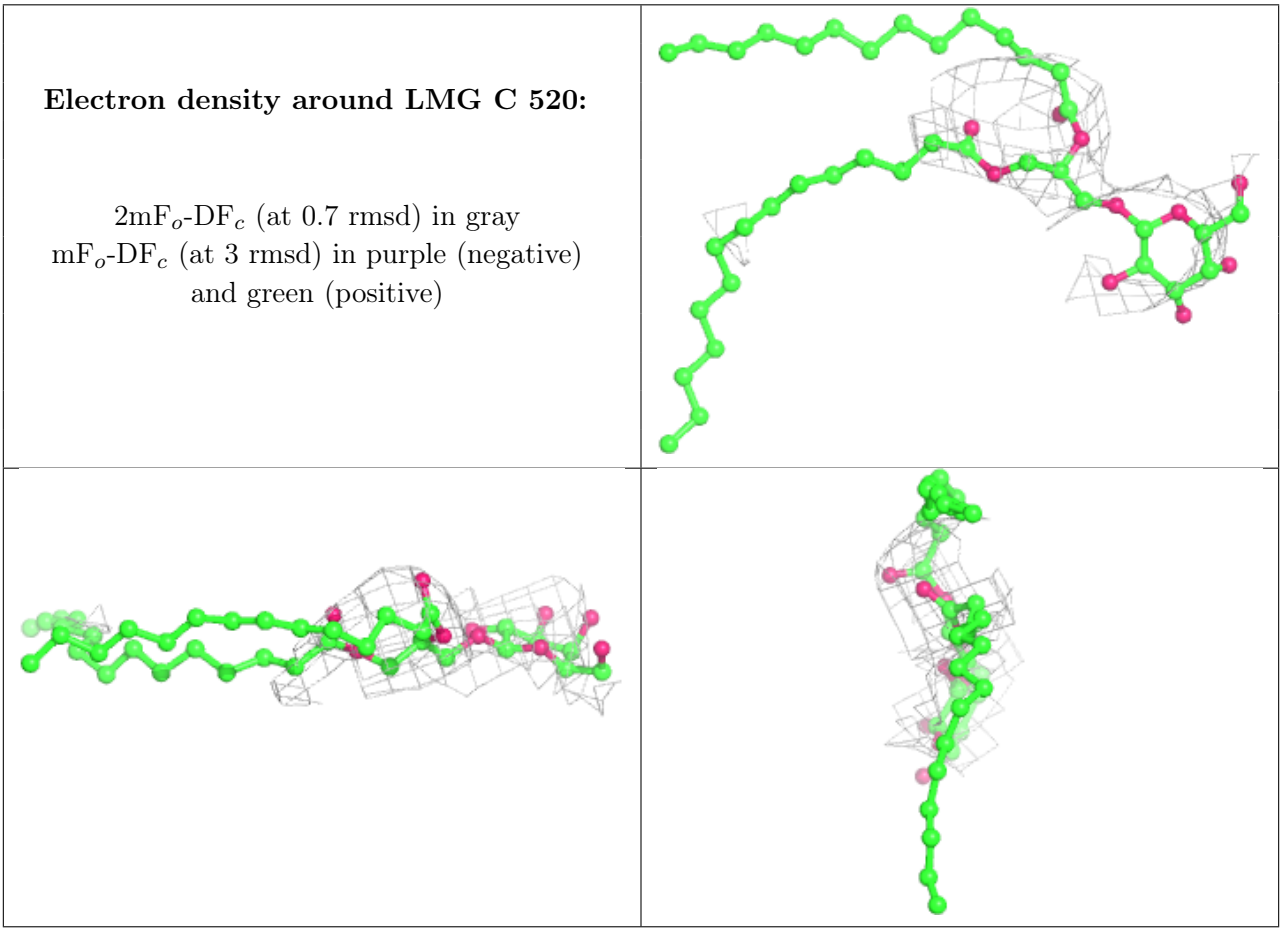
Electron density around LMG b 625:

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



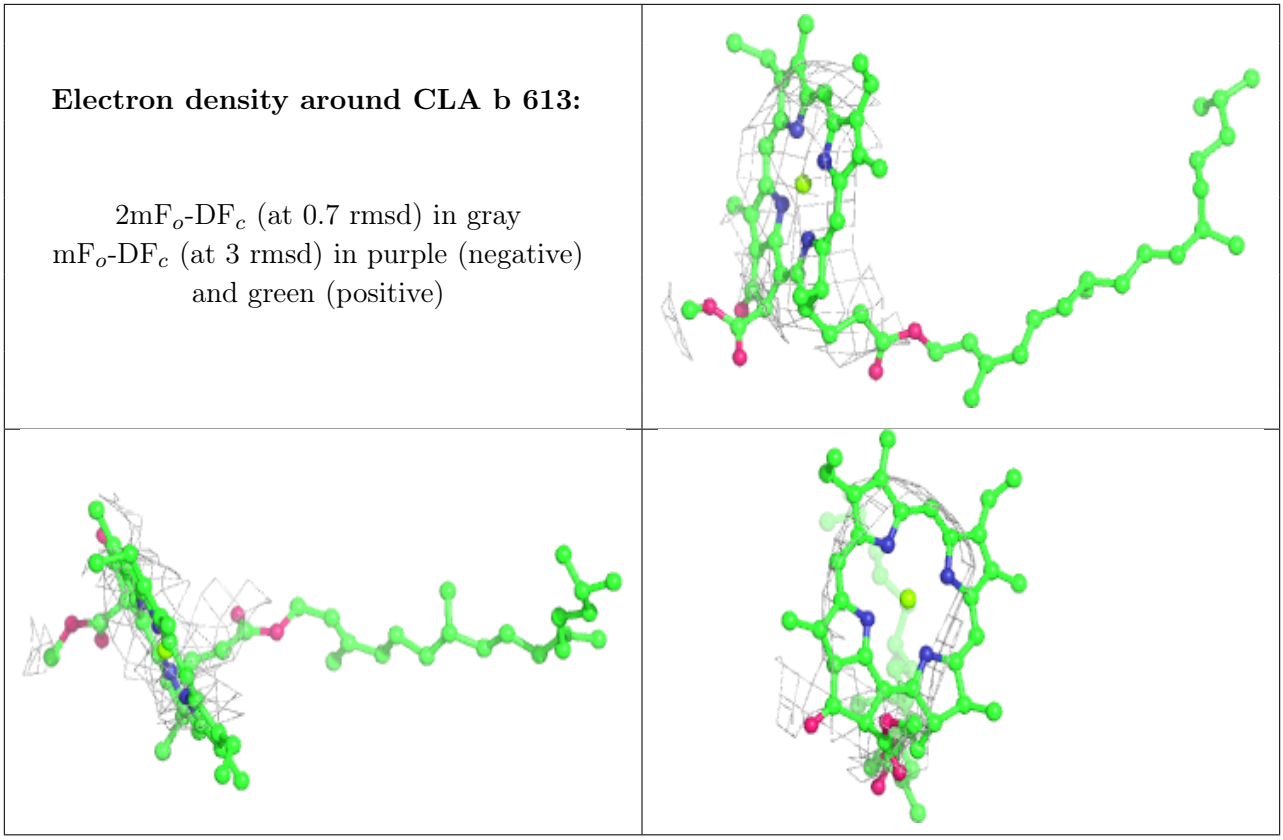
Electron density around LMG C 520:

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



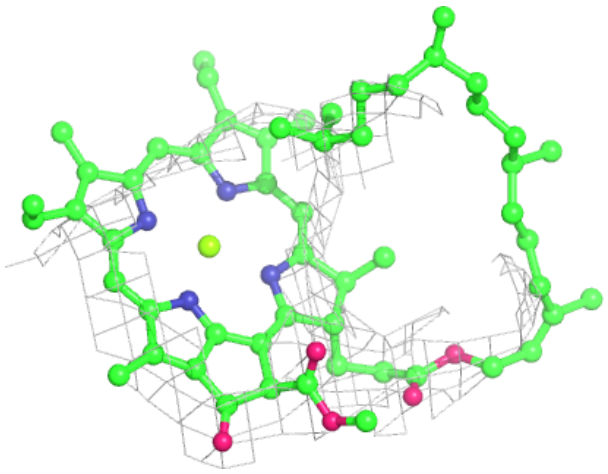
Electron density around CLA b 613:

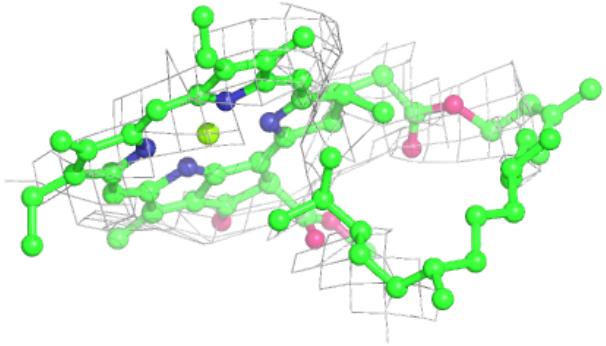
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

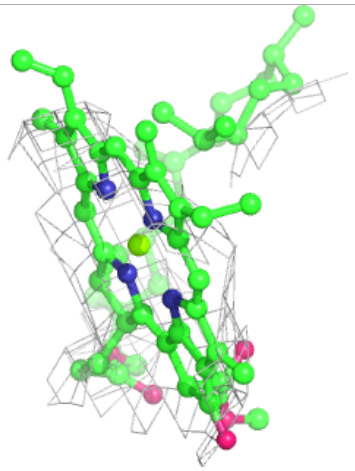


Electron density around CLA b 619:

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

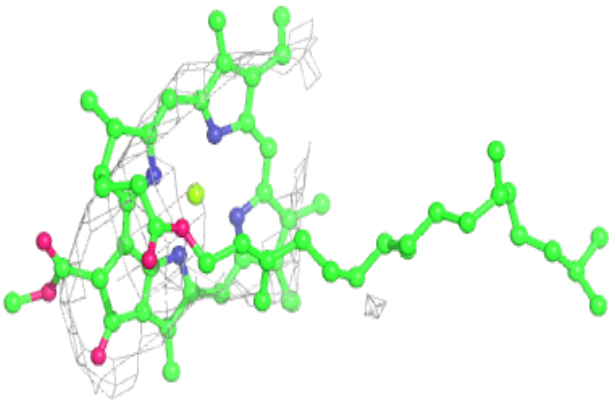


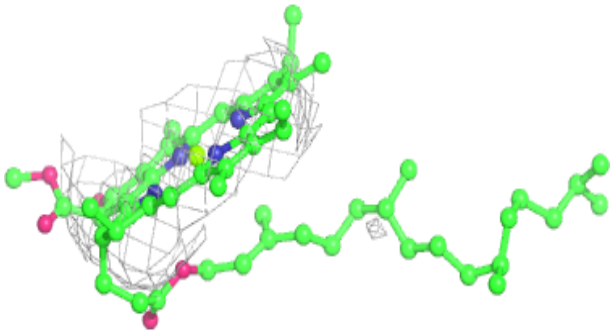


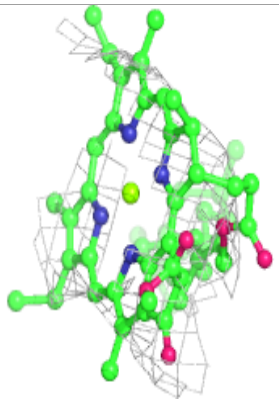


Electron density around CLA b 618:

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

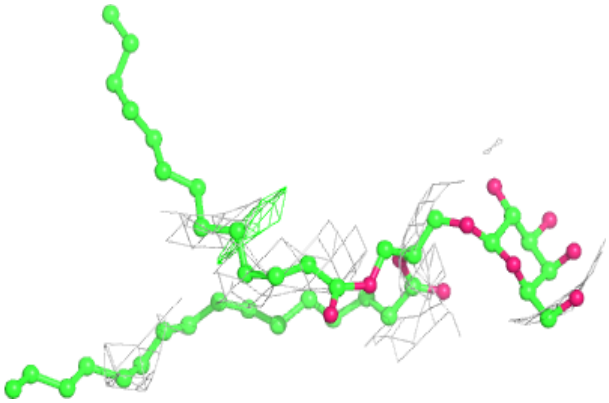


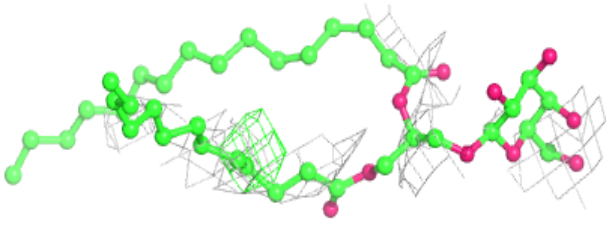


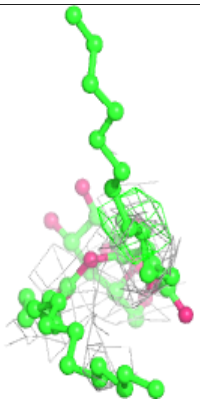


Electron density around LMG d 407:

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

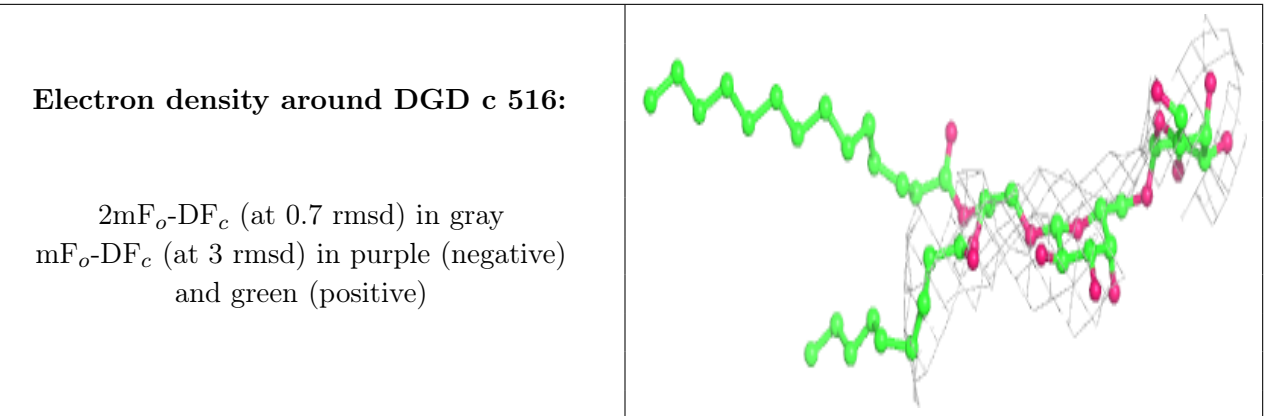


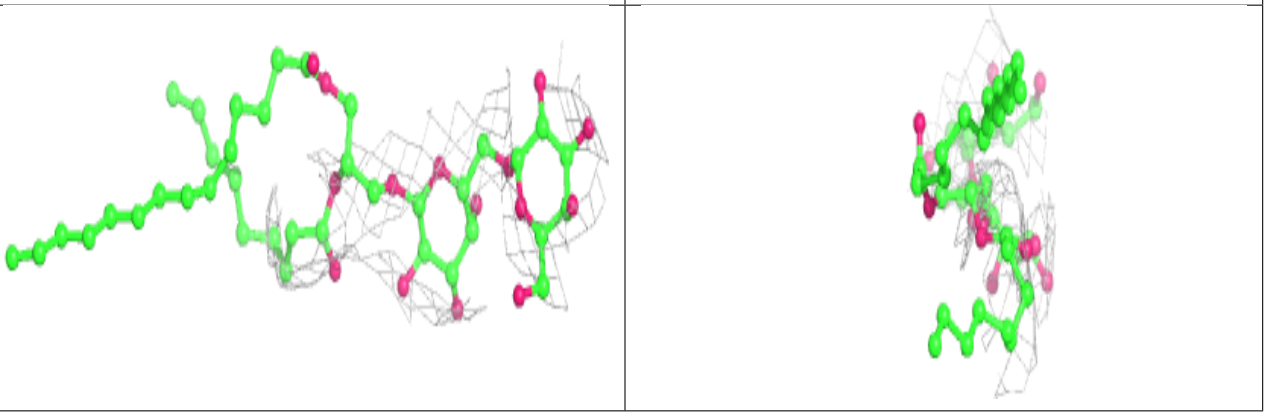




Electron density around DGD c 516:

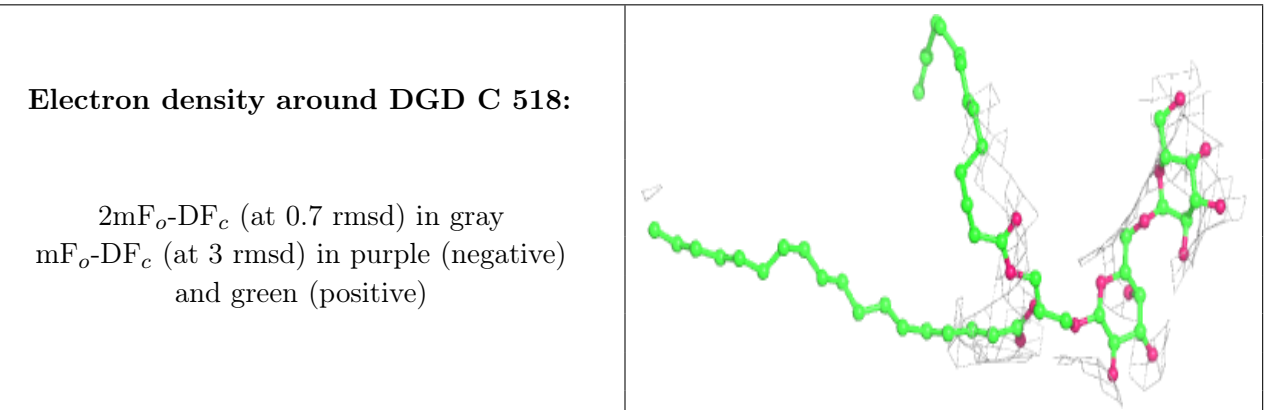
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

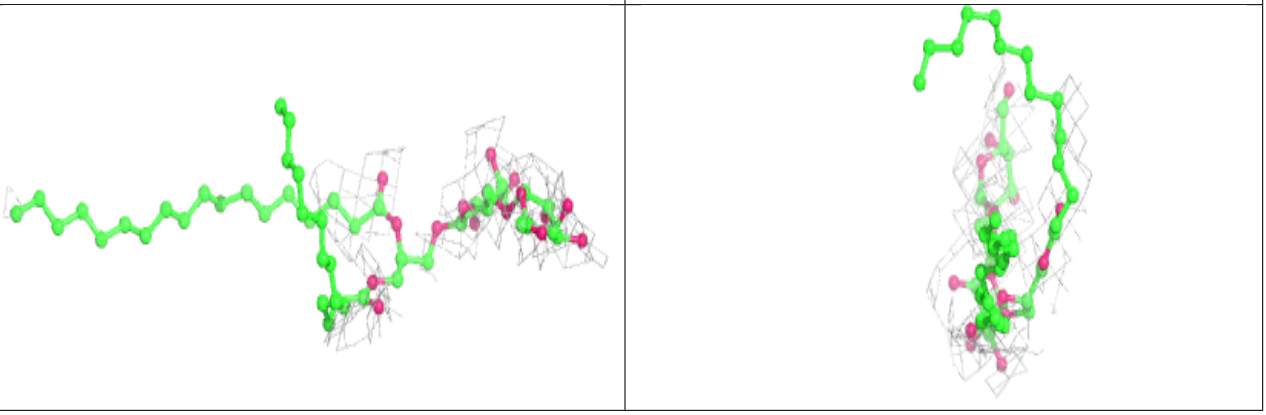




Electron density around DGD C 518:

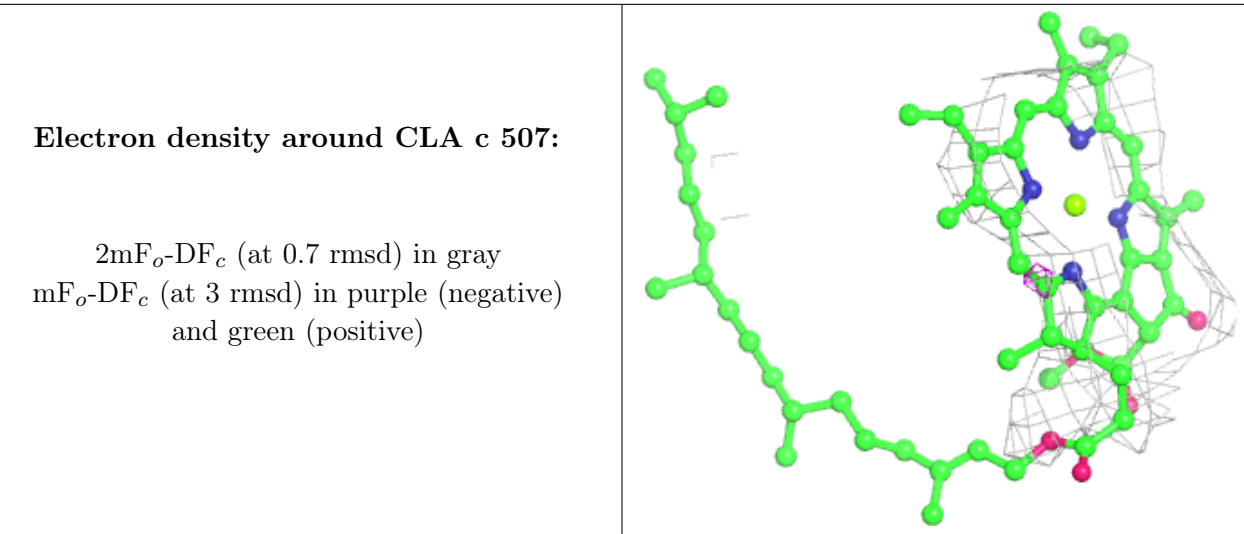
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

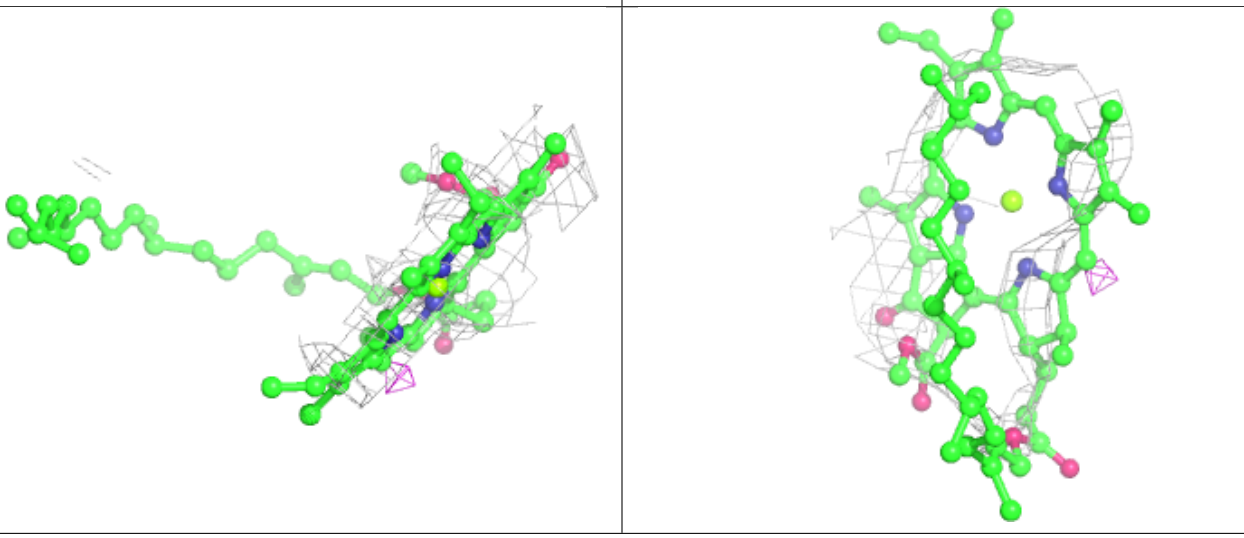




Electron density around CLA c 507:

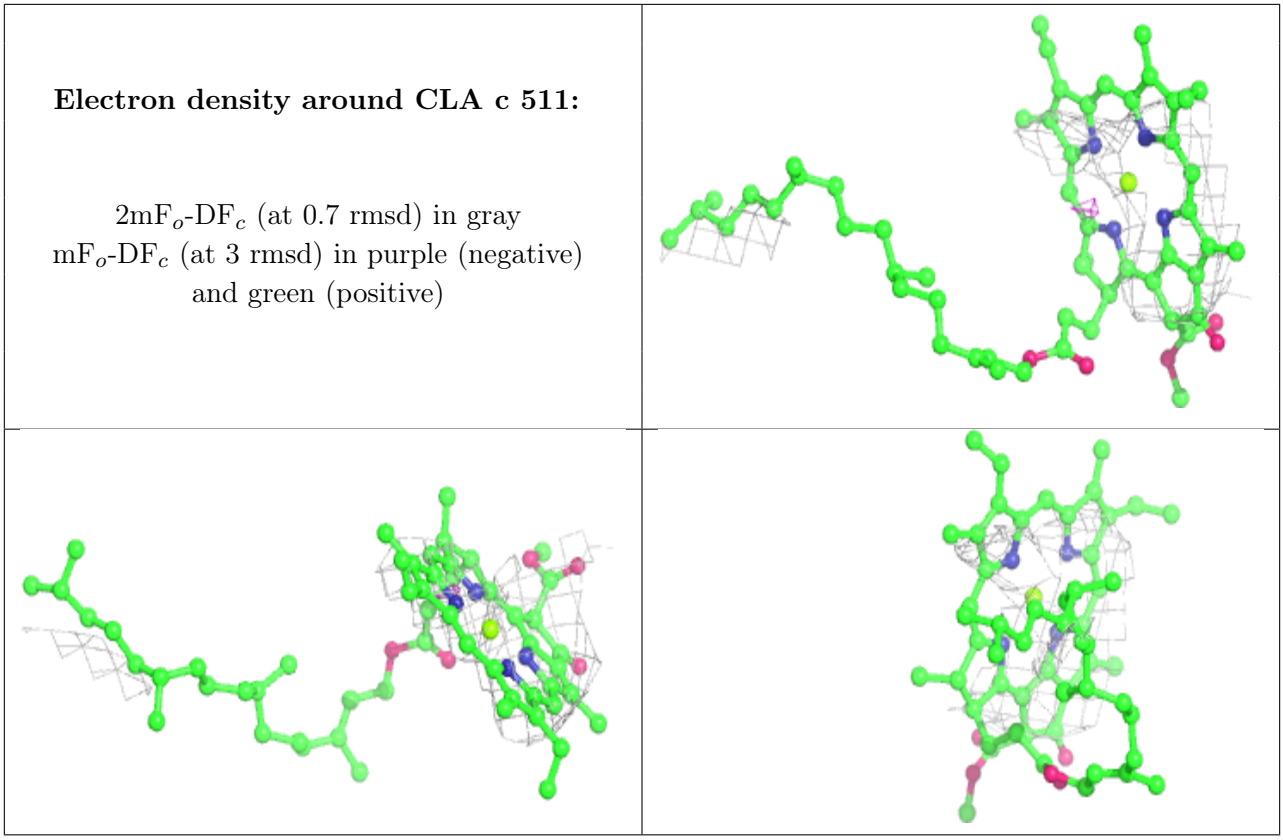
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





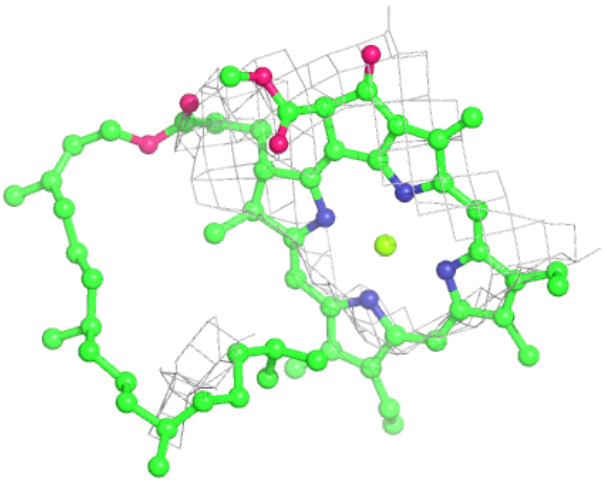
Electron density around CLA c 511:

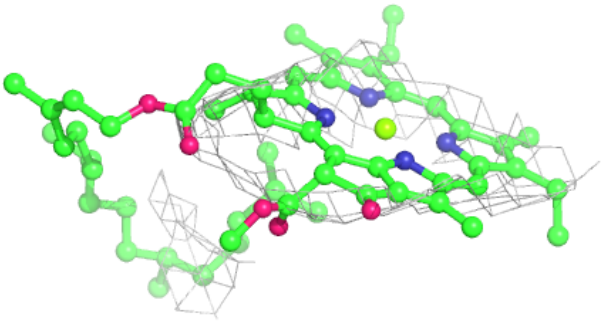
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

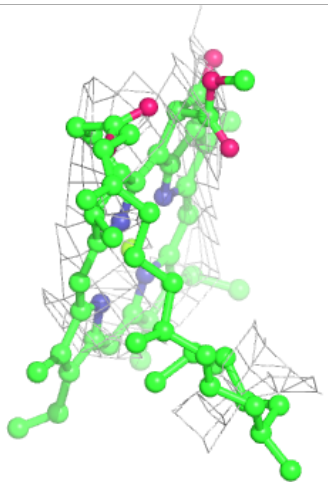


Electron density around CLA B 615:

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

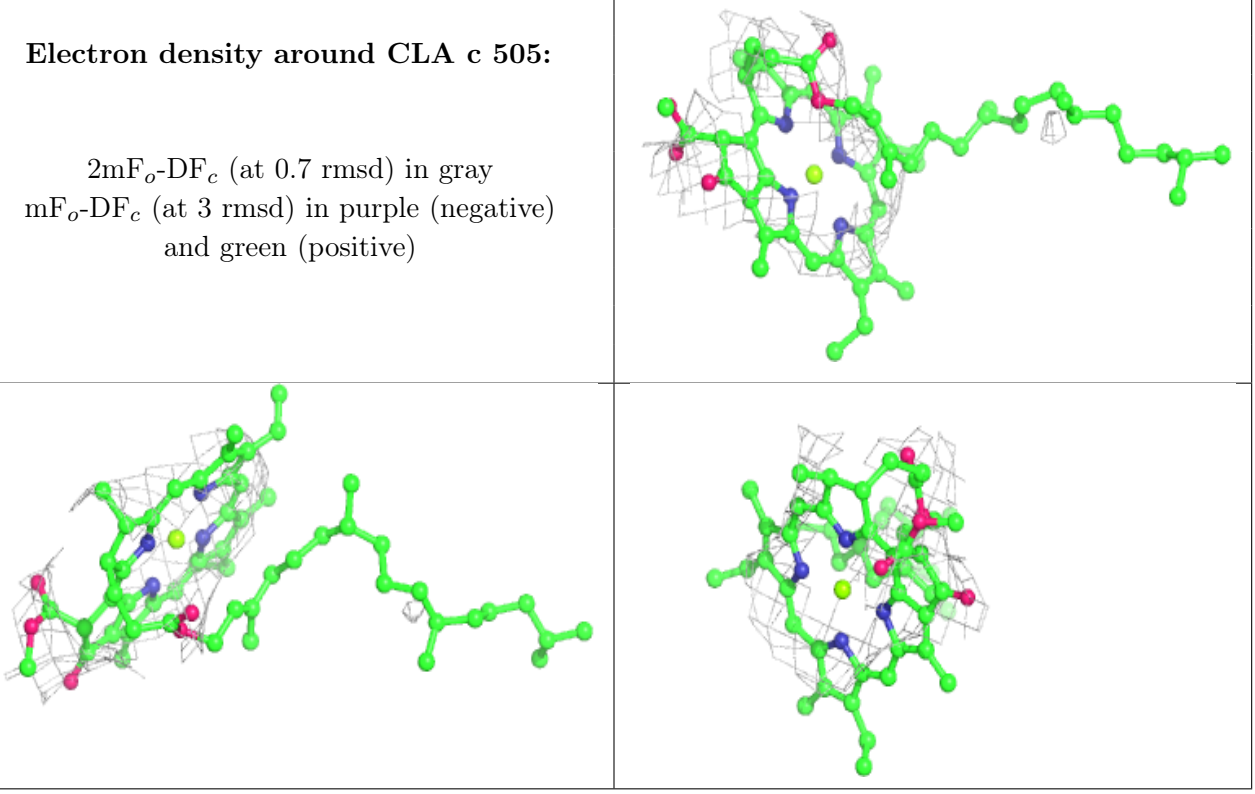






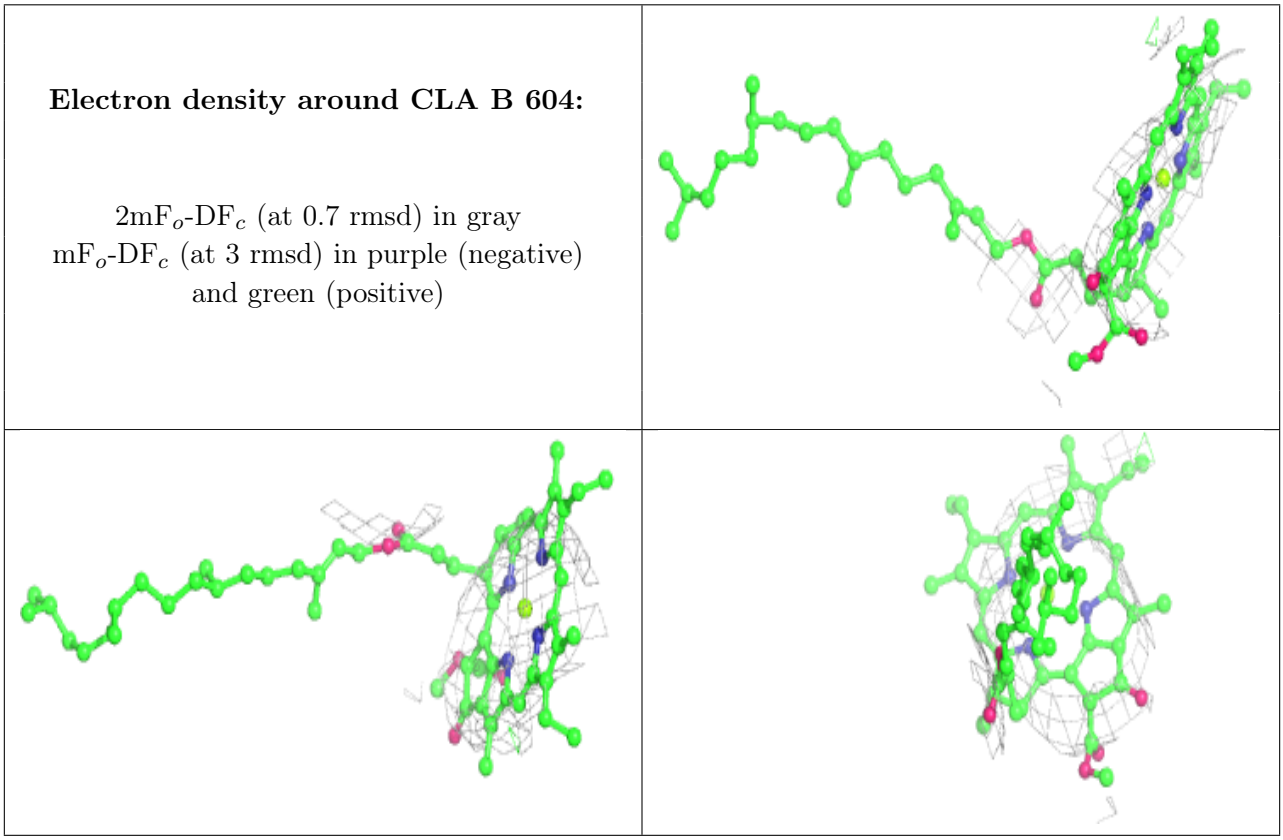
Electron density around CLA c 505:

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



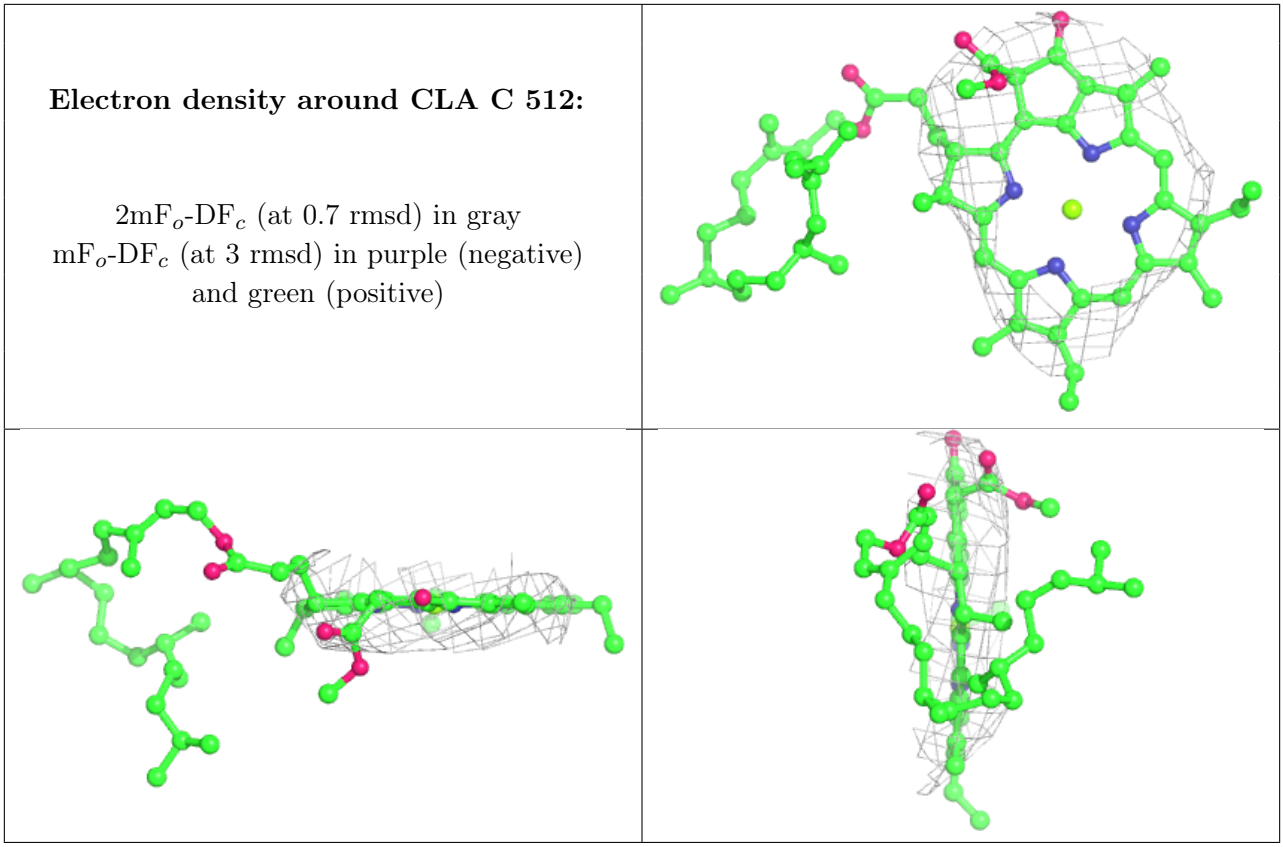
Electron density around CLA B 604:

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



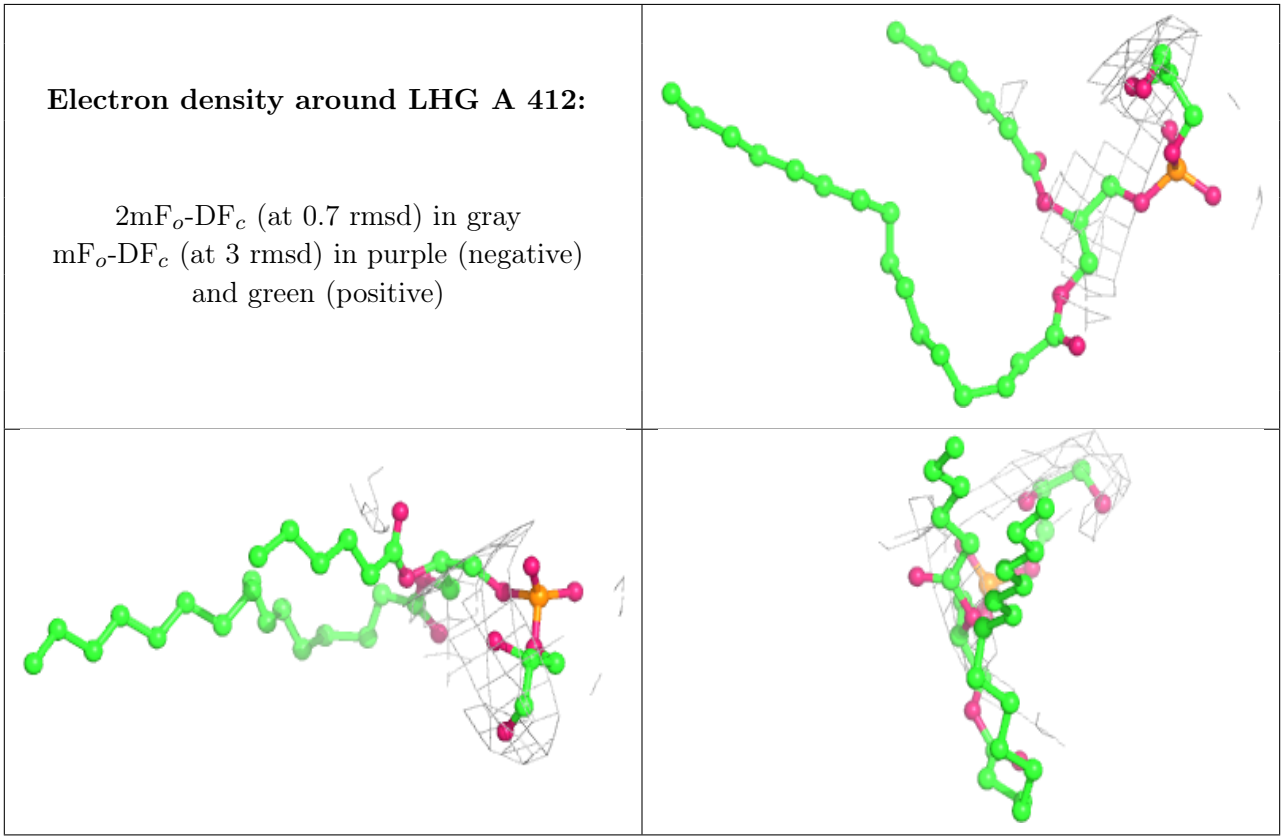
Electron density around CLA C 512:

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



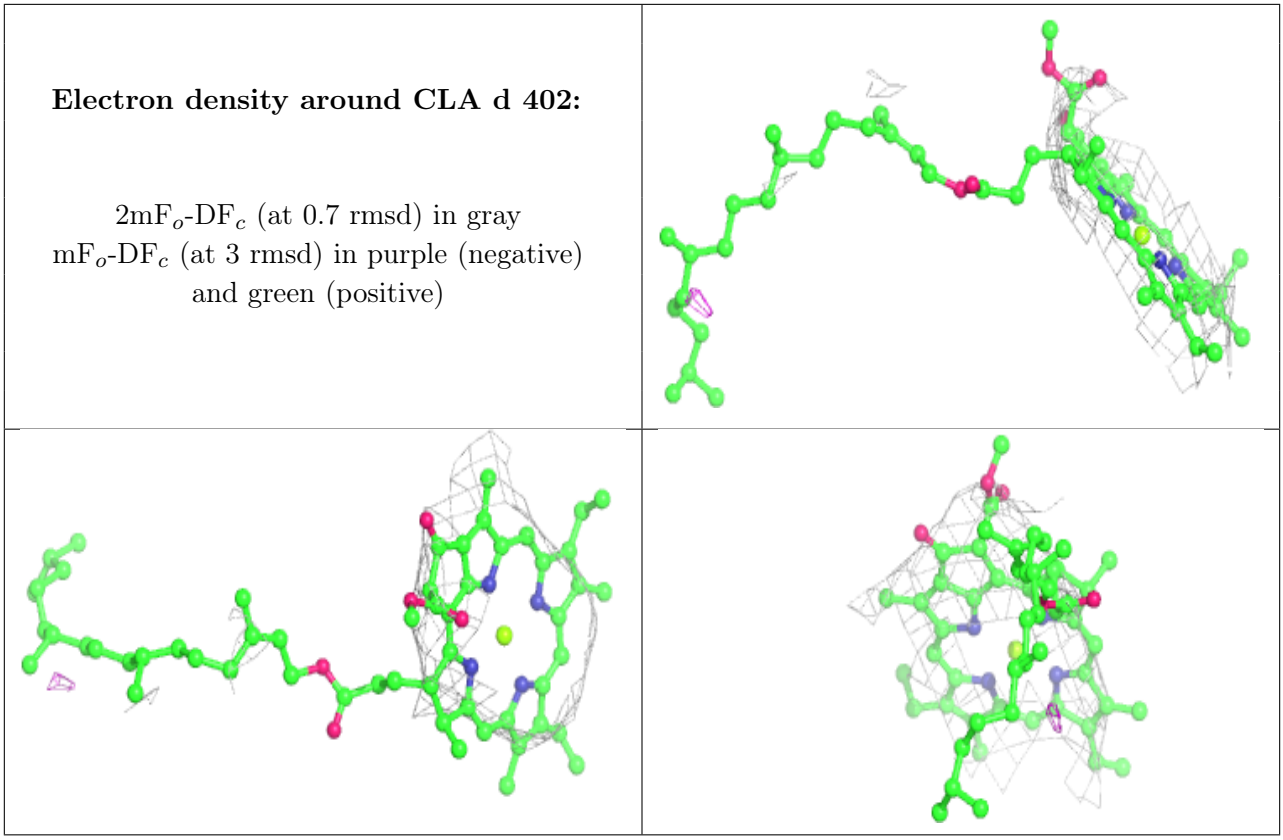
Electron density around LHG A 412:

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



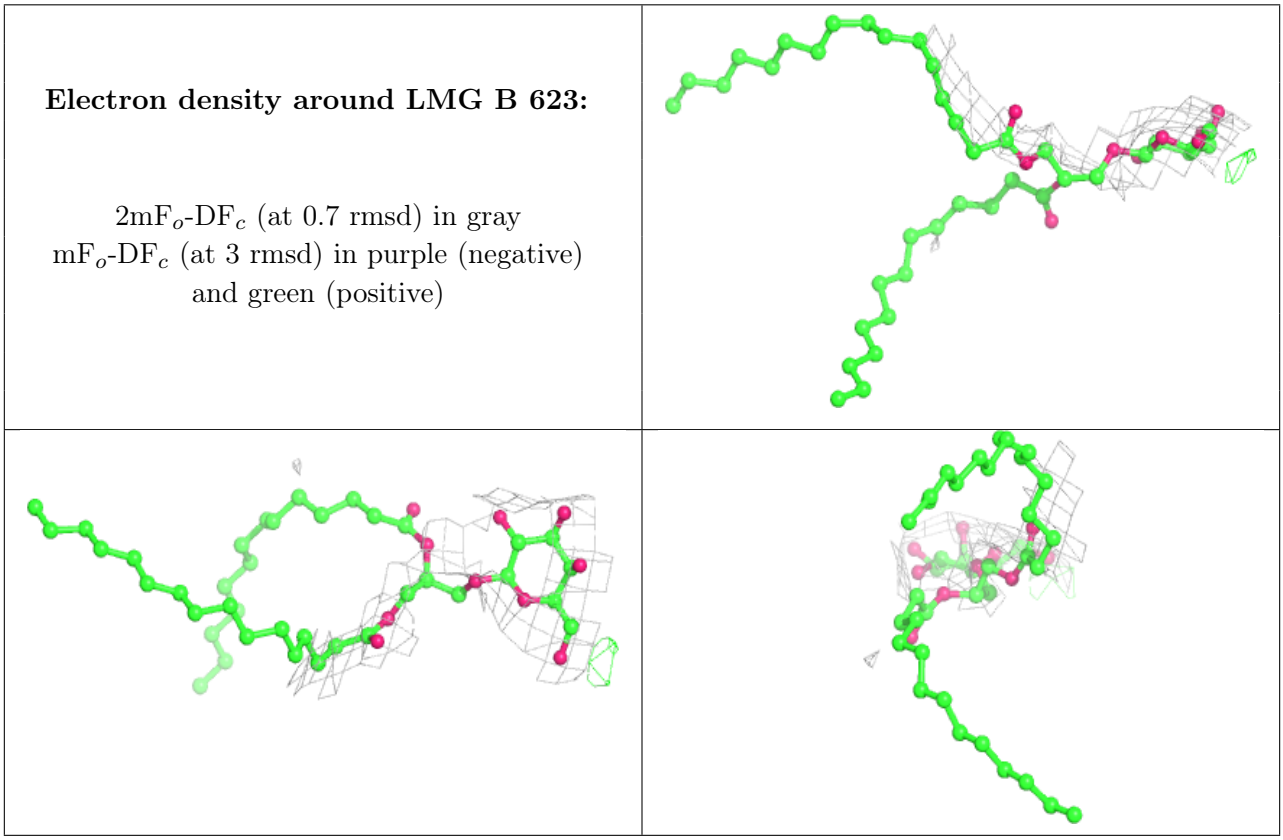
Electron density around CLA d 402:

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



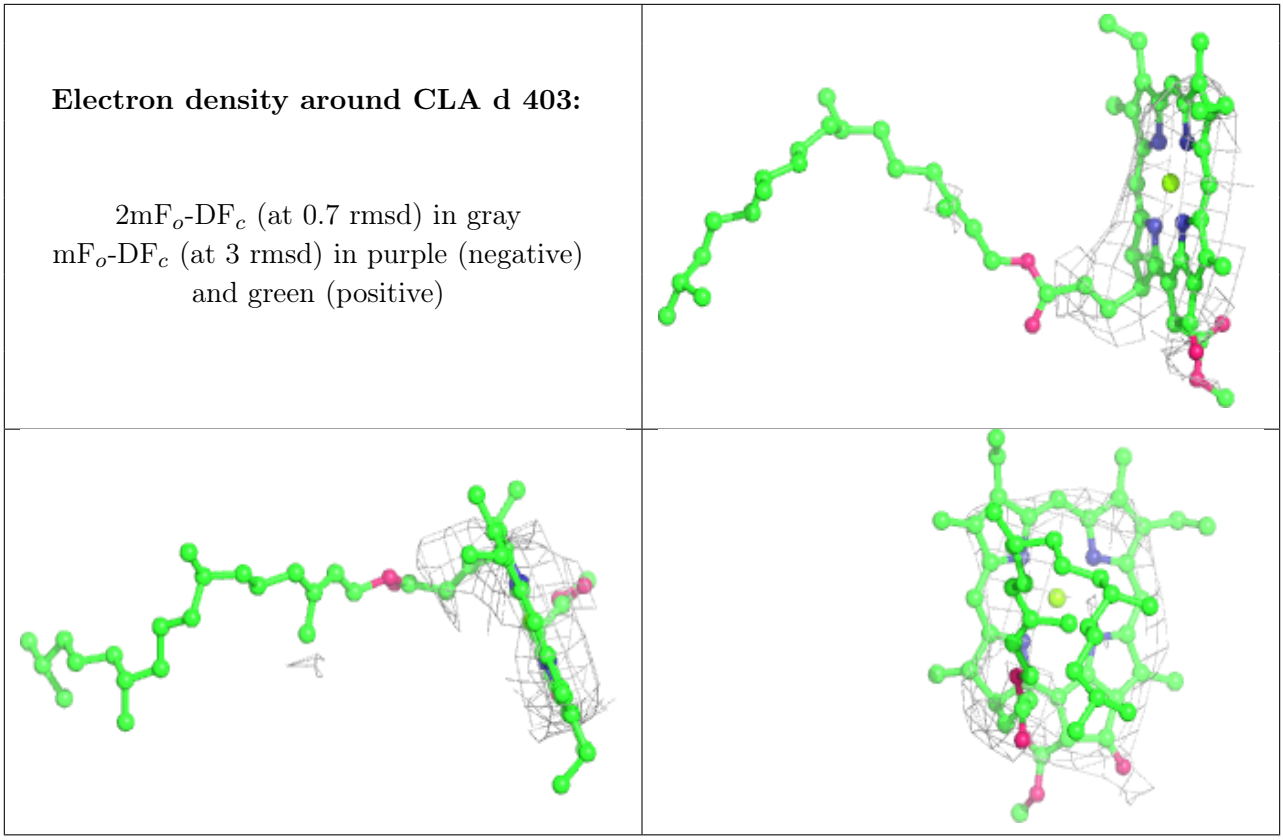
Electron density around LMG B 623:

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



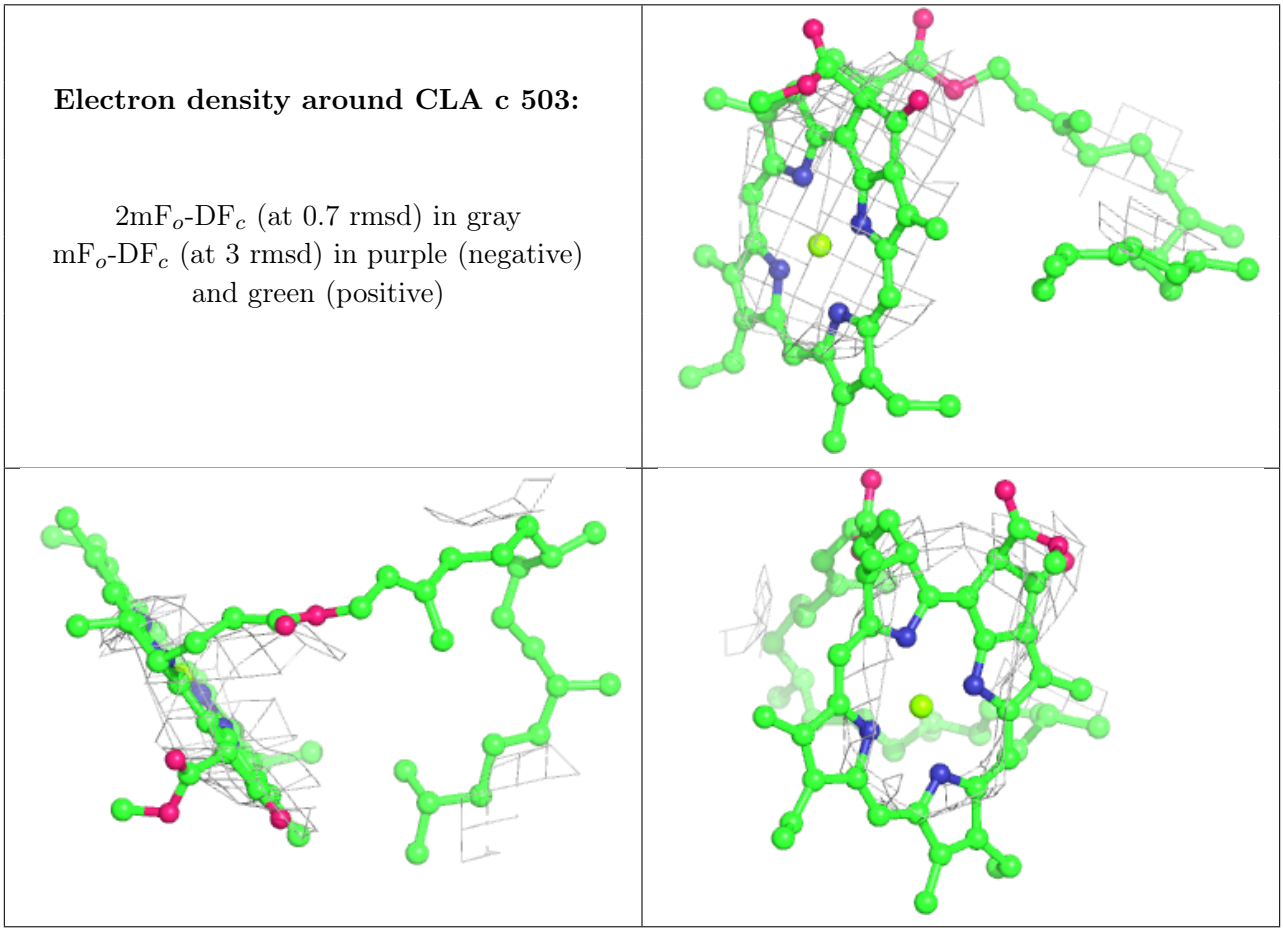
Electron density around CLA d 403:

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



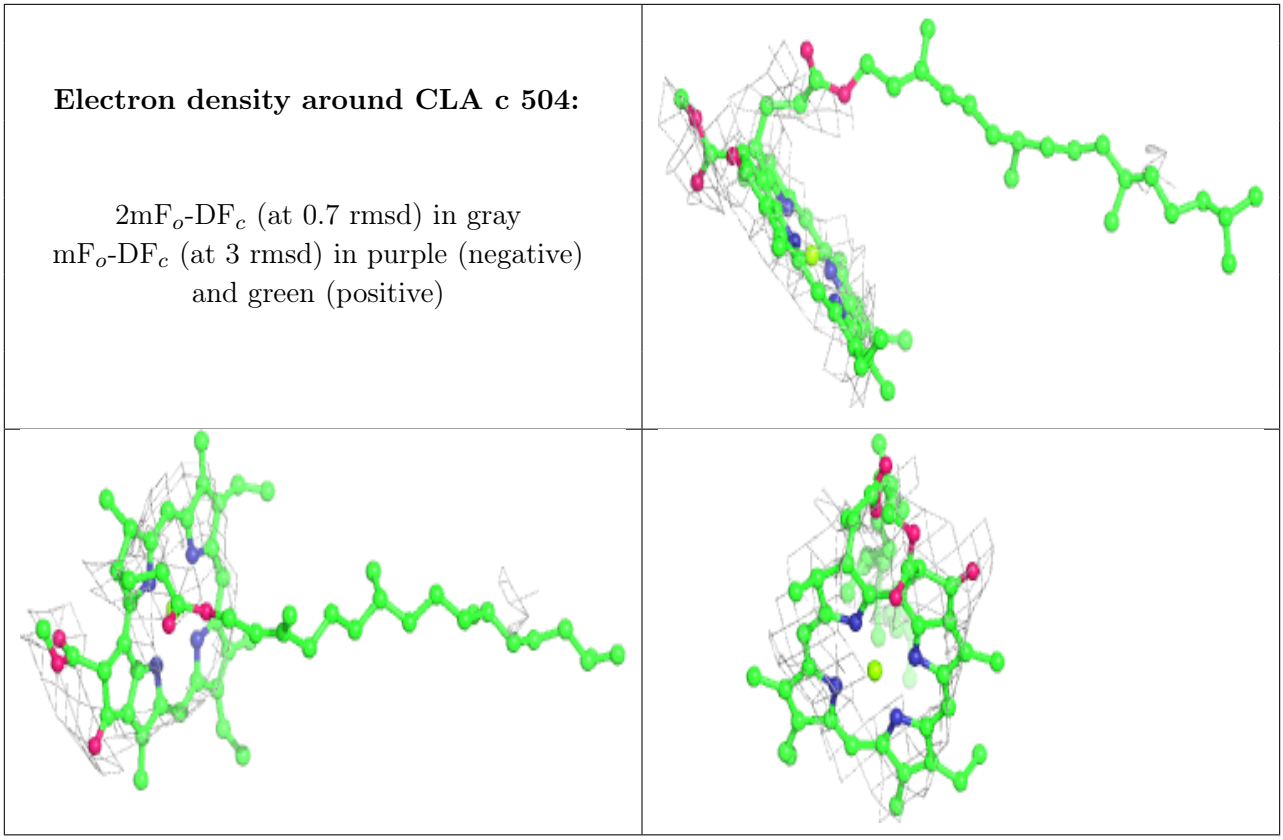
Electron density around CLA c 503:

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



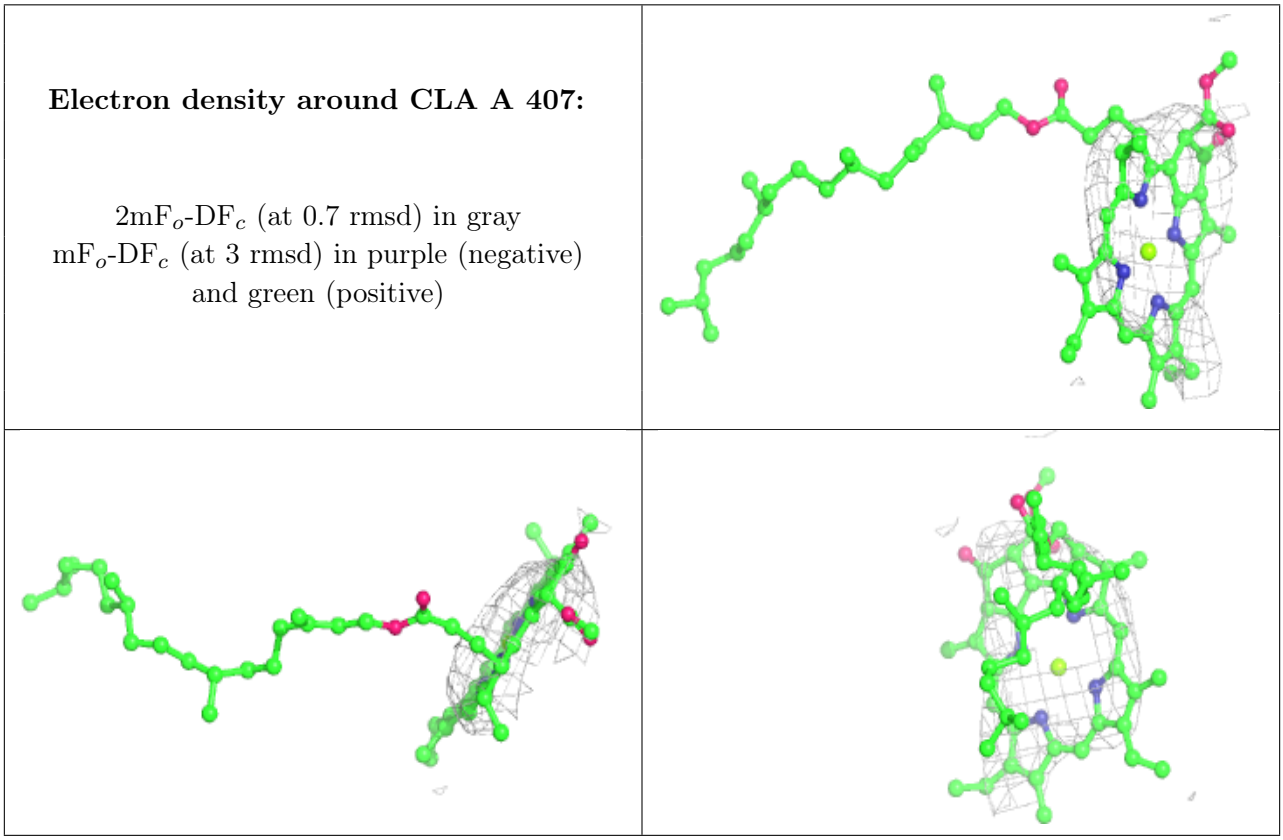
Electron density around CLA c 504:

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



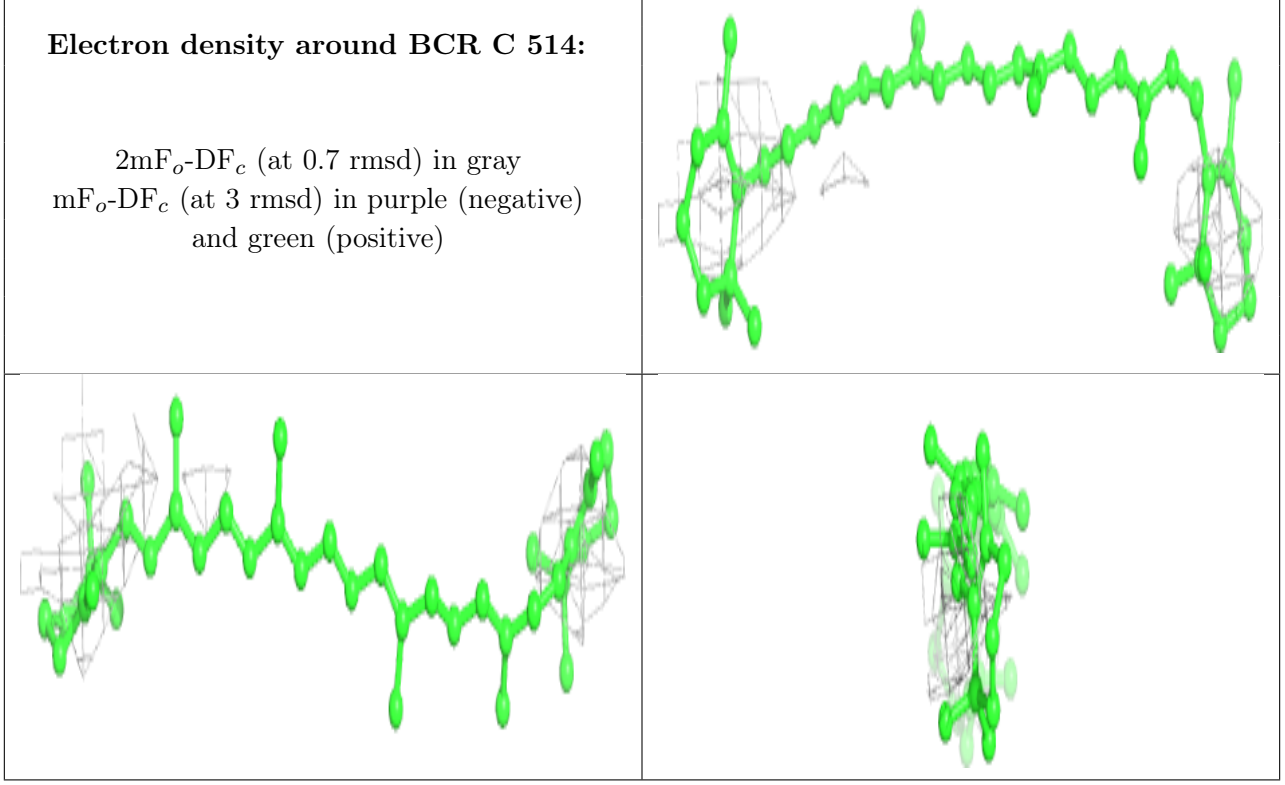
Electron density around CLA A 407:

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



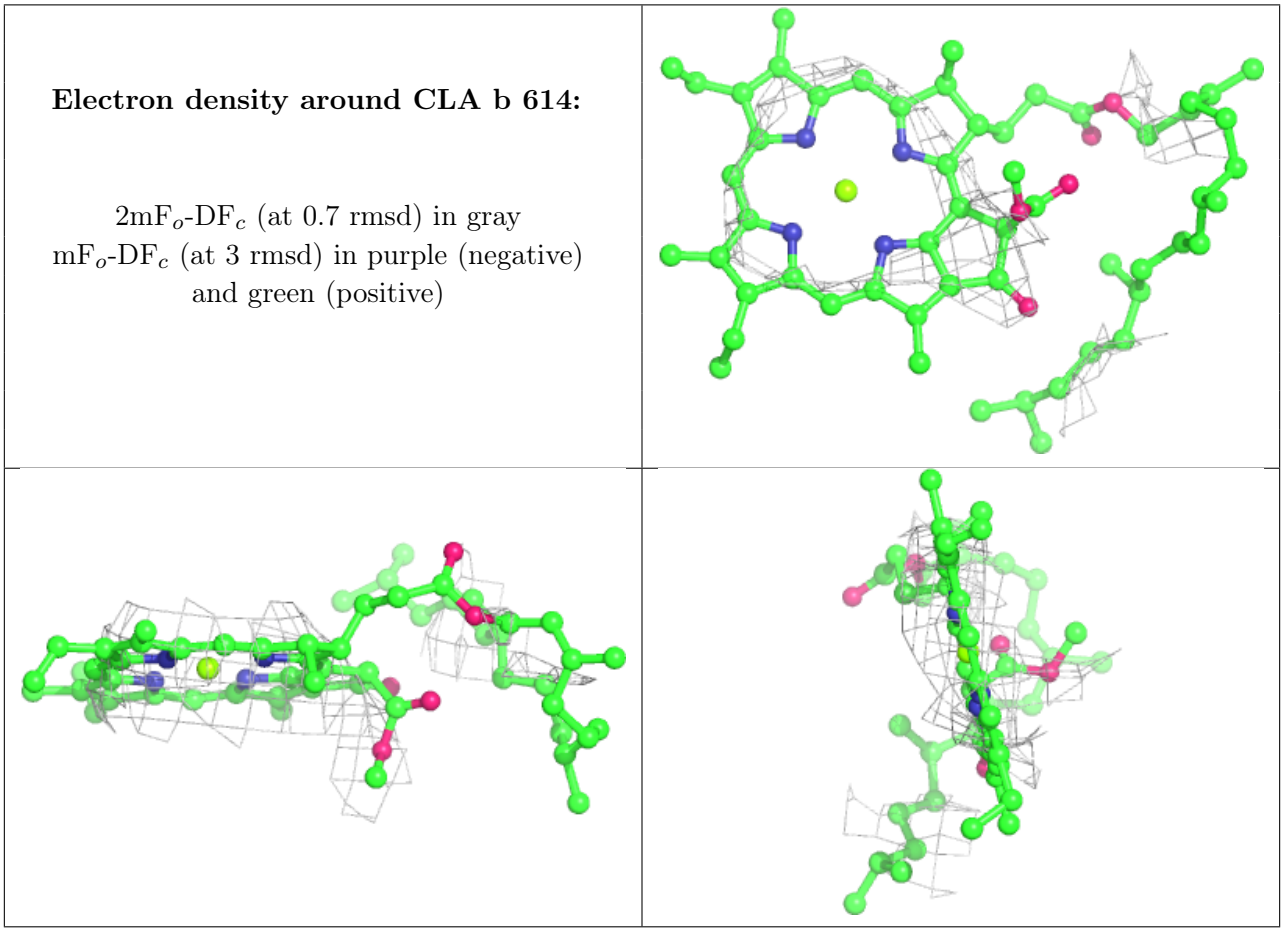
Electron density around BCR C 514:

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



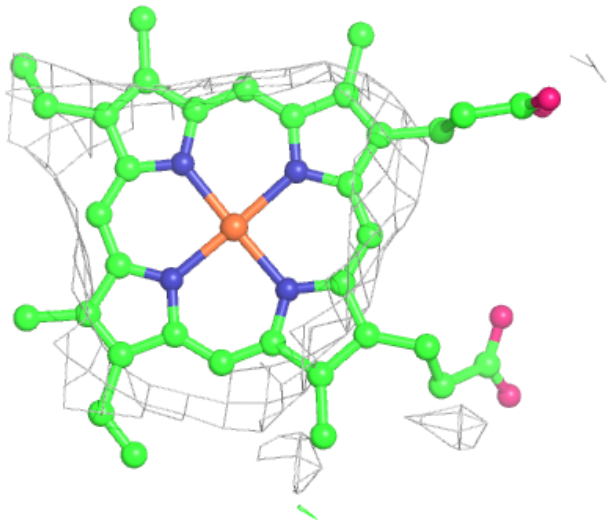
Electron density around CLA b 614:

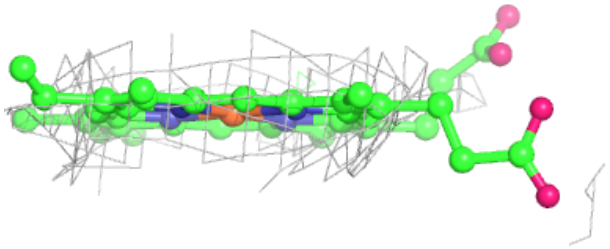
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

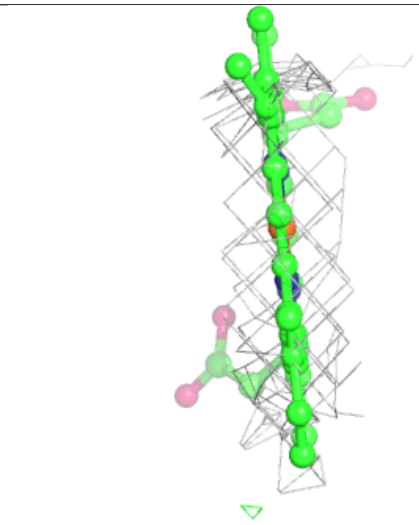


Electron density around HEM v 201:

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

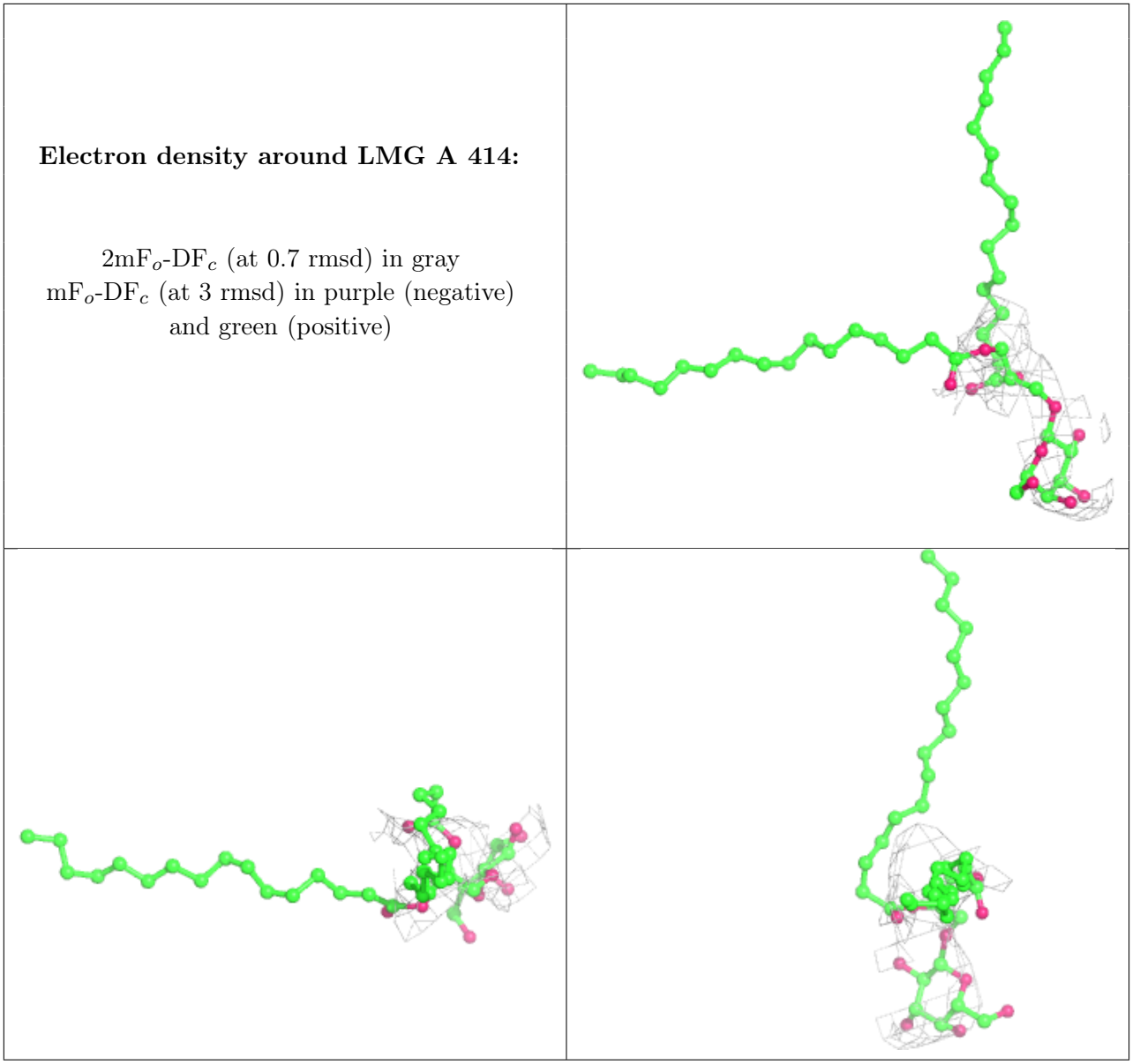






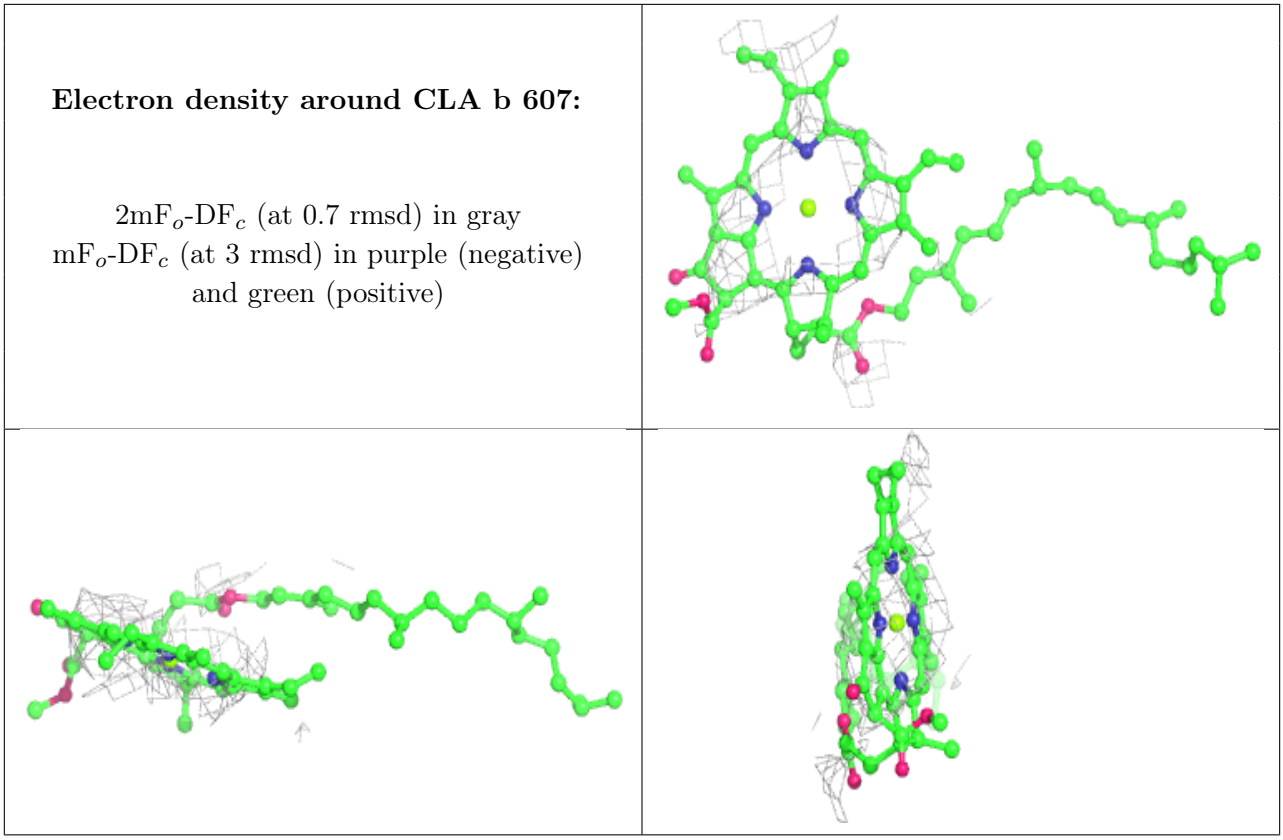
Electron density around LMG A 414:

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



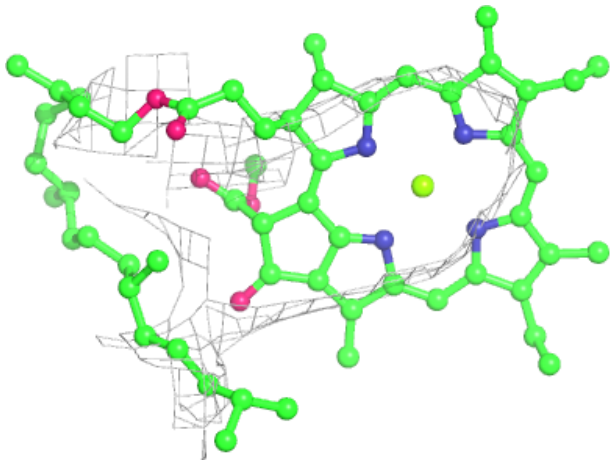
Electron density around CLA b 607:

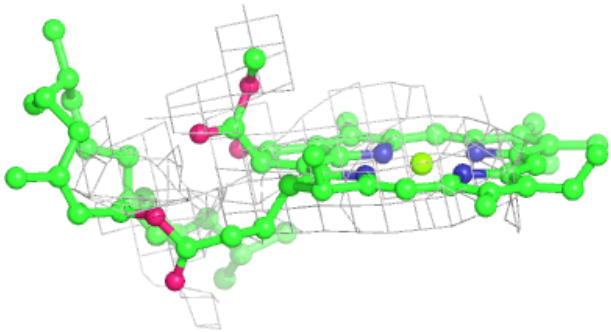
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

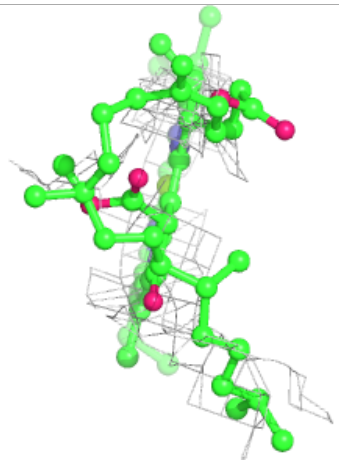


Electron density around CLA B 610:

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

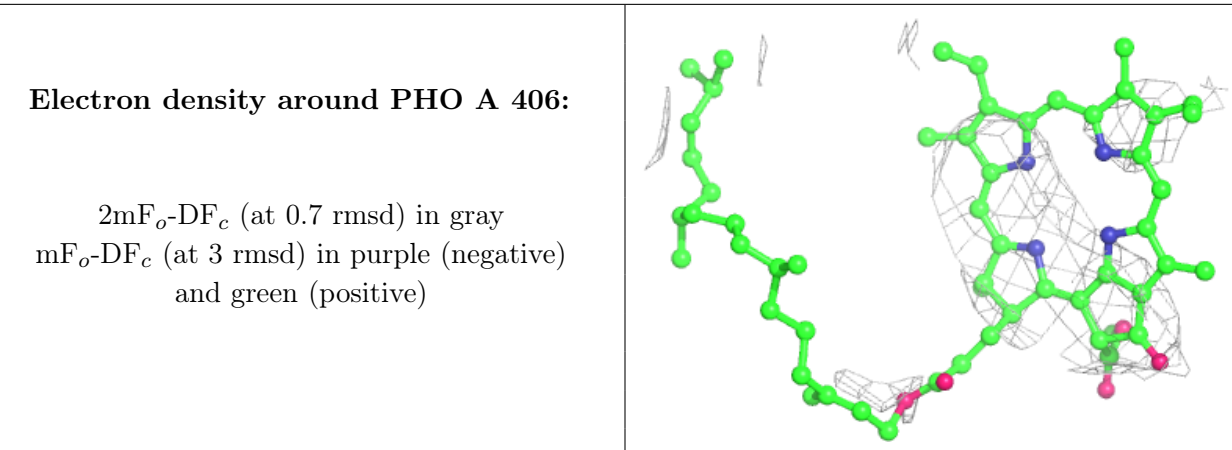






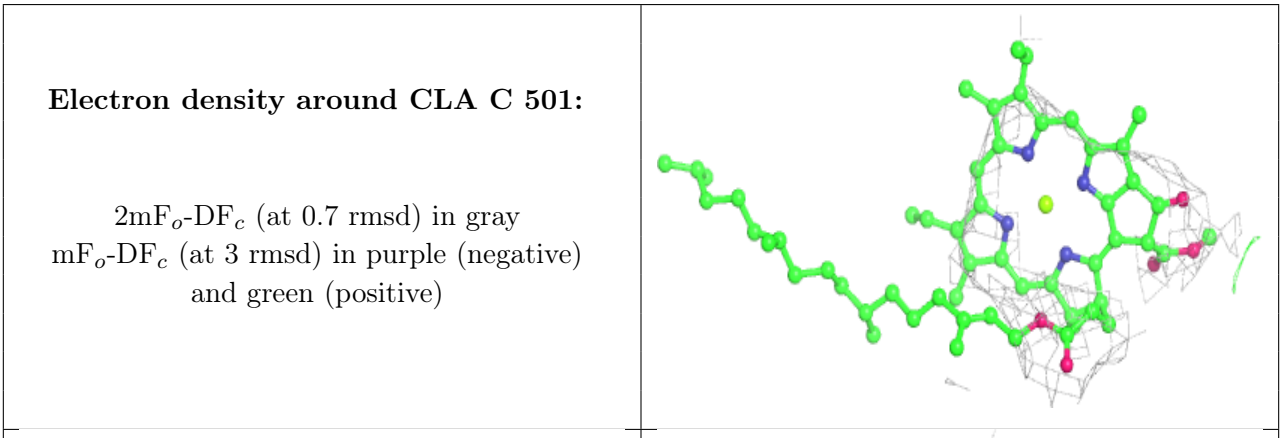
Electron density around PHO A 406:

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



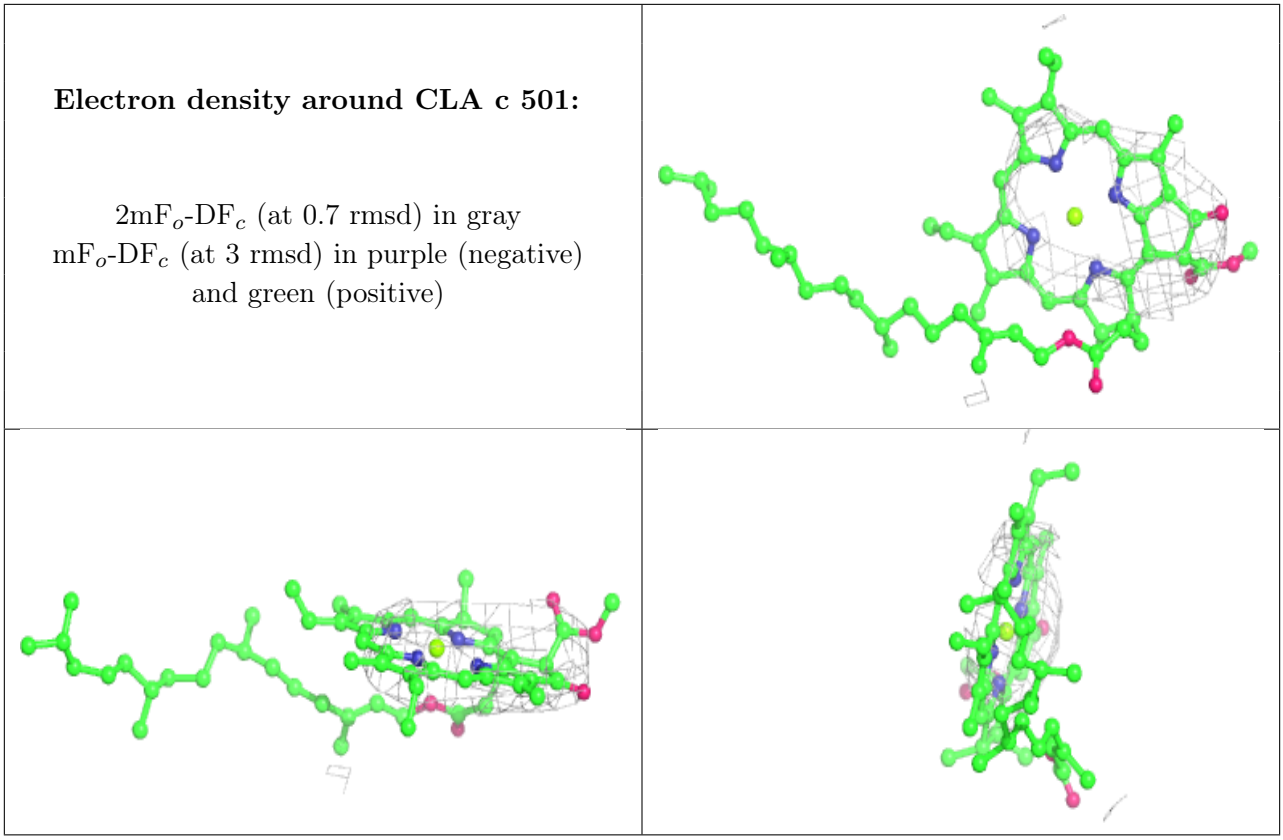
Electron density around CLA C 501:

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



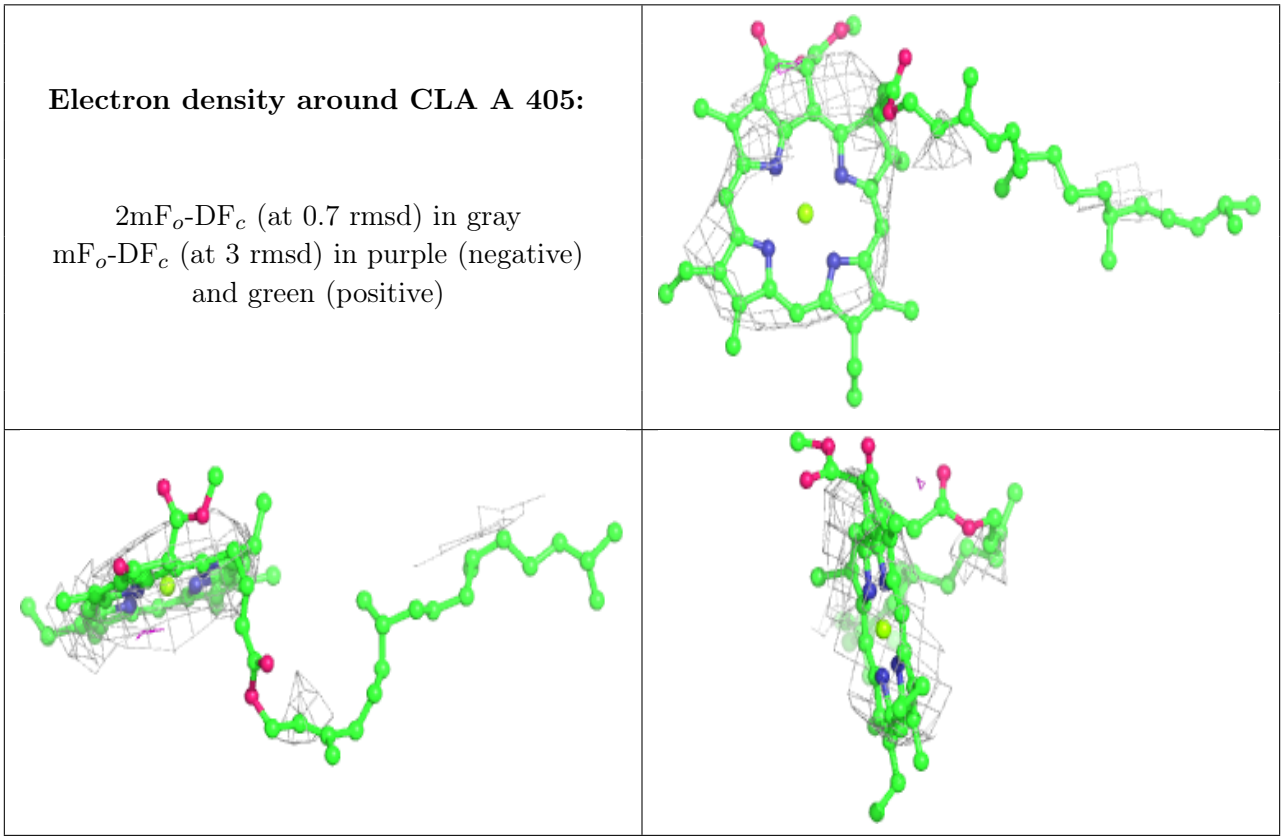
Electron density around CLA c 501:

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



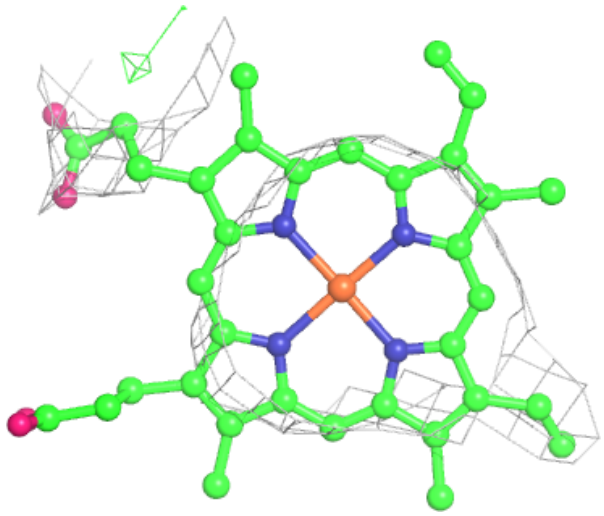
Electron density around CLA A 405:

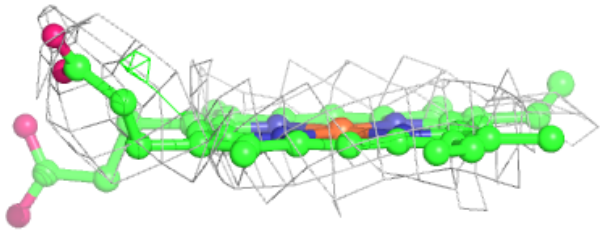
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

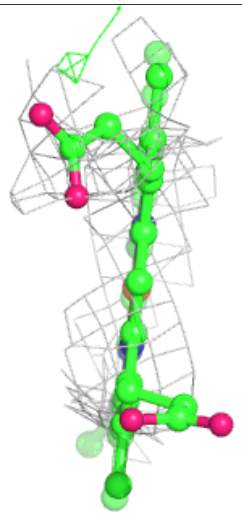


Electron density around HEM V 201:

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

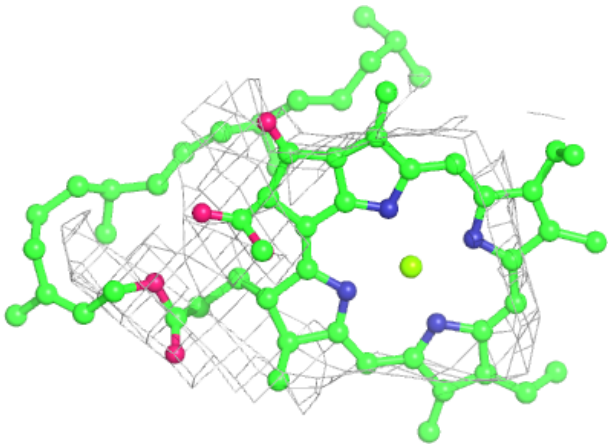


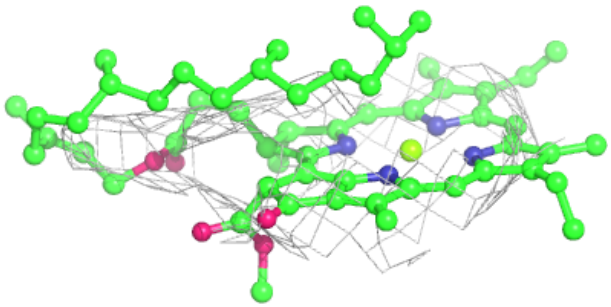


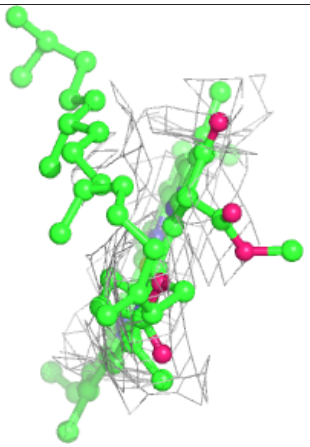


Electron density around CLA c 509:

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

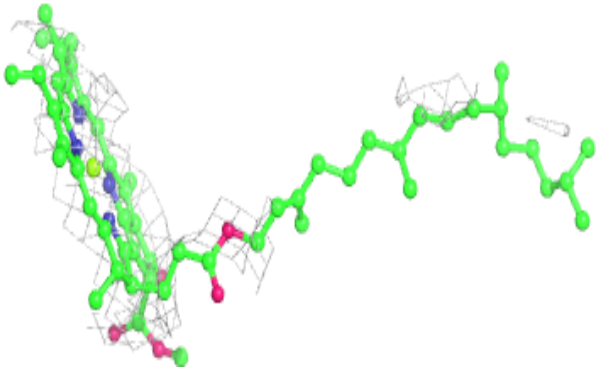


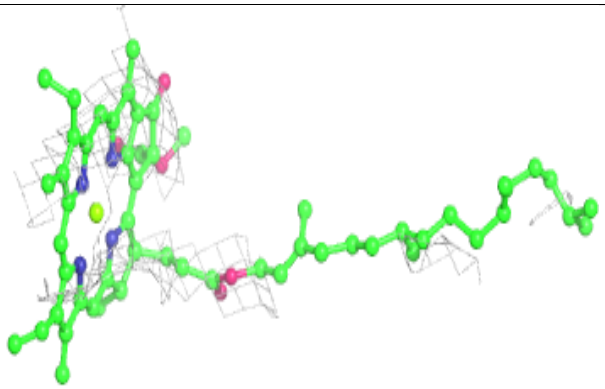


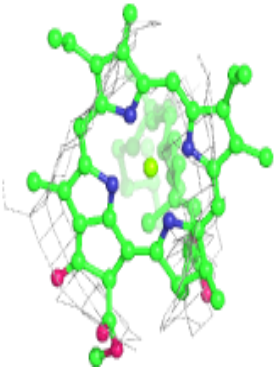


Electron density around CLA b 608:

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

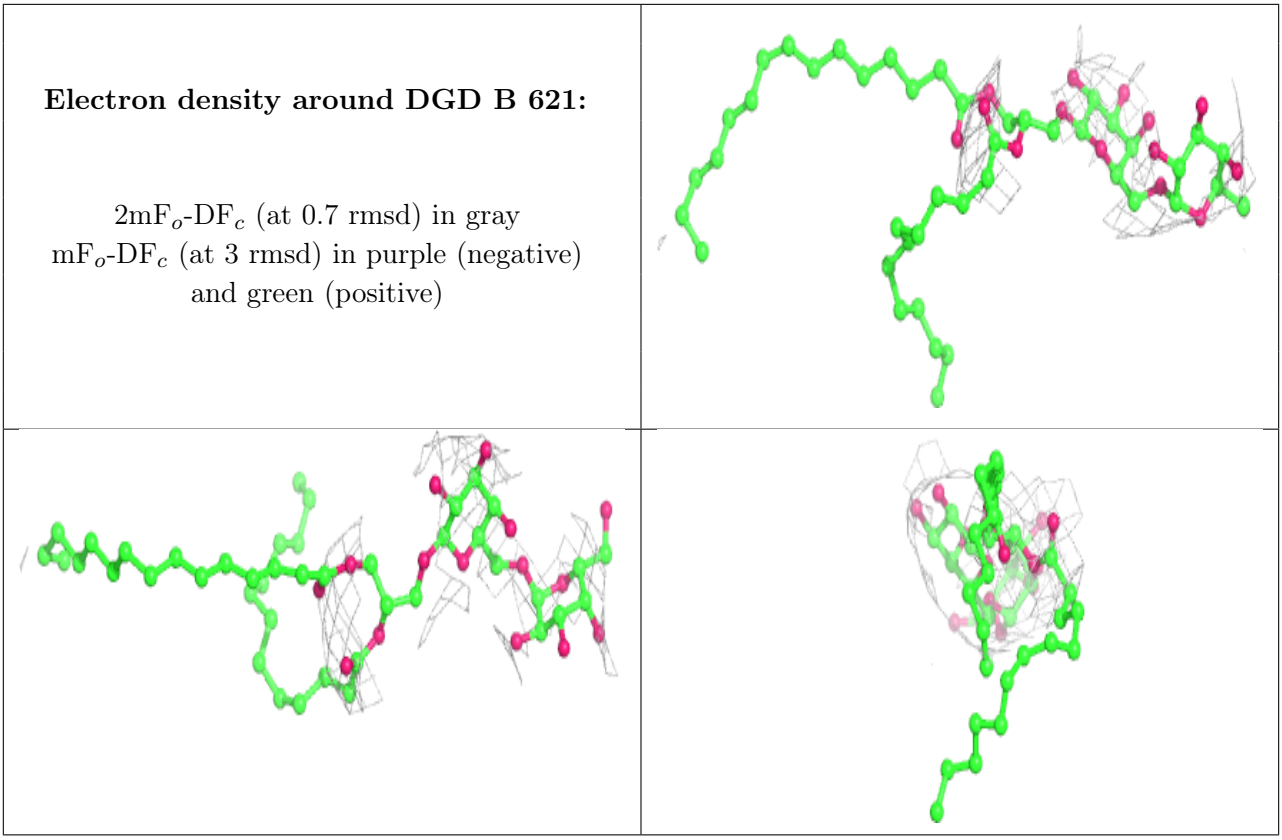






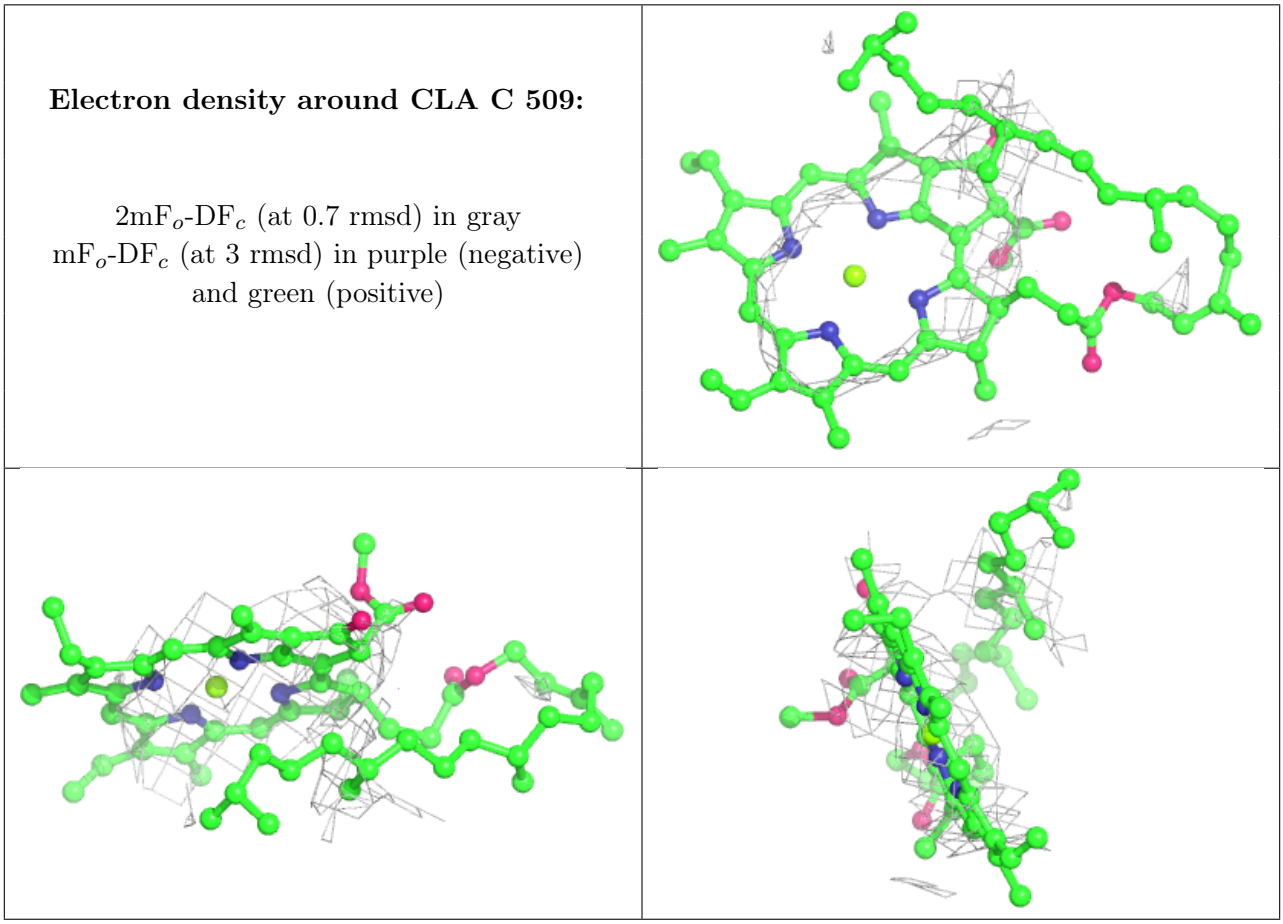
Electron density around DGD B 621:

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



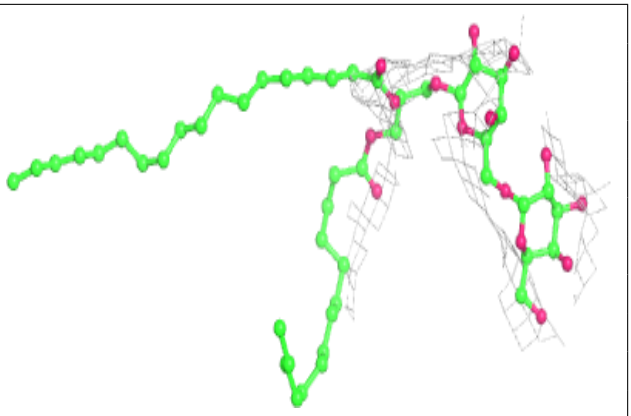
Electron density around CLA C 509:

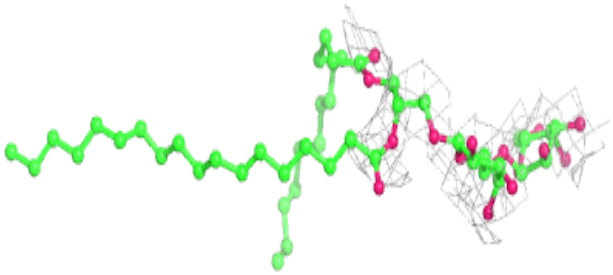
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

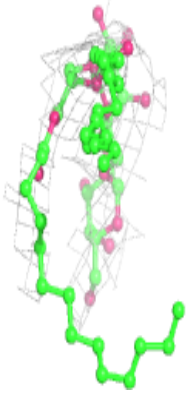


Electron density around DGD c 517:

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

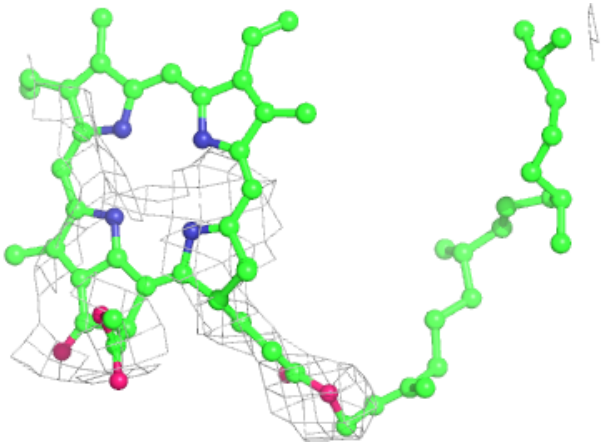


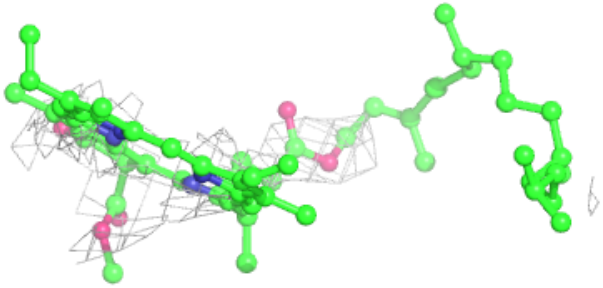


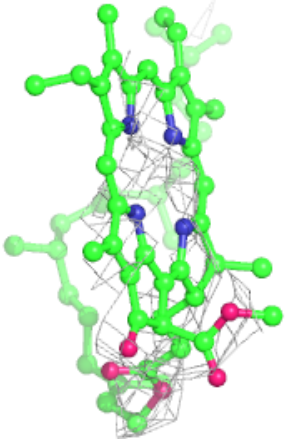


Electron density around PHO a 408:

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

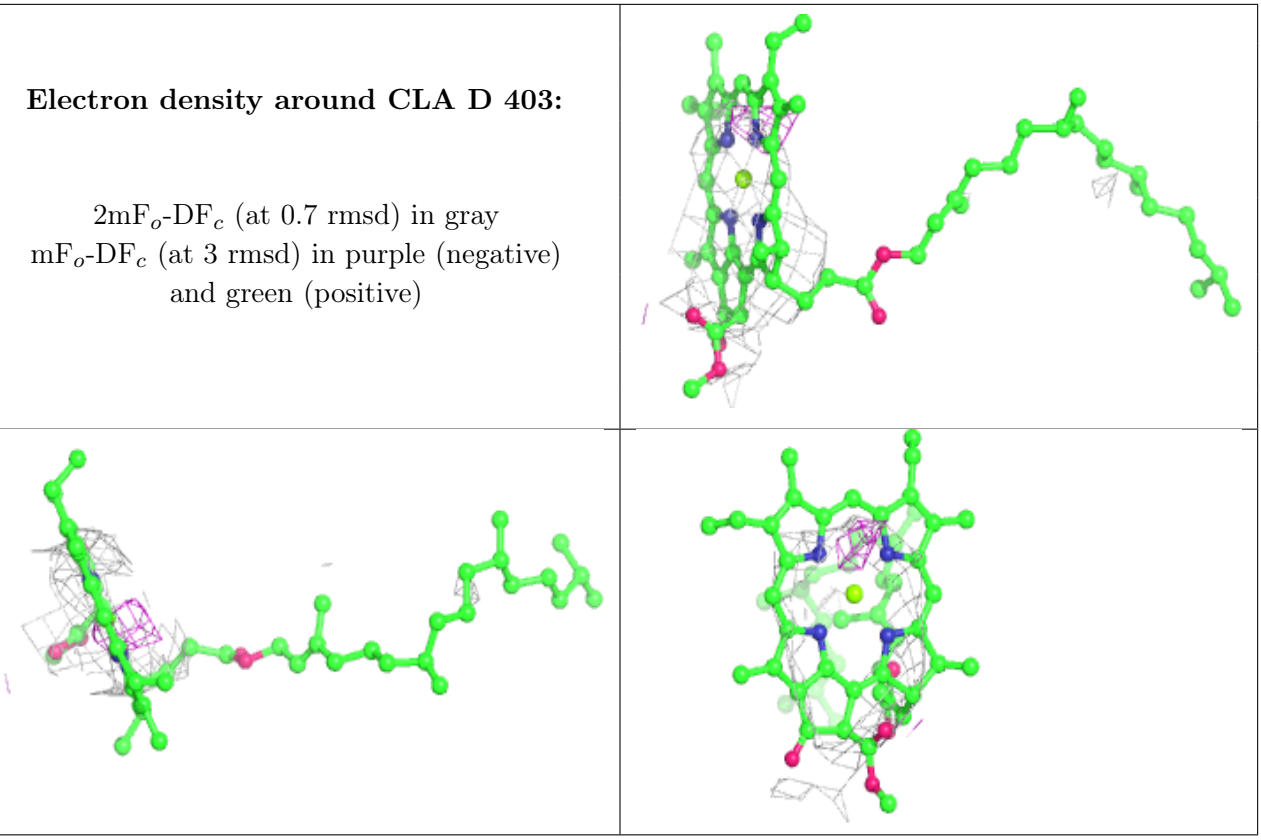






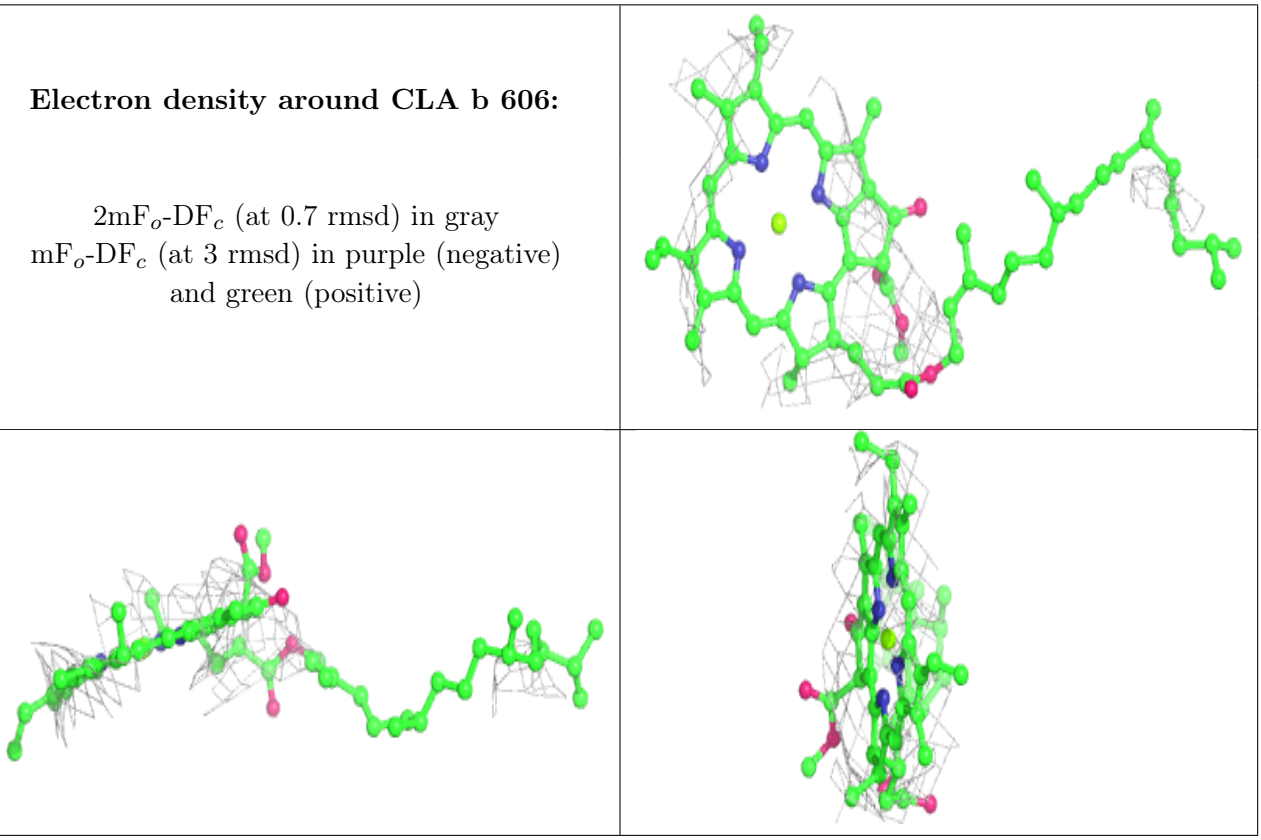
Electron density around CLA D 403:

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



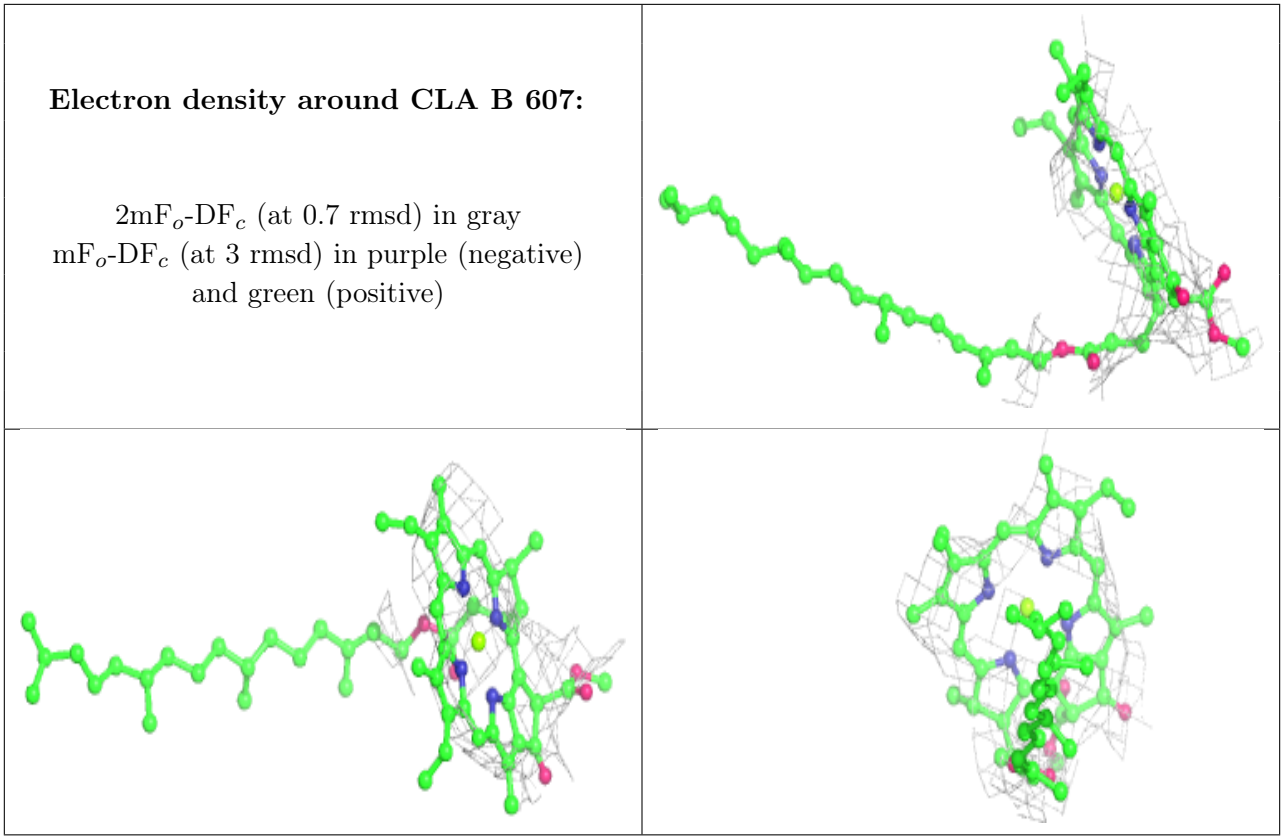
Electron density around CLA b 606:

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



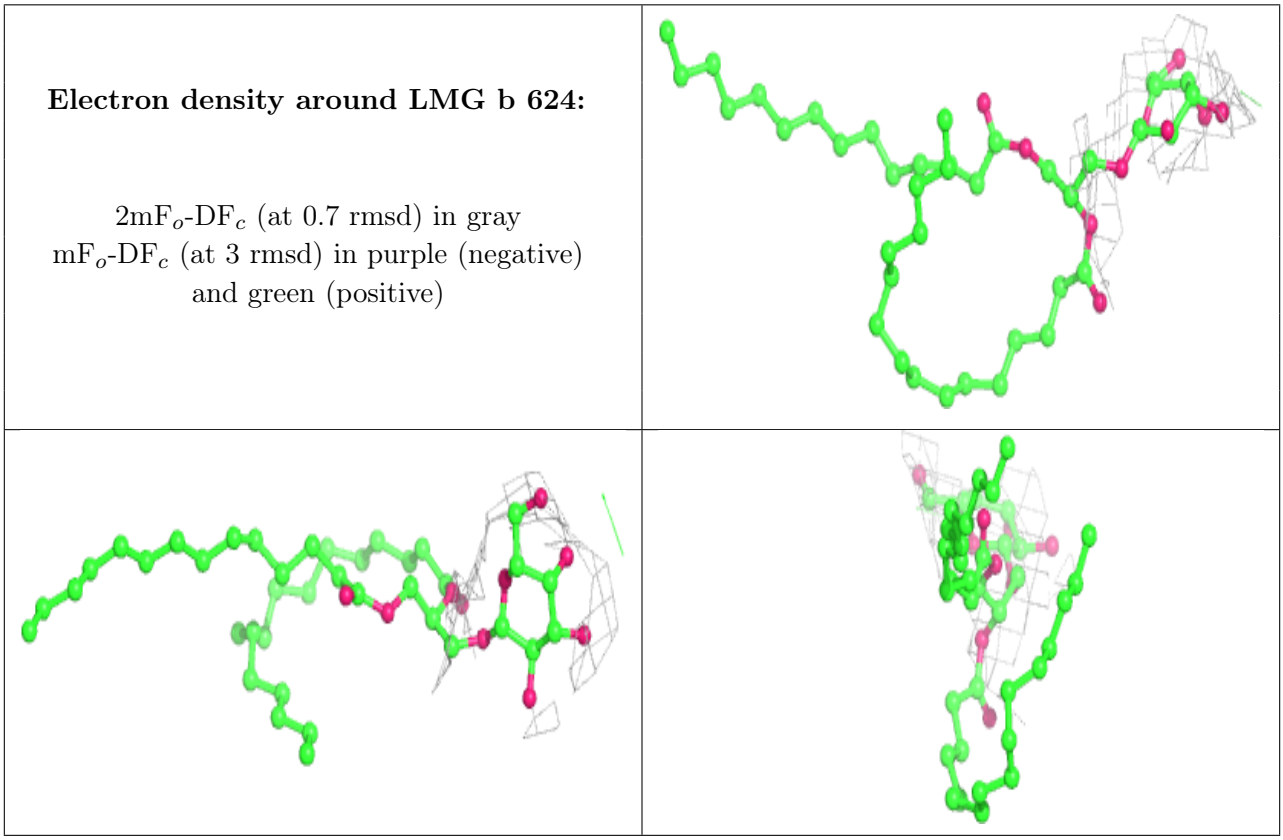
Electron density around CLA B 607:

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



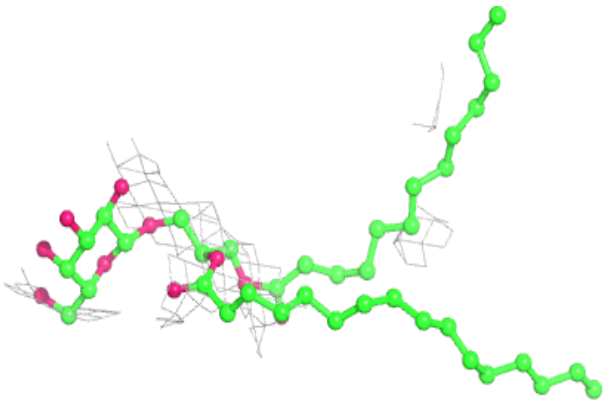
Electron density around LMG b 624:

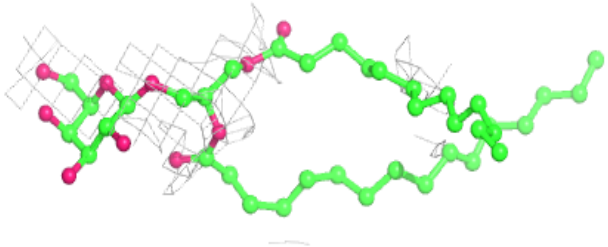
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

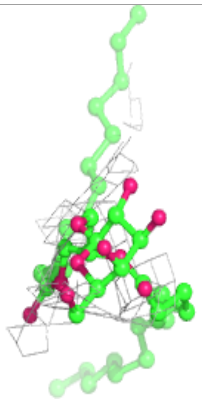


Electron density around LMG D 407:

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

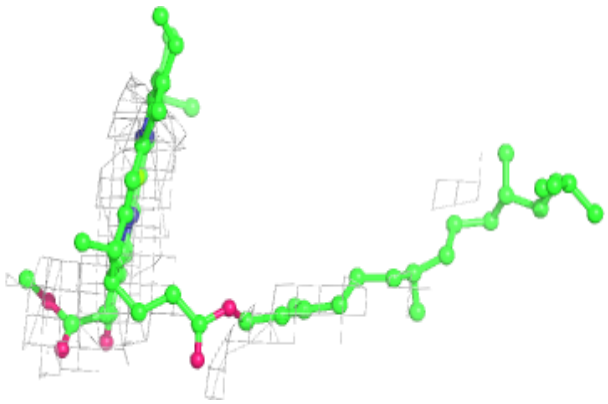


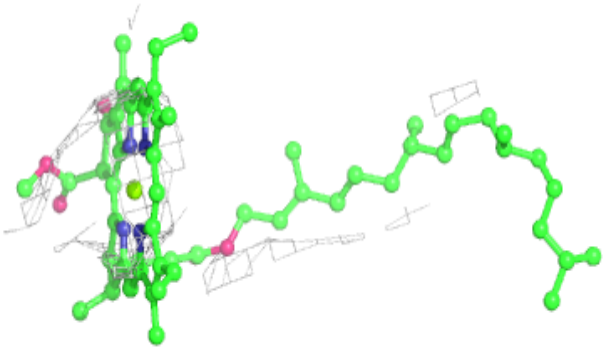


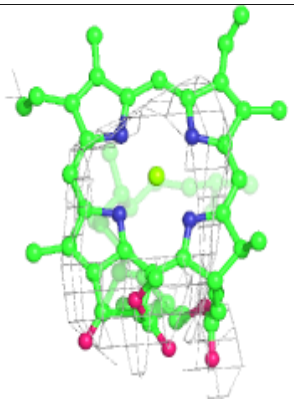


Electron density around CLA B 605:

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

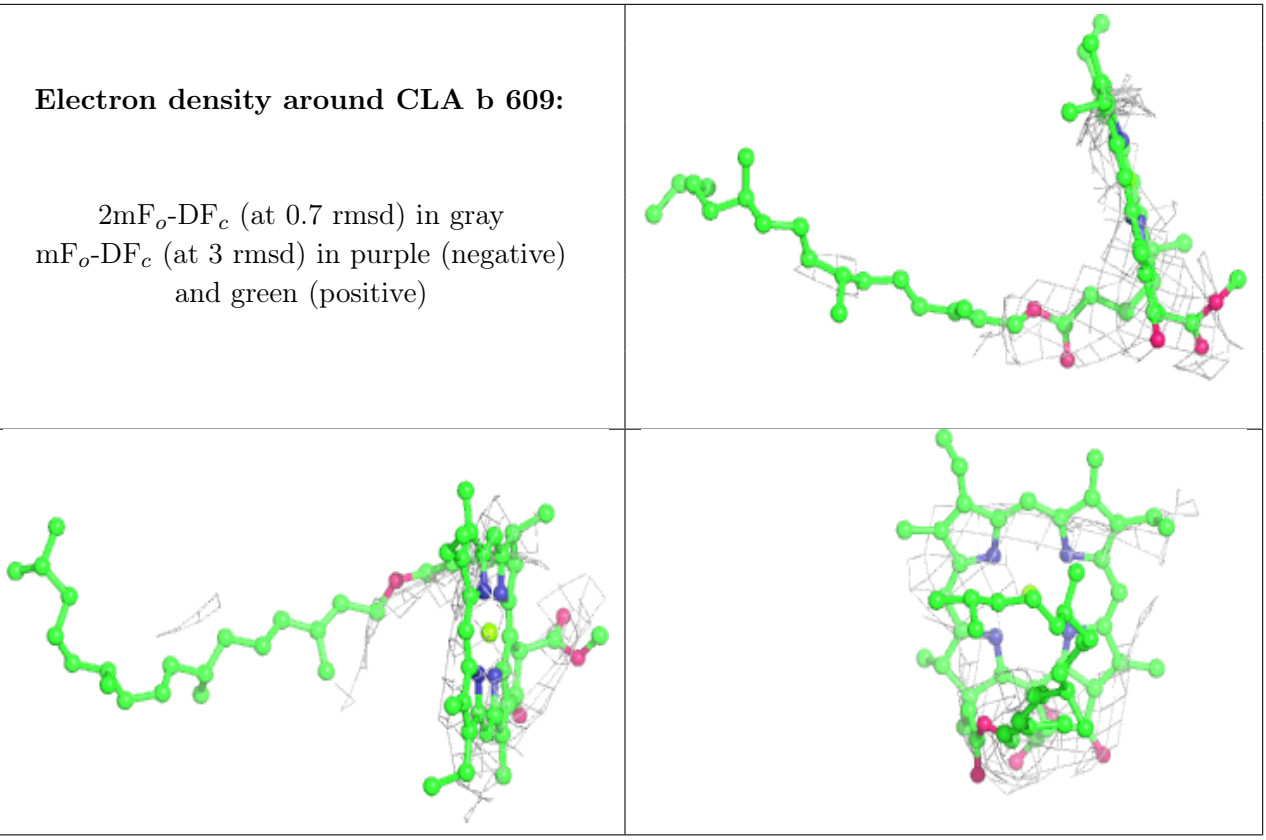






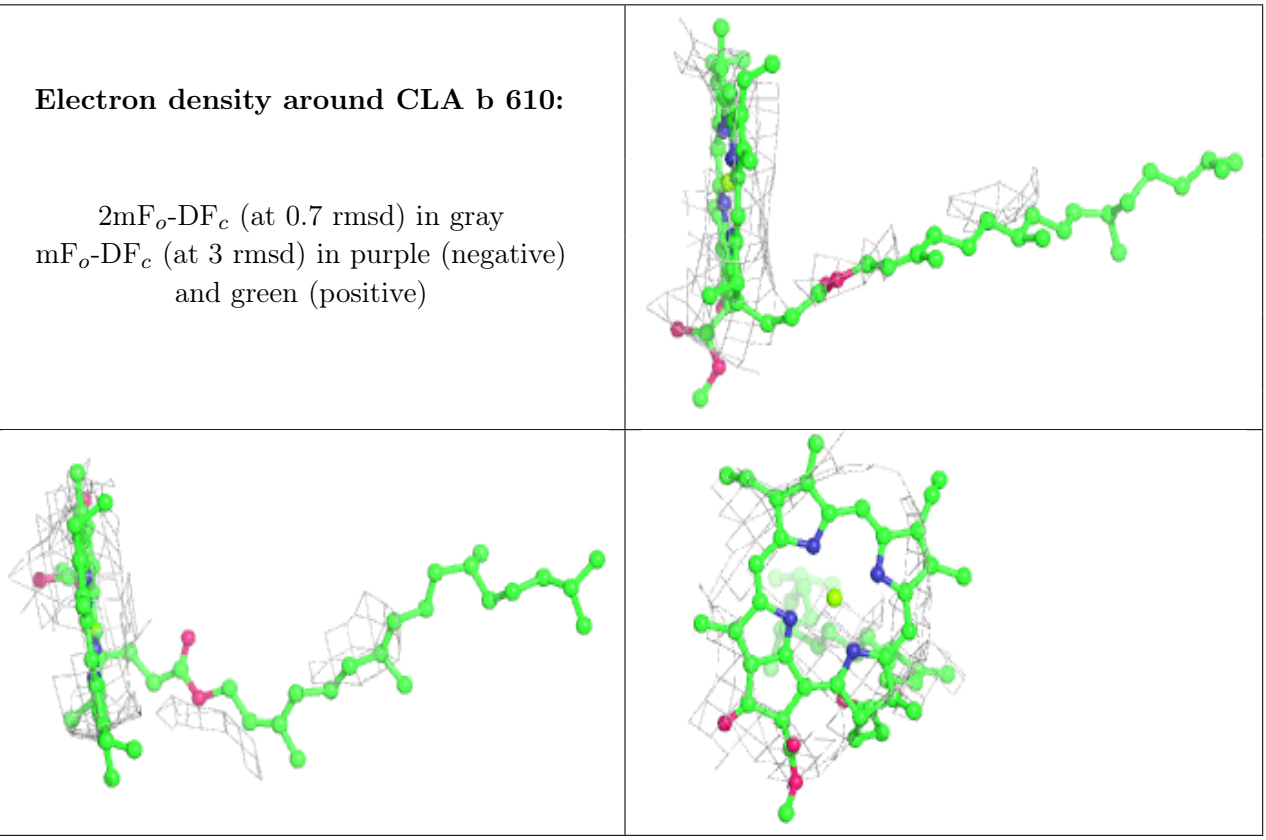
Electron density around CLA b 609:

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



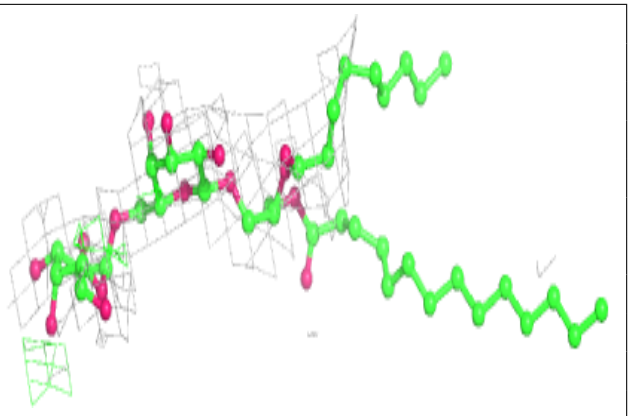
Electron density around CLA b 610:

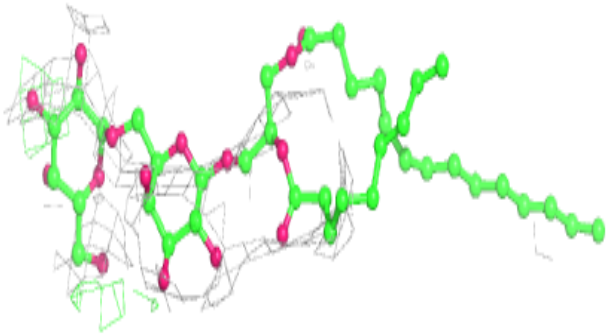
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

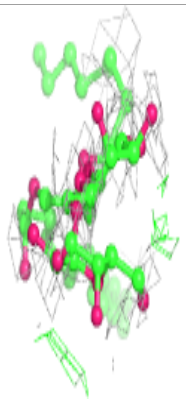


Electron density around DGD C 517:

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

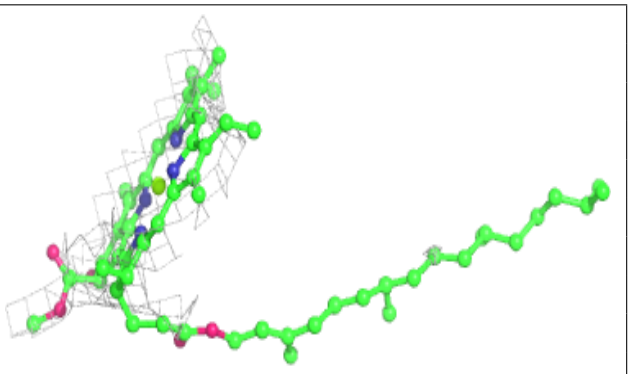


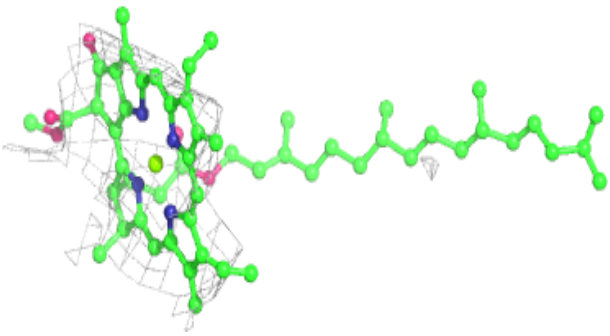


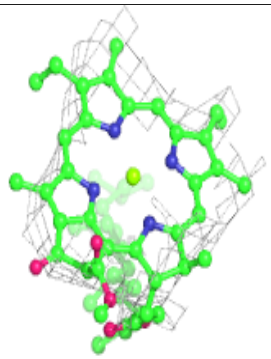


Electron density around CLA b 611:

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

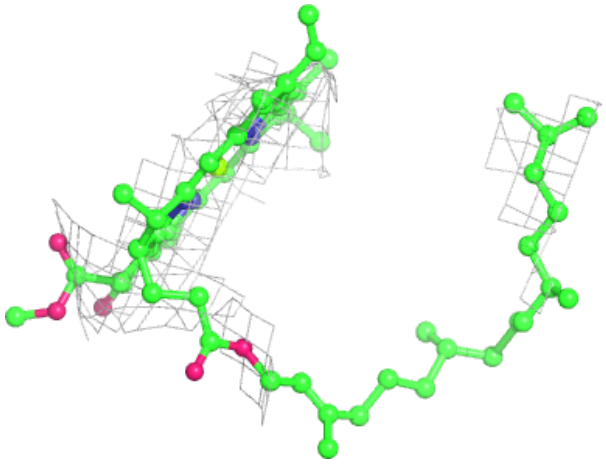


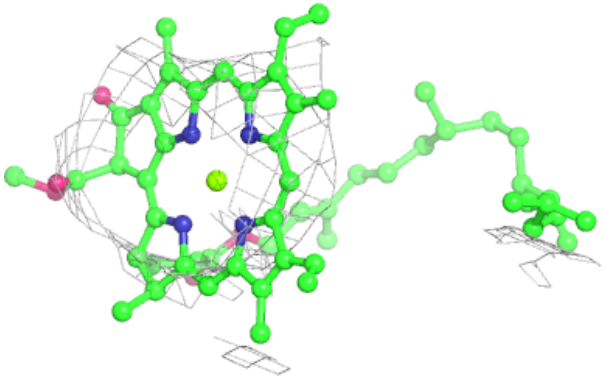


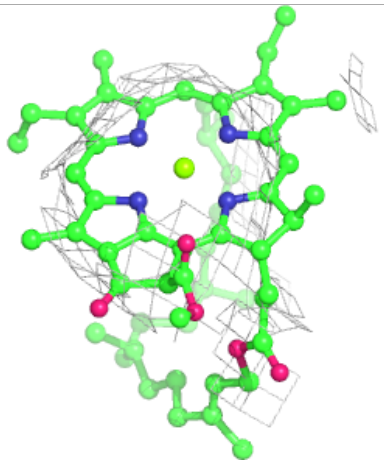


Electron density around CLA B 611:

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

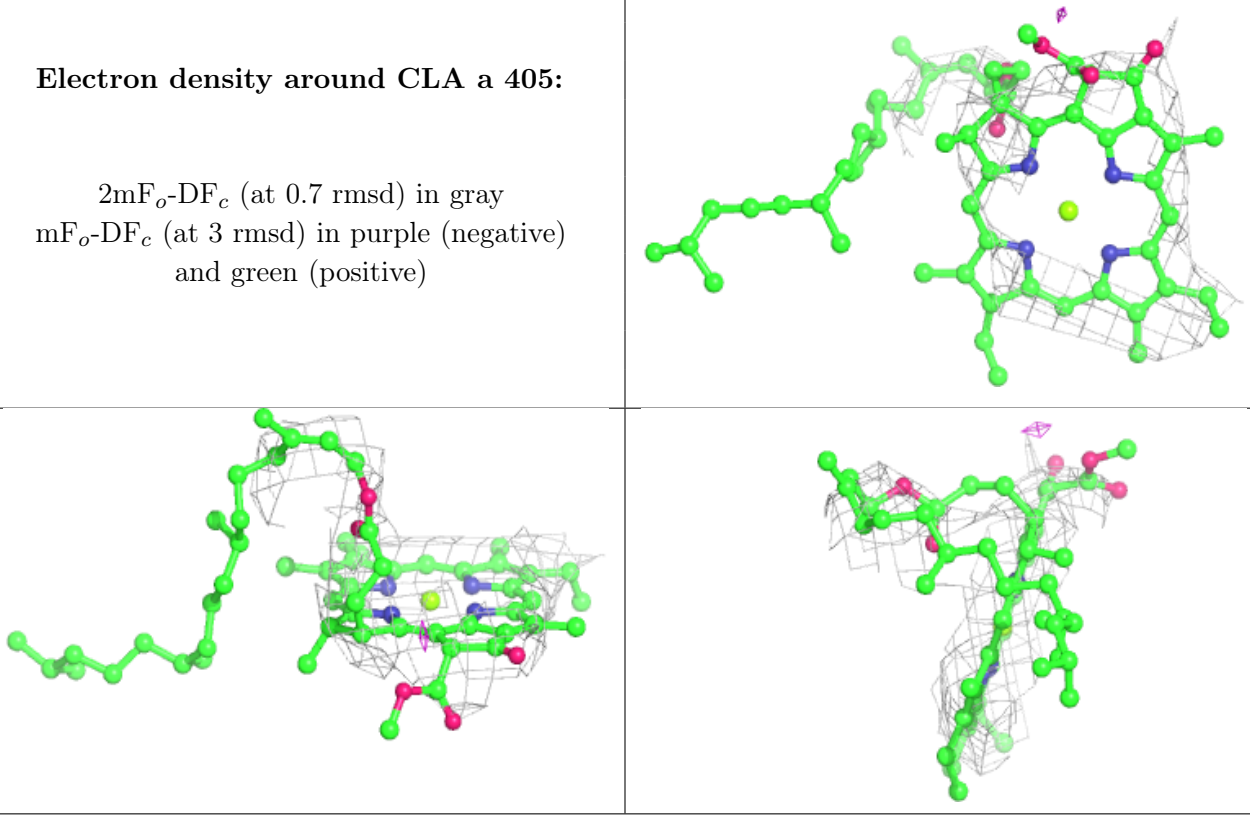






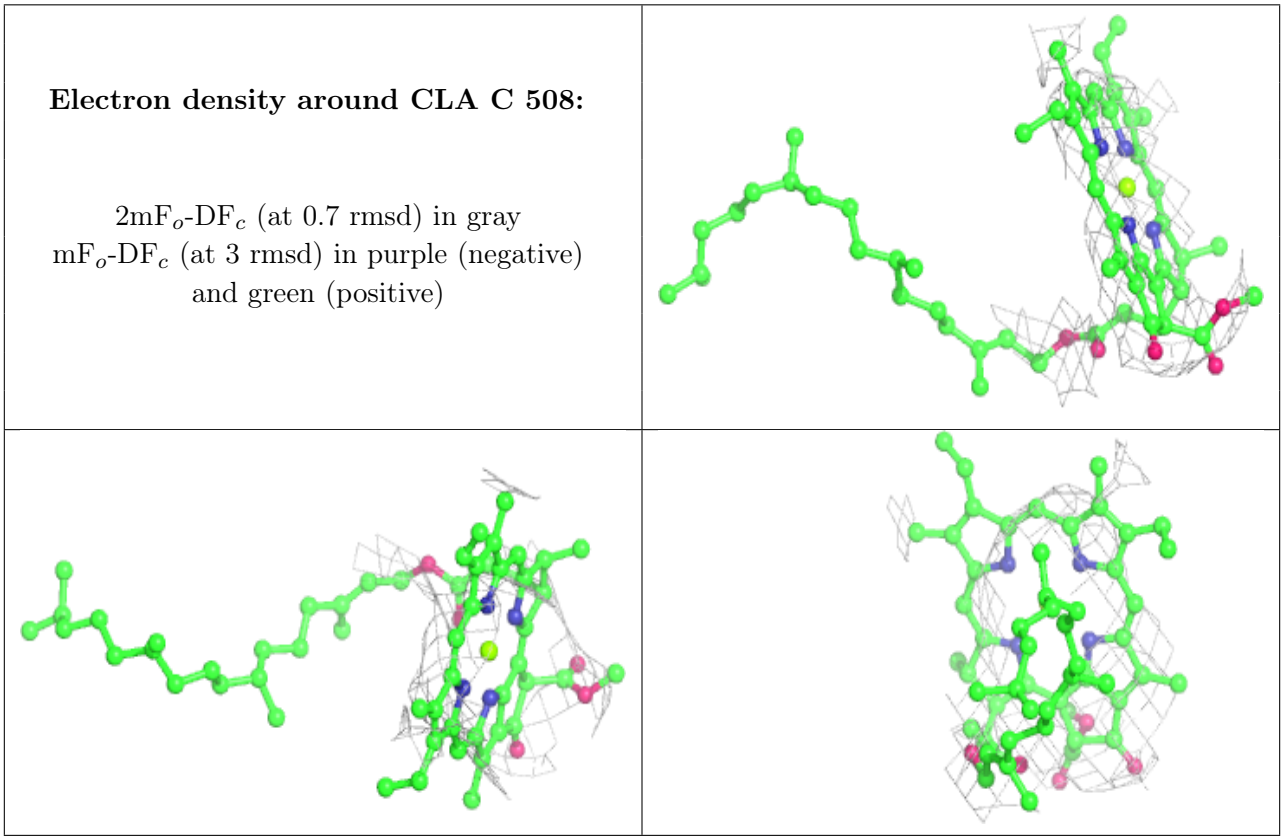
Electron density around CLA a 405:

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



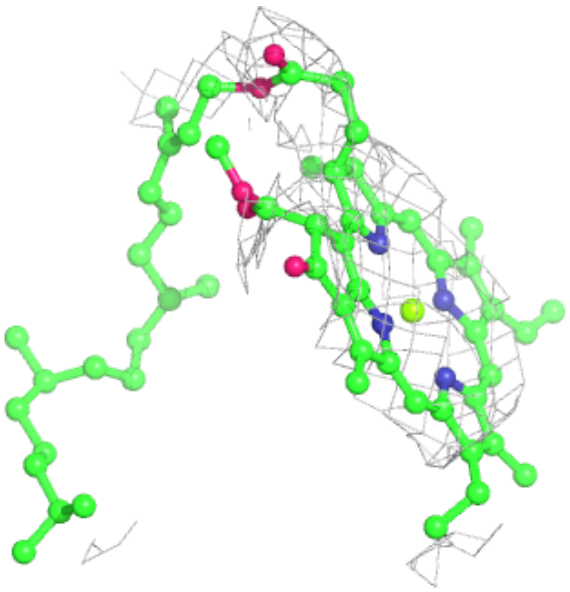
Electron density around CLA C 508:

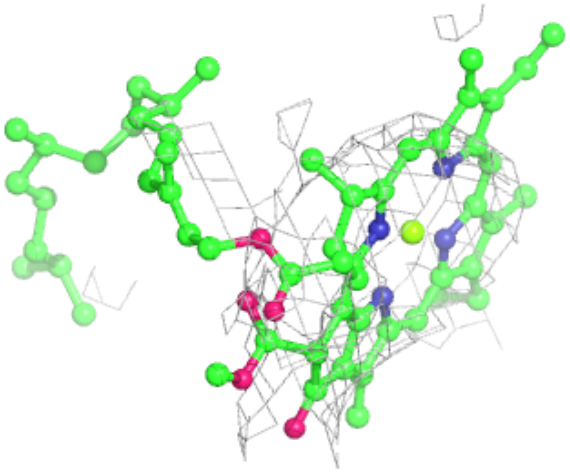
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

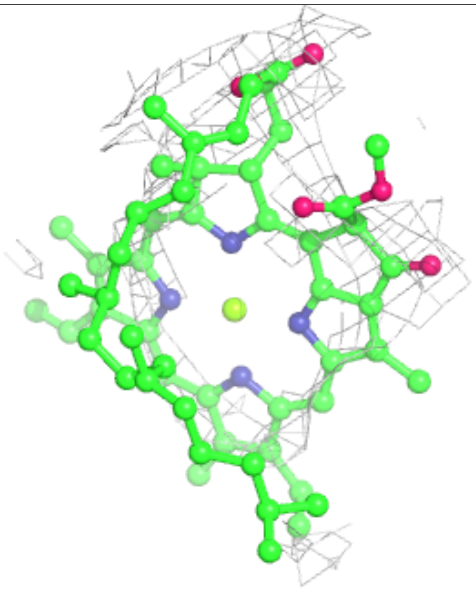


Electron density around CLA B 613:

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

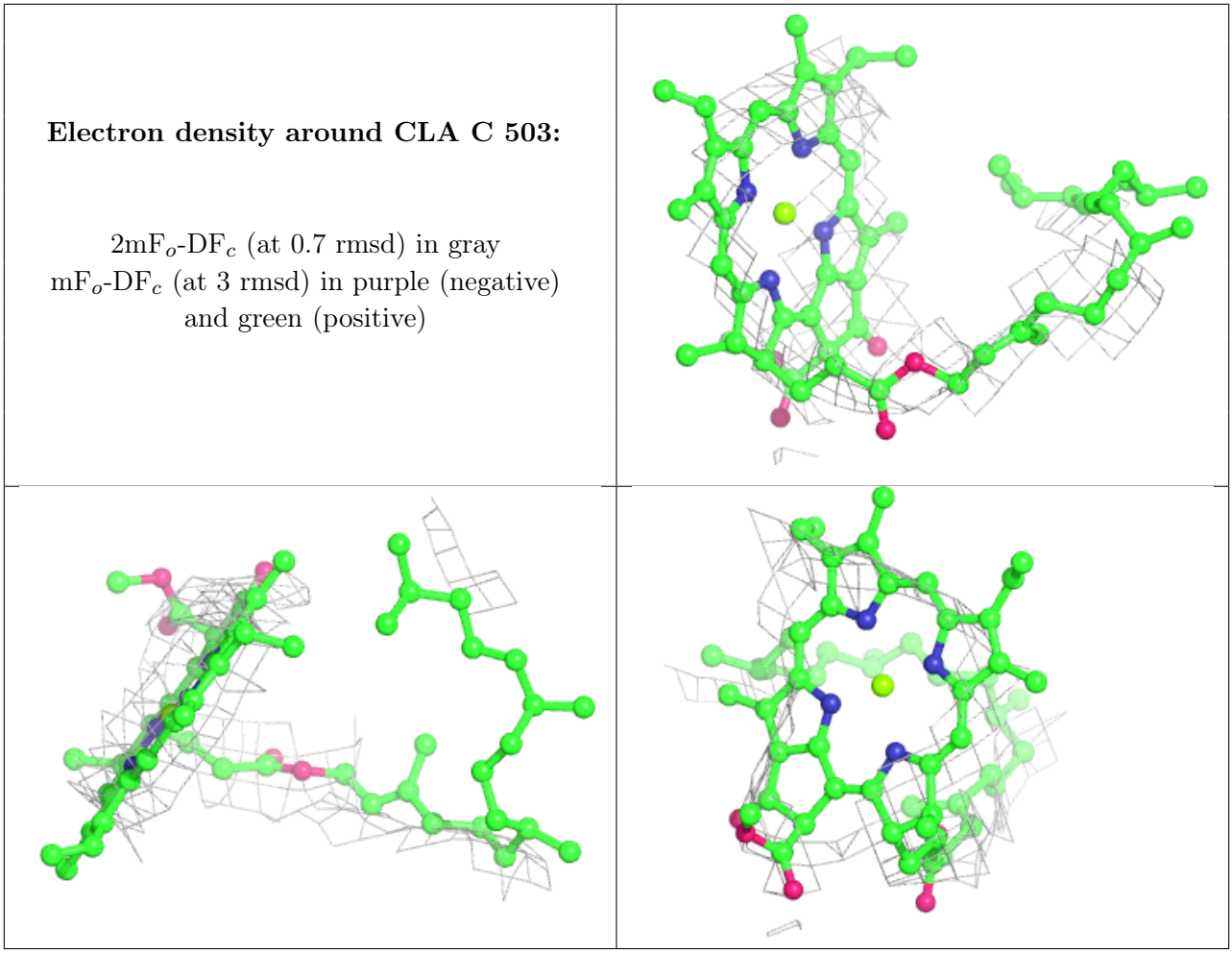






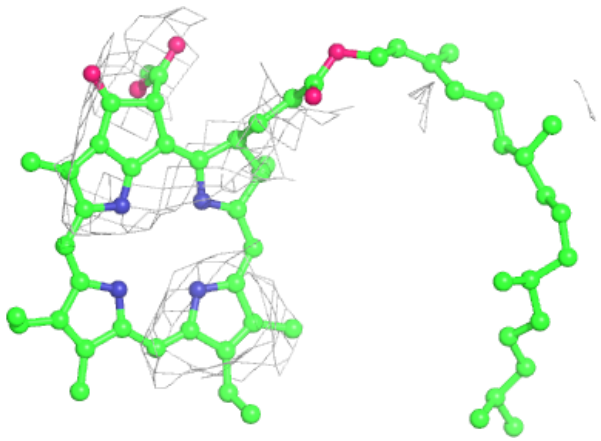
Electron density around CLA C 503:

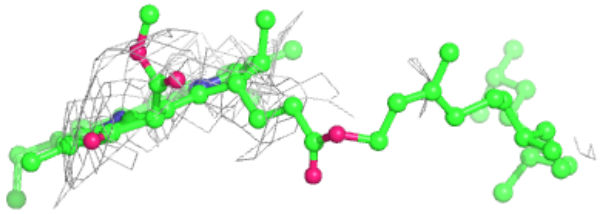
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

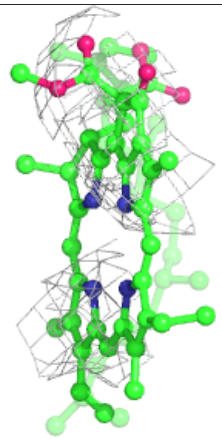


Electron density around PHO a 407:

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

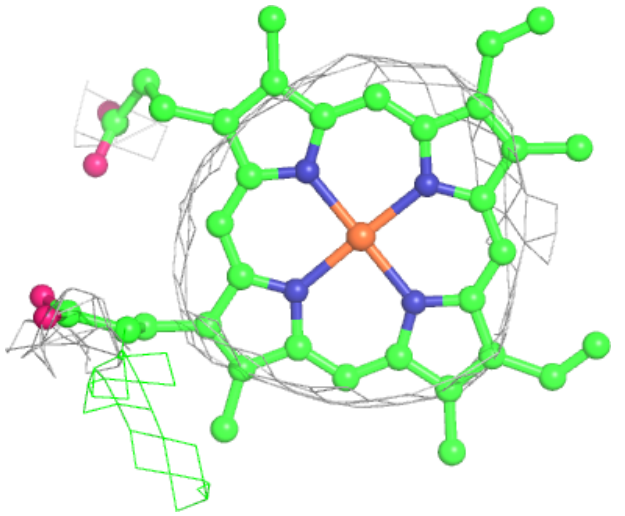


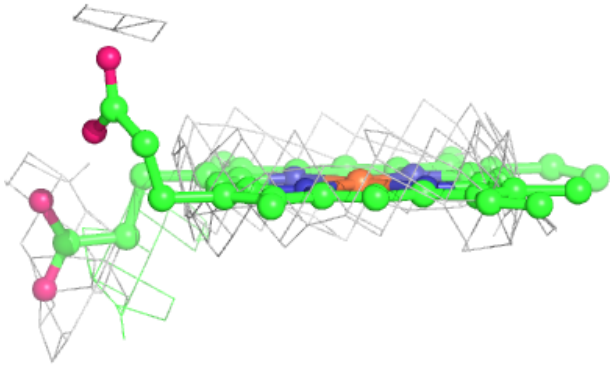


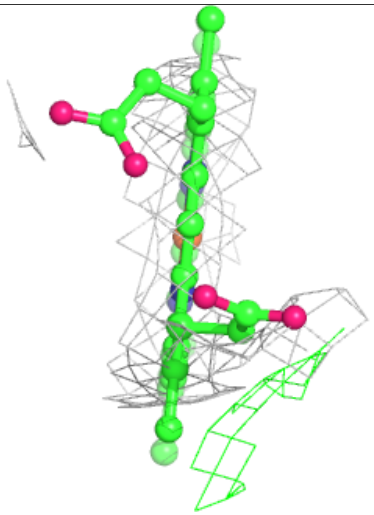


Electron density around HEM F 101:

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

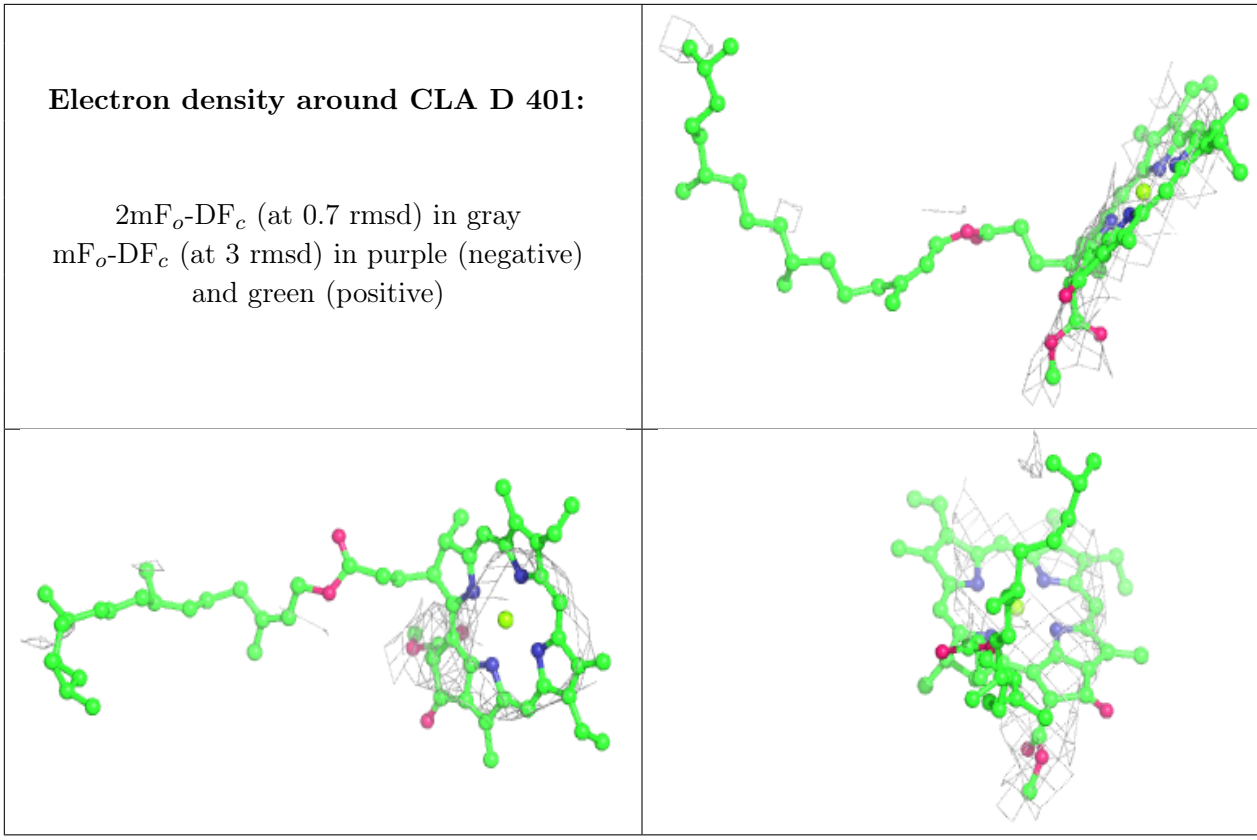






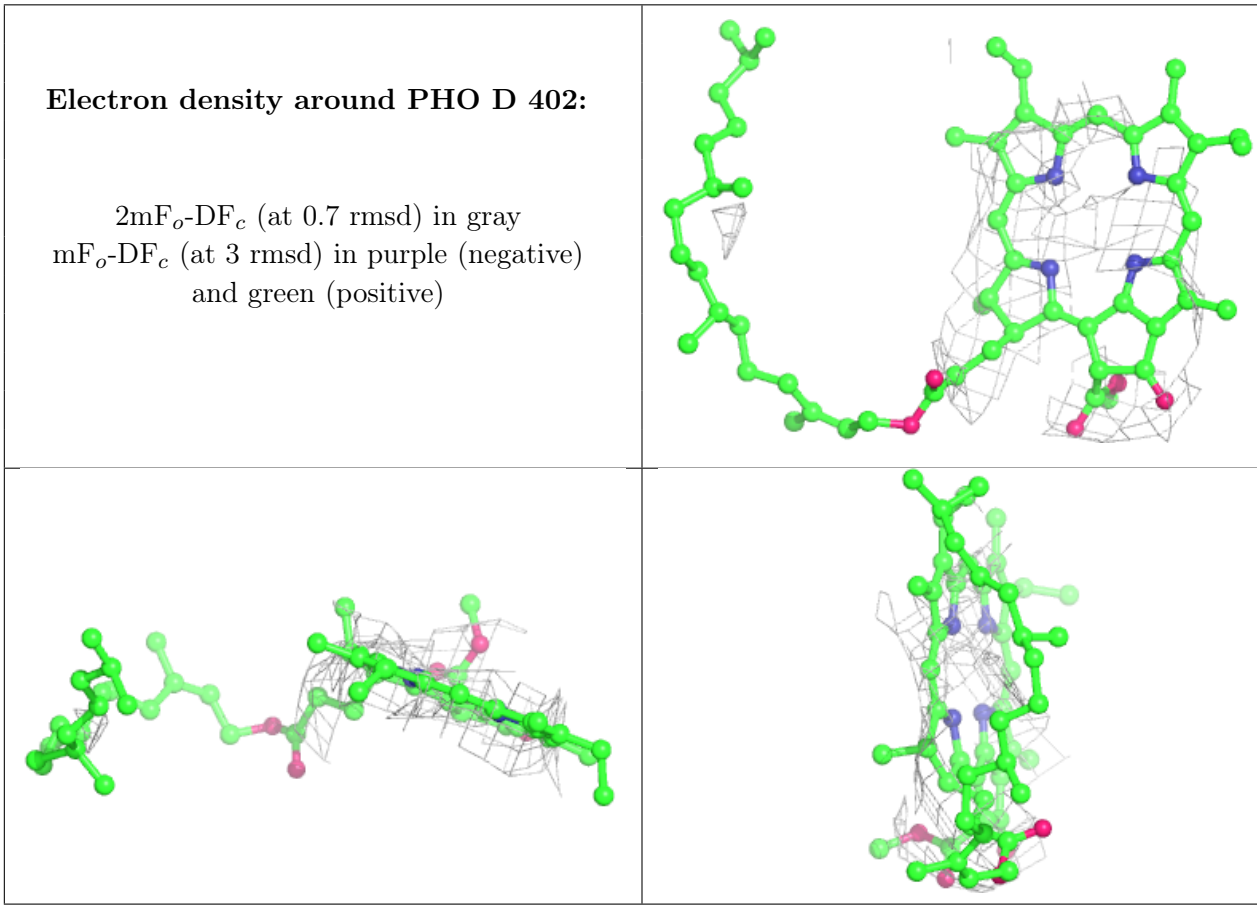
Electron density around CLA D 401:

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



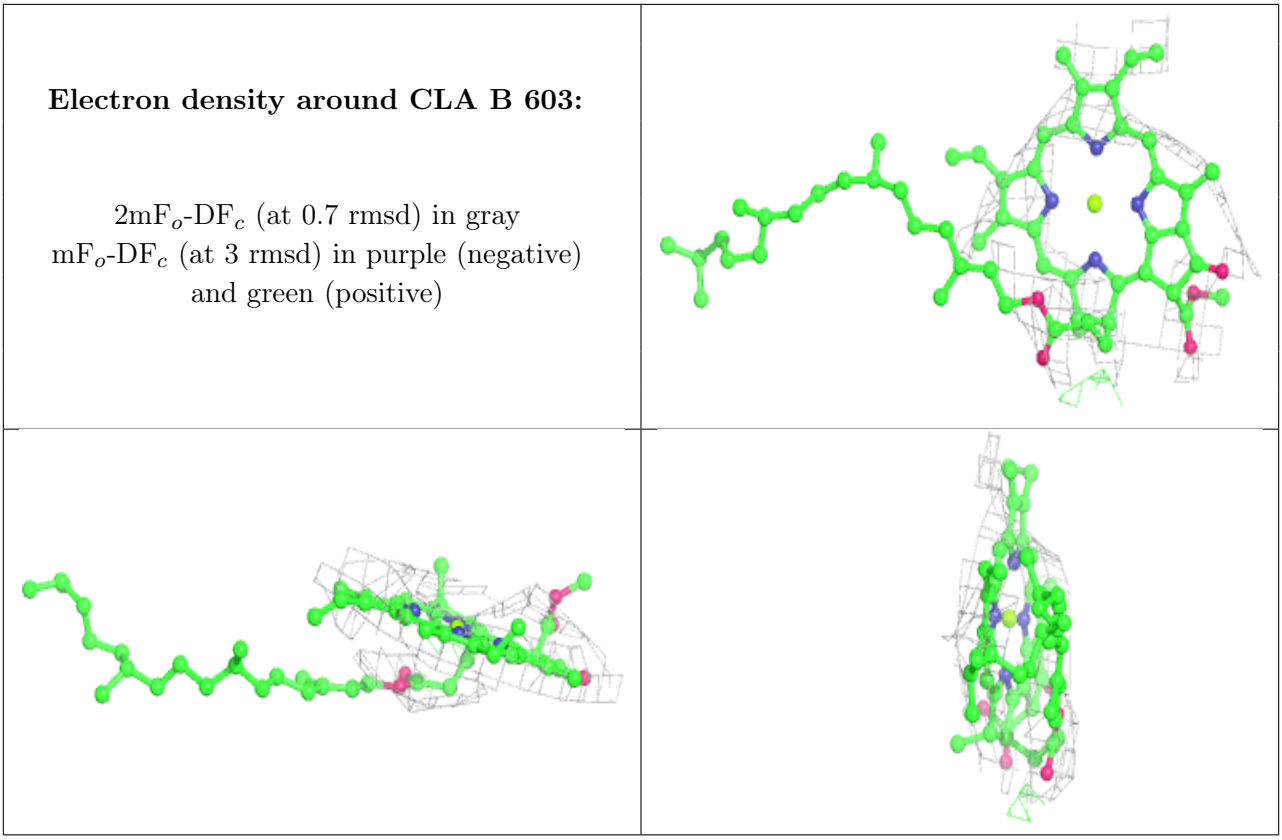
Electron density around PHO D 402:

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



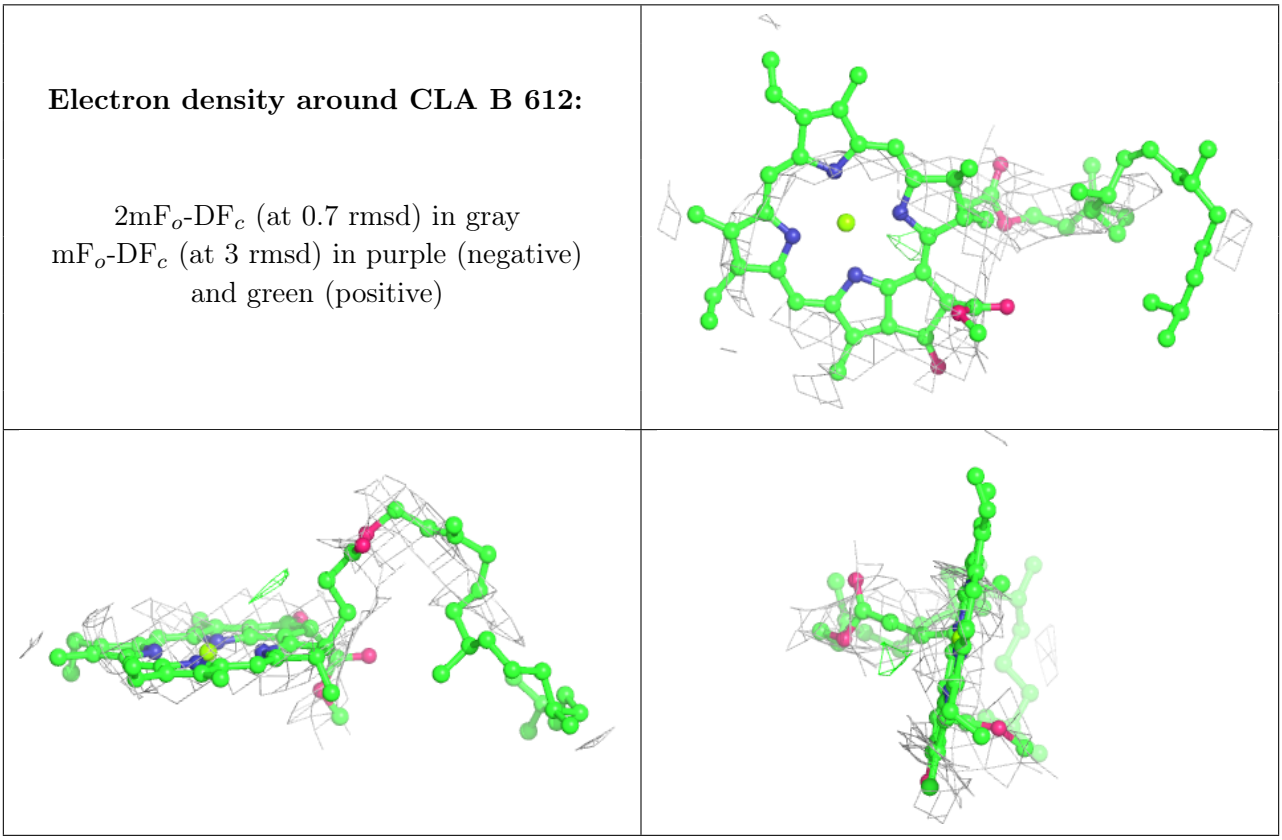
Electron density around CLA B 603:

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



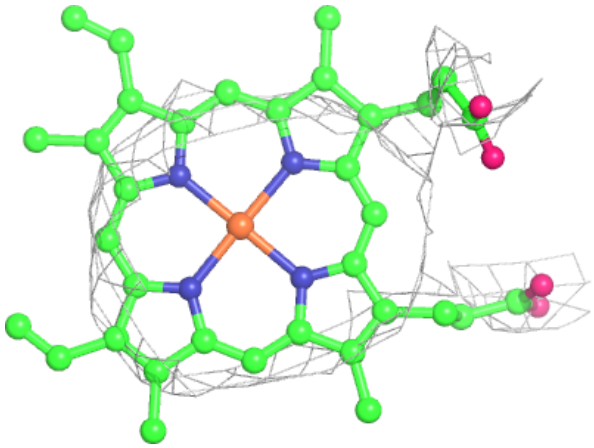
Electron density around CLA B 612:

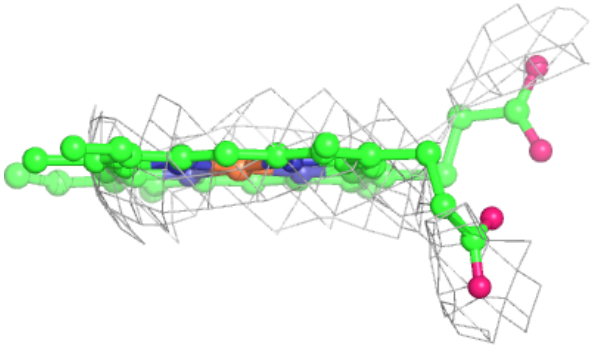
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

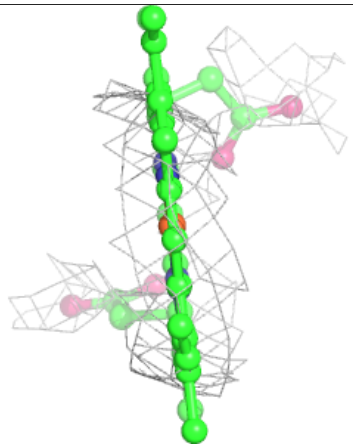


Electron density around HEM f 101:

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

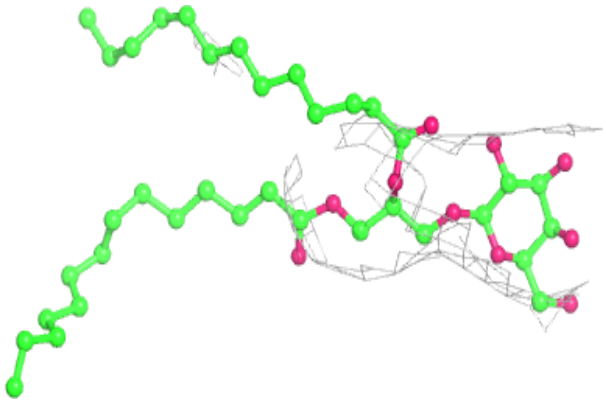


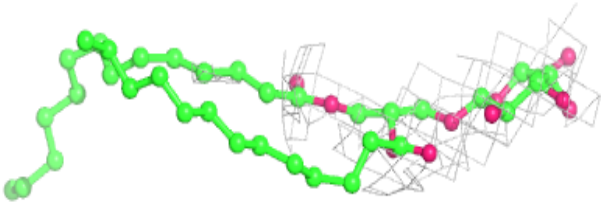


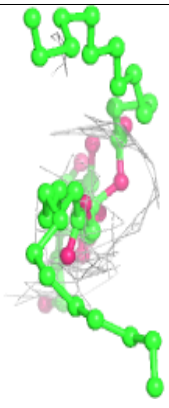


Electron density around LMG d 406:

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

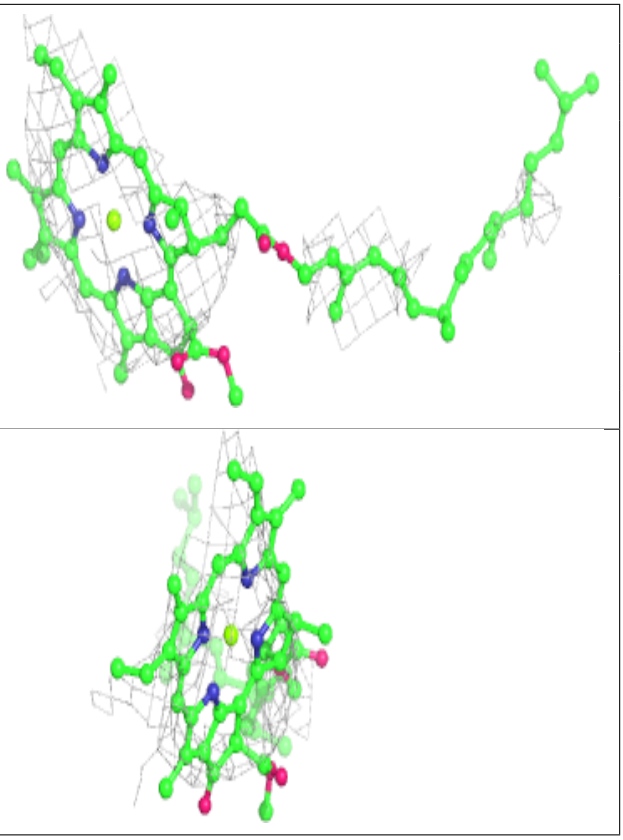


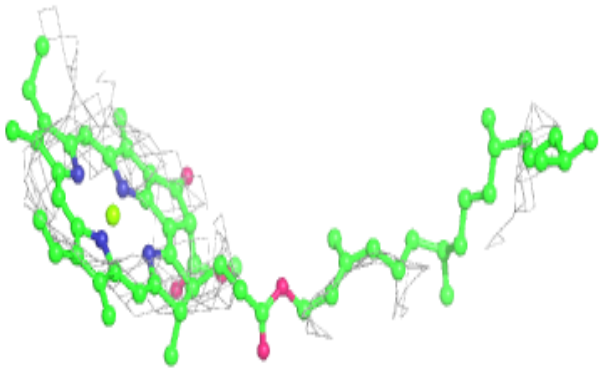




Electron density around CLA a 404:

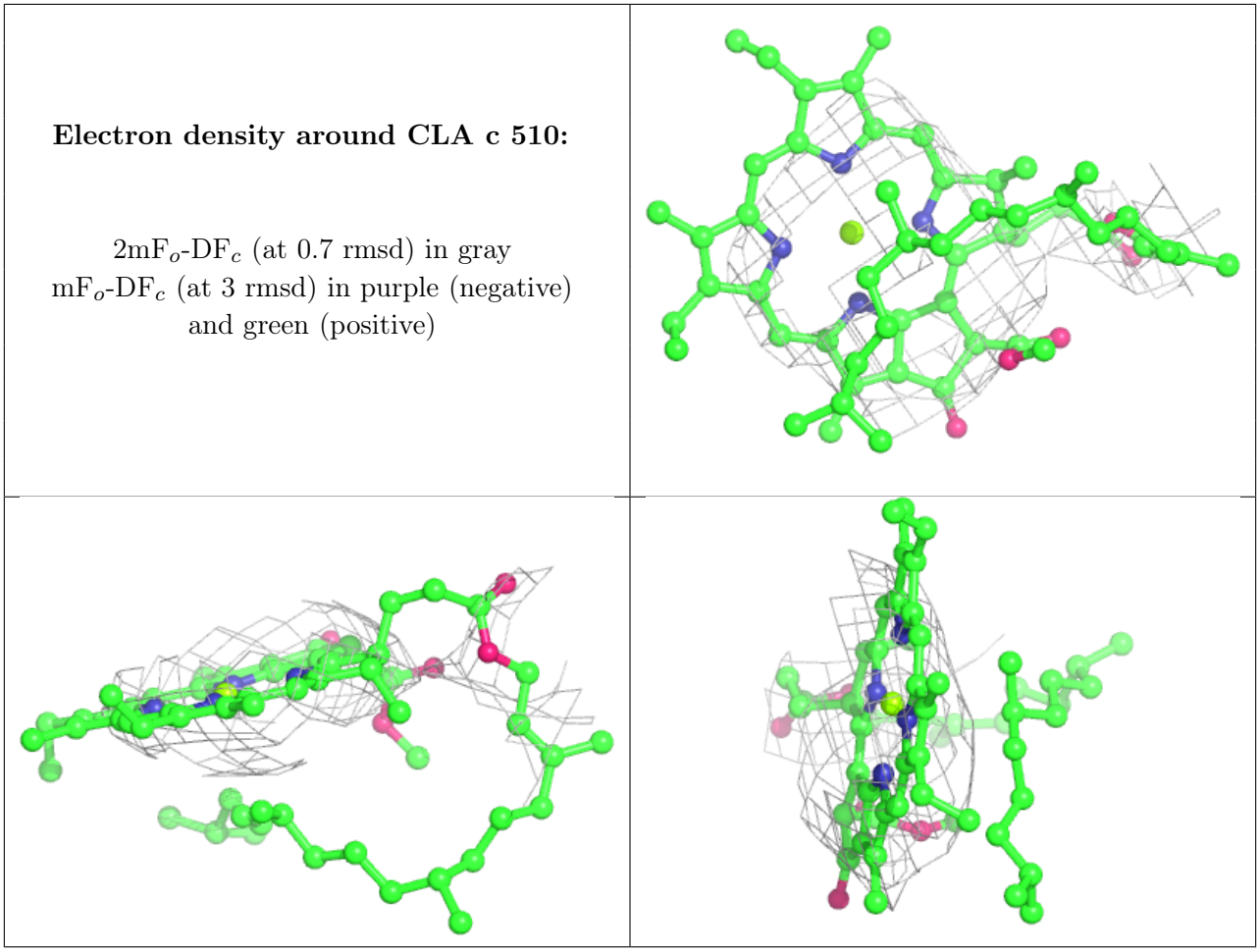
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





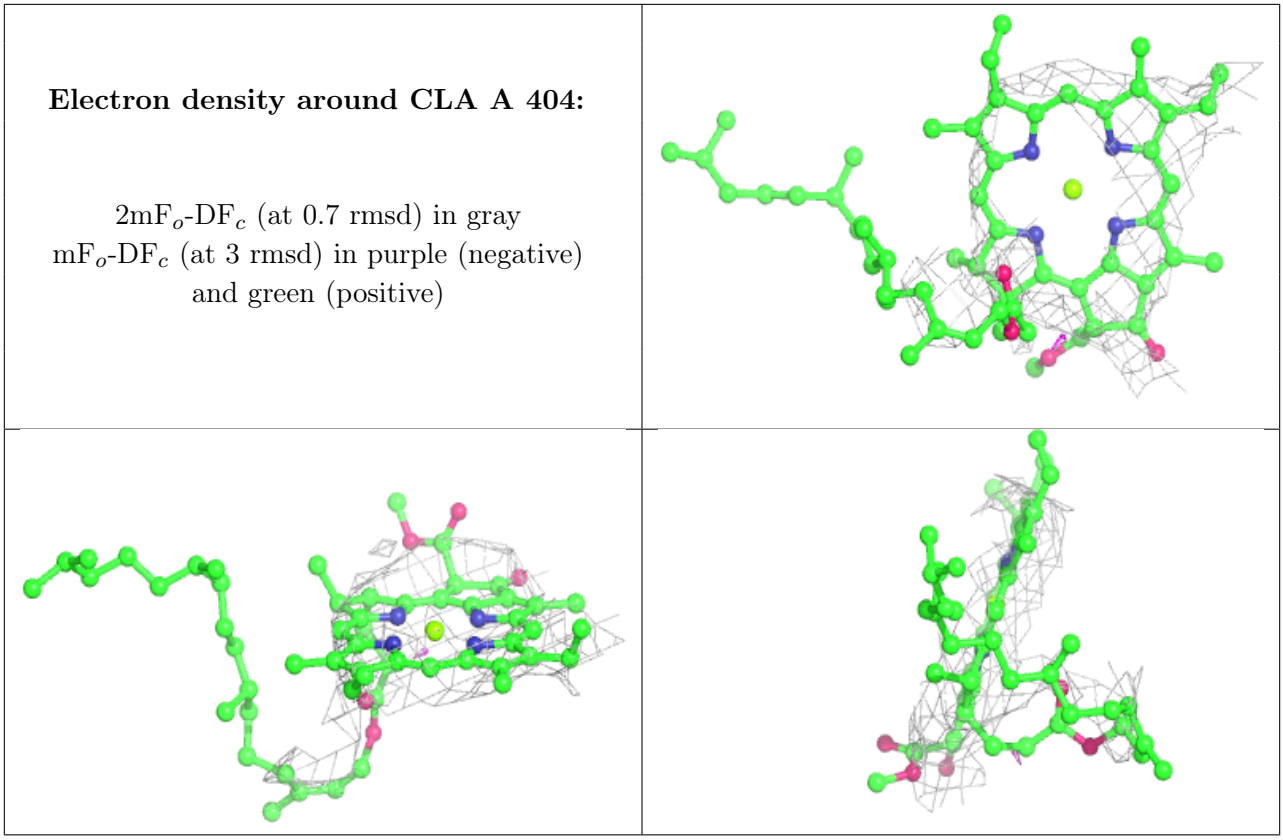
Electron density around CLA c 510:

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



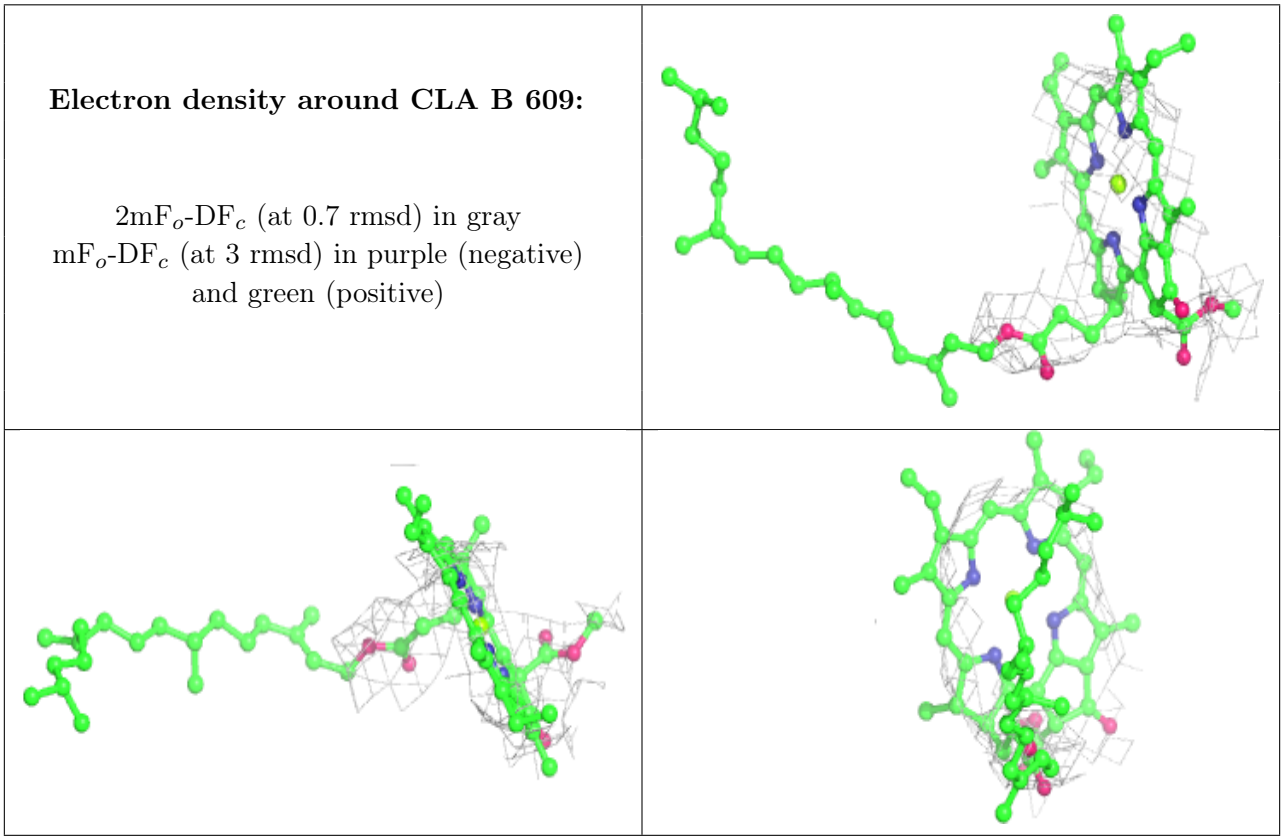
Electron density around CLA A 404:

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



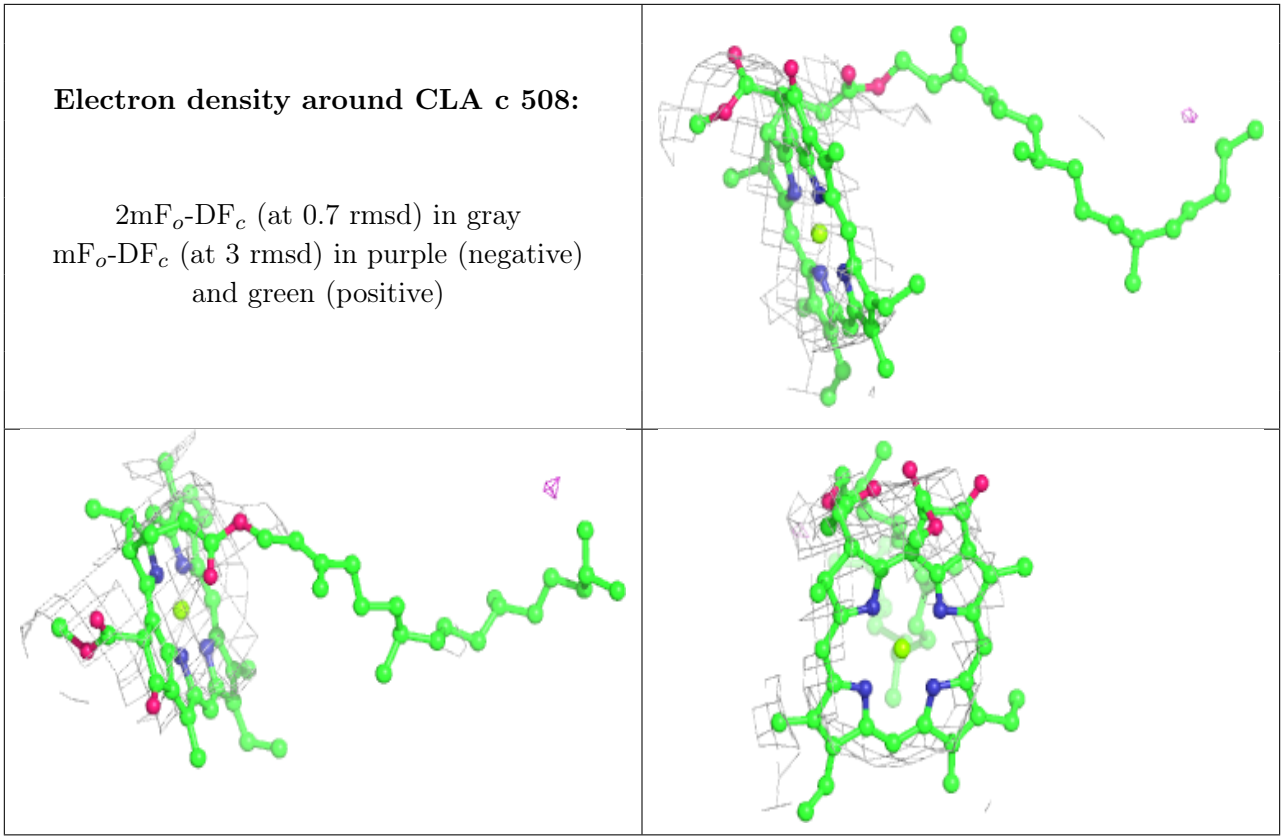
Electron density around CLA B 609:

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



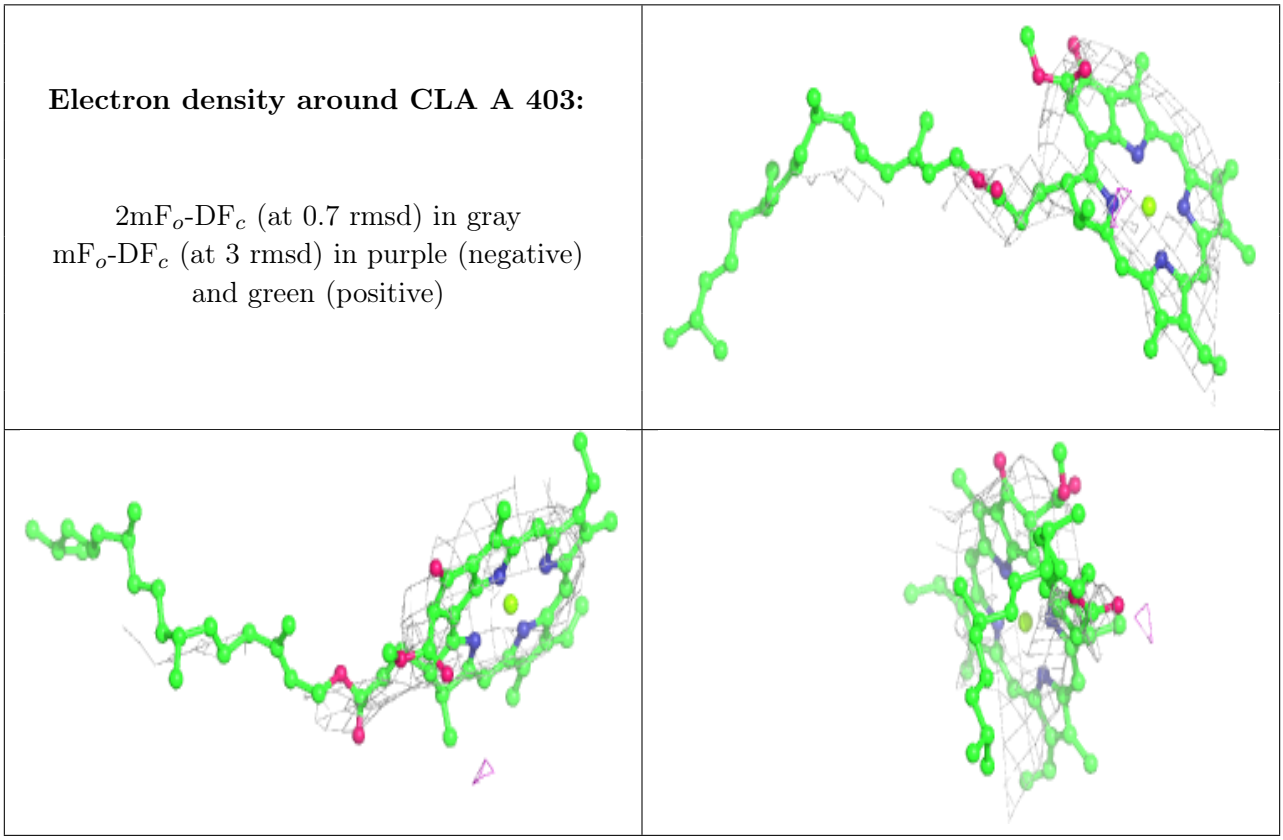
Electron density around CLA c 508:

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



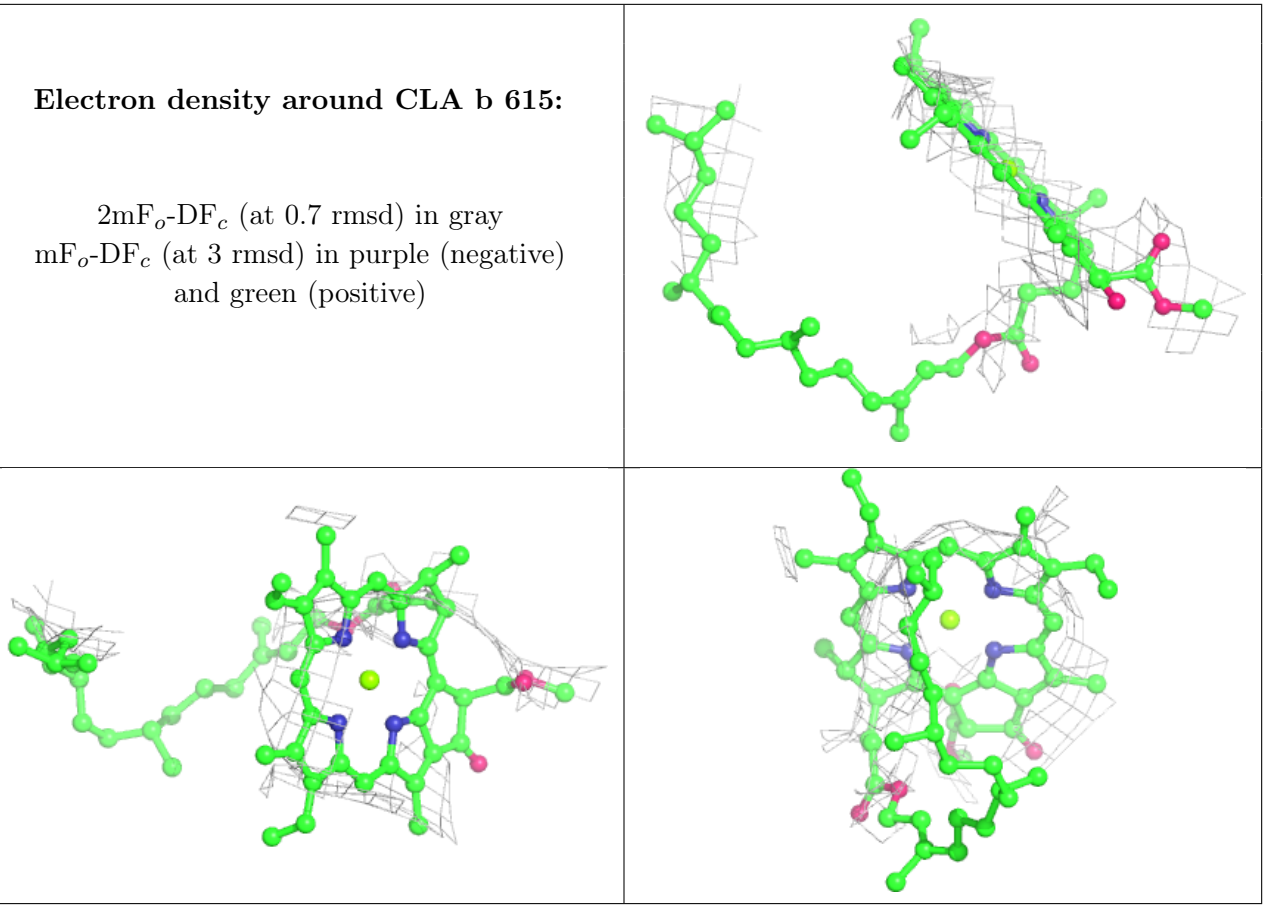
Electron density around CLA A 403:

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



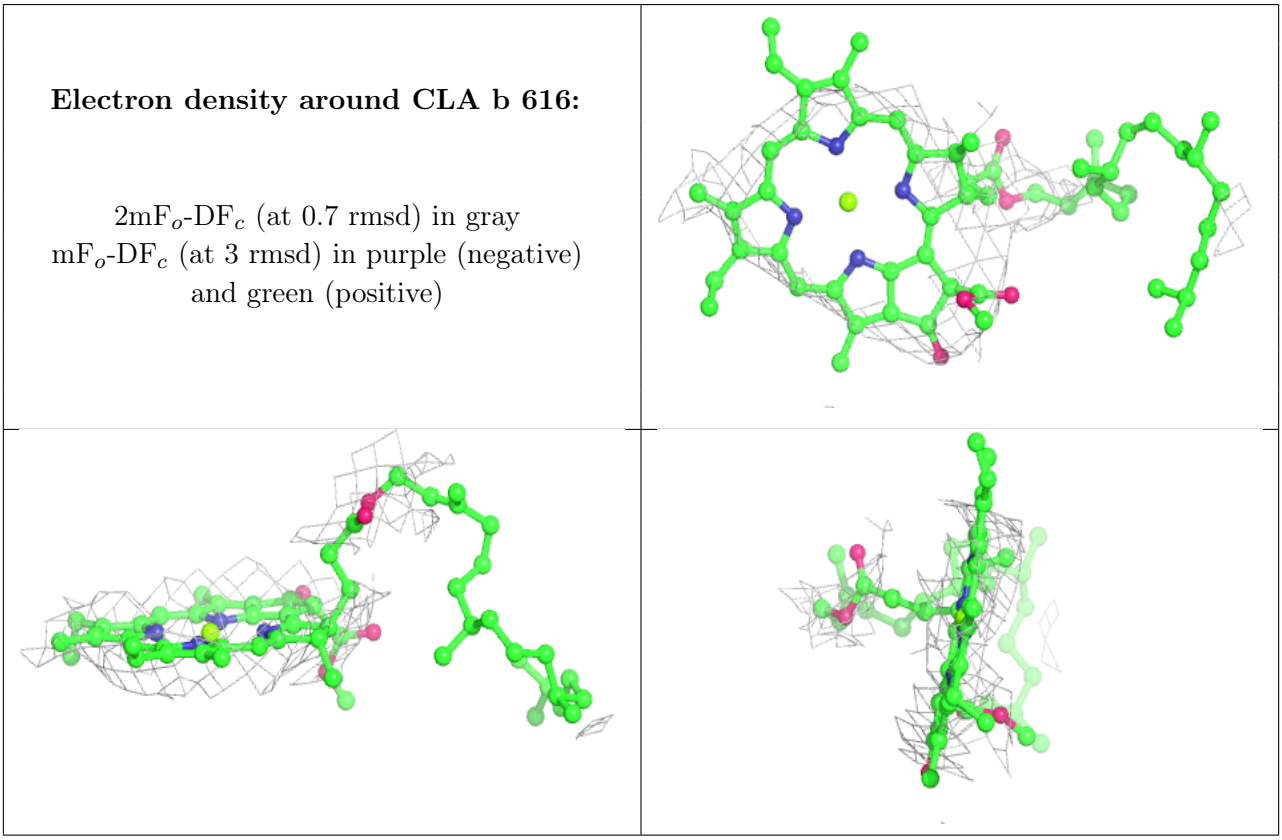
Electron density around CLA b 615:

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



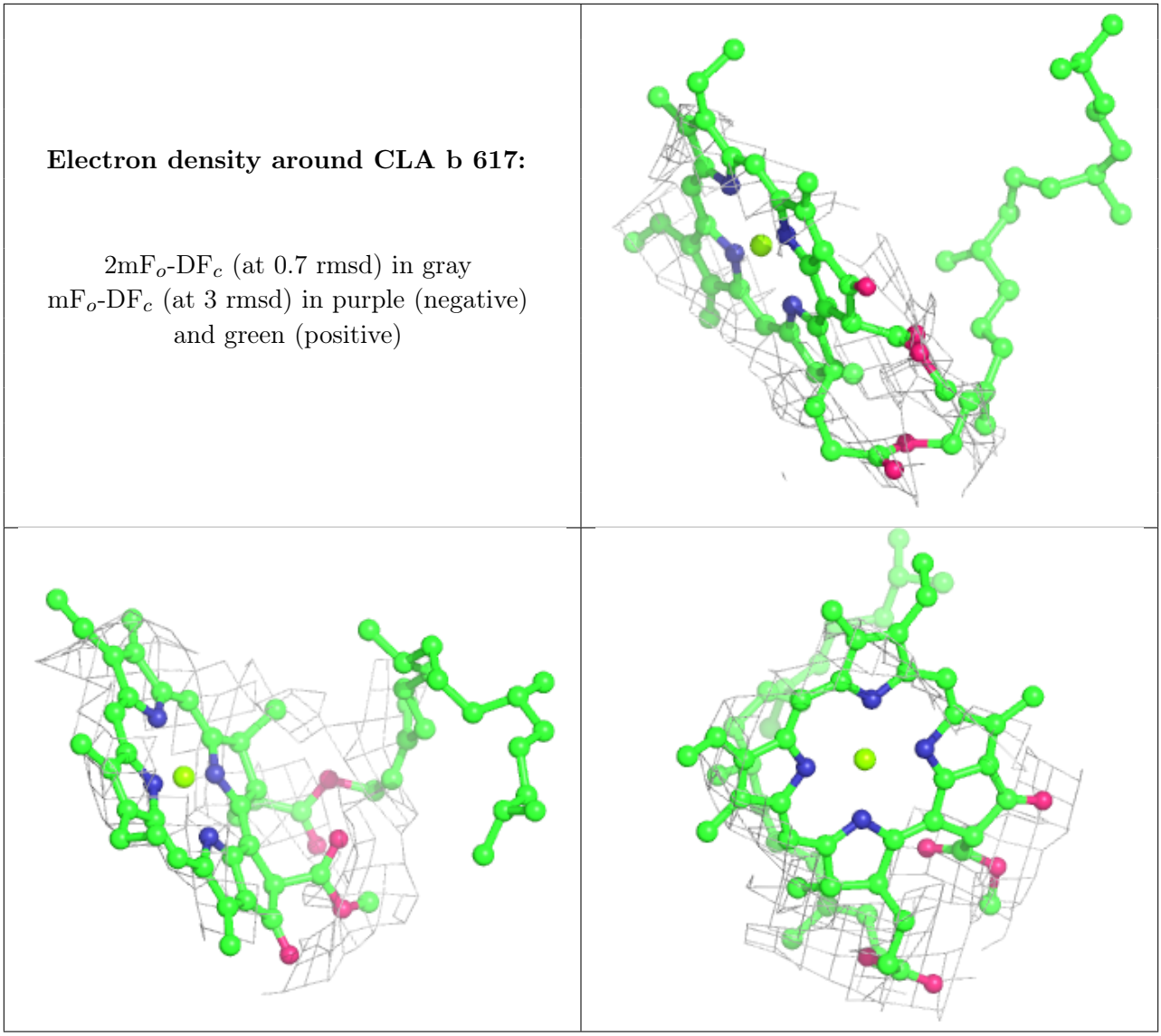
Electron density around CLA b 616:

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



Electron density around CLA b 617:

$2mF_o$-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.