wwPDB X-ray Structure Validation Summary Report (i)

Oct 22, 2023 – 03:45 AM EDT

PDB ID	:	3A0H
Title	:	Crystal structure of I-substituted Photosystem II complex
Authors	:	Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.
Deposited on	:	2009-03-17
Resolution	:	4.00 Å(reported)

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

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

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

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

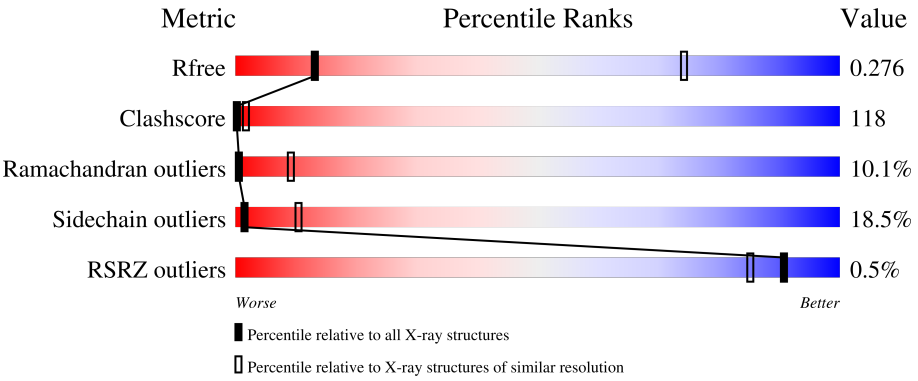
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	344	13% 62% 21%
1	a	344	72% 24%
2	B	488	20% 59% 19%
2	b	488	77% 22%
3	C	447	17% 64% 18%

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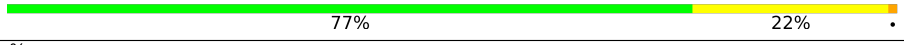
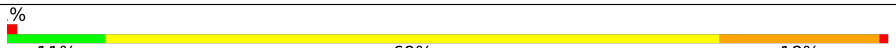
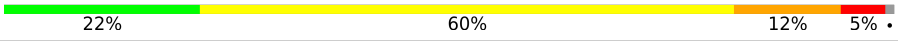
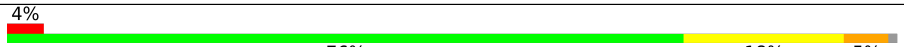
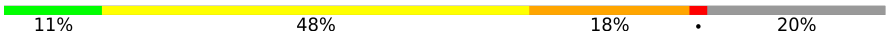
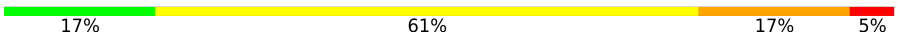
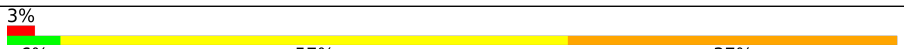
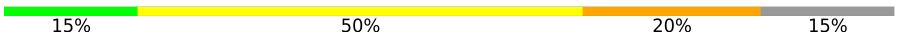
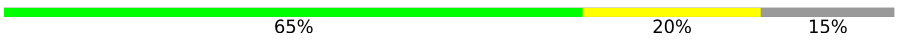
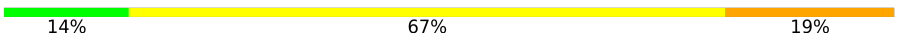
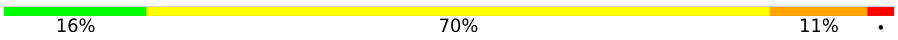
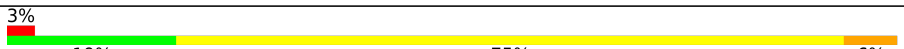
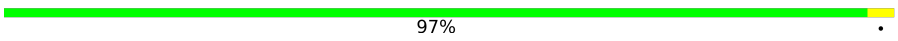
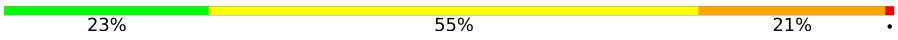
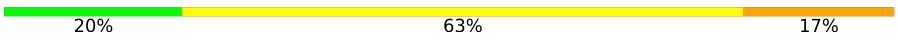
Mol	Chain	Length	Quality of chain
3	c	447	
4	D	340	
4	d	340	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	35	
8	i	35	
9	J	40	
9	j	40	
10	K	36	
10	k	36	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	242	
13	o	242	
14	T	30	
14	t	30	
15	U	98	
15	u	98	

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Mol	Chain	Length	Quality of chain
16	V	137	24% 60% 15%
16	v	137	79% 20%
17	X	34	32% 47% 21%
17	x	34	3% 71% 29%
18	Y	28	29% 29% 36% 7%
18	y	28	57% 36% 7%
19	N	23	70% 30%
19	n	23	100%
20	Z	62	2% 16% 65% 19%
20	z	62	3% 74% 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	1003	X	-	X	-
22	CLA	A	1006	X	-	X	-
22	CLA	A	1007	X	-	X	X
22	CLA	B	1009	X	-	X	-
22	CLA	B	1010	X	-	X	-
22	CLA	B	1011	X	-	X	-
22	CLA	B	1012	X	-	X	-
22	CLA	B	1013	X	-	X	-
22	CLA	B	1014	X	-	X	-
22	CLA	B	1015	X	-	X	-
22	CLA	B	1016	X	-	X	-
22	CLA	B	1018	X	-	X	-
22	CLA	B	1019	X	-	X	-
22	CLA	B	1020	X	-	X	-
22	CLA	B	1021	X	-	X	-
22	CLA	B	1022	X	-	X	-
22	CLA	B	1023	X	-	X	-
22	CLA	B	1024	X	-	X	-
22	CLA	C	1025	X	-	X	-
22	CLA	C	1026	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	1027	X	-	X	X
22	CLA	C	1028	X	-	X	-
22	CLA	C	1029	X	-	X	-
22	CLA	C	1030	X	-	X	-
22	CLA	C	1031	X	-	X	-
22	CLA	C	1032	X	-	X	-
22	CLA	C	1033	X	-	X	-
22	CLA	C	1035	X	-	X	-
22	CLA	C	1036	X	-	X	-
22	CLA	C	1037	X	-	X	X
22	CLA	D	1004	X	-	X	-
22	CLA	D	1005	X	-	X	-
22	CLA	D	1008	X	-	X	X
22	CLA	H	1017	X	-	X	-
22	CLA	K	1034	X	-	X	X
22	CLA	a	6003	X	-	-	-
22	CLA	a	6006	X	-	-	-
22	CLA	a	6007	X	-	-	X
22	CLA	b	6009	X	-	-	X
22	CLA	b	6010	X	-	-	-
22	CLA	b	6011	X	-	-	-
22	CLA	b	6012	X	-	-	-
22	CLA	b	6013	X	-	-	-
22	CLA	b	6014	X	-	-	X
22	CLA	b	6015	X	-	-	-
22	CLA	b	6016	X	-	-	-
22	CLA	b	6018	X	-	-	-
22	CLA	b	6019	X	-	-	-
22	CLA	b	6020	X	-	-	-
22	CLA	b	6021	X	-	-	-
22	CLA	b	6022	X	-	-	-
22	CLA	b	6023	X	-	-	-
22	CLA	b	6024	X	-	-	-
22	CLA	c	6025	X	-	-	-
22	CLA	c	6026	X	-	-	-
22	CLA	c	6027	X	-	-	X
22	CLA	c	6028	X	-	-	-
22	CLA	c	6029	X	-	-	-
22	CLA	c	6030	X	-	-	-
22	CLA	c	6031	X	-	-	X
22	CLA	c	6032	X	-	-	-
22	CLA	c	6033	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	6035	X	-	-	X
22	CLA	c	6036	X	-	-	-
22	CLA	c	6037	X	-	-	X
22	CLA	d	6004	X	-	-	-
22	CLA	d	6005	X	-	-	-
22	CLA	d	6008	X	-	-	X
22	CLA	h	6017	X	-	-	X
22	CLA	k	6034	X	-	-	X
23	PHO	A	1038	X	-	X	-
23	PHO	D	1039	X	-	X	-
23	PHO	a	6038	X	-	-	-
23	PHO	d	6039	X	-	-	-
24	PQ9	A	1043	-	-	X	X
24	PQ9	D	1042	-	-	X	-
24	PQ9	d	6042	-	-	-	X
25	BCR	A	1044	-	-	X	X
25	BCR	B	1045	-	-	X	X
25	BCR	B	1047	-	-	X	-
25	BCR	B	1048	-	-	X	X
25	BCR	C	1052	-	-	X	-
25	BCR	C	1054	-	-	X	X
25	BCR	D	1050	-	-	X	X
25	BCR	H	1049	-	-	X	-
25	BCR	K	1051	-	-	X	X
25	BCR	T	6046	-	-	X	X
25	BCR	T	6048	-	-	-	X
25	BCR	Z	1053	-	-	-	X
25	BCR	a	6044	-	-	-	X
25	BCR	b	6045	-	-	-	X
25	BCR	b	6047	-	-	-	X
25	BCR	c	6054	-	-	-	X
25	BCR	d	6050	-	-	-	X
25	BCR	h	6049	-	-	-	X
25	BCR	k	6051	-	-	-	X
25	BCR	k	6052	-	-	-	X
25	BCR	t	1046	-	-	-	X
25	BCR	z	6053	-	-	-	X
26	LHG	A	1063	-	-	X	X
26	LHG	a	6063	-	-	-	X
27	IOD	B	1067	-	-	X	X
27	IOD	D	1064	-	-	X	-
27	IOD	D	1068	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	IOD	T	1066	-	-	X	-
27	IOD	d	6068	-	-	-	X
28	MGE	B	1060	-	-	X	X
28	MGE	D	1059	-	-	X	X
28	MGE	D	1062	-	-	X	-
28	MGE	L	1061	-	-	X	X
28	MGE	b	6060	-	-	-	X
28	MGE	d	6059	-	-	-	X
28	MGE	d	6062	-	-	-	X
29	DGD	B	1058	-	-	X	-
29	DGD	C	1055	-	-	X	-
29	DGD	C	1056	-	-	X	-
29	DGD	C	1057	-	-	X	-
29	DGD	c	6055	-	-	-	X
29	DGD	c	6056	-	-	-	X

2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 48060 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2630	1720	435	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2630	1720	435	460	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	13			
2	b	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	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
			3455	2264	576	602	13			
3	c	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	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	64	Total 507	C 339	N 81	O 85	S 2	0	0	0
7	h	64	Total 507	C 339	N 81	O 85	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 287	C 195	N 45	O 46	S 1	0	0	0
8	i	35	Total 287	C 195	N 45	O 46	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	36	Total 278	C 195	N 38	O 45	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total 278	C 195	N 38	O 45	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	36	Total 283	C 187	N 42	O 53	S 1	0	0	0
12	m	36	Total 283	C 187	N 42	O 53	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	242	Total 1860	C 1162	N 314	O 380	S 4	0	0	0
13	o	242	Total 1860	C 1162	N 314	O 380	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	30	Total 257	C 180	N 36	O 39	S 2	0	0	0
14	t	30	Total 257	C 180	N 36	O 39	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	98	Total 783	C 496	N 130	O 157	0	0	0
15	u	98	Total 783	C 496	N 130	O 157	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
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	34	Total	C	N	O	0	0	0
			246	166	36	44			
17	x	34	Total	C	N	O	0	0	0
			246	166	36	44			

- Molecule 18 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			
18	y	28	Total	C	N	O	S	0	0	0
			208	137	36	32	3			

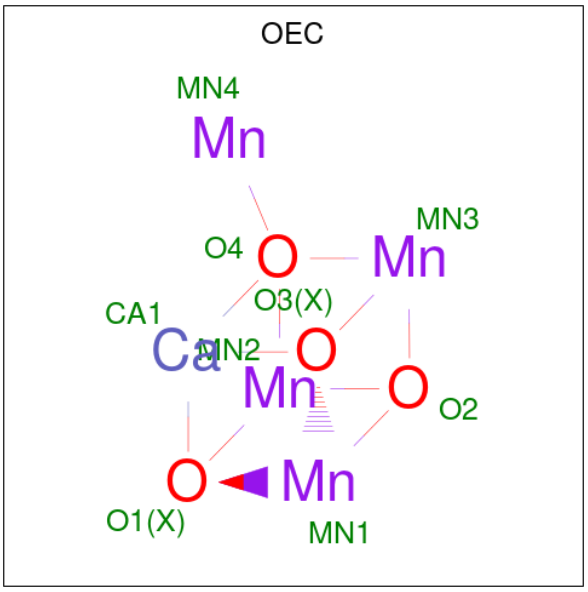
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	23	Total	C	N	O	0	0	0
			116	69	23	24			
19	n	23	Total	C	N	O	0	0	0
			116	69	23	24			

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

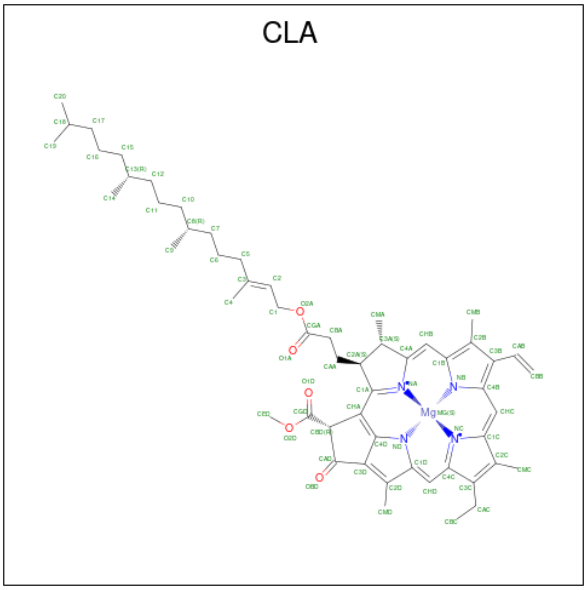
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: $CaMn_4O_4$).



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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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

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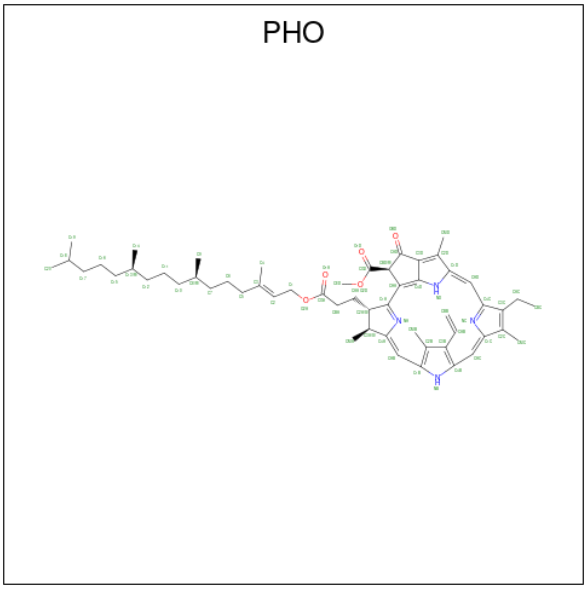
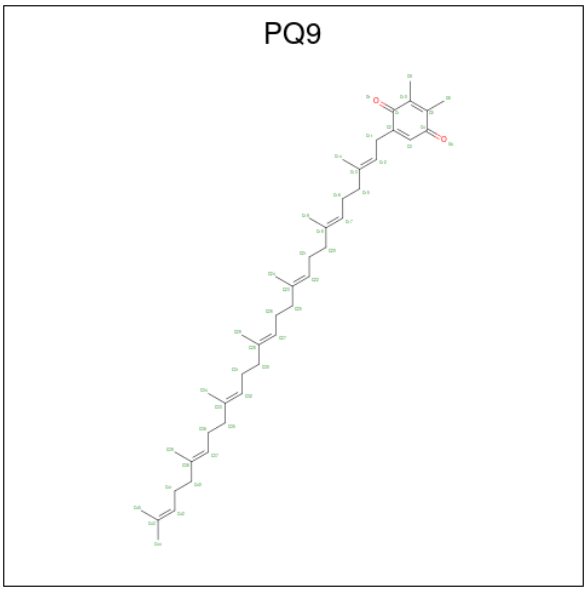
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



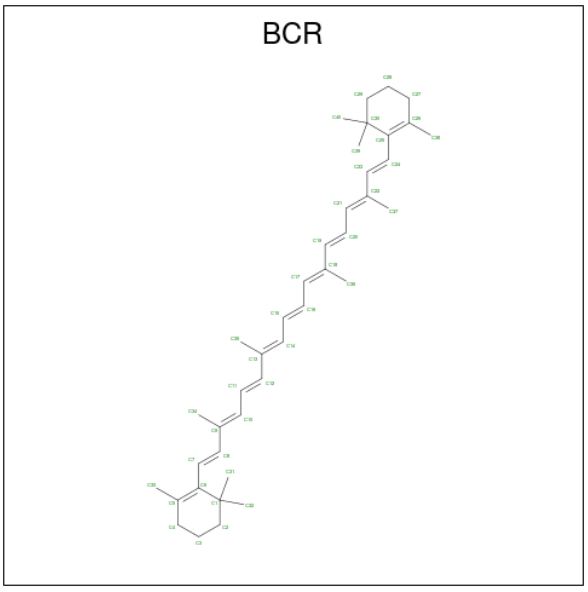
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (three-letter code: PQ9) (formula: $C_{43}H_{64}O_2$).



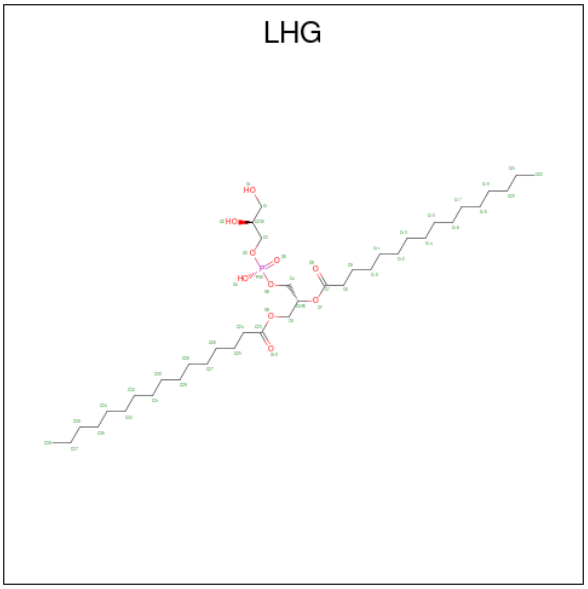
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C O 45 43 2	0	0
24	D	1	Total C O 45 43 2	0	0
24	a	1	Total C O 45 43 2	0	0
24	d	1	Total C O 45 43 2	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Z	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	z	1	Total C 40 40	0	0

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

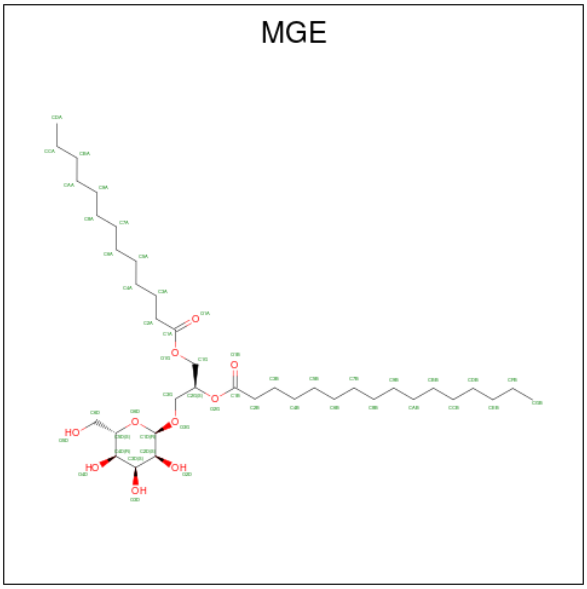


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O P 49 38 10 1	0	0
26	a	1	Total C O P 49 38 10 1	0	0

- Molecule 27 is IODIDE ION (three-letter code: IOD) (formula: I).

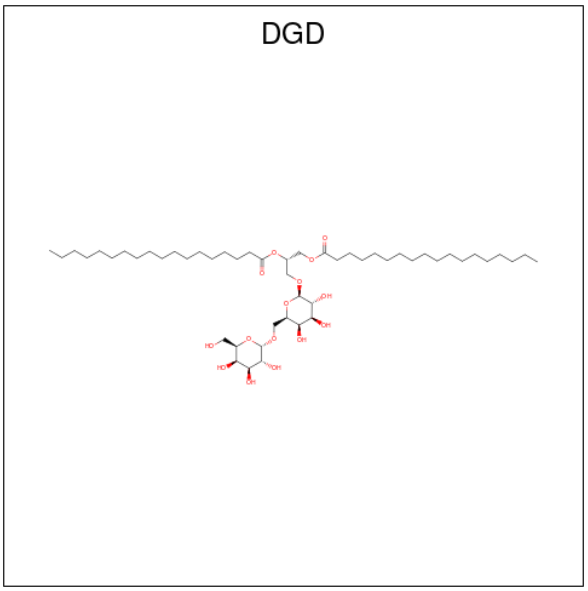
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total I 1 1	0	0
27	B	1	Total I 1 1	0	0
27	D	2	Total I 2 2	0	0
27	T	1	Total I 1 1	0	0
27	a	1	Total I 1 1	0	0
27	b	1	Total I 1 1	0	0
27	d	2	Total I 2 2	0	0
27	t	1	Total I 1 1	0	0

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (three-letter code: MGE) (formula: $C_{38}H_{72}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	B	1	Total C O 48 38 10	0	0
28	D	1	Total C O 48 38 10	0	0
28	D	1	Total C O 48 38 10	0	0
28	L	1	Total C O 48 38 10	0	0
28	b	1	Total C O 48 38 10	0	0
28	d	1	Total C O 48 38 10	0	0
28	d	1	Total C O 48 38 10	0	0
28	l	1	Total C O 48 38 10	0	0

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

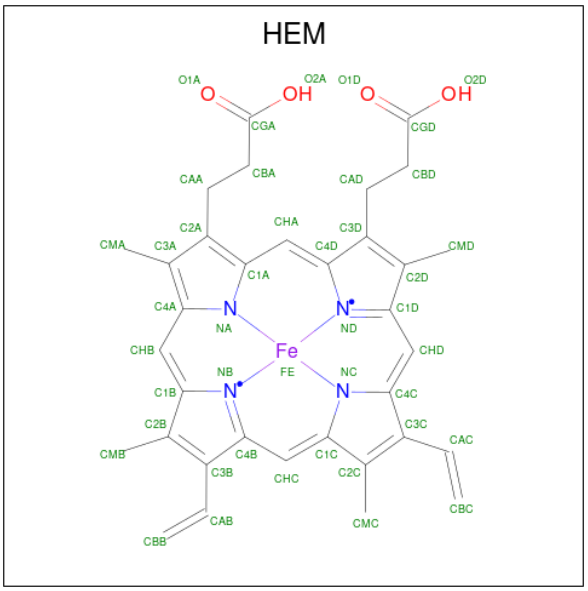


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total C O 66 51 15	0	0
29	C	1	Total C O 66 51 15	0	0
29	C	1	Total C O 66 51 15	0	0
29	C	1	Total C O 66 51 15	0	0
29	b	1	Total C O 66 51 15	0	0
29	c	1	Total C O 66 51 15	0	0
29	c	1	Total C O 66 51 15	0	0
29	c	1	Total C O 66 51 15	0	0

- Molecule 30 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	D	1	Total Fe 1 1	0	0
30	a	1	Total Fe 1 1	0	0

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



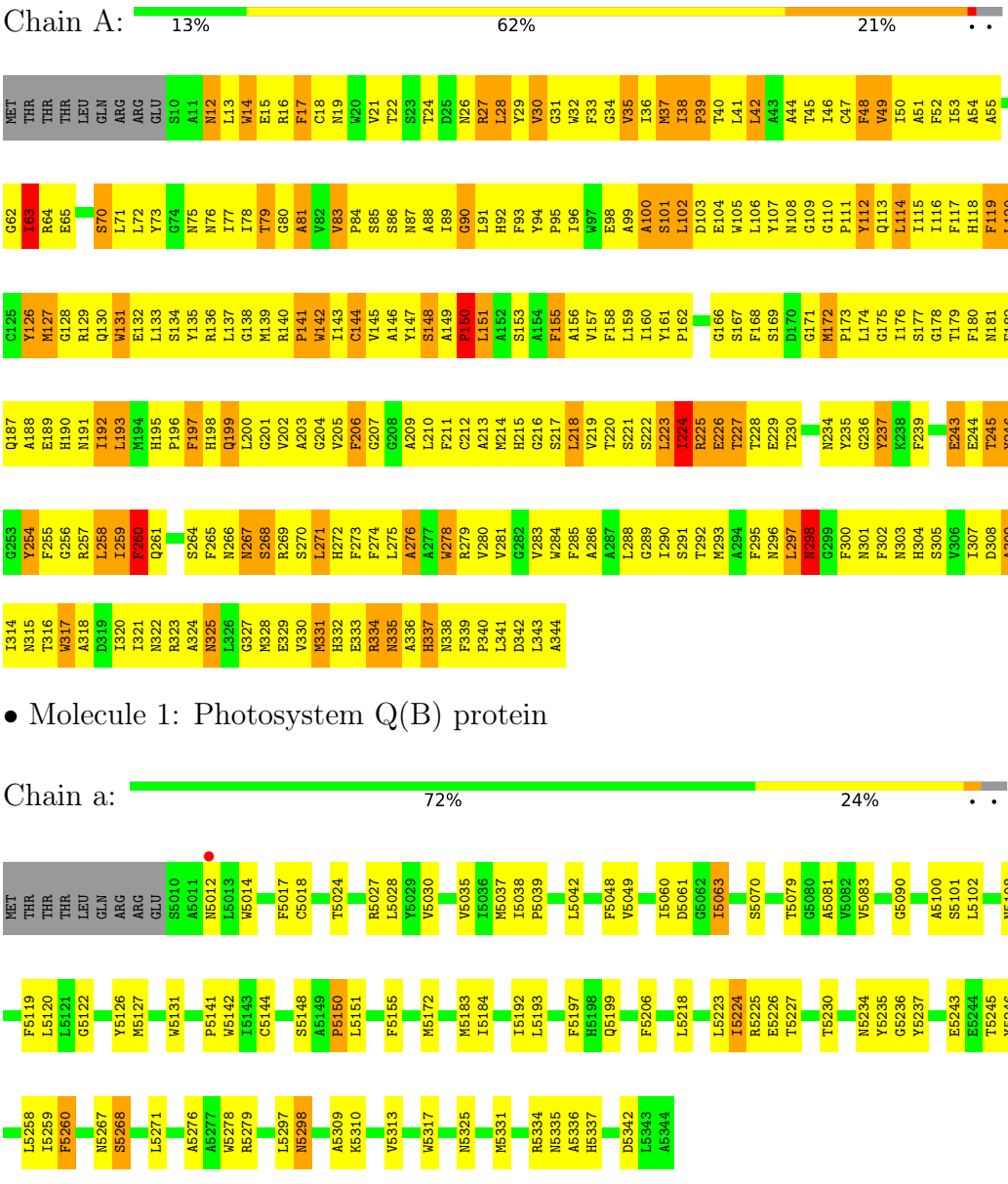
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
31	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
31	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
31	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

Chain A:

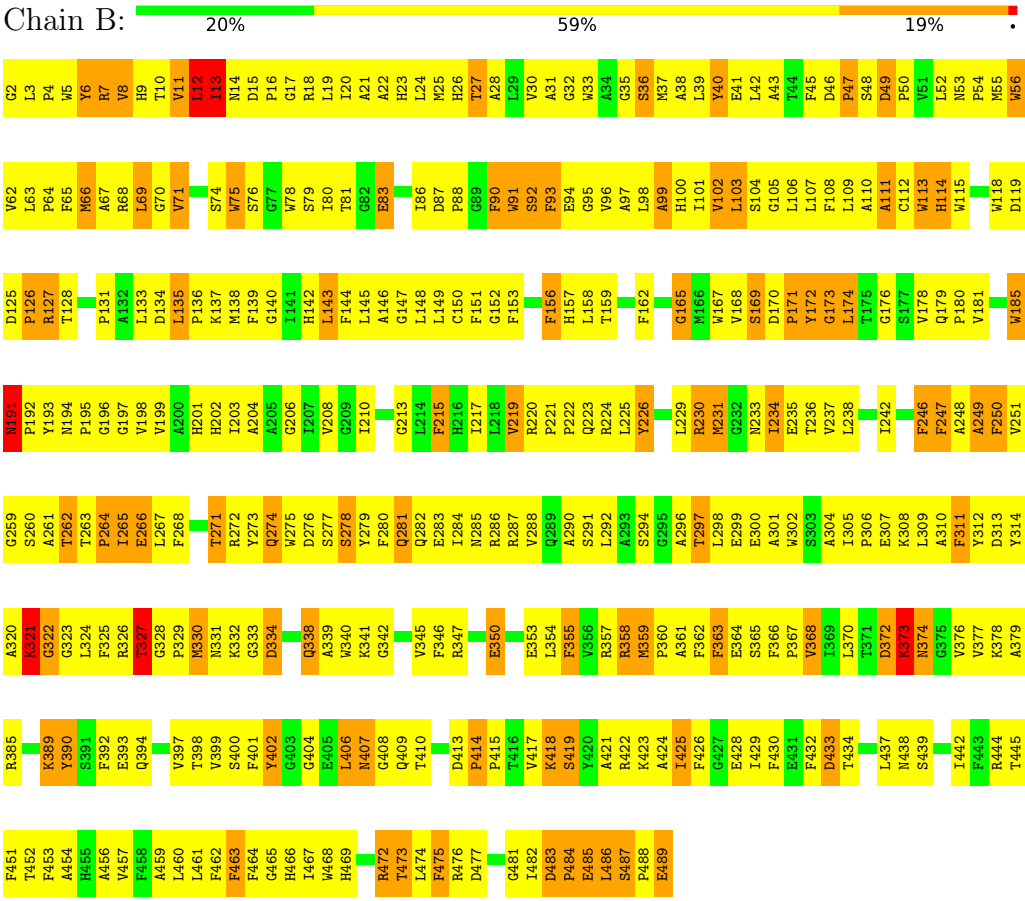


• Molecule 1: Photosystem Q(B) protein

Chain a:

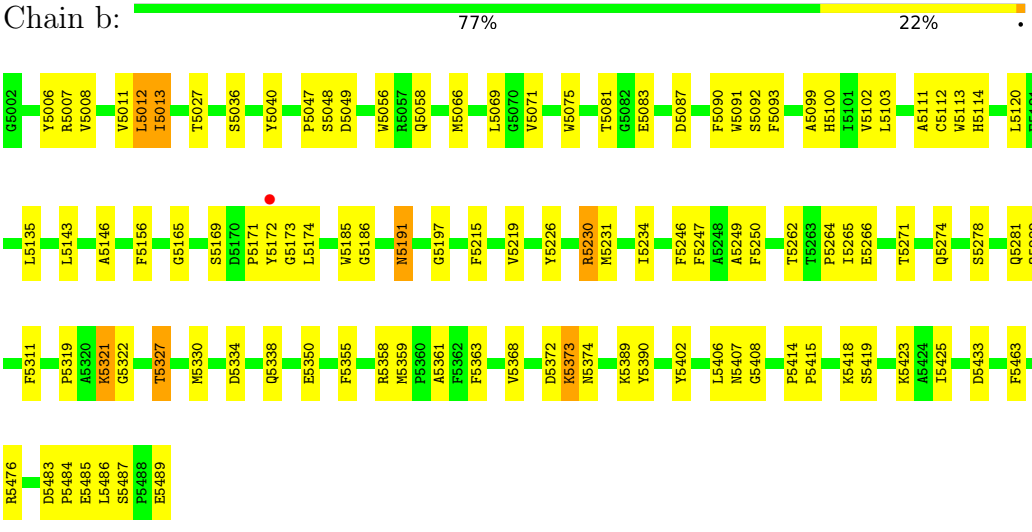
• Molecule 2: Photosystem II core light harvesting protein

Chain B:



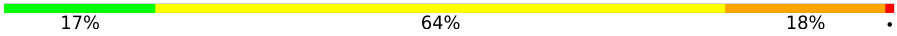
• Molecule 2: Photosystem II core light harvesting protein

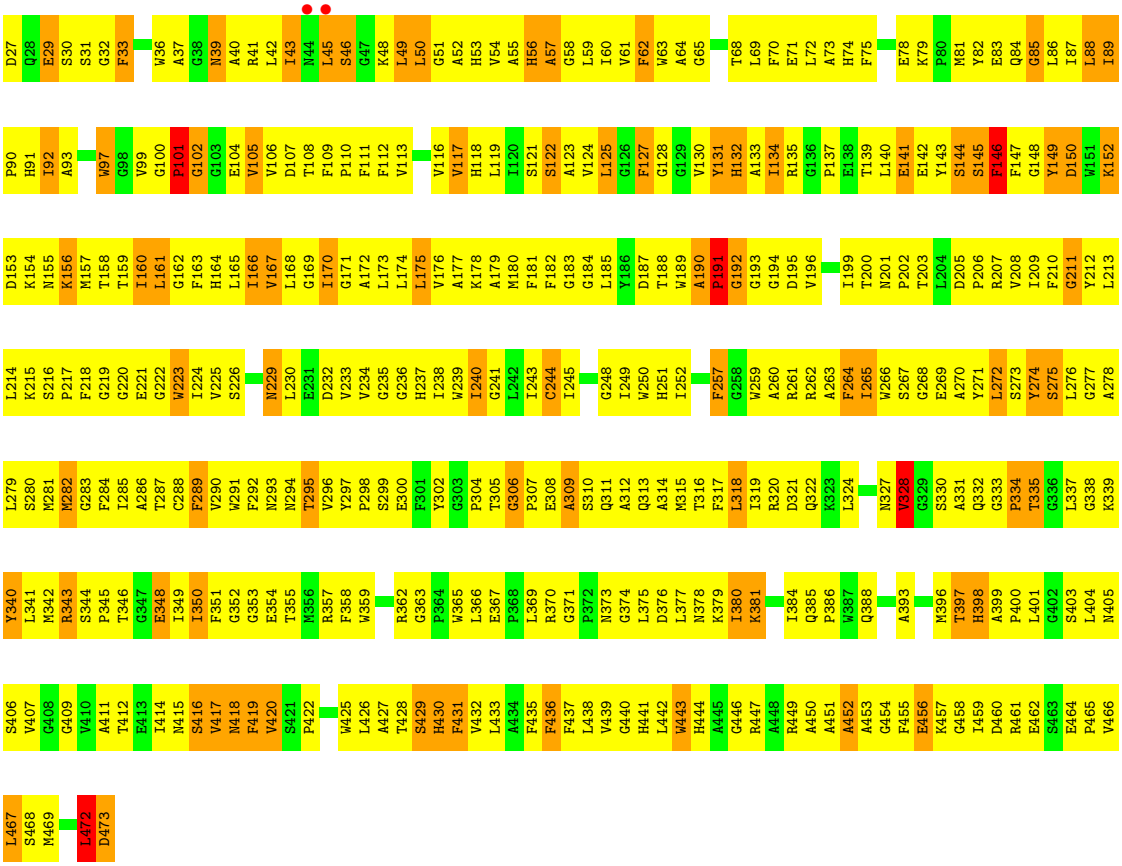
Chain b:



• Molecule 3: Photosystem II CP43 protein

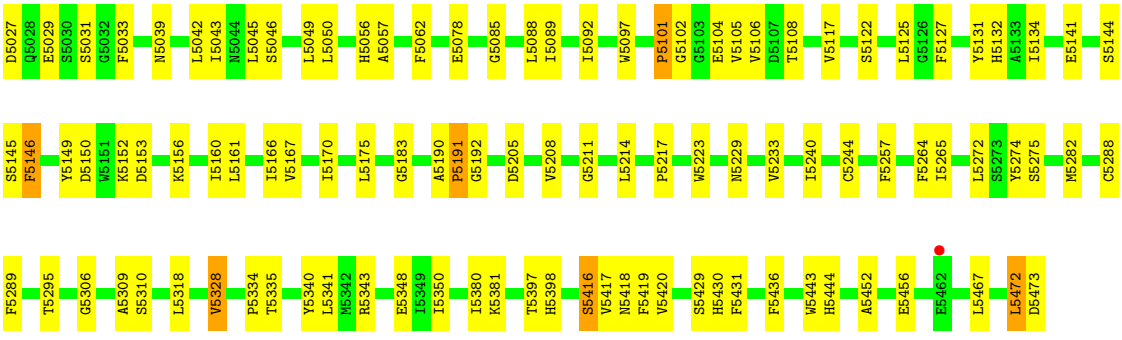
Chain C:





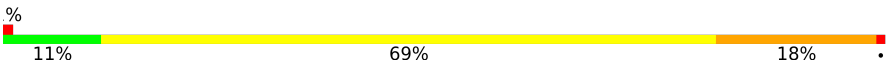
• Molecule 3: Photosystem II CP43 protein

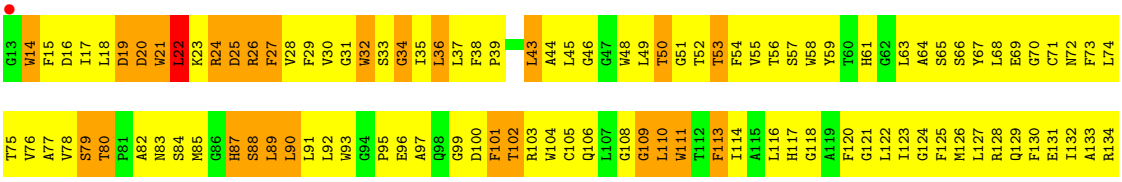
Chain c:

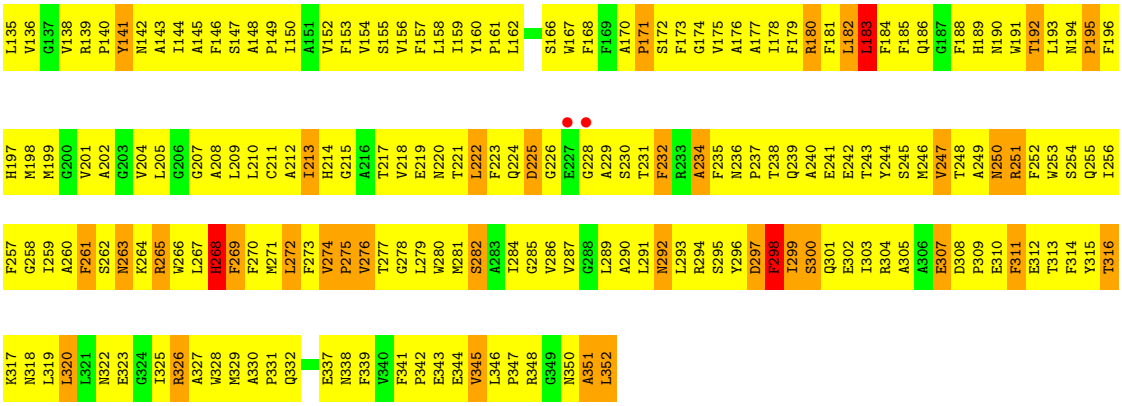


• Molecule 4: Photosystem II D2 protein

Chain D:

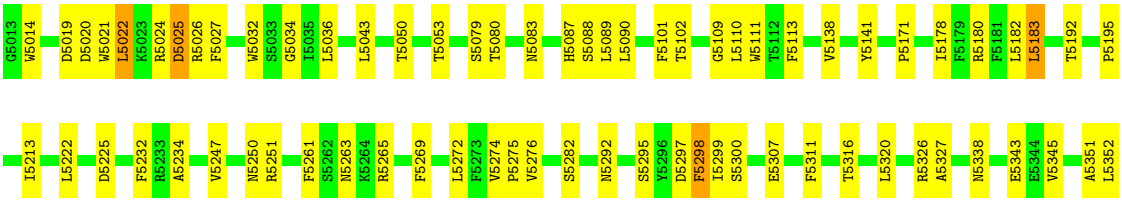






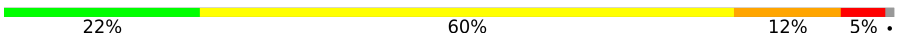
• Molecule 4: Photosystem II D2 protein

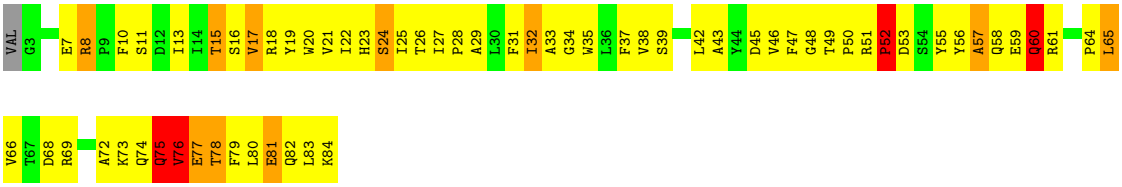
Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

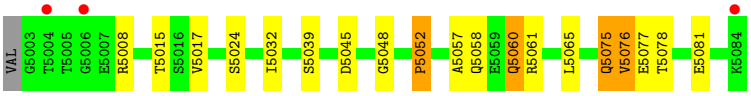
Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

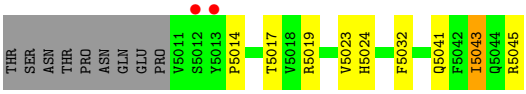


• Molecule 6: Cytochrome b559 subunit beta

Chain F:

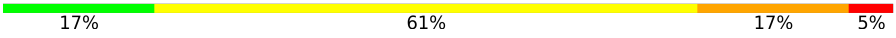
• Molecule 6: Cytochrome b559 subunit beta

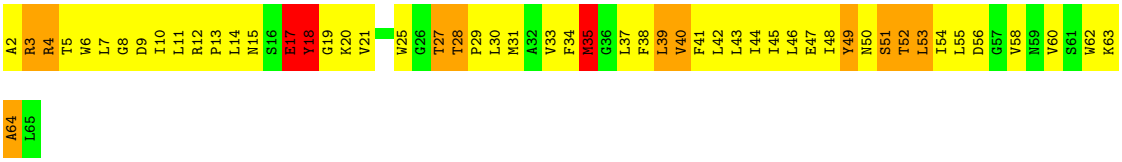
Chain f:



• Molecule 7: Photosystem II reaction center protein H

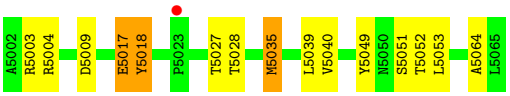
Chain H:





• Molecule 7: Photosystem II reaction center protein H

Chain h:



• Molecule 8: Photosystem II reaction center protein I

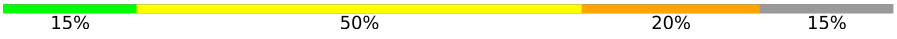
Chain I:

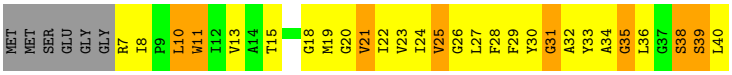
• Molecule 8: Photosystem II reaction center protein I

Chain i:

• Molecule 9: Photosystem II reaction center protein J

Chain J:



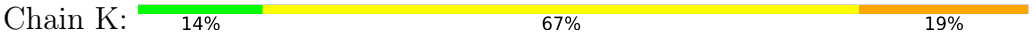


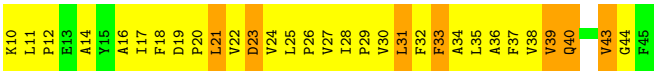
• Molecule 9: Photosystem II reaction center protein J

Chain j:

• Molecule 10: Photosystem II reaction center protein K

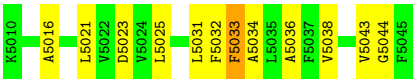
Chain K:





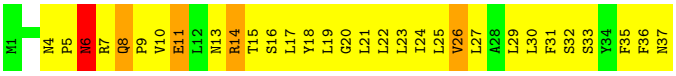
• Molecule 10: Photosystem II reaction center protein K

Chain k:



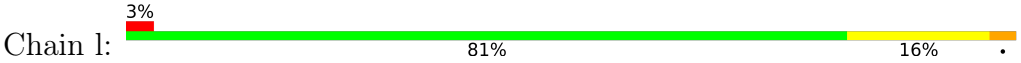
• Molecule 11: Photosystem II reaction center protein L

Chain L:



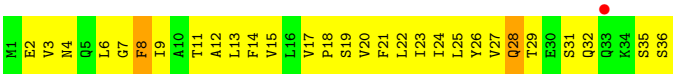
• Molecule 11: Photosystem II reaction center protein L

Chain l:



• Molecule 12: Photosystem II reaction center protein M

Chain M:

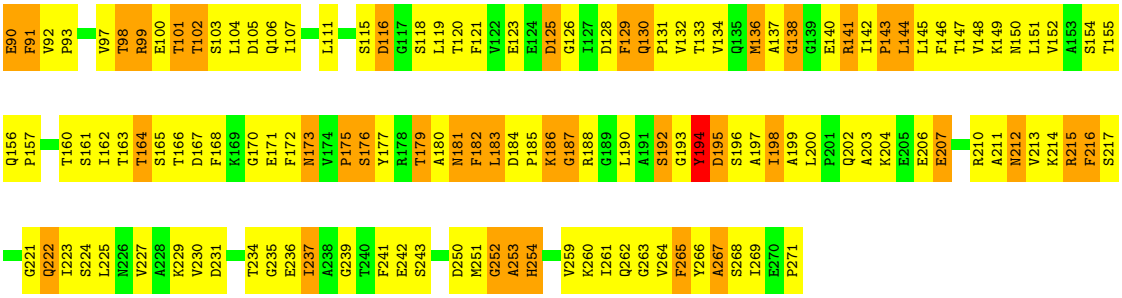


• Molecule 12: Photosystem II reaction center protein M

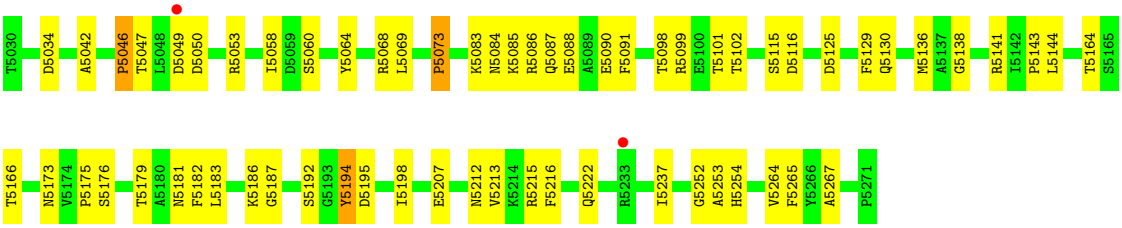
Chain m:

• Molecule 13: Photosystem II manganese-stabilizing polypeptide

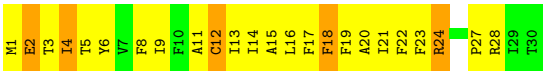
Chain O:



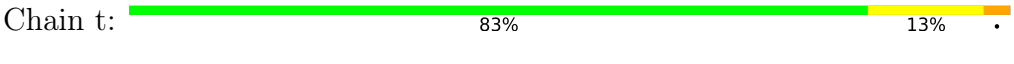
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

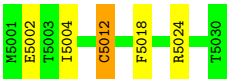


• Molecule 14: Photosystem II reaction center protein T

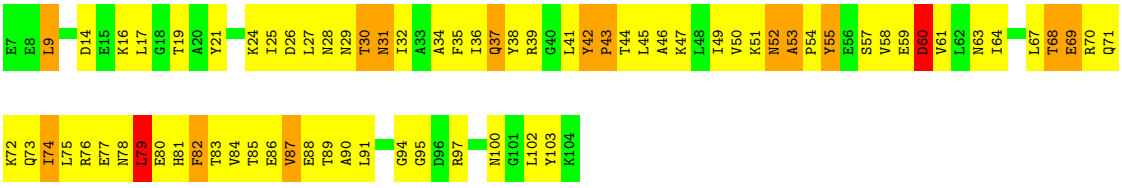


• Molecule 14: Photosystem II reaction center protein T

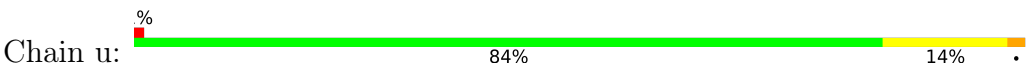


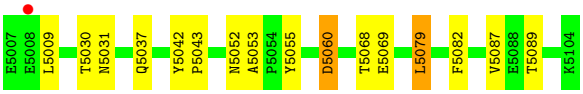


• Molecule 15: Photosystem II 12 kDa extrinsic protein



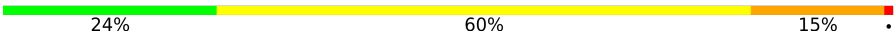
• Molecule 15: Photosystem II 12 kDa extrinsic protein





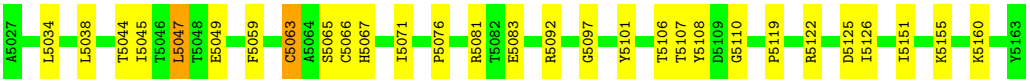
• Molecule 16: Cytochrome c-550

Chain V:



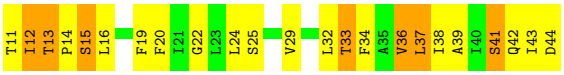
• Molecule 16: Cytochrome c-550

Chain v:



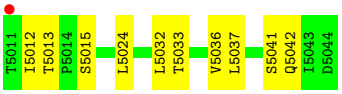
• Molecule 17: Photosystem II reaction center protein X

Chain X:



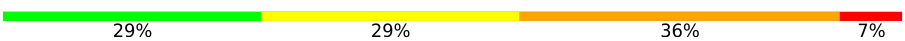
• Molecule 17: Photosystem II reaction center protein X

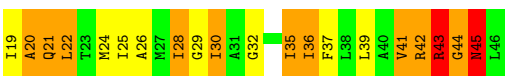
Chain x:



• Molecule 18: Photosystem II reaction center protein ycf12

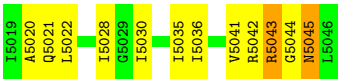
Chain Y:





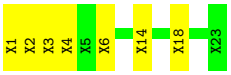
• Molecule 18: Photosystem II reaction center protein ycf12

Chain y:



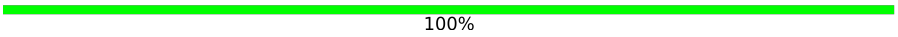
• Molecule 19: Photosystem II reaction center protein Y

Chain N:



• Molecule 19: Photosystem II reaction center protein Y

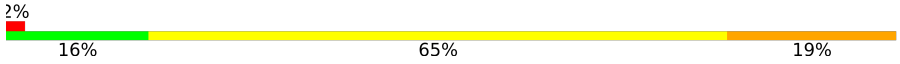
Chain n:

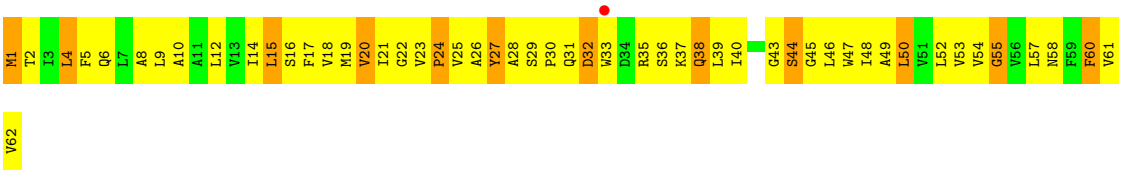


There are no outlier residues recorded for this chain.

• Molecule 20: Photosystem II reaction center protein Z

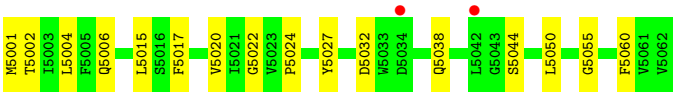
Chain Z:





• Molecule 20: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.50Å 224.70Å 304.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-4.00) 94.8 (20.00-4.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 4.07Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.290 , 0.326 0.275 , 0.276	Depositor DCC
R_{free} test set	3592 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	148.7	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 71.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	48060	wwPDB-VP
Average B, all atoms (Å^2)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PHO, BCR, IOD, HEM, FE2, DGD, PQ9, LHG, CLA, MGE, OEC

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	0.53	0/2714	0.74	0/3699
1	a	0.53	0/2714	0.74	0/3699
2	B	0.55	0/3971	0.80	2/5411 (0.0%)
2	b	0.55	0/3971	0.80	2/5411 (0.0%)
3	C	0.50	0/3568	0.80	2/4858 (0.0%)
3	c	0.50	0/3568	0.80	2/4858 (0.0%)
4	D	0.52	0/2801	0.78	0/3818
4	d	0.52	0/2801	0.78	0/3818
5	E	0.58	0/685	0.79	0/933
5	e	0.58	0/685	0.79	0/933
6	F	0.62	0/291	0.72	0/397
6	f	0.62	0/291	0.72	0/397
7	H	0.54	0/520	0.88	0/708
7	h	0.53	0/520	0.88	0/708
8	I	0.67	0/294	0.75	0/395
8	i	0.67	0/294	0.75	0/395
9	J	0.57	0/255	0.72	0/346
9	j	0.57	0/255	0.71	0/346
10	K	0.52	0/287	0.82	0/394
10	k	0.51	0/287	0.84	0/394
11	L	0.50	0/311	0.76	0/422
11	l	0.50	0/311	0.76	0/422
12	M	0.57	0/287	0.73	0/388
12	m	0.57	0/287	0.73	0/388
13	O	0.51	0/1891	0.83	1/2564 (0.0%)
13	o	0.51	0/1891	0.83	1/2564 (0.0%)
14	T	0.69	0/266	0.83	0/359
14	t	0.66	0/266	0.81	0/359
15	U	0.50	0/794	0.81	0/1076
15	u	0.50	0/794	0.80	0/1076
16	V	0.45	0/1085	0.77	1/1473 (0.1%)
16	v	0.45	0/1085	0.77	1/1473 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	X	0.49	0/249	0.73	0/337
17	x	0.50	0/249	0.73	0/337
18	Y	0.63	0/209	0.94	0/279
18	y	0.63	0/209	0.94	0/279
20	Z	0.61	0/490	0.78	0/669
20	z	0.61	0/490	0.78	0/669
All	All	0.53	0/41936	0.79	12/57052 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	5327	THR	N-CA-C	5.91	126.96	111.00
2	B	327	THR	N-CA-C	5.89	126.91	111.00
3	c	5341	LEU	CA-CB-CG	-5.60	102.43	115.30
3	C	341	LEU	CA-CB-CG	-5.59	102.44	115.30
16	V	110	GLY	N-CA-C	-5.46	99.44	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2630	0	2528	733	0
1	a	2630	0	2528	0	0
2	B	3835	0	3700	797	0
2	b	3835	0	3700	0	0
3	C	3455	0	3376	844	0
3	c	3455	0	3376	0	0
4	D	2706	0	2607	750	0
4	d	2706	0	2608	0	0
5	E	666	0	651	109	0
5	e	666	0	651	0	0
6	F	282	0	291	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	f	282	0	291	0	0
7	H	507	0	529	142	0
7	h	507	0	529	0	0
8	I	287	0	308	65	0
8	i	287	0	305	0	0
9	J	249	0	262	62	0
9	j	249	0	262	0	0
10	K	278	0	289	84	0
10	k	278	0	289	0	0
11	L	304	0	316	76	0
11	l	304	0	313	0	0
12	M	283	0	297	50	0
12	m	283	0	294	0	0
13	O	1860	0	1833	305	0
13	o	1860	0	1833	0	0
14	T	257	0	261	55	0
14	t	257	0	259	0	0
15	U	783	0	779	137	0
15	u	783	0	779	0	0
16	V	1064	0	1072	206	0
16	v	1064	0	1072	0	0
17	X	246	0	269	39	0
17	x	246	0	269	0	0
18	Y	208	0	237	77	0
18	y	208	0	237	0	0
19	N	116	0	26	6	0
19	n	116	0	26	0	0
20	Z	479	0	516	73	0
20	z	479	0	513	0	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	A	195	0	216	139	0
22	B	975	0	1080	668	0
22	C	780	0	864	488	0
22	D	195	0	216	157	0
22	H	65	0	72	45	0
22	K	65	0	72	87	0
22	a	195	0	216	0	0
22	b	975	0	1080	0	0
22	c	780	0	864	0	0
22	d	195	0	216	0	0
22	h	65	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	k	65	0	72	0	0
23	A	64	0	74	63	0
23	D	64	0	74	53	0
23	a	64	0	74	0	0
23	d	64	0	74	0	0
24	A	45	0	64	39	0
24	D	45	0	64	52	0
24	a	45	0	64	0	0
24	d	45	0	64	0	0
25	A	40	0	47	25	0
25	B	120	0	142	74	0
25	C	80	0	96	81	0
25	D	40	0	48	40	0
25	H	40	0	48	36	0
25	K	40	0	47	27	0
25	T	80	0	95	40	0
25	Z	40	0	47	18	0
25	a	40	0	47	0	0
25	b	80	0	95	0	0
25	c	40	0	48	0	0
25	d	40	0	48	0	0
25	h	40	0	48	0	0
25	k	80	0	95	0	0
25	t	40	0	48	0	0
25	z	40	0	47	0	0
26	A	49	0	74	36	0
26	a	49	0	74	0	0
27	A	1	0	0	1	0
27	B	1	0	0	3	0
27	D	2	0	0	10	0
27	T	1	0	0	2	0
27	a	1	0	0	0	0
27	b	1	0	0	0	0
27	d	2	0	0	0	0
27	t	1	0	0	0	0
28	B	48	0	72	39	0
28	D	96	0	144	66	0
28	L	48	0	72	29	0
28	b	48	0	72	0	0
28	d	96	0	144	0	0
28	l	48	0	72	0	0
29	B	66	0	96	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	198	0	288	118	0
29	b	66	0	96	0	0
29	c	198	0	288	0	0
30	D	1	0	0	0	0
30	a	1	0	0	0	0
31	F	43	0	30	17	0
31	V	43	0	30	12	0
31	f	43	0	30	0	0
31	v	43	0	30	0	0
All	All	48060	0	48531	5652	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 118.

The worst 5 of 5652 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:PHE:CE2	22:B:1012:CLA:HMA2	1.39	1.55
22:B:1011:CLA:HED2	22:B:1012:CLA:CED	1.31	1.53
25:C:1052:BCR:H371	25:C:1052:BCR:C26	1.34	1.50
22:B:1016:CLA:H162	22:D:1008:CLA:CMA	1.38	1.49
22:A:1003:CLA:HED2	22:A:1003:CLA:CAA	1.44	1.47

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/344 (97%)	219 (66%)	75 (22%)	39 (12%)	0 6
1	a	333/344 (97%)	216 (65%)	76 (23%)	41 (12%)	0 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0 8
2	b	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0 8
3	C	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1 14
3	c	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1 14
4	D	338/340 (99%)	222 (66%)	78 (23%)	38 (11%)	0 7
4	d	338/340 (99%)	224 (66%)	77 (23%)	37 (11%)	0 7
5	E	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0 6
5	e	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0 6
6	F	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0 5
6	f	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0 5
7	H	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0 4
7	h	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0 4
8	I	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0 2
8	i	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0 2
9	J	32/40 (80%)	29 (91%)	0	3 (9%)	0 11
9	j	32/40 (80%)	29 (91%)	0	3 (9%)	0 11
10	K	34/36 (94%)	23 (68%)	5 (15%)	6 (18%)	0 2
10	k	34/36 (94%)	17 (50%)	8 (24%)	9 (26%)	0 0
11	L	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	1 19
11	l	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	1 19
12	M	34/36 (94%)	23 (68%)	11 (32%)	0	100 100
12	m	34/36 (94%)	23 (68%)	11 (32%)	0	100 100
13	O	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0 6
13	o	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0 6
14	T	28/30 (93%)	22 (79%)	5 (18%)	1 (4%)	3 28
14	t	28/30 (93%)	22 (79%)	4 (14%)	2 (7%)	1 16
15	U	96/98 (98%)	70 (73%)	17 (18%)	9 (9%)	0 11
15	u	96/98 (98%)	70 (73%)	18 (19%)	8 (8%)	1 13
16	V	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1 15
16	v	135/137 (98%)	99 (73%)	26 (19%)	10 (7%)	1 15
17	X	32/34 (94%)	29 (91%)	3 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	x	32/34 (94%)	29 (91%)	3 (9%)	0	100 100
18	Y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0 2
18	y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0 2
20	Z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1 17
20	z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1 17
All	All	5124/5250 (98%)	3622 (71%)	986 (19%)	516 (10%)	0 9

5 of 516 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	61	ASP
1	A	100	ALA
1	A	224	ILE
1	A	226	GLU

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	270/279 (97%)	218 (81%)	52 (19%)	1 9
1	a	270/279 (97%)	217 (80%)	53 (20%)	1 8
2	B	388/388 (100%)	319 (82%)	69 (18%)	2 12
2	b	388/388 (100%)	319 (82%)	69 (18%)	2 12
3	C	349/349 (100%)	277 (79%)	72 (21%)	1 7
3	c	349/349 (100%)	276 (79%)	73 (21%)	1 6
4	D	275/275 (100%)	236 (86%)	39 (14%)	3 19
4	d	275/275 (100%)	237 (86%)	38 (14%)	3 20
5	E	72/73 (99%)	58 (81%)	14 (19%)	1 9
5	e	72/73 (99%)	58 (81%)	14 (19%)	1 9
6	F	29/38 (76%)	23 (79%)	6 (21%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	f	29/38 (76%)	23 (79%)	6 (21%)	1 6
7	H	54/54 (100%)	44 (82%)	10 (18%)	1 10
7	h	54/54 (100%)	44 (82%)	10 (18%)	1 10
8	I	32/32 (100%)	23 (72%)	9 (28%)	0 3
8	i	32/32 (100%)	23 (72%)	9 (28%)	0 3
9	J	24/28 (86%)	19 (79%)	5 (21%)	1 6
9	j	24/28 (86%)	19 (79%)	5 (21%)	1 6
10	K	29/29 (100%)	24 (83%)	5 (17%)	2 13
10	k	29/29 (100%)	25 (86%)	4 (14%)	3 20
11	L	35/35 (100%)	29 (83%)	6 (17%)	2 13
11	l	35/35 (100%)	29 (83%)	6 (17%)	2 13
12	M	33/33 (100%)	31 (94%)	2 (6%)	18 47
12	m	33/33 (100%)	32 (97%)	1 (3%)	41 64
13	O	206/206 (100%)	168 (82%)	38 (18%)	1 10
13	o	206/206 (100%)	168 (82%)	38 (18%)	1 10
14	T	27/27 (100%)	23 (85%)	4 (15%)	3 17
14	t	27/27 (100%)	23 (85%)	4 (15%)	3 17
15	U	85/85 (100%)	74 (87%)	11 (13%)	4 22
15	u	85/85 (100%)	75 (88%)	10 (12%)	5 24
16	V	117/117 (100%)	96 (82%)	21 (18%)	2 11
16	v	117/117 (100%)	97 (83%)	20 (17%)	2 13
17	X	27/27 (100%)	17 (63%)	10 (37%)	0 0
17	x	27/27 (100%)	17 (63%)	10 (37%)	0 0
18	Y	21/21 (100%)	12 (57%)	9 (43%)	0 0
18	y	21/21 (100%)	12 (57%)	9 (43%)	0 0
20	Z	52/52 (100%)	40 (77%)	12 (23%)	1 5
20	z	52/52 (100%)	40 (77%)	12 (23%)	1 5
All	All	4250/4296 (99%)	3465 (82%)	785 (18%)	1 10

5 of 785 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	5092	SER

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Mol	Chain	Res	Type
3	c	5348	GLU
2	b	5215	PHE
2	b	5091	TRP
3	c	5043	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	5374	ASN
7	h	5015	ASN
3	c	5155	ASN
4	d	5197	HIS
13	o	5072	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 136 ligands modelled in this entry, 12 are monoatomic - leaving 124 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	$\#\|Z\|>2$
29	DGD	c	6056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	d	6008	-	65,73,73	1.92	16 (24%)	76,113,113	2.44	26 (34%)
22	CLA	C	1031	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	c	6033	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
26	LHG	a	6063	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	3 (5%)
22	CLA	b	6019	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	a	6007	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	d	6005	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
22	CLA	B	1012	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
26	LHG	A	1063	-	48,48,48	0.95	2 (4%)	51,54,54	1.04	3 (5%)
22	CLA	b	6018	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	b	6022	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
24	PQ9	D	1042	-	45,45,45	0.66	1 (2%)	56,57,57	1.77	17 (30%)
28	MGE	d	6059	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)
29	DGD	b	6058	-	67,67,67	0.85	2 (2%)	81,81,81	0.90	3 (3%)
22	CLA	C	1033	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	B	1023	-	65,73,73	1.91	16 (24%)	76,113,113	2.45	26 (34%)
22	CLA	C	1036	-	65,73,73	1.95	15 (23%)	76,113,113	2.44	24 (31%)
28	MGE	d	6062	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)
22	CLA	A	1006	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	B	1013	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	c	6032	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
25	BCR	K	1051	-	41,41,41	4.26	15 (36%)	56,56,56	4.89	24 (42%)
24	PQ9	d	6042	-	45,45,45	0.66	2 (4%)	56,57,57	1.78	17 (30%)
22	CLA	c	6037	-	65,73,73	1.95	15 (23%)	76,113,113	2.44	25 (32%)
22	CLA	B	1016	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
25	BCR	Z	1053	-	41,41,41	4.26	16 (39%)	56,56,56	5.94	24 (42%)
23	PHO	d	6039	-	51,69,69	2.91	10 (19%)	47,99,99	2.44	11 (23%)
22	CLA	d	6004	-	65,73,73	1.96	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	B	1022	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	D	1004	-	65,73,73	1.96	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	b	6021	2	65,73,73	1.92	16 (24%)	76,113,113	2.46	27 (35%)
22	CLA	b	6024	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	B	1020	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
22	CLA	D	1008	-	65,73,73	1.92	16 (24%)	76,113,113	2.43	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	6026	-	65,73,73	1.95	15 (23%)	76,113,113	2.44	24 (31%)
22	CLA	C	1037	-	65,73,73	1.95	15 (23%)	76,113,113	2.44	24 (31%)
22	CLA	C	1030	-	65,73,73	1.92	16 (24%)	76,113,113	2.43	26 (34%)
22	CLA	B	1019	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	b	6014	-	65,73,73	1.96	15 (23%)	76,113,113	2.45	24 (31%)
29	DGD	C	1057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
28	MGE	b	6060	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)
22	CLA	B	1010	2	65,73,73	1.92	16 (24%)	76,113,113	2.45	25 (32%)
22	CLA	c	6029	-	65,73,73	1.91	16 (24%)	76,113,113	2.45	26 (34%)
22	CLA	c	6030	-	65,73,73	1.92	16 (24%)	76,113,113	2.43	26 (34%)
22	CLA	c	6031	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
25	BCR	h	6049	-	41,41,41	4.25	15 (36%)	56,56,56	5.22	24 (42%)
22	CLA	B	1024	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
22	CLA	b	6012	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
29	DGD	c	6055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	B	1009	-	65,73,73	1.93	16 (24%)	76,113,113	2.43	26 (34%)
25	BCR	C	1054	-	41,41,41	4.26	15 (36%)	56,56,56	5.30	24 (42%)
22	CLA	D	1005	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
22	CLA	b	6010	2	65,73,73	1.92	16 (24%)	76,113,113	2.45	25 (32%)
31	HEM	f	6040	5	41,50,50	1.95	6 (14%)	45,82,82	1.72	5 (11%)
22	CLA	b	6020	-	65,73,73	1.95	15 (23%)	76,113,113	2.46	24 (31%)
31	HEM	F	1040	5	41,50,50	1.96	6 (14%)	45,82,82	1.72	5 (11%)
25	BCR	B	1047	-	41,41,41	4.25	15 (36%)	56,56,56	5.37	28 (50%)
22	CLA	K	1034	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	A	1003	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	b	6013	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
25	BCR	d	6050	-	41,41,41	4.26	15 (36%)	56,56,56	5.08	24 (42%)
25	BCR	D	1050	-	41,41,41	4.26	15 (36%)	56,56,56	5.07	24 (42%)
22	CLA	h	6017	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
22	CLA	C	1029	-	65,73,73	1.91	16 (24%)	76,113,113	2.45	26 (34%)
22	CLA	C	1027	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	c	6028	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
25	BCR	T	6046	-	41,41,41	4.18	17 (41%)	56,56,56	5.95	27 (48%)
28	MGE	l	6061	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)
22	CLA	c	6036	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	HEM	V	1041	16	41,50,50	1.97	6 (14%)	45,82,82	1.73	5 (11%)
22	CLA	C	1025	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	C	1035	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	b	6011	-	65,73,73	1.92	16 (24%)	76,113,113	2.44	27 (35%)
22	CLA	c	6035	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
25	BCR	A	1044	-	41,41,41	4.15	16 (39%)	56,56,56	7.08	30 (53%)
28	MGE	L	1061	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)
31	HEM	v	6041	16	41,50,50	1.97	6 (14%)	45,82,82	1.73	5 (11%)
22	CLA	a	6003	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	b	6023	-	65,73,73	1.91	17 (26%)	76,113,113	2.46	26 (34%)
22	CLA	B	1021	2	65,73,73	1.93	16 (24%)	76,113,113	2.47	27 (35%)
23	PHO	A	1038	-	51,69,69	2.90	10 (19%)	47,99,99	2.45	11 (23%)
25	BCR	k	6051	-	41,41,41	4.26	16 (39%)	56,56,56	4.89	24 (42%)
22	CLA	H	1017	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	k	6034	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
25	BCR	C	1052	-	41,41,41	4.25	16 (39%)	56,56,56	6.82	27 (48%)
25	BCR	a	6044	-	41,41,41	4.15	16 (39%)	56,56,56	7.09	30 (53%)
29	DGD	C	1055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6015	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
25	BCR	T	6048	-	41,41,41	4.25	15 (36%)	56,56,56	6.18	28 (50%)
25	BCR	k	6052	-	41,41,41	4.26	16 (39%)	56,56,56	6.83	27 (48%)
23	PHO	D	1039	-	51,69,69	2.90	10 (19%)	47,99,99	2.44	11 (23%)
22	CLA	b	6016	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
25	BCR	t	1046	-	41,41,41	4.18	17 (41%)	56,56,56	5.94	27 (48%)
22	CLA	C	1026	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
22	CLA	B	1011	-	65,73,73	1.92	17 (26%)	76,113,113	2.44	27 (35%)
29	DGD	C	1056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
24	PQ9	A	1043	-	45,45,45	0.66	1 (2%)	56,57,57	1.77	17 (30%)
28	MGE	D	1062	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)
25	BCR	z	6053	-	41,41,41	4.26	17 (41%)	56,56,56	5.94	24 (42%)
23	PHO	a	6038	-	51,69,69	2.90	10 (19%)	47,99,99	2.44	11 (23%)
24	PQ9	a	6043	-	45,45,45	0.66	2 (4%)	56,57,57	1.77	17 (30%)
22	CLA	B	1014	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
25	BCR	H	1049	-	41,41,41	4.26	16 (39%)	56,56,56	5.22	24 (42%)
29	DGD	B	1058	-	67,67,67	0.85	2 (2%)	81,81,81	0.90	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	DGD	c	6057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6009	-	65,73,73	1.92	16 (24%)	76,113,113	2.43	26 (34%)
22	CLA	B	1015	-	65,73,73	1.95	15 (23%)	76,113,113	2.45	24 (31%)
22	CLA	c	6027	-	65,73,73	1.96	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	B	1018	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	C	1028	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
25	BCR	B	1048	-	41,41,41	4.25	15 (36%)	56,56,56	6.18	28 (50%)
25	BCR	B	1045	-	41,41,41	4.26	16 (39%)	56,56,56	6.04	24 (42%)
25	BCR	b	6047	-	41,41,41	4.25	16 (39%)	56,56,56	5.37	28 (50%)
22	CLA	C	1032	-	65,73,73	1.95	16 (24%)	76,113,113	2.44	24 (31%)
25	BCR	c	6054	-	41,41,41	4.25	15 (36%)	56,56,56	5.30	24 (42%)
28	MGE	B	1060	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)
22	CLA	A	1007	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	c	6025	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
22	CLA	a	6006	-	65,73,73	1.95	16 (24%)	76,113,113	2.45	24 (31%)
25	BCR	b	6045	-	41,41,41	4.26	16 (39%)	56,56,56	6.04	24 (42%)
28	MGE	D	1059	-	48,48,48	0.96	2 (4%)	56,56,56	1.01	3 (5%)

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
29	DGD	c	6056	-	-	32/55/95/95	0/2/2/2
22	CLA	d	6008	-	3/3/15/20	15/37/115/115	-
22	CLA	C	1031	-	2/2/15/20	15/37/115/115	-
22	CLA	c	6033	-	2/2/15/20	18/37/115/115	-
26	LHG	a	6063	-	-	29/53/53/53	-
22	CLA	b	6019	-	2/2/15/20	20/37/115/115	-
22	CLA	a	6007	-	1/1/15/20	23/37/115/115	-
22	CLA	d	6005	-	2/2/15/20	19/37/115/115	-
22	CLA	B	1012	-	2/2/15/20	16/37/115/115	-
26	LHG	A	1063	-	-	29/53/53/53	-
22	CLA	b	6018	-	2/2/15/20	22/37/115/115	-
22	CLA	b	6022	-	3/3/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PQ9	D	1042	-	-	10/41/61/61	0/1/1/1
28	MGE	d	6059	-	-	24/43/63/63	0/1/1/1
29	DGD	b	6058	-	-	31/55/95/95	0/2/2/2
22	CLA	C	1033	-	2/2/15/20	18/37/115/115	-
22	CLA	B	1023	-	3/3/15/20	18/37/115/115	-
22	CLA	C	1036	-	2/2/15/20	24/37/115/115	-
28	MGE	d	6062	-	-	25/43/63/63	0/1/1/1
22	CLA	A	1006	-	2/2/15/20	22/37/115/115	-
22	CLA	B	1013	-	2/2/15/20	22/37/115/115	-
22	CLA	c	6032	-	3/3/15/20	18/37/115/115	-
25	BCR	K	1051	-	-	15/29/63/63	0/2/2/2
24	PQ9	d	6042	-	-	10/41/61/61	0/1/1/1
22	CLA	c	6037	-	2/2/15/20	17/37/115/115	-
22	CLA	B	1016	-	1/1/15/20	20/37/115/115	-
25	BCR	Z	1053	-	-	15/29/63/63	0/2/2/2
23	PHO	d	6039	-	3/3/17/22	17/37/103/103	0/5/6/6
22	CLA	d	6004	-	2/2/15/20	12/37/115/115	-
22	CLA	B	1022	-	3/3/15/20	19/37/115/115	-
22	CLA	D	1004	-	2/2/15/20	12/37/115/115	-
22	CLA	b	6021	2	2/2/15/20	22/37/115/115	-
22	CLA	b	6024	-	1/1/15/20	15/37/115/115	-
22	CLA	B	1020	-	3/3/15/20	14/37/115/115	-
22	CLA	D	1008	-	3/3/15/20	15/37/115/115	-
22	CLA	c	6026	-	1/1/15/20	20/37/115/115	-
22	CLA	C	1037	-	2/2/15/20	17/37/115/115	-
22	CLA	C	1030	-	2/2/15/20	17/37/115/115	-
22	CLA	B	1019	-	2/2/15/20	20/37/115/115	-
22	CLA	b	6014	-	2/2/15/20	18/37/115/115	-
29	DGD	C	1057	-	-	32/55/95/95	0/2/2/2
28	MGE	b	6060	-	-	30/43/63/63	0/1/1/1
22	CLA	B	1010	2	2/2/15/20	16/37/115/115	-
22	CLA	c	6029	-	3/3/15/20	16/37/115/115	-
22	CLA	c	6030	-	2/2/15/20	17/37/115/115	-
22	CLA	c	6031	-	2/2/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	h	6049	-	-	13/29/63/63	0/2/2/2
22	CLA	B	1024	-	1/1/15/20	15/37/115/115	-
22	CLA	b	6012	-	2/2/15/20	16/37/115/115	-
29	DGD	c	6055	-	-	33/55/95/95	0/2/2/2
22	CLA	B	1009	-	2/2/15/20	19/37/115/115	-
25	BCR	C	1054	-	-	14/29/63/63	0/2/2/2
22	CLA	D	1005	-	2/2/15/20	19/37/115/115	-
22	CLA	b	6010	2	2/2/15/20	16/37/115/115	-
31	HEM	f	6040	5	-	8/12/54/54	-
22	CLA	b	6020	-	3/3/15/20	14/37/115/115	-
31	HEM	F	1040	5	-	8/12/54/54	-
25	BCR	B	1047	-	-	17/29/63/63	0/2/2/2
22	CLA	K	1034	-	5/5/15/20	23/37/115/115	-
22	CLA	A	1003	-	2/2/15/20	22/37/115/115	-
22	CLA	b	6013	-	2/2/15/20	22/37/115/115	-
25	BCR	d	6050	-	-	21/29/63/63	0/2/2/2
25	BCR	D	1050	-	-	21/29/63/63	0/2/2/2
22	CLA	h	6017	-	2/2/15/20	22/37/115/115	-
22	CLA	C	1029	-	3/3/15/20	16/37/115/115	-
22	CLA	C	1027	-	3/3/15/20	18/37/115/115	-
22	CLA	c	6028	-	2/2/15/20	24/37/115/115	-
25	BCR	T	6046	-	-	11/29/63/63	0/2/2/2
28	MGE	l	6061	-	-	26/43/63/63	0/1/1/1
22	CLA	c	6036	-	2/2/15/20	24/37/115/115	-
31	HEM	V	1041	16	-	5/12/54/54	-
22	CLA	C	1025	-	2/2/15/20	20/37/115/115	-
22	CLA	C	1035	-	2/2/15/20	17/37/115/115	-
22	CLA	b	6011	-	3/3/15/20	19/37/115/115	-
22	CLA	c	6035	-	2/2/15/20	17/37/115/115	-
25	BCR	A	1044	-	-	12/29/63/63	0/2/2/2
28	MGE	L	1061	-	-	26/43/63/63	0/1/1/1
31	HEM	v	6041	16	-	5/12/54/54	-
22	CLA	a	6003	-	2/2/15/20	23/37/115/115	-
22	CLA	b	6023	-	3/3/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1021	2	2/2/15/20	22/37/115/115	-
23	PHO	A	1038	-	1/1/17/22	19/37/103/103	0/5/6/6
25	BCR	k	6051	-	-	15/29/63/63	0/2/2/2
22	CLA	H	1017	-	2/2/15/20	22/37/115/115	-
22	CLA	k	6034	-	5/5/15/20	23/37/115/115	-
25	BCR	C	1052	-	-	14/29/63/63	0/2/2/2
25	BCR	a	6044	-	-	12/29/63/63	0/2/2/2
29	DGD	C	1055	-	-	33/55/95/95	0/2/2/2
22	CLA	b	6015	-	2/2/15/20	21/37/115/115	-
25	BCR	T	6048	-	-	10/29/63/63	0/2/2/2
25	BCR	k	6052	-	-	14/29/63/63	0/2/2/2
23	PHO	D	1039	-	3/3/17/22	17/37/103/103	0/5/6/6
22	CLA	b	6016	-	1/1/15/20	20/37/115/115	-
25	BCR	t	1046	-	-	11/29/63/63	0/2/2/2
22	CLA	C	1026	-	1/1/15/20	20/37/115/115	-
22	CLA	B	1011	-	3/3/15/20	19/37/115/115	-
29	DGD	C	1056	-	-	32/55/95/95	0/2/2/2
24	PQ9	A	1043	-	-	16/41/61/61	0/1/1/1
28	MGE	D	1062	-	-	25/43/63/63	0/1/1/1
25	BCR	z	6053	-	-	15/29/63/63	0/2/2/2
23	PHO	a	6038	-	1/1/17/22	19/37/103/103	0/5/6/6
24	PQ9	a	6043	-	-	16/41/61/61	0/1/1/1
22	CLA	B	1014	-	2/2/15/20	18/37/115/115	-
25	BCR	H	1049	-	-	13/29/63/63	0/2/2/2
29	DGD	B	1058	-	-	31/55/95/95	0/2/2/2
29	DGD	c	6057	-	-	32/55/95/95	0/2/2/2
22	CLA	b	6009	-	2/2/15/20	19/37/115/115	-
22	CLA	B	1015	-	2/2/15/20	21/37/115/115	-
22	CLA	c	6027	-	3/3/15/20	18/37/115/115	-
22	CLA	B	1018	-	2/2/15/20	22/37/115/115	-
22	CLA	C	1028	-	2/2/15/20	24/37/115/115	-
25	BCR	B	1048	-	-	10/29/63/63	0/2/2/2
25	BCR	B	1045	-	-	20/29/63/63	0/2/2/2
25	BCR	b	6047	-	-	17/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	1032	-	3/3/15/20	18/37/115/115	-
25	BCR	c	6054	-	-	14/29/63/63	0/2/2/2
28	MGE	B	1060	-	-	30/43/63/63	0/1/1/1
22	CLA	A	1007	-	1/1/15/20	23/37/115/115	-
22	CLA	c	6025	-	2/2/15/20	20/37/115/115	-
22	CLA	a	6006	-	2/2/15/20	22/37/115/115	-
25	BCR	b	6045	-	-	20/29/63/63	0/2/2/2
28	MGE	D	1059	-	-	24/43/63/63	0/1/1/1

The worst 5 of 1556 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	6039	PHO	OBD-CAD	13.72	1.41	1.22
23	D	1039	PHO	OBD-CAD	13.71	1.41	1.22
23	A	1038	PHO	OBD-CAD	13.70	1.41	1.22
23	a	6038	PHO	OBD-CAD	13.70	1.41	1.22
25	b	6047	BCR	C19-C18	-9.35	1.25	1.45

The worst 5 of 2469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	6045	BCR	C16-C17-C18	28.75	168.34	127.31
25	B	1045	BCR	C16-C17-C18	28.73	168.32	127.31
25	T	6048	BCR	C15-C16-C17	26.43	177.62	123.47
25	B	1048	BCR	C15-C16-C17	26.41	177.57	123.47
25	Z	1053	BCR	C15-C16-C17	26.10	176.94	123.47

5 of 162 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	1003	CLA	C8
22	A	1003	CLA	ND
22	A	1006	CLA	C8
22	A	1006	CLA	ND
22	A	1007	CLA	ND

5 of 2325 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1003	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	1003	CLA	C2A-CAA-CBA-CGA
22	A	1003	CLA	CHA-CBD-CGD-O1D
22	A	1003	CLA	CHA-CBD-CGD-O2D
22	A	1003	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

62 monomers are involved in 2123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	1031	CLA	63	0
22	B	1012	CLA	61	0
26	A	1063	LHG	36	0
24	D	1042	PQ9	52	0
22	C	1033	CLA	65	0
22	B	1023	CLA	70	0
22	C	1036	CLA	24	0
22	A	1006	CLA	45	0
22	B	1013	CLA	67	0
25	K	1051	BCR	27	0
22	B	1016	CLA	49	0
25	Z	1053	BCR	18	0
22	B	1022	CLA	75	0
22	D	1004	CLA	57	0
22	B	1020	CLA	54	0
22	D	1008	CLA	48	0
22	C	1037	CLA	23	0
22	C	1030	CLA	38	0
22	B	1019	CLA	40	0
29	C	1057	DGD	41	0
22	B	1010	CLA	38	0
22	B	1024	CLA	45	0
22	B	1009	CLA	63	0
25	C	1054	BCR	41	0
22	D	1005	CLA	58	0
31	F	1040	HEM	17	0
25	B	1047	BCR	31	0
22	K	1034	CLA	87	0
22	A	1003	CLA	55	0
25	D	1050	BCR	40	0
22	C	1029	CLA	62	0
22	C	1027	CLA	37	0
25	T	6046	BCR	25	0

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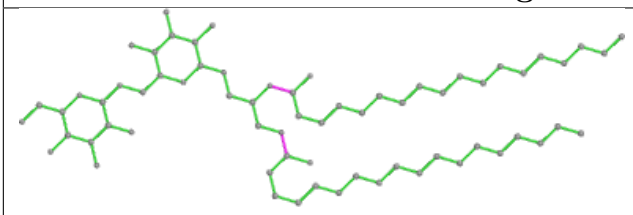
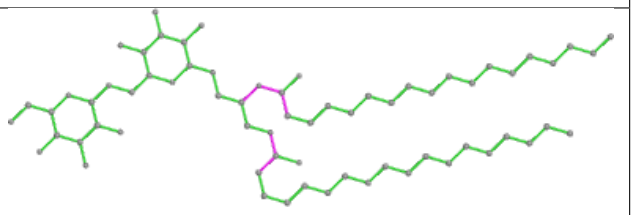
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	V	1041	HEM	12	0
22	C	1025	CLA	67	0
22	C	1035	CLA	56	0
25	A	1044	BCR	25	0
28	L	1061	MGE	29	0
22	B	1021	CLA	63	0
23	A	1038	PHO	63	0
22	H	1017	CLA	45	0
25	C	1052	BCR	40	0
29	C	1055	DGD	26	0
25	T	6048	BCR	15	0
23	D	1039	PHO	53	0
22	C	1026	CLA	29	0
22	B	1011	CLA	89	0
29	C	1056	DGD	55	0
24	A	1043	PQ9	39	0
28	D	1062	MGE	21	0
22	B	1014	CLA	49	0
25	H	1049	BCR	36	0
29	B	1058	DGD	32	0
22	B	1015	CLA	45	0
22	B	1018	CLA	34	0
22	C	1028	CLA	34	0
25	B	1048	BCR	23	0
25	B	1045	BCR	21	0
22	C	1032	CLA	43	0
28	B	1060	MGE	39	0
22	A	1007	CLA	40	0
28	D	1059	MGE	45	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

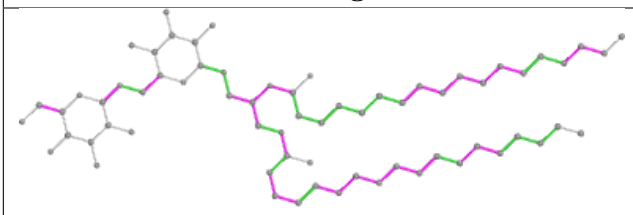
Ligand DGD c 6056



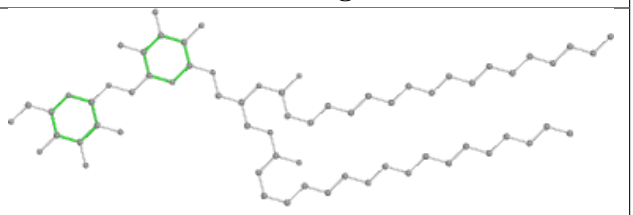
Bond lengths



Bond angles

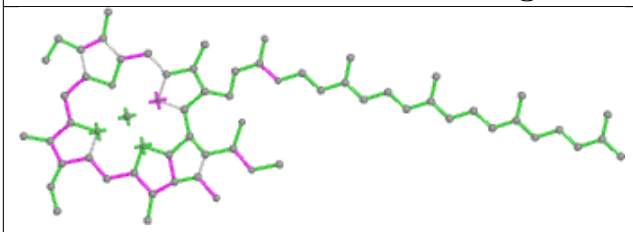


Torsions

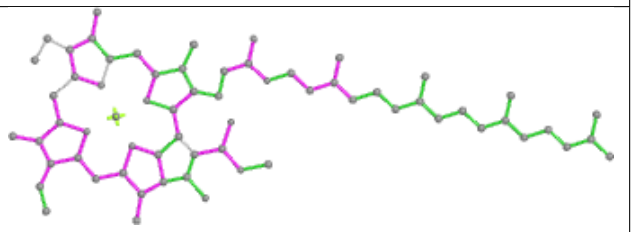


Rings

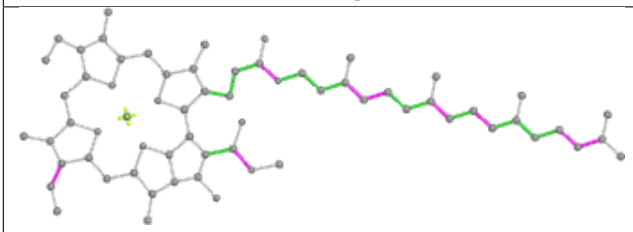
Ligand CLA d 6008



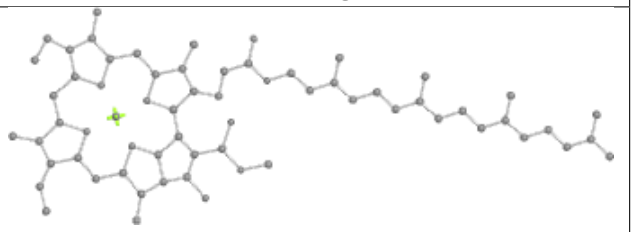
Bond lengths



Bond angles

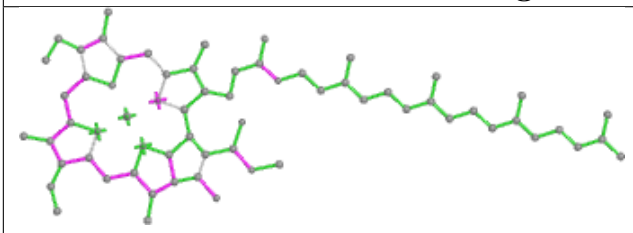


Torsions

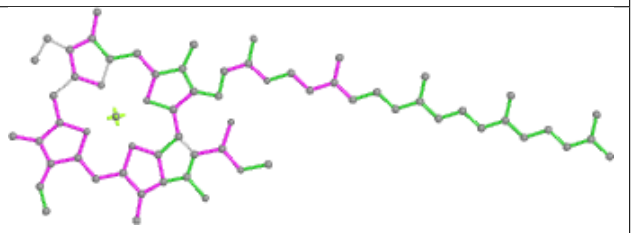


Rings

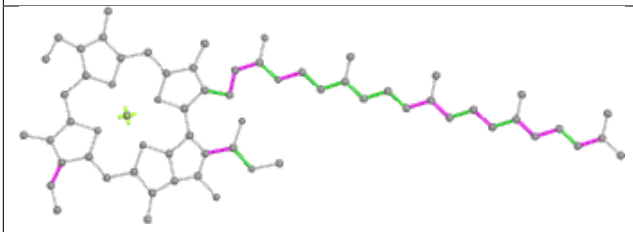
Ligand CLA C 1031



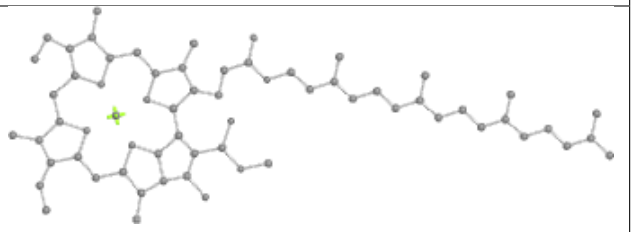
Bond lengths



Bond angles

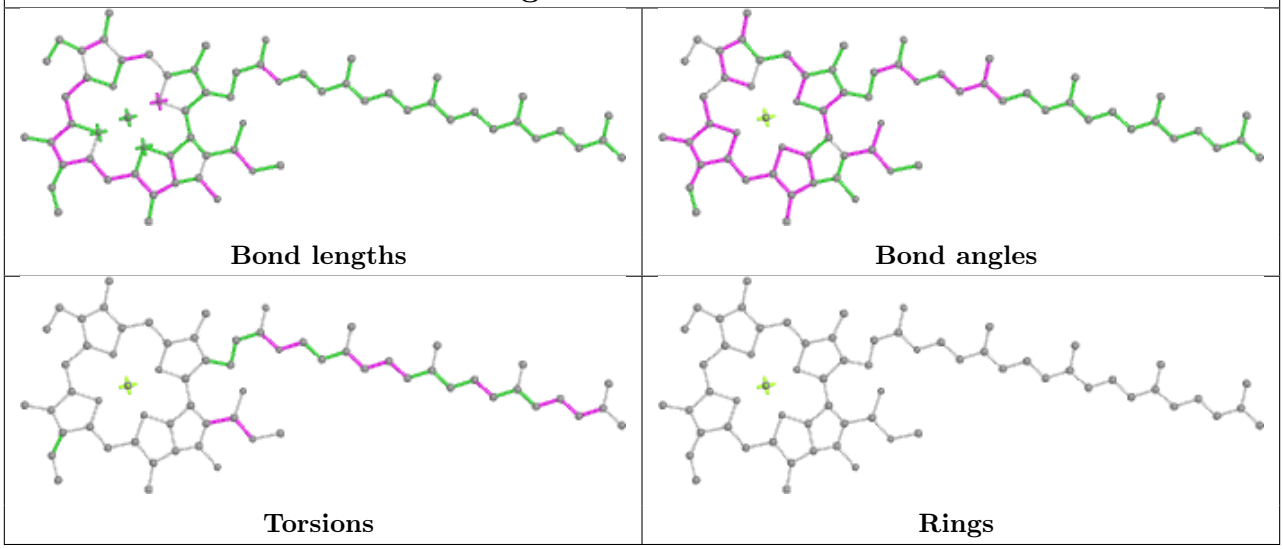


Torsions

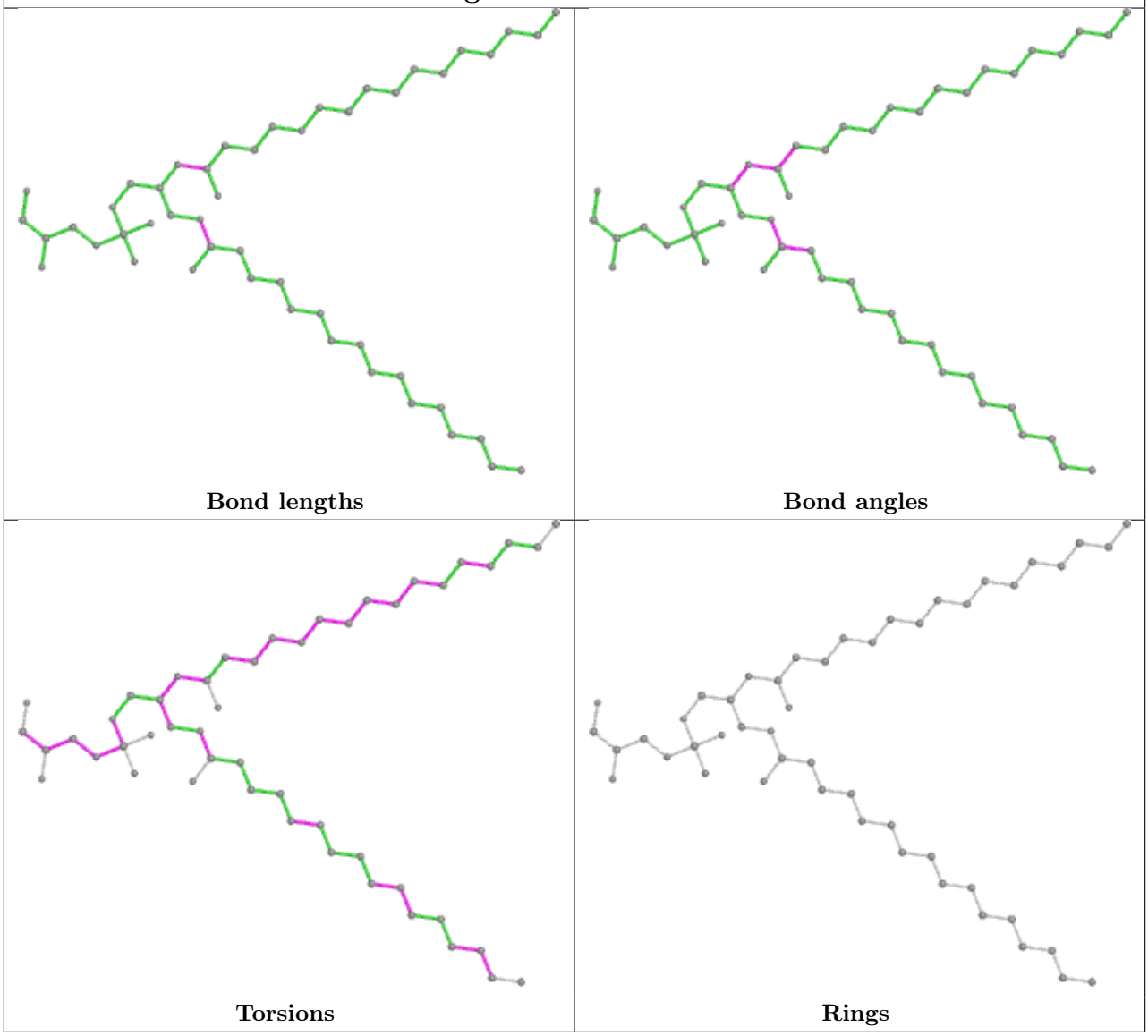


Rings

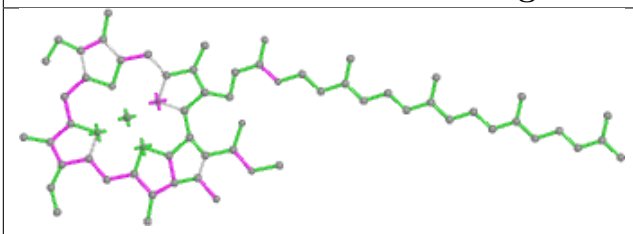
Ligand CLA c 6033



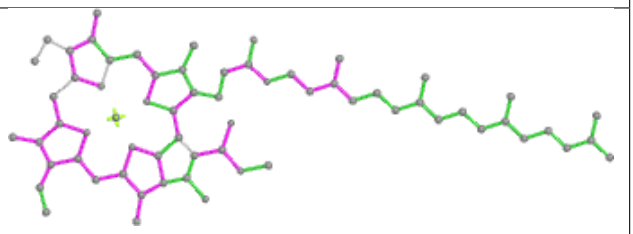
Ligand LHG a 6063



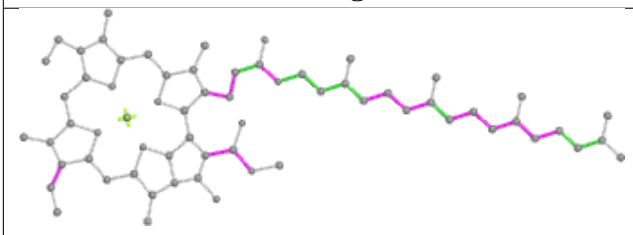
Ligand CLA b 6019



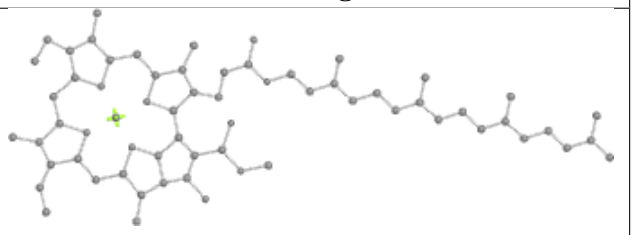
Bond lengths



Bond angles

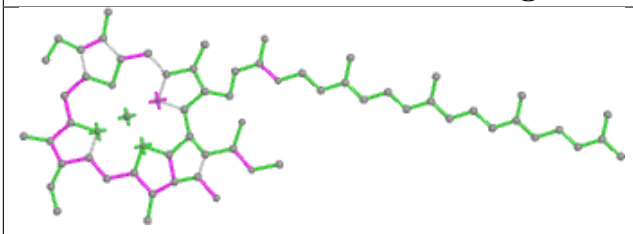


Torsions

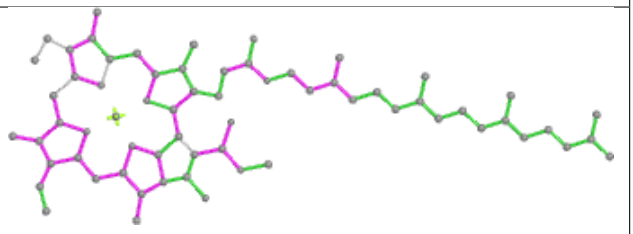


Rings

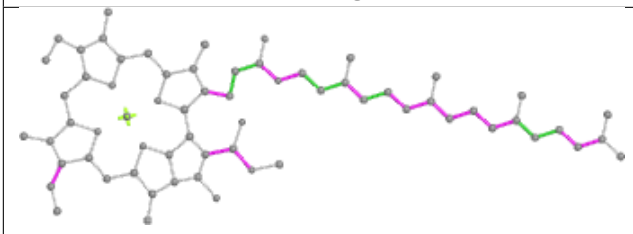
Ligand CLA a 6007



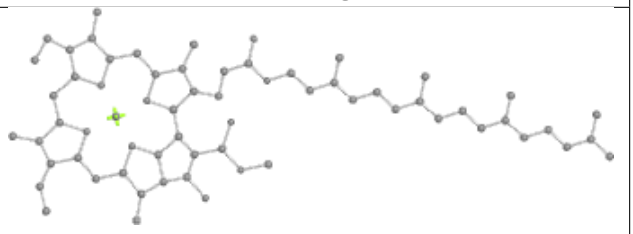
Bond lengths



Bond angles

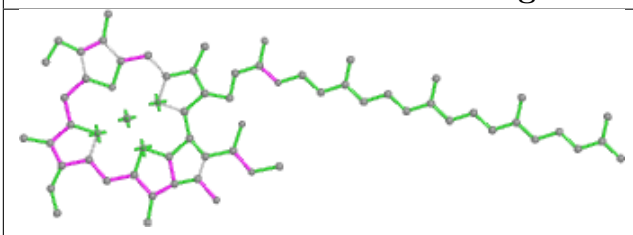


Torsions

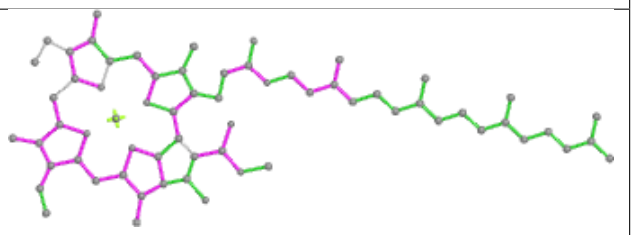


Rings

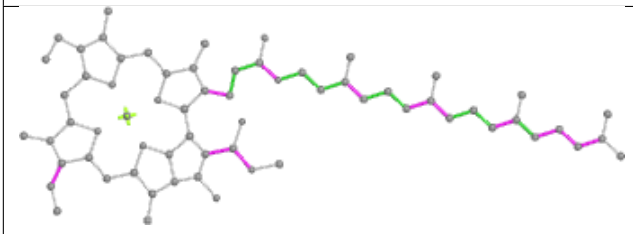
Ligand CLA d 6005



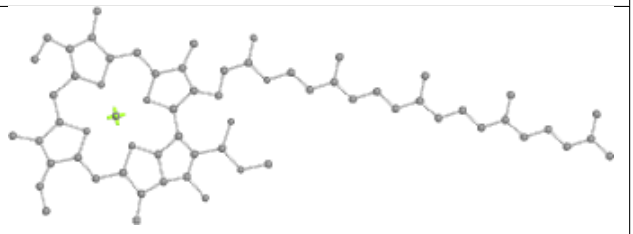
Bond lengths



Bond angles

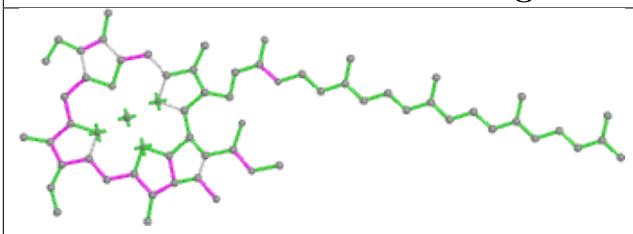


Torsions

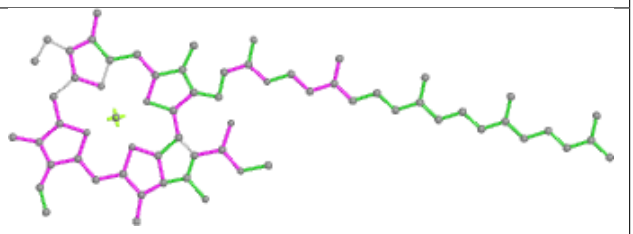


Rings

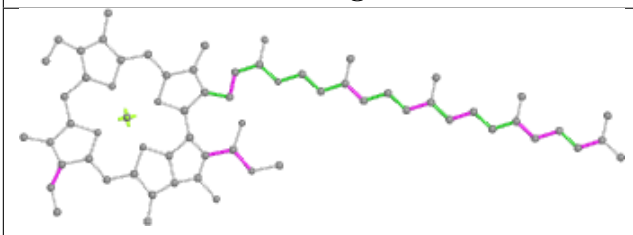
Ligand CLA B 1012



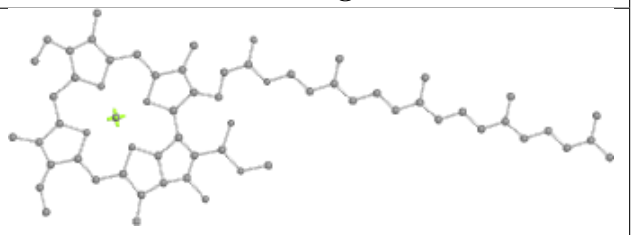
Bond lengths



Bond angles

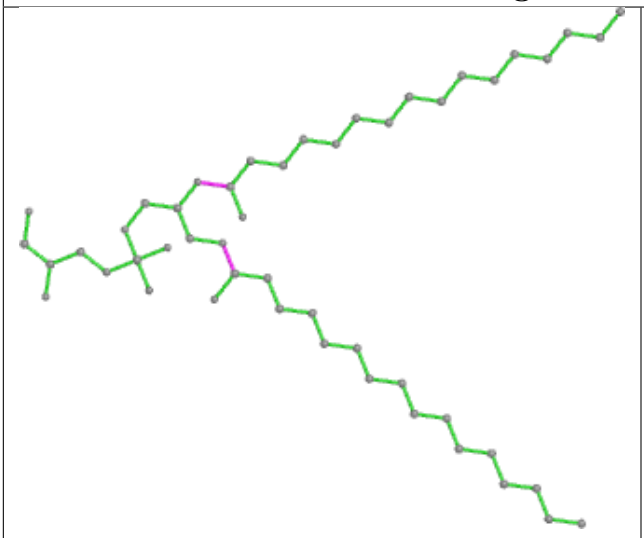


Torsions



Rings

Ligand LHG A 1063



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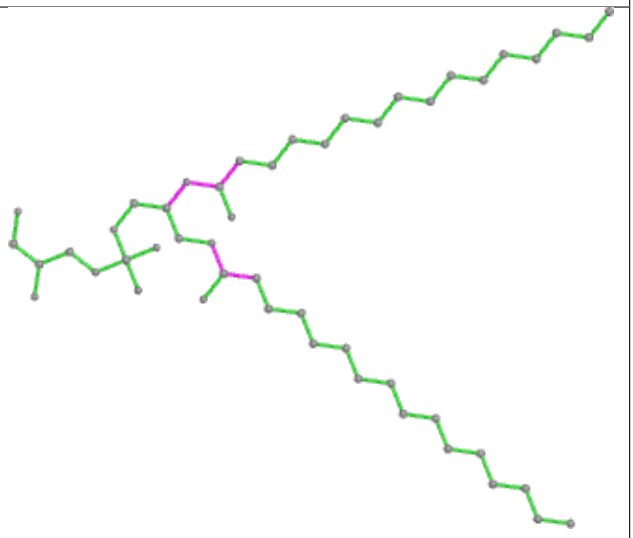
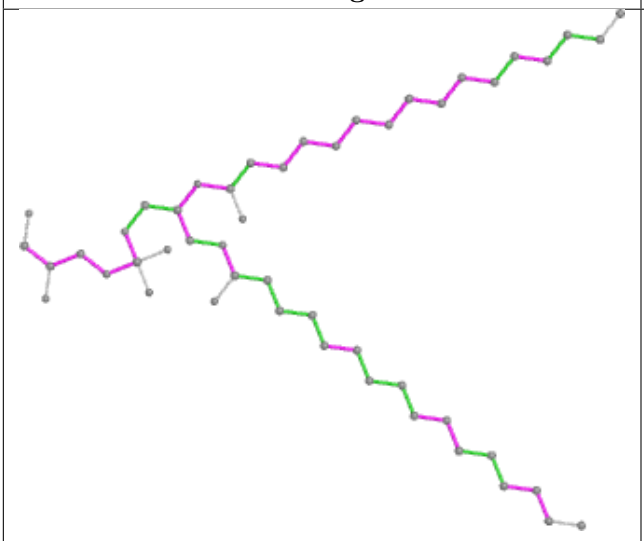
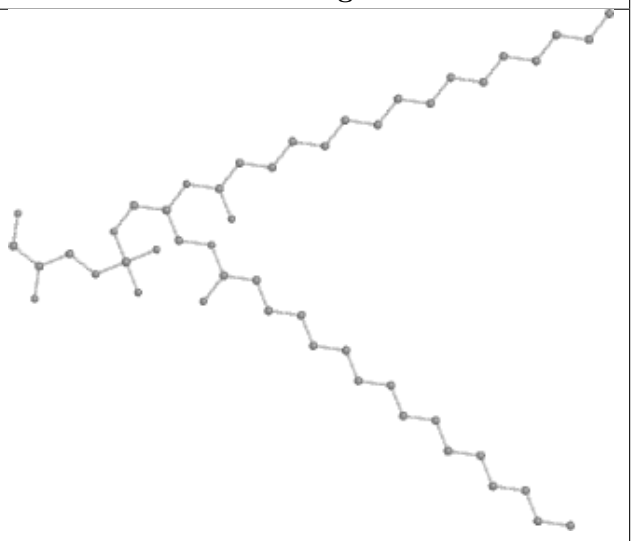


Bond angles

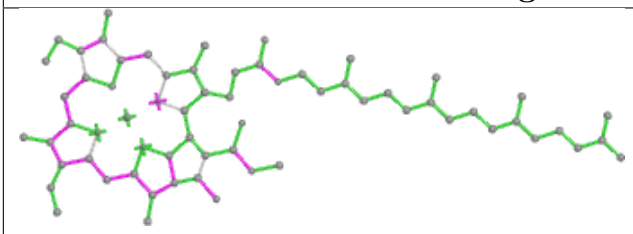


Torsions

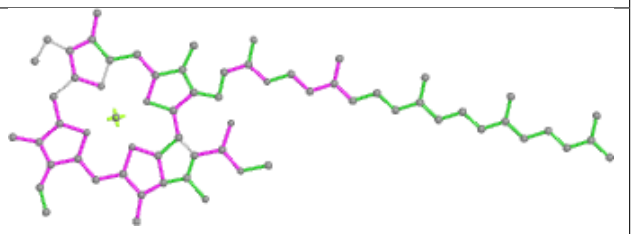


Rings

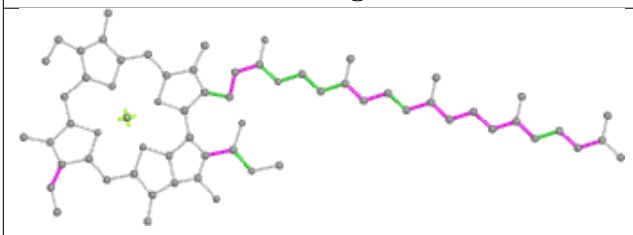
Ligand CLA b 6018



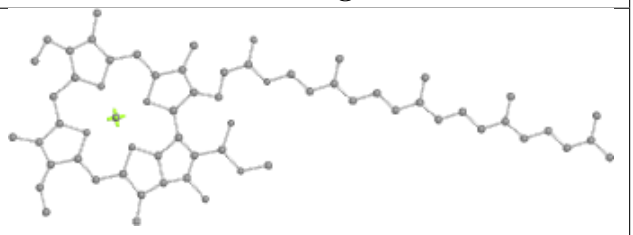
Bond lengths



Bond angles

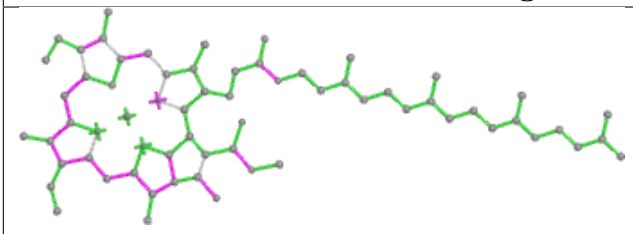


Torsions

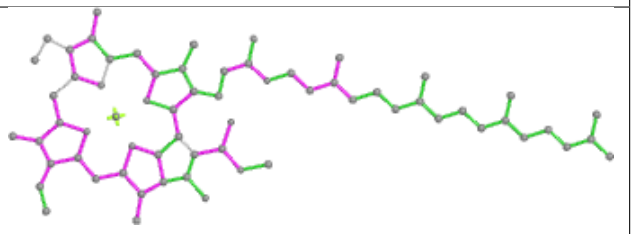


Rings

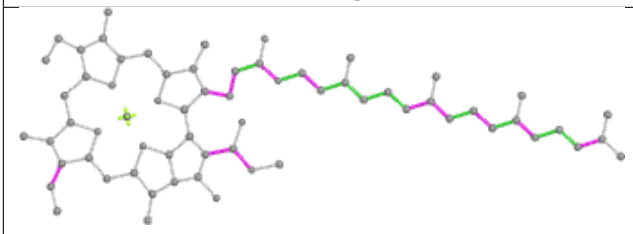
Ligand CLA b 6022



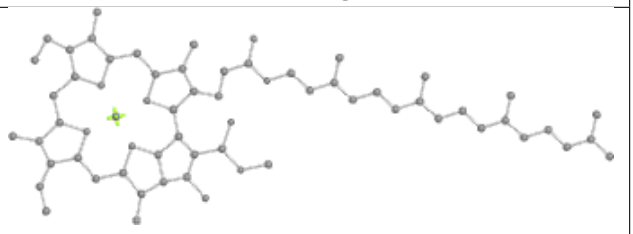
Bond lengths



Bond angles

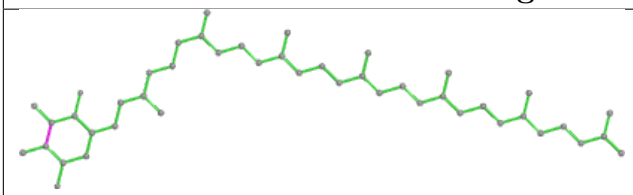


Torsions

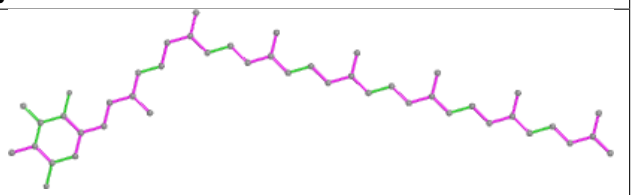


Rings

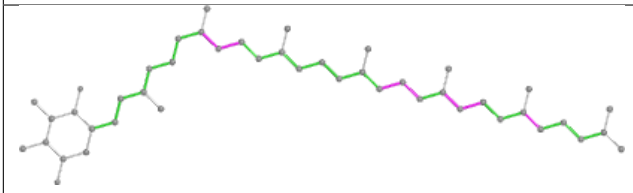
Ligand PQ9 D 1042



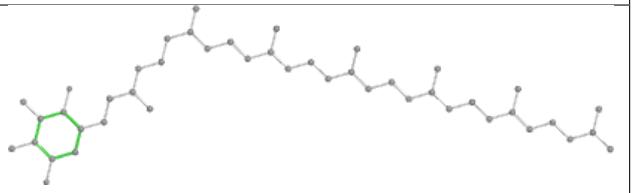
Bond lengths



Bond angles

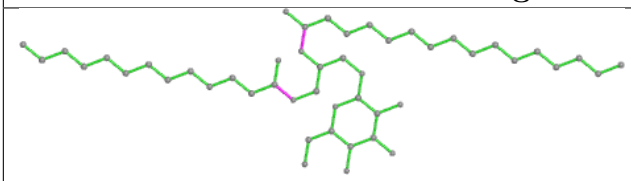


Torsions

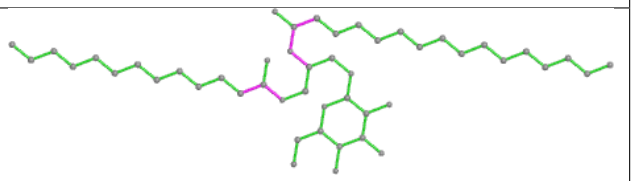


Rings

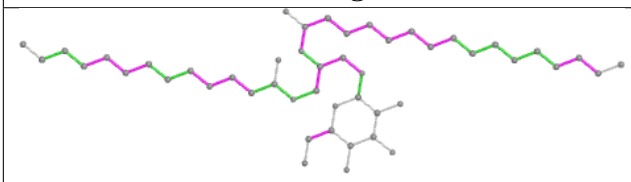
Ligand MGE d 6059



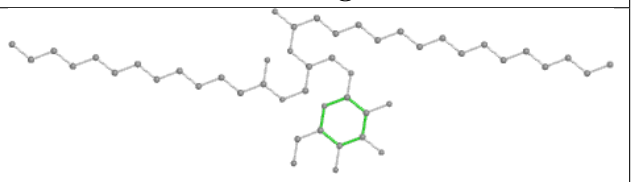
Bond lengths



Bond angles

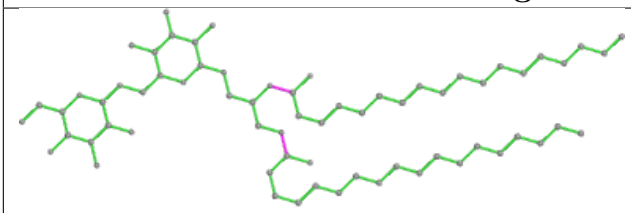


Torsions



Rings

Ligand DGD b 6058



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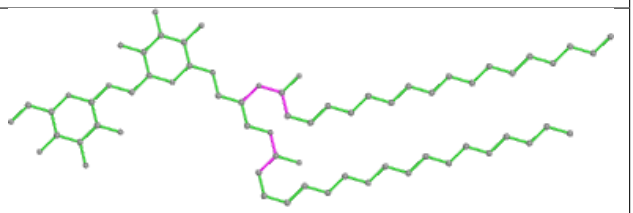
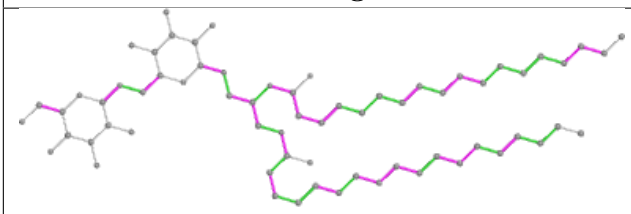
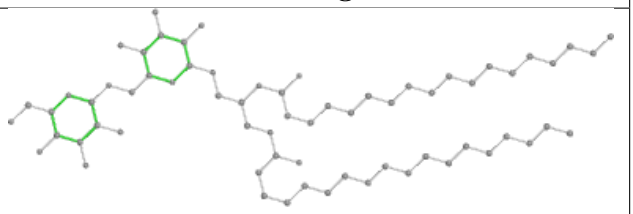


Bond angles

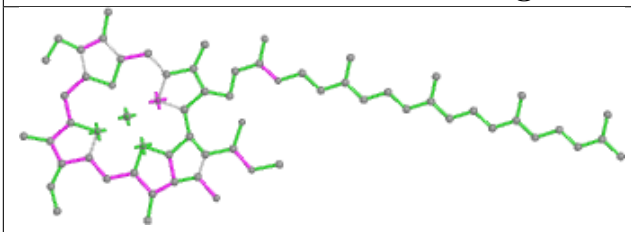


Torsions

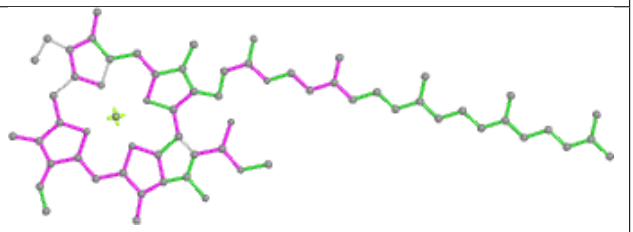


Rings

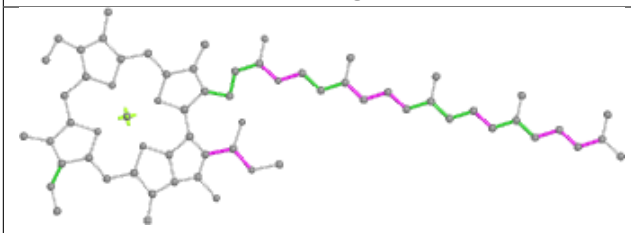
Ligand CLA C 1033



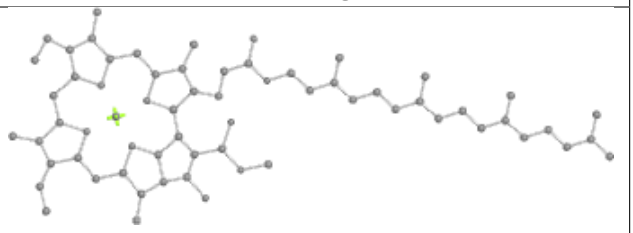
Bond lengths



Bond angles

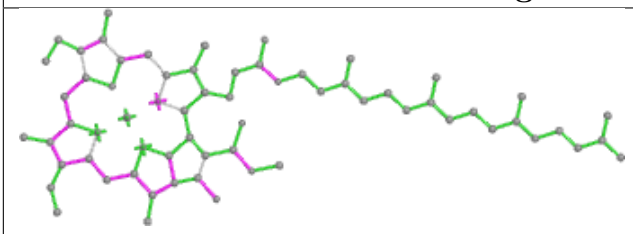


Torsions

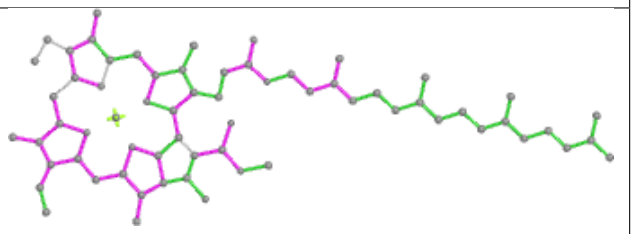


Rings

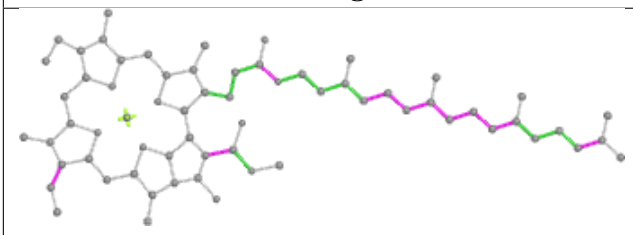
Ligand CLA B 1023



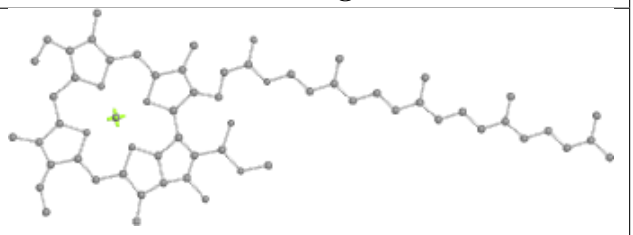
Bond lengths



Bond angles

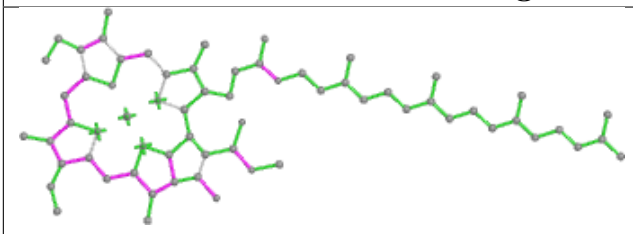


Torsions

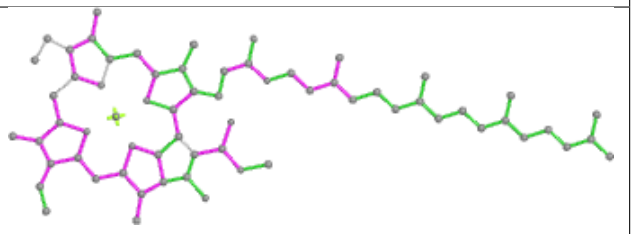


Rings

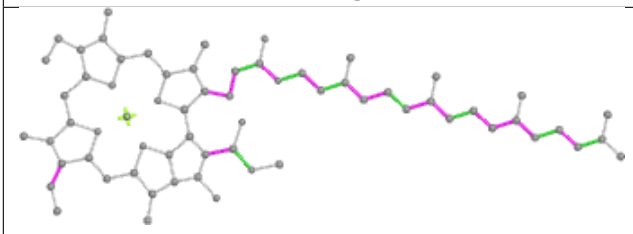
Ligand CLA C 1036



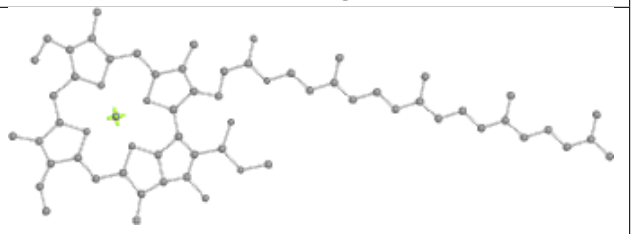
Bond lengths



Bond angles

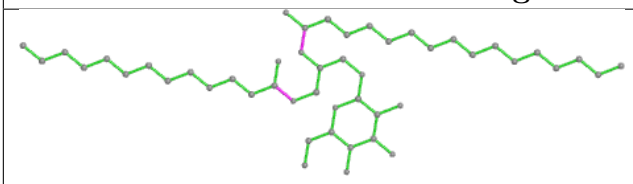


Torsions

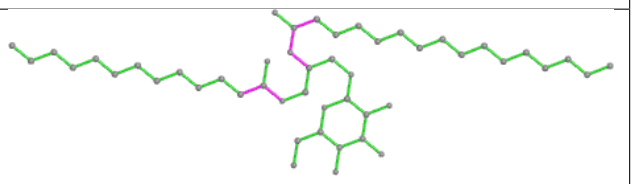


Rings

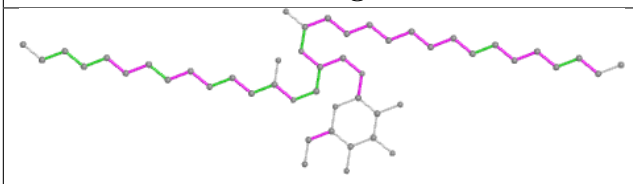
Ligand MGE d 6062



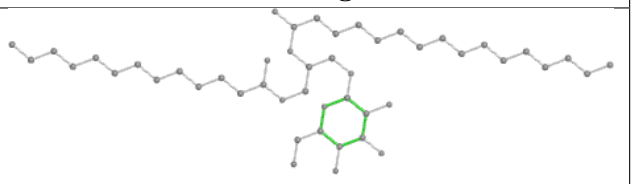
Bond lengths



Bond angles

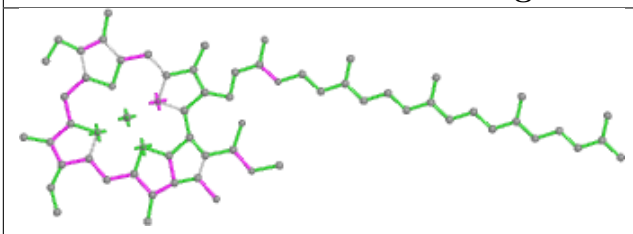


Torsions

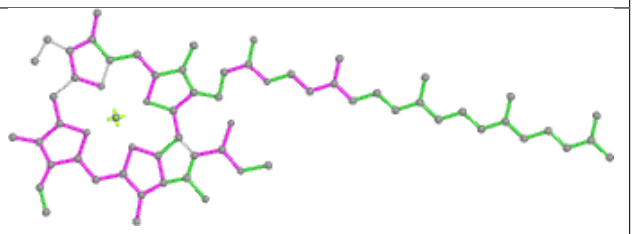


Rings

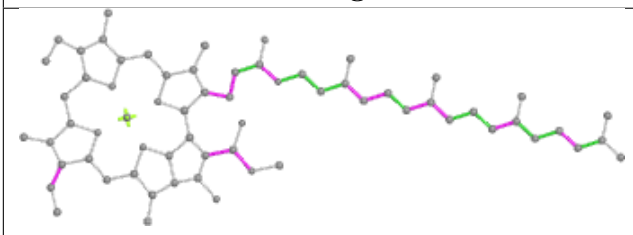
Ligand CLA A 1006



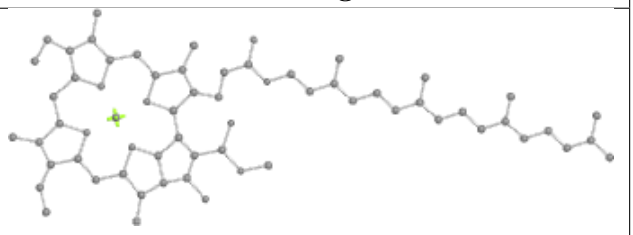
Bond lengths



Bond angles

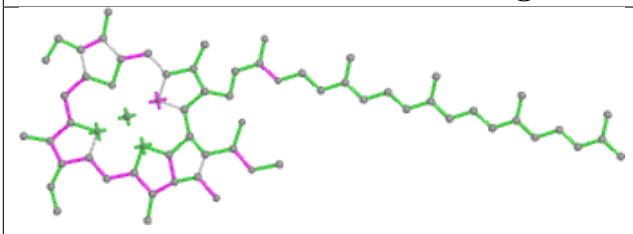


Torsions

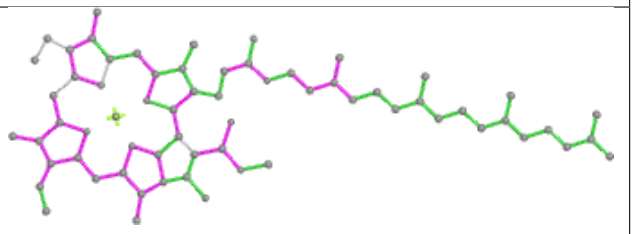


Rings

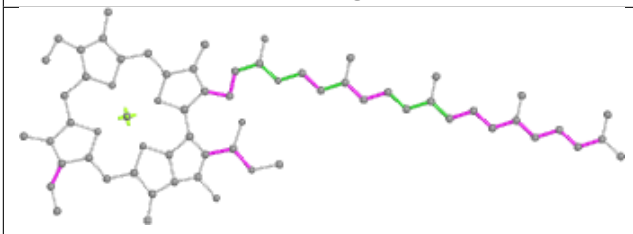
Ligand CLA B 1013



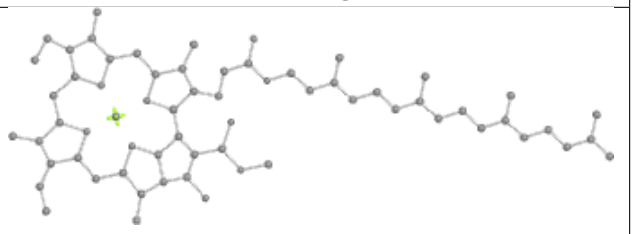
Bond lengths



Bond angles

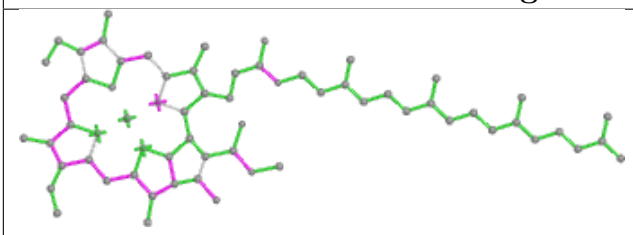


Torsions

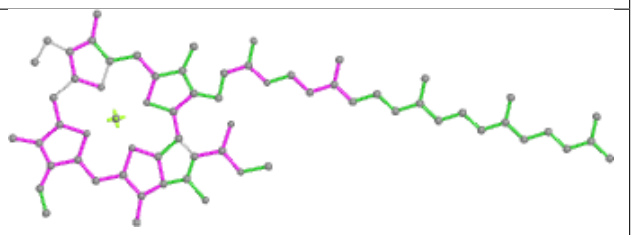


Rings

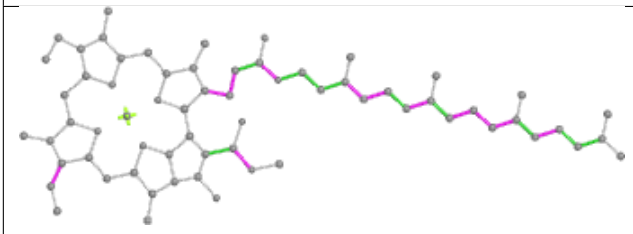
Ligand CLA c 6032



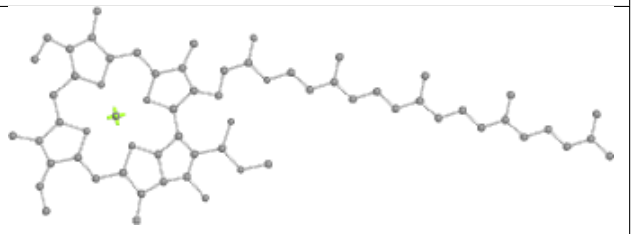
Bond lengths



Bond angles

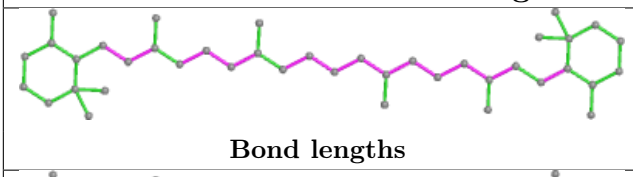


Torsions

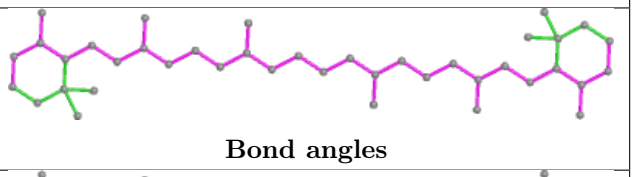


Rings

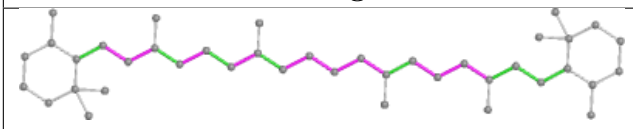
Ligand BCR K 1051



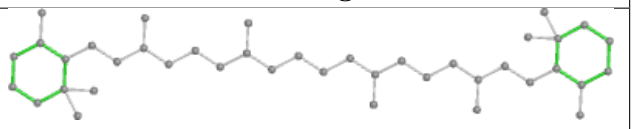
Bond lengths



Bond angles

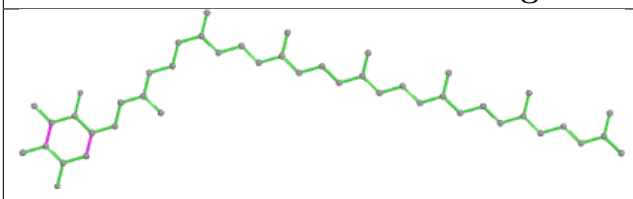


Torsions



Rings

Ligand PQ9 d 6042



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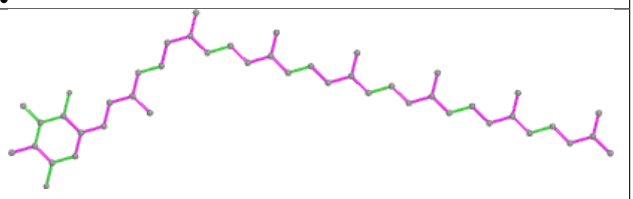
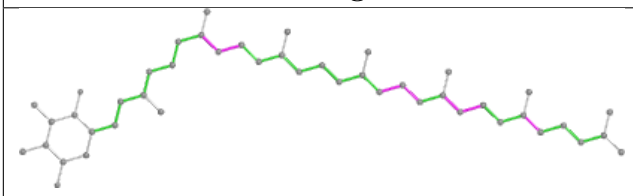
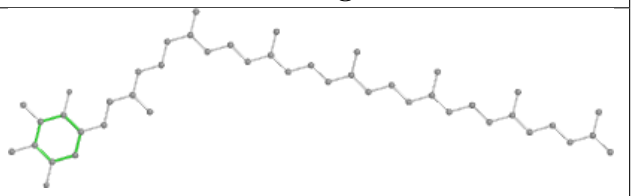


Bond angles

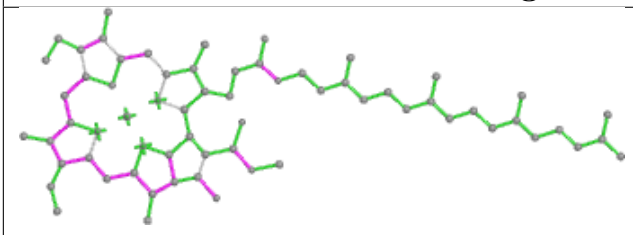


Torsions

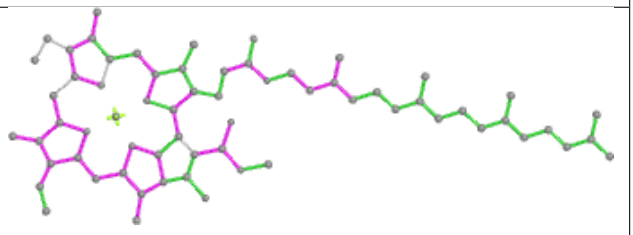


Rings

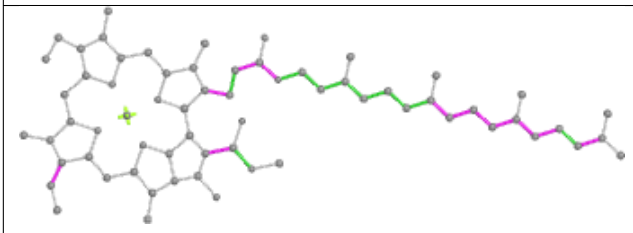
Ligand CLA c 6037



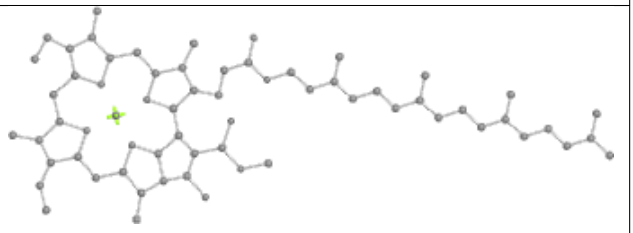
Bond lengths



Bond angles

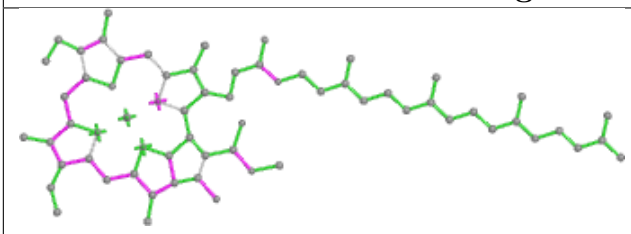


Torsions

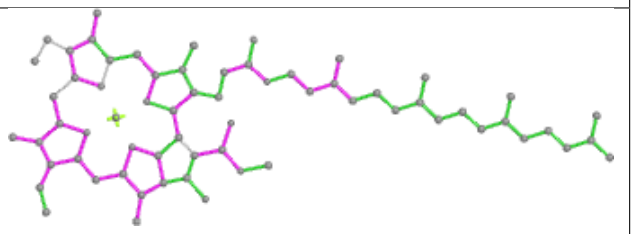


Rings

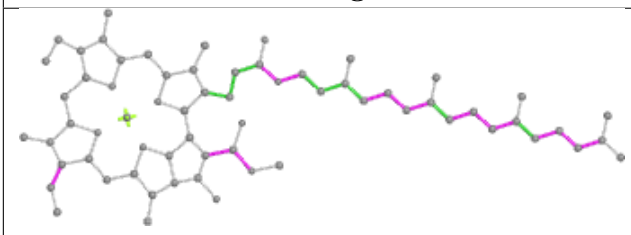
Ligand CLA B 1016



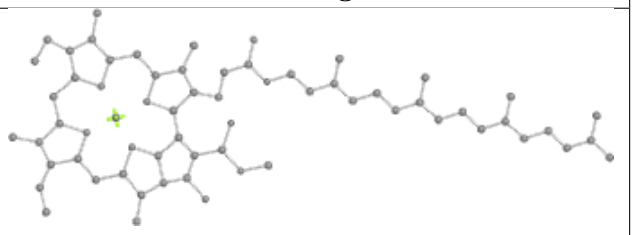
Bond lengths



Bond angles

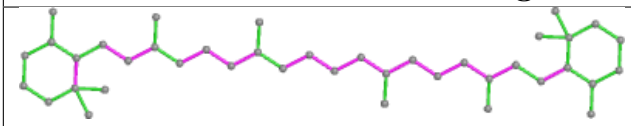


Torsions

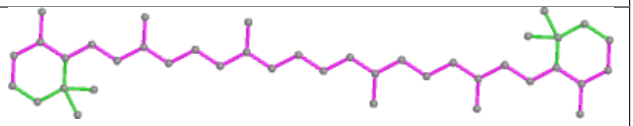


Rings

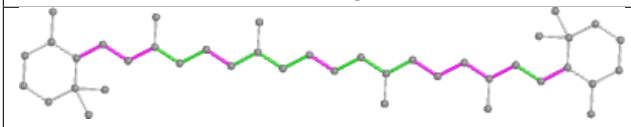
Ligand BCR Z 1053



Bond lengths



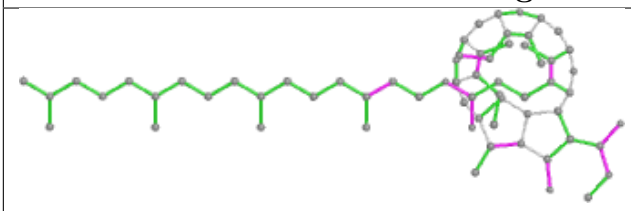
Bond angles



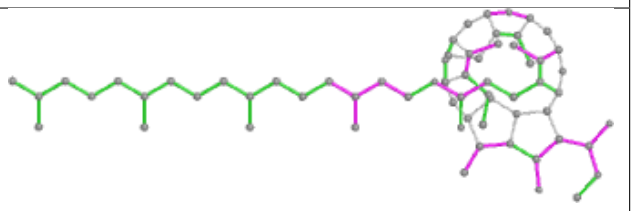
Torsions

Rings

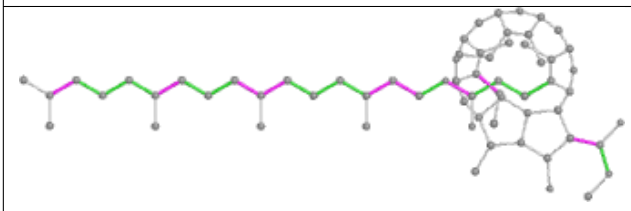
Ligand PHO d 6039



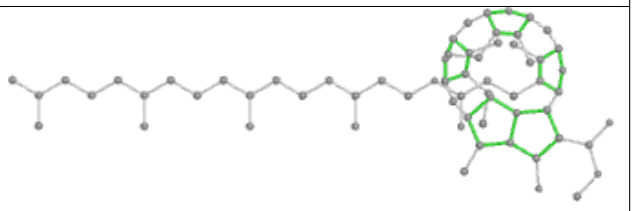
Bond lengths



Bond angles

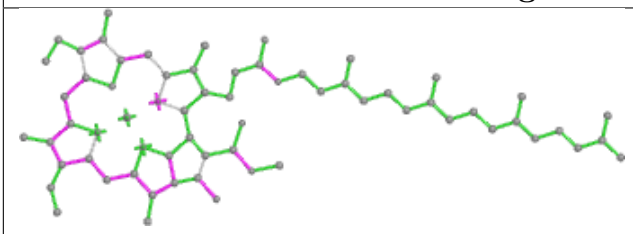


Torsions



Rings

Ligand CLA d 6004



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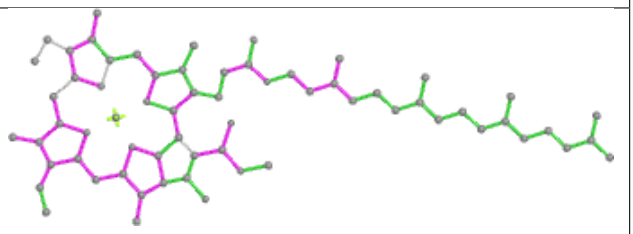
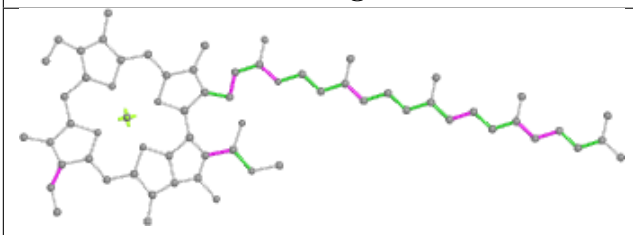
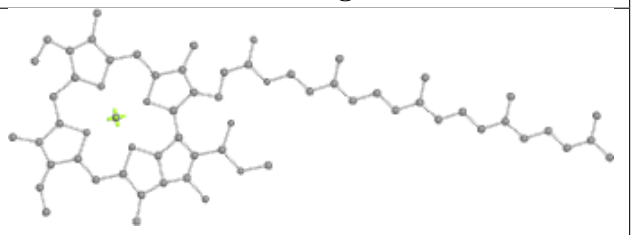


Bond angles

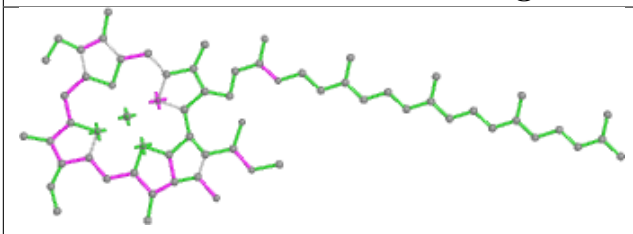


Torsions

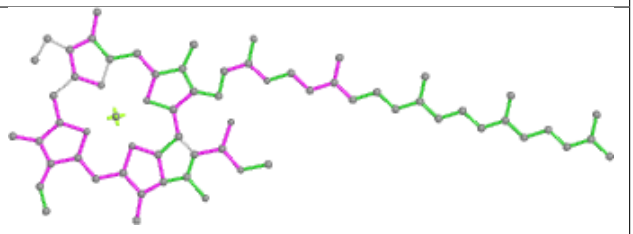


Rings

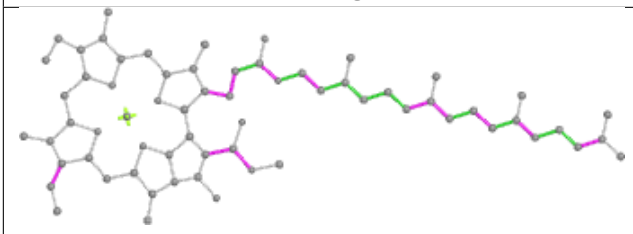
Ligand CLA B 1022



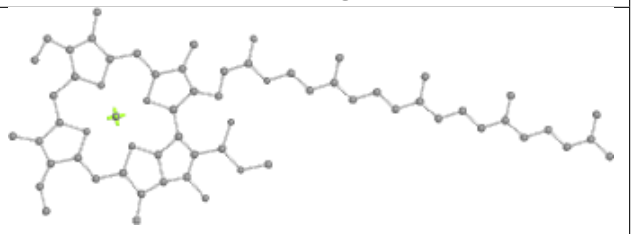
Bond lengths



Bond angles

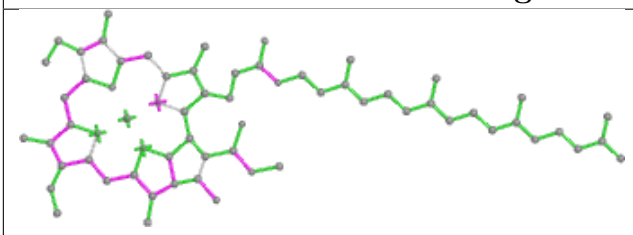


Torsions

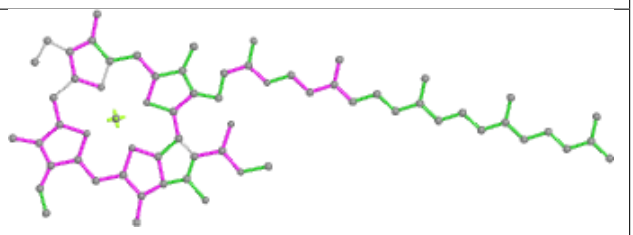


Rings

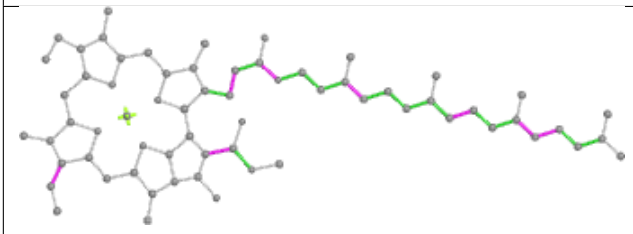
Ligand CLA D 1004



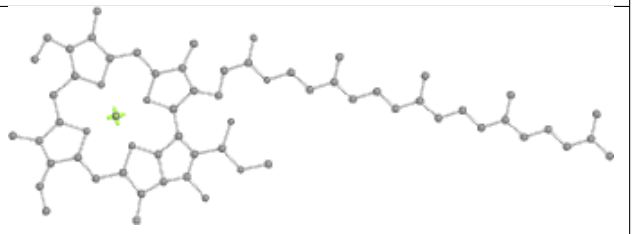
Bond lengths



Bond angles

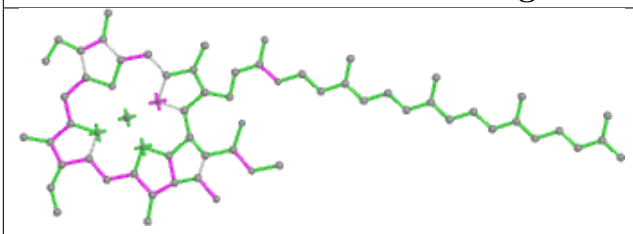


Torsions

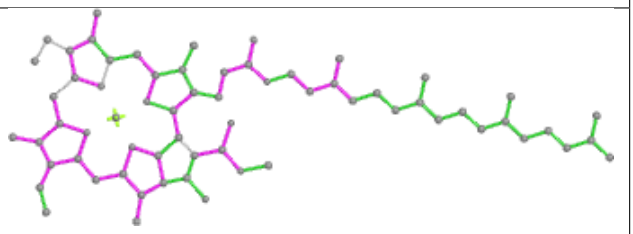


Rings

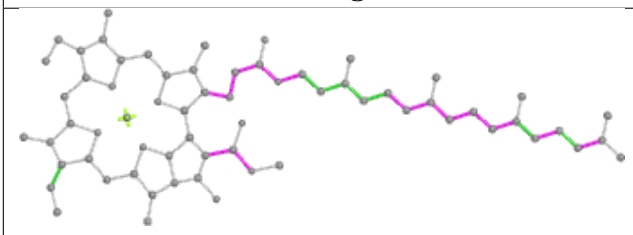
Ligand CLA b 6021



Bond lengths



Bond angles



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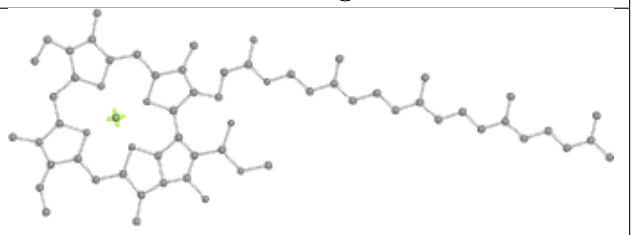
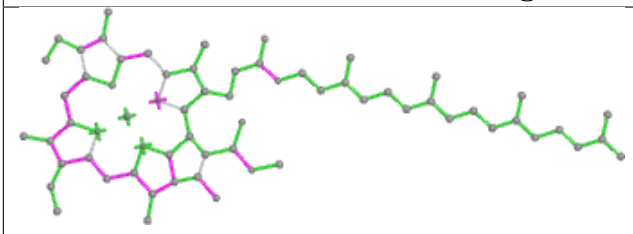
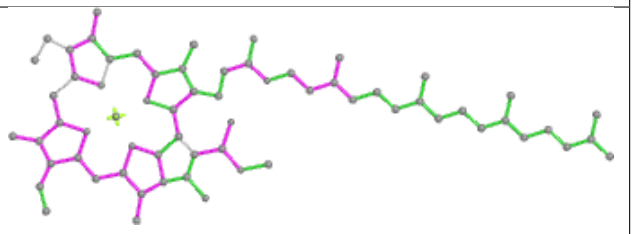


Rings

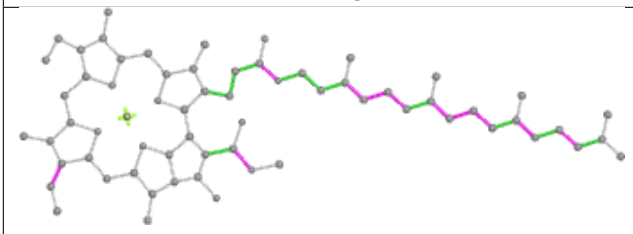
Ligand CLA b 6024



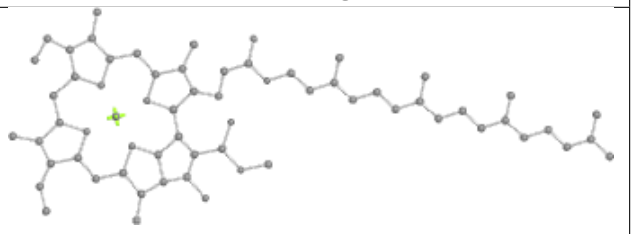
Bond lengths



Bond angles

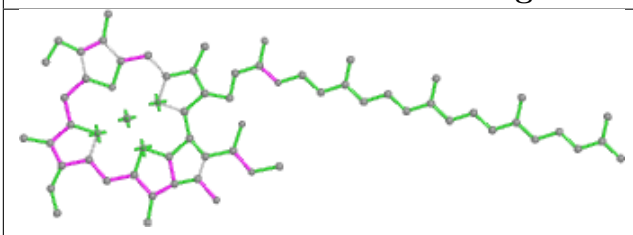


Torsions

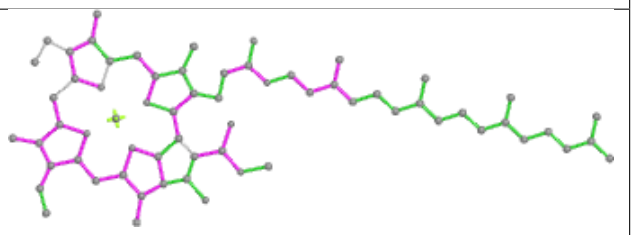


Rings

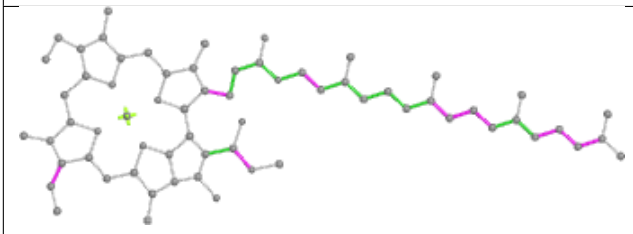
Ligand CLA B 1020



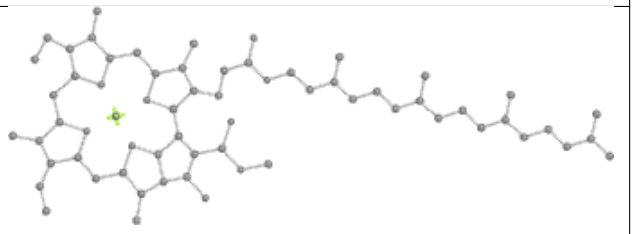
Bond lengths



Bond angles

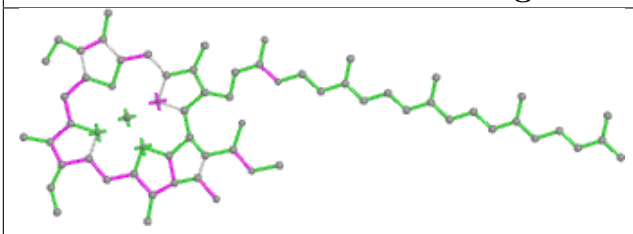


Torsions

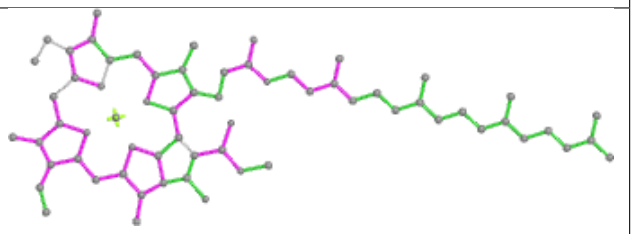


Rings

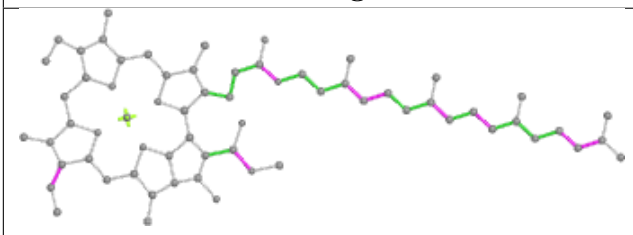
Ligand CLA D 1008



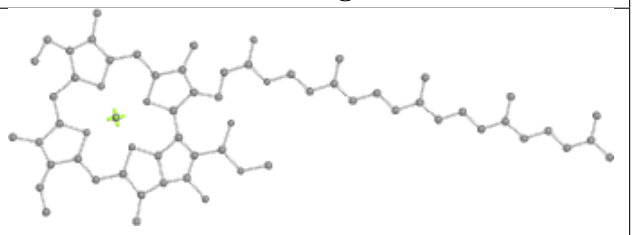
Bond lengths



Bond angles

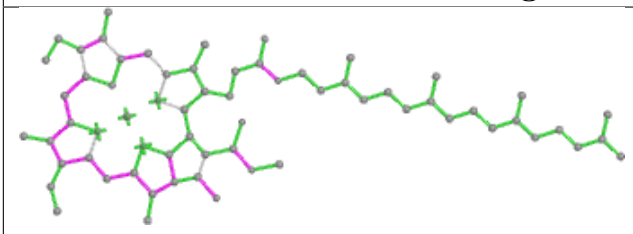


Torsions

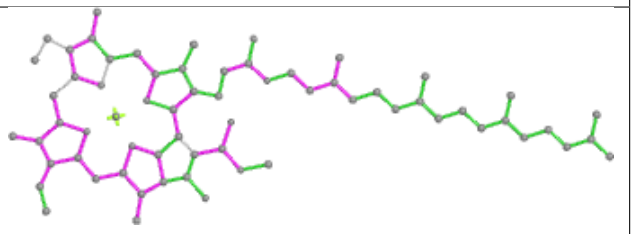


Rings

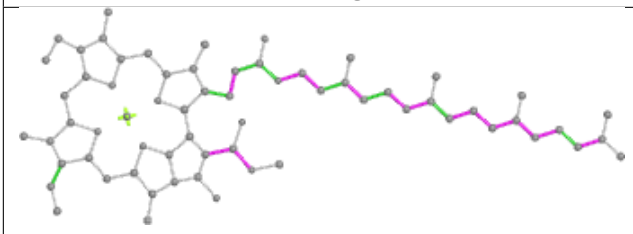
Ligand CLA c 6026



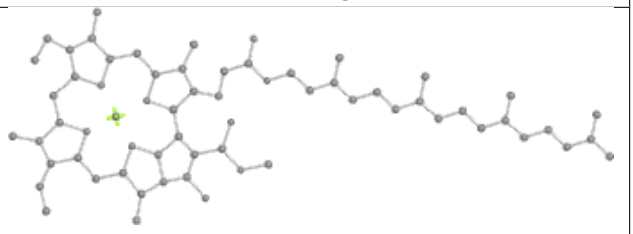
Bond lengths



Bond angles

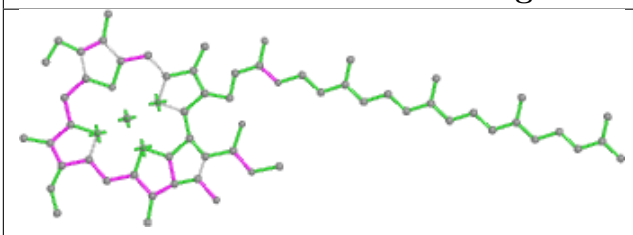


Torsions

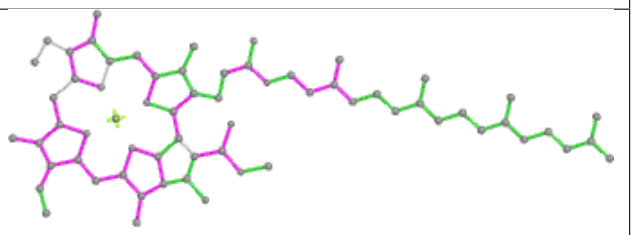


Rings

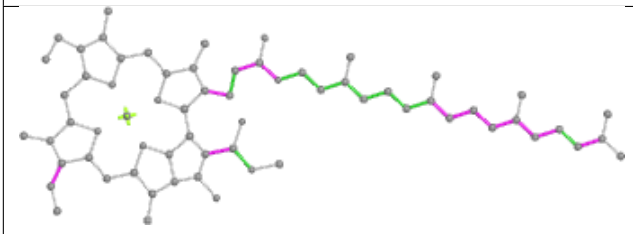
Ligand CLA C 1037



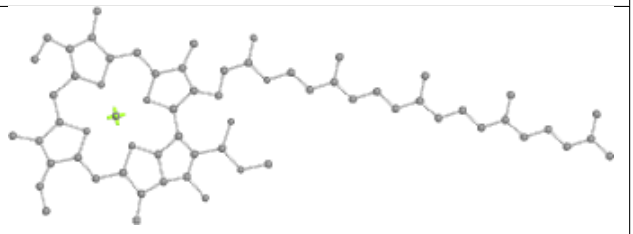
Bond lengths



Bond angles

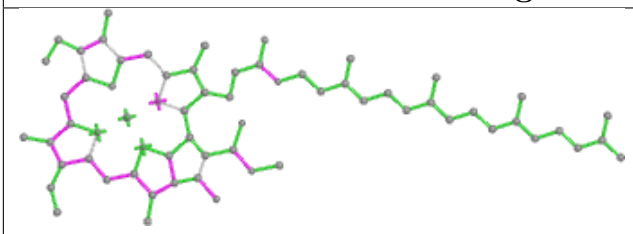


Torsions



Rings

Ligand CLA C 1030



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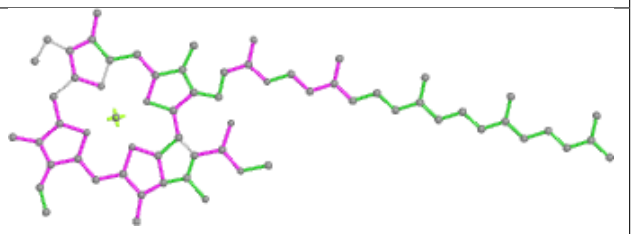
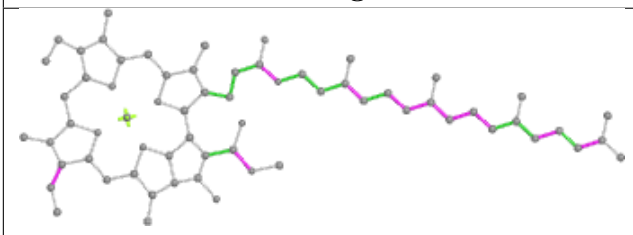
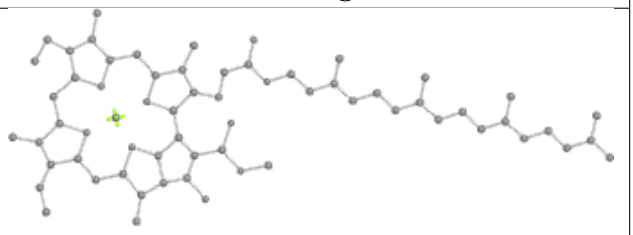


Bond angles

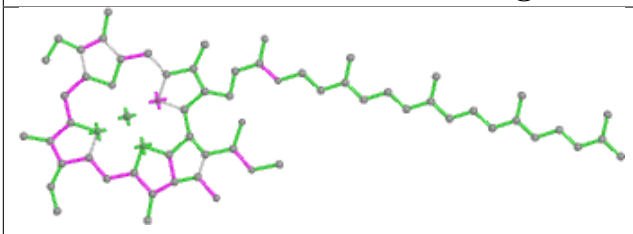


Torsions



Rings

Ligand CLA B 1019



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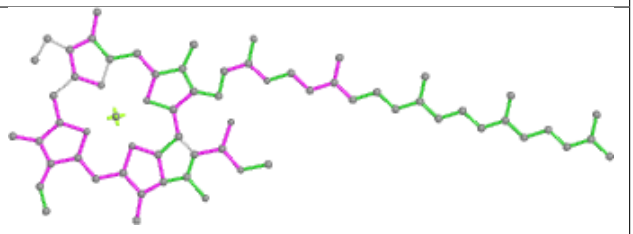
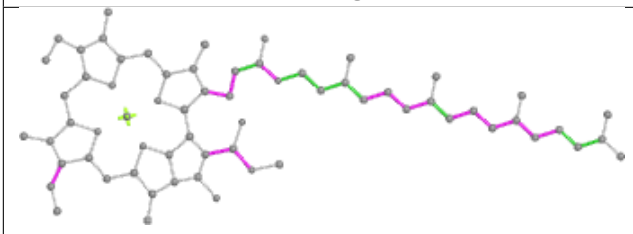


Bond angles



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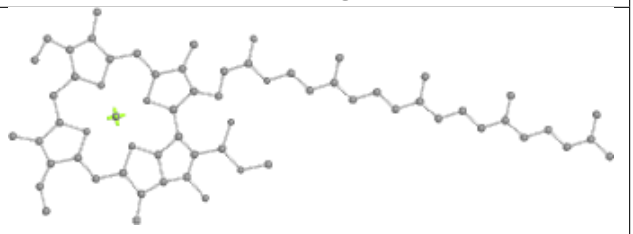
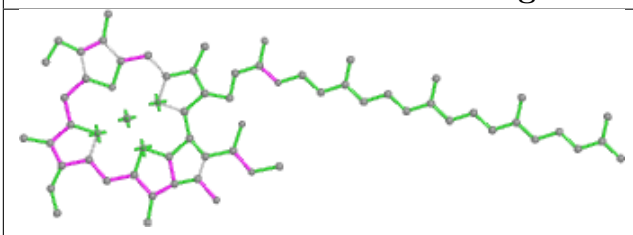


Rings

Ligand CLA b 6014



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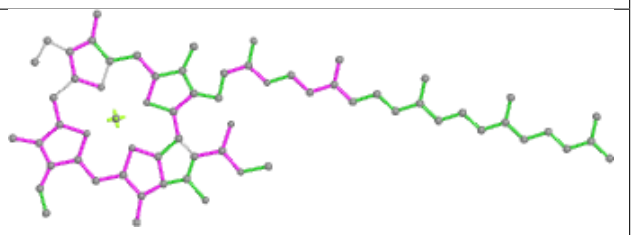
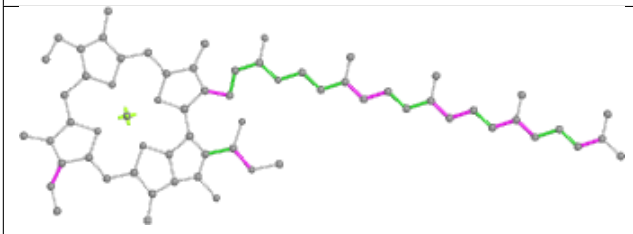


Bond angles



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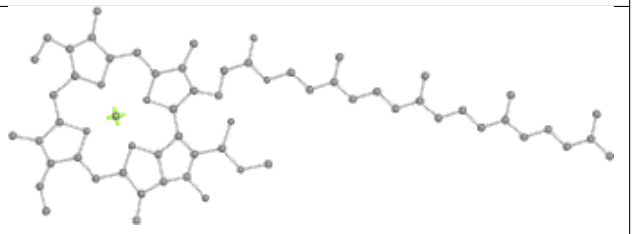
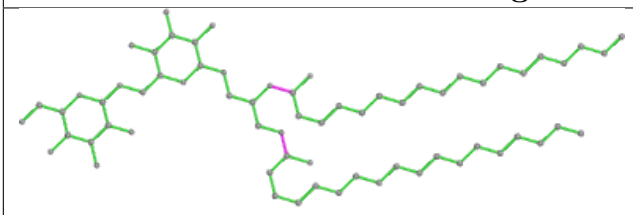


Rings

Ligand DGD C 1057



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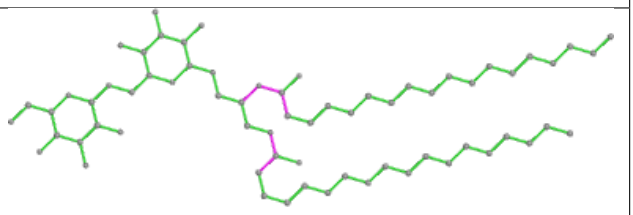
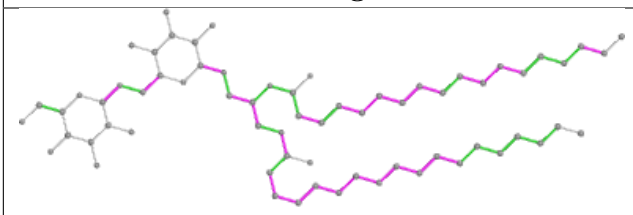


Bond angles



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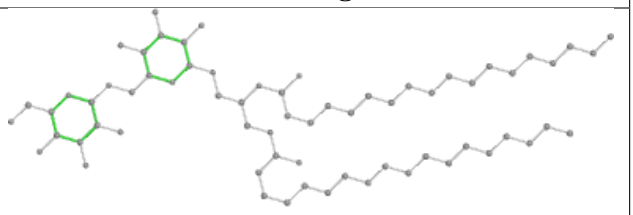
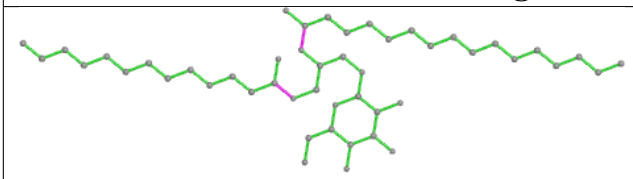


Rings

Ligand MGE b 6060



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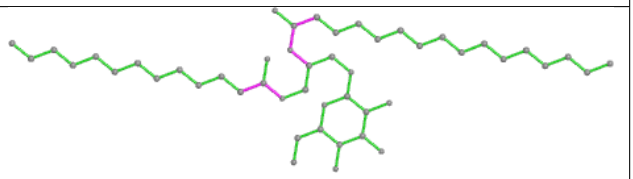
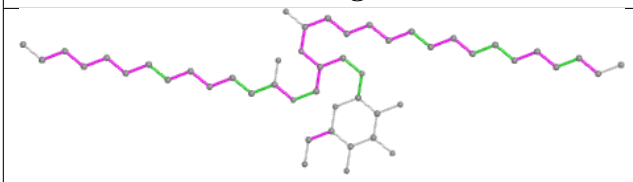
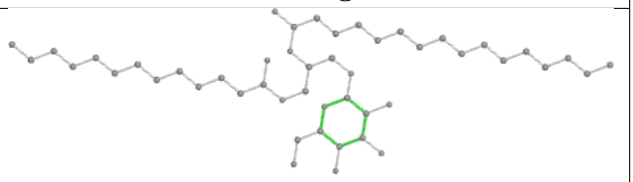


Bond angles

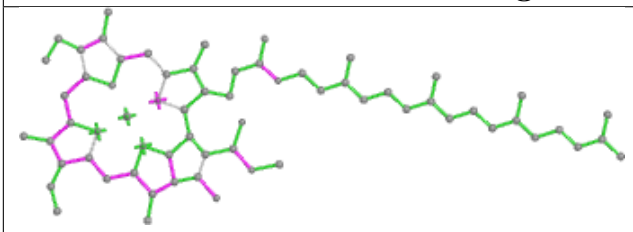


Torsions

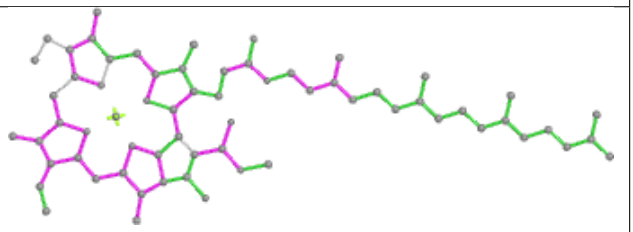


Rings

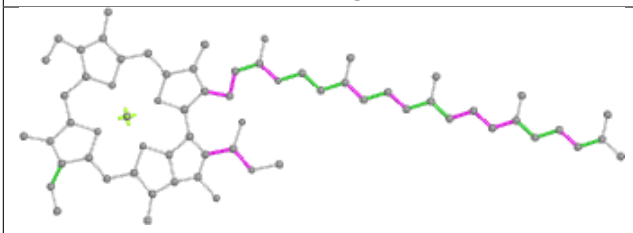
Ligand CLA B 1010



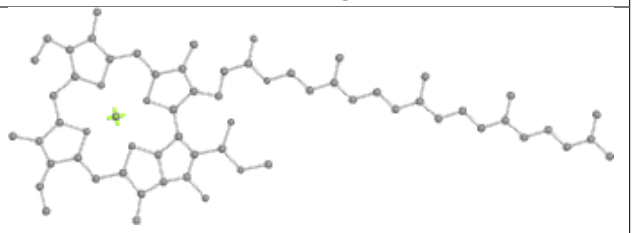
Bond lengths



Bond angles

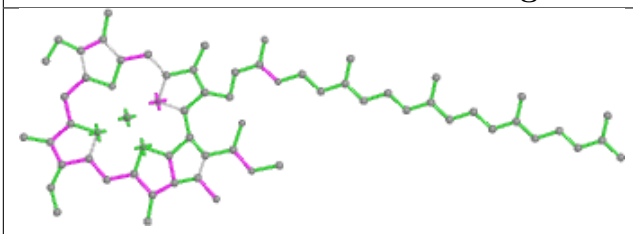


Torsions

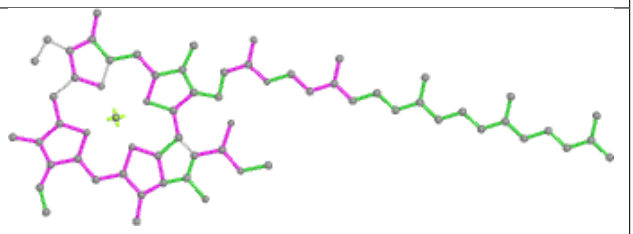


Rings

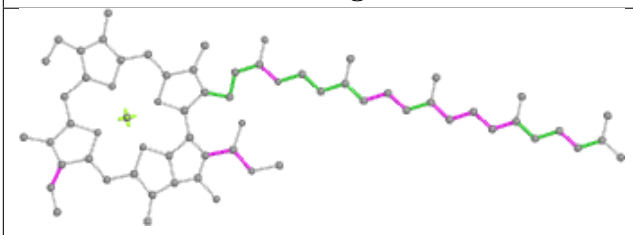
Ligand CLA c 6029



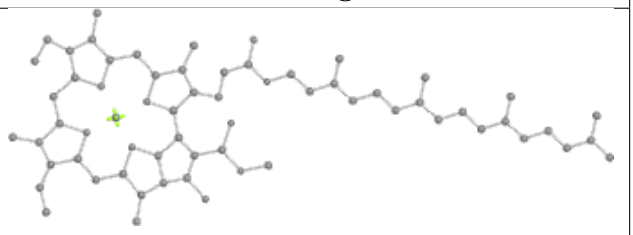
Bond lengths



Bond angles

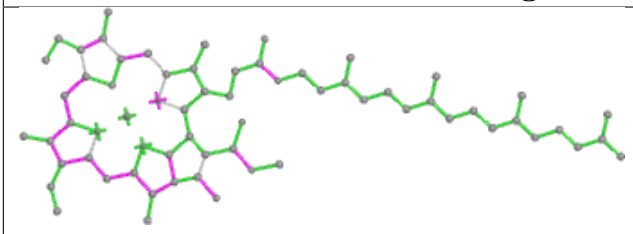


Torsions



Rings

Ligand CLA c 6030



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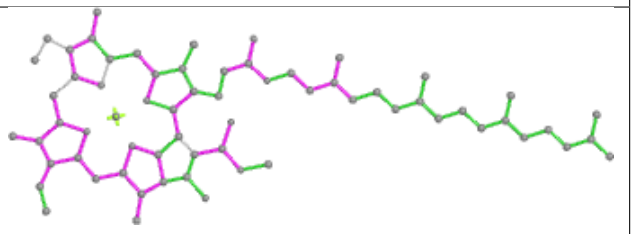
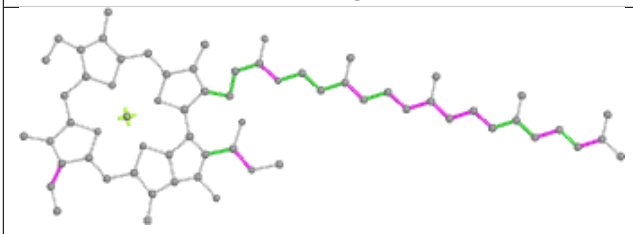
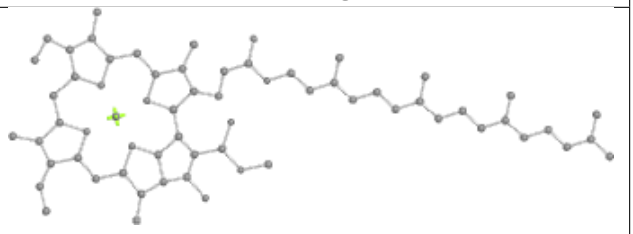


Bond angles

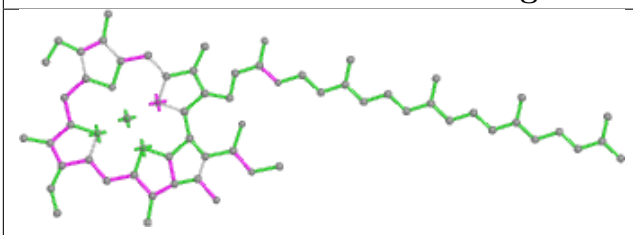


Torsions

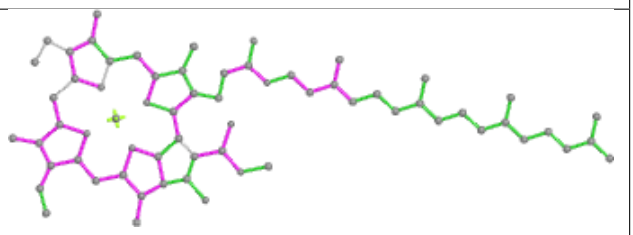


Rings

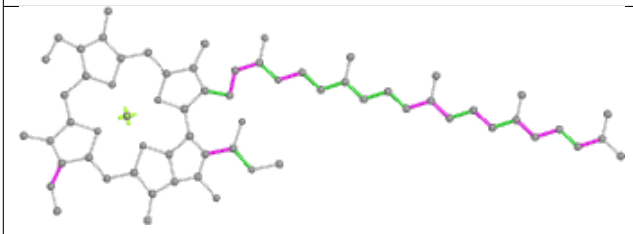
Ligand CLA c 6031



Bond lengths



Bond angles



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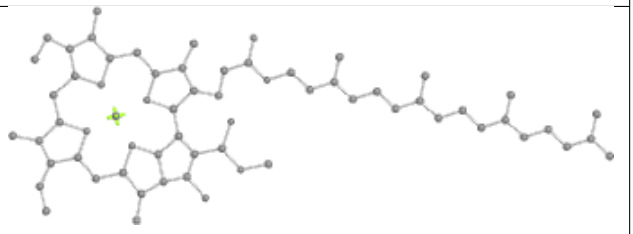
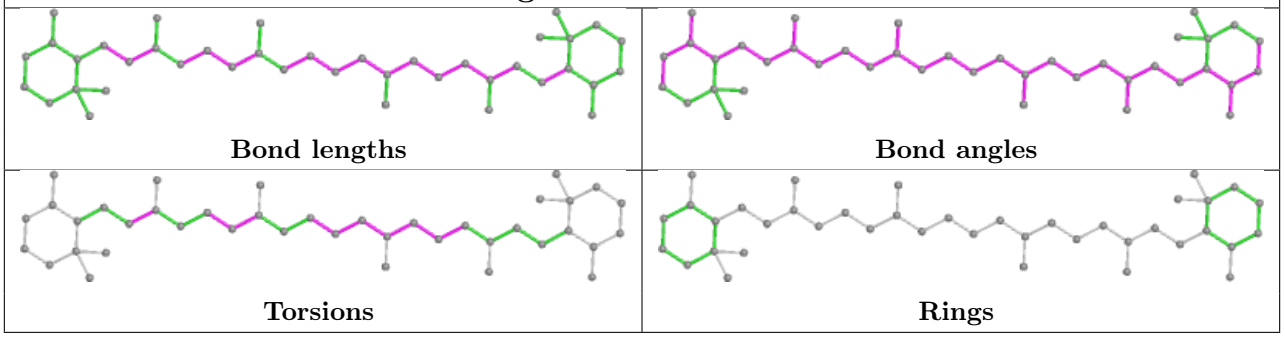
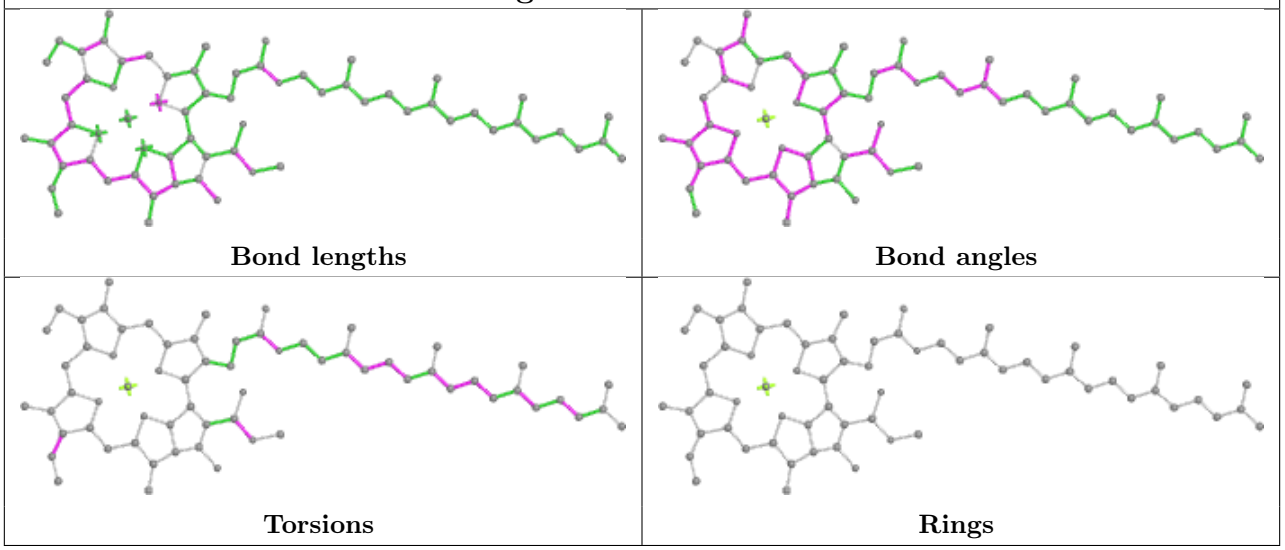


Rings

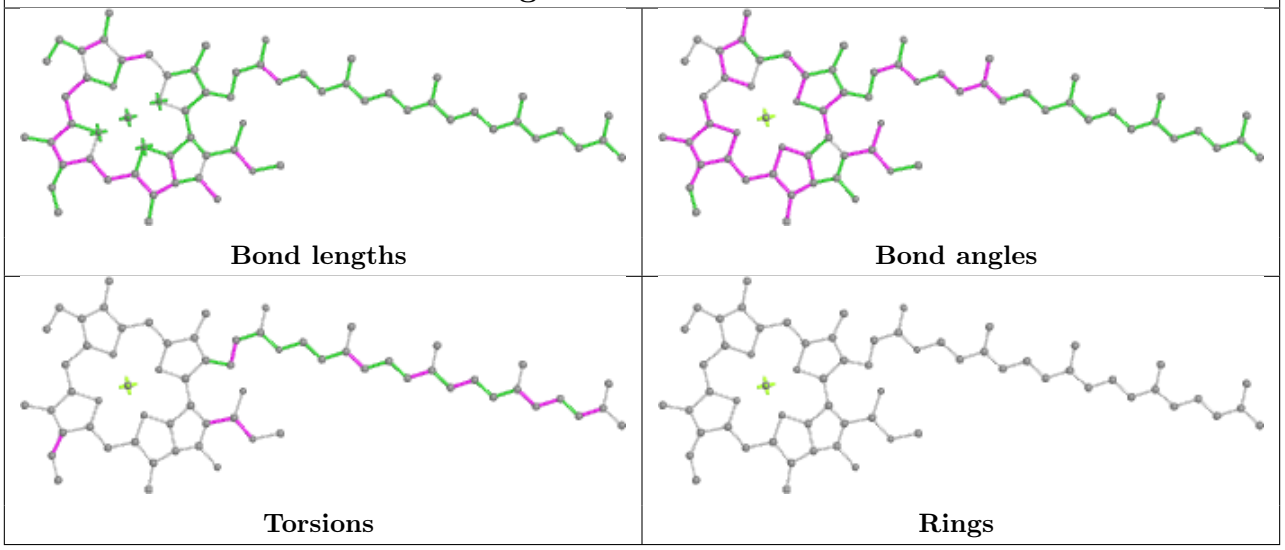
Ligand BCR h 6049



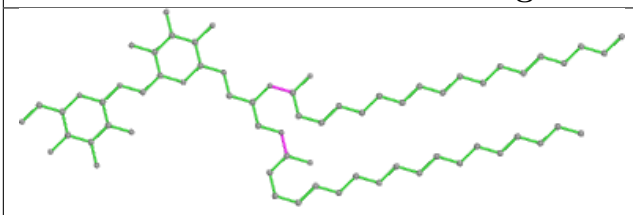
Ligand CLA B 1024



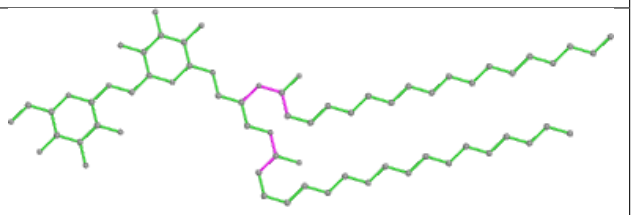
Ligand CLA b 6012



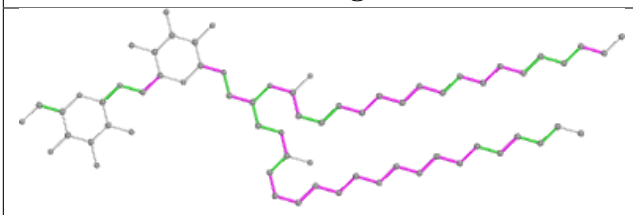
Ligand DGD c 6055



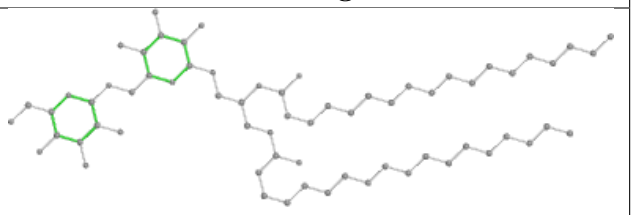
Bond lengths



Bond angles

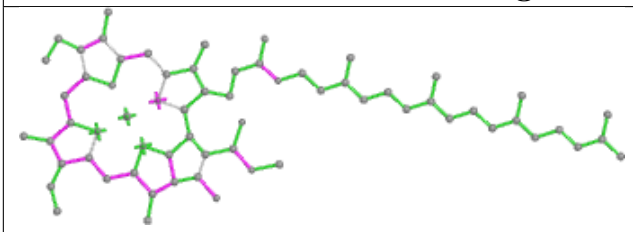


Torsions

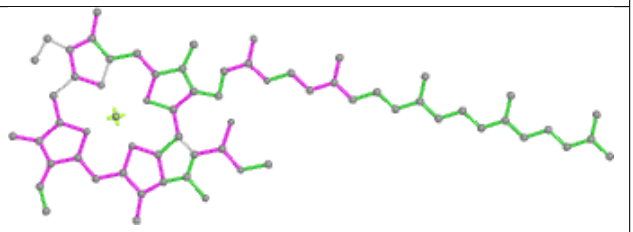


Rings

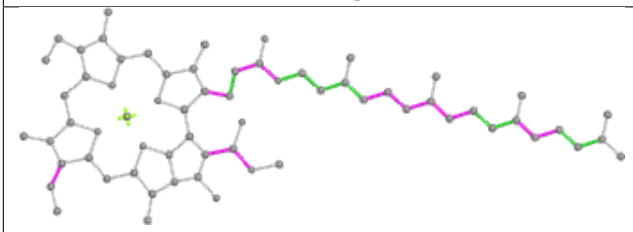
Ligand CLA B 1009



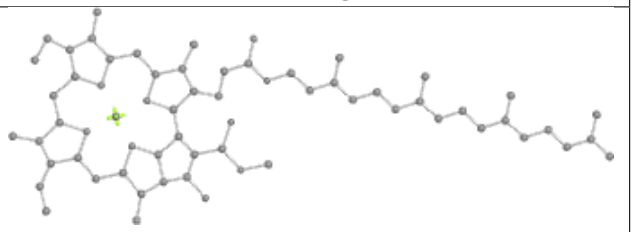
Bond lengths



Bond angles

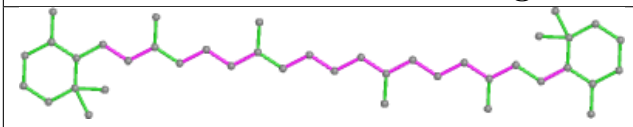


Torsions

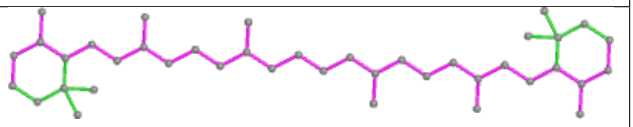


Rings

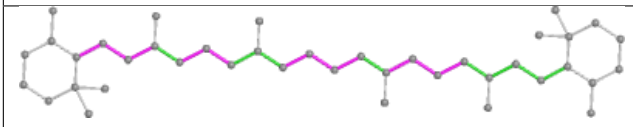
Ligand BCR C 1054



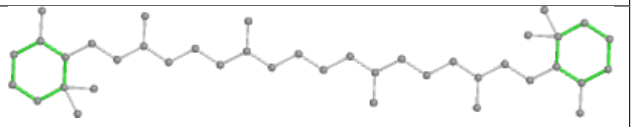
Bond lengths



Bond angles

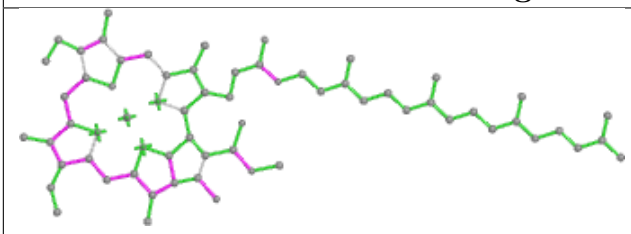


Torsions

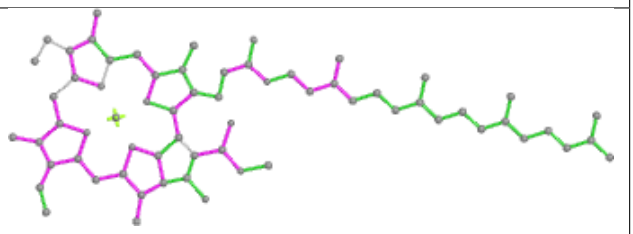


Rings

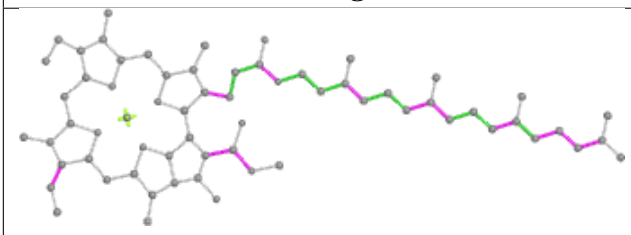
Ligand CLA D 1005



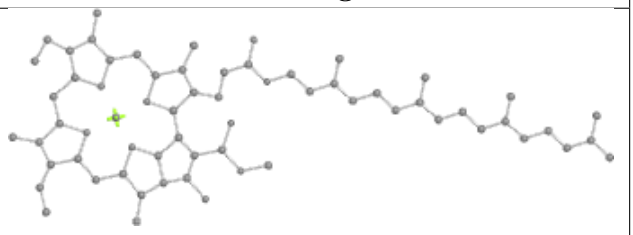
Bond lengths



Bond angles

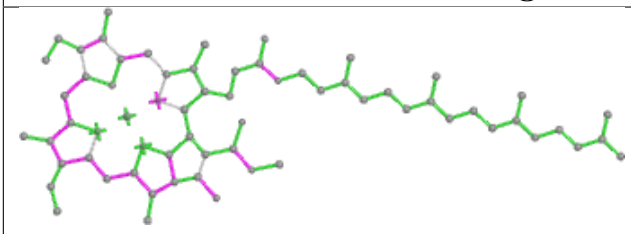


Torsions

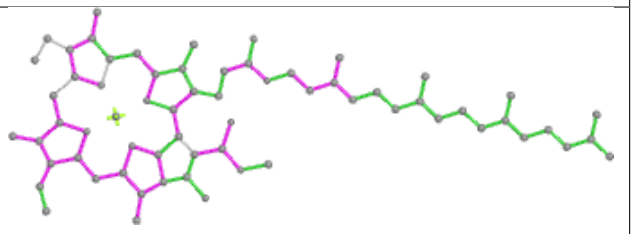


Rings

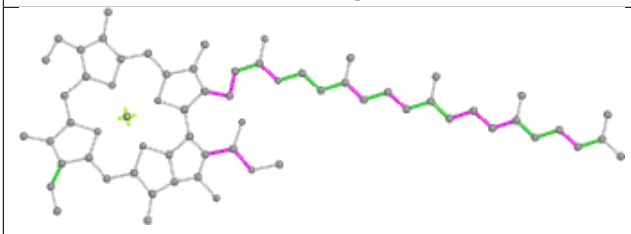
Ligand CLA b 6010



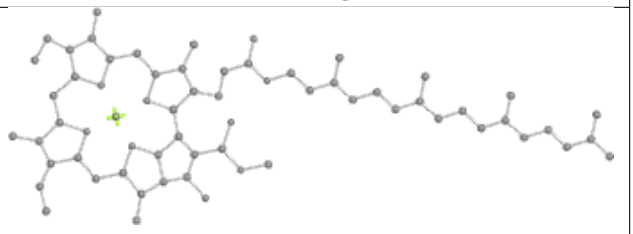
Bond lengths



Bond angles

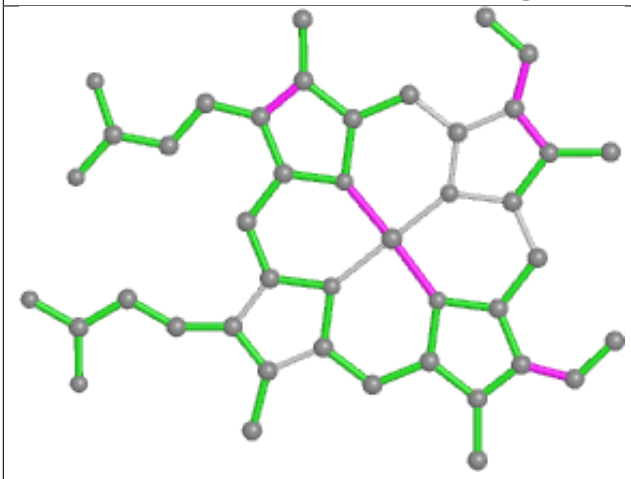


Torsions



Rings

Ligand HEM f 6040



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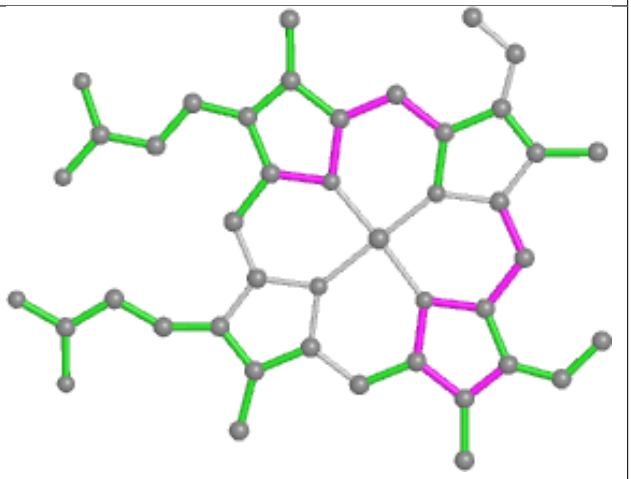
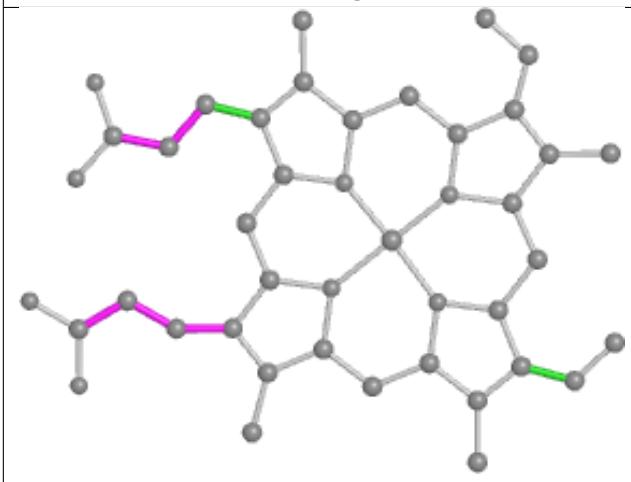
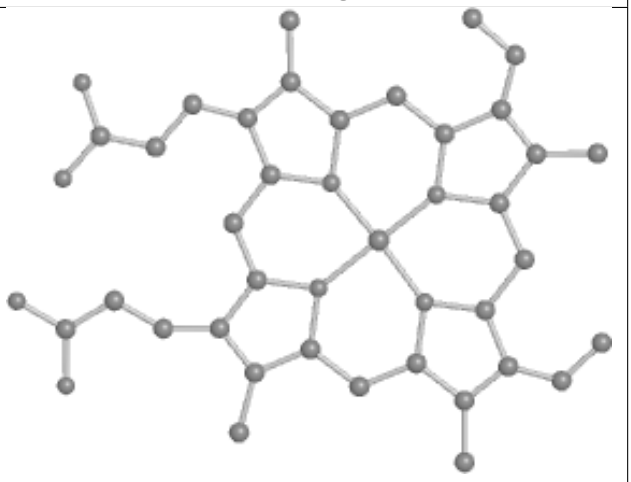


Bond angles

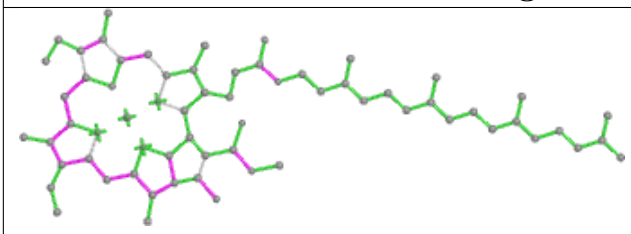


Torsions

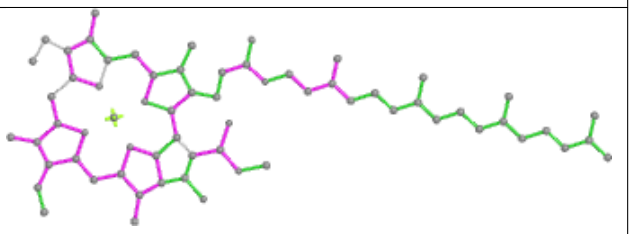


Rings

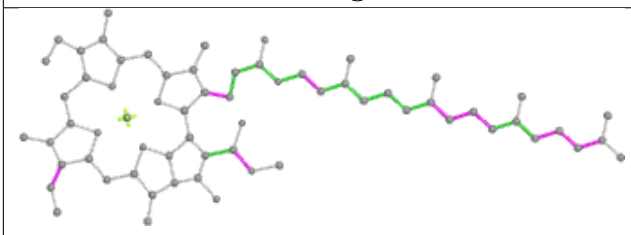
Ligand CLA b 6020



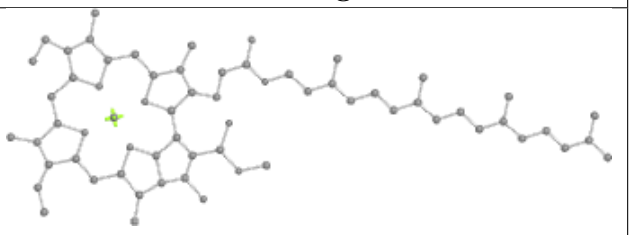
Bond lengths



Bond angles

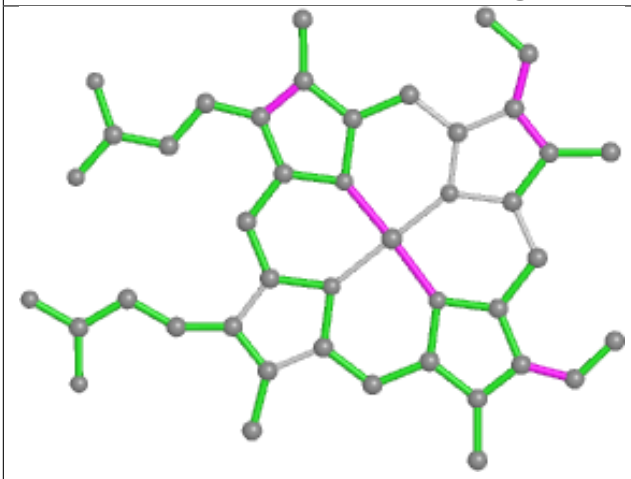


Torsions



Rings

Ligand HEM F 1040



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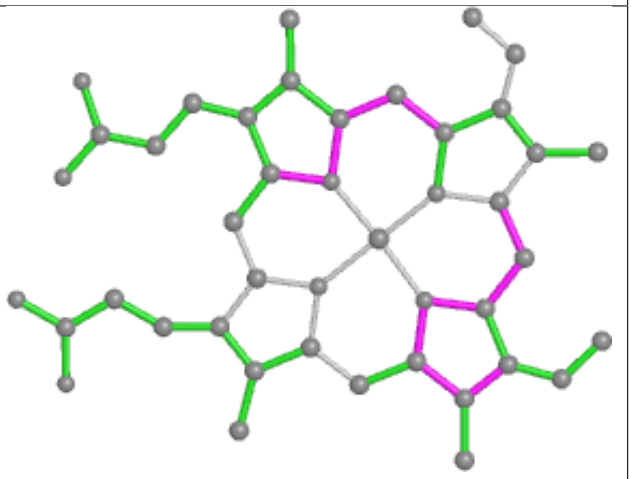
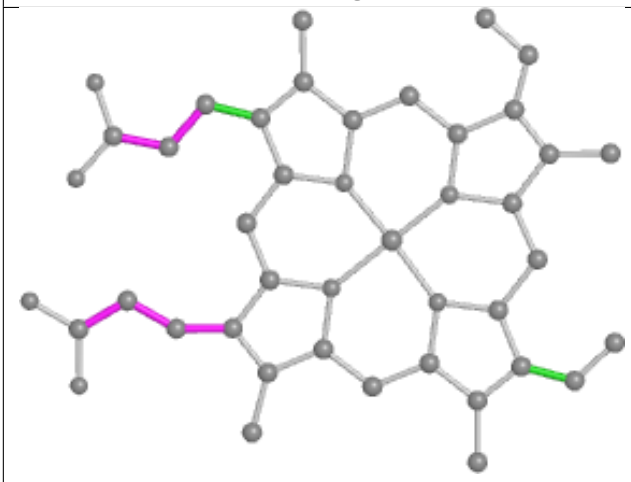
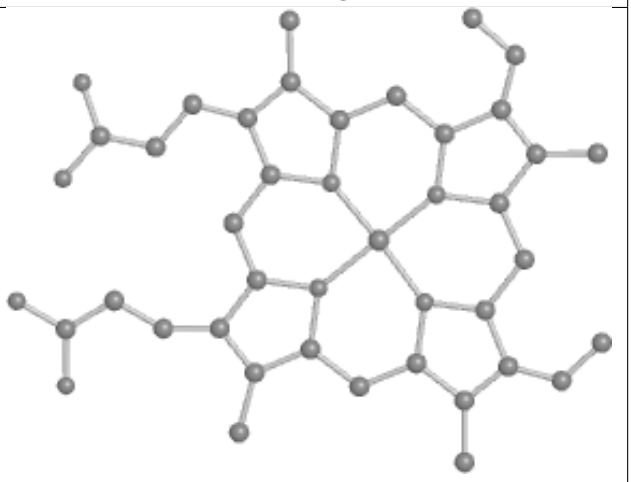


Bond angles

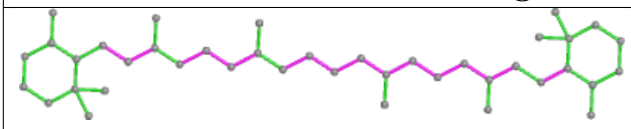


Torsions

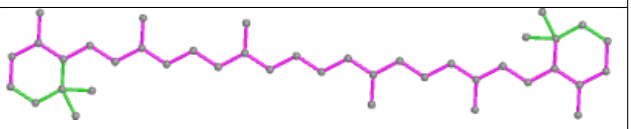


Rings

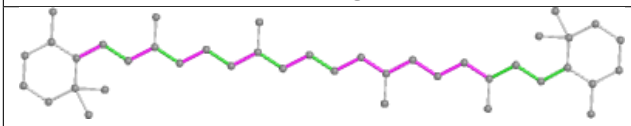
Ligand BCR B 1047



Bond lengths



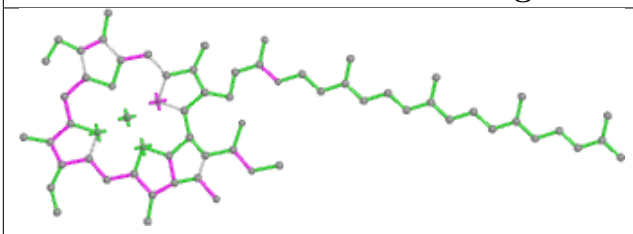
Bond angles



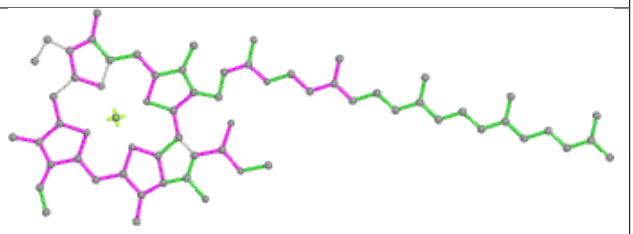
Torsions

Rings

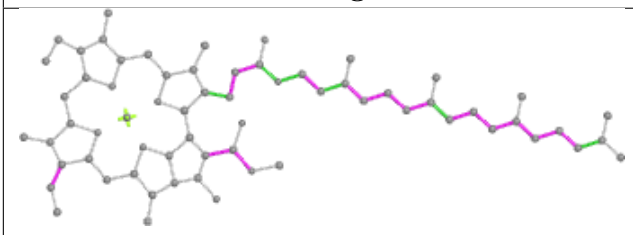
Ligand CLA K 1034



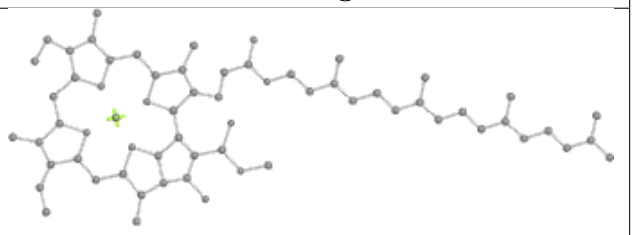
Bond lengths



Bond angles

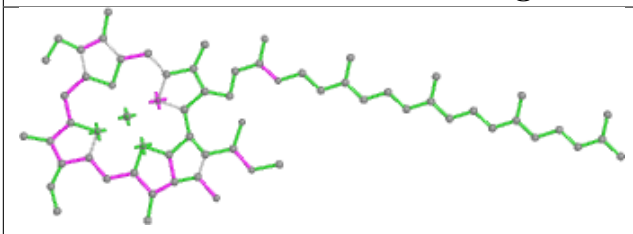


Torsions

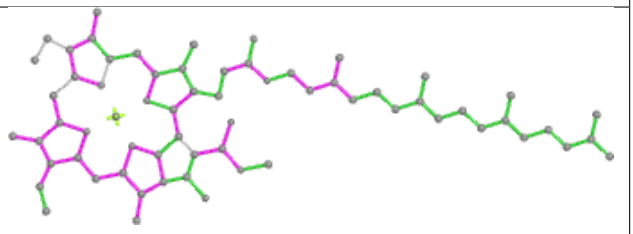


Rings

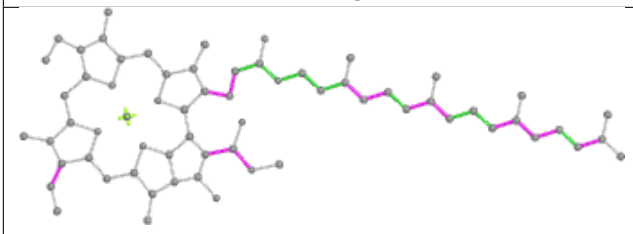
Ligand CLA A 1003



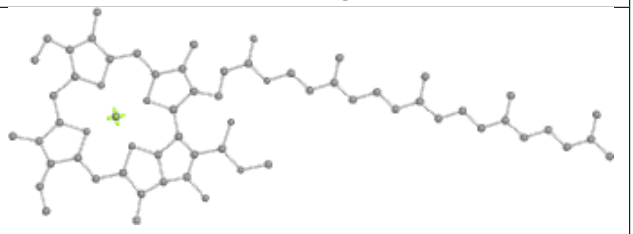
Bond lengths



Bond angles

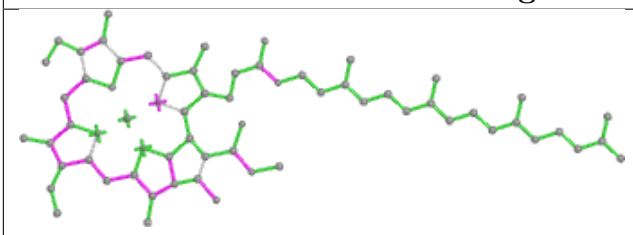


Torsions

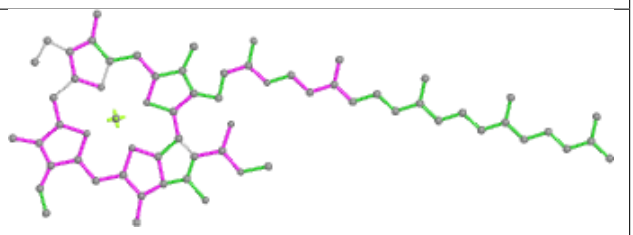


Rings

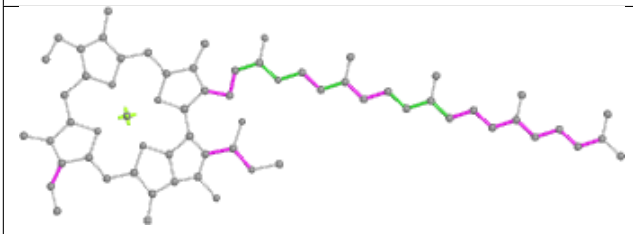
Ligand CLA b 6013



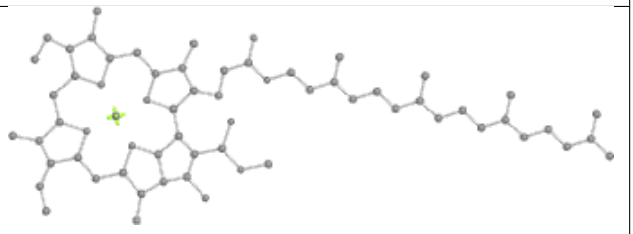
Bond lengths



Bond angles

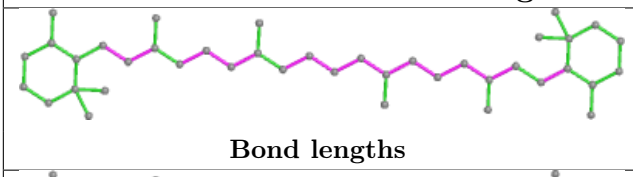


Torsions

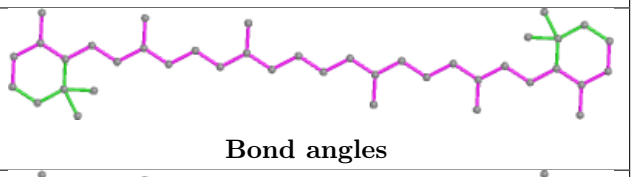


Rings

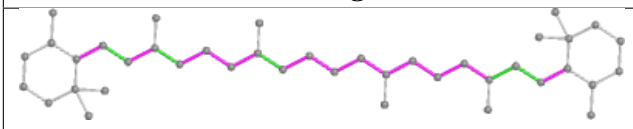
Ligand BCR d 6050



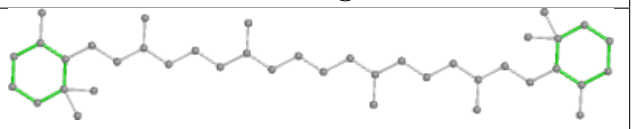
Bond lengths



Bond angles

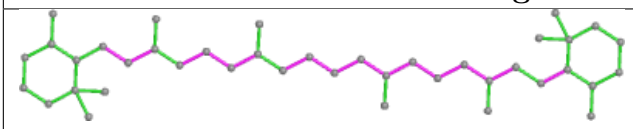


Torsions

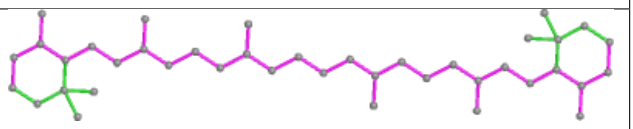


Rings

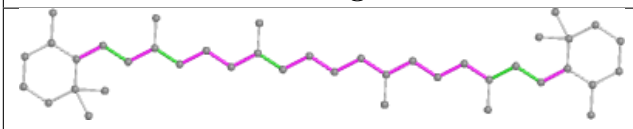
Ligand BCR D 1050



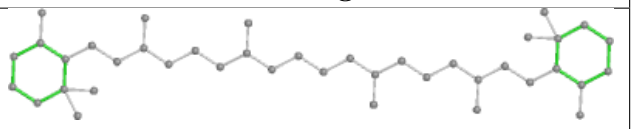
Bond lengths



Bond angles

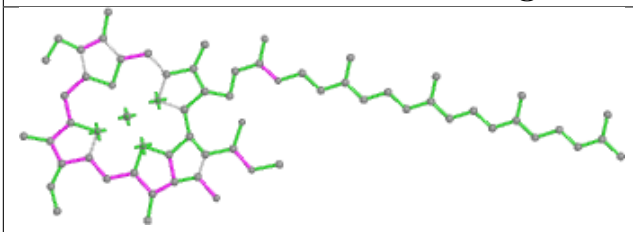


Torsions

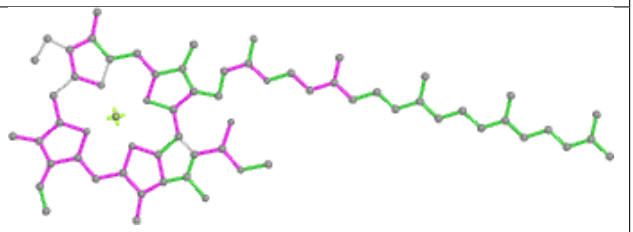


Rings

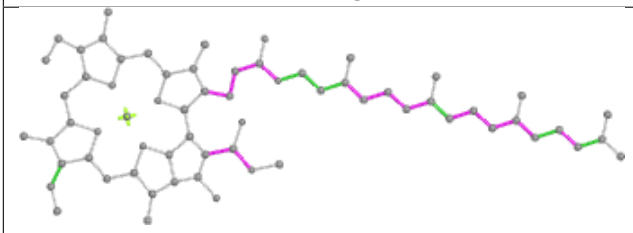
Ligand CLA h 6017



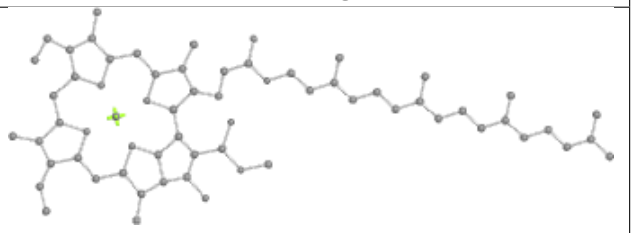
Bond lengths



Bond angles

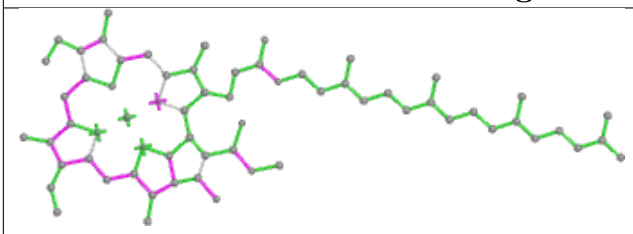


Torsions

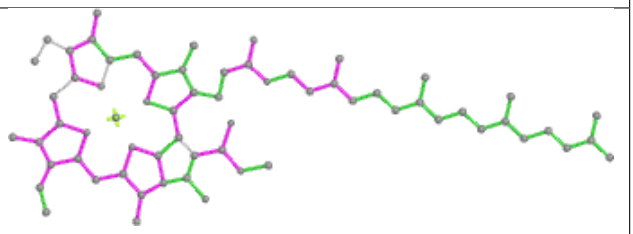


Rings

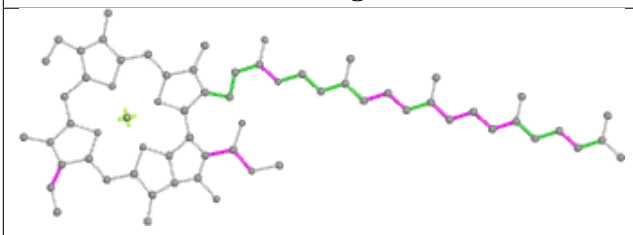
Ligand CLA C 1029



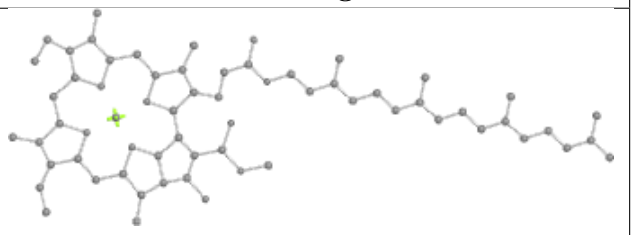
Bond lengths



Bond angles

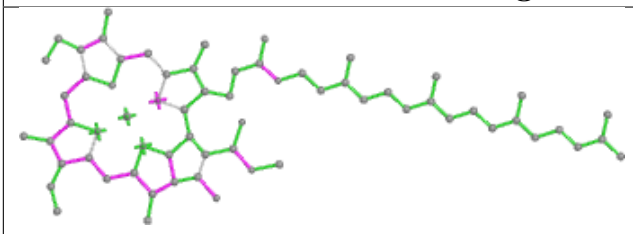


Torsions

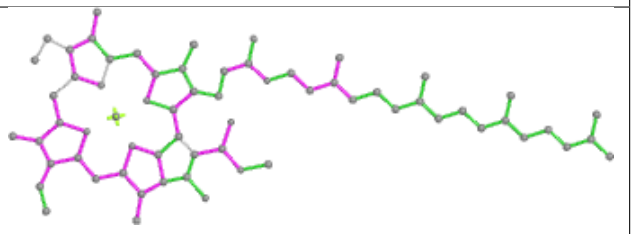


Rings

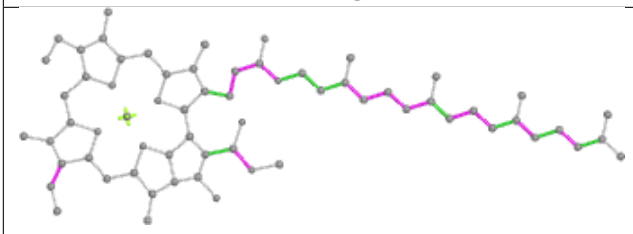
Ligand CLA C 1027



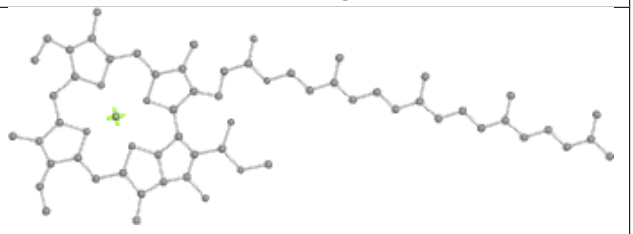
Bond lengths



Bond angles

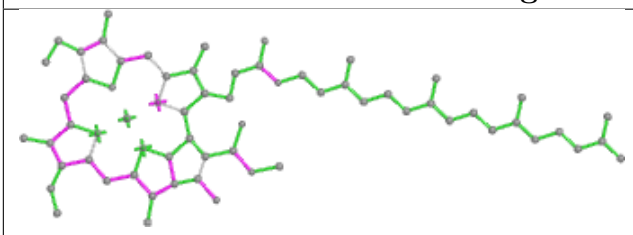


Torsions

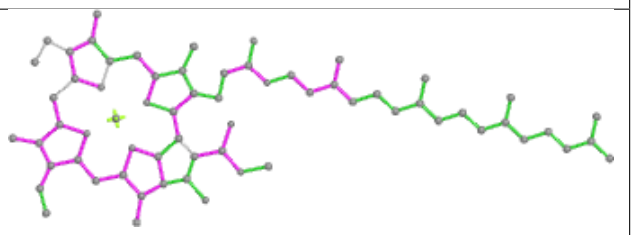


Rings

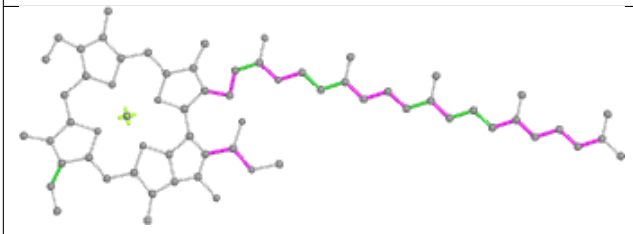
Ligand CLA c 6028



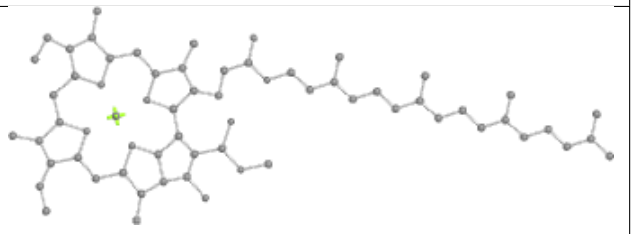
Bond lengths



Bond angles

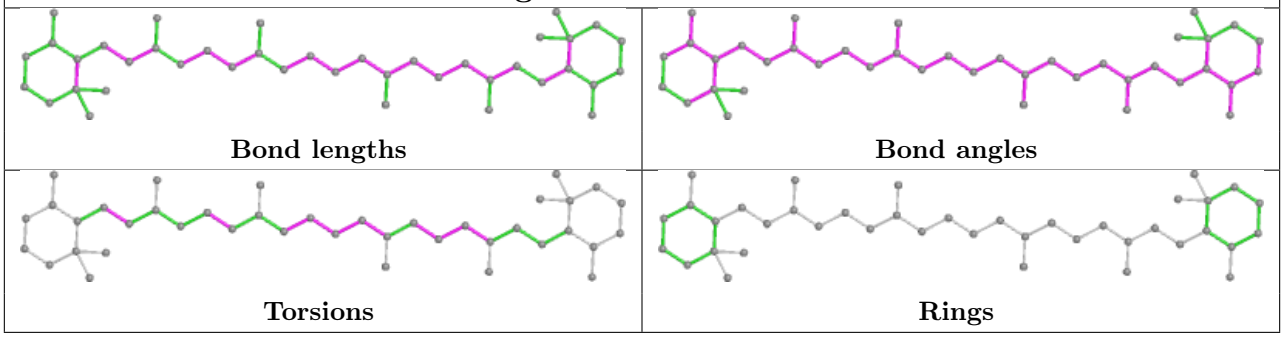


Torsions

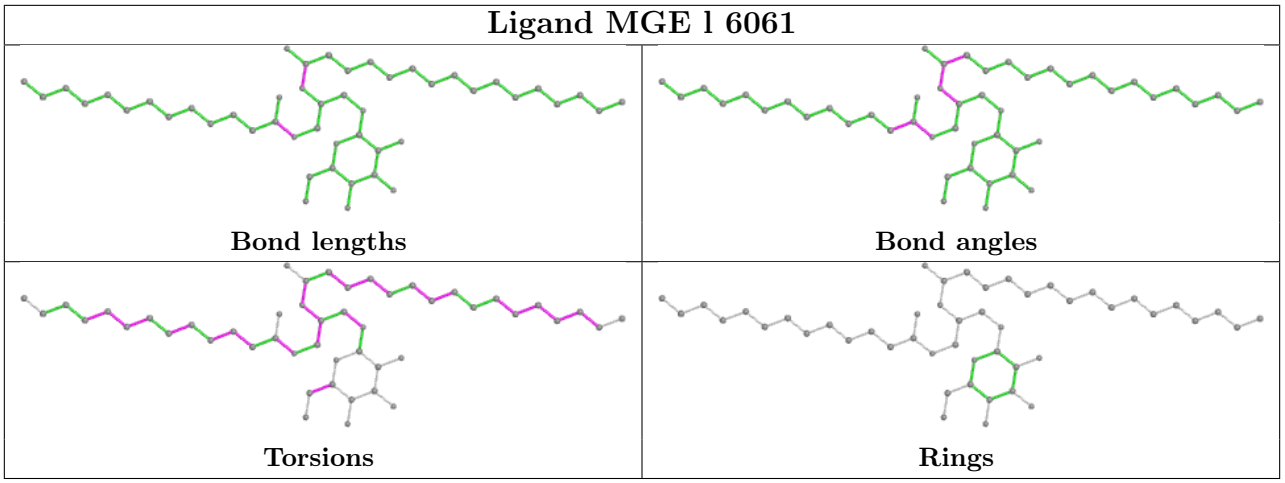


Rings

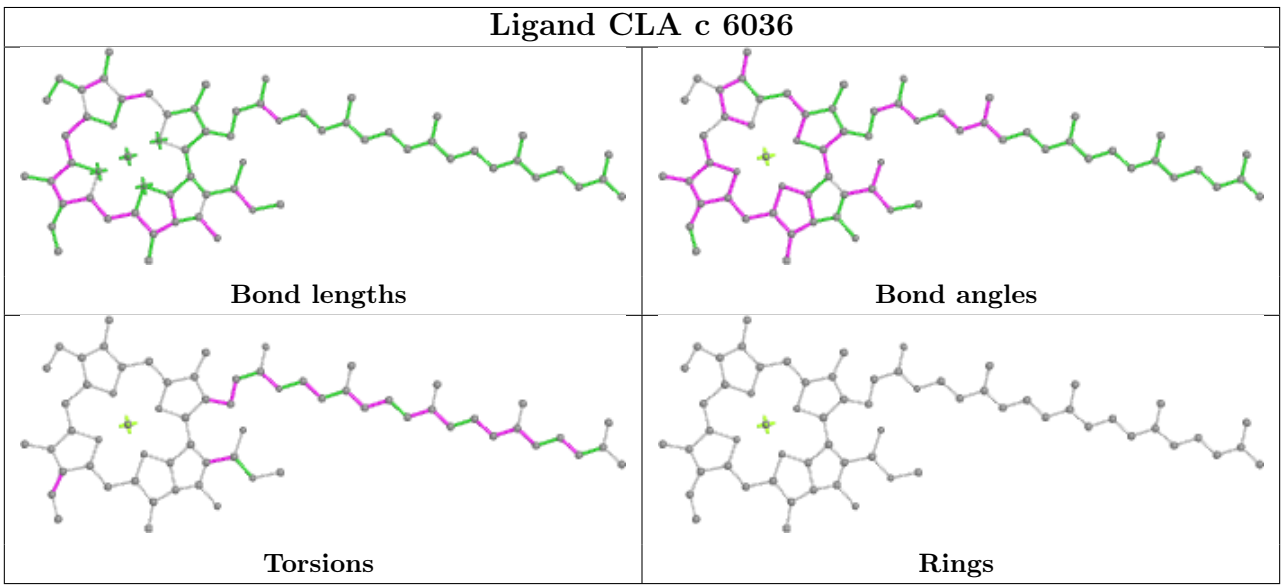
Ligand BCR T 6046



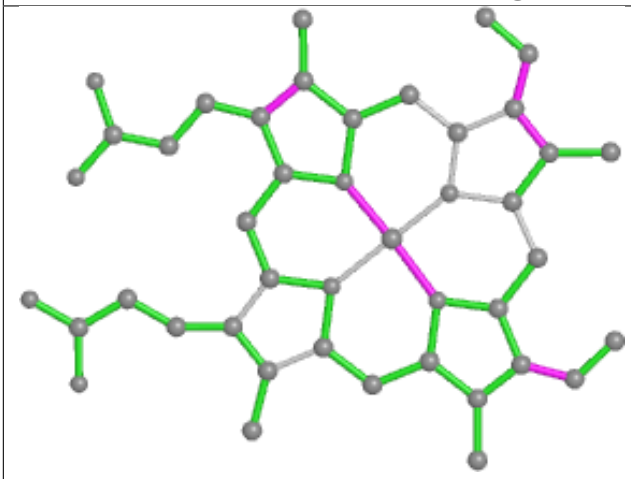
Ligand MGE l 6061



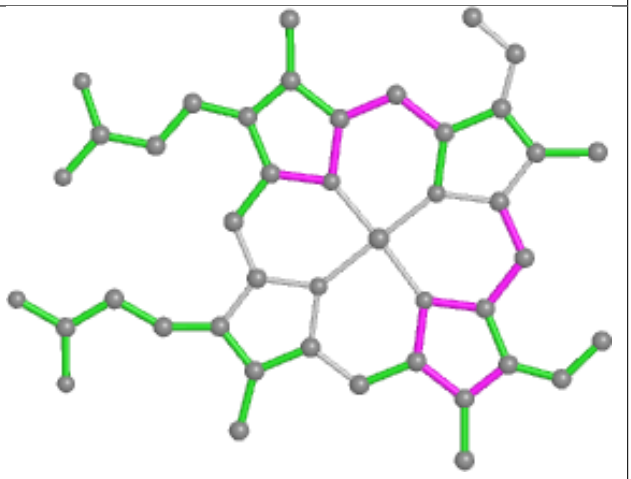
Ligand CLA c 6036



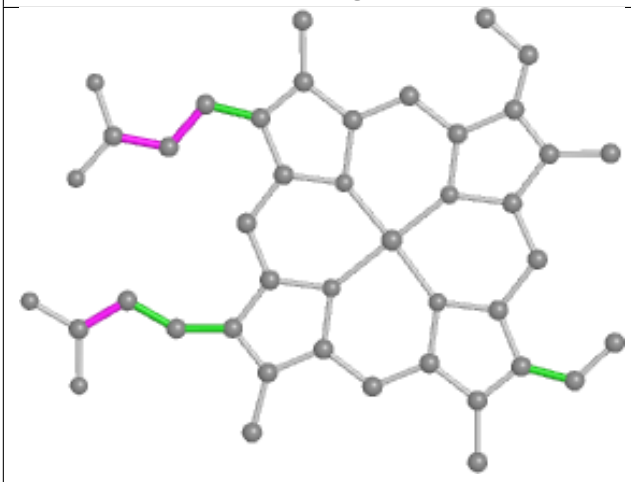
Ligand HEM V 1041



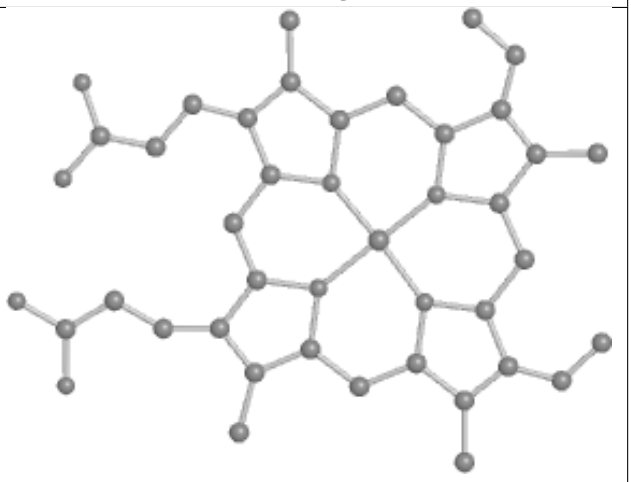
Bond lengths



Bond angles

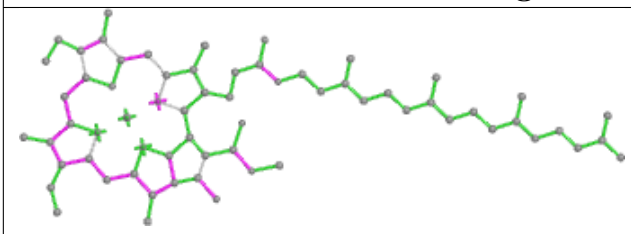


Torsions

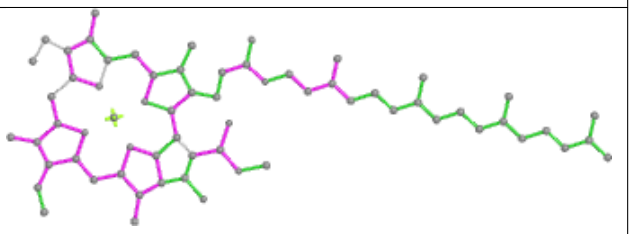


Rings

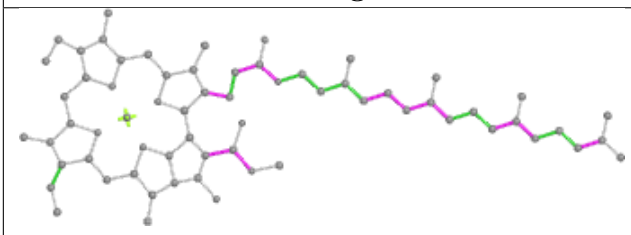
Ligand CLA C 1025



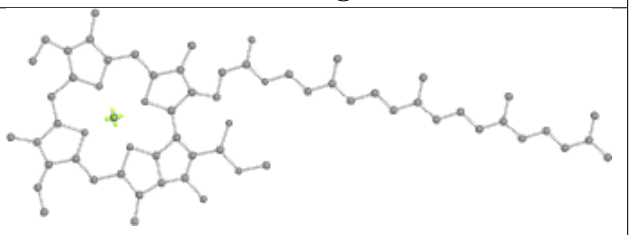
Bond lengths



Bond angles

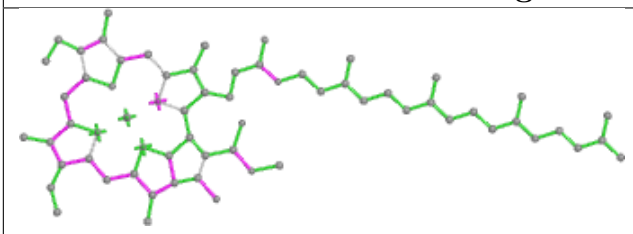


Torsions

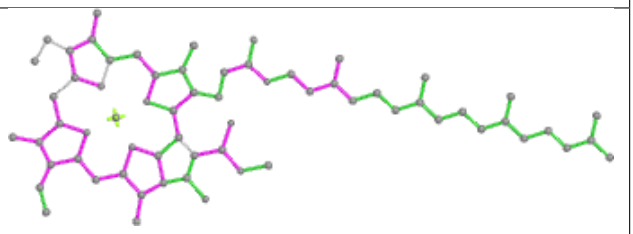


Rings

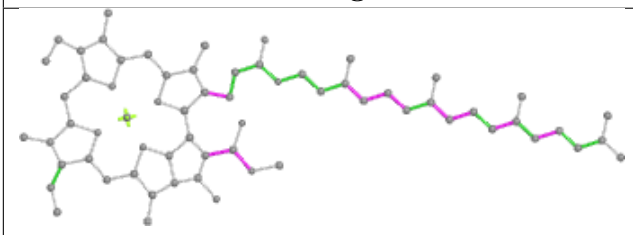
Ligand CLA C 1035



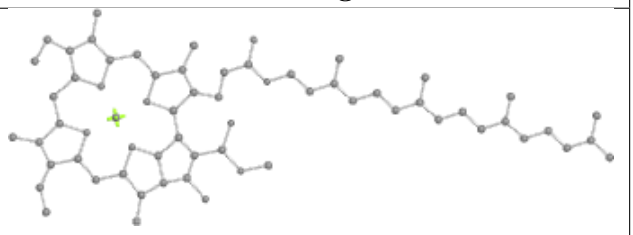
Bond lengths



Bond angles

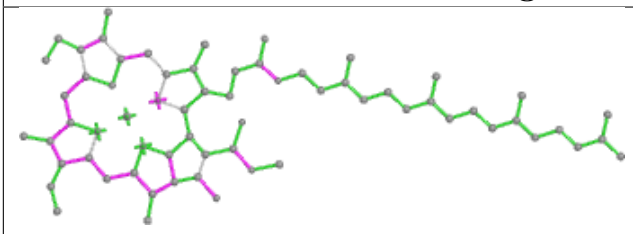


Torsions

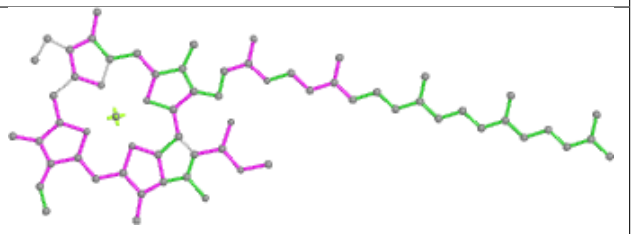


Rings

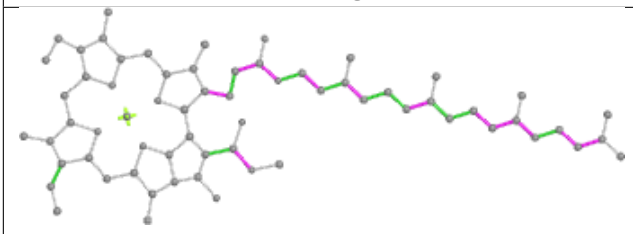
Ligand CLA b 6011



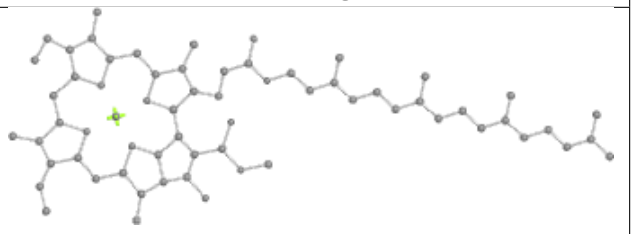
Bond lengths



Bond angles

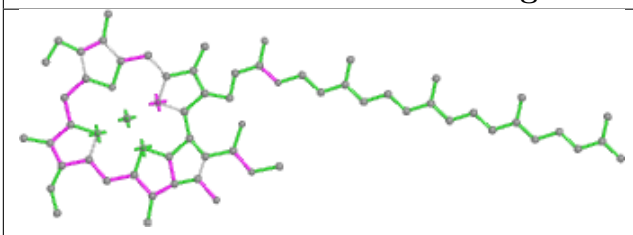


Torsions



Rings

Ligand CLA c 6035



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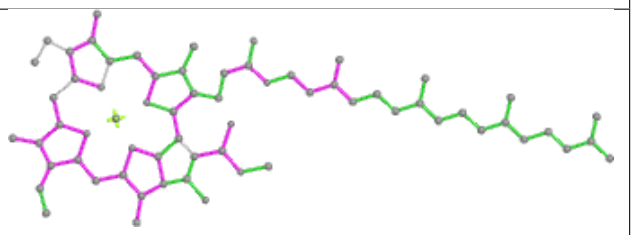
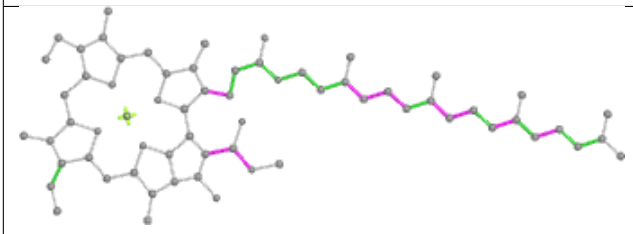
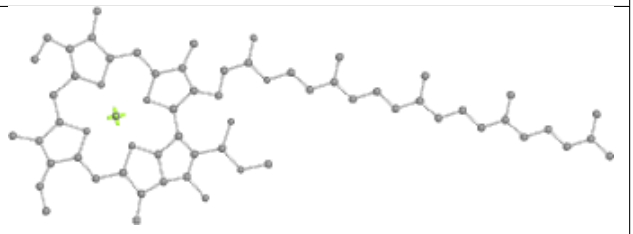


Bond angles

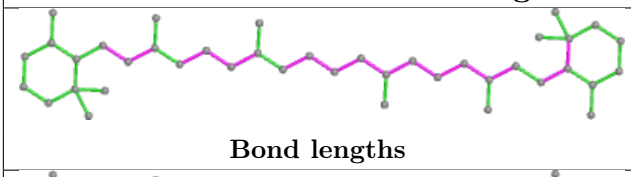


Torsions

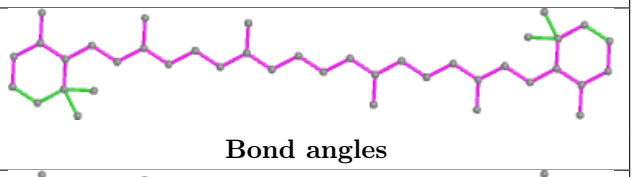


Rings

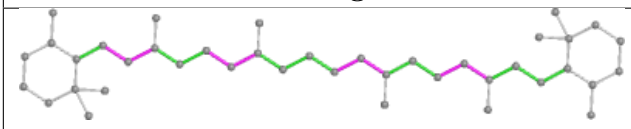
Ligand BCR A 1044



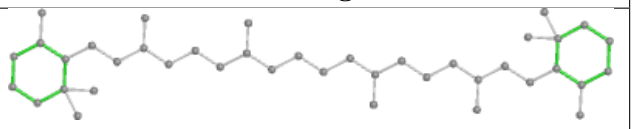
Bond lengths



Bond angles

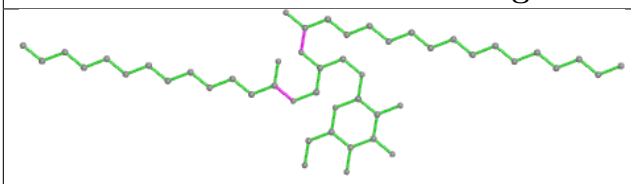


Torsions



Rings

Ligand MGE L 1061



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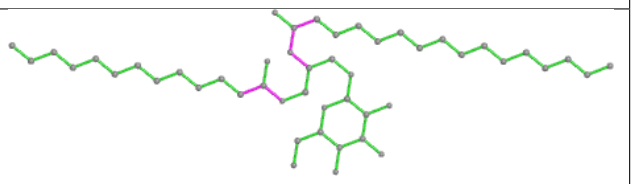
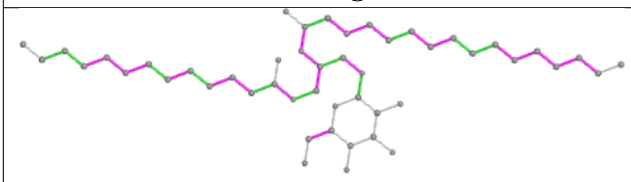
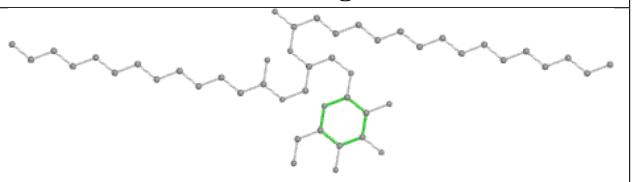


Bond angles

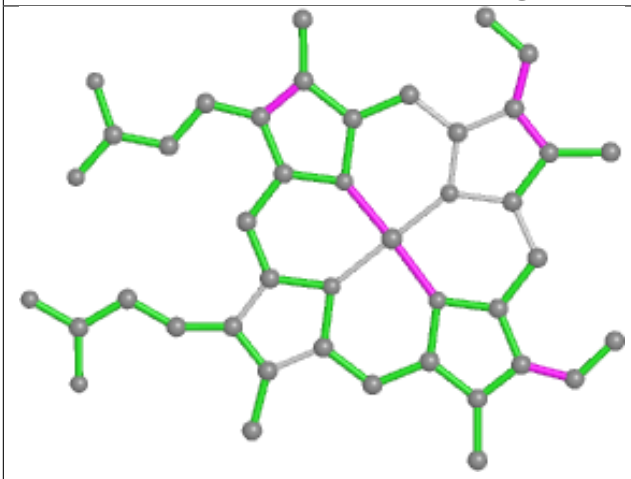


Torsions

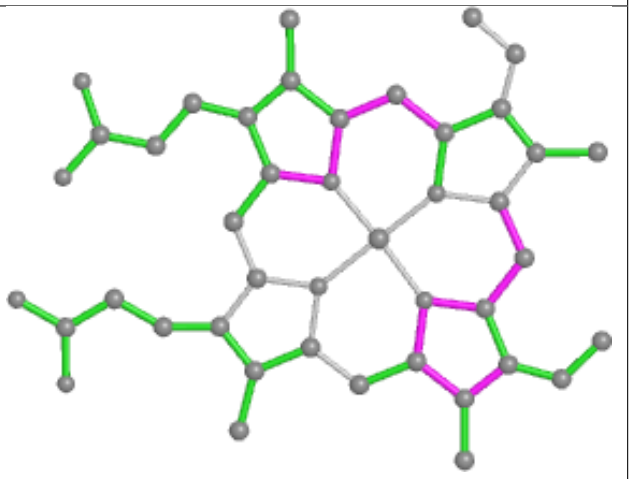


Rings

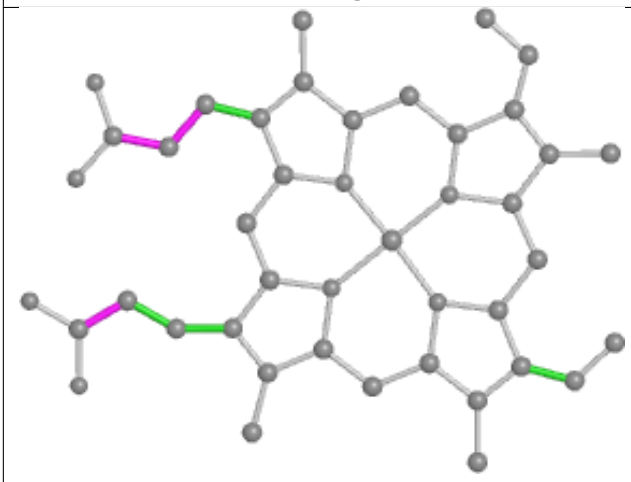
Ligand HEM v 6041



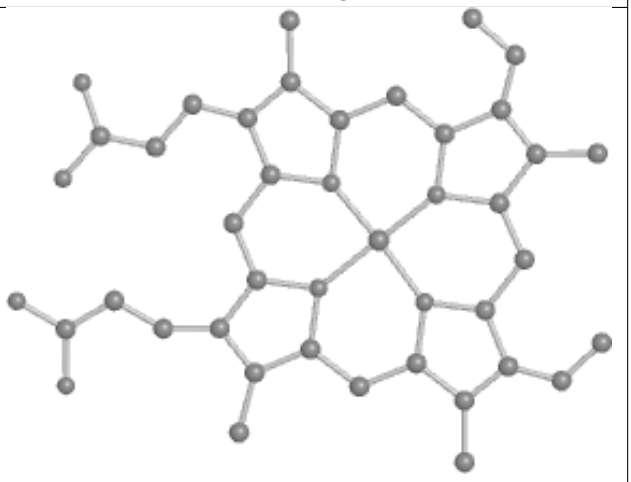
Bond lengths



Bond angles

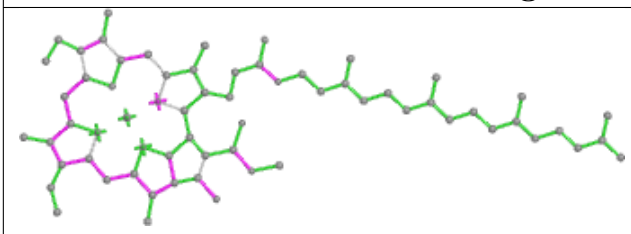


Torsions

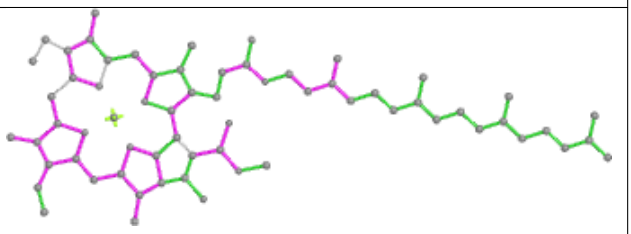


Rings

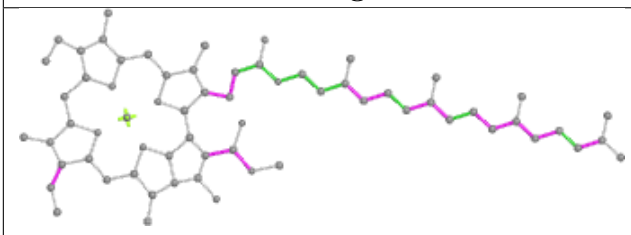
Ligand CLA a 6003



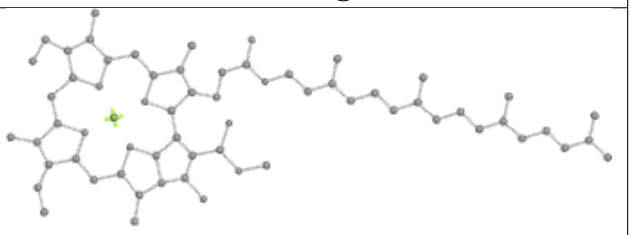
Bond lengths



Bond angles

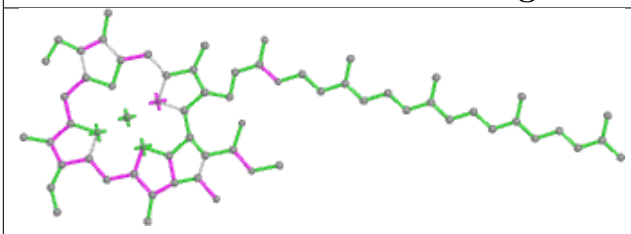


Torsions

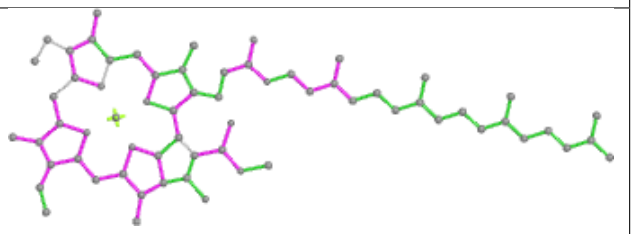


Rings

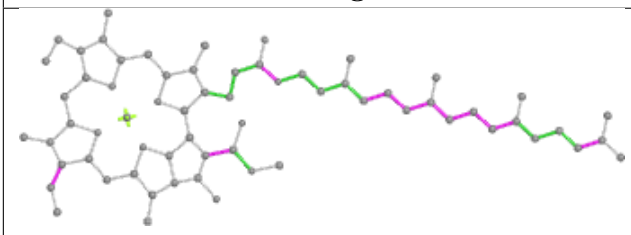
Ligand CLA b 6023



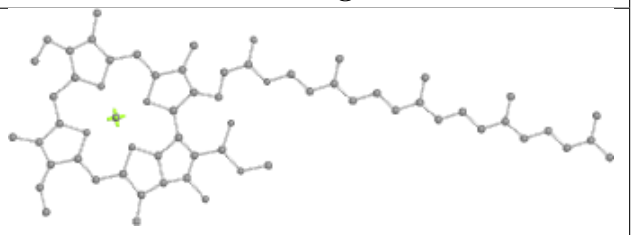
Bond lengths



Bond angles

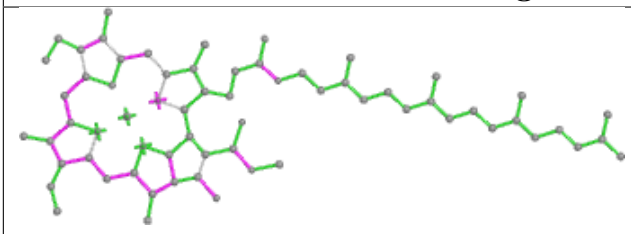


Torsions

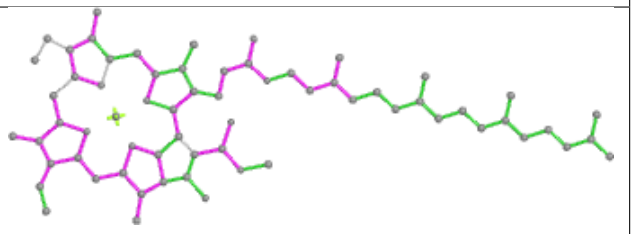


Rings

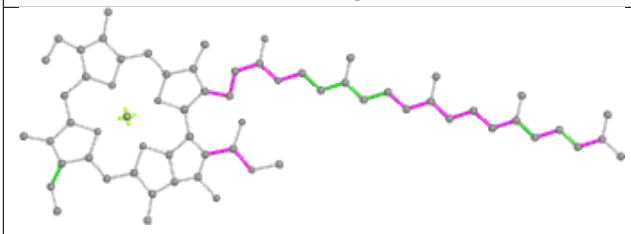
Ligand CLA B 1021



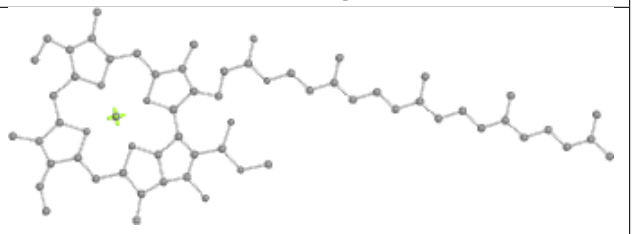
Bond lengths



Bond angles

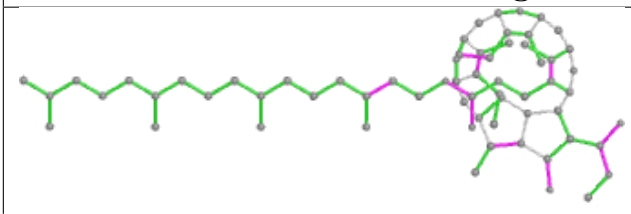


Torsions

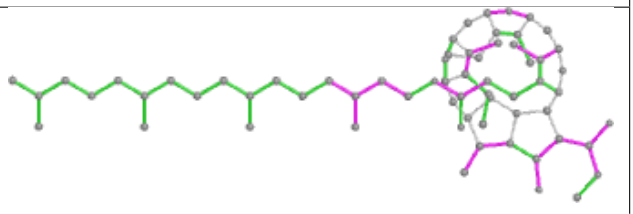


Rings

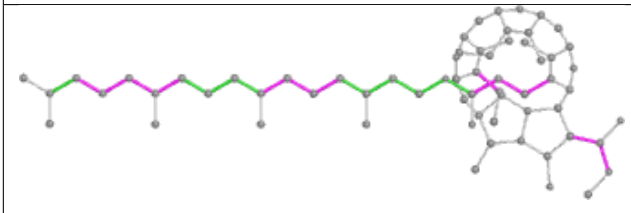
Ligand PHO A 1038



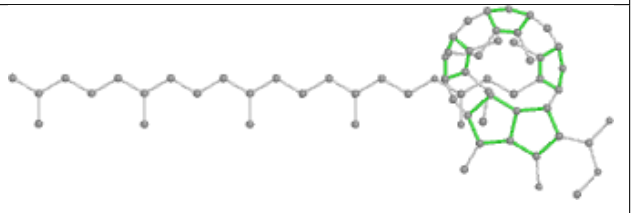
Bond lengths



Bond angles

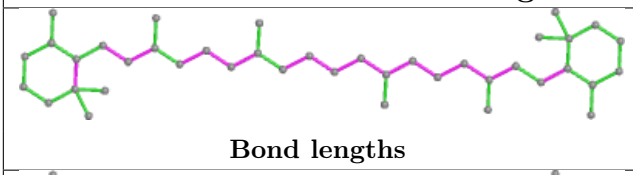


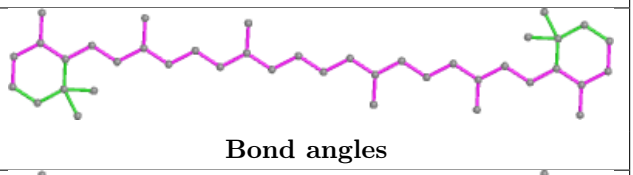
Torsions

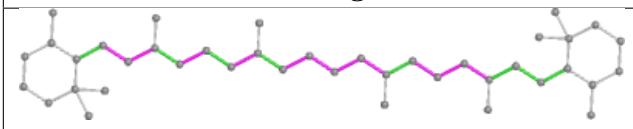


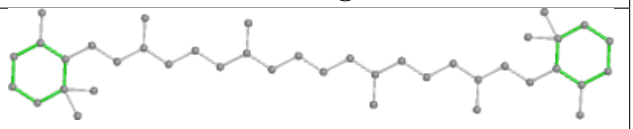
Rings

Ligand BCR k 6051

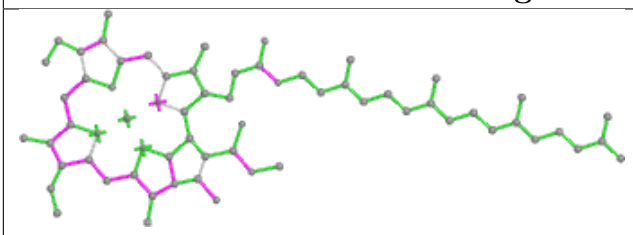

Bond lengths

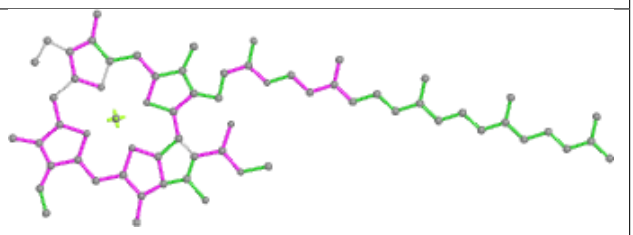

Bond angles

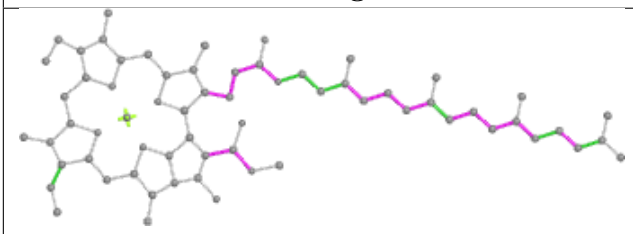

Torsions

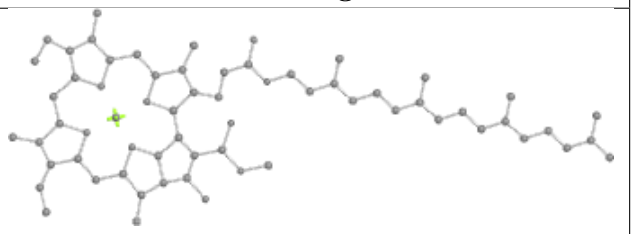

Rings

Ligand CLA H 1017

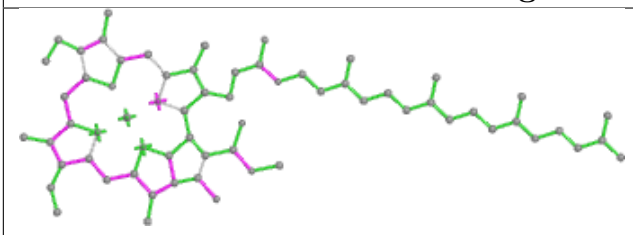

Bond lengths

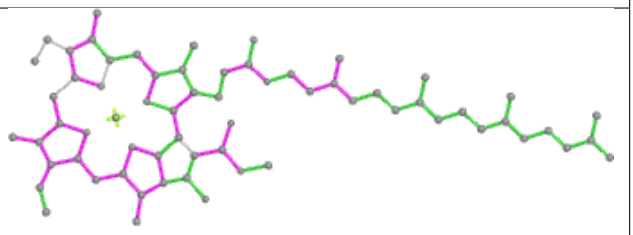

Bond angles

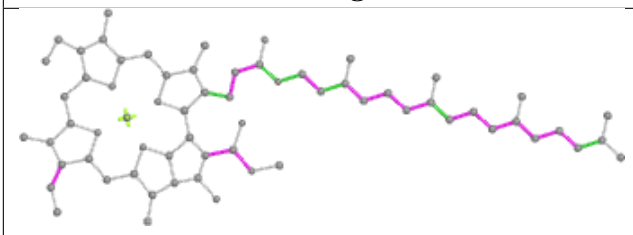

Torsions

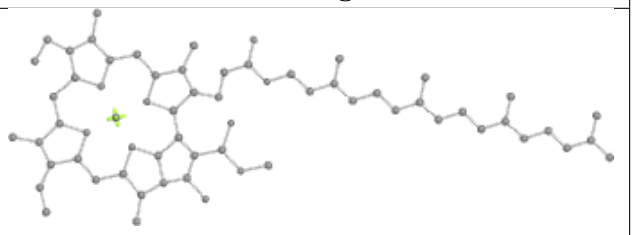

Rings

Ligand CLA k 6034

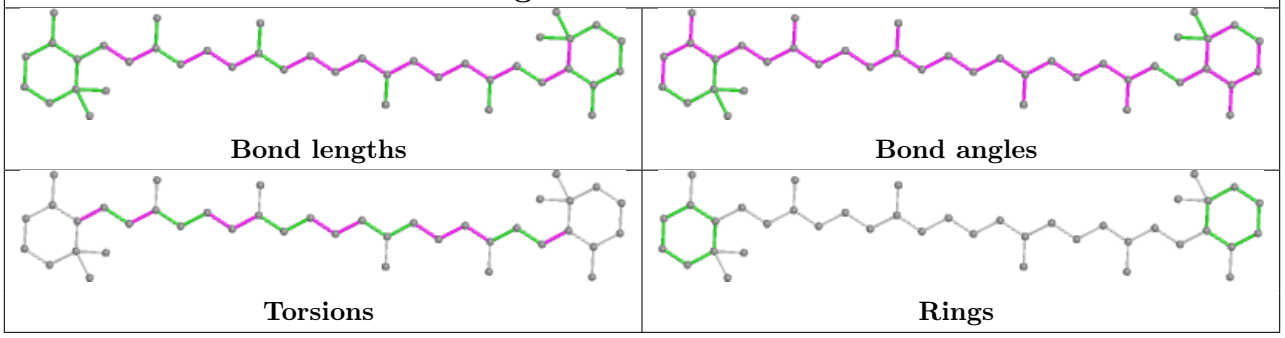

Bond lengths


Bond angles

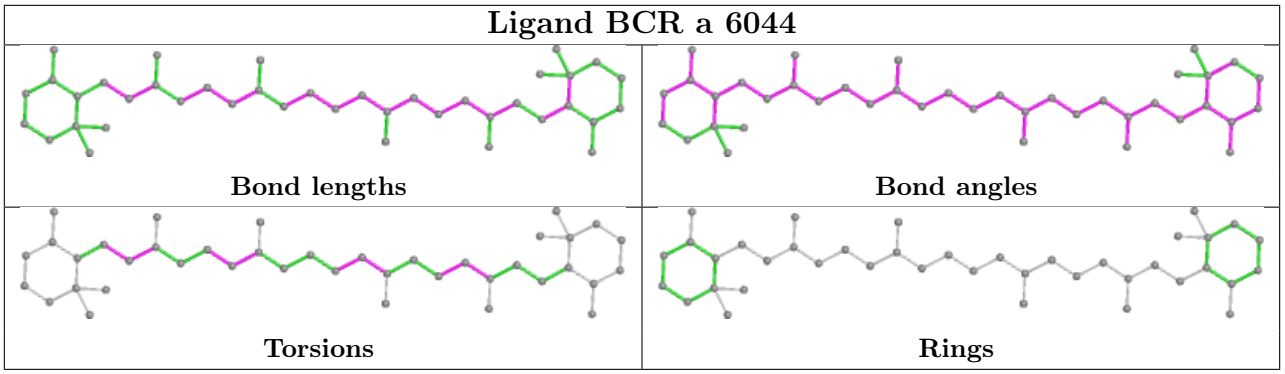

Torsions


Rings

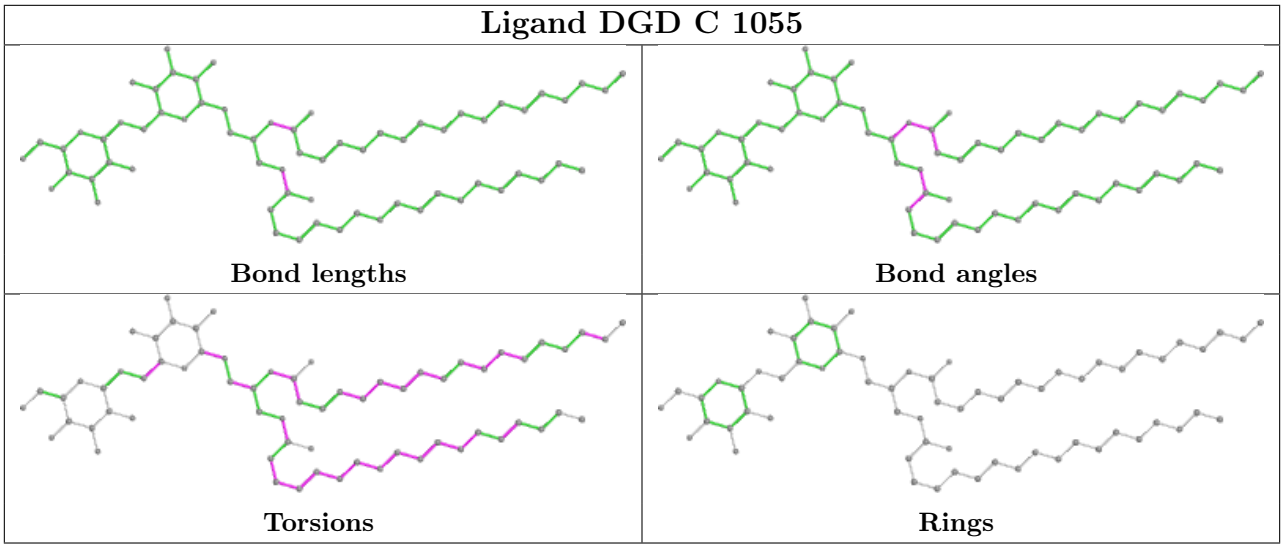
Ligand BCR C 1052



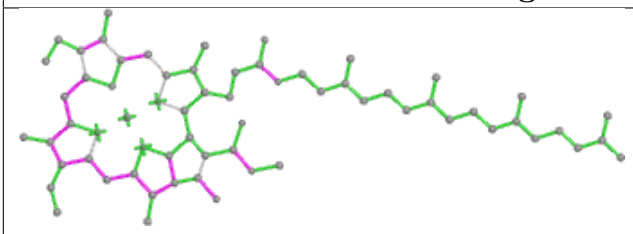
Ligand BCR a 6044



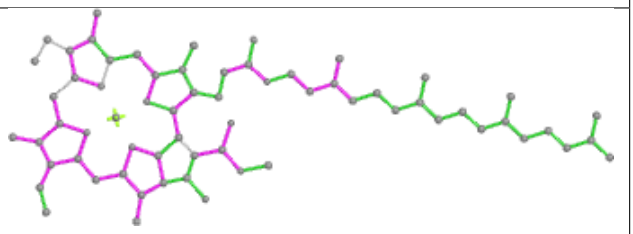
Ligand DGD C 1055



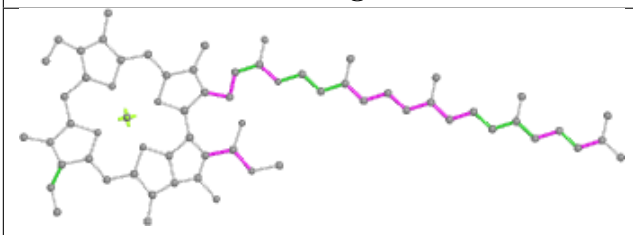
Ligand CLA b 6015



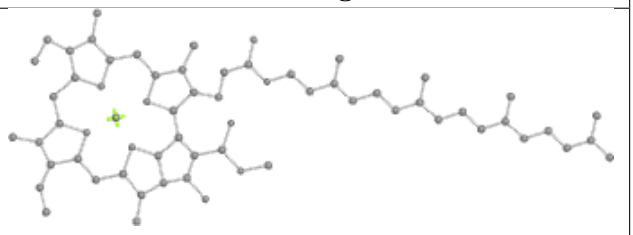
Bond lengths



Bond angles

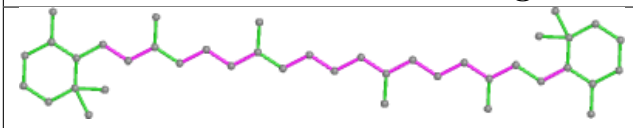


Torsions

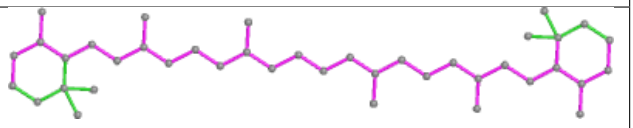


Rings

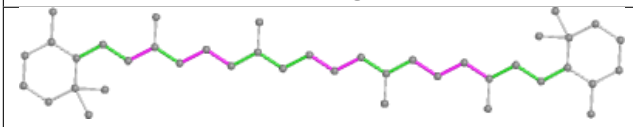
Ligand BCR T 6048



Bond lengths



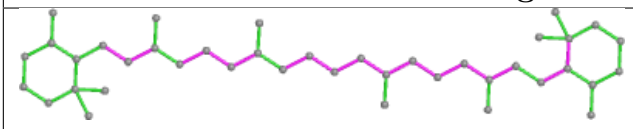
Bond angles



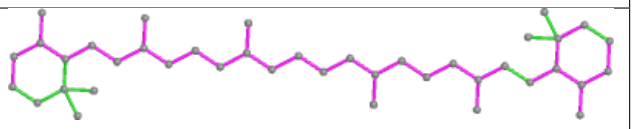
Torsions

Rings

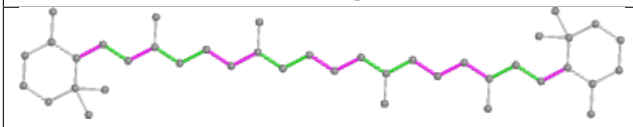
Ligand BCR k 6052



Bond lengths



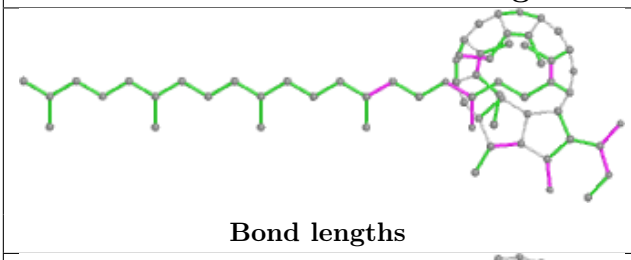
Bond angles



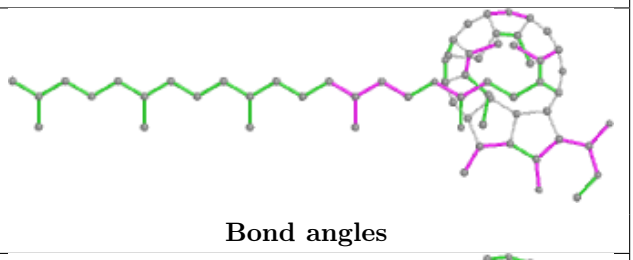
Torsions

Rings

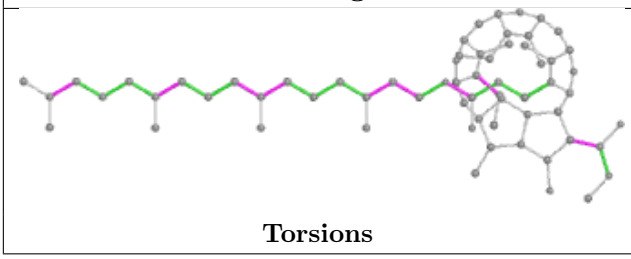
Ligand PHO D 1039



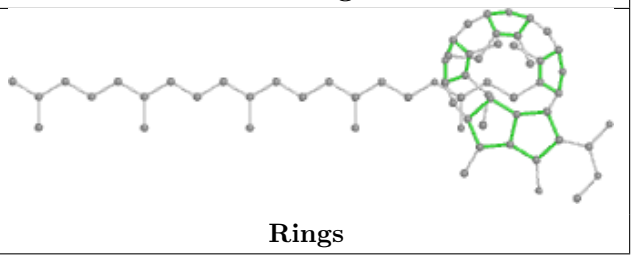
Bond lengths



Bond angles

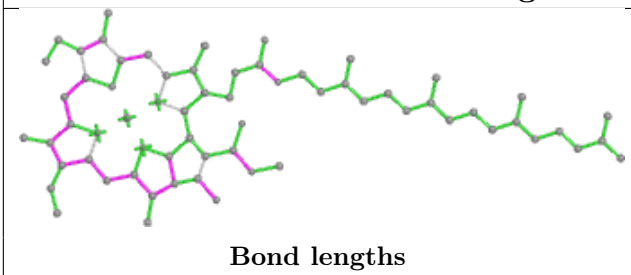


Torsions

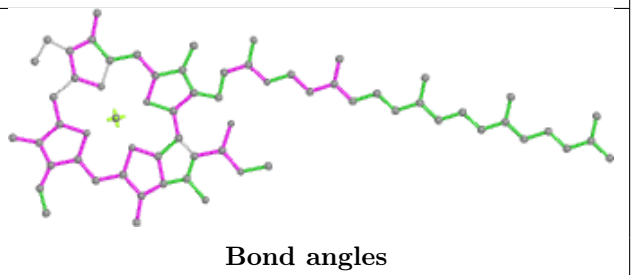


Rings

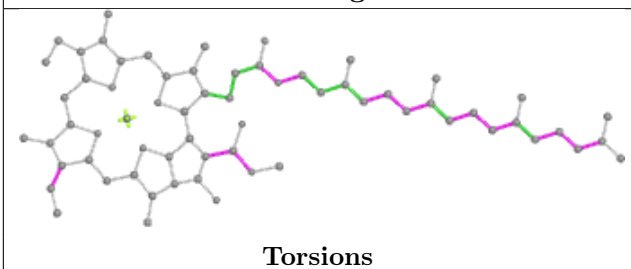
Ligand CLA b 6016



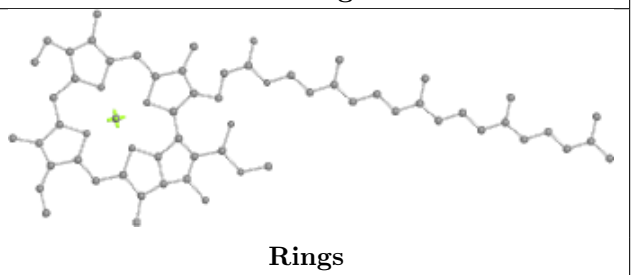
Bond lengths



Bond angles

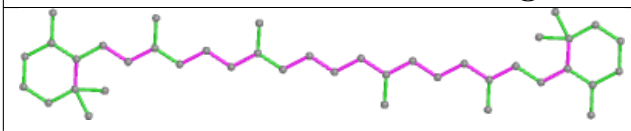


Torsions

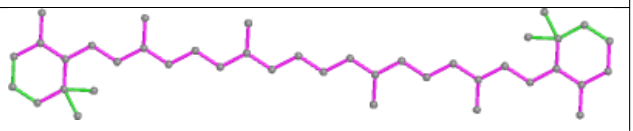


Rings

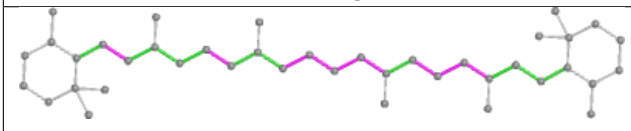
Ligand BCR t 1046



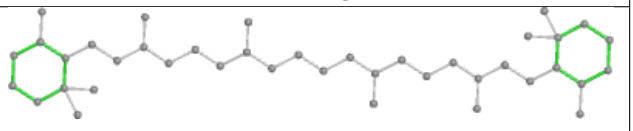
Bond lengths



Bond angles

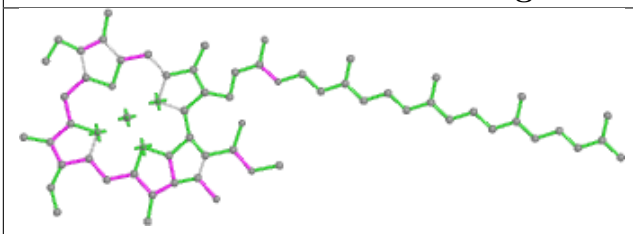


Torsions

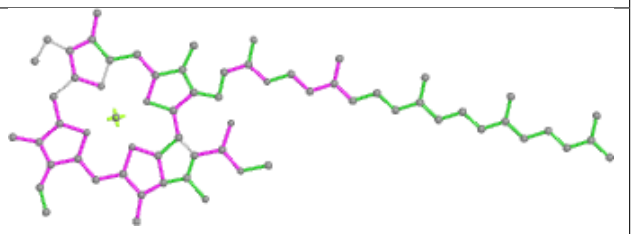


Rings

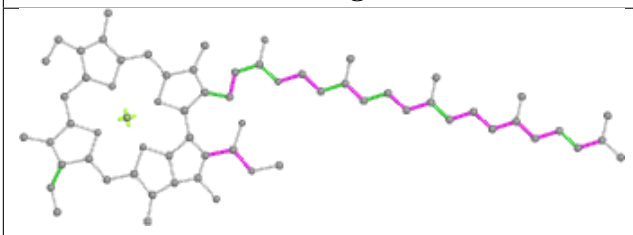
Ligand CLA C 1026



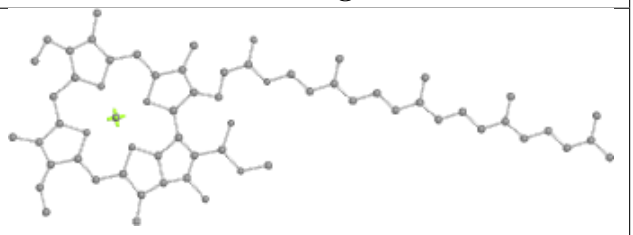
Bond lengths



Bond angles

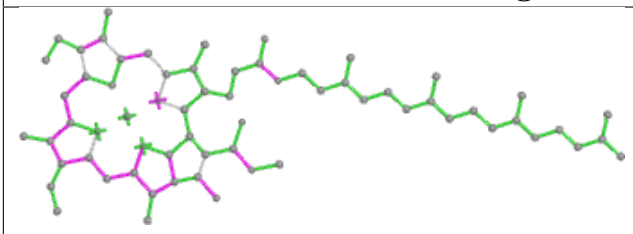


Torsions

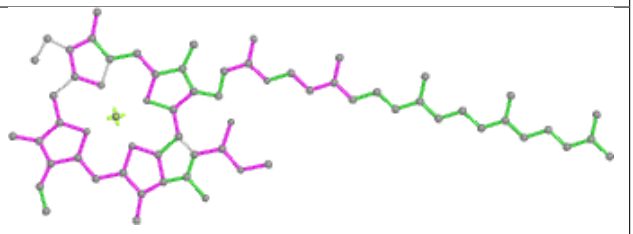


Rings

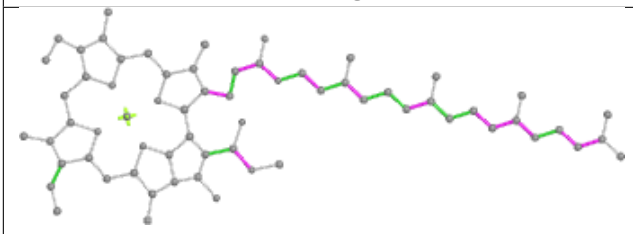
Ligand CLA B 1011



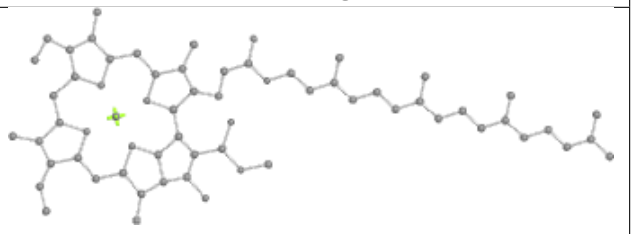
Bond lengths



Bond angles

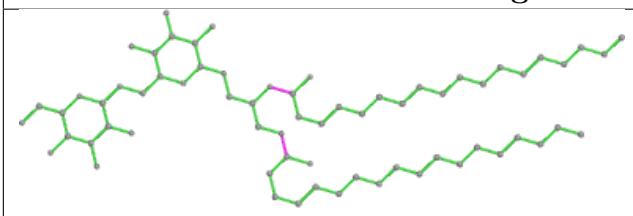


Torsions

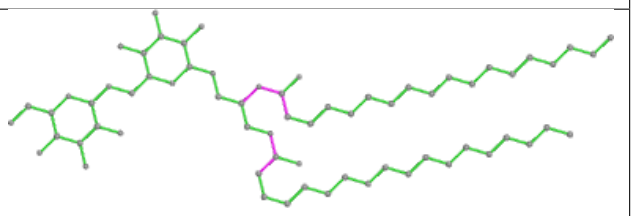


Rings

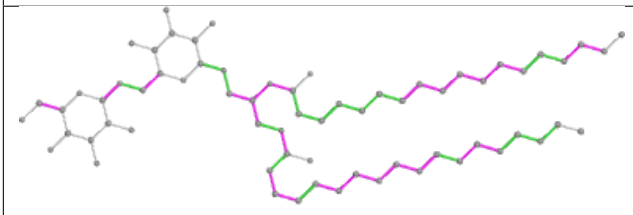
Ligand DGD C 1056



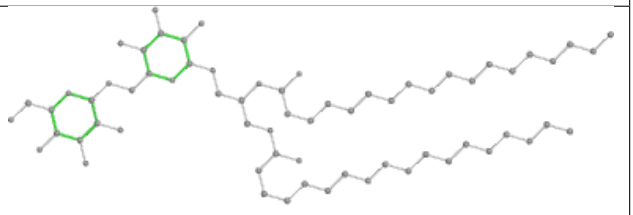
Bond lengths



Bond angles

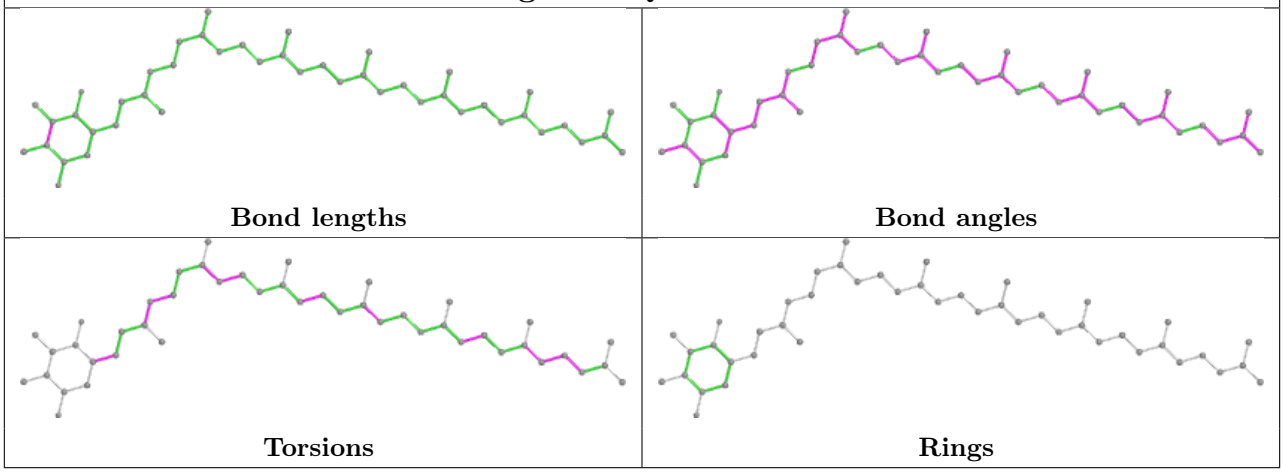


Torsions

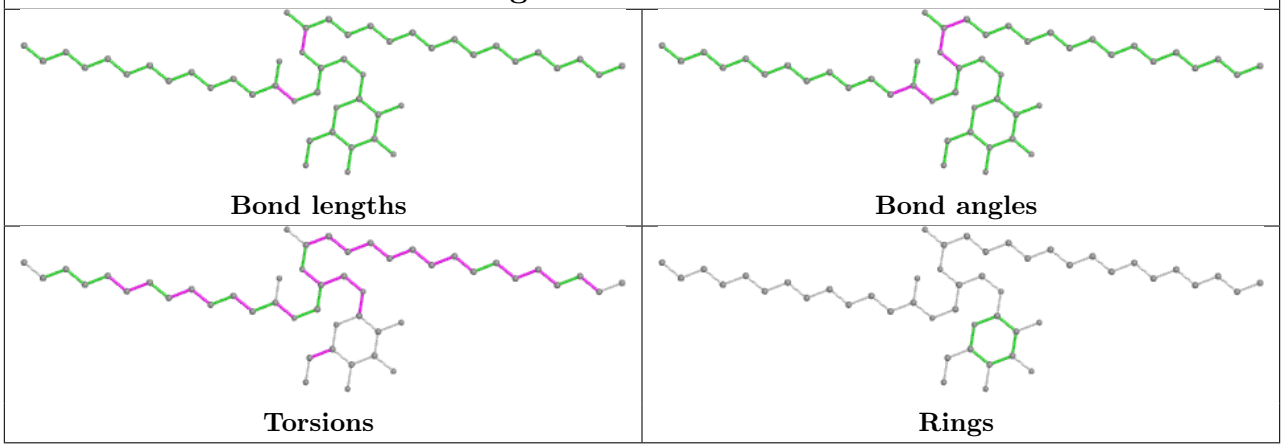


Rings

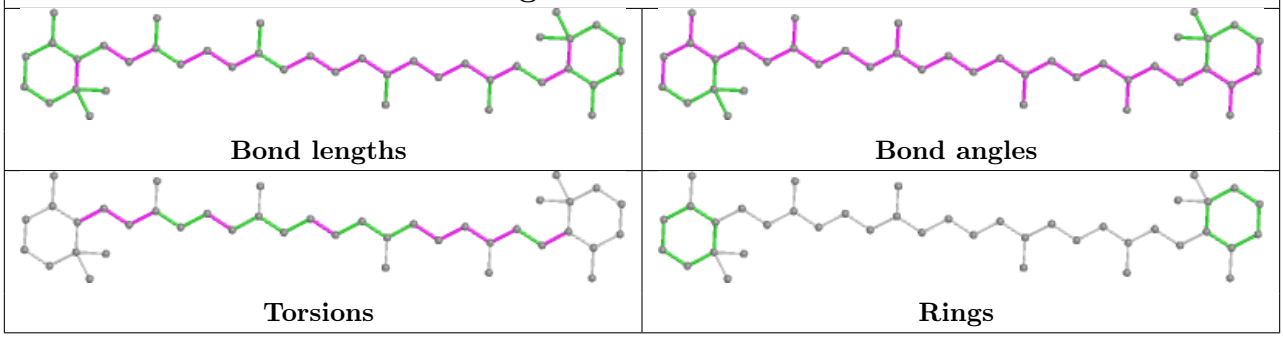
Ligand PQ9 A 1043



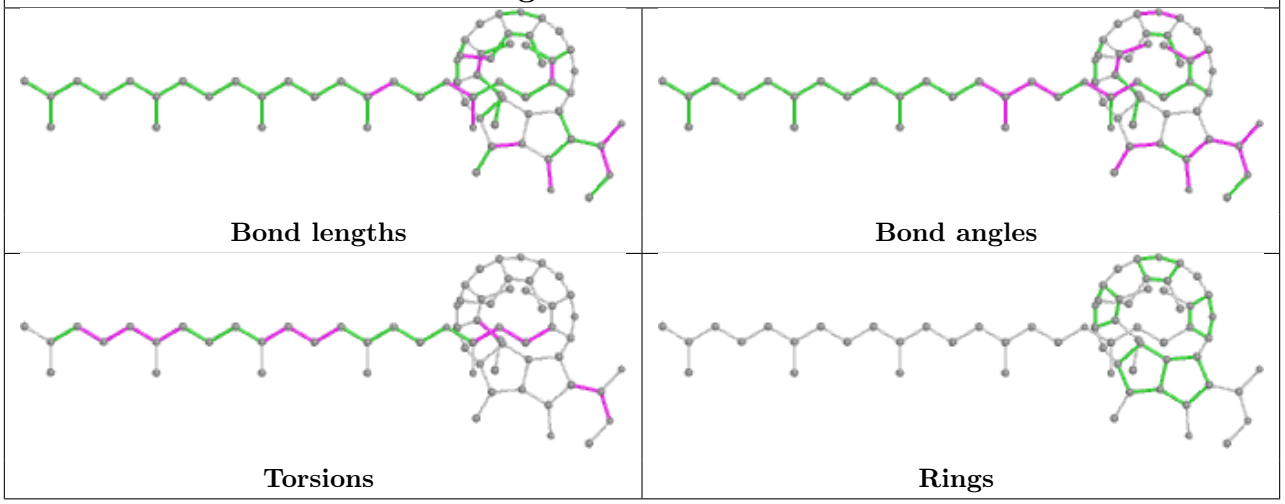
Ligand MGE D 1062



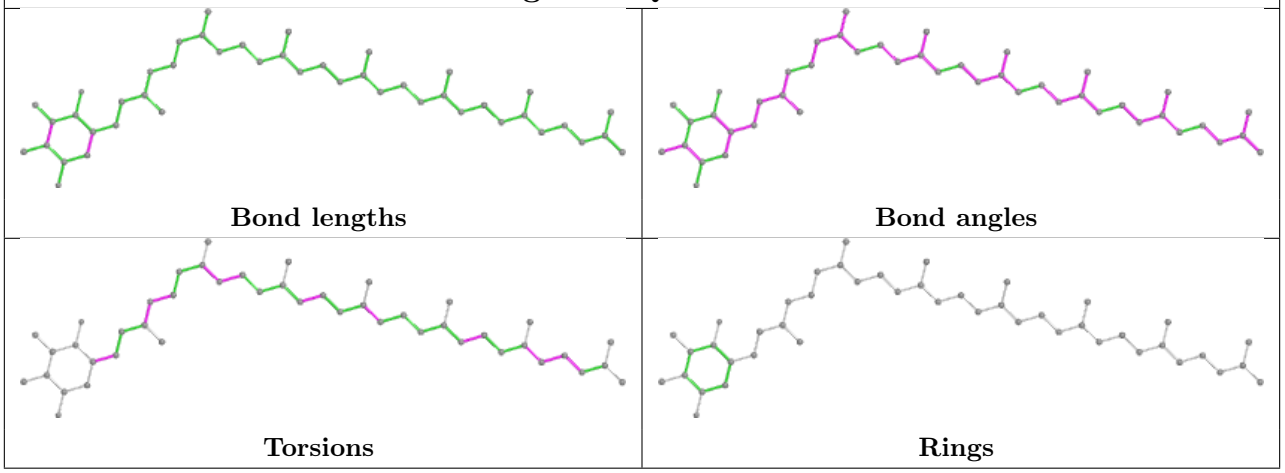
Ligand BCR z 6053



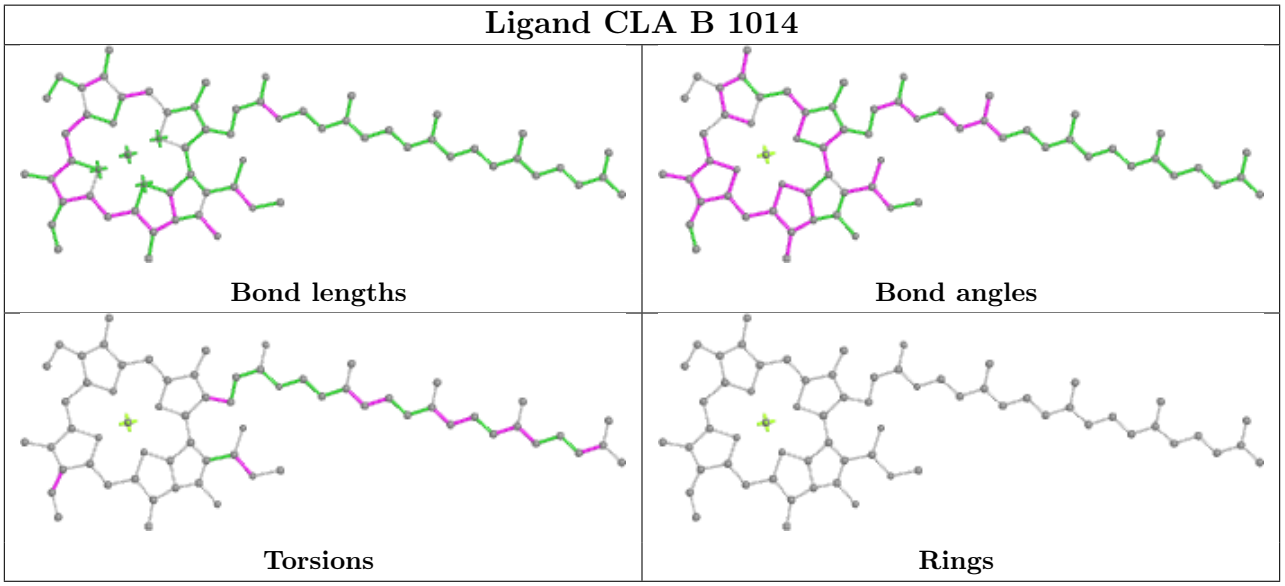
Ligand PHO a 6038



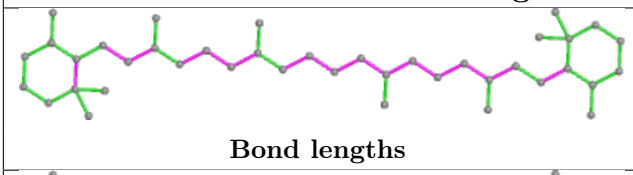
Ligand PQ9 a 6043

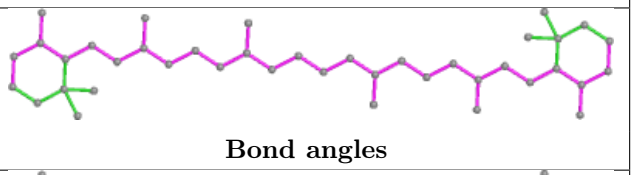


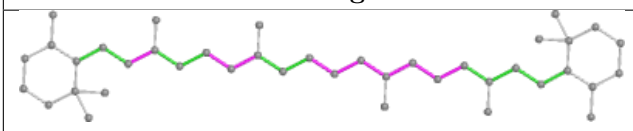
Ligand CLA B 1014

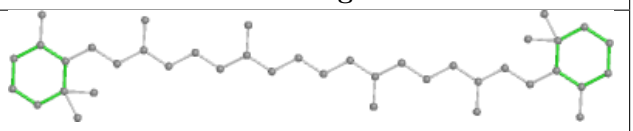


Ligand BCR H 1049

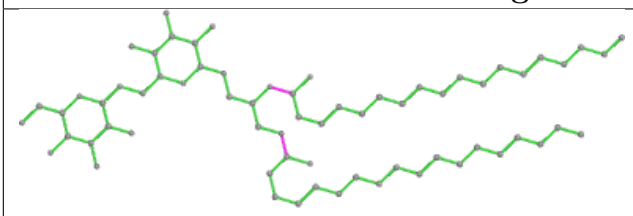

Bond lengths

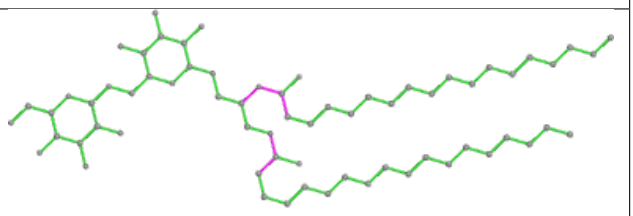

Bond angles

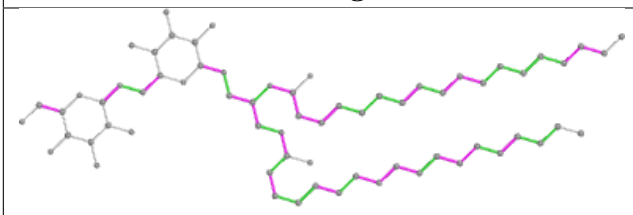

Torsions

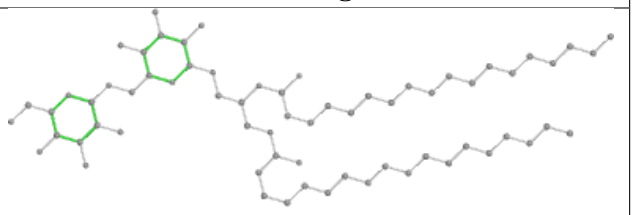

Rings

Ligand DGD B 1058

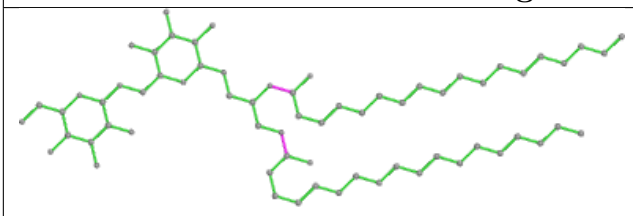

Bond lengths

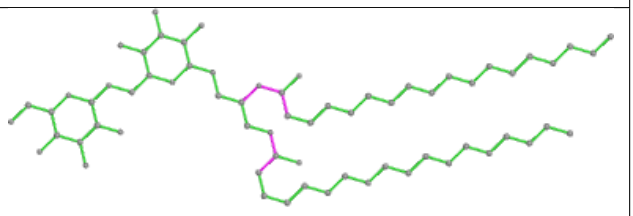

Bond angles

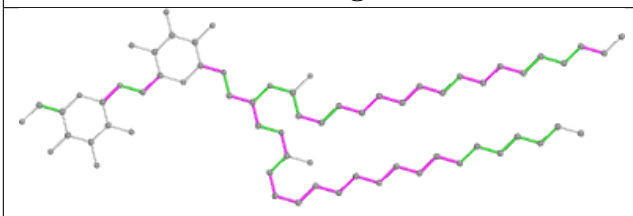

Torsions

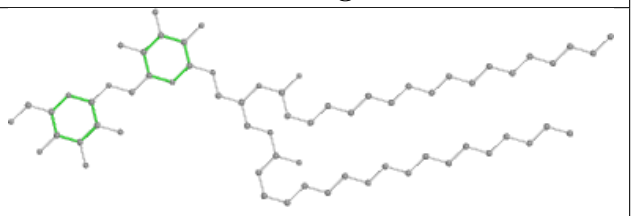

Rings

Ligand DGD c 6057

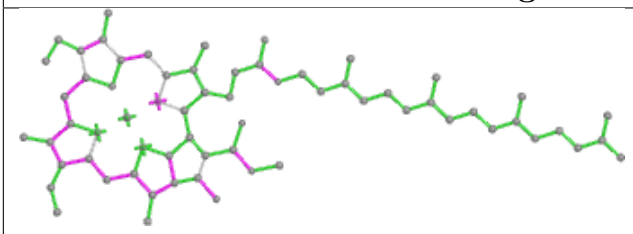

Bond lengths


Bond angles

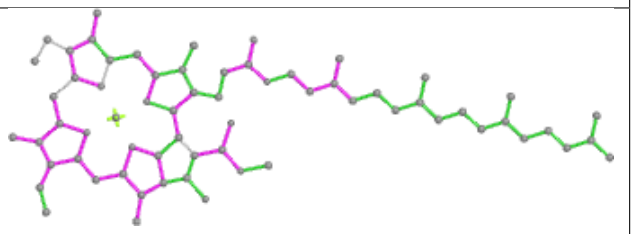

Torsions


Rings

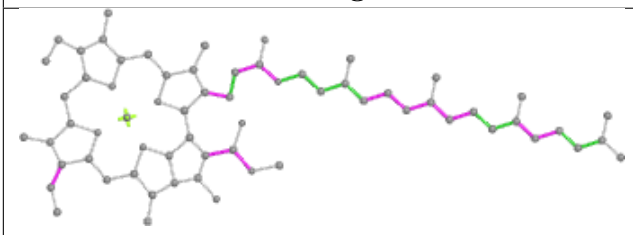
Ligand CLA b 6009



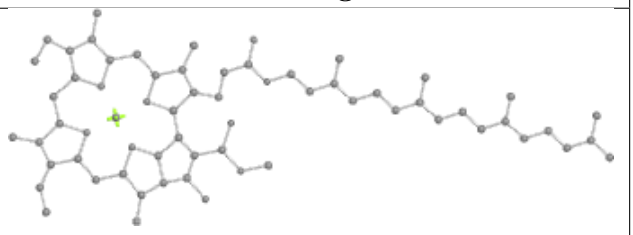
Bond lengths



Bond angles

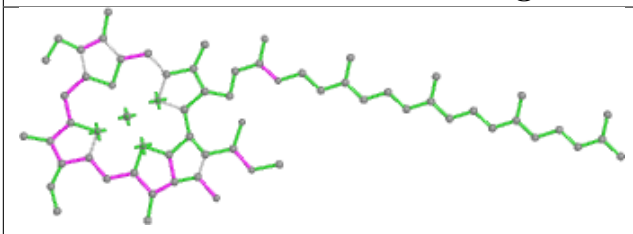


Torsions

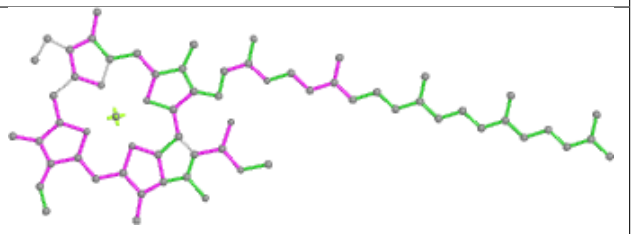


Rings

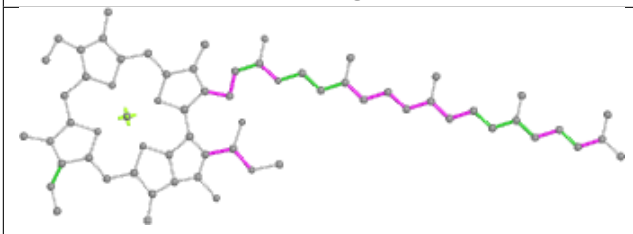
Ligand CLA B 1015



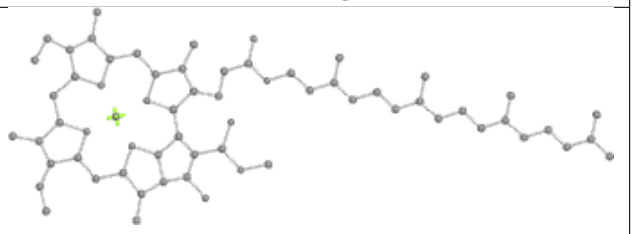
Bond lengths



Bond angles

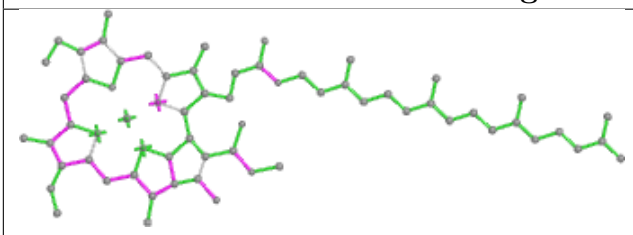


Torsions

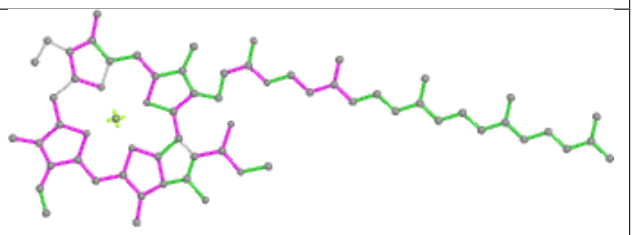


Rings

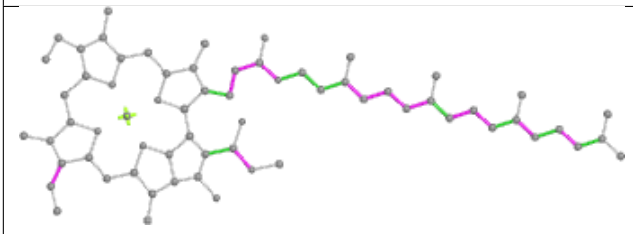
Ligand CLA c 6027



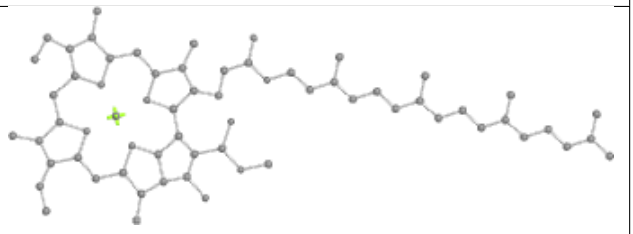
Bond lengths



Bond angles

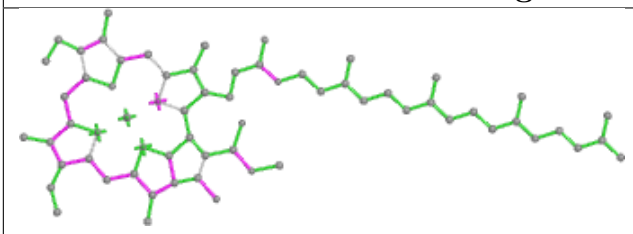


Torsions

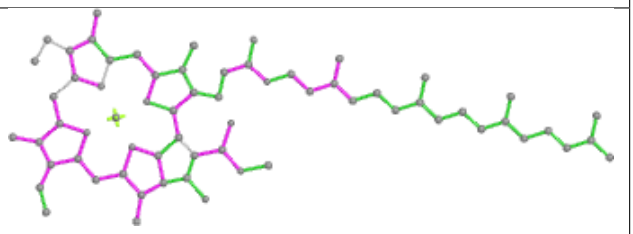


Rings

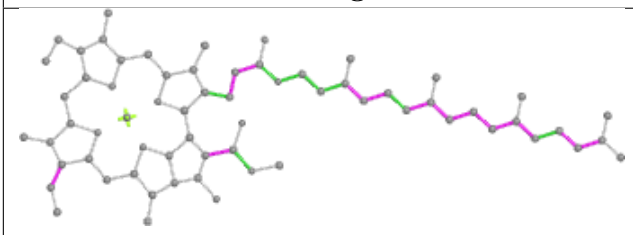
Ligand CLA B 1018



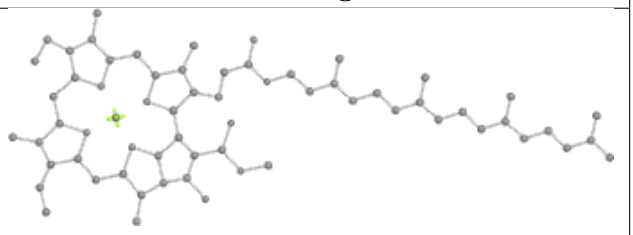
Bond lengths



Bond angles

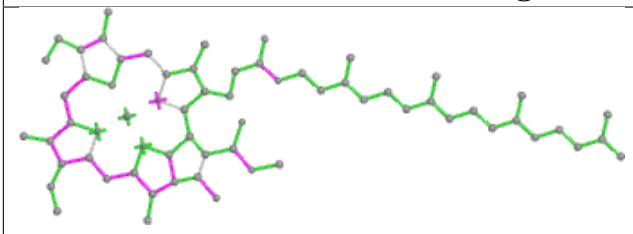


Torsions

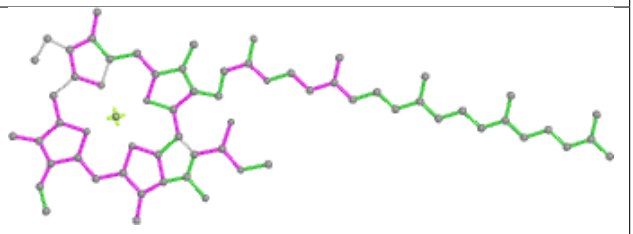


Rings

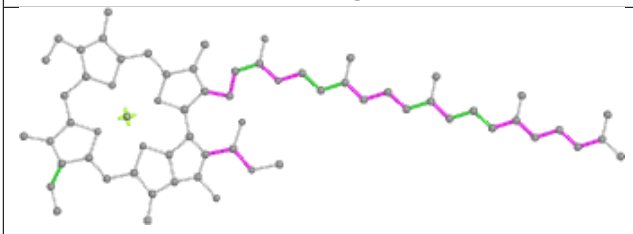
Ligand CLA C 1028



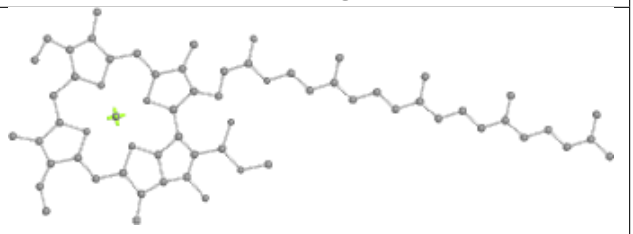
Bond lengths



Bond angles

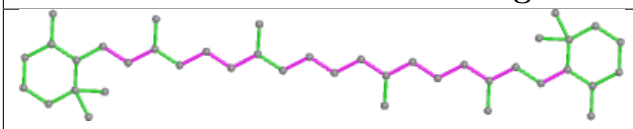


Torsions

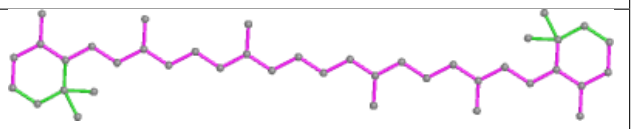


Rings

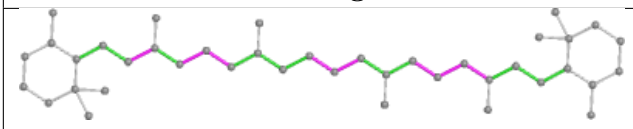
Ligand BCR B 1048



Bond lengths



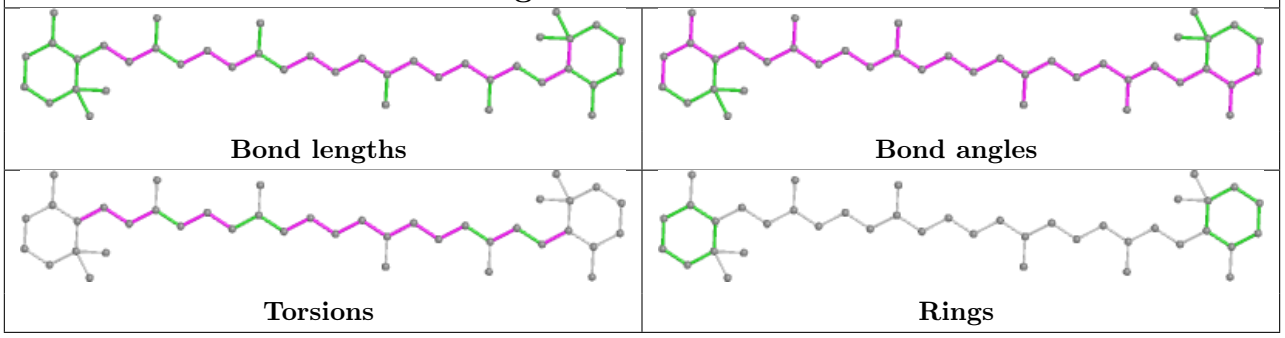
Bond angles



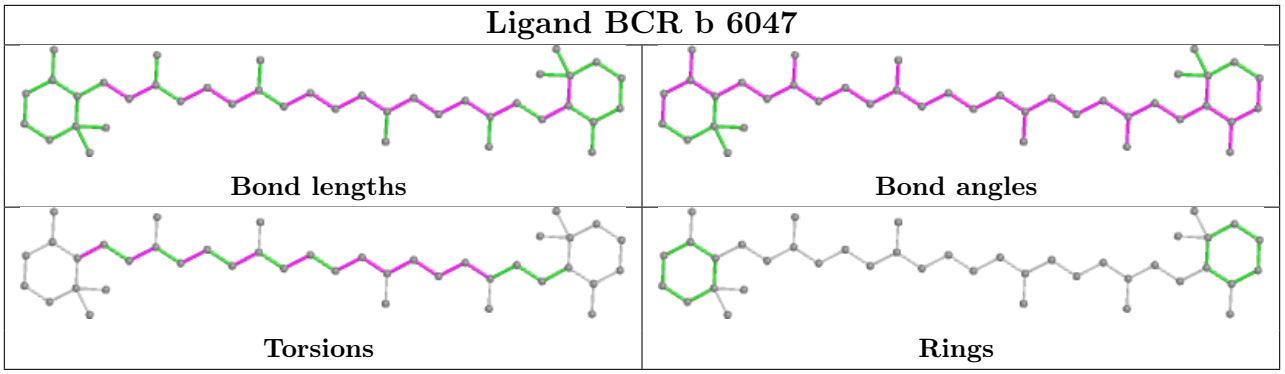
Torsions

Rings

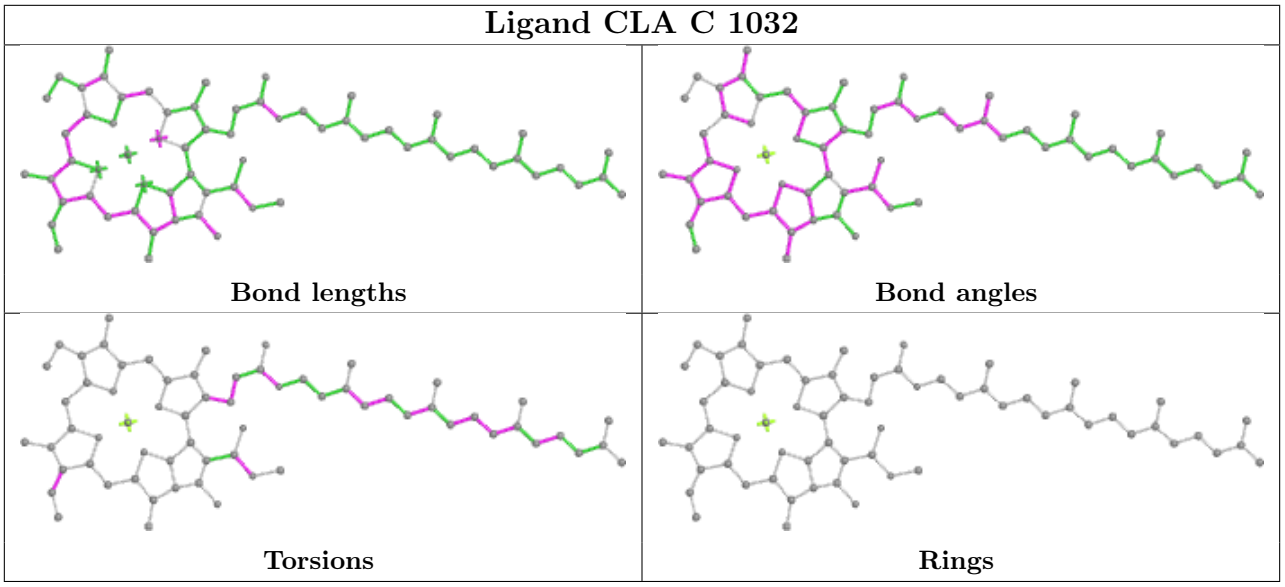
Ligand BCR B 1045



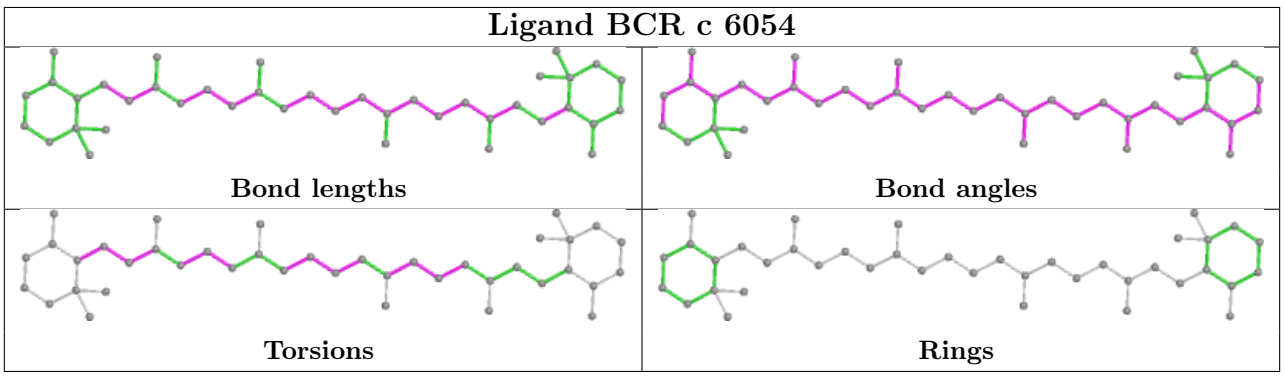
Ligand BCR b 6047



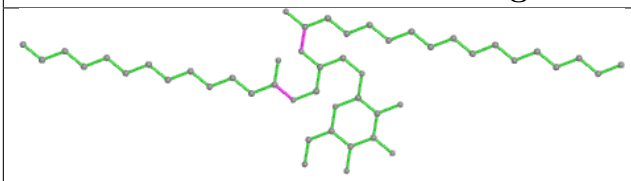
Ligand CLA C 1032



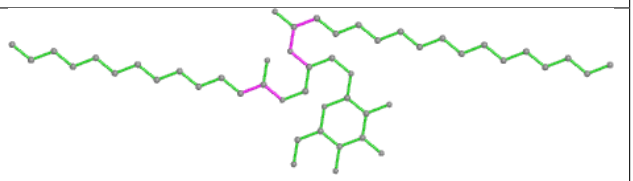
Ligand BCR c 6054



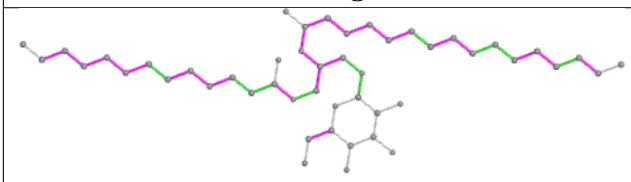
Ligand MGE B 1060



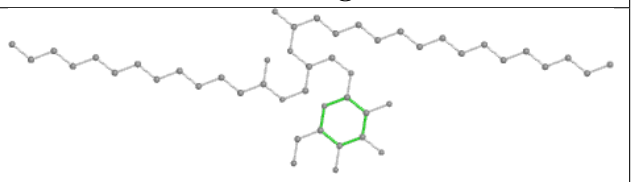
Bond lengths



Bond angles

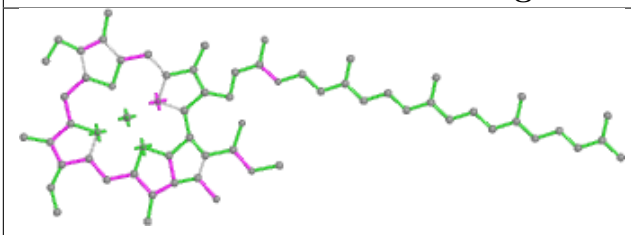


Torsions

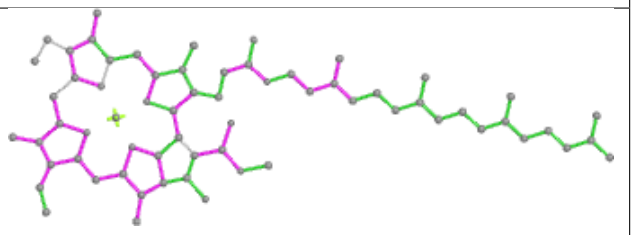


Rings

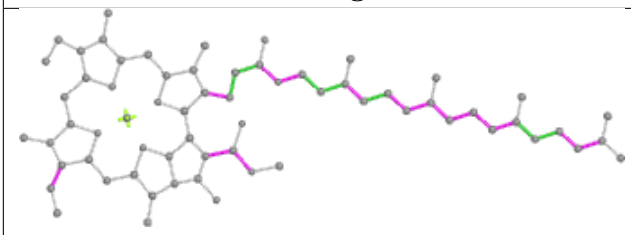
Ligand CLA A 1007



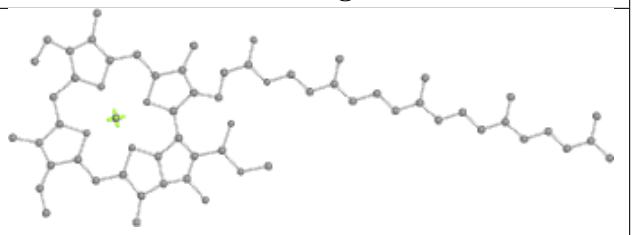
Bond lengths



Bond angles

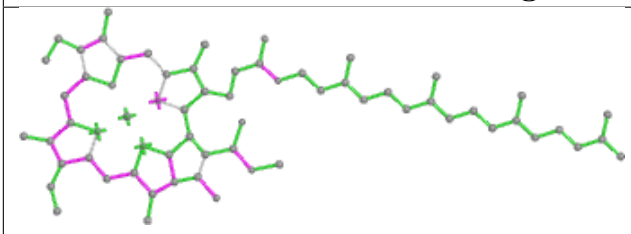


Torsions

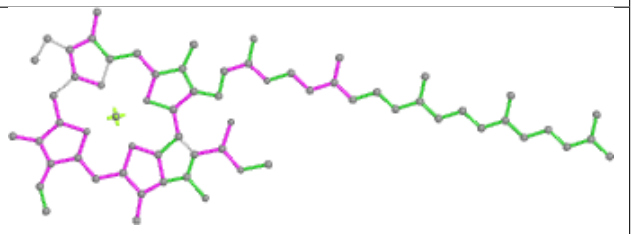


Rings

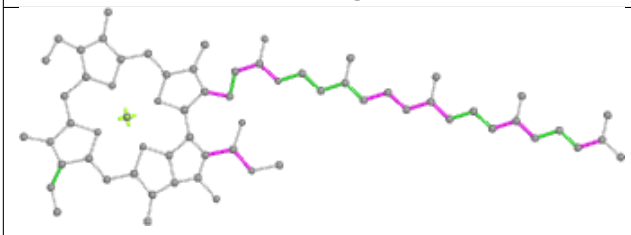
Ligand CLA c 6025



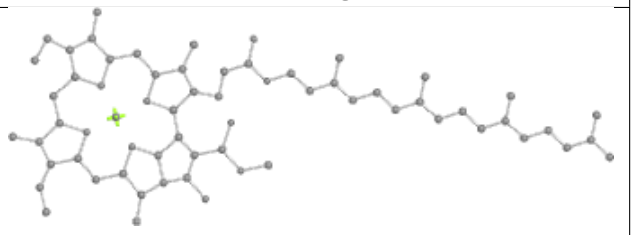
Bond lengths



Bond angles

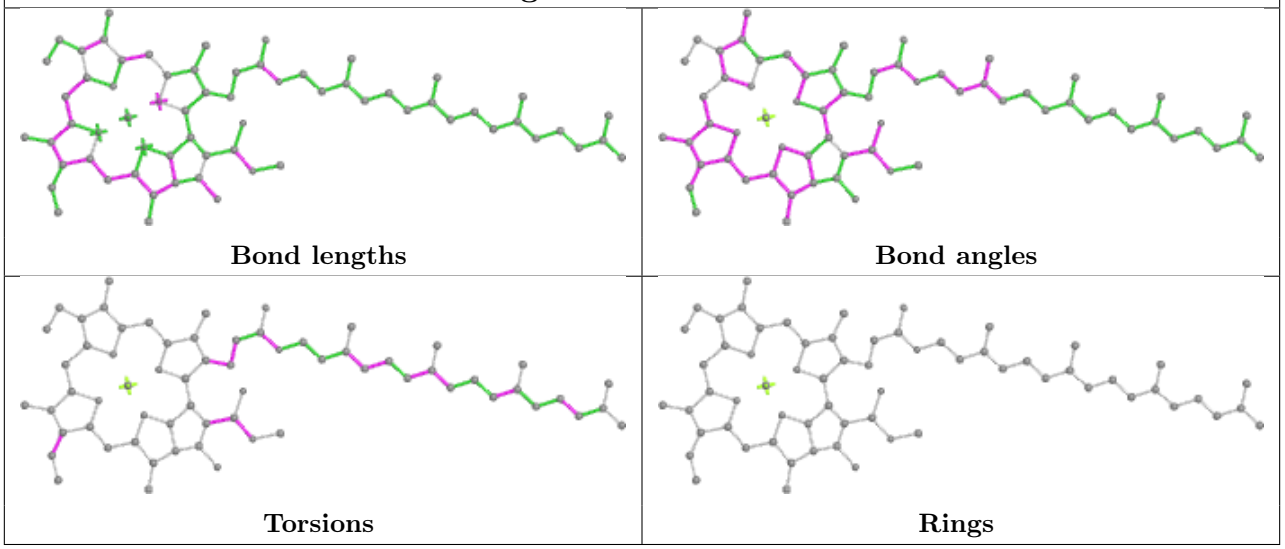


Torsions

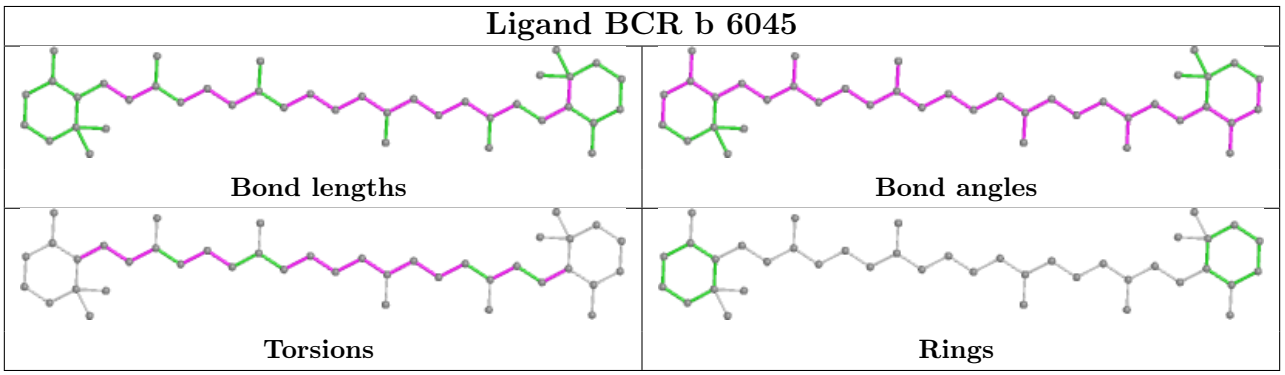


Rings

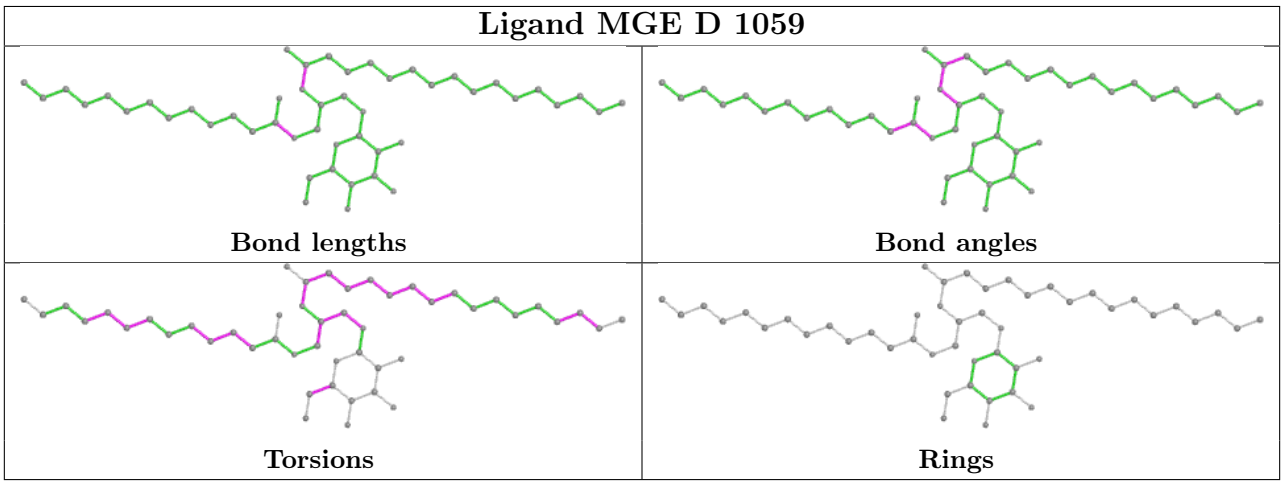
Ligand CLA a 6006



Ligand BCR b 6045



Ligand MGE D 1059



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/344 (97%)	-0.57	0 100 100	135, 156, 186, 200	0
1	a	335/344 (97%)	-0.63	1 (0%) 94 90	135, 156, 186, 200	0
2	B	488/488 (100%)	-0.57	0 100 100	133, 156, 180, 191	0
2	b	488/488 (100%)	-0.55	1 (0%) 95 93	133, 156, 180, 191	0
3	C	447/447 (100%)	-0.56	2 (0%) 92 87	138, 165, 181, 193	0
3	c	447/447 (100%)	-0.44	1 (0%) 95 93	138, 165, 181, 193	0
4	D	340/340 (100%)	-0.60	3 (0%) 84 77	134, 156, 179, 192	0
4	d	340/340 (100%)	-0.61	0 100 100	134, 156, 179, 192	0
5	E	82/83 (98%)	-0.50	0 100 100	153, 172, 191, 198	0
5	e	82/83 (98%)	-0.33	3 (3%) 41 32	153, 172, 191, 198	0
6	F	35/44 (79%)	-0.43	0 100 100	153, 167, 187, 191	0
6	f	35/44 (79%)	-0.37	2 (5%) 23 20	153, 167, 187, 191	0
7	H	64/64 (100%)	-0.49	0 100 100	154, 163, 175, 185	0
7	h	64/64 (100%)	-0.34	1 (1%) 72 62	154, 163, 175, 185	0
8	I	35/35 (100%)	-0.14	1 (2%) 51 41	152, 169, 196, 201	0
8	i	35/35 (100%)	-0.09	0 100 100	152, 169, 196, 201	0
9	J	34/40 (85%)	-0.66	0 100 100	155, 162, 184, 192	0
9	j	34/40 (85%)	-0.66	0 100 100	155, 162, 184, 192	0
10	K	36/36 (100%)	-0.67	0 100 100	144, 168, 182, 185	0
10	k	36/36 (100%)	-0.53	0 100 100	156, 170, 182, 192	0
11	L	37/37 (100%)	-0.43	0 100 100	138, 160, 191, 197	0
11	l	37/37 (100%)	-0.30	1 (2%) 54 44	138, 160, 191, 197	0
12	M	36/36 (100%)	-0.36	1 (2%) 53 42	131, 146, 188, 194	0
12	m	36/36 (100%)	-0.57	0 100 100	131, 146, 188, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	242/242 (100%)	-0.46	1 (0%) 92 87	139, 160, 181, 187	0
13	o	242/242 (100%)	-0.46	2 (0%) 86 79	139, 160, 181, 187	0
14	T	30/30 (100%)	-0.67	0 100 100	124, 143, 186, 191	0
14	t	30/30 (100%)	-0.79	0 100 100	131, 143, 186, 191	0
15	U	98/98 (100%)	-0.58	0 100 100	139, 155, 165, 173	0
15	u	98/98 (100%)	-0.63	1 (1%) 82 74	139, 155, 165, 173	0
16	V	137/137 (100%)	-0.54	0 100 100	144, 162, 173, 178	0
16	v	137/137 (100%)	-0.56	0 100 100	144, 162, 173, 178	0
17	X	34/34 (100%)	-0.77	0 100 100	173, 181, 198, 201	0
17	x	34/34 (100%)	-0.48	1 (2%) 51 41	173, 181, 198, 201	0
18	Y	28/28 (100%)	0.06	0 100 100	187, 199, 208, 210	0
18	y	28/28 (100%)	-0.30	0 100 100	187, 199, 208, 210	0
19	N	0/23	-	-	-	-
19	n	0/23	-	-	-	-
20	Z	62/62 (100%)	-0.56	1 (1%) 72 62	159, 173, 188, 196	0
20	z	62/62 (100%)	-0.38	2 (3%) 47 37	159, 173, 188, 196	0
All	All	5200/5296 (98%)	-0.53	25 (0%) 91 85	124, 161, 185, 210	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	45	LEU	6.6
3	C	44	ASN	5.2
4	D	228	GLY	3.3
5	e	5006	GLY	3.1
13	o	5233	ARG	3.1

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
26	LHG	A	1063	49/49	0.52	0.60	199,213,216,216	0
25	BCR	k	6052	40/40	0.58	0.41	191,195,202,203	0
26	LHG	a	6063	49/49	0.58	0.52	199,213,216,216	0
27	IOD	B	1067	1/1	0.59	0.51	198,198,198,198	0
25	BCR	Z	1053	40/40	0.60	0.60	190,214,216,216	0
25	BCR	z	6053	40/40	0.64	0.53	190,214,216,216	0
22	CLA	c	6037	65/65	0.64	0.55	201,211,214,216	0
22	CLA	K	1034	65/65	0.65	0.47	138,189,216,216	0
22	CLA	C	1027	65/65	0.65	0.50	192,198,204,216	0
27	IOD	T	1066	1/1	0.65	0.23	199,199,199,199	0
22	CLA	a	6007	65/65	0.66	0.49	129,174,204,205	0
28	MGE	d	6059	48/48	0.66	0.47	179,190,215,216	0
22	CLA	c	6027	65/65	0.67	0.51	192,198,204,216	0
25	BCR	K	1051	40/40	0.67	0.46	192,202,210,210	0
28	MGE	d	6062	48/48	0.67	0.42	187,202,208,210	0
24	PQ9	d	6042	45/45	0.68	0.43	171,173,185,187	0
25	BCR	C	1054	40/40	0.69	0.43	197,201,216,216	0
28	MGE	B	1060	48/48	0.69	0.50	186,199,213,216	0
22	CLA	k	6034	65/65	0.69	0.43	138,189,216,216	0
27	IOD	D	1068	1/1	0.69	1.29	198,198,198,198	0
25	BCR	T	6046	40/40	0.70	0.51	179,185,188,189	0
25	BCR	c	6054	40/40	0.70	0.41	197,201,216,216	0
25	BCR	k	6051	40/40	0.71	0.42	192,202,210,210	0
22	CLA	d	6008	65/65	0.71	0.47	184,188,216,216	0
22	CLA	C	1037	65/65	0.71	0.49	201,211,214,216	0
28	MGE	D	1059	48/48	0.71	0.41	179,190,215,216	0
25	BCR	h	6049	40/40	0.71	0.44	177,182,188,189	0
22	CLA	b	6014	65/65	0.71	0.41	178,187,197,216	0
25	BCR	H	1049	40/40	0.72	0.40	177,182,188,189	0
25	BCR	a	6044	40/40	0.72	0.52	155,177,185,185	0
22	CLA	h	6017	65/65	0.72	0.42	169,197,201,208	0
24	PQ9	A	1043	45/45	0.72	0.41	171,172,193,197	30
22	CLA	b	6024	65/65	0.73	0.37	165,193,197,198	0
22	CLA	C	1036	65/65	0.73	0.38	186,190,203,216	0
22	CLA	B	1024	65/65	0.73	0.40	165,193,197,198	0
25	BCR	A	1044	40/40	0.73	0.61	155,177,185,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	6009	65/65	0.73	0.44	143,192,213,213	0
22	CLA	D	1008	65/65	0.73	0.45	184,188,216,216	0
28	MGE	D	1062	48/48	0.74	0.37	187,202,208,210	0
28	MGE	L	1061	48/48	0.74	0.46	177,191,195,199	0
22	CLA	A	1007	65/65	0.74	0.45	129,174,204,205	0
25	BCR	T	6048	40/40	0.74	0.65	179,184,203,204	0
29	DGD	C	1056	66/66	0.74	0.38	190,201,216,216	0
29	DGD	c	6055	66/66	0.74	0.41	184,192,202,203	0
25	BCR	B	1048	40/40	0.75	0.58	179,184,203,204	0
25	BCR	b	6045	40/40	0.75	0.49	163,196,216,216	0
28	MGE	b	6060	48/48	0.76	0.41	186,199,213,216	0
24	PQ9	a	6043	45/45	0.76	0.38	171,172,193,197	30
22	CLA	B	1014	65/65	0.76	0.37	178,187,197,216	0
25	BCR	t	1046	40/40	0.76	0.41	179,185,188,189	0
27	IOD	d	6068	1/1	0.76	0.61	199,199,199,199	0
29	DGD	c	6056	66/66	0.76	0.42	190,201,216,216	0
22	CLA	c	6035	65/65	0.77	0.42	189,202,210,216	0
25	BCR	C	1052	40/40	0.77	0.27	191,195,202,203	0
28	MGE	l	6061	48/48	0.77	0.39	177,191,195,199	0
25	BCR	b	6047	40/40	0.77	0.43	155,171,200,202	0
22	CLA	c	6036	65/65	0.77	0.37	186,190,203,216	0
25	BCR	B	1045	40/40	0.77	0.51	163,196,216,216	0
29	DGD	c	6057	66/66	0.78	0.36	177,190,206,207	0
25	BCR	d	6050	40/40	0.79	0.47	184,193,198,199	0
22	CLA	c	6031	65/65	0.79	0.41	181,185,202,216	0
22	CLA	C	1030	65/65	0.79	0.34	185,197,216,216	0
22	CLA	H	1017	65/65	0.79	0.35	169,197,201,208	0
29	DGD	C	1055	66/66	0.80	0.35	184,192,202,203	0
22	CLA	c	6030	65/65	0.80	0.29	185,197,216,216	0
25	BCR	B	1047	40/40	0.80	0.35	155,171,200,202	0
25	BCR	D	1050	40/40	0.80	0.49	184,193,198,199	0
22	CLA	B	1009	65/65	0.80	0.35	143,192,213,213	0
30	FE2	a	6002	1/1	0.80	0.23	148,148,148,148	0
24	PQ9	D	1042	45/45	0.81	0.32	171,173,185,187	0
23	PHO	D	1039	64/64	0.81	0.33	184,187,196,198	0
22	CLA	C	1032	65/65	0.81	0.37	184,188,192,216	0
29	DGD	b	6058	66/66	0.82	0.32	175,188,196,203	0
22	CLA	b	6015	65/65	0.82	0.31	177,182,185,216	0
22	CLA	c	6032	65/65	0.82	0.34	186,189,200,216	0
22	CLA	C	1035	65/65	0.82	0.36	189,202,210,216	0
29	DGD	C	1057	66/66	0.82	0.33	177,190,206,207	0
22	CLA	C	1031	65/65	0.83	0.33	181,185,202,216	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	d	6005	65/65	0.83	0.33	135,162,169,173	0
22	CLA	D	1005	65/65	0.83	0.35	135,162,169,173	0
31	HEM	F	1040	43/43	0.83	0.37	186,215,216,216	0
22	CLA	c	6033	65/65	0.84	0.33	138,185,199,200	0
22	CLA	A	1006	65/65	0.84	0.33	166,181,211,213	0
27	IOD	b	6067	1/1	0.84	0.51	199,199,199,199	0
22	CLA	b	6021	65/65	0.85	0.30	154,164,172,176	0
22	CLA	B	1010	65/65	0.85	0.29	160,183,186,189	0
22	CLA	c	6026	65/65	0.85	0.34	138,171,178,183	0
22	CLA	b	6012	65/65	0.85	0.33	160,167,172,174	0
23	PHO	a	6038	64/64	0.85	0.35	166,176,178,181	0
31	HEM	f	6040	43/43	0.85	0.36	186,215,216,216	0
22	CLA	B	1018	65/65	0.86	0.30	172,186,191,192	0
22	CLA	b	6011	65/65	0.86	0.31	168,178,184,188	0
23	PHO	A	1038	64/64	0.86	0.31	166,176,178,181	0
22	CLA	C	1026	65/65	0.86	0.28	138,171,178,183	0
22	CLA	c	6029	65/65	0.87	0.36	177,187,190,201	0
22	CLA	c	6025	65/65	0.87	0.26	156,187,191,194	0
22	CLA	b	6023	65/65	0.87	0.28	174,179,181,191	0
22	CLA	B	1012	65/65	0.87	0.28	160,167,172,174	0
29	DGD	B	1058	66/66	0.87	0.29	175,188,196,203	0
22	CLA	B	1021	65/65	0.88	0.25	154,164,172,176	0
22	CLA	B	1023	65/65	0.88	0.25	174,179,181,191	0
22	CLA	C	1028	65/65	0.88	0.29	178,182,201,202	0
23	PHO	d	6039	64/64	0.88	0.24	184,187,196,198	0
22	CLA	b	6018	65/65	0.88	0.28	172,186,191,192	0
22	CLA	B	1019	65/65	0.88	0.31	167,172,175,180	0
22	CLA	c	6028	65/65	0.88	0.27	178,182,201,202	0
22	CLA	a	6006	65/65	0.89	0.24	166,181,211,213	0
22	CLA	b	6019	65/65	0.89	0.25	167,172,175,180	0
22	CLA	B	1011	65/65	0.89	0.25	168,178,184,188	0
22	CLA	C	1025	65/65	0.89	0.27	156,187,191,194	0
22	CLA	b	6010	65/65	0.89	0.26	160,183,186,189	0
22	CLA	C	1033	65/65	0.89	0.32	138,185,199,200	0
22	CLA	C	1029	65/65	0.89	0.31	177,187,190,201	0
22	CLA	b	6013	65/65	0.89	0.29	146,173,183,184	0
22	CLA	B	1015	65/65	0.89	0.27	177,182,185,216	0
22	CLA	a	6003	65/65	0.89	0.29	160,169,175,212	0
22	CLA	b	6016	65/65	0.89	0.29	130,172,175,180	0
22	CLA	A	1003	65/65	0.90	0.25	160,169,175,212	0
22	CLA	b	6022	65/65	0.90	0.25	138,180,198,200	0
22	CLA	D	1004	65/65	0.91	0.27	130,168,179,181	0

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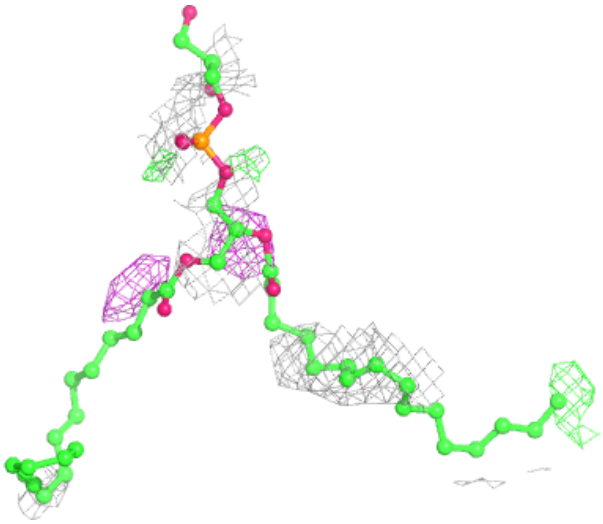
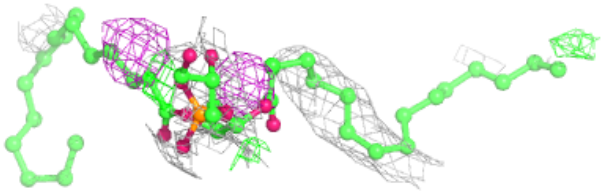
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	B	1022	65/65	0.91	0.22	138,180,198,200	0
22	CLA	B	1013	65/65	0.91	0.23	146,173,183,184	0
22	CLA	d	6004	65/65	0.92	0.24	130,168,179,181	0
22	CLA	b	6020	65/65	0.92	0.24	167,175,180,197	0
30	FE2	D	1002	1/1	0.93	0.17	148,148,148,148	0
22	CLA	B	1016	65/65	0.93	0.21	130,172,175,180	0
31	HEM	v	6041	43/43	0.93	0.25	131,181,185,187	0
22	CLA	B	1020	65/65	0.94	0.24	167,175,180,197	0
31	HEM	V	1041	43/43	0.94	0.28	131,181,185,187	0
21	OEC	A	1001	5/9	0.97	0.14	132,148,162,172	0
27	IOD	d	6064	1/1	0.98	0.12	160,160,160,160	0
27	IOD	A	1065	1/1	0.98	0.13	158,158,158,158	0
27	IOD	t	6066	1/1	0.98	0.09	199,199,199,199	0
21	OEC	a	6001	5/9	0.98	0.17	132,148,162,172	0
27	IOD	D	1064	1/1	0.98	0.04	160,160,160,160	0
27	IOD	a	6065	1/1	0.99	0.13	158,158,158,158	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 LHG A 1063:

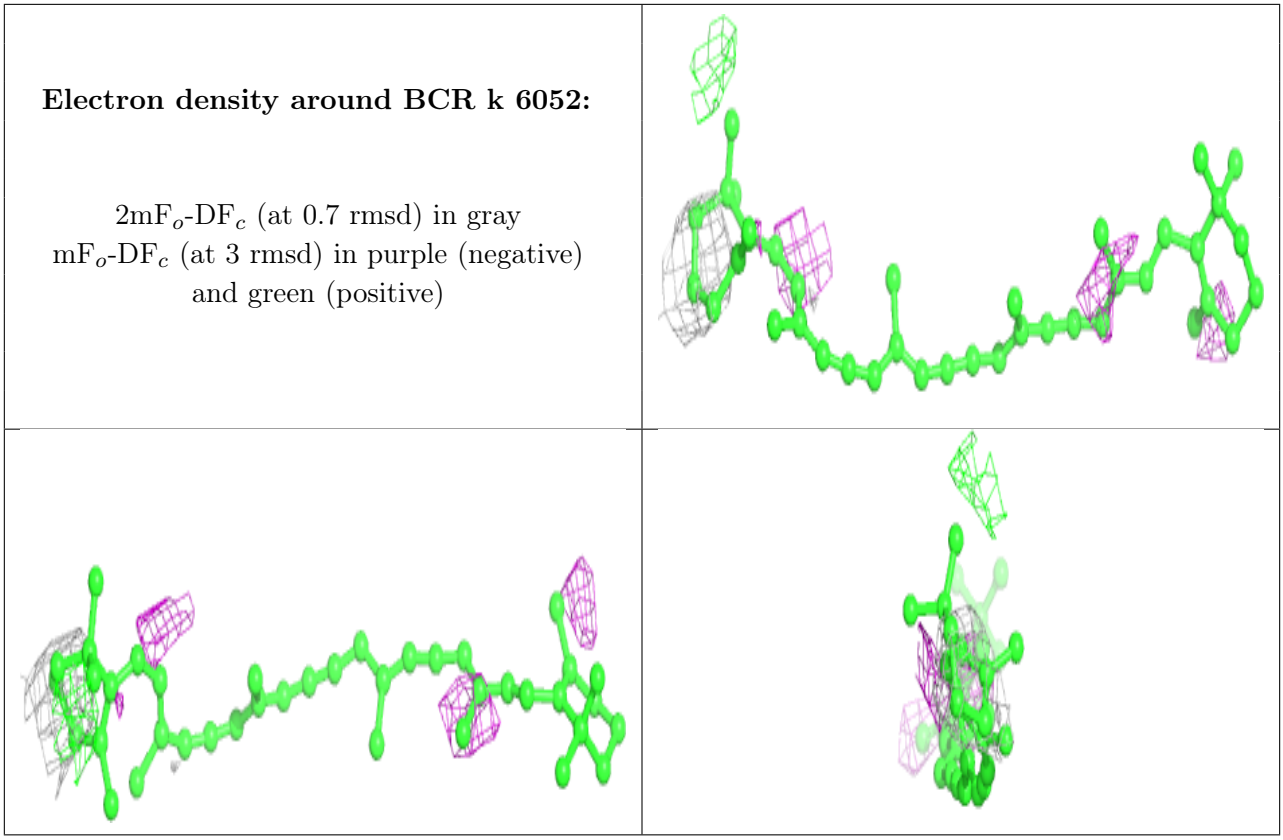
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





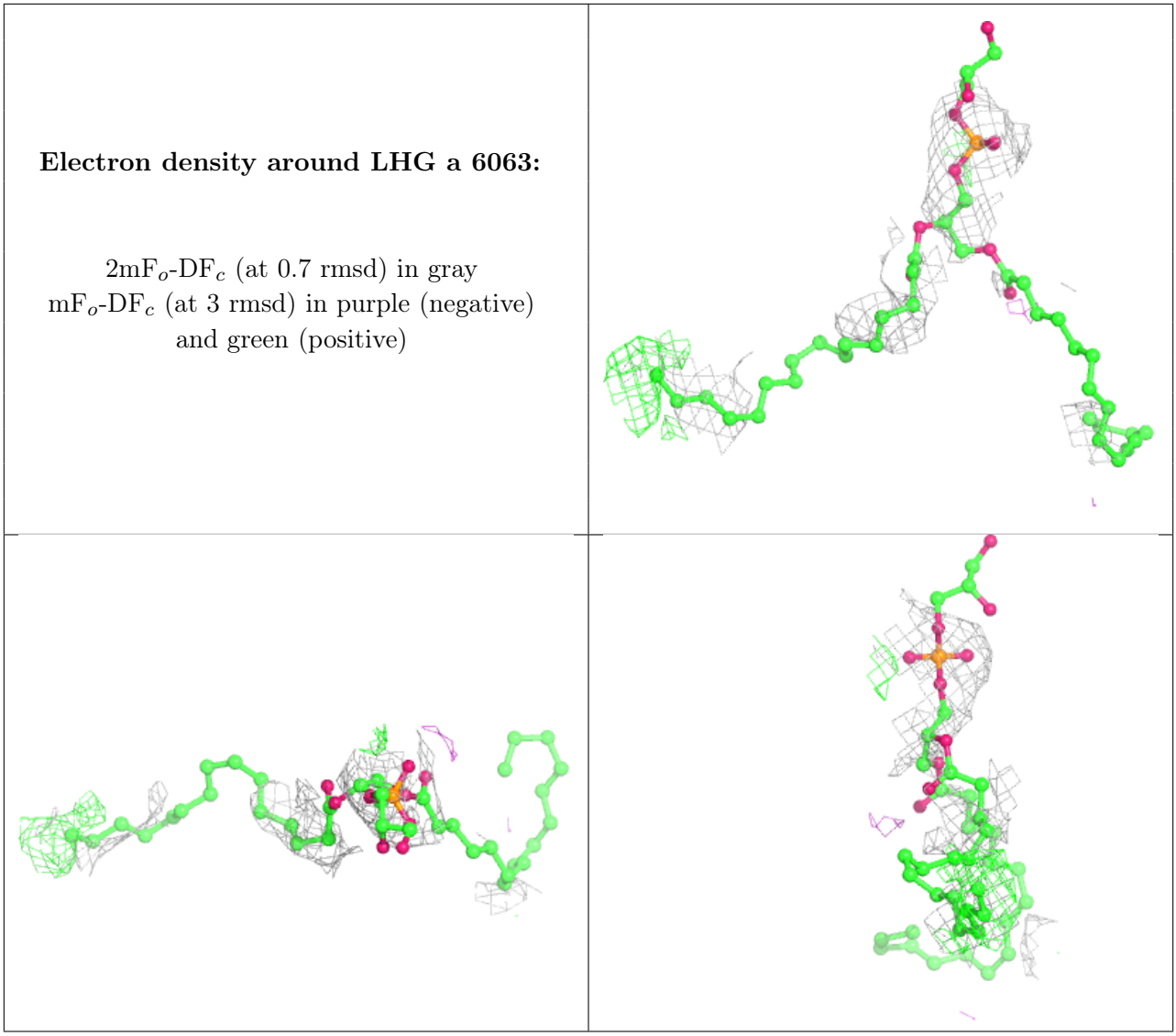
Electron density around BCR k 6052:

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



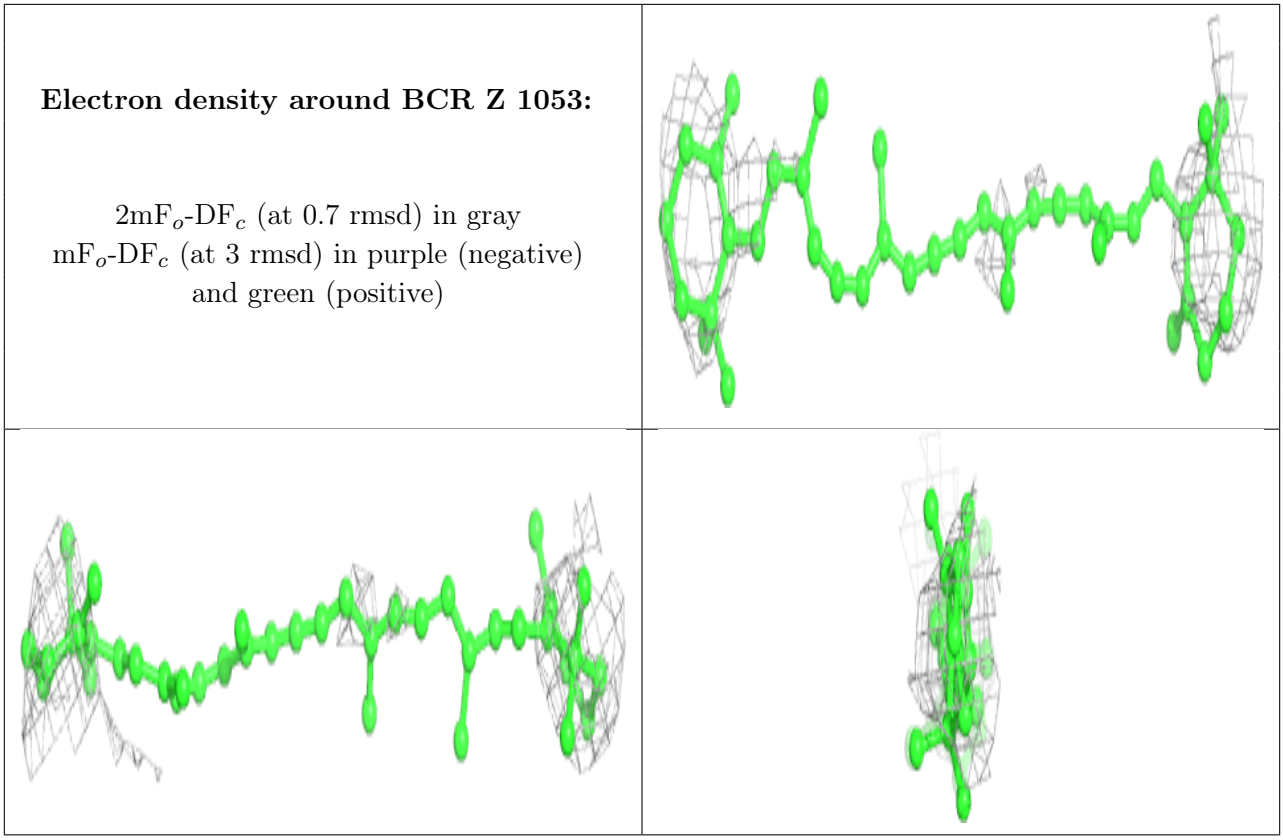
Electron density around LHG a 6063:

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



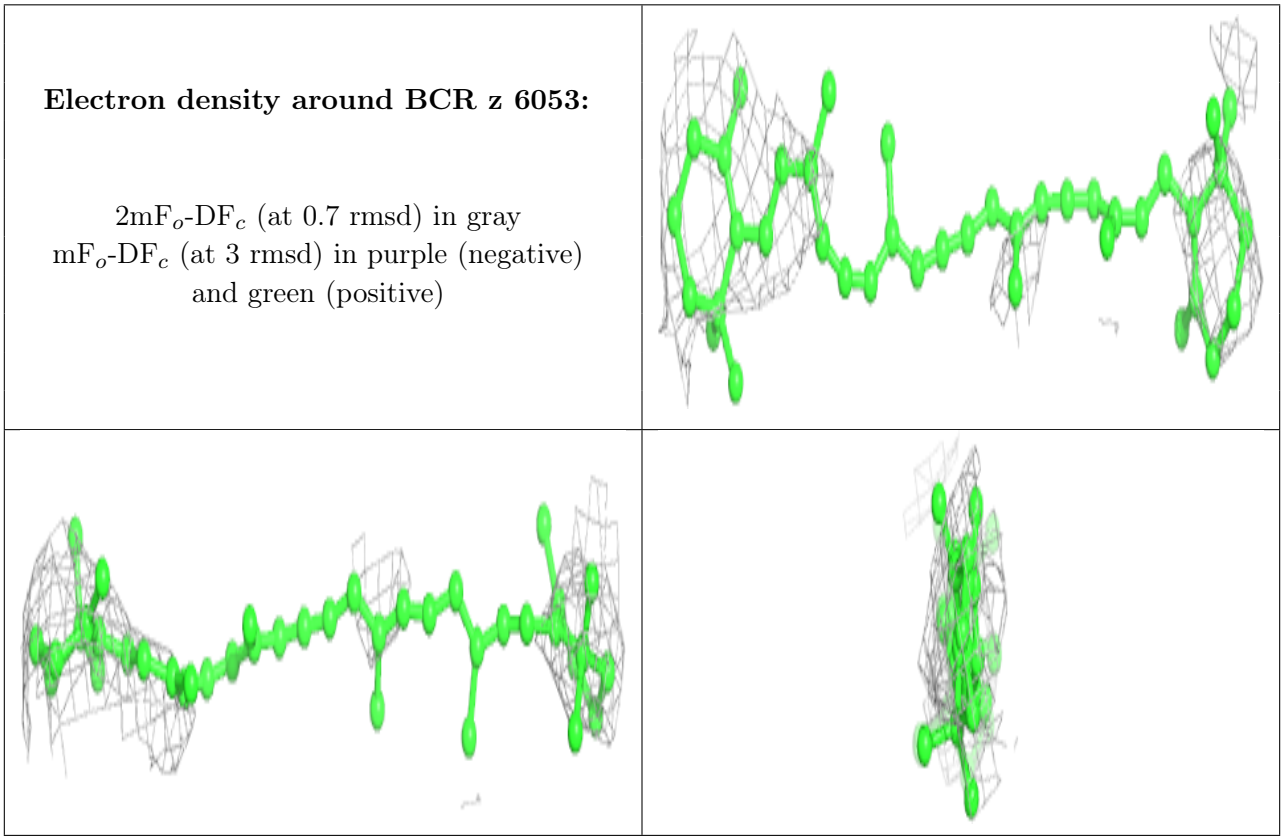
Electron density around BCR Z 1053:

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



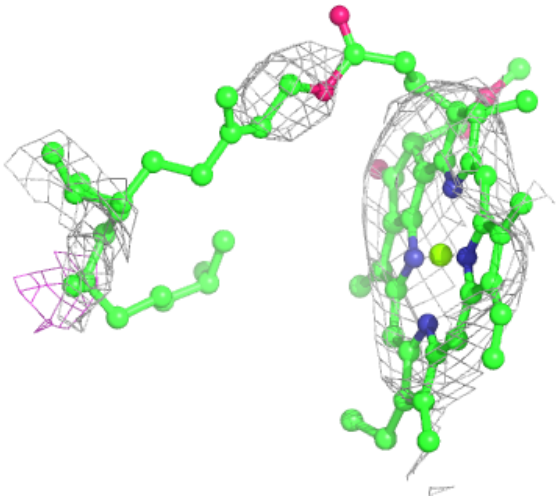
Electron density around BCR z 6053:

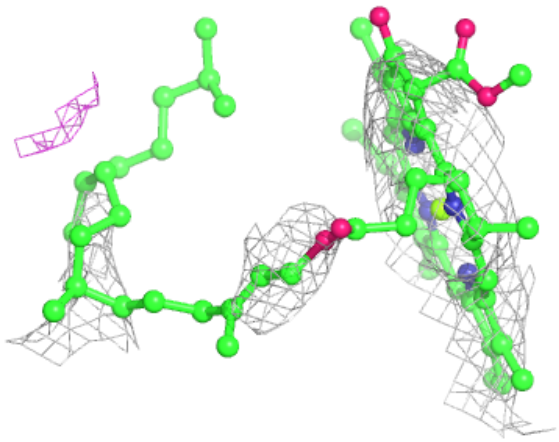
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

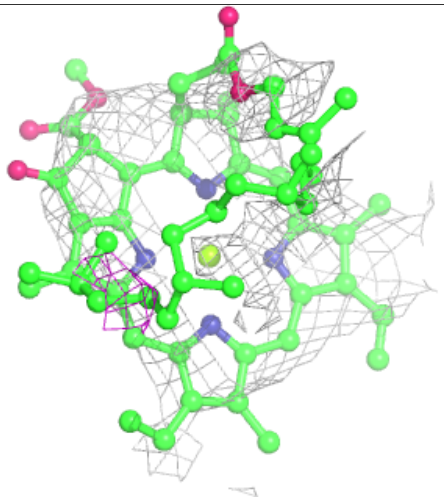


Electron density around CLA c 6037:

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

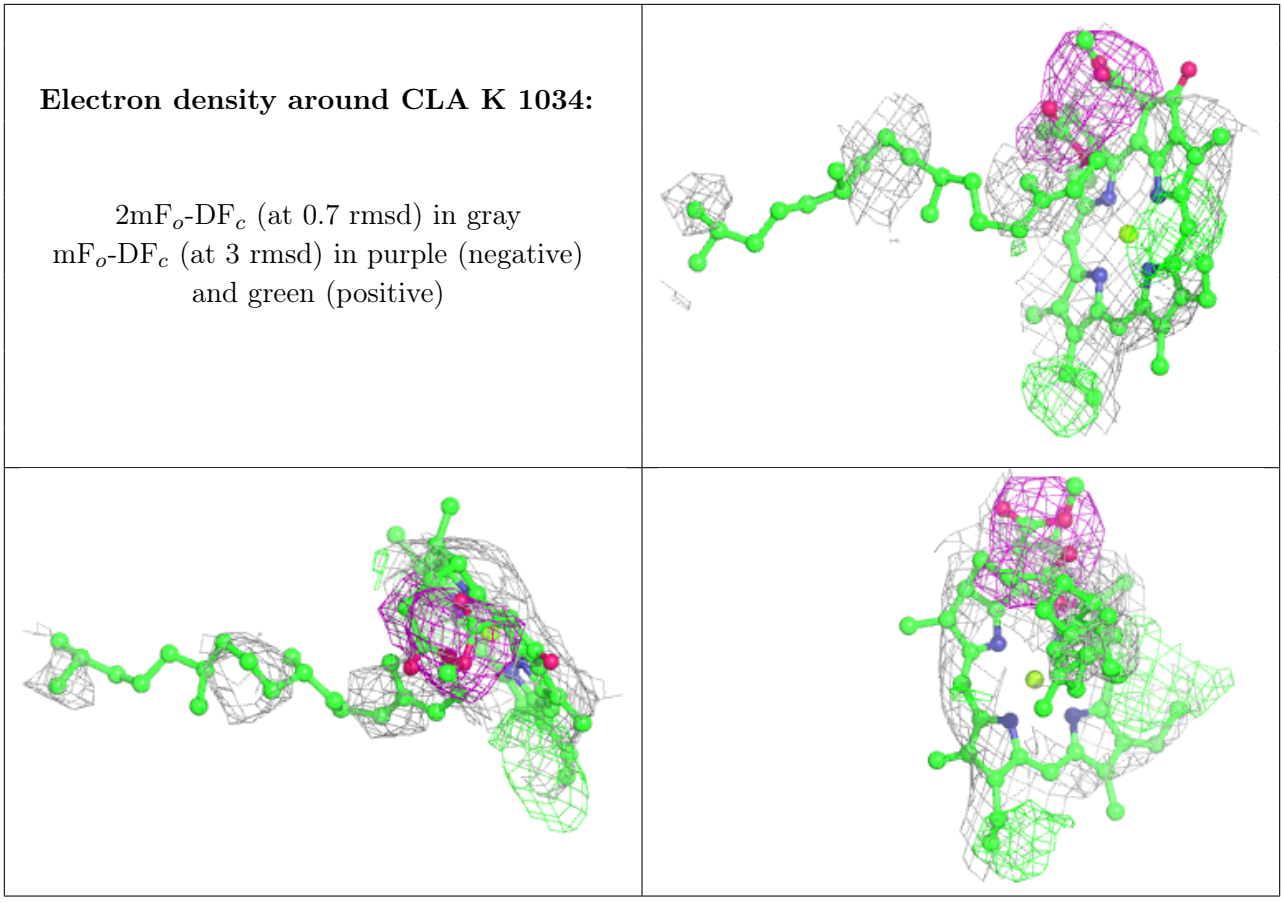






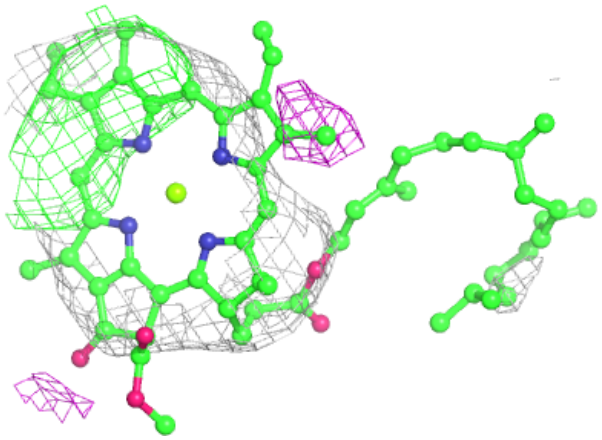
Electron density around CLA K 1034:

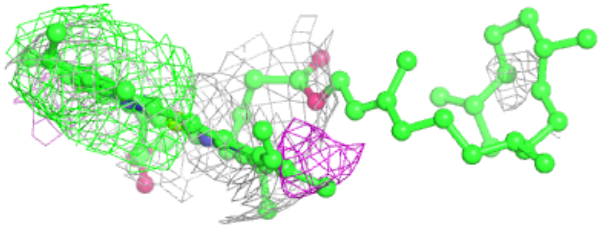
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

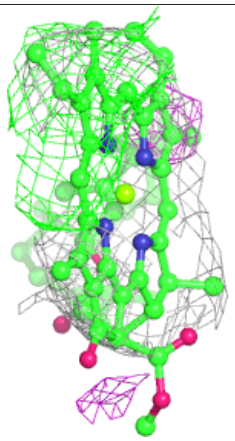


Electron density around CLA C 1027:

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

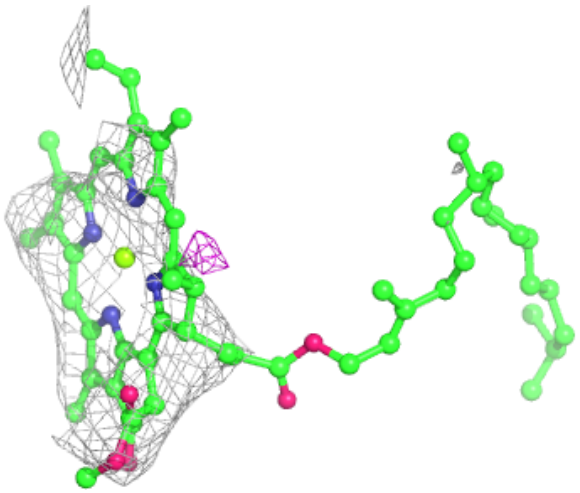


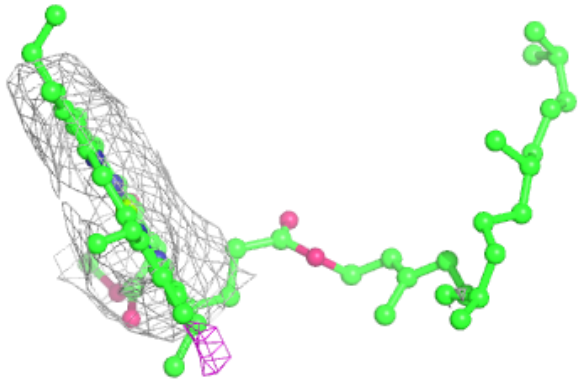


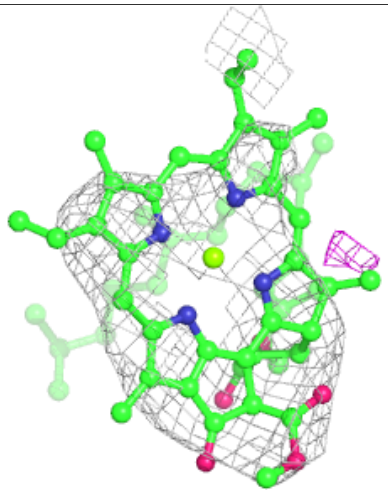


Electron density around CLA a 6007:

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

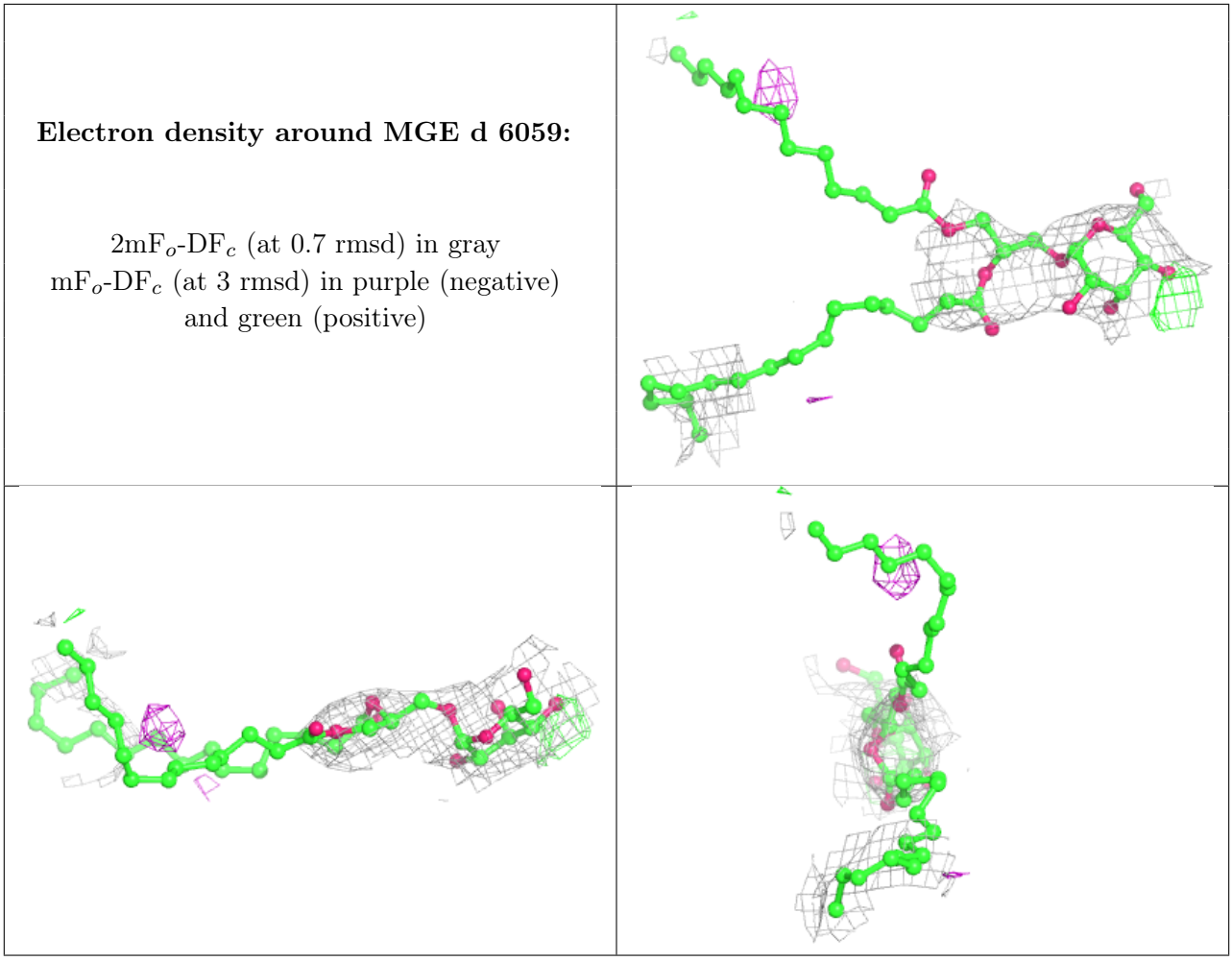






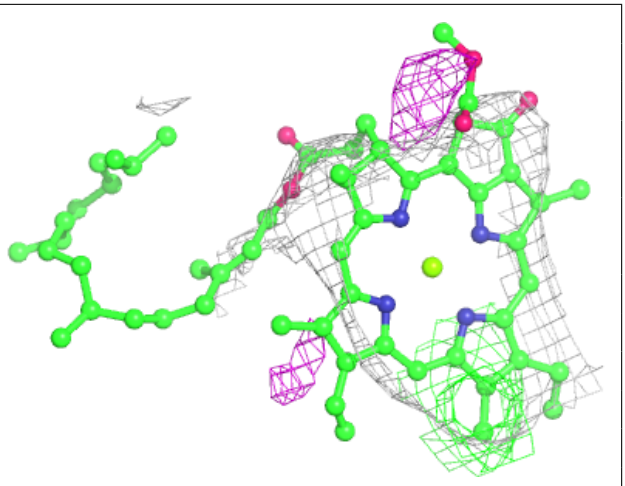
Electron density around MGE d 6059:

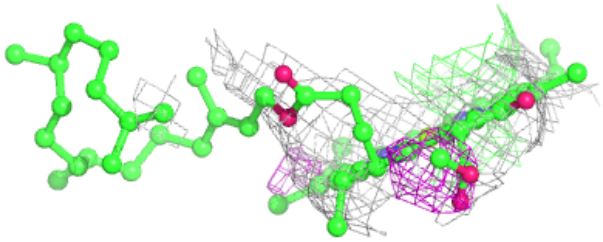
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

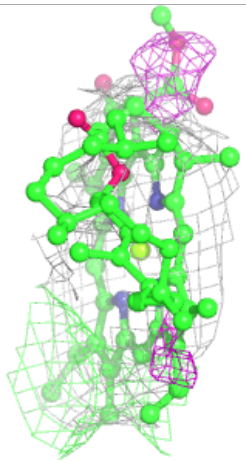


Electron density around CLA c 6027:

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

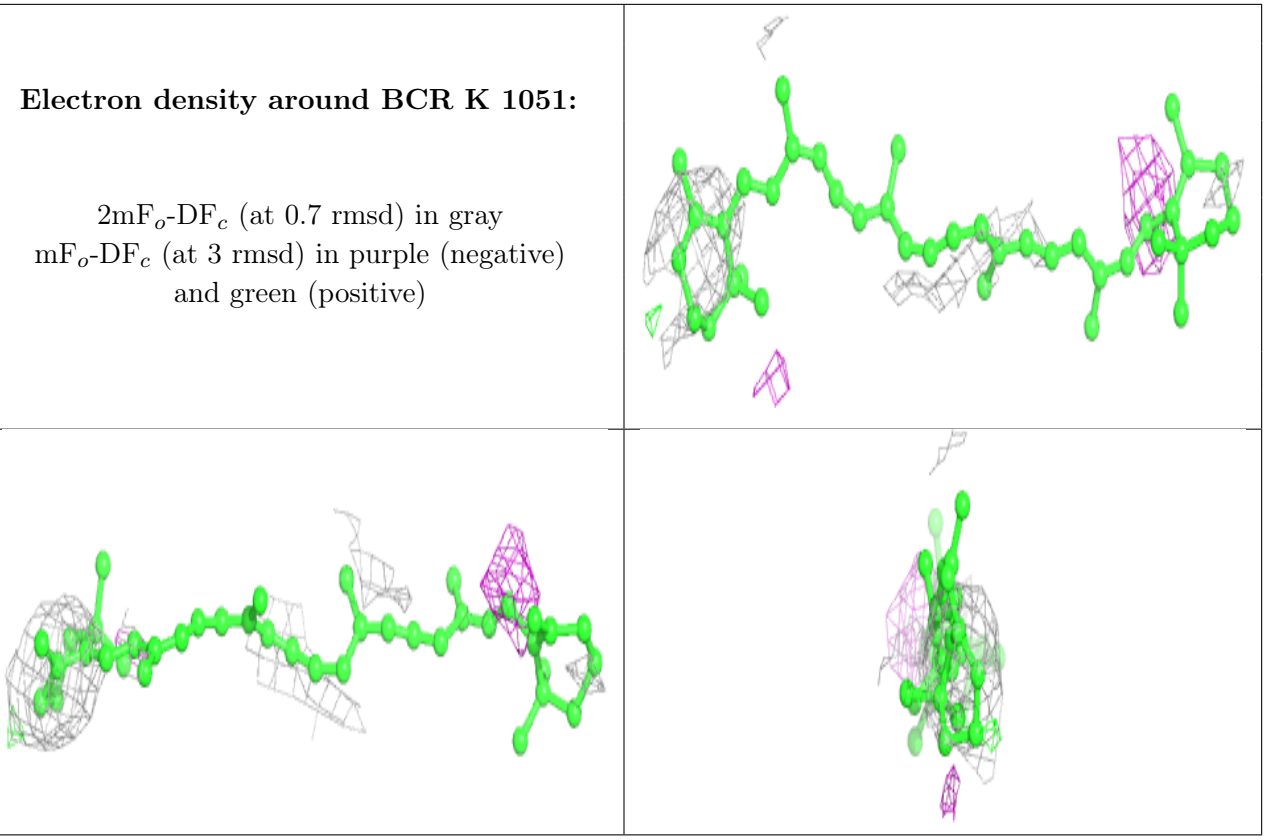






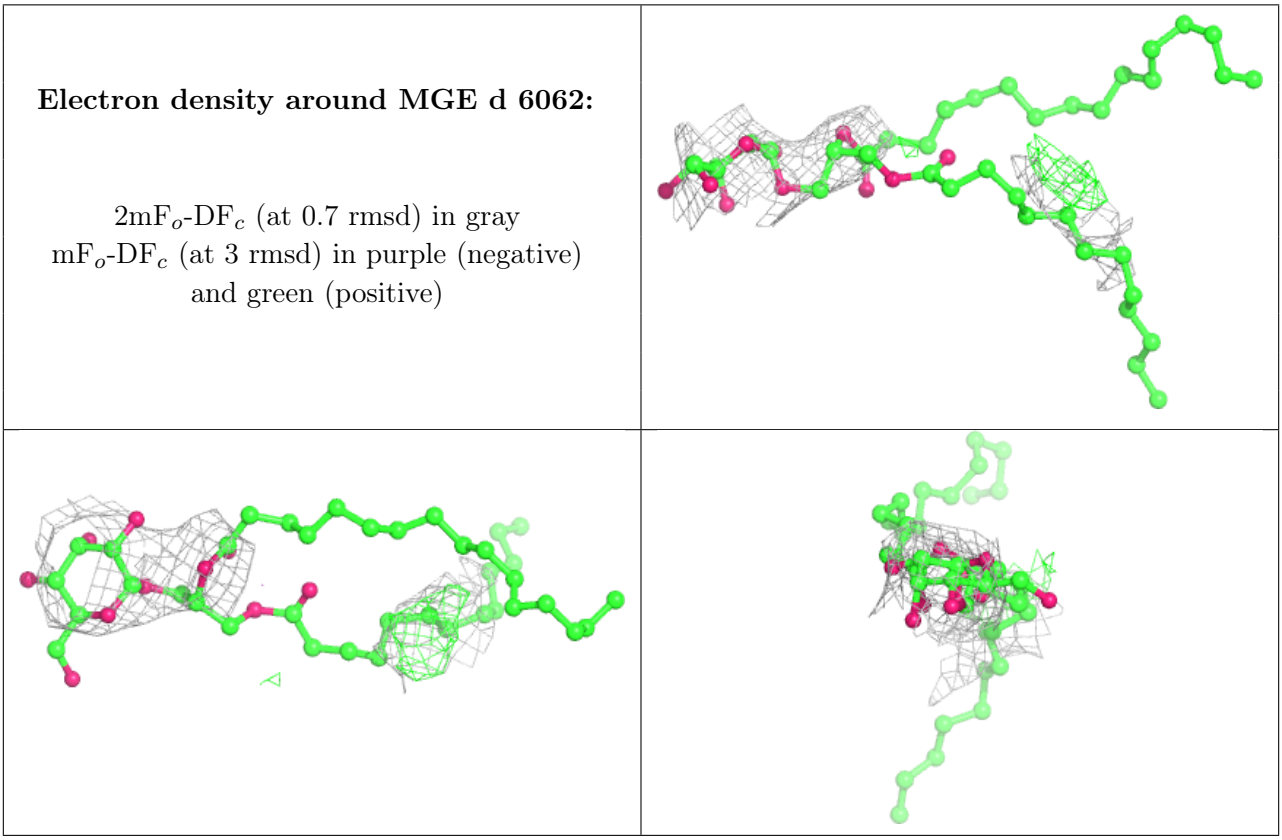
Electron density around BCR K 1051:

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



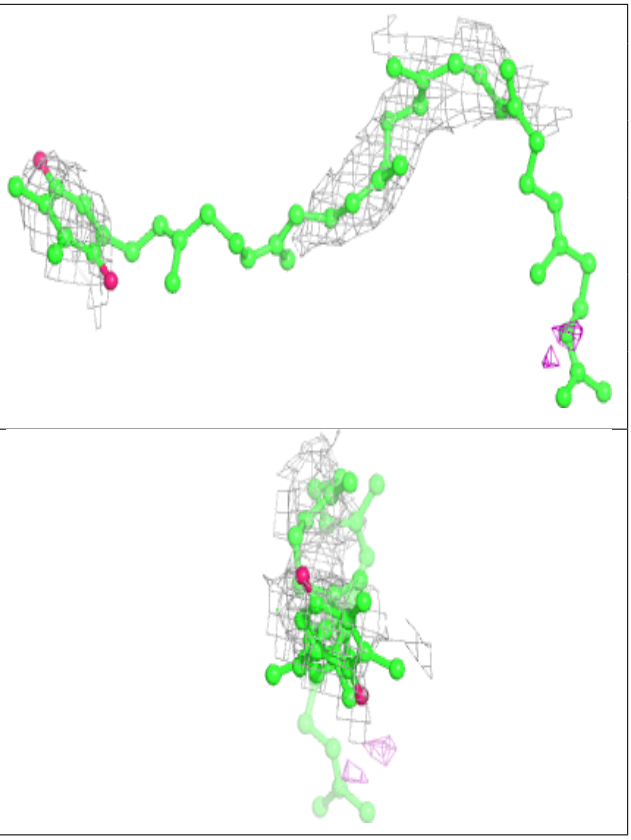
Electron density around MGE d 6062:

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



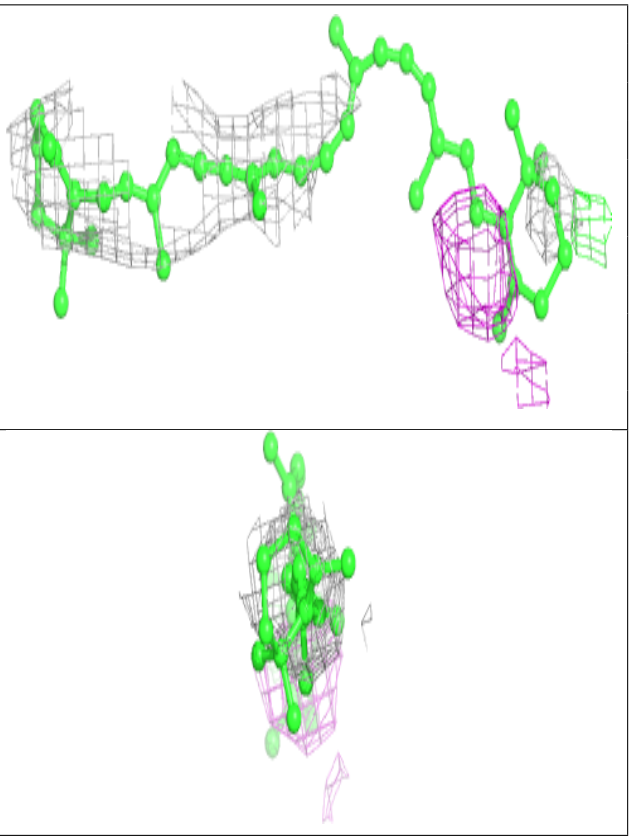
Electron density around PQ9 d 6042:

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



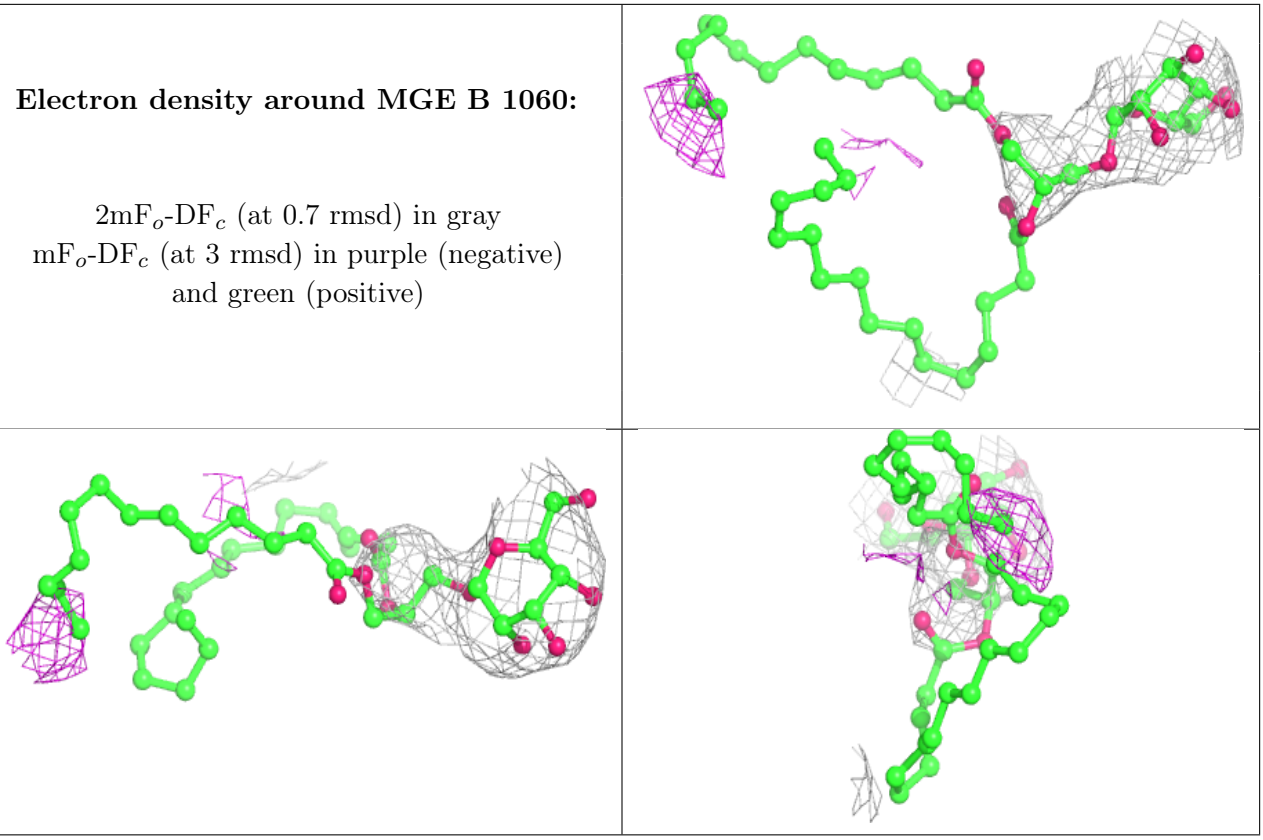
Electron density around BCR C 1054:

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



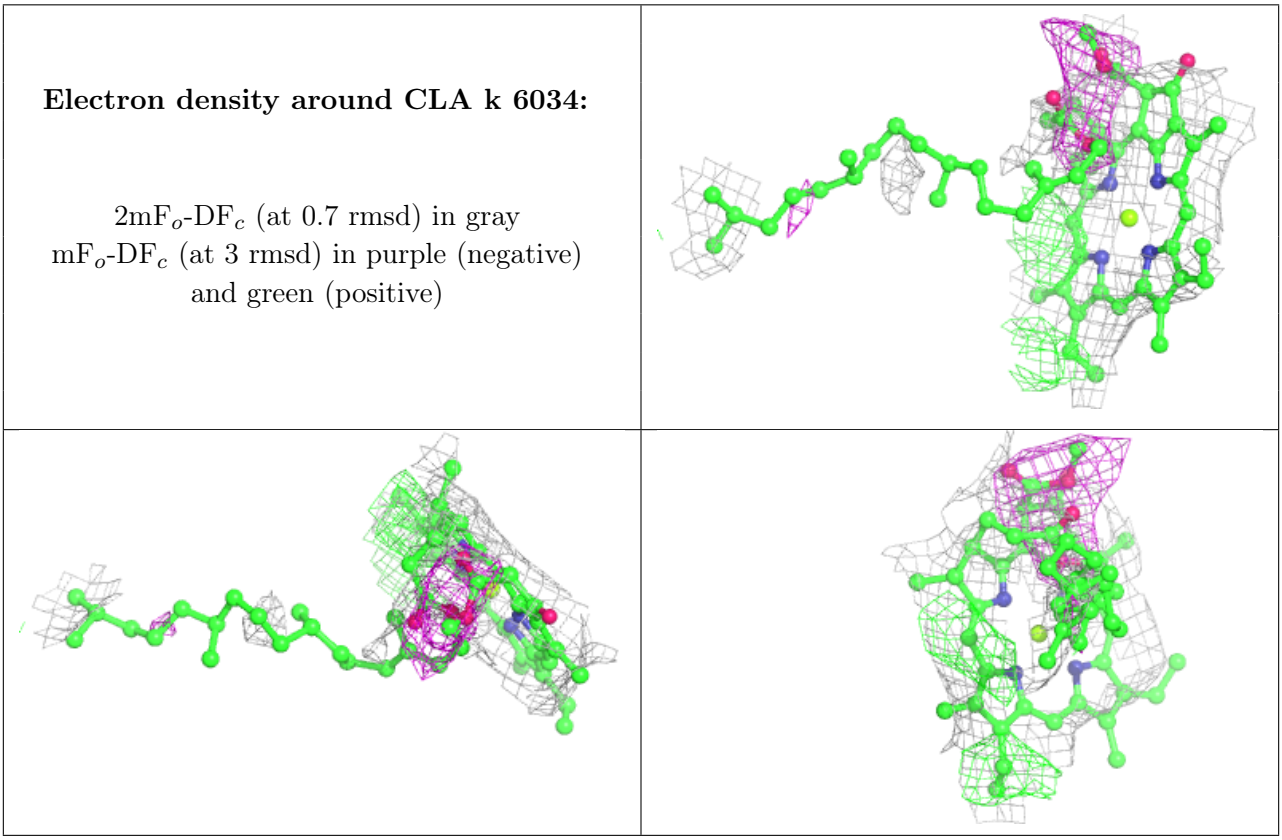
Electron density around MGE B 1060:

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



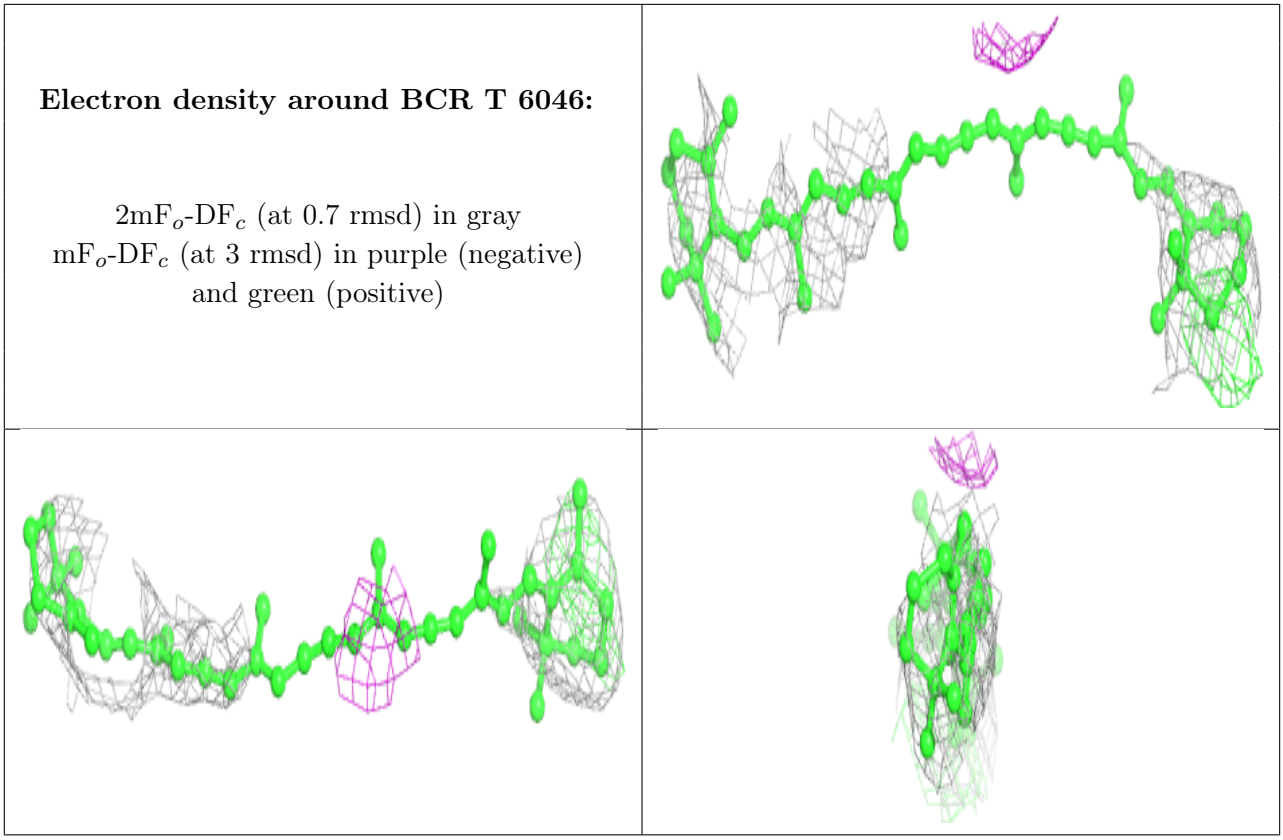
Electron density around CLA k 6034:

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



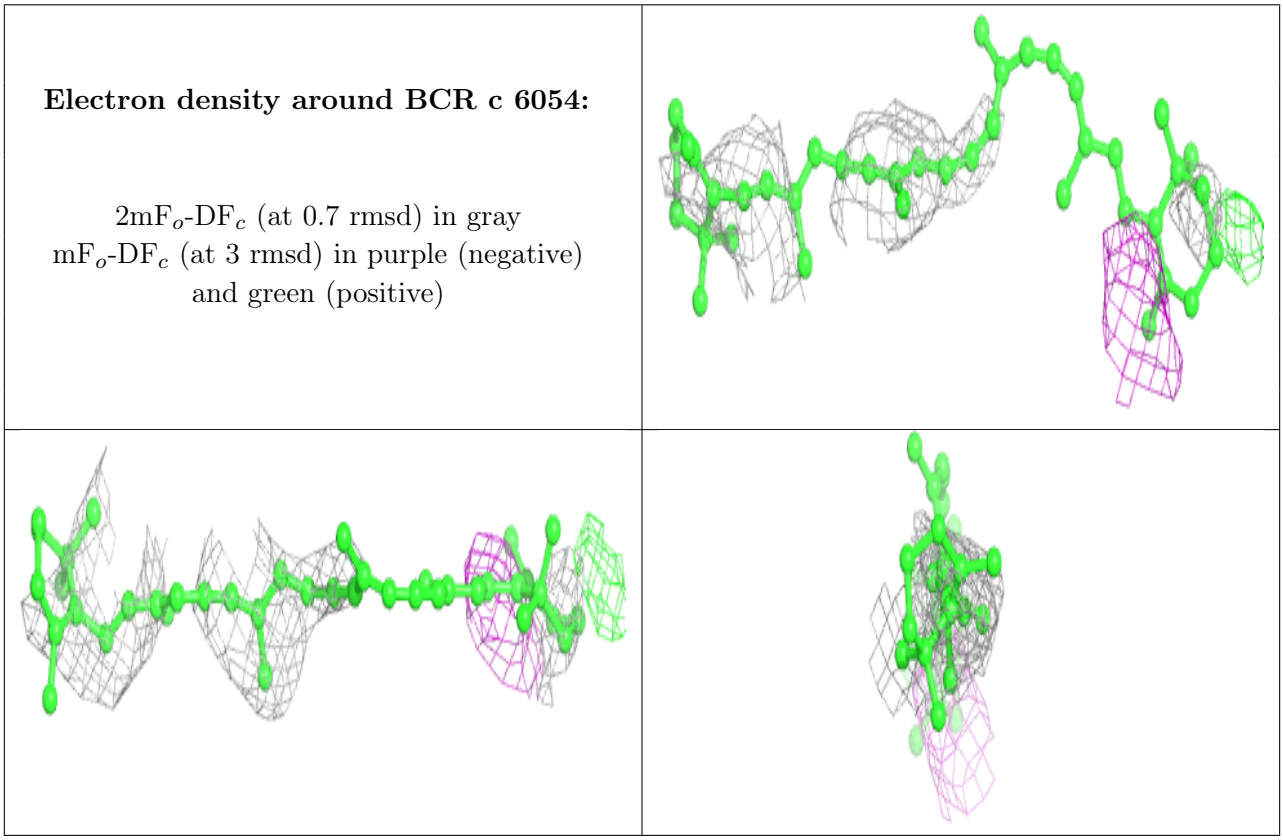
Electron density around BCR T 6046:

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



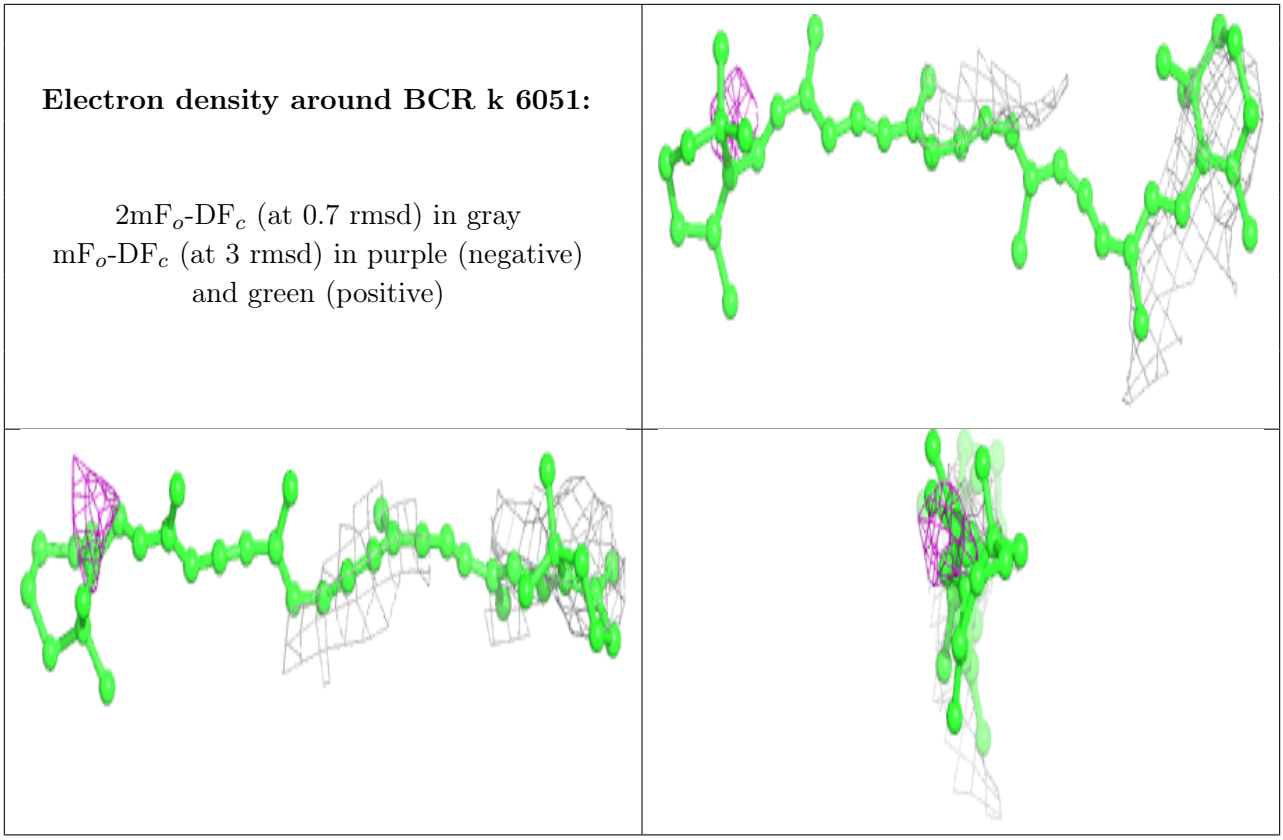
Electron density around BCR c 6054:

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



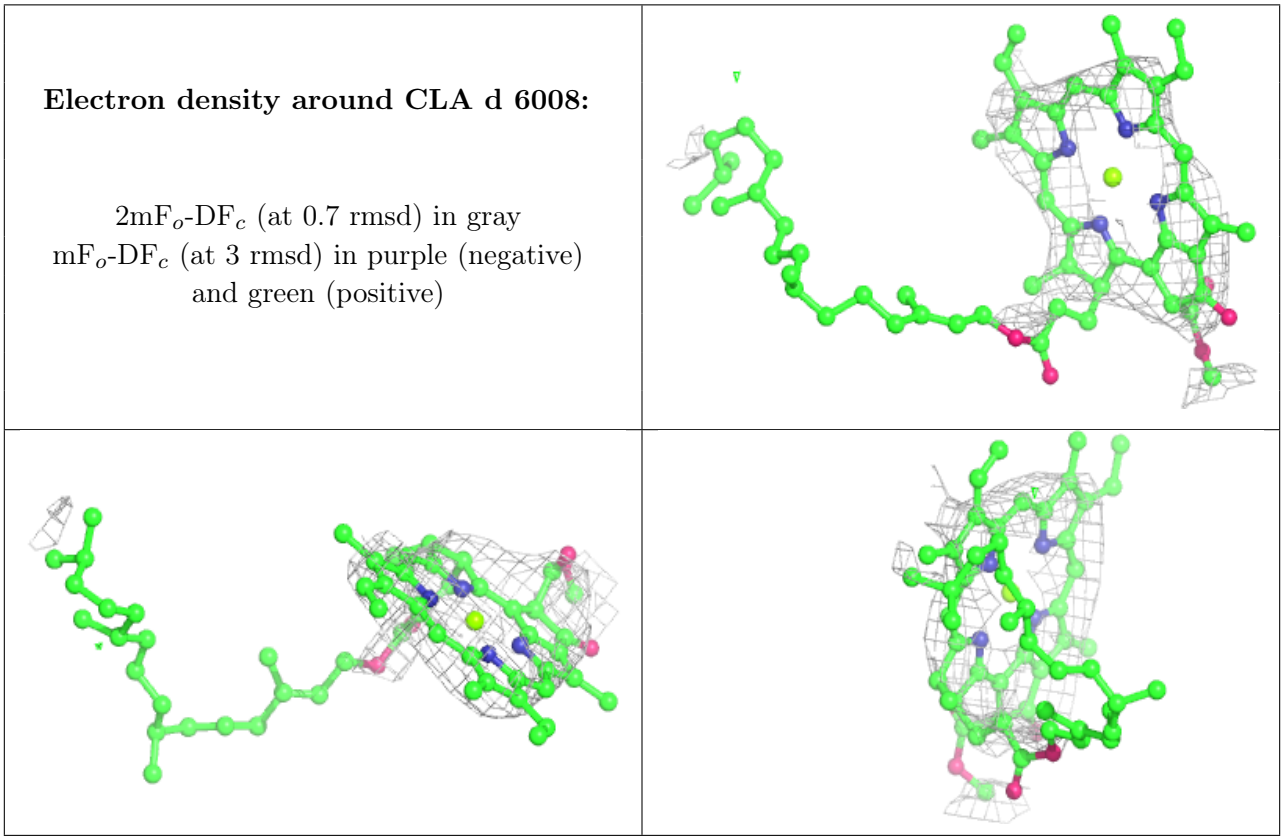
Electron density around BCR k 6051:

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



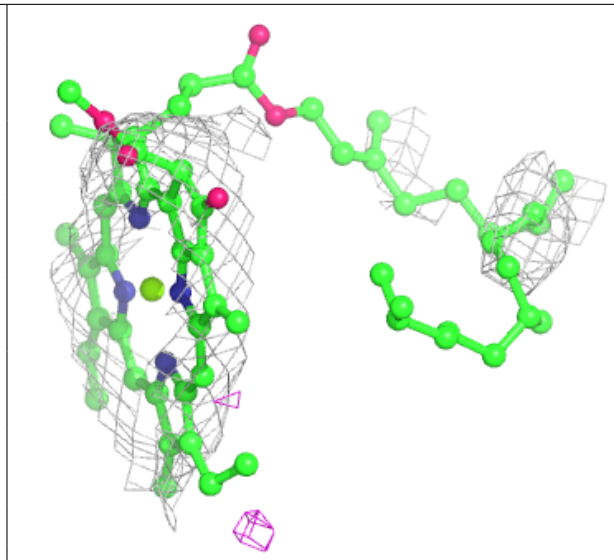
Electron density around CLA d 6008:

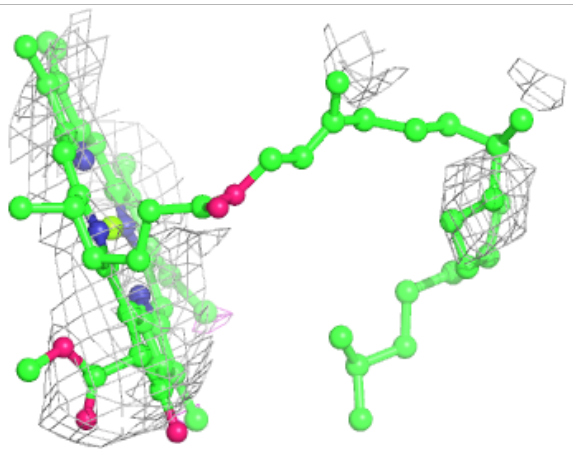
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

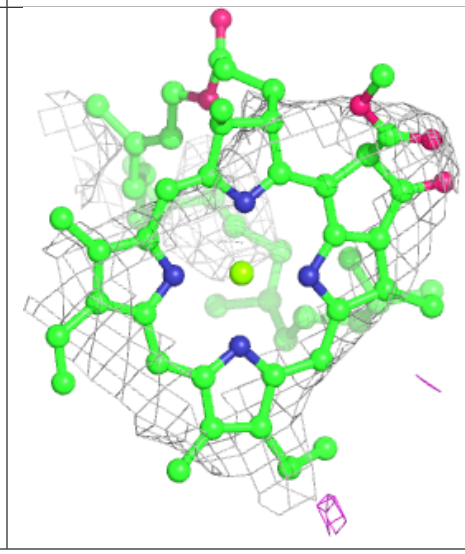


Electron density around CLA C 1037:

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

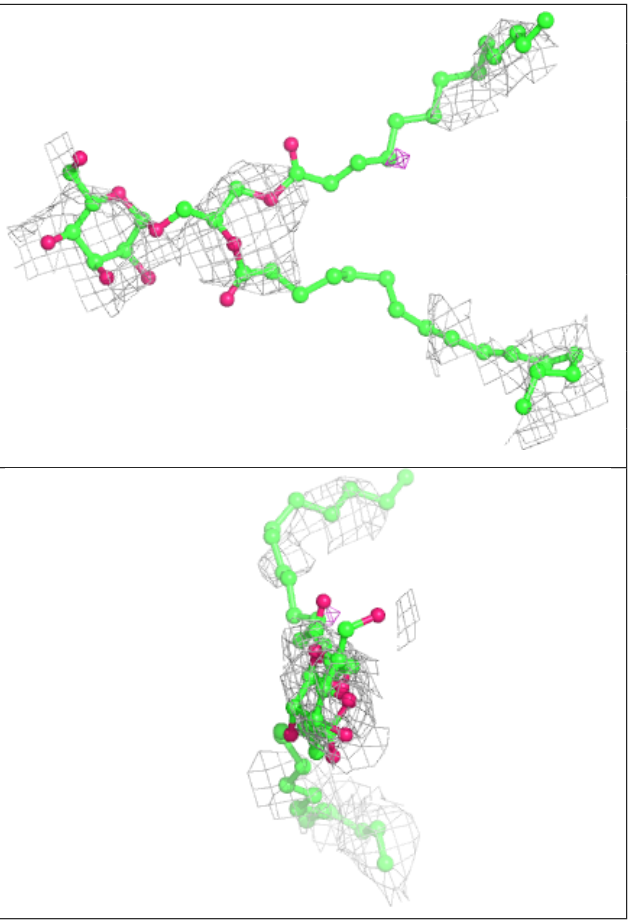






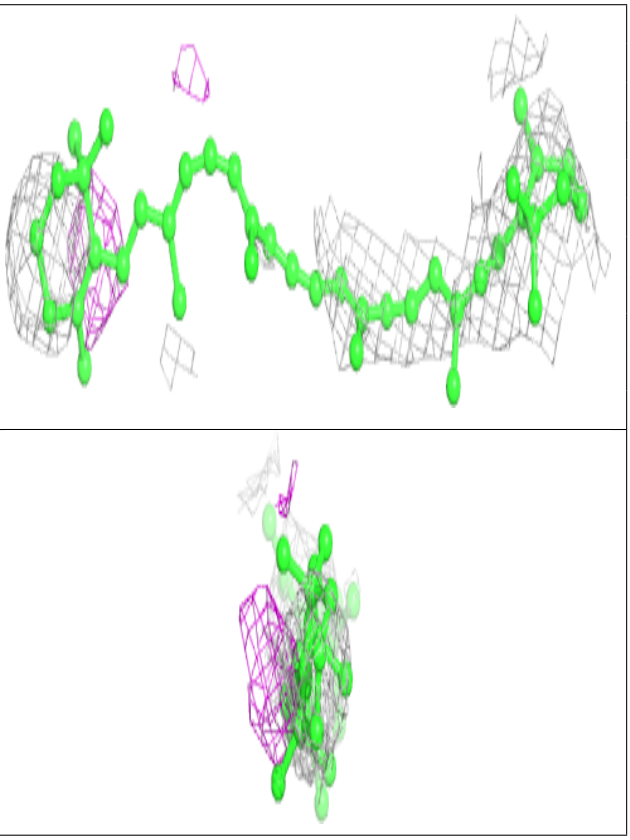
Electron density around MGE D 1059:

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



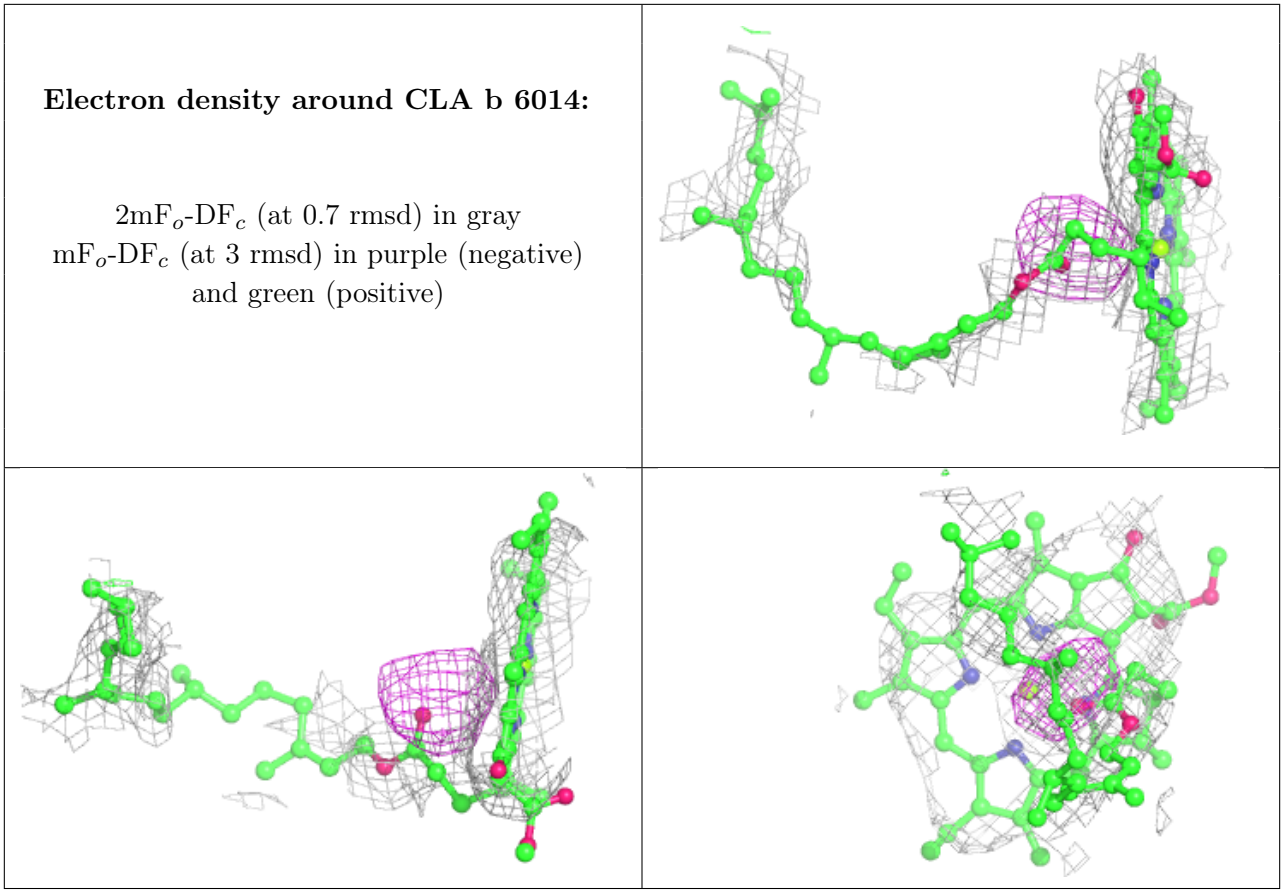
Electron density around BCR h 6049:

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



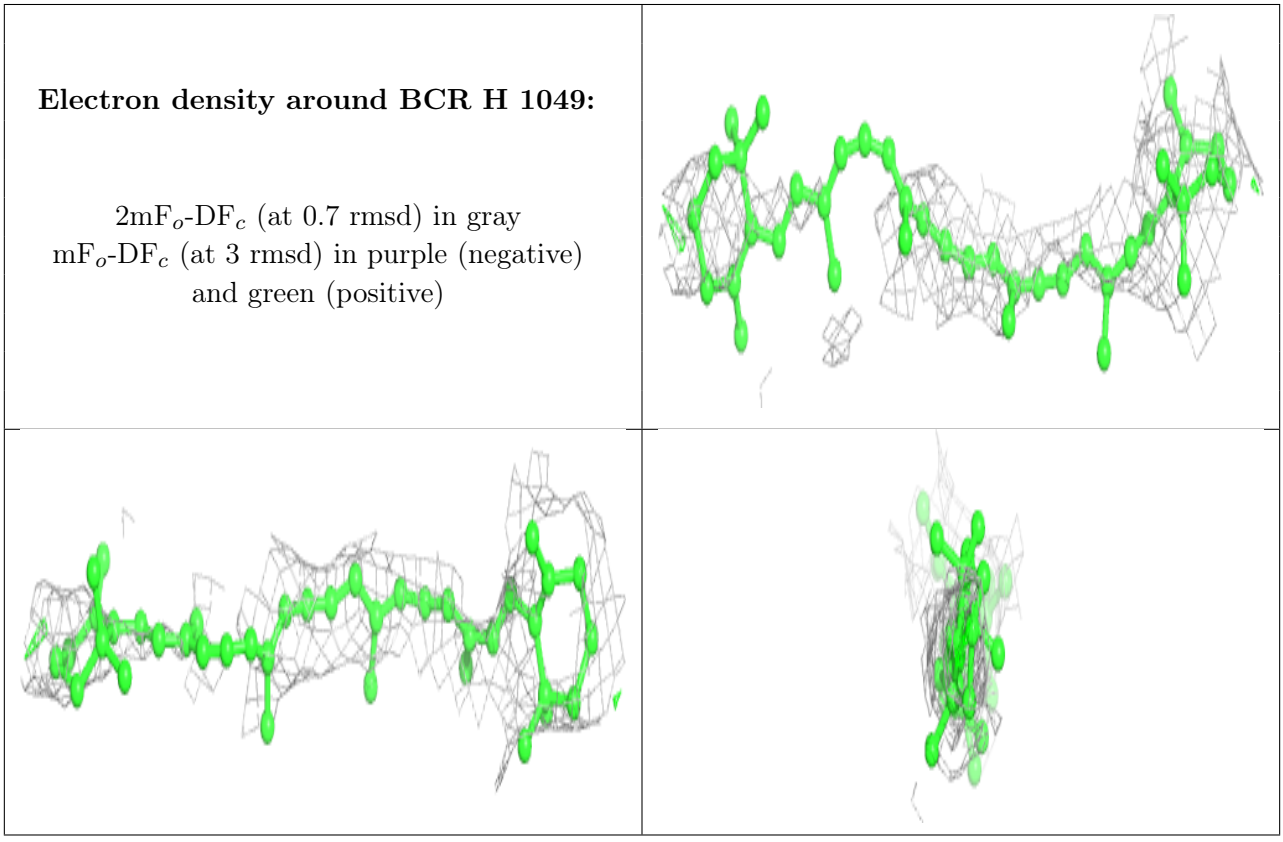
Electron density around CLA b 6014:

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



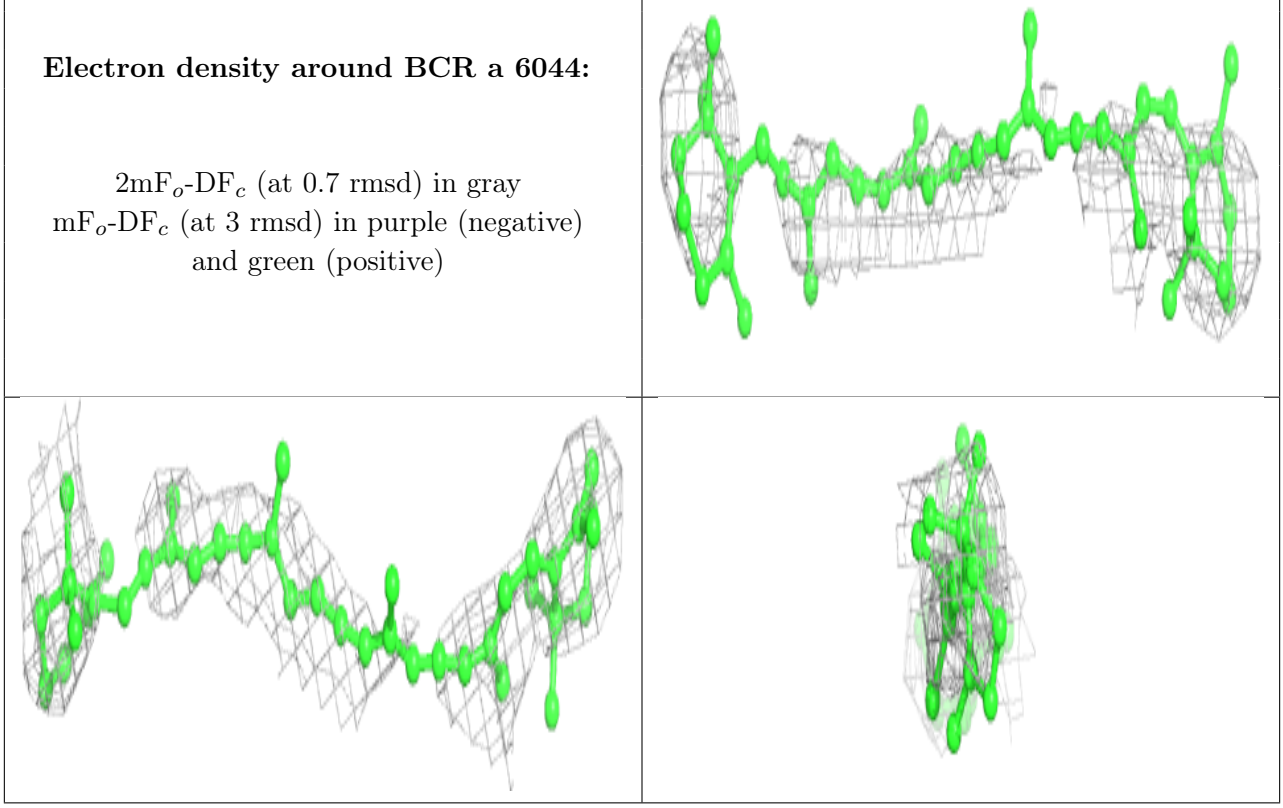
Electron density around BCR H 1049:

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



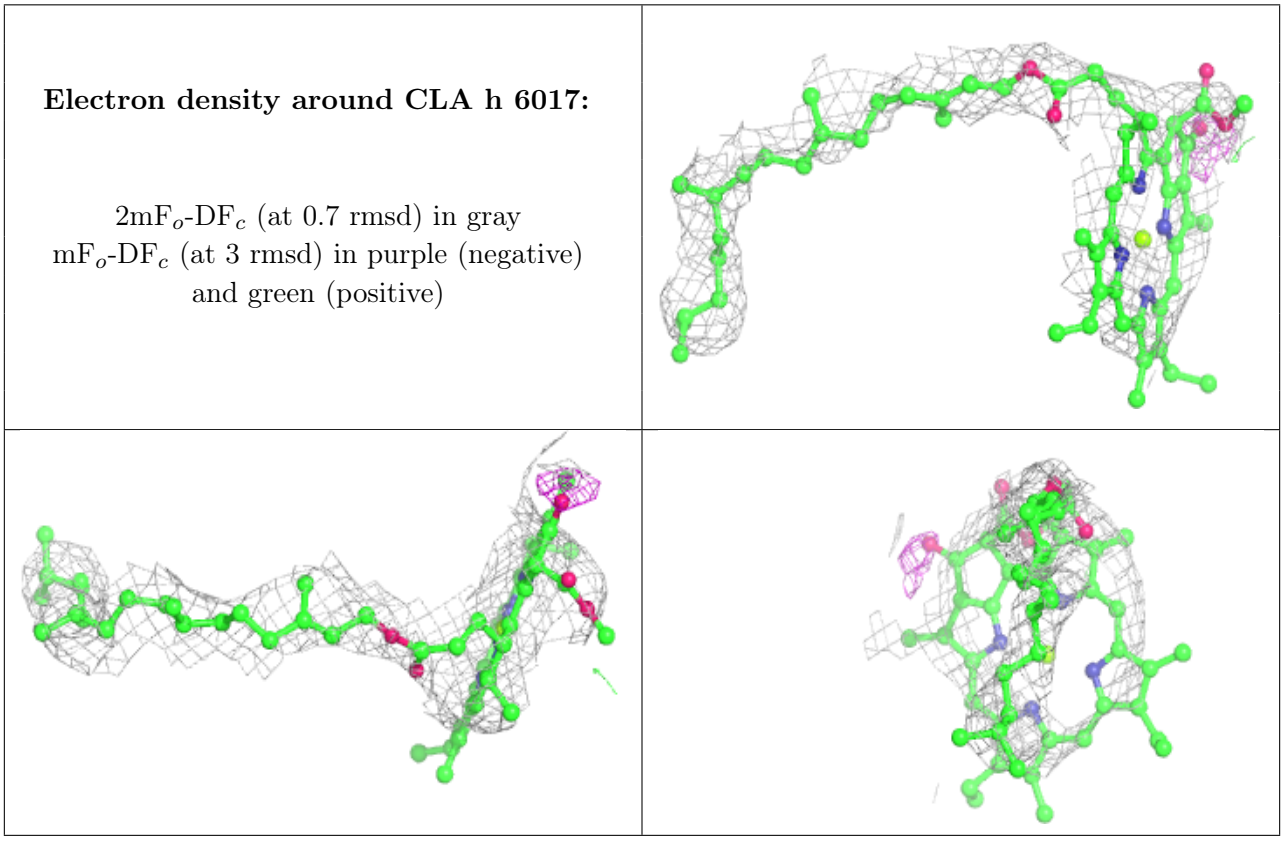
Electron density around BCR a 6044:

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



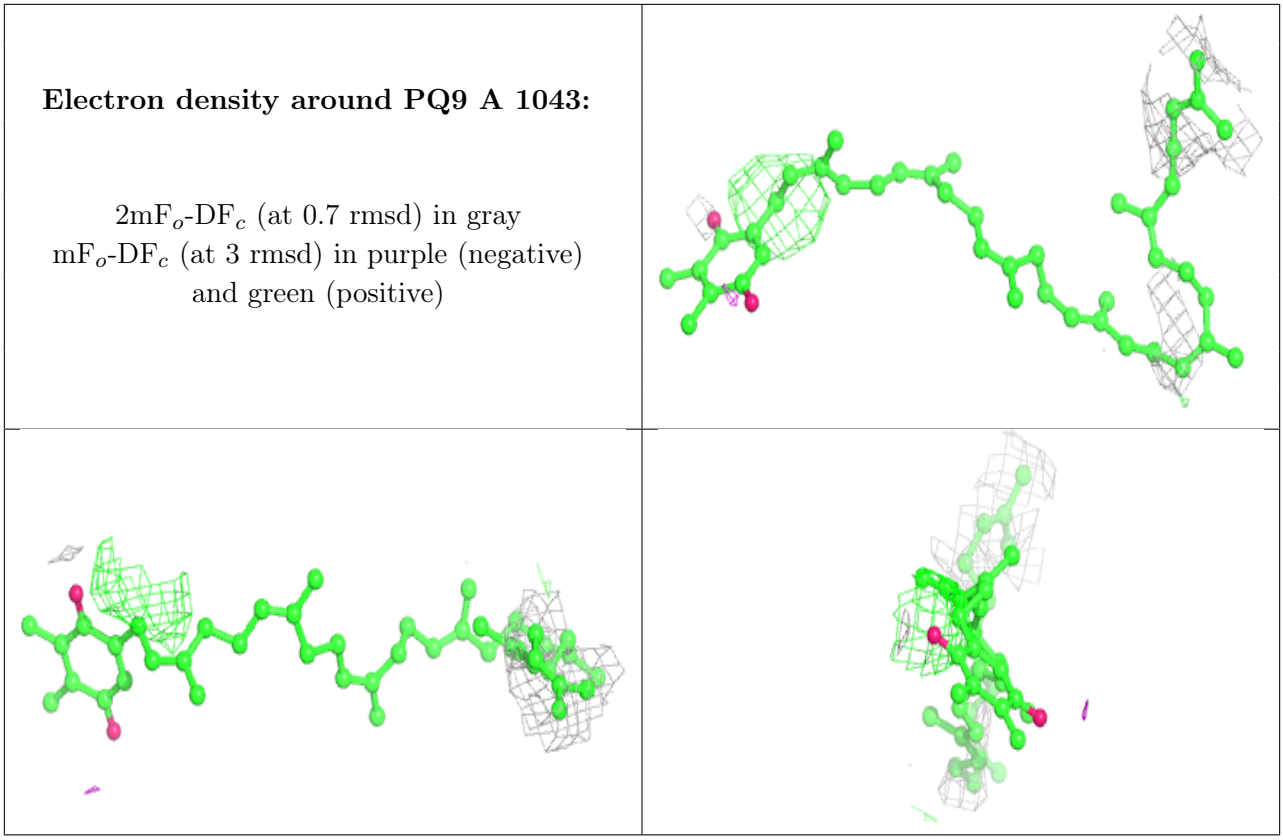
Electron density around CLA h 6017:

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



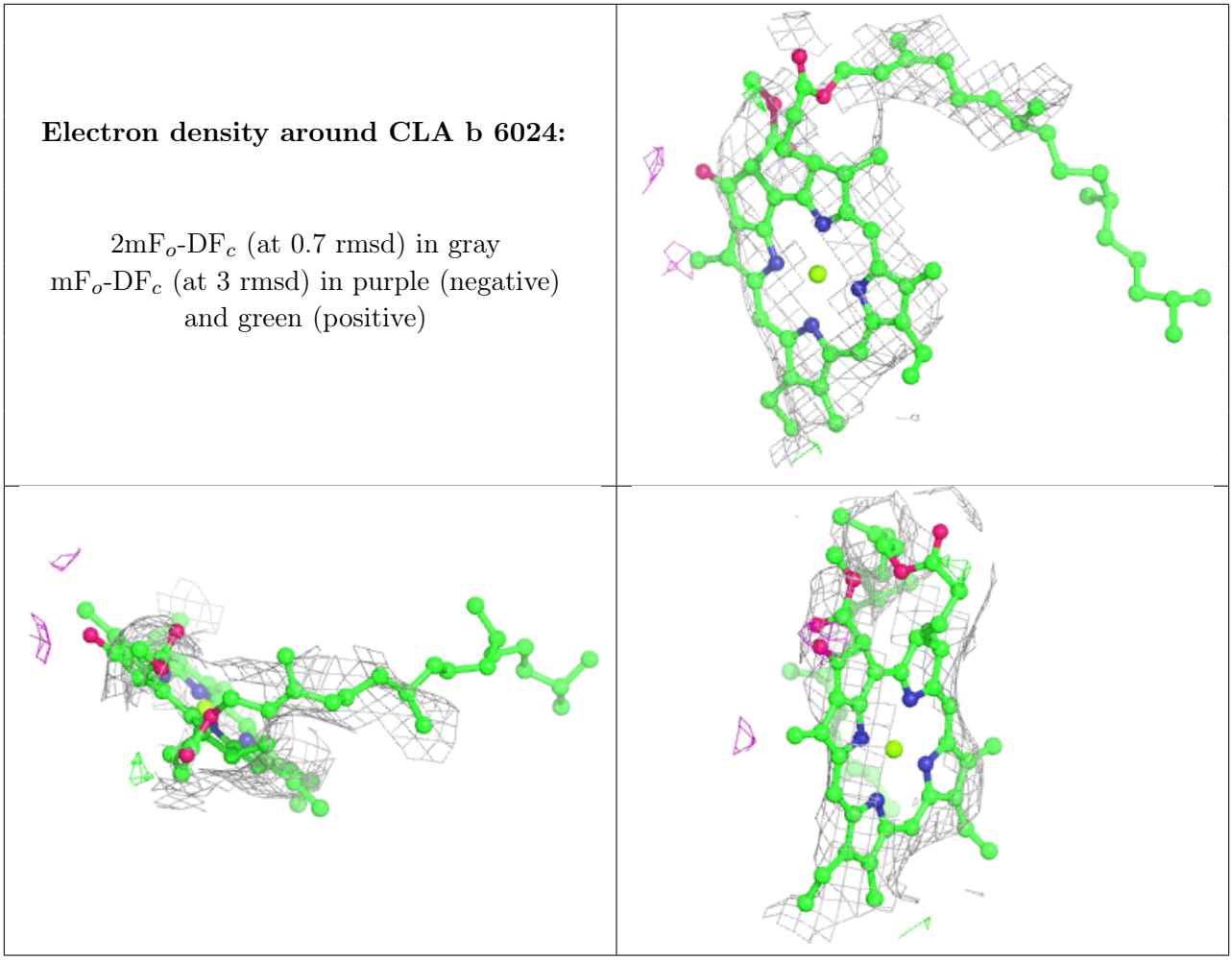
Electron density around PQ9 A 1043:

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



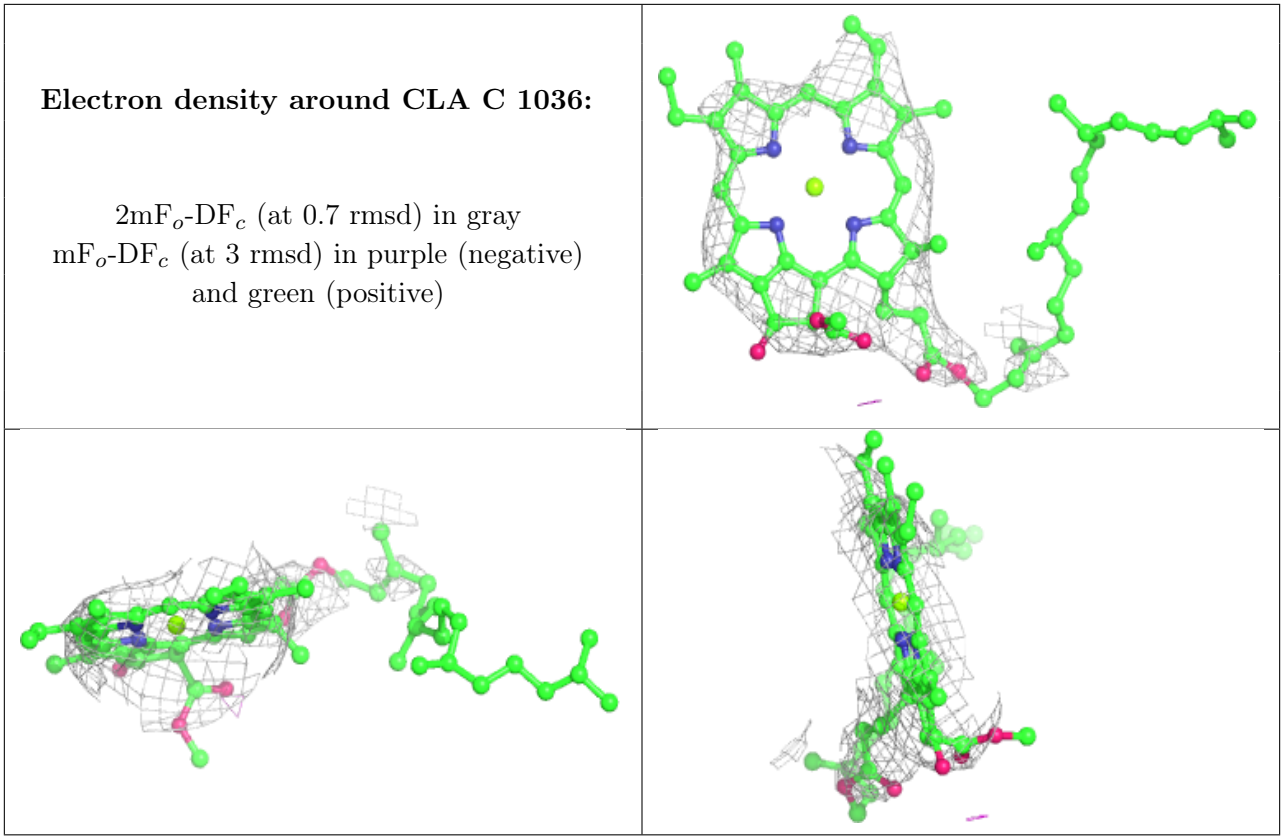
Electron density around CLA b 6024:

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



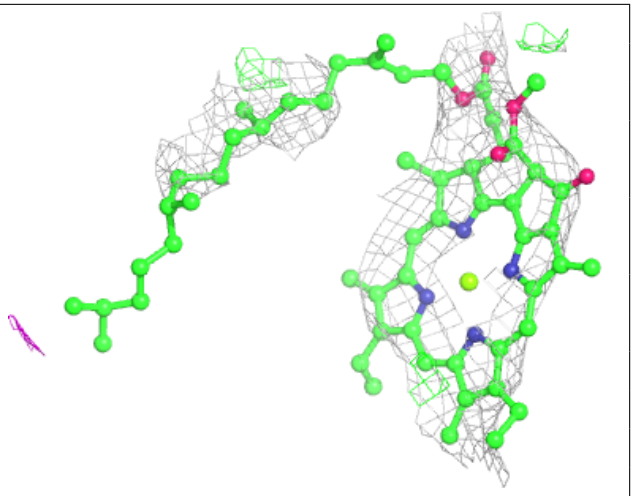
Electron density around CLA C 1036:

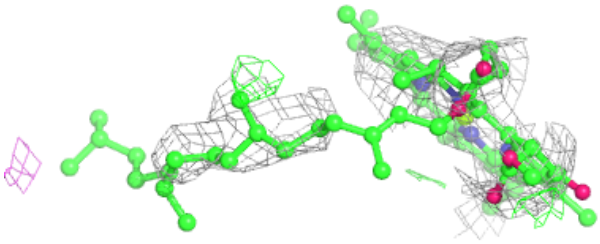
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

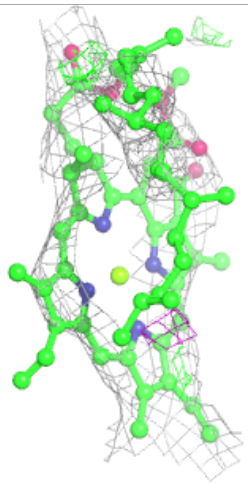


Electron density around CLA B 1024:

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

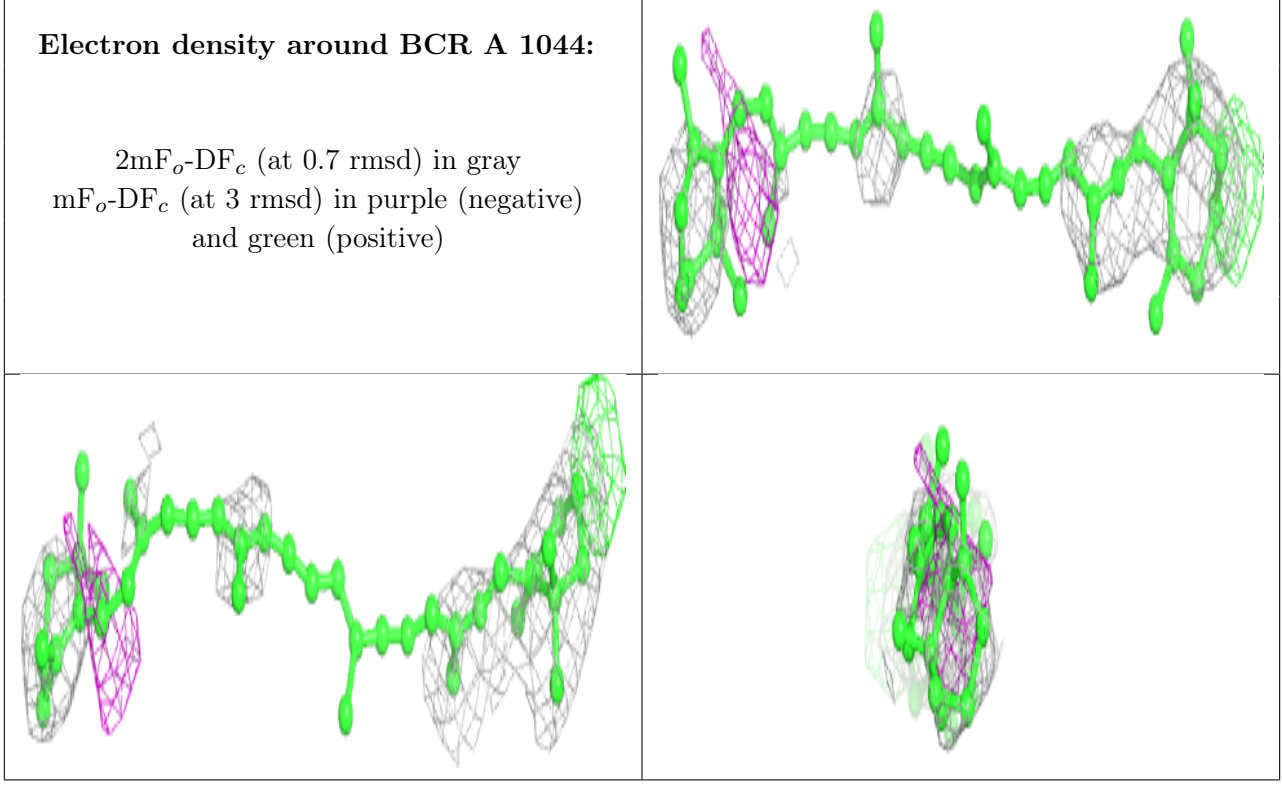






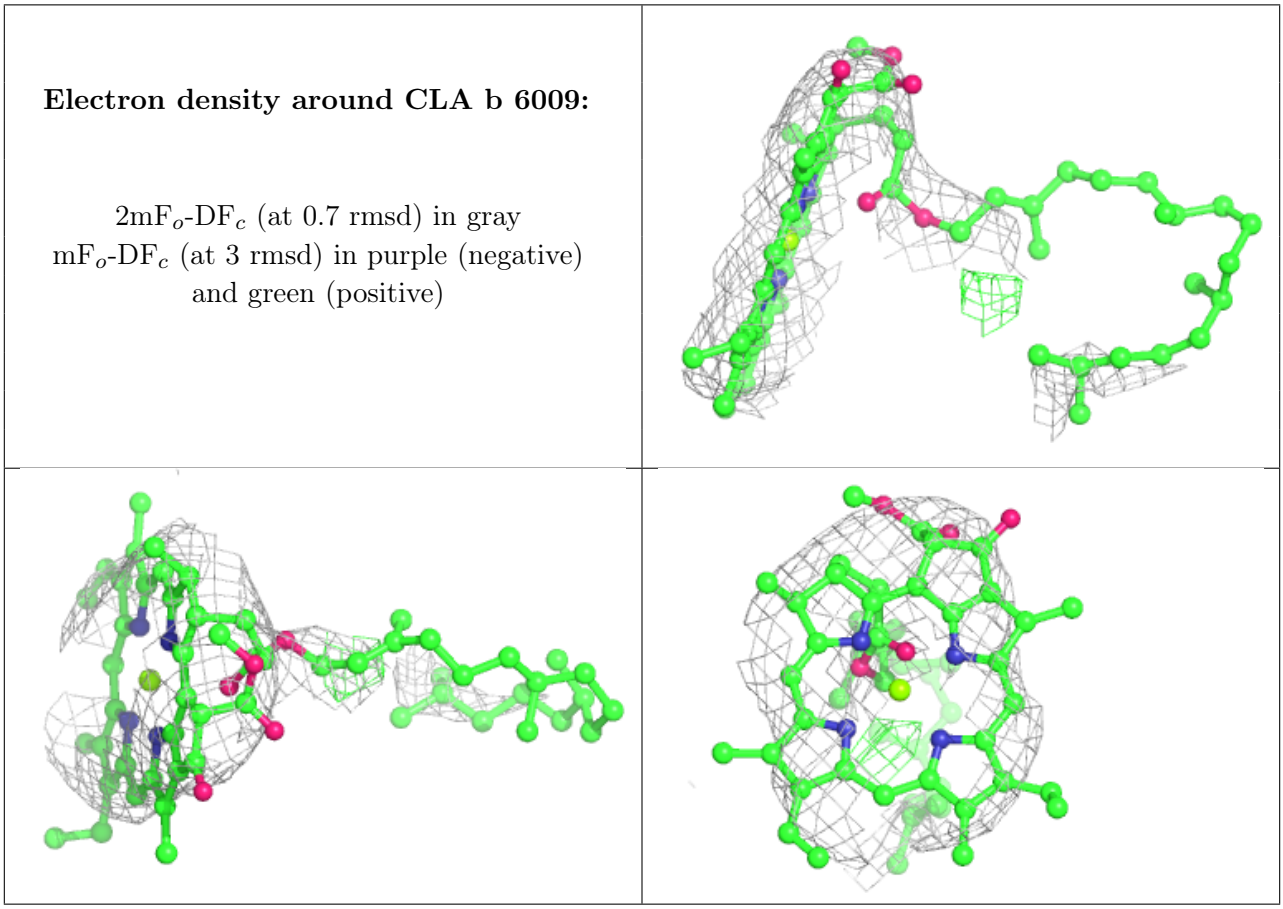
Electron density around BCR A 1044:

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



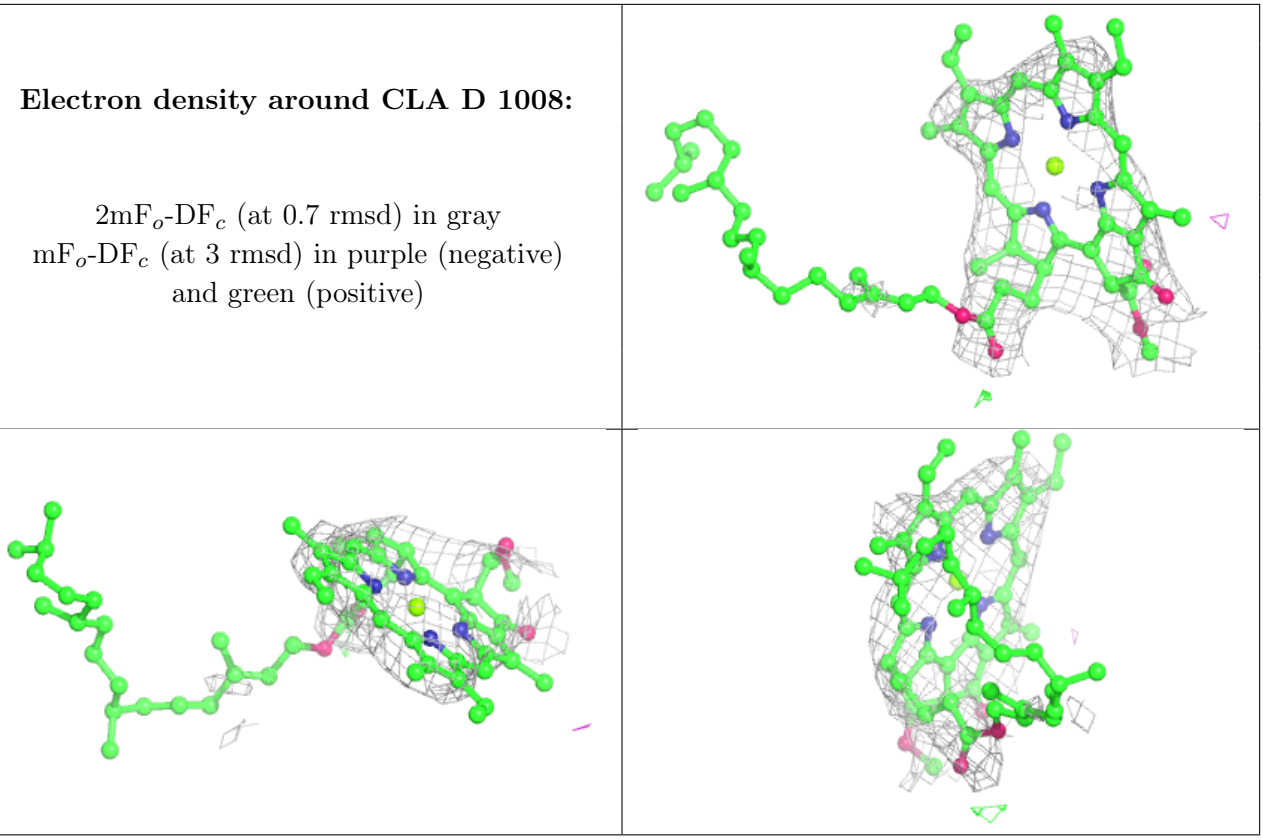
Electron density around CLA b 6009:

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



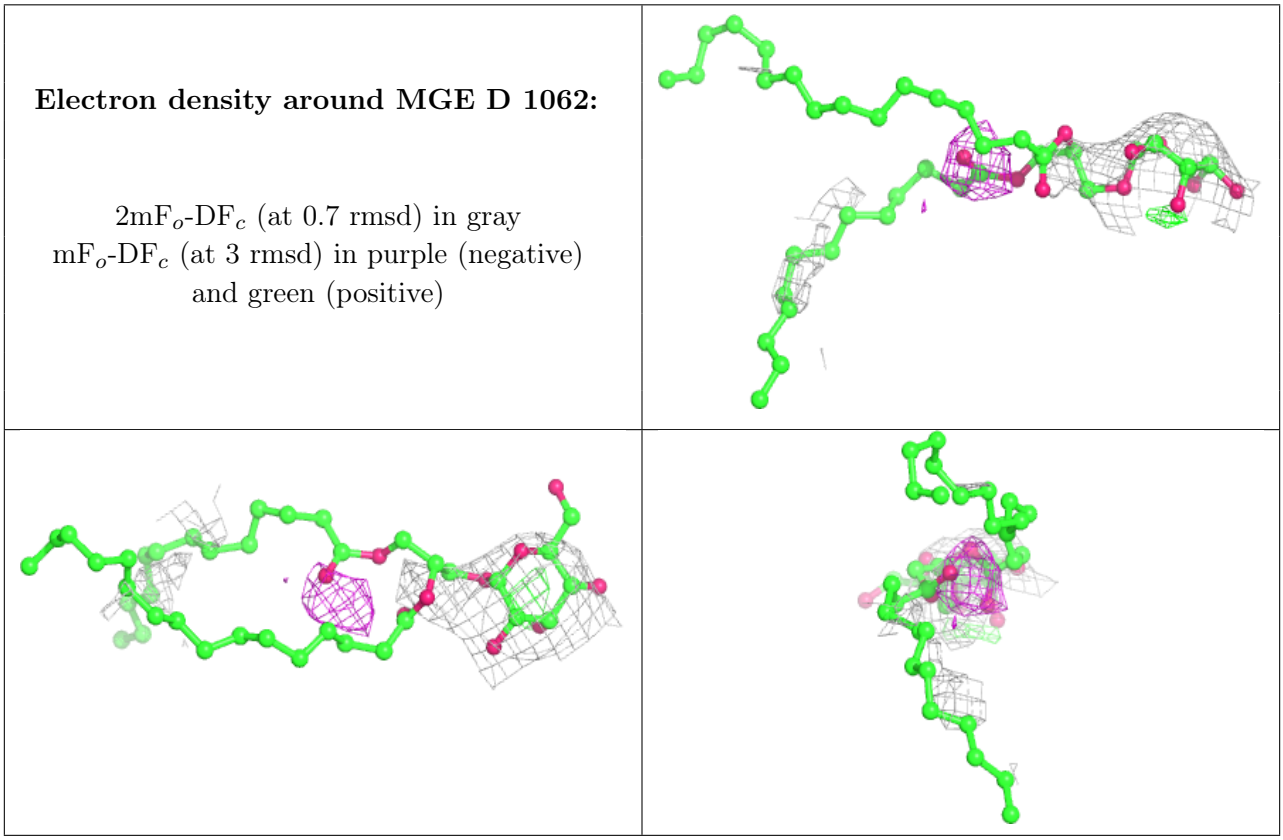
Electron density around CLA D 1008:

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



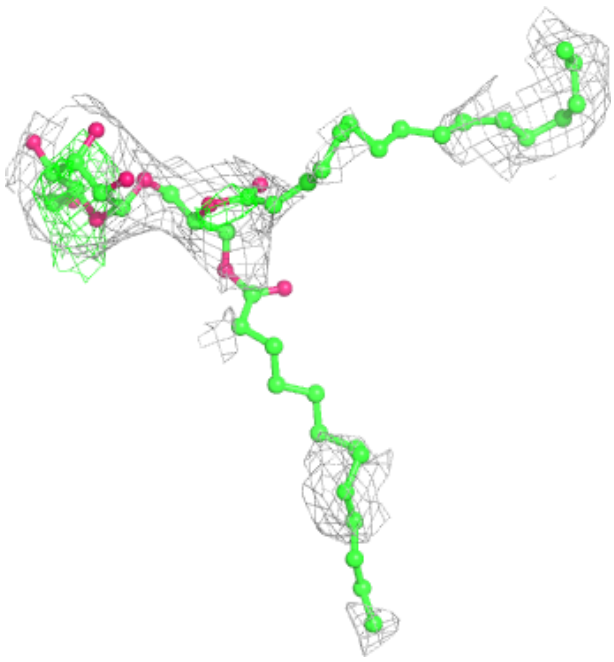
Electron density around MGE D 1062:

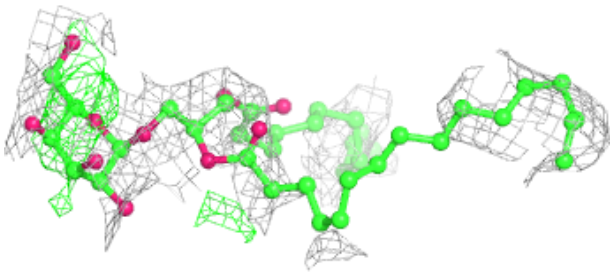
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

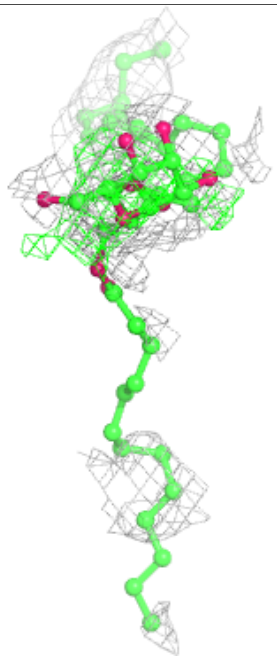


Electron density around MGE L 1061:

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

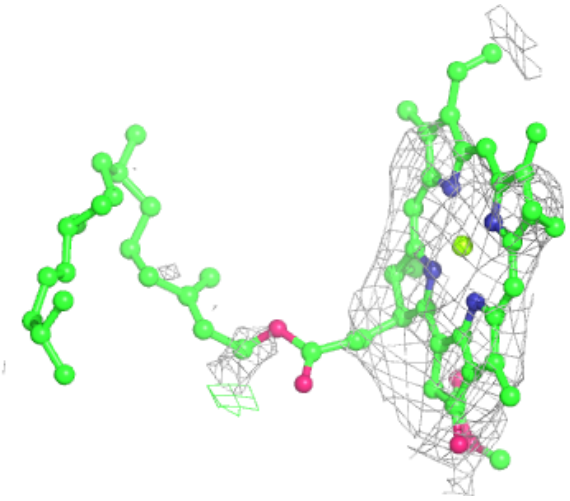


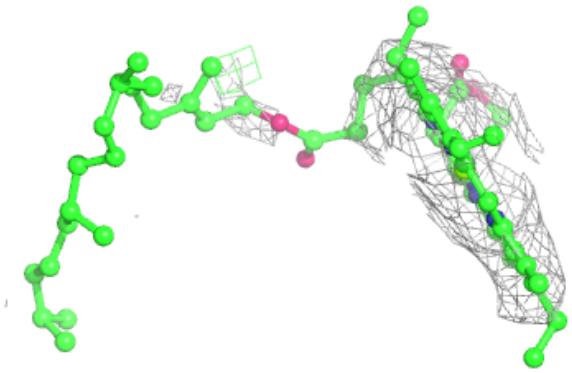


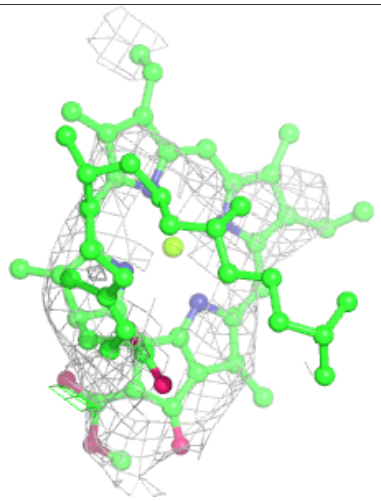


Electron density around CLA A 1007:

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

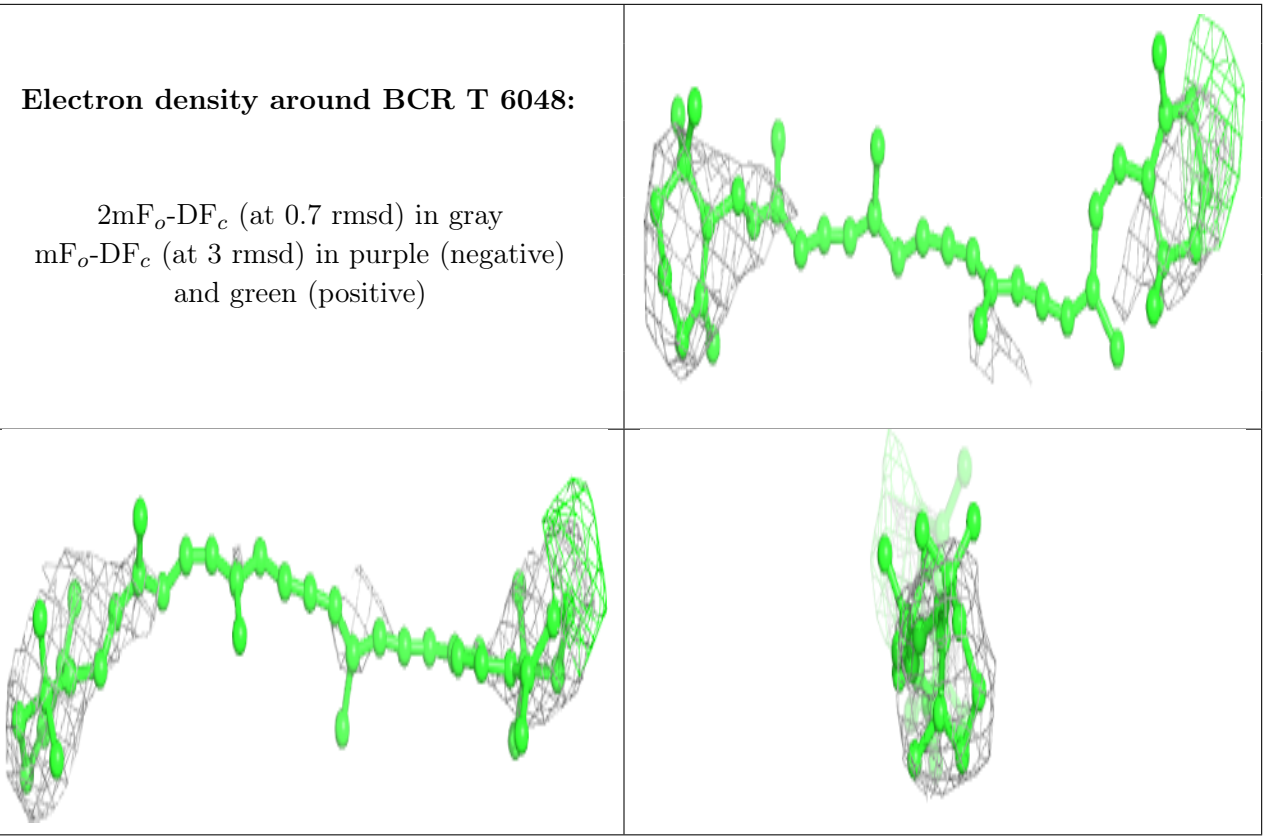






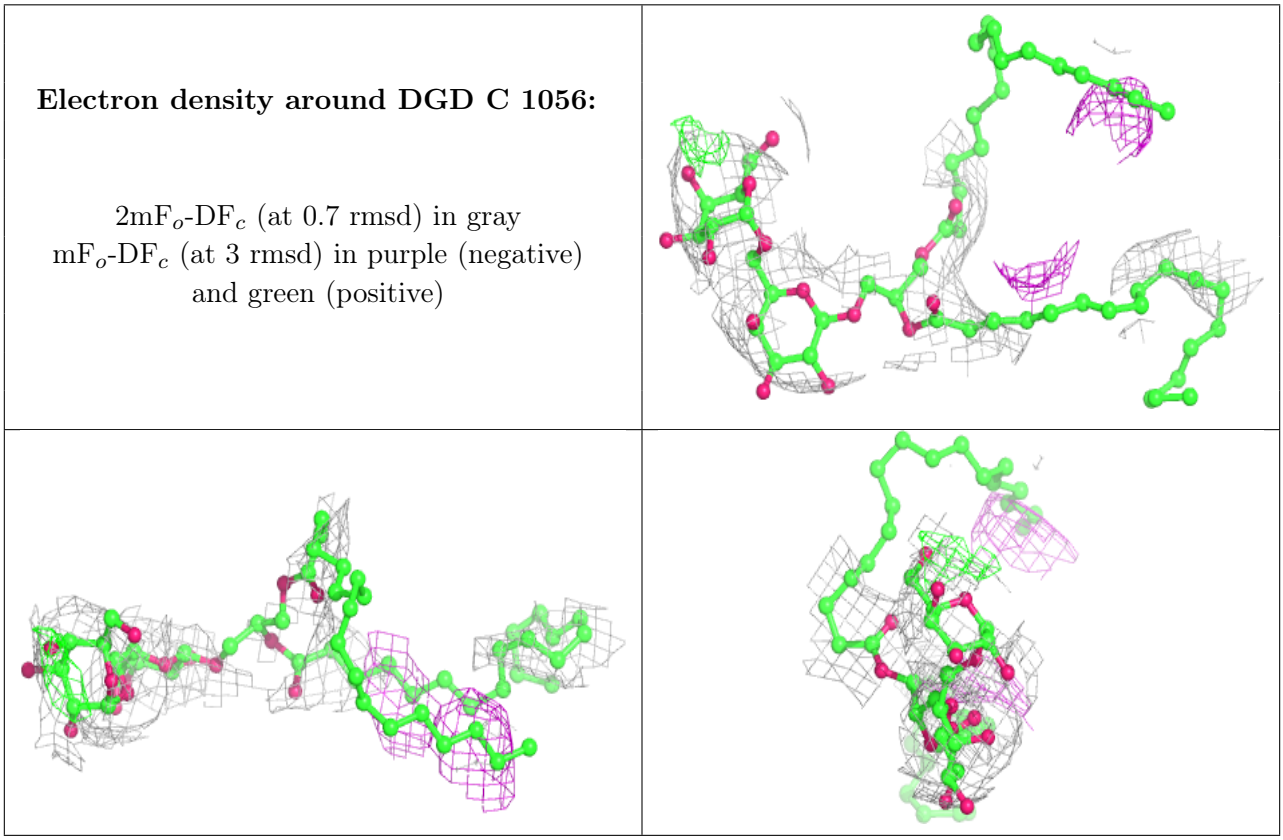
Electron density around BCR T 6048:

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



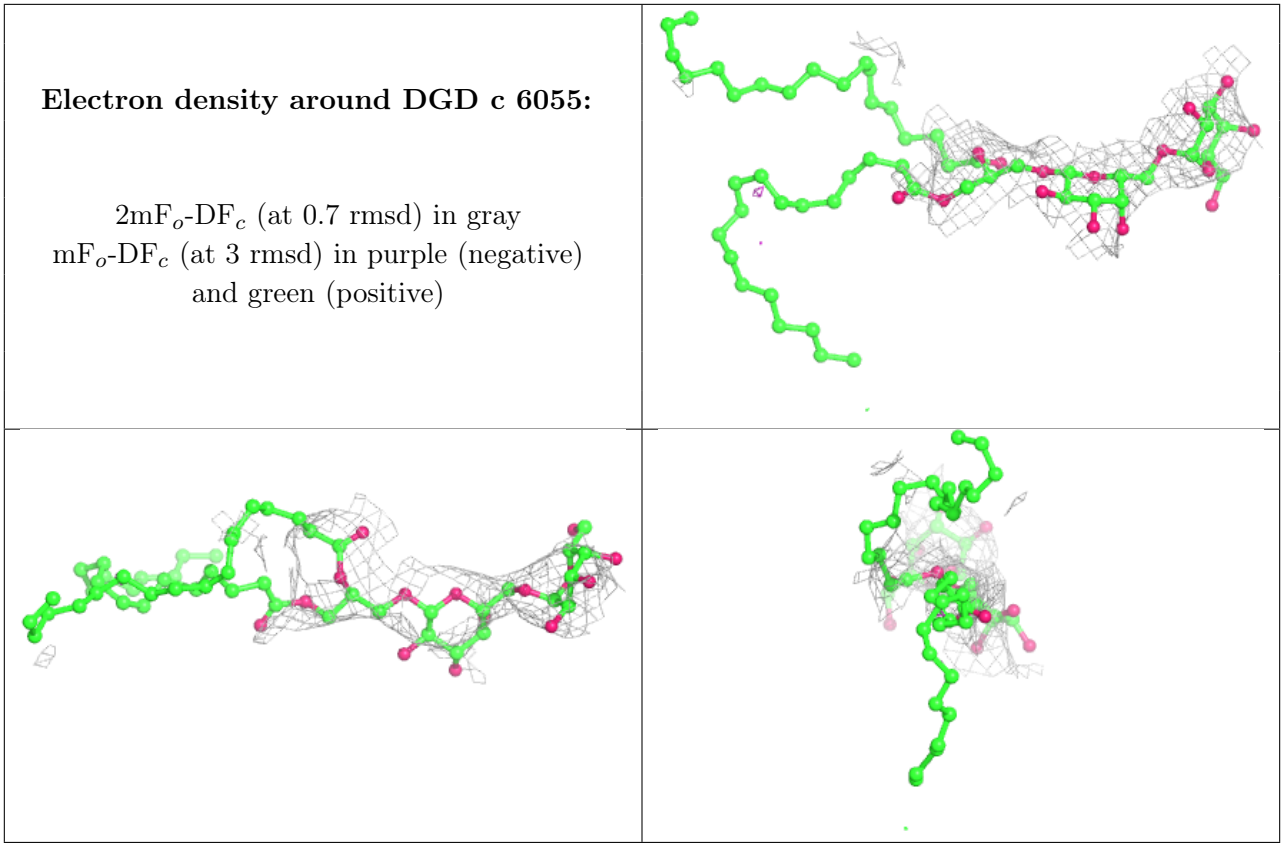
Electron density around DGD C 1056:

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



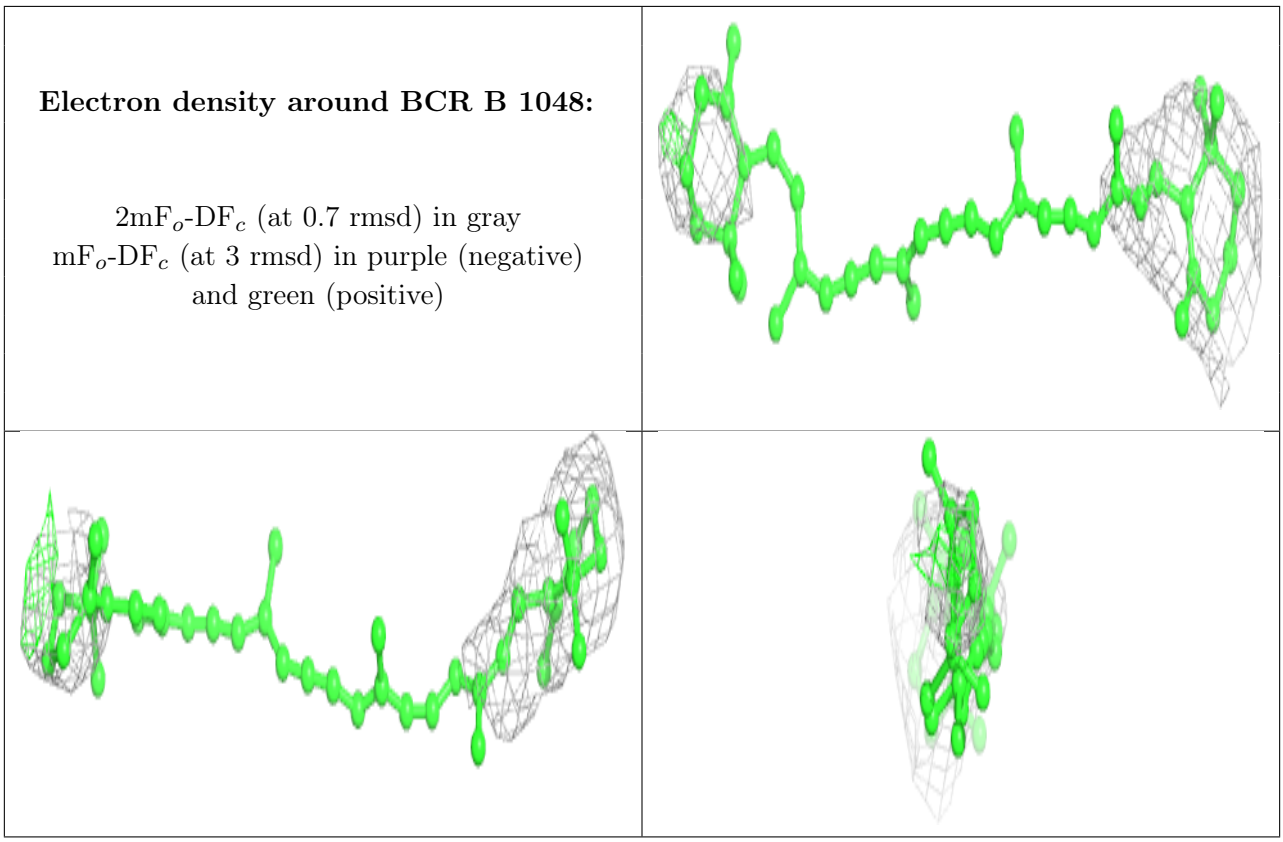
Electron density around DGD c 6055:

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



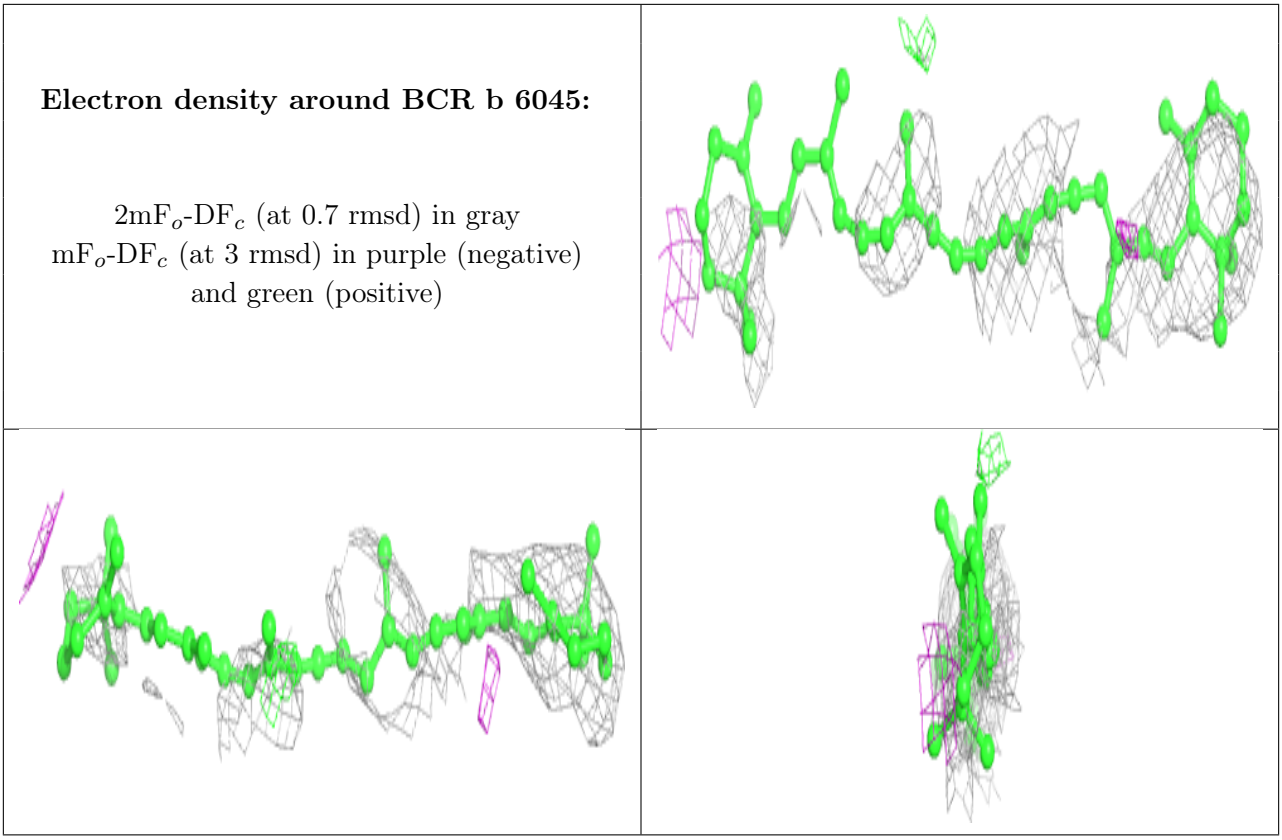
Electron density around BCR B 1048:

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



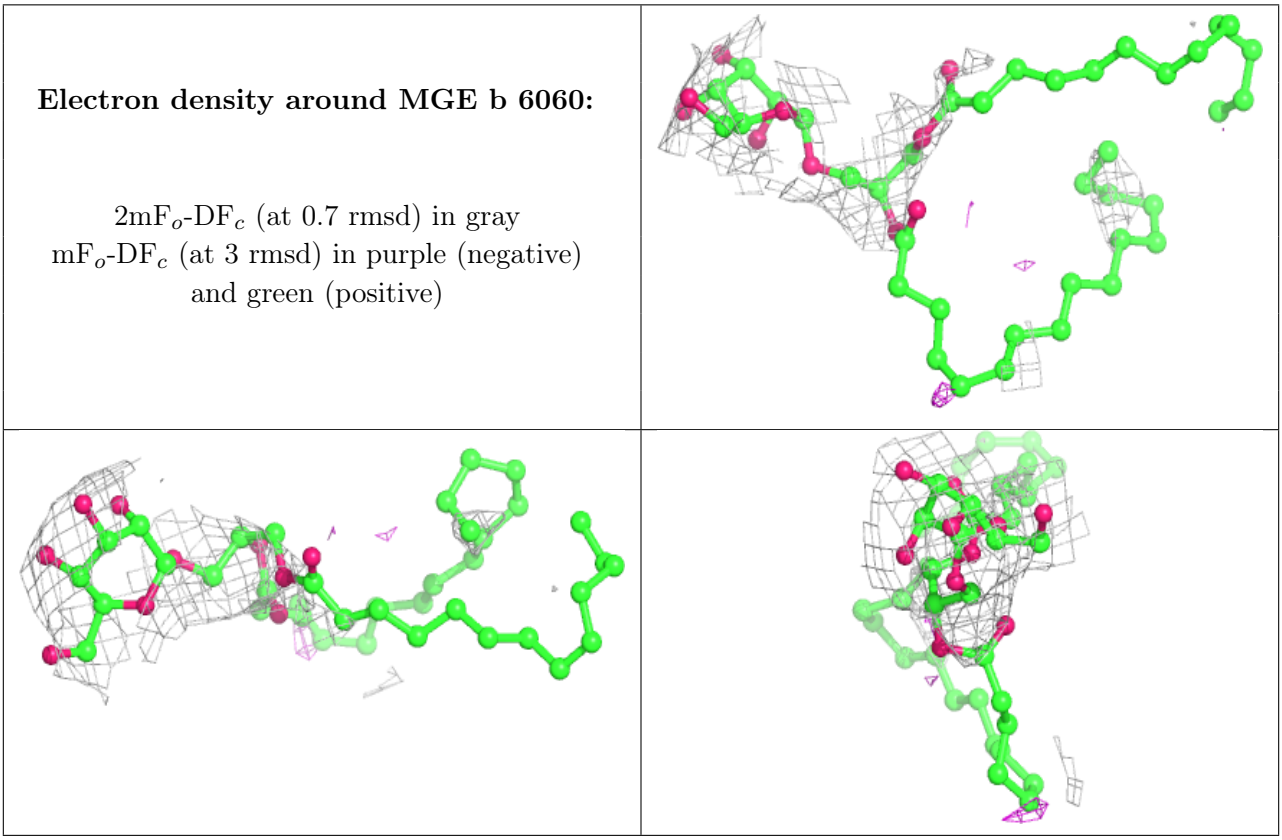
Electron density around BCR b 6045:

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



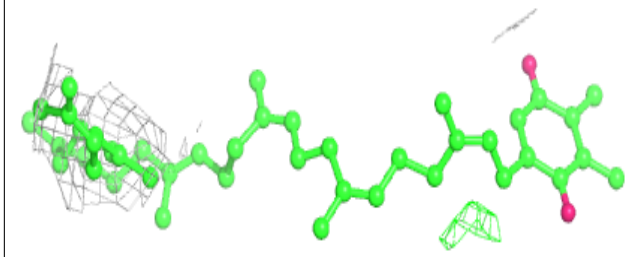
Electron density around MGE b 6060:

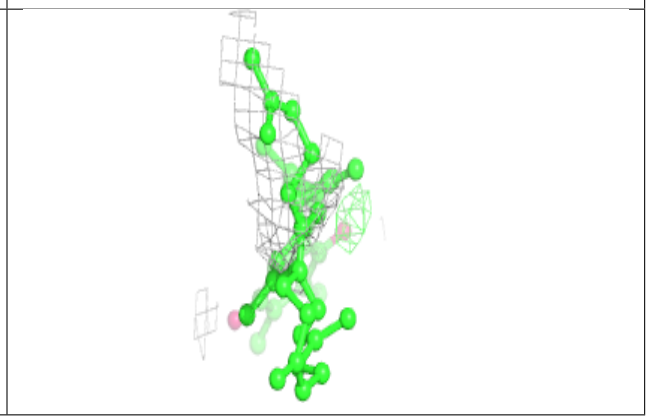
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PQ9 a 6043:

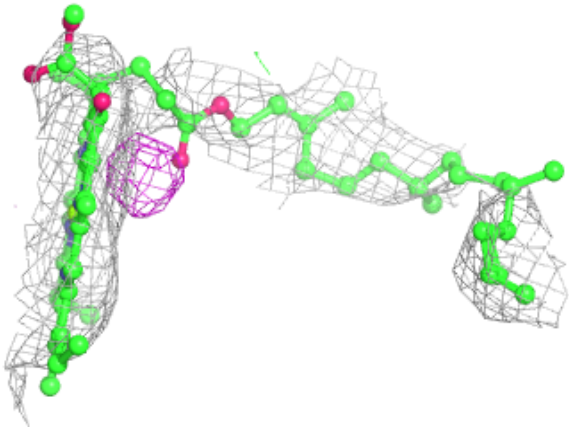
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

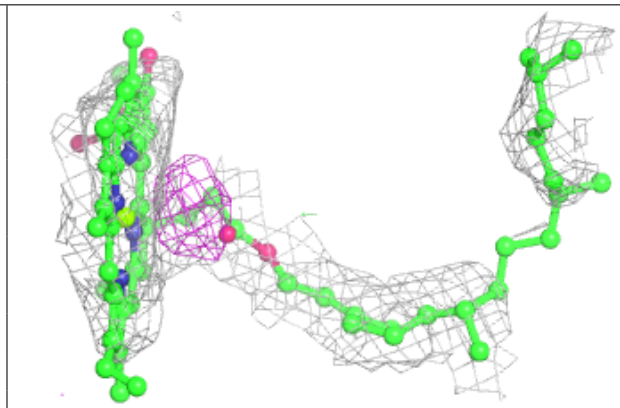




Electron density around CLA B 1014:

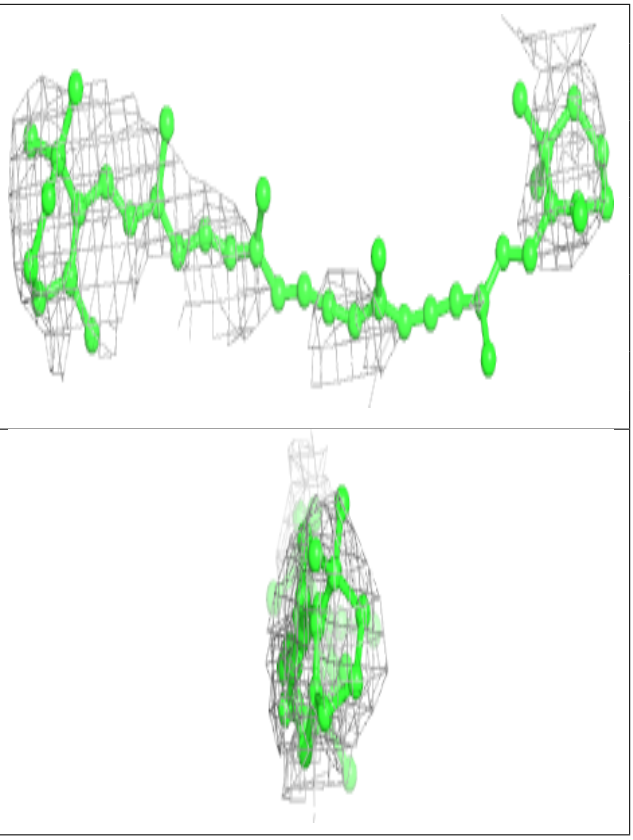
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





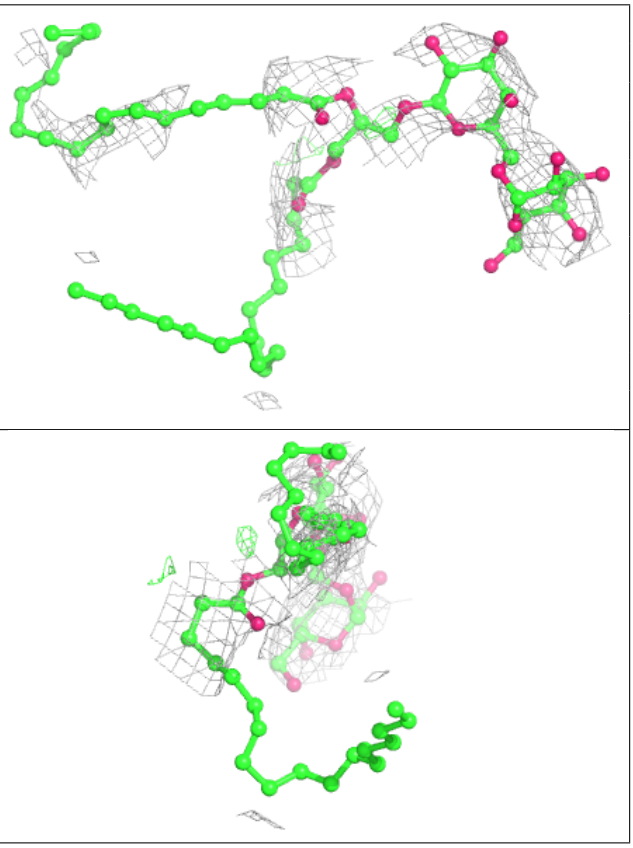
Electron density around BCR t 1046:

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



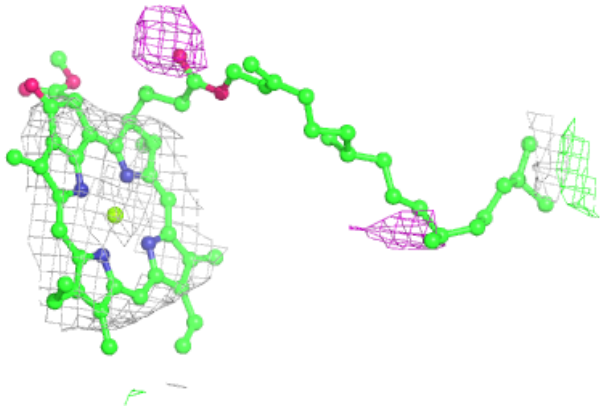
Electron density around DGD c 6056:

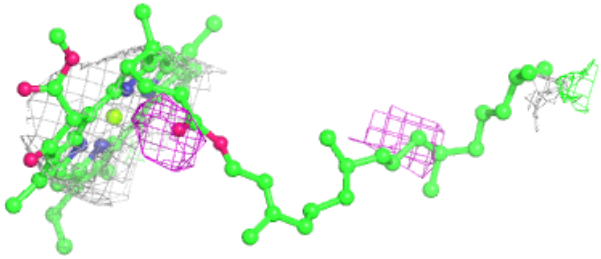
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

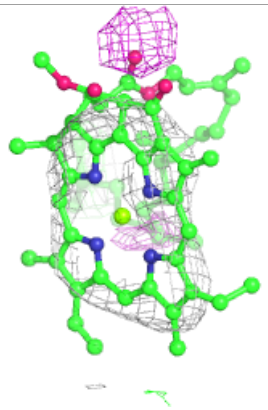


Electron density around CLA c 6035:

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

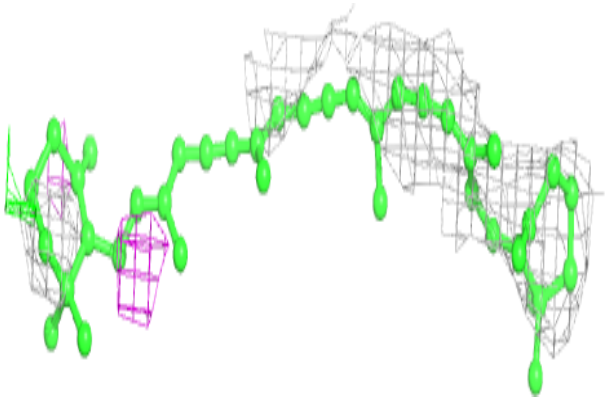


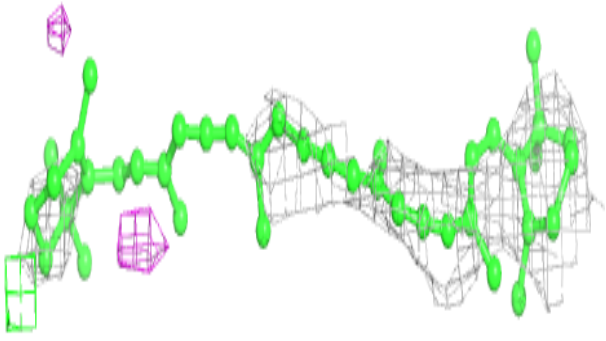


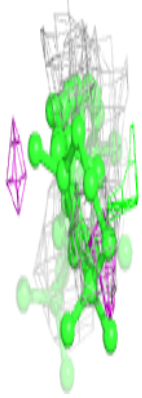


Electron density around BCR C 1052:

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

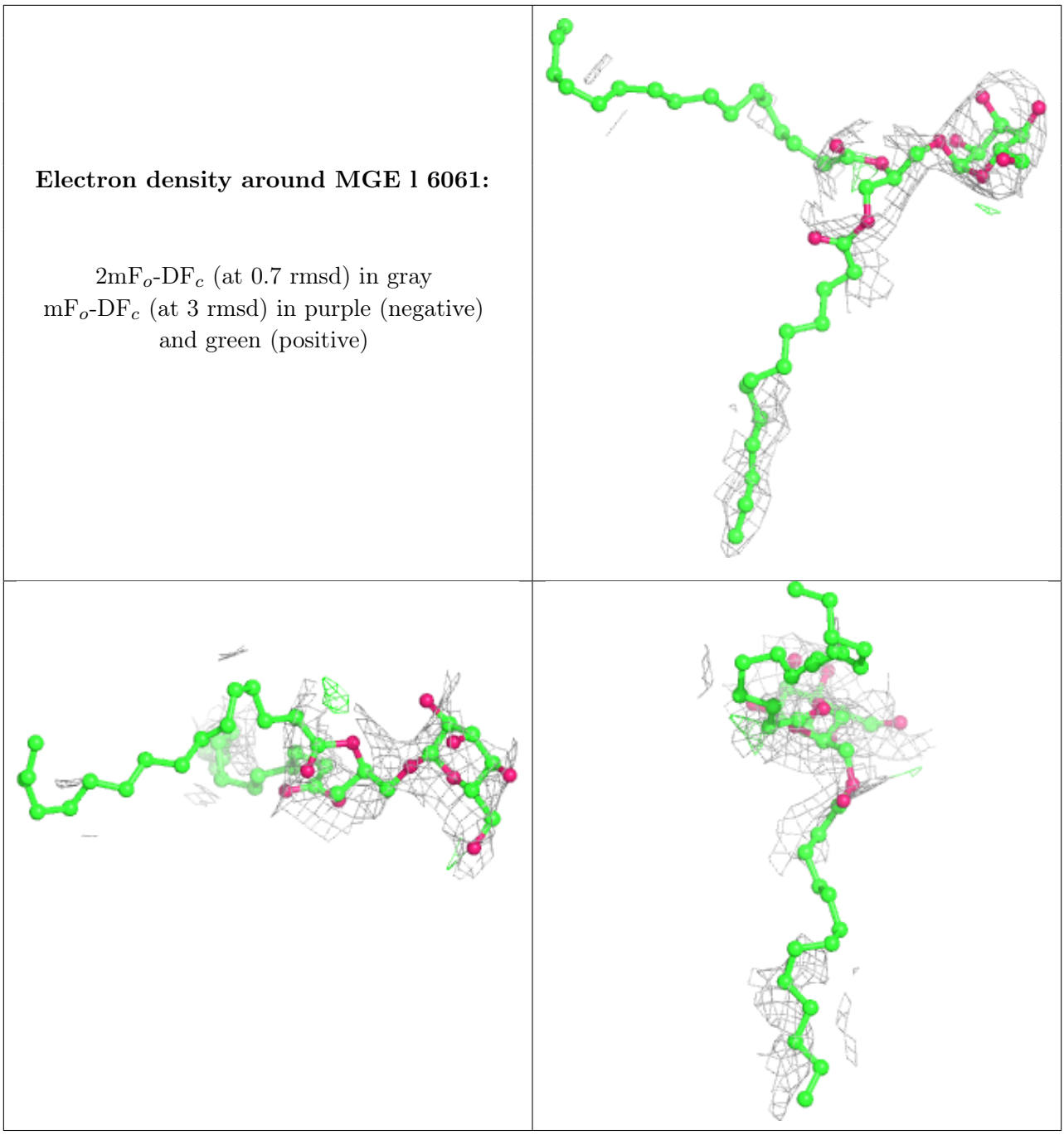






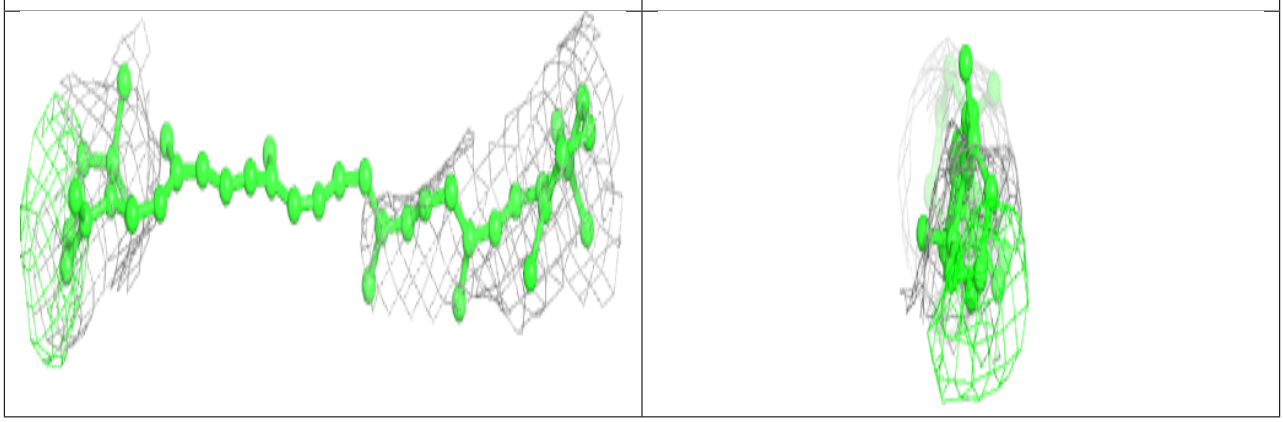
Electron density around MGE l 6061:

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



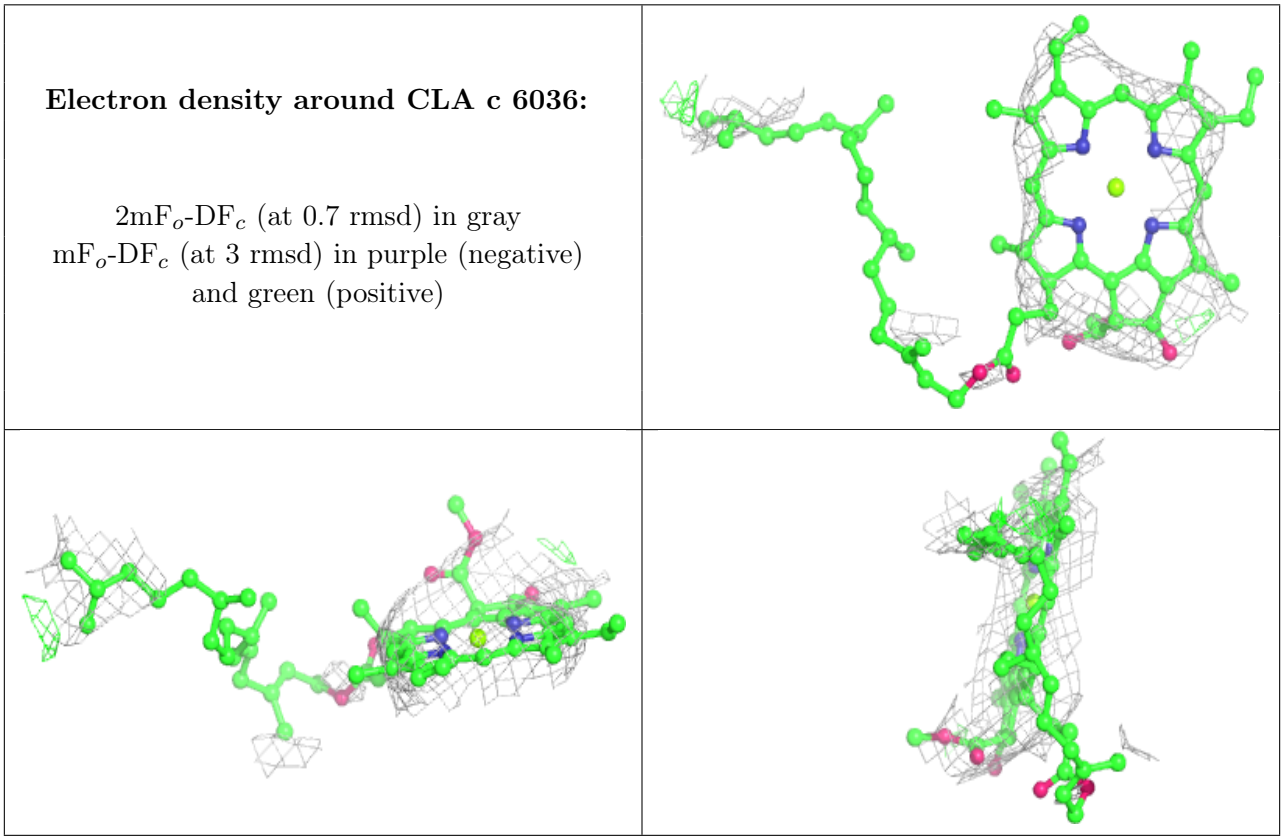
Electron density around BCR b 6047:

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



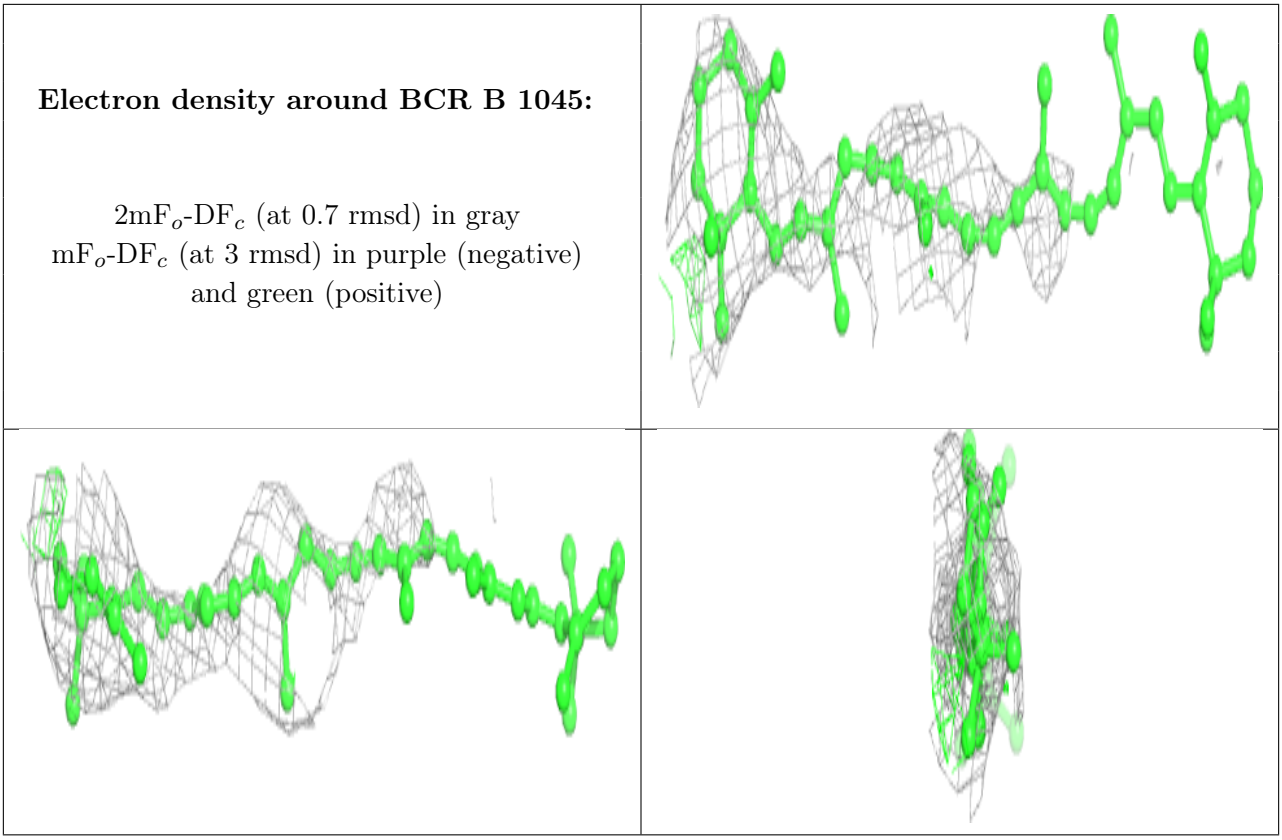
Electron density around CLA c 6036:

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



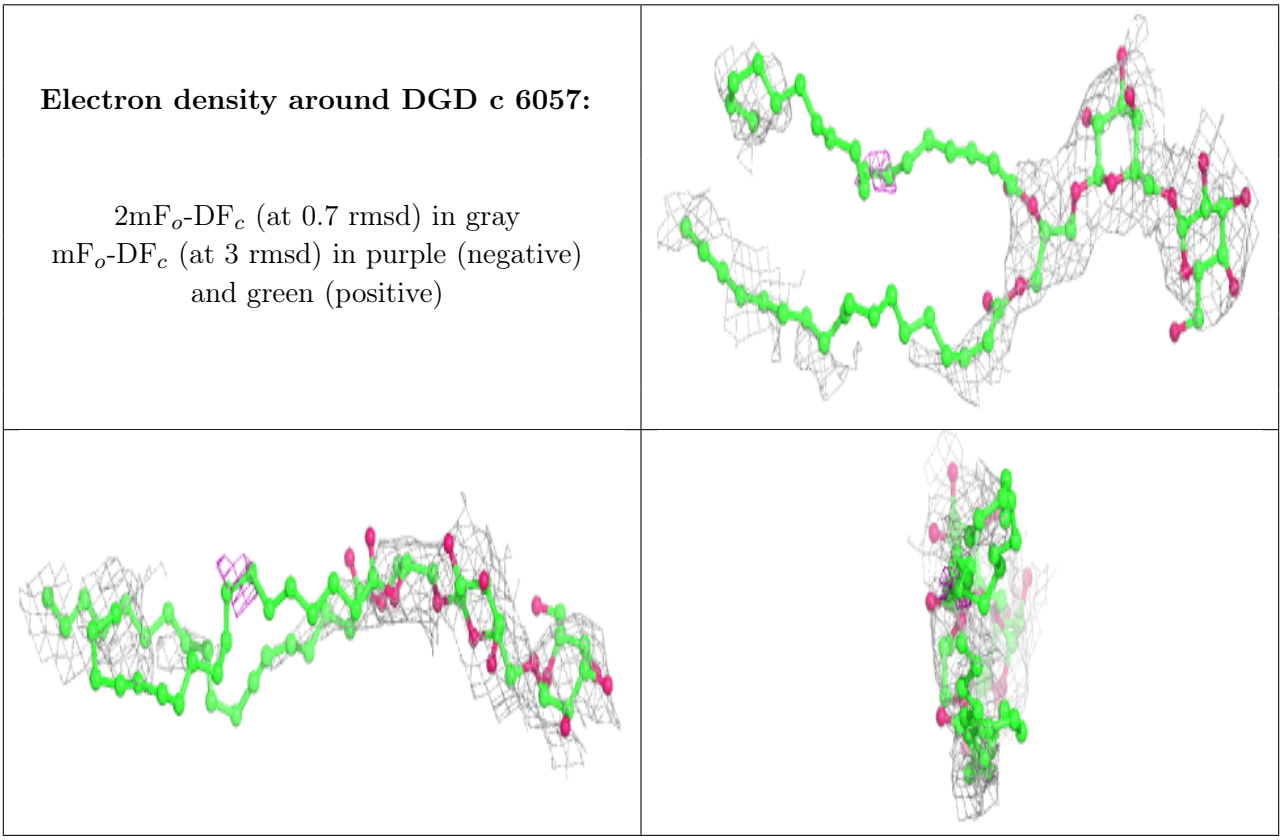
Electron density around BCR B 1045:

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



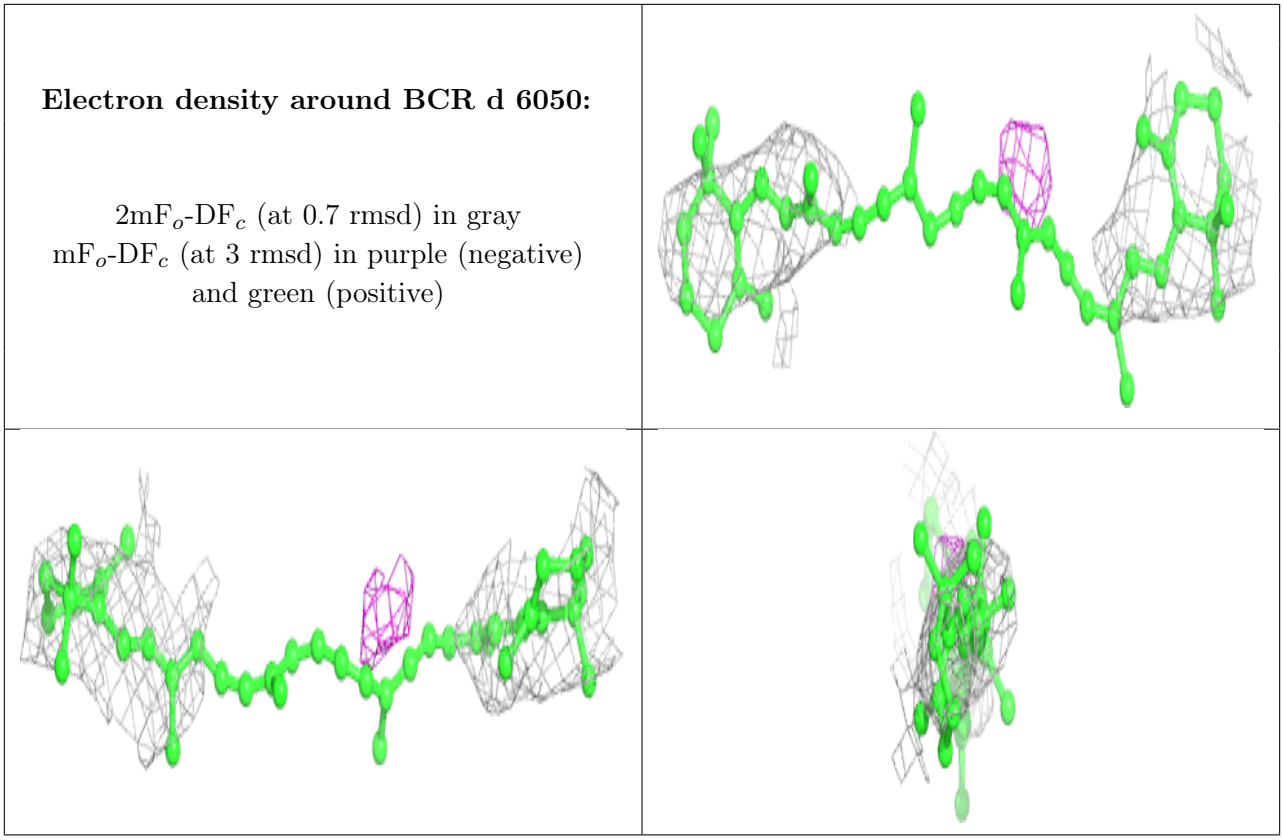
Electron density around DGD c 6057:

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



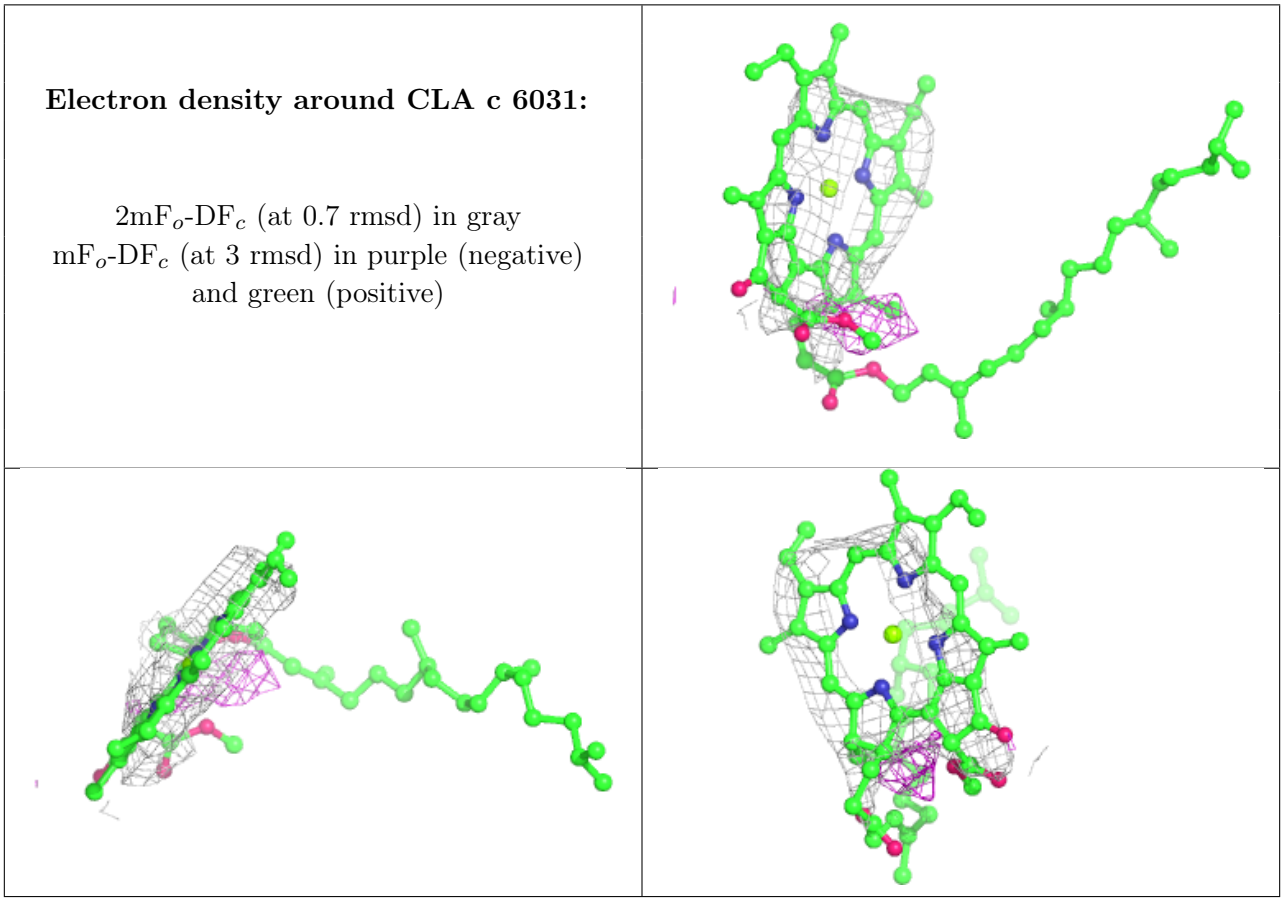
Electron density around BCR d 6050:

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



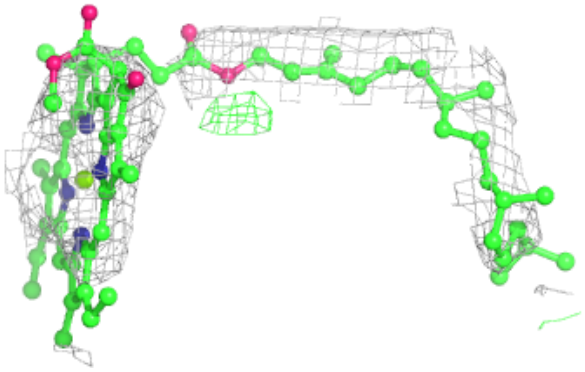
Electron density around CLA c 6031:

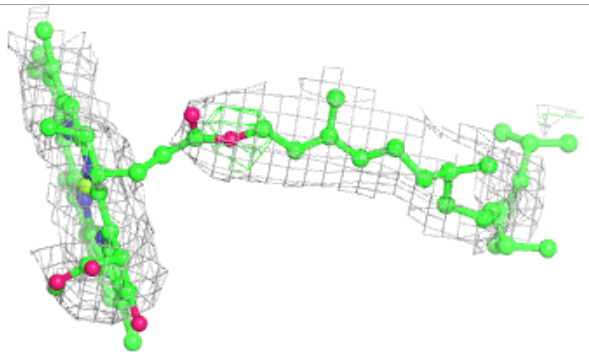
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

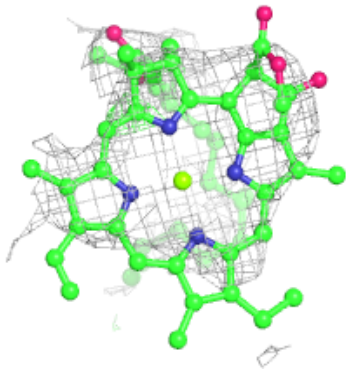


Electron density around CLA C 1030:

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

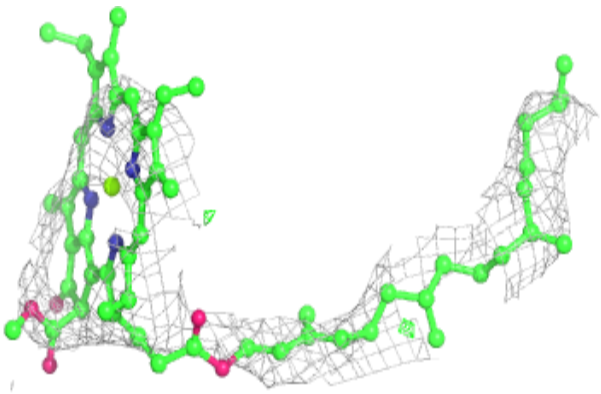


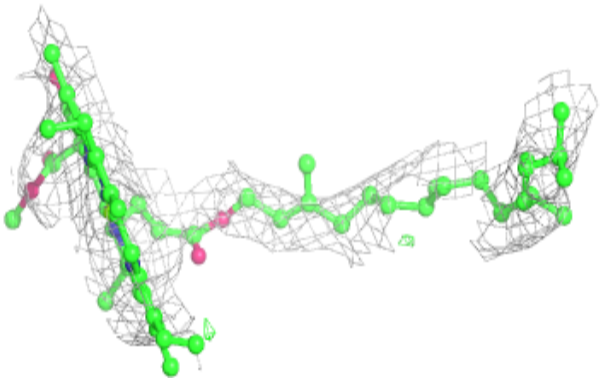


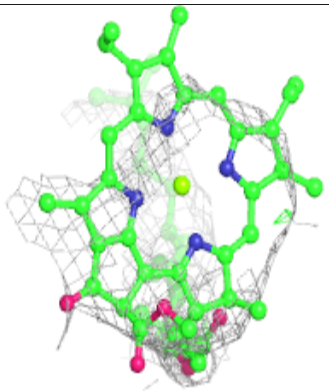


Electron density around CLA H 1017:

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

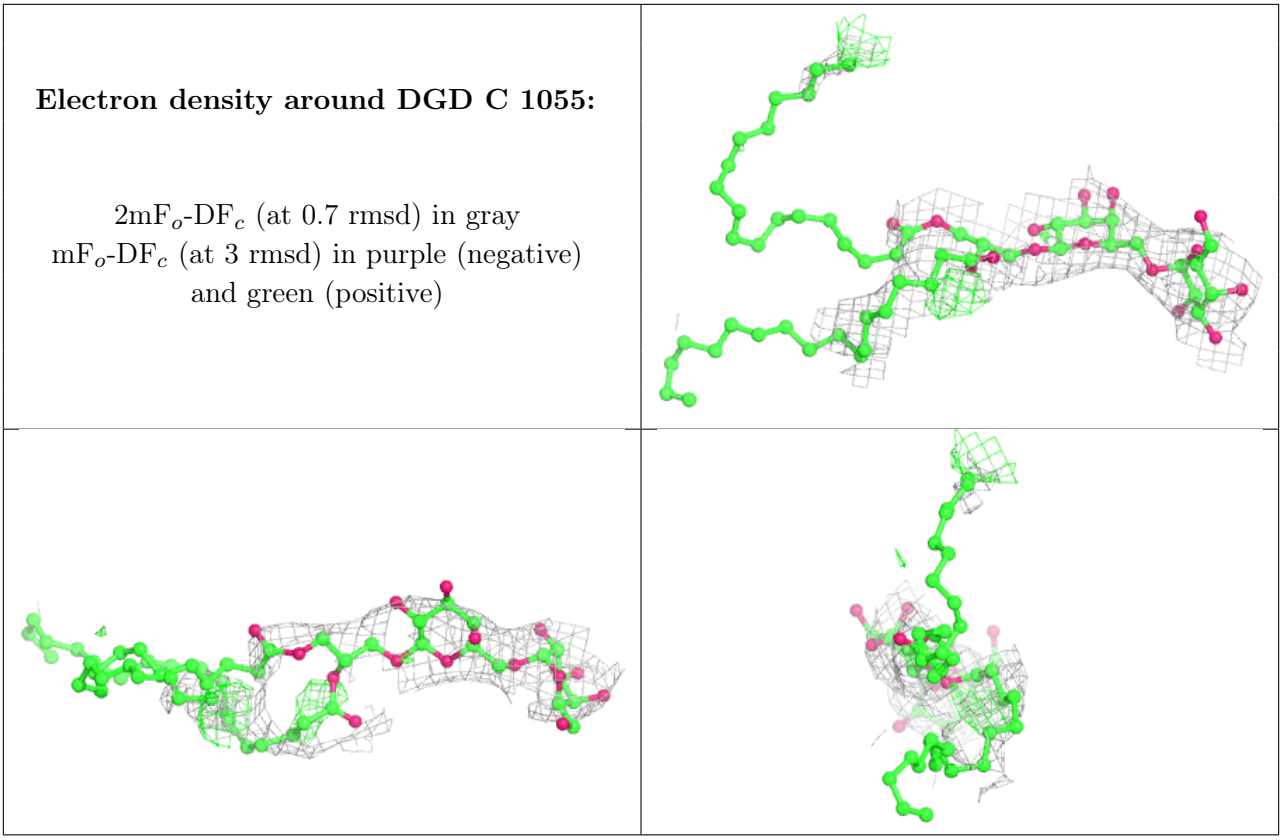






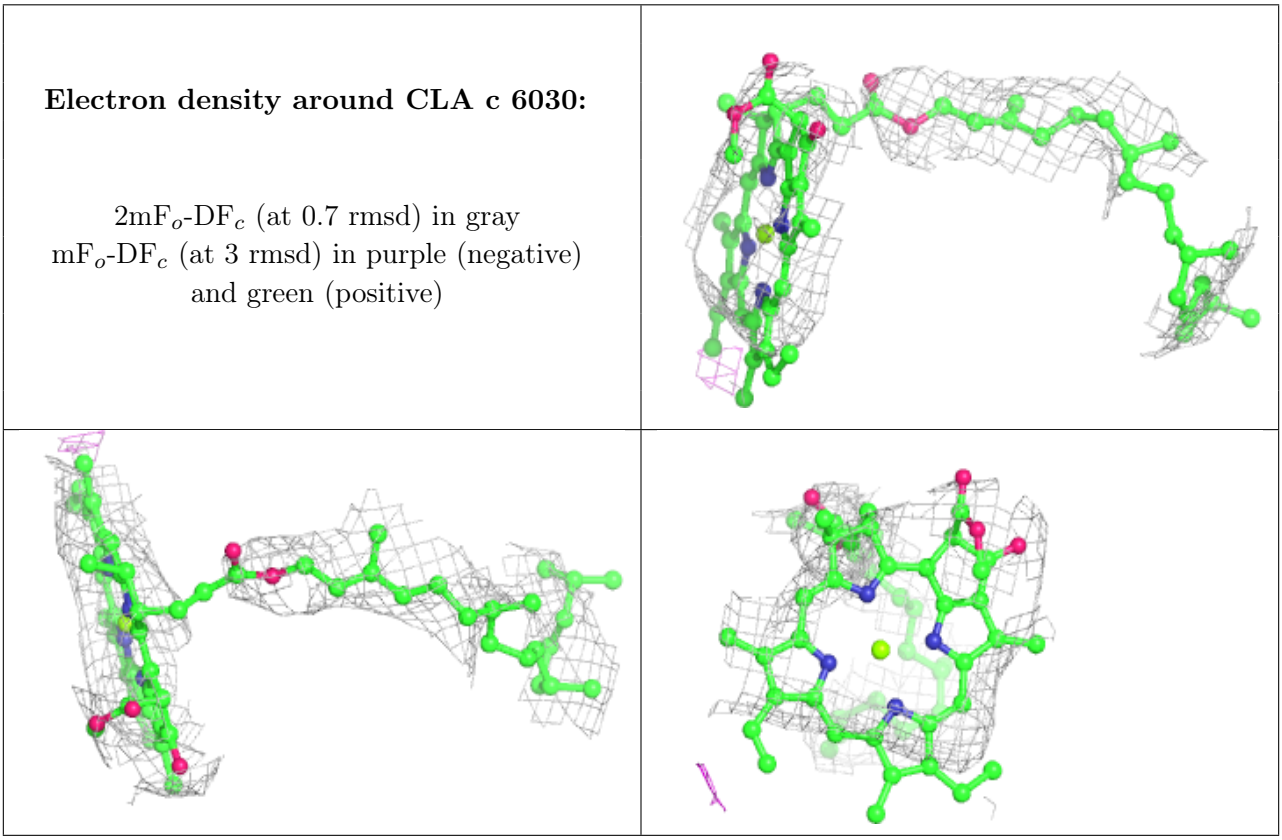
Electron density around DGD C 1055:

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



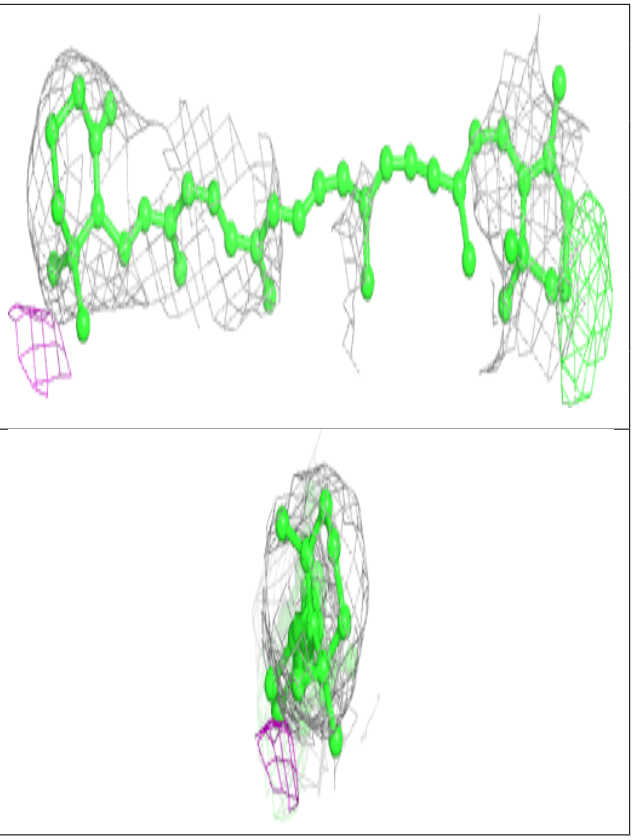
Electron density around CLA c 6030:

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



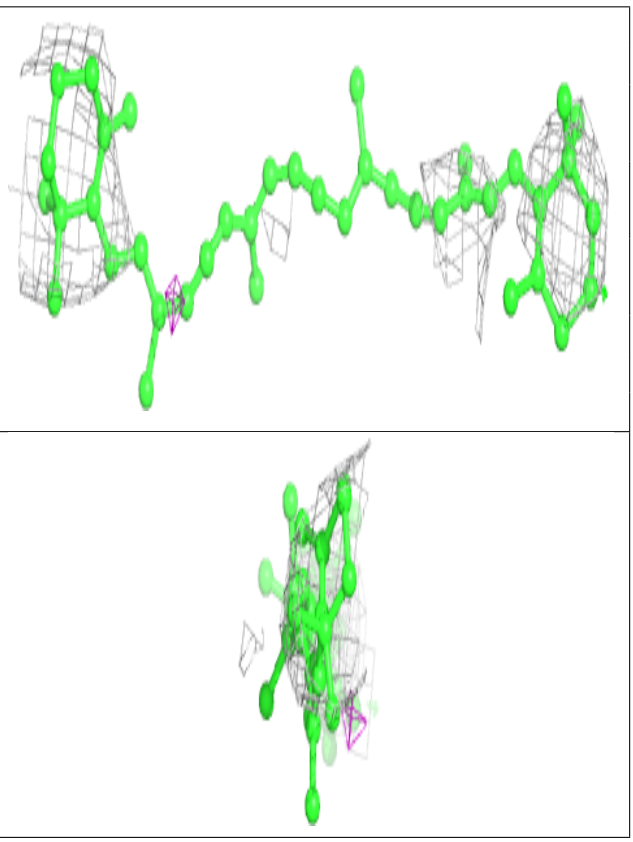
Electron density around BCR B 1047:

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



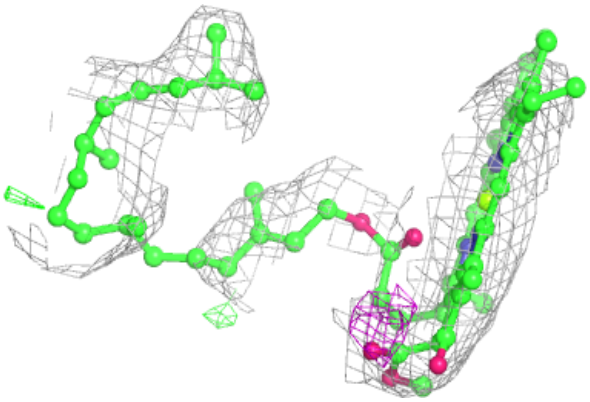
Electron density around BCR D 1050:

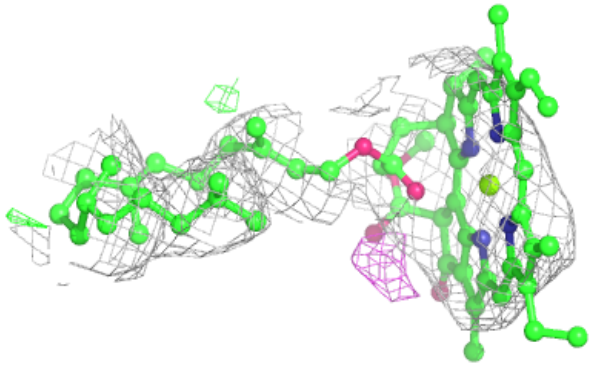
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

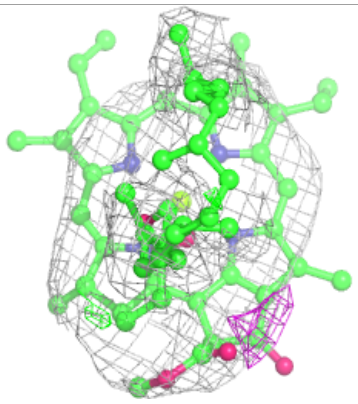


Electron density around CLA B 1009:

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

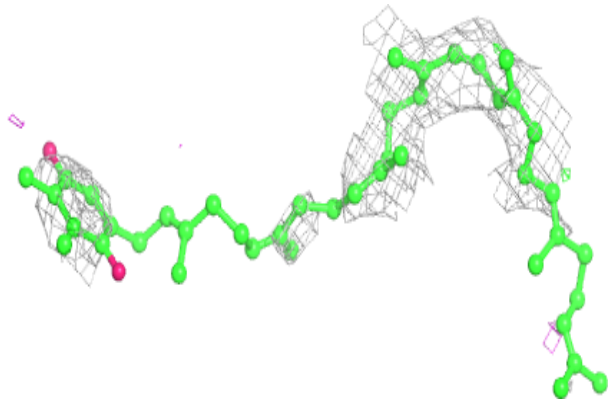


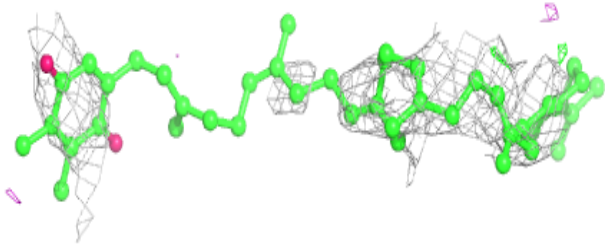


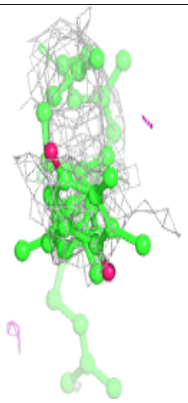


Electron density around PQ9 D 1042:

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

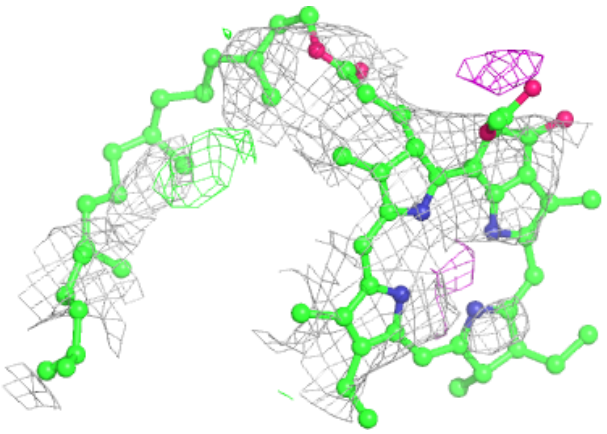


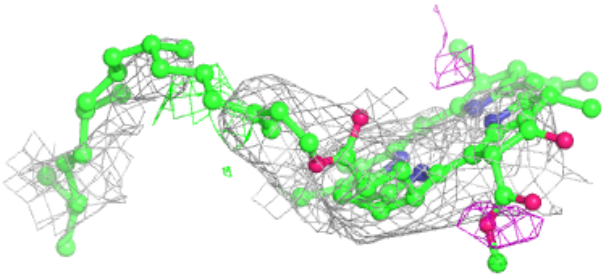


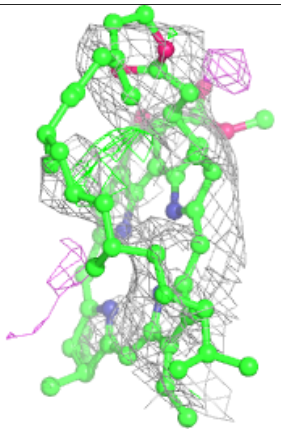


Electron density around PHO D 1039:

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

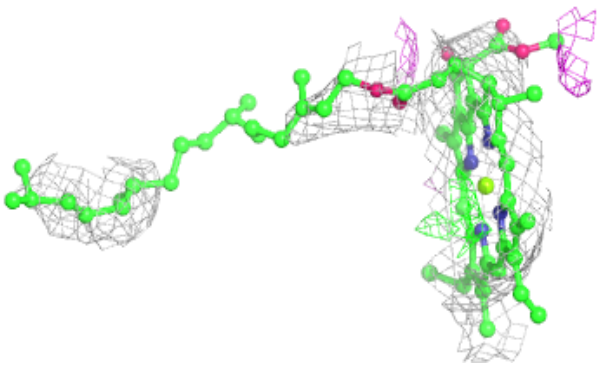


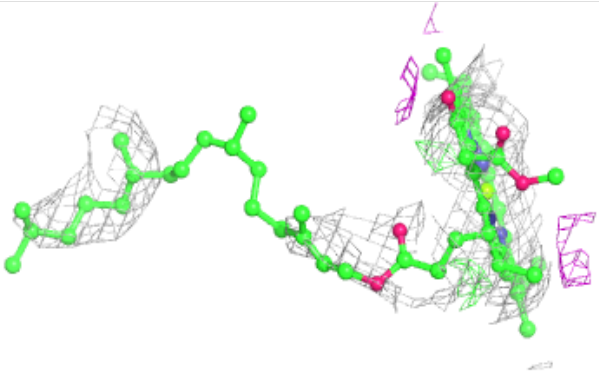


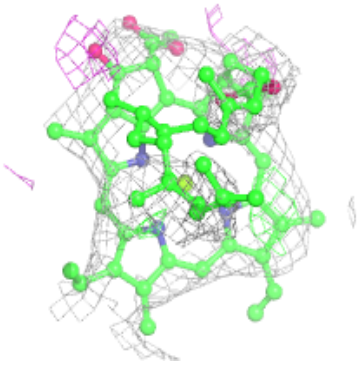


Electron density around CLA C 1032:

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

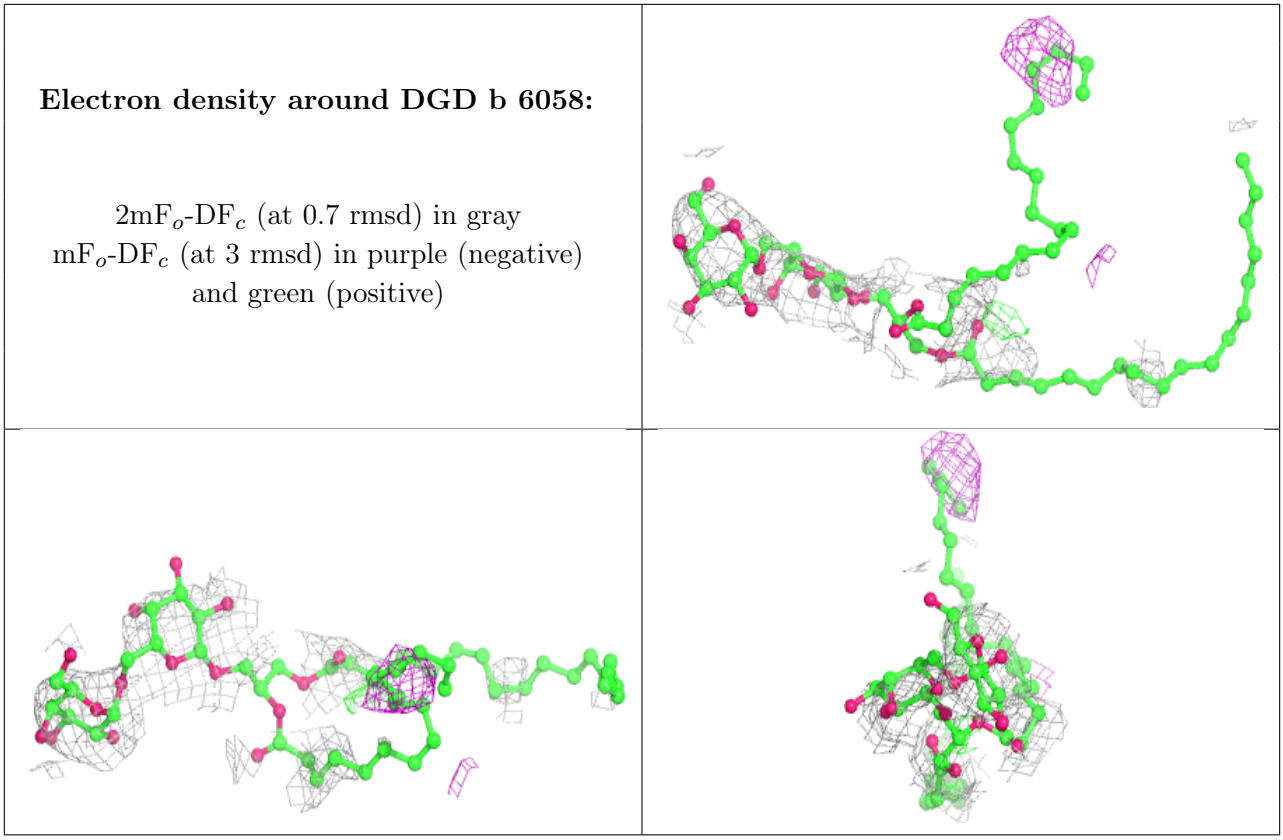






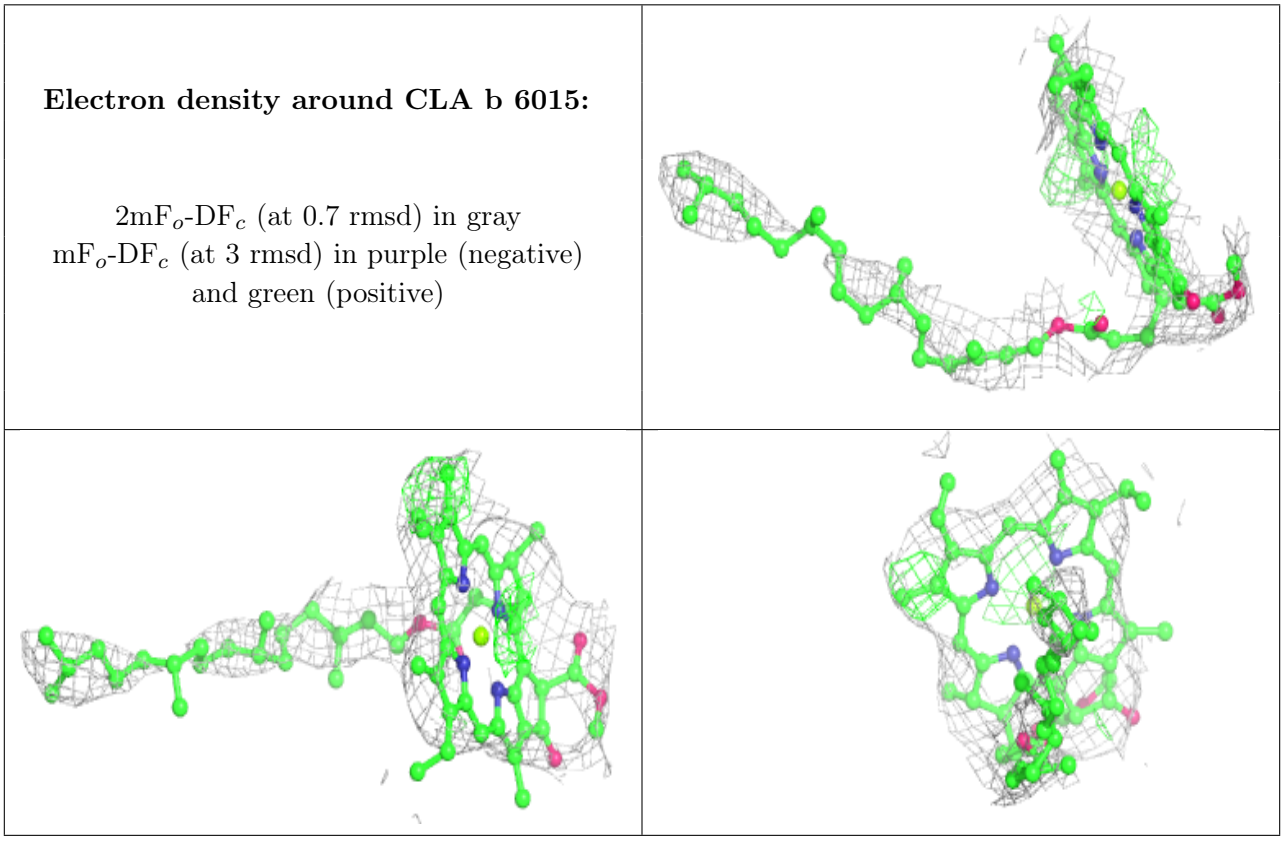
Electron density around DGD b 6058:

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



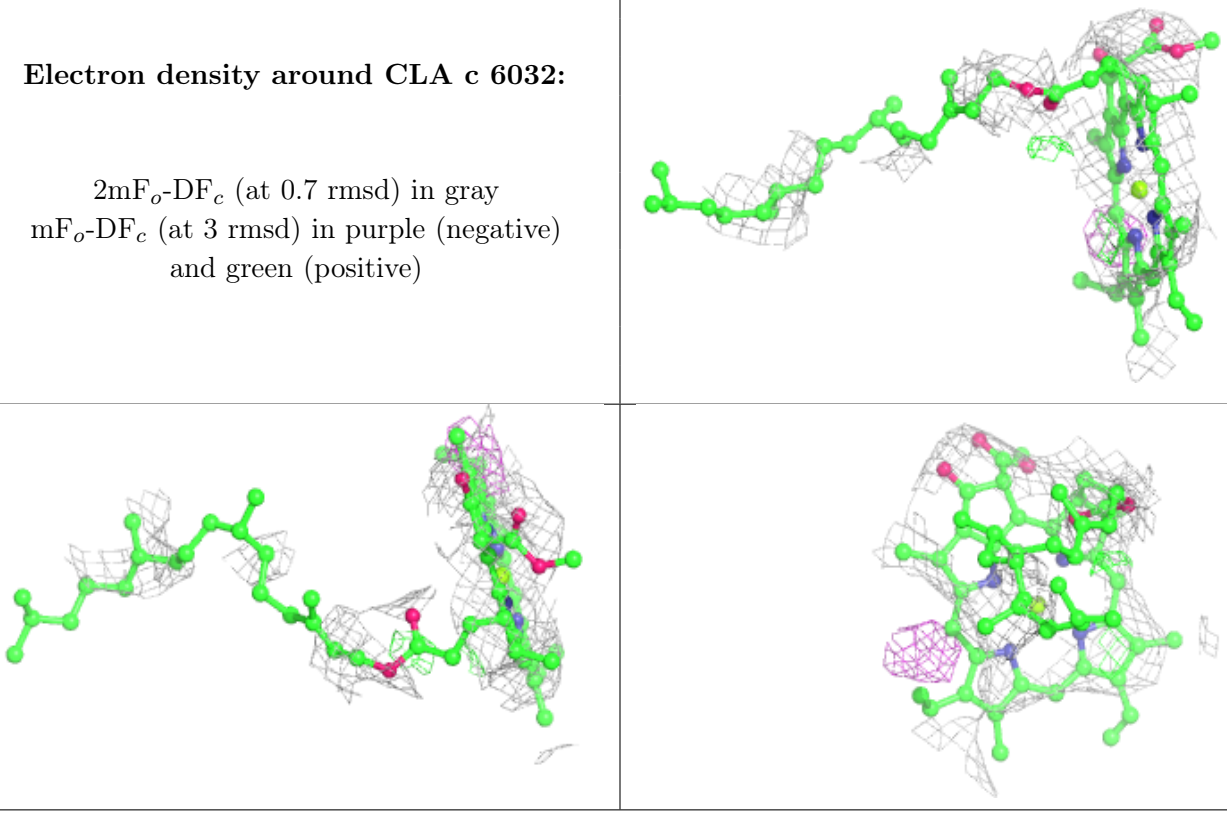
Electron density around CLA b 6015:

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



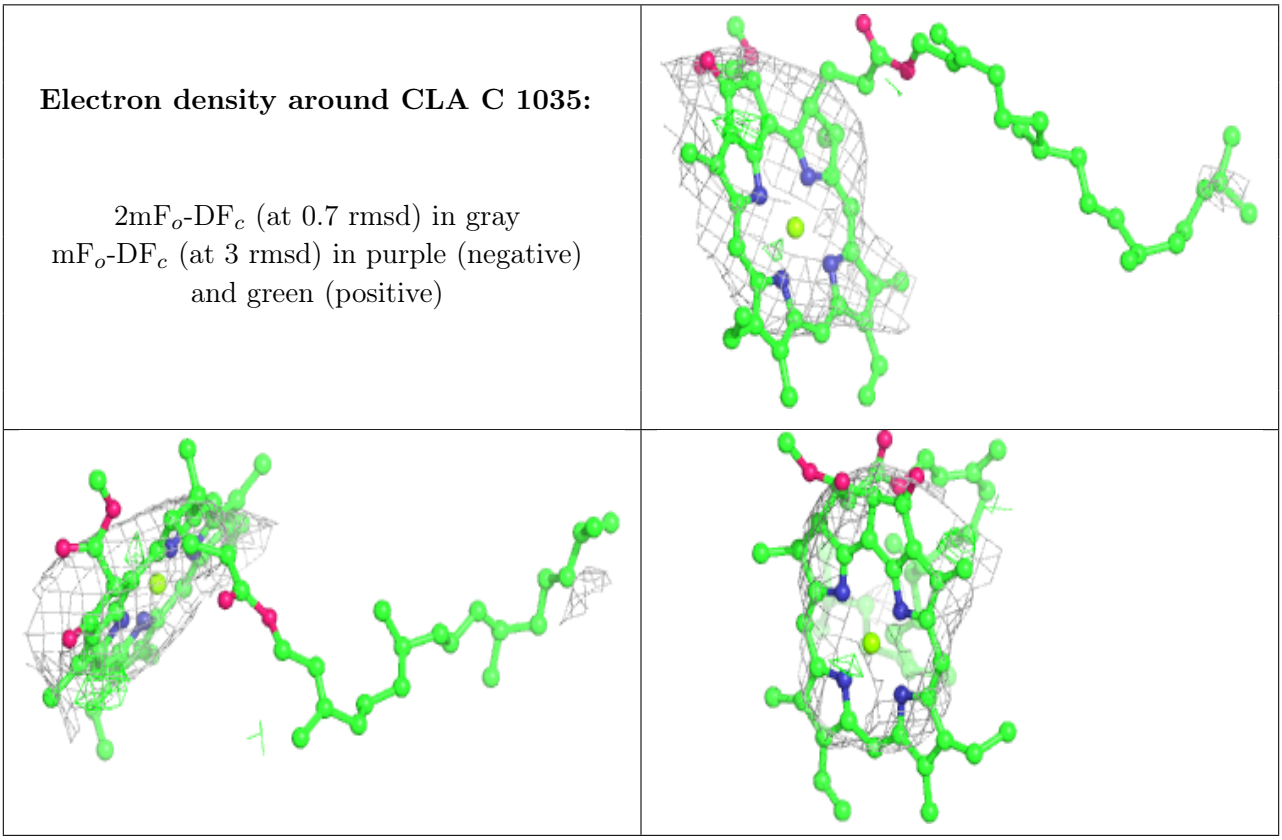
Electron density around CLA c 6032:

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



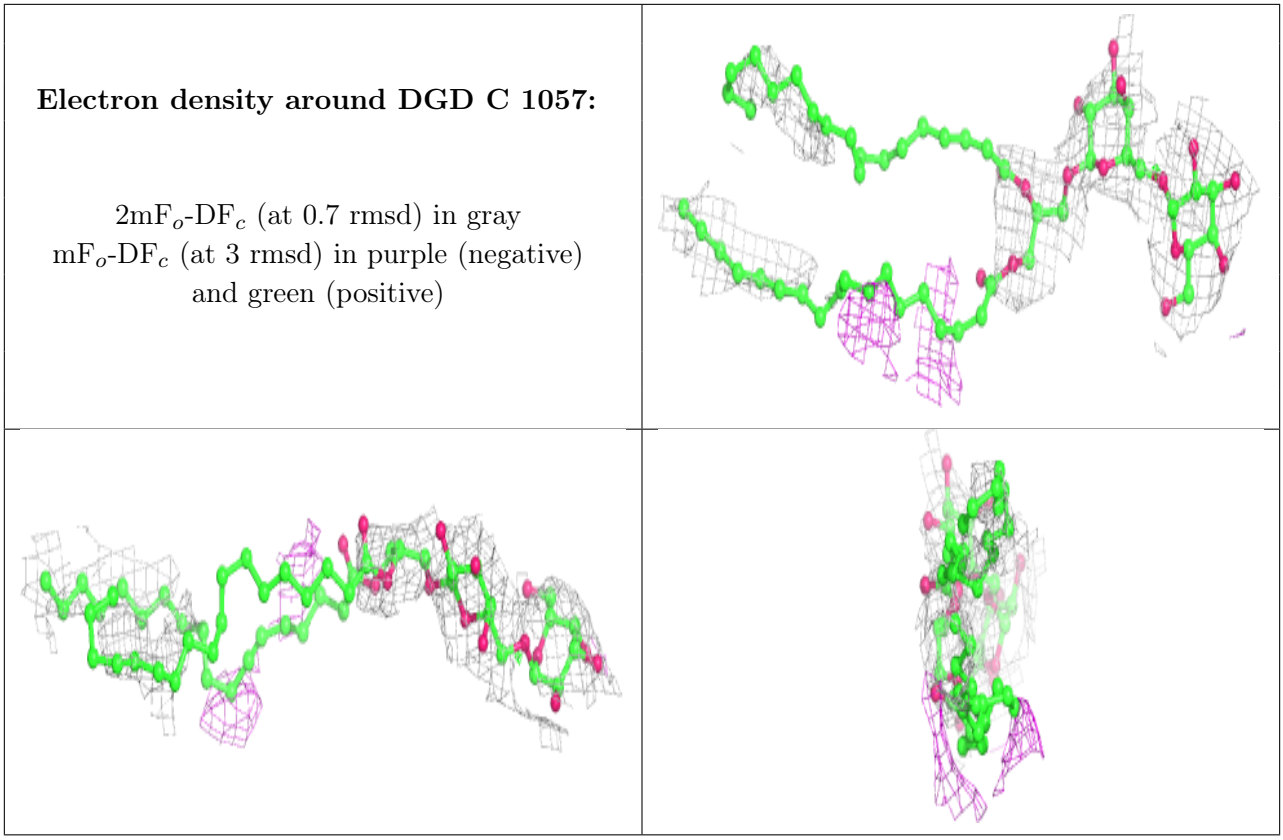
Electron density around CLA C 1035:

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



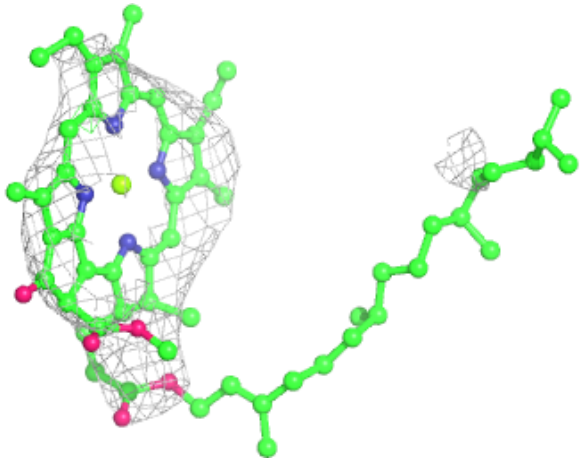
Electron density around DGD C 1057:

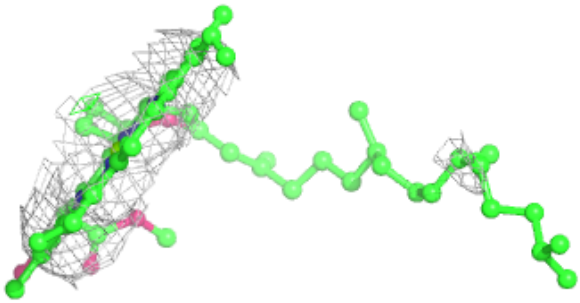
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

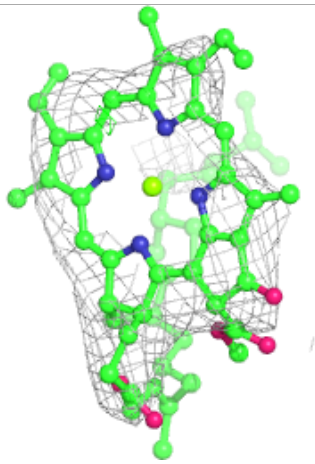


Electron density around CLA C 1031:

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

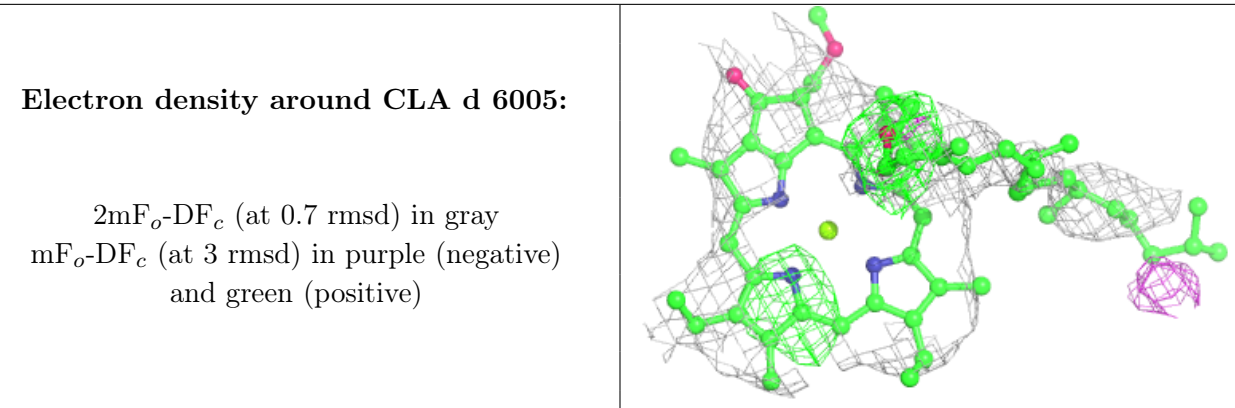






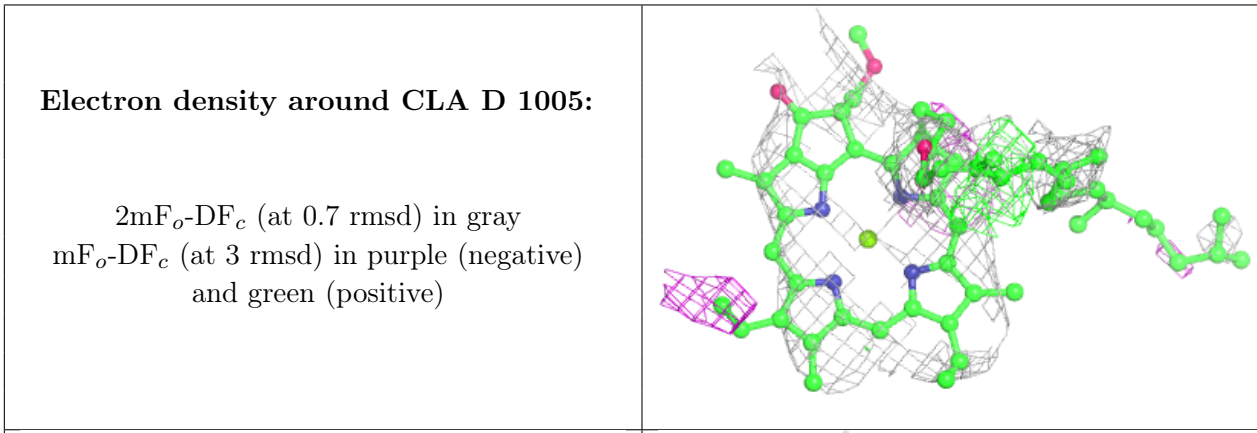
Electron density around CLA d 6005:

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



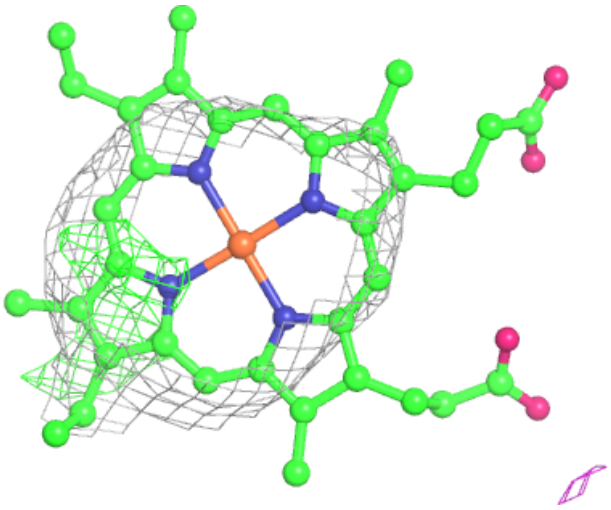
Electron density around CLA D 1005:

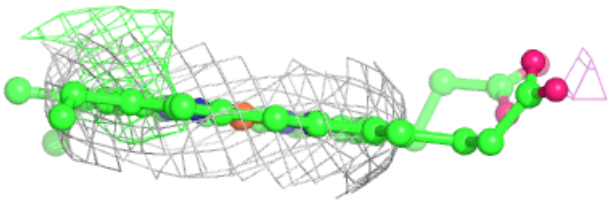
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

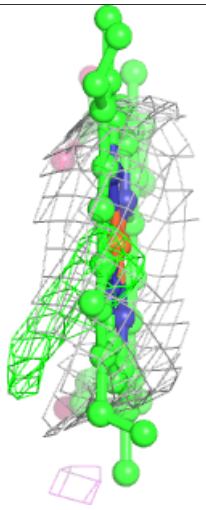


Electron density around HEM F 1040:

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

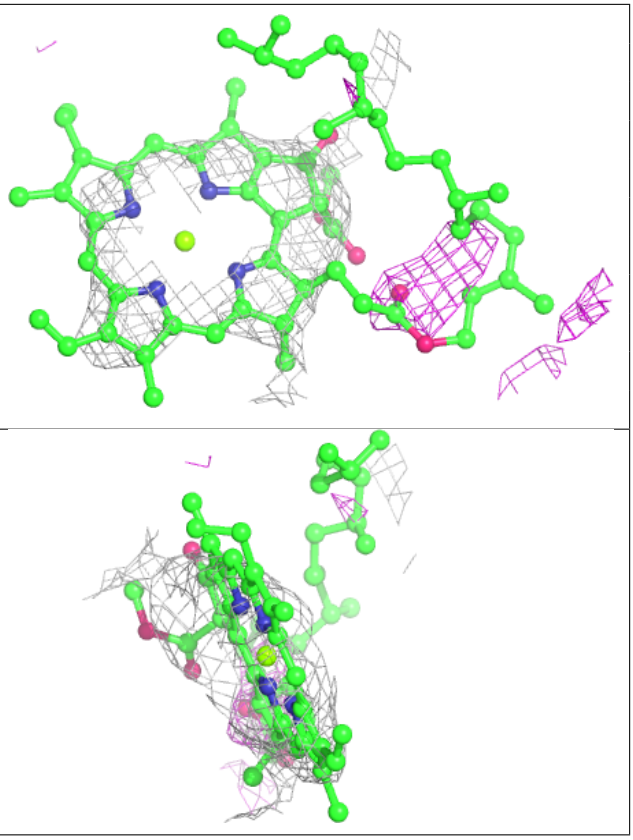






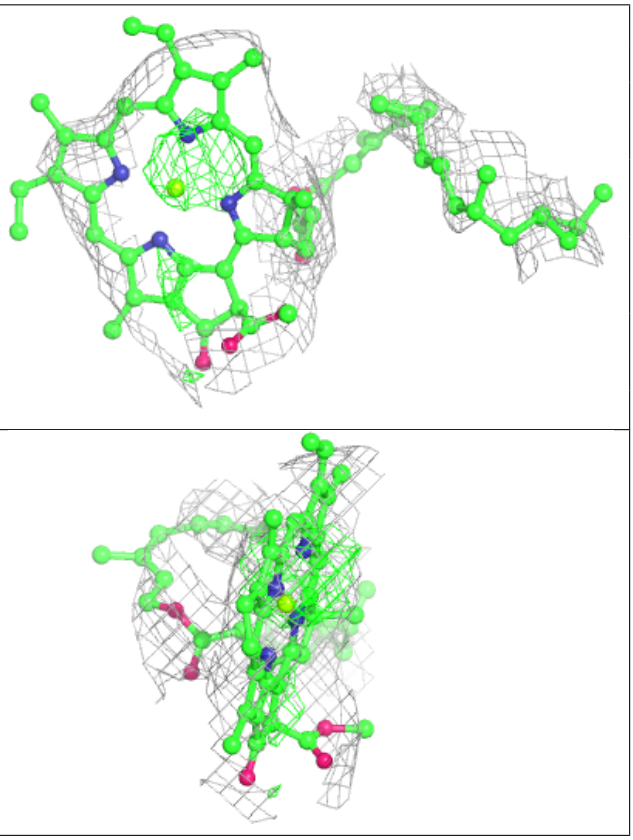
Electron density around CLA c 6033:

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



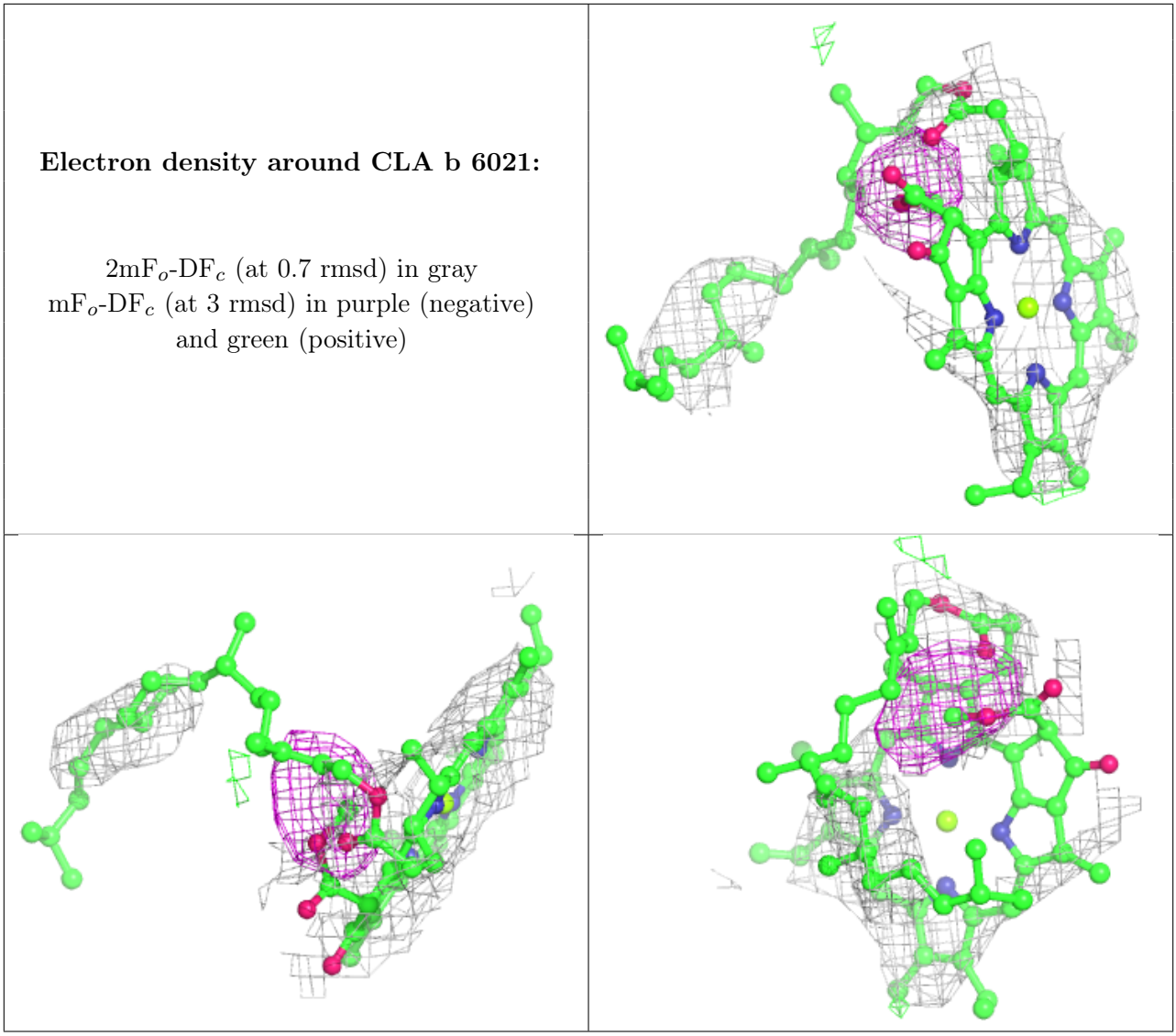
Electron density around CLA A 1006:

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



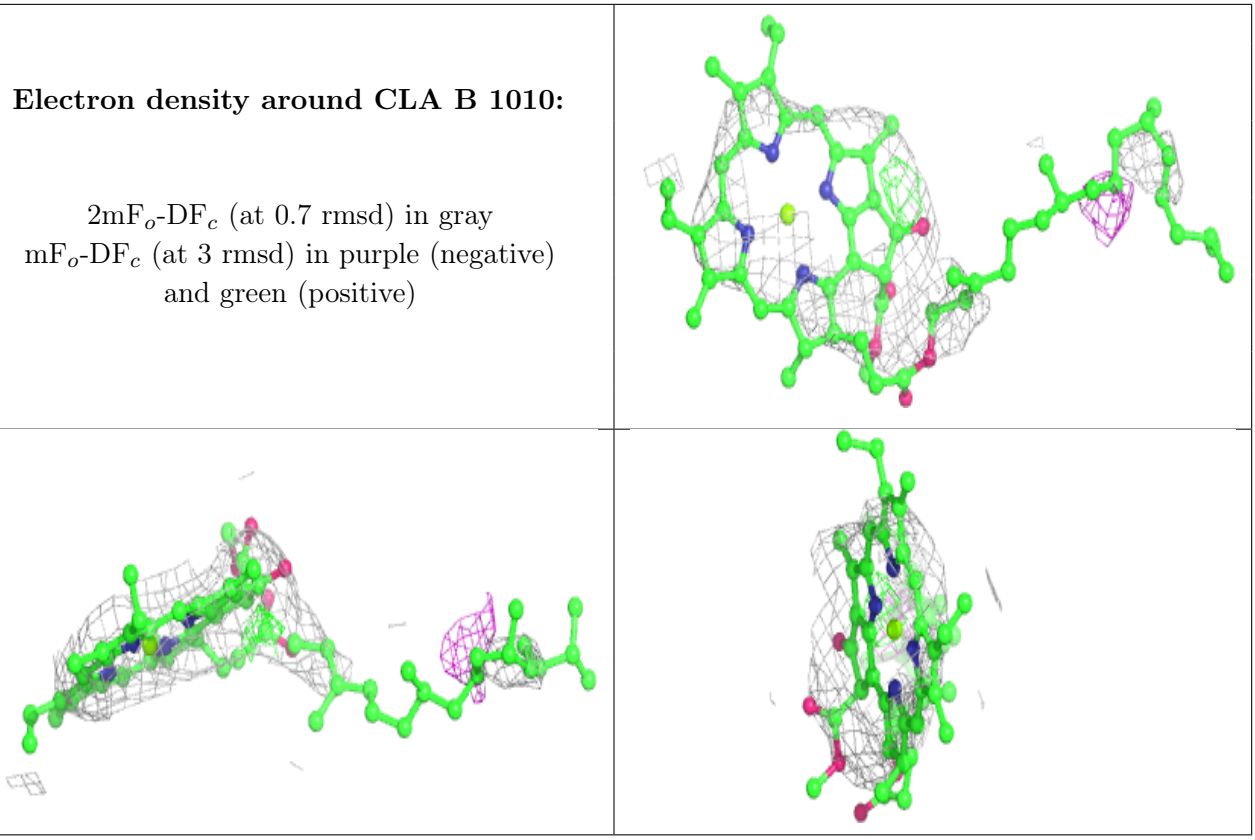
Electron density around CLA b 6021:

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



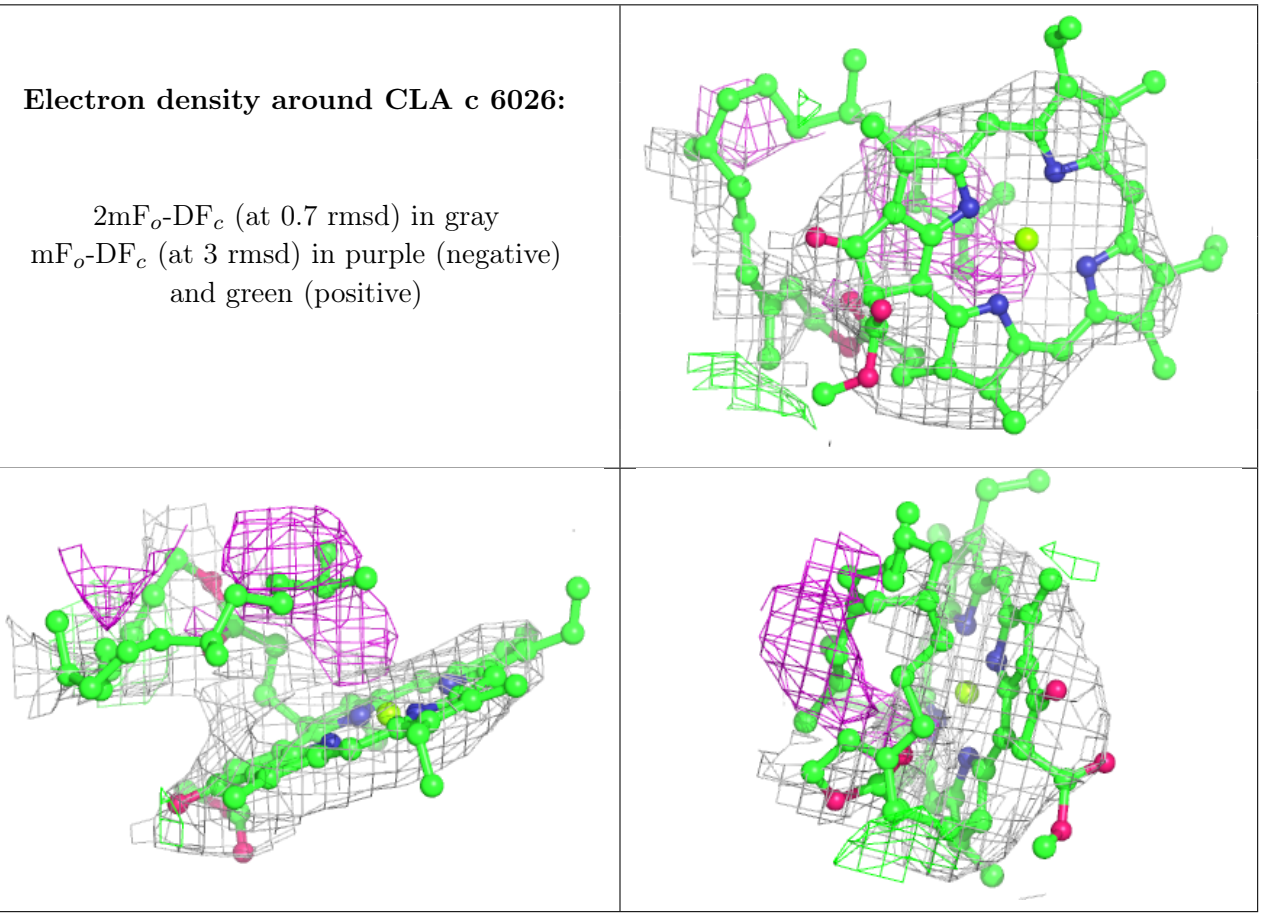
Electron density around CLA B 1010:

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



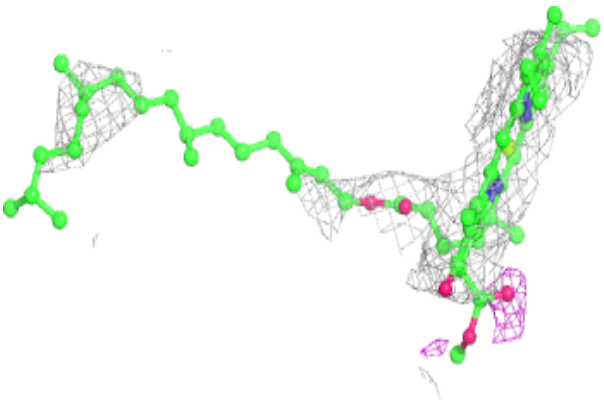
Electron density around CLA c 6026:

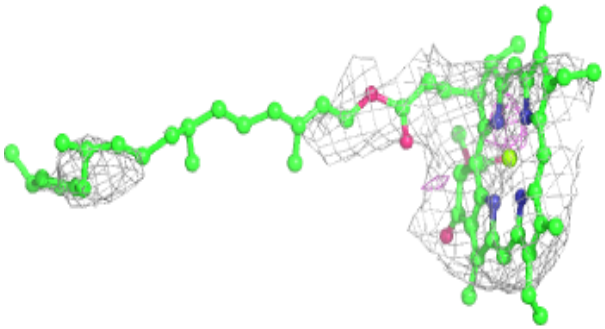
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

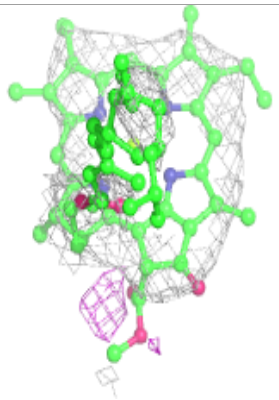


Electron density around CLA b 6012:

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

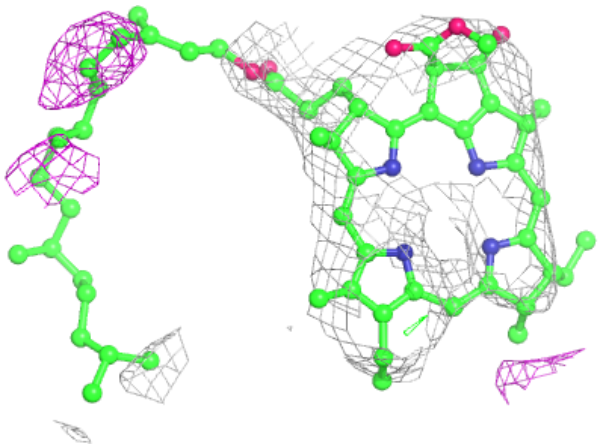


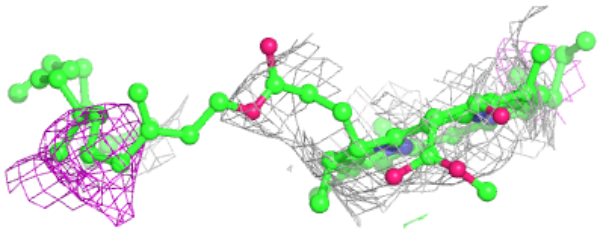


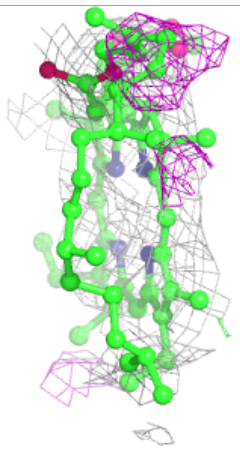


Electron density around PHO a 6038:

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

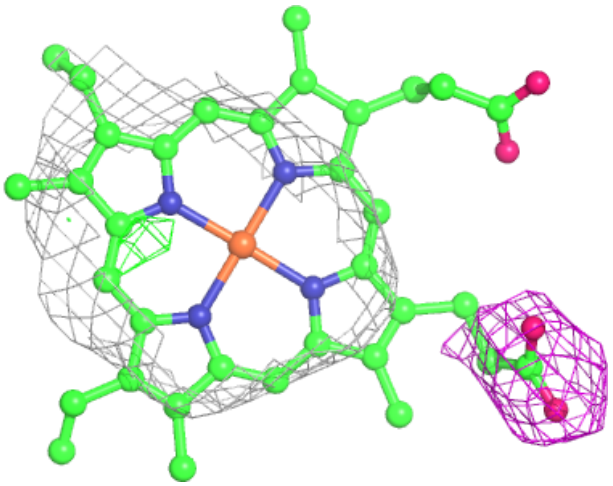


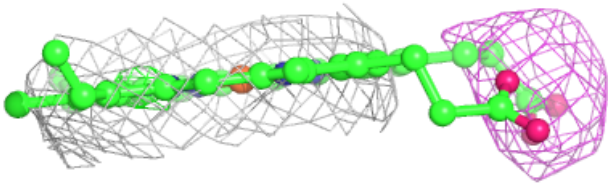


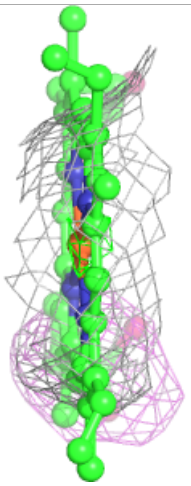


Electron density around HEM f 6040:

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

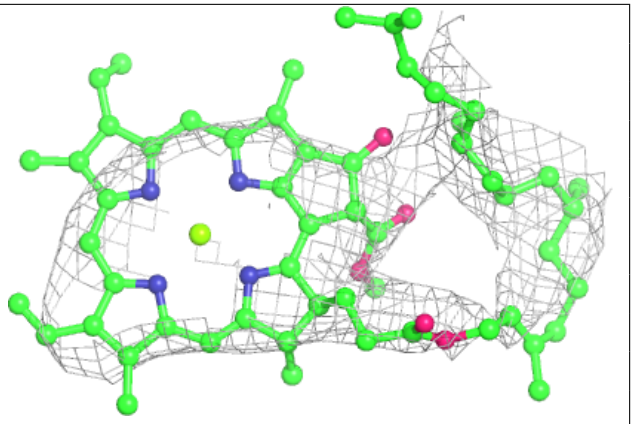


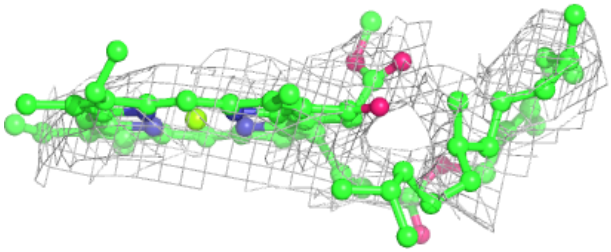


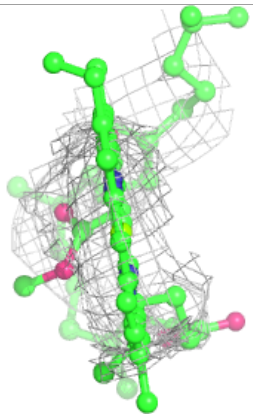


Electron density around CLA B 1018:

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

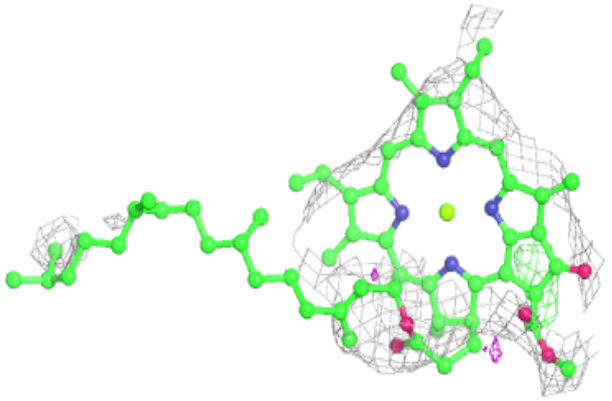


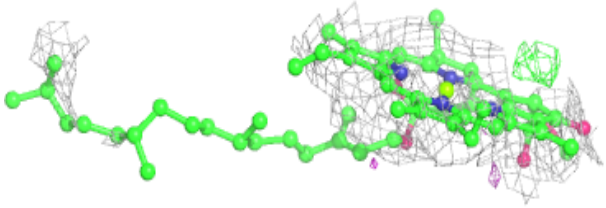


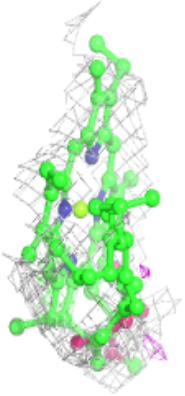


Electron density around CLA b 6011:

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

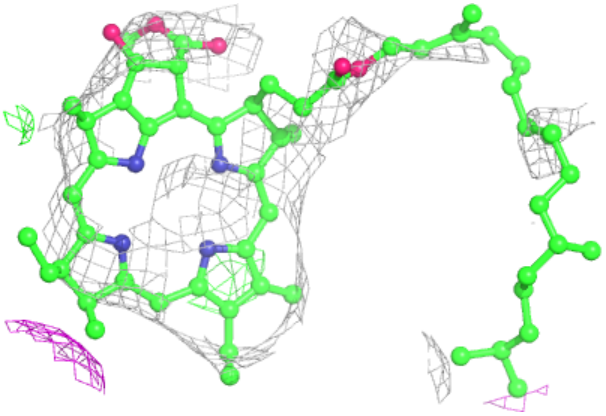


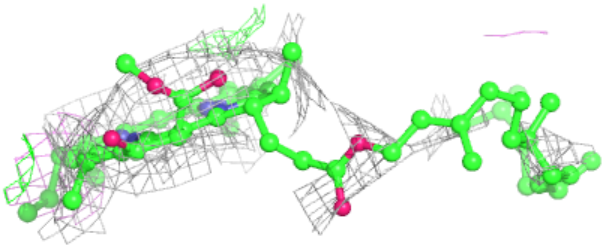


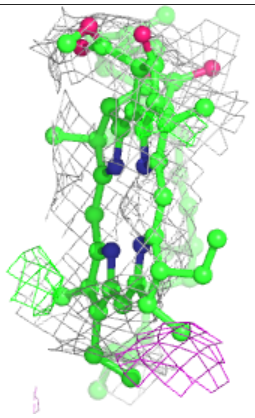


Electron density around PHO A 1038:

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

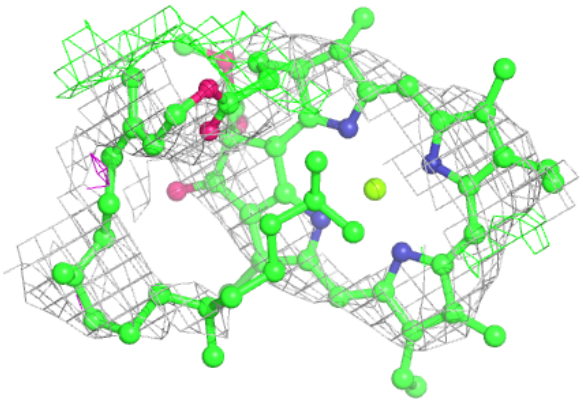


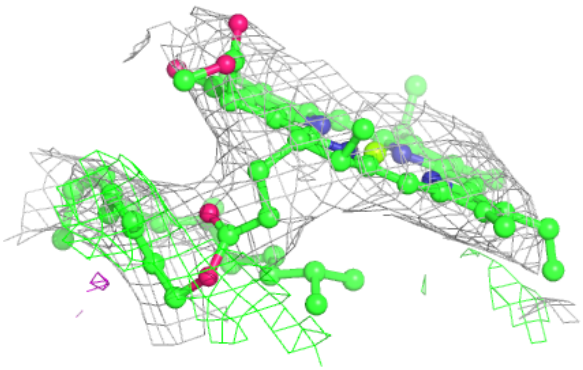


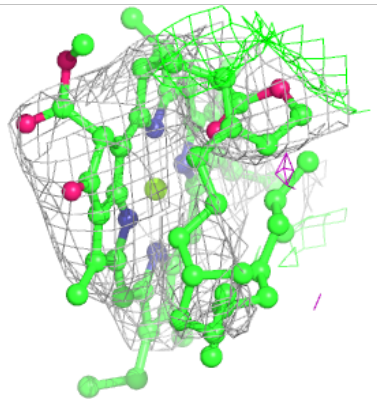


Electron density around CLA C 1026:

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

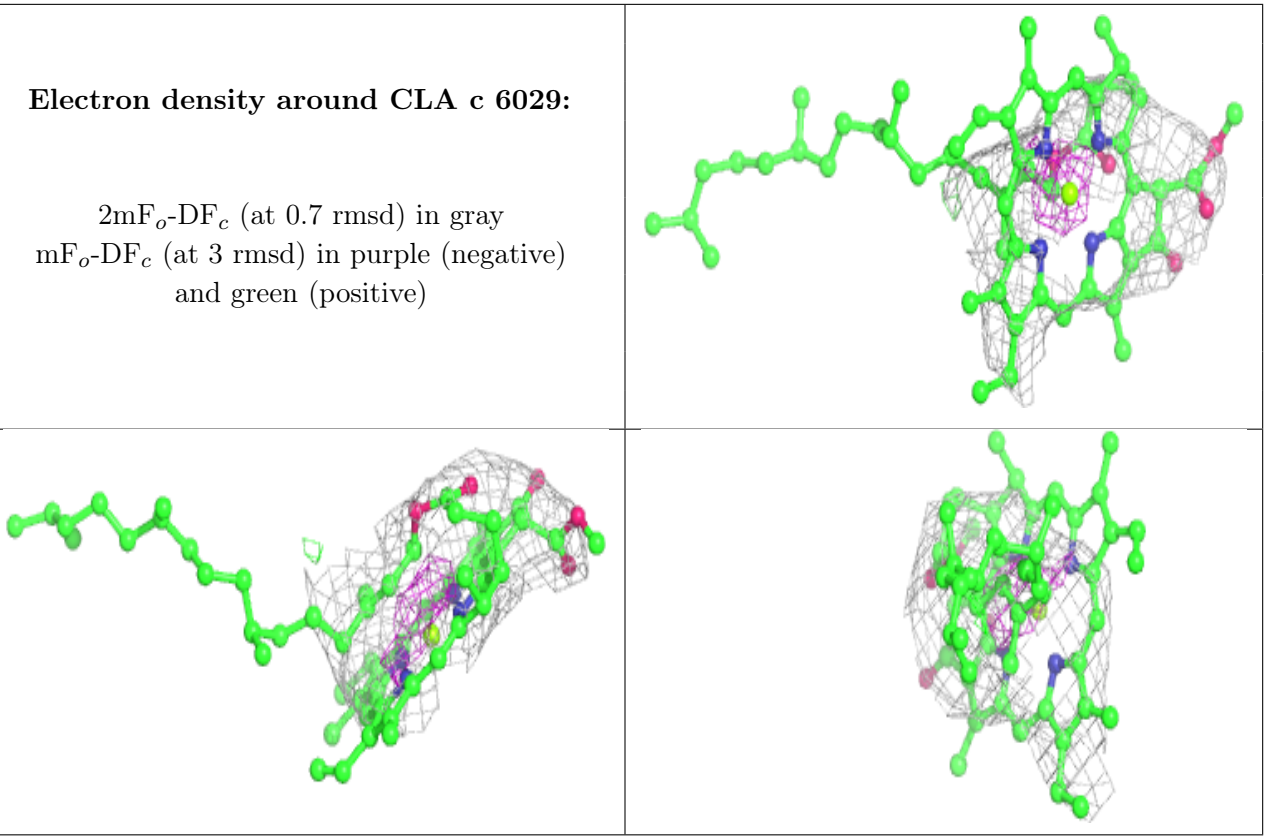






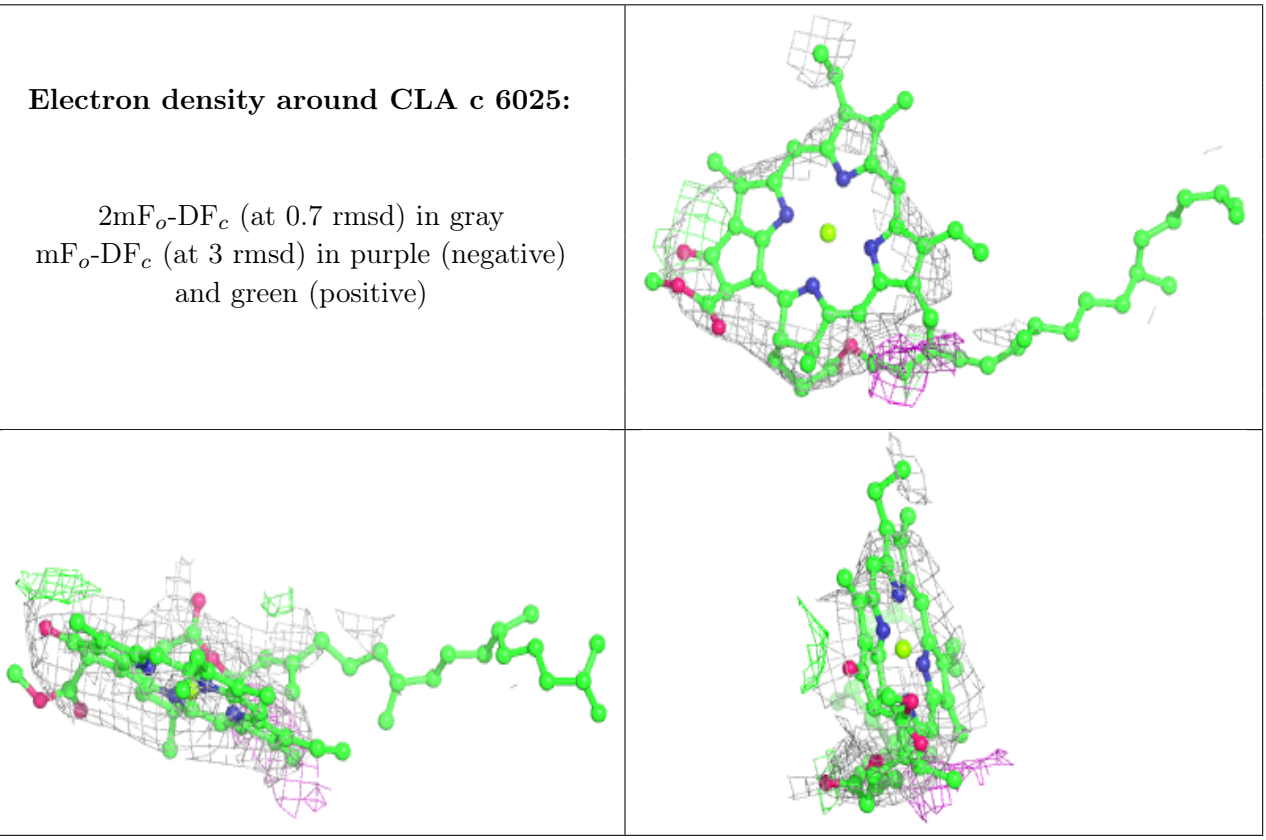
Electron density around CLA c 6029:

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



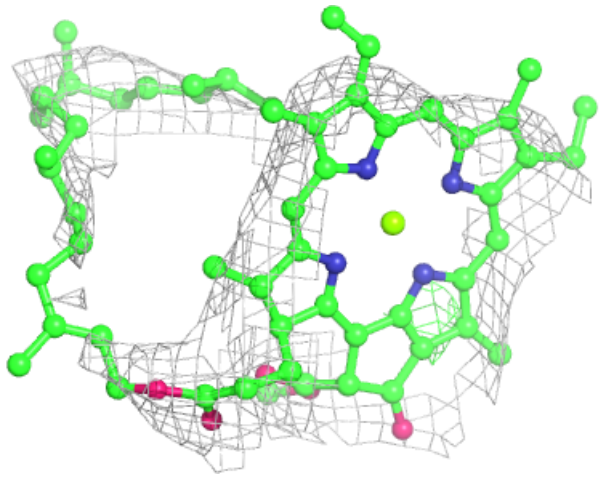
Electron density around CLA c 6025:

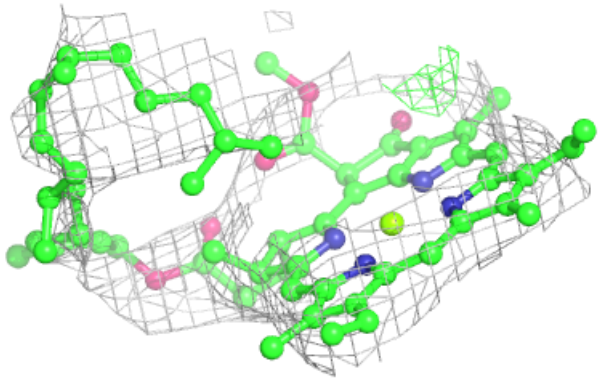
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

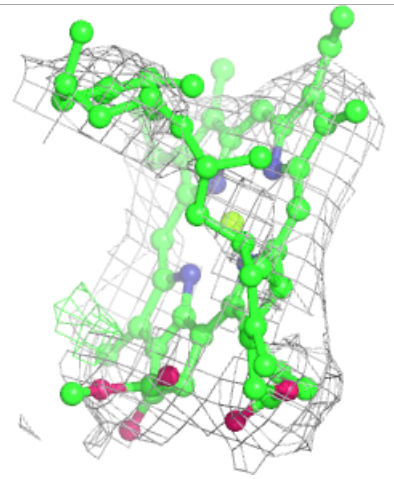


Electron density around CLA b 6023:

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

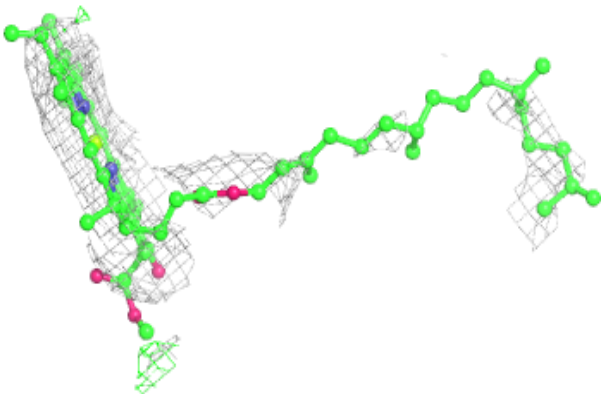


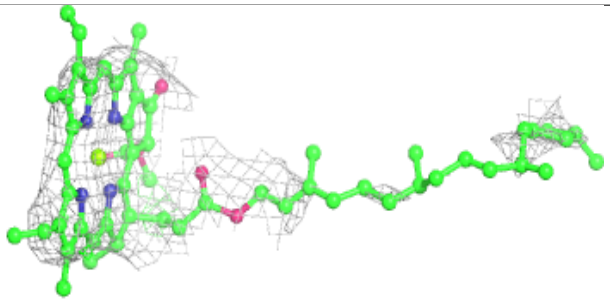


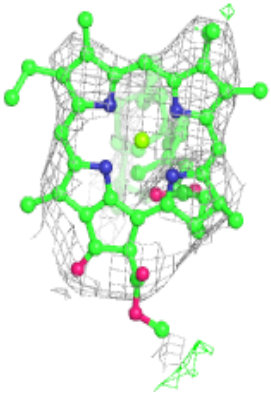


Electron density around CLA B 1012:

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

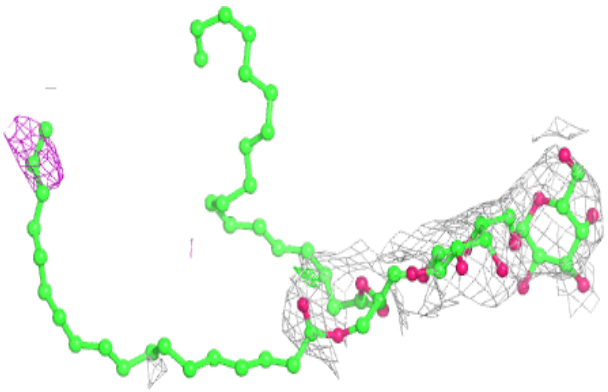


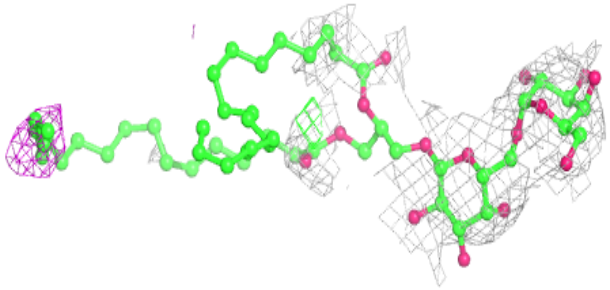


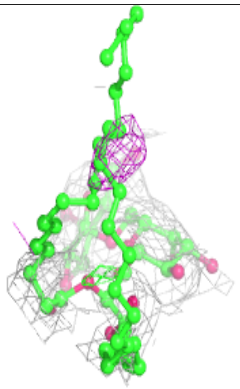


Electron density around DGD B 1058:

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

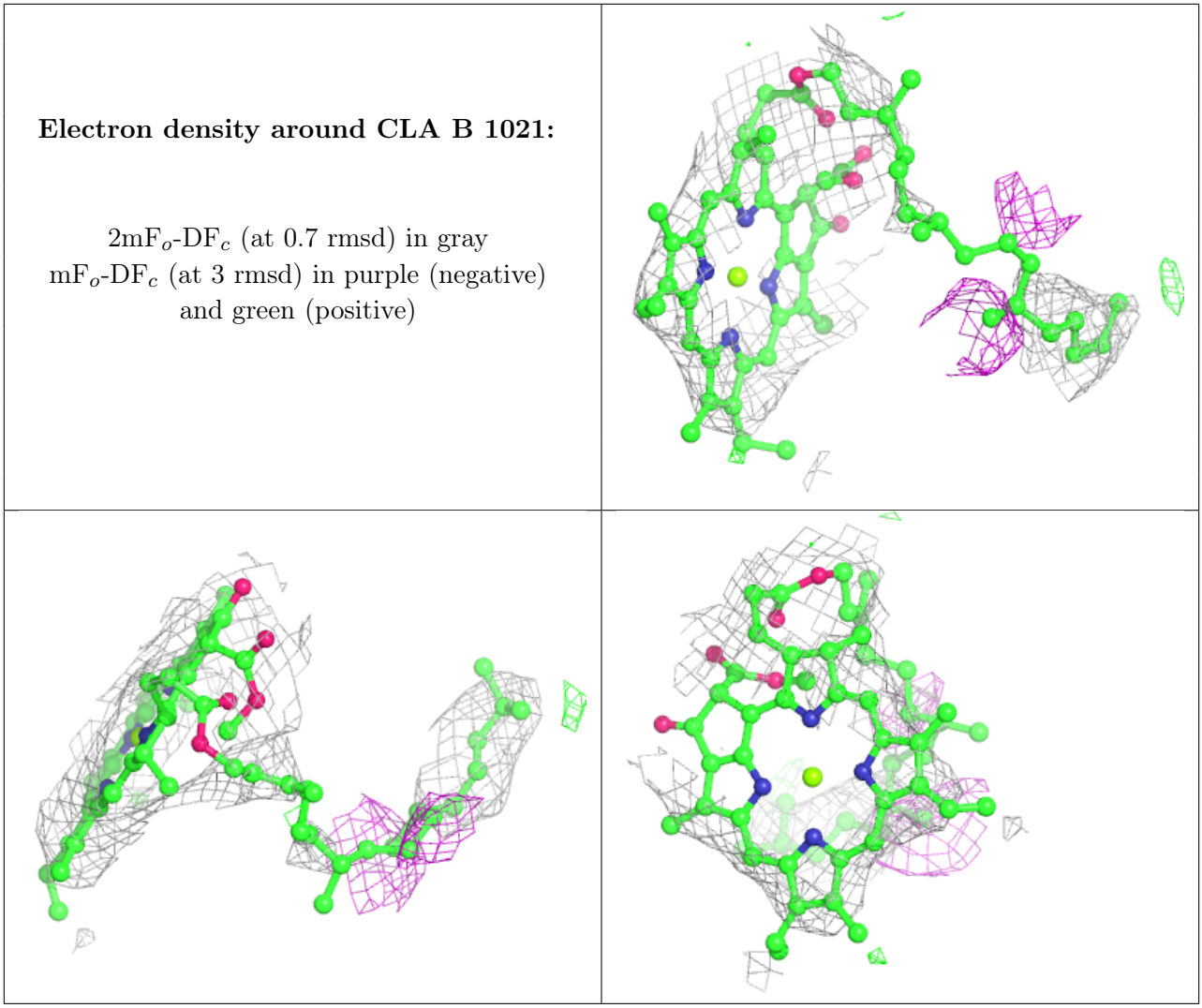






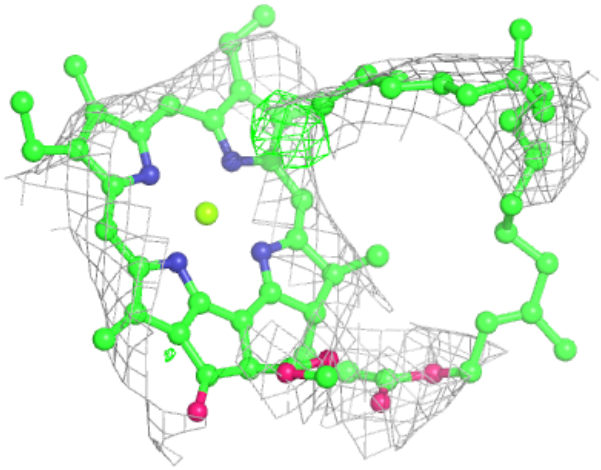
Electron density around CLA B 1021:

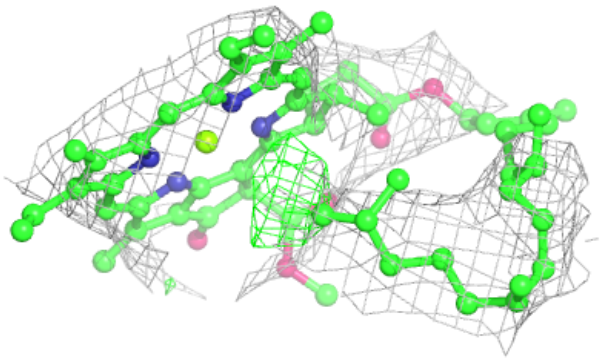
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

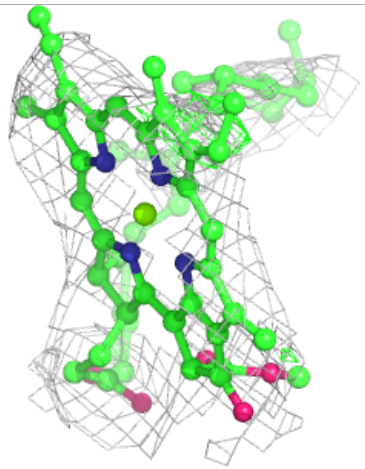


Electron density around CLA B 1023:

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

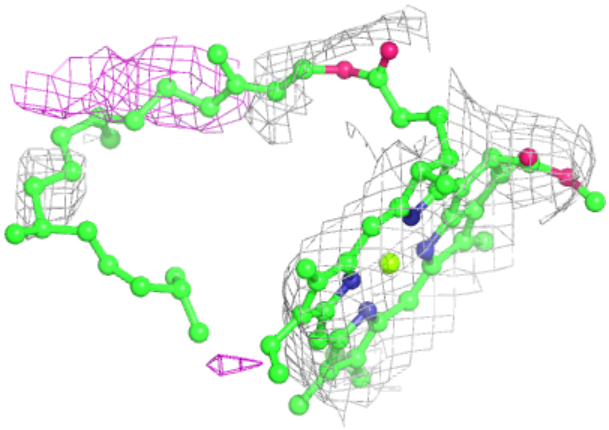


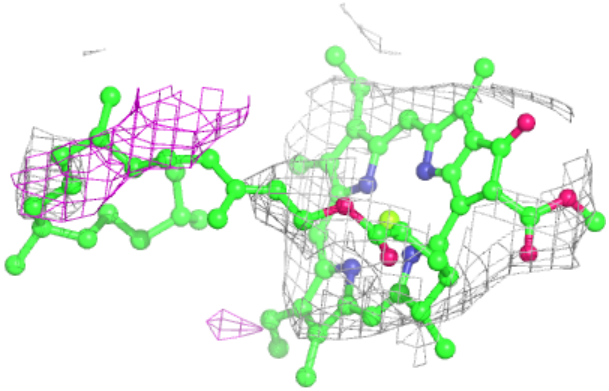


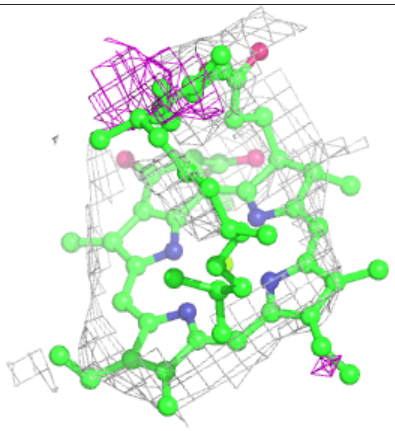


Electron density around CLA C 1028:

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

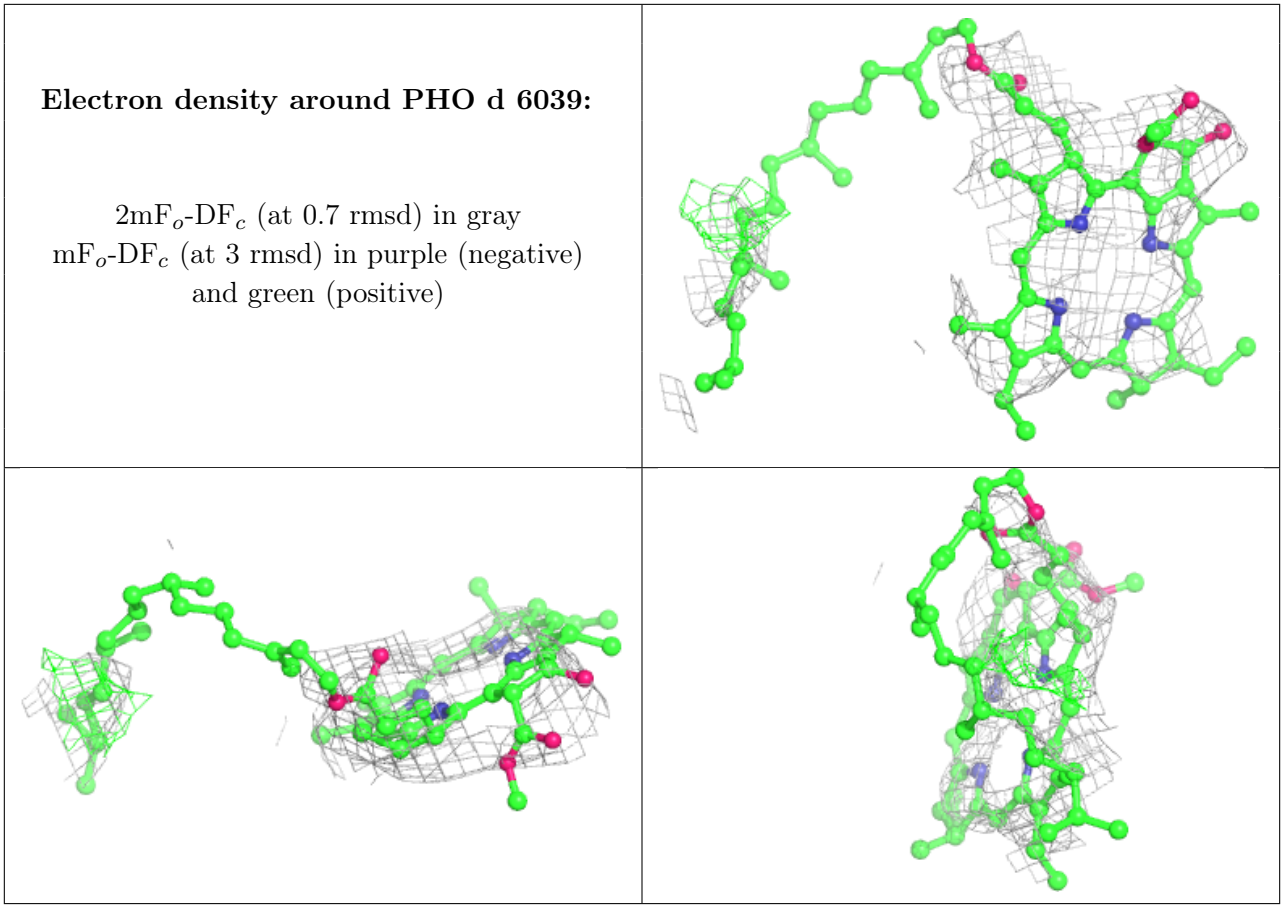






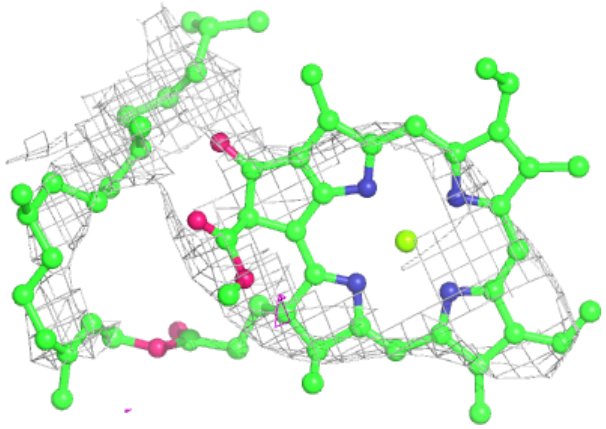
Electron density around PHO d 6039:

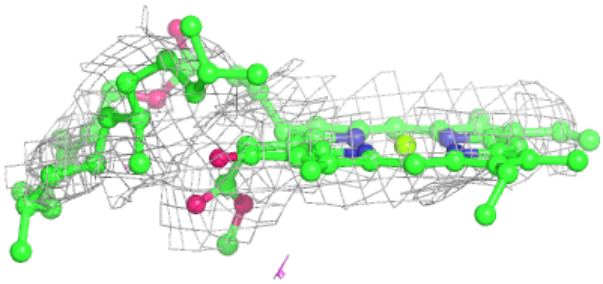
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

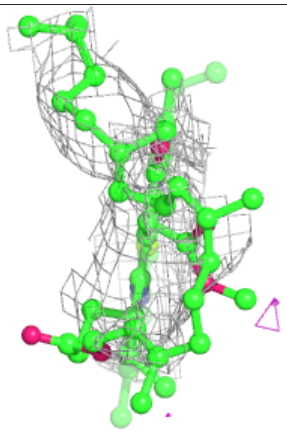


Electron density around CLA b 6018:

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

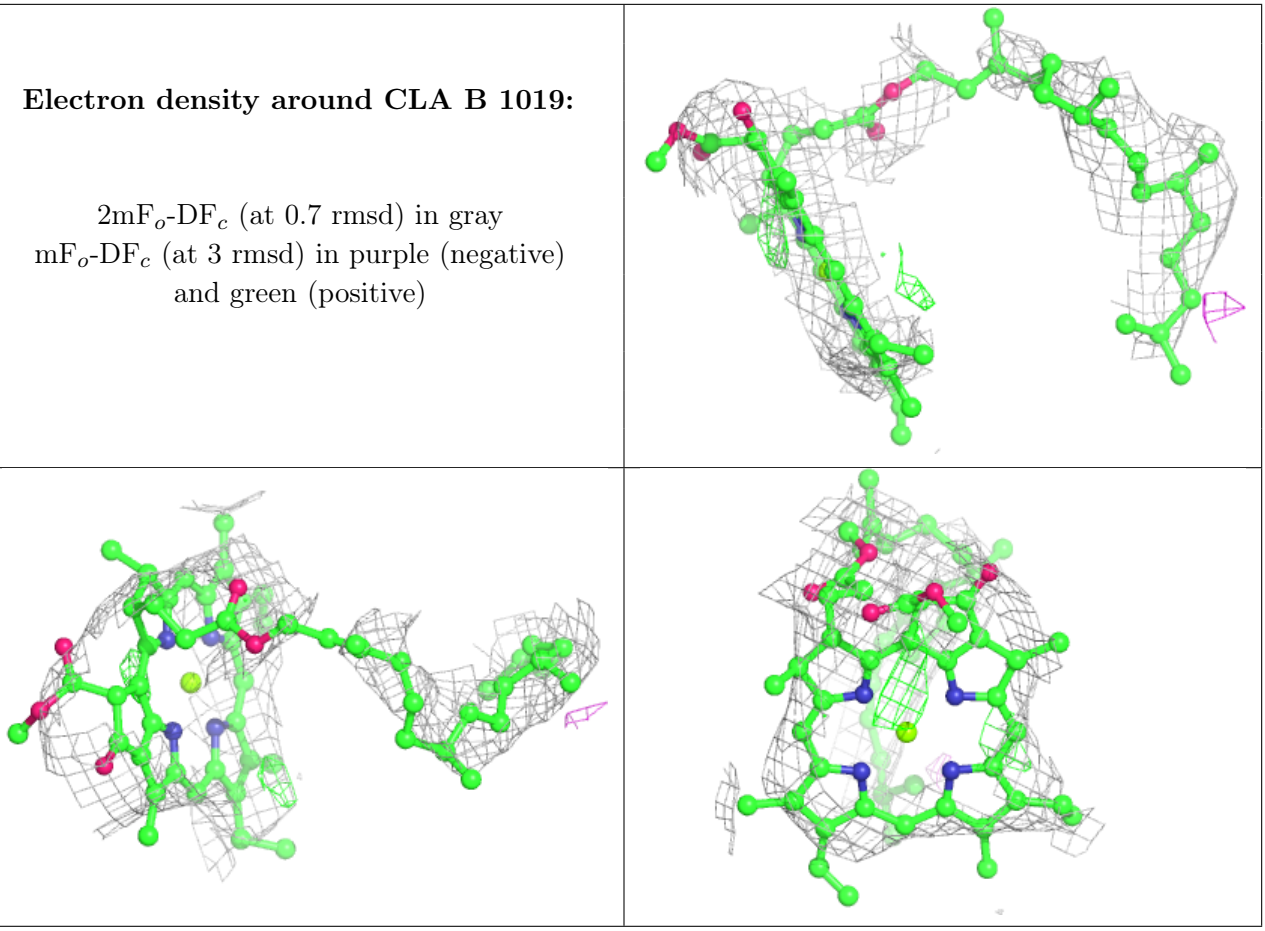






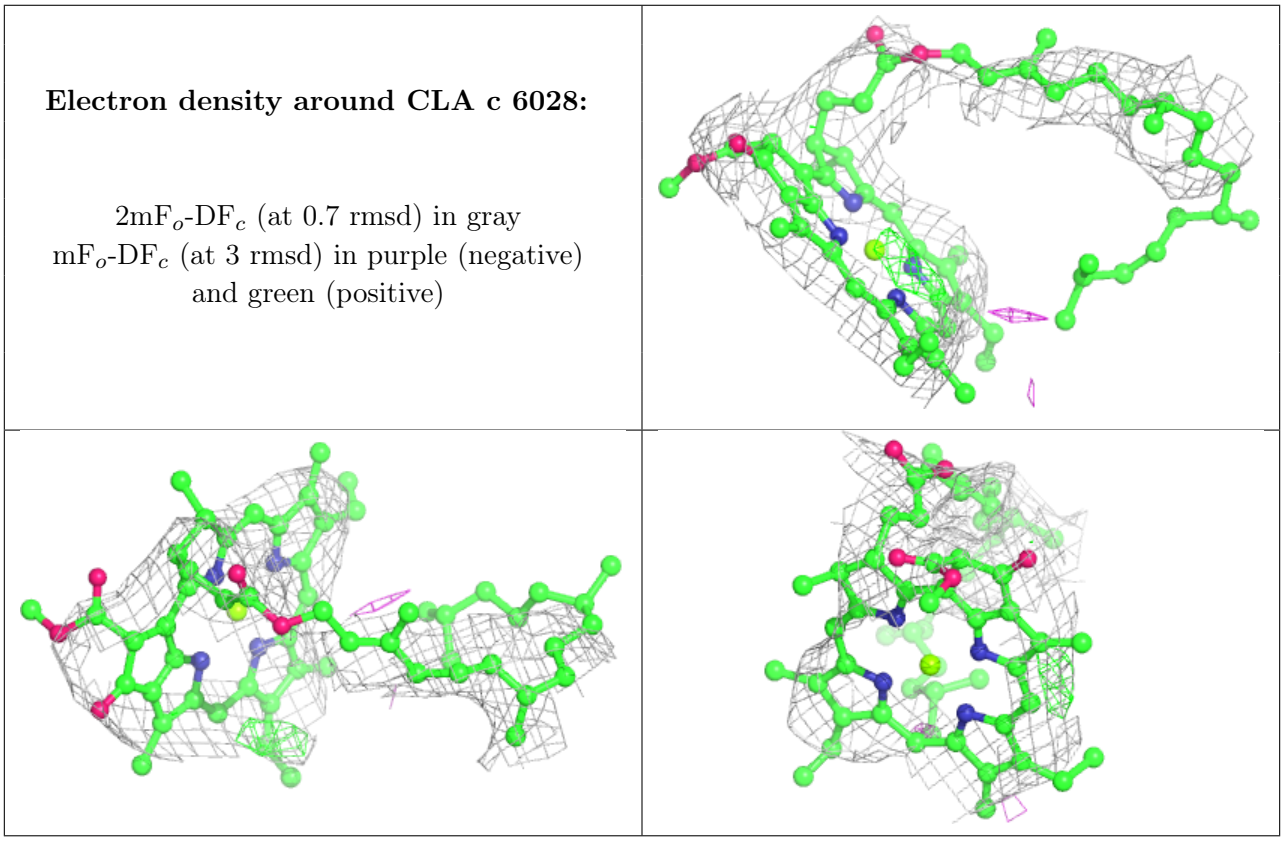
Electron density around CLA B 1019:

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



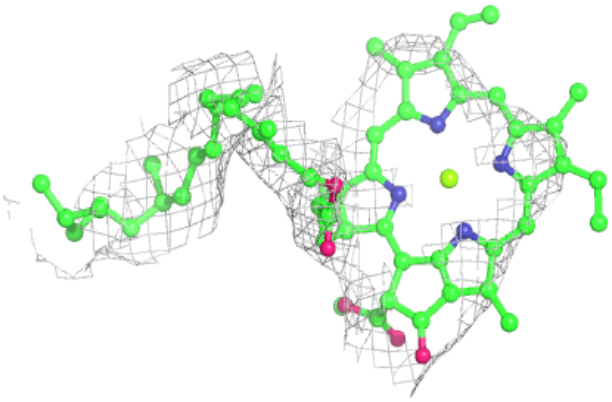
Electron density around CLA c 6028:

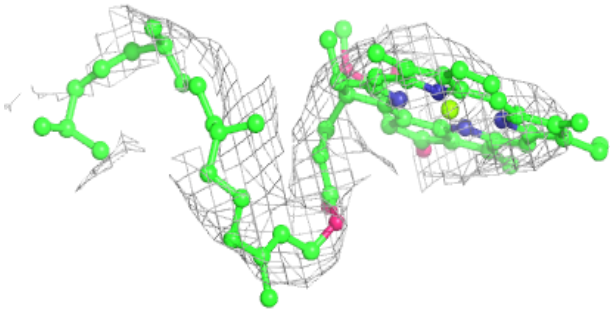
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

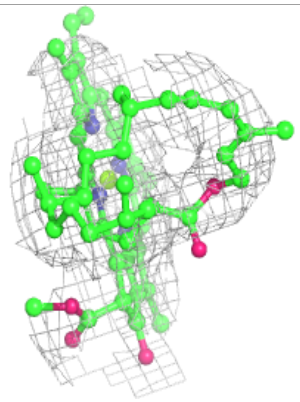


Electron density around CLA a 6006:

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

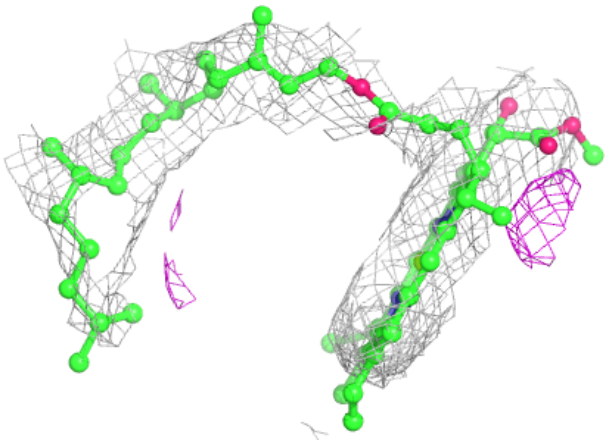


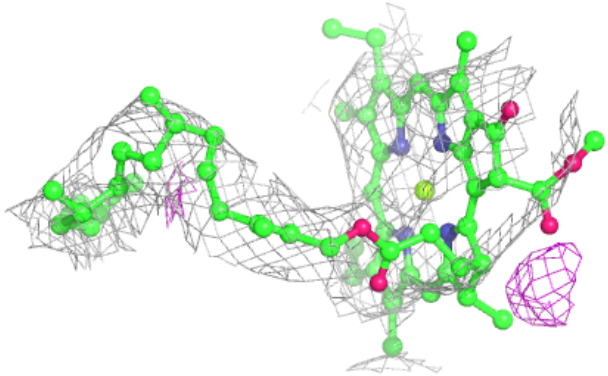


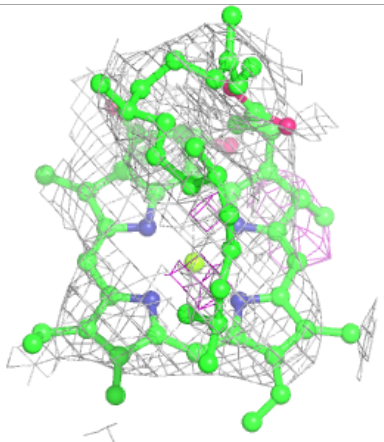


Electron density around CLA b 6019:

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

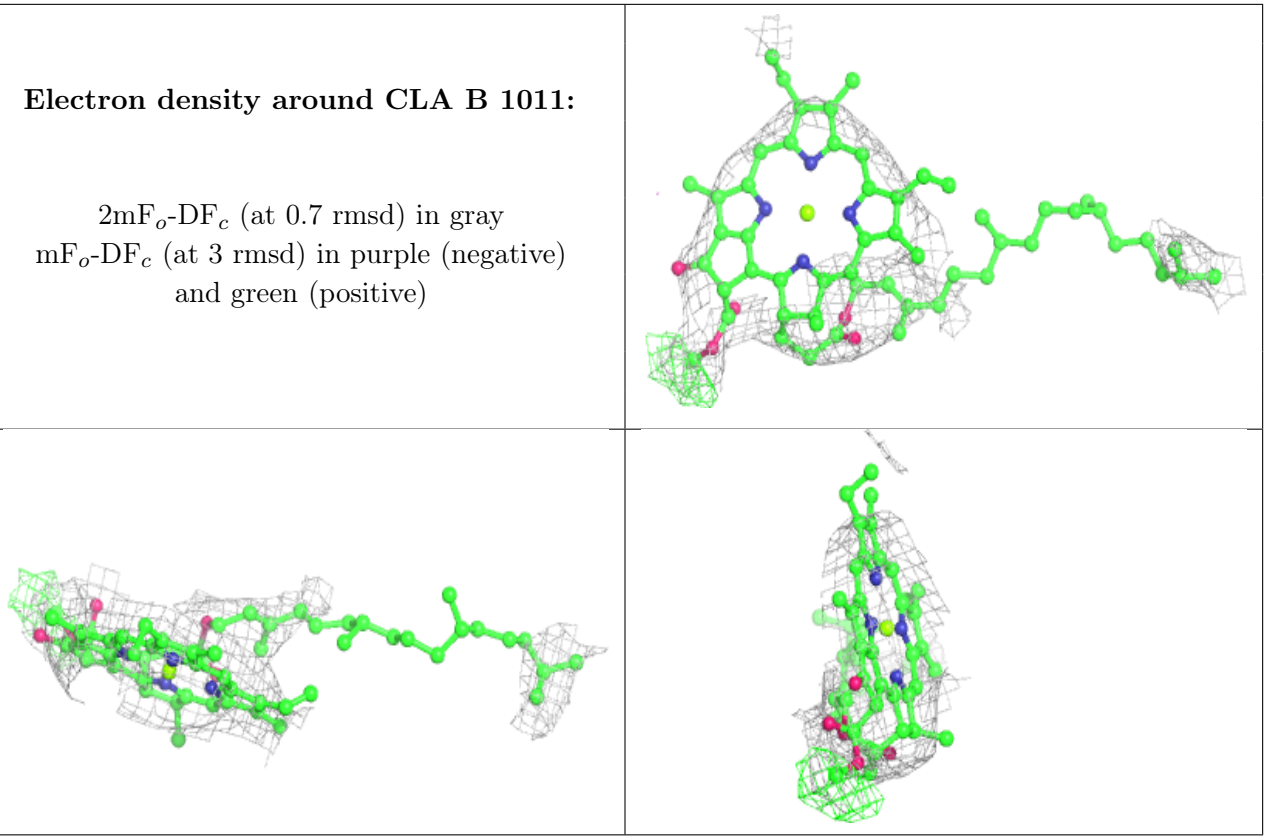






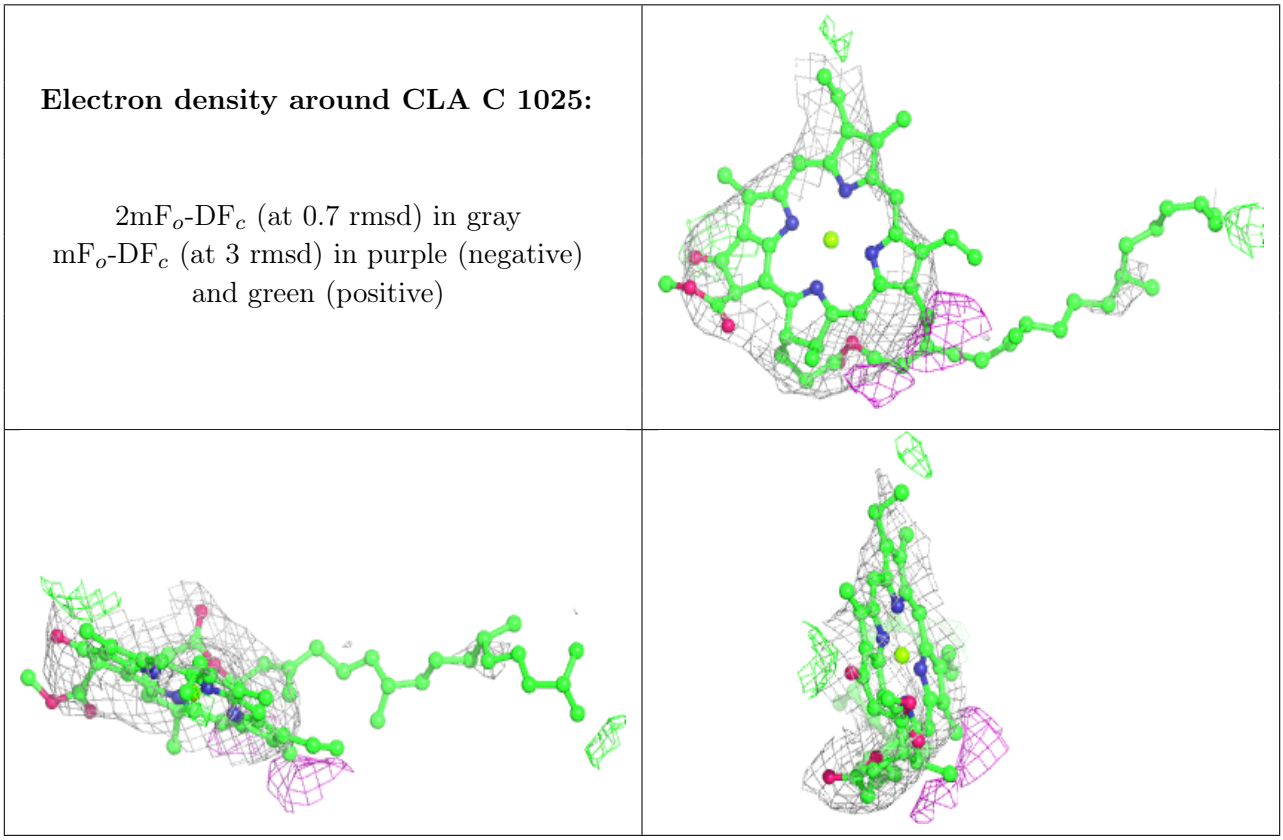
Electron density around CLA B 1011:

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



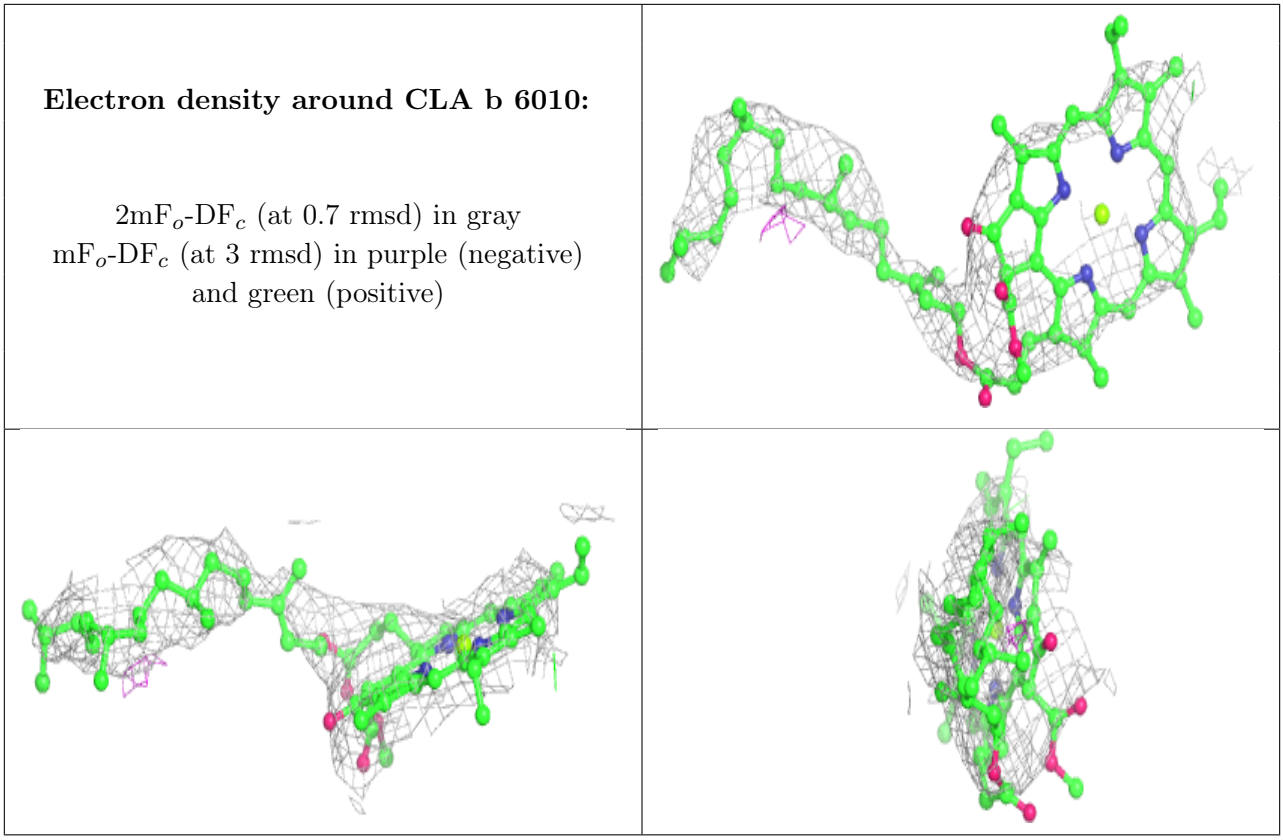
Electron density around CLA C 1025:

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



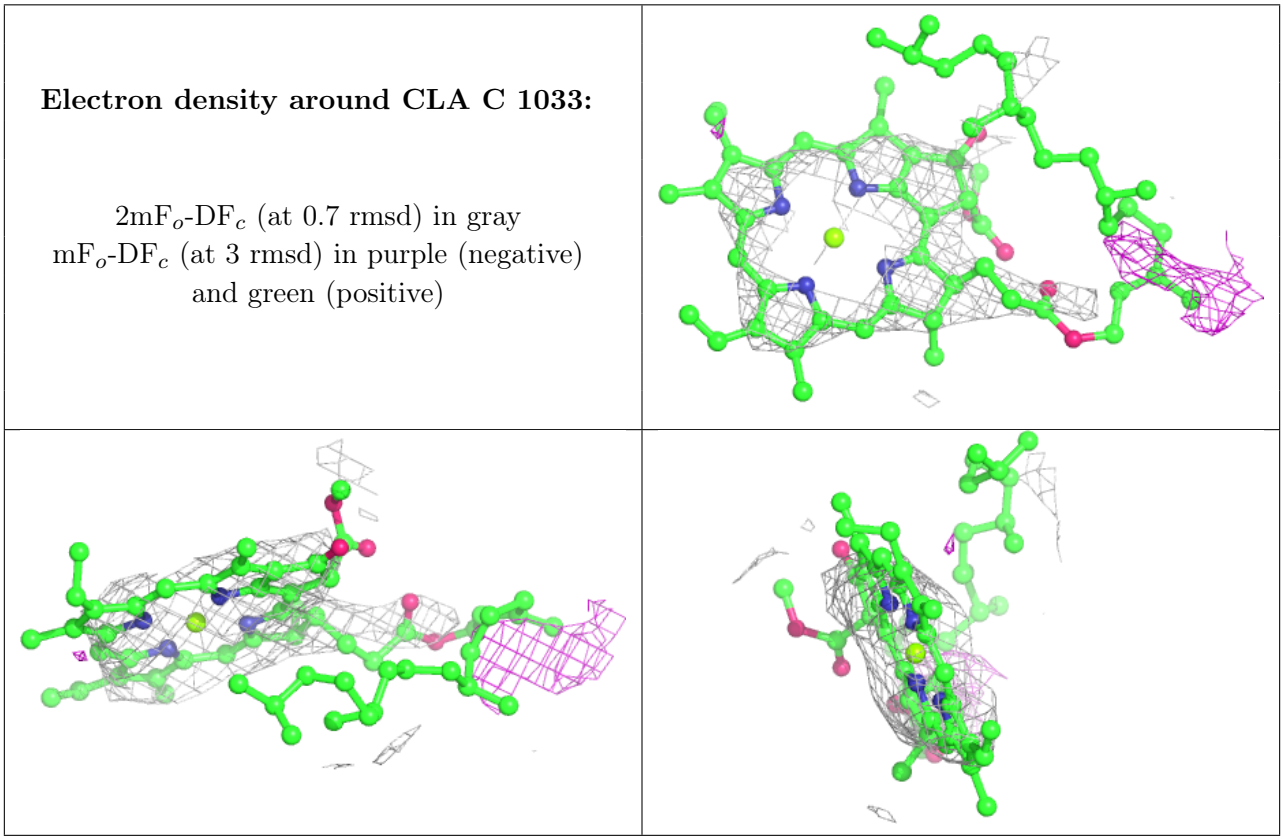
Electron density around CLA b 6010:

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



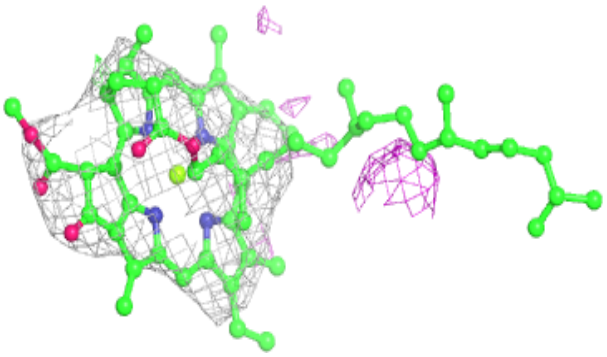
Electron density around CLA C 1033:

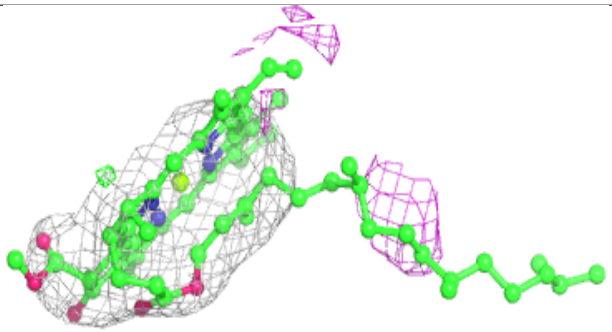
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

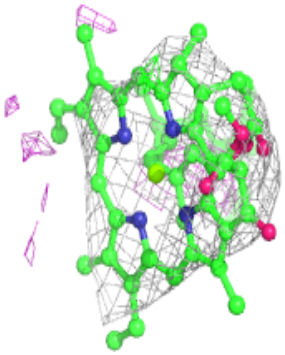


Electron density around CLA C 1029:

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

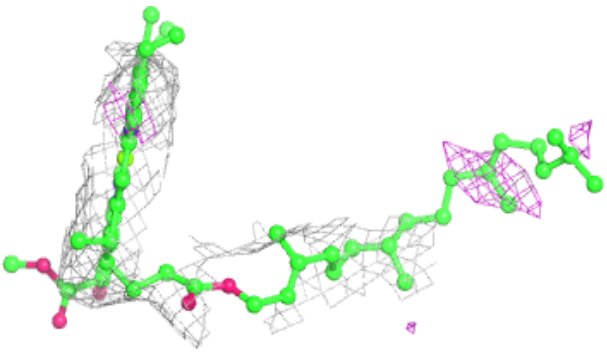


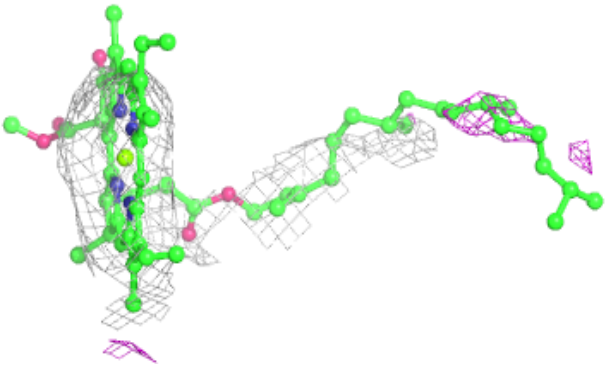


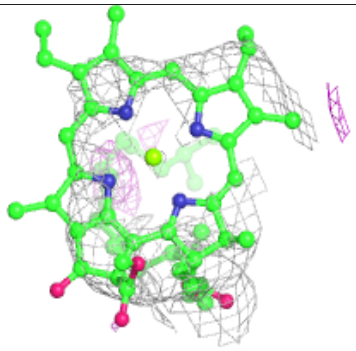


Electron density around CLA b 6013:

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

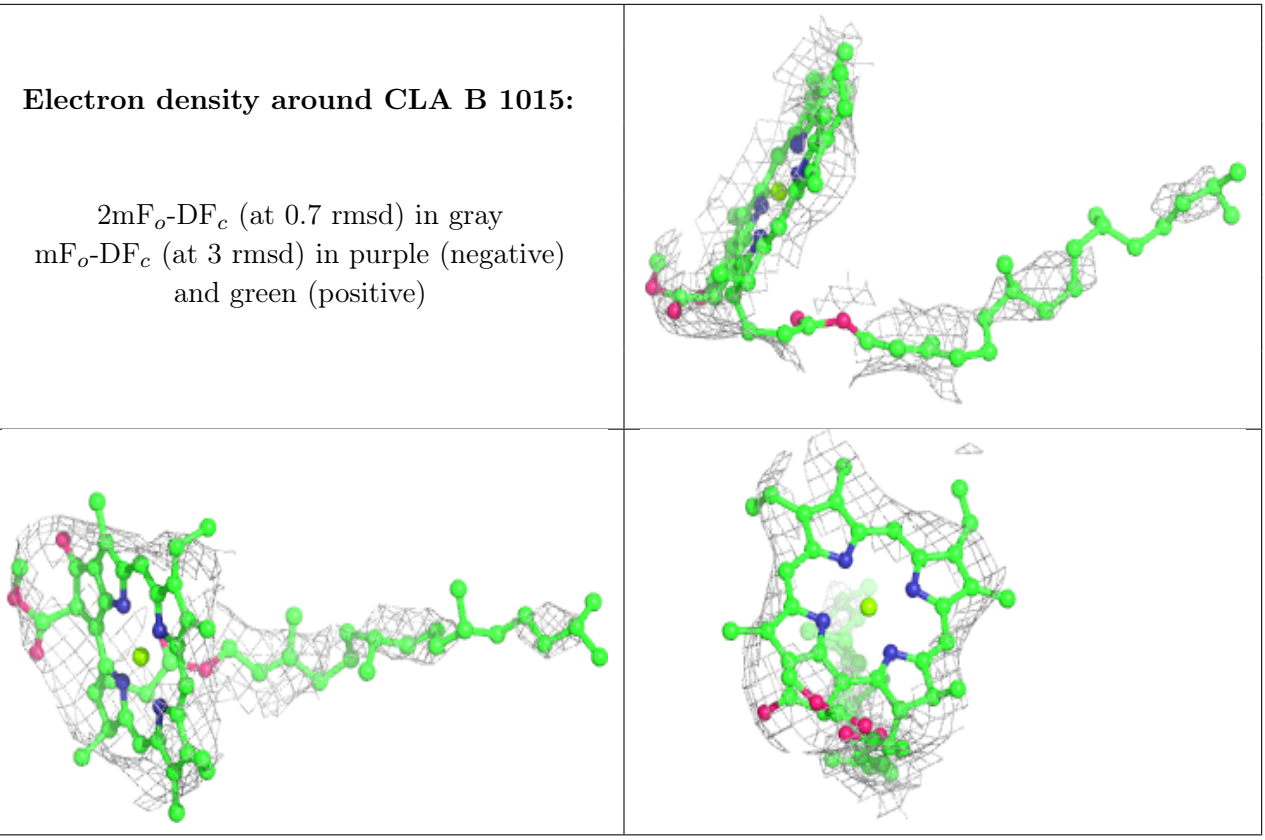






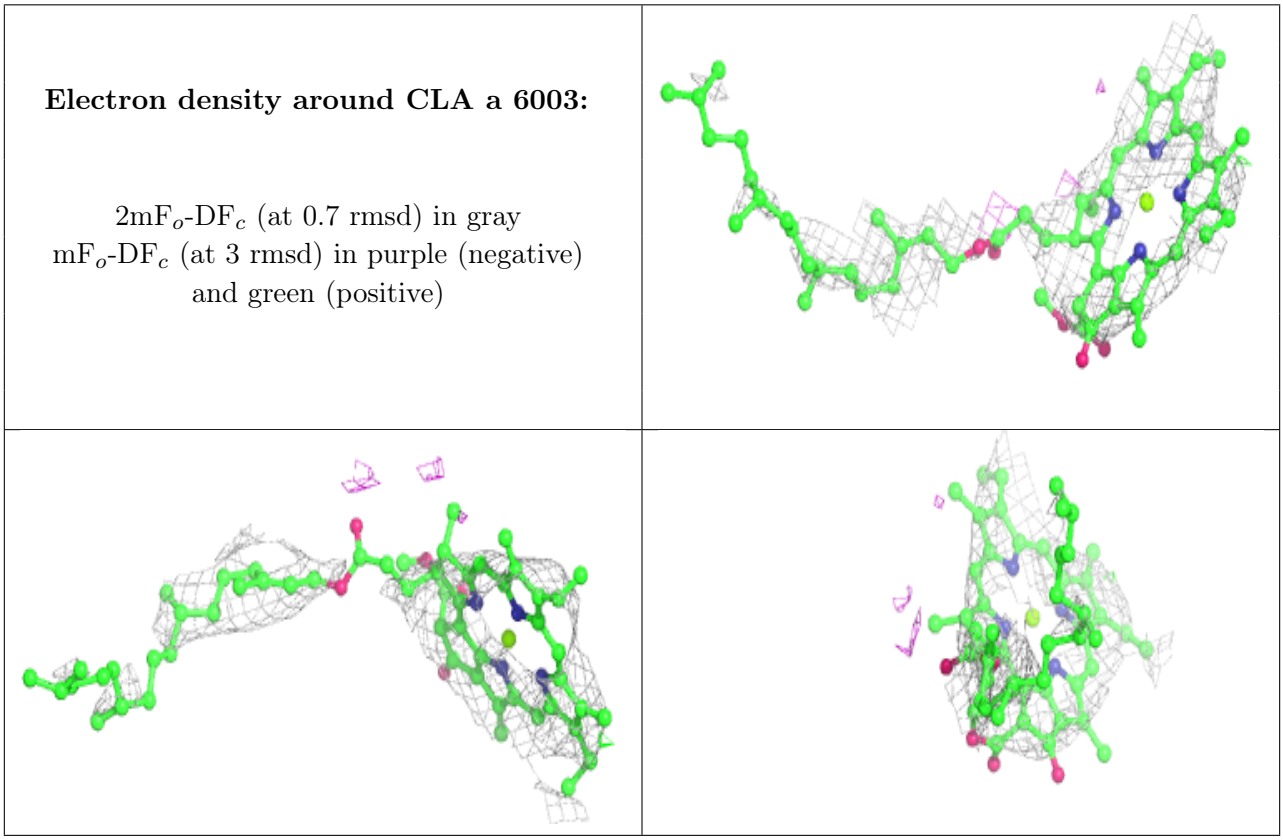
Electron density around CLA B 1015:

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



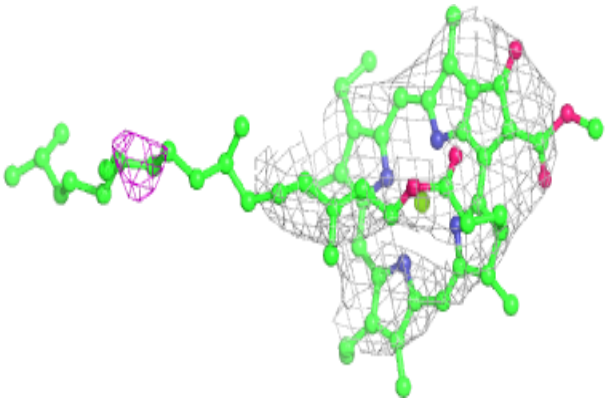
Electron density around CLA a 6003:

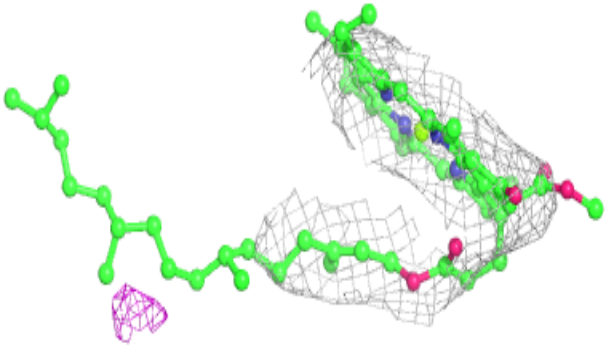
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

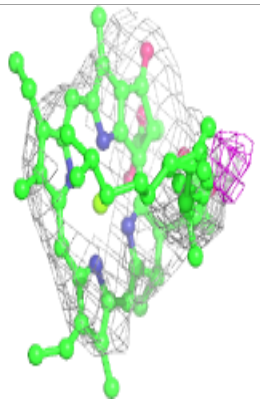


Electron density around CLA b 6016:

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

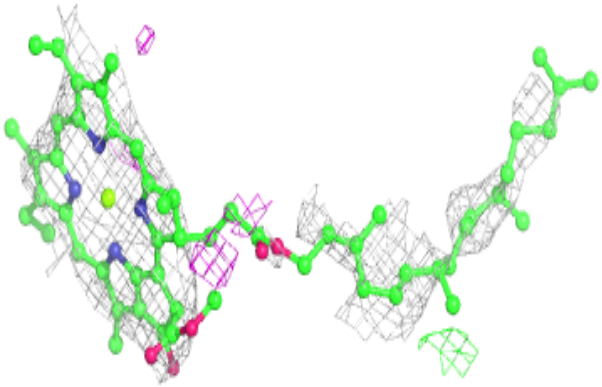


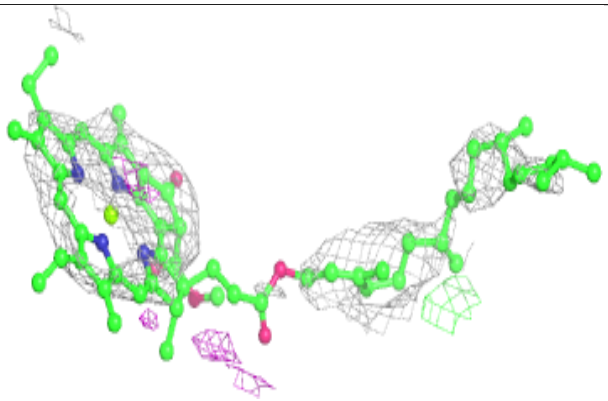


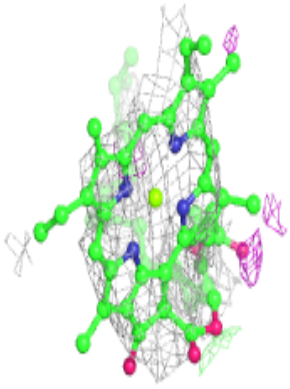


Electron density around CLA A 1003:

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

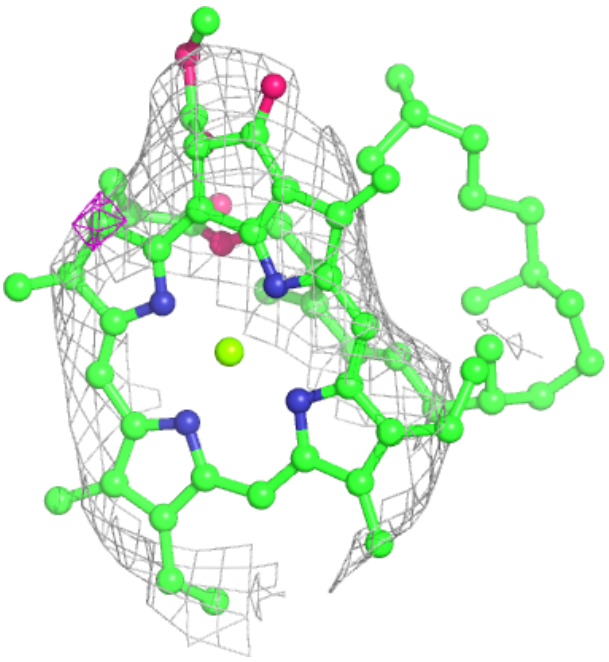


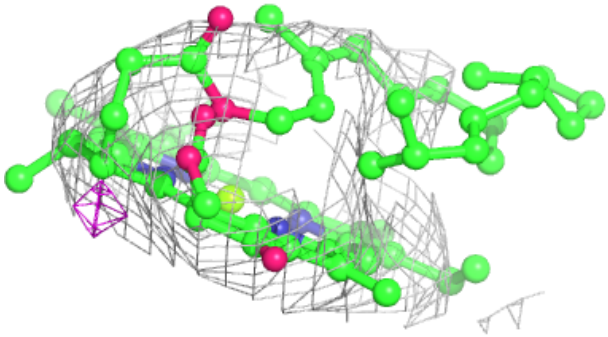


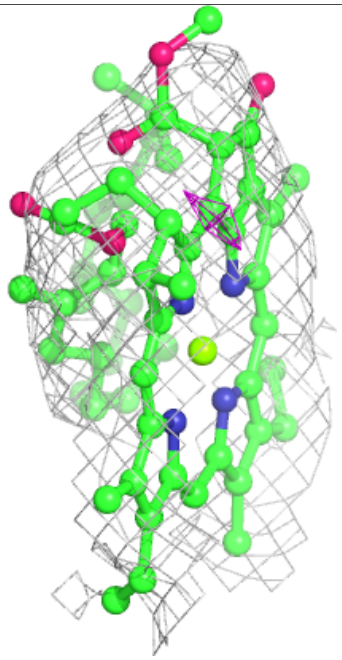


Electron density around CLA b 6022:

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

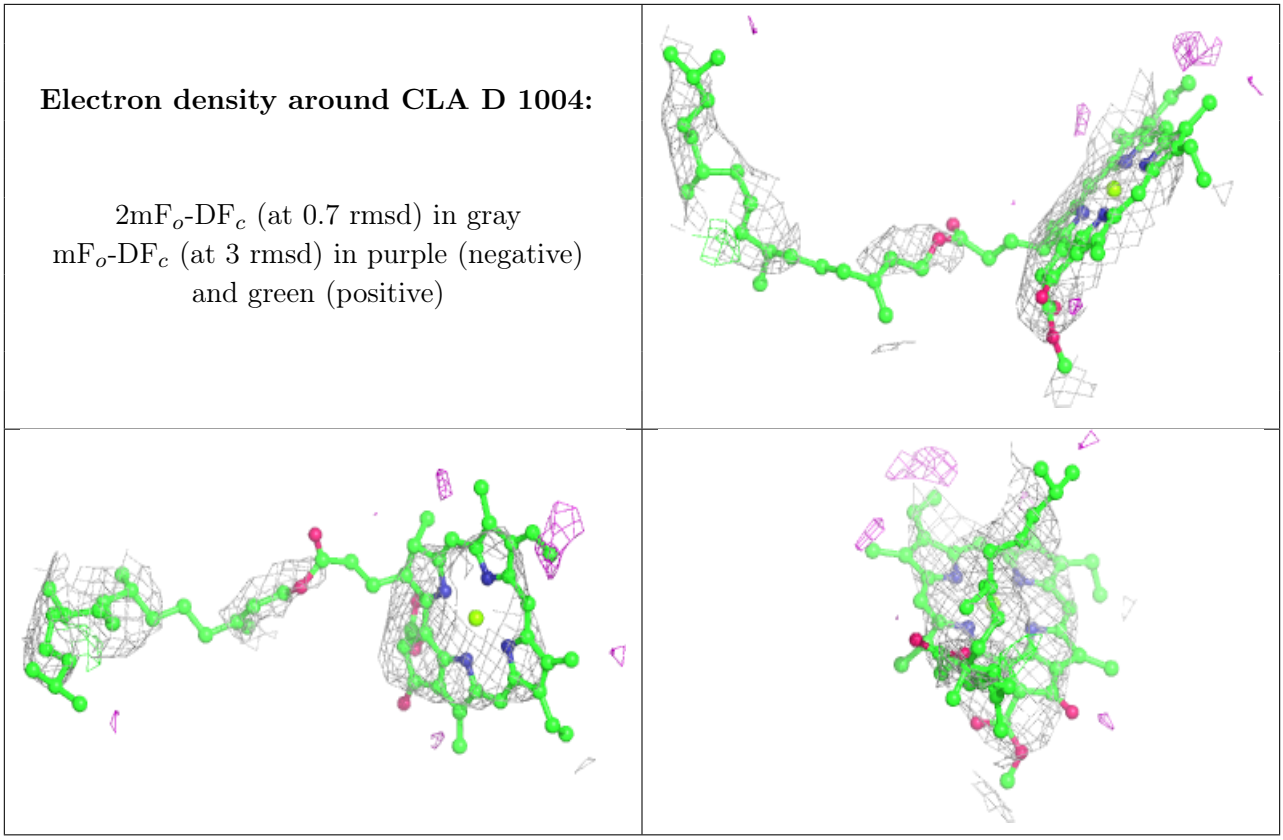






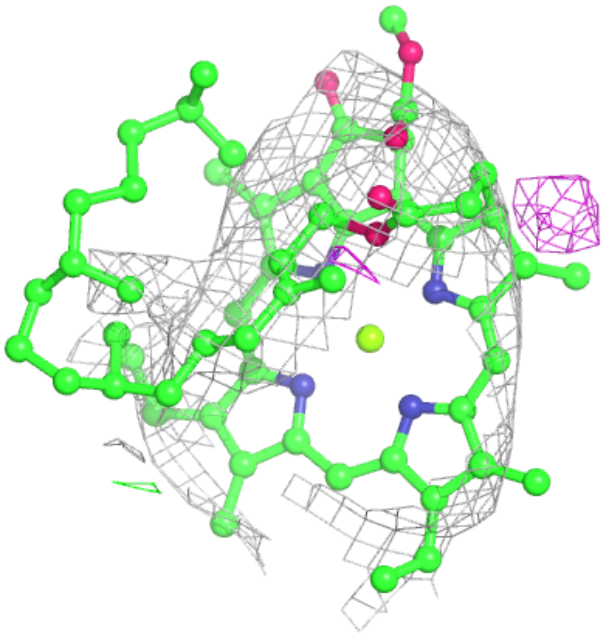
Electron density around CLA D 1004:

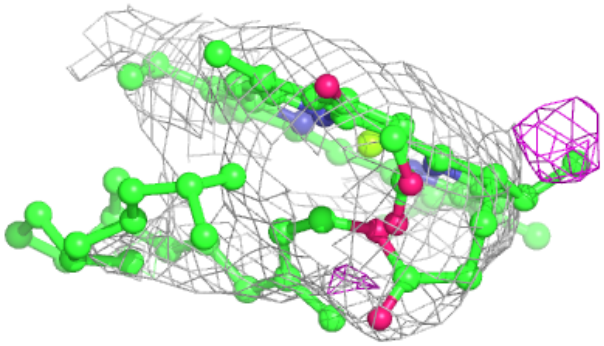
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

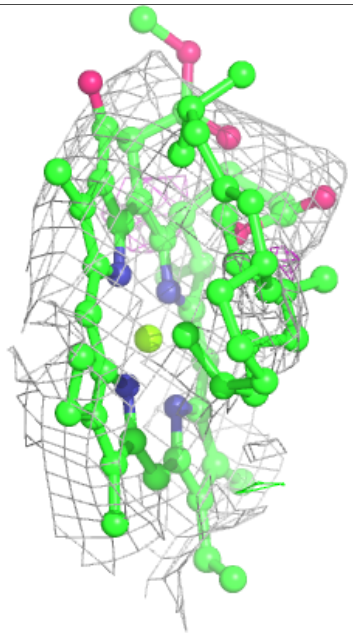


Electron density around CLA B 1022:

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

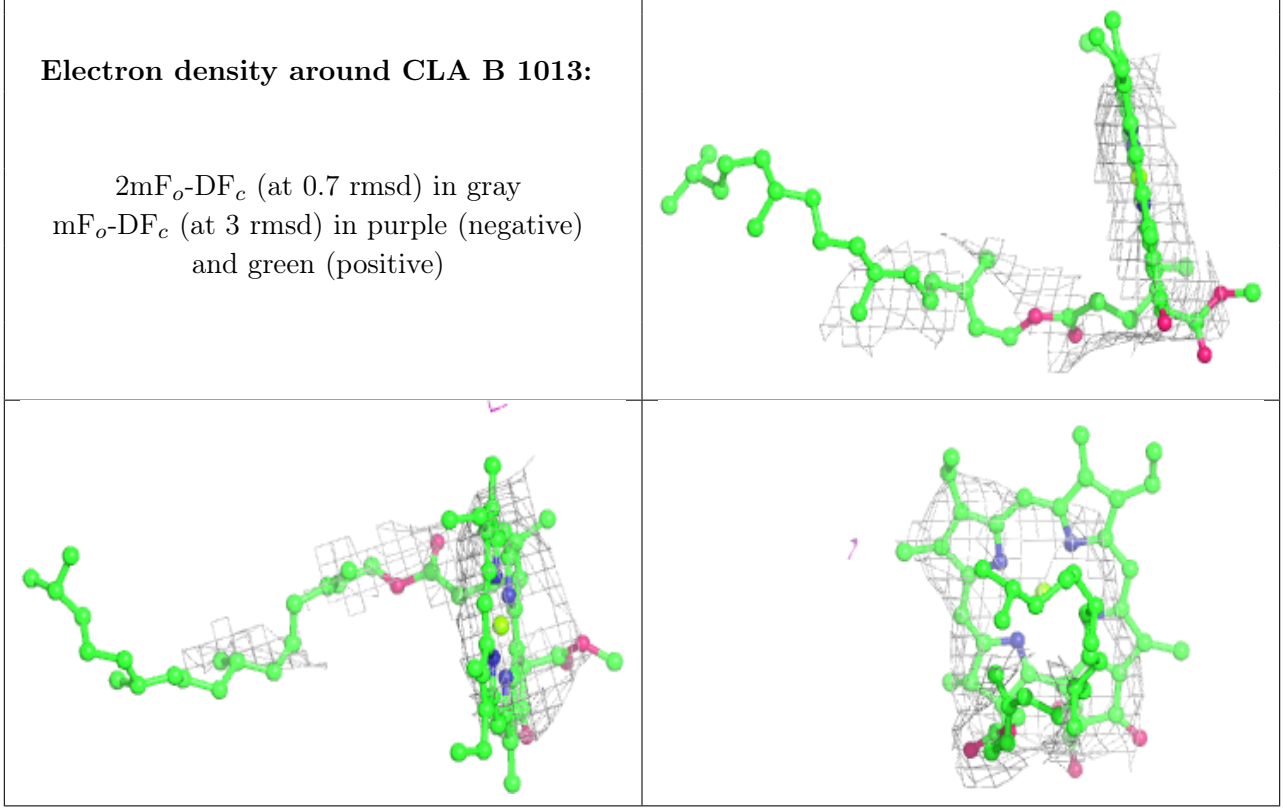






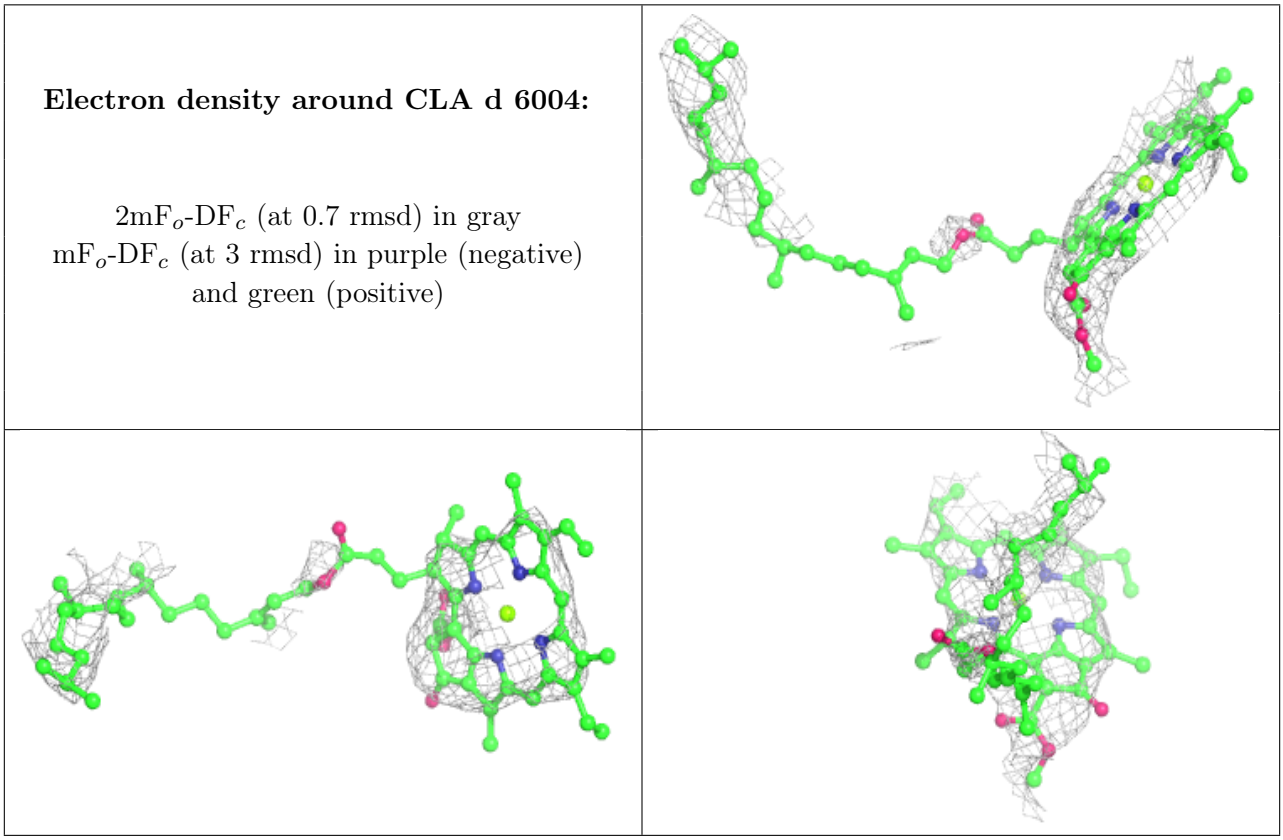
Electron density around CLA B 1013:

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



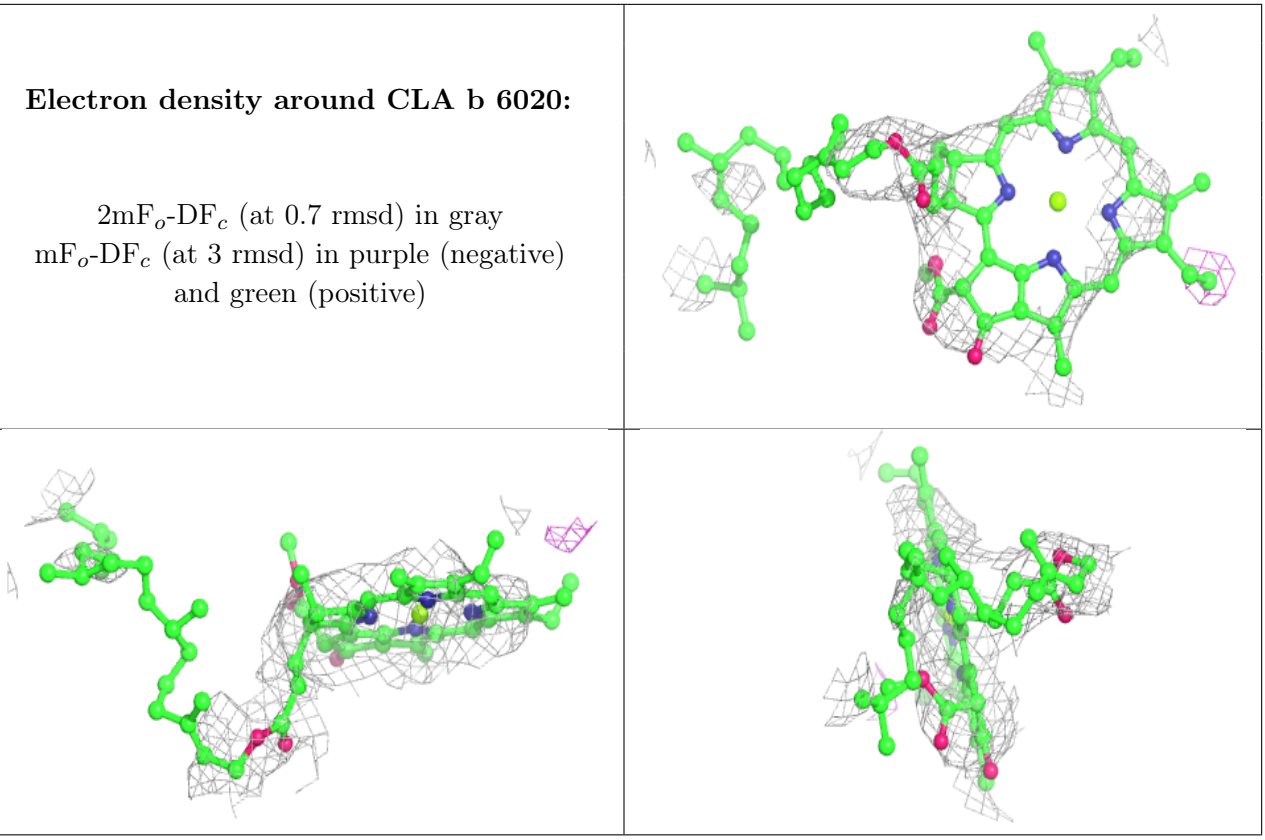
Electron density around CLA d 6004:

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



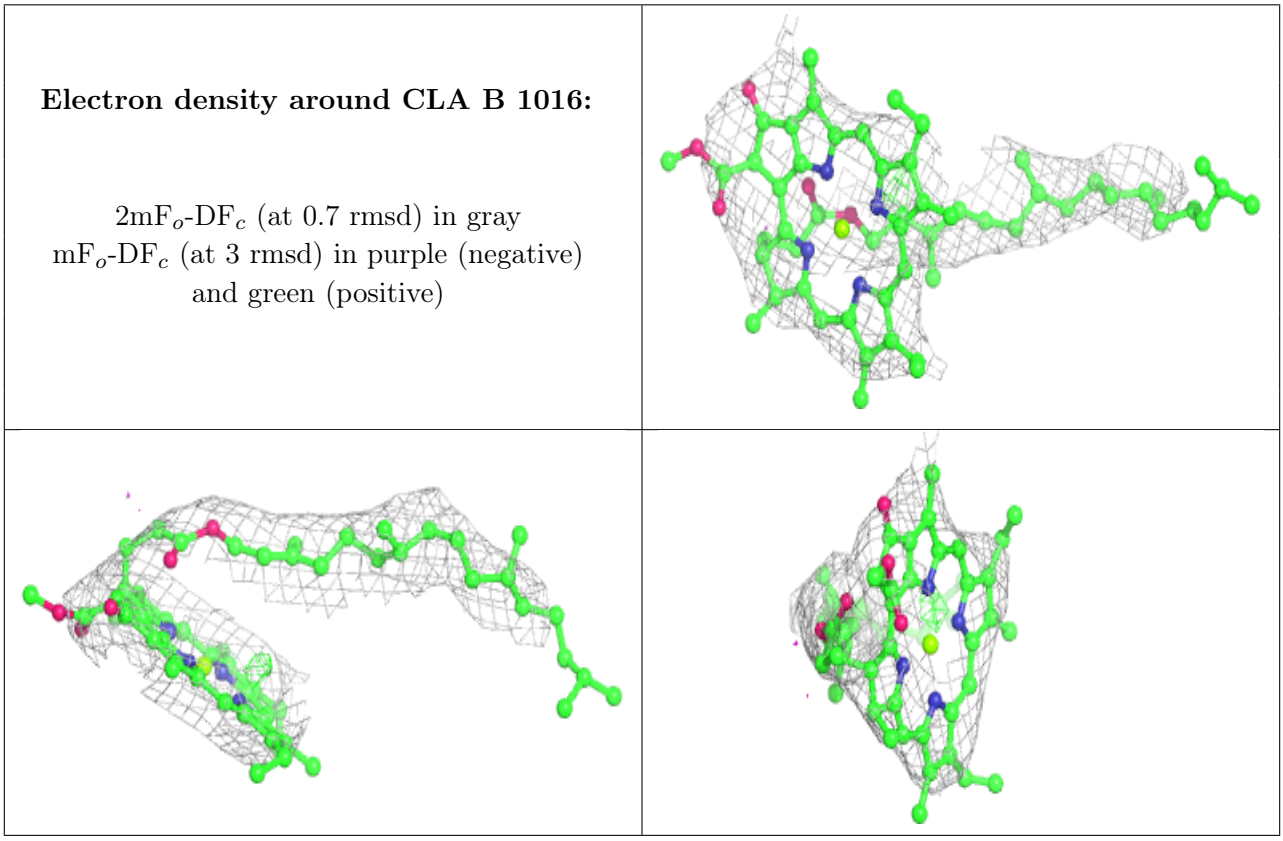
Electron density around CLA b 6020:

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



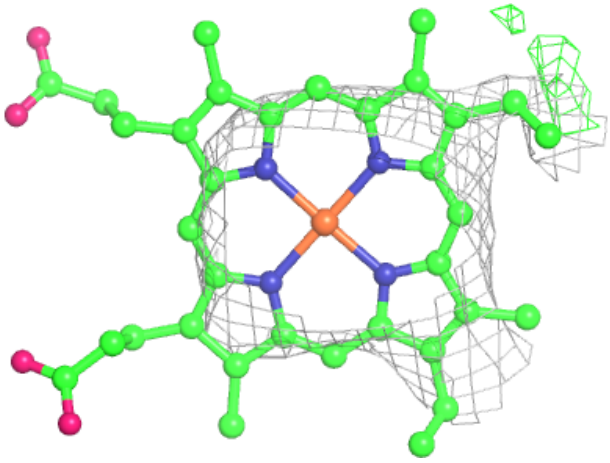
Electron density around CLA B 1016:

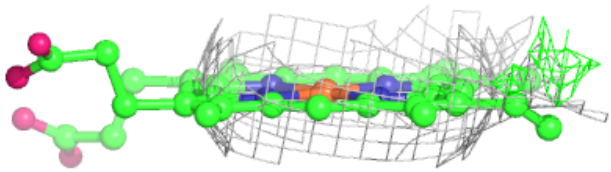
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

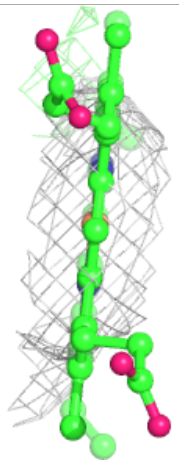


Electron density around HEM v 6041:

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

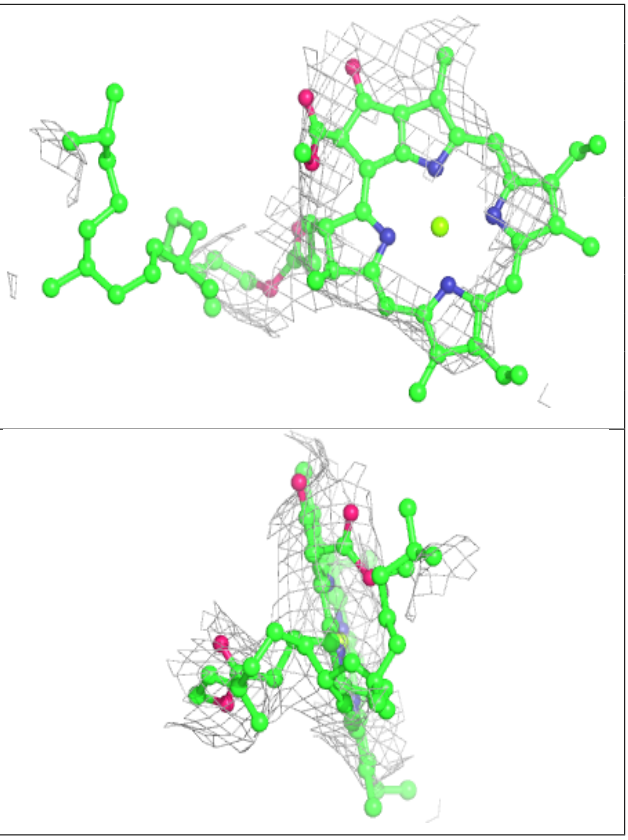


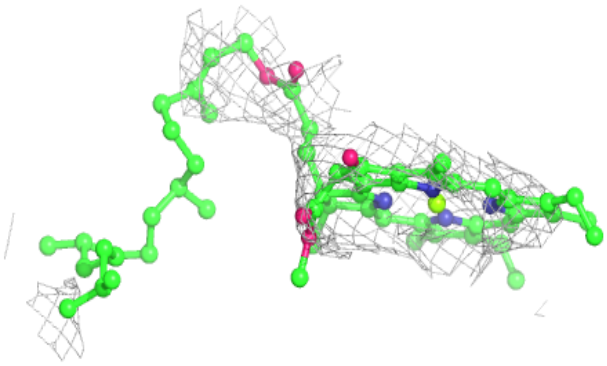




Electron density around CLA B 1020:

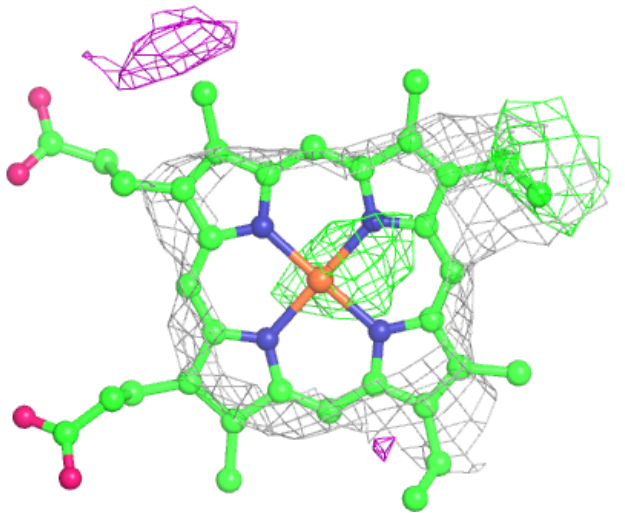
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

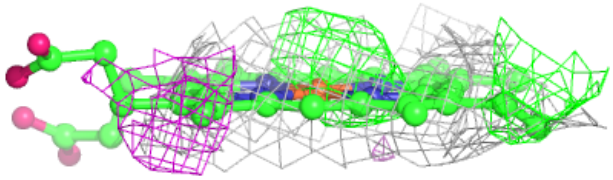


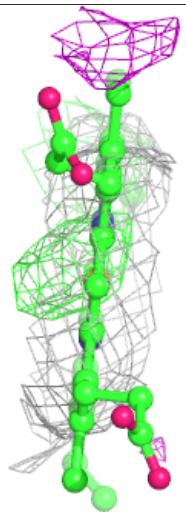


Electron density around HEM V 1041:

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







6.5 Other polymers

There are no such residues in this entry.