wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 09:30 PM EDT

PDB ID	:	3A0H / pdb_00003a0h
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:

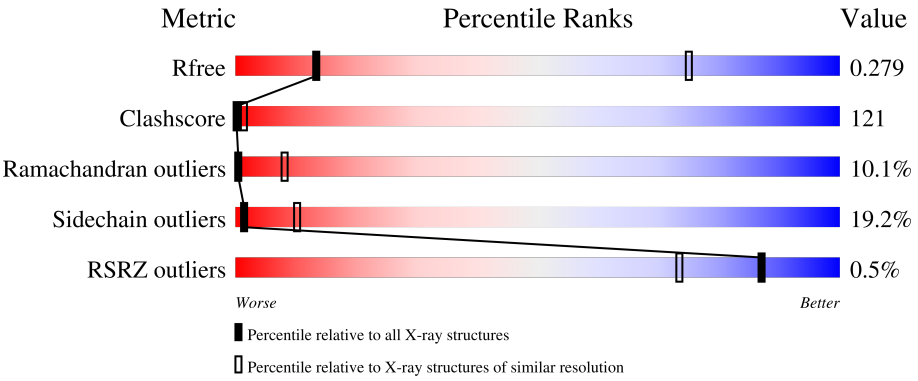
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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.



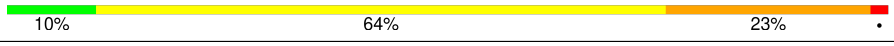
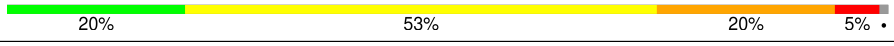
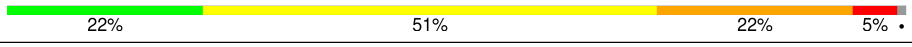
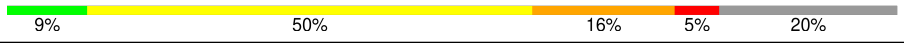
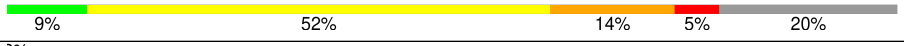
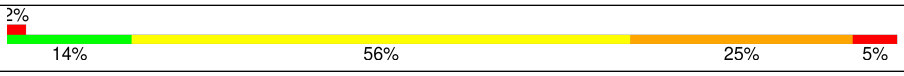
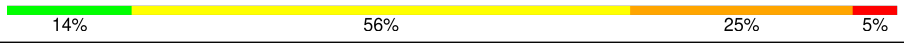
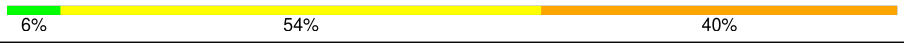
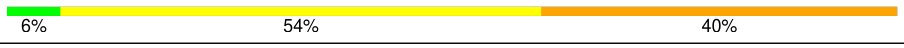
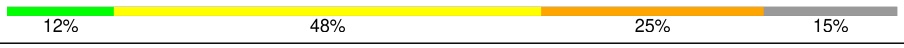
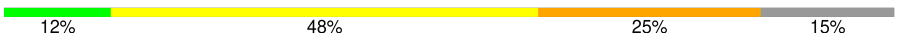
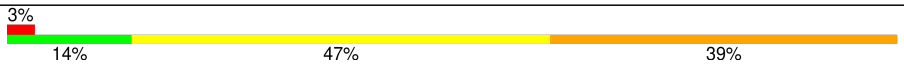
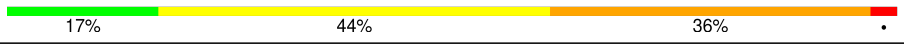
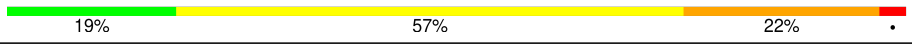
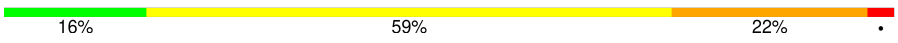
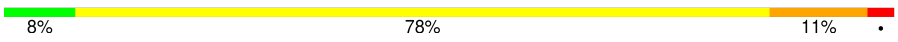
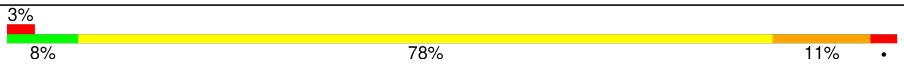
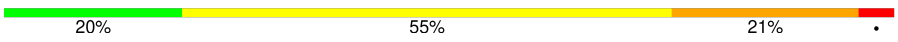
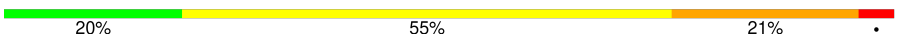
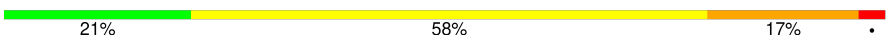
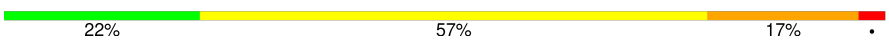
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	% 11% 56% 26%
1	a	344	% 11% 56% 26%
2	B	488	% 17% 56% 24%
2	b	488	17% 56% 24%
3	C	447	% 14% 59% 23%

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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	2% 19% 60% 20%
16	v	137	21% 57% 20%
17	X	34	3% 32% 44% 24%
17	x	34	29% 47% 24%
18	Y	28	29% 25% 36% 11%
18	y	28	29% 25% 36% 11%
19	N	23	70% 30%
19	n	23	70% 30%
20	Z	62	15% 60% 26%
20	z	62	2% 15% 60% 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	-
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	-
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	-
22	CLA	C	1025	X	-	X	-
22	CLA	C	1026	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	1027	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	-
22	CLA	D	1004	X	-	X	-
22	CLA	D	1005	X	-	X	-
22	CLA	D	1008	X	-	X	-
22	CLA	H	1017	X	-	X	-
22	CLA	K	1034	X	-	X	-
22	CLA	a	6003	X	-	X	-
22	CLA	a	6006	X	-	X	-
22	CLA	a	6007	-	-	X	-
22	CLA	b	6009	X	-	X	-
22	CLA	b	6010	X	-	X	-
22	CLA	b	6011	X	-	X	-
22	CLA	b	6012	X	-	X	-
22	CLA	b	6013	X	-	X	-
22	CLA	b	6014	X	-	X	-
22	CLA	b	6015	X	-	X	-
22	CLA	b	6016	-	-	X	-
22	CLA	b	6018	X	-	X	-
22	CLA	b	6019	X	-	X	-
22	CLA	b	6020	X	-	X	-
22	CLA	b	6021	X	-	X	-
22	CLA	b	6022	X	-	X	-
22	CLA	b	6023	X	-	X	-
22	CLA	b	6024	-	-	X	-
22	CLA	c	6025	X	-	X	-
22	CLA	c	6026	-	-	X	-
22	CLA	c	6027	X	-	X	-
22	CLA	c	6028	X	-	X	-
22	CLA	c	6029	X	-	X	-
22	CLA	c	6030	X	-	X	-
22	CLA	c	6031	X	-	X	-
22	CLA	c	6032	X	-	X	-
22	CLA	c	6033	X	-	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	-	X	-
22	CLA	c	6037	X	-	X	-
22	CLA	d	6004	X	-	X	-
22	CLA	d	6005	X	-	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	-	X	-
23	PHO	d	6039	X	-	X	-
24	PQ9	A	1043	-	-	X	-
24	PQ9	D	1042	-	-	X	-
24	PQ9	a	6043	-	-	X	-
24	PQ9	d	6042	-	-	X	-
25	BCR	A	1044	-	-	X	-
25	BCR	B	1045	-	-	X	-
25	BCR	B	1047	-	-	X	-
25	BCR	B	1048	-	-	X	-
25	BCR	C	1052	-	-	X	-
25	BCR	C	1054	-	-	X	-
25	BCR	D	1050	-	-	X	-
25	BCR	H	1049	-	-	X	-
25	BCR	K	1051	-	-	X	-
25	BCR	T	6046	-	-	X	-
25	BCR	T	6048	-	-	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	-
26	LHG	A	1063	-	-	X	-
26	LHG	a	6063	-	-	X	-
27	IOD	B	1067	-	-	X	X
27	IOD	D	1064	-	-	X	-
27	IOD	D	1068	-	-	X	X
27	IOD	T	1066	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	IOD	b	6067	-	-	-	X
27	IOD	d	6064	-	-	X	-
27	IOD	d	6068	-	-	X	-
27	IOD	t	6066	-	-	X	-
28	MGE	B	1060	-	-	X	-
28	MGE	D	1059	-	-	X	-
28	MGE	D	1062	-	-	X	-
28	MGE	L	1061	-	-	X	-
28	MGE	b	6060	-	-	X	-
28	MGE	d	6059	-	-	X	-
28	MGE	d	6062	-	-	X	-
28	MGE	l	6061	-	-	X	-
29	DGD	B	1058	-	-	X	-
29	DGD	C	1055	-	-	X	-
29	DGD	C	1056	-	-	X	-
29	DGD	C	1057	-	-	X	-
29	DGD	b	6058	-	-	X	-
29	DGD	c	6055	-	-	X	-
29	DGD	c	6056	-	-	X	-
29	DGD	c	6057	-	-	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			

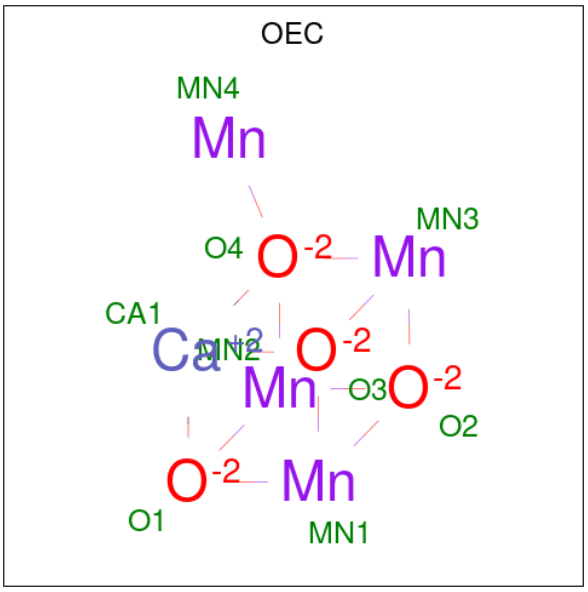
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

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.

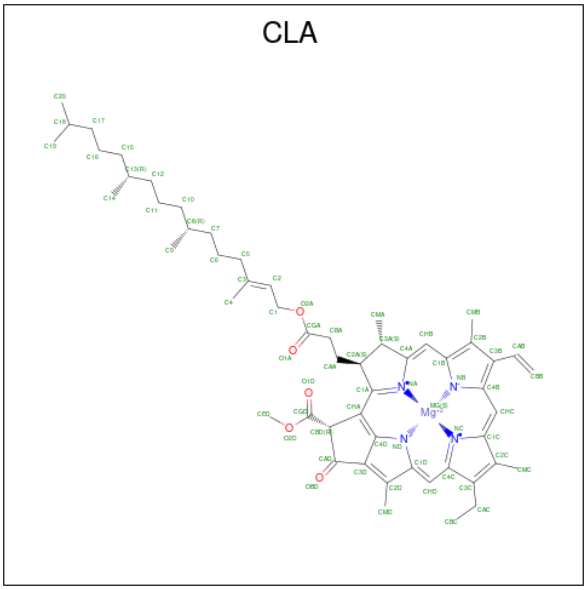
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is OXYGEN EVOLVING SYSTEM (CCD ID: 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 (CCD ID: 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	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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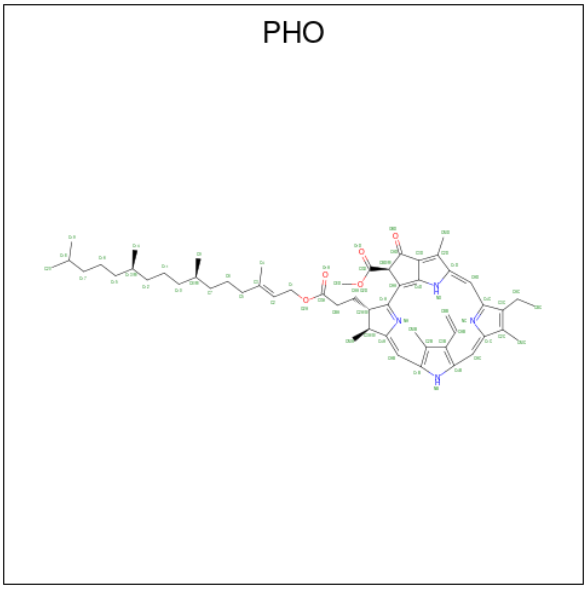
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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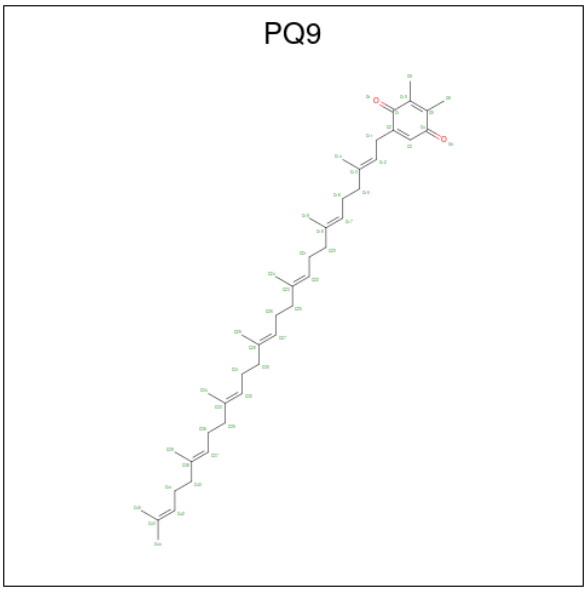
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



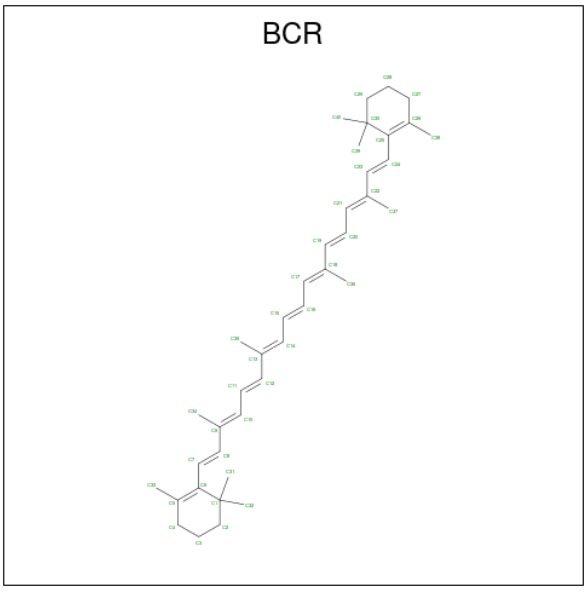
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- 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 (CCD ID: PQ9) (formula: $C_{43}H_{64}O_2$).



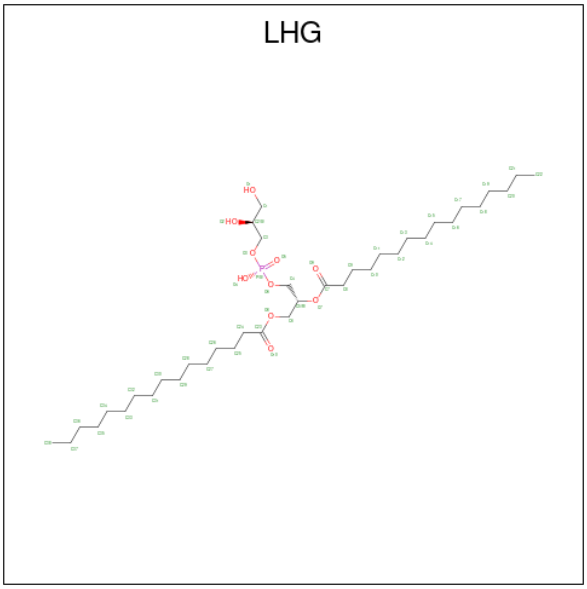
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C O 45 43 2	0	0
24	D	1	Total C O 45 43 2	0	0
24	a	1	Total C O 45 43 2	0	0
24	d	1	Total C O 45 43 2	0	0

- Molecule 25 is BETA-CAROTENE (CCD ID: 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 (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).

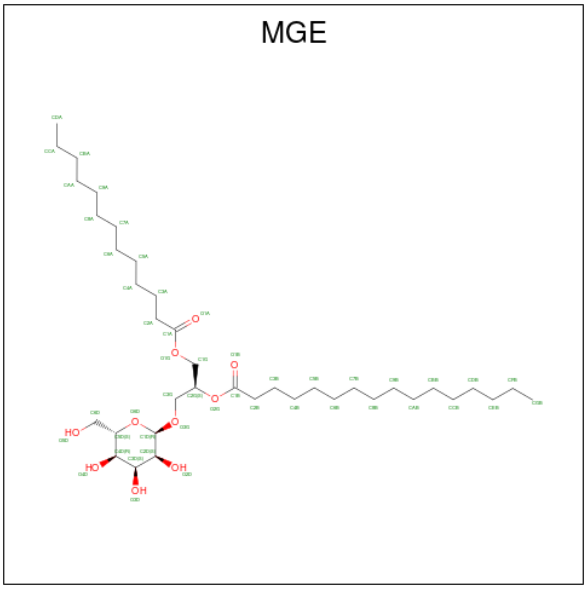


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O P 49 38 10 1	0	0
26	a	1	Total C O P 49 38 10 1	0	0

- Molecule 27 is IODIDE ION (CCD ID: IOD) (formula: I).

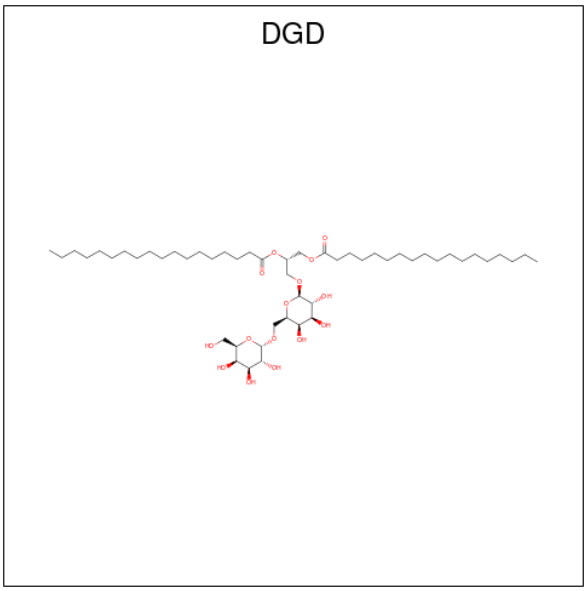
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total I 1 1	0	0
27	B	1	Total I 1 1	0	0
27	D	2	Total I 2 2	0	0
27	T	1	Total I 1 1	0	0
27	a	1	Total I 1 1	0	0
27	b	1	Total I 1 1	0	0
27	d	2	Total I 2 2	0	0
27	t	1	Total I 1 1	0	0

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: 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) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

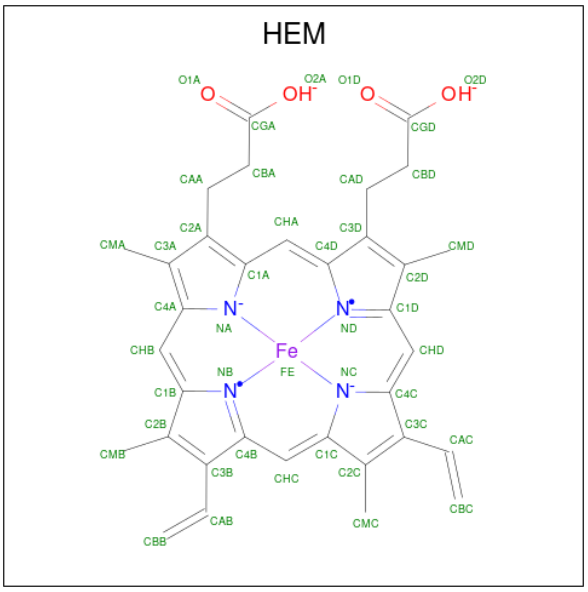


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	1	Total C O 66 51 15	0	0
29	C	1	Total C O 66 51 15	0	0
29	C	1	Total C O 66 51 15	0	0
29	C	1	Total C O 66 51 15	0	0
29	b	1	Total C O 66 51 15	0	0
29	c	1	Total C O 66 51 15	0	0
29	c	1	Total C O 66 51 15	0	0
29	c	1	Total C O 66 51 15	0	0

- Molecule 30 is FE (II) ION (CCD ID: 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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



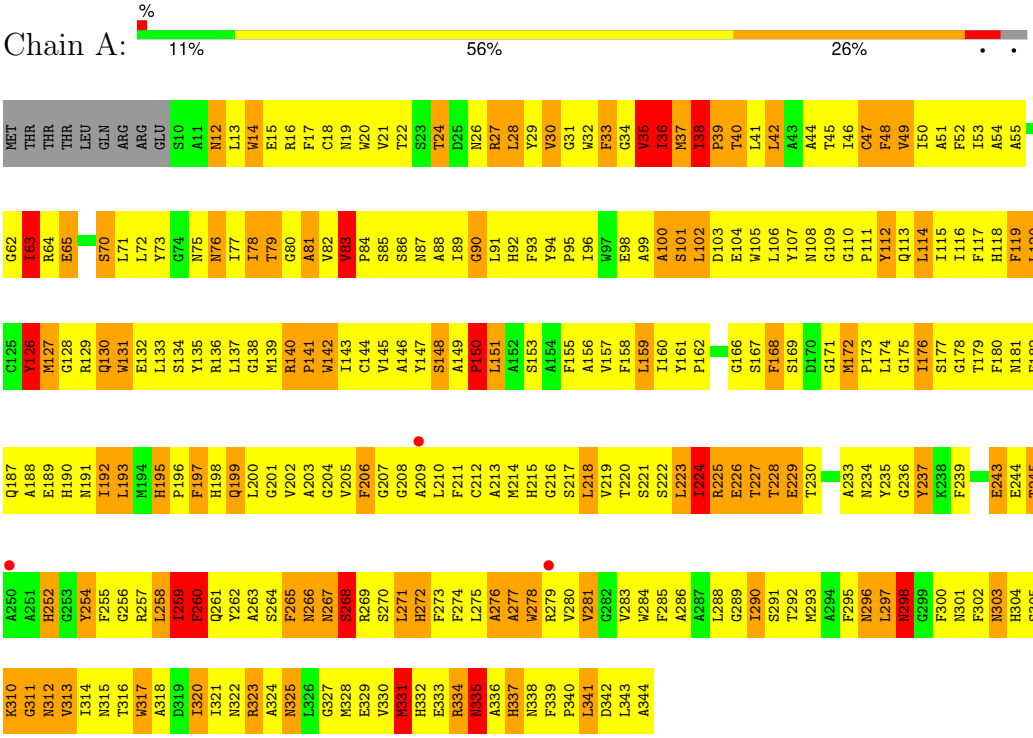
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
31	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
31	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
31	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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.

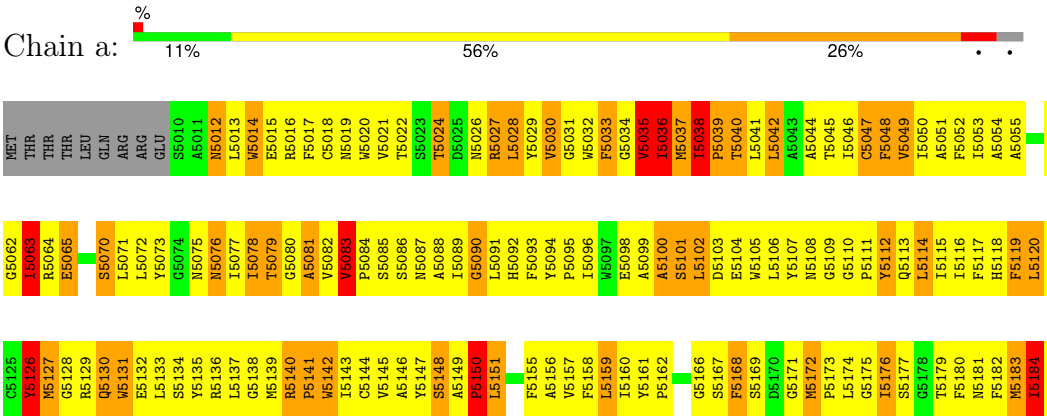
• Molecule 1: Photosystem Q(B) protein

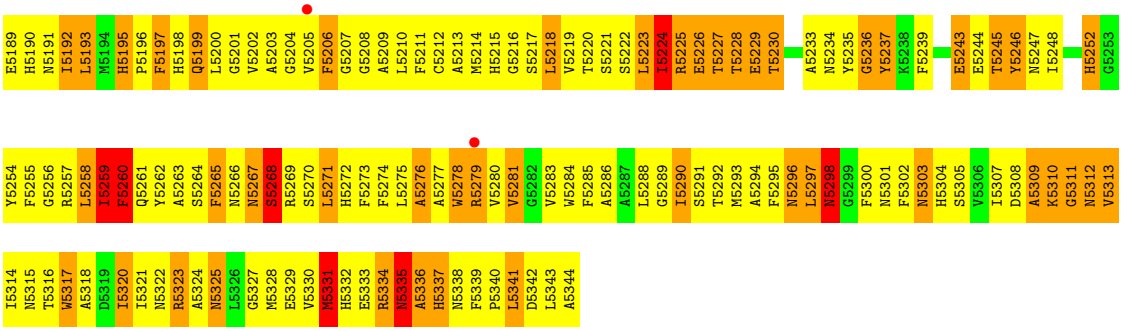
Chain A:



• Molecule 1: Photosystem Q(B) protein

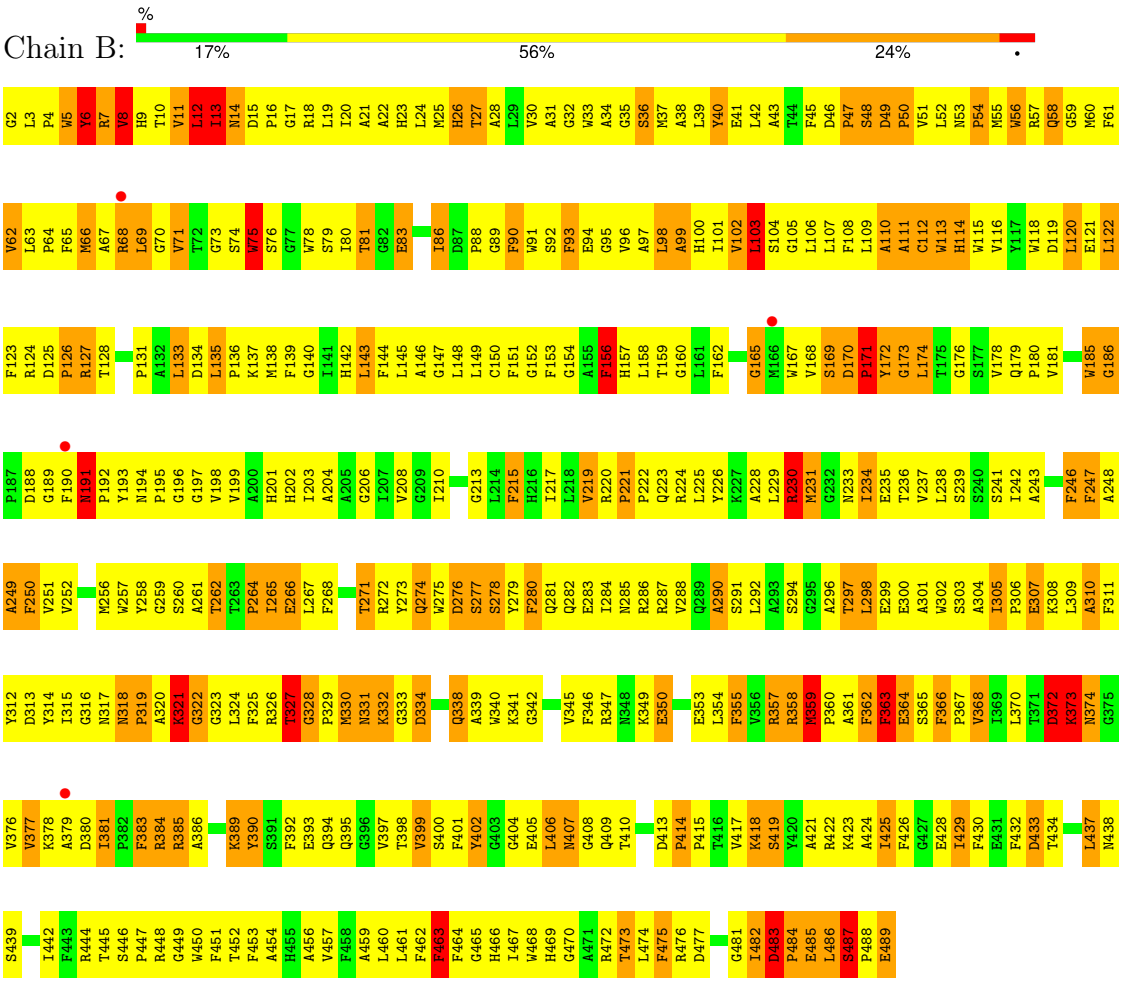
Chain a:





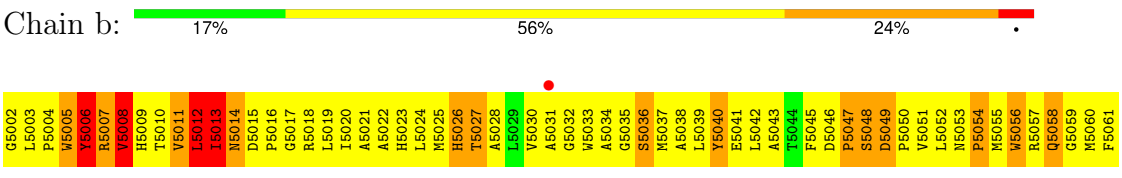
• Molecule 2: Photosystem II core light harvesting protein

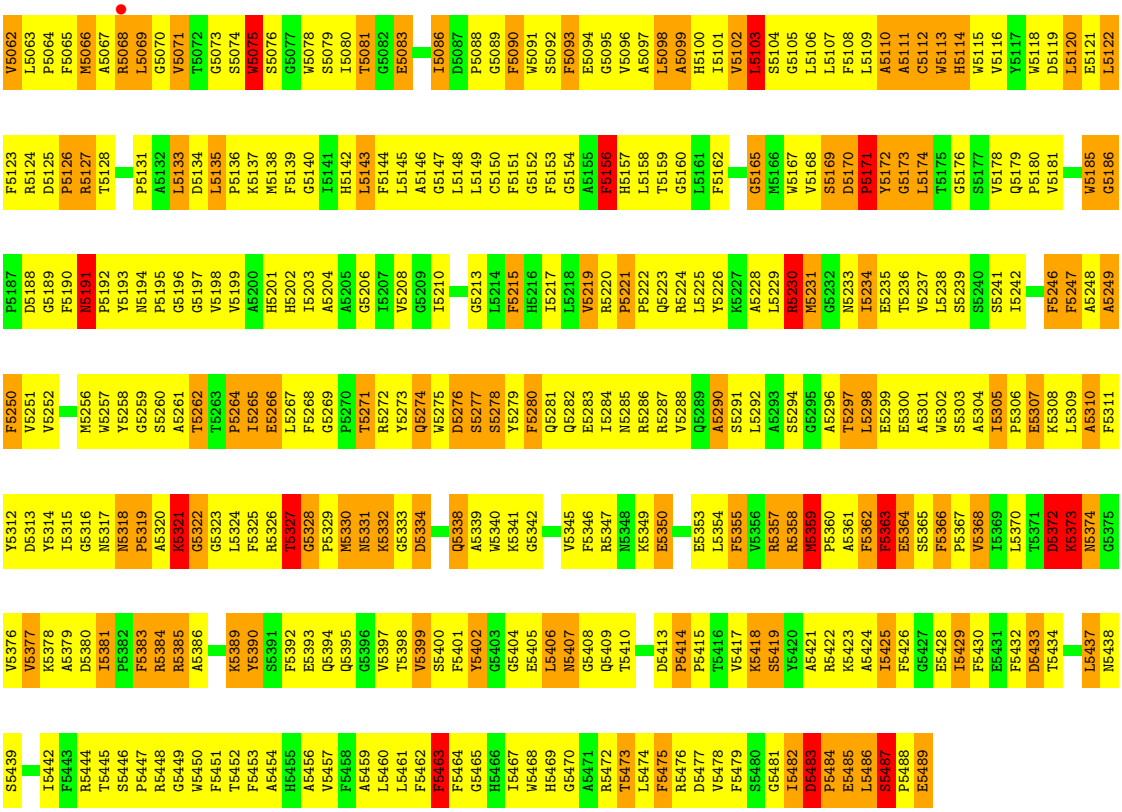
Chain B:



• Molecule 2: Photosystem II core light harvesting protein

Chain b:

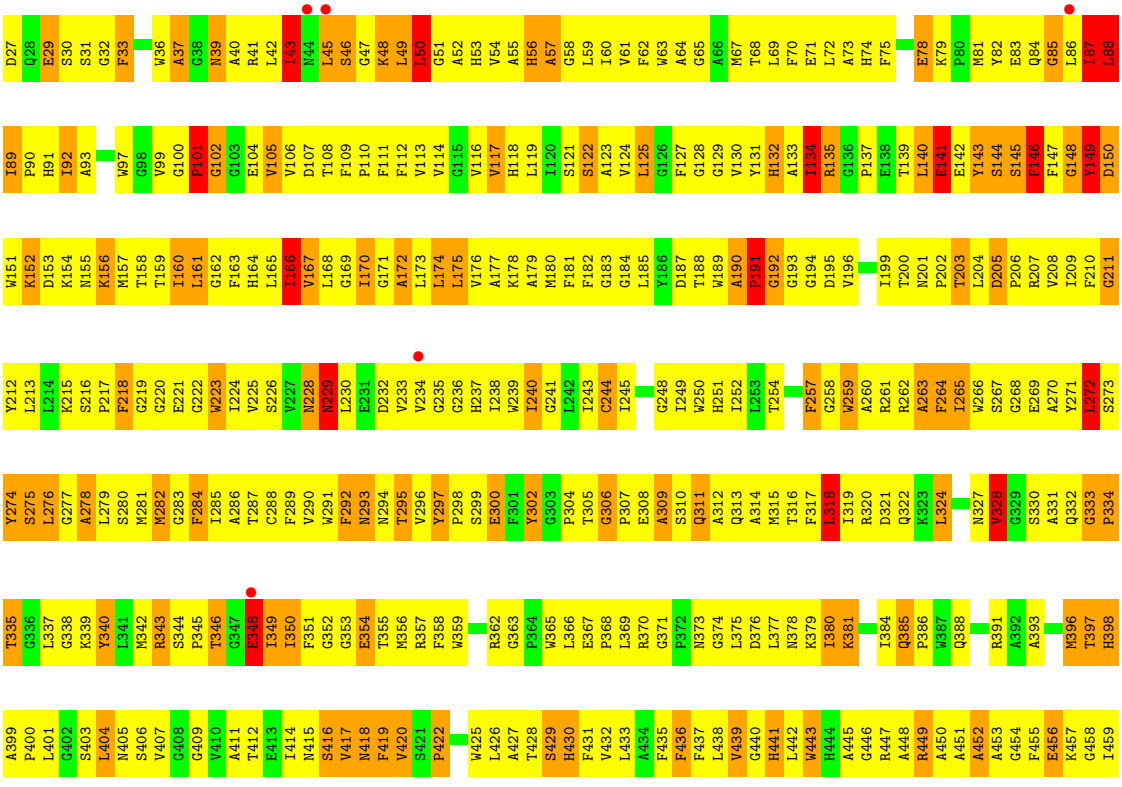




• Molecule 3: Photosystem II CP43 protein

Chain C:

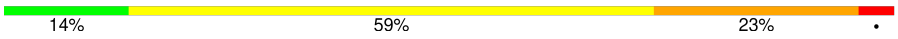


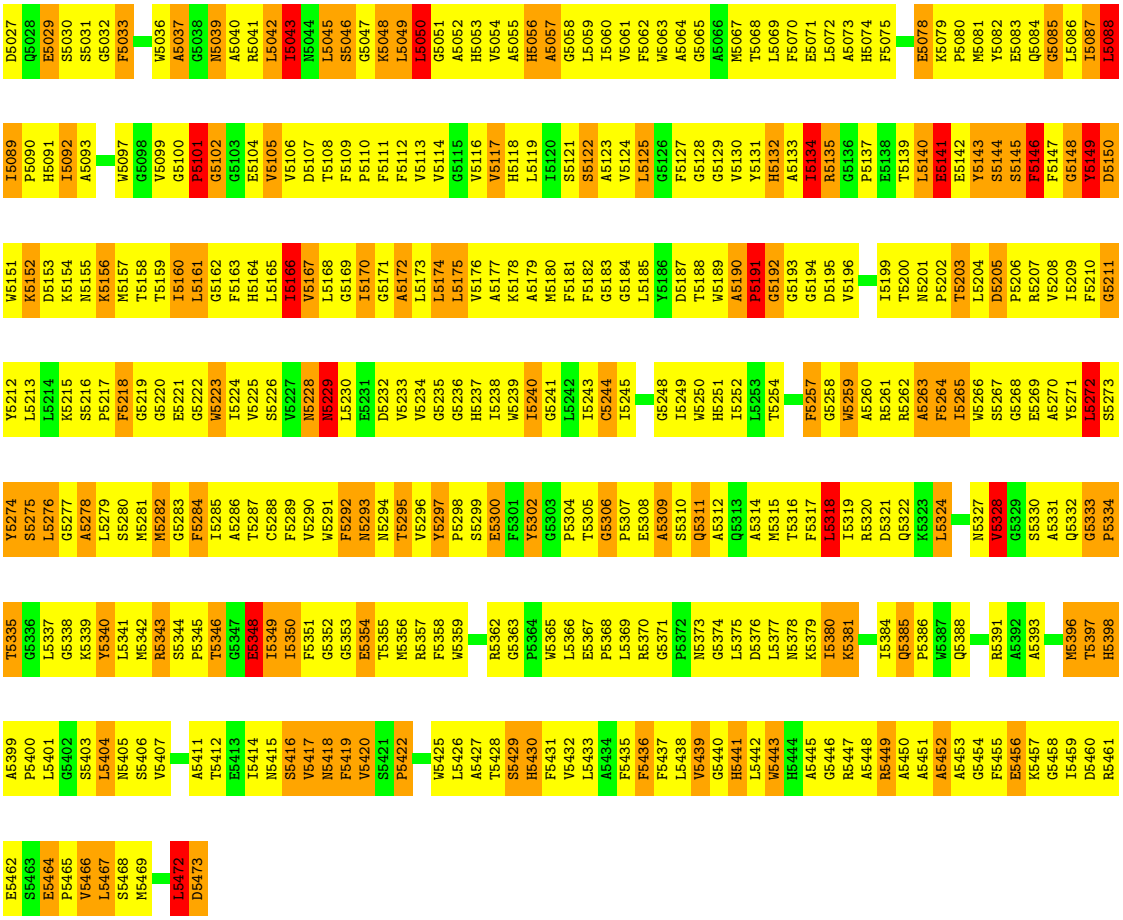




• Molecule 3: Photosystem II CP43 protein

Chain c:

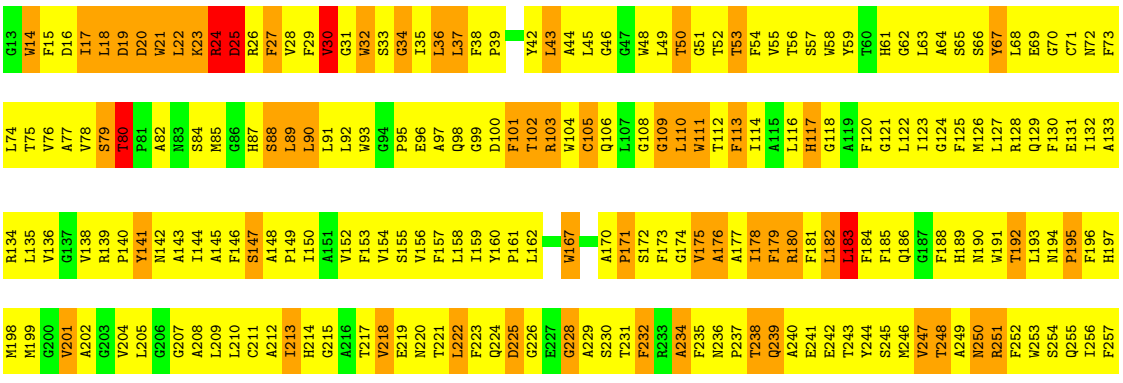


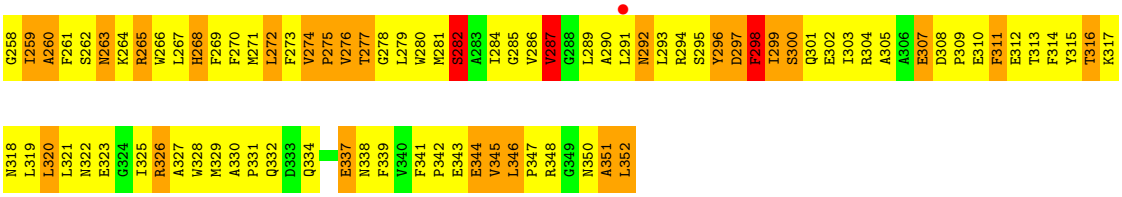


• Molecule 4: Photosystem II D2 protein

Chain D:

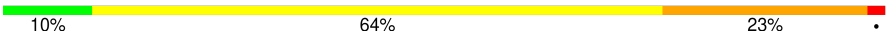






• Molecule 4: Photosystem II D2 protein

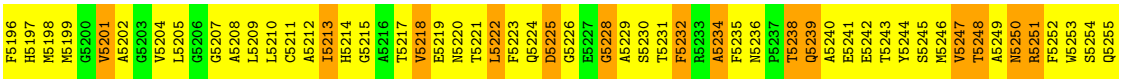
Chain d:

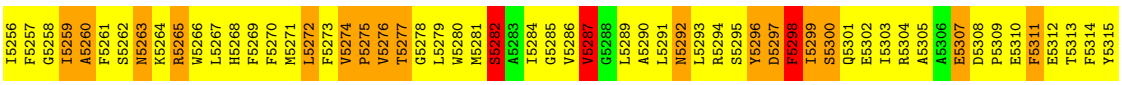


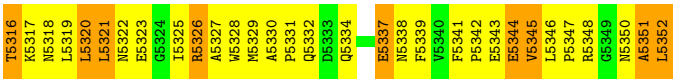






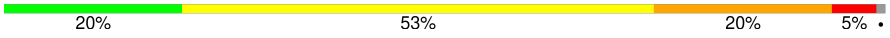


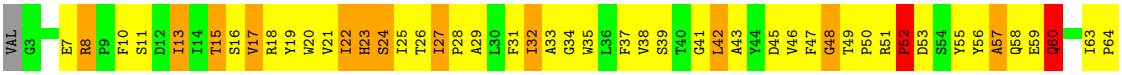


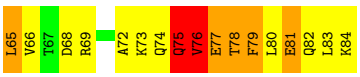


• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

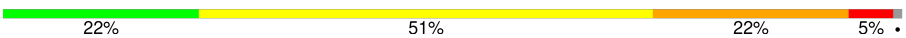


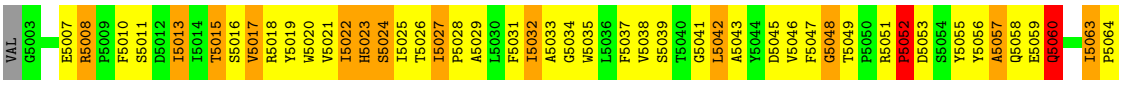




• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

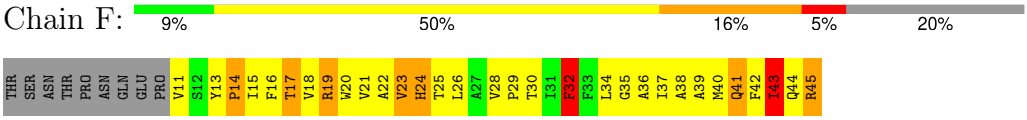






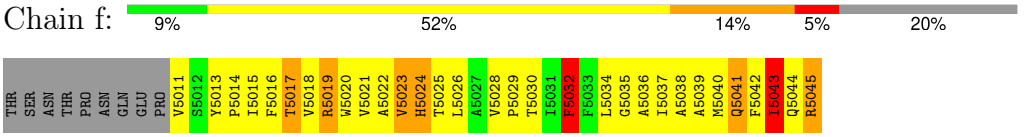
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



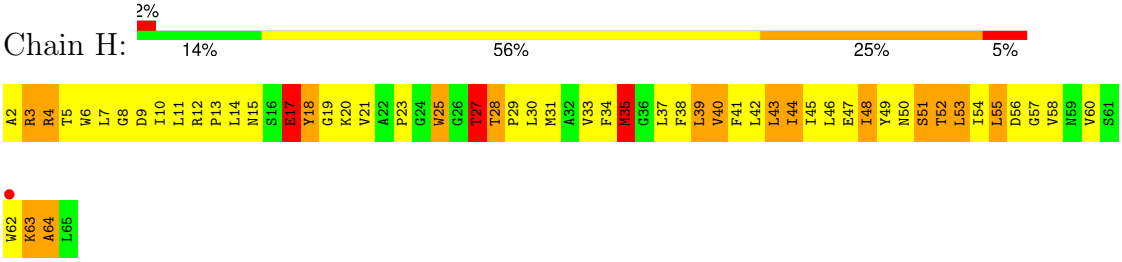
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



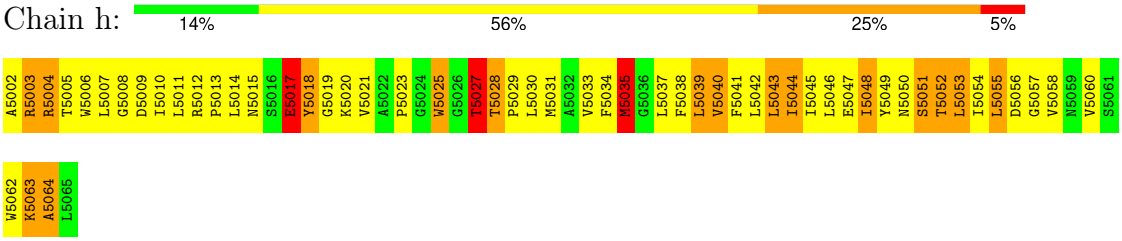
• Molecule 7: Photosystem II reaction center protein H

Chain H:



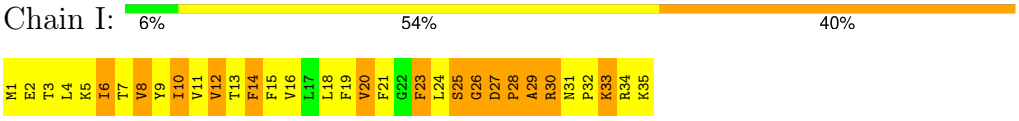
• Molecule 7: Photosystem II reaction center protein H

Chain h:



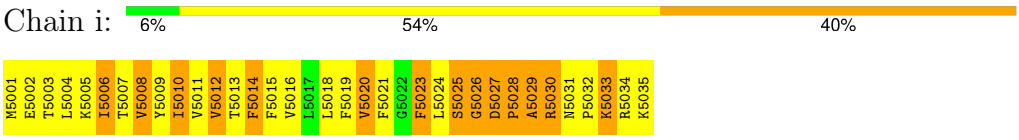
• Molecule 8: Photosystem II reaction center protein I

Chain I:



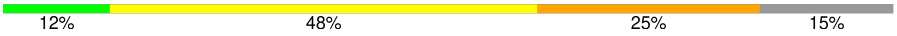
• Molecule 8: Photosystem II reaction center protein I

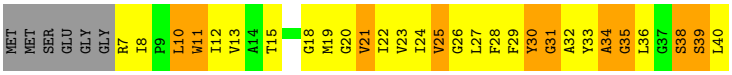
Chain i:



• Molecule 9: Photosystem II reaction center protein J

Chain J:



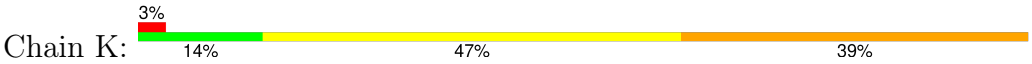


• Molecule 9: Photosystem II reaction center protein J



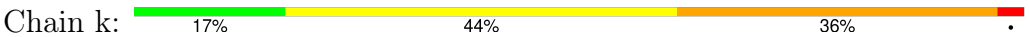


• Molecule 10: Photosystem II reaction center protein K





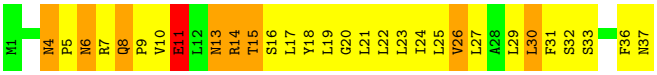
• Molecule 10: Photosystem II reaction center protein K



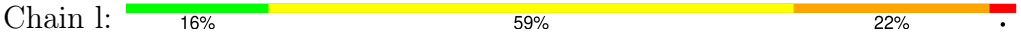


• Molecule 11: Photosystem II reaction center protein L



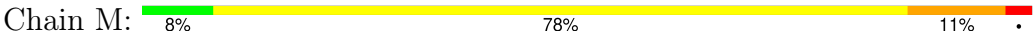


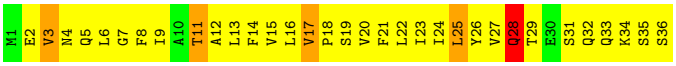
• Molecule 11: Photosystem II reaction center protein L



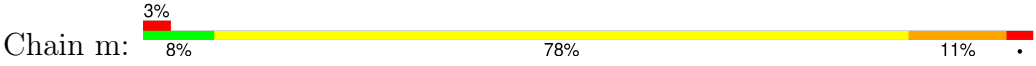


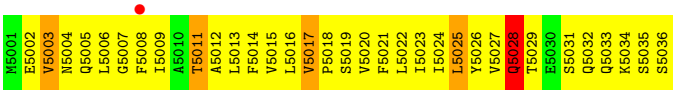
• Molecule 12: Photosystem II reaction center protein M





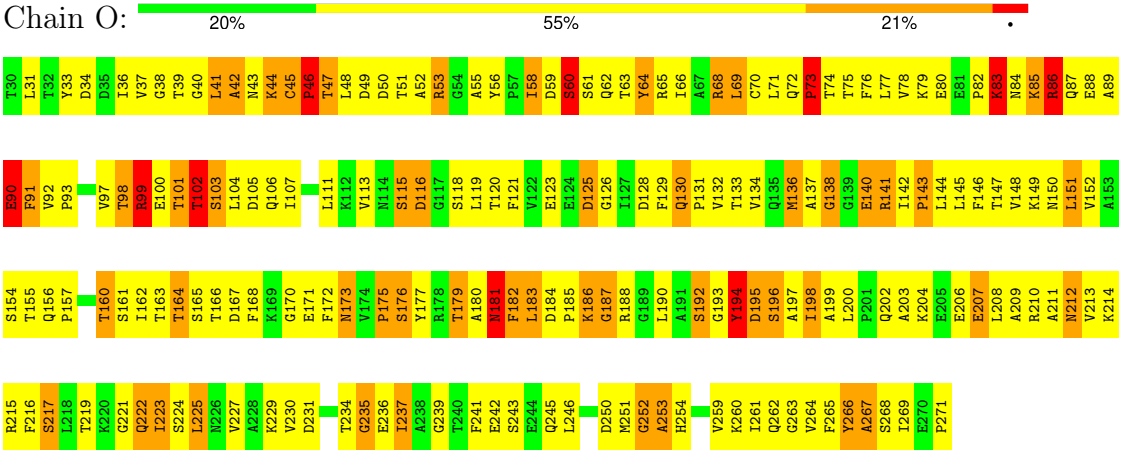
• Molecule 12: Photosystem II reaction center protein M





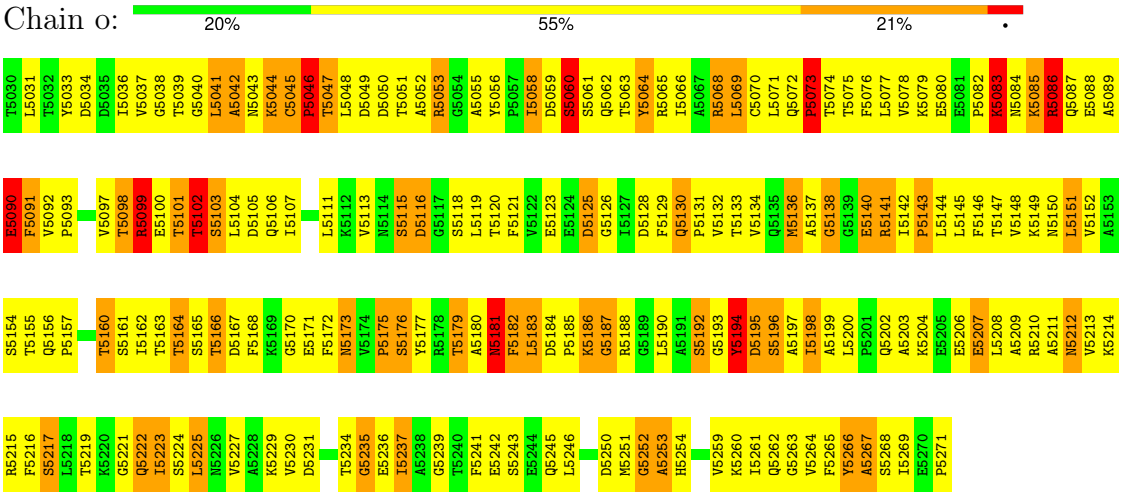
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



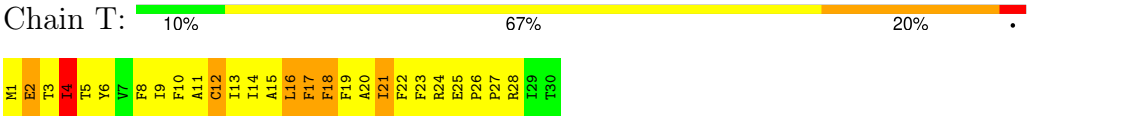
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



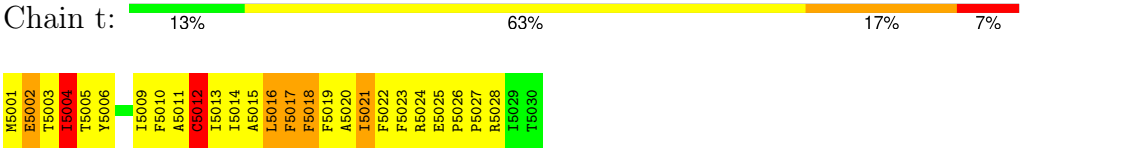
• Molecule 14: Photosystem II reaction center protein T

Chain T:



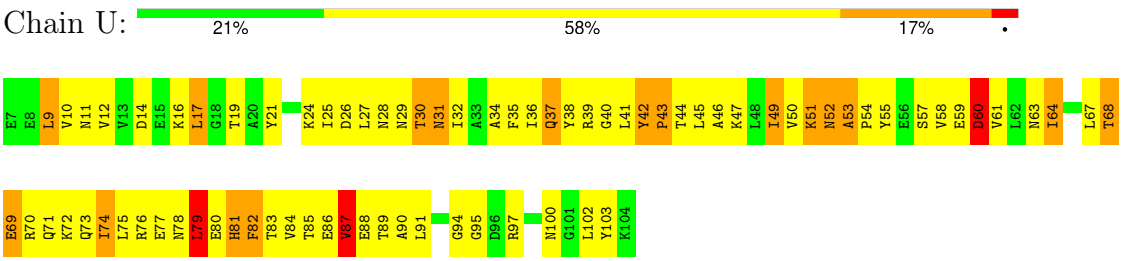
• Molecule 14: Photosystem II reaction center protein T

Chain t:



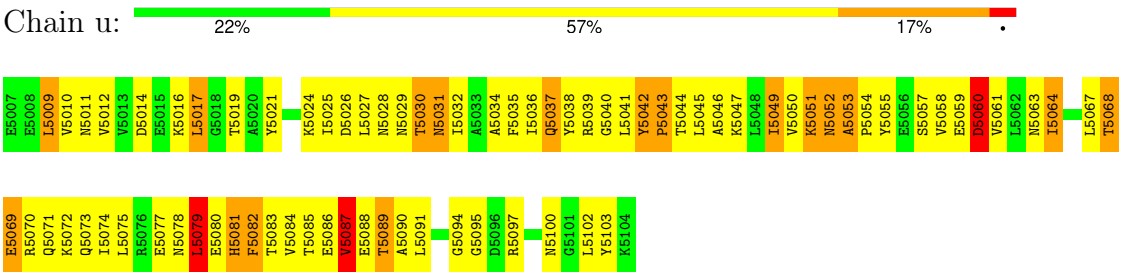
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



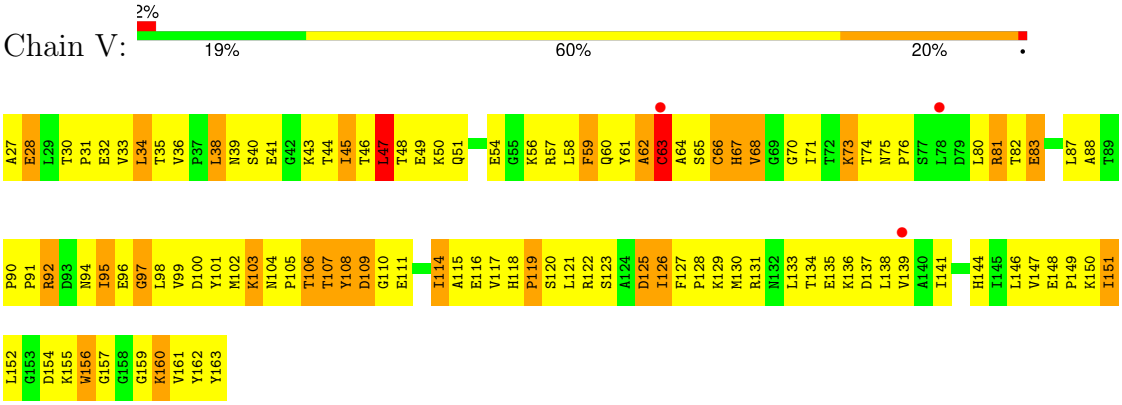
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



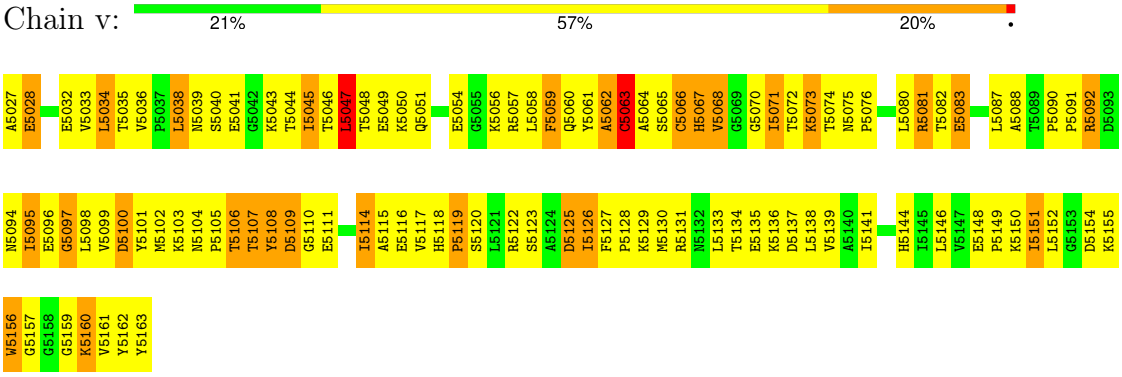
• Molecule 16: Cytochrome c-550

Chain V:



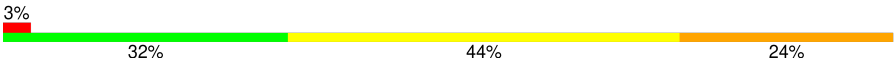
• Molecule 16: Cytochrome c-550

Chain v:



• Molecule 17: Photosystem II reaction center protein X

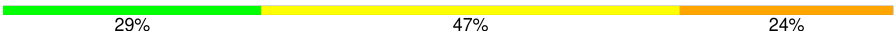
Chain X:

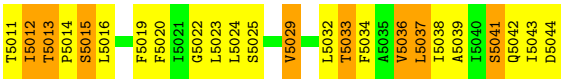




• Molecule 17: Photosystem II reaction center protein X

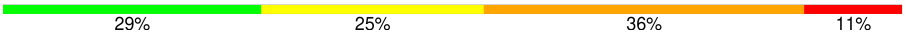
Chain x:

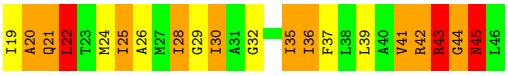




• Molecule 18: Photosystem II reaction center protein ycf12

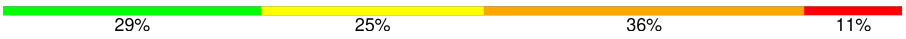
Chain Y:

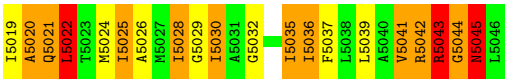




• Molecule 18: Photosystem II reaction center protein ycf12

Chain y:

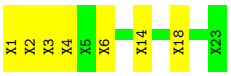




• Molecule 19: Photosystem II reaction center protein Y

Chain N:

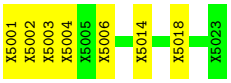




• Molecule 19: Photosystem II reaction center protein Y

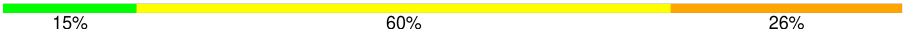
Chain n:





• Molecule 20: Photosystem II reaction center protein Z

Chain Z:

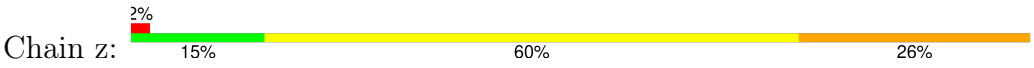


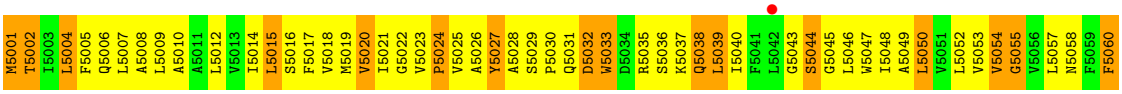


V62

• Molecule 20: Photosystem II reaction center protein Z

Chain z:





V5061
V5062

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) 93.9 (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 0.278 , 0.279	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)	0.23 , 71.4	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: FE2, PQ9, MGE, DGD, OEC, LHG, IOD, PHO, CLA, BCR, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.66	0/2714	1.19	38/3699 (1.0%)
1	a	0.66	0/2714	1.19	37/3699 (1.0%)
2	B	0.68	0/3971	1.27	59/5411 (1.1%)
2	b	0.68	0/3971	1.27	59/5411 (1.1%)
3	C	0.62	1/3568 (0.0%)	1.28	52/4858 (1.1%)
3	c	0.63	1/3568 (0.0%)	1.28	52/4858 (1.1%)
4	D	0.65	0/2801	1.22	34/3818 (0.9%)
4	d	0.65	0/2801	1.22	33/3818 (0.9%)
5	E	0.66	0/685	1.32	7/933 (0.8%)
5	e	0.66	0/685	1.32	7/933 (0.8%)
6	F	0.69	0/291	1.07	1/397 (0.3%)
6	f	0.69	0/291	1.07	1/397 (0.3%)
7	H	0.70	1/520 (0.2%)	1.27	8/708 (1.1%)
7	h	0.70	1/520 (0.2%)	1.27	8/708 (1.1%)
8	I	0.80	0/294	1.07	2/395 (0.5%)
8	i	0.80	0/294	1.07	2/395 (0.5%)
9	J	0.78	0/255	1.22	2/346 (0.6%)
9	j	0.78	0/255	1.22	2/346 (0.6%)
10	K	0.66	0/287	1.25	2/394 (0.5%)
10	k	0.66	0/287	1.27	3/394 (0.8%)
11	L	0.69	0/311	1.12	3/422 (0.7%)
11	l	0.69	0/311	1.11	3/422 (0.7%)
12	M	0.70	0/287	1.10	3/388 (0.8%)
12	m	0.70	0/287	1.09	3/388 (0.8%)
13	O	0.66	0/1891	1.24	23/2564 (0.9%)
13	o	0.66	0/1891	1.24	23/2564 (0.9%)
14	T	0.77	0/266	1.47	7/359 (1.9%)
14	t	0.74	0/266	1.45	7/359 (1.9%)
15	U	0.60	0/794	1.19	8/1076 (0.7%)
15	u	0.59	0/794	1.18	8/1076 (0.7%)
16	V	0.58	0/1085	1.18	13/1473 (0.9%)
16	v	0.58	0/1085	1.18	13/1473 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	X	0.62	0/249	1.16	0/337
17	x	0.62	0/249	1.16	0/337
18	Y	0.84	0/209	1.35	1/279 (0.4%)
18	y	0.84	0/209	1.35	1/279 (0.4%)
20	Z	0.64	0/490	1.19	6/669 (0.9%)
20	z	0.64	0/490	1.19	6/669 (0.9%)
All	All	0.66	4/41936 (0.0%)	1.24	537/57052 (0.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	5346	THR	CA-CB	5.83	1.60	1.53
3	C	346	THR	CA-CB	5.81	1.60	1.53
7	h	5035	MET	SD-CE	5.24	1.92	1.79
7	H	35	MET	SD-CE	5.23	1.92	1.79

The worst 5 of 537 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	170	ASP	CA-C-N	15.15	138.78	119.84
2	B	170	ASP	C-N-CA	15.15	138.78	119.84
2	b	5170	ASP	CA-C-N	15.15	138.78	119.84
2	b	5170	ASP	C-N-CA	15.15	138.78	119.84
3	c	5050	LEU	N-CA-C	-12.24	97.93	111.28

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	776	0
1	a	2630	0	2528	771	0
2	B	3835	0	3700	851	0
2	b	3835	0	3700	836	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3455	0	3376	877	0
3	c	3455	0	3376	878	0
4	D	2706	0	2607	781	0
4	d	2706	0	2608	776	0
5	E	666	0	651	111	0
5	e	666	0	651	112	0
6	F	282	0	291	84	0
6	f	282	0	291	83	0
7	H	507	0	529	146	0
7	h	507	0	529	155	0
8	I	287	0	308	65	0
8	i	287	0	305	64	0
9	J	249	0	262	64	0
9	j	249	0	262	63	0
10	K	278	0	289	88	0
10	k	278	0	289	118	0
11	L	304	0	316	82	0
11	l	304	0	313	87	0
12	M	283	0	297	81	0
12	m	283	0	294	82	0
13	O	1860	0	1833	325	0
13	o	1860	0	1833	334	0
14	T	257	0	261	60	0
14	t	257	0	259	61	0
15	U	783	0	779	143	0
15	u	783	0	779	148	0
16	V	1064	0	1072	218	0
16	v	1064	0	1072	209	0
17	X	246	0	269	39	0
17	x	246	0	269	36	0
18	Y	208	0	237	77	0
18	y	208	0	237	76	0
19	N	116	0	26	5	0
19	n	116	0	26	5	0
20	Z	479	0	516	74	0
20	z	479	0	513	74	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	A	195	0	216	133	0
22	B	975	0	1080	648	0
22	C	780	0	864	478	0
22	D	195	0	216	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	65	0	72	46	0
22	K	65	0	72	89	0
22	a	195	0	216	135	0
22	b	975	0	1080	640	0
22	c	780	0	864	473	0
22	d	195	0	216	149	0
22	h	65	0	72	47	0
22	k	65	0	72	93	0
23	A	64	0	74	63	0
23	D	64	0	74	51	0
23	a	64	0	74	63	0
23	d	64	0	74	52	0
24	A	45	0	64	36	0
24	D	45	0	64	56	0
24	a	45	0	64	35	0
24	d	45	0	64	55	0
25	A	40	0	47	25	0
25	B	120	0	142	86	0
25	C	80	0	96	76	0
25	D	40	0	48	40	0
25	H	40	0	48	34	0
25	K	40	0	47	27	0
25	T	80	0	95	67	0
25	Z	40	0	47	17	0
25	a	40	0	47	26	0
25	b	80	0	95	62	0
25	c	40	0	48	36	0
25	d	40	0	48	39	0
25	h	40	0	48	34	0
25	k	80	0	95	74	0
25	t	40	0	48	44	0
25	z	40	0	47	19	0
26	A	49	0	74	36	0
26	a	49	0	74	36	0
27	A	1	0	0	1	0
27	B	1	0	0	3	0
27	D	2	0	0	9	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	9	0
27	t	1	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	38	0
28	d	96	0	144	67	0
28	l	48	0	72	27	0
29	B	66	0	96	32	0
29	C	198	0	288	118	0
29	b	66	0	96	34	0
29	c	198	0	288	121	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	17	0
31	v	43	0	30	10	0
All	All	48060	0	48531	11725	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 121.

The worst 5 of 11725 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)
4:d:5169:PHE:HB3	27:d:6068:IOD:I	1.69	1.61
14:t:5012:CYS:SG	27:t:6066:IOD:I	1.65	1.58
25:k:6052:BCR:H371	25:k:6052:BCR:C26	1.34	1.56
22:B:1011:CLA:HED2	22:B:1012:CLA:CED	1.31	1.53
22:b:6011:CLA:HED2	22:b:6012:CLA:CED	1.31	1.53

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	5
1	a	333/344 (97%)	216 (65%)	76 (23%)	41 (12%)	0	4
2	B	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	7
2	b	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	7
3	C	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	12
3	c	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	12
4	D	338/340 (99%)	222 (66%)	78 (23%)	38 (11%)	0	6
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	5
5	e	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0	5
6	F	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	4
6	f	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	4
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	10
9	j	32/40 (80%)	29 (91%)	0	3 (9%)	0	10
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	17
11	l	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	1	17
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	5
13	o	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0	5
14	T	28/30 (93%)	22 (79%)	5 (18%)	1 (4%)	2	23
14	t	28/30 (93%)	22 (79%)	4 (14%)	2 (7%)	1	14
15	U	96/98 (98%)	70 (73%)	17 (18%)	9 (9%)	0	10
15	u	96/98 (98%)	70 (73%)	18 (19%)	8 (8%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	V	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1 13
16	v	135/137 (98%)	99 (73%)	26 (19%)	10 (7%)	1 13
17	X	32/34 (94%)	29 (91%)	3 (9%)	0	100 100
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 15
20	z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1 15
All	All	5124/5250 (98%)	3622 (71%)	986 (19%)	516 (10%)	0 8

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%)	213 (79%)	57 (21%)	1 7
1	a	270/279 (97%)	213 (79%)	57 (21%)	1 7
2	B	388/388 (100%)	315 (81%)	73 (19%)	1 11
2	b	388/388 (100%)	315 (81%)	73 (19%)	1 11
3	C	349/349 (100%)	276 (79%)	73 (21%)	1 7
3	c	349/349 (100%)	276 (79%)	73 (21%)	1 7
4	D	275/275 (100%)	235 (86%)	40 (14%)	3 16
4	d	275/275 (100%)	235 (86%)	40 (14%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	72/73 (99%)	57 (79%)	15 (21%)	1 7
5	e	72/73 (99%)	57 (79%)	15 (21%)	1 7
6	F	29/38 (76%)	22 (76%)	7 (24%)	1 5
6	f	29/38 (76%)	22 (76%)	7 (24%)	1 5
7	H	54/54 (100%)	45 (83%)	9 (17%)	2 13
7	h	54/54 (100%)	45 (83%)	9 (17%)	2 13
8	I	32/32 (100%)	24 (75%)	8 (25%)	0 4
8	i	32/32 (100%)	24 (75%)	8 (25%)	0 4
9	J	24/28 (86%)	18 (75%)	6 (25%)	0 4
9	j	24/28 (86%)	18 (75%)	6 (25%)	0 4
10	K	29/29 (100%)	21 (72%)	8 (28%)	0 3
10	k	29/29 (100%)	23 (79%)	6 (21%)	1 7
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%)	28 (85%)	5 (15%)	3 15
12	m	33/33 (100%)	28 (85%)	5 (15%)	3 15
13	O	206/206 (100%)	170 (82%)	36 (18%)	2 13
13	o	206/206 (100%)	170 (82%)	36 (18%)	2 13
14	T	27/27 (100%)	24 (89%)	3 (11%)	6 23
14	t	27/27 (100%)	24 (89%)	3 (11%)	6 23
15	U	85/85 (100%)	74 (87%)	11 (13%)	4 19
15	u	85/85 (100%)	75 (88%)	10 (12%)	5 21
16	V	117/117 (100%)	96 (82%)	21 (18%)	2 12
16	v	117/117 (100%)	97 (83%)	20 (17%)	2 13
17	X	27/27 (100%)	16 (59%)	11 (41%)	0 0
17	x	27/27 (100%)	16 (59%)	11 (41%)	0 0
18	Y	21/21 (100%)	11 (52%)	10 (48%)	0 0
18	y	21/21 (100%)	11 (52%)	10 (48%)	0 0
20	Z	52/52 (100%)	41 (79%)	11 (21%)	1 7
20	z	52/52 (100%)	41 (79%)	11 (21%)	1 7
All	All	4250/4296 (99%)	3434 (81%)	816 (19%)	1 10

5 of 816 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	5317	TRP
3	c	5167	VAL
18	y	5035	ILE
2	b	5066	MET
1	a	5313	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 202 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	5267	ASN
3	c	5294	ASN
20	z	5006	GLN
1	a	5312	ASN
2	b	5274	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 oligosaccharides 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	$\#\|Z\|>2$
22	CLA	C	1031	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	A	1006	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	a	6007	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	b	6011	2	69,73,73	1.92	17 (24%)	82,113,113	2.48	30 (36%)
23	PHO	D	1039	-	58,69,69	2.94	13 (22%)	55,99,99	3.52	19 (34%)
24	PQ9	A	1043	-	45,45,45	0.68	2 (4%)	56,57,57	1.79	17 (30%)
25	BCR	B	1045	-	41,41,41	4.02	17 (41%)	56,56,56	6.17	21 (37%)
25	BCR	A	1044	-	41,41,41	3.93	16 (39%)	56,56,56	7.23	28 (50%)
31	HEM	F	1040	6,5	50,50,50	1.87	8 (16%)	67,82,82	1.34	5 (7%)
22	CLA	b	6021	2	69,73,73	1.92	16 (23%)	82,113,113	2.49	30 (36%)
22	CLA	B	1019	2	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	T	6048	-	41,41,41	4.01	17 (41%)	56,56,56	6.30	27 (48%)
22	CLA	B	1022	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	DGD	C	1055	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
25	BCR	d	6050	-	41,41,41	4.02	17 (41%)	56,56,56	5.17	21 (37%)
22	CLA	C	1026	3	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
25	BCR	C	1052	-	41,41,41	4.02	17 (41%)	56,56,56	6.97	24 (42%)
29	DGD	C	1056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
23	PHO	a	6038	-	58,69,69	2.94	13 (22%)	55,99,99	3.53	19 (34%)
22	CLA	B	1009	-	69,73,73	1.92	15 (21%)	82,113,113	2.47	29 (35%)
22	CLA	D	1008	4	69,73,73	1.92	17 (24%)	82,113,113	2.48	29 (35%)
25	BCR	D	1050	-	41,41,41	4.02	17 (41%)	56,56,56	5.17	22 (39%)
25	BCR	z	6053	-	41,41,41	4.03	17 (41%)	56,56,56	6.02	22 (39%)
22	CLA	b	6022	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1023	2	69,73,73	1.91	16 (23%)	82,113,113	2.48	29 (35%)
22	CLA	b	6024	2	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
22	CLA	b	6014	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	c	6030	3	69,73,73	1.91	17 (24%)	82,113,113	2.48	29 (35%)
22	CLA	C	1032	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	H	1017	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	C	1025	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	a	6003	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	b	6015	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	b	6012	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
23	PHO	d	6039	-	58,69,69	2.94	13 (22%)	55,99,99	3.52	19 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	MGE	b	6060	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	B	1011	2	69,73,73	1.92	16 (23%)	82,113,113	2.47	30 (36%)
22	CLA	A	1003	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	c	6028	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
25	BCR	t	1046	-	41,41,41	3.96	17 (41%)	56,56,56	6.06	26 (46%)
25	BCR	Z	1053	-	41,41,41	4.03	17 (41%)	56,56,56	6.02	21 (37%)
22	CLA	c	6031	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	a	6006	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	c	6029	3	69,73,73	1.91	16 (23%)	82,113,113	2.48	29 (35%)
22	CLA	c	6026	3	69,73,73	1.93	15 (21%)	82,113,113	2.48	28 (34%)
24	PQ9	a	6043	-	45,45,45	0.69	2 (4%)	56,57,57	1.79	17 (30%)
22	CLA	d	6005	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	c	6025	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	b	6047	-	41,41,41	4.02	17 (41%)	56,56,56	5.46	27 (48%)
31	HEM	V	1041	16	50,50,50	1.88	8 (16%)	67,82,82	1.35	5 (7%)
29	DGD	c	6056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6009	-	69,73,73	1.91	15 (21%)	82,113,113	2.47	29 (35%)
22	CLA	C	1037	3	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
28	MGE	D	1059	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	A	1007	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	C	1054	-	41,41,41	4.02	16 (39%)	56,56,56	5.42	21 (37%)
22	CLA	d	6008	4	69,73,73	1.92	18 (26%)	82,113,113	2.48	29 (35%)
22	CLA	C	1033	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	PHO	A	1038	-	58,69,69	2.94	13 (22%)	55,99,99	3.53	19 (34%)
22	CLA	c	6032	3	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
22	CLA	b	6023	2	69,73,73	1.91	16 (23%)	82,113,113	2.48	29 (35%)
31	HEM	v	6041	16	50,50,50	1.88	8 (16%)	67,82,82	1.36	5 (7%)
22	CLA	B	1015	-	69,73,73	1.93	15 (21%)	82,113,113	2.48	28 (34%)
25	BCR	b	6045	-	41,41,41	4.02	17 (41%)	56,56,56	6.17	20 (35%)
24	PQ9	d	6042	-	45,45,45	0.68	2 (4%)	56,57,57	1.79	17 (30%)
24	PQ9	D	1042	-	45,45,45	0.68	2 (4%)	56,57,57	1.79	17 (30%)
25	BCR	K	1051	-	41,41,41	4.03	17 (41%)	56,56,56	4.97	20 (35%)
29	DGD	C	1057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	c	6036	3	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	HEM	f	6040	6,5	50,50,50	1.87	9 (18%)	67,82,82	1.34	5 (7%)
25	BCR	T	6046	-	41,41,41	3.96	17 (41%)	56,56,56	6.06	26 (46%)
22	CLA	B	1016	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1021	2	69,73,73	1.92	16 (23%)	82,113,113	2.49	30 (36%)
22	CLA	b	6010	2	69,73,73	1.91	16 (23%)	82,113,113	2.49	29 (35%)
22	CLA	D	1004	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	k	6034	-	69,73,73	1.93	16 (23%)	82,113,113	2.49	28 (34%)
25	BCR	k	6051	-	41,41,41	4.03	17 (41%)	56,56,56	4.97	20 (35%)
28	MGE	B	1060	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
29	DGD	B	1058	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6013	2	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	B	1048	-	41,41,41	4.01	17 (41%)	56,56,56	6.30	27 (48%)
22	CLA	B	1012	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	B	1014	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
29	DGD	c	6057	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	C	1027	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	C	1028	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	27 (32%)
22	CLA	C	1035	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	LHG	A	1063	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
28	MGE	l	6061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	c	6027	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	c	6035	3	69,73,73	1.94	16 (23%)	82,113,113	2.49	28 (34%)
28	MGE	L	1061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
25	BCR	a	6044	-	41,41,41	3.92	16 (39%)	56,56,56	7.23	28 (50%)
22	CLA	B	1020	2	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	D	1005	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	b	6020	2	69,73,73	1.94	15 (21%)	82,113,113	2.49	28 (34%)
22	CLA	C	1029	3	69,73,73	1.91	17 (24%)	82,113,113	2.48	29 (35%)
25	BCR	B	1047	-	41,41,41	4.01	17 (41%)	56,56,56	5.46	26 (46%)
22	CLA	c	6037	3	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
25	BCR	H	1049	-	41,41,41	4.02	16 (39%)	56,56,56	5.30	20 (35%)
22	CLA	b	6016	2	69,73,73	1.93	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	c	6033	3	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
25	BCR	k	6052	-	41,41,41	4.02	17 (41%)	56,56,56	6.97	24 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	LHG	a	6063	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
22	CLA	C	1036	3	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	B	1013	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
28	MGE	d	6062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	d	6004	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	DGD	b	6058	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6019	2	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	K	1034	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1024	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1010	2	69,73,73	1.92	16 (23%)	82,113,113	2.49	29 (35%)
28	MGE	D	1062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	h	6017	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
29	DGD	c	6055	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
25	BCR	h	6049	-	41,41,41	4.02	17 (41%)	56,56,56	5.30	20 (35%)
22	CLA	C	1030	3	69,73,73	1.91	17 (24%)	82,113,113	2.48	29 (35%)
28	MGE	d	6059	-	48,48,48	0.97	2 (4%)	56,56,56	1.01	3 (5%)
25	BCR	c	6054	-	41,41,41	4.02	16 (39%)	56,56,56	5.43	21 (37%)

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
22	CLA	C	1031	3	1/1/15/20	14/39/115/115	-
22	CLA	A	1006	-	1/1/15/20	19/39/115/115	-
22	CLA	a	6007	-	-	25/39/115/115	-
22	CLA	b	6011	2	2/2/15/20	21/39/115/115	-
23	PHO	D	1039	-	3/3/17/22	16/37/103/103	0/5/6/6
24	PQ9	A	1043	-	-	16/41/61/61	0/1/1/1
25	BCR	B	1045	-	-	20/29/63/63	0/2/2/2
25	BCR	A	1044	-	-	12/29/63/63	0/2/2/2
31	HEM	F	1040	6,5	-	10/14/54/54	-
22	CLA	b	6021	2	1/1/15/20	24/39/115/115	-
22	CLA	B	1019	2	1/1/15/20	19/39/115/115	-
25	BCR	T	6048	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1022	2	2/2/15/20	20/39/115/115	-
29	DGD	C	1055	-	-	33/55/95/95	0/2/2/2
25	BCR	d	6050	-	-	21/29/63/63	0/2/2/2
22	CLA	C	1026	3	-	18/39/115/115	-
25	BCR	C	1052	-	-	13/29/63/63	0/2/2/2
29	DGD	C	1056	-	-	32/55/95/95	0/2/2/2
23	PHO	a	6038	-	1/1/17/22	18/37/103/103	0/5/6/6
22	CLA	B	1009	-	1/1/15/20	17/39/115/115	-
22	CLA	D	1008	4	2/2/15/20	15/39/115/115	-
25	BCR	D	1050	-	-	21/29/63/63	0/2/2/2
25	BCR	z	6053	-	-	15/29/63/63	0/2/2/2
22	CLA	b	6022	2	2/2/15/20	20/39/115/115	-
22	CLA	B	1023	2	2/2/15/20	16/39/115/115	-
22	CLA	b	6024	2	-	17/39/115/115	-
22	CLA	b	6014	-	1/1/15/20	18/39/115/115	-
22	CLA	c	6030	3	1/1/15/20	18/39/115/115	-
22	CLA	C	1032	3	2/2/15/20	19/39/115/115	-
22	CLA	H	1017	-	1/1/15/20	24/39/115/115	-
22	CLA	C	1025	3	1/1/15/20	17/39/115/115	-
22	CLA	a	6003	-	1/1/15/20	23/39/115/115	-
22	CLA	b	6015	-	1/1/15/20	18/39/115/115	-
22	CLA	b	6012	-	1/1/15/20	18/39/115/115	-
23	PHO	d	6039	-	3/3/17/22	16/37/103/103	0/5/6/6
28	MGE	b	6060	-	-	31/43/63/63	0/1/1/1
22	CLA	B	1011	2	2/2/15/20	21/39/115/115	-
22	CLA	A	1003	-	1/1/15/20	23/39/115/115	-
22	CLA	c	6028	-	1/1/15/20	24/39/115/115	-
25	BCR	t	1046	-	-	11/29/63/63	0/2/2/2
25	BCR	Z	1053	-	-	15/29/63/63	0/2/2/2
22	CLA	c	6031	3	1/1/15/20	14/39/115/115	-
22	CLA	a	6006	-	1/1/15/20	19/39/115/115	-
22	CLA	c	6029	3	2/2/15/20	15/39/115/115	-
22	CLA	c	6026	3	-	18/39/115/115	-
24	PQ9	a	6043	-	-	16/41/61/61	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	6005	-	1/1/15/20	20/39/115/115	-
22	CLA	c	6025	3	1/1/15/20	17/39/115/115	-
25	BCR	b	6047	-	-	17/29/63/63	0/2/2/2
31	HEM	V	1041	16	-	6/14/54/54	-
29	DGD	c	6056	-	-	32/55/95/95	0/2/2/2
22	CLA	b	6009	-	1/1/15/20	17/39/115/115	-
22	CLA	C	1037	3	1/1/15/20	16/39/115/115	-
28	MGE	D	1059	-	-	23/43/63/63	0/1/1/1
22	CLA	A	1007	-	-	25/39/115/115	-
25	BCR	C	1054	-	-	14/29/63/63	0/2/2/2
22	CLA	d	6008	4	2/2/15/20	15/39/115/115	-
22	CLA	C	1033	3	1/1/15/20	16/39/115/115	-
23	PHO	A	1038	-	1/1/17/22	18/37/103/103	0/5/6/6
22	CLA	c	6032	3	2/2/15/20	19/39/115/115	-
22	CLA	b	6023	2	2/2/15/20	16/39/115/115	-
31	HEM	v	6041	16	-	5/14/54/54	-
22	CLA	B	1015	-	1/1/15/20	18/39/115/115	-
25	BCR	b	6045	-	-	20/29/63/63	0/2/2/2
24	PQ9	d	6042	-	-	11/41/61/61	0/1/1/1
24	PQ9	D	1042	-	-	11/41/61/61	0/1/1/1
25	BCR	K	1051	-	-	15/29/63/63	0/2/2/2
29	DGD	C	1057	-	-	32/55/95/95	0/2/2/2
22	CLA	b	6018	-	1/1/15/20	23/39/115/115	-
22	CLA	c	6036	3	1/1/15/20	23/39/115/115	-
31	HEM	f	6040	6,5	-	10/14/54/54	-
25	BCR	T	6046	-	-	11/29/63/63	0/2/2/2
22	CLA	B	1021	2	1/1/15/20	24/39/115/115	-
22	CLA	B	1016	2	-	20/39/115/115	-
22	CLA	b	6010	2	1/1/15/20	15/39/115/115	-
22	CLA	D	1004	-	1/1/15/20	12/39/115/115	-
22	CLA	B	1018	-	1/1/15/20	23/39/115/115	-
22	CLA	k	6034	-	4/4/15/20	24/39/115/115	-
25	BCR	k	6051	-	-	15/29/63/63	0/2/2/2
28	MGE	B	1060	-	-	31/43/63/63	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	B	1058	-	-	32/55/95/95	0/2/2/2
22	CLA	b	6013	2	1/1/15/20	24/39/115/115	-
25	BCR	B	1048	-	-	10/29/63/63	0/2/2/2
22	CLA	B	1012	-	1/1/15/20	18/39/115/115	-
22	CLA	B	1014	-	1/1/15/20	18/39/115/115	-
29	DGD	c	6057	-	-	32/55/95/95	0/2/2/2
22	CLA	C	1027	3	2/2/15/20	18/39/115/115	-
22	CLA	C	1028	-	1/1/15/20	24/39/115/115	-
22	CLA	C	1035	3	1/1/15/20	14/39/115/115	-
26	LHG	A	1063	-	-	27/53/53/53	-
28	MGE	l	6061	-	-	26/43/63/63	0/1/1/1
22	CLA	c	6027	3	2/2/15/20	18/39/115/115	-
22	CLA	c	6035	3	1/1/15/20	14/39/115/115	-
28	MGE	L	1061	-	-	26/43/63/63	0/1/1/1
25	BCR	a	6044	-	-	12/29/63/63	0/2/2/2
22	CLA	B	1020	2	2/2/15/20	18/39/115/115	-
22	CLA	D	1005	-	1/1/15/20	20/39/115/115	-
22	CLA	b	6020	2	2/2/15/20	18/39/115/115	-
22	CLA	C	1029	3	2/2/15/20	15/39/115/115	-
25	BCR	B	1047	-	-	17/29/63/63	0/2/2/2
22	CLA	c	6037	3	1/1/15/20	16/39/115/115	-
25	BCR	H	1049	-	-	13/29/63/63	0/2/2/2
22	CLA	c	6033	3	1/1/15/20	16/39/115/115	-
22	CLA	b	6016	2	-	20/39/115/115	-
25	BCR	k	6052	-	-	13/29/63/63	0/2/2/2
26	LHG	a	6063	-	-	28/53/53/53	-
22	CLA	C	1036	3	1/1/15/20	23/39/115/115	-
22	CLA	B	1013	2	1/1/15/20	24/39/115/115	-
28	MGE	d	6062	-	-	24/43/63/63	0/1/1/1
22	CLA	d	6004	-	1/1/15/20	12/39/115/115	-
29	DGD	b	6058	-	-	32/55/95/95	0/2/2/2
22	CLA	b	6019	2	1/1/15/20	19/39/115/115	-
22	CLA	K	1034	-	4/4/15/20	24/39/115/115	-
22	CLA	B	1024	2	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1010	2	1/1/15/20	15/39/115/115	-
28	MGE	D	1062	-	-	24/43/63/63	0/1/1/1
22	CLA	h	6017	-	1/1/15/20	24/39/115/115	-
29	DGD	c	6055	-	-	33/55/95/95	0/2/2/2
25	BCR	h	6049	-	-	13/29/63/63	0/2/2/2
22	CLA	C	1030	3	1/1/15/20	18/39/115/115	-
28	MGE	d	6059	-	-	23/43/63/63	0/1/1/1
25	BCR	c	6054	-	-	14/29/63/63	0/2/2/2

The worst 5 of 1605 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	6039	PHO	OBD-CAD	14.60	1.41	1.22
23	D	1039	PHO	OBD-CAD	14.58	1.41	1.22
23	A	1038	PHO	OBD-CAD	14.57	1.41	1.22
23	a	6038	PHO	OBD-CAD	14.57	1.41	1.22
25	b	6047	BCR	C19-C18	-9.39	1.25	1.46

The worst 5 of 2709 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	6045	BCR	C16-C17-C18	29.28	168.34	127.28
25	B	1045	BCR	C16-C17-C18	29.26	168.32	127.28
25	T	6048	BCR	C15-C16-C17	26.44	177.62	123.52
25	B	1048	BCR	C15-C16-C17	26.42	177.57	123.52
25	Z	1053	BCR	C15-C16-C17	26.11	176.94	123.52

5 of 92 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	1003	CLA	C8
22	A	1006	CLA	C8
22	B	1009	CLA	CBD
22	B	1010	CLA	C8
22	B	1011	CLA	CBD

5 of 2320 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	C2B-C3B-CAB-CBB
22	A	1003	CLA	C4B-C3B-CAB-CBB
22	A	1003	CLA	CBD-CGD-O2D-CED
22	A	1003	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

122 monomers are involved in 4181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	1031	CLA	63	0
22	A	1006	CLA	44	0
22	a	6007	CLA	38	0
22	b	6011	CLA	87	0
23	D	1039	PHO	51	0
24	A	1043	PQ9	36	0
25	B	1045	BCR	21	0
25	A	1044	BCR	25	0
31	F	1040	HEM	17	0
22	b	6021	CLA	57	0
22	B	1019	CLA	40	0
25	T	6048	BCR	23	0
22	B	1022	CLA	74	0
29	C	1055	DGD	26	0
25	d	6050	BCR	39	0
22	C	1026	CLA	27	0
25	C	1052	BCR	38	0
29	C	1056	DGD	55	0
23	a	6038	PHO	63	0
22	B	1009	CLA	59	0
22	D	1008	CLA	48	0
25	D	1050	BCR	40	0
25	z	6053	BCR	19	0
22	b	6022	CLA	76	0
22	B	1023	CLA	68	0
22	b	6024	CLA	45	0
22	b	6014	CLA	41	0
22	c	6030	CLA	37	0
22	C	1032	CLA	42	0
22	H	1017	CLA	46	0
22	C	1025	CLA	64	0
22	a	6003	CLA	51	0
22	b	6015	CLA	46	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	b	6012	CLA	61	0
23	d	6039	PHO	52	0
28	b	6060	MGE	38	0
22	B	1011	CLA	86	0
22	A	1003	CLA	51	0
22	c	6028	CLA	37	0
25	t	1046	BCR	44	0
25	Z	1053	BCR	17	0
22	c	6031	CLA	61	0
22	a	6006	CLA	47	0
22	c	6029	CLA	59	0
22	c	6026	CLA	28	0
24	a	6043	PQ9	35	0
22	d	6005	CLA	57	0
22	c	6025	CLA	65	0
25	b	6047	BCR	42	0
31	V	1041	HEM	12	0
29	c	6056	DGD	59	0
22	b	6009	CLA	62	0
22	C	1037	CLA	21	0
28	D	1059	MGE	45	0
22	A	1007	CLA	39	0
25	C	1054	BCR	38	0
22	d	6008	CLA	46	0
22	C	1033	CLA	66	0
23	A	1038	PHO	63	0
22	c	6032	CLA	39	0
22	b	6023	CLA	67	0
31	v	6041	HEM	10	0
22	B	1015	CLA	47	0
25	b	6045	BCR	21	0
24	d	6042	PQ9	55	0
24	D	1042	PQ9	56	0
25	K	1051	BCR	27	0
29	C	1057	DGD	41	0
22	b	6018	CLA	35	0
22	c	6036	CLA	21	0
31	f	6040	HEM	17	0
25	T	6046	BCR	44	0
22	B	1016	CLA	46	0
22	B	1021	CLA	60	0
22	b	6010	CLA	37	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	1004	CLA	51	0
22	B	1018	CLA	34	0
22	k	6034	CLA	93	0
25	k	6051	BCR	26	0
28	B	1060	MGE	39	0
29	B	1058	DGD	32	0
22	b	6013	CLA	63	0
25	B	1048	BCR	23	0
22	B	1012	CLA	61	0
22	B	1014	CLA	44	0
29	c	6057	DGD	41	0
22	C	1027	CLA	35	0
22	C	1028	CLA	37	0
22	C	1035	CLA	53	0
26	A	1063	LHG	36	0
28	l	6061	MGE	27	0
22	c	6027	CLA	37	0
22	c	6035	CLA	49	0
28	L	1061	MGE	29	0
25	a	6044	BCR	26	0
22	B	1020	CLA	52	0
22	D	1005	CLA	58	0
22	b	6020	CLA	52	0
22	C	1029	CLA	62	0
25	B	1047	BCR	43	0
22	c	6037	CLA	21	0
25	H	1049	BCR	34	0
22	b	6016	CLA	43	0
22	c	6033	CLA	68	0
25	k	6052	BCR	51	0
26	a	6063	LHG	36	0
22	C	1036	CLA	22	0
22	B	1013	CLA	65	0
28	d	6062	MGE	21	0
22	d	6004	CLA	52	0
29	b	6058	DGD	34	0
22	b	6019	CLA	37	0
22	K	1034	CLA	89	0
22	B	1024	CLA	45	0
22	B	1010	CLA	38	0
28	D	1062	MGE	21	0
22	h	6017	CLA	47	0

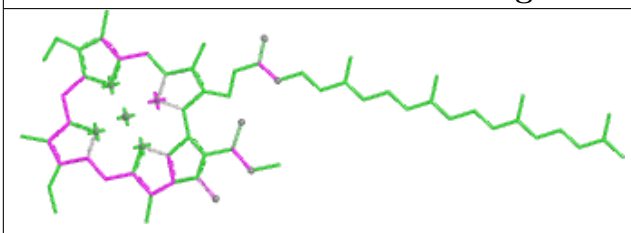
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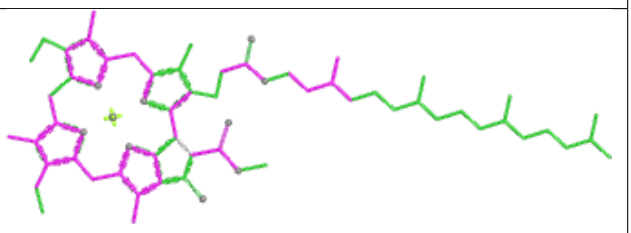
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c	6055	DGD	25	0
25	h	6049	BCR	34	0
22	C	1030	CLA	37	0
28	d	6059	MGE	46	0
25	c	6054	BCR	36	0

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.

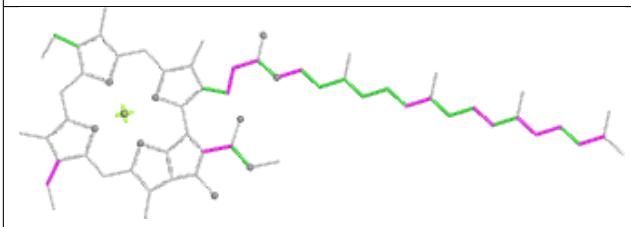
Ligand CLA C 1031



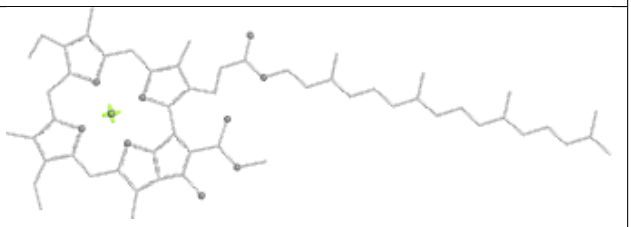
Bond lengths



Bond angles

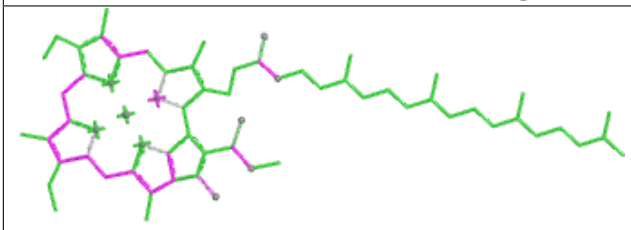


Torsions

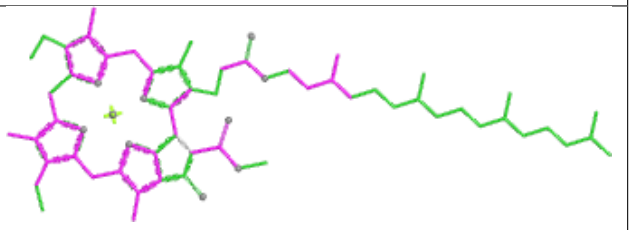


Rings

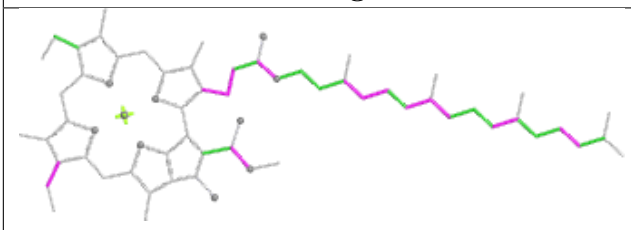
Ligand CLA A 1006



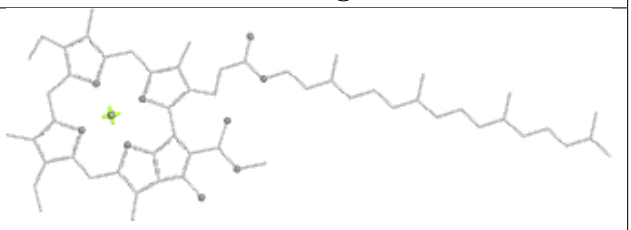
Bond lengths



Bond angles

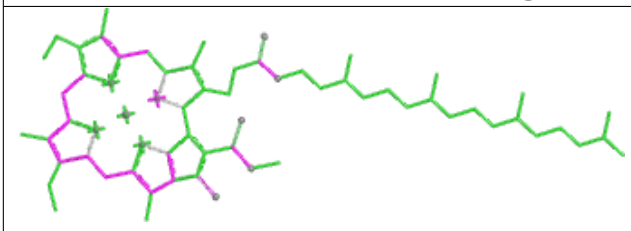


Torsions

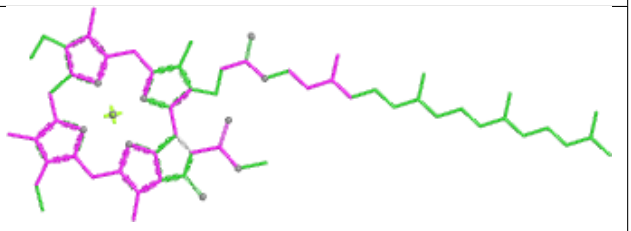


Rings

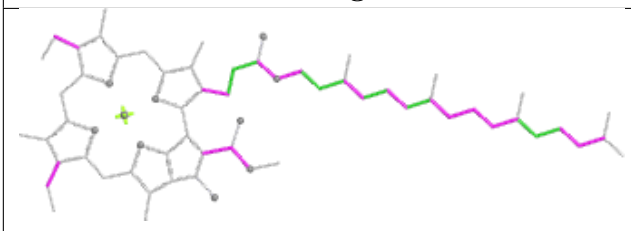
Ligand CLA a 6007



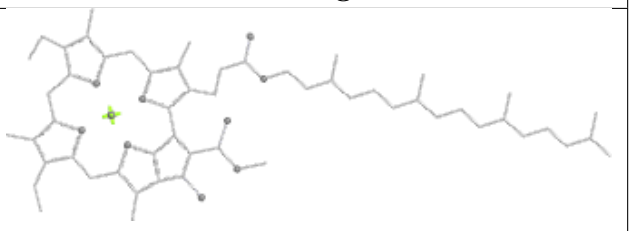
Bond lengths



Bond angles

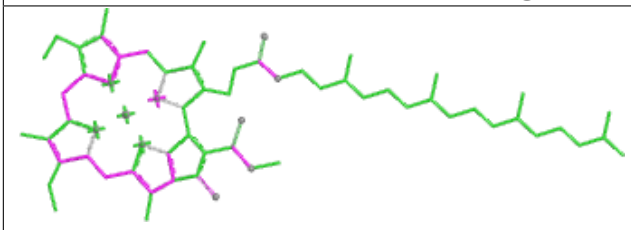


Torsions

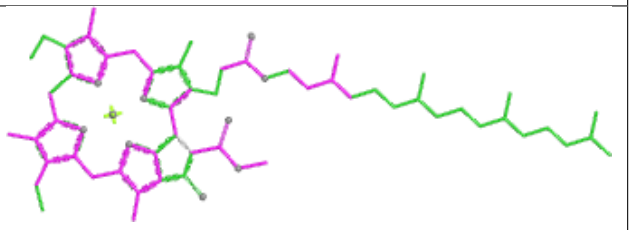


Rings

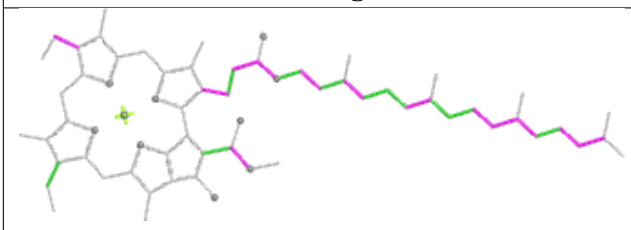
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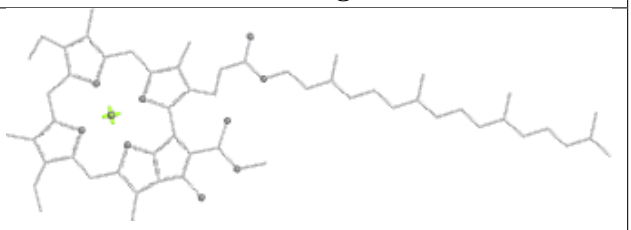
Bond lengths



Bond angles

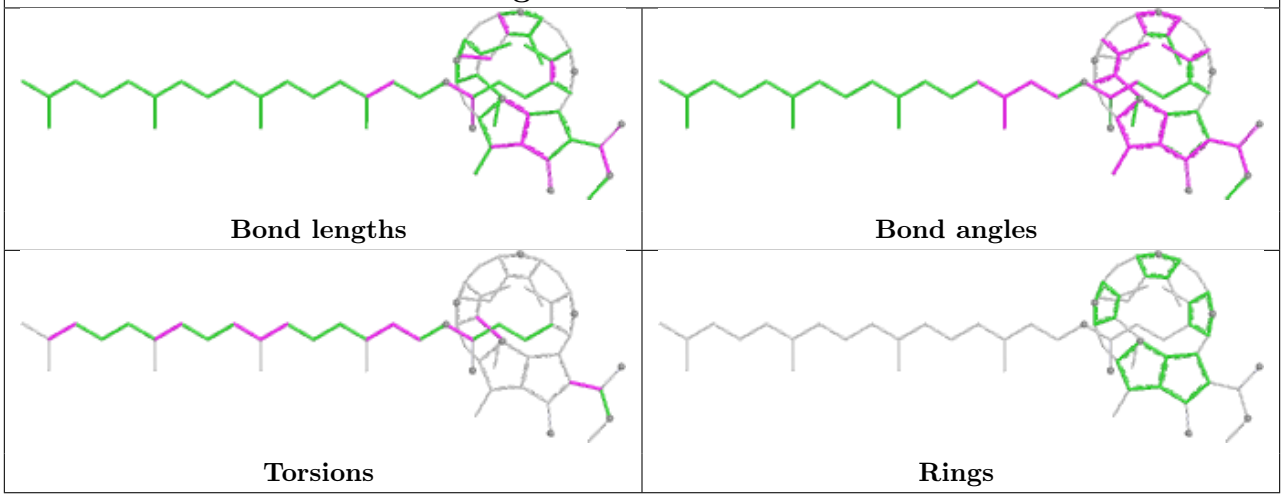


Torsions

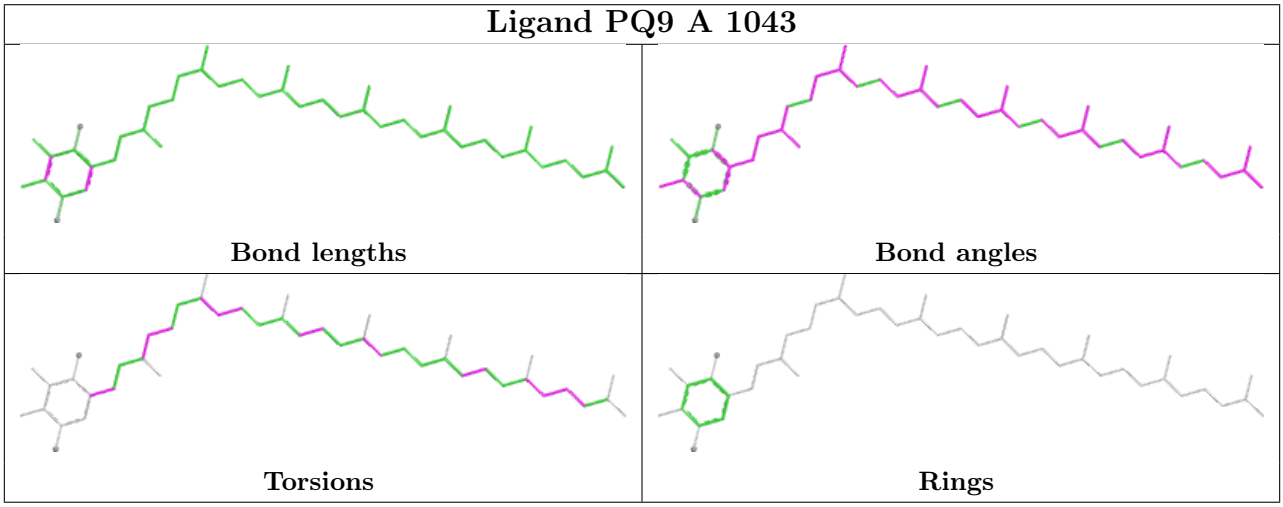


Rings

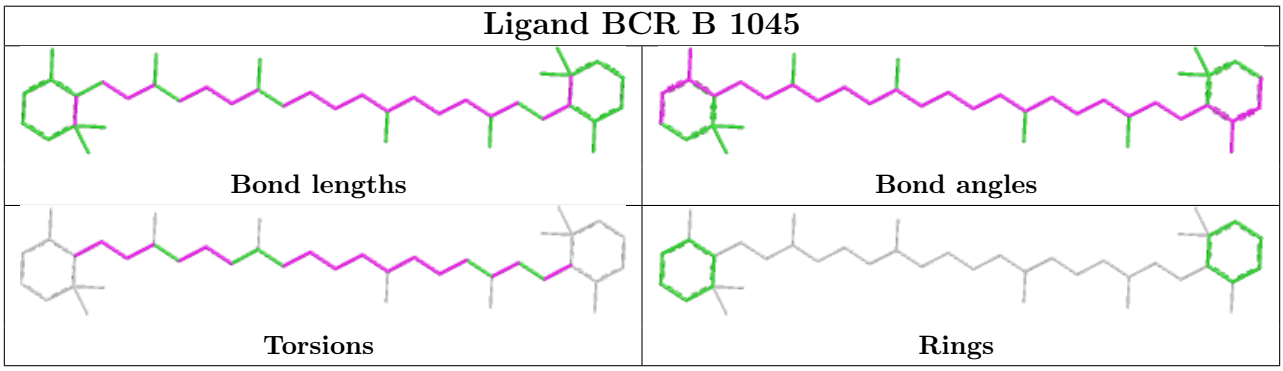
Ligand PHO D 1039



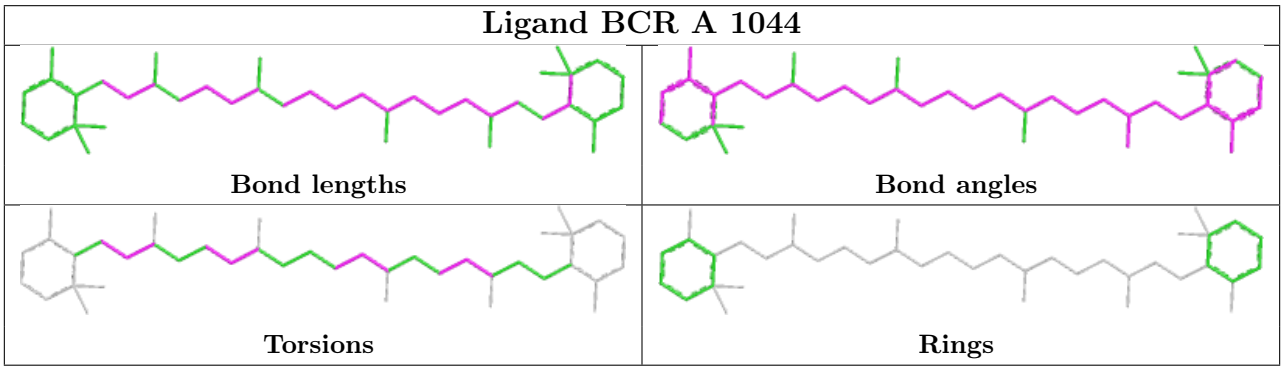
Ligand PQ9 A 1043



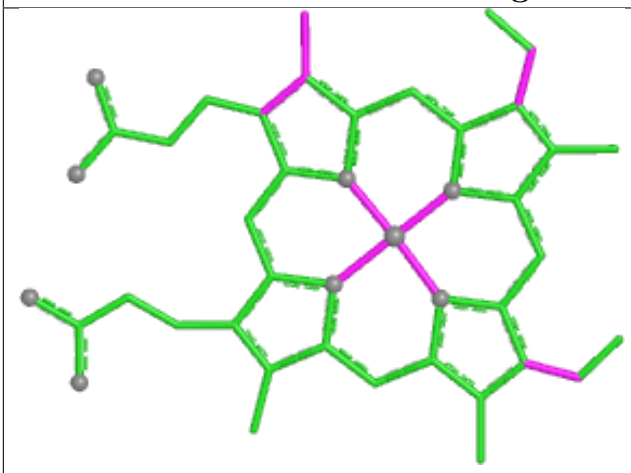
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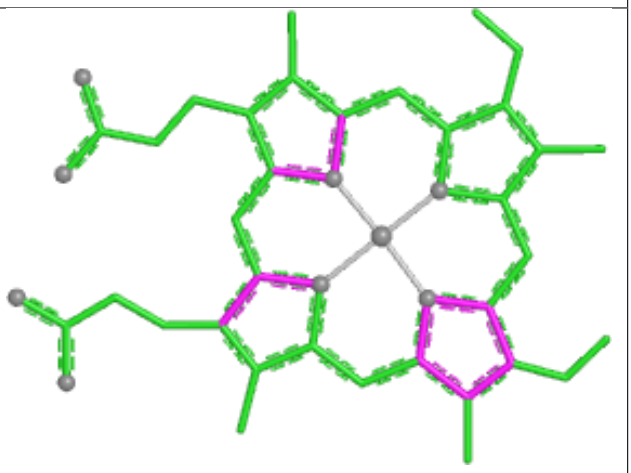
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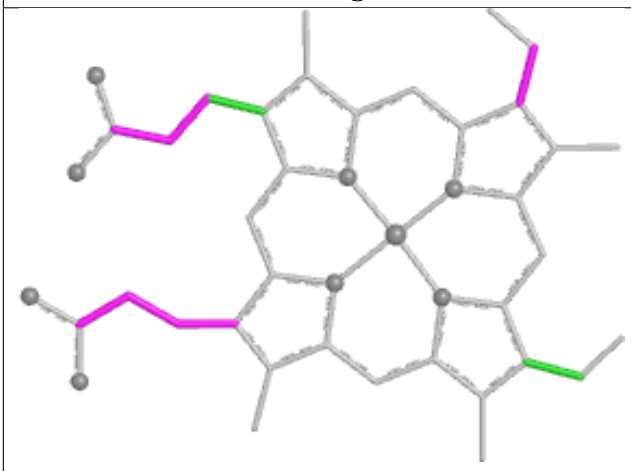
Ligand HEM F 1040



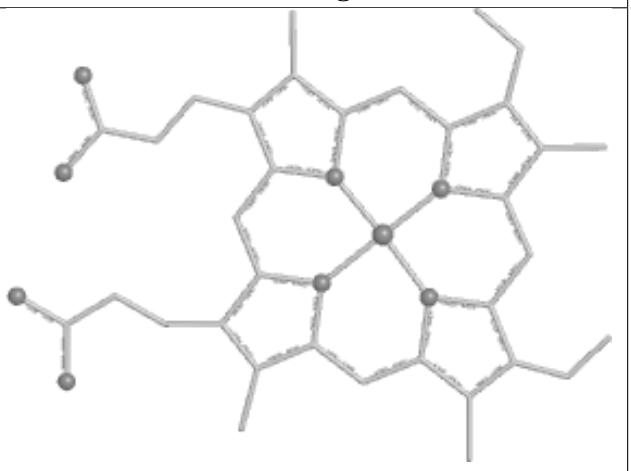
Bond lengths



Bond angles

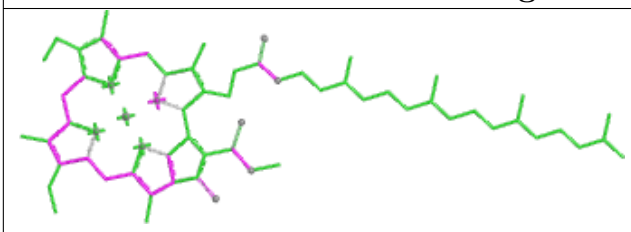


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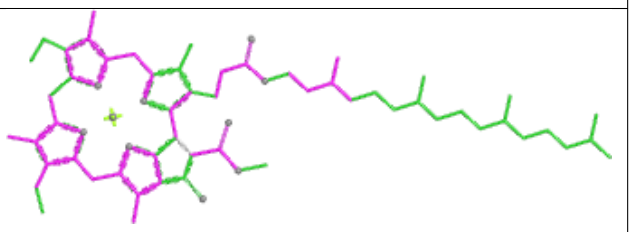


Rings

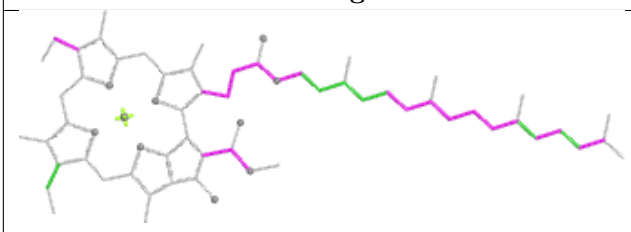
Ligand CLA b 6021



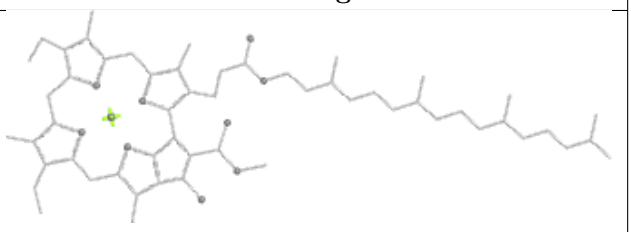
Bond lengths



Bond angles

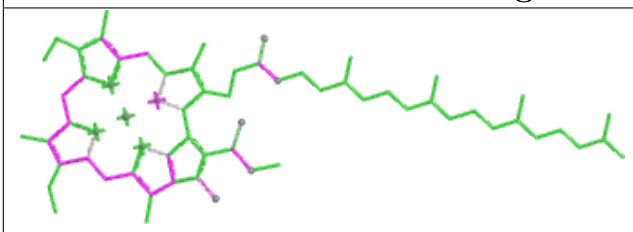


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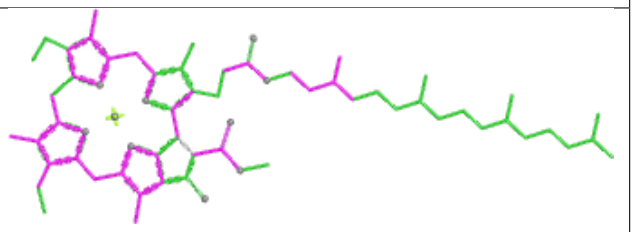


Rings

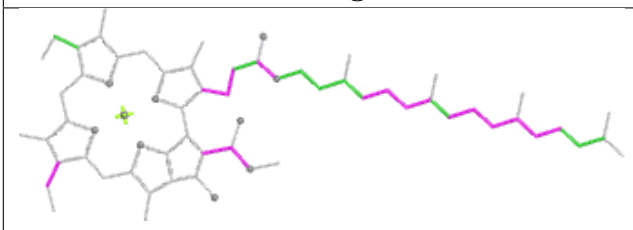
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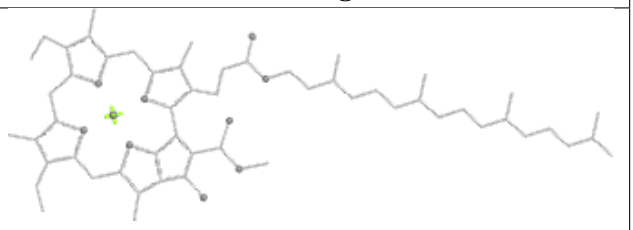
Bond lengths



Bond angles

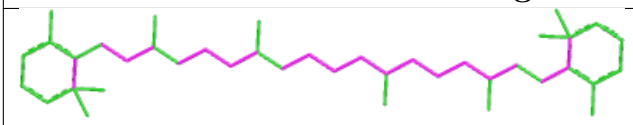


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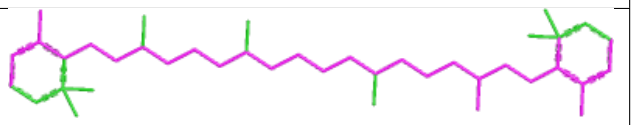


Rings

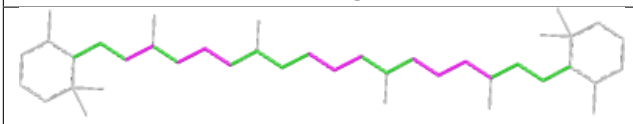
Ligand BCR T 6048



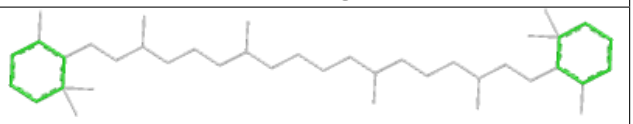
Bond lengths



Bond angles

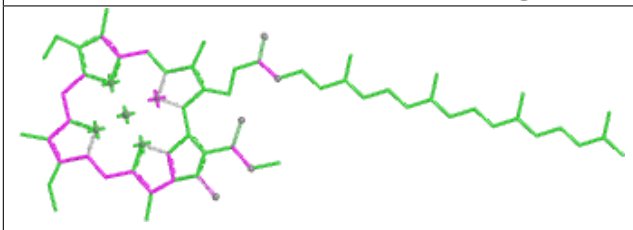


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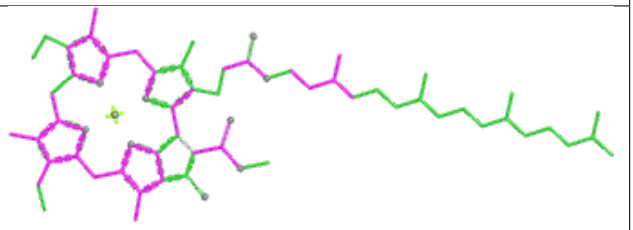


Rings

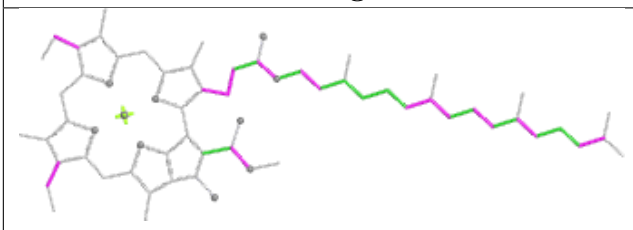
Ligand CLA B 1022



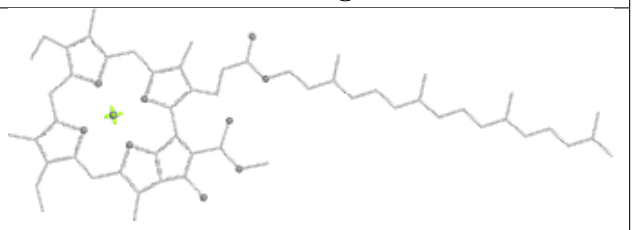
Bond lengths



Bond angles

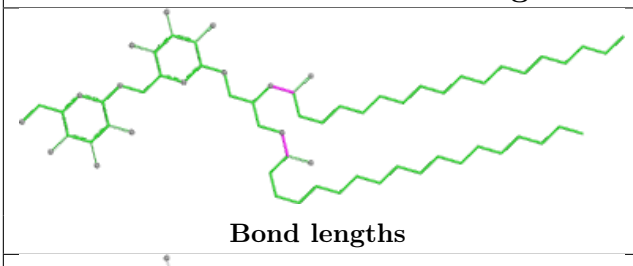


Torsions

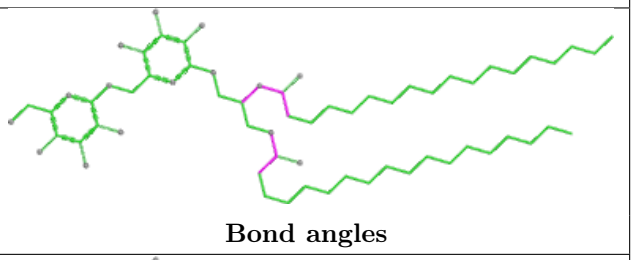


Rings

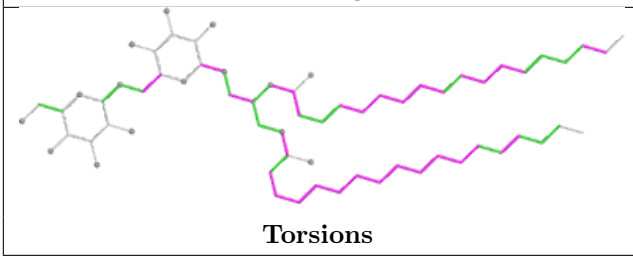
Ligand DGD C 1055



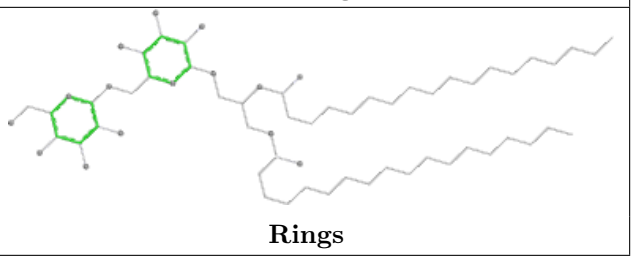
Bond lengths



Bond angles

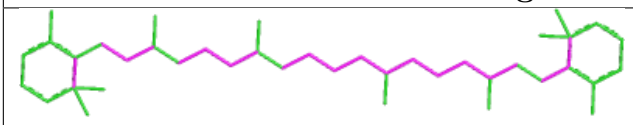


Torsions

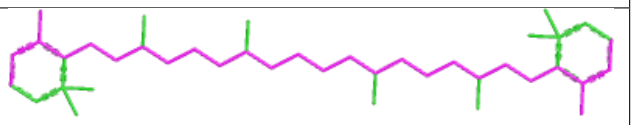


Rings

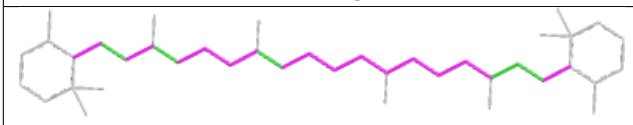
Ligand BCR d 6050



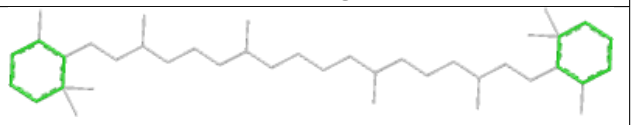
Bond lengths



Bond angles

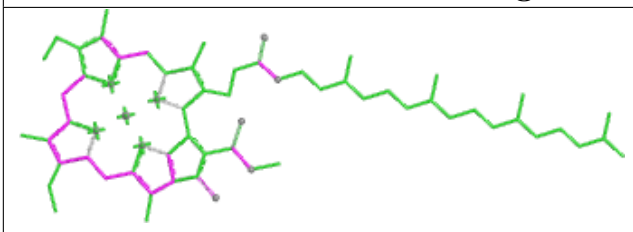


Torsions

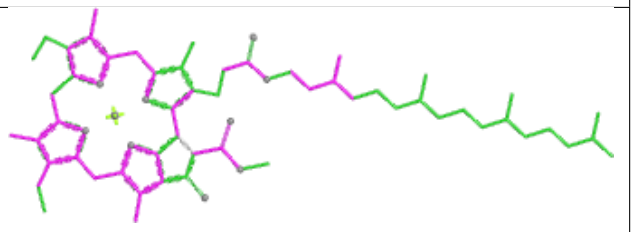


Rings

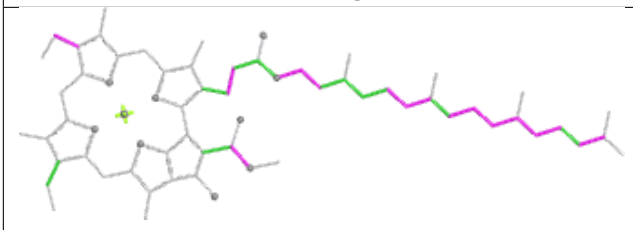
Ligand CLA C 1026



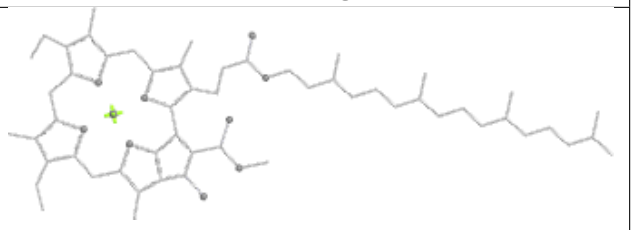
Bond lengths



Bond angles



Torsions

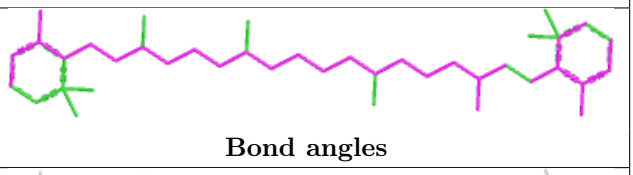


Rings

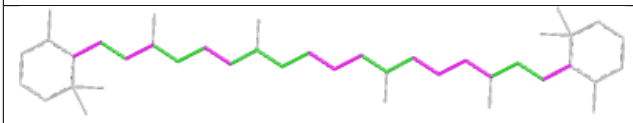
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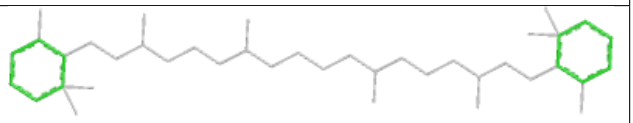
Bond lengths



Bond angles

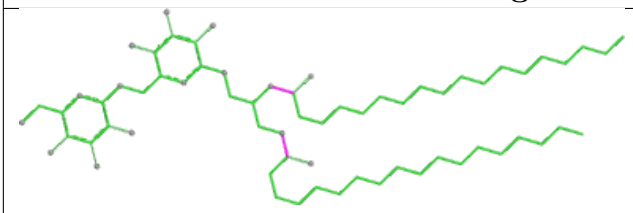


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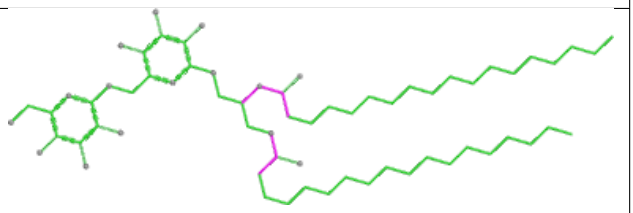


Rings

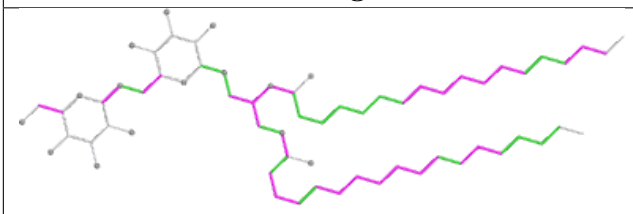
Ligand DGD C 1056



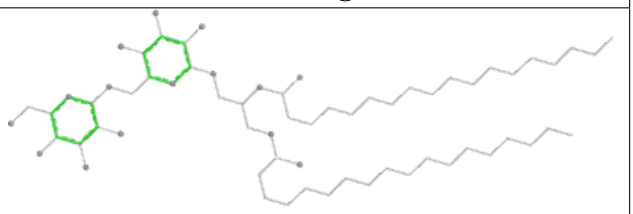
Bond lengths



Bond angles

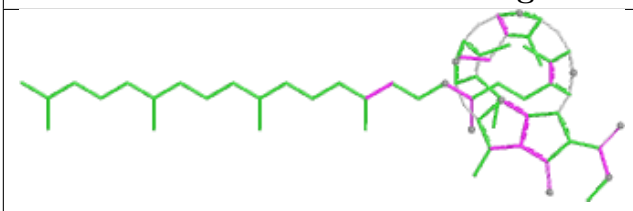


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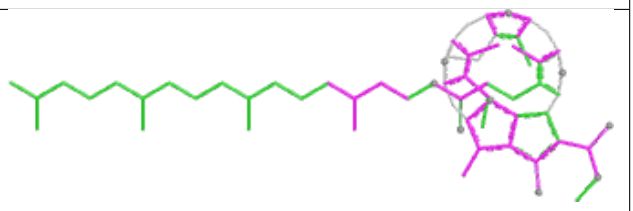


Rings

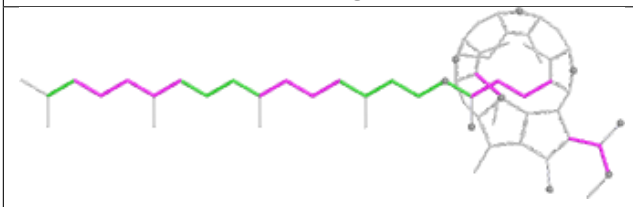
Ligand PHO a 6038



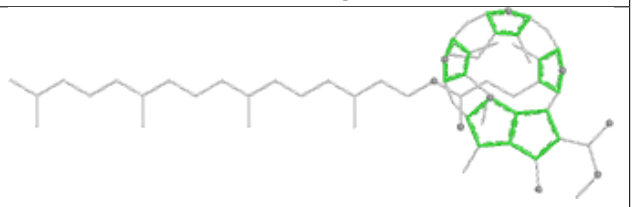
Bond lengths



Bond angles

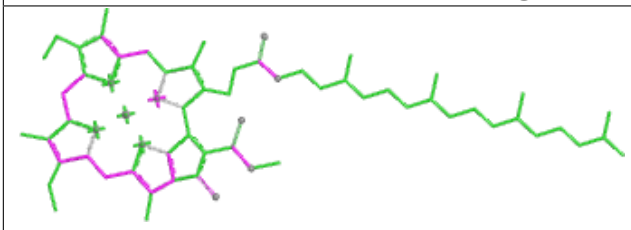


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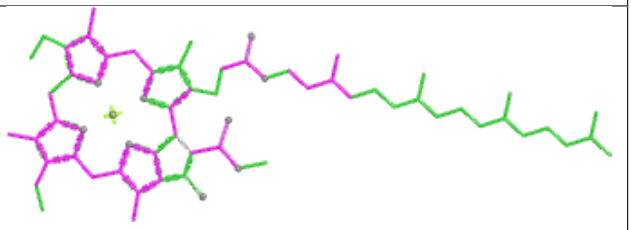


Rings

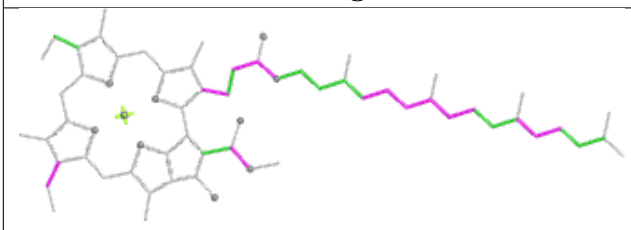
Ligand CLA B 1009



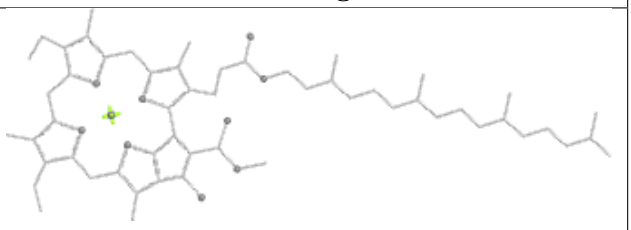
Bond lengths



Bond angles

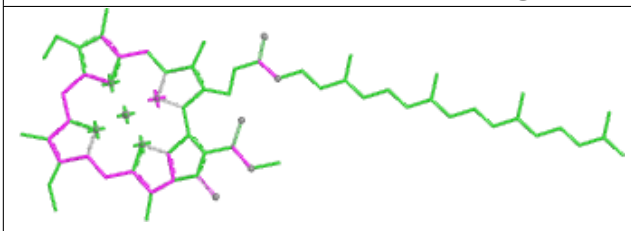


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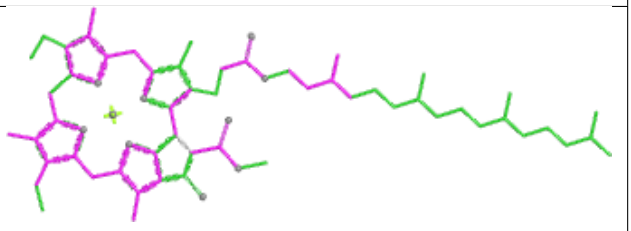


Rings

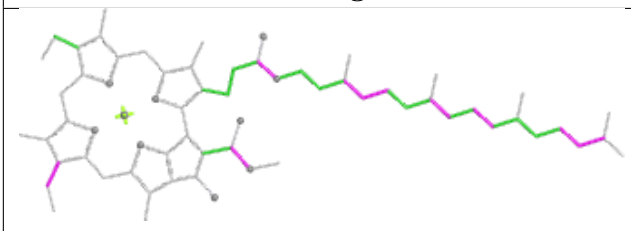
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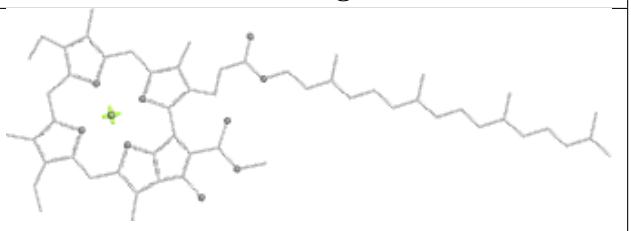
Bond lengths



Bond angles

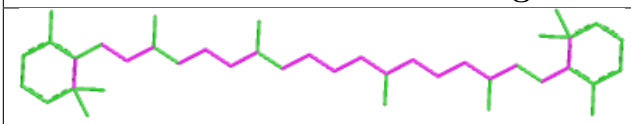


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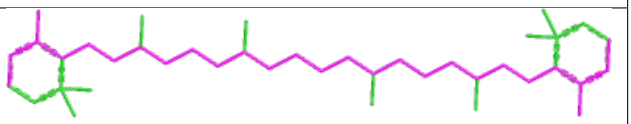


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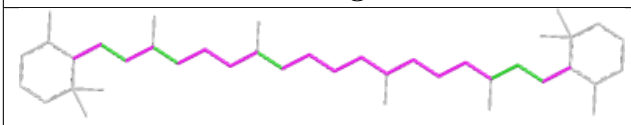
Ligand BCR D 1050



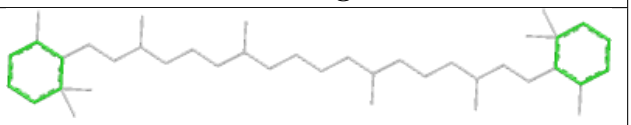
Bond lengths



Bond angles



Torsions

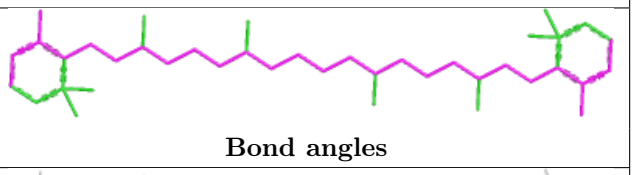


Rings

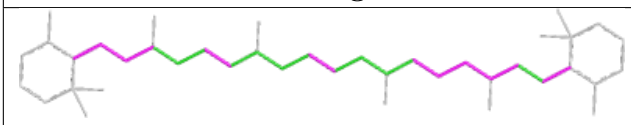
Ligand BCR z 6053



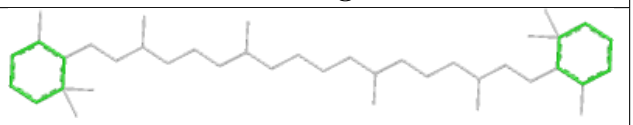
Bond lengths



Bond angles

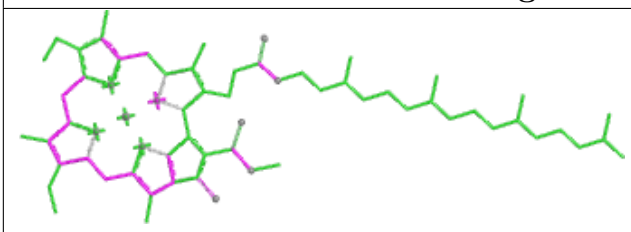


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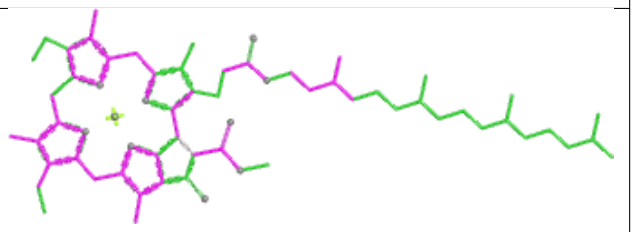


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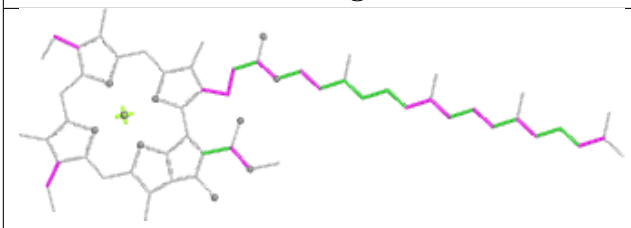
Ligand CLA b 6022



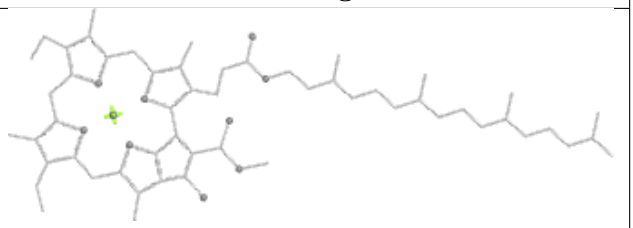
Bond lengths



Bond angles

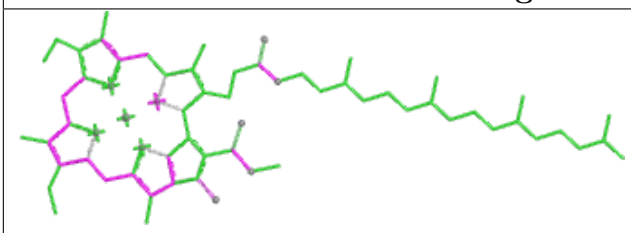


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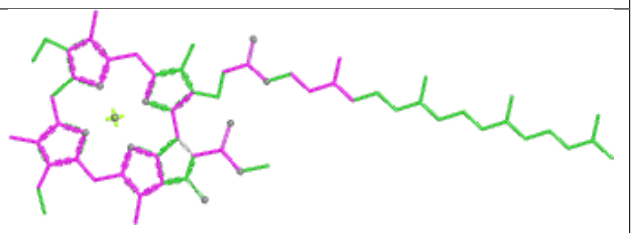


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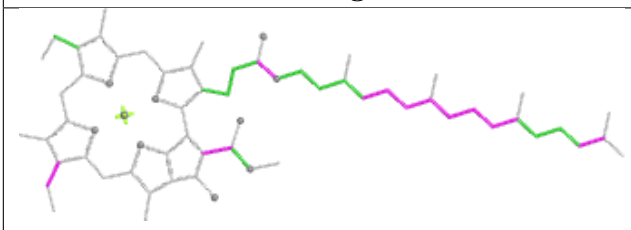
Ligand CLA B 1023



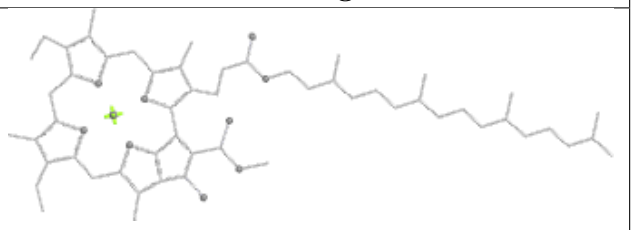
Bond lengths



Bond angles

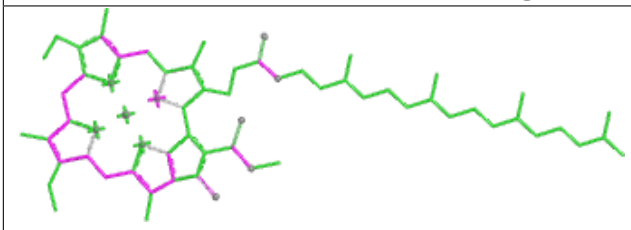


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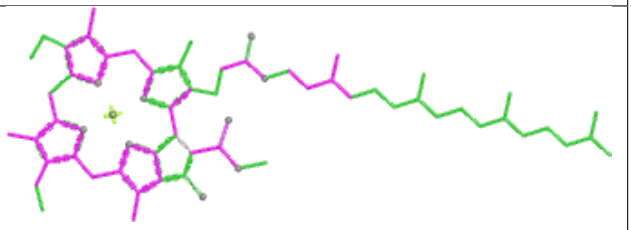


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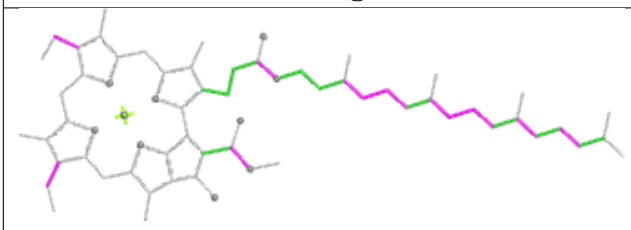
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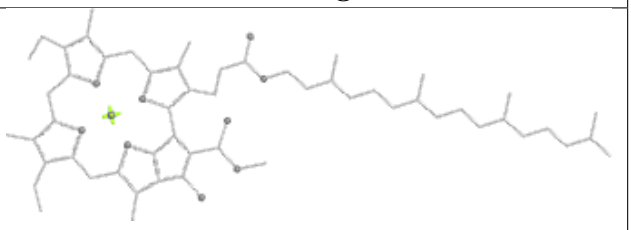
Bond lengths



Bond angles

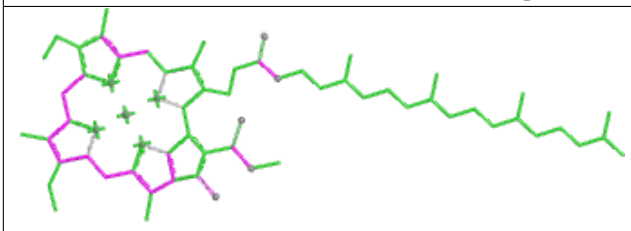


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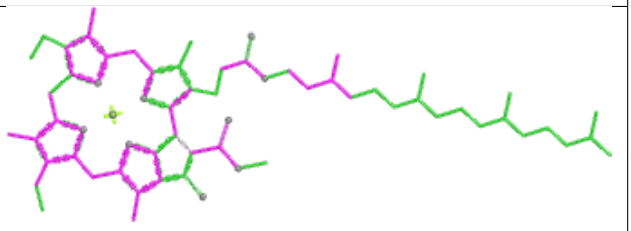


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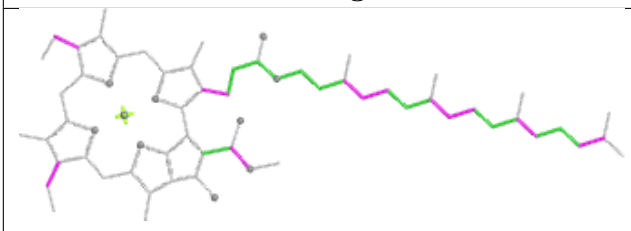
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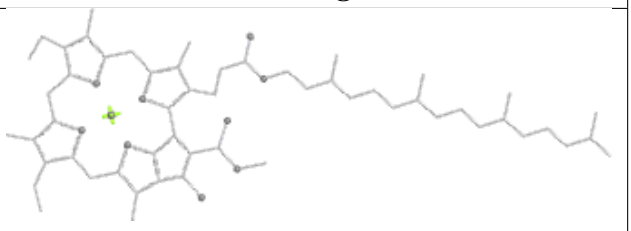
Bond lengths



Bond angles

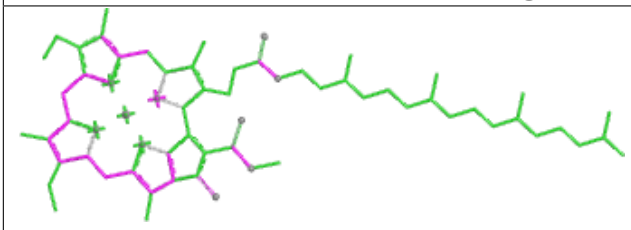


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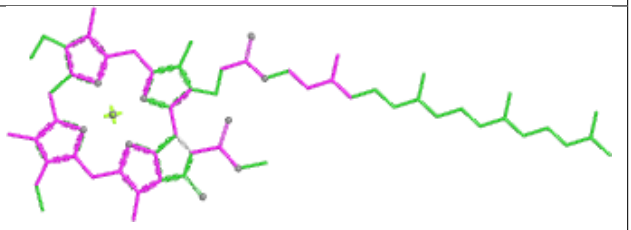


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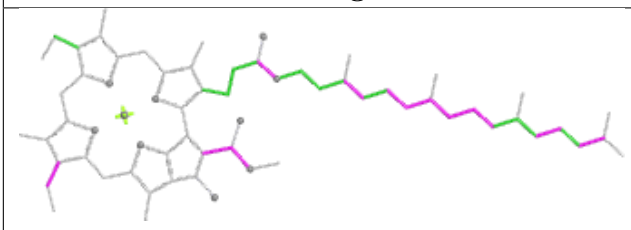
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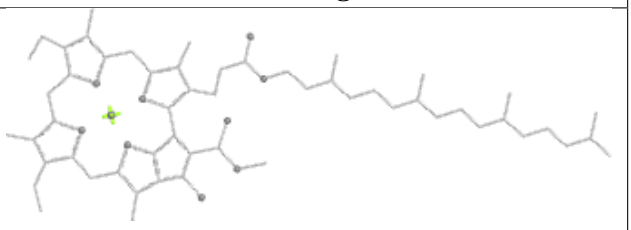
Bond lengths



Bond angles

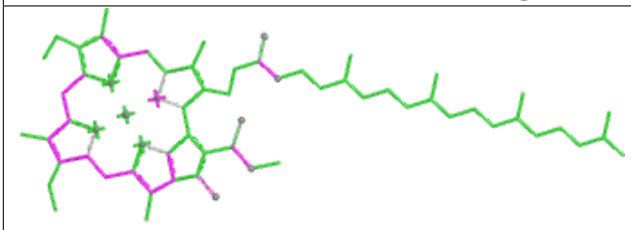


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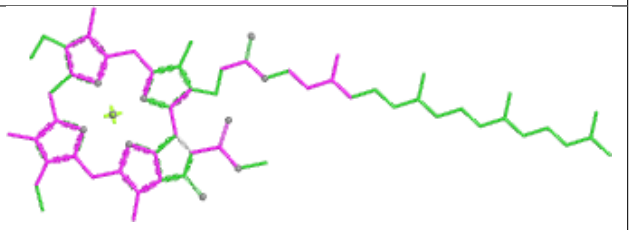


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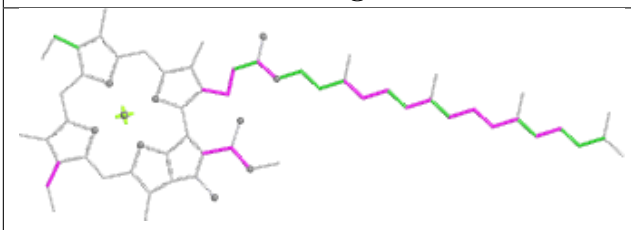
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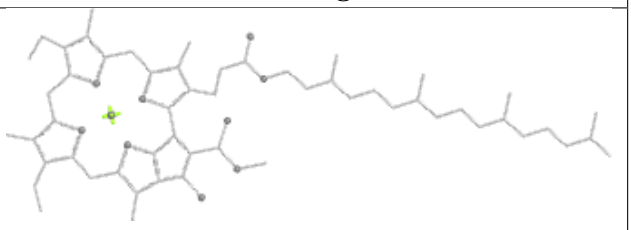
Bond lengths



Bond angles

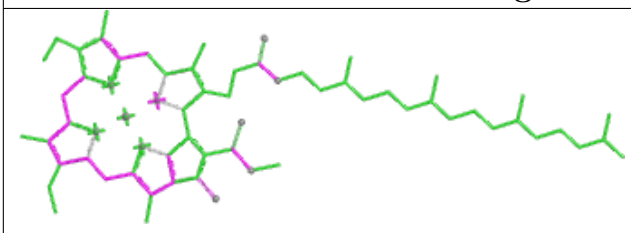


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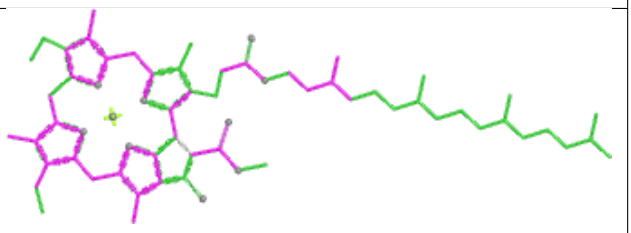


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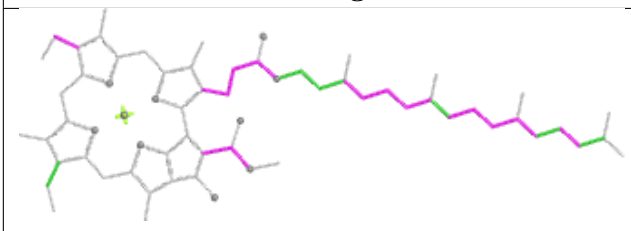
Ligand CLA H 1017



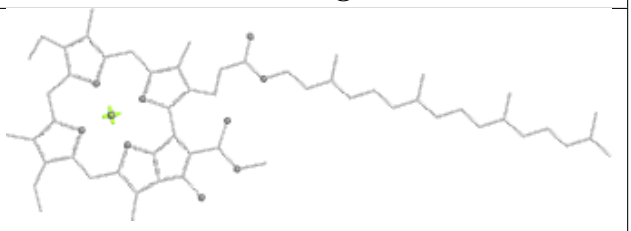
Bond lengths



Bond angles

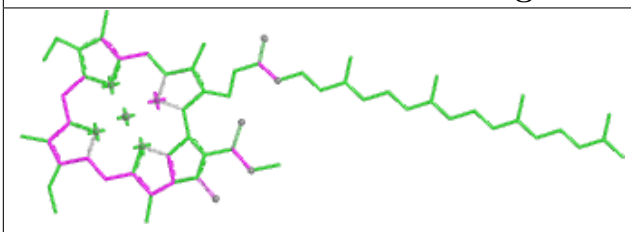


Torsions

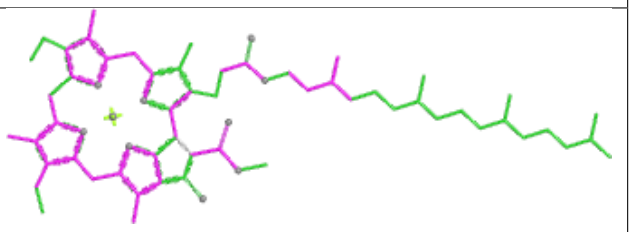


Rings

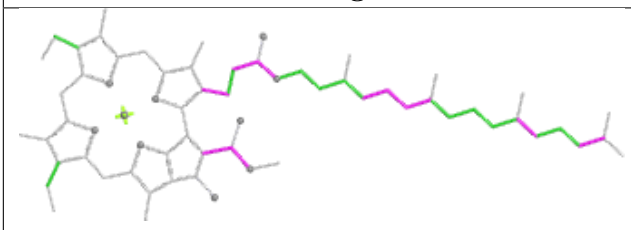
Ligand CLA C 1025



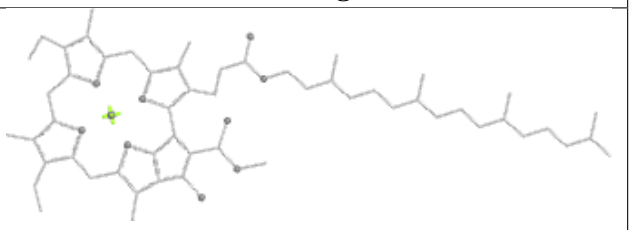
Bond lengths



Bond angles

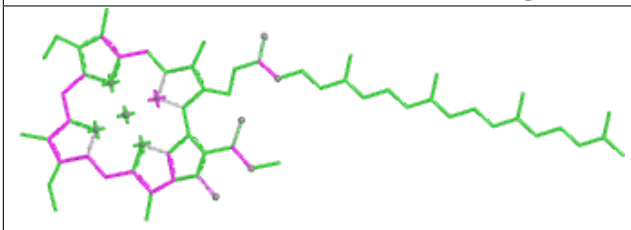


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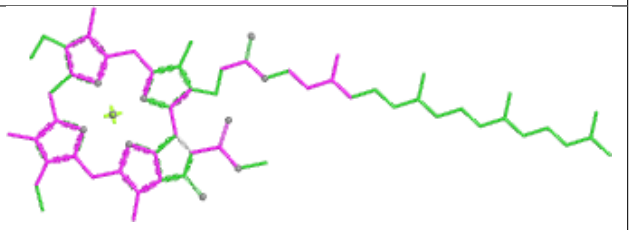


Rings

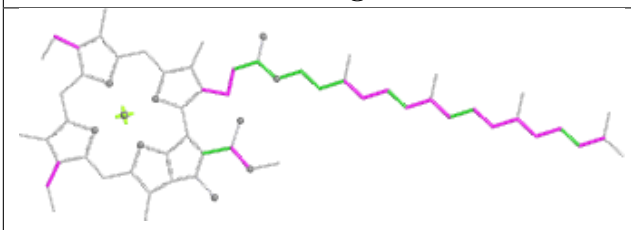
Ligand CLA a 6003



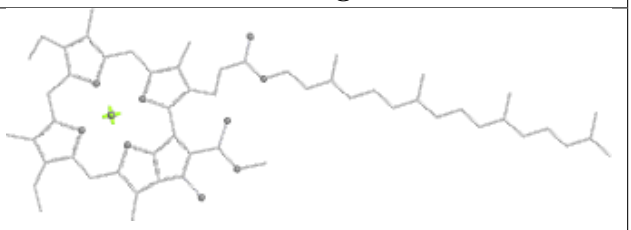
Bond lengths



Bond angles

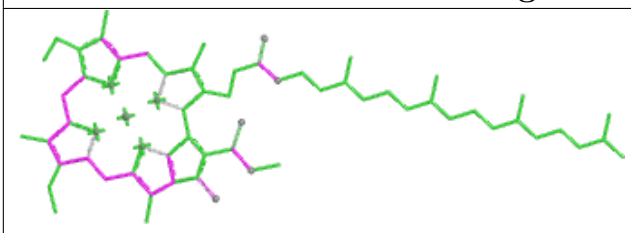


Torsions

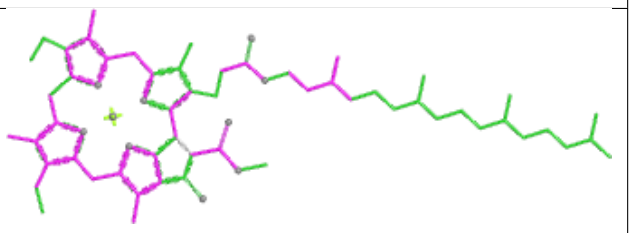


Rings

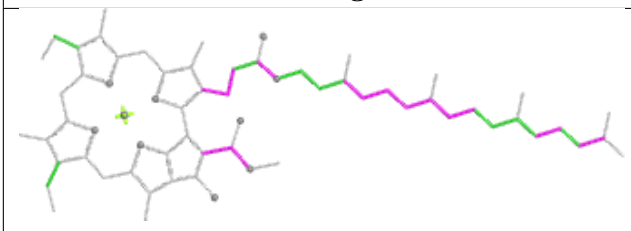
Ligand CLA b 6015



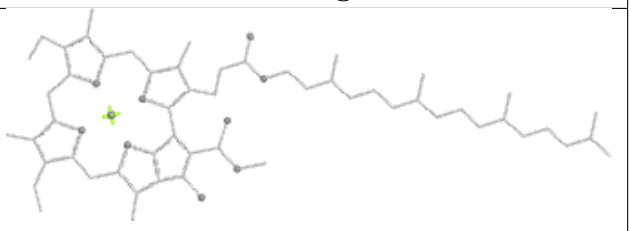
Bond lengths



Bond angles

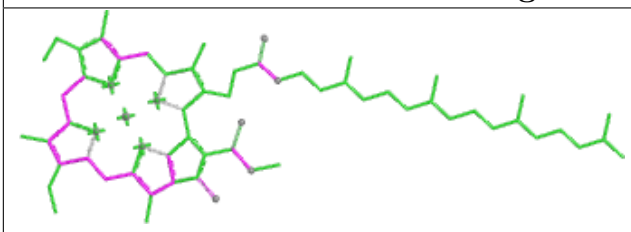


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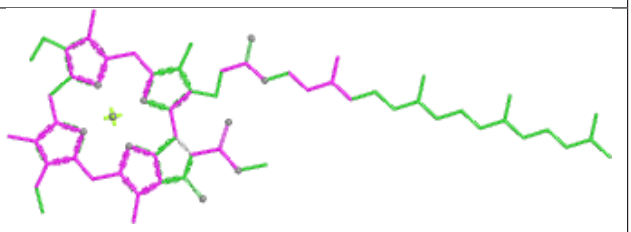


Rings

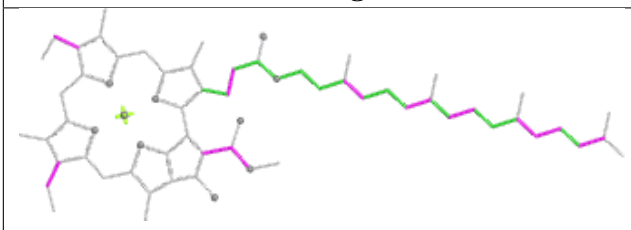
Ligand CLA b 6012



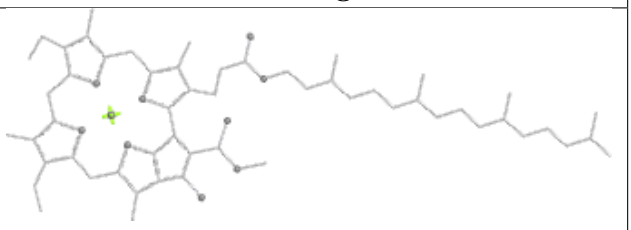
Bond lengths



Bond angles

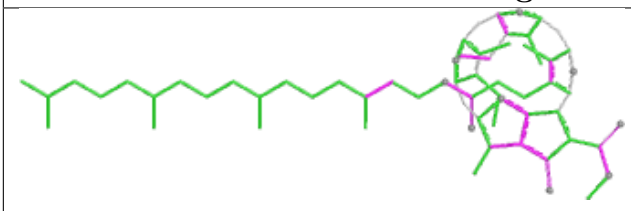


Torsions

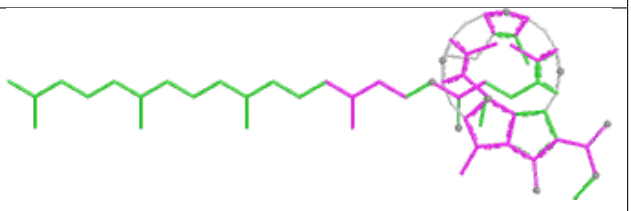


Rings

Ligand PHO d 6039



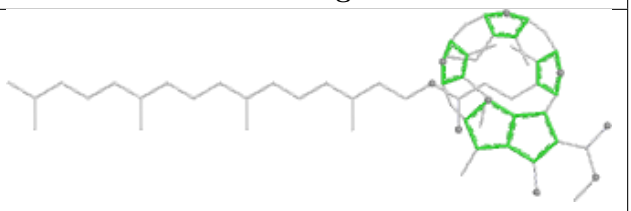
Bond lengths



Bond angles

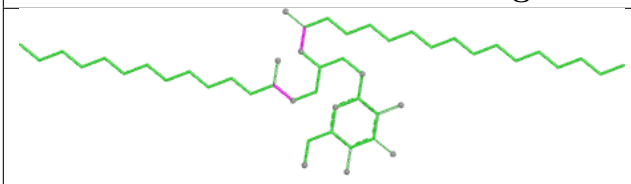


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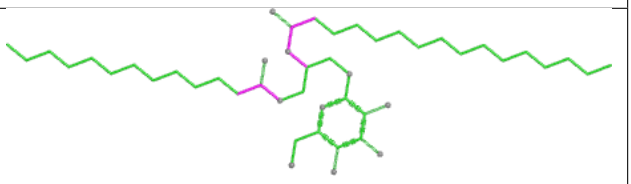


Rings

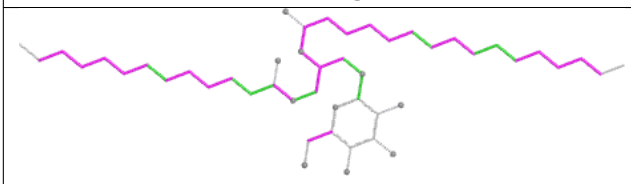
Ligand MGE b 6060



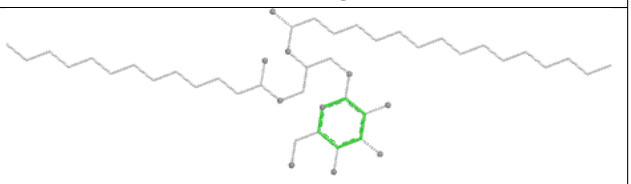
Bond lengths



Bond angles

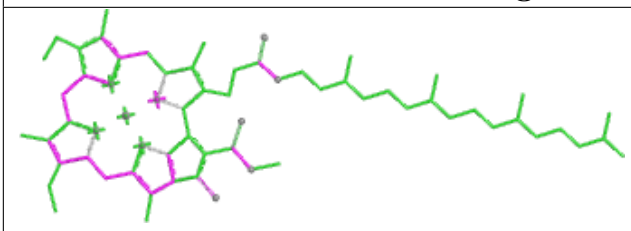


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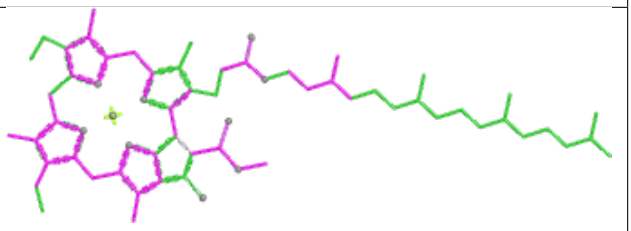


Rings

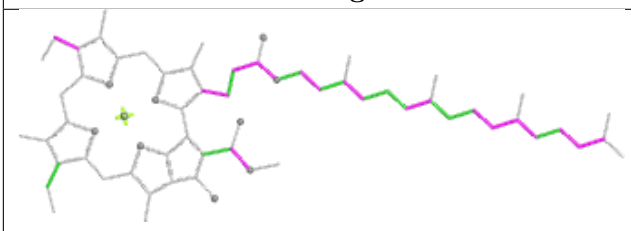
Ligand CLA B 1011



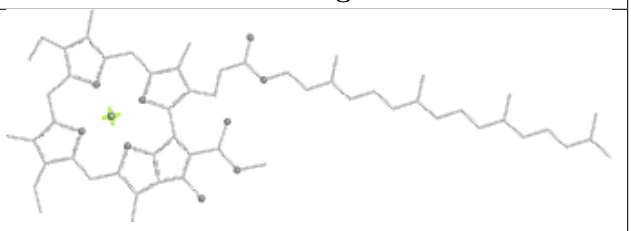
Bond lengths



Bond angles

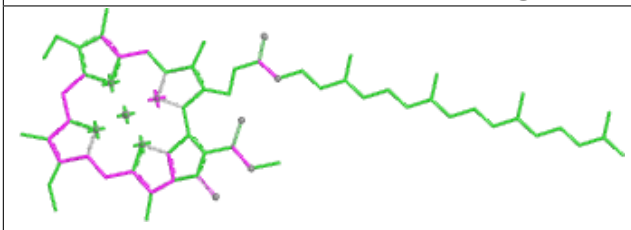


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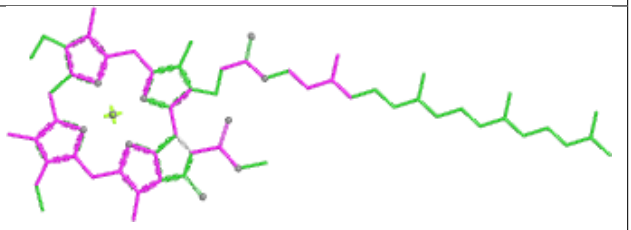


Rings

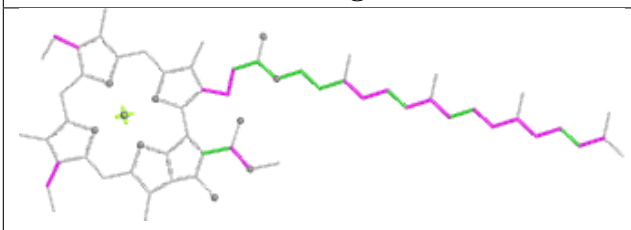
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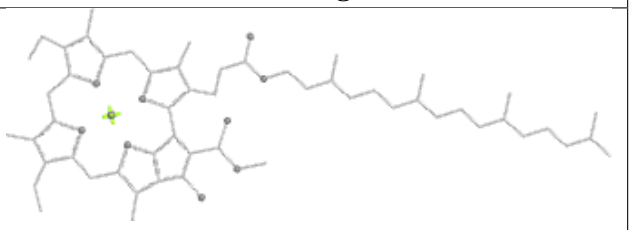
Bond lengths



Bond angles

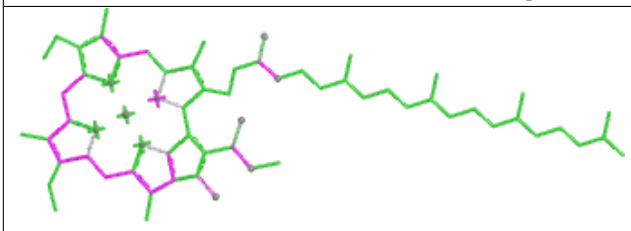


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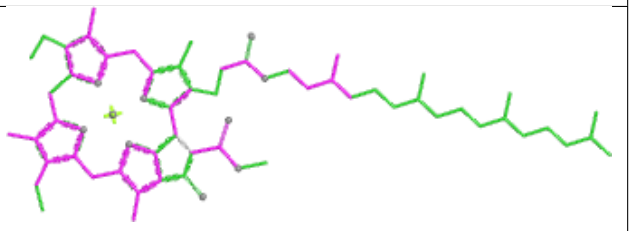


Rings

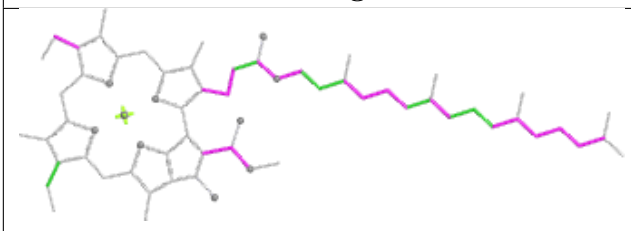
Ligand CLA c 6028



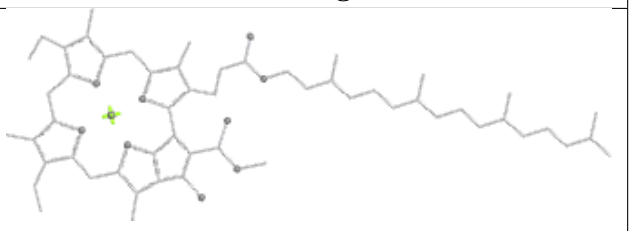
Bond lengths



Bond angles

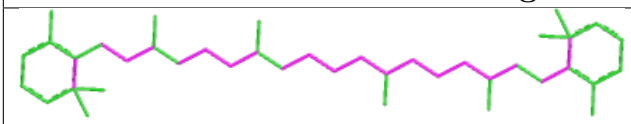


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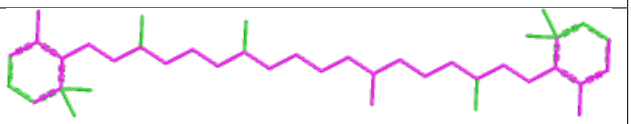


Rings

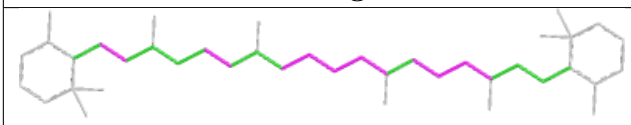
Ligand BCR t 1046



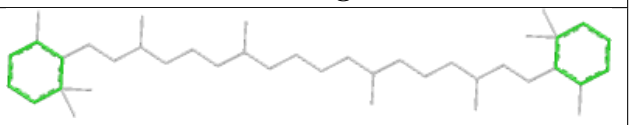
Bond lengths



Bond angles



Torsions

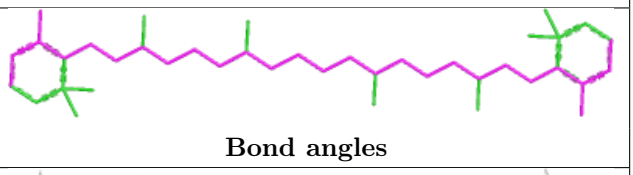


Rings

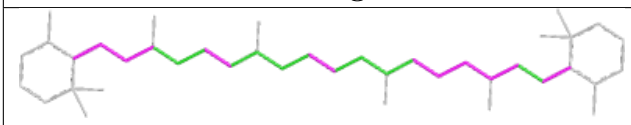
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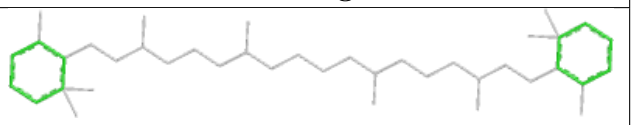
Bond lengths



Bond angles

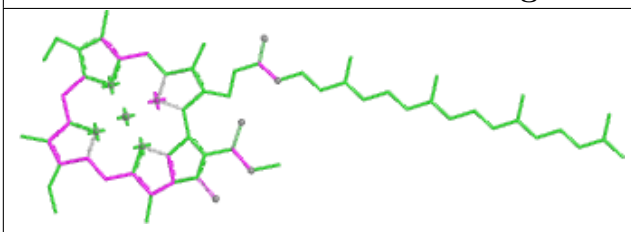


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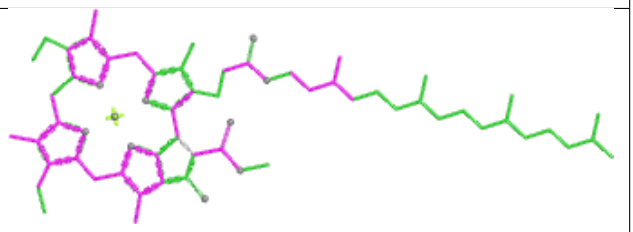


Rings

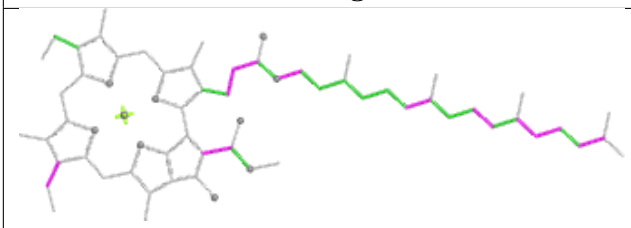
Ligand CLA c 6031



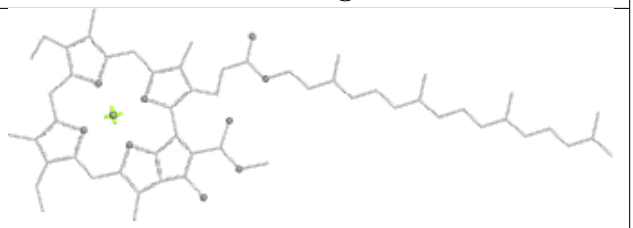
Bond lengths



Bond angles

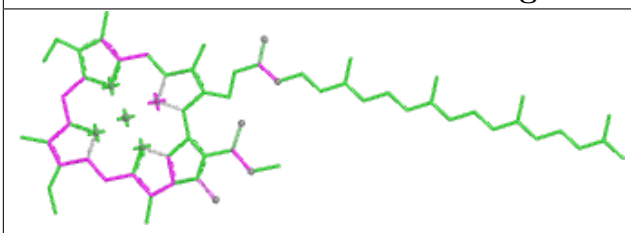


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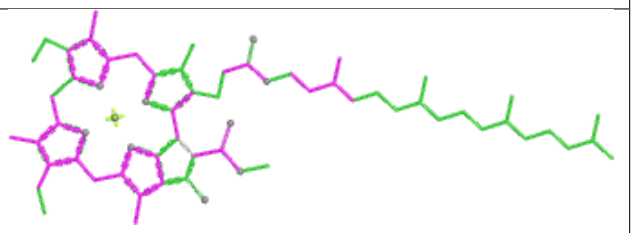


Rings

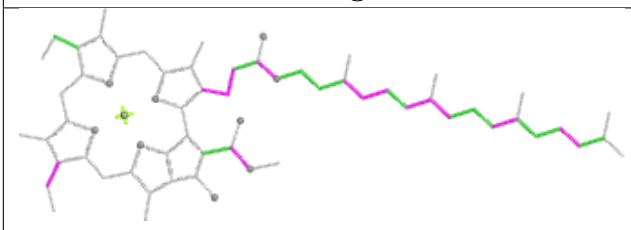
Ligand CLA a 6006



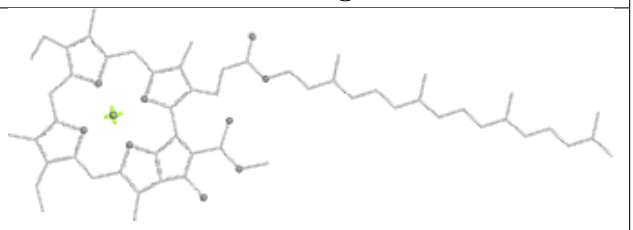
Bond lengths



Bond angles

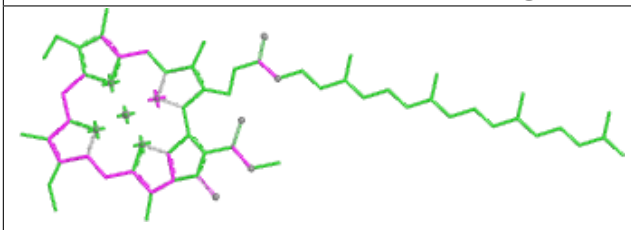


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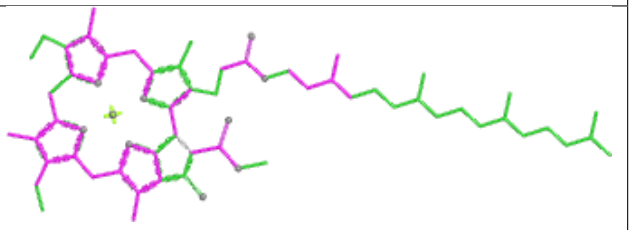


Rings

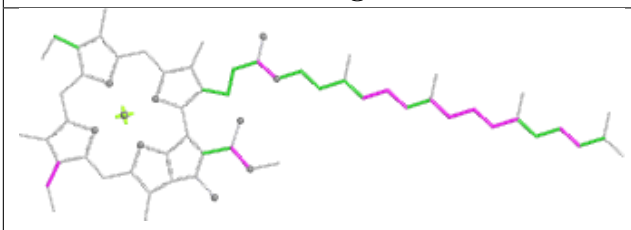
Ligand CLA c 6029



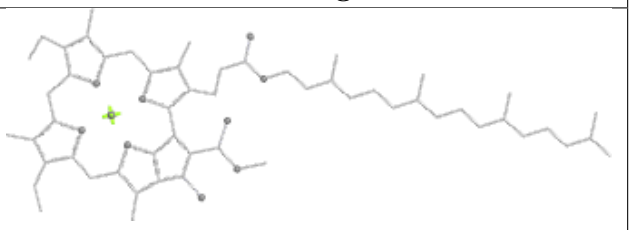
Bond lengths



Bond angles

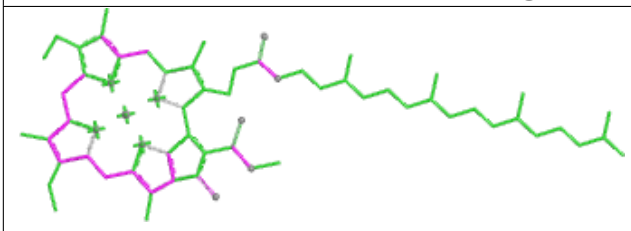


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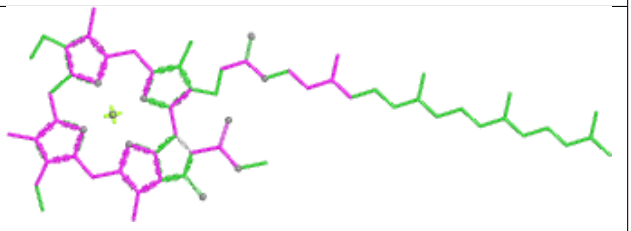


Rings

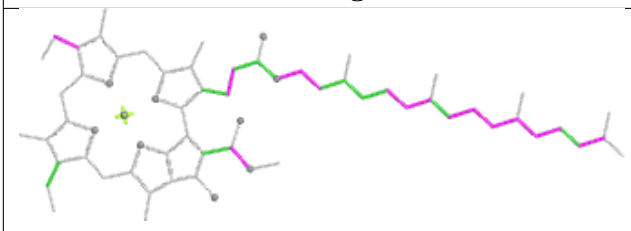
Ligand CLA c 6026



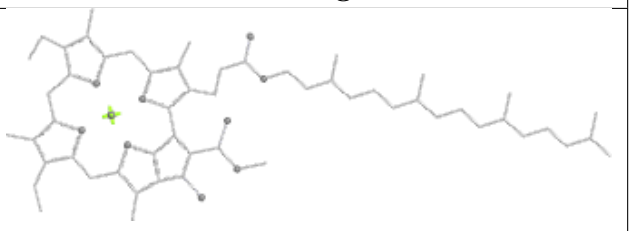
Bond lengths



Bond angles

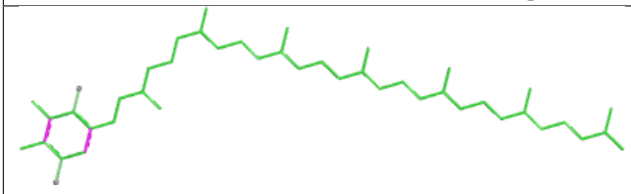


Torsions

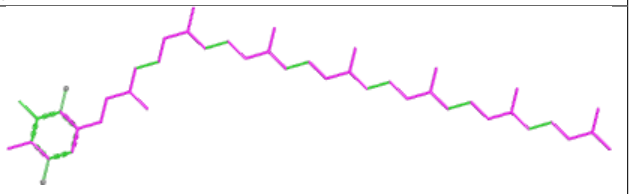


Rings

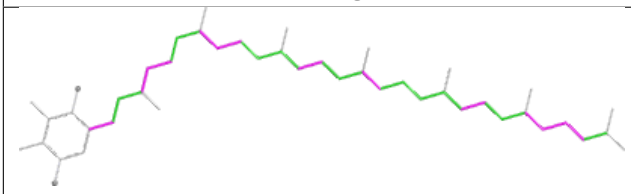
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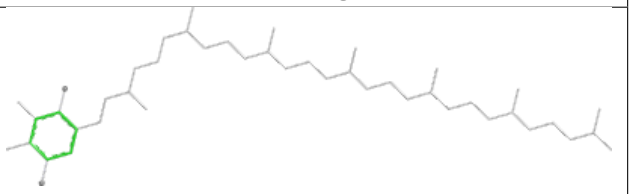
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Bond angles

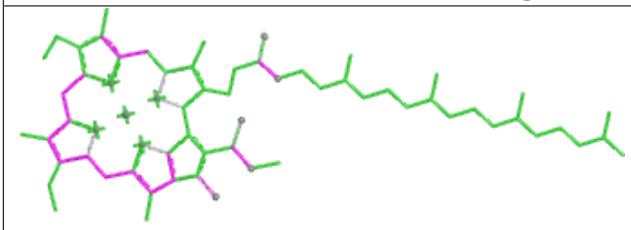


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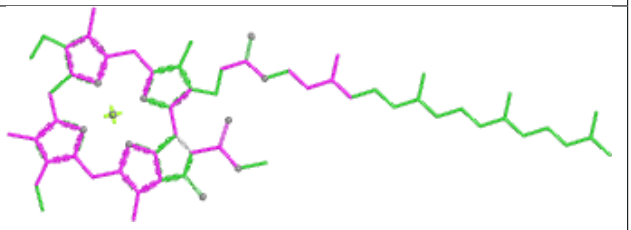


Rings

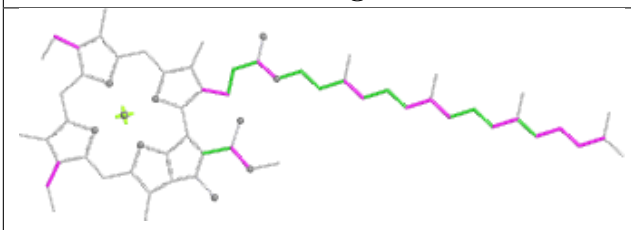
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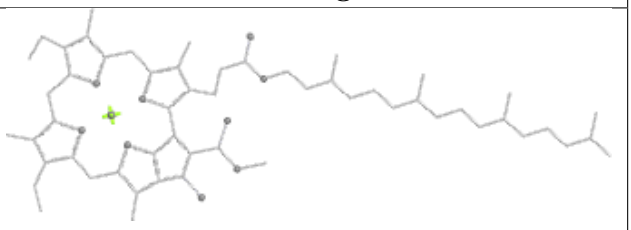
Bond lengths



Bond angles

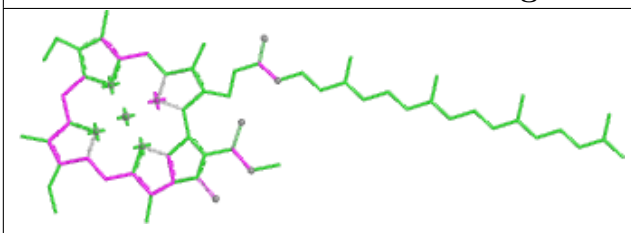


Torsions

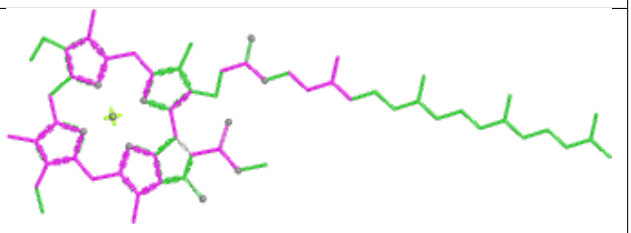


Rings

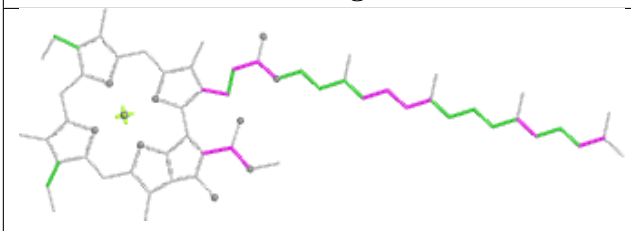
Ligand CLA c 6025



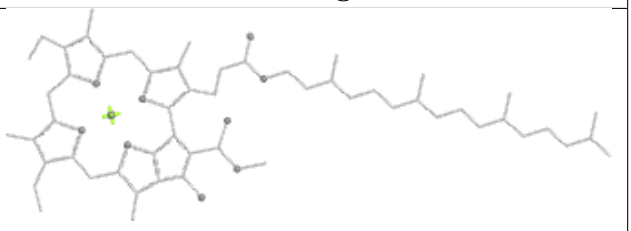
Bond lengths



Bond angles

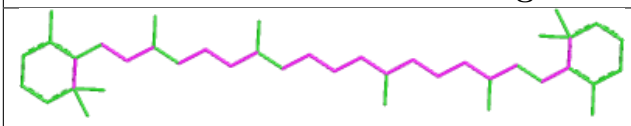


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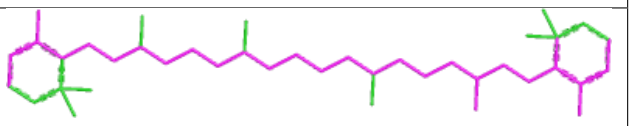


Rings

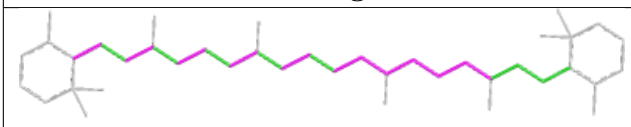
Ligand BCR b 6047



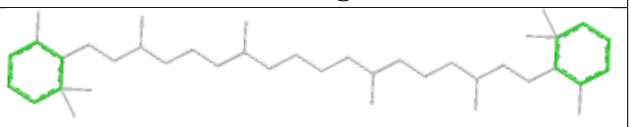
Bond lengths



Bond angles

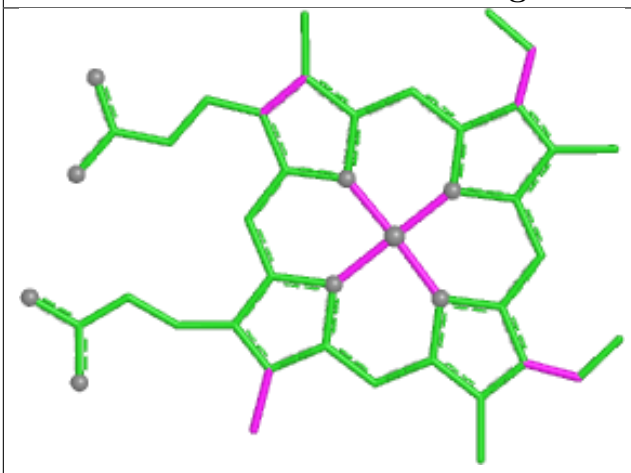


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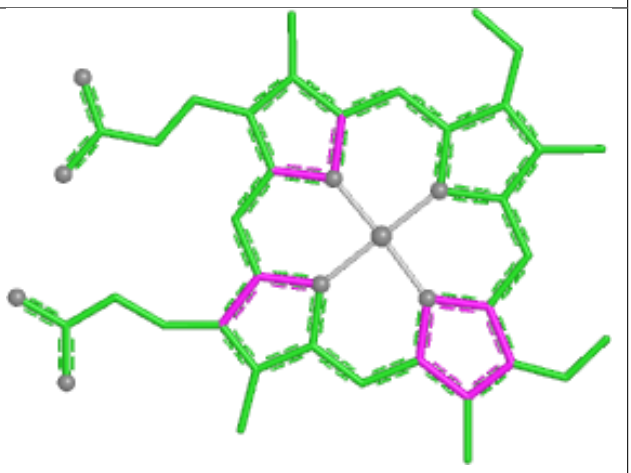


Rings

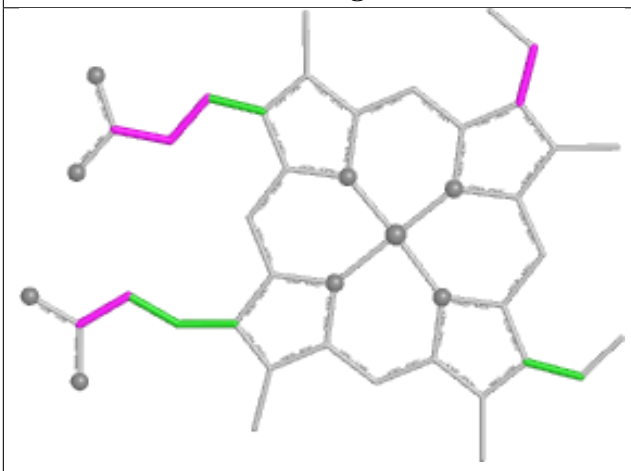
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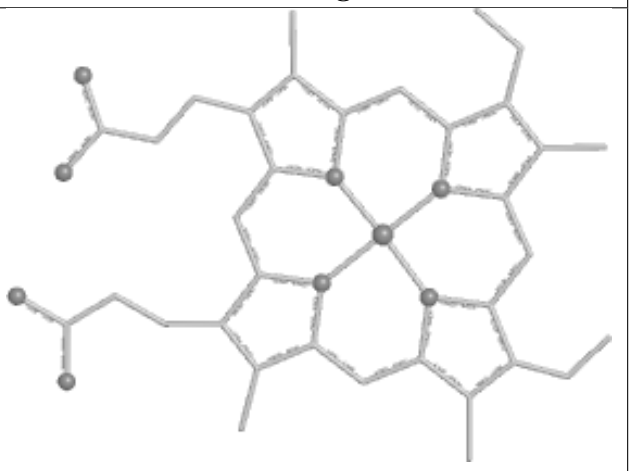
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Bond angles

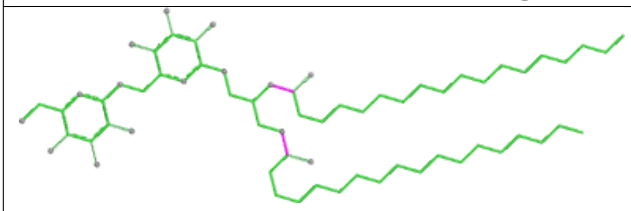


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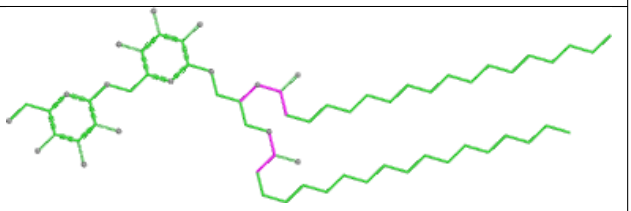


Rings

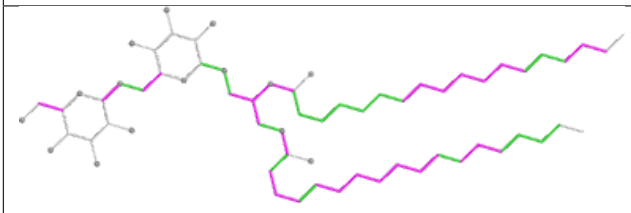
Ligand DGD c 6056



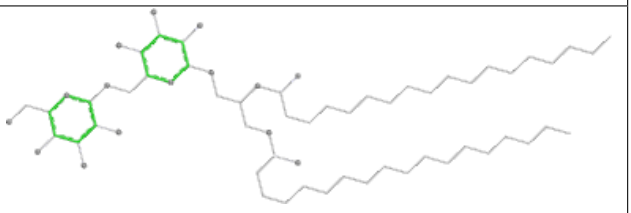
Bond lengths



Bond angles

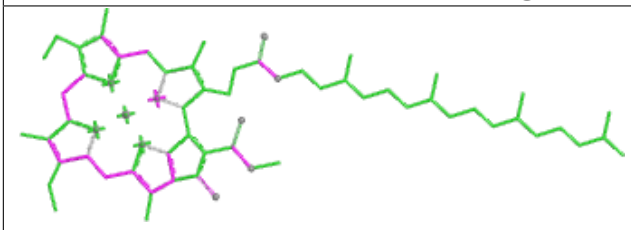


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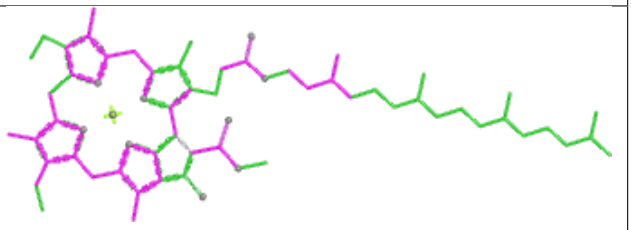


Rings

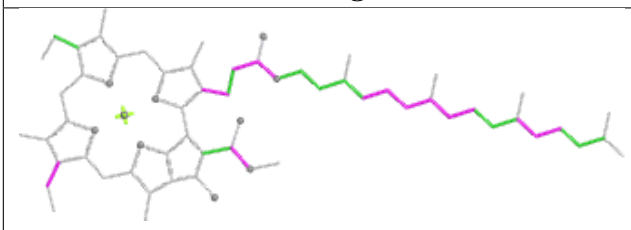
Ligand CLA b 6009



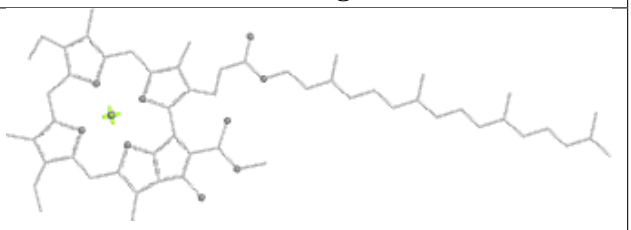
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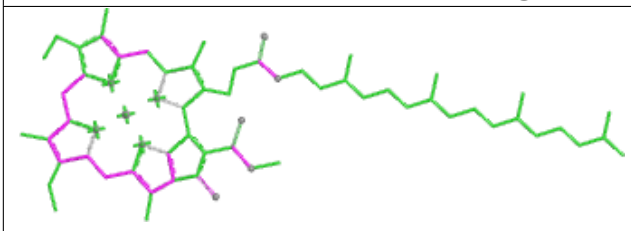


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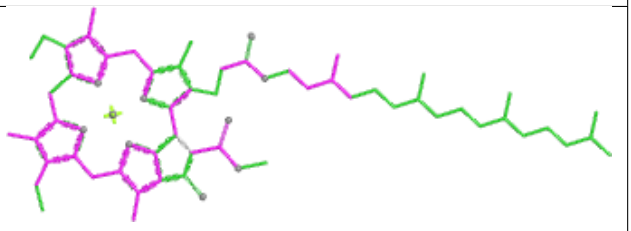


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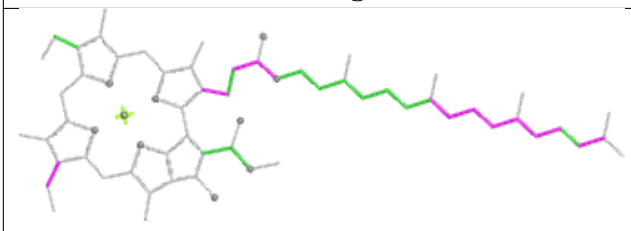
Ligand CLA C 1037



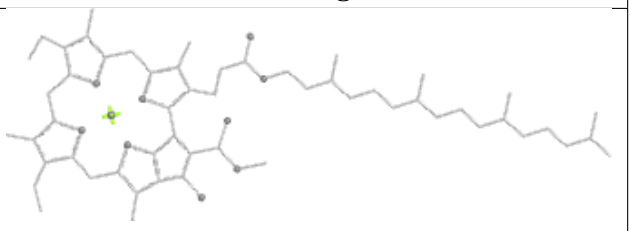
Bond lengths



Bond angles

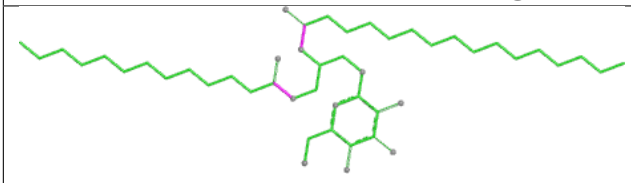


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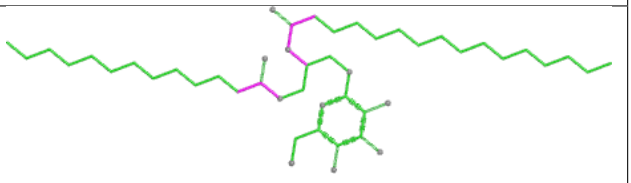


Rings

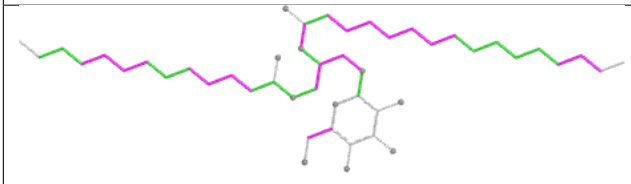
Ligand MGE D 1059



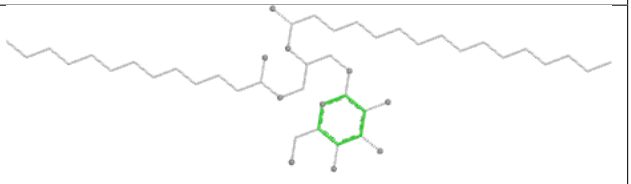
Bond lengths



Bond angles

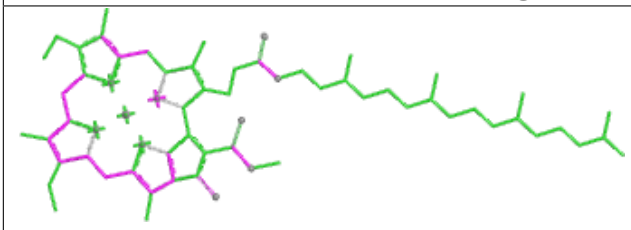


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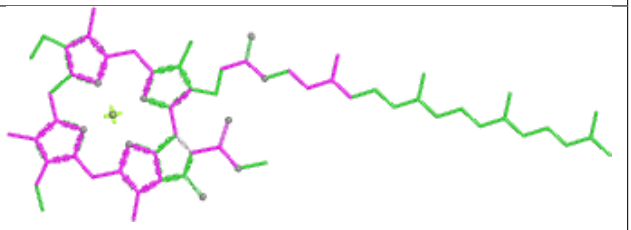


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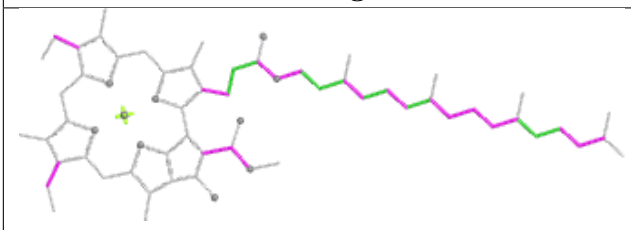
Ligand CLA A 1007



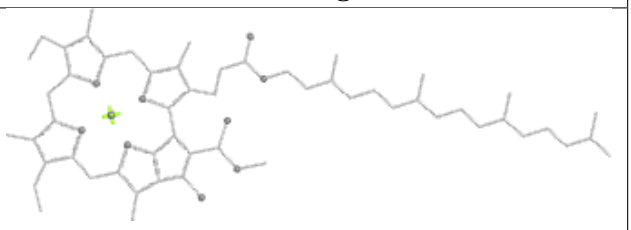
Bond lengths



Bond angles

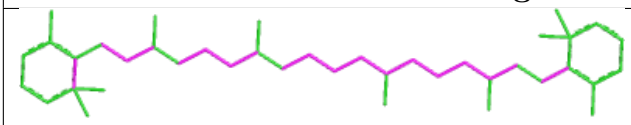


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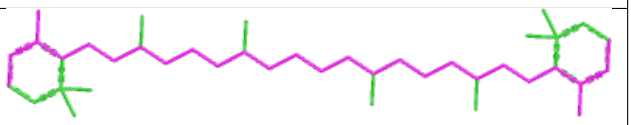


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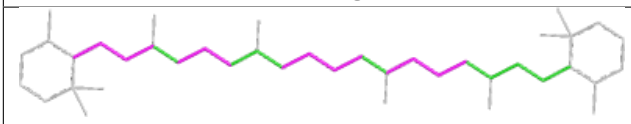
Ligand BCR C 1054



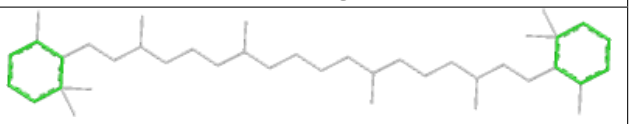
Bond lengths



Bond angles

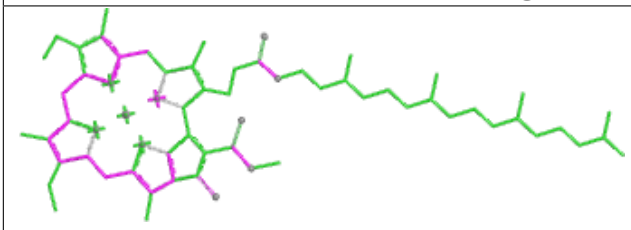


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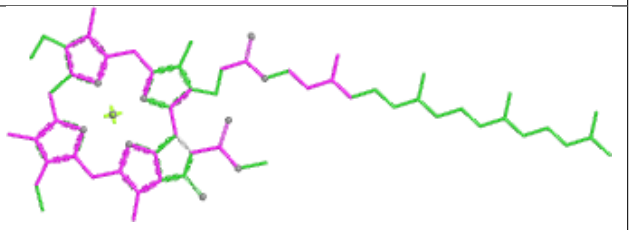


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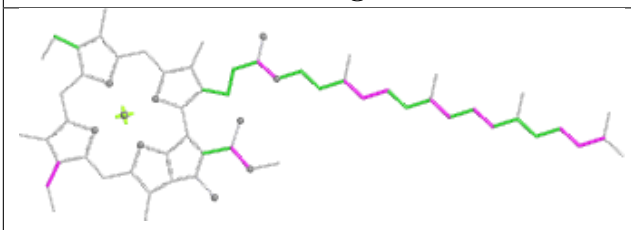
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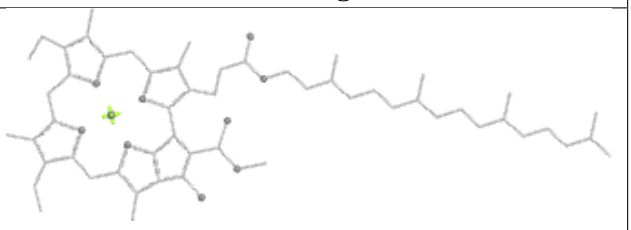
Bond lengths



Bond angles

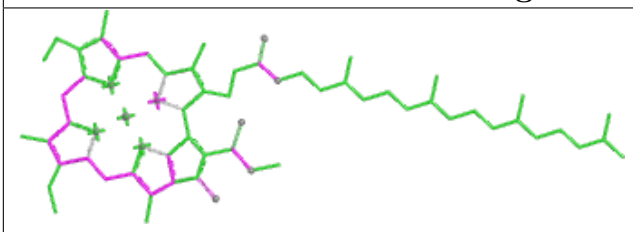


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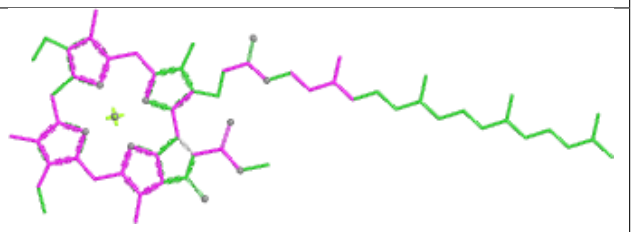


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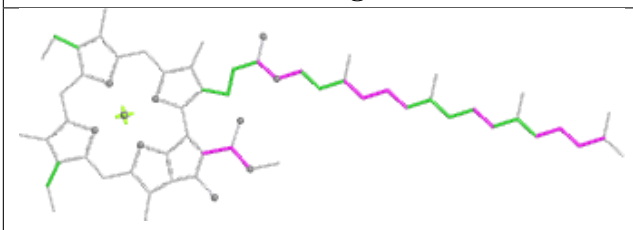
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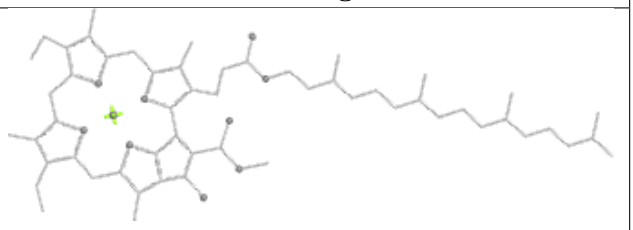
Bond lengths



Bond angles

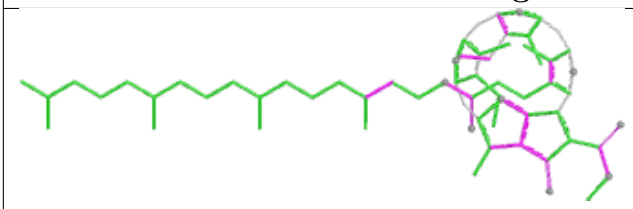


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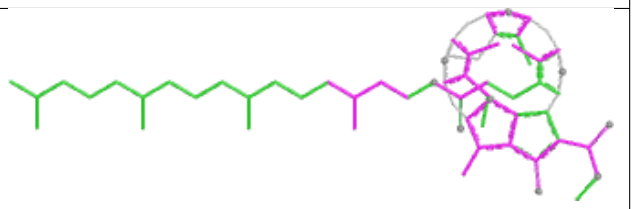


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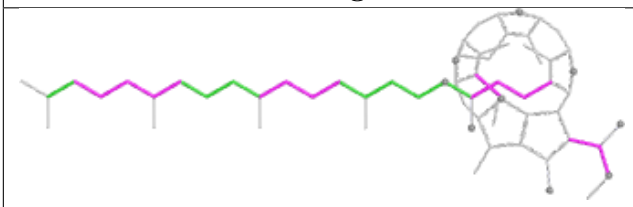
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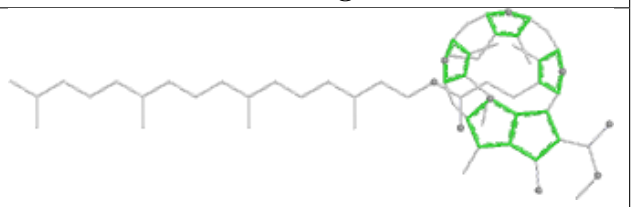
Bond lengths



Bond angles

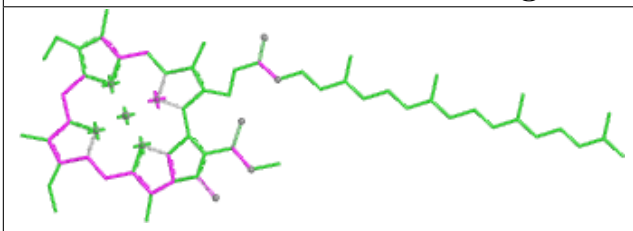


Torsions

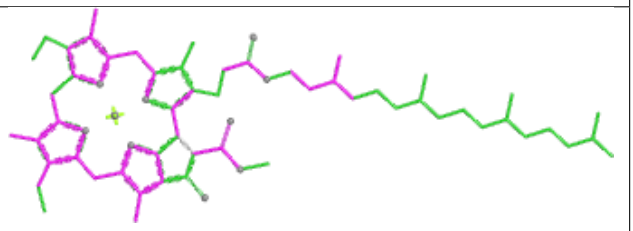


Rings

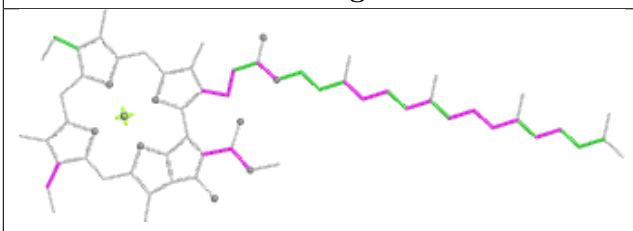
Ligand CLA c 6032



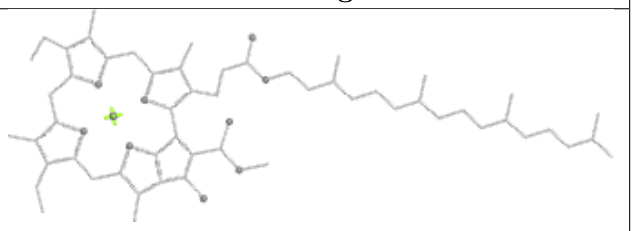
Bond lengths



Bond angles

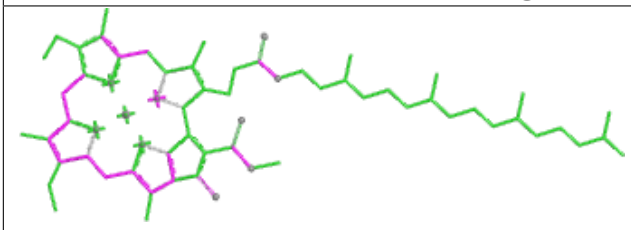


Torsions

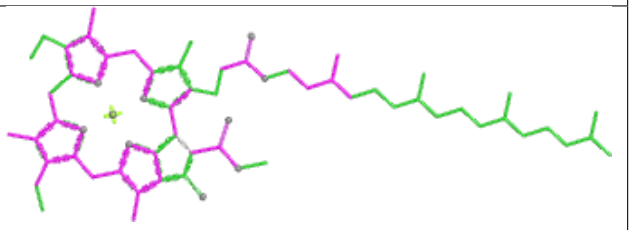


Rings

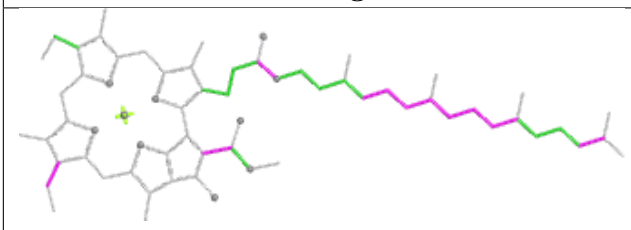
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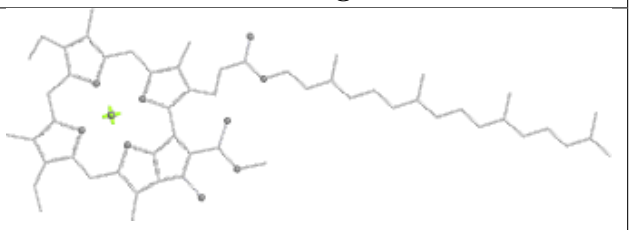
Bond lengths



Bond angles

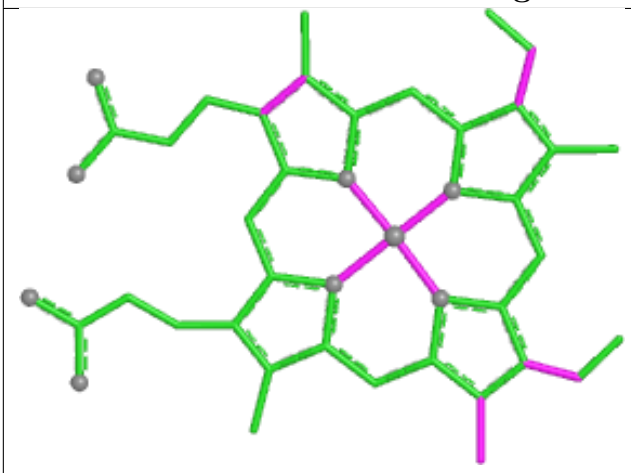


Torsions

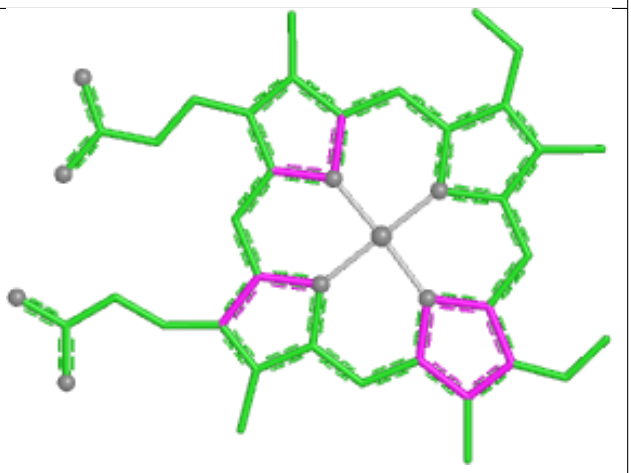


Rings

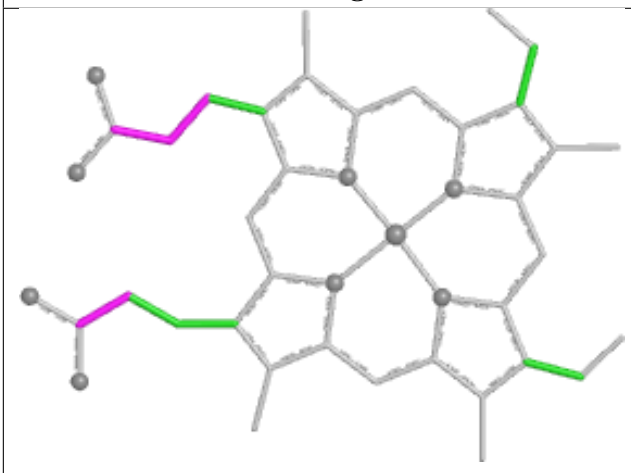
Ligand HEM v 6041



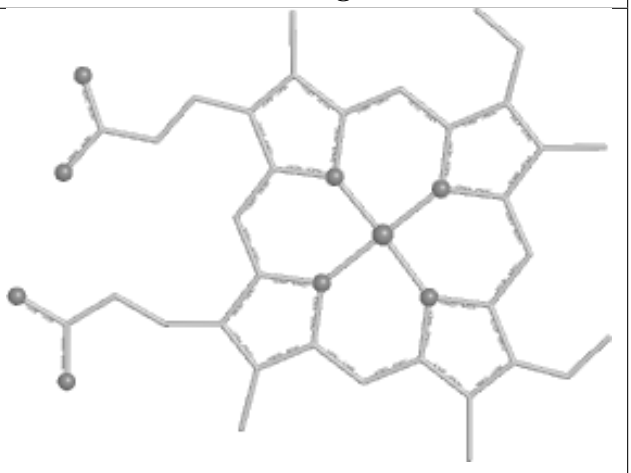
Bond lengths



Bond angles

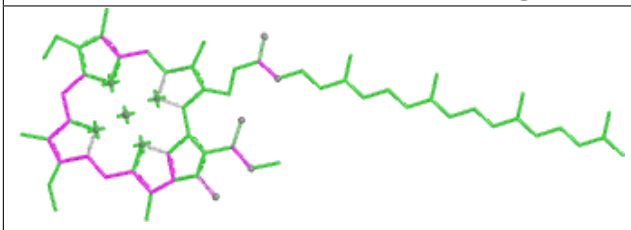


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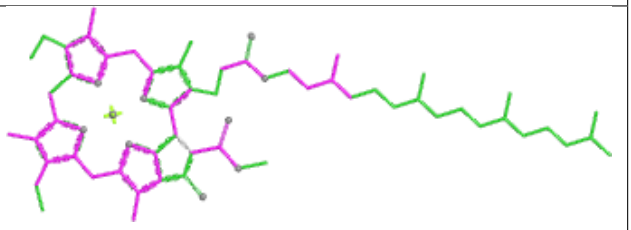


Rings

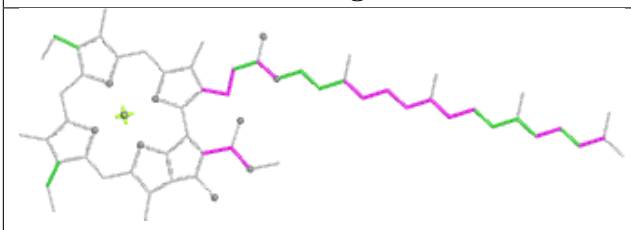
Ligand CLA B 1015



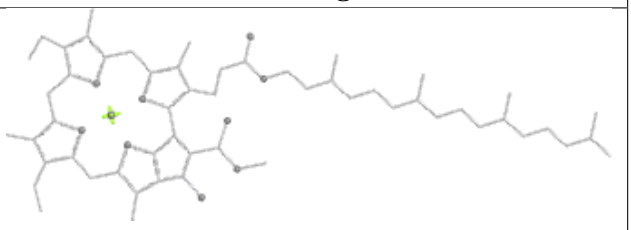
Bond lengths



Bond angles

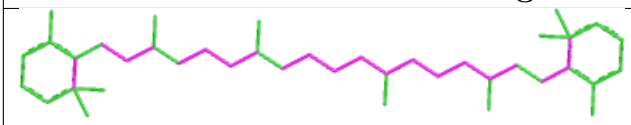


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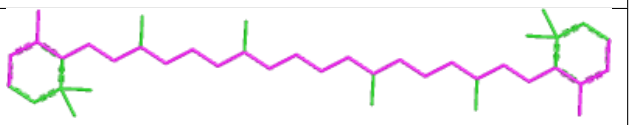


Rings

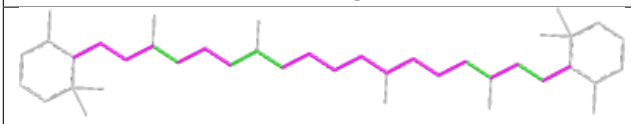
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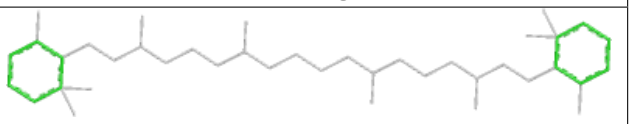
Bond lengths



Bond angles

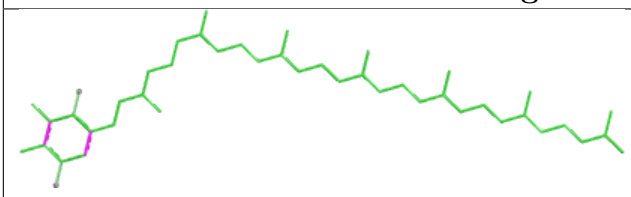


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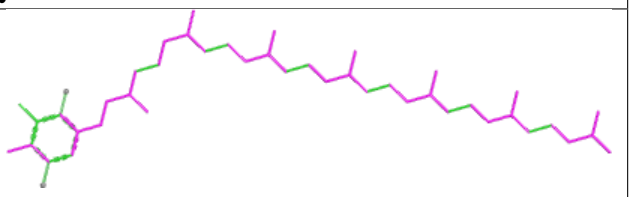


Rings

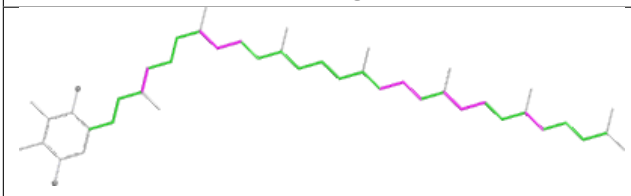
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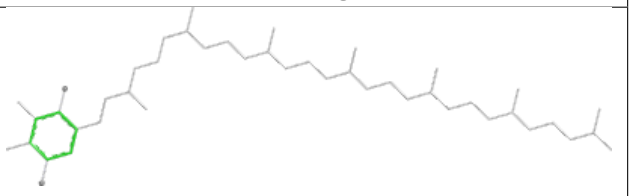
Bond lengths



Bond angles

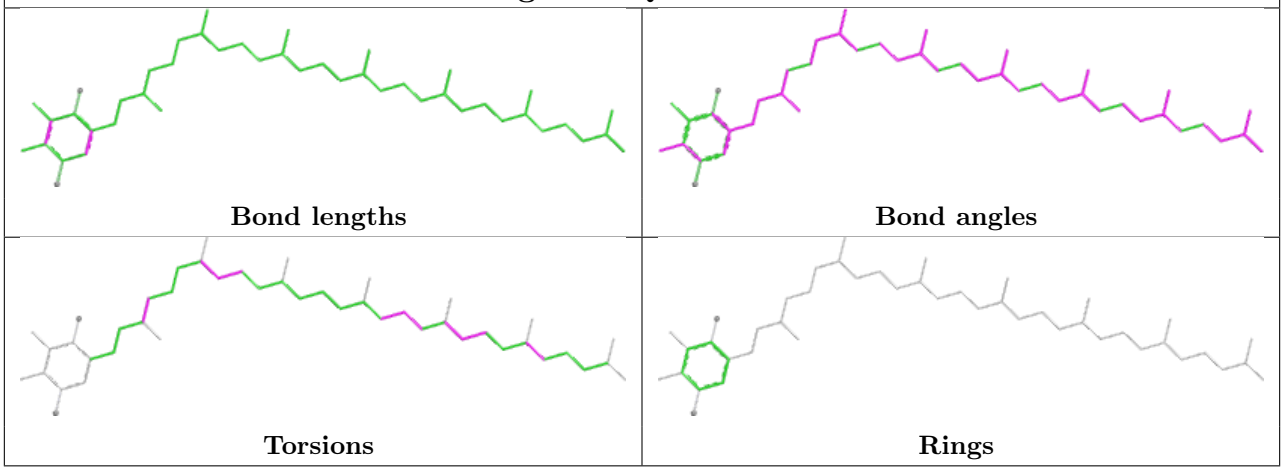


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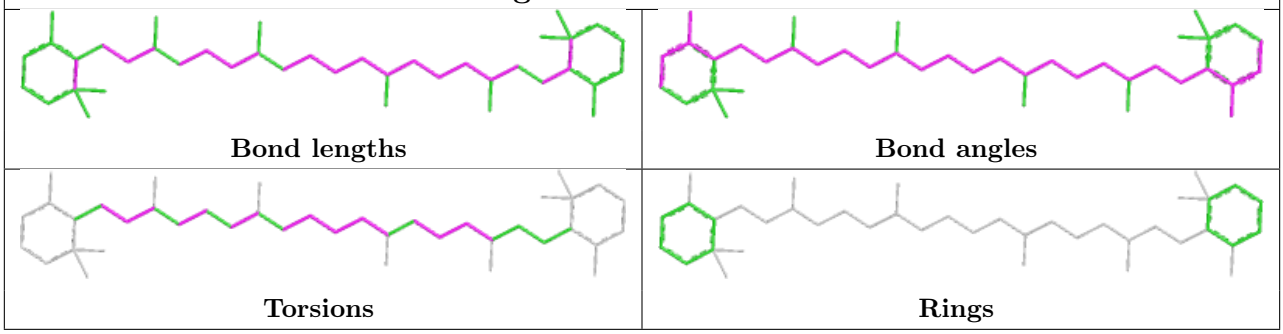


Rings

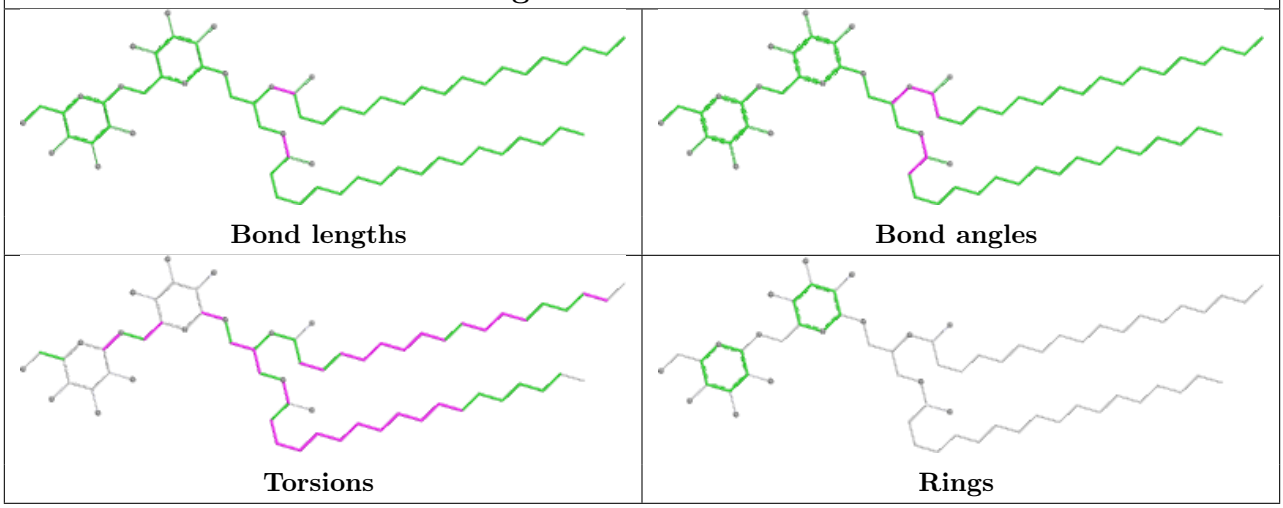
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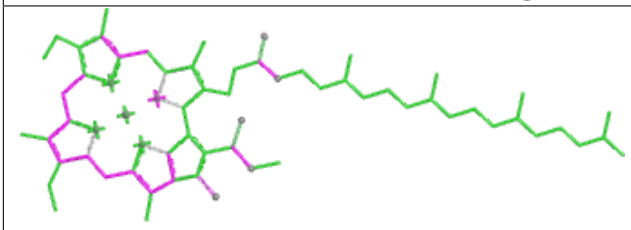
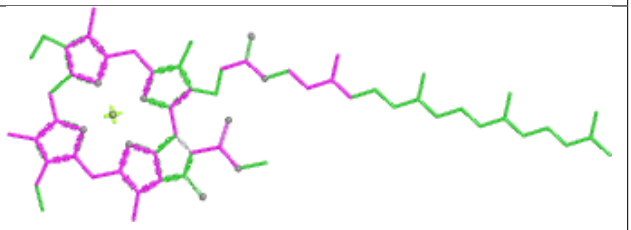
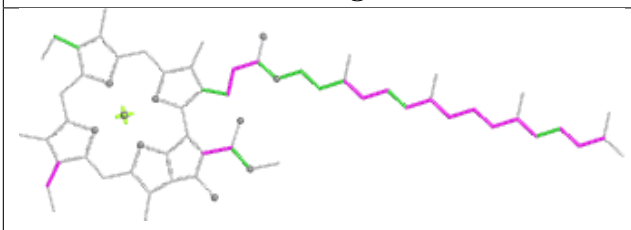
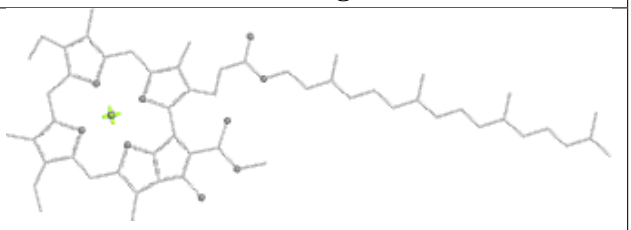


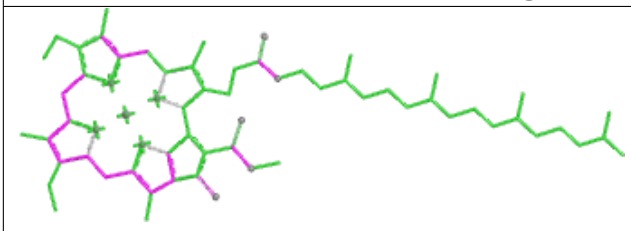
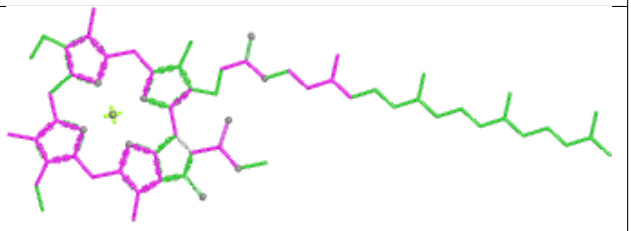
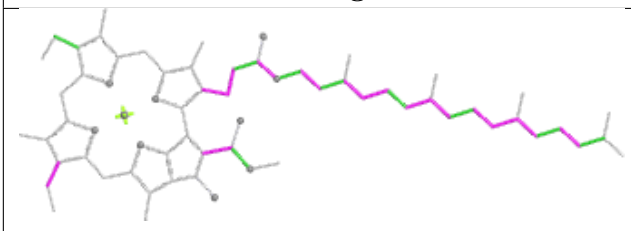
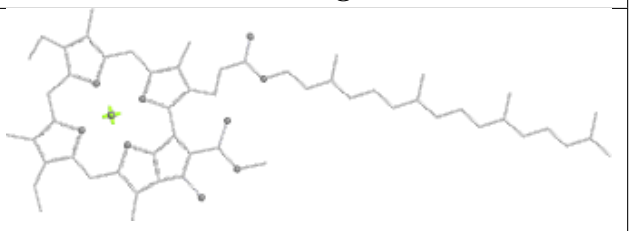
Ligand BCR K 1051



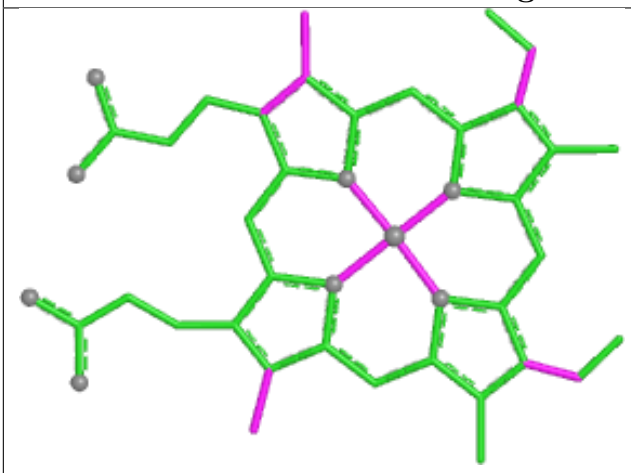
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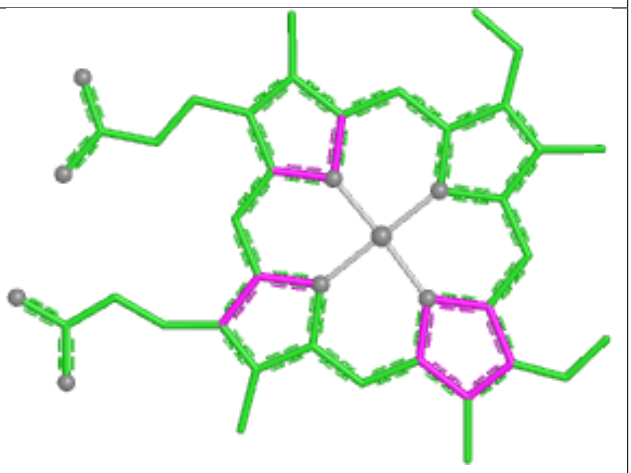
Ligand CLA b 6018	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 6036	
	
Bond lengths	Bond angles
	
Torsions	Rings

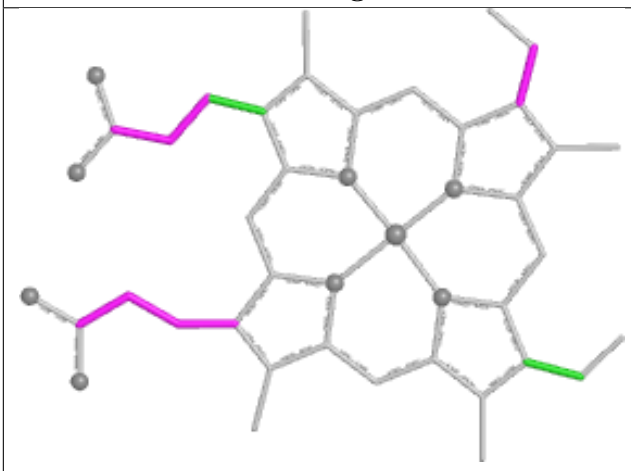
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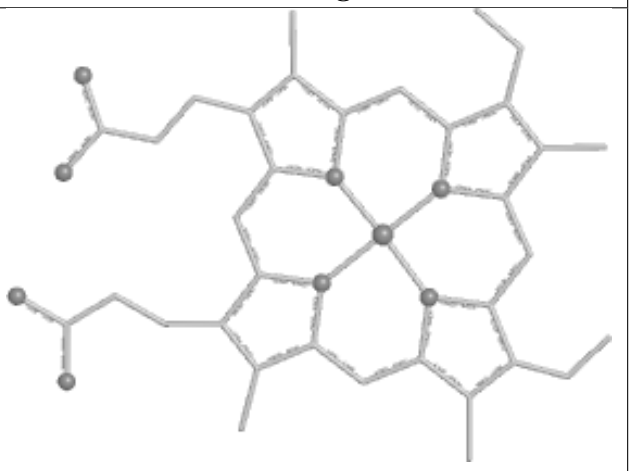
Bond lengths



Bond angles

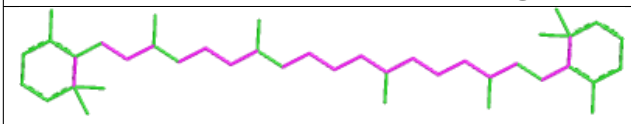


Torsions

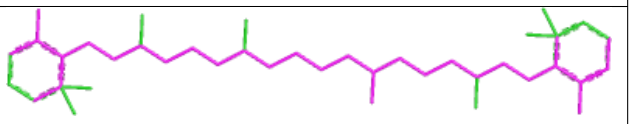


Rings

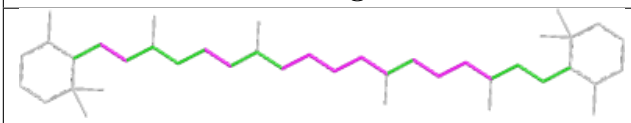
Ligand BCR T 6046



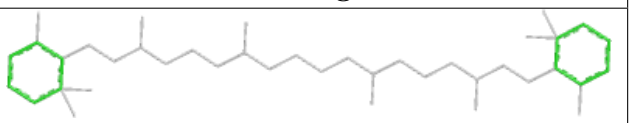
Bond lengths



Bond angles

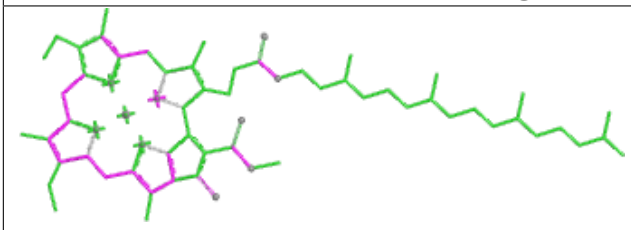


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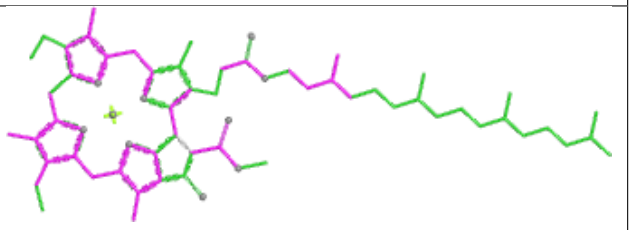


Rings

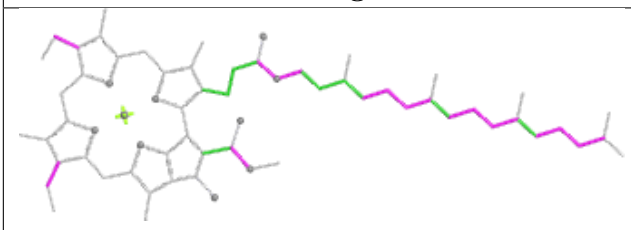
Ligand CLA B 1016



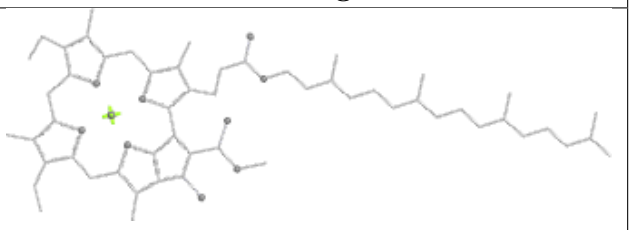
Bond lengths



Bond angles

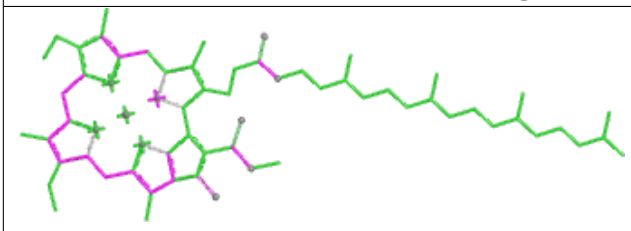


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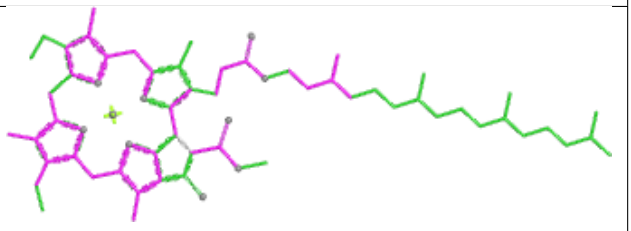


Rings

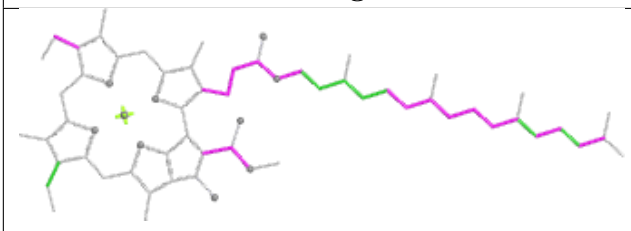
Ligand CLA B 1021



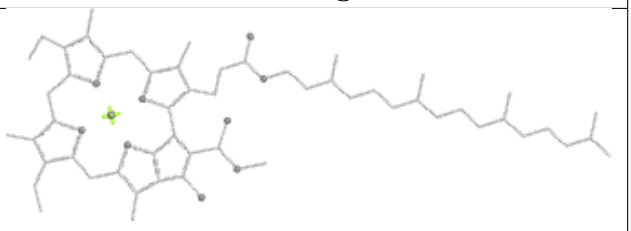
Bond lengths



Bond angles

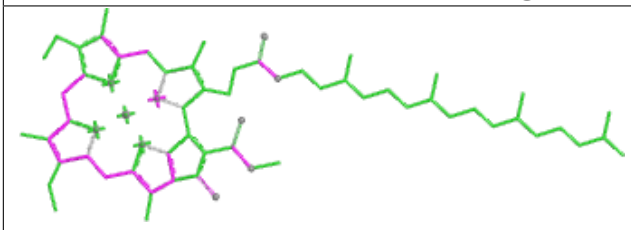


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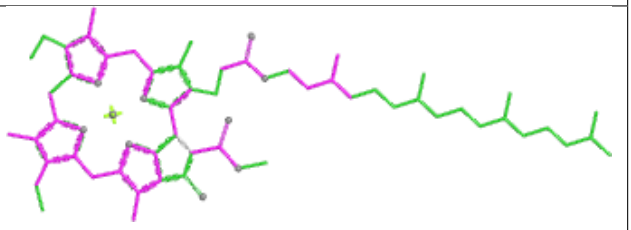


Rings

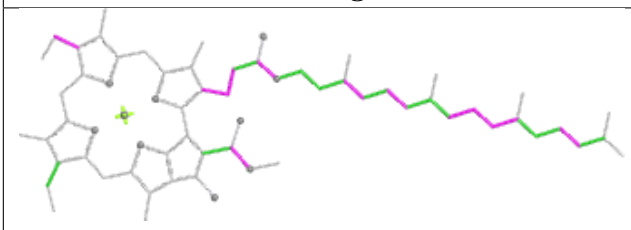
Ligand CLA b 6010



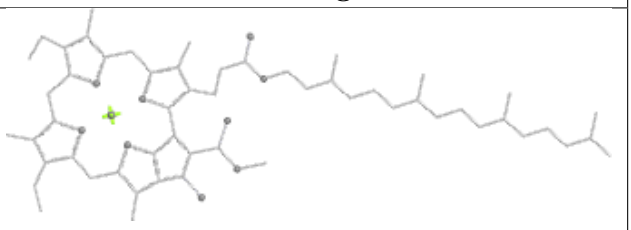
Bond lengths



Bond angles

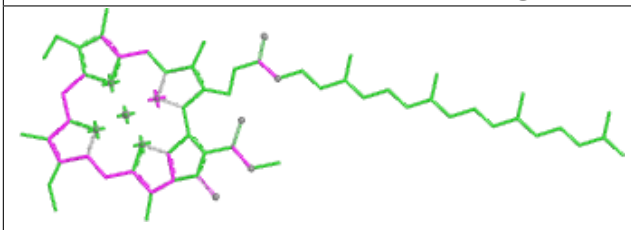


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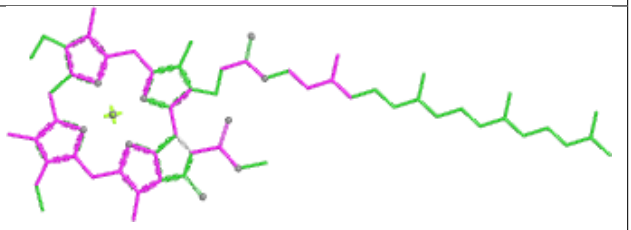


Rings

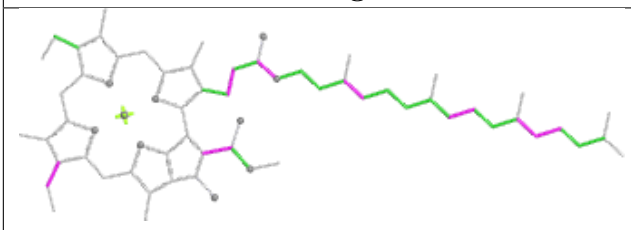
Ligand CLA D 1004



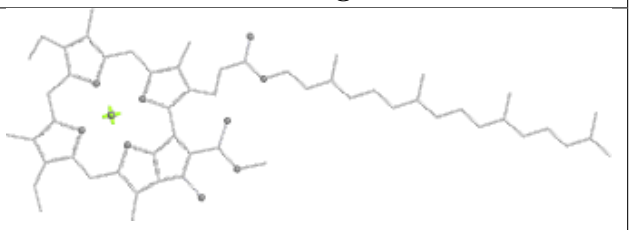
Bond lengths



Bond angles

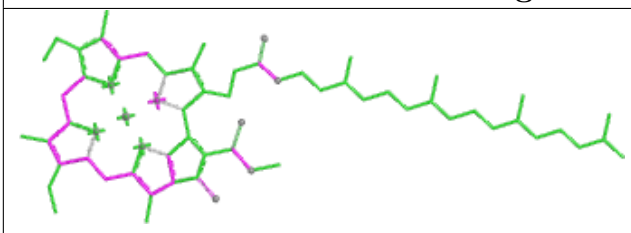


Torsions

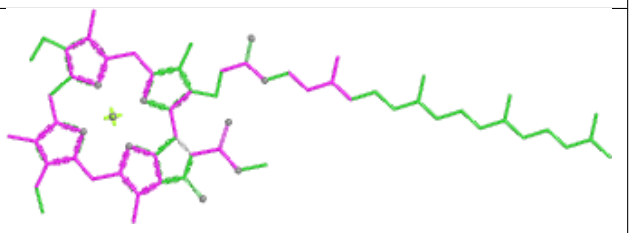


Rings

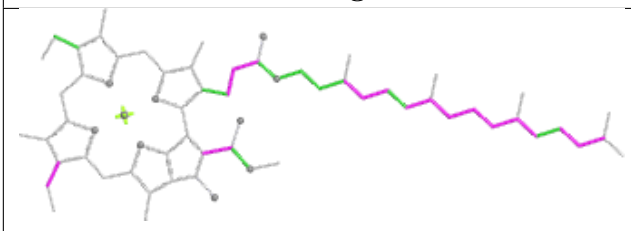
Ligand CLA B 1018



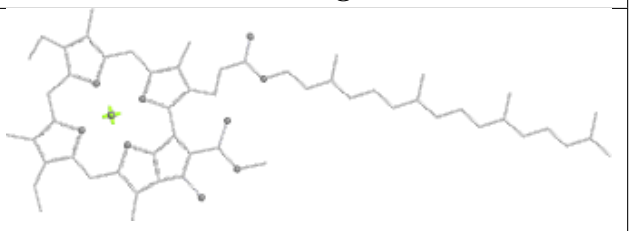
Bond lengths



Bond angles

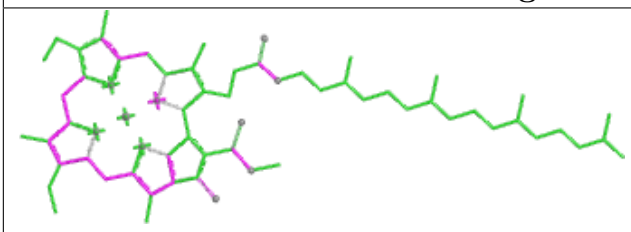


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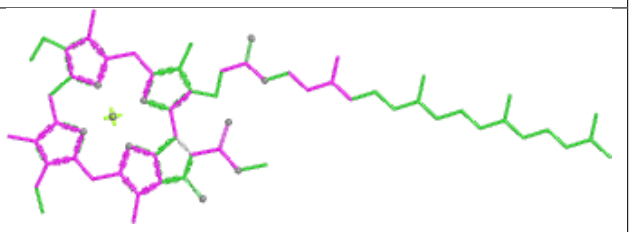


Rings

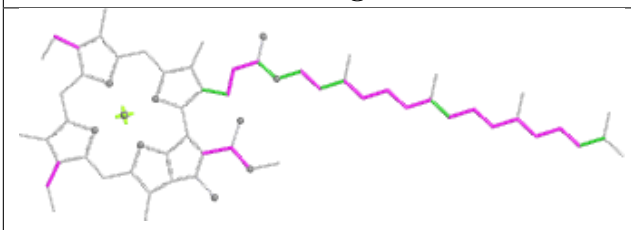
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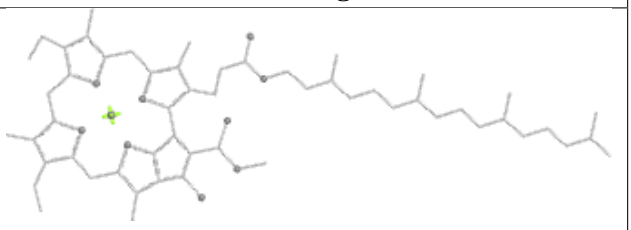
Bond lengths



Bond angles



Torsions

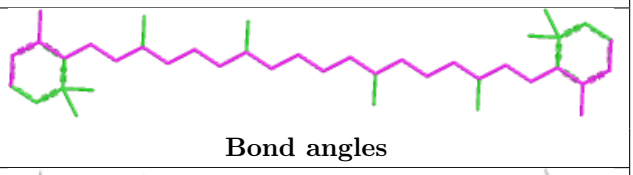


Rings

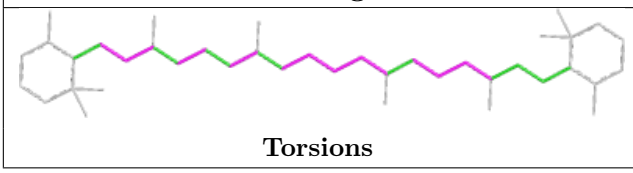
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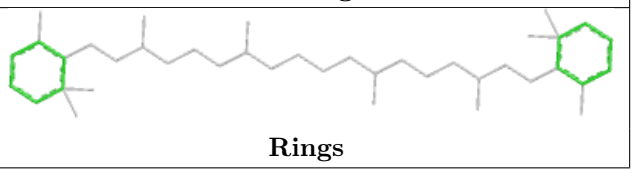
Bond lengths



Bond angles

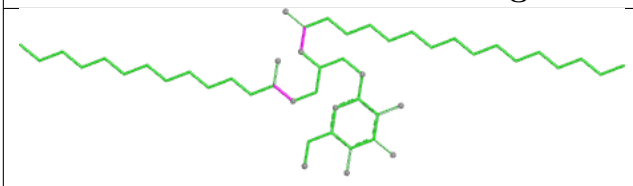


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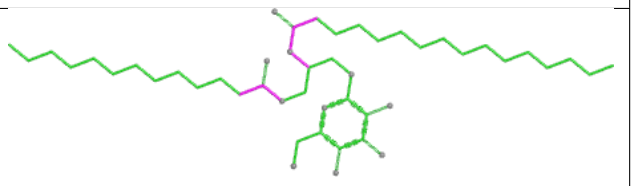


Rings

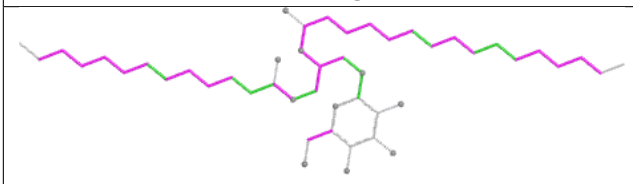
Ligand MGE B 1060



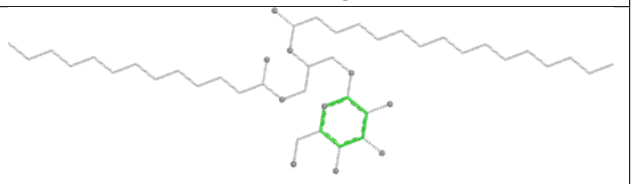
Bond lengths



Bond angles

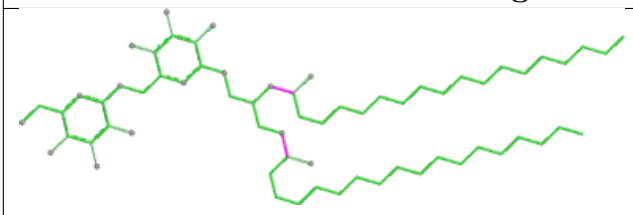


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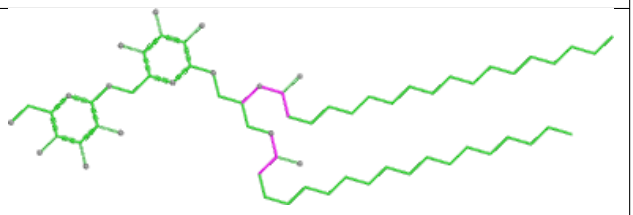


Rings

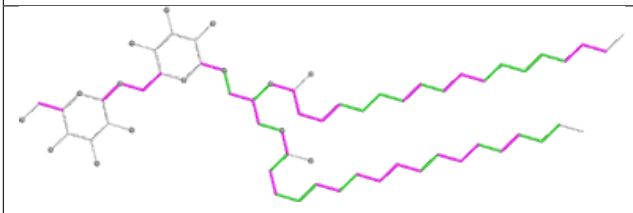
Ligand DGD B 1058



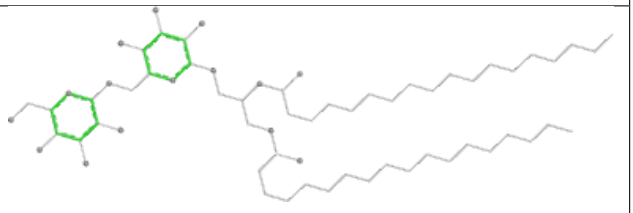
Bond lengths



Bond angles

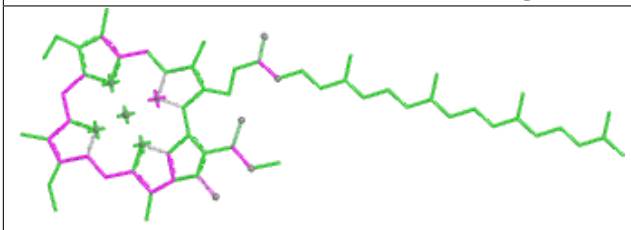


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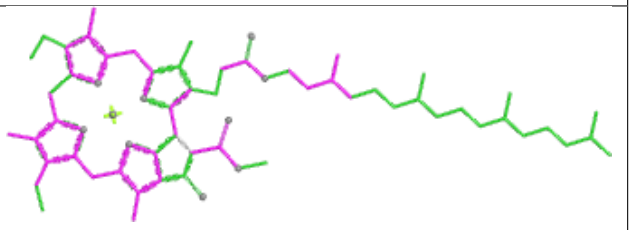


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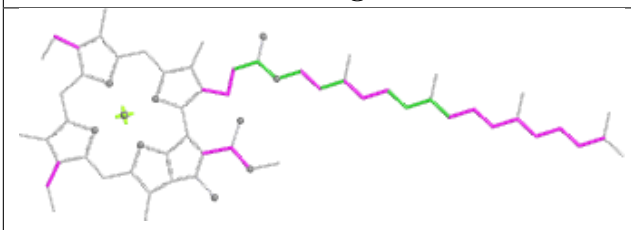
Ligand CLA b 6013



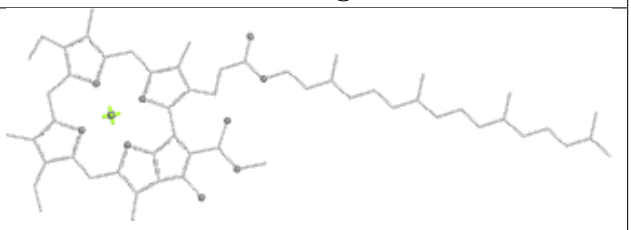
Bond lengths



Bond angles

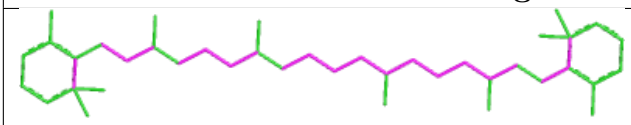


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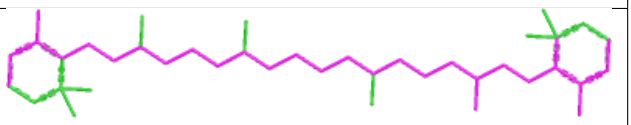


Rings

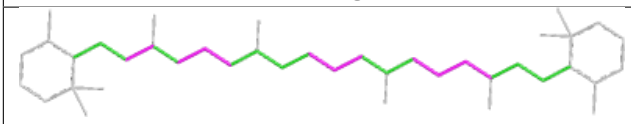
Ligand BCR B 1048



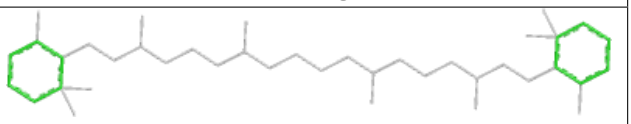
Bond lengths



Bond angles

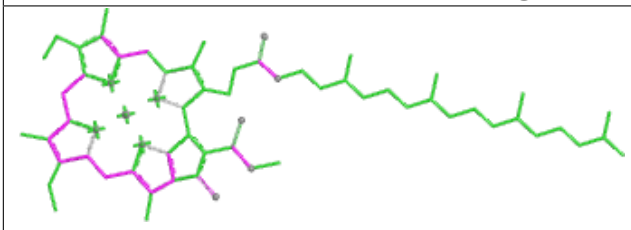


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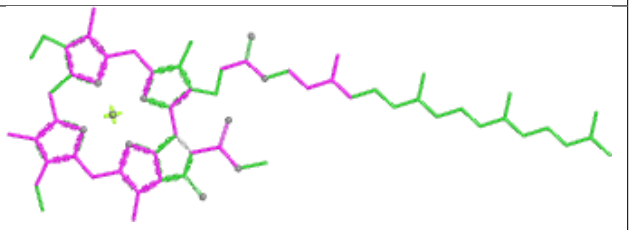


Rings

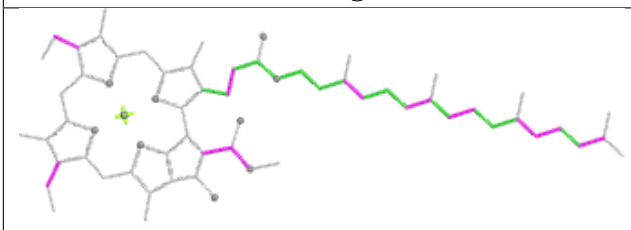
Ligand CLA B 1012



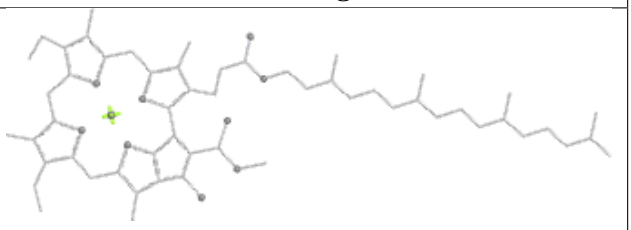
Bond lengths



Bond angles

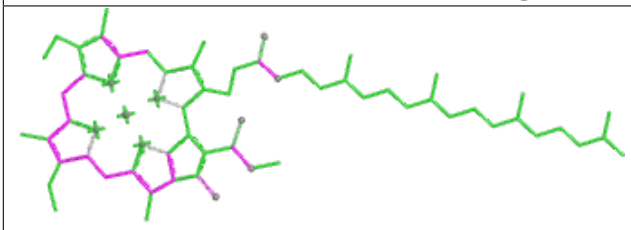


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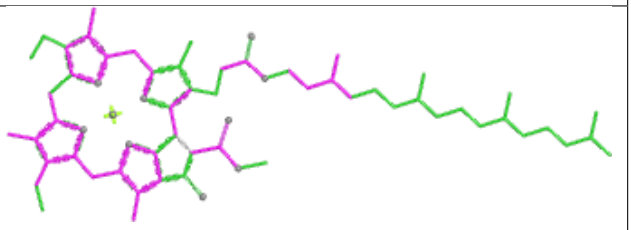


Rings

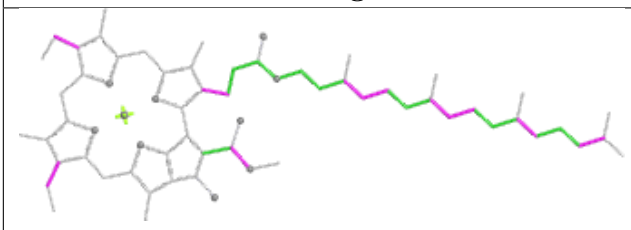
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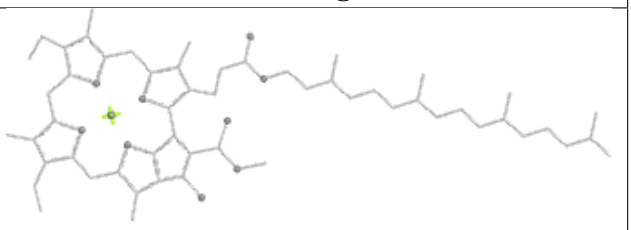
Bond lengths



Bond angles

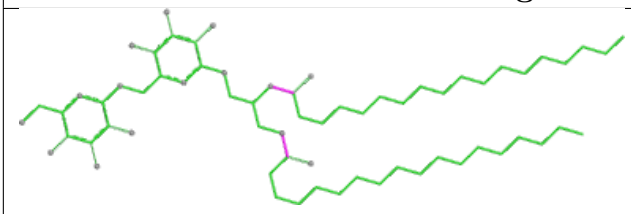


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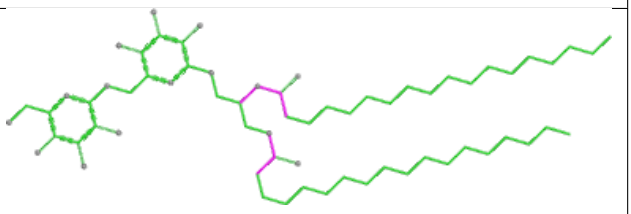


Rings

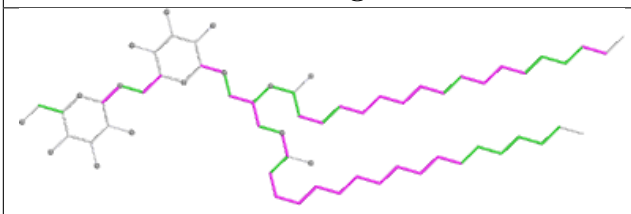
Ligand DGD c 6057



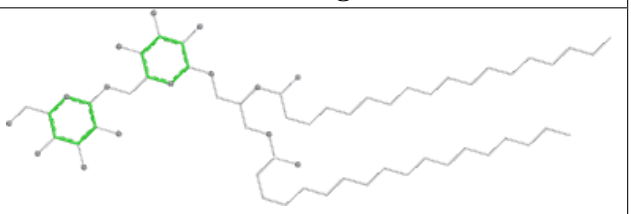
Bond lengths



Bond angles

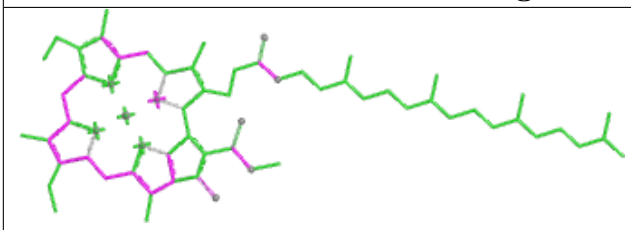


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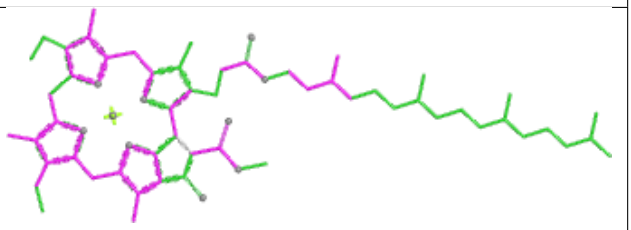


Rings

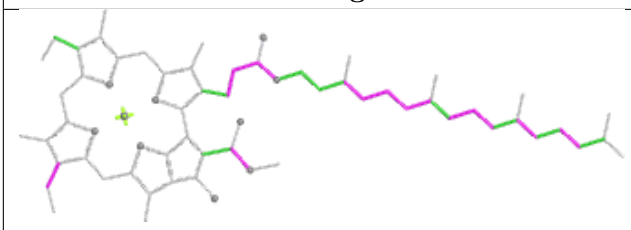
Ligand CLA C 1027



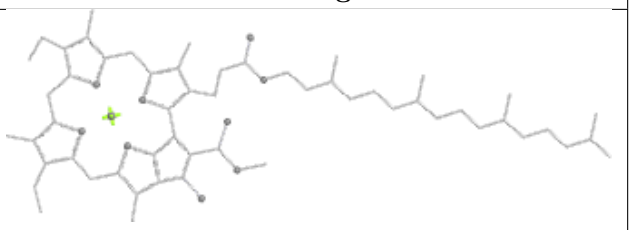
Bond lengths



Bond angles

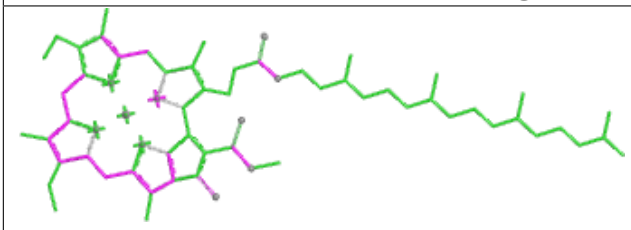


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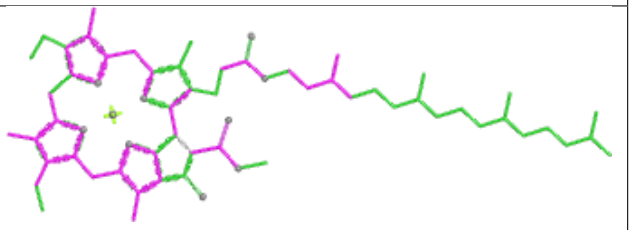


Rings

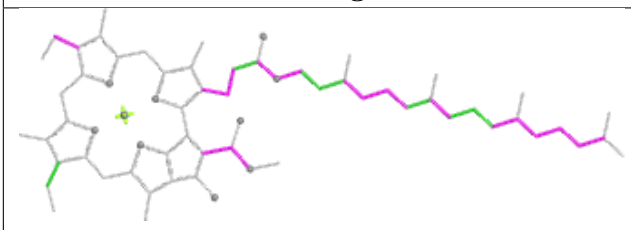
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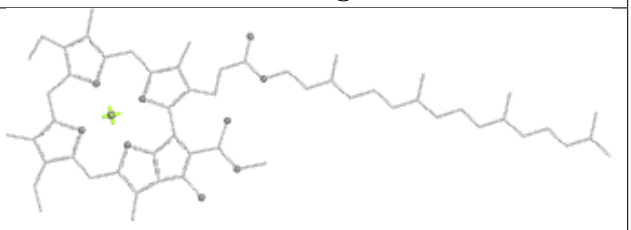
Bond lengths



Bond angles

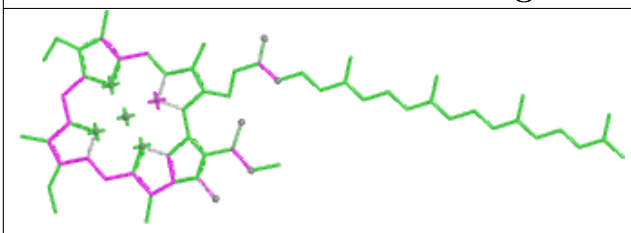


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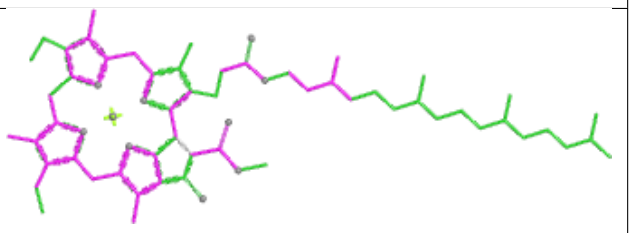


Rings

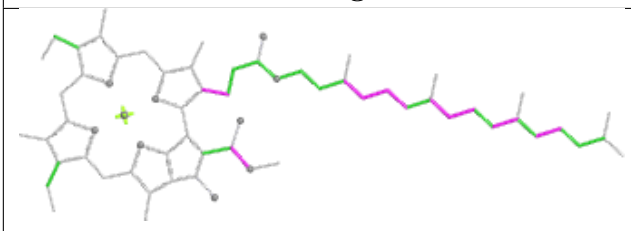
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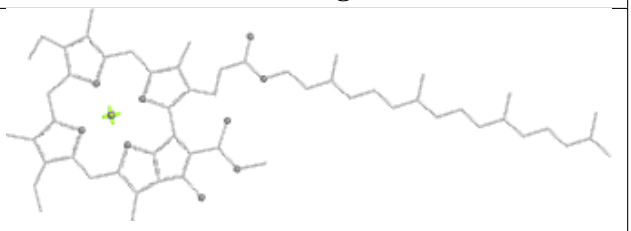
Bond lengths



Bond angles

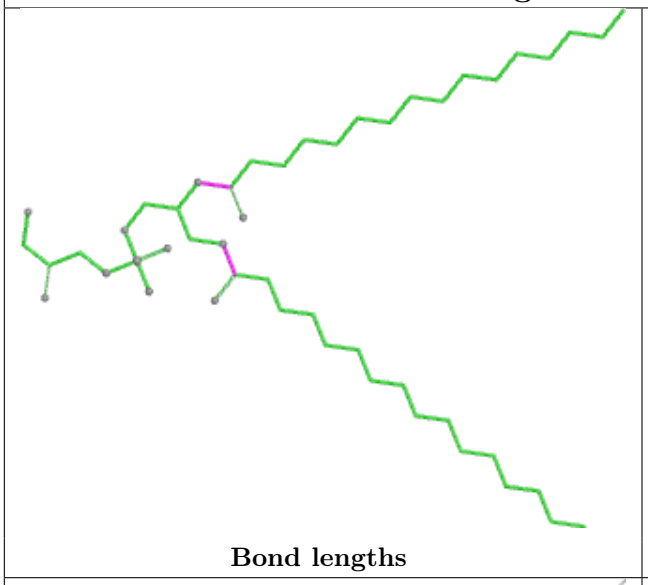


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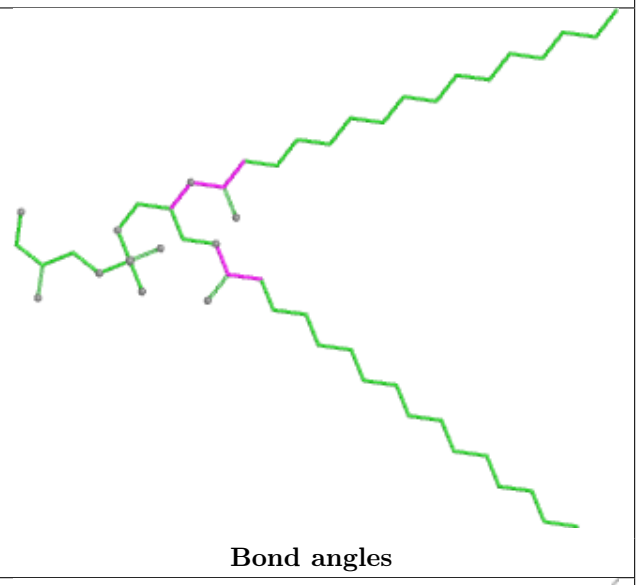


Rings

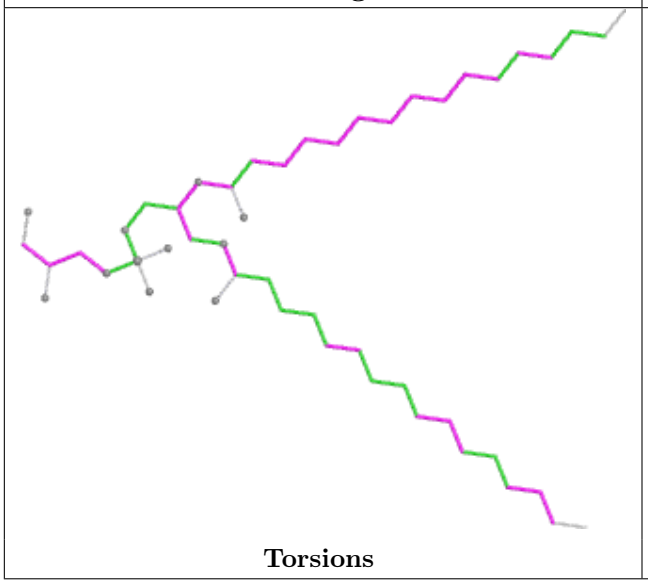
Ligand LHG A 1063



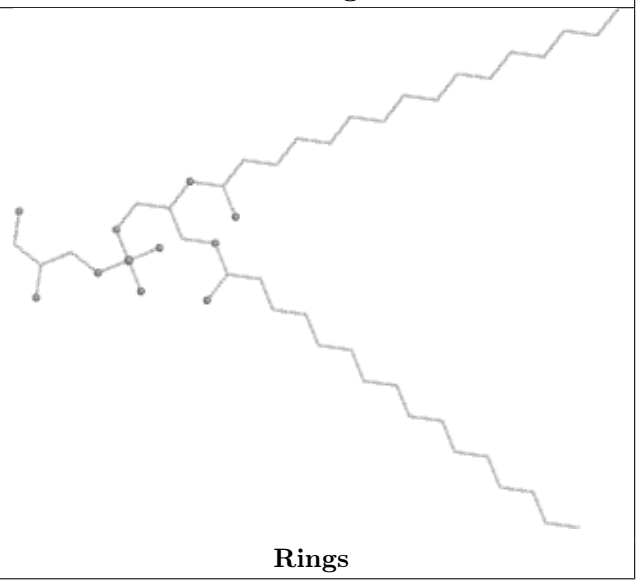
Bond lengths



Bond angles

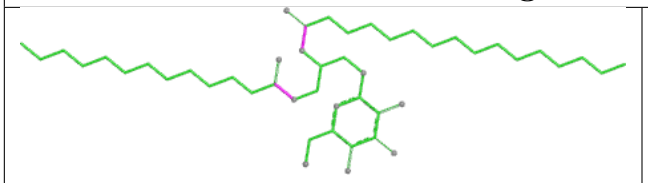


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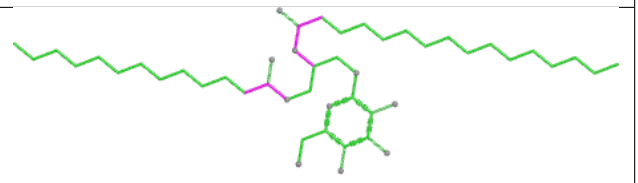


Rings

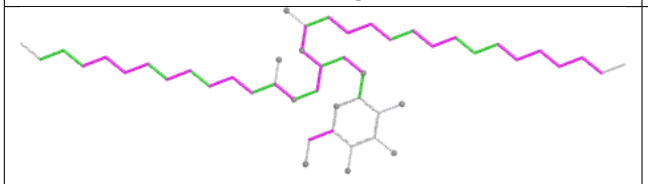
Ligand MGE l 6061



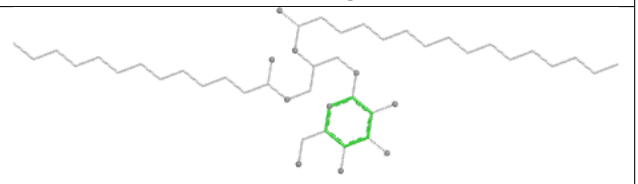
Bond lengths



Bond angles

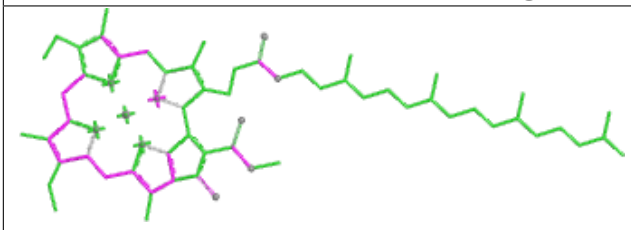


Torsions

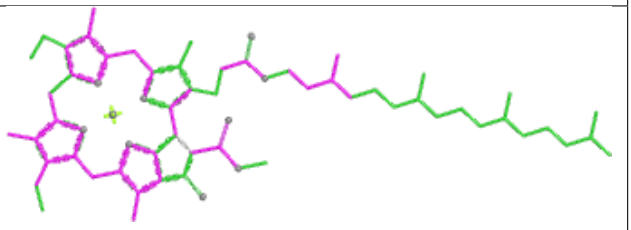


Rings

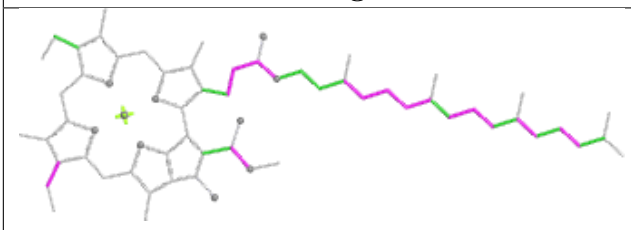
Ligand CLA c 6027



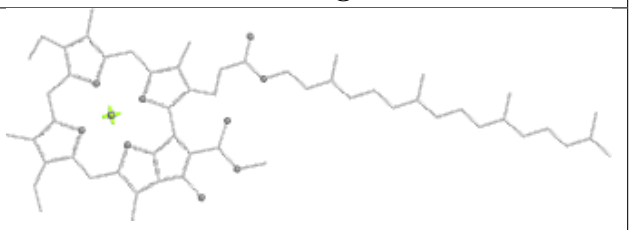
Bond lengths



Bond angles

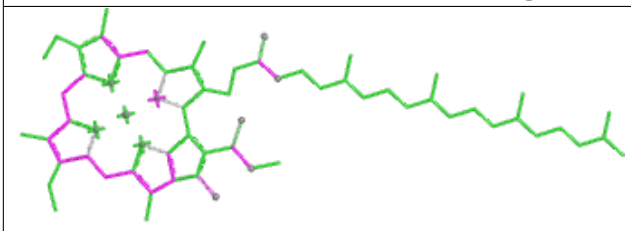


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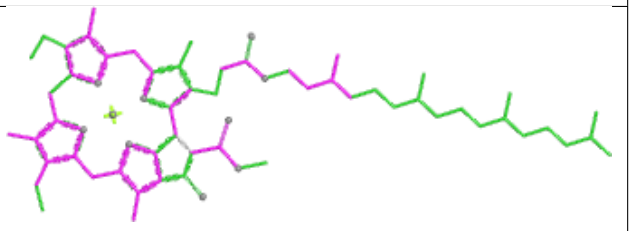


Rings

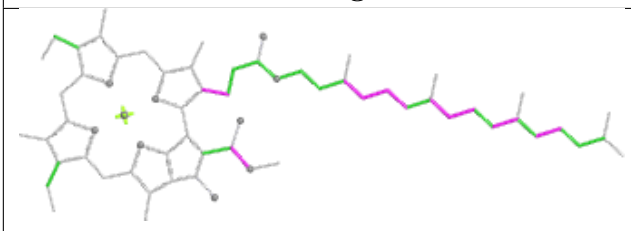
Ligand CLA c 6035



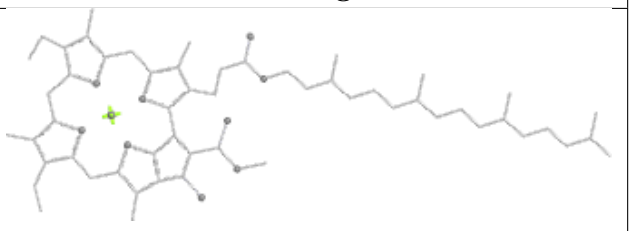
Bond lengths



Bond angles

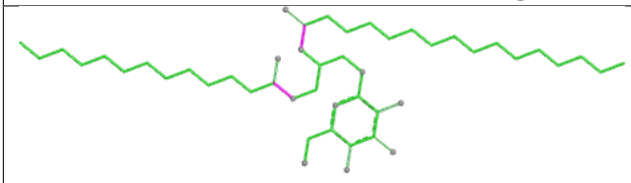


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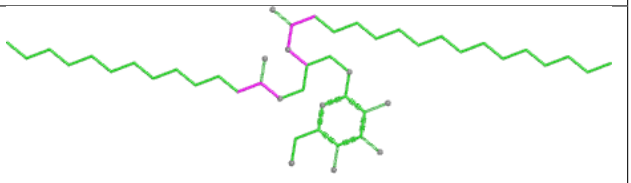


Rings

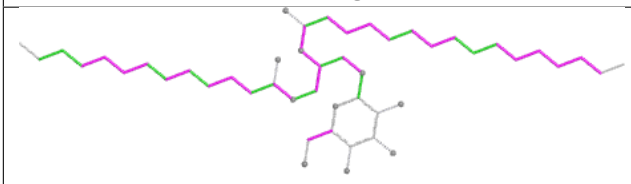
Ligand MGE L 1061



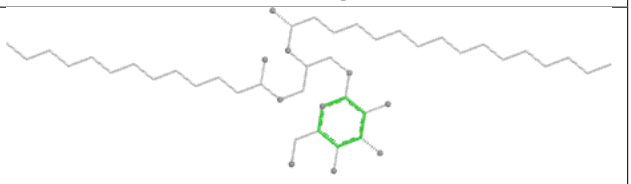
Bond lengths



Bond angles



Torsions

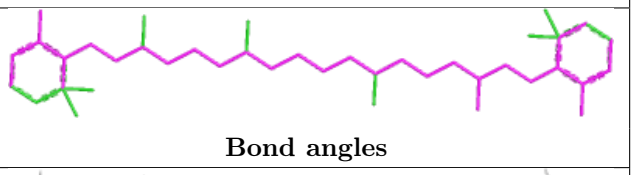


Rings

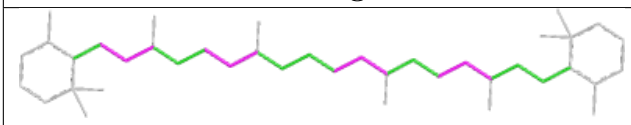
Ligand BCR a 6044



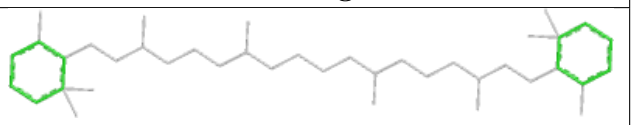
Bond lengths



Bond angles

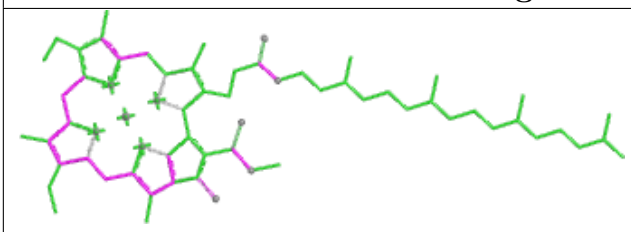


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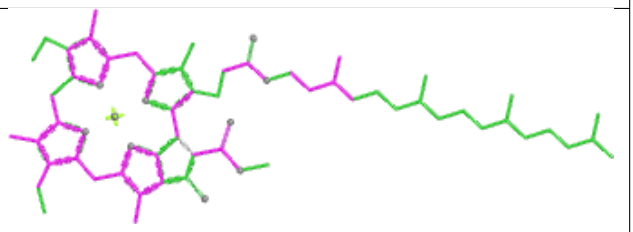


Rings

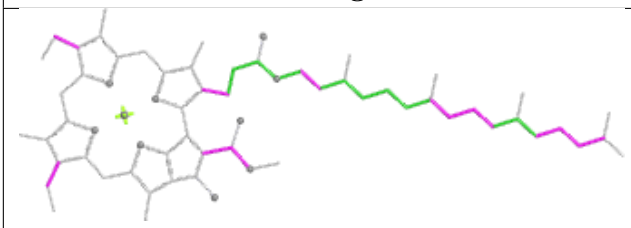
Ligand CLA B 1020



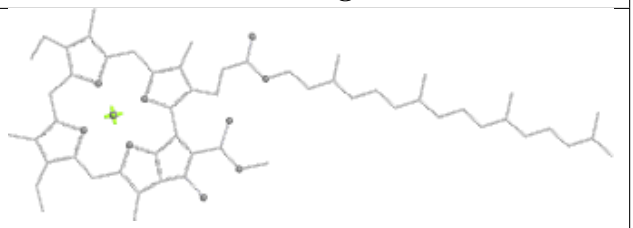
Bond lengths



Bond angles

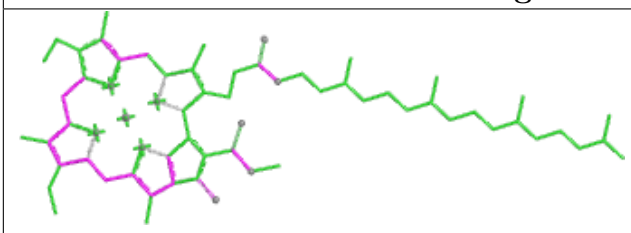


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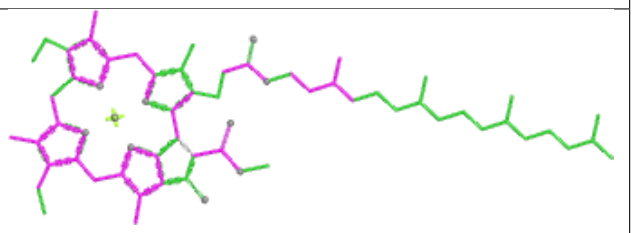


Rings

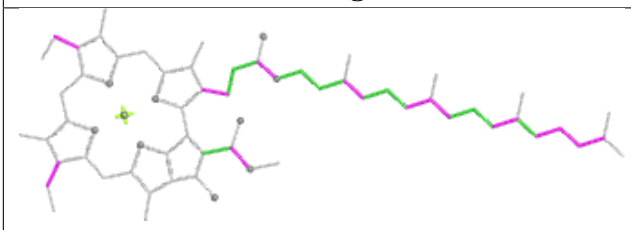
Ligand CLA D 1005



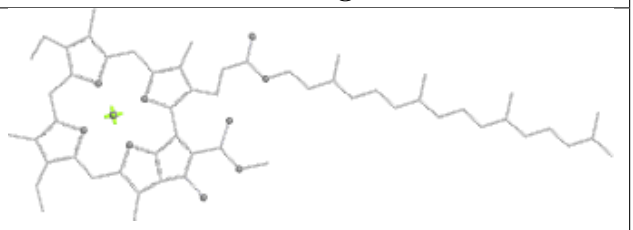
Bond lengths



Bond angles

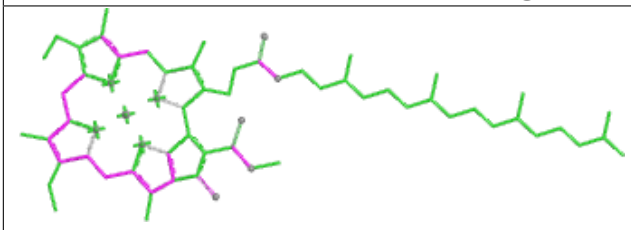


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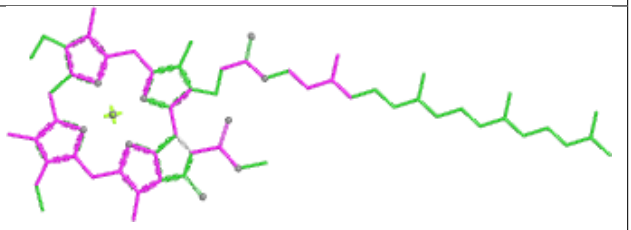


Rings

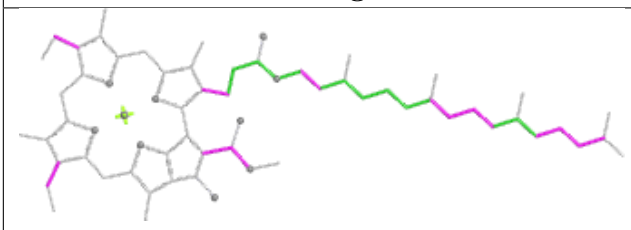
Ligand CLA b 6020



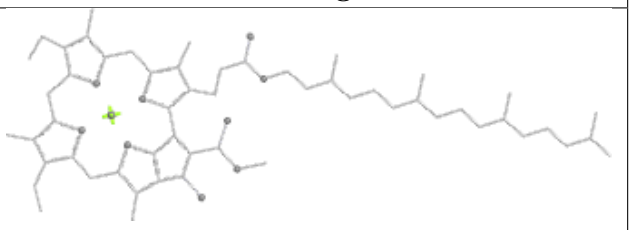
Bond lengths



Bond angles

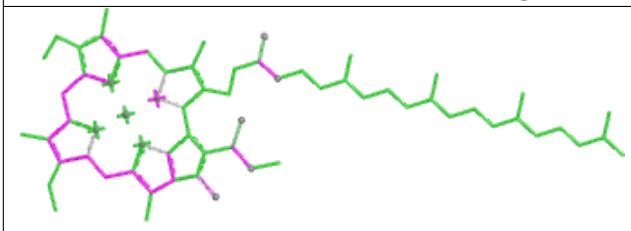


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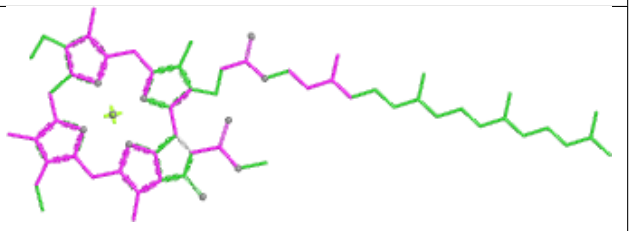


Rings

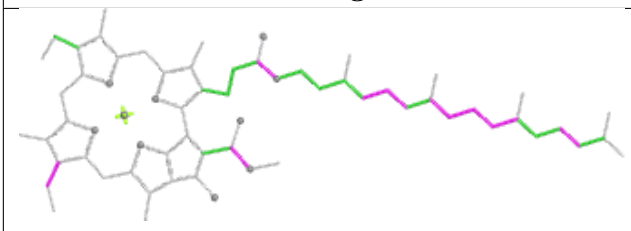
Ligand CLA C 1029



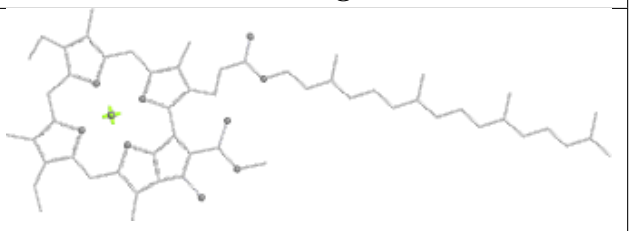
Bond lengths



Bond angles

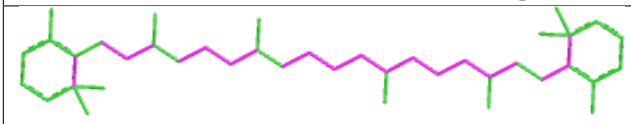


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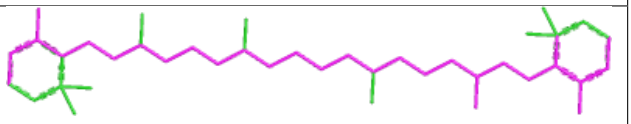


Rings

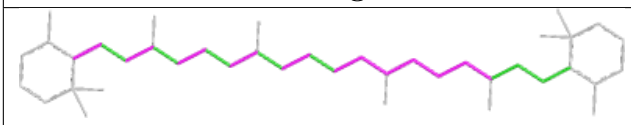
Ligand BCR B 1047



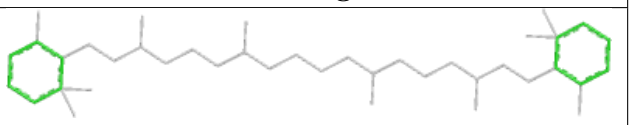
Bond lengths



Bond angles

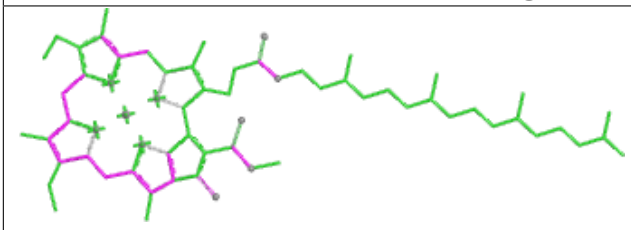


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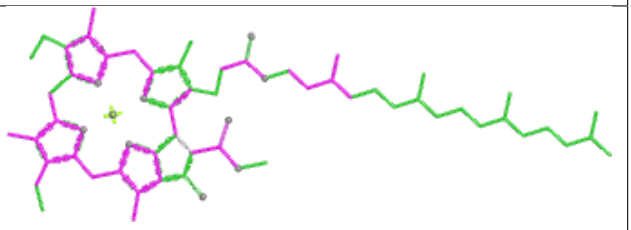


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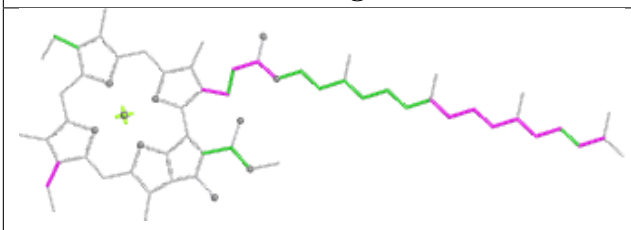
Ligand CLA c 6037



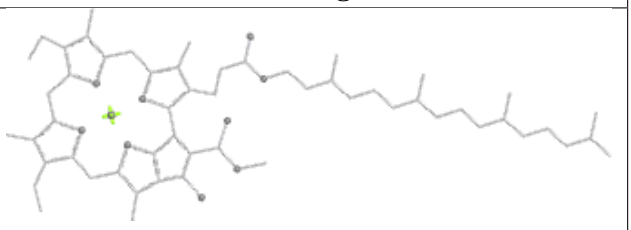
Bond lengths



Bond angles

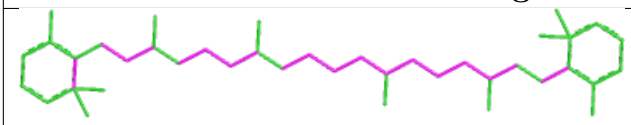


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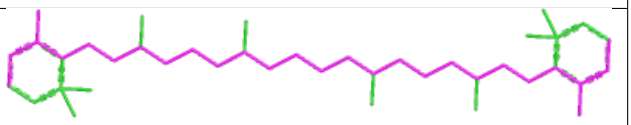


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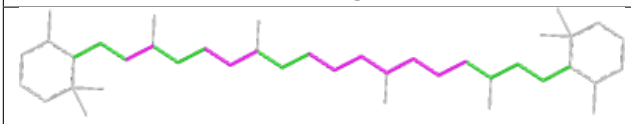
Ligand BCR H 1049



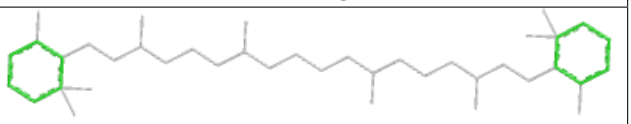
Bond lengths



Bond angles

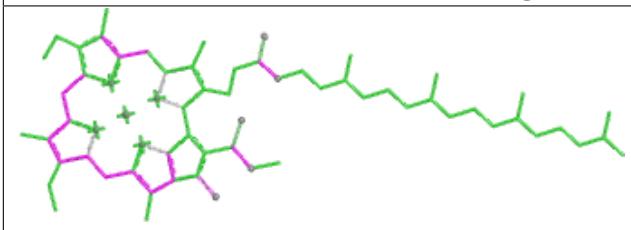


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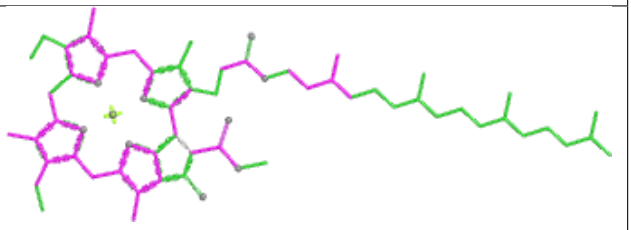


Rings

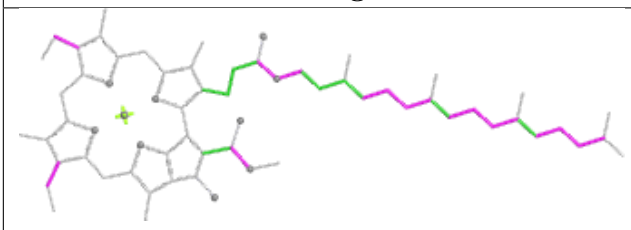
Ligand CLA b 6016



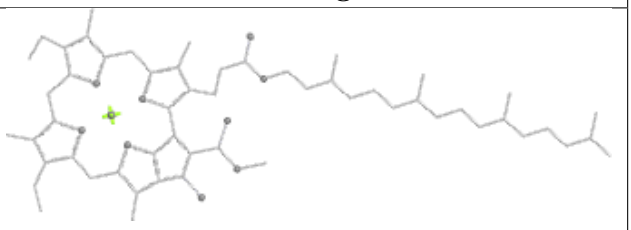
Bond lengths



Bond angles

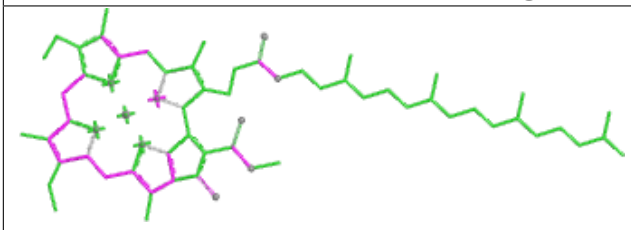


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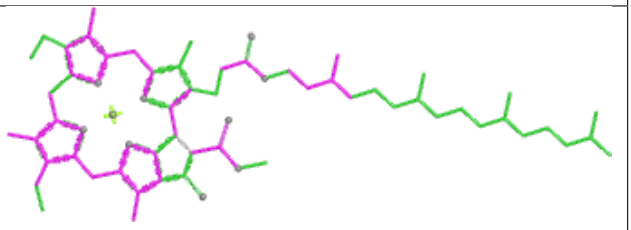


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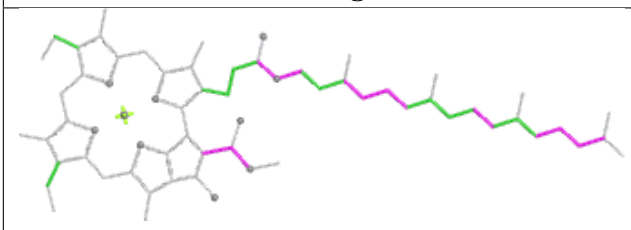
Ligand CLA c 6033



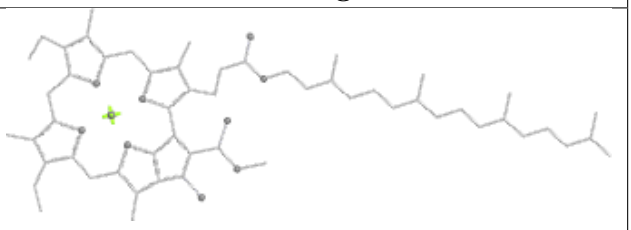
Bond lengths



Bond angles

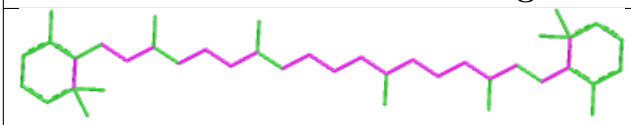


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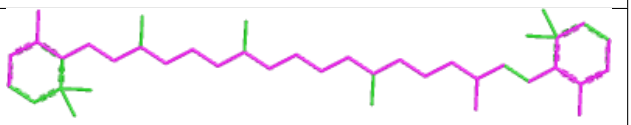


Rings

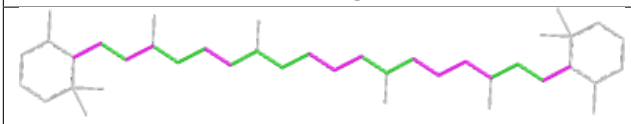
Ligand BCR k 6052



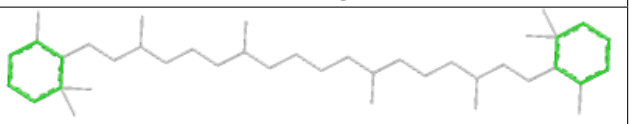
Bond lengths



Bond angles

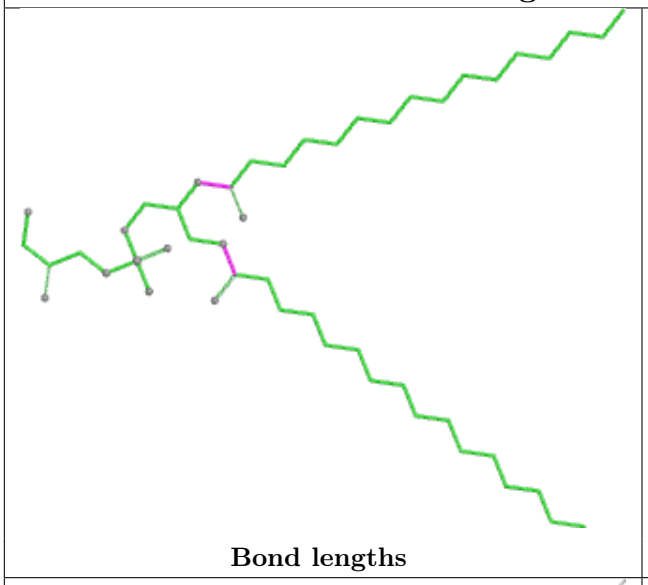


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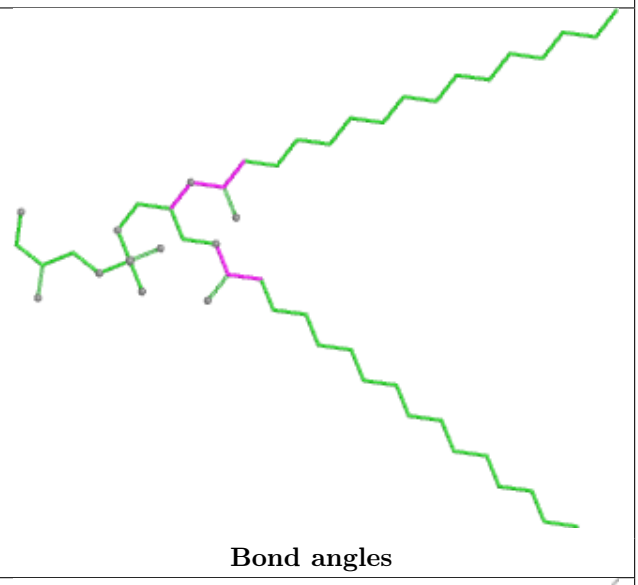


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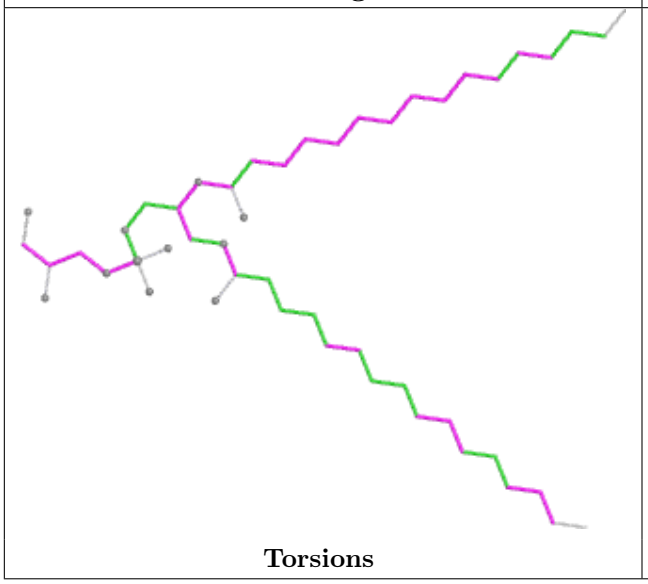
Ligand LHG a 6063



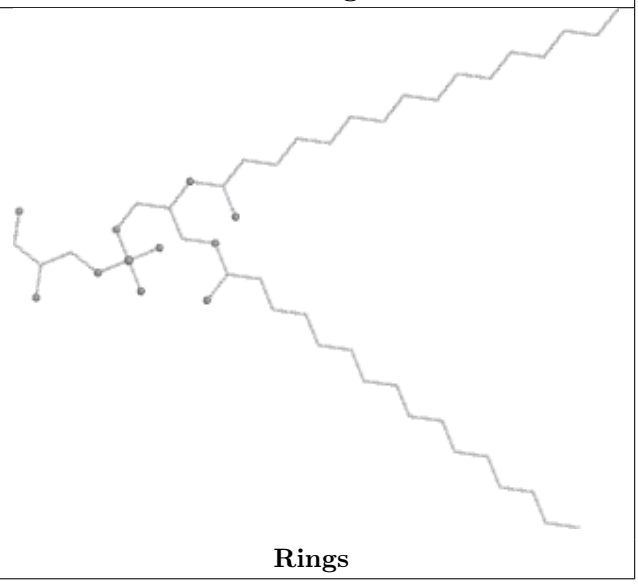
Bond lengths



Bond angles

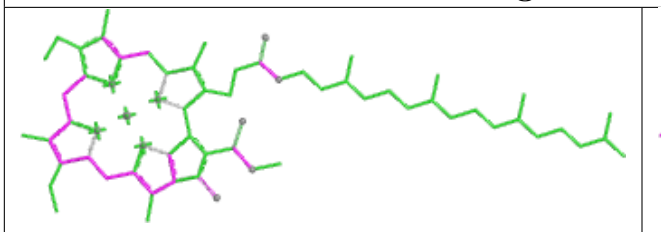


Torsions

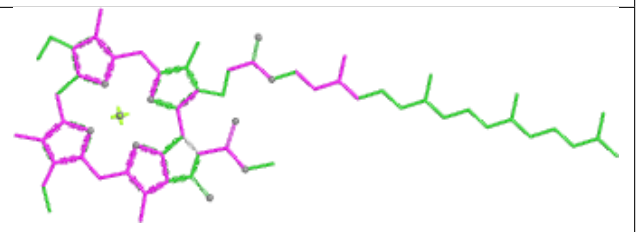


Rings

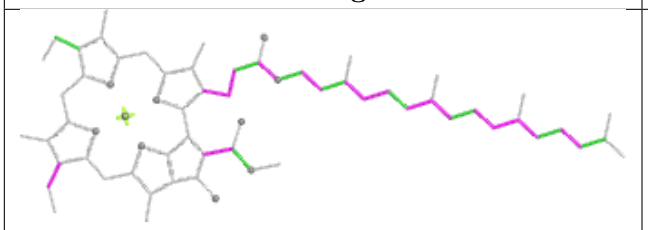
Ligand CLA C 1036



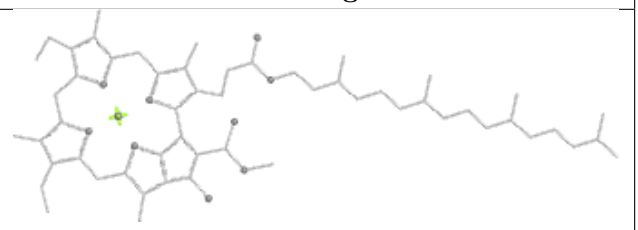
Bond lengths



Bond angles

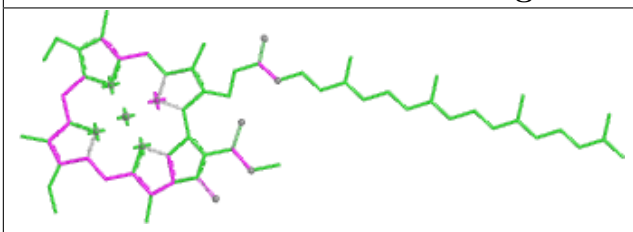


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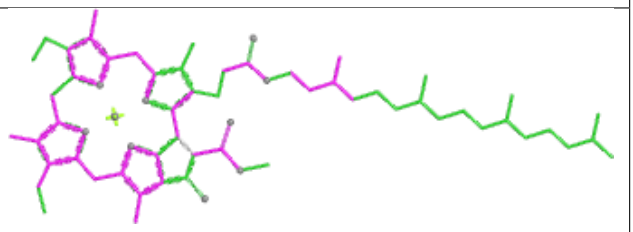


Rings

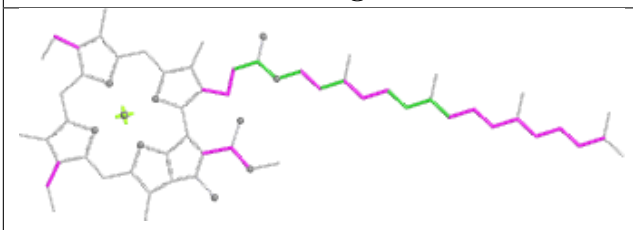
Ligand CLA B 1013



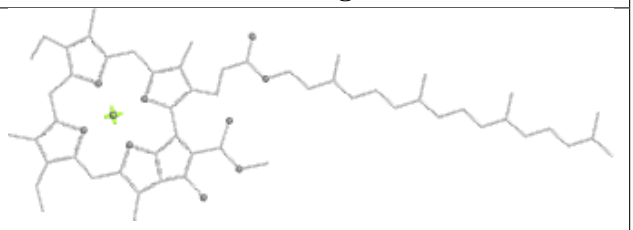
Bond lengths



Bond angles

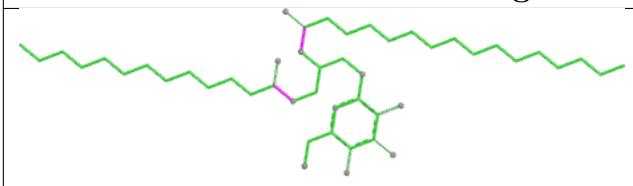


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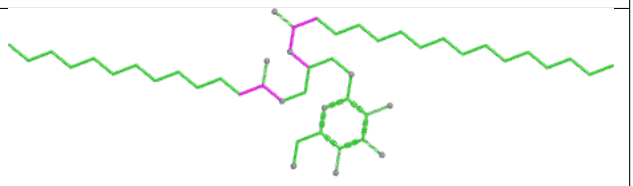


Rings

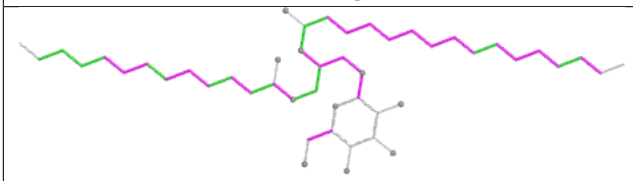
Ligand MGE d 6062



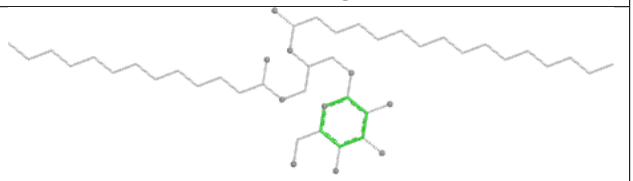
Bond lengths



Bond angles

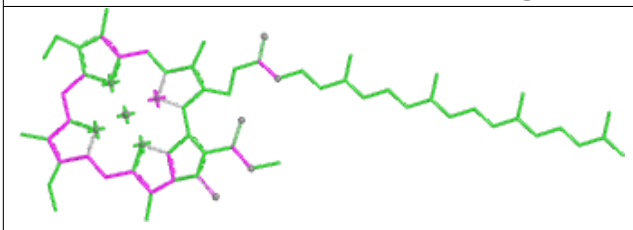


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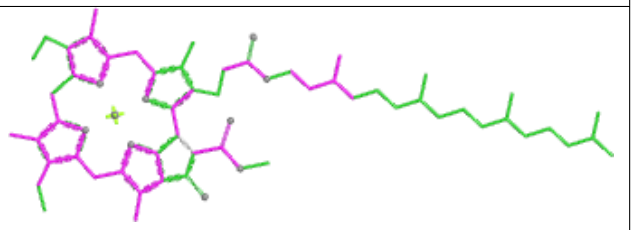


Rings

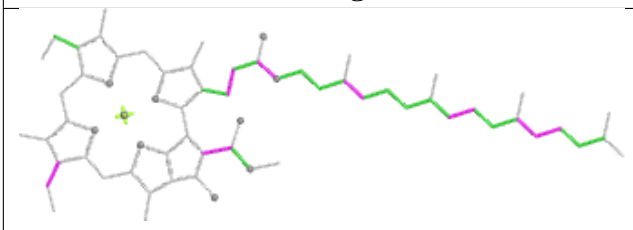
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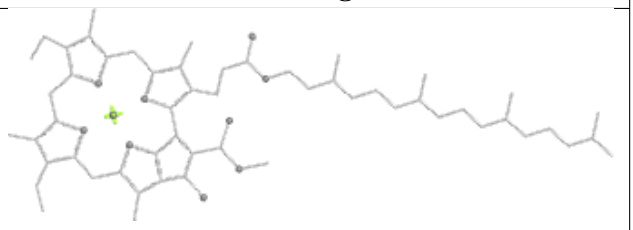
Bond lengths



Bond angles

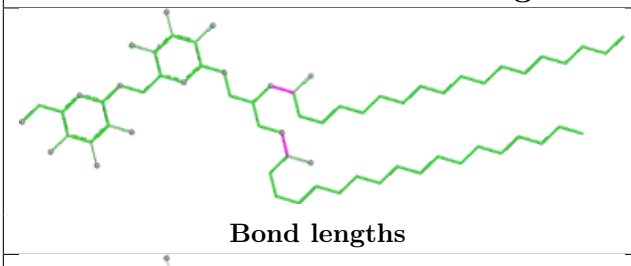


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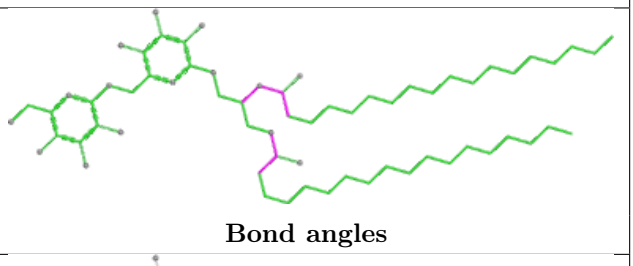


Rings

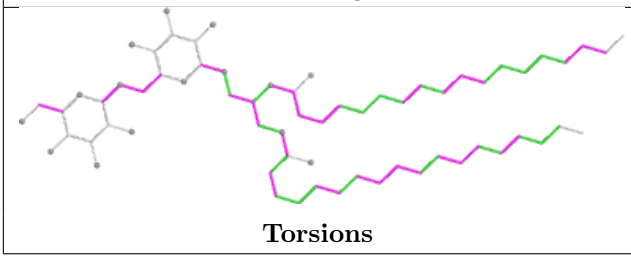
Ligand DGD b 6058



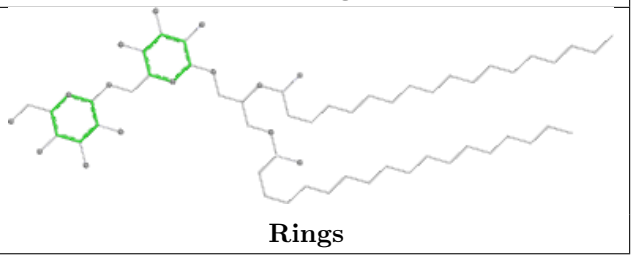
Bond lengths



Bond angles

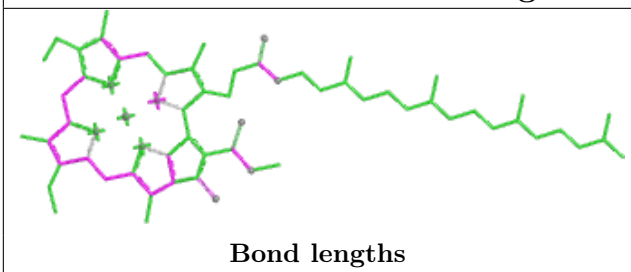


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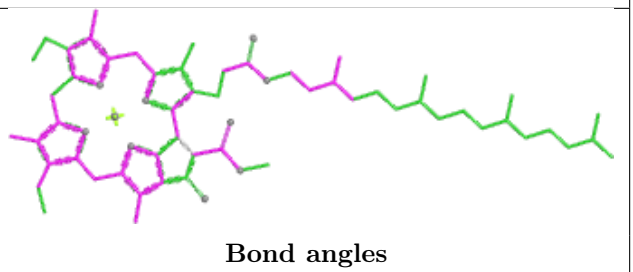


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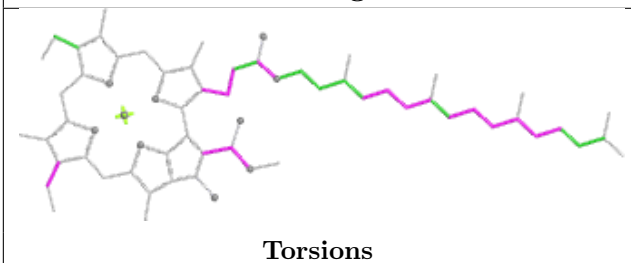
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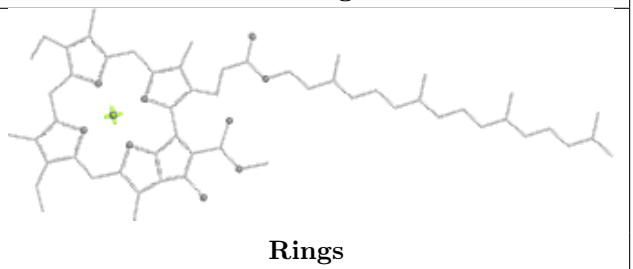
Bond lengths



Bond angles

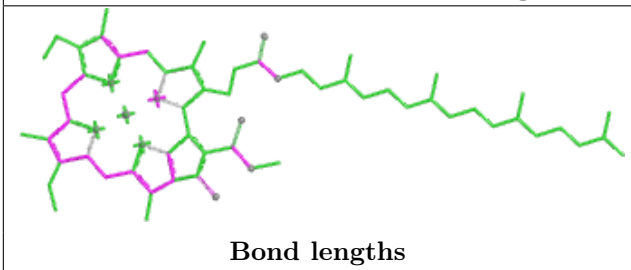


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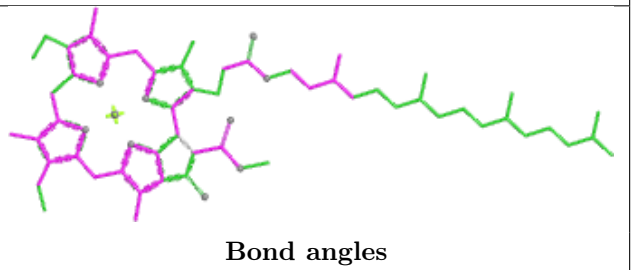


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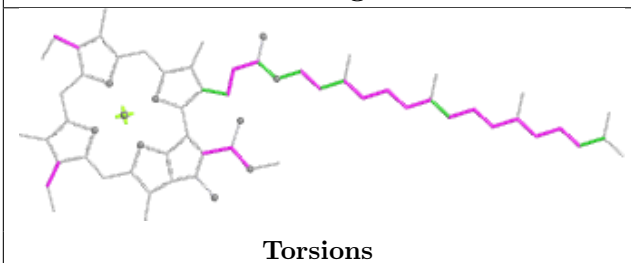
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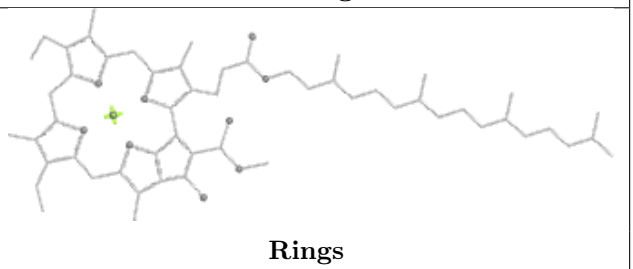
Bond lengths



Bond angles

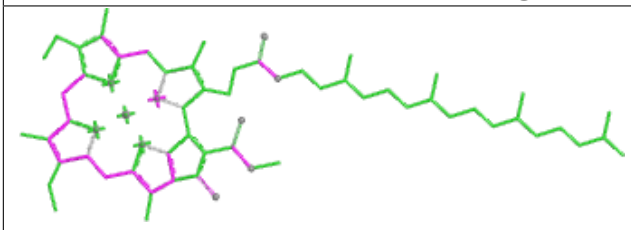


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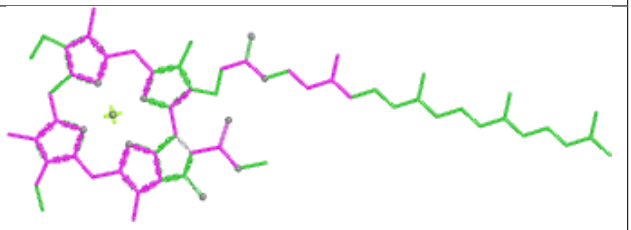


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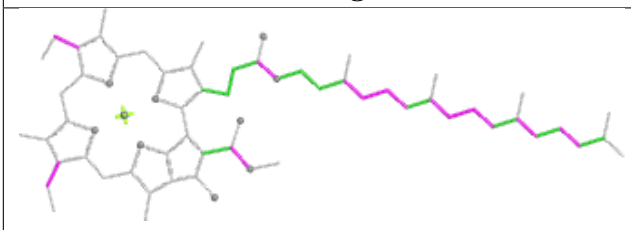
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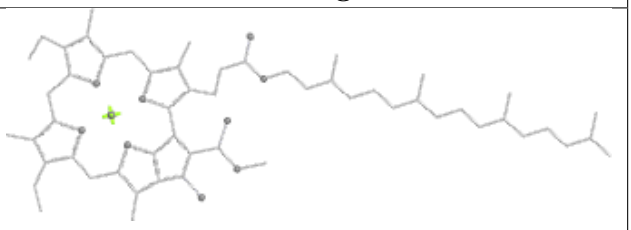
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Bond angles

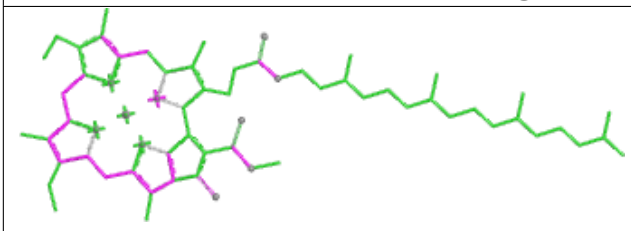


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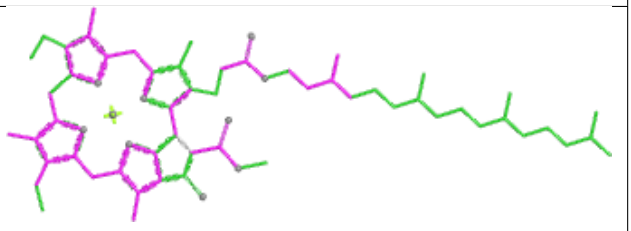


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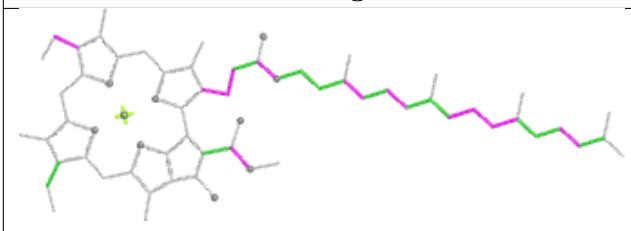
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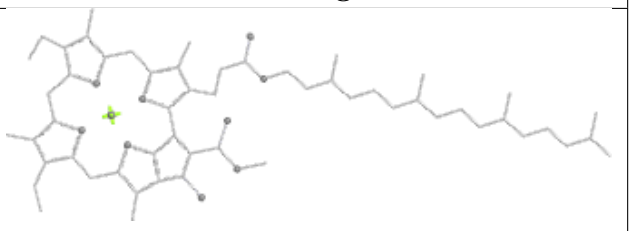
Bond lengths



Bond angles

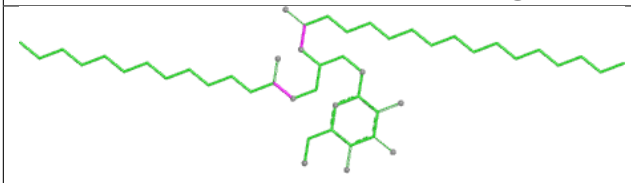


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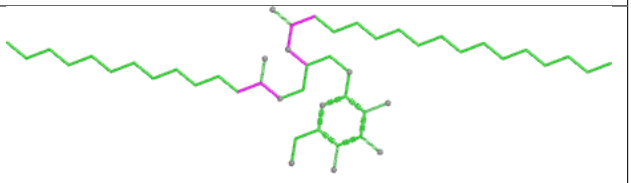


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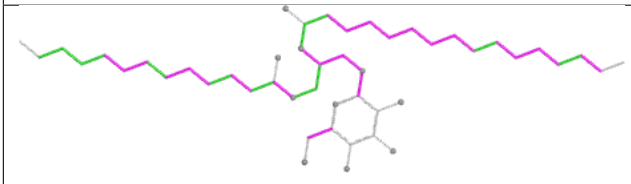
Ligand MGE D 1062



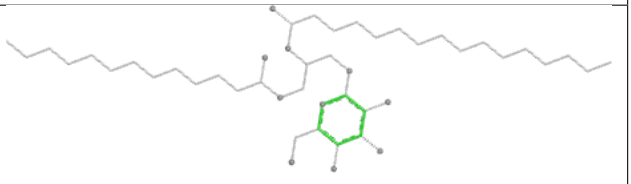
Bond lengths



Bond angles

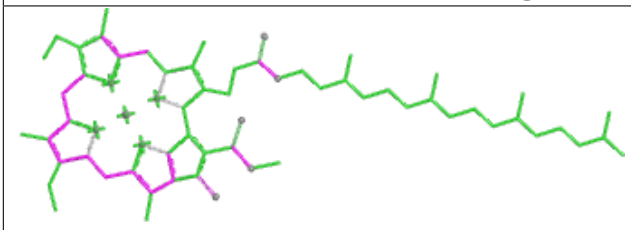


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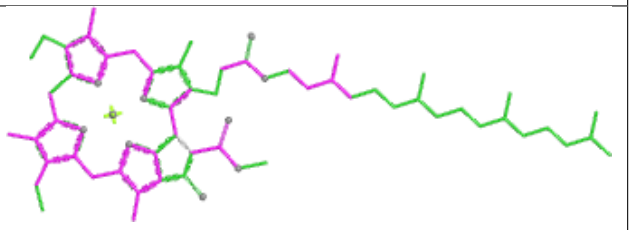


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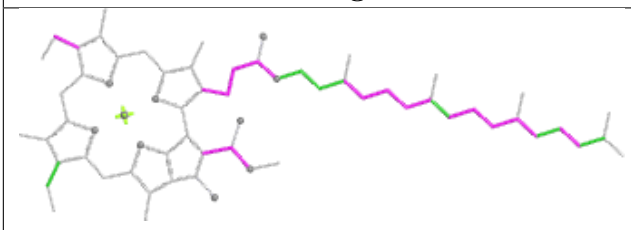
Ligand CLA h 6017



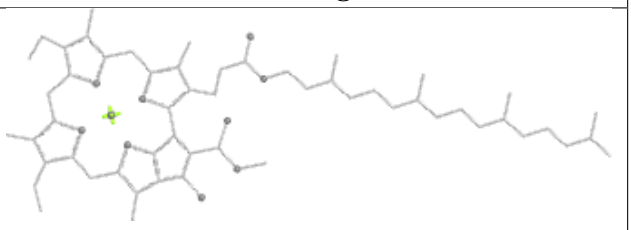
Bond lengths



Bond angles

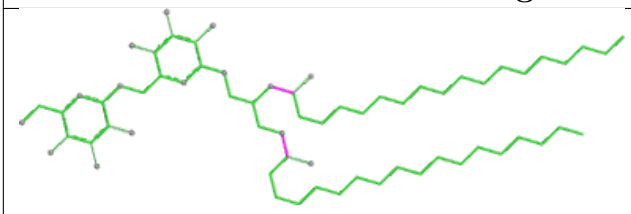


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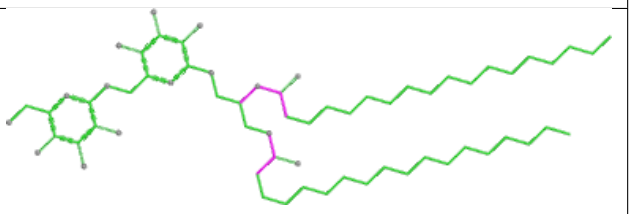


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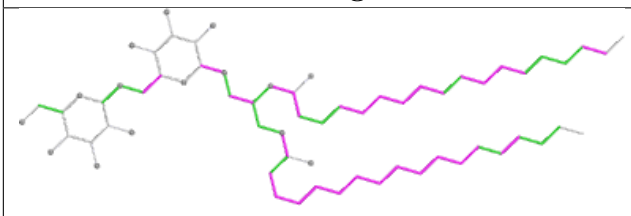
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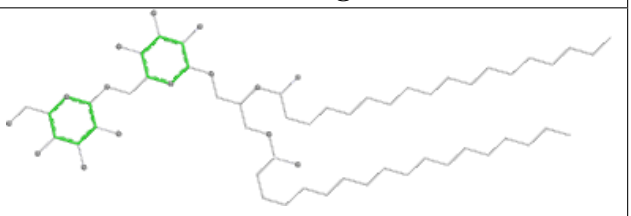
Bond lengths



Bond angles

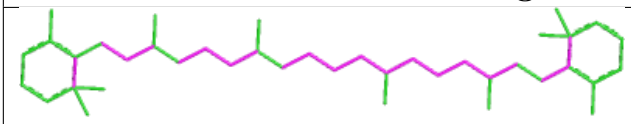


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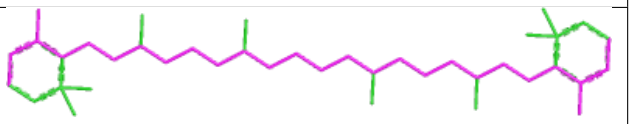


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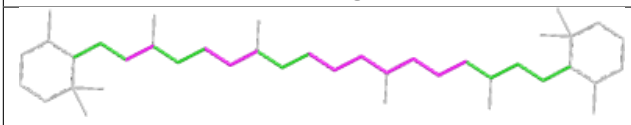
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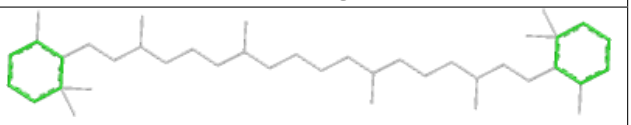
Bond lengths



Bond angles

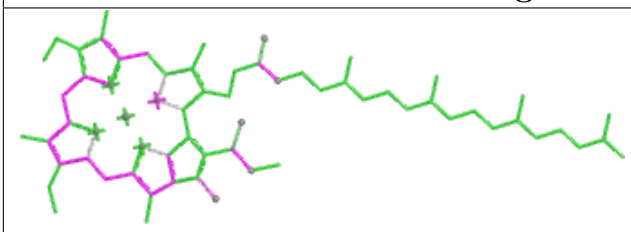


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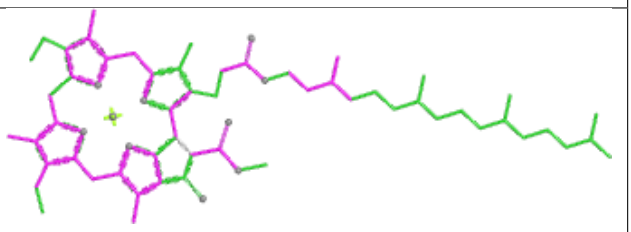


Rings

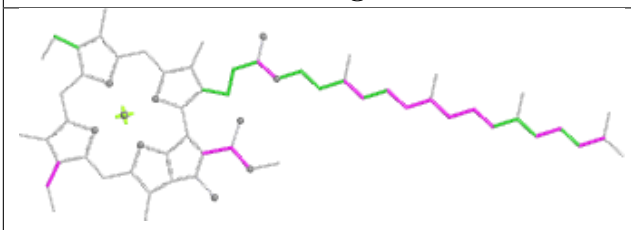
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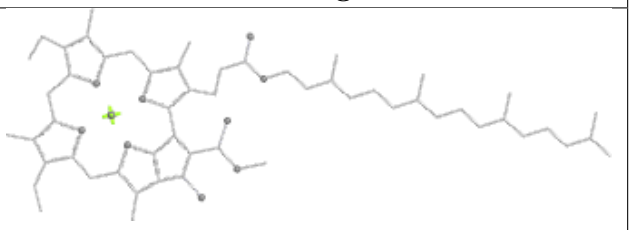
Bond lengths



Bond angles

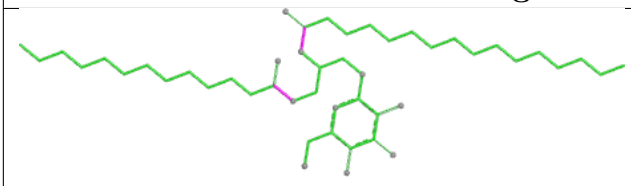


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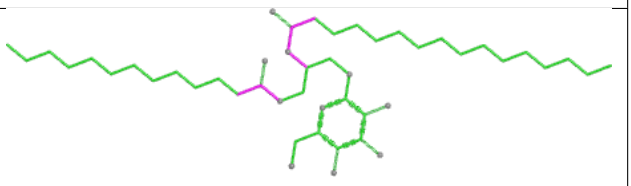


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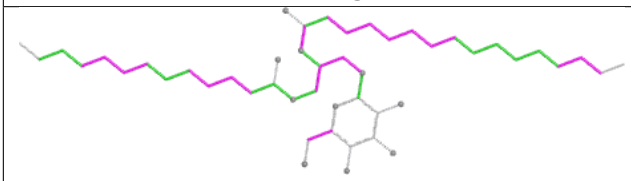
Ligand MGE d 6059



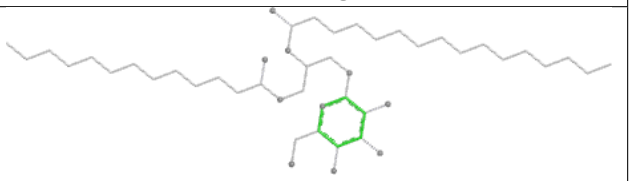
Bond lengths



Bond angles

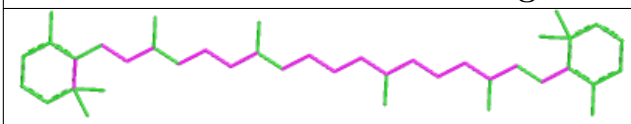


Torsions

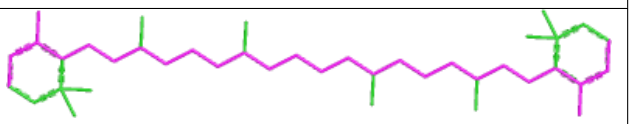


Rings

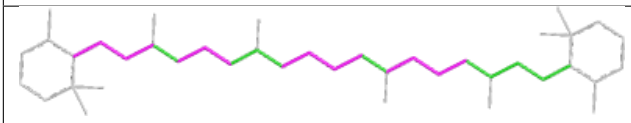
Ligand BCR c 6054



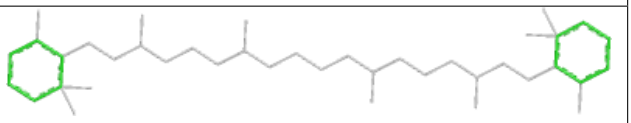
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/344 (97%)	-0.18	3 (0%) 81 64	135, 156, 186, 200	0
1	a	335/344 (97%)	-0.30	2 (0%) 85 71	135, 156, 186, 200	0
2	B	488/488 (100%)	-0.28	4 (0%) 82 65	133, 156, 180, 191	0
2	b	488/488 (100%)	-0.29	2 (0%) 88 75	133, 156, 180, 191	0
3	C	447/447 (100%)	-0.24	5 (1%) 78 60	138, 165, 181, 193	0
3	c	447/447 (100%)	-0.27	0 100 100	138, 165, 181, 193	0
4	D	340/340 (100%)	-0.24	1 (0%) 90 78	134, 156, 179, 192	0
4	d	340/340 (100%)	-0.28	1 (0%) 90 78	134, 156, 179, 192	0
5	E	82/83 (98%)	-0.35	0 100 100	153, 172, 191, 198	0
5	e	82/83 (98%)	-0.41	0 100 100	153, 172, 191, 198	0
6	F	35/44 (79%)	-0.47	0 100 100	153, 167, 187, 191	0
6	f	35/44 (79%)	-0.32	0 100 100	153, 167, 187, 191	0
7	H	64/64 (100%)	-0.36	1 (1%) 70 52	154, 163, 175, 185	0
7	h	64/64 (100%)	-0.38	0 100 100	154, 163, 175, 185	0
8	I	35/35 (100%)	-0.38	0 100 100	152, 169, 196, 201	0
8	i	35/35 (100%)	-0.18	0 100 100	152, 169, 196, 201	0
9	J	34/40 (85%)	-0.57	0 100 100	155, 162, 184, 192	0
9	j	34/40 (85%)	-0.45	0 100 100	155, 162, 184, 192	0
10	K	36/36 (100%)	-0.19	1 (2%) 55 40	144, 168, 182, 185	0
10	k	36/36 (100%)	-0.16	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%)	-0.38	0 100 100	138, 160, 191, 197	0
12	M	36/36 (100%)	-0.23	0 100 100	131, 146, 188, 194	0
12	m	36/36 (100%)	-0.29	1 (2%) 55 40	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%)	-0.38	0 100 100	139, 160, 181, 187	0
13	o	242/242 (100%)	-0.38	0 100 100	139, 160, 181, 187	0
14	T	30/30 (100%)	-0.58	0 100 100	124, 143, 186, 191	0
14	t	30/30 (100%)	-0.39	0 100 100	131, 143, 186, 191	0
15	U	98/98 (100%)	-0.46	0 100 100	139, 155, 165, 173	0
15	u	98/98 (100%)	-0.52	0 100 100	139, 155, 165, 173	0
16	V	137/137 (100%)	-0.17	3 (2%) 62 46	144, 162, 173, 178	0
16	v	137/137 (100%)	-0.33	0 100 100	144, 162, 173, 178	0
17	X	34/34 (100%)	-0.25	1 (2%) 53 39	173, 181, 198, 201	0
17	x	34/34 (100%)	-0.39	0 100 100	173, 181, 198, 201	0
18	Y	28/28 (100%)	-0.18	0 100 100	187, 199, 208, 210	0
18	y	28/28 (100%)	-0.27	0 100 100	187, 199, 208, 210	0
19	N	0/23	-	-	-	-
19	n	0/23	-	-	-	-
20	Z	62/62 (100%)	-0.45	0 100 100	159, 173, 188, 196	0
20	z	62/62 (100%)	-0.33	1 (1%) 70 52	159, 173, 188, 196	0
All	All	5200/5296 (98%)	-0.30	26 (0%) 87 73	124, 161, 185, 210	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	ARG	6.3
1	a	5279	ARG	6.1
3	C	44	ASN	3.9
2	B	166	MET	3.2
3	C	45	LEU	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 oligosaccharides 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
27	IOD	D	1068	1/1	0.20	0.60	198,198,198,198	0
27	IOD	B	1067	1/1	0.47	0.43	198,198,198,198	0
22	CLA	K	1034	65/65	0.56	0.18	138,189,216,216	0
26	LHG	a	6063	49/49	0.57	0.19	199,213,216,216	0
22	CLA	B	1009	65/65	0.57	0.17	143,192,213,213	0
26	LHG	A	1063	49/49	0.57	0.20	199,213,216,216	0
22	CLA	k	6034	65/65	0.63	0.18	138,189,216,216	0
25	BCR	T	6048	40/40	0.63	0.16	179,184,203,204	0
27	IOD	b	6067	1/1	0.67	0.42	199,199,199,199	0
25	BCR	A	1044	40/40	0.70	0.18	155,177,185,185	0
25	BCR	B	1048	40/40	0.70	0.16	179,184,203,204	0
25	BCR	b	6047	40/40	0.71	0.13	155,171,200,202	0
22	CLA	b	6009	65/65	0.71	0.14	143,192,213,213	0
22	CLA	c	6037	65/65	0.71	0.13	201,211,214,216	0
22	CLA	c	6027	65/65	0.72	0.17	192,198,204,216	0
29	DGD	C	1056	66/66	0.72	0.14	190,201,216,216	0
27	IOD	T	1066	1/1	0.73	0.23	199,199,199,199	0
22	CLA	C	1027	65/65	0.73	0.19	192,198,204,216	0
25	BCR	c	6054	40/40	0.73	0.19	197,201,216,216	0
25	BCR	k	6052	40/40	0.75	0.27	191,195,202,203	0
27	IOD	d	6068	1/1	0.75	0.39	199,199,199,199	0
22	CLA	d	6008	65/65	0.75	0.16	184,188,216,216	0
25	BCR	Z	1053	40/40	0.76	0.15	190,214,216,216	0
22	CLA	c	6026	65/65	0.77	0.16	138,171,178,183	0
25	BCR	z	6053	40/40	0.77	0.13	190,214,216,216	0
25	BCR	b	6045	40/40	0.77	0.19	163,196,216,216	0
25	BCR	C	1054	40/40	0.77	0.22	197,201,216,216	0
28	MGE	d	6062	48/48	0.77	0.19	187,202,208,210	0
25	BCR	B	1047	40/40	0.77	0.13	155,171,200,202	0
29	DGD	c	6056	66/66	0.77	0.12	190,201,216,216	0
22	CLA	b	6014	65/65	0.78	0.16	178,187,197,216	0
28	MGE	B	1060	48/48	0.79	0.20	186,199,213,216	0
28	MGE	D	1059	48/48	0.79	0.16	179,190,215,216	0
25	BCR	T	6046	40/40	0.79	0.15	179,185,188,189	0
22	CLA	C	1037	65/65	0.79	0.13	201,211,214,216	0
25	BCR	d	6050	40/40	0.79	0.17	184,193,198,199	0
22	CLA	B	1014	65/65	0.80	0.14	178,187,197,216	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	MGE	d	6059	48/48	0.80	0.15	179,190,215,216	0
25	BCR	h	6049	40/40	0.80	0.17	177,182,188,189	0
25	BCR	D	1050	40/40	0.80	0.18	184,193,198,199	0
25	BCR	K	1051	40/40	0.80	0.23	192,202,210,210	0
25	BCR	a	6044	40/40	0.81	0.15	155,177,185,185	0
24	PQ9	A	1043	45/45	0.81	0.26	171,172,193,197	30
22	CLA	b	6021	65/65	0.81	0.15	154,164,172,176	0
28	MGE	b	6060	48/48	0.82	0.19	186,199,213,216	0
22	CLA	d	6005	65/65	0.82	0.17	135,162,169,173	0
24	PQ9	d	6042	45/45	0.82	0.24	171,173,185,187	0
28	MGE	l	6061	48/48	0.82	0.17	177,191,195,199	0
22	CLA	c	6035	65/65	0.82	0.19	189,202,210,216	0
29	DGD	C	1057	66/66	0.82	0.15	177,190,206,207	0
22	CLA	C	1030	65/65	0.82	0.13	185,197,216,216	0
29	DGD	c	6057	66/66	0.82	0.15	177,190,206,207	0
22	CLA	B	1021	65/65	0.83	0.12	154,164,172,176	0
23	PHO	D	1039	64/64	0.83	0.16	184,187,196,198	0
22	CLA	D	1005	65/65	0.83	0.15	135,162,169,173	0
28	MGE	L	1061	48/48	0.83	0.19	177,191,195,199	0
22	CLA	b	6015	65/65	0.84	0.13	177,182,185,216	0
25	BCR	H	1049	40/40	0.84	0.17	177,182,188,189	0
29	DGD	c	6055	66/66	0.84	0.17	184,192,202,203	0
28	MGE	D	1062	48/48	0.84	0.19	187,202,208,210	0
22	CLA	C	1036	65/65	0.84	0.14	186,190,203,216	0
25	BCR	B	1045	40/40	0.85	0.15	163,196,216,216	0
22	CLA	C	1026	65/65	0.85	0.16	138,171,178,183	0
25	BCR	k	6051	40/40	0.85	0.18	192,202,210,210	0
22	CLA	b	6024	65/65	0.85	0.13	165,193,197,198	0
22	CLA	c	6025	65/65	0.85	0.11	156,187,191,194	0
22	CLA	c	6036	65/65	0.85	0.12	186,190,203,216	0
24	PQ9	a	6043	45/45	0.86	0.23	171,172,193,197	30
22	CLA	C	1028	65/65	0.86	0.15	178,182,201,202	0
22	CLA	c	6032	65/65	0.86	0.14	186,189,200,216	0
22	CLA	B	1024	65/65	0.87	0.12	165,193,197,198	0
22	CLA	b	6019	65/65	0.87	0.12	167,172,175,180	0
29	DGD	C	1055	66/66	0.87	0.19	184,192,202,203	0
22	CLA	a	6007	65/65	0.87	0.17	129,174,204,205	0
22	CLA	C	1025	65/65	0.88	0.12	156,187,191,194	0
25	BCR	t	1046	40/40	0.88	0.12	179,185,188,189	0
29	DGD	B	1058	66/66	0.88	0.20	175,188,196,203	0
22	CLA	C	1032	65/65	0.88	0.16	184,188,192,216	0
22	CLA	b	6012	65/65	0.88	0.14	160,167,172,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PHO	a	6038	64/64	0.88	0.14	166,176,178,181	0
29	DGD	b	6058	66/66	0.88	0.20	175,188,196,203	0
23	PHO	d	6039	64/64	0.88	0.12	184,187,196,198	0
22	CLA	C	1029	65/65	0.88	0.14	177,187,190,201	0
25	BCR	C	1052	40/40	0.88	0.29	191,195,202,203	0
22	CLA	a	6003	65/65	0.89	0.17	160,169,175,212	0
22	CLA	c	6031	65/65	0.89	0.16	181,185,202,216	0
22	CLA	b	6022	65/65	0.89	0.13	138,180,198,200	0
22	CLA	D	1008	65/65	0.89	0.13	184,188,216,216	0
22	CLA	B	1011	65/65	0.89	0.12	168,178,184,188	0
22	CLA	b	6011	65/65	0.89	0.15	168,178,184,188	0
31	HEM	f	6040	43/43	0.89	0.20	186,215,216,216	0
22	CLA	a	6006	65/65	0.90	0.11	166,181,211,213	0
24	PQ9	D	1042	45/45	0.90	0.19	171,173,185,187	0
22	CLA	c	6028	65/65	0.90	0.13	178,182,201,202	0
22	CLA	c	6029	65/65	0.90	0.13	177,187,190,201	0
22	CLA	h	6017	65/65	0.90	0.14	169,197,201,208	0
22	CLA	B	1019	65/65	0.90	0.13	167,172,175,180	0
23	PHO	A	1038	64/64	0.90	0.13	166,176,178,181	0
22	CLA	A	1006	65/65	0.90	0.14	166,181,211,213	0
22	CLA	b	6016	65/65	0.90	0.12	130,172,175,180	0
22	CLA	C	1035	65/65	0.90	0.18	189,202,210,216	0
22	CLA	B	1023	65/65	0.91	0.11	174,179,181,191	0
22	CLA	c	6030	65/65	0.91	0.10	185,197,216,216	0
22	CLA	B	1012	65/65	0.91	0.11	160,167,172,174	0
22	CLA	A	1007	65/65	0.91	0.14	129,174,204,205	0
22	CLA	B	1022	65/65	0.91	0.11	138,180,198,200	0
22	CLA	A	1003	65/65	0.92	0.14	160,169,175,212	0
22	CLA	C	1031	65/65	0.92	0.14	181,185,202,216	0
22	CLA	B	1015	65/65	0.92	0.12	177,182,185,216	0
22	CLA	c	6033	65/65	0.92	0.14	138,185,199,200	0
22	CLA	C	1033	65/65	0.92	0.16	138,185,199,200	0
22	CLA	H	1017	65/65	0.92	0.15	169,197,201,208	0
27	IOD	t	6066	1/1	0.92	0.08	199,199,199,199	0
22	CLA	B	1010	65/65	0.92	0.15	160,183,186,189	0
22	CLA	b	6018	65/65	0.93	0.14	172,186,191,192	0
22	CLA	b	6010	65/65	0.93	0.12	160,183,186,189	0
22	CLA	b	6020	65/65	0.93	0.15	167,175,180,197	0
22	CLA	D	1004	65/65	0.93	0.15	130,168,179,181	0
22	CLA	B	1016	65/65	0.93	0.12	130,172,175,180	0
30	FE2	a	6002	1/1	0.93	0.14	148,148,148,148	0
31	HEM	F	1040	43/43	0.93	0.17	186,215,216,216	0

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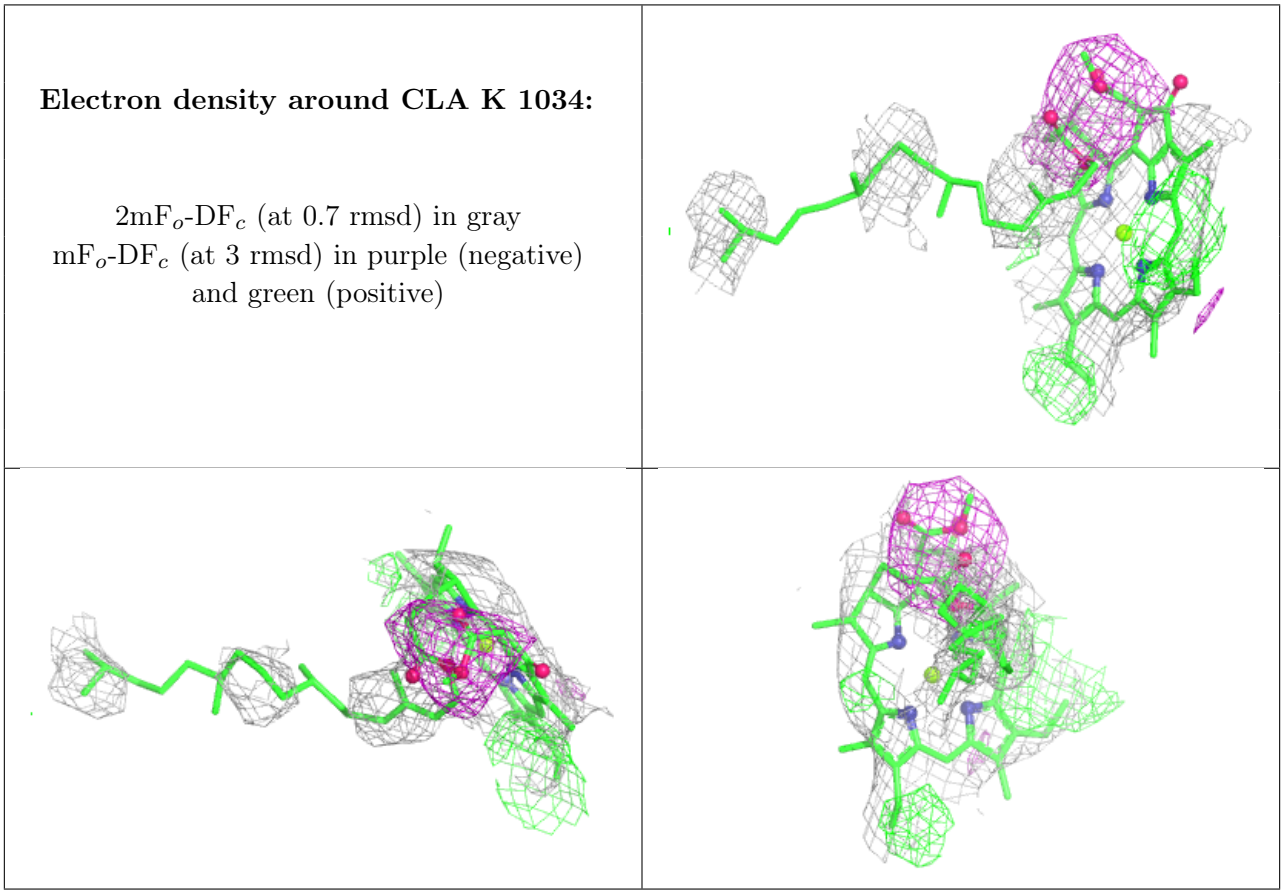
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CLA	b	6023	65/65	0.93	0.11	174,179,181,191	0
22	CLA	b	6013	65/65	0.94	0.17	146,173,183,184	0
22	CLA	B	1018	65/65	0.94	0.13	172,186,191,192	0
31	HEM	V	1041	43/43	0.94	0.23	131,181,185,187	0
22	CLA	B	1013	65/65	0.94	0.14	146,173,183,184	0
31	HEM	v	6041	43/43	0.94	0.15	131,181,185,187	0
30	FE2	D	1002	1/1	0.95	0.09	148,148,148,148	0
22	CLA	d	6004	65/65	0.95	0.13	130,168,179,181	0
27	IOD	a	6065	1/1	0.96	0.06	158,158,158,158	0
22	CLA	B	1020	65/65	0.96	0.13	167,175,180,197	0
21	OEC	a	6001	5/9	0.98	0.09	132,148,162,172	0
27	IOD	A	1065	1/1	0.98	0.04	158,158,158,158	0
21	OEC	A	1001	5/9	0.98	0.07	132,148,162,172	0
27	IOD	D	1064	1/1	0.98	0.03	160,160,160,160	0
27	IOD	d	6064	1/1	0.99	0.04	160,160,160,160	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.

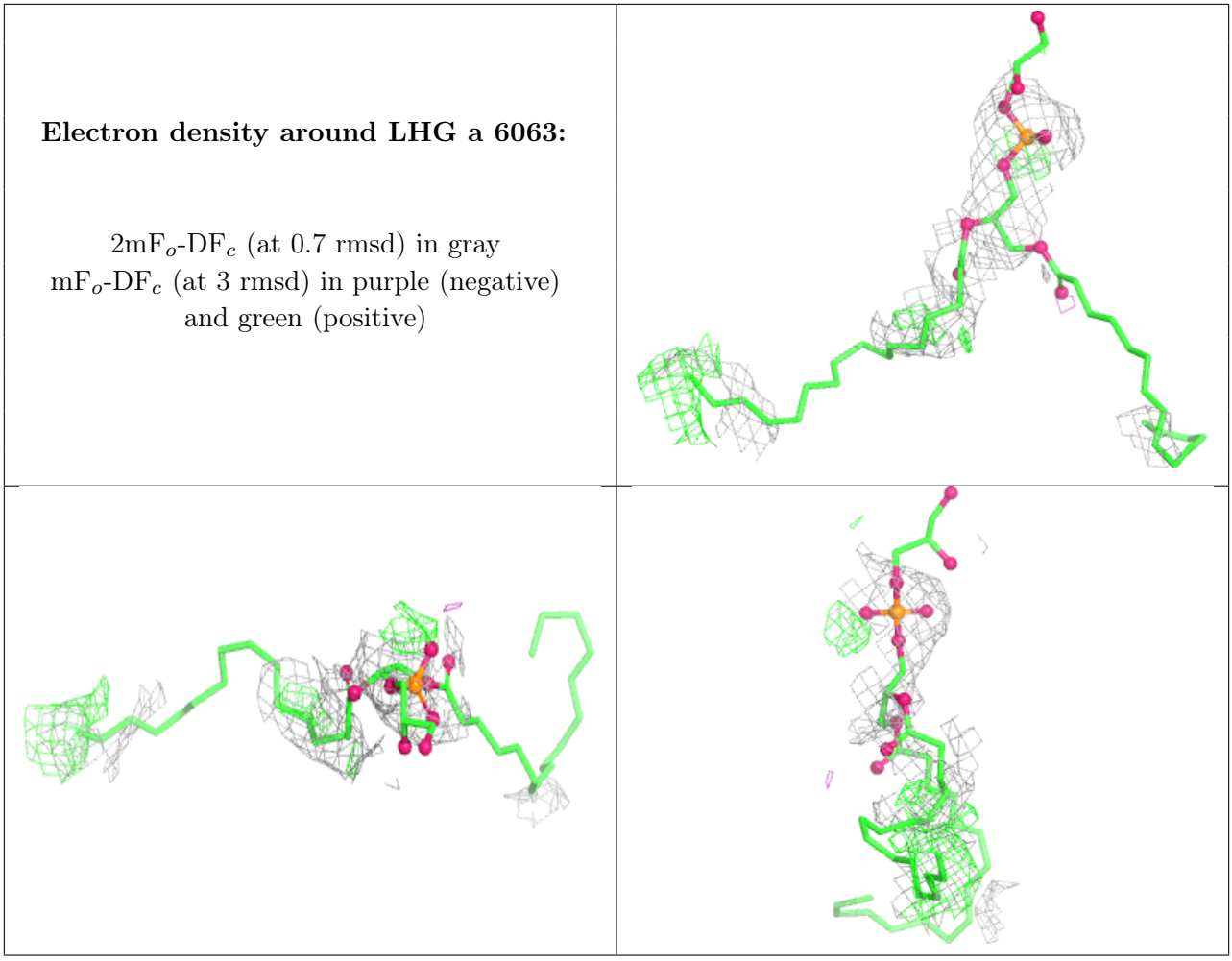
Electron density around CLA K 1034:

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



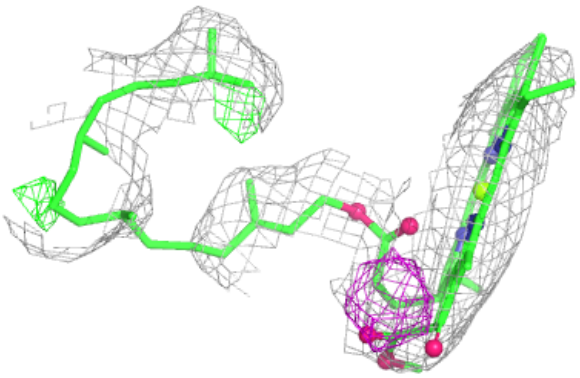
Electron density around LHG a 6063:

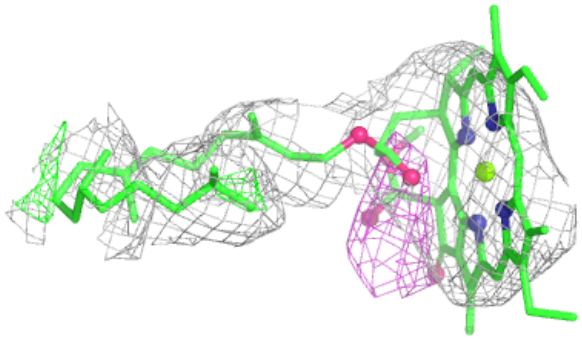
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

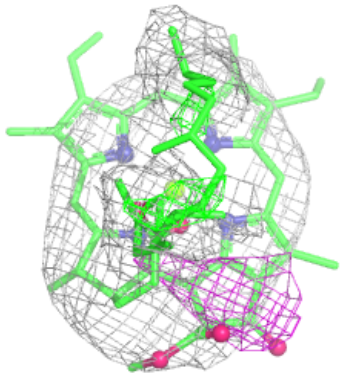


Electron density around CLA B 1009:

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

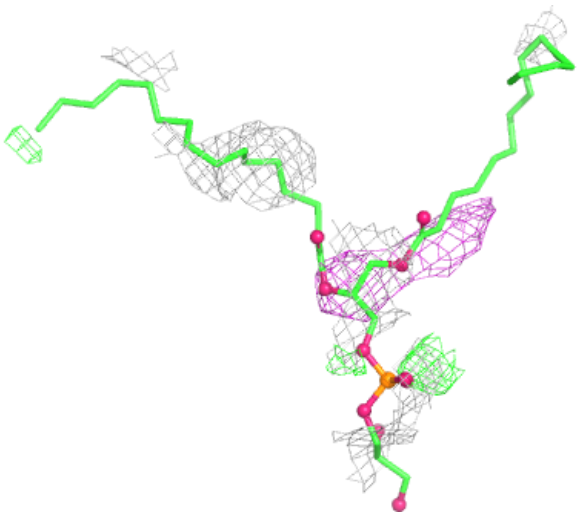


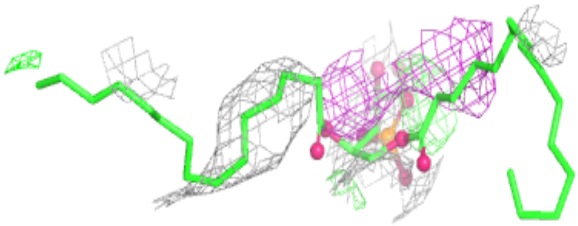


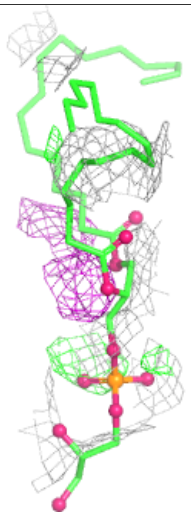


Electron density around LHG A 1063:

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

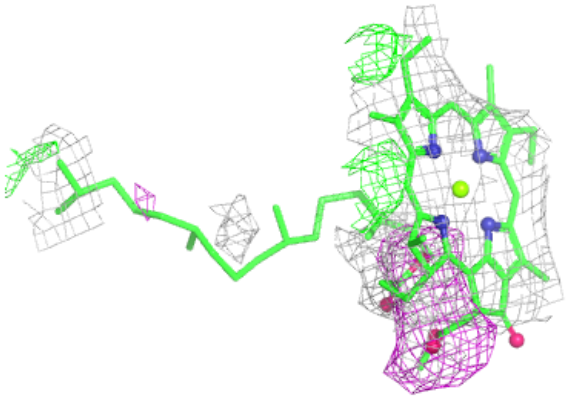


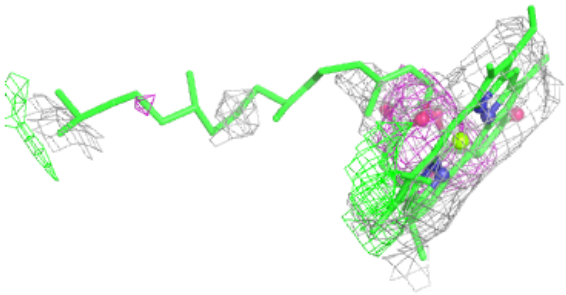


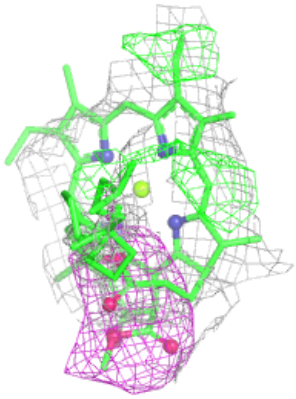


Electron density around CLA k 6034:

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

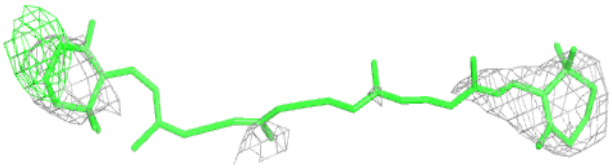




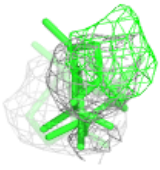


Electron density around BCR T 6048:

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

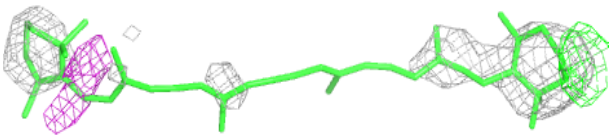


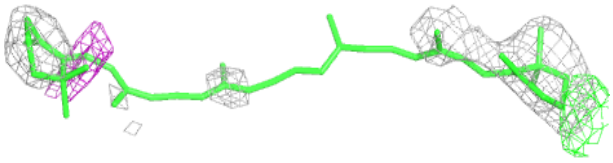


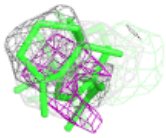


Electron density around BCR A 1044:

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

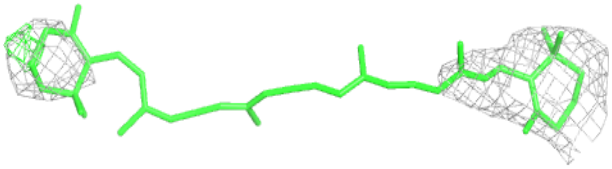


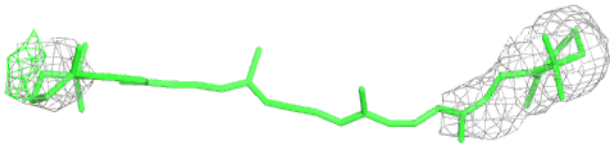


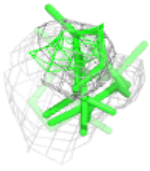


Electron density around BCR B 1048:

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

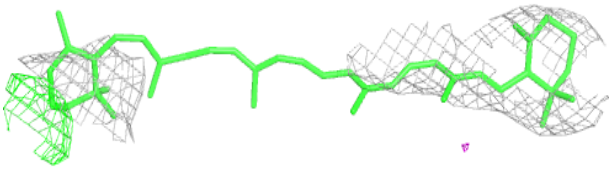


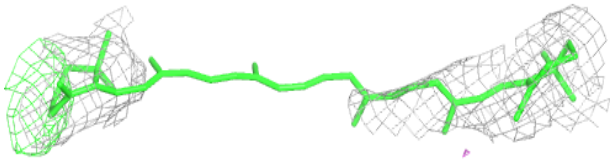


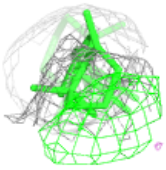


Electron density around BCR b 6047:

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

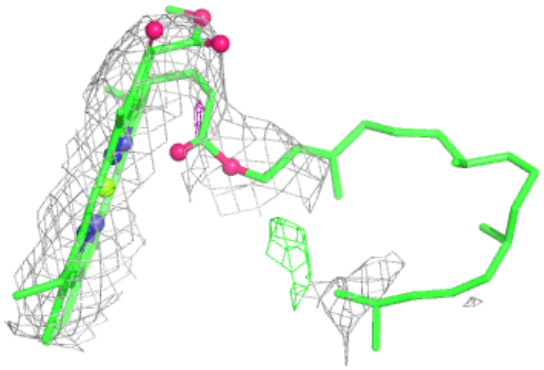


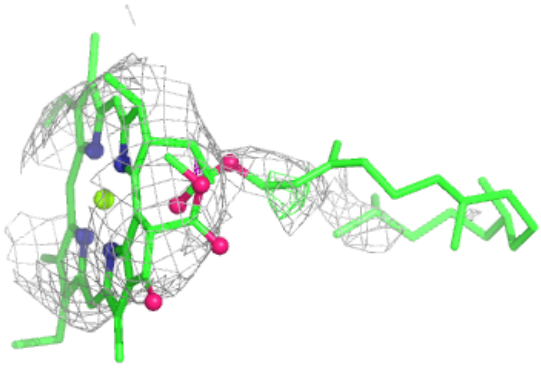


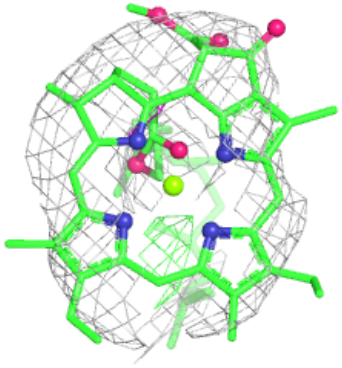


Electron density around CLA b 6009:

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

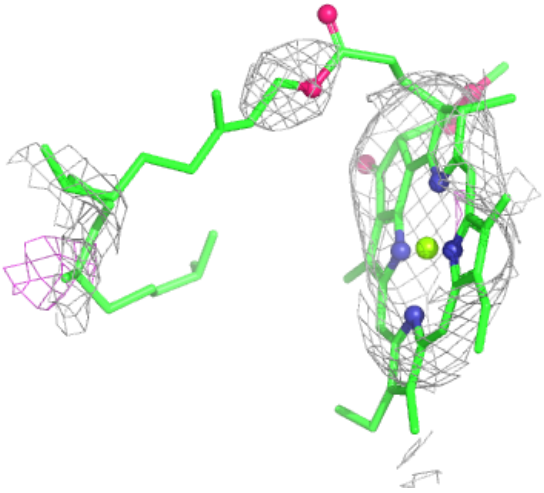


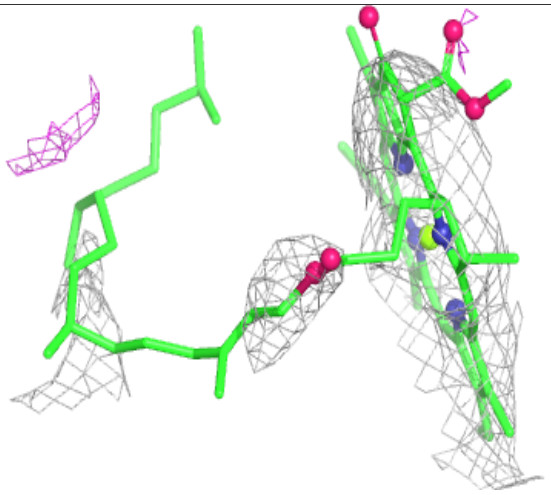


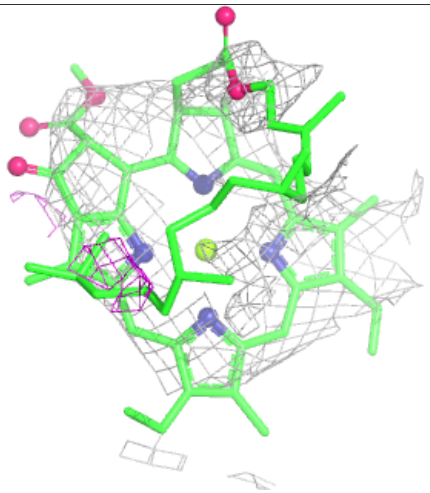


Electron density around CLA c 6037:

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

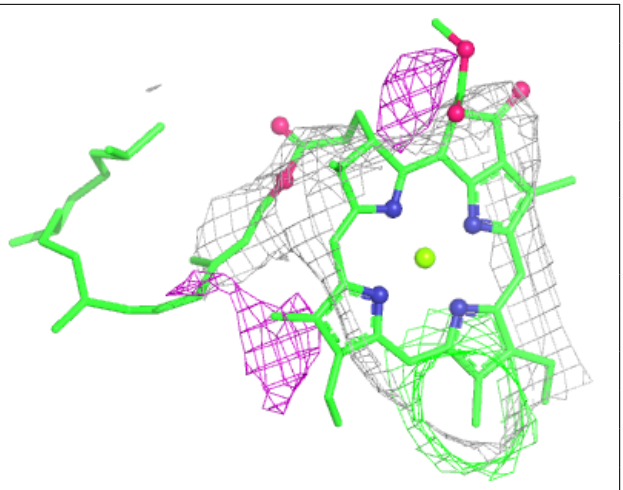


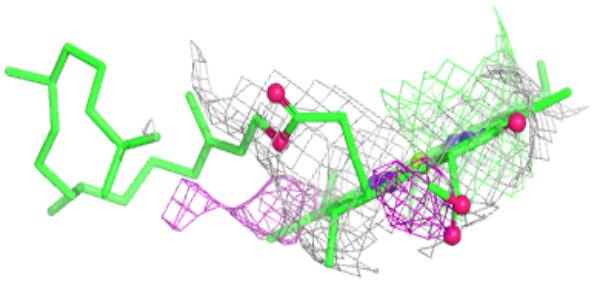


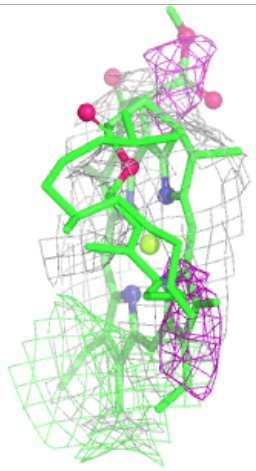


Electron density around CLA c 6027:

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

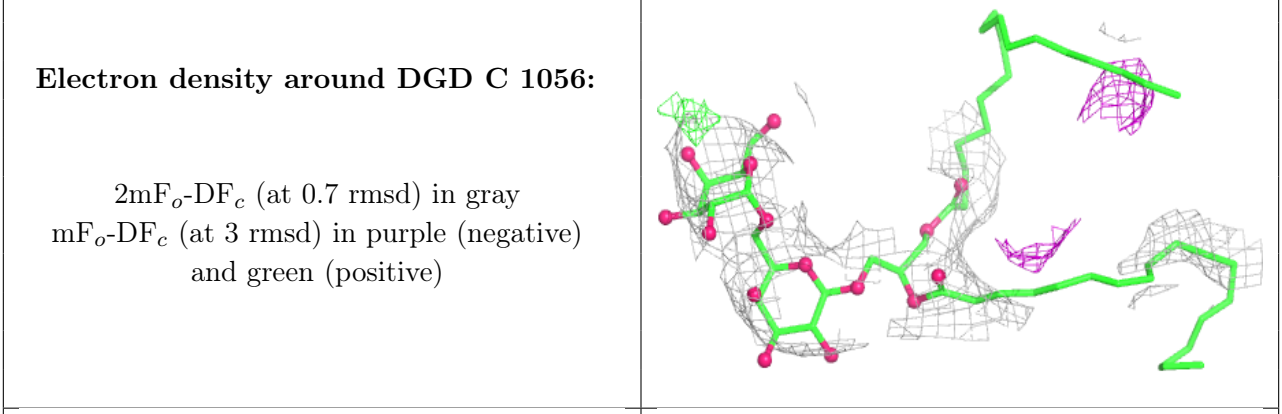






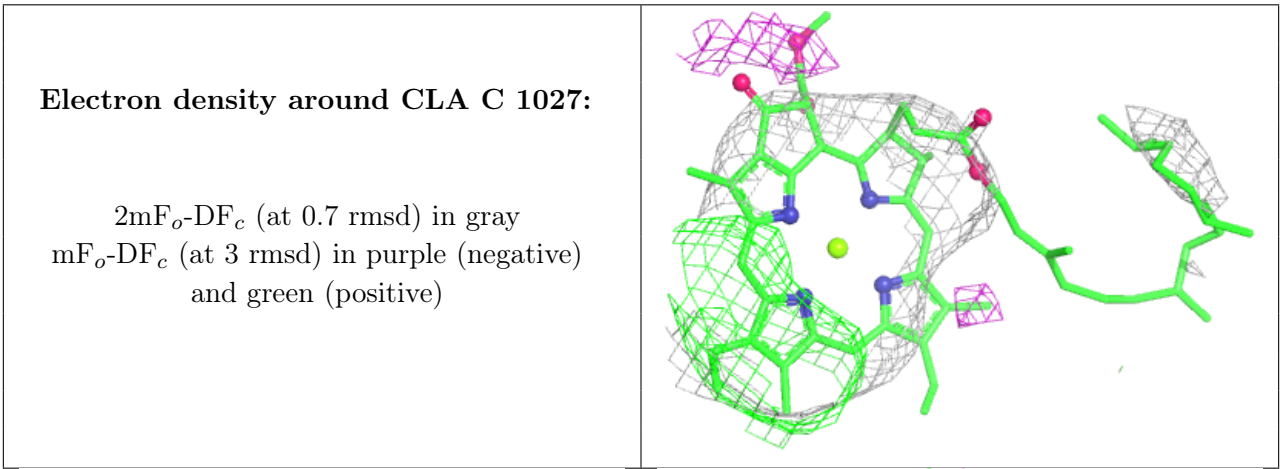
Electron density around DGD C 1056:

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



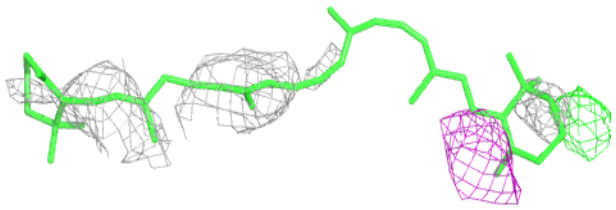
Electron density around CLA C 1027:

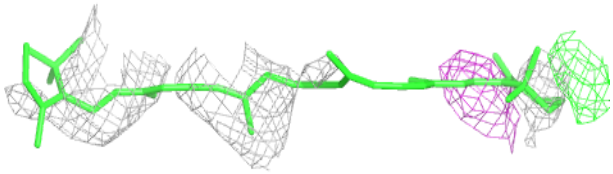
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

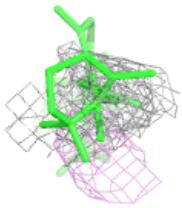


Electron density around BCR c 6054:

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

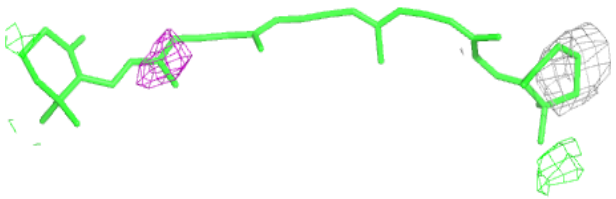


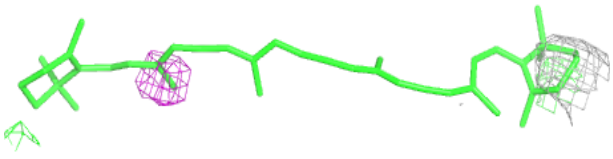


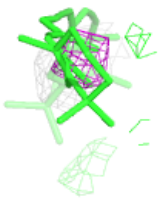


Electron density around BCR k 6052:

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

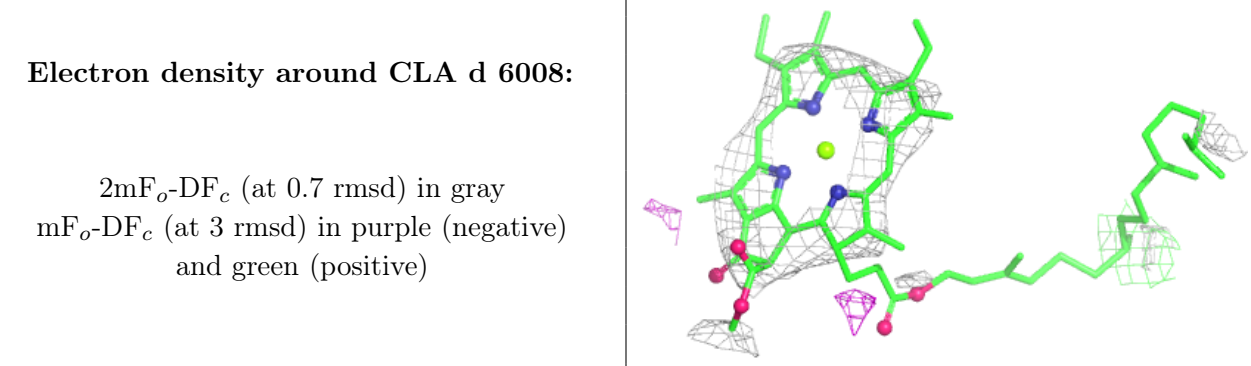


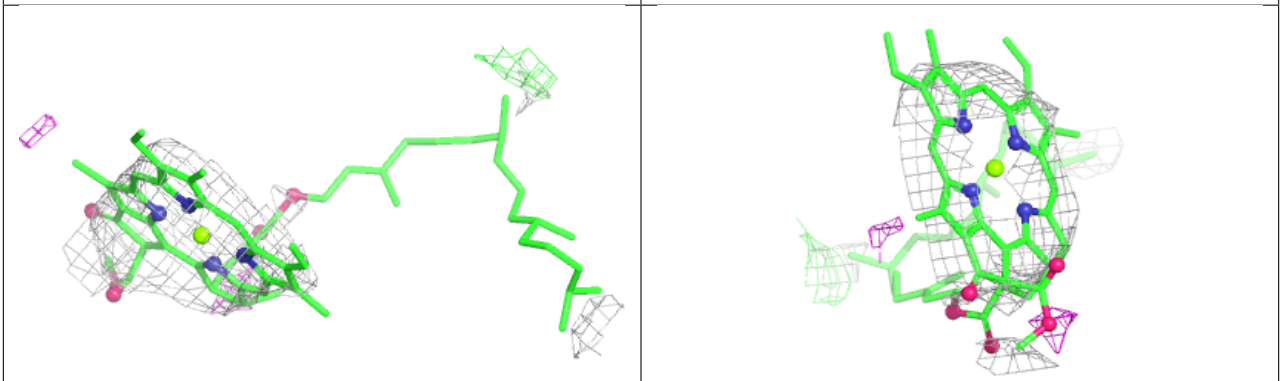




Electron density around CLA d 6008:

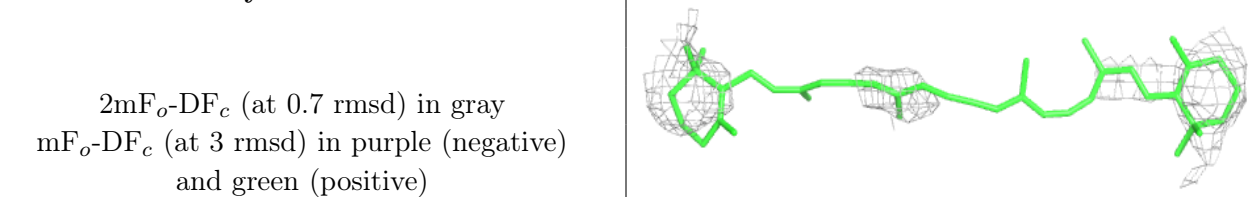
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

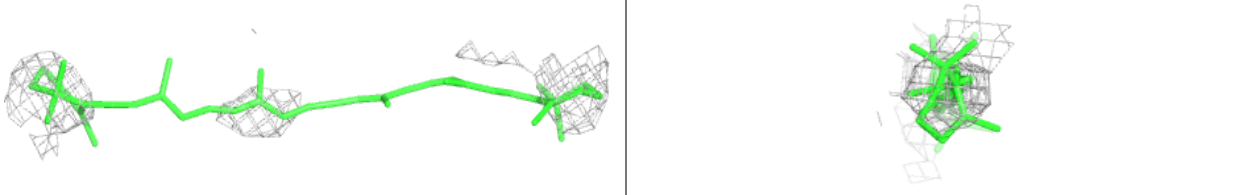




Electron density around BCR Z 1053:

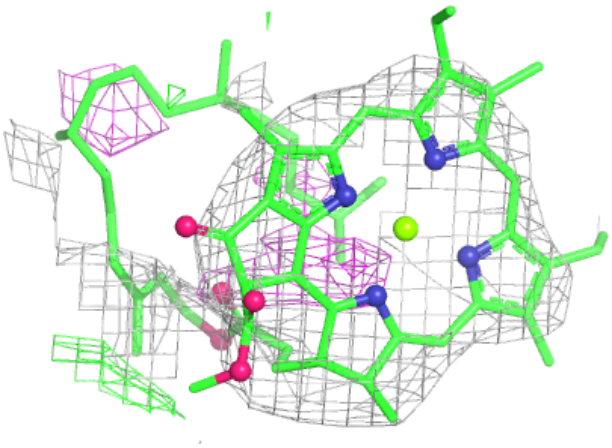
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

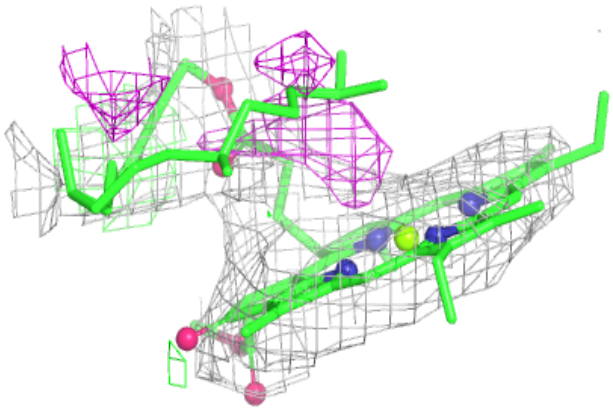


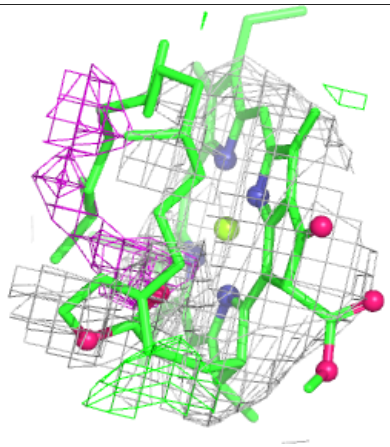


Electron density around CLA c 6026:

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

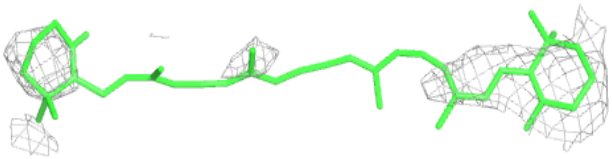


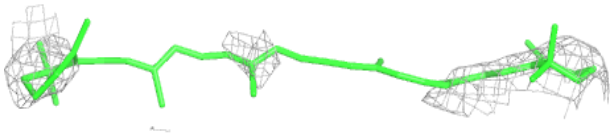


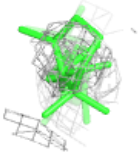


Electron density around BCR z 6053:

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

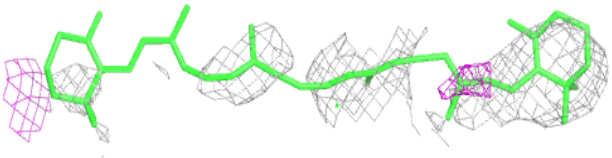


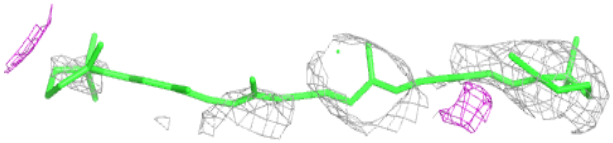


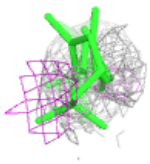


Electron density around BCR b 6045:

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



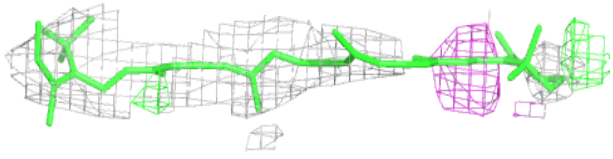


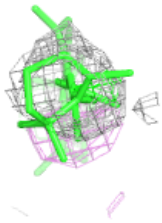


Electron density around BCR C 1054:

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

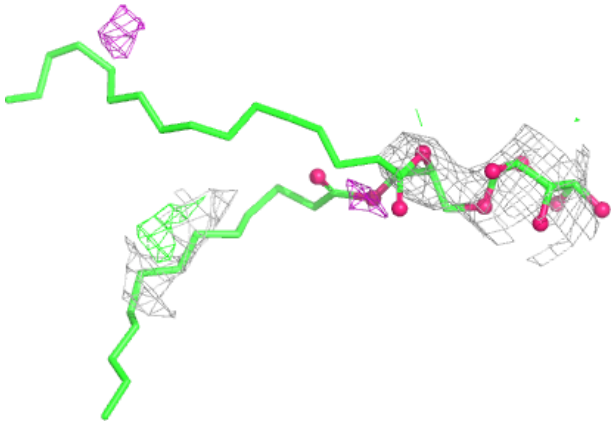


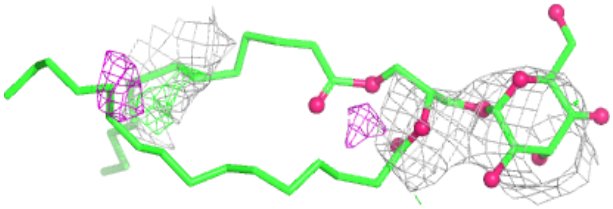


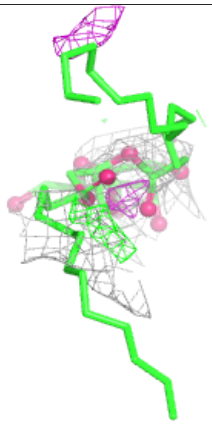


Electron density around MGE d 6062:

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

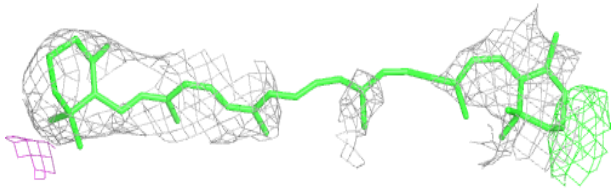


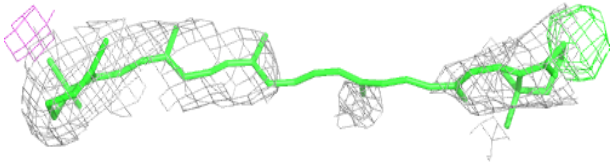


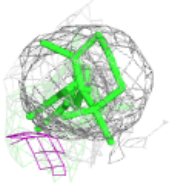


Electron density around BCR B 1047:

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

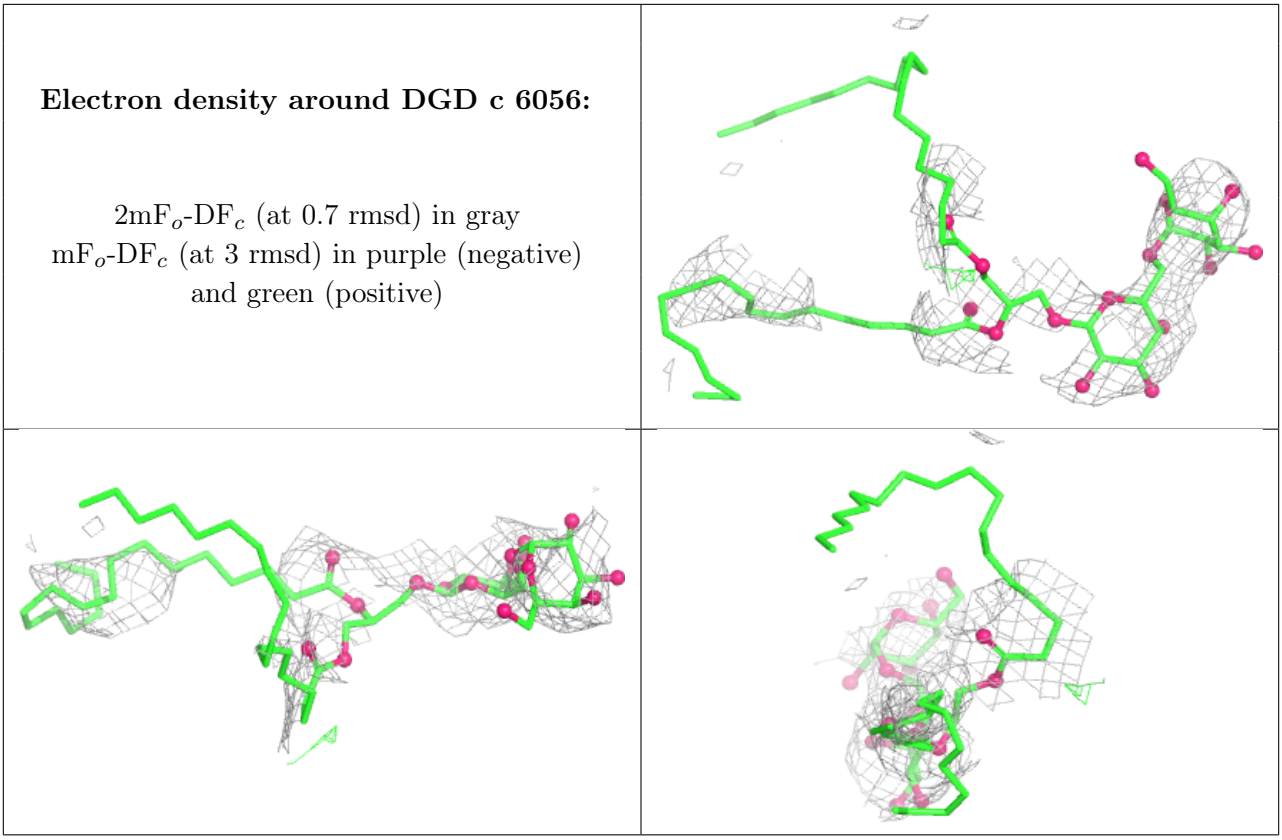






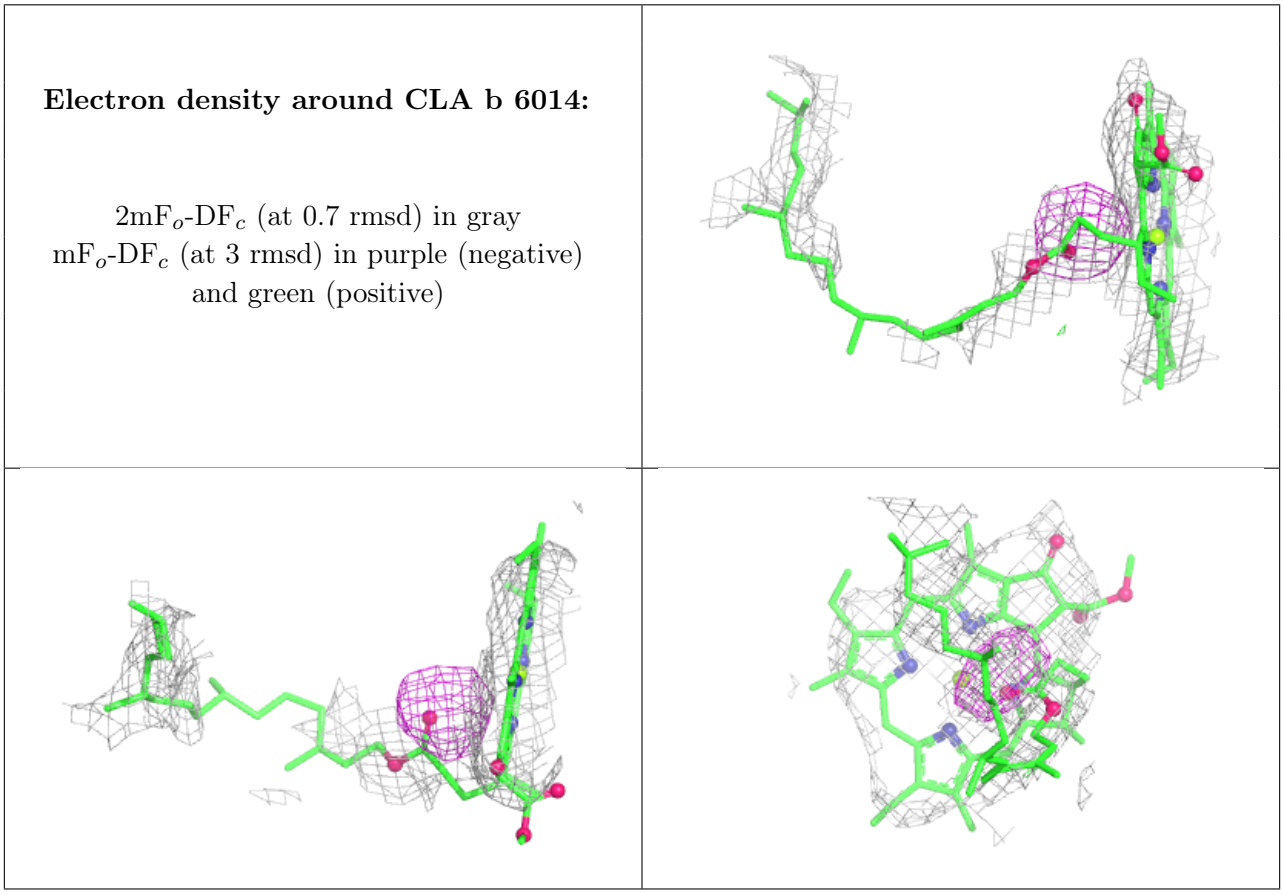
Electron density around DGD c 6056:

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



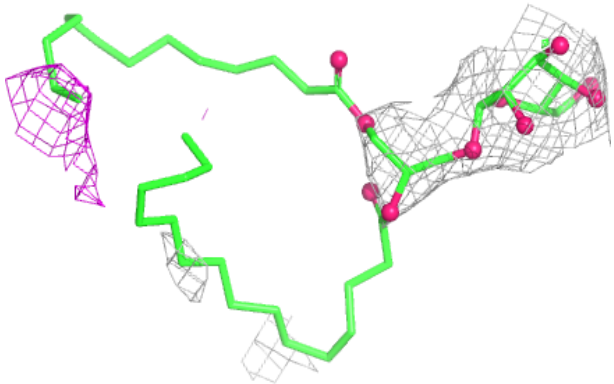
Electron density around CLA b 6014:

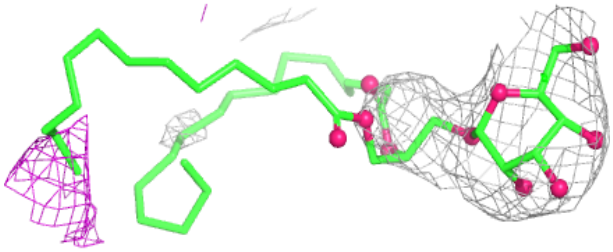
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 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)

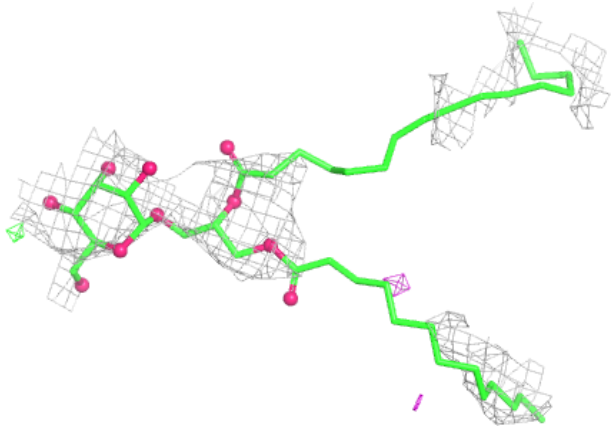


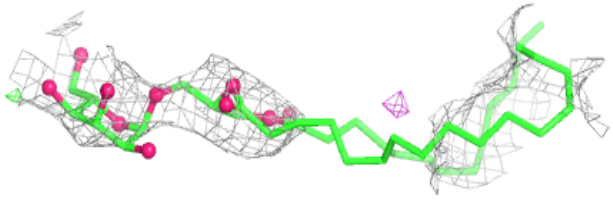


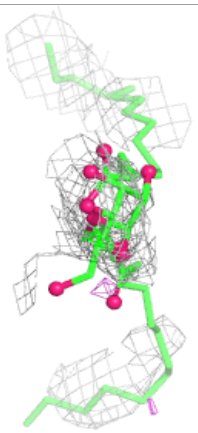


Electron density around MGE D 1059:

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

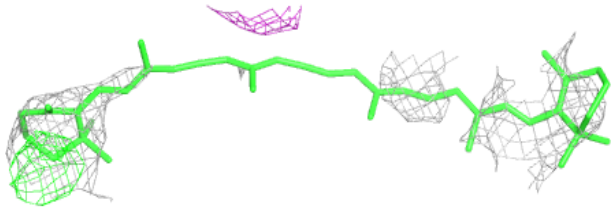


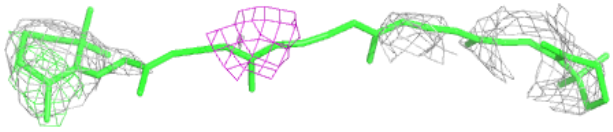


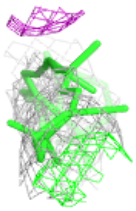


Electron density around BCR T 6046:

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

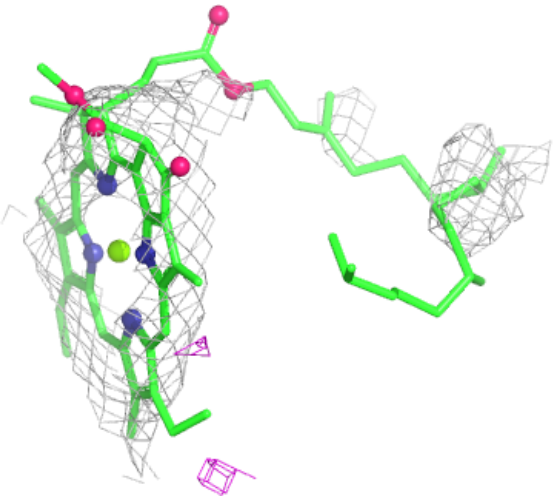


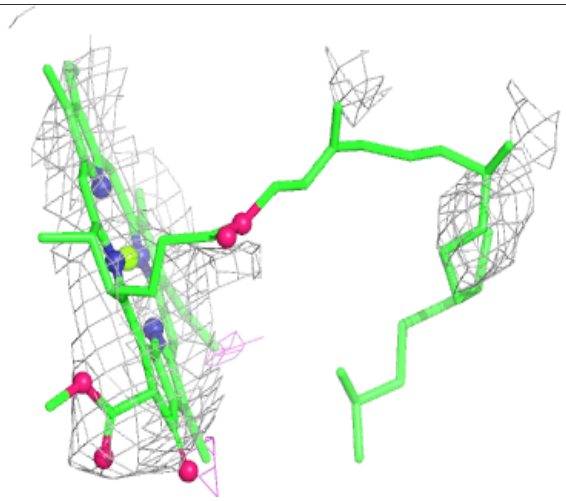


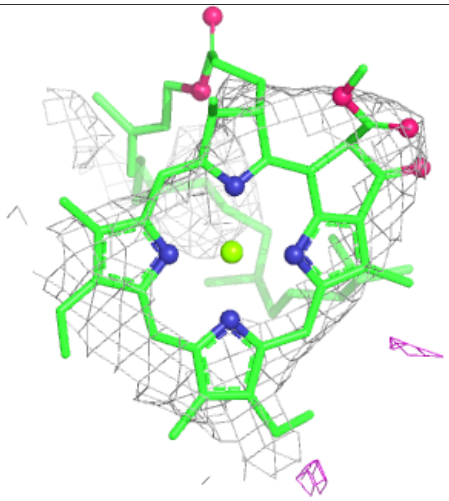


Electron density around CLA C 1037:

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

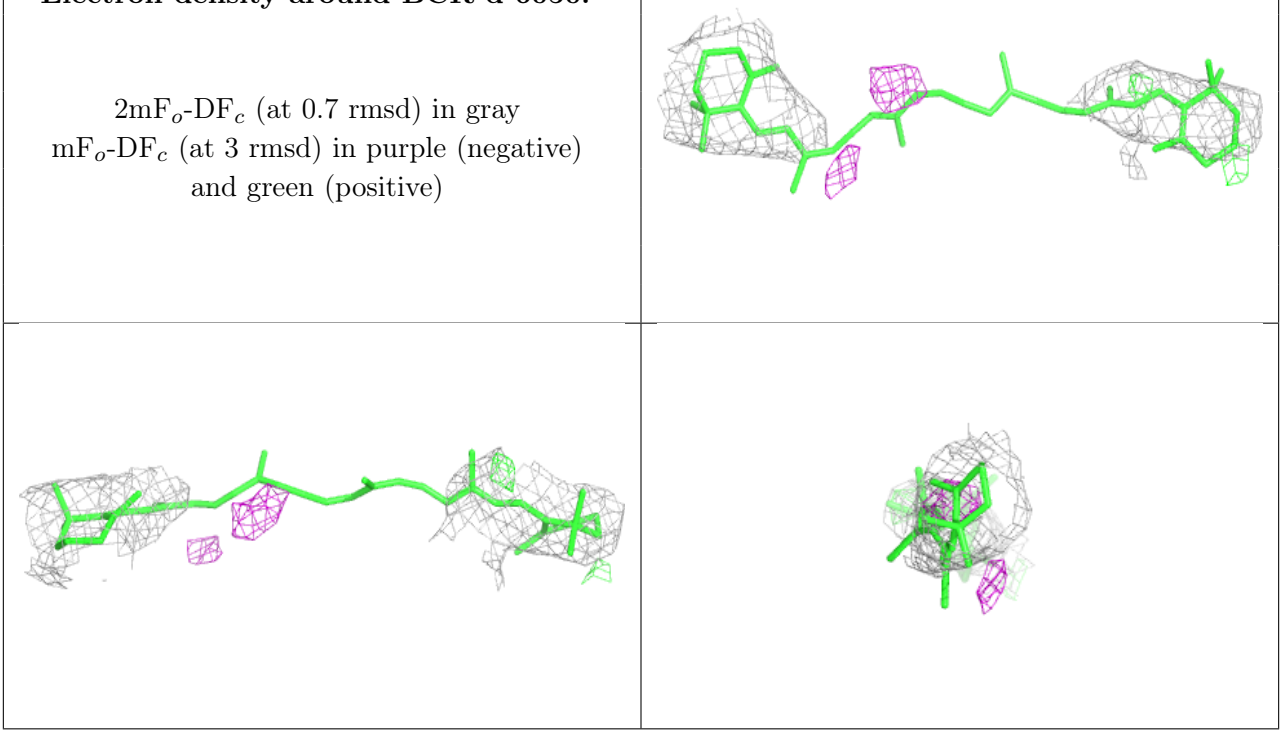






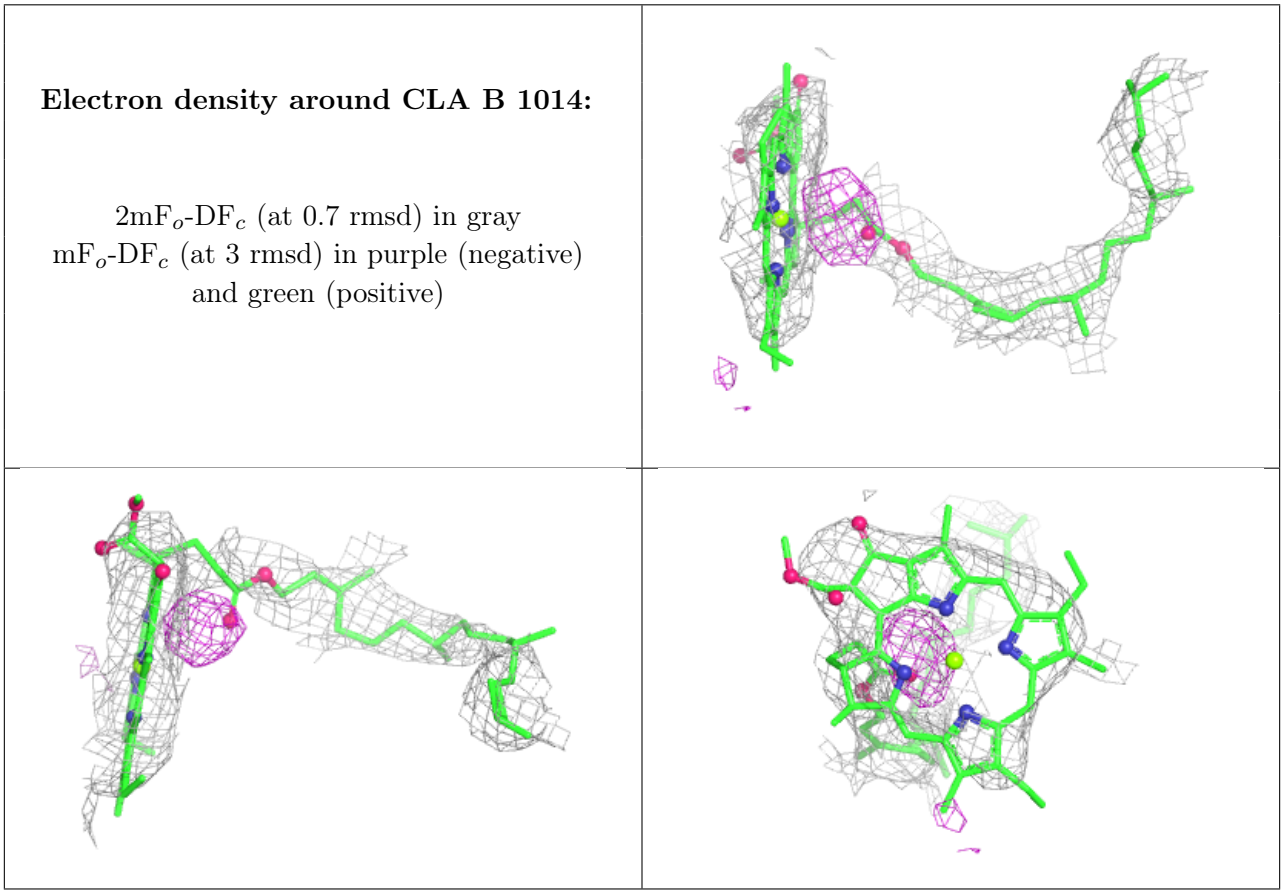
Electron density around BCR d 6050:

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



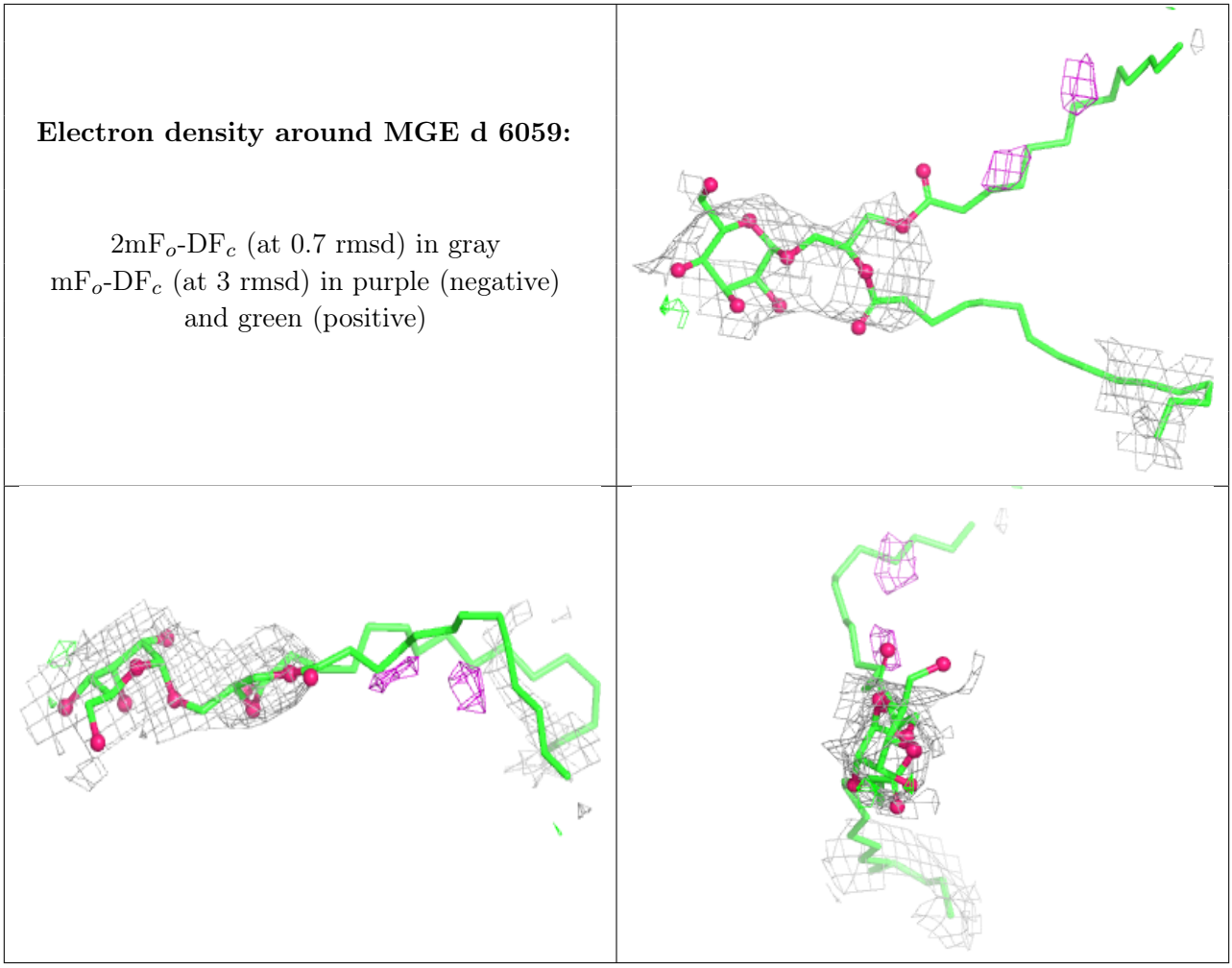
Electron density around CLA B 1014:

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



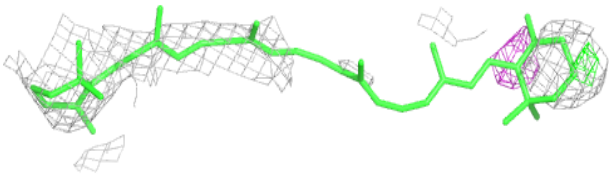
Electron density around MGE d 6059:

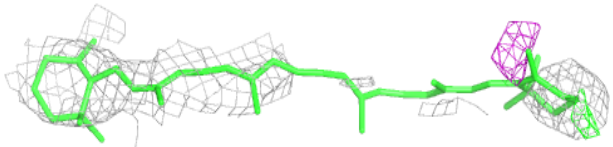
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

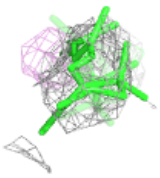


Electron density around BCR h 6049:

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

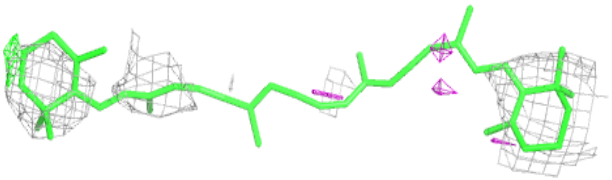


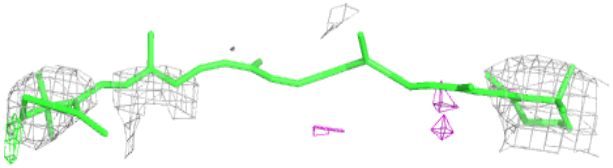


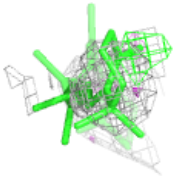


Electron density around BCR D 1050:

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

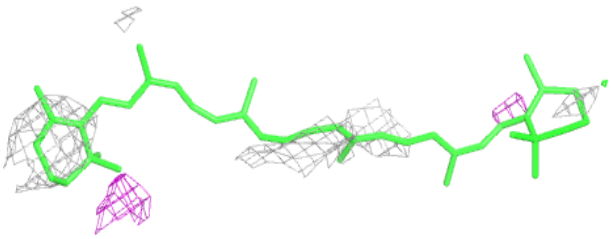




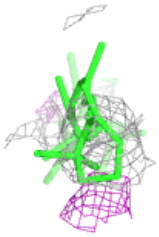


Electron density around BCR K 1051:

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

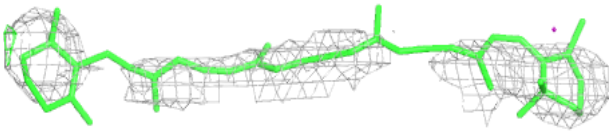


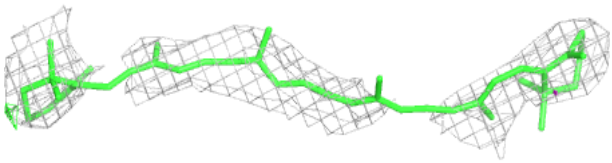


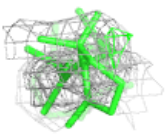


Electron density around BCR a 6044:

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

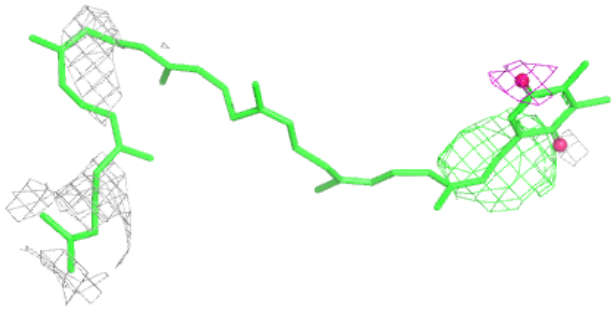


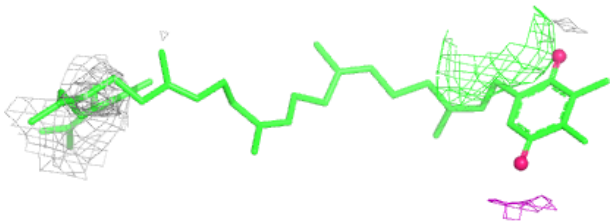


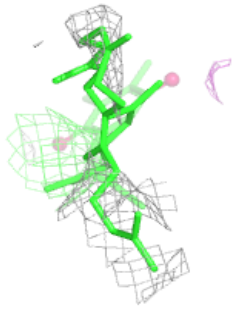


Electron density around PQ9 A 1043:

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

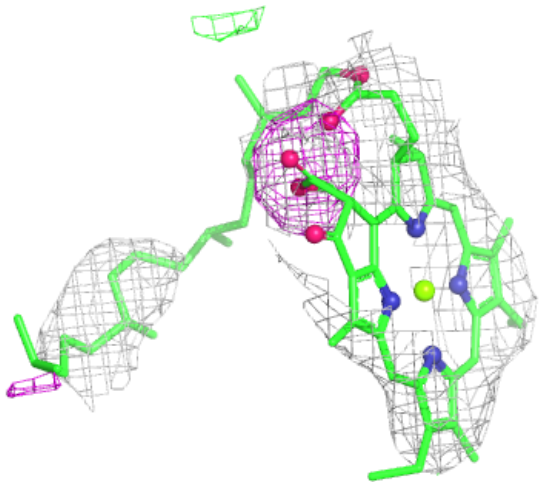


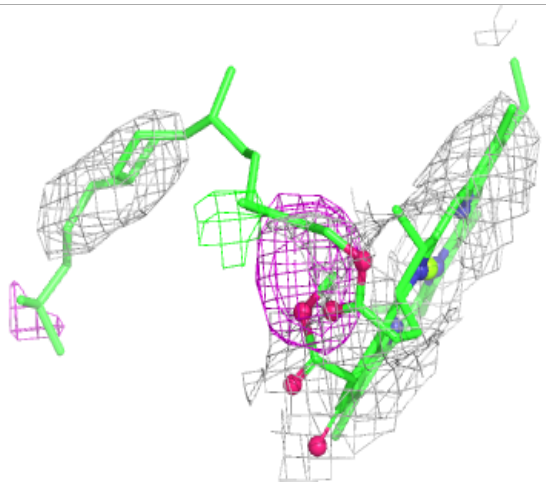


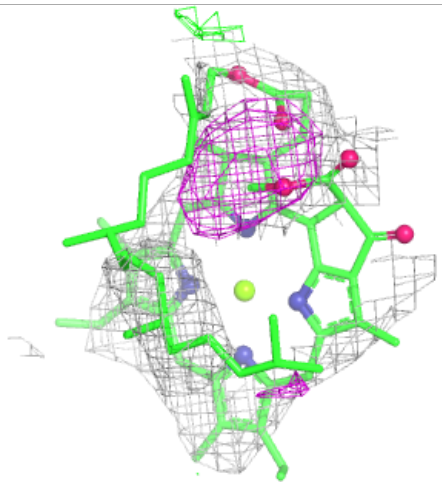


Electron density around CLA b 6021:

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

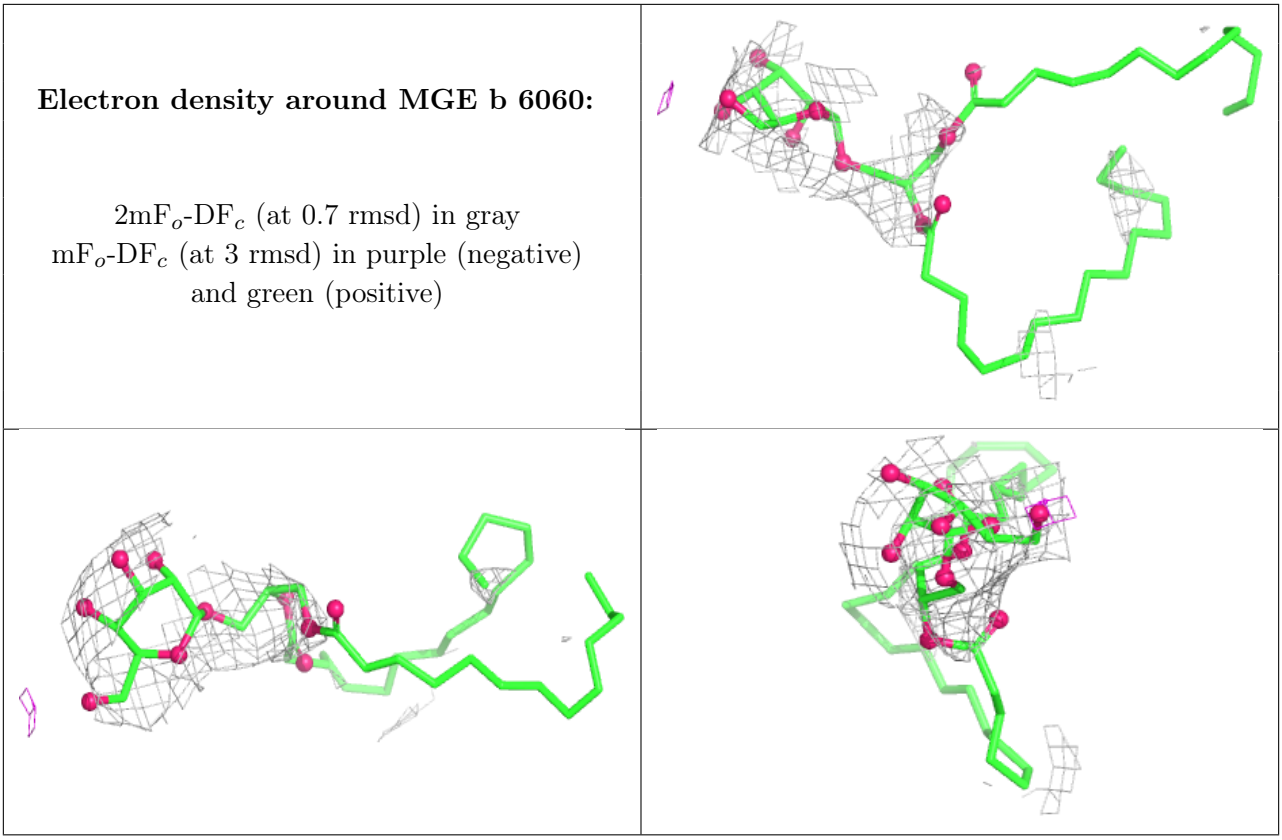






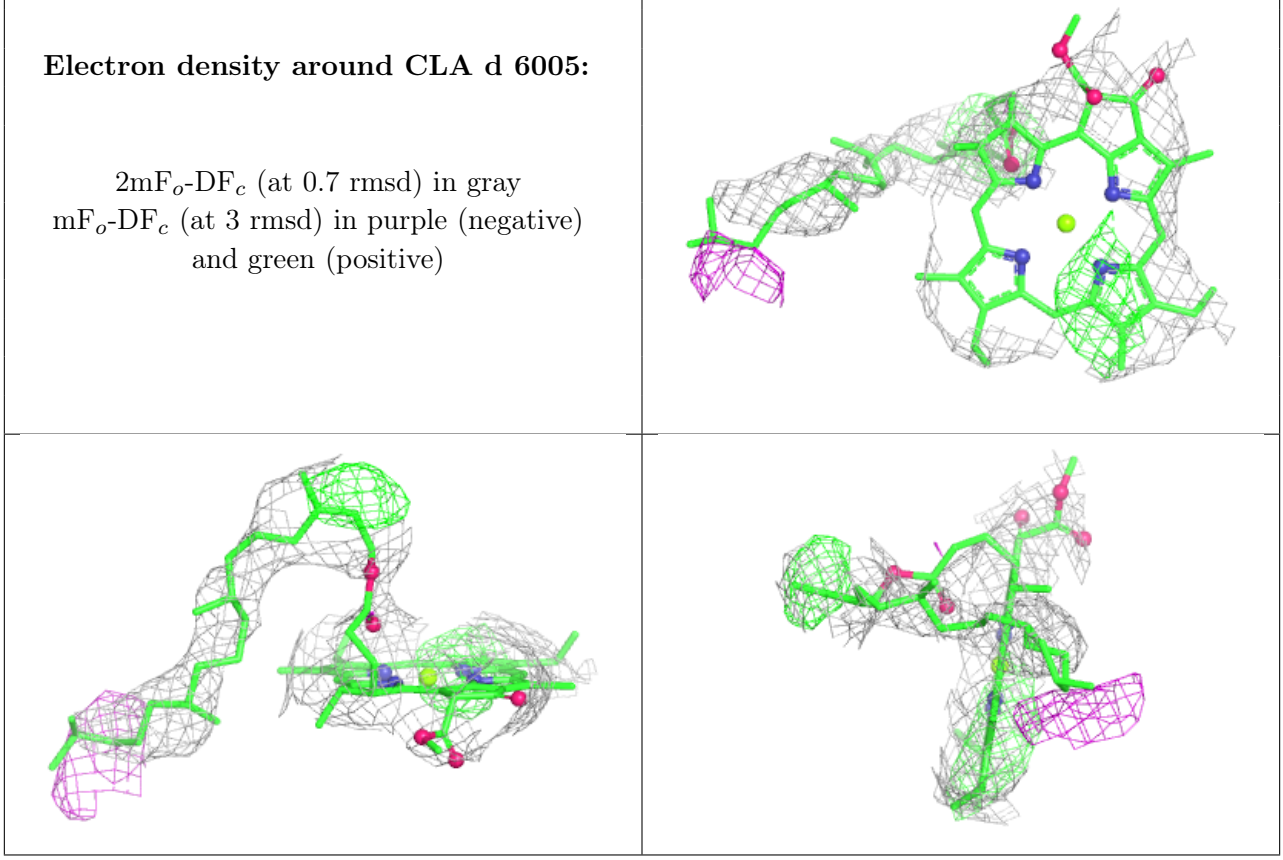
Electron density around MGE b 6060:

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



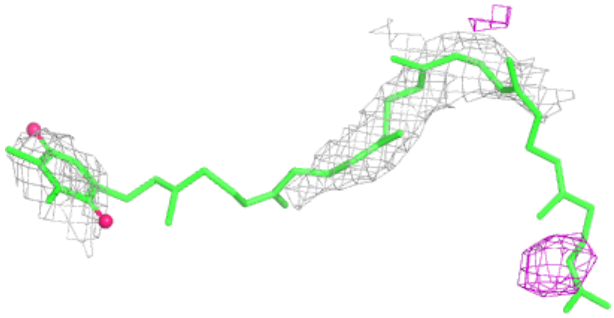
Electron density around CLA d 6005:

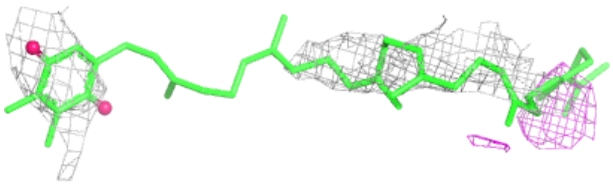
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

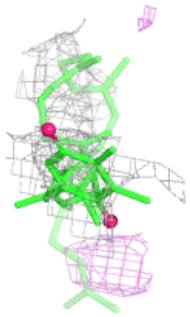


Electron density around PQ9 d 6042:

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



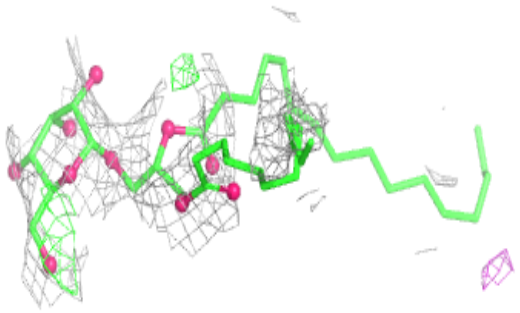




Electron density around MGE l 6061:

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

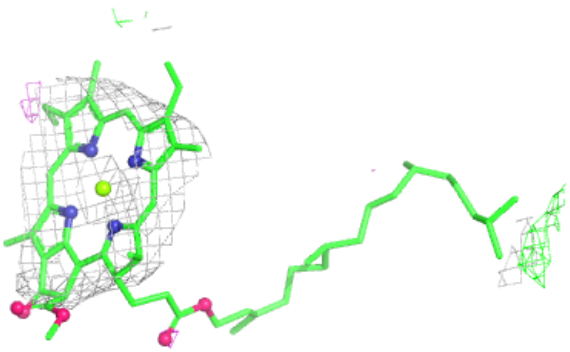


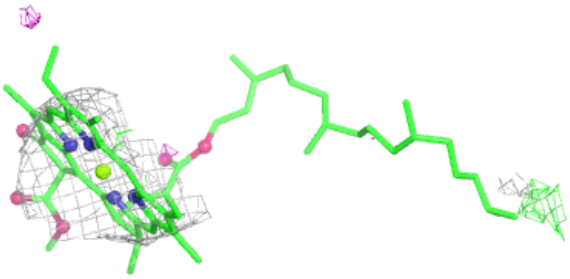


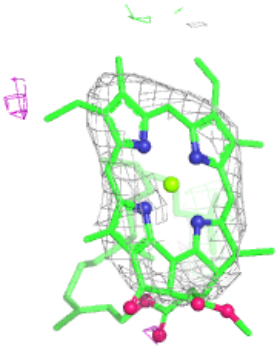


Electron density around CLA c 6035:

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



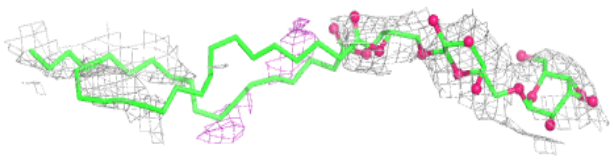


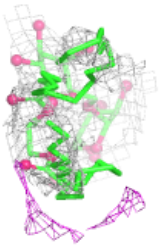


Electron density around DGD C 1057:

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

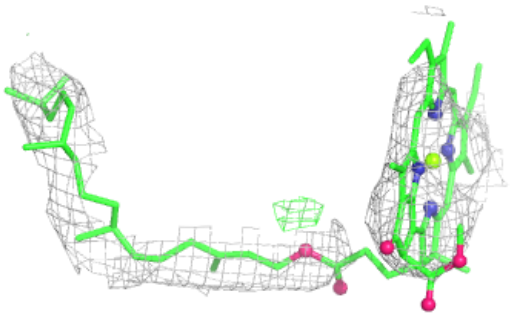


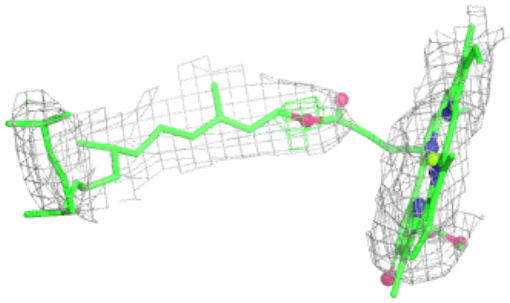




Electron density around CLA C 1030:

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



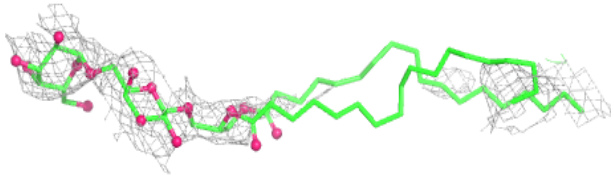


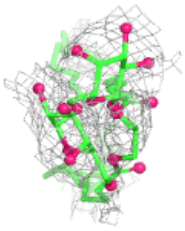


Electron density around DGD c 6057:

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

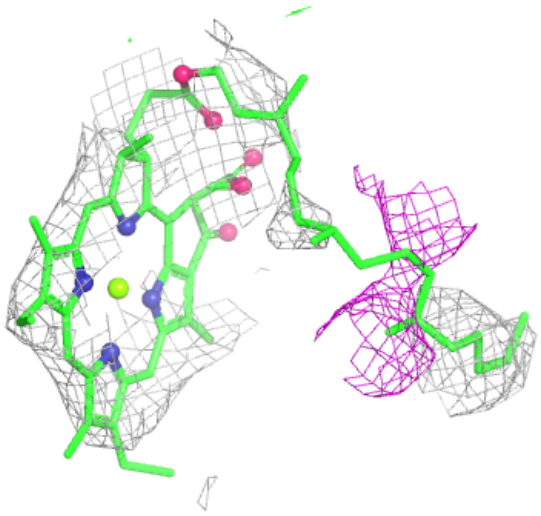


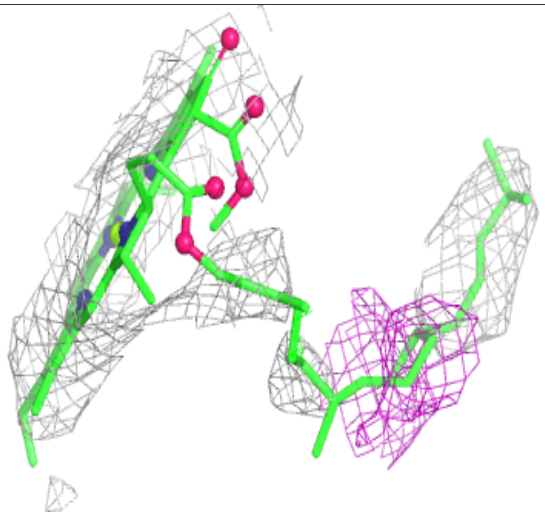


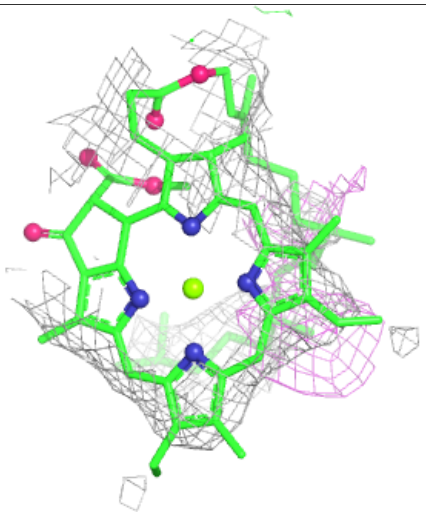


Electron density around CLA B 1021:

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

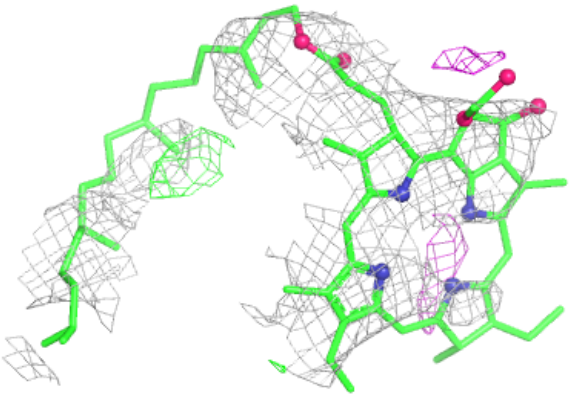


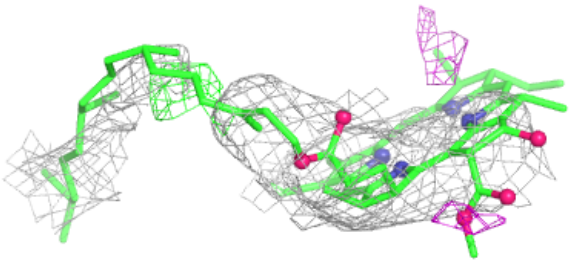


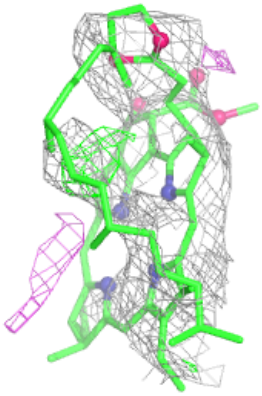


Electron density around PHO D 1039:

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

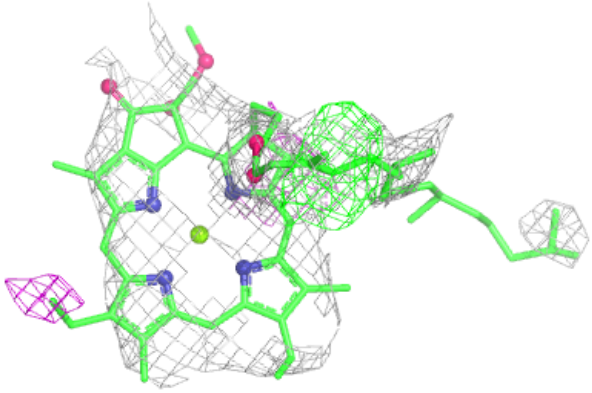


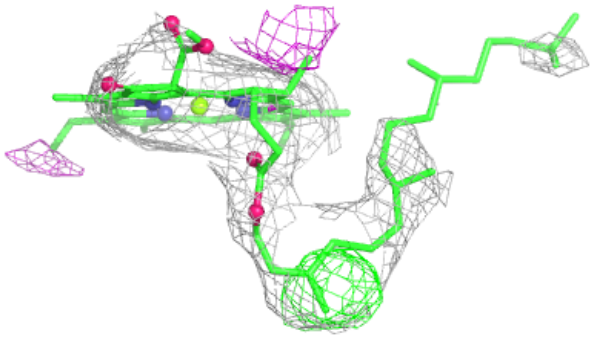


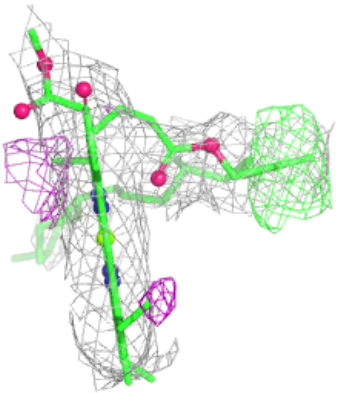


Electron density around CLA D 1005:

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

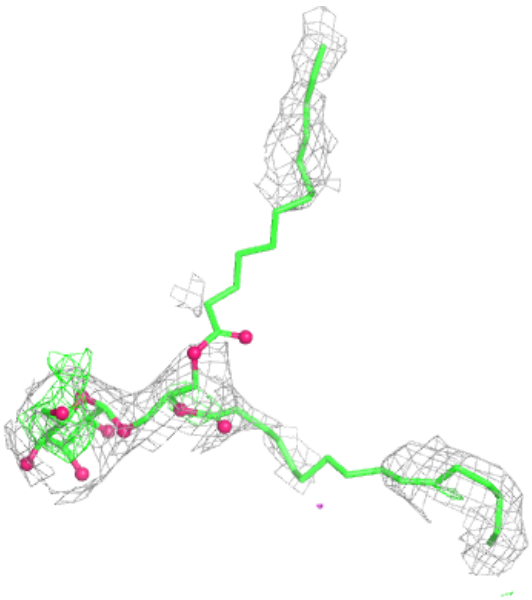


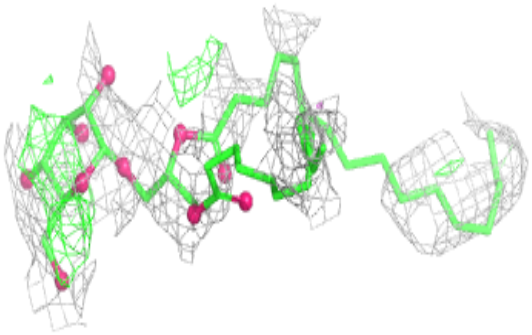




Electron density around MGE L 1061:

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

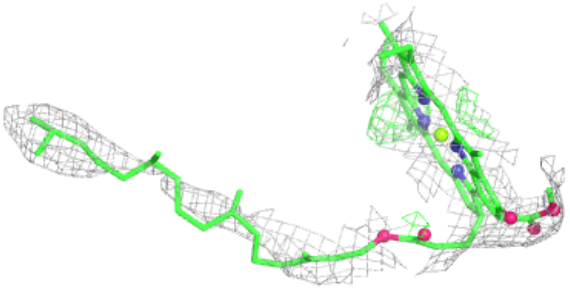


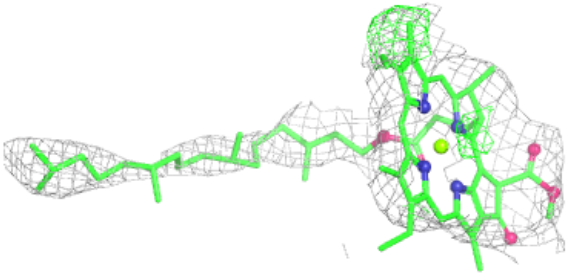


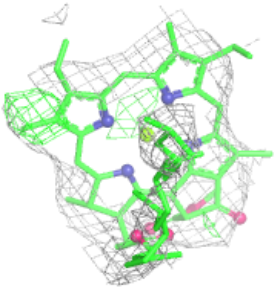


Electron density around CLA b 6015:

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

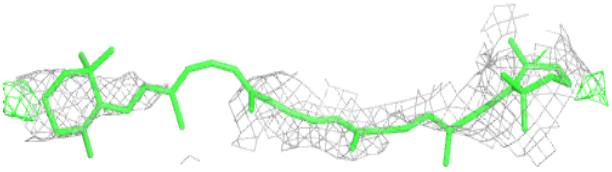


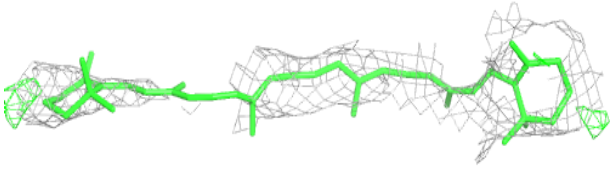


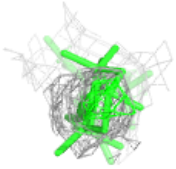


Electron density around BCR H 1049:

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

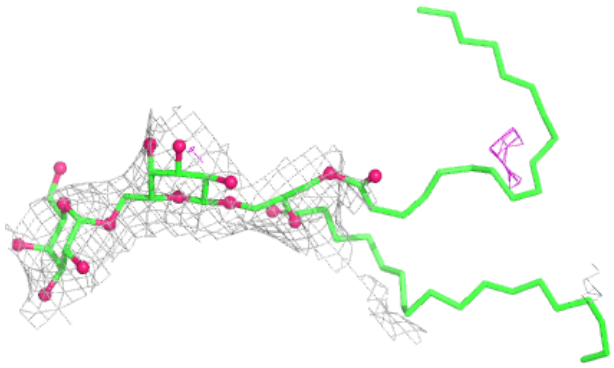


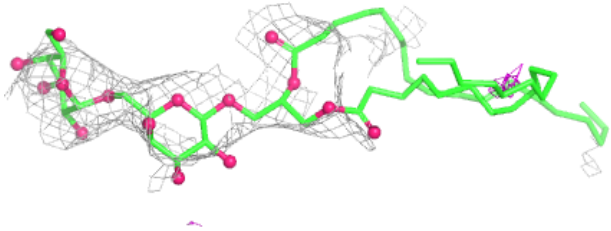


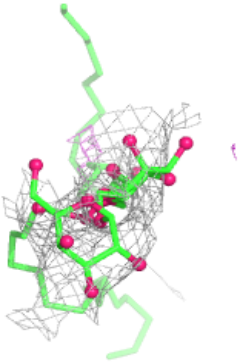


Electron density around DGD c 6055:

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

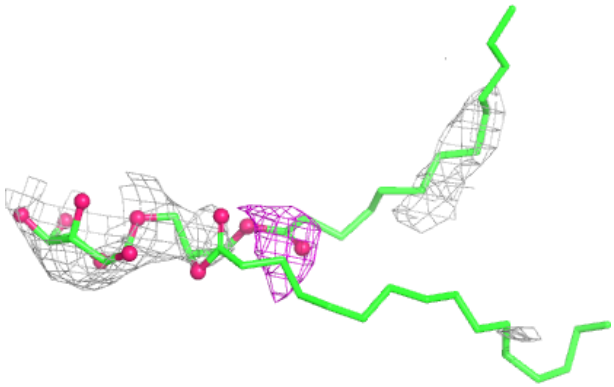


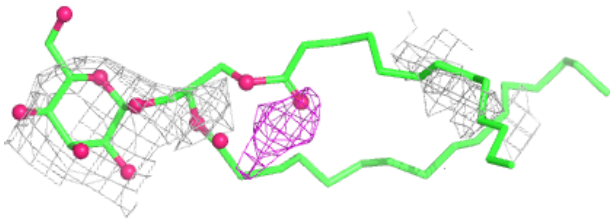


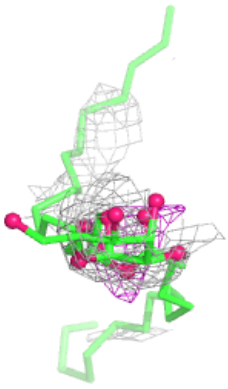


Electron density around MGE D 1062:

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

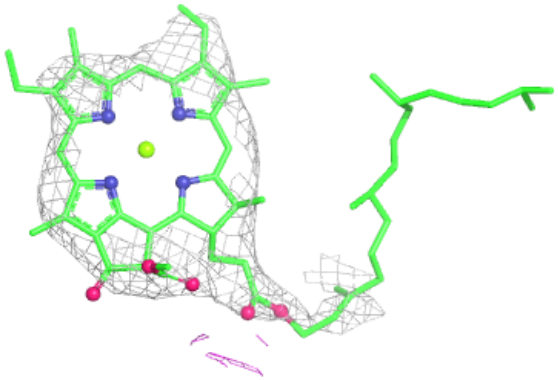


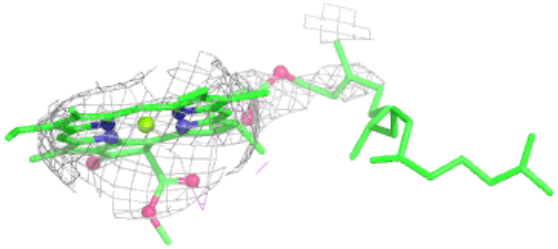


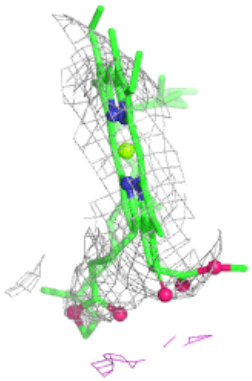


Electron density around CLA C 1036:

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

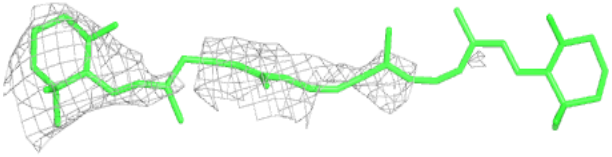


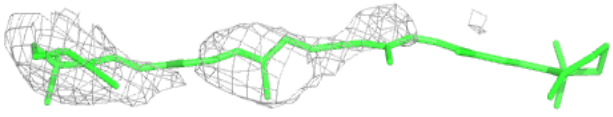


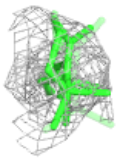


Electron density around BCR B 1045:

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

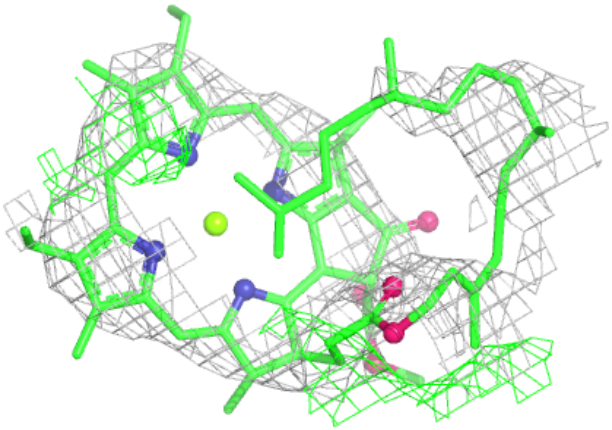


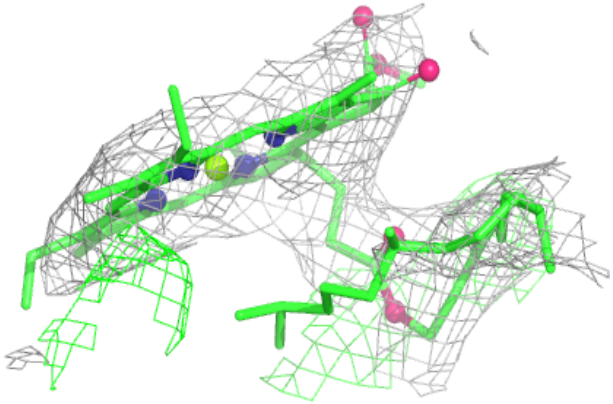


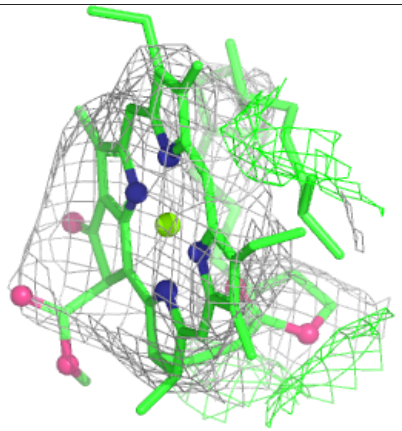


Electron density around CLA C 1026:

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

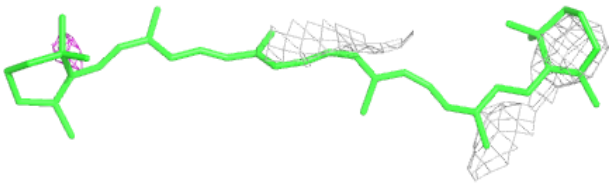




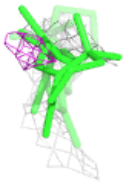


Electron density around BCR k 6051:

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

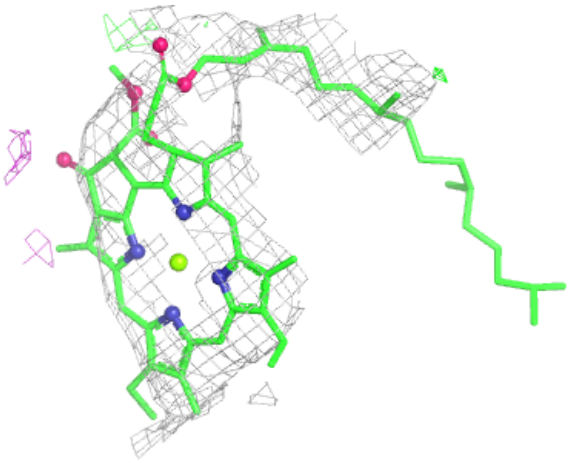


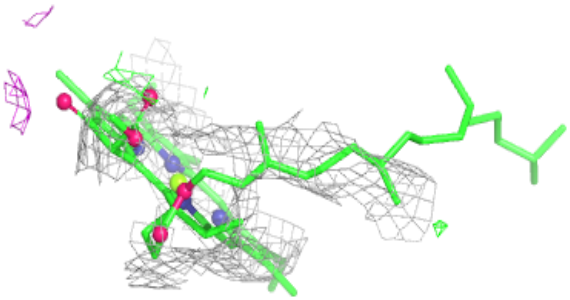


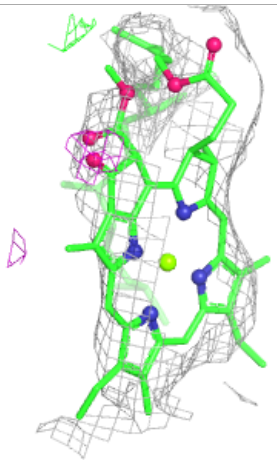


Electron density around CLA b 6024:

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

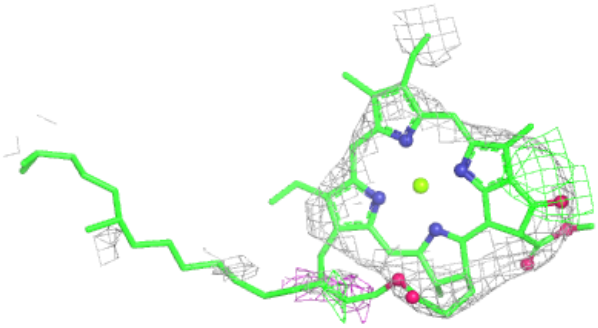


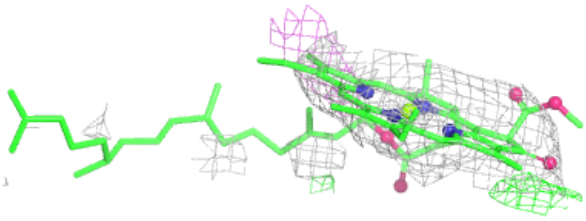




Electron density around CLA c 6025:

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

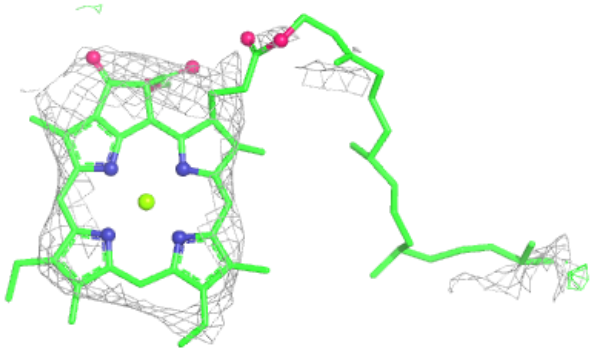


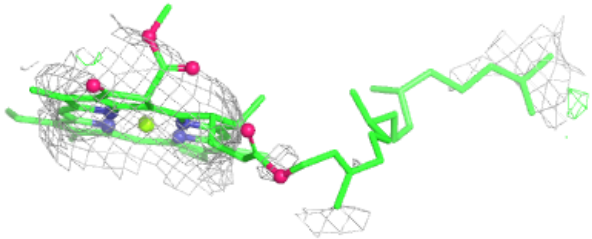


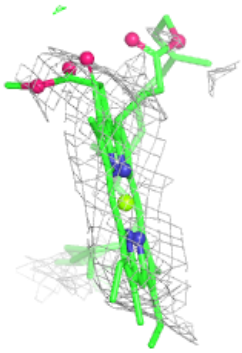


Electron density around CLA c 6036:

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

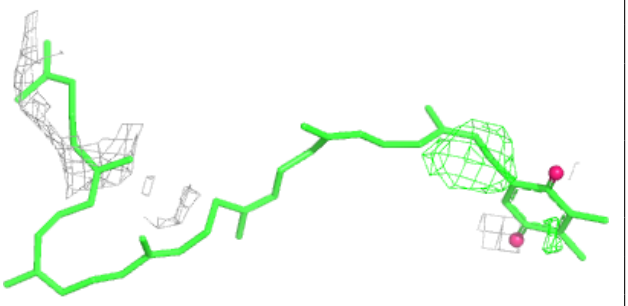


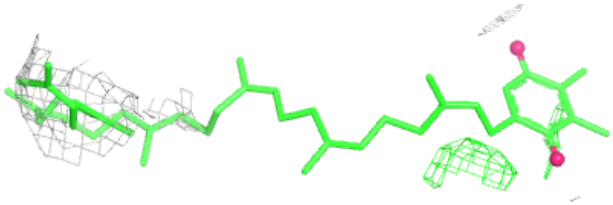


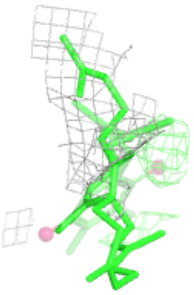


Electron density around PQ9 a 6043:

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

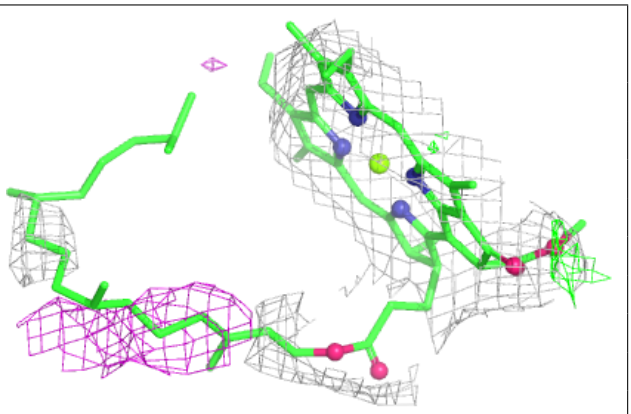


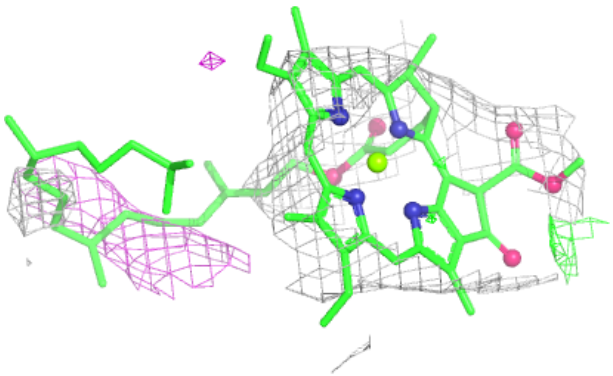




Electron density around CLA C 1028:

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

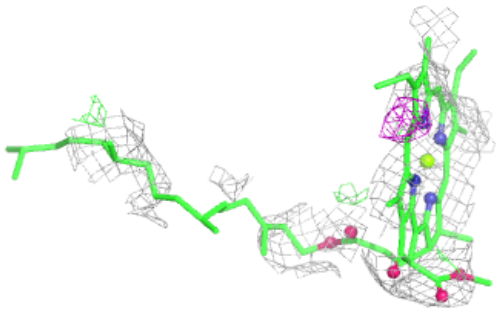


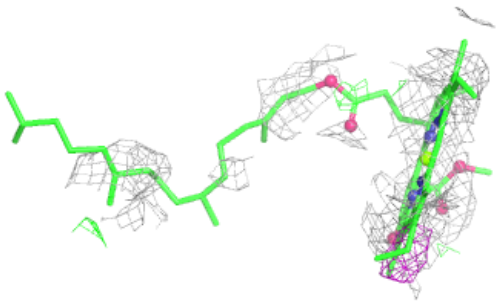


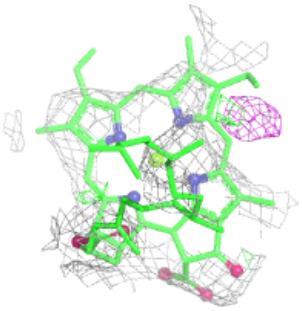


Electron density around CLA c 6032:

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

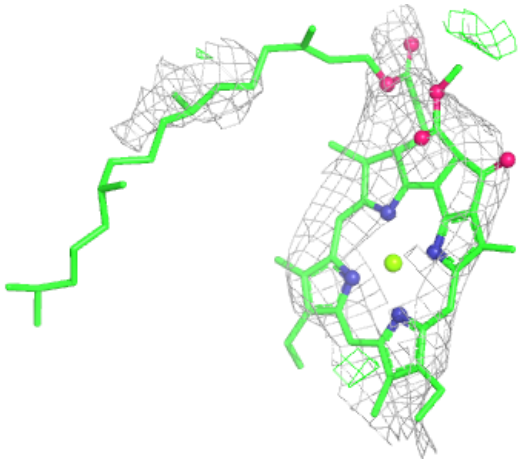


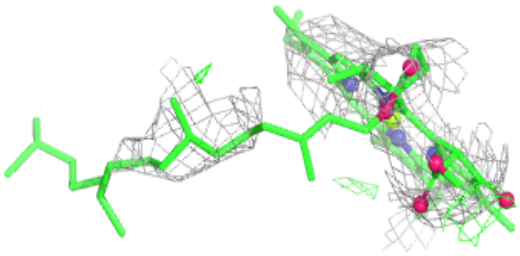


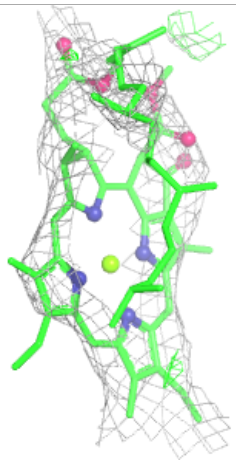


Electron density around CLA B 1024:

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

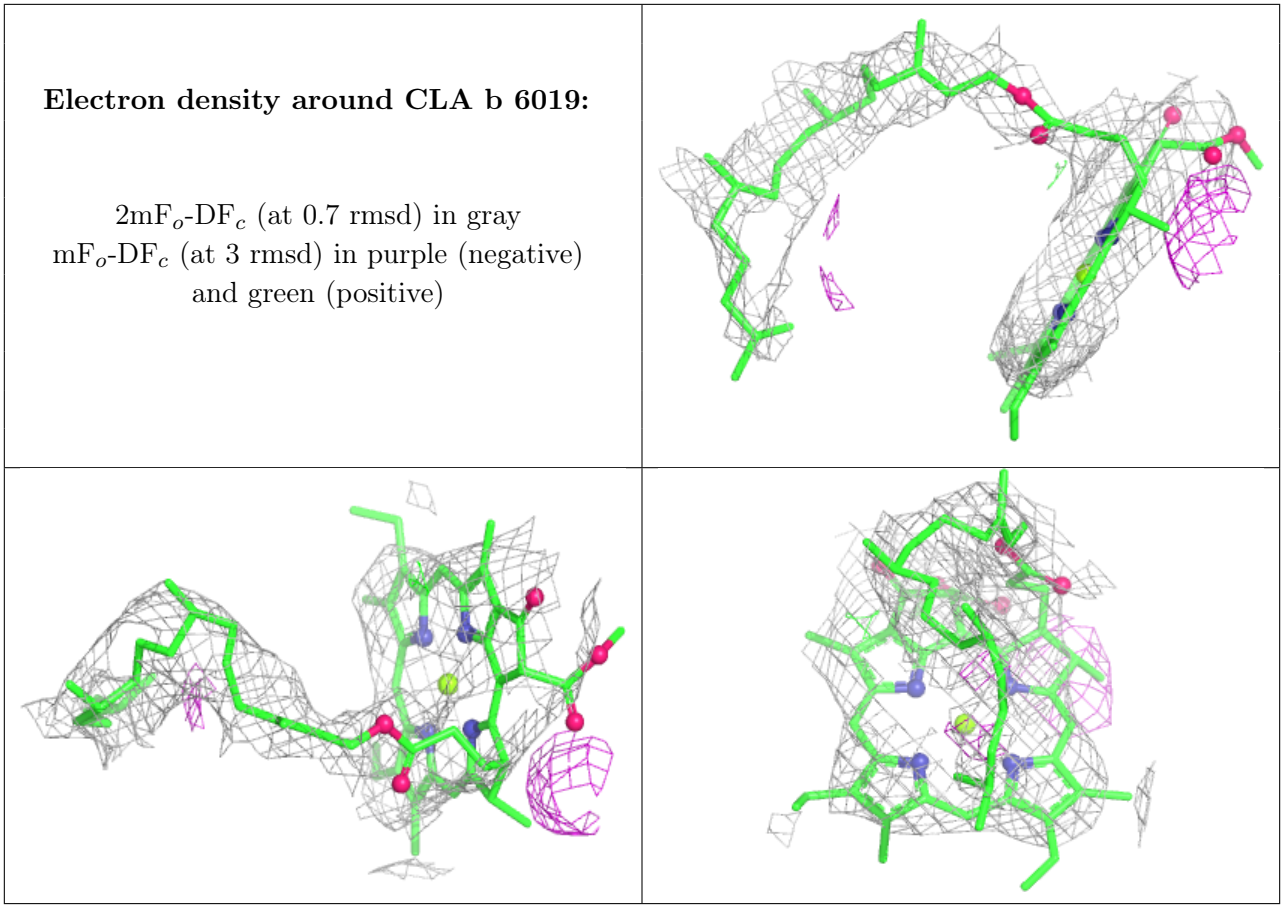






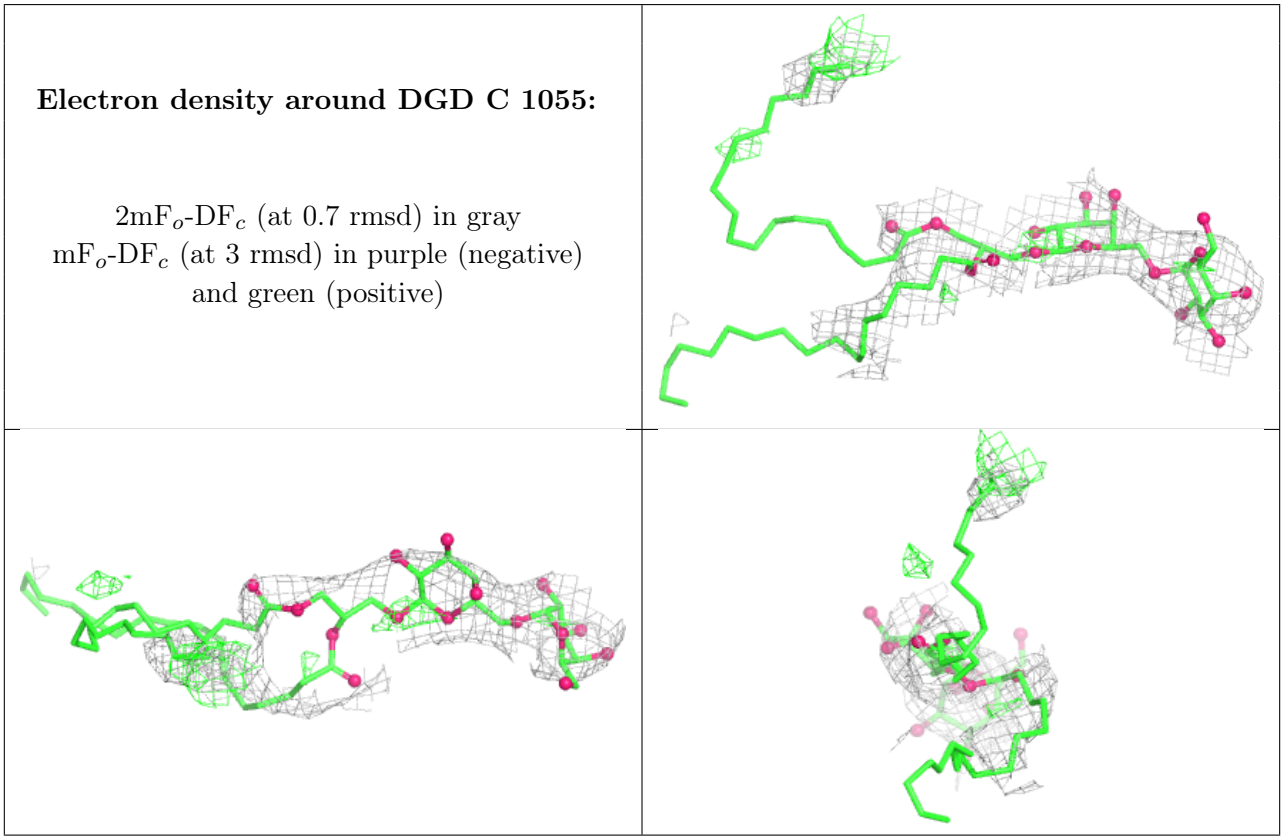
Electron density around CLA b 6019:

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



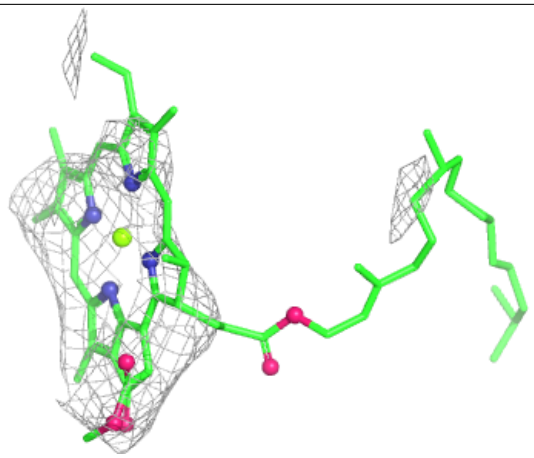
Electron density around DGD C 1055:

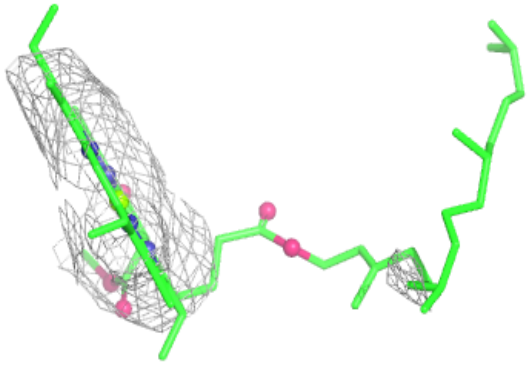
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

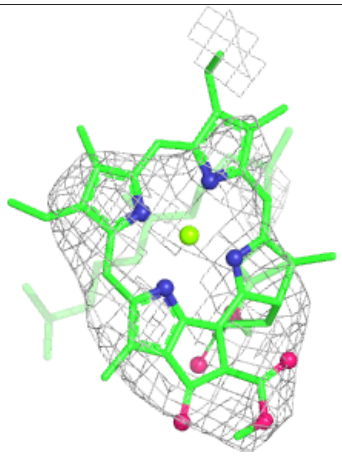


Electron density around CLA a 6007:

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

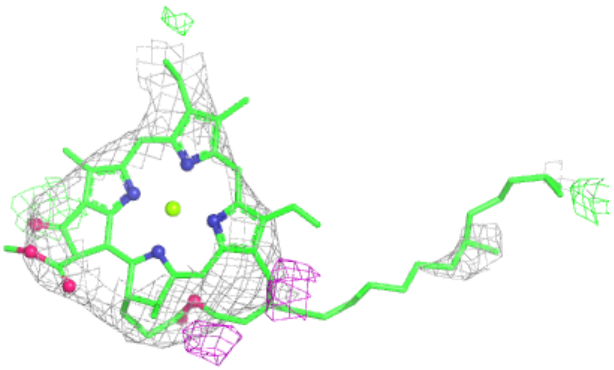


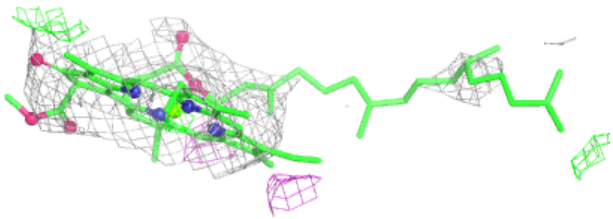


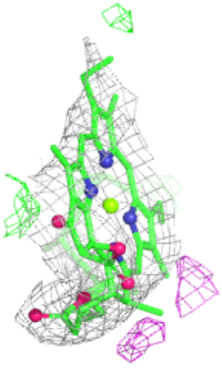


Electron density around CLA C 1025:

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

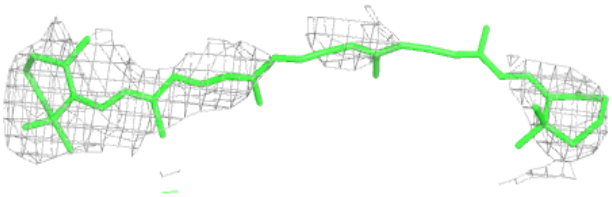


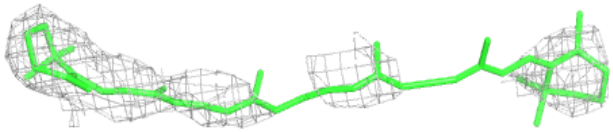


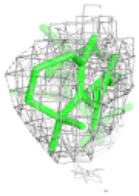


Electron density around BCR t 1046:

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



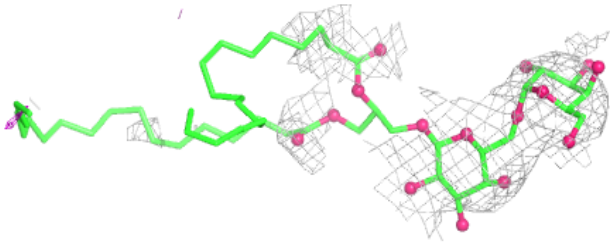


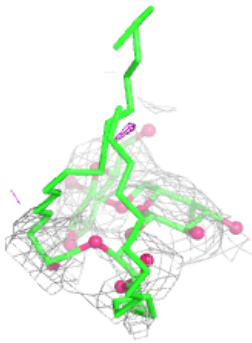


Electron density around DGD B 1058:

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

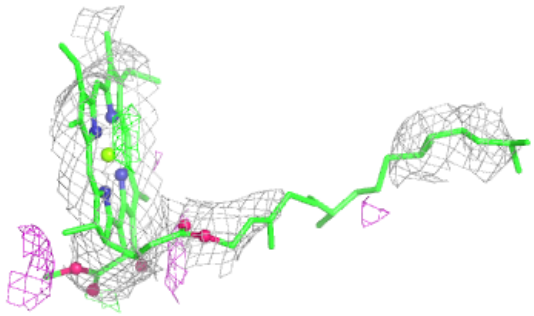


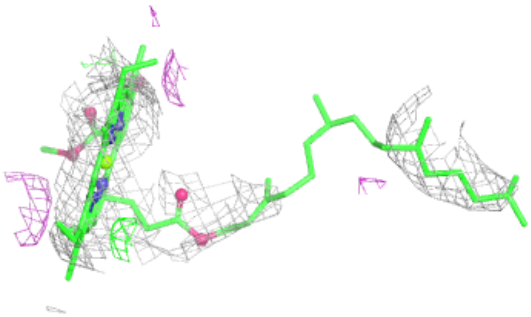


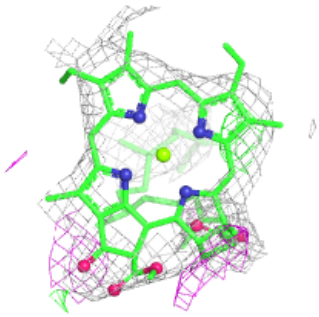


Electron density around CLA C 1032:

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



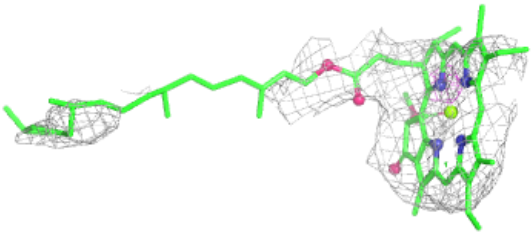


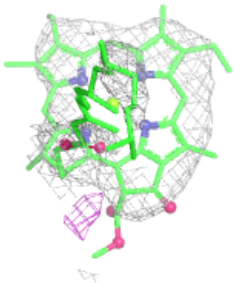


Electron density around CLA b 6012:

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

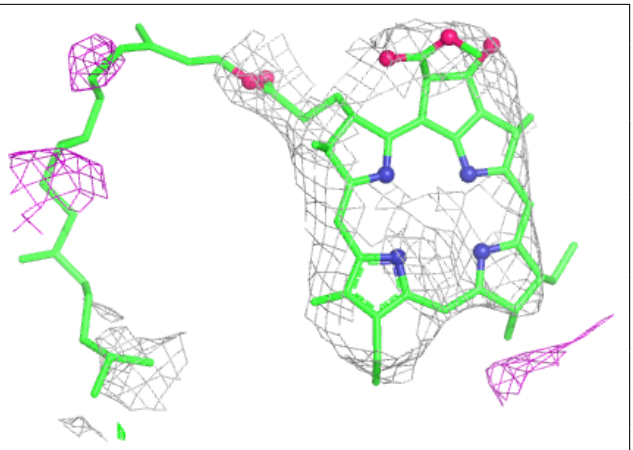


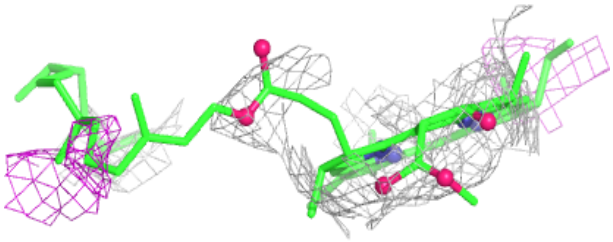




Electron density around PHO a 6038:

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

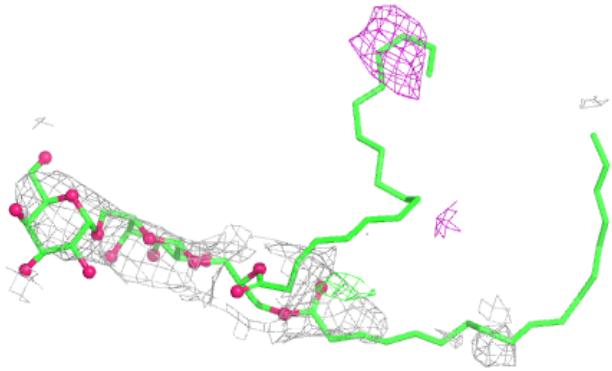


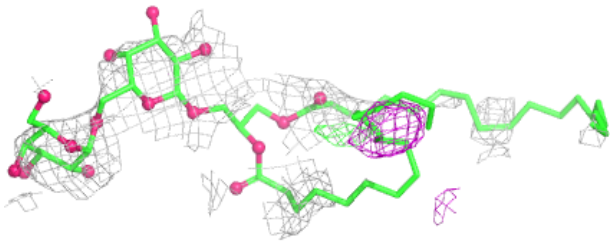


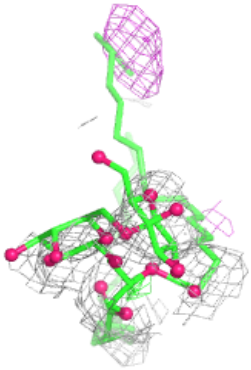


Electron density around DGD b 6058:

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

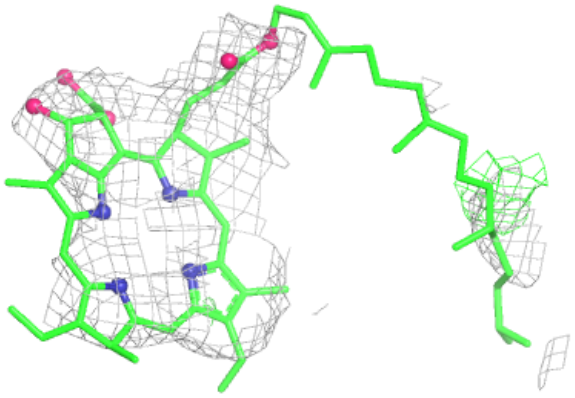


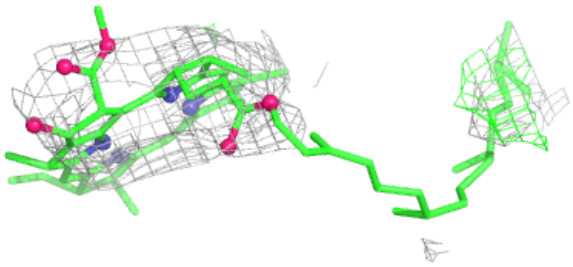


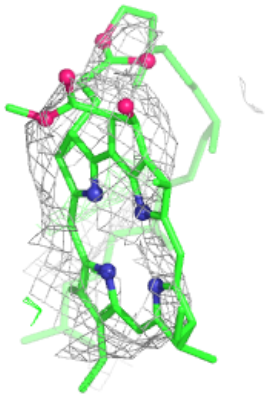


Electron density around PHO d 6039:

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

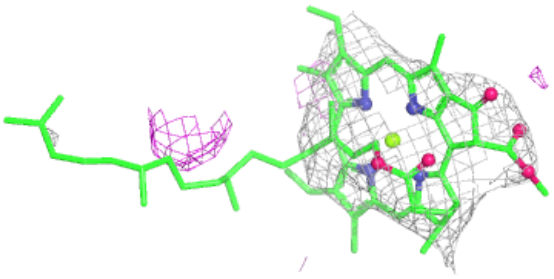


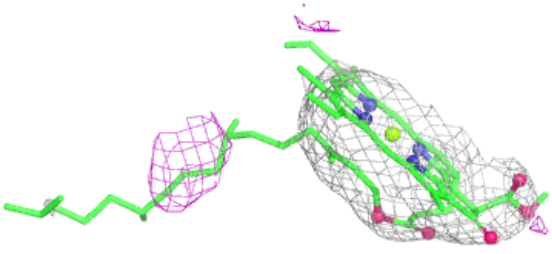


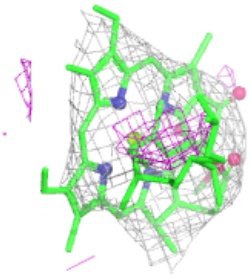


Electron density around CLA C 1029:

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

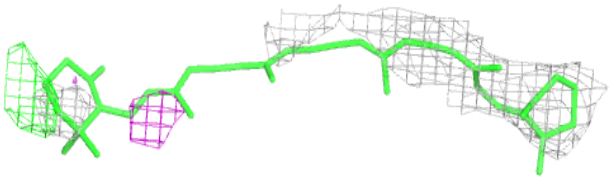


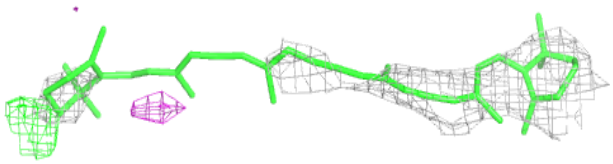


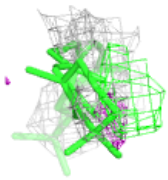


Electron density around BCR C 1052:

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

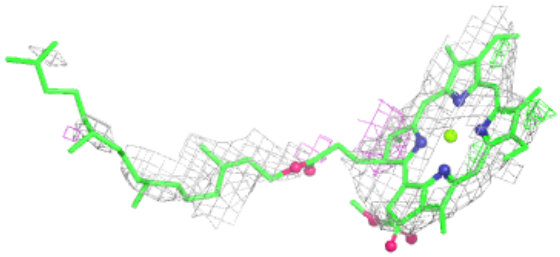


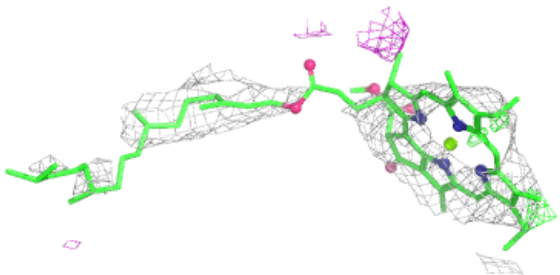


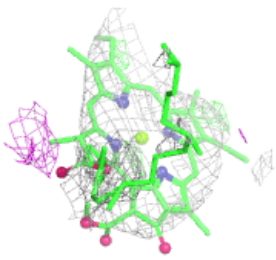


Electron density around CLA a 6003:

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

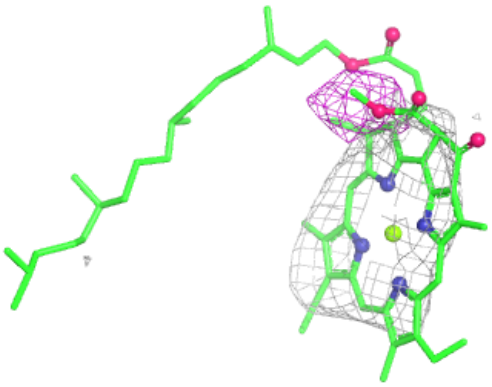


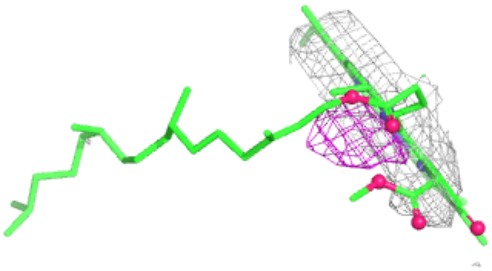


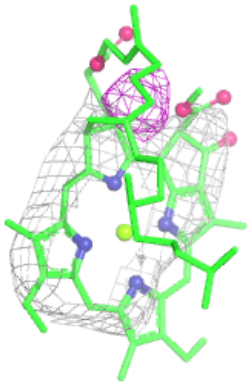


Electron density around CLA c 6031:

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

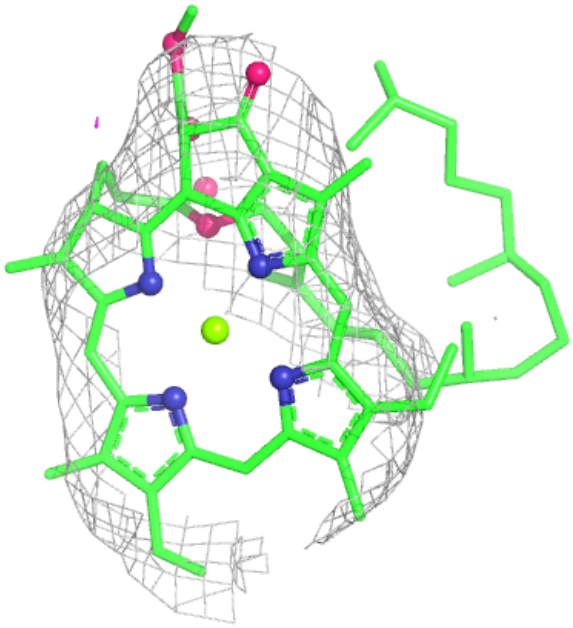


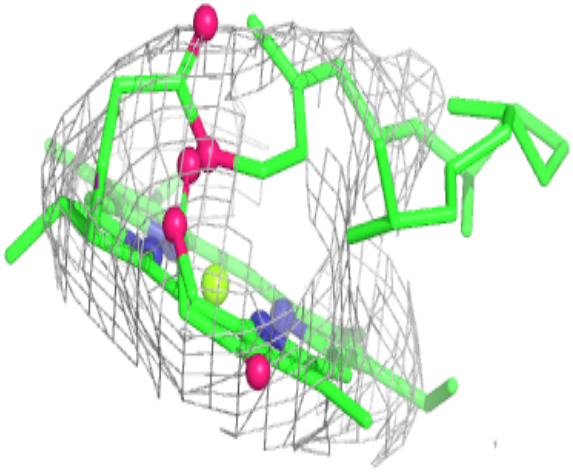


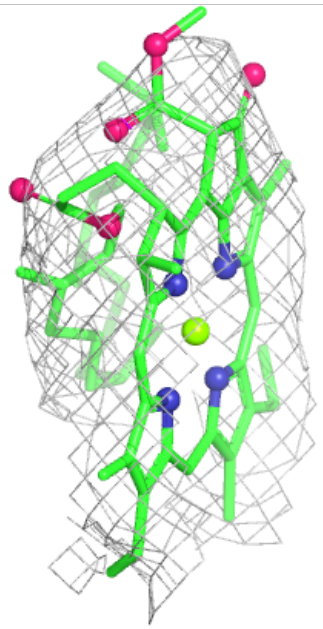


Electron density around CLA b 6022:

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

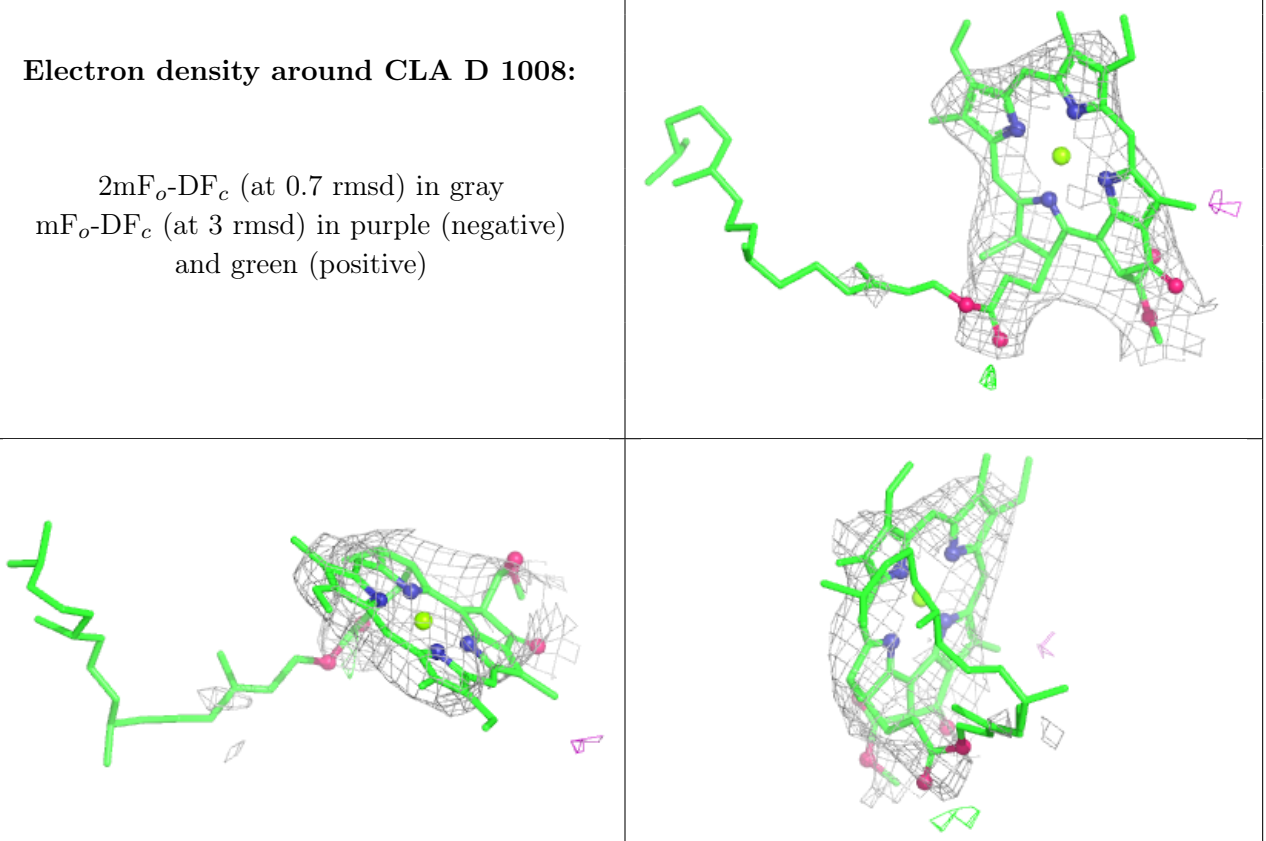






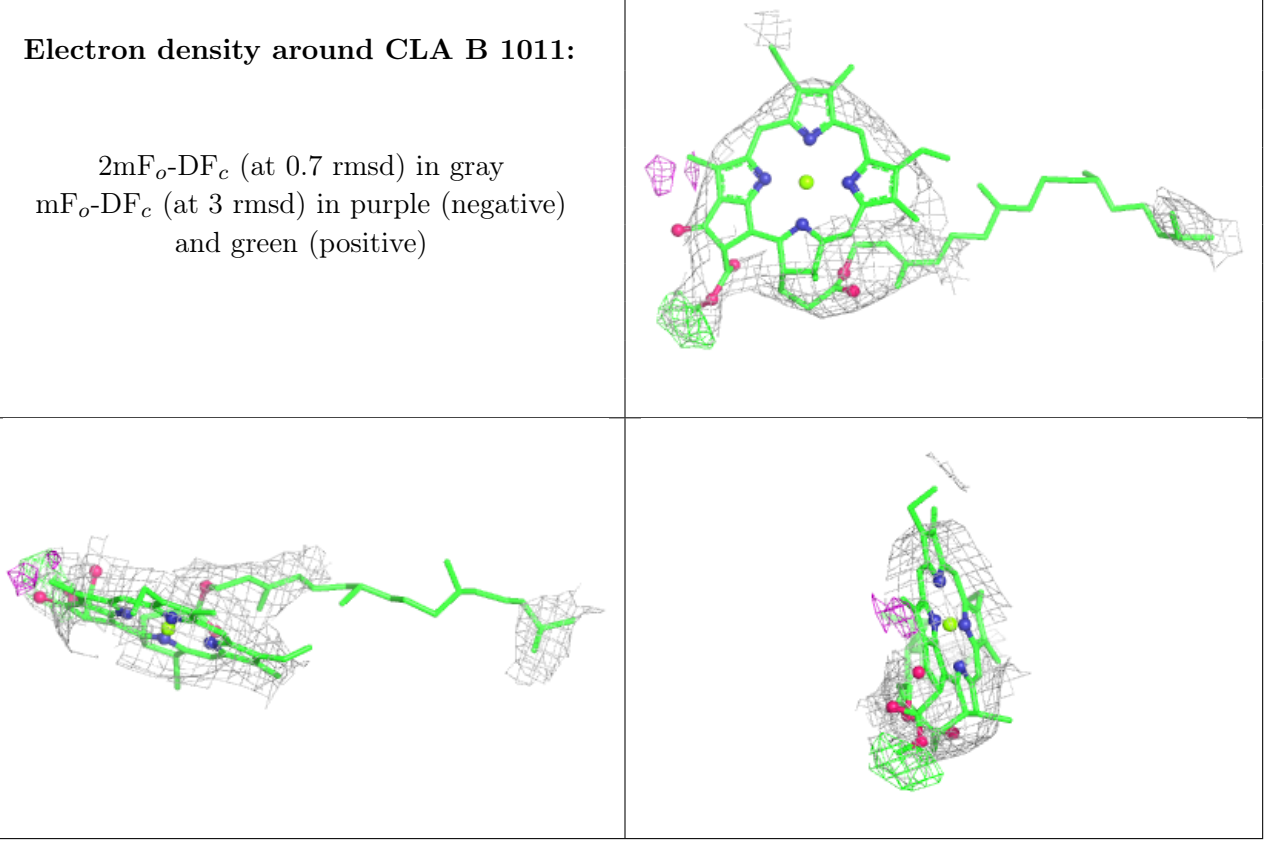
Electron density around CLA D 1008:

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



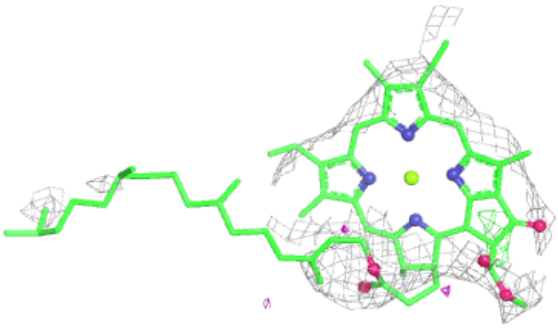
Electron density around CLA B 1011:

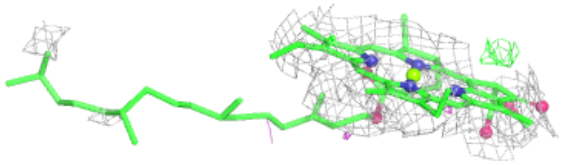
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

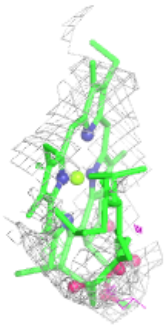


Electron density around CLA b 6011:

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

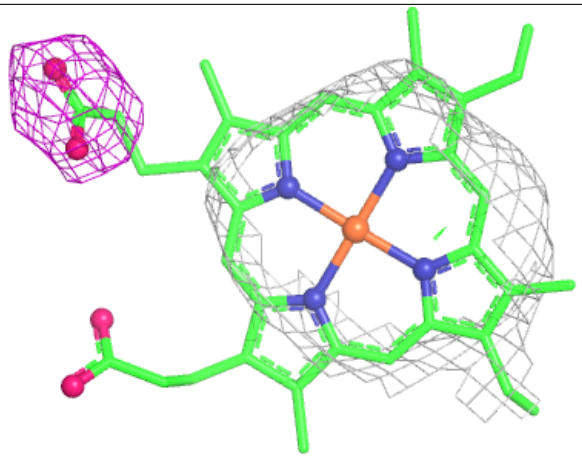


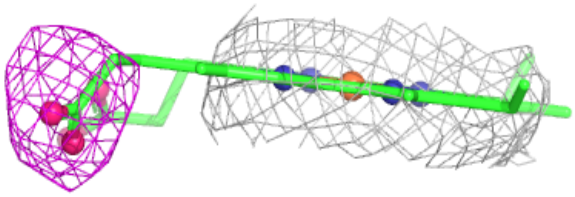


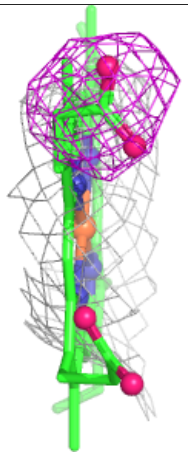


Electron density around HEM f 6040:

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

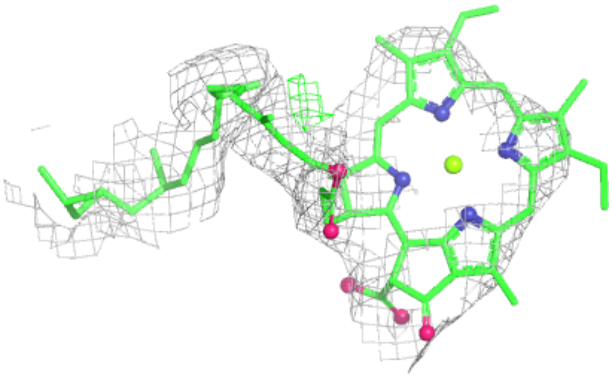


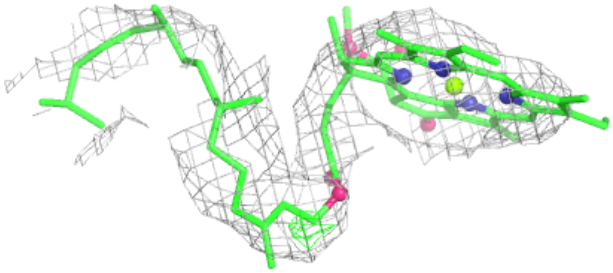




Electron density around CLA a 6006:

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

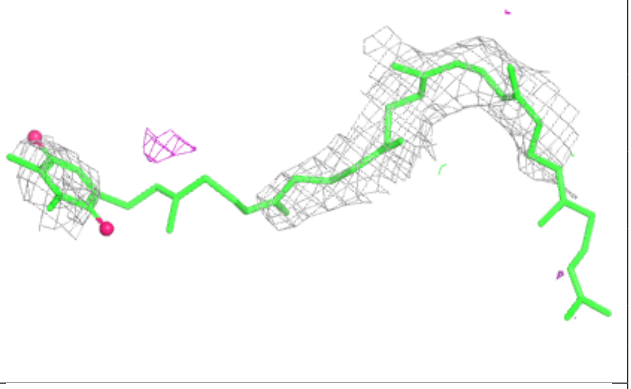


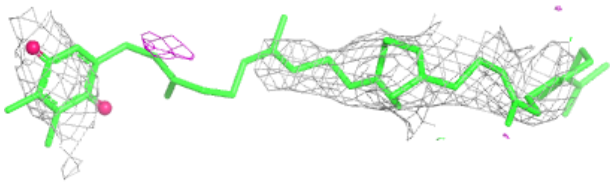


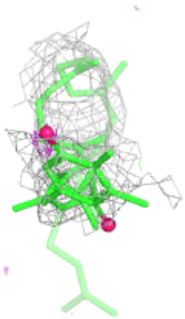


Electron density around PQ9 D 1042:

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

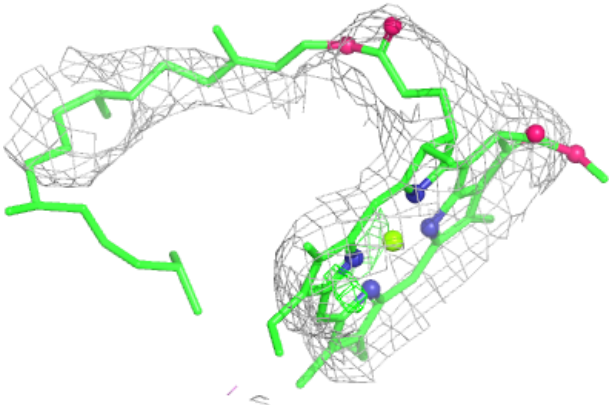


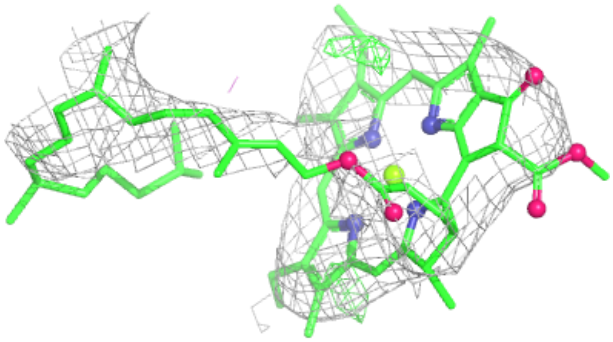




Electron density around CLA c 6028:

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

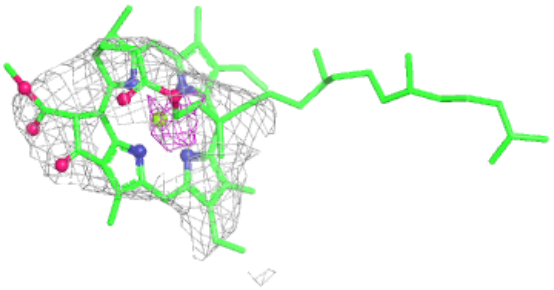


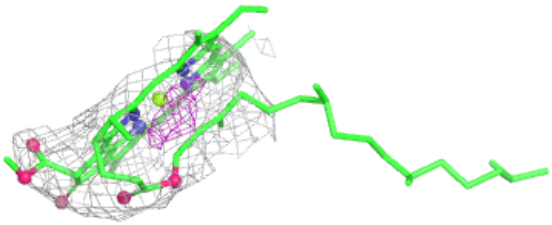


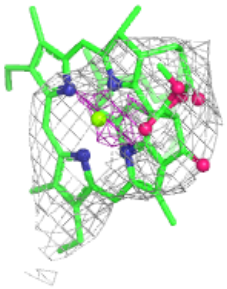


Electron density around CLA c 6029:

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

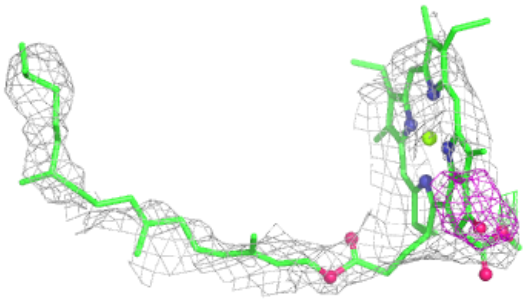


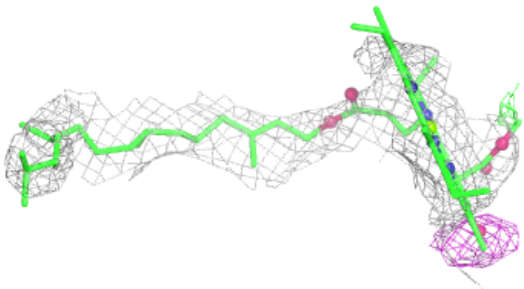


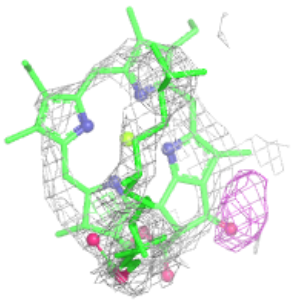


Electron density around CLA h 6017:

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

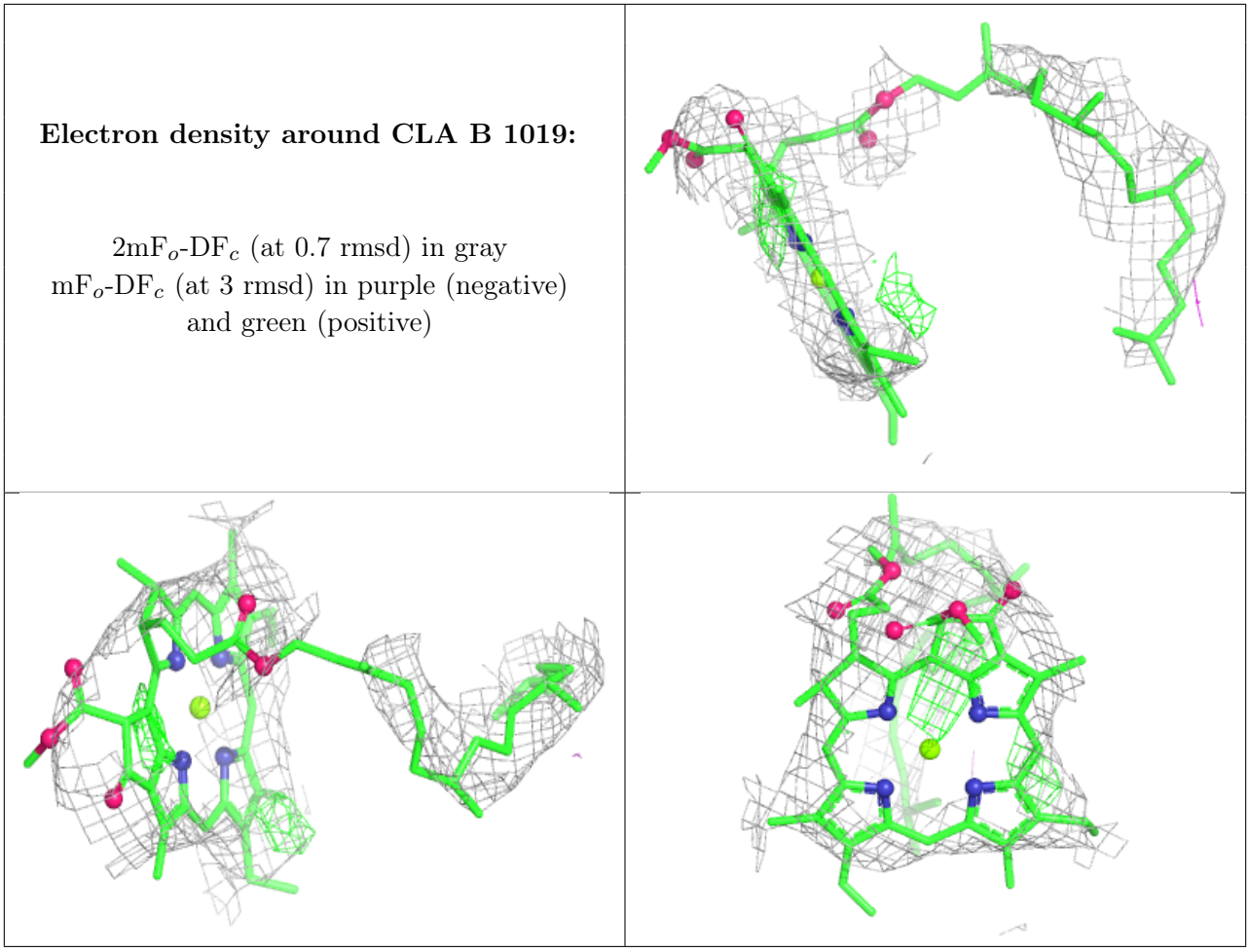






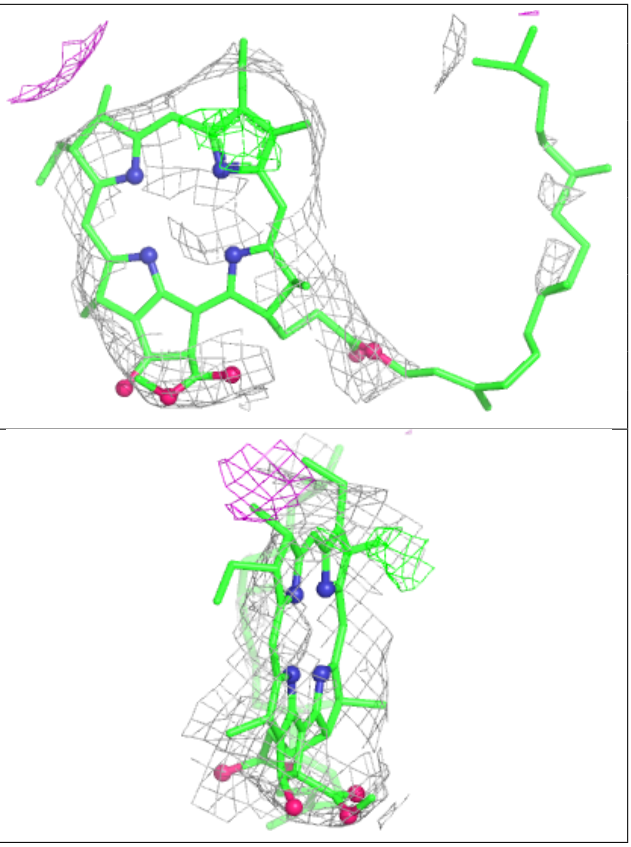
Electron density around CLA B 1019:

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



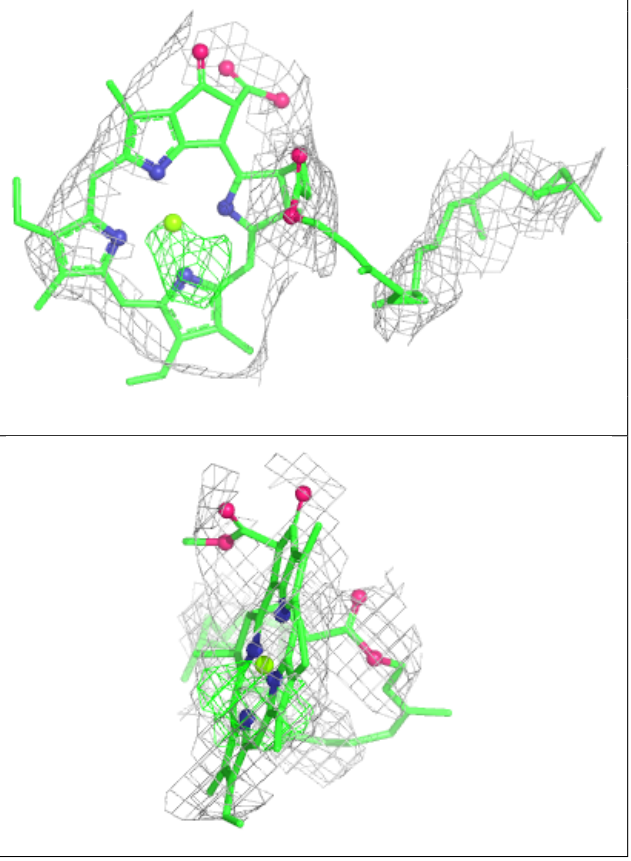
Electron density around PHO A 1038:

$2mF_o$-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 A 1006:

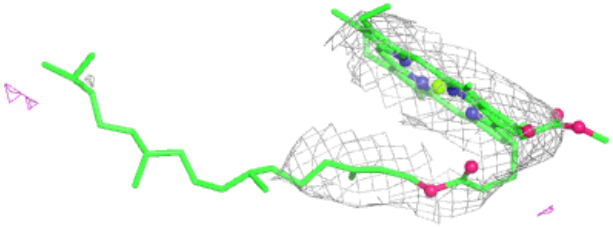
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

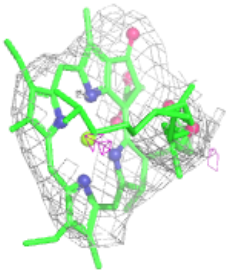


Electron density around CLA b 6016:

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

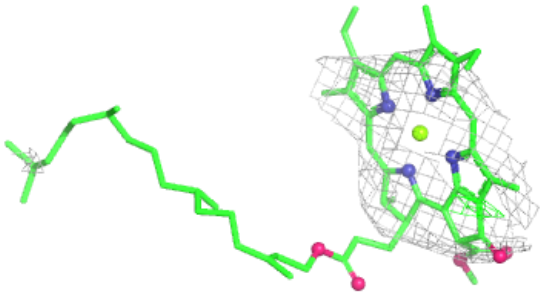


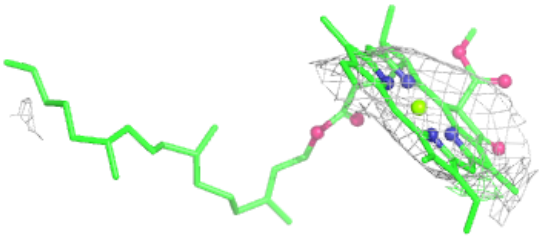


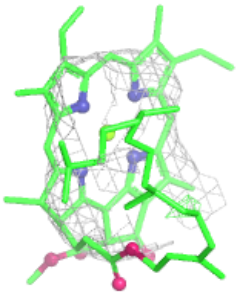


Electron density around CLA C 1035:

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

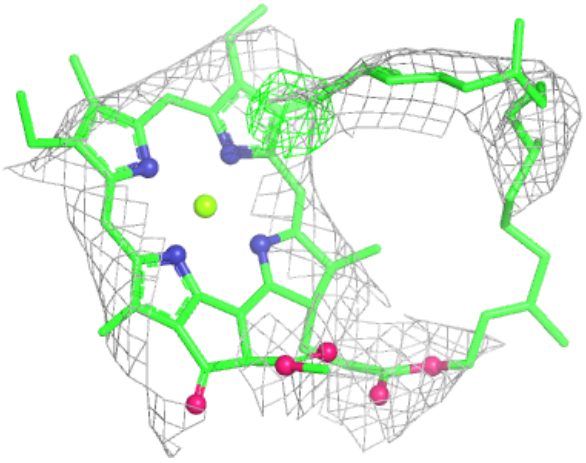


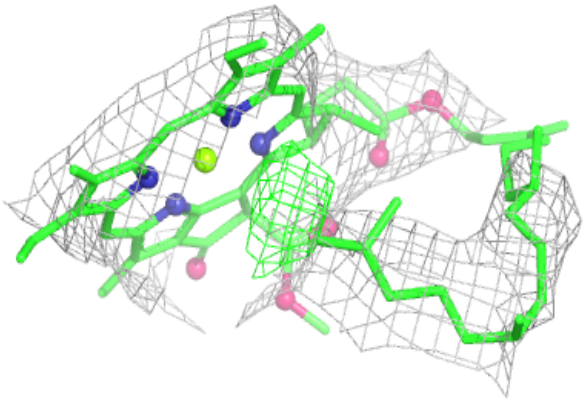


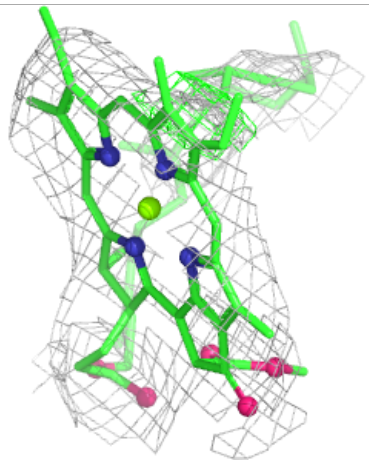


Electron density around CLA B 1023:

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

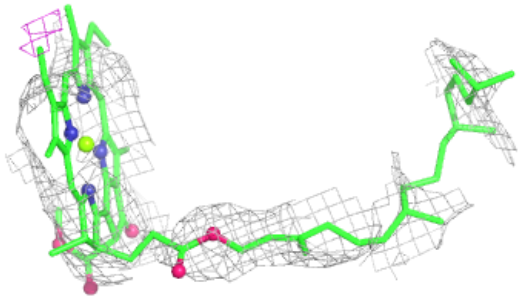


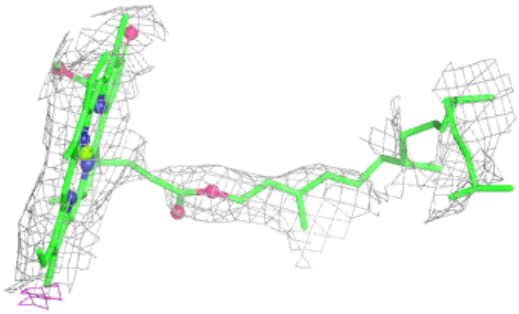


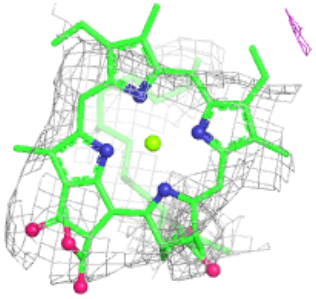


Electron density around CLA c 6030:

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

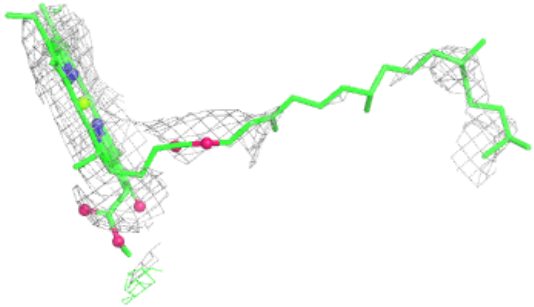


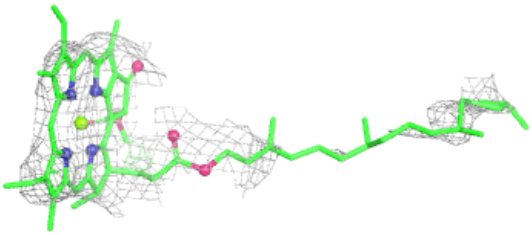


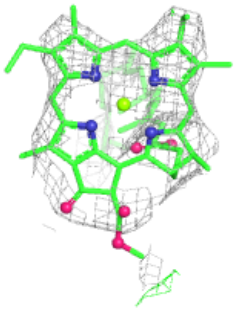


Electron density around CLA B 1012:

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

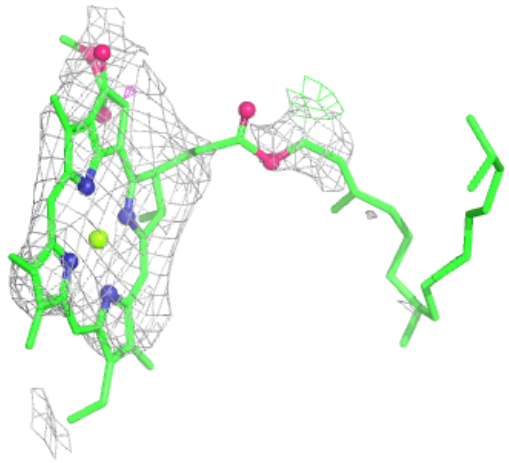


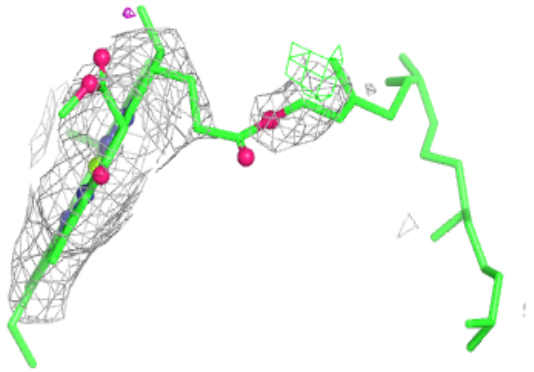


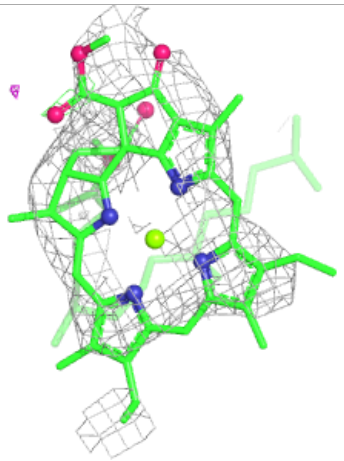


Electron density around CLA A 1007:

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

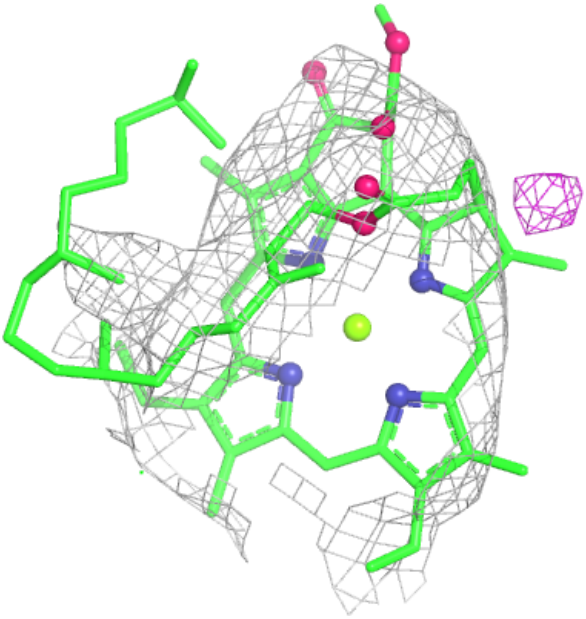


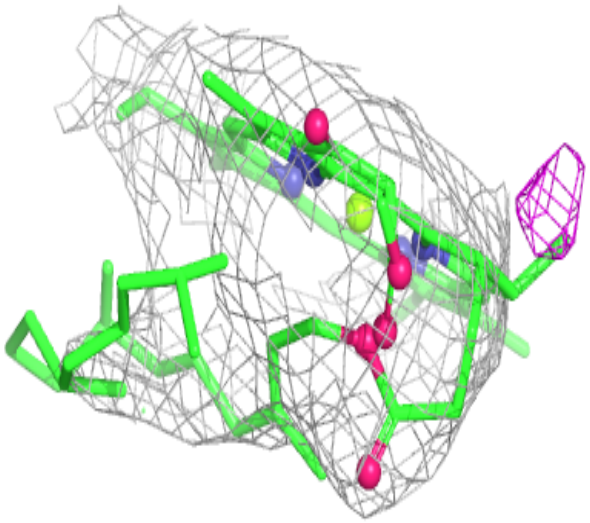


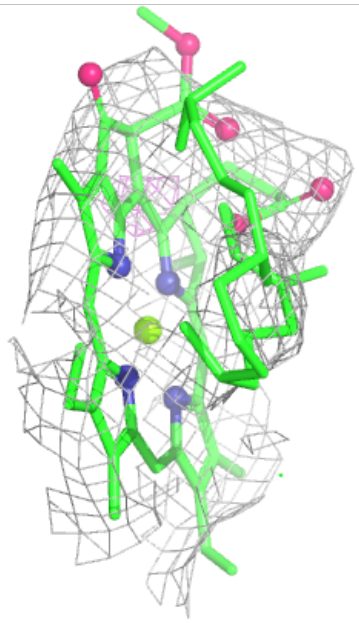


Electron density around CLA B 1022:

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

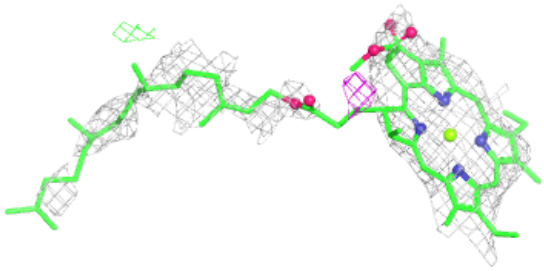


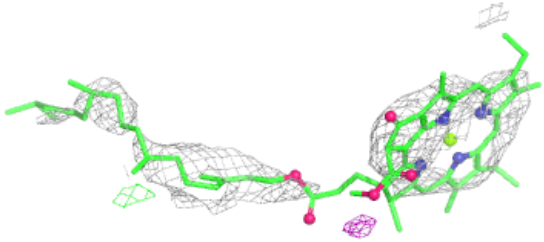


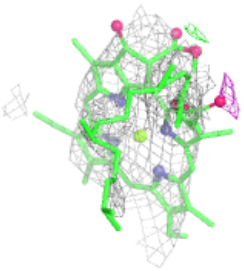


Electron density around CLA A 1003:

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

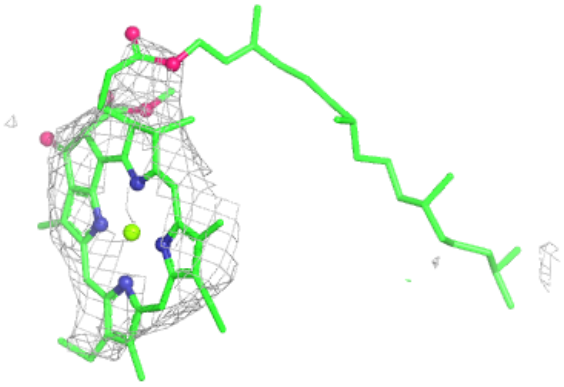


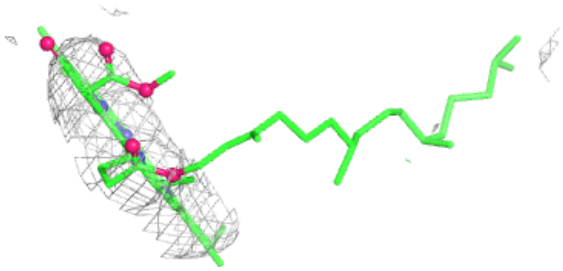


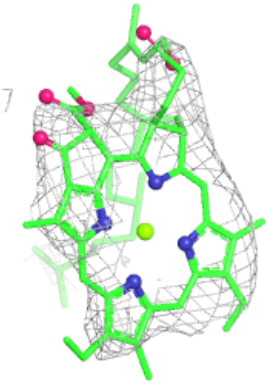


Electron density around CLA C 1031:

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

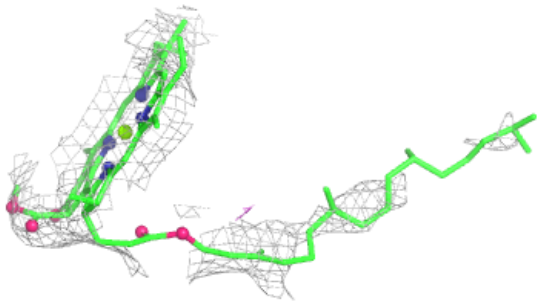


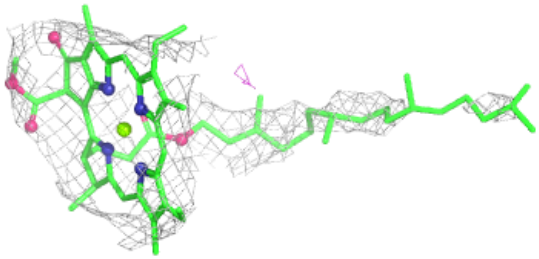


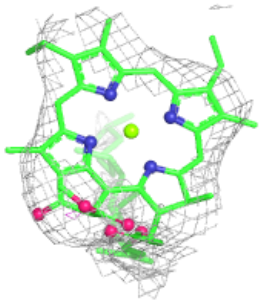


Electron density around CLA B 1015:

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

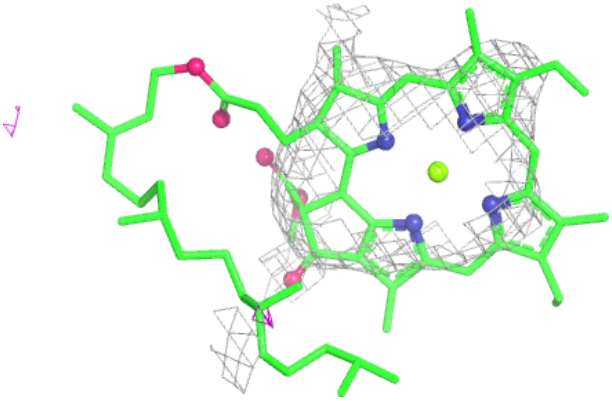


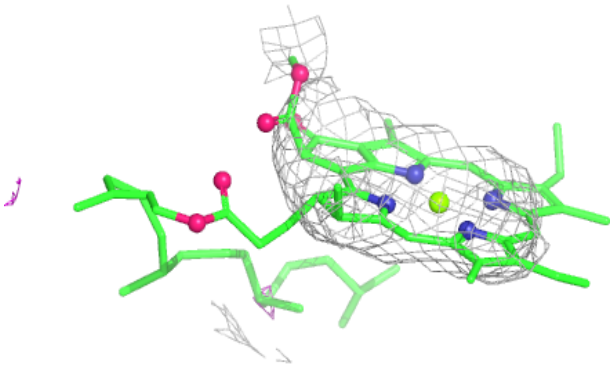




Electron density around CLA c 6033:

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

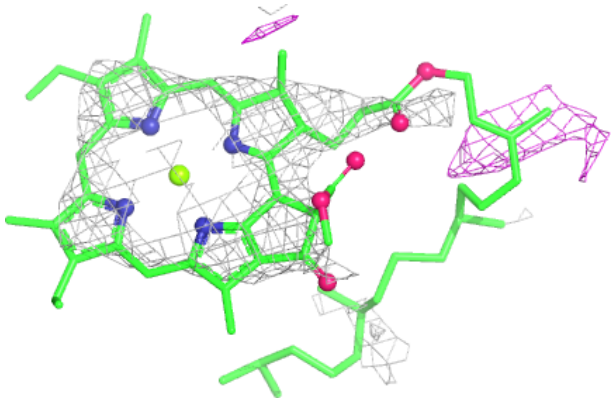


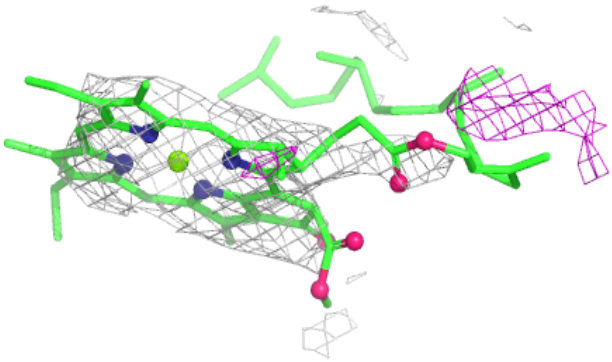


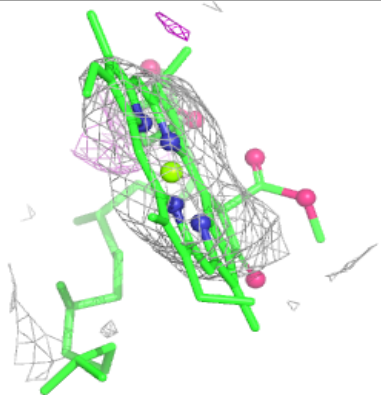


Electron density around CLA C 1033:

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

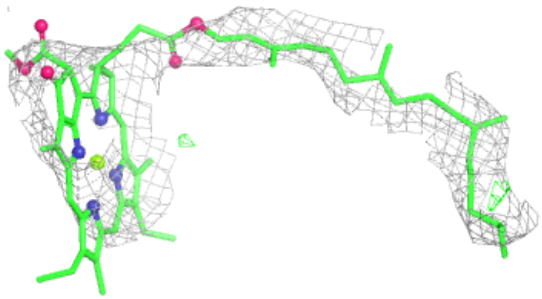


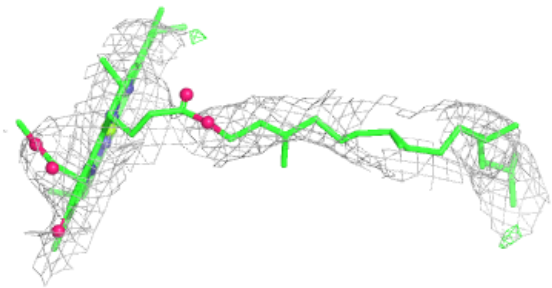


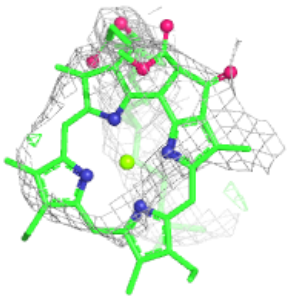


Electron density around CLA H 1017:

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

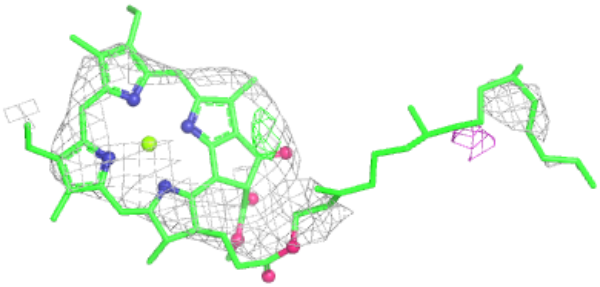


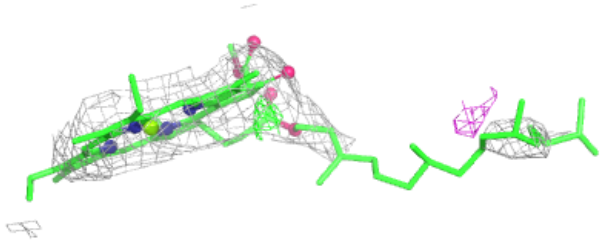


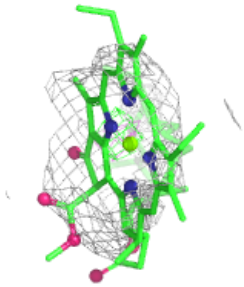


Electron density around CLA B 1010:

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

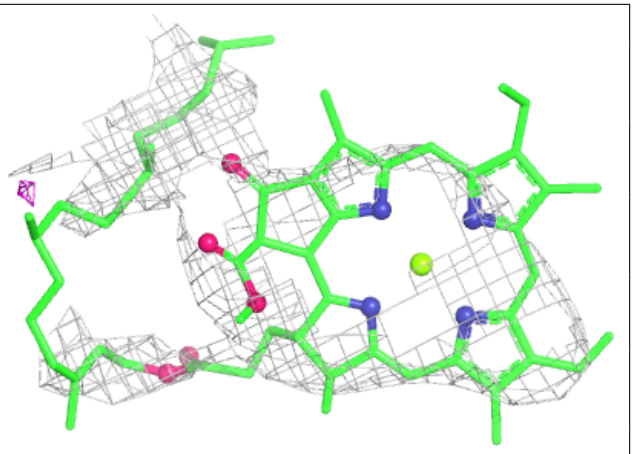


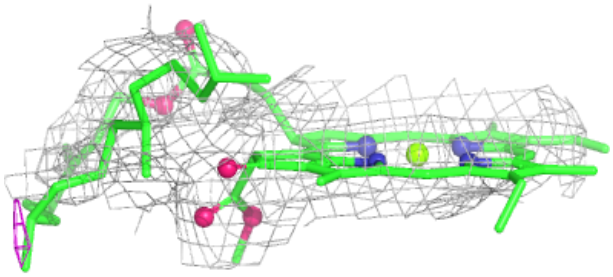




Electron density around CLA b 6018:

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

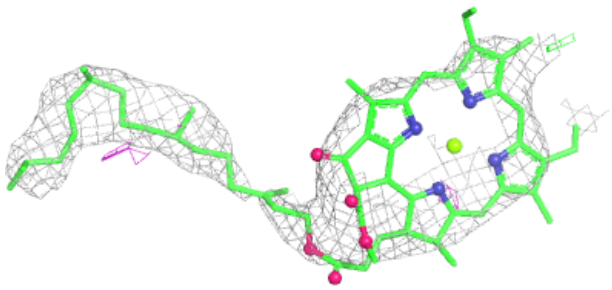


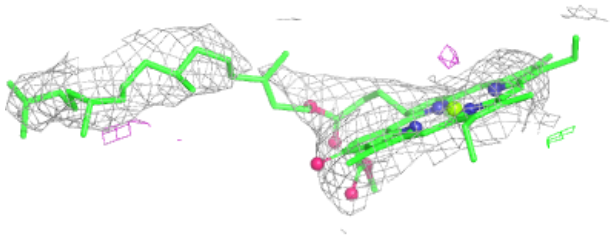


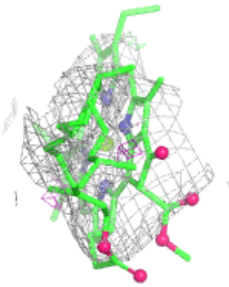


Electron density around CLA b 6010:

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

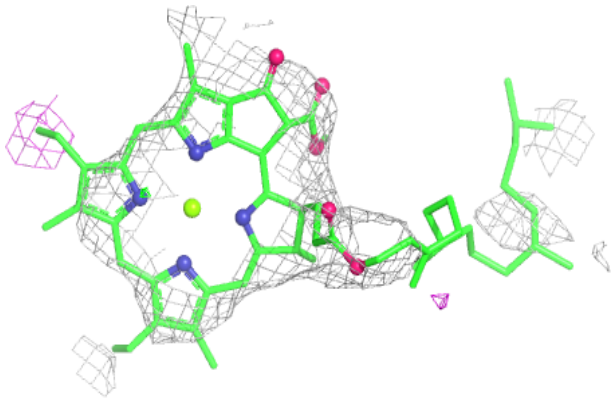


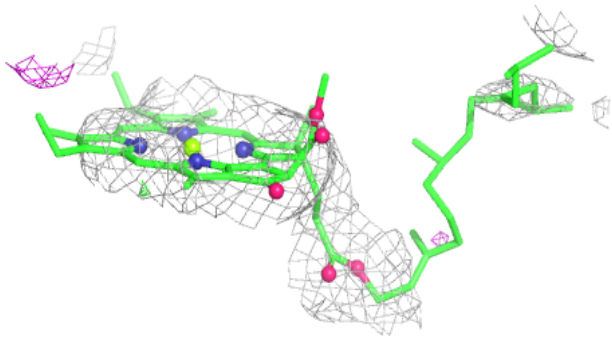


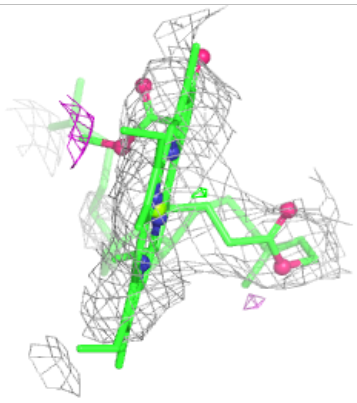


Electron density around CLA b 6020:

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

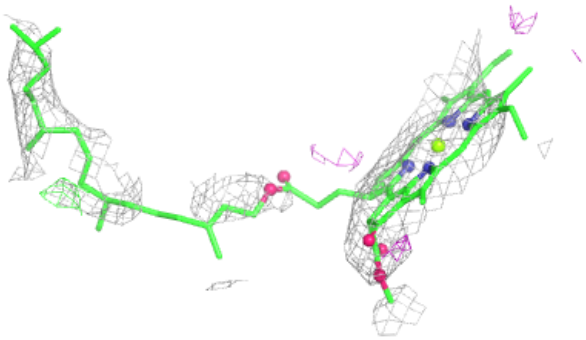


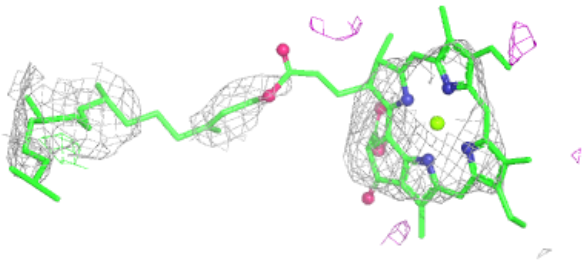




Electron density around CLA D 1004:

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

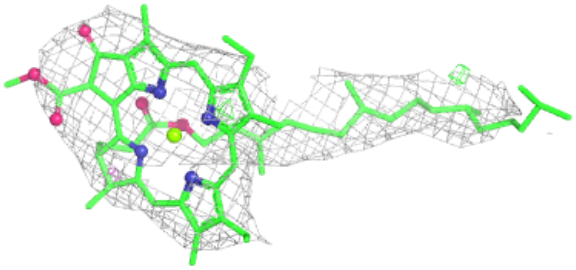


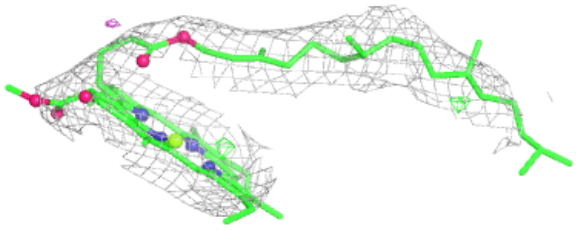


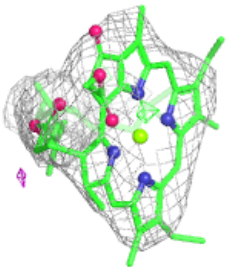


Electron density around CLA B 1016:

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

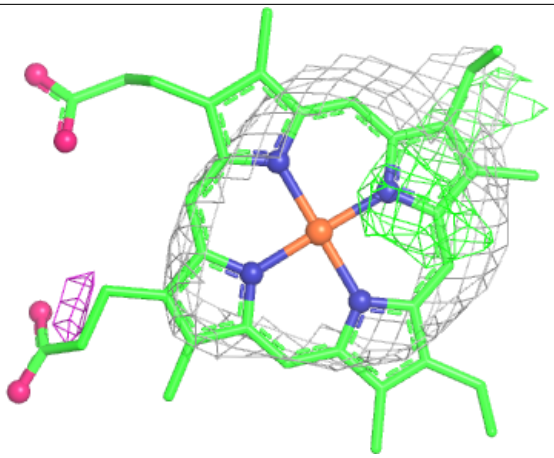


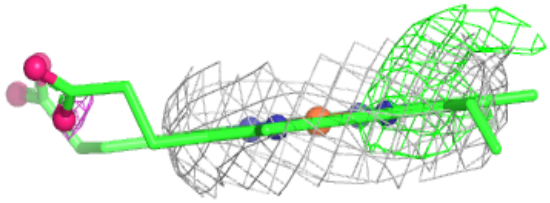


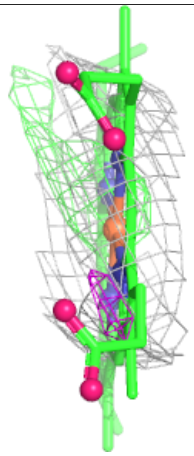


Electron density around HEM F 1040:

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

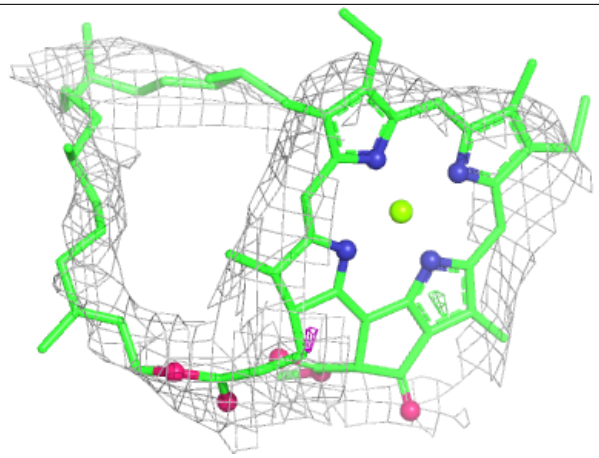


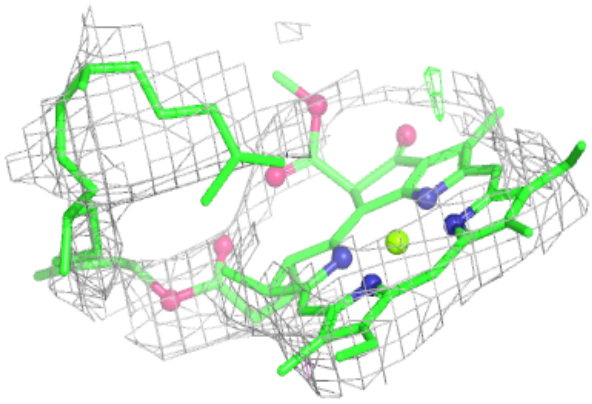




Electron density around CLA b 6023:

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

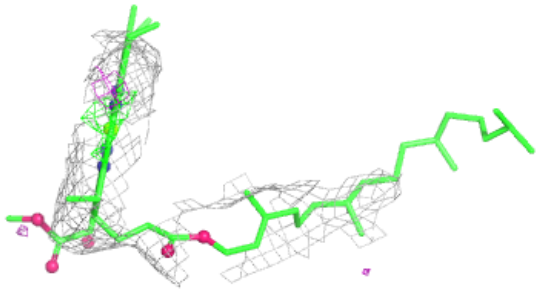


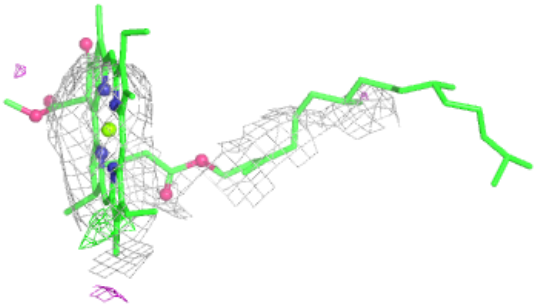


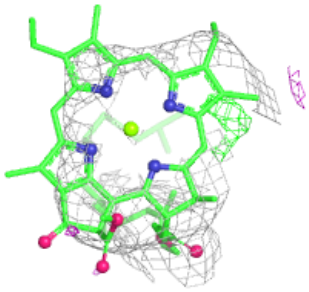


Electron density around CLA b 6013:

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

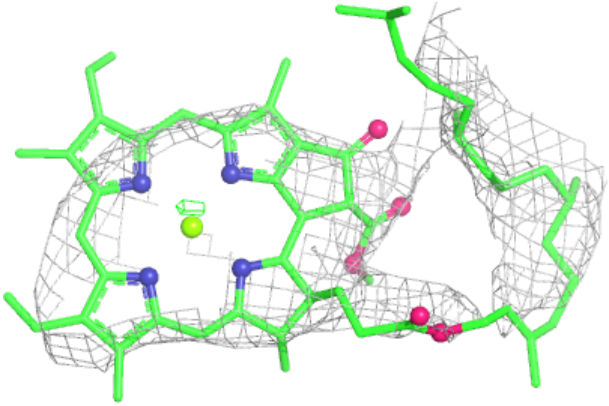


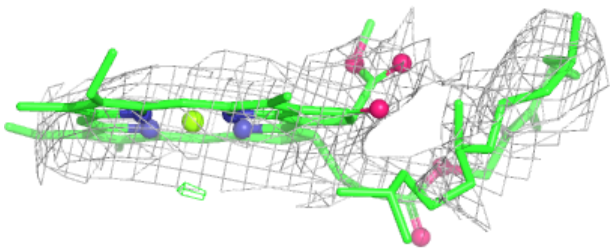


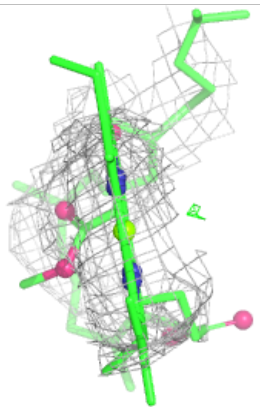


Electron density around CLA B 1018:

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

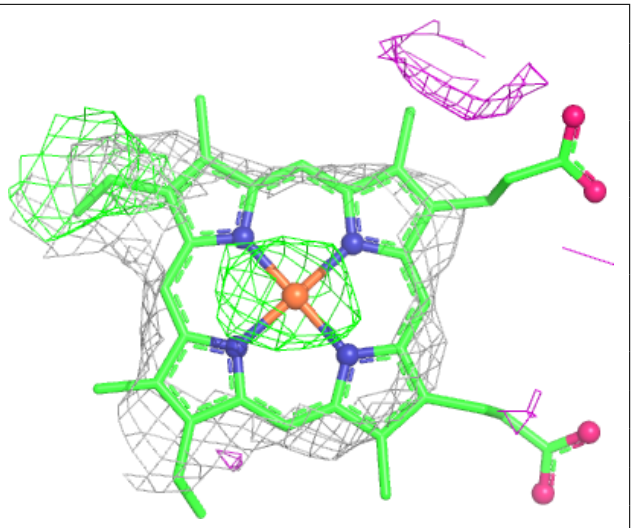


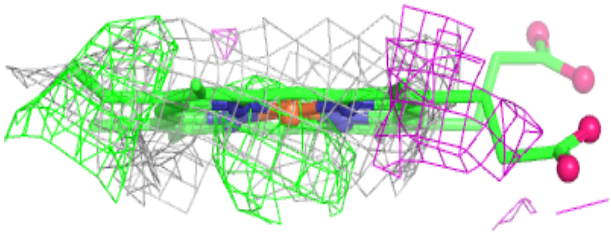


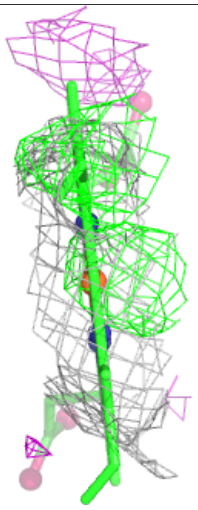


Electron density around HEM V 1041:

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





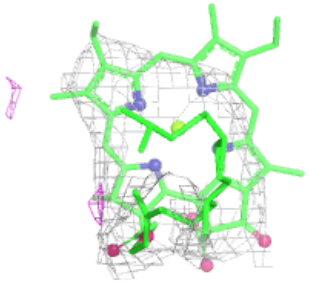


Electron density around CLA B 1013:

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

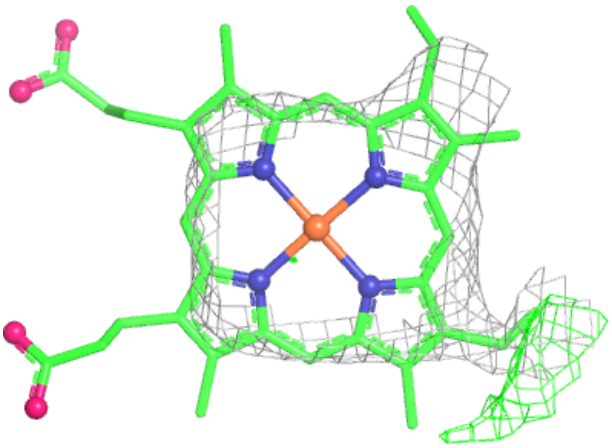


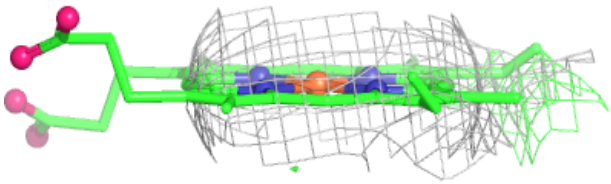


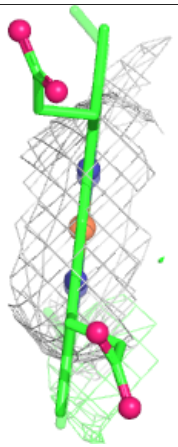


Electron density around HEM v 6041:

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

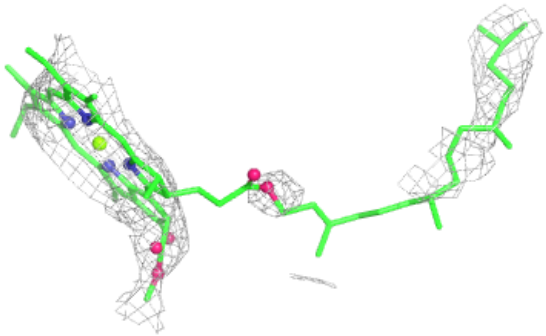


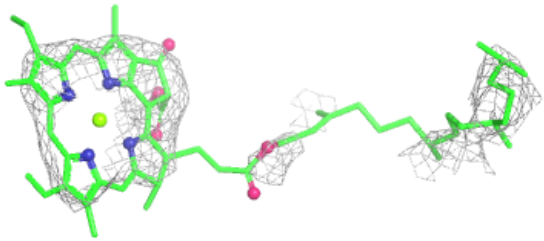


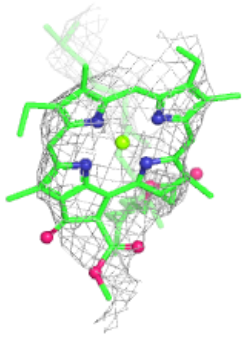


Electron density around CLA d 6004:

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

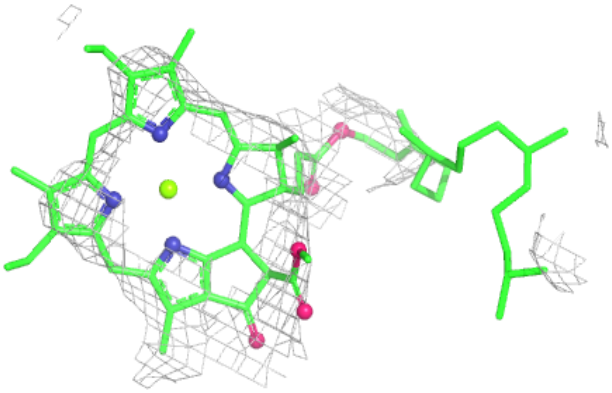


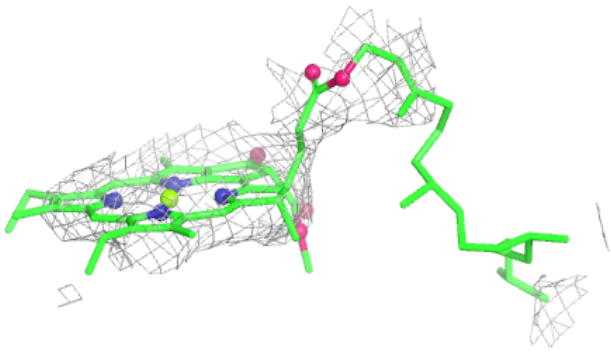


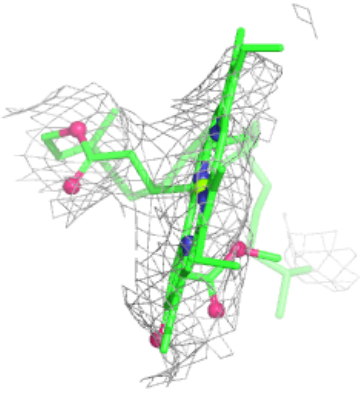


Electron density around CLA B 1020:

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







6.5 Other polymers (i)

There are no such residues in this entry.