wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 07:25 AM EDT

PDB ID	:	4V82 / pdb_00004v82
Title	:	Crystal structure of cyanobacterial Photosystem II in complex with terbutryn
Authors	:	Gabdulkhakov, A.; Broser, M.; Guskov, A.; Kern, J.; Glockner, C.; Muh, F.; Saenger, W.; Zouni, A.
Deposited on	:	2010-11-30
Resolution	:	3.20 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:

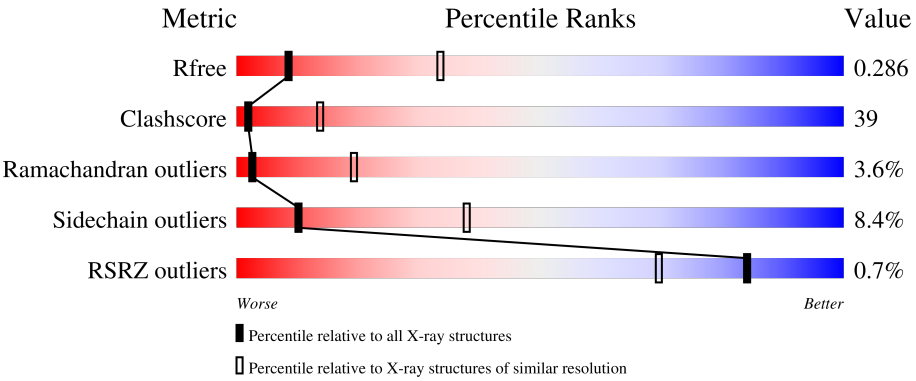
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.20 Å.

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



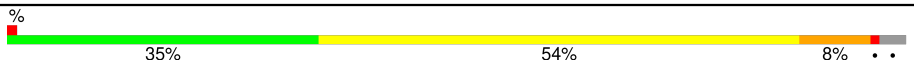
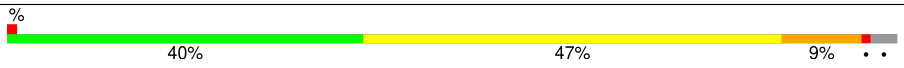
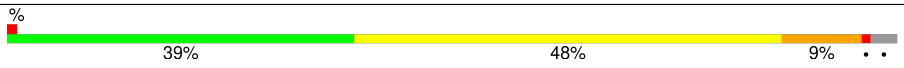
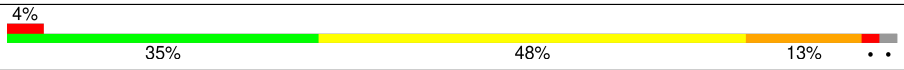
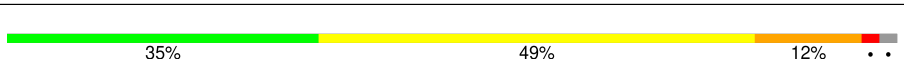
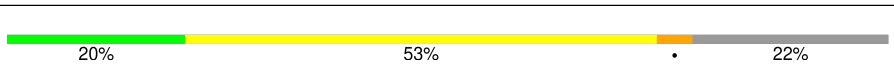
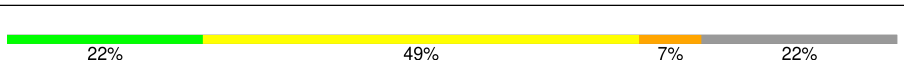
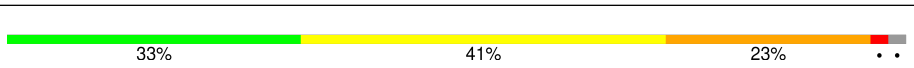
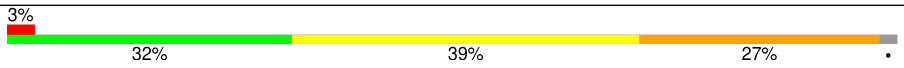
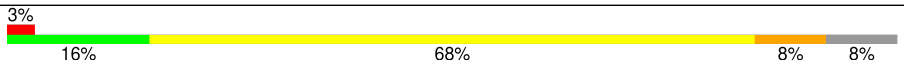
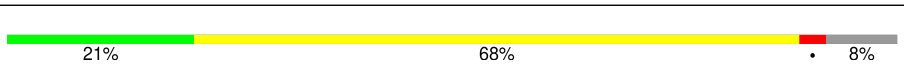
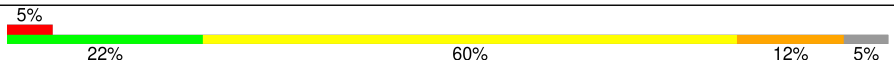
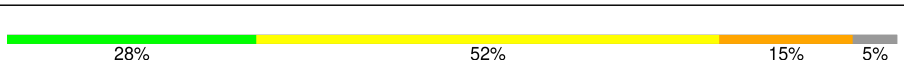
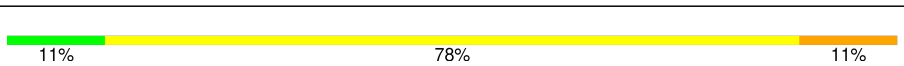
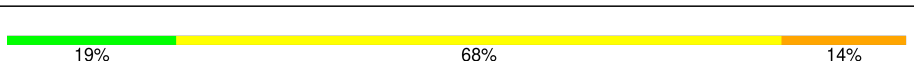
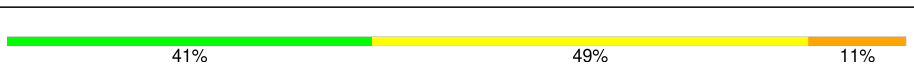
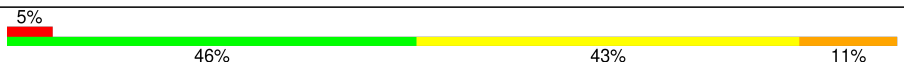
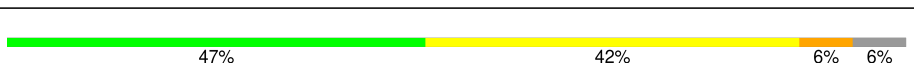
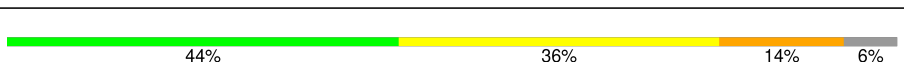
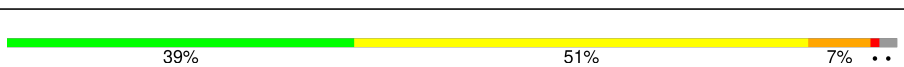
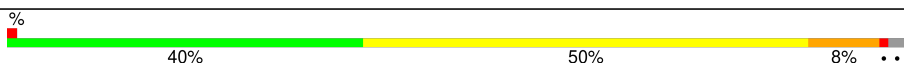
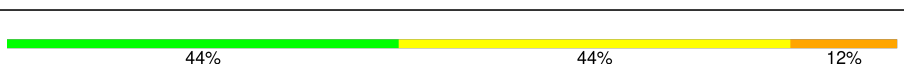
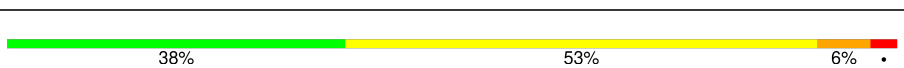
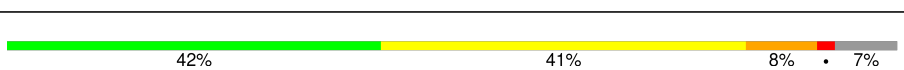
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	AA	344	36% 52% 8%
1	BA	344	35% 53% 8%
2	AB	510	% 43% 45% 8%
2	BB	510	% 42% 45% 8%
3	AC	461	% 36% 53% 7%

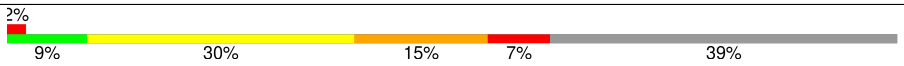
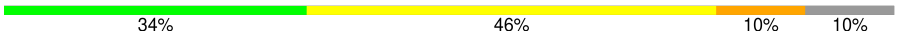
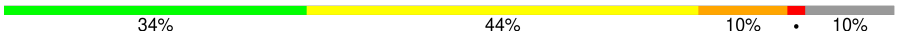
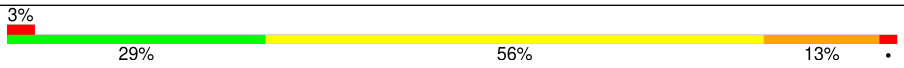
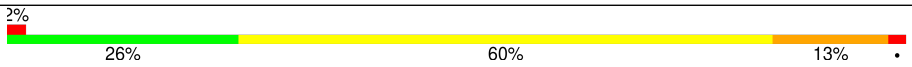
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Mol	Chain	Length	Quality of chain
3	BC	461	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	

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Mol	Chain	Length	Quality of chain
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	41	
18	BX	41	
19	AY	28	
19	BY	28	
20	AZ	62	
20	BZ	62	

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
24	CLA	AA	404	X	-	-	-
24	CLA	AA	405	X	-	-	-
24	CLA	AA	406	X	-	-	-
24	CLA	AA	407	X	-	-	-
24	CLA	AB	601	X	-	-	-
24	CLA	AB	602	X	-	-	-
24	CLA	AB	603	X	-	-	-
24	CLA	AB	604	X	-	-	-
24	CLA	AB	605	X	-	-	-
24	CLA	AB	606	X	-	-	-
24	CLA	AB	607	X	-	-	-
24	CLA	AB	608	X	-	-	-
24	CLA	AB	609	X	-	-	-
24	CLA	AB	610	X	-	-	-
24	CLA	AB	611	X	-	-	-
24	CLA	AB	612	X	-	-	-
24	CLA	AB	613	X	-	-	-
24	CLA	AB	614	X	-	-	-
24	CLA	AB	615	X	-	-	-
24	CLA	AB	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	AC	501	X	-	-	-
24	CLA	AC	502	X	-	-	-
24	CLA	AC	503	X	-	-	-
24	CLA	AC	504	X	-	-	-
24	CLA	AC	505	X	-	-	-
24	CLA	AC	506	X	-	-	-
24	CLA	AC	507	X	-	-	-
24	CLA	AC	508	X	-	-	-
24	CLA	AC	509	X	-	-	-
24	CLA	AC	510	X	-	-	-
24	CLA	AC	511	X	-	-	-
24	CLA	AC	512	X	-	-	-
24	CLA	AC	513	X	-	-	-
24	CLA	AD	401	X	-	-	-
24	CLA	AD	404	X	-	-	-
24	CLA	BA	5405	X	-	-	-
24	CLA	BA	5406	X	-	-	-
24	CLA	BA	5407	X	-	-	-
24	CLA	BA	5408	X	-	-	-
24	CLA	BB	5605	X	-	-	-
24	CLA	BB	5606	X	-	-	-
24	CLA	BB	5607	X	-	-	-
24	CLA	BB	5608	X	-	-	-
24	CLA	BB	5609	X	-	-	-
24	CLA	BB	5610	X	-	-	-
24	CLA	BB	5611	X	-	-	-
24	CLA	BB	5612	X	-	-	-
24	CLA	BB	5613	X	-	-	-
24	CLA	BB	5614	X	-	-	-
24	CLA	BB	5615	X	-	-	-
24	CLA	BB	5616	X	-	-	-
24	CLA	BB	5617	X	-	-	-
24	CLA	BB	5618	X	-	-	-
24	CLA	BB	5619	X	-	-	-
24	CLA	BB	5620	X	-	-	-
24	CLA	BC	5501	X	-	-	-
24	CLA	BC	5502	X	-	-	-
24	CLA	BC	5503	X	-	-	-
24	CLA	BC	5504	X	-	-	-
24	CLA	BC	5505	X	-	-	-
24	CLA	BC	5506	X	-	-	-
24	CLA	BC	5507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	BC	5508	X	-	-	-
24	CLA	BC	5509	X	-	-	-
24	CLA	BC	5510	X	-	-	-
24	CLA	BC	5511	X	-	-	-
24	CLA	BC	5512	X	-	-	-
24	CLA	BC	5513	X	-	-	-
24	CLA	BD	5402	X	-	-	-
24	CLA	BD	5405	X	-	-	-
25	MST	AA	408	-	-	X	-
25	MST	BA	5409	-	-	X	-
28	DGD	AC	518	X	-	-	-
28	DGD	AC	519	X	-	X	-
28	DGD	BC	5518	X	-	-	-
28	DGD	BC	5519	X	-	X	-
30	SQD	AA	413	-	X	-	-
34	PHO	AD	402	X	-	-	-
34	PHO	AD	403	X	-	-	-
34	PHO	BD	5403	X	-	-	-
34	PHO	BD	5404	X	-	-	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 50266 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	BA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			
4	BD	341	Total	C	N	O	S	0	0	0
			2711	1797	441	461	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AE	82	Total 666	C 434	N 108	O 124	0	0	0
5	BE	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	AF	35	Total 282	C 192	N 46	O 43	S 1	0	0	0
6	BF	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	AH	65	Total 507	C 338	N 81	O 86	S 2	0	0	0
7	BH	65	Total 507	C 338	N 81	O 86	S 2	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	38	Total 271	C 182	N 42	O 46	S 1	0	0	0
9	BJ	38	Total 271	C 182	N 42	O 46	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	AK	37	Total 293	C 204	N 43	O 46	0	0	0

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	37	Total 304	C 202	N 48	O 53	S 1	0	0	0
11	BL	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	AM	34	Total 267	C 178	N 40	O 48	S 1	0	0	0
12	BM	34	Total 267	C 178	N 40	O 48	S 1	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 19 is a protein called PHOTOSYSTEM II PSBX PROTEIN.

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

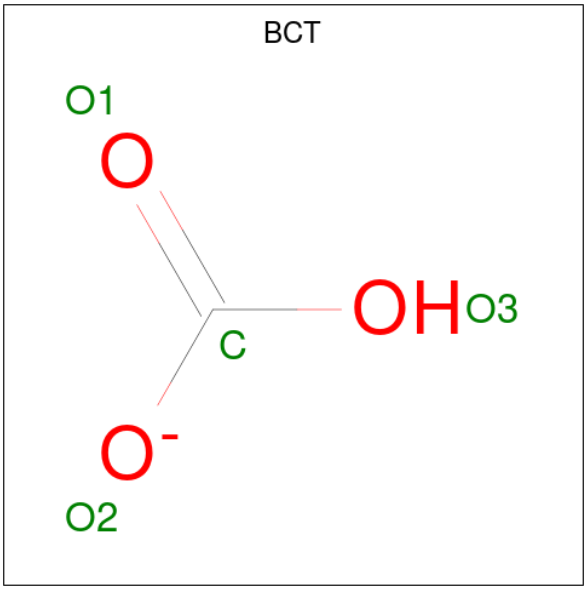
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	AA	1	Total Fe 1 1	0	0
21	BD	1	Total Fe 1 1	0	0

- Molecule 22 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).

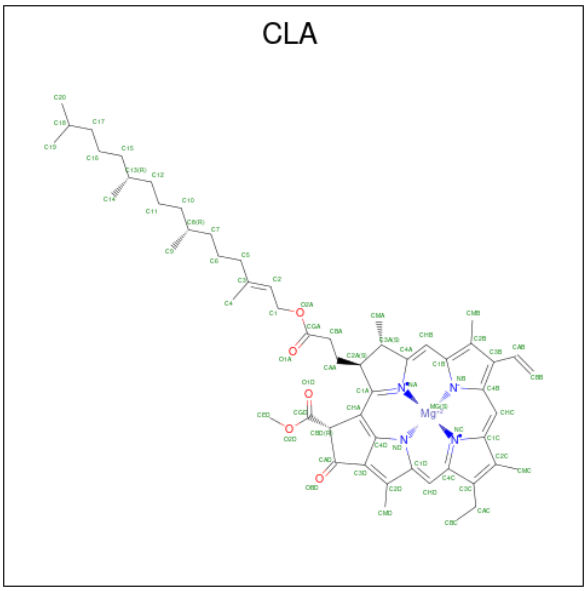


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	AA	1	Total C O 4 1 3	0	0
22	BA	1	Total C O 4 1 3	0	0

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	AA	1	Total Cl 2 2	0	1
23	BA	1	Total Cl 2 2	0	1

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	AD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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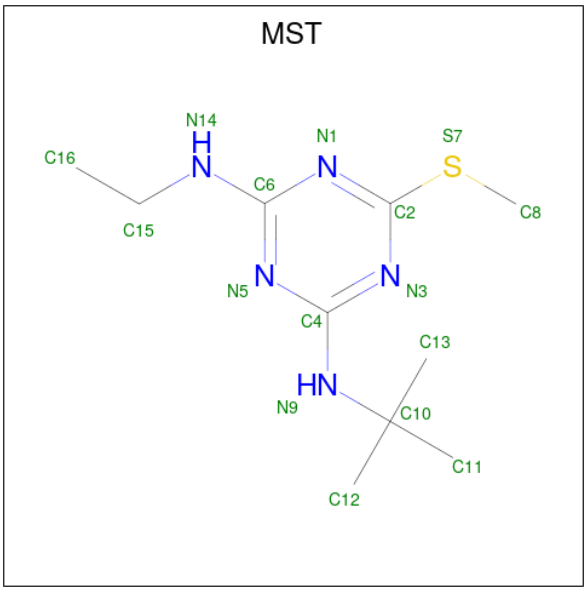
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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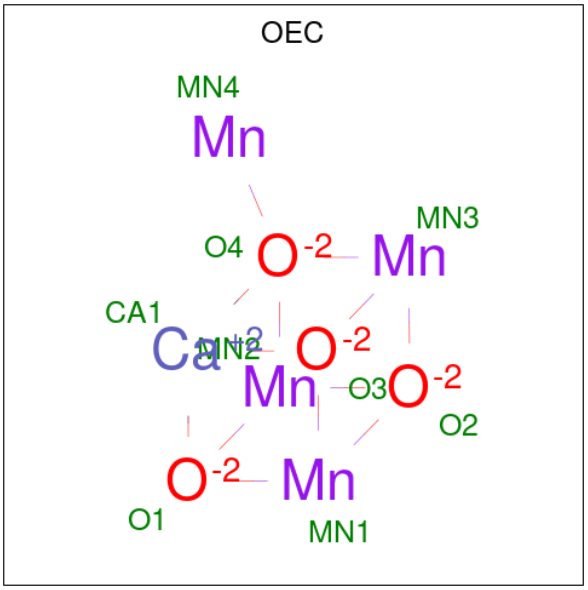
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is 2-T-BUTYLAMINO-4-ETHYLAMINO-6-METHYLTHIO-S-TRIAZINE (CCD ID: MST) (formula: $C_{10}H_{19}N_5S$).



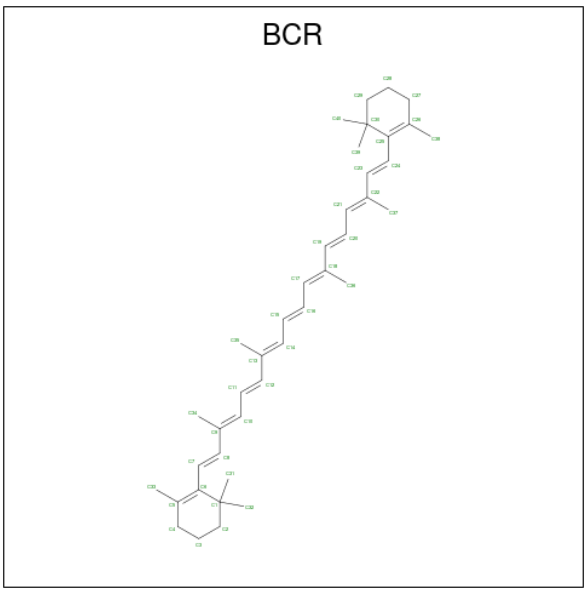
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	AA	1	Total	C	N	S	0	0
			16	10	5	1		
25	BA	1	Total	C	N	S	0	0
			16	10	5	1		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: $CaMn_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	AA	1	Total	Ca	Mn	0	0
			5	1	4		
26	BA	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



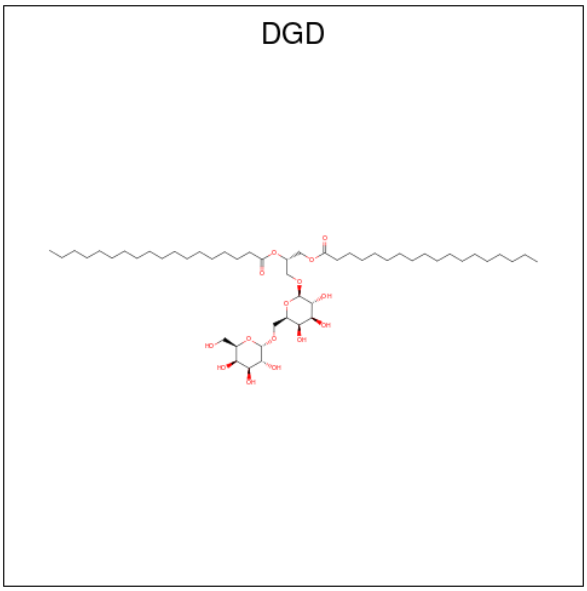
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AB	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AC	1	Total C 40 40	0	0
27	AD	1	Total C 40 40	0	0
27	AJ	1	Total C 40 40	0	0
27	AK	1	Total C 40 40	0	0
27	AT	1	Total C 40 40	0	0
27	AX	1	Total C 40 40	0	0
27	BA	1	Total C 40 40	0	0

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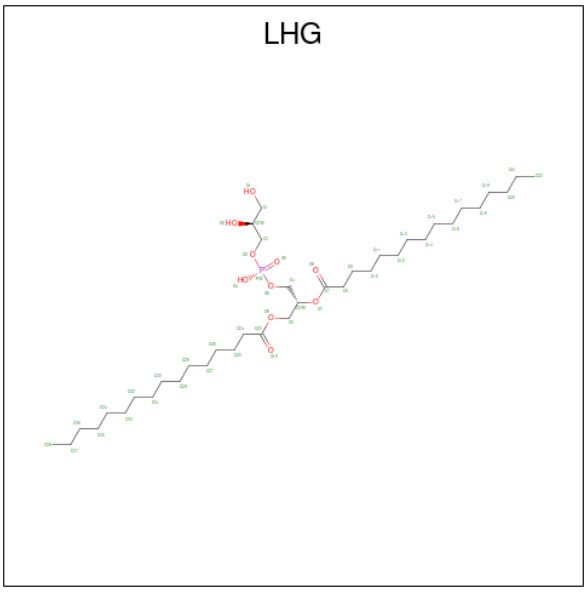
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BB	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BC	1	Total C 40 40	0	0
27	BD	1	Total C 40 40	0	0
27	BJ	1	Total C 40 40	0	0
27	BK	1	Total C 40 40	0	0
27	BT	1	Total C 40 40	0	0
27	BX	1	Total C 40 40	0	0

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



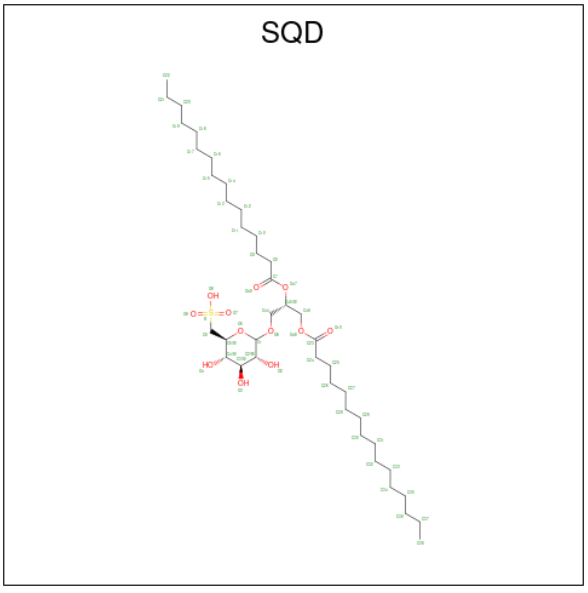
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	AA	1	Total C O 56 41 15	0	0
28	AB	1	Total C O 52 37 15	0	0
28	AC	1	Total C O 53 38 15	0	0
28	AC	1	Total C O 62 47 15	0	0
28	AC	1	Total C O 66 51 15	0	0
28	AE	1	Total C O 63 48 15	0	0
28	AH	1	Total C O 58 43 15	0	0
28	BA	1	Total C O 56 41 15	0	0
28	BB	1	Total C O 52 37 15	0	0
28	BC	1	Total C O 53 38 15	0	0
28	BC	1	Total C O 62 47 15	0	0
28	BC	1	Total C O 66 51 15	0	0
28	BE	1	Total C O 63 48 15	0	0
28	BH	1	Total C O 58 43 15	0	0

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



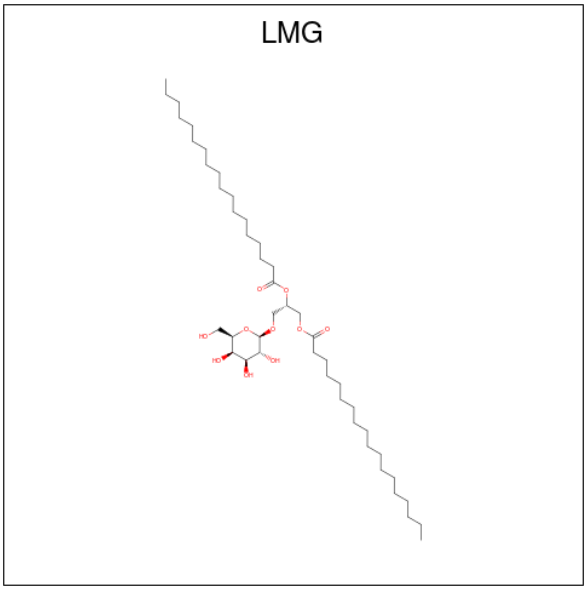
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	P	0	0
			39	28	10	1		
29	AA	1	Total	C	O	P	0	0
			37	26	10	1		
29	BA	1	Total	C	O	P	0	0
			39	28	10	1		
29	BA	1	Total	C	O	P	0	0
			37	26	10	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	AA	1	Total	C	O	S	0	0
			51	38	12	1		
30	AA	1	Total	C	O	S	0	0
			54	41	12	1		
30	AB	1	Total	C	O	S	0	0
			43	30	12	1		
30	AB	1	Total	C	O	S	0	0
			47	34	12	1		
30	AF	1	Total	C	O	S	0	0
			45	32	12	1		
30	BA	1	Total	C	O	S	0	0
			54	41	12	1		
30	BA	1	Total	C	O	S	0	0
			51	38	12	1		
30	BB	1	Total	C	O	S	0	0
			47	34	12	1		
30	BB	1	Total	C	O	S	0	0
			43	30	12	1		
30	BF	1	Total	C	O	S	0	0
			45	32	12	1		

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



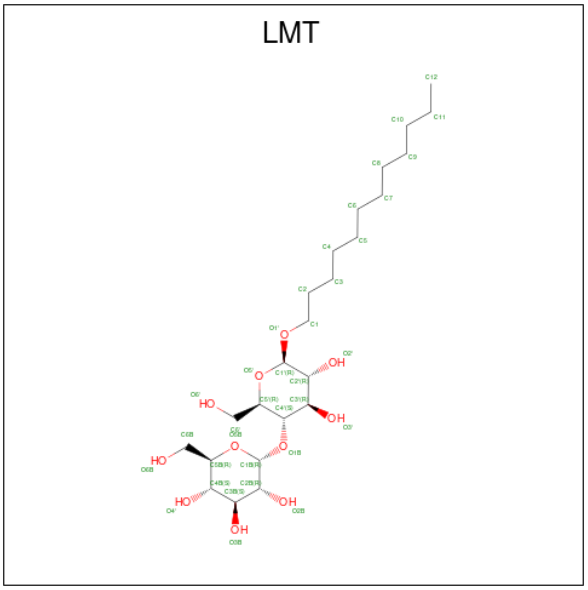
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	AA	1	Total	C	O	0	0
			44	34	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	AA	1	Total C O 42 32 10	0	0
31	AB	1	Total C O 51 41 10	0	0
31	AB	1	Total C O 49 39 10	0	0
31	AC	1	Total C O 48 38 10	0	0
31	AC	1	Total C O 45 35 10	0	0
31	AD	1	Total C O 49 39 10	0	0
31	AD	1	Total C O 48 38 10	0	0
31	AI	1	Total C O 43 33 10	0	0
31	AJ	1	Total C O 46 36 10	0	0
31	AM	1	Total C O 42 32 10	0	0
31	BA	1	Total C O 42 32 10	0	0
31	BB	1	Total C O 49 39 10	0	0
31	BC	1	Total C O 48 38 10	0	0
31	BC	1	Total C O 45 35 10	0	0
31	BD	1	Total C O 46 36 10	0	0
31	BD	1	Total C O 49 39 10	0	0
31	BD	1	Total C O 48 38 10	0	0
31	BE	1	Total C O 44 34 10	0	0
31	BI	1	Total C O 43 33 10	0	0
31	BL	1	Total C O 51 41 10	0	0
31	BM	1	Total C O 42 32 10	0	0

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



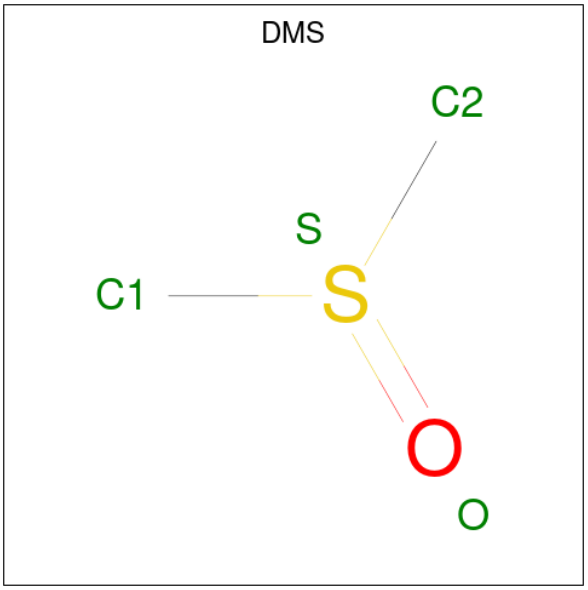
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AB	1	Total C O 35 24 11	0	0
32	AD	1	Total C O 31 20 11	0	0
32	AI	1	Total C O 35 24 11	0	0
32	AI	1	Total C O 35 24 11	0	0
32	AM	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BB	1	Total C O 35 24 11	0	0
32	BC	1	Total C O 35 24 11	0	0

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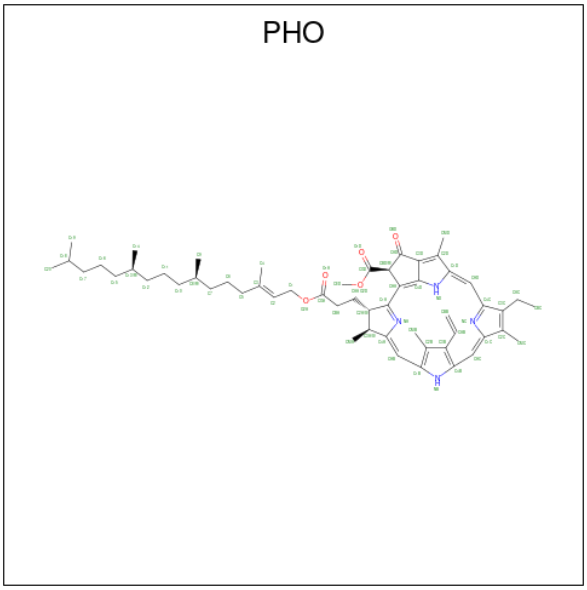
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	BD	1	Total C O 31 20 11	0	0
32	BI	1	Total C O 35 24 11	0	0
32	BM	1	Total C O 35 24 11	0	0

- Molecule 33 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



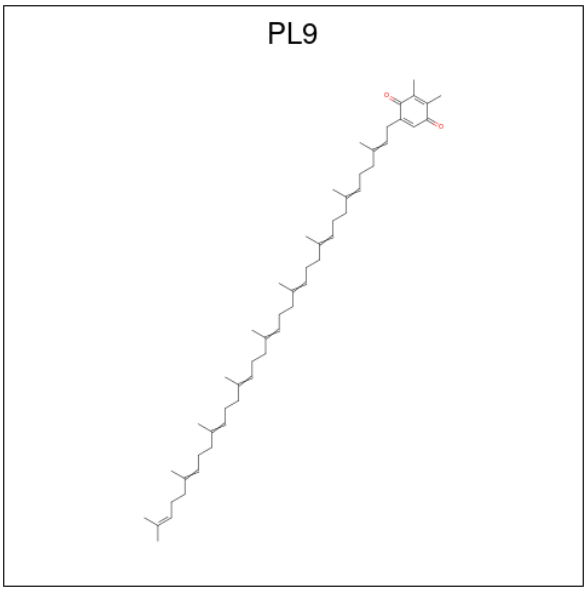
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	AB	1	Total C O S 4 2 1 1	0	0
33	AB	1	Total C O S 4 2 1 1	0	0
33	AU	1	Total C O S 4 2 1 1	0	0
33	AV	1	Total C O S 4 2 1 1	0	0
33	BB	1	Total C O S 4 2 1 1	0	0
33	BB	1	Total C O S 4 2 1 1	0	0
33	BV	1	Total C O S 4 2 1 1	0	0
33	BV	1	Total C O S 4 2 1 1	0	0

- Molecule 34 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



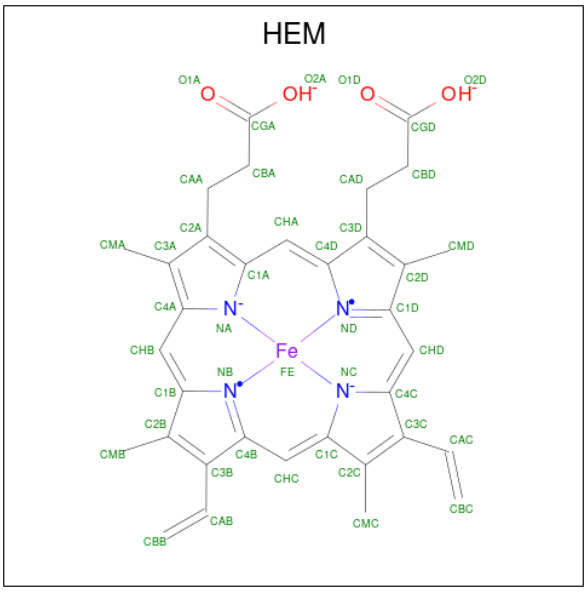
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	AD	1	Total C N O 64 55 4 5	0	0
34	AD	1	Total C N O 64 55 4 5	0	0
34	BD	1	Total C N O 64 55 4 5	0	0
34	BD	1	Total C N O 64 55 4 5	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	AD	1	Total C O 55 53 2	0	0
35	BD	1	Total C O 55 53 2	0	0

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	AF	1	Total C Fe N O 43 34 1 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	AV	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
36	BF	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
36	BV	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

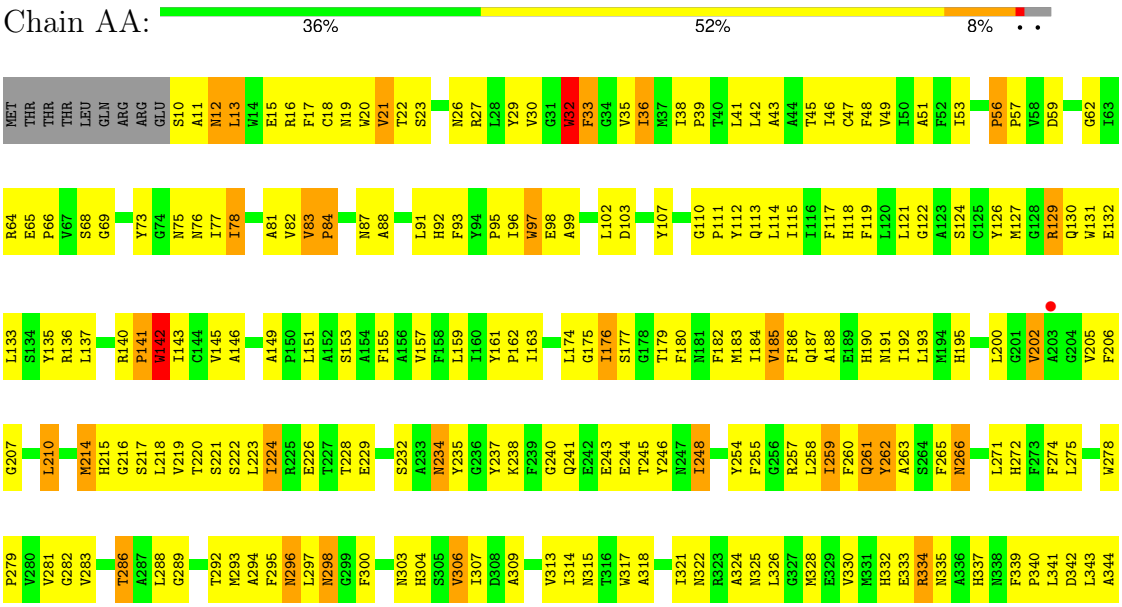
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	AF	1	Total	Ca	0	0
			1	1		
37	AK	1	Total	Ca	0	0
			1	1		
37	AO	1	Total	Ca	0	0
			1	1		
37	BF	1	Total	Ca	0	0
			1	1		
37	BK	1	Total	Ca	0	0
			1	1		
37	BO	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

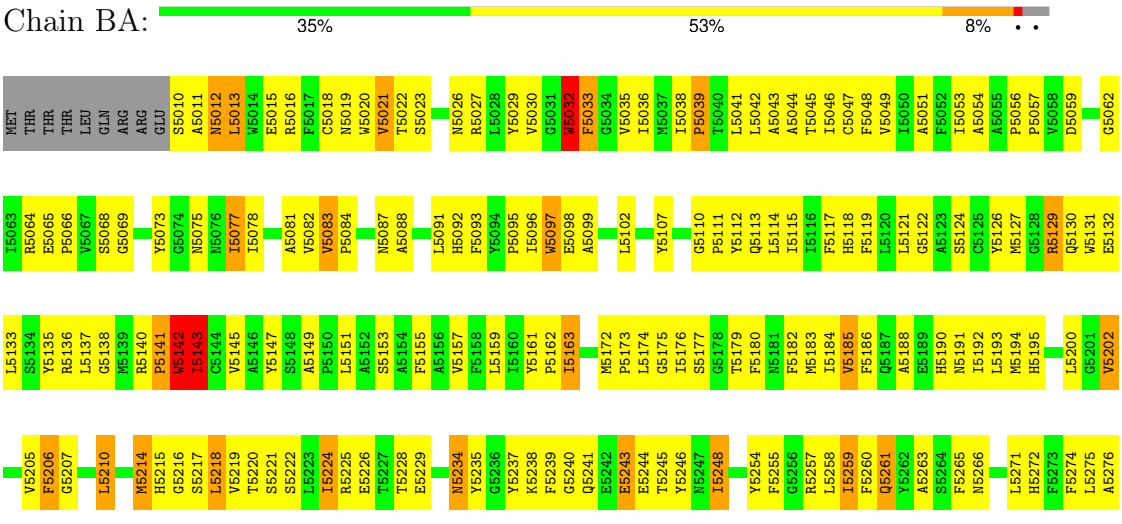
• Molecule 1: Photosystem Q(B) protein 1

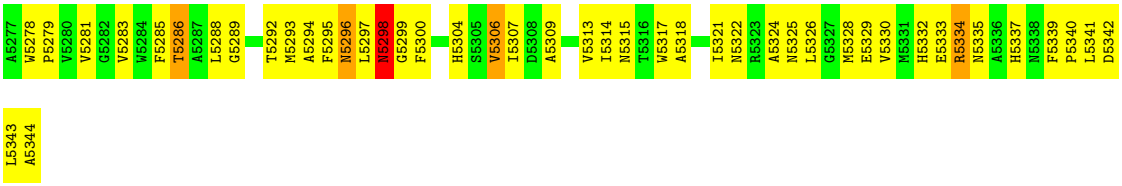
Chain AA:



• Molecule 1: Photosystem Q(B) protein 1

Chain BA:

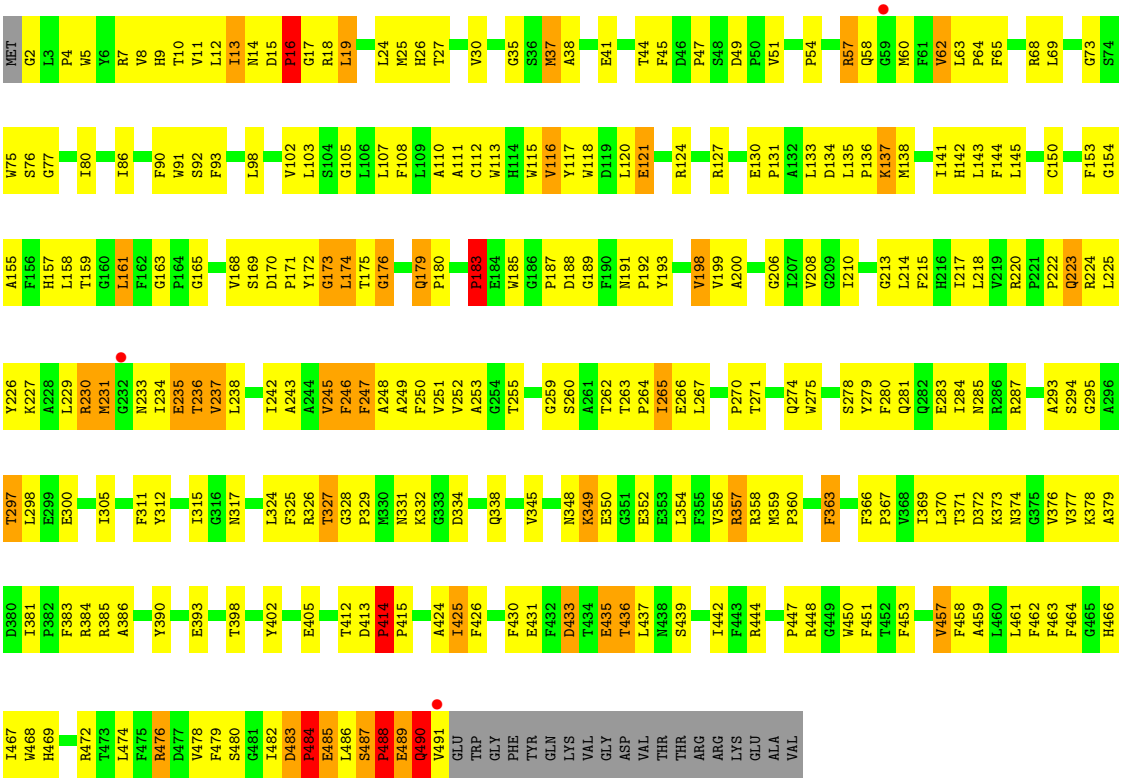




• Molecule 2: Photosystem II core light harvesting protein

Chain AB:

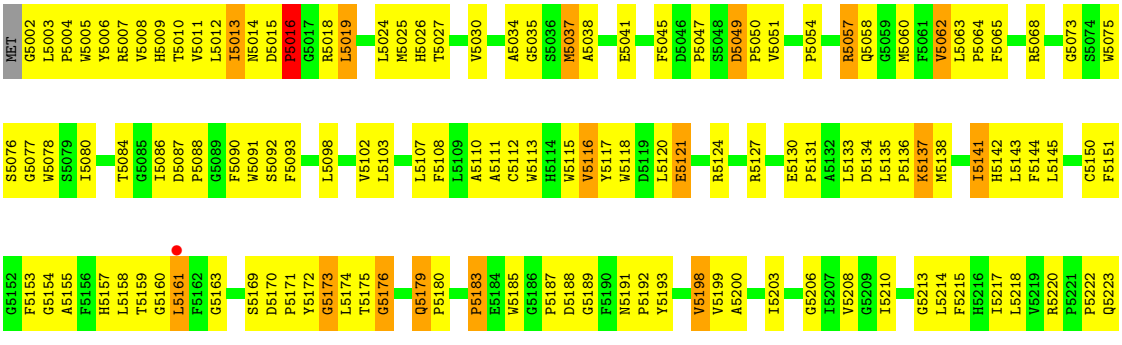


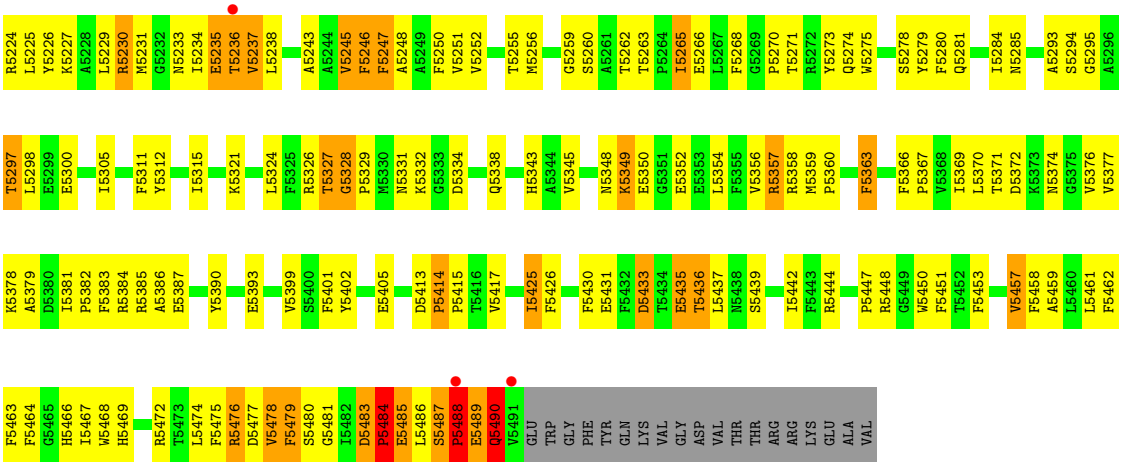


• Molecule 2: Photosystem II core light harvesting protein

Chain BB:



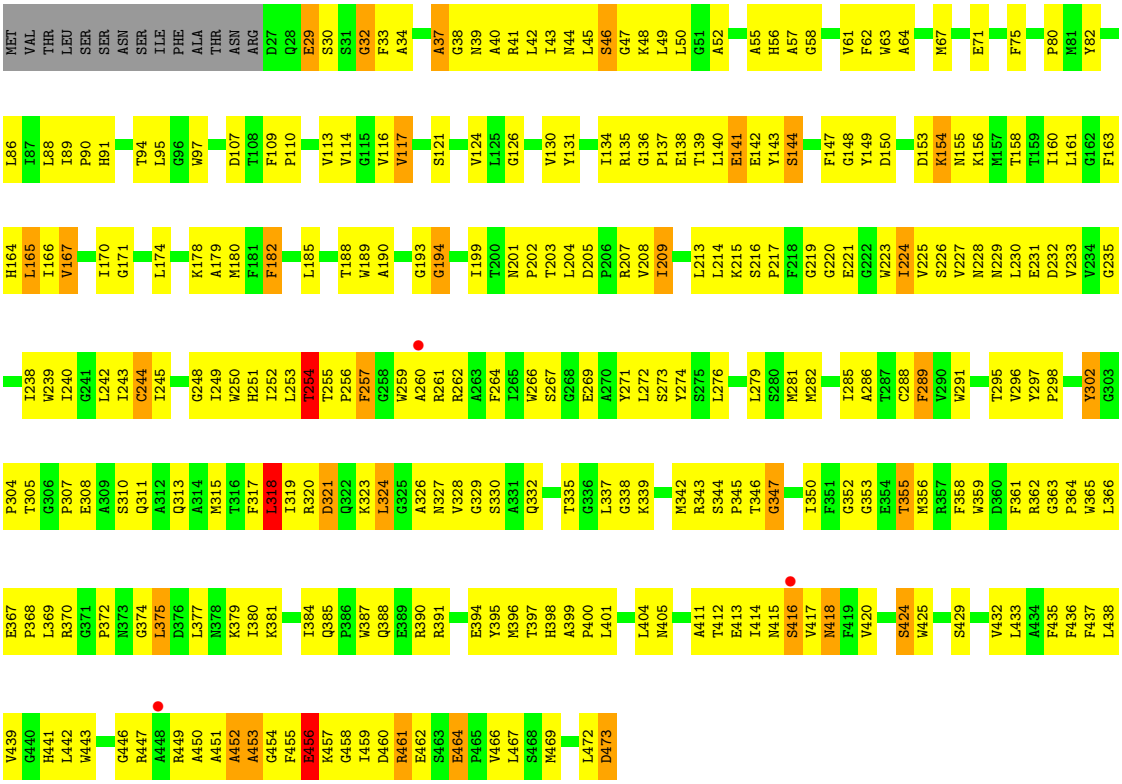




• Molecule 3: Photosystem II CP43 protein

Chain AC:

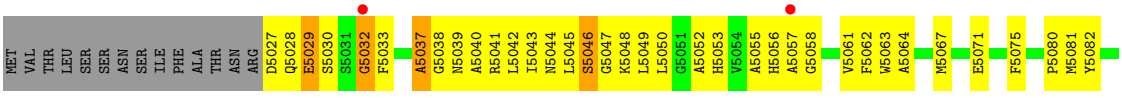


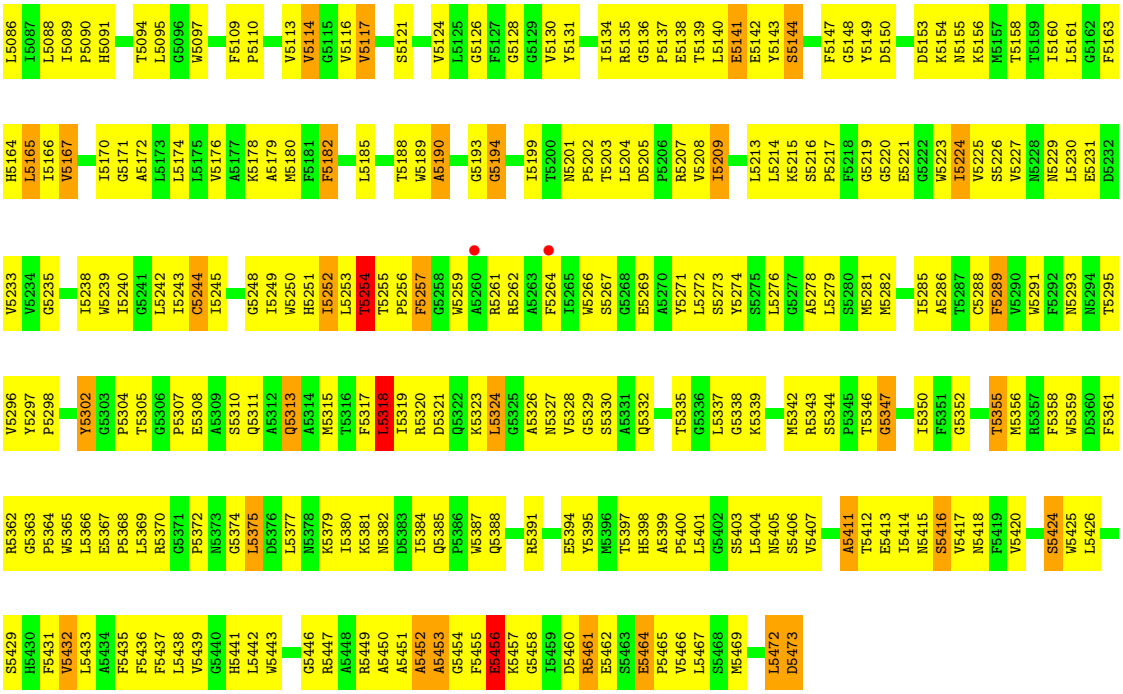


• Molecule 3: Photosystem II CP43 protein

Chain BC:



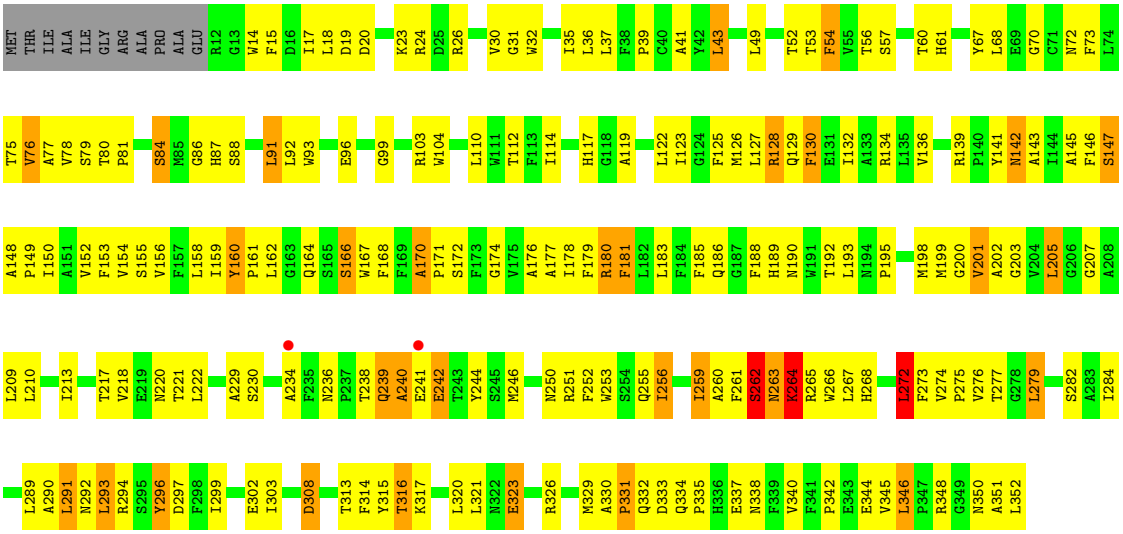




• Molecule 4: Photosystem II D2 protein

Chain AD:

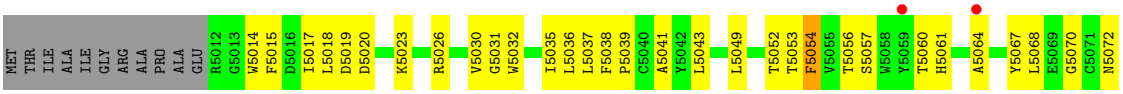


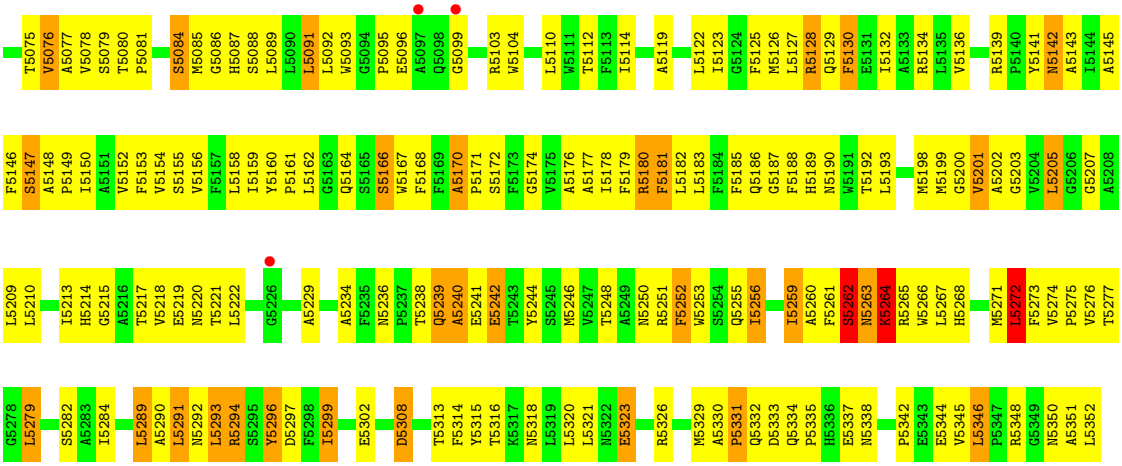


• Molecule 4: Photosystem II D2 protein

Chain BD:



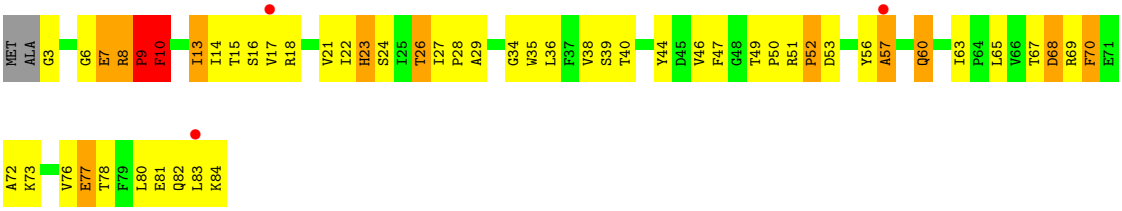




• Molecule 5: Cytochrome b559 subunit alpha

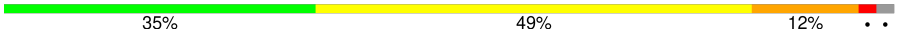
Chain AE:

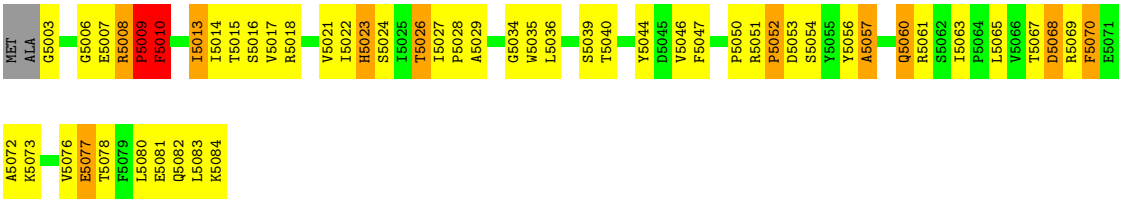




• Molecule 5: Cytochrome b559 subunit alpha

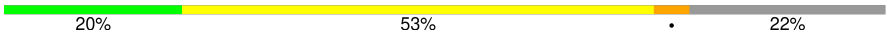
Chain BE:

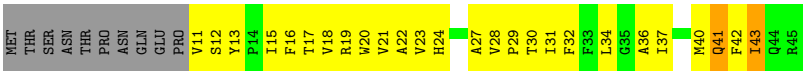




• Molecule 6: Cytochrome b559 subunit beta

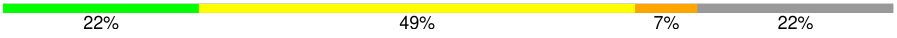
Chain AF:





• Molecule 6: Cytochrome b559 subunit beta

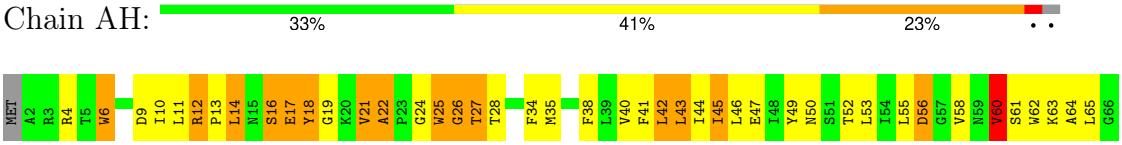
Chain BF:





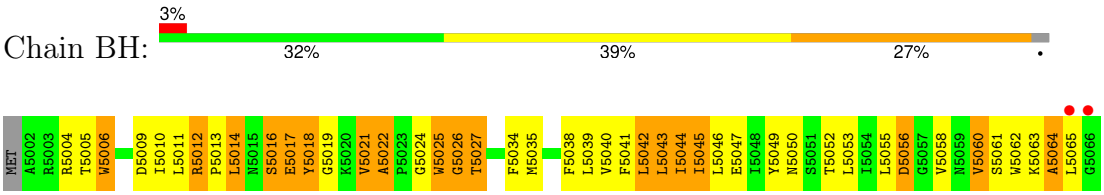
• Molecule 7: Photosystem II reaction center protein H

Chain AH:



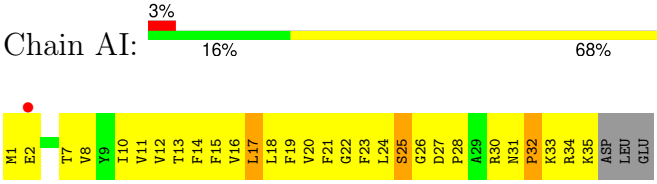
• Molecule 7: Photosystem II reaction center protein H

Chain BH:



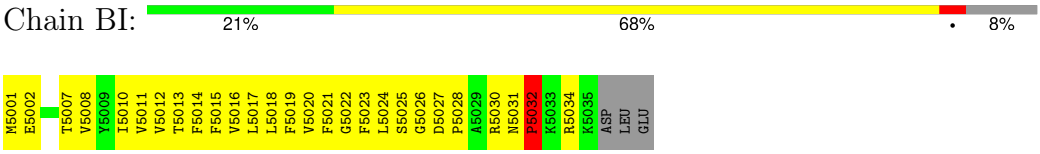
• Molecule 8: Photosystem II reaction center protein I

Chain AI:



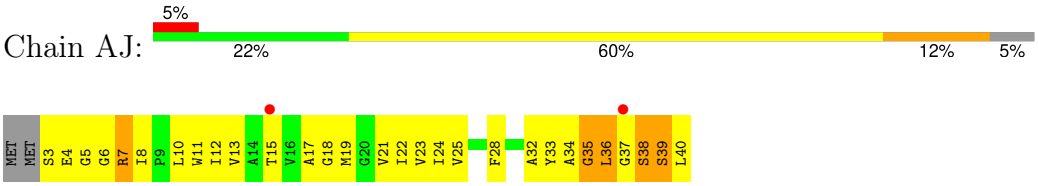
• Molecule 8: Photosystem II reaction center protein I

Chain BI:



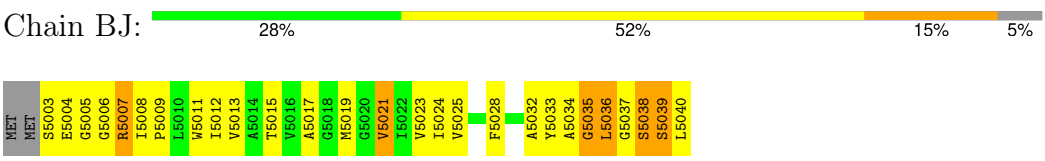
• Molecule 9: Photosystem II reaction center protein J

Chain AJ:



• Molecule 9: Photosystem II reaction center protein J

Chain BJ:



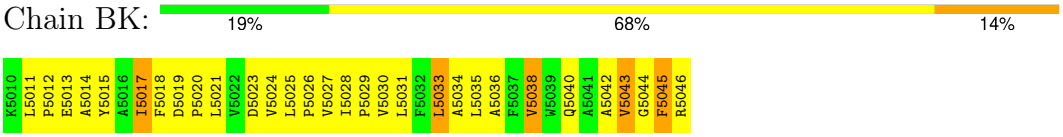
• Molecule 10: Photosystem II reaction center protein K

Chain AK:



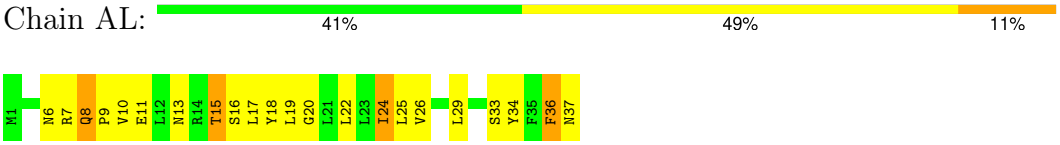
• Molecule 10: Photosystem II reaction center protein K

Chain BK:



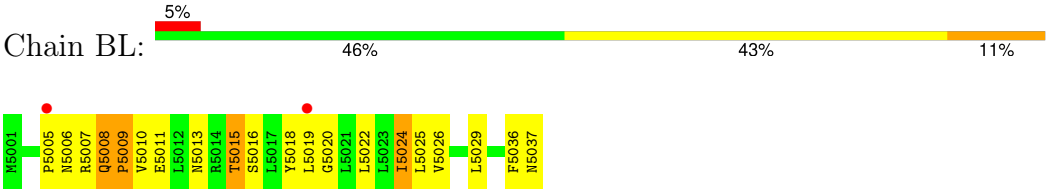
• Molecule 11: Photosystem II reaction center protein L

Chain AL:



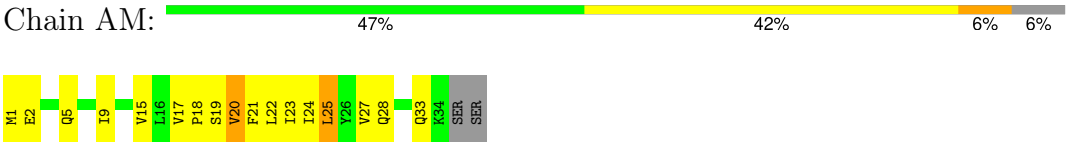
• Molecule 11: Photosystem II reaction center protein L

Chain BL:



• Molecule 12: Photosystem II reaction center protein M

Chain AM:



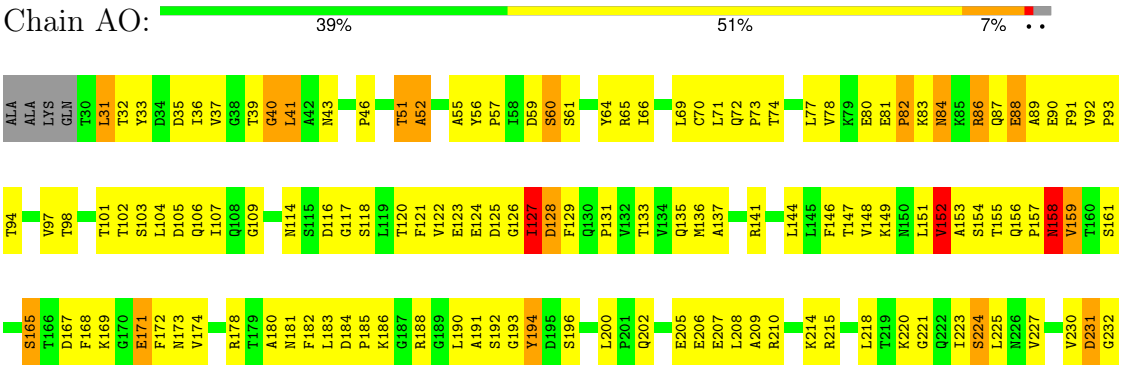
• Molecule 12: Photosystem II reaction center protein M

Chain BM:



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

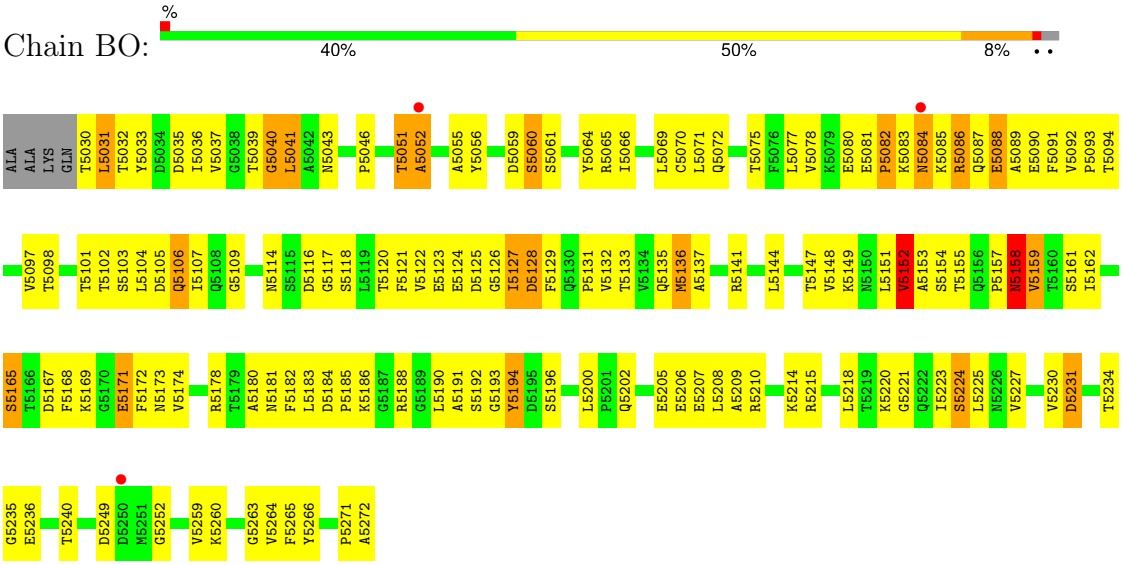
Chain AO:





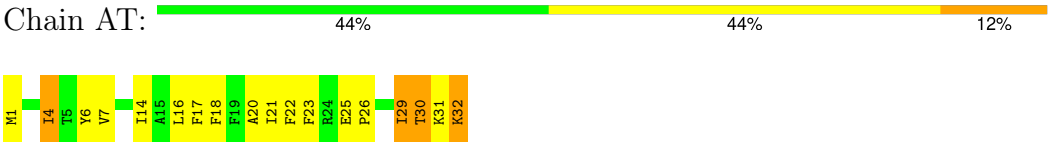
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain BO:



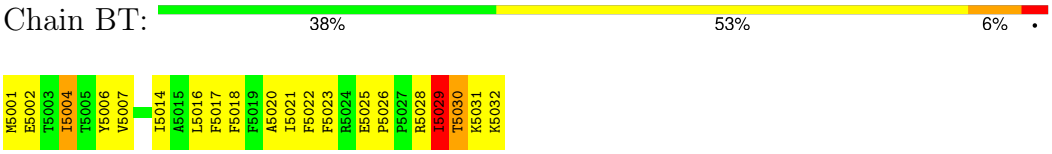
• Molecule 14: Photosystem II reaction center protein T

Chain AT:



• Molecule 14: Photosystem II reaction center protein T

Chain BT:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

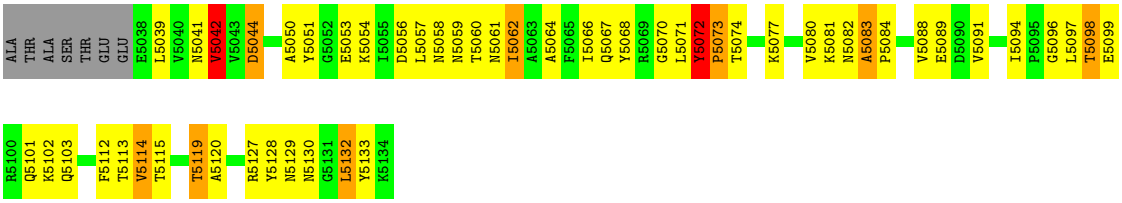
Chain AU:



• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain BU:

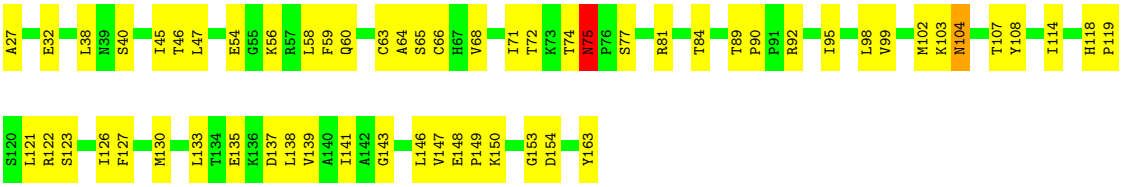




• Molecule 16: Cytochrome c-550

Chain AV:

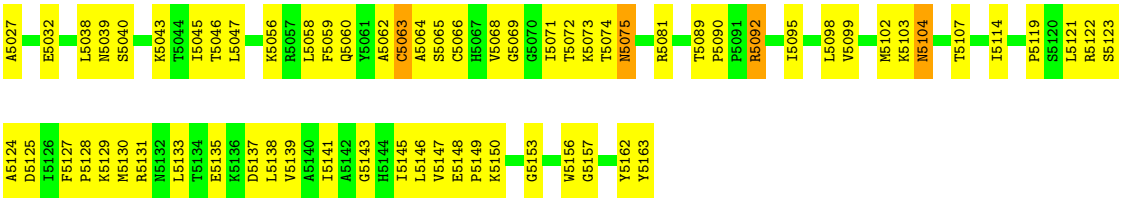




• Molecule 16: Cytochrome c-550

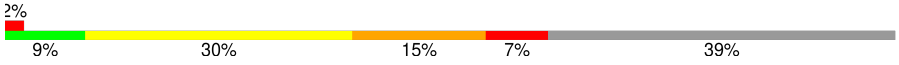
Chain BV:





• Molecule 17: Photosystem II reaction center protein ycf12

Chain Ay:





• Molecule 17: Photosystem II reaction center protein ycf12

Chain By:

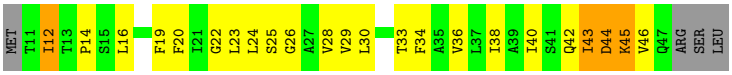




• Molecule 18: Photosystem II reaction center X protein

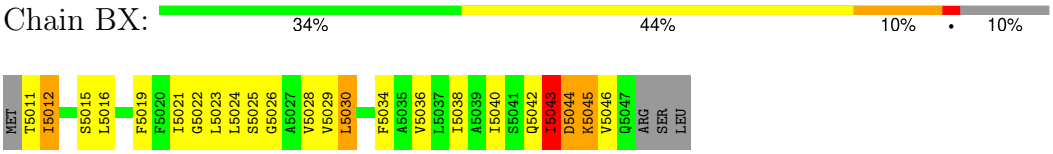
Chain AX:





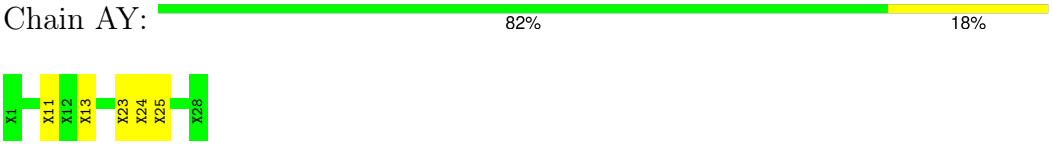
• Molecule 18: Photosystem II reaction center X protein

Chain BX:



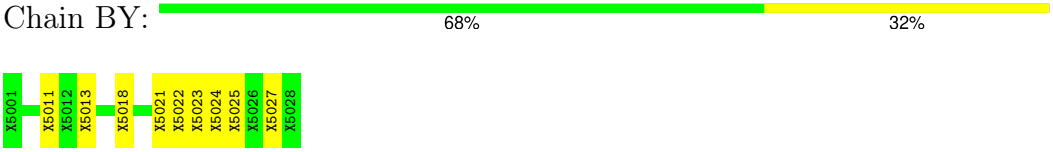
• Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain AY:



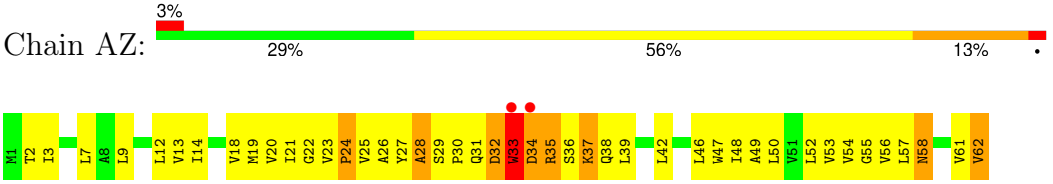
• Molecule 19: PHOTOSYSTEM II PSBX PROTEIN

Chain BY:



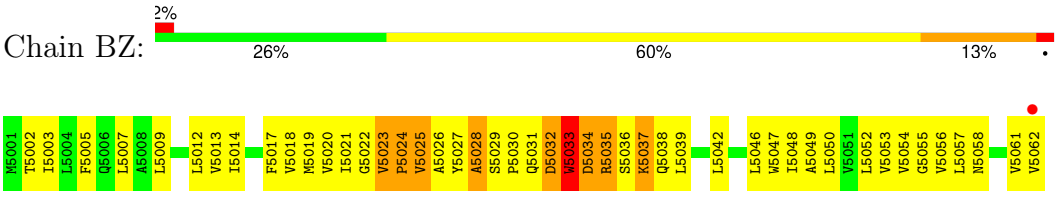
• Molecule 20: Photosystem II reaction center protein Z

Chain AZ:



• Molecule 20: Photosystem II reaction center protein Z

Chain BZ:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	128.08Å 225.37Å 305.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-3.20) 99.2 (20.00-3.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.12Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.269 , 0.299 0.264 , 0.286	Depositor DCC
R_{free} test set	3179 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	95.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 82.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	50266	wwPDB-VP
Average B, all atoms (Å^2)	119.0	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

5.1 Standard geometry

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

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	AA	0.63	0/2713	1.11	21/3700 (0.6%)
1	BA	0.59	0/2713	1.10	22/3700 (0.6%)
2	AB	0.60	0/3986	1.09	31/5433 (0.6%)
2	BB	0.60	1/3986 (0.0%)	1.09	34/5433 (0.6%)
3	AC	0.55	0/3556	1.06	14/4842 (0.3%)
3	BC	0.52	0/3556	1.06	20/4842 (0.4%)
4	AD	0.63	0/2806	1.06	11/3825 (0.3%)
4	BD	0.60	0/2806	1.05	15/3825 (0.4%)
5	AE	0.60	0/685	1.23	11/933 (1.2%)
5	BE	0.60	0/685	1.23	10/933 (1.1%)
6	AF	0.89	1/291 (0.3%)	1.04	0/397
6	BF	0.90	1/291 (0.3%)	0.96	0/397
7	AH	0.54	0/520	1.08	3/709 (0.4%)
7	BH	0.57	0/520	1.09	4/709 (0.6%)
8	AI	0.61	0/293	1.17	2/395 (0.5%)
8	BI	0.67	0/293	1.17	2/395 (0.5%)
9	AJ	0.70	0/277	1.32	2/375 (0.5%)
9	BJ	0.73	0/277	1.27	3/375 (0.8%)
10	AK	0.61	0/303	1.02	1/416 (0.2%)
10	BK	0.74	1/303 (0.3%)	1.02	1/416 (0.2%)
11	AL	0.72	0/311	1.07	1/422 (0.2%)
11	BL	0.71	0/311	1.09	0/422
12	AM	0.79	0/270	1.07	1/367 (0.3%)
12	BM	0.88	2/270 (0.7%)	1.07	0/367
13	AO	0.59	0/1876	1.07	11/2548 (0.4%)
13	BO	0.57	0/1876	1.07	13/2548 (0.5%)
14	AT	0.92	1/284 (0.4%)	1.17	1/381 (0.3%)
14	BT	0.96	2/284 (0.7%)	1.25	3/381 (0.8%)
15	AU	0.67	0/785	1.19	6/1064 (0.6%)
15	BU	0.62	0/785	1.17	6/1064 (0.6%)
16	AV	0.59	0/1081	1.01	5/1468 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	BV	0.54	0/1081	0.99	4/1468 (0.3%)
17	Ay	1.52	3/202 (1.5%)	1.52	3/272 (1.1%)
17	By	1.48	4/202 (2.0%)	1.60	2/272 (0.7%)
18	AX	0.69	0/273	1.10	1/370 (0.3%)
18	BX	0.84	2/273 (0.7%)	1.04	2/370 (0.5%)
20	AZ	0.62	0/490	1.14	4/669 (0.6%)
20	BZ	0.67	0/490	1.23	4/669 (0.6%)
All	All	0.63	18/42004 (0.0%)	1.09	274/57172 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
2	BB	0	1
All	All	0	2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	By	5030	ILE	CA-CB	-11.38	1.41	1.54
17	Ay	35	ILE	CA-CB	-8.76	1.42	1.54
6	BF	5017	THR	CA-CB	8.33	1.66	1.53
14	BT	5029	ILE	CA-CB	7.72	1.65	1.54
17	Ay	31	ALA	CA-CB	-6.35	1.43	1.53

The worst 5 of 274 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BB	5489	GLU	N-CA-C	10.04	126.27	110.70
20	AZ	34	ASP	N-CA-C	-9.33	101.68	113.43
20	BZ	5034	ASP	N-CA-C	-9.08	101.99	113.43
17	By	5022	LEU	N-CA-C	-8.95	101.63	112.54
3	AC	182	PHE	N-CA-C	8.88	123.94	113.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	262	TYR	Sidechain
2	BB	5273	TYR	Sidechain

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	AA	2628	0	2524	314	0
1	BA	2628	0	2524	330	0
2	AB	3850	0	3718	352	0
2	BB	3850	0	3718	359	0
3	AC	3444	0	3365	365	0
3	BC	3444	0	3365	371	0
4	AD	2711	0	2610	262	0
4	BD	2711	0	2610	274	0
5	AE	666	0	651	70	0
5	BE	666	0	651	76	0
6	AF	282	0	291	40	0
6	BF	282	0	291	38	0
7	AH	507	0	521	71	0
7	BH	507	0	521	76	0
8	AI	286	0	308	40	0
8	BI	286	0	305	40	0
9	AJ	271	0	276	37	0
9	BJ	271	0	276	40	0
10	AK	293	0	305	56	0
10	BK	293	0	305	51	0
11	AL	304	0	316	35	0
11	BL	304	0	313	36	0
12	AM	267	0	289	27	0
12	BM	267	0	286	27	0
13	AO	1845	0	1801	144	0
13	BO	1845	0	1801	150	0
14	AT	275	0	288	30	0
14	BT	275	0	285	29	0
15	AU	774	0	773	53	0
15	BU	774	0	773	57	0
16	AV	1060	0	1068	55	0
16	BV	1060	0	1068	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Ay	201	0	226	37	0
17	By	201	0	226	37	0
18	AX	270	0	299	32	0
18	BX	270	0	299	29	0
19	AY	140	0	32	3	0
19	BY	140	0	32	7	0
20	AZ	479	0	516	64	0
20	BZ	479	0	513	64	0
21	AA	1	0	0	0	0
21	BD	1	0	0	0	0
22	AA	4	0	0	0	0
22	BA	4	0	0	0	0
23	AA	2	0	0	1	0
23	BA	2	0	0	0	0
24	AA	260	0	288	35	0
24	AB	1040	0	1152	115	0
24	AC	845	0	936	86	0
24	AD	130	0	144	15	0
24	BA	260	0	288	40	0
24	BB	1040	0	1152	124	0
24	BC	845	0	936	88	0
24	BD	130	0	144	16	0
25	AA	16	0	19	10	0
25	BA	16	0	19	11	0
26	AA	5	0	0	0	0
26	BA	5	0	0	0	0
27	AA	40	0	56	4	0
27	AB	120	0	168	9	0
27	AC	120	0	168	22	0
27	AD	40	0	56	2	0
27	AJ	40	0	56	4	0
27	AK	40	0	56	5	0
27	AT	40	0	56	9	0
27	AX	40	0	56	6	0
27	BA	40	0	56	3	0
27	BB	120	0	168	9	0
27	BC	120	0	168	24	0
27	BD	40	0	56	2	0
27	BJ	40	0	56	3	0
27	BK	40	0	56	5	0
27	BT	40	0	56	5	0
27	BX	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AA	56	0	70	7	0
28	AB	52	0	62	0	0
28	AC	181	0	243	63	0
28	AE	63	0	87	1	0
28	AH	58	0	74	10	0
28	BA	56	0	70	7	0
28	BB	52	0	62	5	0
28	BC	181	0	243	63	0
28	BE	63	0	87	1	0
28	BH	58	0	74	10	0
29	AA	76	0	95	7	0
29	BA	76	0	95	9	0
30	AA	105	0	145	2	0
30	AB	90	0	109	9	0
30	AF	45	0	53	1	0
30	BA	105	0	145	3	0
30	BB	90	0	109	11	0
30	BF	45	0	53	1	0
31	AA	86	0	111	15	0
31	AB	100	0	139	21	0
31	AC	93	0	125	11	0
31	AD	97	0	134	14	0
31	AI	43	0	56	3	0
31	AJ	46	0	61	2	0
31	AM	42	0	54	6	0
31	BA	42	0	53	3	0
31	BB	49	0	68	4	0
31	BC	93	0	125	10	0
31	BD	143	0	195	15	0
31	BE	44	0	58	3	0
31	BI	43	0	56	4	0
31	BL	51	0	71	18	0
31	BM	42	0	54	4	0
32	AB	140	0	184	15	0
32	AD	31	0	35	0	0
32	AI	70	0	92	9	0
32	AM	35	0	46	2	0
32	BB	140	0	184	15	0
32	BC	35	0	46	3	0
32	BD	31	0	35	1	0
32	BI	35	0	46	5	0
32	BM	35	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	AB	8	0	12	1	0
33	AU	4	0	6	0	0
33	AV	4	0	6	1	0
33	BB	8	0	12	1	0
33	BV	8	0	12	1	0
34	AD	128	0	148	11	0
34	BD	128	0	148	13	0
35	AD	55	0	80	15	0
35	BD	55	0	80	15	0
36	AF	43	0	30	8	0
36	AV	43	0	30	5	0
36	BF	43	0	30	7	0
36	BV	43	0	30	7	0
37	AF	1	0	0	0	0
37	AK	1	0	0	0	0
37	AO	1	0	0	0	0
37	BF	1	0	0	0	0
37	BK	1	0	0	0	0
37	BO	1	0	0	0	0
All	All	50266	0	51335	3946	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 39.

The worst 5 of 3946 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)
1:AA:278:TRP:CE3	28:AC:519:DGD:HAG2	1.69	1.27
1:BA:5278:TRP:CE3	28:BC:5519:DGD:HAG2	1.78	1.17
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.25	1.15
24:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.29	1.14
24:BB:5612:CLA:H42	4:BD:5127:LEU:HD11	1.29	1.14

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	AA	333/344 (97%)	284 (85%)	42 (13%)	7 (2%)	5 31
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	5 31
2	AB	488/510 (96%)	418 (86%)	54 (11%)	16 (3%)	3 21
2	BB	488/510 (96%)	422 (86%)	51 (10%)	15 (3%)	3 22
3	AC	445/461 (96%)	371 (83%)	58 (13%)	16 (4%)	2 19
3	BC	445/461 (96%)	372 (84%)	56 (13%)	17 (4%)	2 18
4	AD	339/352 (96%)	286 (84%)	44 (13%)	9 (3%)	4 25
4	BD	339/352 (96%)	288 (85%)	43 (13%)	8 (2%)	4 28
5	AE	80/84 (95%)	71 (89%)	6 (8%)	3 (4%)	2 18
5	BE	80/84 (95%)	70 (88%)	7 (9%)	3 (4%)	2 18
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	3 23
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	3 23
7	AH	63/66 (96%)	47 (75%)	11 (18%)	5 (8%)	1 5
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	1 8
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1 9
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	1 9
9	AJ	36/40 (90%)	27 (75%)	6 (17%)	3 (8%)	0 4
9	BJ	36/40 (90%)	25 (69%)	8 (22%)	3 (8%)	0 4
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 11
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1 11
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	AM	32/36 (89%)	24 (75%)	8 (25%)	0	100 100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100 100
13	AO	241/247 (98%)	198 (82%)	31 (13%)	12 (5%)	1 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	2 15
14	AT	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	3 21
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	3 21
15	AU	95/104 (91%)	78 (82%)	12 (13%)	5 (5%)	1 12
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	2 16
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	18 52
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	18 52
17	Ay	26/46 (56%)	15 (58%)	7 (27%)	4 (15%)	0 0
17	By	26/46 (56%)	14 (54%)	9 (35%)	3 (12%)	0 1
18	AX	35/41 (85%)	26 (74%)	5 (14%)	4 (11%)	0 2
18	BX	35/41 (85%)	27 (77%)	4 (11%)	4 (11%)	0 2
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1 13
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1 13
All	All	5148/5438 (95%)	4279 (83%)	686 (13%)	183 (4%)	2 19

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG

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	AA	271/280 (97%)	247 (91%)	24 (9%)	9 34
1	BA	271/280 (97%)	247 (91%)	24 (9%)	9 34
2	AB	390/407 (96%)	362 (93%)	28 (7%)	13 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	BB	390/407 (96%)	364 (93%)	26 (7%)	15 47
3	AC	347/362 (96%)	327 (94%)	20 (6%)	18 51
3	BC	347/362 (96%)	325 (94%)	22 (6%)	16 48
4	AD	275/283 (97%)	248 (90%)	27 (10%)	7 31
4	BD	275/283 (97%)	247 (90%)	28 (10%)	7 29
5	AE	72/73 (99%)	65 (90%)	7 (10%)	8 32
5	BE	72/73 (99%)	65 (90%)	7 (10%)	8 32
6	AF	29/39 (74%)	28 (97%)	1 (3%)	32 64
6	BF	29/39 (74%)	28 (97%)	1 (3%)	32 64
7	AH	53/55 (96%)	41 (77%)	12 (23%)	1 5
7	BH	53/55 (96%)	41 (77%)	12 (23%)	1 5
8	AI	32/35 (91%)	31 (97%)	1 (3%)	35 66
8	BI	32/35 (91%)	31 (97%)	1 (3%)	35 66
9	AJ	25/28 (89%)	24 (96%)	1 (4%)	28 61
9	BJ	25/28 (89%)	24 (96%)	1 (4%)	28 61
10	AK	30/30 (100%)	28 (93%)	2 (7%)	15 47
10	BK	30/30 (100%)	28 (93%)	2 (7%)	15 47
11	AL	35/35 (100%)	31 (89%)	4 (11%)	5 24
11	BL	35/35 (100%)	30 (86%)	5 (14%)	3 16
12	AM	31/33 (94%)	29 (94%)	2 (6%)	15 47
12	BM	31/33 (94%)	28 (90%)	3 (10%)	8 32
13	AO	202/208 (97%)	183 (91%)	19 (9%)	8 33
13	BO	202/208 (97%)	184 (91%)	18 (9%)	9 34
14	AT	29/29 (100%)	27 (93%)	2 (7%)	14 45
14	BT	29/29 (100%)	27 (93%)	2 (7%)	14 45
15	AU	84/89 (94%)	75 (89%)	9 (11%)	6 27
15	BU	84/89 (94%)	75 (89%)	9 (11%)	6 27
16	AV	116/117 (99%)	112 (97%)	4 (3%)	32 64
16	BV	116/117 (99%)	109 (94%)	7 (6%)	17 50
17	Ay	20/37 (54%)	15 (75%)	5 (25%)	0 3
17	By	20/37 (54%)	14 (70%)	6 (30%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	AX	30/34 (88%)	28 (93%)	2 (7%)	15 47
18	BX	30/34 (88%)	30 (100%)	0	100 100
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	8 32
20	BZ	52/52 (100%)	46 (88%)	6 (12%)	5 24
All	All	4246/4452 (95%)	3891 (92%)	355 (8%)	10 38

5 of 355 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	BC	5165	LEU
7	BH	5021	VAL
3	BC	5313	GLN
4	BD	5259	ILE
11	BL	5009	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
13	AO	222	GLN
13	BO	5087	GLN
1	BA	5315	ASN
13	BO	5084	ASN
16	BV	5060	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 196 ligands modelled in this entry, 12 are monoatomic - leaving 184 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
29	LHG	AA	415	-	36,36,48	1.08	2 (5%)	39,42,54	1.14	3 (7%)
27	BCR	BB	5621	-	41,41,41	1.52	7 (17%)	56,56,56	2.15	21 (37%)
30	SQD	AA	413	-	49,51,54	2.55	28 (57%)	59,62,65	2.70	20 (33%)
34	PHO	BD	5404	-	58,69,69	3.07	16 (27%)	55,99,99	2.25	13 (23%)
30	SQD	AA	416	-	52,54,54	2.57	30 (57%)	62,65,65	2.68	20 (32%)
32	LMT	AI	103	-	36,36,36	1.46	7 (19%)	47,47,47	1.81	9 (19%)
27	BCR	BD	5407	-	41,41,41	1.85	8 (19%)	56,56,56	2.38	24 (42%)
31	LMG	BM	5102	-	42,42,55	1.02	3 (7%)	50,50,63	1.65	8 (16%)
27	BCR	BB	5622	-	41,41,41	1.92	7 (17%)	56,56,56	2.11	17 (30%)
32	LMT	BI	5102	-	36,36,36	1.66	8 (22%)	47,47,47	1.01	2 (4%)
24	CLA	AC	503	3	69,73,73	2.23	17 (24%)	82,113,113	2.32	16 (19%)
27	BCR	BB	5623	-	41,41,41	1.78	8 (19%)	56,56,56	1.99	18 (32%)
30	SQD	BB	5625	-	41,43,54	2.68	20 (48%)	51,54,65	2.74	15 (29%)
32	LMT	AM	102	-	36,36,36	1.76	10 (27%)	47,47,47	0.91	2 (4%)
24	CLA	BB	5607	2	69,73,73	2.54	19 (27%)	82,113,113	2.18	22 (26%)
27	BCR	AD	406	-	41,41,41	1.68	7 (17%)	56,56,56	2.40	25 (44%)
24	CLA	AB	602	2	69,73,73	2.21	16 (23%)	82,113,113	2.08	13 (15%)
24	CLA	AB	615	2	69,73,73	2.21	16 (23%)	82,113,113	2.18	13 (15%)
24	CLA	AC	504	-	69,73,73	2.20	18 (26%)	82,113,113	2.16	15 (18%)
24	CLA	BA	5407	-	69,73,73	2.32	20 (28%)	82,113,113	2.23	14 (17%)
31	LMG	BL	5101	-	51,51,55	1.43	3 (5%)	59,59,63	1.96	13 (22%)
31	LMG	AD	408	-	48,48,55	0.97	4 (8%)	56,56,63	2.08	11 (19%)
32	LMT	AI	102	-	36,36,36	1.62	7 (19%)	47,47,47	1.02	2 (4%)
27	BCR	BJ	5101	-	41,41,41	2.34	10 (24%)	56,56,56	3.33	24 (42%)
27	BCR	BC	5515	-	41,41,41	1.97	8 (19%)	56,56,56	2.29	25 (44%)
24	CLA	BB	5617	2	69,73,73	2.12	16 (23%)	82,113,113	2.00	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	BB	5612	2	69,73,73	2.39	20 (28%)	82,113,113	2.32	15 (18%)
32	LMT	BB	5604	-	36,36,36	1.72	10 (27%)	47,47,47	1.01	1 (2%)
27	BCR	AC	515	-	41,41,41	1.81	7 (17%)	56,56,56	2.29	23 (41%)
33	DMS	BV	5203	-	3,3,3	0.85	0	3,3,3	1.24	0
24	CLA	AC	502	3	69,73,73	2.23	17 (24%)	82,113,113	2.11	14 (17%)
34	PHO	AD	402	-	58,69,69	2.97	16 (27%)	55,99,99	2.08	12 (21%)
33	DMS	BV	5202	-	3,3,3	0.88	0	3,3,3	1.03	0
24	CLA	BB	5608	2	69,73,73	2.20	16 (23%)	82,113,113	2.10	16 (19%)
31	LMG	AD	407	-	49,49,55	0.77	1 (2%)	57,57,63	2.74	19 (33%)
28	DGD	BC	5518	-	63,63,67	1.29	6 (9%)	77,77,81	2.72	24 (31%)
36	HEM	BF	5101	6,5	50,50,50	3.08	23 (46%)	67,82,82	2.52	19 (28%)
24	CLA	AB	613	2	69,73,73	2.09	14 (20%)	82,113,113	2.00	12 (14%)
24	CLA	BB	5620	2	69,73,73	2.28	15 (21%)	82,113,113	2.09	10 (12%)
24	CLA	AB	607	-	69,73,73	2.29	16 (23%)	82,113,113	2.22	17 (20%)
24	CLA	AC	512	3	69,73,73	2.31	19 (27%)	82,113,113	2.19	13 (15%)
24	CLA	AD	404	-	69,73,73	2.31	18 (26%)	82,113,113	2.20	14 (17%)
24	CLA	BB	5606	2	69,73,73	2.21	16 (23%)	82,113,113	2.11	15 (18%)
24	CLA	BB	5618	2	69,73,73	2.73	20 (28%)	82,113,113	2.14	15 (18%)
29	LHG	BA	5415	-	36,36,48	1.09	2 (5%)	39,42,54	1.14	3 (7%)
30	SQD	BF	5102	-	43,45,54	2.61	22 (51%)	53,56,65	2.82	20 (37%)
31	LMG	BB	5624	-	49,49,55	0.81	1 (2%)	57,57,63	1.93	14 (24%)
28	DGD	BA	5412	-	57,57,67	1.85	12 (21%)	71,71,81	3.54	23 (32%)
33	DMS	BB	5629	-	3,3,3	0.69	0	3,3,3	1.27	0
24	CLA	BB	5615	-	69,73,73	2.20	16 (23%)	82,113,113	2.22	20 (24%)
31	LMG	AM	101	-	42,42,55	0.97	2 (4%)	50,50,63	1.65	8 (16%)
27	BCR	BC	5514	-	41,41,41	1.89	6 (14%)	56,56,56	2.15	25 (44%)
28	DGD	AE	101	-	64,64,67	1.58	13 (20%)	78,78,81	1.43	11 (14%)
28	DGD	BE	5102	-	64,64,67	1.55	14 (21%)	78,78,81	1.41	10 (12%)
27	BCR	BC	5516	-	41,41,41	1.84	7 (17%)	56,56,56	2.27	20 (35%)
24	CLA	AB	604	2	69,73,73	2.21	17 (24%)	82,113,113	2.06	15 (18%)
24	CLA	BB	5610	2	69,73,73	2.39	17 (24%)	82,113,113	2.13	14 (17%)
34	PHO	AD	403	-	58,69,69	2.99	17 (29%)	55,99,99	2.21	13 (23%)
35	PL9	BD	5406	-	55,55,55	4.08	19 (34%)	68,69,69	2.77	22 (32%)
28	DGD	BC	5517	-	54,54,67	1.45	8 (14%)	68,68,81	2.70	22 (32%)
24	CLA	AC	507	-	69,73,73	2.13	16 (23%)	82,113,113	2.12	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	BA	5406	-	69,73,73	2.20	19 (27%)	82,113,113	2.37	19 (23%)
24	CLA	AB	608	2	69,73,73	2.38	20 (28%)	82,113,113	2.31	16 (19%)
24	CLA	BC	5504	-	69,73,73	2.30	18 (26%)	82,113,113	2.15	12 (14%)
27	BCR	AB	618	-	41,41,41	1.96	7 (17%)	56,56,56	2.12	17 (30%)
28	DGD	AB	628	-	53,53,67	1.47	7 (13%)	67,67,81	2.04	13 (19%)
32	LMT	BB	5603	-	36,36,36	1.59	7 (19%)	47,47,47	1.41	7 (14%)
28	DGD	BH	5101	-	59,59,67	1.33	8 (13%)	73,73,81	2.07	18 (24%)
35	PL9	AD	405	-	55,55,55	3.97	18 (32%)	68,69,69	2.77	23 (33%)
30	SQD	BA	5401	-	52,54,54	2.60	30 (57%)	62,65,65	2.68	22 (35%)
31	LMG	BD	5409	-	49,49,55	0.74	1 (2%)	57,57,63	2.75	20 (35%)
24	CLA	BB	5613	2	69,73,73	2.31	20 (28%)	82,113,113	2.06	14 (17%)
31	LMG	AB	621	-	49,49,55	0.79	1 (2%)	57,57,63	1.93	14 (24%)
24	CLA	BB	5605	-	69,73,73	2.56	20 (28%)	82,113,113	2.19	12 (14%)
24	CLA	BC	5503	3	69,73,73	2.27	17 (24%)	82,113,113	2.25	16 (19%)
32	LMT	AD	409	-	32,32,36	1.74	7 (21%)	43,43,47	1.29	2 (4%)
31	LMG	BC	5520	-	48,48,55	1.11	3 (6%)	56,56,63	1.90	18 (32%)
29	LHG	BA	5413	-	38,38,48	2.05	5 (13%)	41,44,54	1.45	5 (12%)
30	SQD	BA	5414	-	49,51,54	2.62	27 (55%)	59,62,65	2.68	19 (32%)
24	CLA	BC	5513	3	69,73,73	2.81	23 (33%)	82,113,113	1.99	13 (15%)
32	LMT	AB	629	-	36,36,36	1.59	7 (19%)	47,47,47	1.41	6 (12%)
31	LMG	BD	5410	-	48,48,55	0.95	3 (6%)	56,56,63	2.08	11 (19%)
33	DMS	BB	5628	-	3,3,3	0.72	0	3,3,3	1.19	0
24	CLA	BB	5611	-	69,73,73	2.25	19 (27%)	82,113,113	2.26	17 (20%)
29	LHG	AA	412	-	38,38,48	2.06	5 (13%)	41,44,54	1.48	5 (12%)
24	CLA	AB	609	2	69,73,73	2.29	17 (24%)	82,113,113	2.04	14 (17%)
31	LMG	BE	5101	-	44,44,55	1.10	2 (4%)	52,52,63	1.52	6 (11%)
27	BCR	AK	102	-	41,41,41	1.83	7 (17%)	56,56,56	2.53	25 (44%)
25	MST	BA	5409	-	16,16,16	0.48	0	22,22,22	3.70	9 (40%)
22	BCT	AA	402	21	3,3,3	1.92	1 (33%)	2,3,3	0.09	0
27	BCR	AB	617	-	41,41,41	1.59	7 (17%)	56,56,56	2.16	21 (37%)
31	LMG	AA	417	-	42,42,55	1.09	5 (11%)	50,50,63	2.31	11 (22%)
24	CLA	BC	5508	3	69,73,73	2.27	18 (26%)	82,113,113	2.29	15 (18%)
27	BCR	AB	619	-	41,41,41	1.92	8 (19%)	56,56,56	2.01	20 (35%)
27	BCR	AT	101	-	41,41,41	1.69	7 (17%)	56,56,56	2.29	24 (42%)
24	CLA	BC	5506	-	69,73,73	2.37	21 (30%)	82,113,113	2.14	14 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	SQD	AF	102	-	43,45,54	2.61	22 (51%)	53,56,65	2.81	18 (33%)
24	CLA	BC	5512	3	69,73,73	2.38	18 (26%)	82,113,113	2.18	11 (13%)
22	BCT	BA	5403	21	3,3,3	2.30	1 (33%)	2,3,3	0.38	0
24	CLA	AC	501	3	69,73,73	2.28	18 (26%)	82,113,113	2.28	15 (18%)
27	BCR	AJ	101	-	41,41,41	2.38	11 (26%)	56,56,56	3.35	24 (42%)
24	CLA	AB	605	2	69,73,73	2.36	21 (30%)	82,113,113	2.11	16 (19%)
31	LMG	BA	5402	-	42,42,55	1.09	3 (7%)	50,50,63	2.32	11 (22%)
32	LMT	BB	5627	-	36,36,36	1.64	8 (22%)	47,47,47	0.93	2 (4%)
24	CLA	AB	612	2	69,73,73	2.43	19 (27%)	82,113,113	2.00	13 (15%)
24	CLA	BB	5614	-	69,73,73	2.15	15 (21%)	82,113,113	2.06	14 (17%)
28	DGD	BB	5602	-	53,53,67	1.52	7 (13%)	67,67,81	2.06	13 (19%)
24	CLA	AA	405	-	69,73,73	2.20	19 (27%)	82,113,113	2.32	18 (21%)
24	CLA	BC	5502	3	69,73,73	2.30	17 (24%)	82,113,113	2.21	15 (18%)
32	LMT	AB	630	-	36,36,36	1.74	9 (25%)	47,47,47	1.02	1 (2%)
30	SQD	BB	5601	-	45,47,54	2.59	23 (51%)	55,58,65	2.62	16 (29%)
31	LMG	AI	101	-	43,43,55	1.04	3 (6%)	51,51,63	1.69	8 (15%)
31	LMG	BI	5101	-	43,43,55	1.03	3 (6%)	51,51,63	1.68	8 (15%)
27	BCR	AA	410	-	41,41,41	1.67	8 (19%)	56,56,56	2.11	22 (39%)
24	CLA	AC	506	-	69,73,73	2.36	21 (30%)	82,113,113	2.12	13 (15%)
24	CLA	AC	510	3	69,73,73	2.17	16 (23%)	82,113,113	2.08	13 (15%)
24	CLA	BB	5616	2	69,73,73	2.50	21 (30%)	82,113,113	2.06	13 (15%)
24	CLA	BC	5507	-	69,73,73	2.19	17 (24%)	82,113,113	2.12	14 (17%)
24	CLA	BA	5405	1	69,73,73	2.17	15 (21%)	82,113,113	1.97	15 (18%)
24	CLA	BC	5511	3	69,73,73	2.79	23 (33%)	82,113,113	2.14	17 (20%)
25	MST	AA	408	-	16,16,16	0.51	0	22,22,22	3.77	9 (40%)
28	DGD	AH	101	-	59,59,67	1.35	9 (15%)	73,73,81	2.06	18 (24%)
33	DMS	AB	626	-	3,3,3	0.69	0	3,3,3	1.10	0
28	DGD	AC	519	-	67,67,67	1.52	12 (17%)	81,81,81	3.23	30 (37%)
32	LMT	BD	5411	-	32,32,36	1.73	8 (25%)	43,43,47	1.30	2 (4%)
24	CLA	AB	601	-	69,73,73	2.57	22 (31%)	82,113,113	2.23	11 (13%)
24	CLA	BC	5505	3	69,73,73	2.50	20 (28%)	82,113,113	2.25	14 (17%)
24	CLA	AA	406	-	69,73,73	2.21	18 (26%)	82,113,113	2.18	15 (18%)
28	DGD	AA	411	-	57,57,67	1.82	12 (21%)	71,71,81	3.53	24 (33%)
31	LMG	AB	620	-	51,51,55	1.38	3 (5%)	59,59,63	1.98	12 (20%)
30	SQD	AB	627	-	45,47,54	2.60	24 (53%)	55,58,65	2.61	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	PHO	BD	5403	-	58,69,69	3.11	17 (29%)	55,99,99	2.09	12 (21%)
27	BCR	BA	5411	-	41,41,41	1.74	7 (17%)	56,56,56	2.13	22 (39%)
24	CLA	AA	407	1	69,73,73	2.19	16 (23%)	82,113,113	2.20	15 (18%)
36	HEM	AV	201	16	50,50,50	2.84	20 (40%)	67,82,82	2.40	18 (26%)
24	CLA	BA	5408	1	69,73,73	2.27	18 (26%)	82,113,113	2.15	15 (18%)
24	CLA	AA	404	1	69,73,73	2.22	15 (21%)	82,113,113	1.96	15 (18%)
24	CLA	BB	5619	2	69,73,73	2.19	15 (21%)	82,113,113	2.22	12 (14%)
31	LMG	BC	5521	-	45,45,55	1.04	2 (4%)	53,53,63	1.91	13 (24%)
27	BCR	BT	5101	-	41,41,41	1.83	7 (17%)	56,56,56	2.28	24 (42%)
33	DMS	AU	201	-	3,3,3	0.94	0	3,3,3	1.17	0
24	CLA	BC	5510	3	69,73,73	2.20	17 (24%)	82,113,113	2.09	12 (14%)
24	CLA	AC	513	3	69,73,73	2.73	20 (28%)	82,113,113	1.97	13 (15%)
24	CLA	BD	5402	4	69,73,73	2.23	16 (23%)	82,113,113	2.14	17 (20%)
24	CLA	BB	5609	2	69,73,73	2.28	19 (27%)	82,113,113	2.11	16 (19%)
27	BCR	AX	101	-	41,41,41	1.90	7 (17%)	56,56,56	2.27	23 (41%)
28	DGD	BC	5519	-	67,67,67	1.55	12 (17%)	81,81,81	3.23	30 (37%)
30	SQD	AB	622	-	41,43,54	2.66	19 (46%)	51,54,65	2.73	15 (29%)
24	CLA	AB	614	2	69,73,73	2.80	22 (31%)	82,113,113	2.17	15 (18%)
24	CLA	AB	606	2	69,73,73	2.38	18 (26%)	82,113,113	2.11	15 (18%)
28	DGD	AC	517	-	54,54,67	1.37	7 (12%)	68,68,81	2.70	22 (32%)
24	CLA	AC	508	3	69,73,73	2.19	17 (24%)	82,113,113	2.21	14 (17%)
31	LMG	AC	520	-	48,48,55	1.07	5 (10%)	56,56,63	1.93	18 (32%)
36	HEM	AF	101	6,5	50,50,50	3.00	23 (46%)	67,82,82	2.49	20 (29%)
24	CLA	AB	610	-	69,73,73	2.18	15 (21%)	82,113,113	2.07	13 (15%)
24	CLA	AB	603	2	69,73,73	2.56	18 (26%)	82,113,113	2.20	22 (26%)
27	BCR	BK	5102	-	41,41,41	1.95	8 (19%)	56,56,56	2.48	26 (46%)
24	CLA	AC	511	3	69,73,73	2.68	20 (28%)	82,113,113	2.12	17 (20%)
24	CLA	AB	611	-	69,73,73	2.17	16 (23%)	82,113,113	2.22	18 (21%)
32	LMT	BB	5626	-	36,36,36	1.78	9 (25%)	47,47,47	1.03	2 (4%)
31	LMG	AJ	102	-	46,46,55	1.00	3 (6%)	54,54,63	2.58	16 (29%)
32	LMT	AB	624	-	36,36,36	1.67	8 (22%)	47,47,47	0.94	2 (4%)
32	LMT	BM	5101	-	36,36,36	1.77	9 (25%)	47,47,47	0.90	2 (4%)
24	CLA	AD	401	4	69,73,73	2.16	17 (24%)	82,113,113	2.12	17 (20%)
31	LMG	AA	414	-	44,44,55	1.12	3 (6%)	52,52,63	1.51	6 (11%)
31	LMG	AC	521	-	45,45,55	1.09	2 (4%)	53,53,63	1.91	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	DGD	AC	518	-	63,63,67	1.26	6 (9%)	77,77,81	2.74	23 (29%)
24	CLA	BC	5509	3	69,73,73	2.59	21 (30%)	82,113,113	2.12	12 (14%)
33	DMS	AB	625	-	3,3,3	0.74	0	3,3,3	1.51	1 (33%)
32	LMT	AB	623	-	36,36,36	1.78	8 (22%)	47,47,47	1.01	2 (4%)
27	BCR	BX	5101	-	41,41,41	1.92	7 (17%)	56,56,56	2.30	22 (39%)
27	BCR	AC	516	-	41,41,41	1.68	9 (21%)	56,56,56	2.31	22 (39%)
31	LMG	BD	5408	-	46,46,55	1.00	3 (6%)	54,54,63	2.57	16 (29%)
24	CLA	AB	616	2	69,73,73	2.26	15 (21%)	82,113,113	2.09	12 (14%)
24	CLA	AC	509	3	69,73,73	2.48	13 (18%)	82,113,113	2.13	14 (17%)
27	BCR	AC	514	-	41,41,41	1.67	7 (17%)	56,56,56	2.19	24 (42%)
24	CLA	AC	505	3	69,73,73	2.51	20 (28%)	82,113,113	2.25	13 (15%)
33	DMS	AV	202	-	3,3,3	0.77	0	3,3,3	1.10	0
24	CLA	BD	5405	-	69,73,73	2.34	16 (23%)	82,113,113	2.19	15 (18%)
32	LMT	BC	5522	-	36,36,36	1.53	7 (19%)	47,47,47	1.80	10 (21%)
24	CLA	BC	5501	3	69,73,73	2.33	20 (28%)	82,113,113	2.31	15 (18%)
36	HEM	BV	5201	16	50,50,50	2.95	25 (50%)	67,82,82	2.39	18 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	AA	415	-	-	21/41/41/53	-
34	PHO	BD	5404	-	1/1/17/22	10/37/103/103	0/5/6/6
27	BCR	BB	5621	-	-	1/29/63/63	0/2/2/2
30	SQD	AA	413	-	-	24/46/66/69	0/1/1/1
30	SQD	AA	416	-	-	20/49/69/69	0/1/1/1
32	LMT	AI	103	-	-	1/21/61/61	0/2/2/2
27	BCR	BD	5407	-	-	5/29/63/63	0/2/2/2
31	LMG	BM	5102	-	-	3/37/57/70	0/1/1/1
27	BCR	BB	5622	-	-	1/29/63/63	0/2/2/2
32	LMT	BI	5102	-	-	3/21/61/61	0/2/2/2
24	CLA	AC	503	3	1/1/15/20	15/39/115/115	-
27	BCR	BB	5623	-	-	4/29/63/63	0/2/2/2
30	SQD	BB	5625	-	-	18/38/58/69	0/1/1/1
32	LMT	AM	102	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	BB	5607	2	1/1/15/20	11/39/115/115	-
27	BCR	AD	406	-	-	5/29/63/63	0/2/2/2
24	CLA	AB	602	2	1/1/15/20	7/39/115/115	-
24	CLA	AB	615	2	1/1/15/20	5/39/115/115	-
24	CLA	AC	504	-	1/1/15/20	8/39/115/115	-
24	CLA	BA	5407	-	1/1/15/20	3/39/115/115	-
31	LMG	BL	5101	-	-	5/46/66/70	0/1/1/1
31	LMG	AD	408	-	-	5/43/63/70	0/1/1/1
32	LMT	AI	102	-	-	3/21/61/61	0/2/2/2
27	BCR	BJ	5101	-	-	1/29/63/63	0/2/2/2
27	BCR	BC	5515	-	-	3/29/63/63	0/2/2/2
24	CLA	BB	5617	2	1/1/15/20	10/39/115/115	-
24	CLA	BB	5612	2	1/1/15/20	10/39/115/115	-
32	LMT	BB	5604	-	-	3/21/61/61	0/2/2/2
27	BCR	AC	515	-	-	3/29/63/63	0/2/2/2
24	CLA	AC	502	3	1/1/15/20	7/39/115/115	-
34	PHO	AD	402	-	1/1/17/22	10/37/103/103	0/5/6/6
24	CLA	BB	5608	2	1/1/15/20	10/39/115/115	-
31	LMG	AD	407	-	-	7/44/64/70	0/1/1/1
28	DGD	BC	5518	-	1/1/13/13	8/51/91/95	0/2/2/2
36	HEM	BF	5101	6,5	-	8/14/54/54	-
24	CLA	AB	613	2	1/1/15/20	9/39/115/115	-
24	CLA	BB	5620	2	1/1/15/20	11/39/115/115	-
24	CLA	AB	607	-	1/1/15/20	5/39/115/115	-
24	CLA	AC	512	3	1/1/15/20	11/39/115/115	-
24	CLA	AD	404	-	1/1/15/20	10/39/115/115	-
24	CLA	BB	5606	2	1/1/15/20	7/39/115/115	-
24	CLA	BB	5618	2	1/1/15/20	7/39/115/115	-
29	LHG	BA	5415	-	-	21/41/41/53	-
30	SQD	BF	5102	-	-	22/40/60/69	0/1/1/1
31	LMG	BB	5624	-	-	4/44/64/70	0/1/1/1
28	DGD	BA	5412	-	-	8/45/85/95	0/2/2/2
24	CLA	BB	5615	-	1/1/15/20	8/39/115/115	-
31	LMG	AM	101	-	-	3/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	BCR	BC	5514	-	-	5/29/63/63	0/2/2/2
28	DGD	AE	101	-	-	5/52/92/95	0/2/2/2
28	DGD	BE	5102	-	-	6/52/92/95	0/2/2/2
27	BCR	BC	5516	-	-	4/29/63/63	0/2/2/2
24	CLA	AB	604	2	1/1/15/20	9/39/115/115	-
24	CLA	BB	5610	2	1/1/15/20	10/39/115/115	-
34	PHO	AD	403	-	1/1/17/22	10/37/103/103	0/5/6/6
35	PL9	BD	5406	-	-	17/53/73/73	0/1/1/1
28	DGD	BC	5517	-	-	4/42/82/95	0/2/2/2
24	CLA	AC	507	-	1/1/15/20	6/39/115/115	-
24	CLA	BA	5406	-	1/1/15/20	14/39/115/115	-
24	CLA	AB	608	2	1/1/15/20	10/39/115/115	-
24	CLA	BC	5504	-	1/1/15/20	9/39/115/115	-
27	BCR	AB	618	-	-	1/29/63/63	0/2/2/2
28	DGD	AB	628	-	-	7/41/81/95	0/2/2/2
32	LMT	BB	5603	-	-	3/21/61/61	0/2/2/2
28	DGD	BH	5101	-	-	3/47/87/95	0/2/2/2
35	PL9	AD	405	-	-	16/53/73/73	0/1/1/1
30	SQD	BA	5401	-	-	21/49/69/69	0/1/1/1
31	LMG	BD	5409	-	-	7/44/64/70	0/1/1/1
24	CLA	BB	5613	2	1/1/15/20	7/39/115/115	-
31	LMG	AB	621	-	-	4/44/64/70	0/1/1/1
24	CLA	BB	5605	-	1/1/15/20	13/39/115/115	-
24	CLA	BC	5503	3	1/1/15/20	15/39/115/115	-
32	LMT	AD	409	-	-	1/17/57/61	0/2/2/2
31	LMG	BC	5520	-	-	5/43/63/70	0/1/1/1
29	LHG	BA	5413	-	-	19/43/43/53	-
30	SQD	BA	5414	-	-	24/46/66/69	0/1/1/1
24	CLA	BC	5513	3	1/1/15/20	7/39/115/115	-
32	LMT	AB	629	-	-	3/21/61/61	0/2/2/2
31	LMG	BD	5410	-	-	5/43/63/70	0/1/1/1
24	CLA	BB	5611	-	1/1/15/20	5/39/115/115	-
29	LHG	AA	412	-	-	18/43/43/53	-
24	CLA	AB	609	2	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	BE	5101	-	-	5/39/59/70	0/1/1/1
27	BCR	AK	102	-	-	2/29/63/63	0/2/2/2
25	MST	BA	5409	-	-	2/10/10/10	0/1/1/1
27	BCR	AB	617	-	-	1/29/63/63	0/2/2/2
31	LMG	AA	417	-	-	3/37/57/70	0/1/1/1
24	CLA	BC	5508	3	1/1/15/20	8/39/115/115	-
27	BCR	AB	619	-	-	4/29/63/63	0/2/2/2
27	BCR	AT	101	-	-	4/29/63/63	0/2/2/2
24	CLA	BC	5506	-	1/1/15/20	4/39/115/115	-
30	SQD	AF	102	-	-	21/40/60/69	0/1/1/1
24	CLA	BC	5512	3	1/1/15/20	10/39/115/115	-
24	CLA	AC	501	3	1/1/15/20	11/39/115/115	-
27	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
24	CLA	AB	605	2	1/1/15/20	8/39/115/115	-
31	LMG	BA	5402	-	-	3/37/57/70	0/1/1/1
32	LMT	BB	5627	-	-	3/21/61/61	0/2/2/2
24	CLA	AB	612	2	1/1/15/20	10/39/115/115	-
24	CLA	BB	5614	-	1/1/15/20	10/39/115/115	-
28	DGD	BB	5602	-	-	6/41/81/95	0/2/2/2
24	CLA	AA	405	-	1/1/15/20	13/39/115/115	-
24	CLA	BC	5502	3	1/1/15/20	8/39/115/115	-
32	LMT	AB	630	-	-	3/21/61/61	0/2/2/2
30	SQD	BB	5601	-	-	23/42/62/69	0/1/1/1
31	LMG	AI	101	-	-	2/38/58/70	0/1/1/1
31	LMG	BI	5101	-	-	2/38/58/70	0/1/1/1
25	MST	AA	408	-	-	2/10/10/10	0/1/1/1
24	CLA	AC	506	-	1/1/15/20	5/39/115/115	-
24	CLA	AC	510	3	1/1/15/20	10/39/115/115	-
24	CLA	BB	5616	2	1/1/15/20	9/39/115/115	-
24	CLA	BC	5507	-	1/1/15/20	6/39/115/115	-
24	CLA	BA	5405	1	1/1/15/20	14/39/115/115	-
24	CLA	BC	5511	3	1/1/15/20	15/39/115/115	-
27	BCR	AA	410	-	-	5/29/63/63	0/2/2/2
28	DGD	AH	101	-	-	3/47/87/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DGD	AC	519	-	1/1/13/13	9/55/95/95	0/2/2/2
32	LMT	BD	5411	-	-	1/17/57/61	0/2/2/2
24	CLA	AB	601	-	1/1/15/20	13/39/115/115	-
24	CLA	BC	5505	3	1/1/15/20	9/39/115/115	-
24	CLA	AA	406	-	1/1/15/20	3/39/115/115	-
28	DGD	AA	411	-	-	7/45/85/95	0/2/2/2
31	LMG	AB	620	-	-	5/46/66/70	0/1/1/1
34	PHO	BD	5403	-	1/1/17/22	10/37/103/103	0/5/6/6
30	SQD	AB	627	-	-	24/42/62/69	0/1/1/1
27	BCR	BA	5411	-	-	5/29/63/63	0/2/2/2
24	CLA	AA	407	1	1/1/15/20	11/39/115/115	-
36	HEM	AV	201	16	-	6/14/54/54	-
24	CLA	BA	5408	1	1/1/15/20	11/39/115/115	-
24	CLA	AA	404	1	1/1/15/20	13/39/115/115	-
24	CLA	BB	5619	2	1/1/15/20	5/39/115/115	-
31	LMG	BC	5521	-	-	6/40/60/70	0/1/1/1
27	BCR	BT	5101	-	-	4/29/63/63	0/2/2/2
24	CLA	BC	5510	3	1/1/15/20	10/39/115/115	-
24	CLA	AC	513	3	1/1/15/20	8/39/115/115	-
24	CLA	BD	5402	4	1/1/15/20	10/39/115/115	-
24	CLA	BB	5609	2	1/1/15/20	8/39/115/115	-
27	BCR	AX	101	-	-	1/29/63/63	0/2/2/2
28	DGD	BC	5519	-	1/1/13/13	7/55/95/95	0/2/2/2
30	SQD	AB	622	-	-	20/38/58/69	0/1/1/1
24	CLA	AB	614	2	1/1/15/20	7/39/115/115	-
24	CLA	AB	606	2	1/1/15/20	11/39/115/115	-
28	DGD	AC	517	-	-	4/42/82/95	0/2/2/2
24	CLA	AC	508	3	1/1/15/20	7/39/115/115	-
31	LMG	AC	520	-	-	5/43/63/70	0/1/1/1
36	HEM	AF	101	6,5	-	8/14/54/54	-
24	CLA	AB	610	-	1/1/15/20	10/39/115/115	-
24	CLA	AB	603	2	1/1/15/20	10/39/115/115	-
27	BCR	BK	5102	-	-	2/29/63/63	0/2/2/2
24	CLA	AC	511	3	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	AB	611	-	1/1/15/20	9/39/115/115	-
32	LMT	BB	5626	-	-	1/21/61/61	0/2/2/2
31	LMG	AJ	102	-	-	5/41/61/70	0/1/1/1
32	LMT	AB	624	-	-	3/21/61/61	0/2/2/2
32	LMT	BM	5101	-	-	3/21/61/61	0/2/2/2
24	CLA	AD	401	4	1/1/15/20	10/39/115/115	-
31	LMG	AA	414	-	-	5/39/59/70	0/1/1/1
31	LMG	AC	521	-	-	6/40/60/70	0/1/1/1
28	DGD	AC	518	-	1/1/13/13	8/51/91/95	0/2/2/2
24	CLA	BC	5509	3	1/1/15/20	3/39/115/115	-
32	LMT	AB	623	-	-	1/21/61/61	0/2/2/2
27	BCR	BX	5101	-	-	1/29/63/63	0/2/2/2
27	BCR	AC	516	-	-	4/29/63/63	0/2/2/2
31	LMG	BD	5408	-	-	5/41/61/70	0/1/1/1
24	CLA	AB	616	2	1/1/15/20	10/39/115/115	-
24	CLA	AC	509	3	1/1/15/20	5/39/115/115	-
27	BCR	AC	514	-	-	5/29/63/63	0/2/2/2
24	CLA	AC	505	3	1/1/15/20	8/39/115/115	-
24	CLA	BD	5405	-	1/1/15/20	10/39/115/115	-
32	LMT	BC	5522	-	-	1/21/61/61	0/2/2/2
24	CLA	BC	5501	3	1/1/15/20	11/39/115/115	-
36	HEM	BV	5201	16	-	6/14/54/54	-

The worst 5 of 2213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AB	614	CLA	MG-NA	12.11	2.35	2.06
24	BC	5513	CLA	MG-NA	12.03	2.34	2.06
24	BC	5511	CLA	MG-NA	11.84	2.34	2.06
24	AC	513	CLA	MG-NA	11.69	2.34	2.06
24	AC	511	CLA	MG-NA	11.67	2.34	2.06

The worst 5 of 2556 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	AB	601	CLA	C4A-NA-C1A	14.17	113.14	106.68
24	BB	5605	CLA	C4A-NA-C1A	13.73	112.94	106.68
24	AC	512	CLA	C4A-NA-C1A	13.38	112.78	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	BC	5512	CLA	C4A-NA-C1A	13.37	112.78	106.68
24	BB	5619	CLA	C4A-NA-C1A	13.28	112.74	106.68

5 of 78 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	AA	404	CLA	C8
24	AA	405	CLA	C8
24	AA	406	CLA	C8
24	AA	407	CLA	C8
24	AB	601	CLA	C8

5 of 1327 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AA	405	CLA	C6-C7-C8-C9
24	AB	607	CLA	C4-C3-C5-C6
24	AB	610	CLA	CHA-CBD-CGD-O2D
24	AB	610	CLA	C14-C13-C15-C16
24	AC	503	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

171 monomers are involved in 1019 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	AA	415	LHG	2	0
27	BB	5621	BCR	4	0
34	BD	5404	PHO	4	0
30	AA	416	SQD	2	0
32	AI	103	LMT	4	0
27	BD	5407	BCR	2	0
31	BM	5102	LMG	4	0
27	BB	5622	BCR	1	0
32	BI	5102	LMT	5	0
24	AC	503	CLA	5	0
27	BB	5623	BCR	4	0
30	BB	5625	SQD	6	0
32	AM	102	LMT	2	0
24	BB	5607	CLA	13	0
27	AD	406	BCR	2	0
24	AB	602	CLA	8	0
24	AB	615	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AC	504	CLA	12	0
24	BA	5407	CLA	1	0
31	BL	5101	LMG	18	0
31	AD	408	LMG	11	0
32	AI	102	LMT	5	0
27	BJ	5101	BCR	3	0
27	BC	5515	BCR	5	0
24	BB	5617	CLA	7	0
24	BB	5612	CLA	14	0
32	BB	5604	LMT	2	0
27	AC	515	BCR	5	0
24	AC	502	CLA	5	0
34	AD	402	PHO	8	0
33	BV	5202	DMS	1	0
24	BB	5608	CLA	11	0
31	AD	407	LMG	3	0
28	BC	5518	DGD	10	0
36	BF	5101	HEM	7	0
24	AB	613	CLA	8	0
24	BB	5620	CLA	3	0
24	AB	607	CLA	7	0
24	AC	512	CLA	4	0
24	AD	404	CLA	7	0
24	BB	5606	CLA	8	0
24	BB	5618	CLA	14	0
29	BA	5415	LHG	3	0
30	BF	5102	SQD	1	0
31	BB	5624	LMG	4	0
28	BA	5412	DGD	7	0
24	BB	5615	CLA	18	0
31	AM	101	LMG	6	0
27	BC	5514	BCR	6	0
28	AE	101	DGD	1	0
28	BE	5102	DGD	1	0
27	BC	5516	BCR	13	0
24	AB	604	CLA	10	0
24	BB	5610	CLA	8	0
34	AD	403	PHO	3	0
35	BD	5406	PL9	15	0
28	BC	5517	DGD	10	0
24	AC	507	CLA	6	0
24	BA	5406	CLA	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AB	608	CLA	16	0
24	BC	5504	CLA	10	0
27	AB	618	BCR	2	0
32	BB	5603	LMT	2	0
28	BH	5101	DGD	10	0
35	AD	405	PL9	15	0
30	BA	5401	SQD	3	0
31	BD	5409	LMG	3	0
24	BB	5613	CLA	4	0
31	AB	621	LMG	4	0
24	BB	5605	CLA	3	0
24	BC	5503	CLA	3	0
31	BC	5520	LMG	3	0
29	BA	5413	LHG	6	0
24	BC	5513	CLA	4	0
32	AB	629	LMT	4	0
31	BD	5410	LMG	11	0
33	BB	5628	DMS	1	0
24	BB	5611	CLA	8	0
29	AA	412	LHG	5	0
24	AB	609	CLA	4	0
31	BE	5101	LMG	3	0
27	AK	102	BCR	5	0
25	BA	5409	MST	11	0
27	AB	617	BCR	4	0
31	AA	417	LMG	6	0
24	BC	5508	CLA	8	0
27	AB	619	BCR	3	0
27	AT	101	BCR	9	0
24	BC	5506	CLA	4	0
30	AF	102	SQD	1	0
24	BC	5512	CLA	5	0
24	AC	501	CLA	6	0
27	AJ	101	BCR	4	0
24	AB	605	CLA	11	0
31	BA	5402	LMG	3	0
32	BB	5627	LMT	9	0
24	AB	612	CLA	7	0
24	BB	5614	CLA	8	0
28	BB	5602	DGD	5	0
24	AA	405	CLA	17	0
24	BC	5502	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	AB	630	LMT	2	0
30	BB	5601	SQD	5	0
31	AI	101	LMG	3	0
31	BI	5101	LMG	4	0
27	AA	410	BCR	4	0
24	AC	506	CLA	5	0
24	AC	510	CLA	4	0
24	BB	5616	CLA	7	0
24	BC	5507	CLA	8	0
24	BA	5405	CLA	11	0
24	BC	5511	CLA	20	0
25	AA	408	MST	10	0
28	AH	101	DGD	10	0
28	AC	519	DGD	42	0
32	BD	5411	LMT	1	0
24	AB	601	CLA	3	0
24	BC	5505	CLA	9	0
24	AA	406	CLA	1	0
28	AA	411	DGD	7	0
31	AB	620	LMG	17	0
30	AB	627	SQD	3	0
34	BD	5403	PHO	9	0
27	BA	5411	BCR	3	0
24	AA	407	CLA	7	0
36	AV	201	HEM	5	0
24	BA	5408	CLA	9	0
24	AA	404	CLA	11	0
24	BB	5619	CLA	9	0
31	BC	5521	LMG	7	0
27	BT	5101	BCR	5	0
24	BC	5510	CLA	4	0
24	AC	513	CLA	2	0
24	BD	5402	CLA	9	0
24	BB	5609	CLA	13	0
27	AX	101	BCR	6	0
28	BC	5519	DGD	44	0
30	AB	622	SQD	6	0
24	AB	614	CLA	9	0
24	AB	606	CLA	8	0
28	AC	517	DGD	10	0
24	AC	508	CLA	10	0
31	AC	520	LMG	4	0

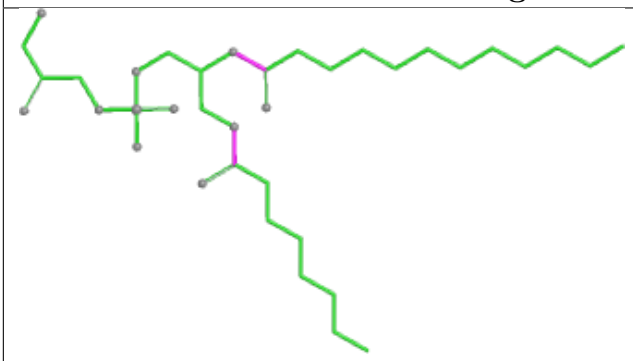
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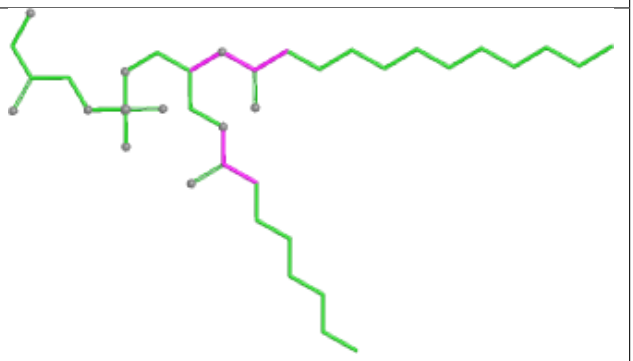
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	AF	101	HEM	8	0
24	AB	610	CLA	7	0
24	AB	603	CLA	15	0
27	BK	5102	BCR	5	0
24	AC	511	CLA	19	0
24	AB	611	CLA	14	0
32	BB	5626	LMT	2	0
31	AJ	102	LMG	2	0
32	AB	624	LMT	9	0
32	BM	5101	LMT	3	0
24	AD	401	CLA	8	0
31	AA	414	LMG	9	0
31	AC	521	LMG	7	0
28	AC	518	DGD	12	0
24	BC	5509	CLA	6	0
33	AB	625	DMS	1	0
27	BX	5101	BCR	2	0
27	AC	516	BCR	11	0
31	BD	5408	LMG	1	0
24	AB	616	CLA	3	0
24	AC	509	CLA	4	0
27	AC	514	BCR	6	0
24	AC	505	CLA	9	0
33	AV	202	DMS	1	0
24	BD	5405	CLA	7	0
32	BC	5522	LMT	3	0
24	BC	5501	CLA	8	0
36	BV	5201	HEM	7	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.

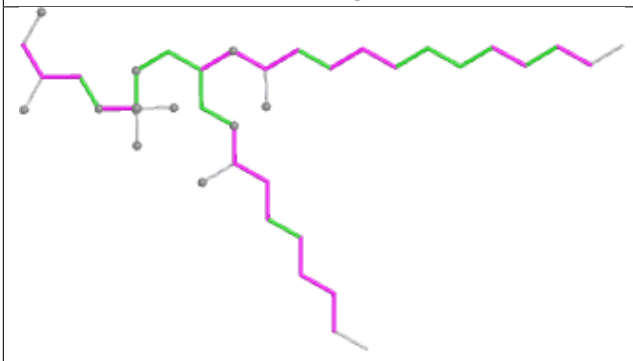
Ligand LHG AA 415



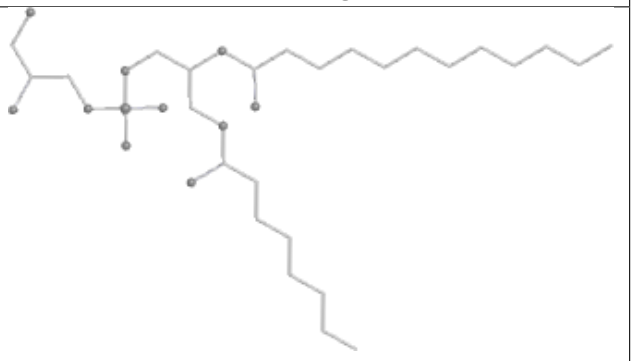
Bond lengths



Bond angles

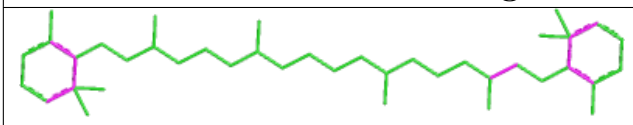


Torsions

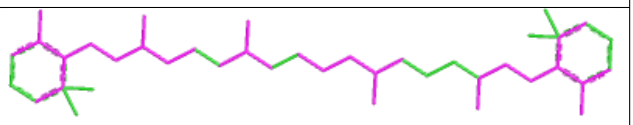


Rings

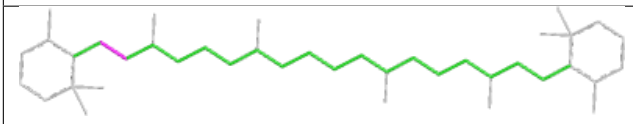
Ligand BCR BB 5621



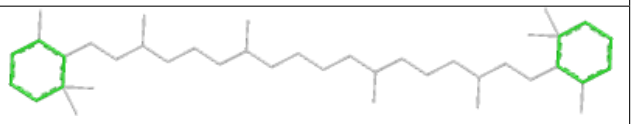
Bond lengths



Bond angles

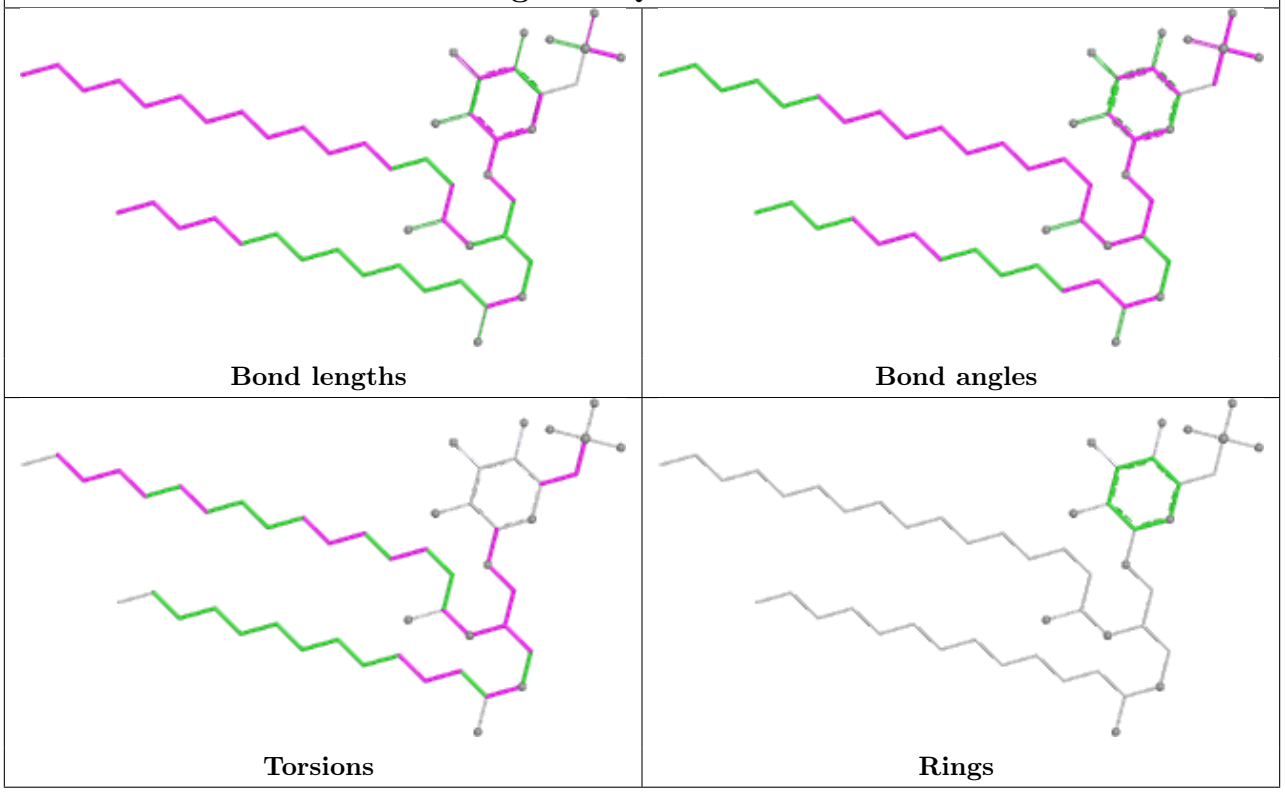


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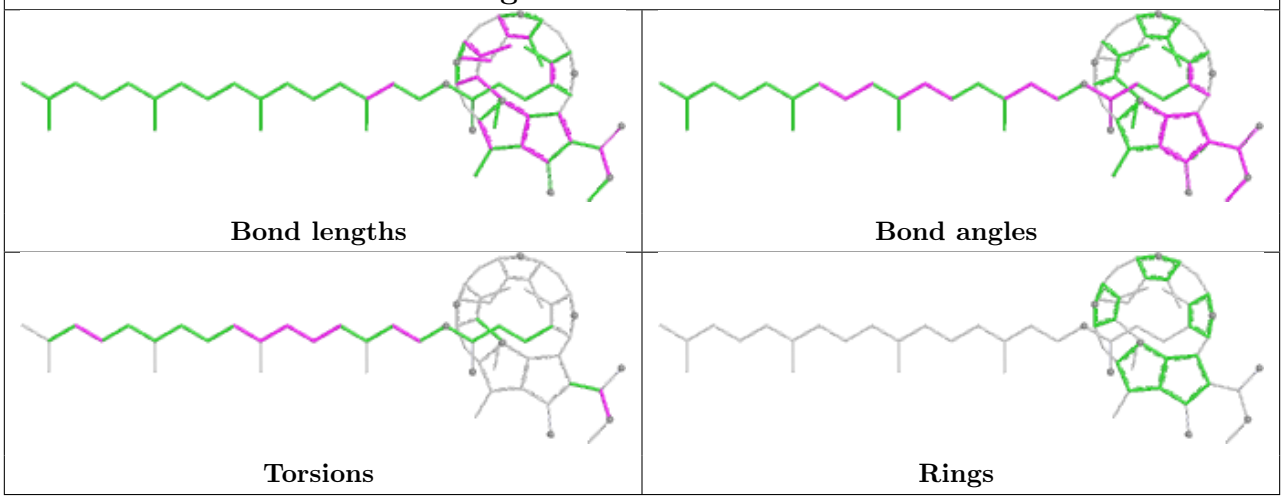


Rings

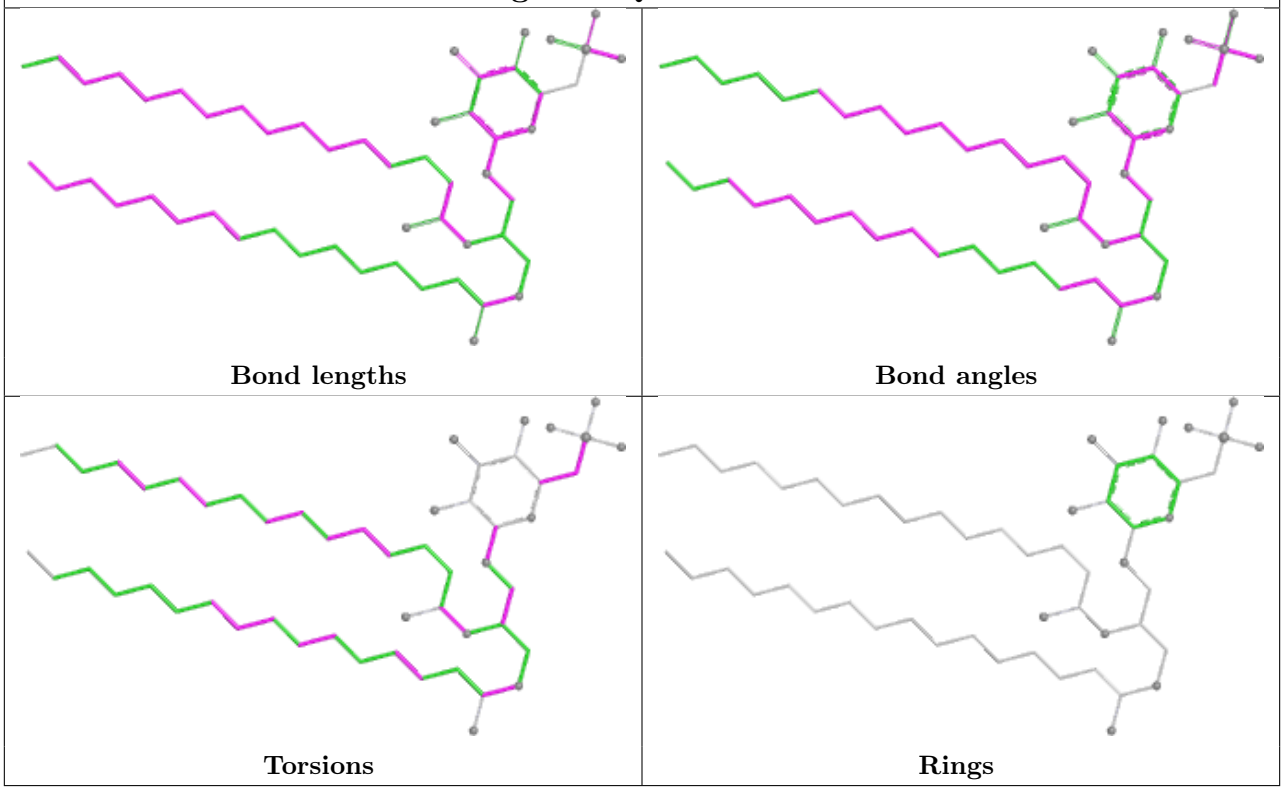
Ligand SQD AA 413



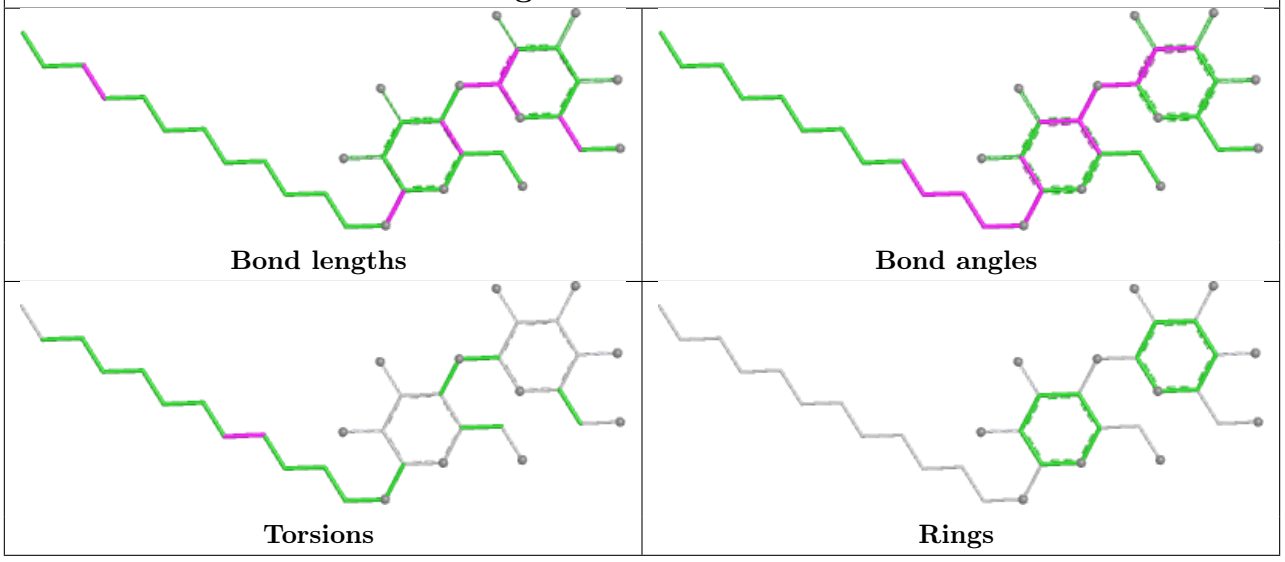
Ligand PHO BD 5404



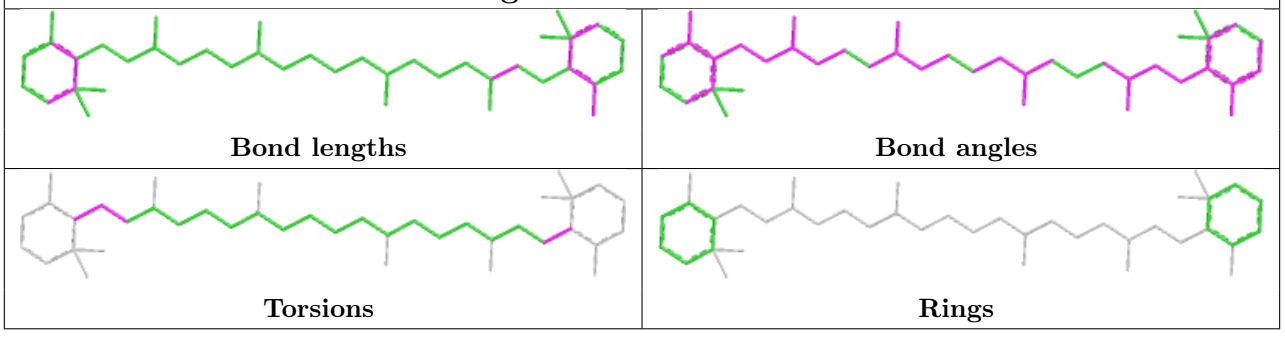
Ligand SQD AA 416



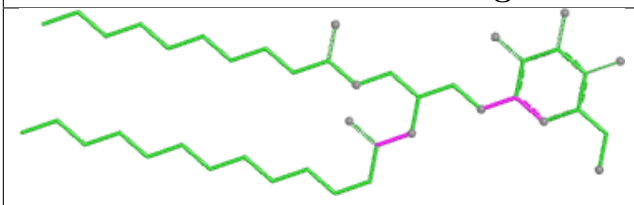
Ligand LMT AI 103



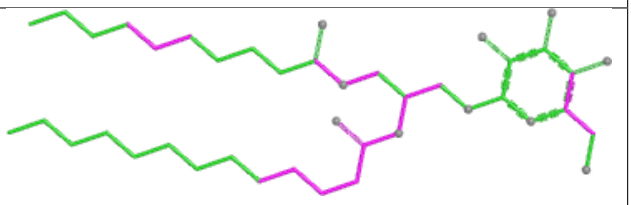
Ligand BCR BD 5407



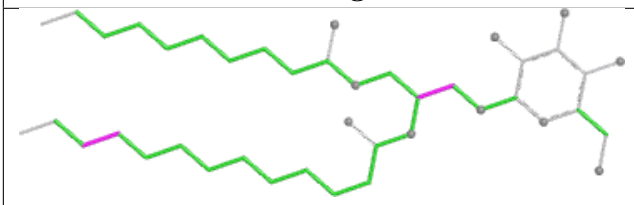
Ligand LMG BM 5102



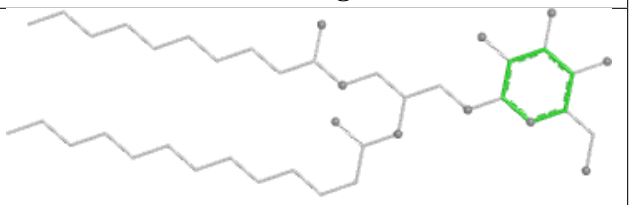
Bond lengths



Bond angles

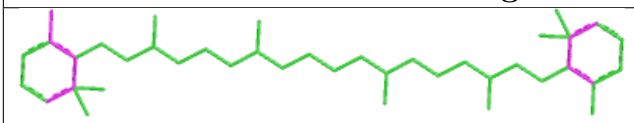


Torsions

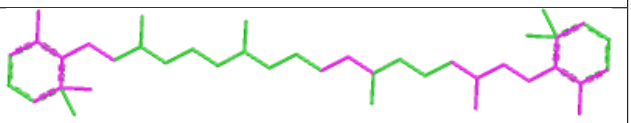


Rings

Ligand BCR BB 5622



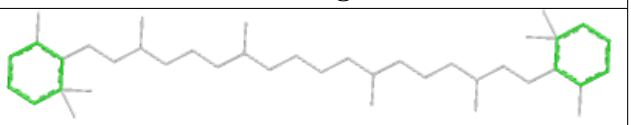
Bond lengths



Bond angles

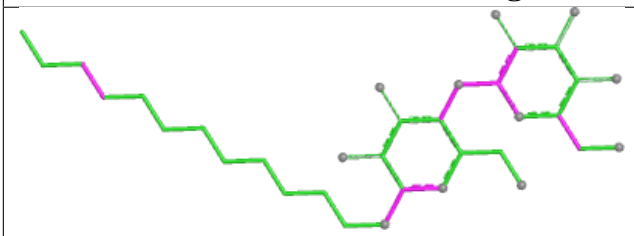


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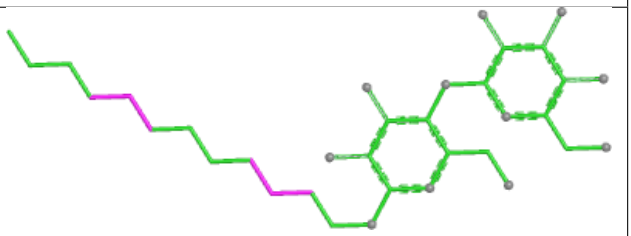


Rings

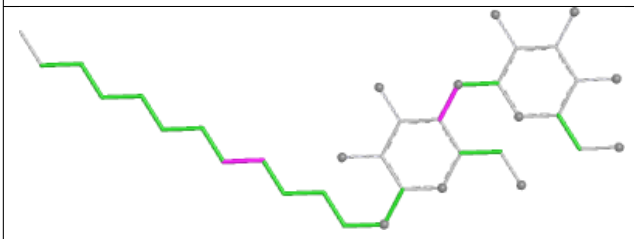
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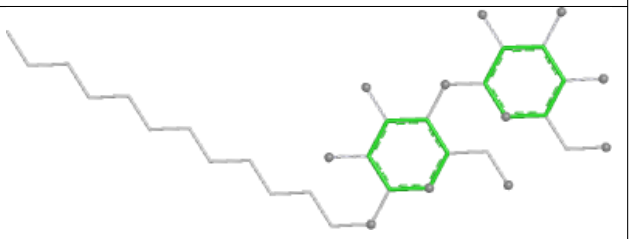
Bond lengths



Bond angles

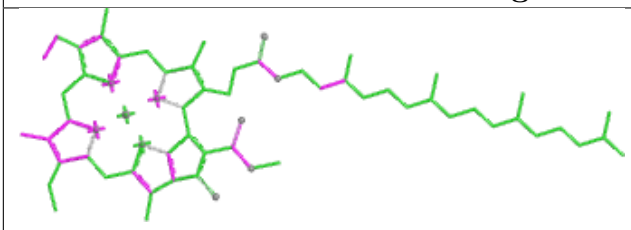


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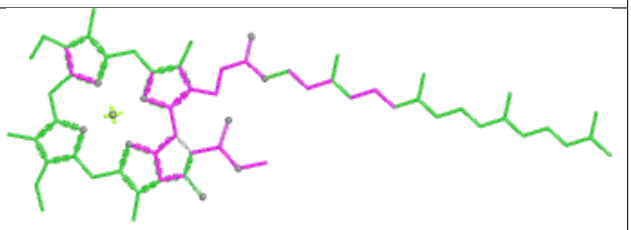


Rings

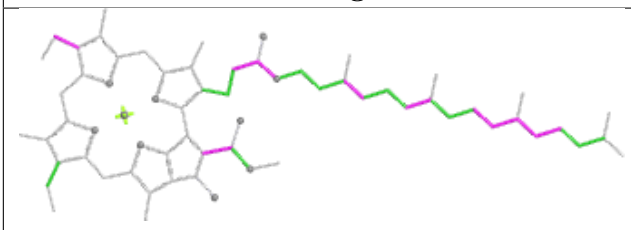
Ligand CLA AC 503



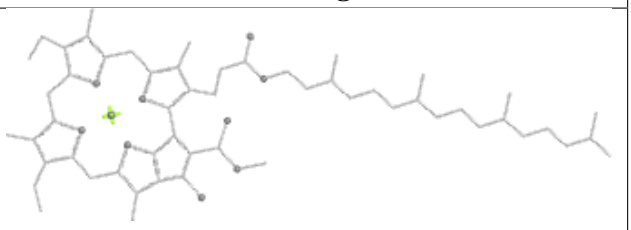
Bond lengths



Bond angles

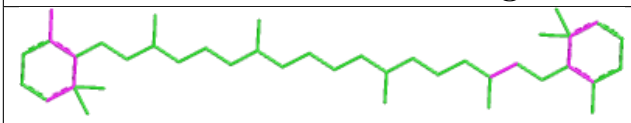


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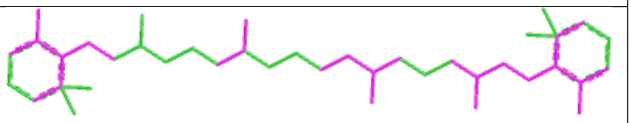


Rings

Ligand BCR BB 5623



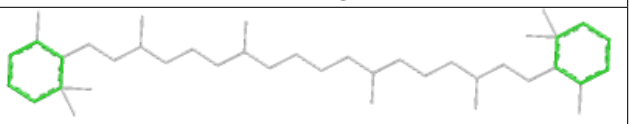
Bond lengths



Bond angles

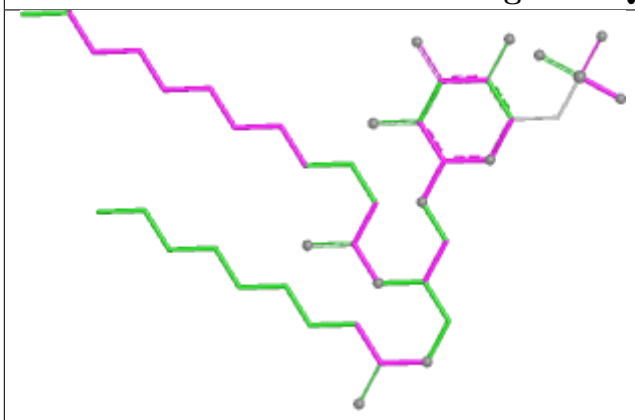


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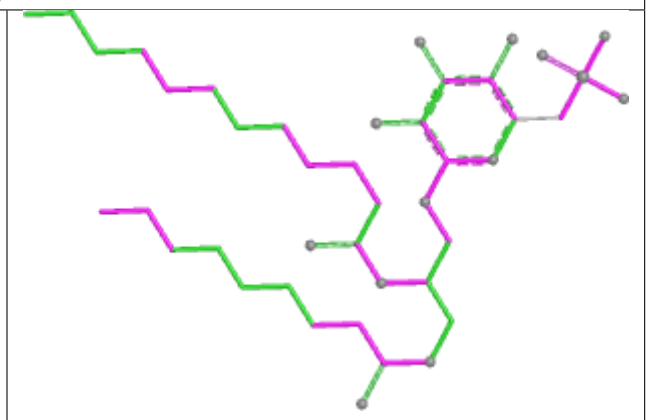


Rings

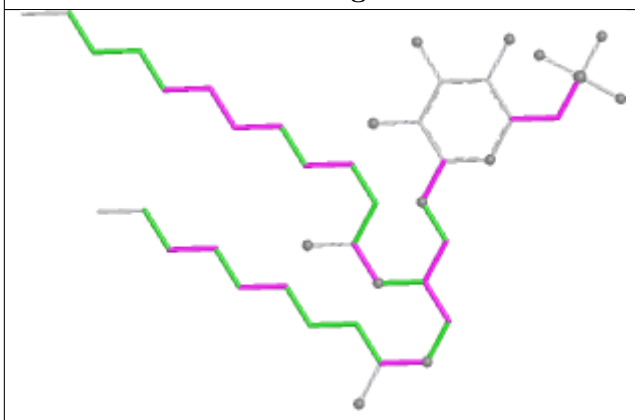
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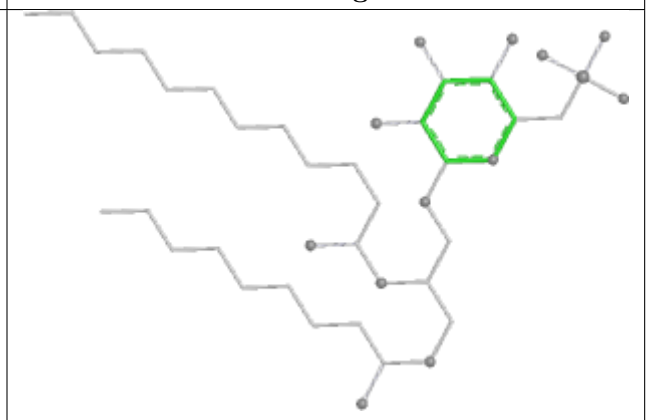
Bond lengths



Bond angles

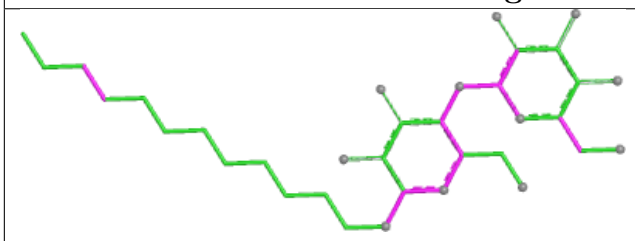


Torsions

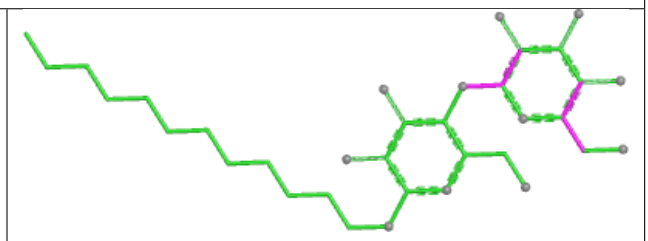


Rings

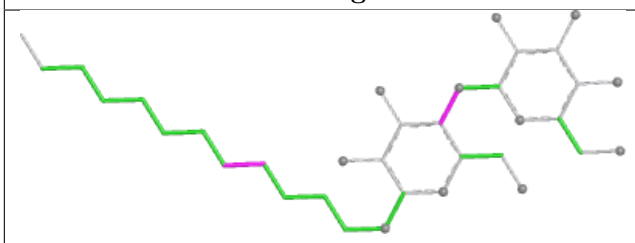
Ligand LMT AM 102



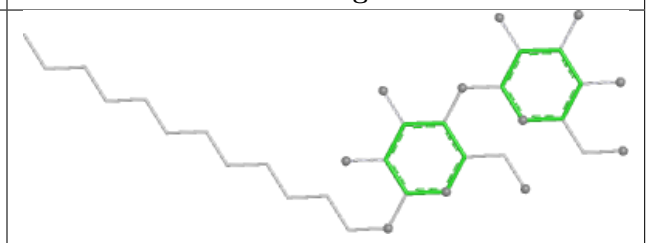
Bond lengths



Bond angles

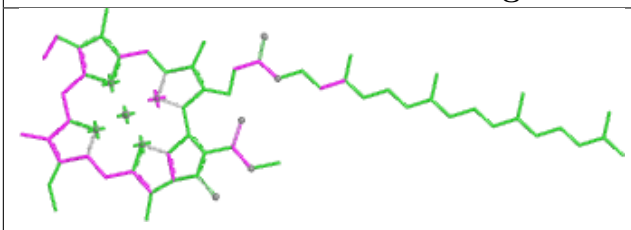


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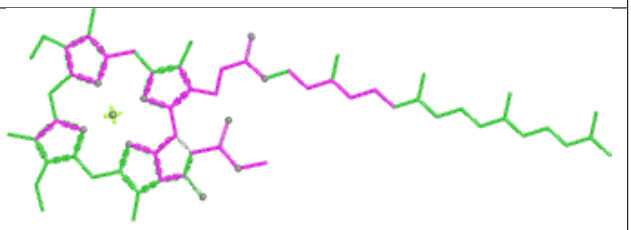


Rings

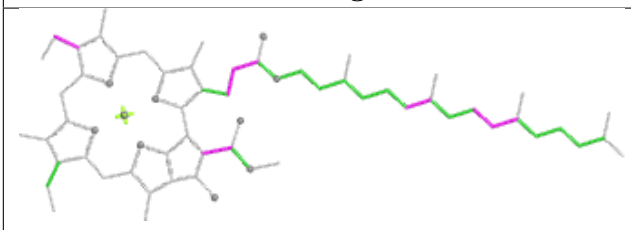
Ligand CLA BB 5607



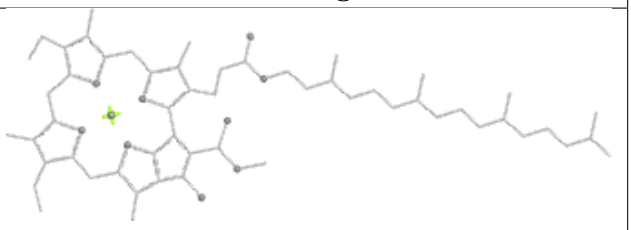
Bond lengths



Bond angles

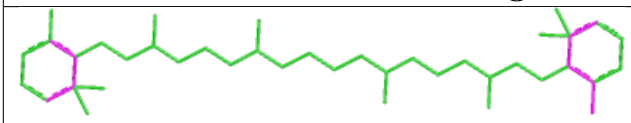


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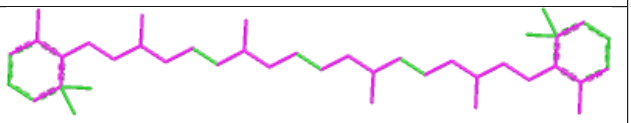


Rings

Ligand BCR AD 406



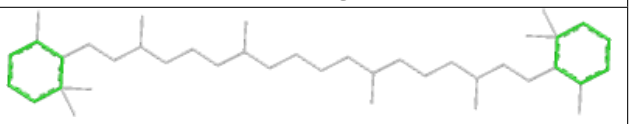
Bond lengths



Bond angles

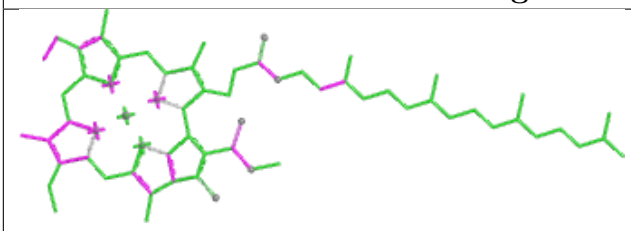


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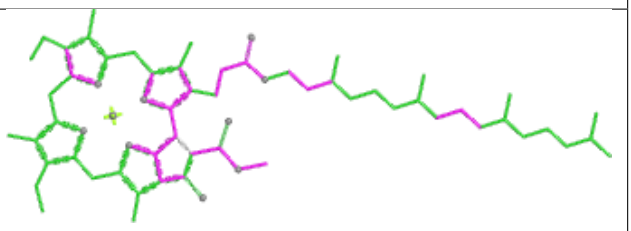


Rings

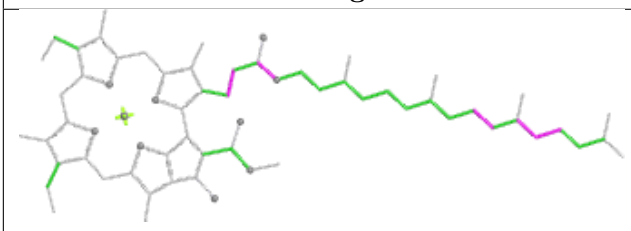
Ligand CLA AB 602



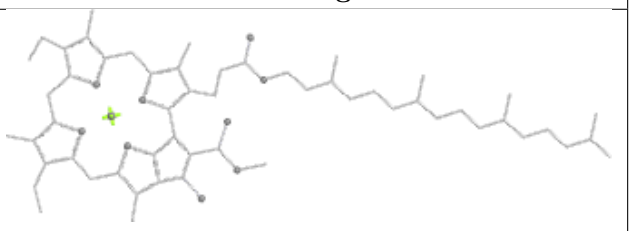
Bond lengths



Bond angles

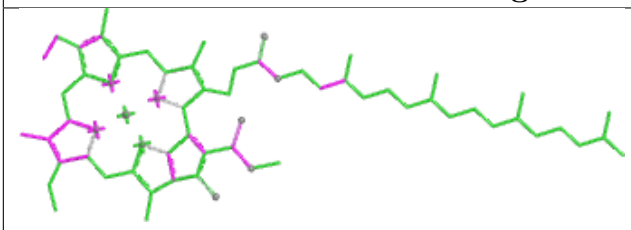


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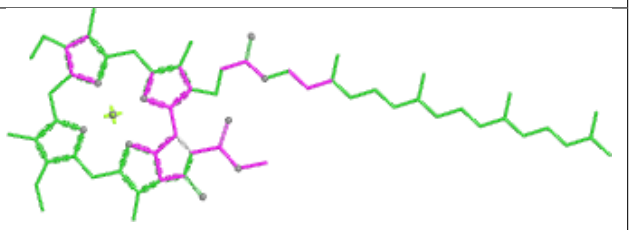


Rings

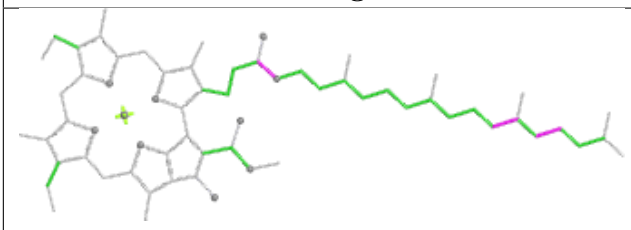
Ligand CLA AB 615



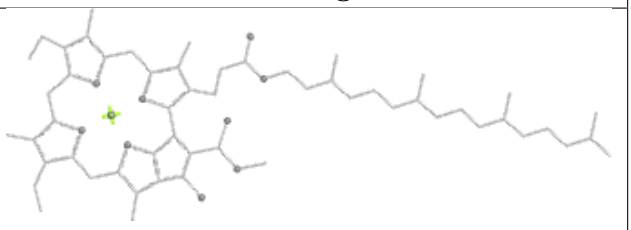
Bond lengths



Bond angles

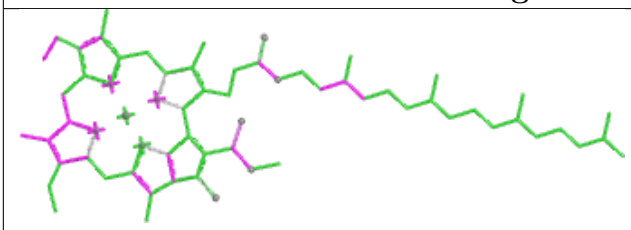


Torsions

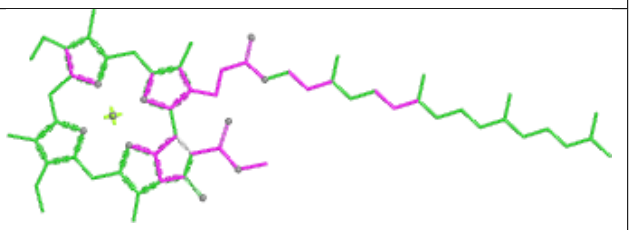


Rings

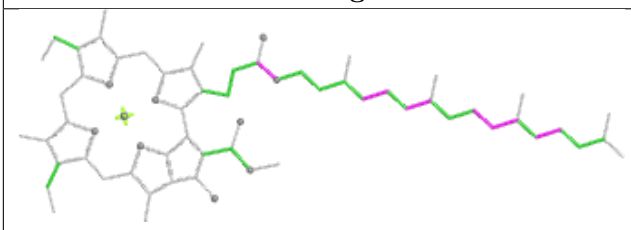
Ligand CLA AC 504



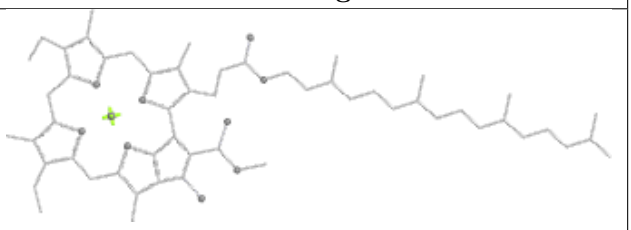
Bond lengths



Bond angles

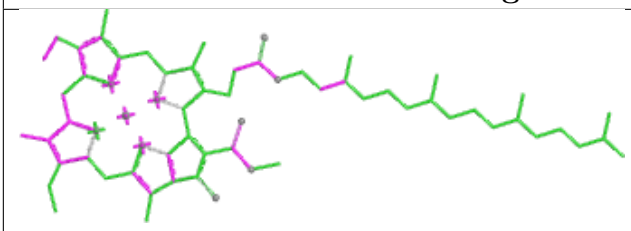


Torsions

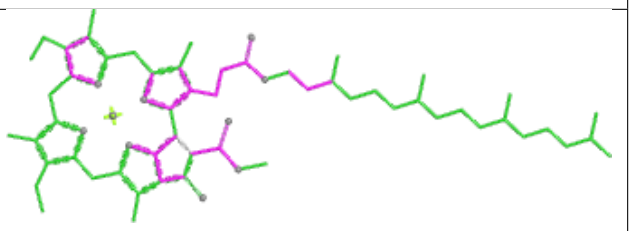


Rings

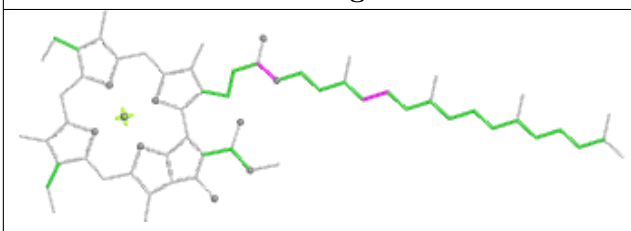
Ligand CLA BA 5407



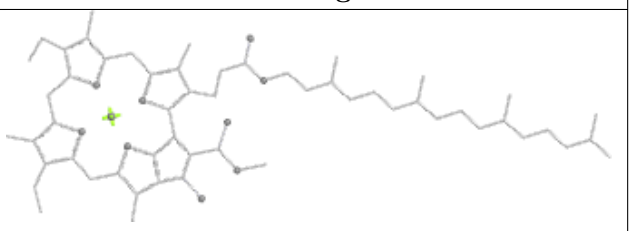
Bond lengths



Bond angles

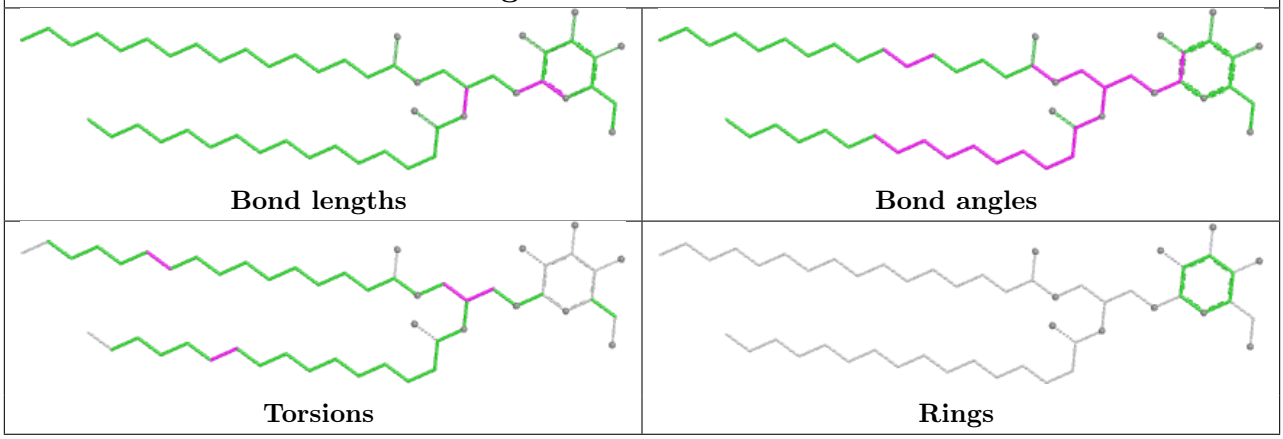


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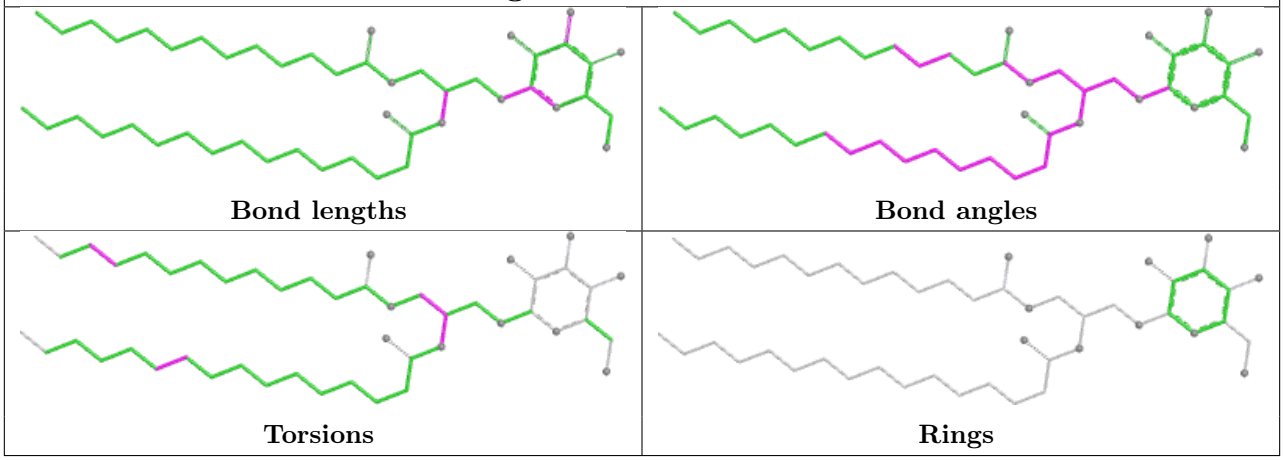


Rings

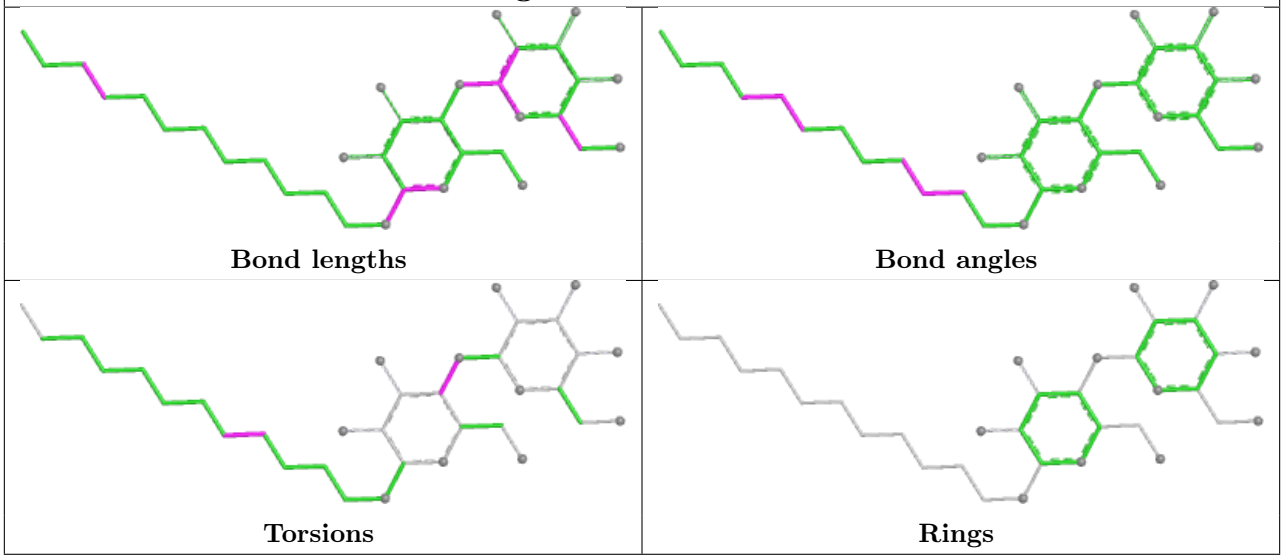
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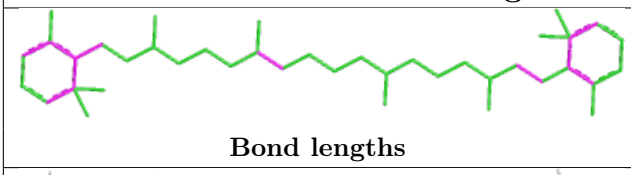
Ligand LMG AD 408



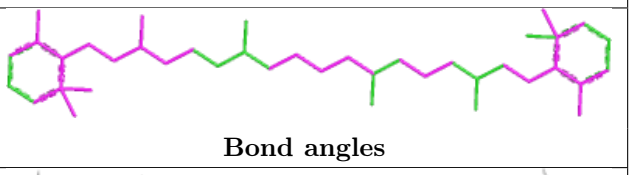
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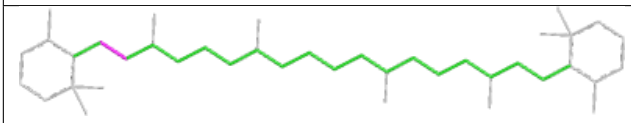
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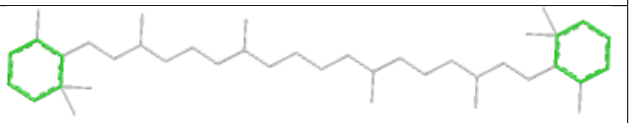
Bond lengths



Bond angles



Torsions

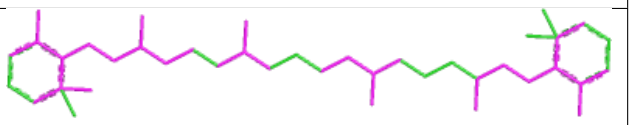


Rings

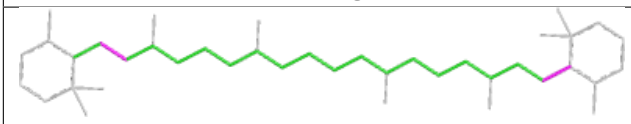
Ligand BCR BC 5515



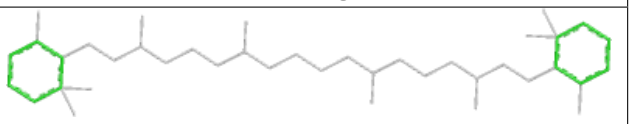
Bond lengths



Bond angles

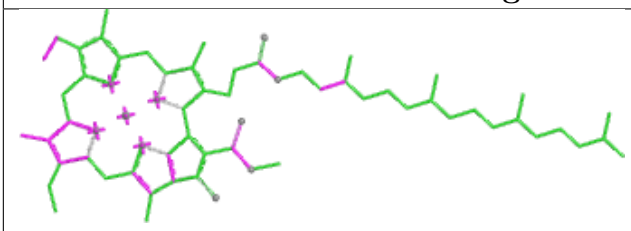


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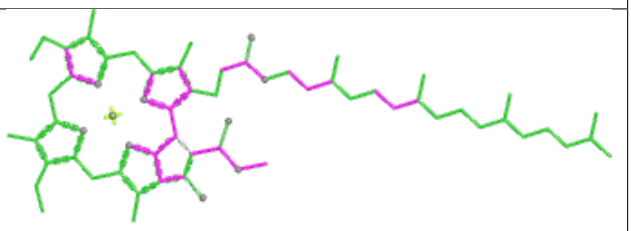


Rings

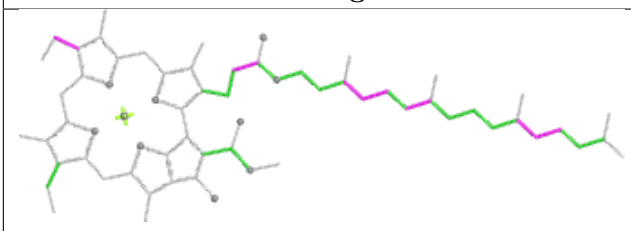
Ligand CLA BB 5617



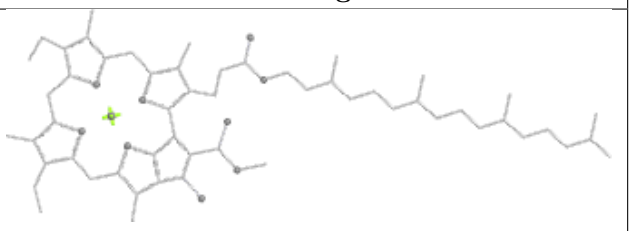
Bond lengths



Bond angles

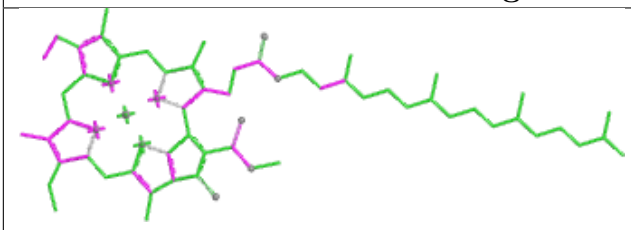


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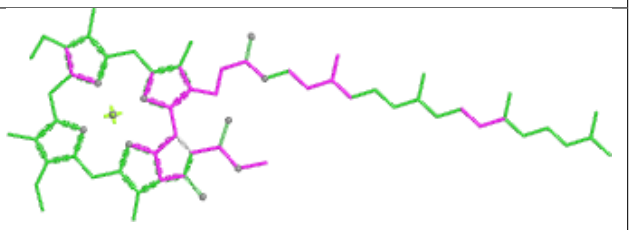


Rings

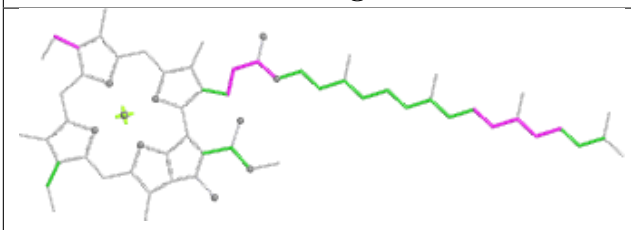
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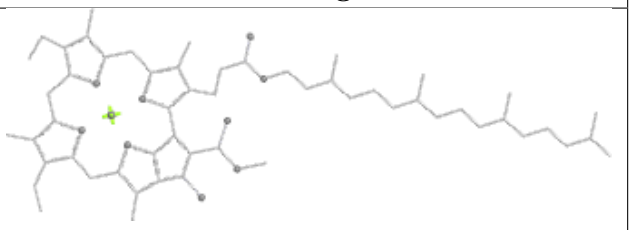
Bond lengths



Bond angles

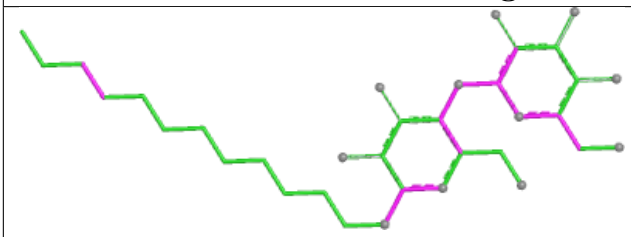


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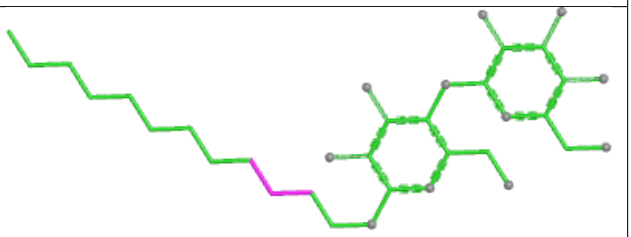


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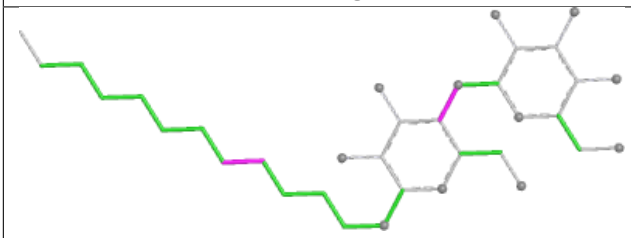
Ligand LMT BB 5604



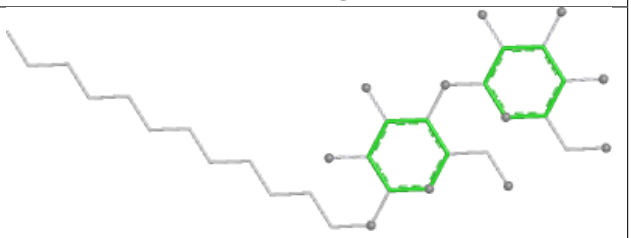
Bond lengths



Bond angles



Torsions

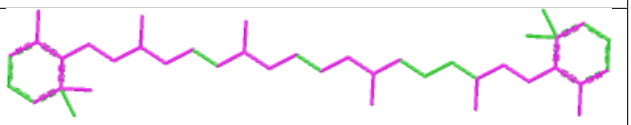


Rings

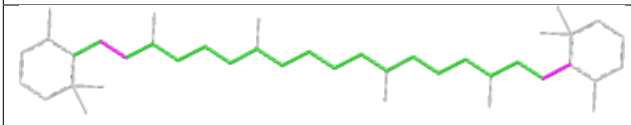
Ligand BCR AC 515



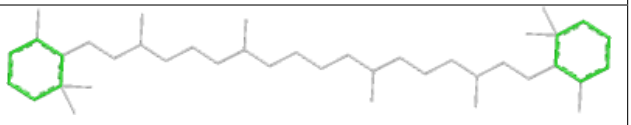
Bond lengths



Bond angles

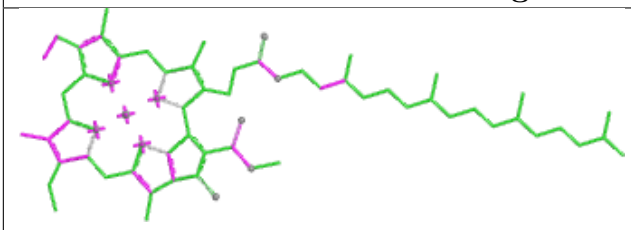


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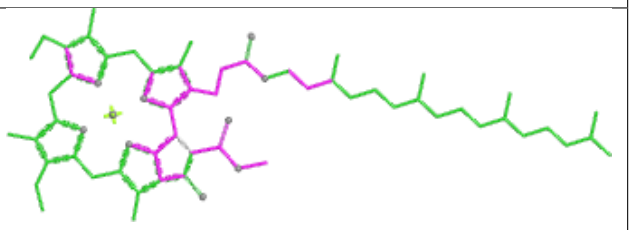


Rings

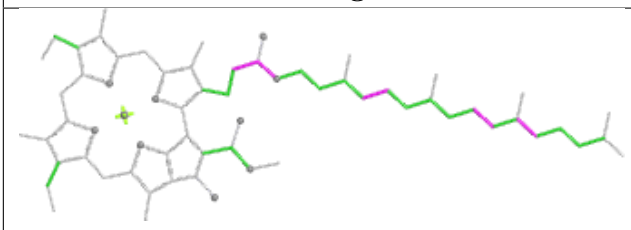
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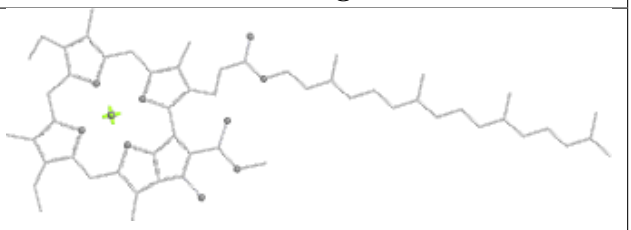
Bond lengths



Bond angles

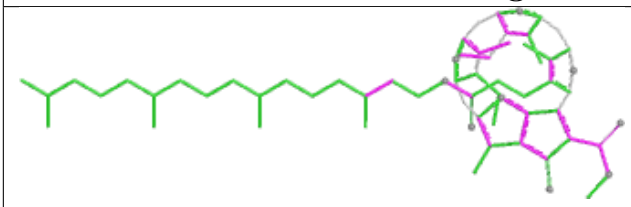


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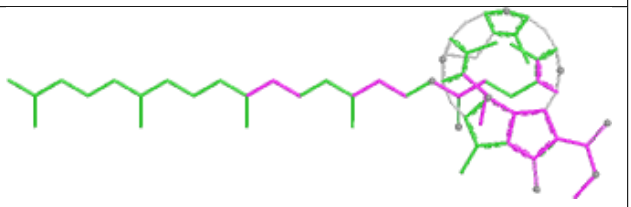


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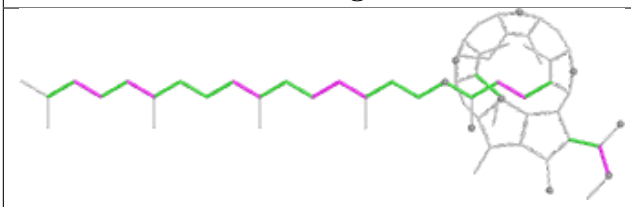
Ligand PHO AD 402



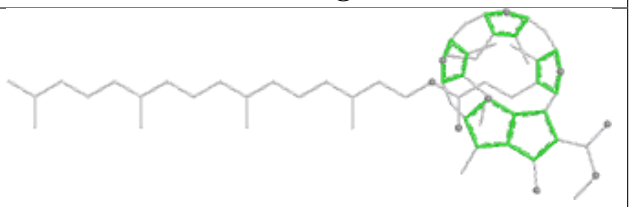
Bond lengths



Bond angles

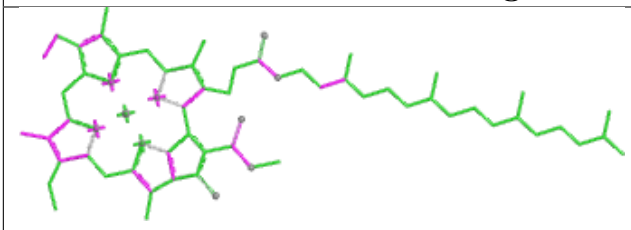


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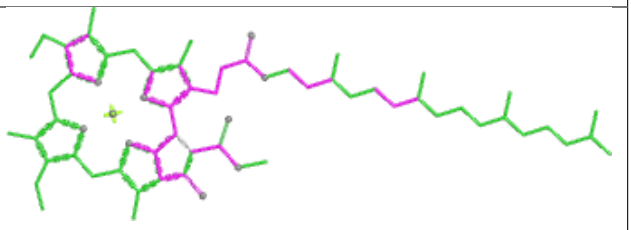


Rings

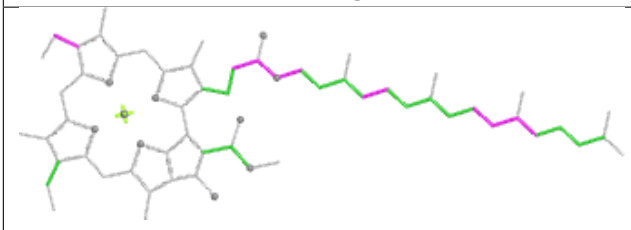
Ligand CLA BB 5608



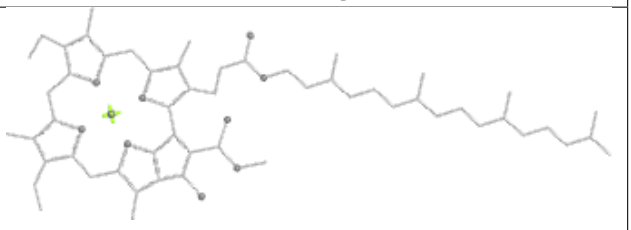
Bond lengths



Bond angles

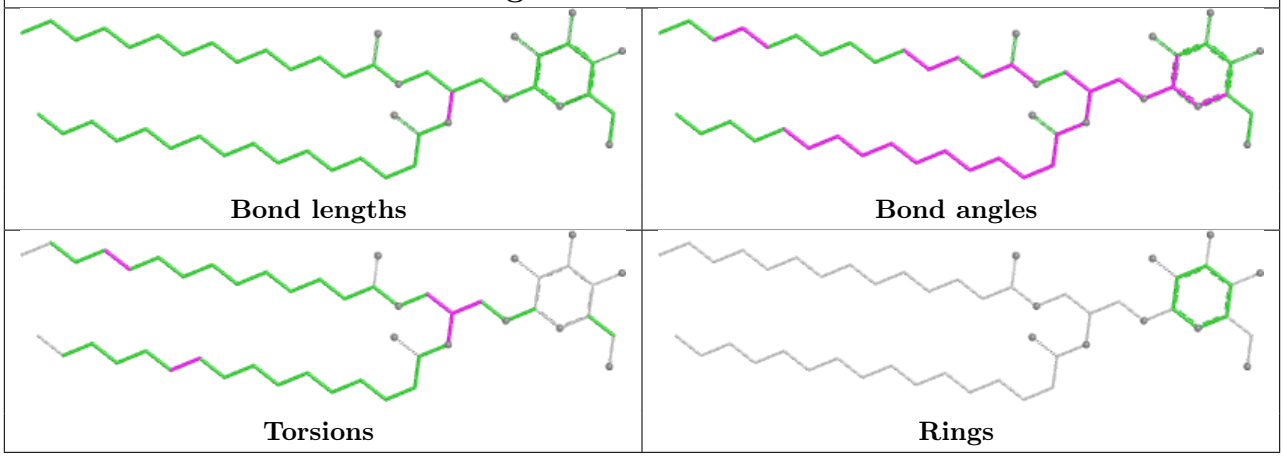


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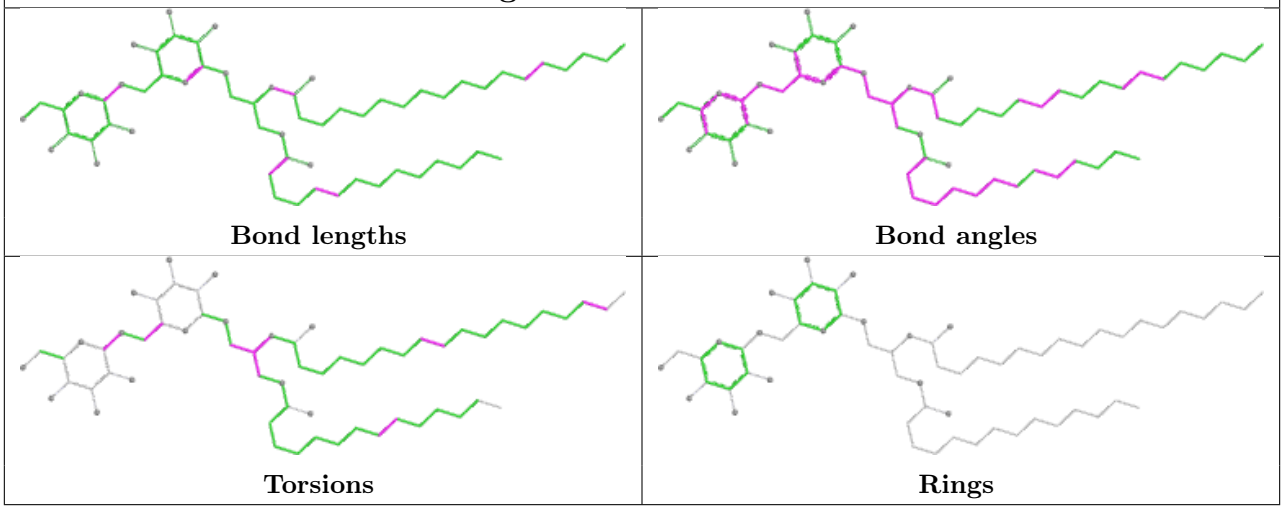


Rings

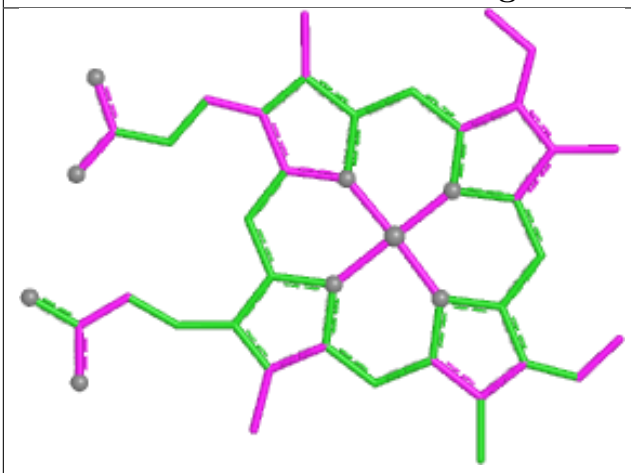
Ligand LMG AD 407



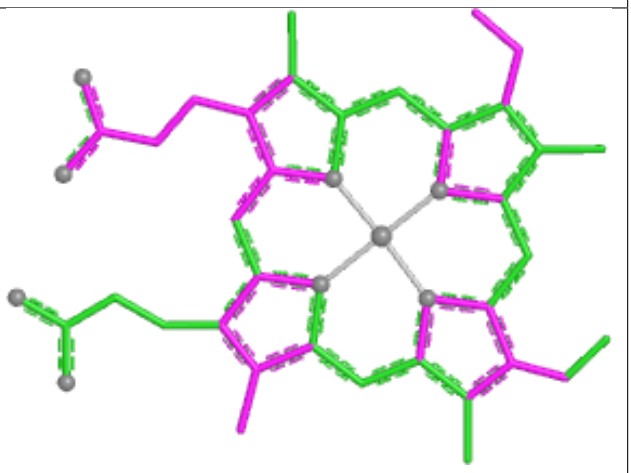
Ligand DGD BC 5518



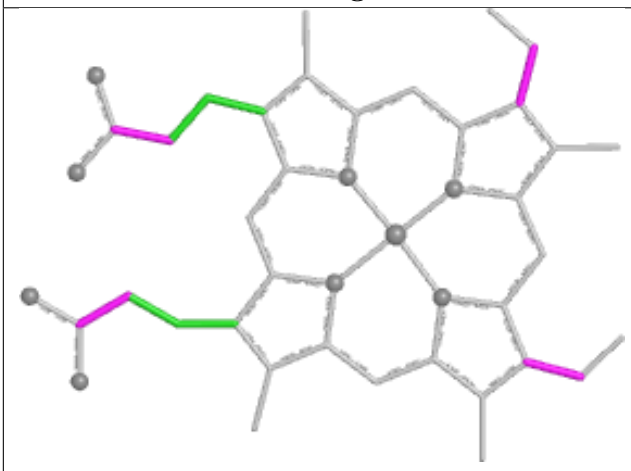
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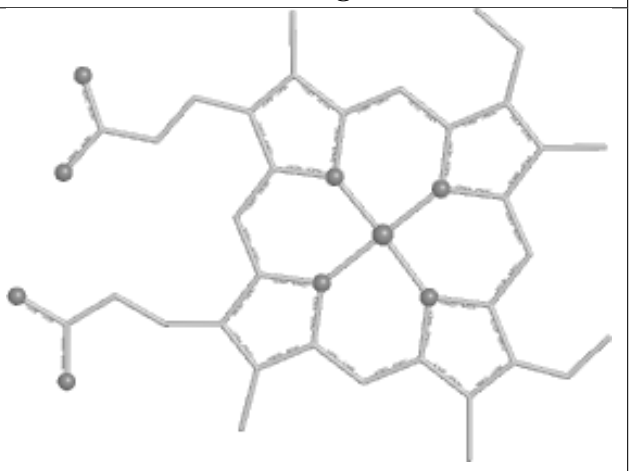
Bond lengths



Bond angles

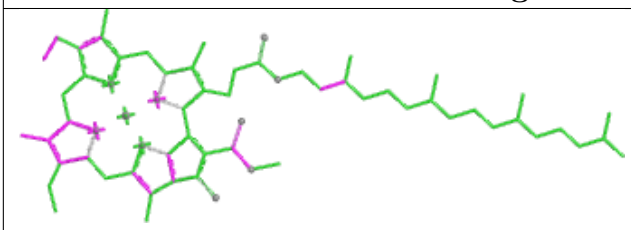


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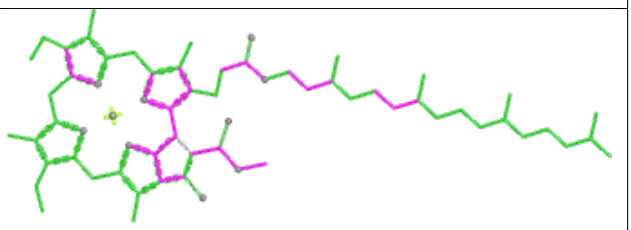


Rings

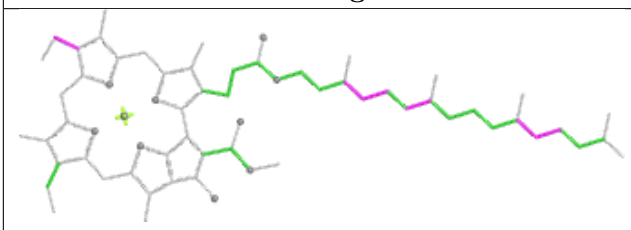
Ligand CLA AB 613



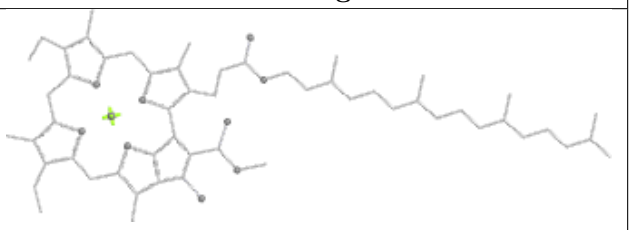
Bond lengths



Bond angles

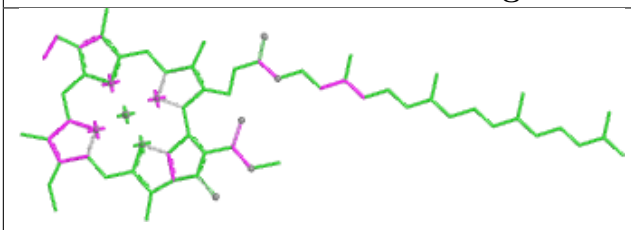


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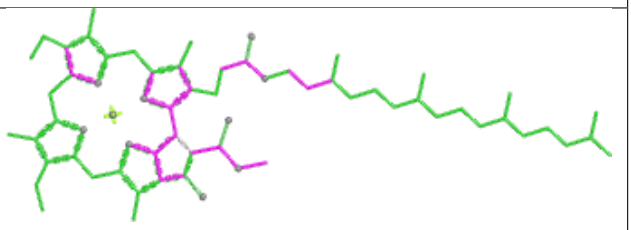


Rings

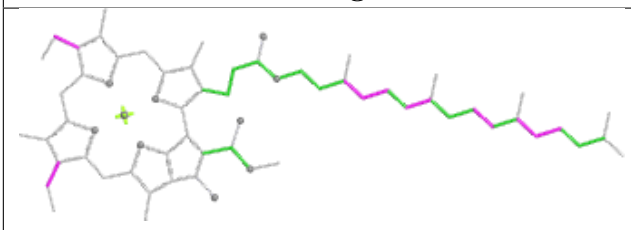
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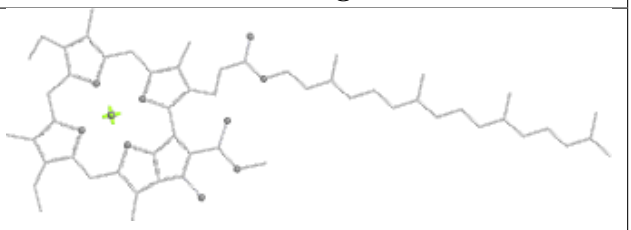
Bond lengths



Bond angles

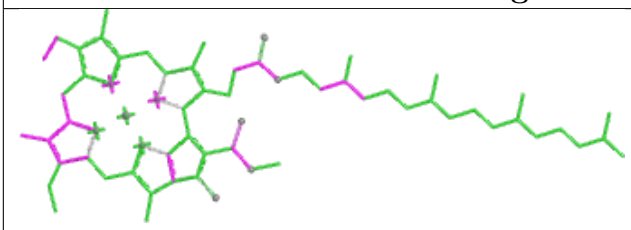


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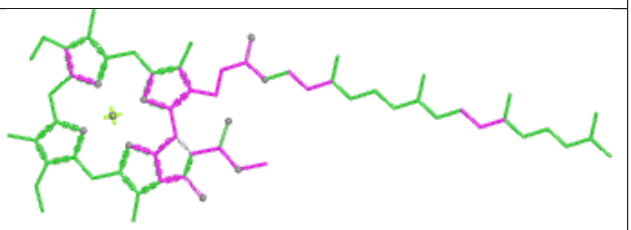


Rings

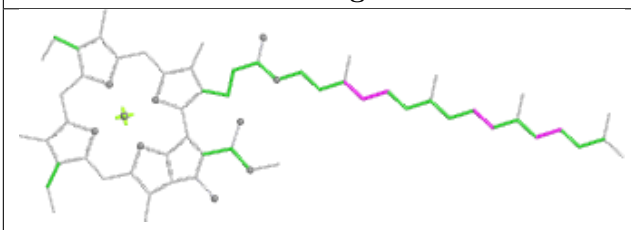
Ligand CLA AB 607



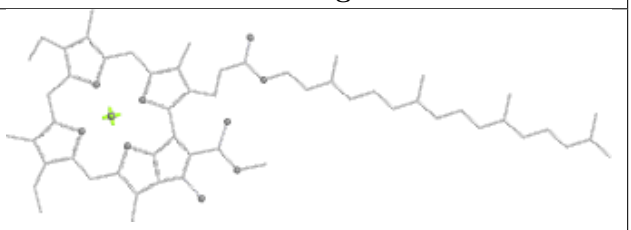
Bond lengths



Bond angles

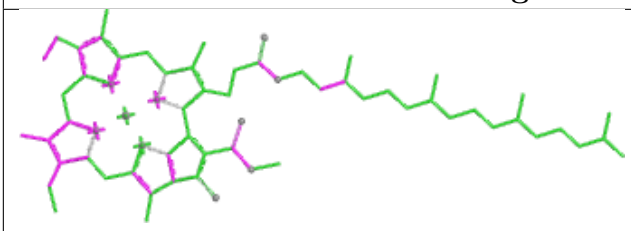


Torsions

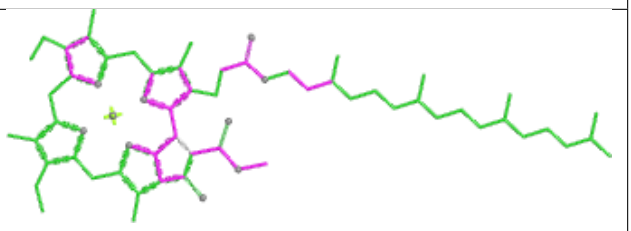


Rings

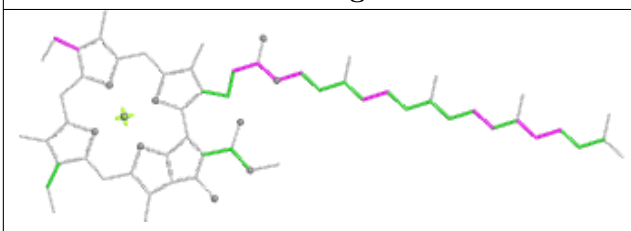
Ligand CLA AC 512



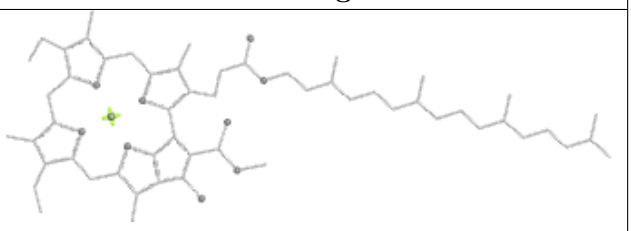
Bond lengths



Bond angles

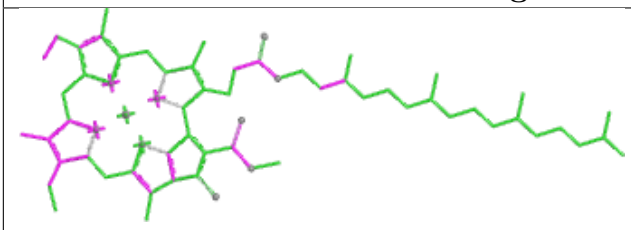


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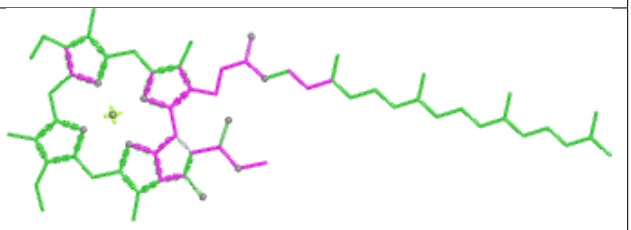


Rings

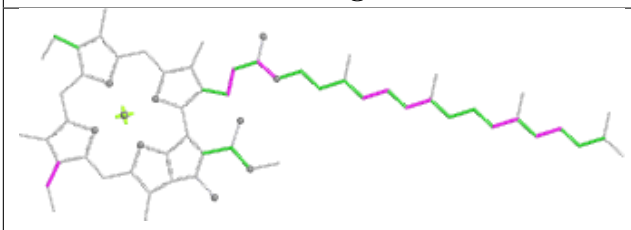
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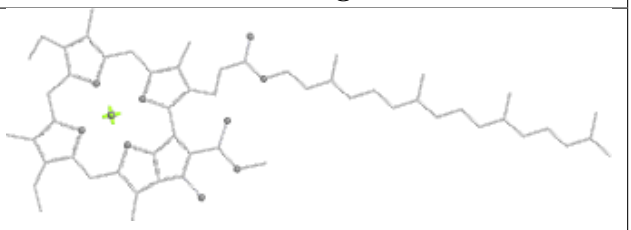
Bond lengths



Bond angles

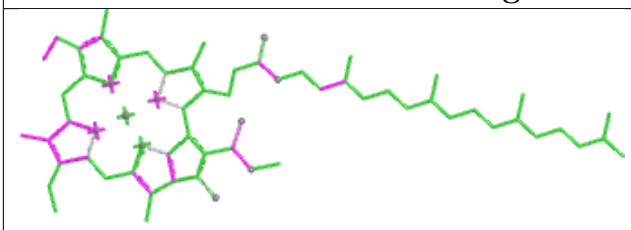


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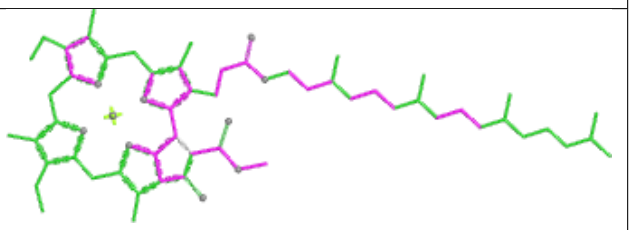


Rings

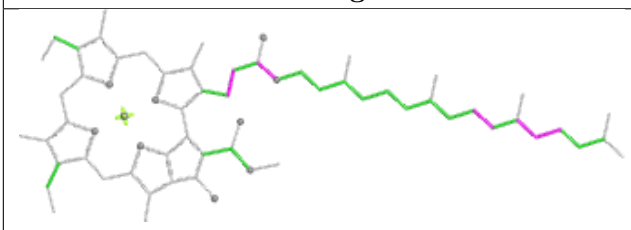
Ligand CLA BB 5606



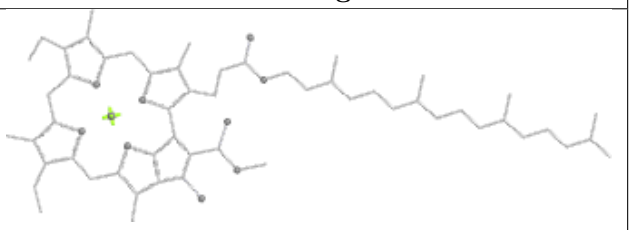
Bond lengths



Bond angles

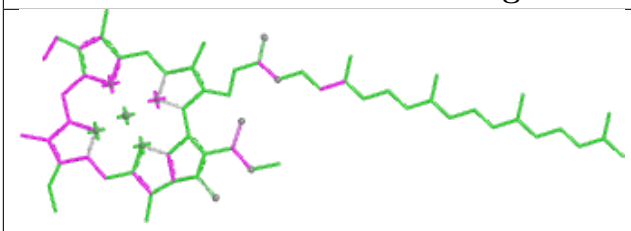


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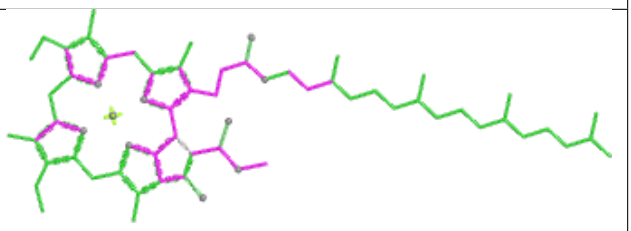


Rings

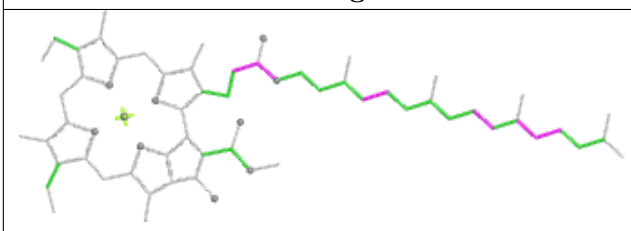
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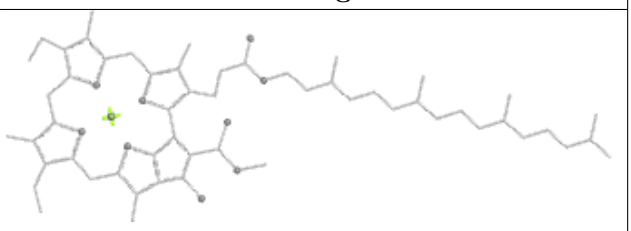
Bond lengths



Bond angles

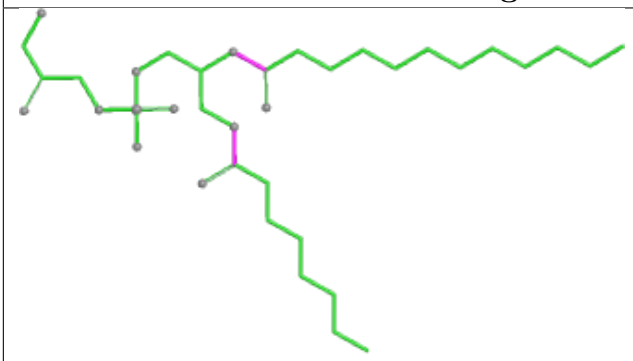


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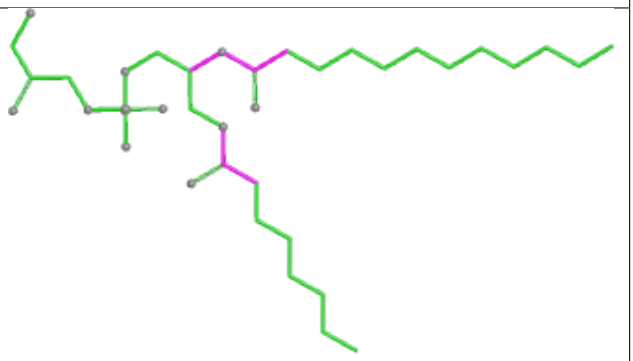


Rings

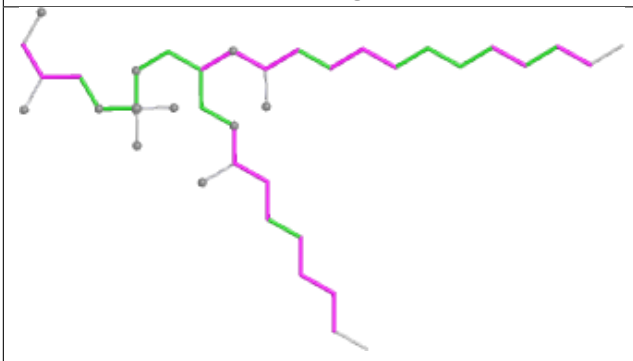
Ligand LHG BA 5415



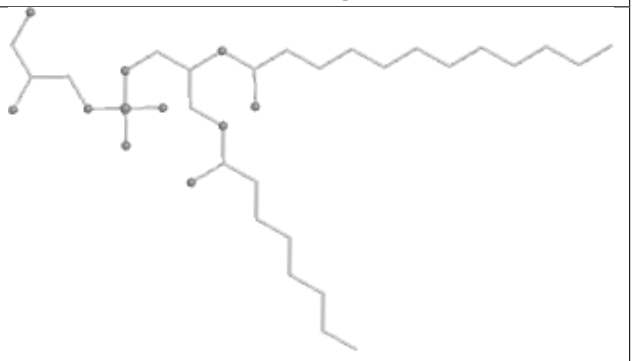
Bond lengths



Bond angles

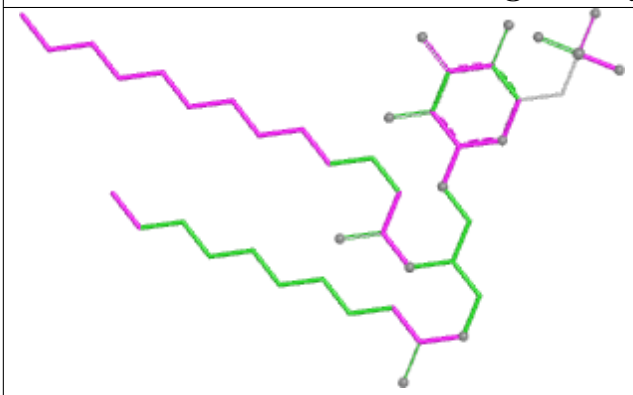


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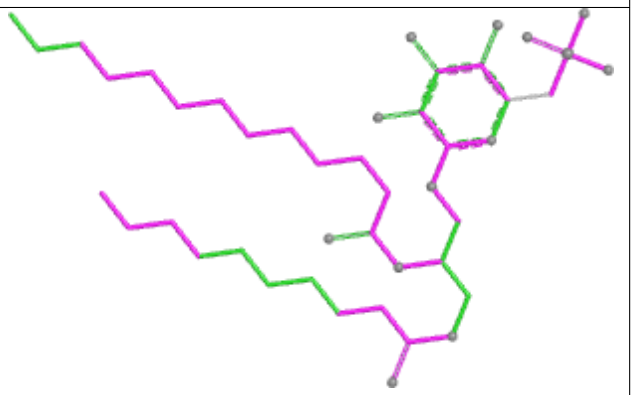


Rings

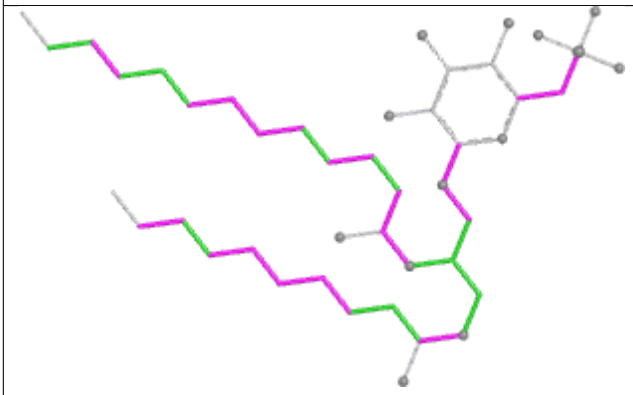
Ligand SQD BF 5102



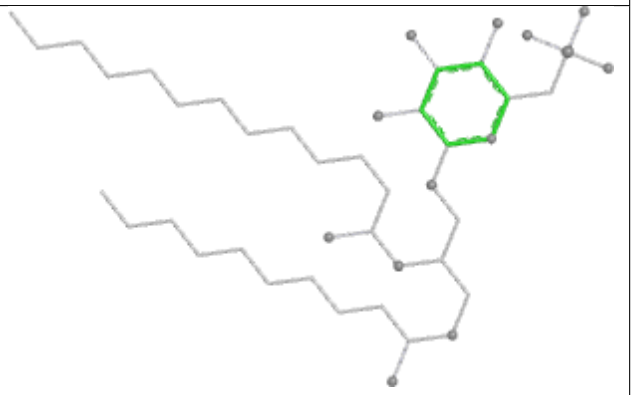
Bond lengths



Bond angles

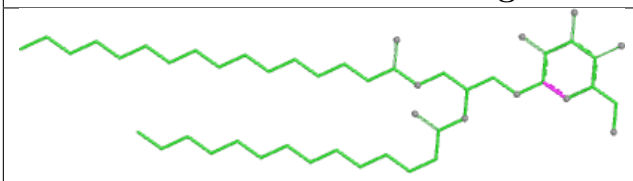


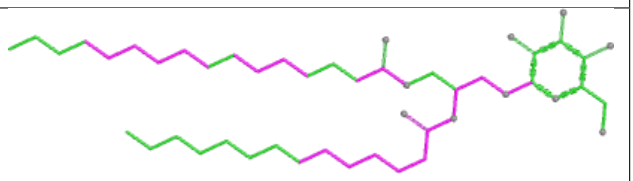
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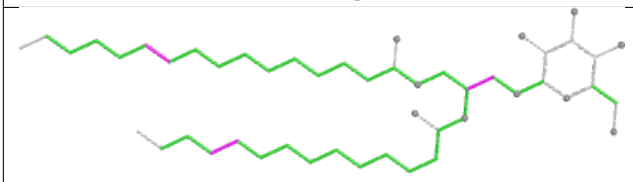


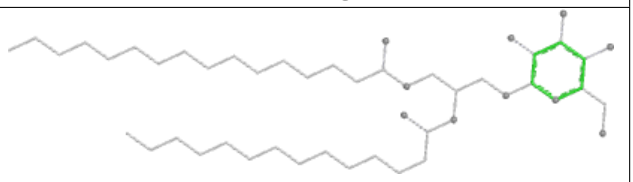
Rings

Ligand LMG BB 5624

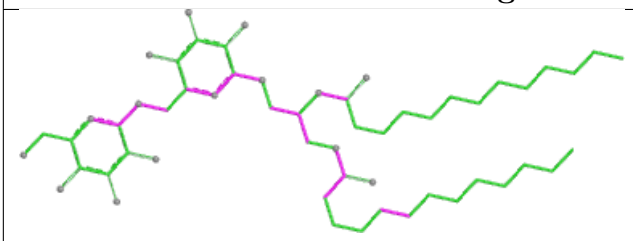

Bond lengths

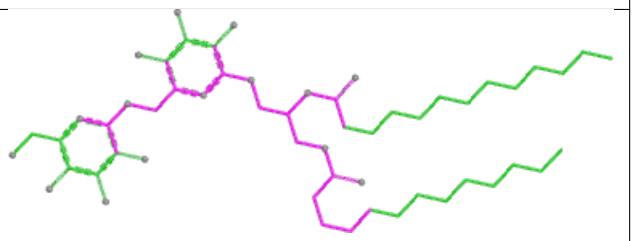

Bond angles

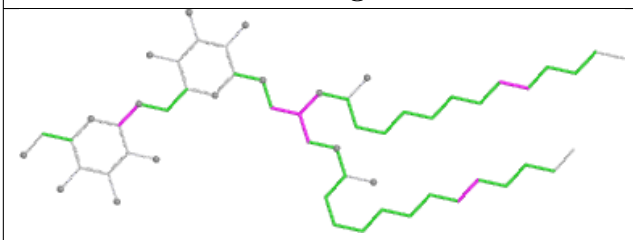

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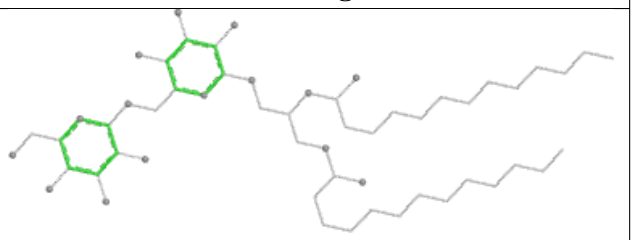

Rings

Ligand DGD BA 5412

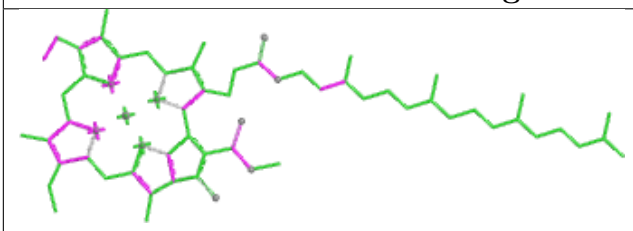

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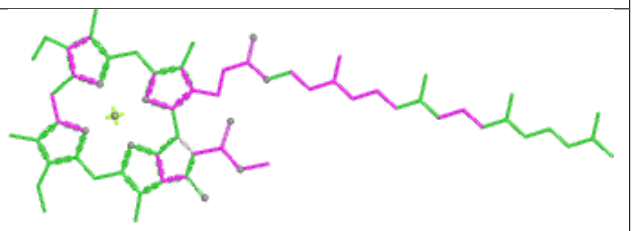

Bond angles

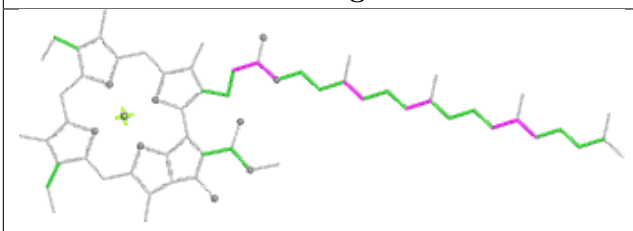

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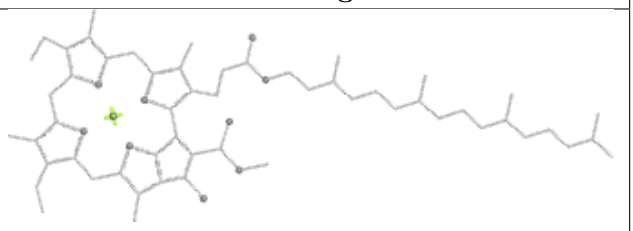

Rings

Ligand CLA BB 5615

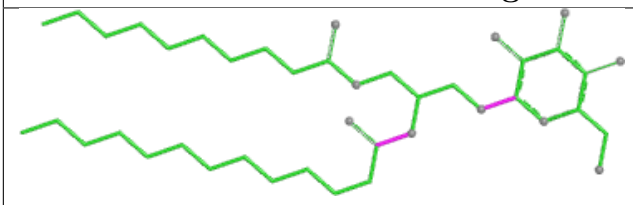

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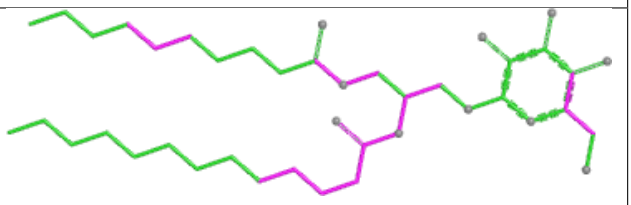

Bond angles

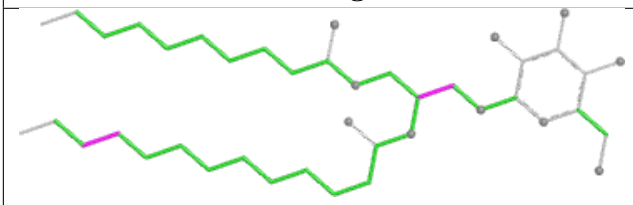

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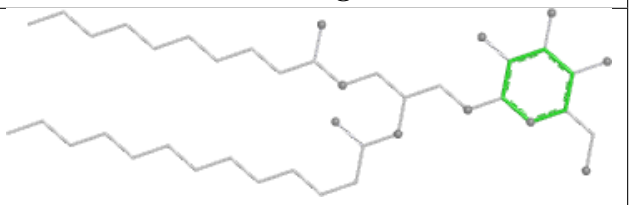

Rings

Ligand LMG AM 101

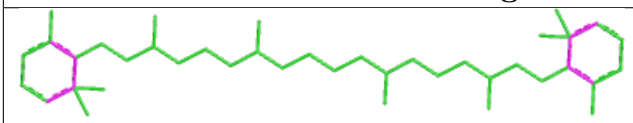

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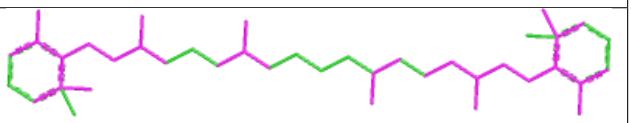

Bond angles


Torsions

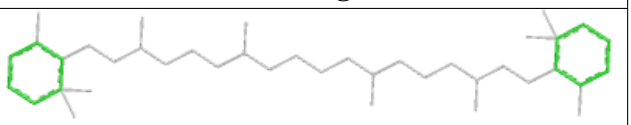

Rings

Ligand BCR BC 5514

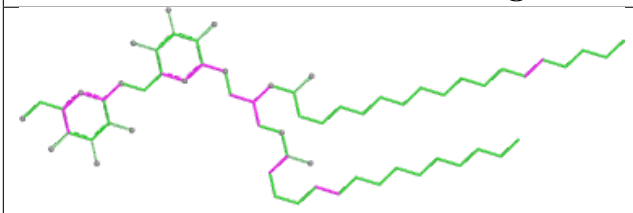

Bond lengths

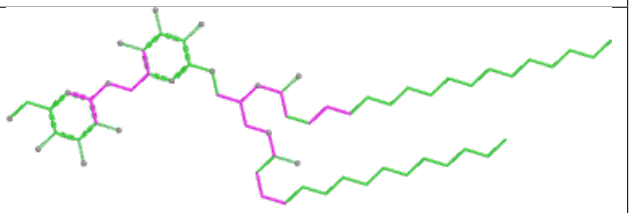

Bond angles

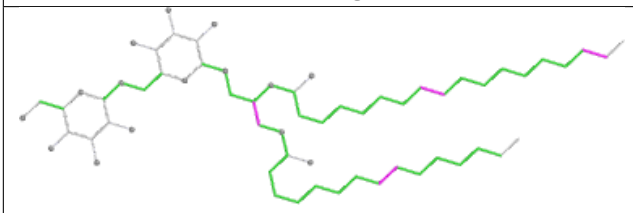

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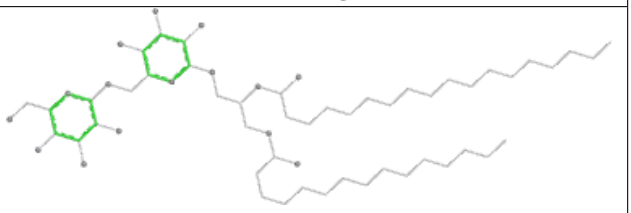

Rings

Ligand DGD AE 101

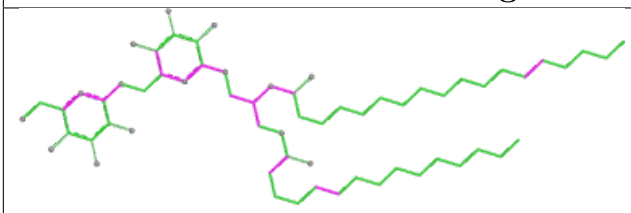

Bond lengths


Bond angles

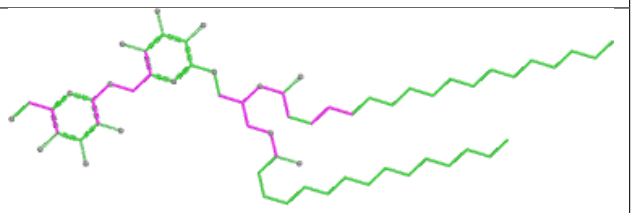

Torsions


Rings

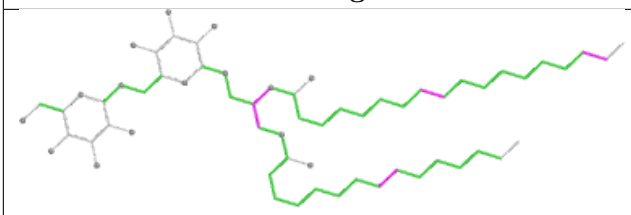
Ligand DGD BE 5102



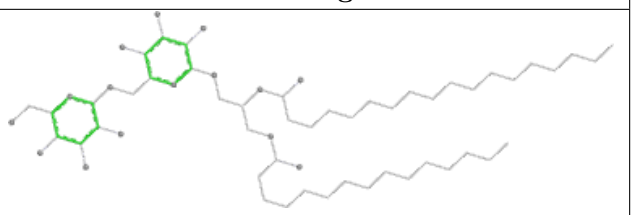
Bond lengths



Bond angles



Torsions

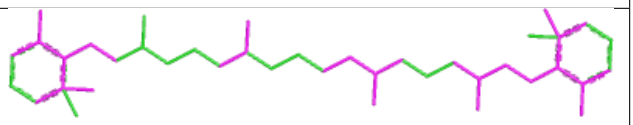


Rings

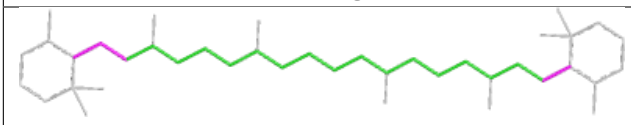
Ligand BCR BC 5516



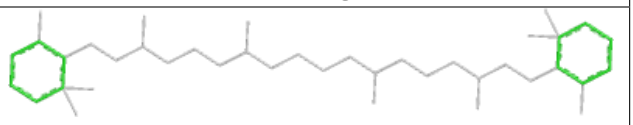
Bond lengths



Bond angles

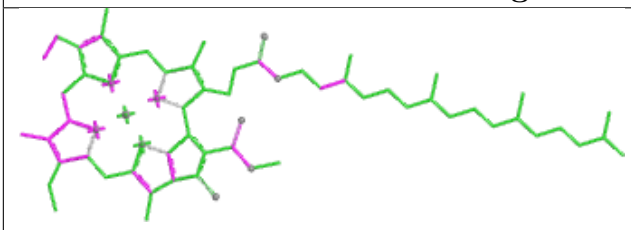


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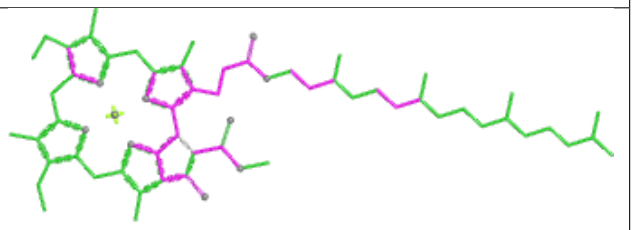


Rings

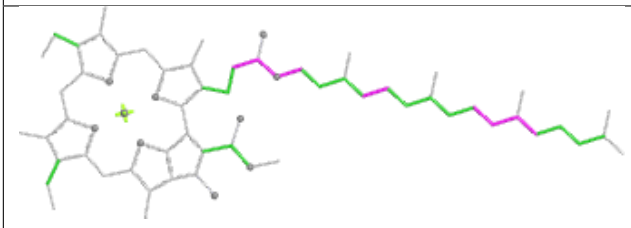
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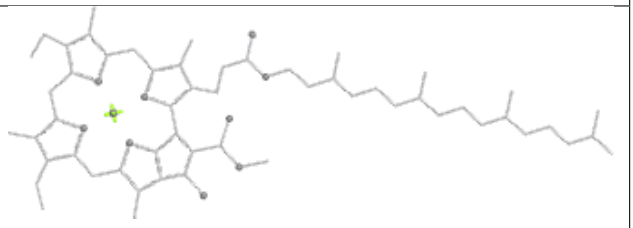
Bond lengths



Bond angles

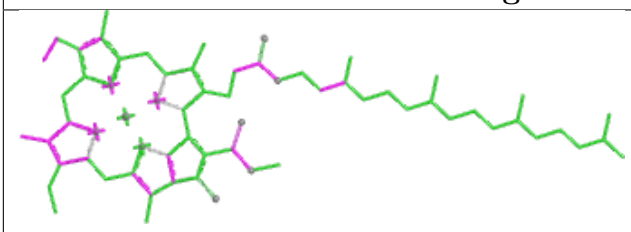


Torsions

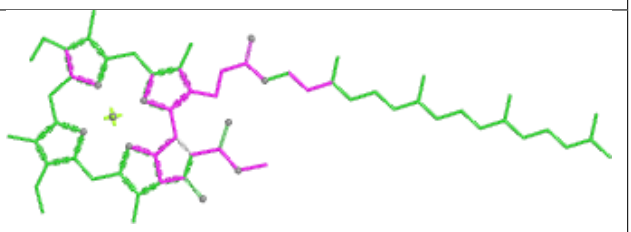


Rings

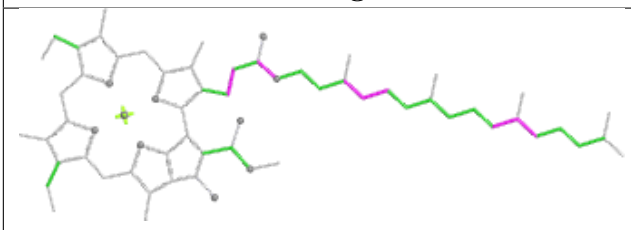
Ligand CLA BB 5610



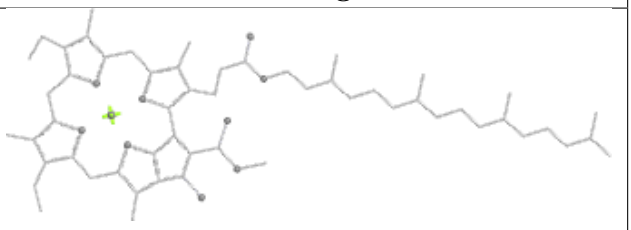
Bond lengths



Bond angles

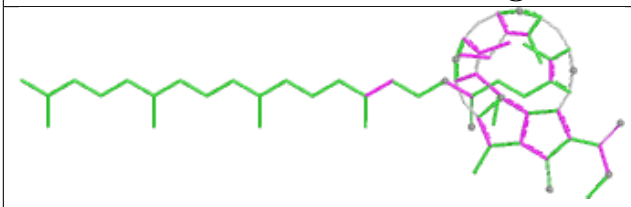


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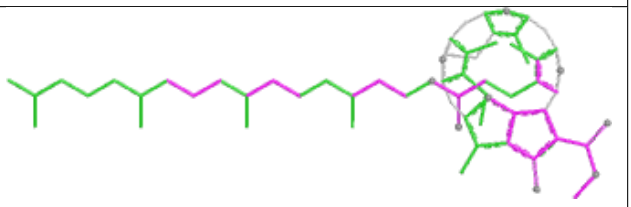


Rings

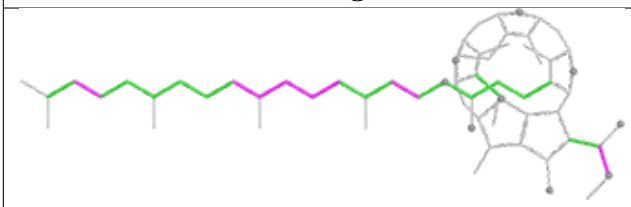
Ligand PHO AD 403



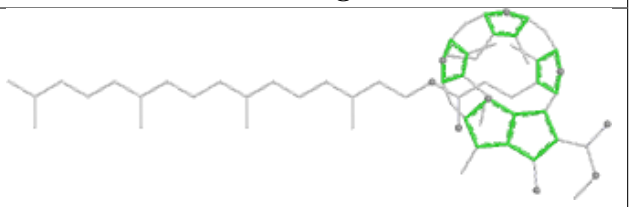
Bond lengths



Bond angles

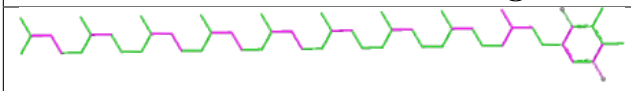


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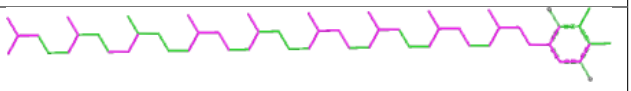


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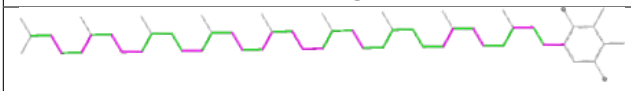
Ligand PL9 BD 5406



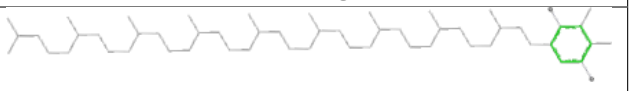
Bond lengths



Bond angles

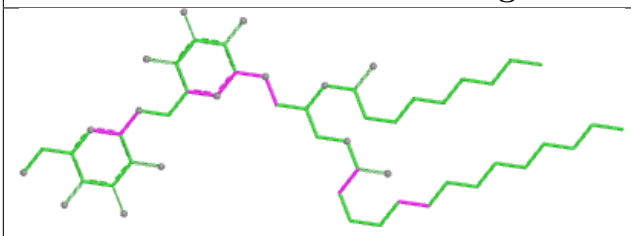


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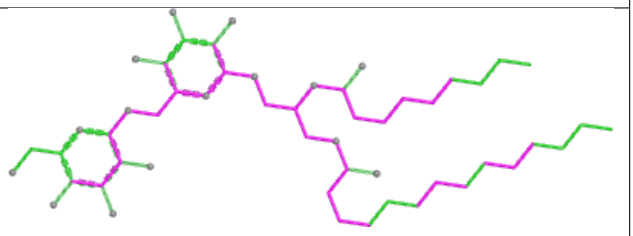


Rings

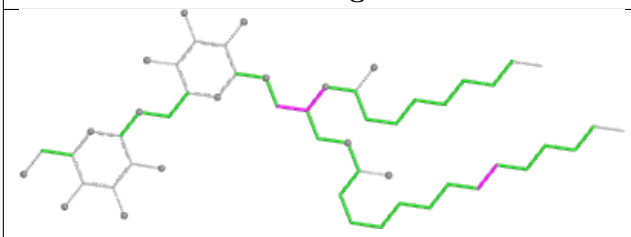
Ligand DGD BC 5517



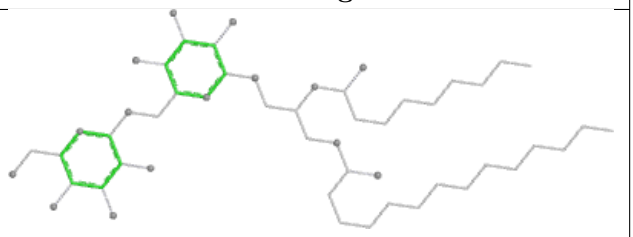
Bond lengths



Bond angles

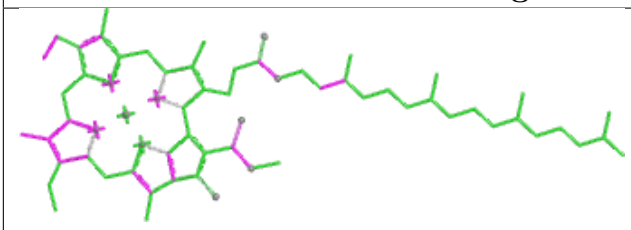


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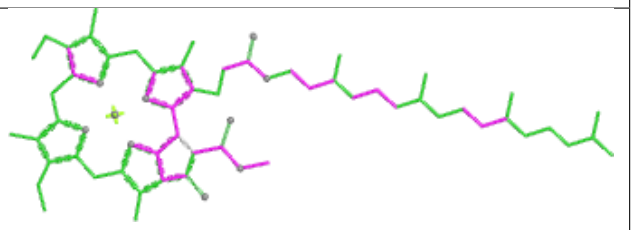


Rings

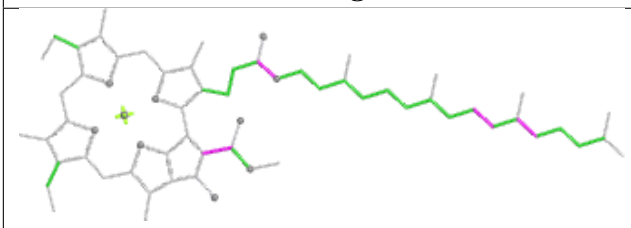
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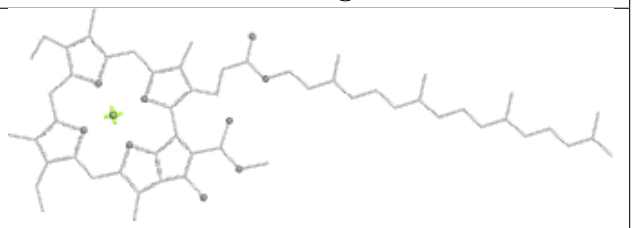
Bond lengths



Bond angles

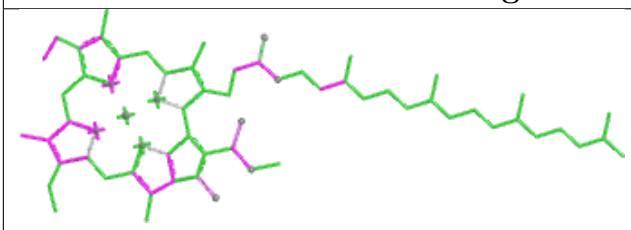


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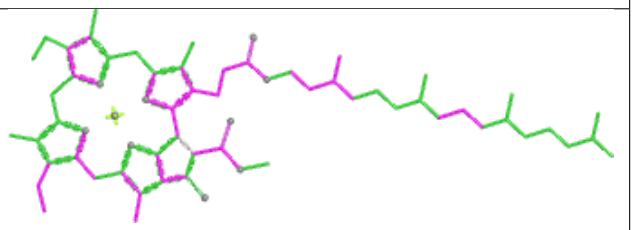


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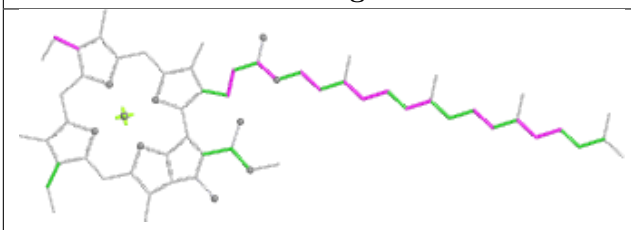
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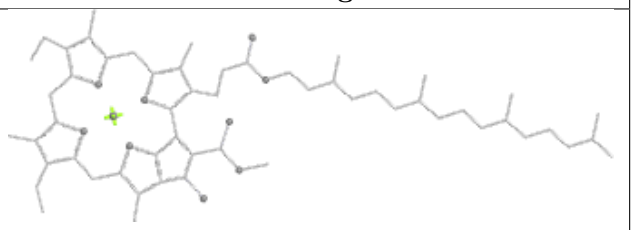
Bond lengths



Bond angles

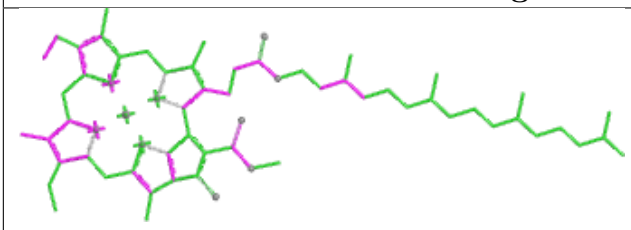


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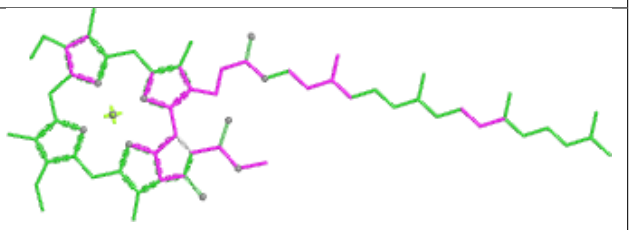


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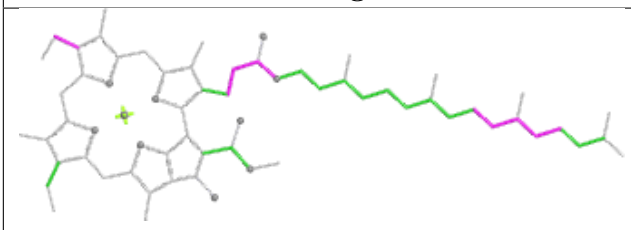
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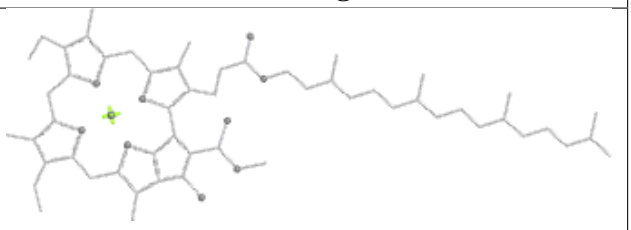
Bond lengths



Bond angles

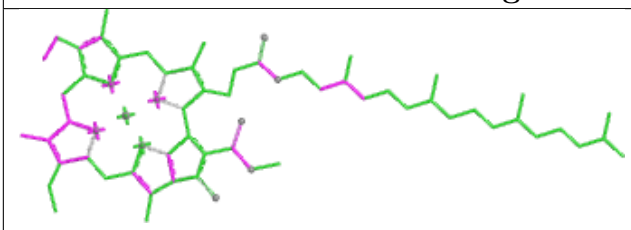


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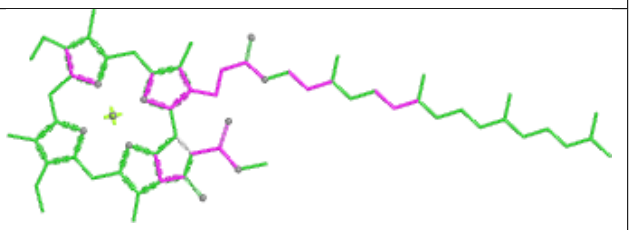


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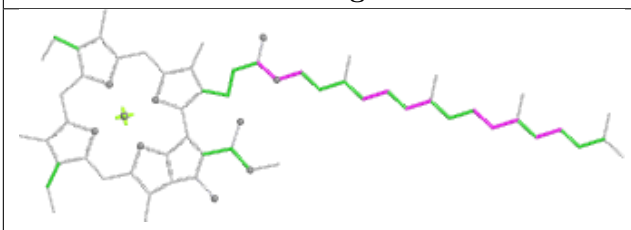
Ligand CLA BC 5504



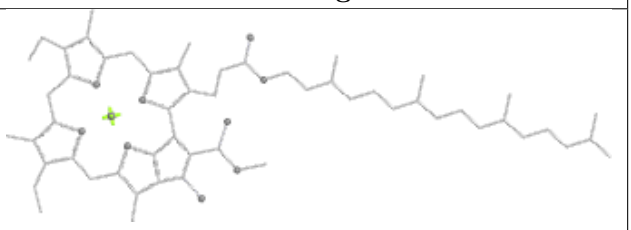
Bond lengths



Bond angles



Torsions

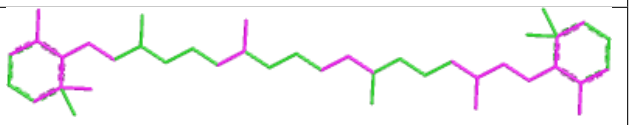


Rings

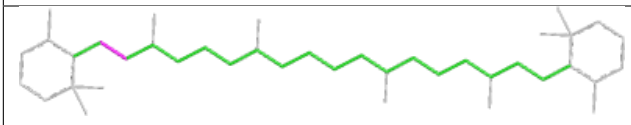
Ligand BCR AB 618



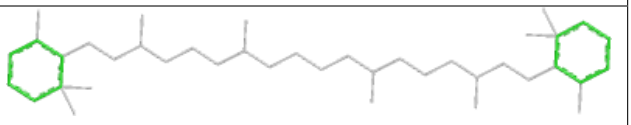
Bond lengths



Bond angles

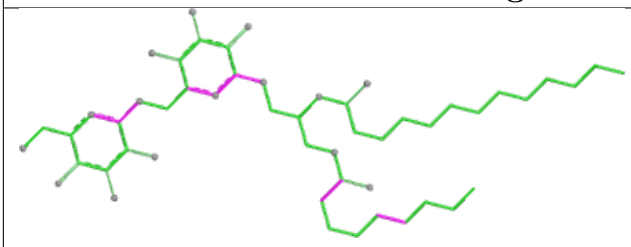


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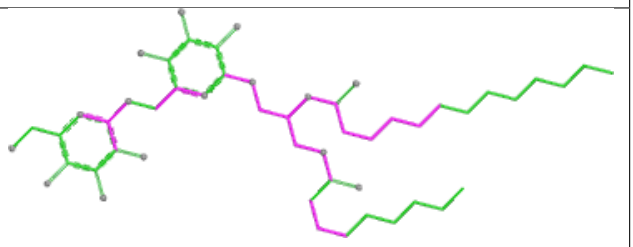


Rings

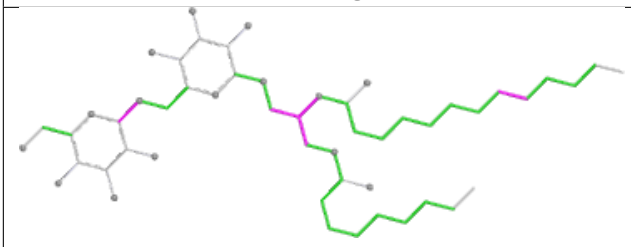
Ligand DGD AB 628



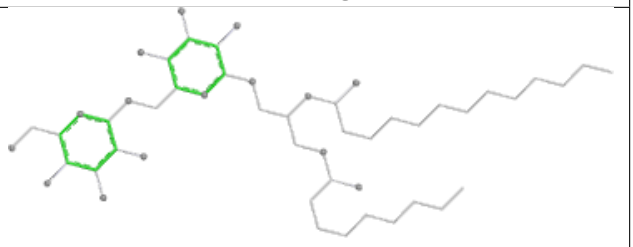
Bond lengths



Bond angles

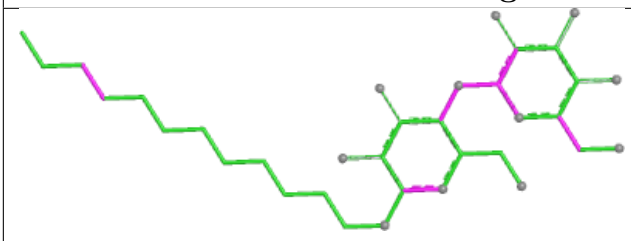


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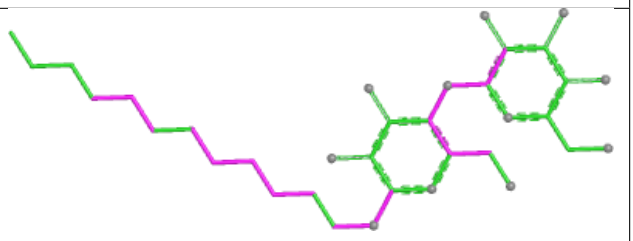


Rings

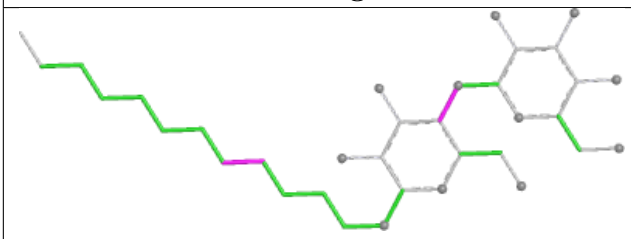
Ligand LMT BB 5603



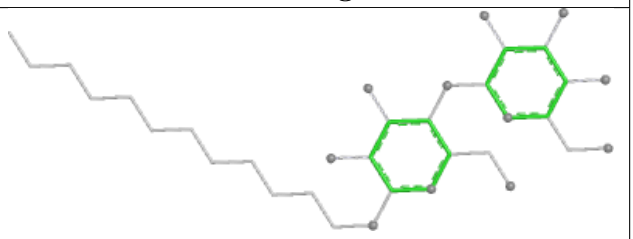
Bond lengths



Bond angles

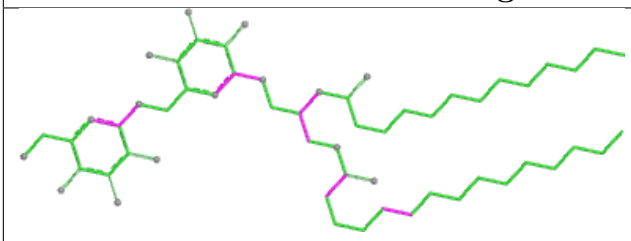


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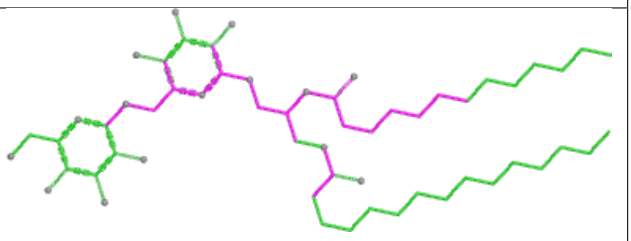


Rings

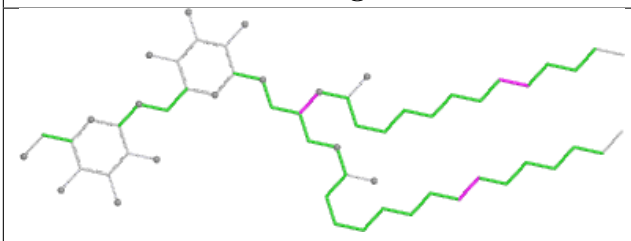
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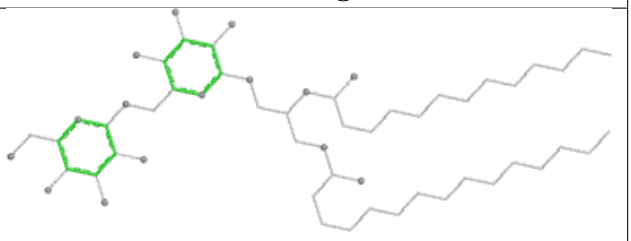
Bond lengths



Bond angles

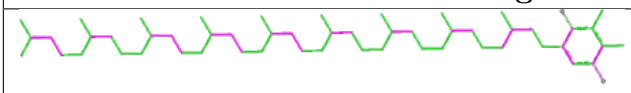


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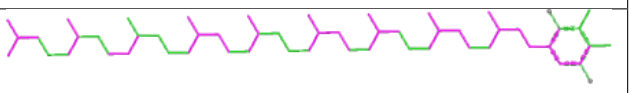


Rings

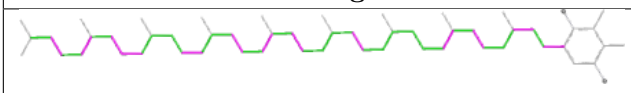
Ligand PL9 AD 405



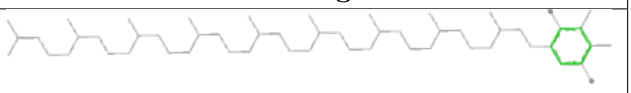
Bond lengths



Bond angles

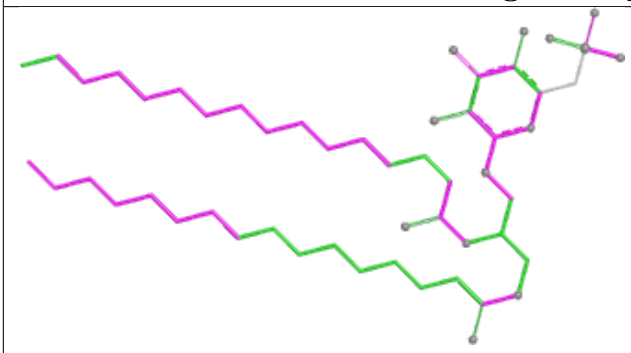


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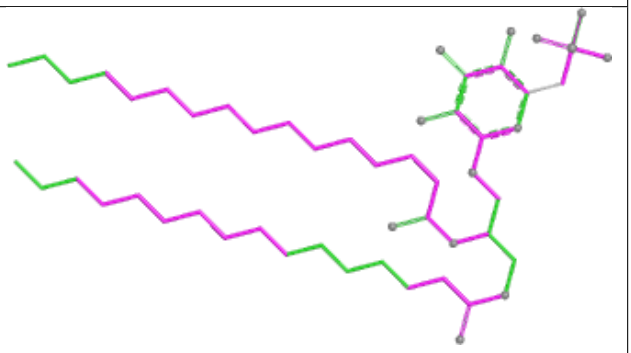


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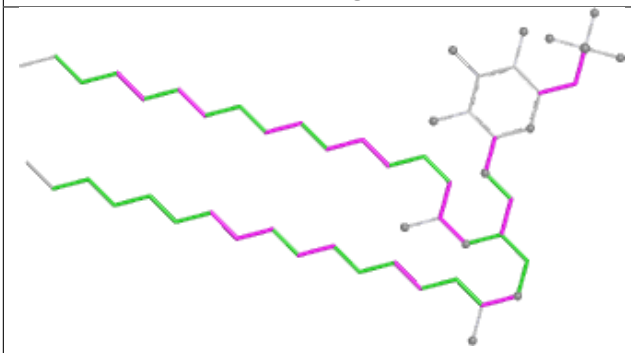
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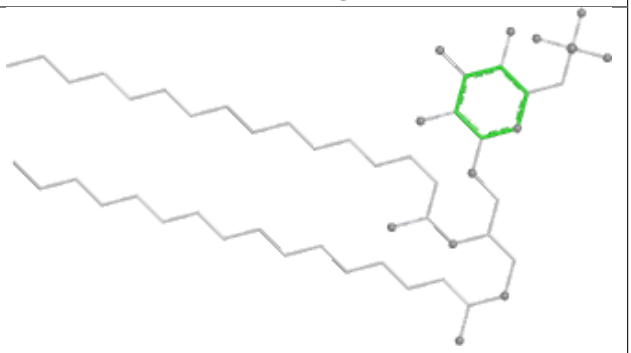
Bond lengths



Bond angles

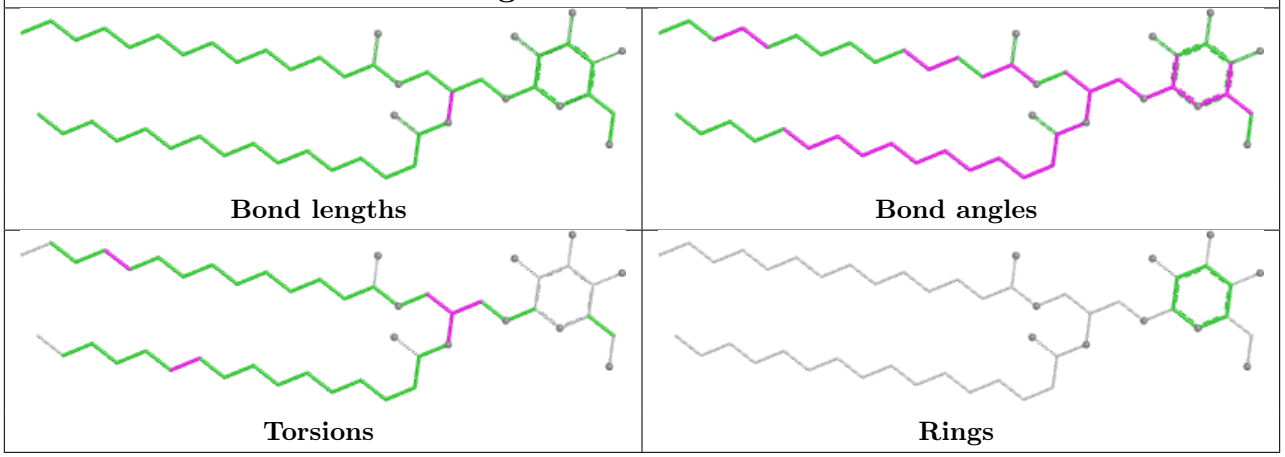


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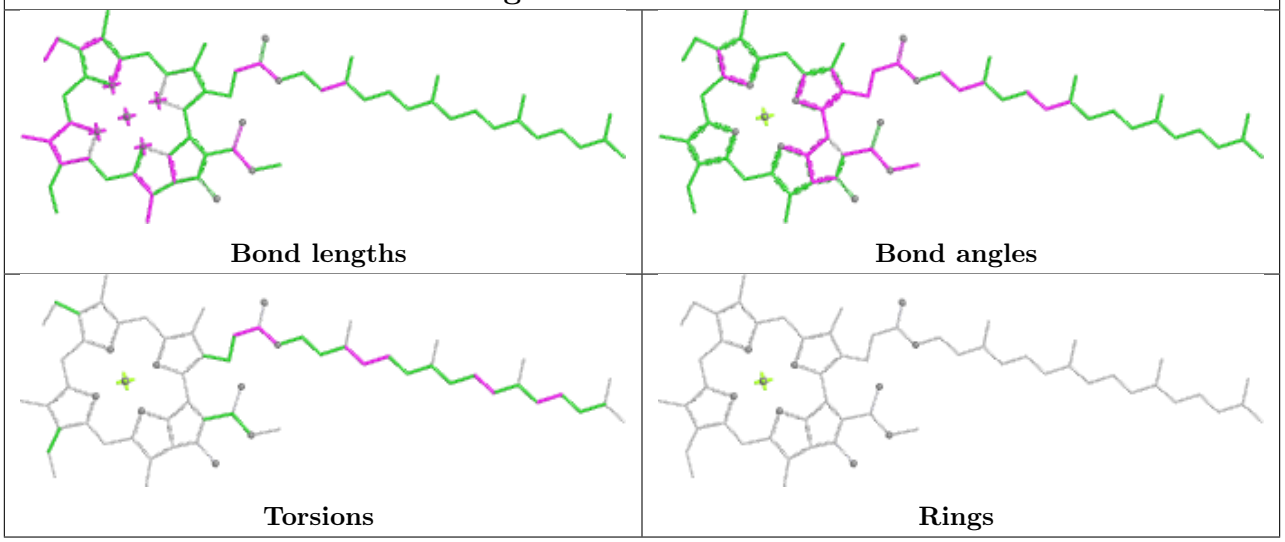


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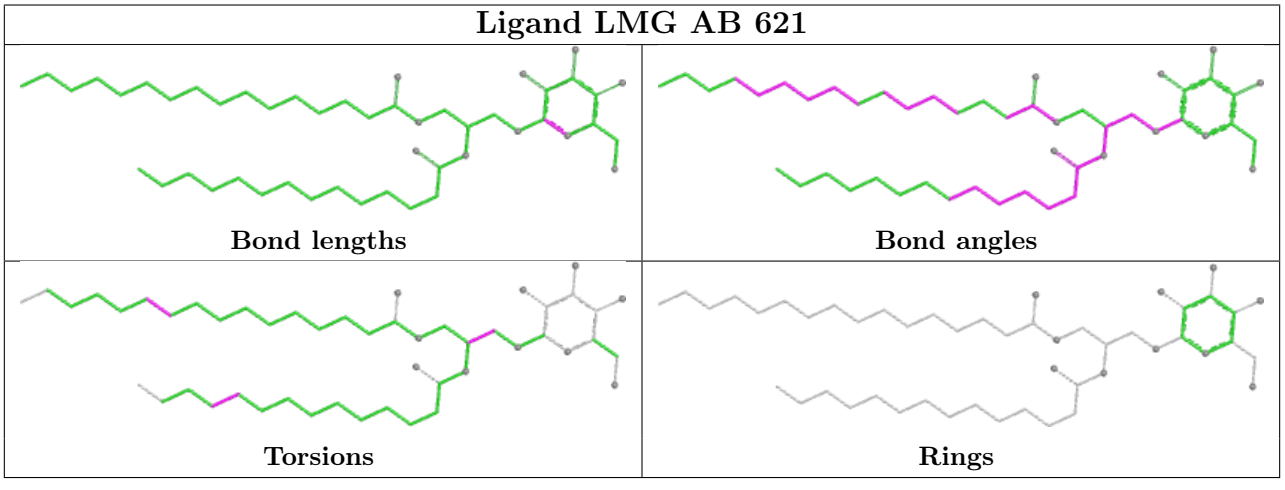
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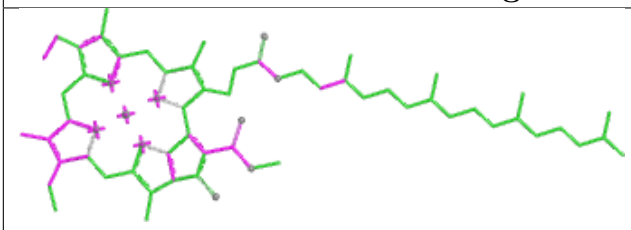
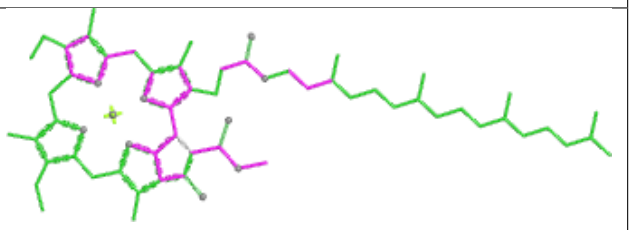
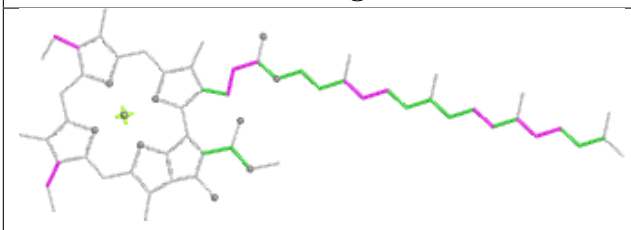
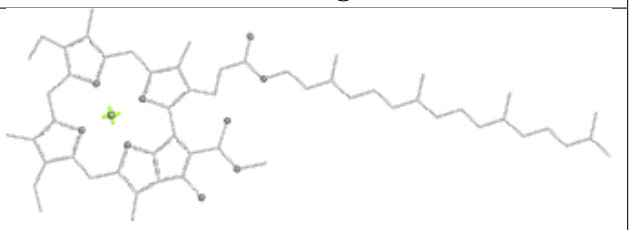


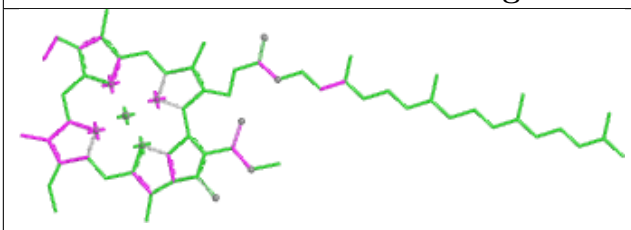
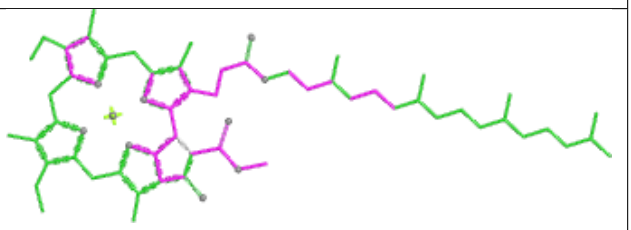
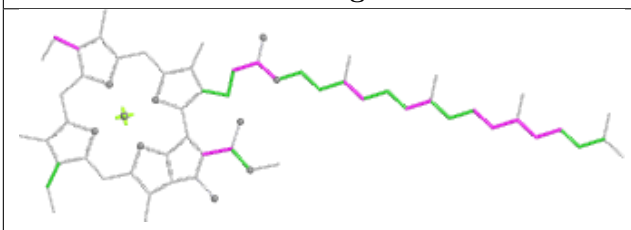
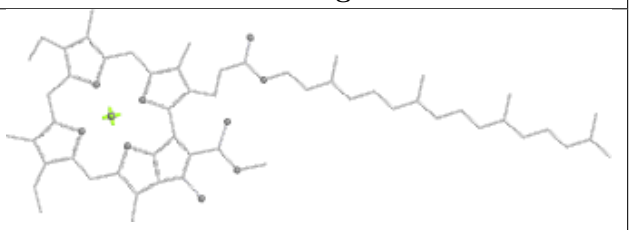
Ligand CLA BB 5613



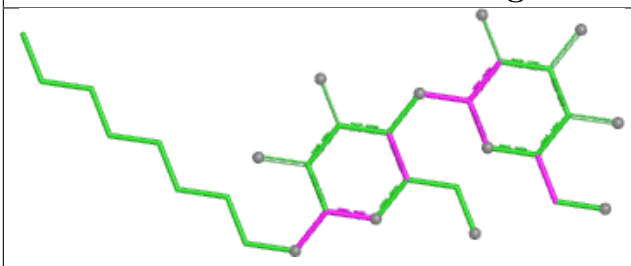
Ligand LMG AB 621



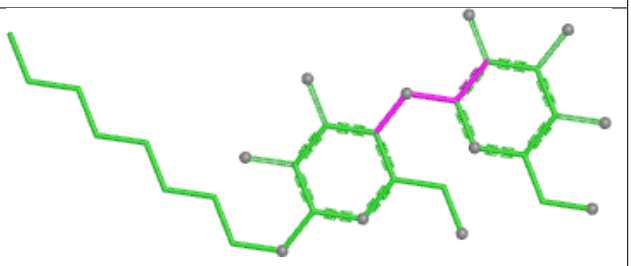
Ligand CLA BB 5605	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA BC 5503	
 Bond lengths	 Bond angles
 Torsions	 Rings

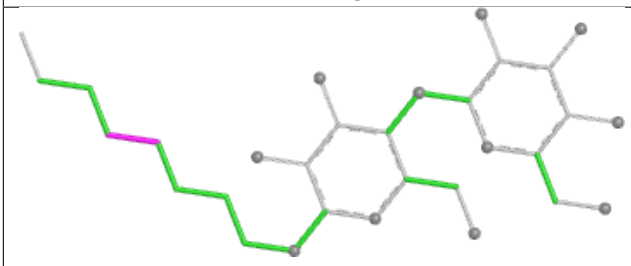
Ligand LMT AD 409



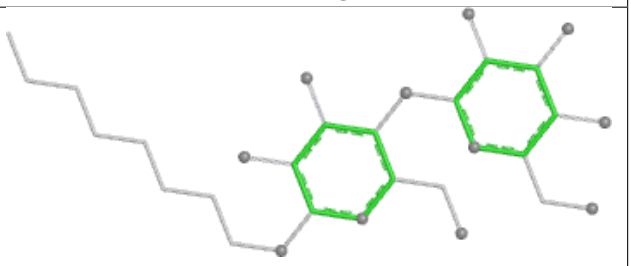
Bond lengths



Bond angles

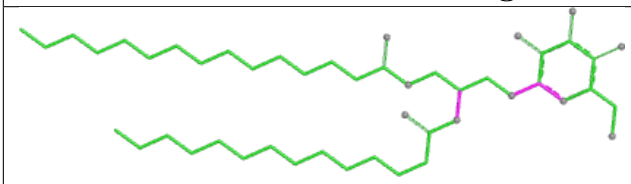


Torsions

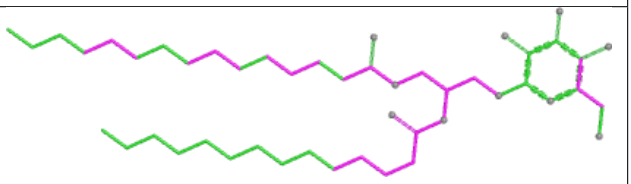


Rings

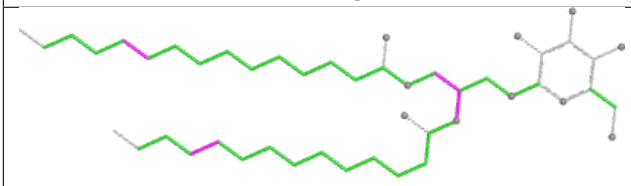
Ligand LMG BC 5520



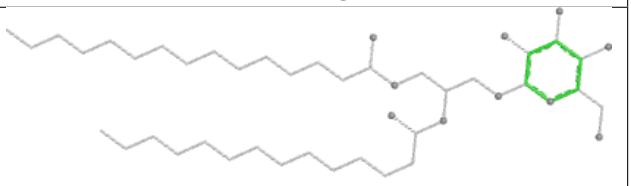
Bond lengths



Bond angles

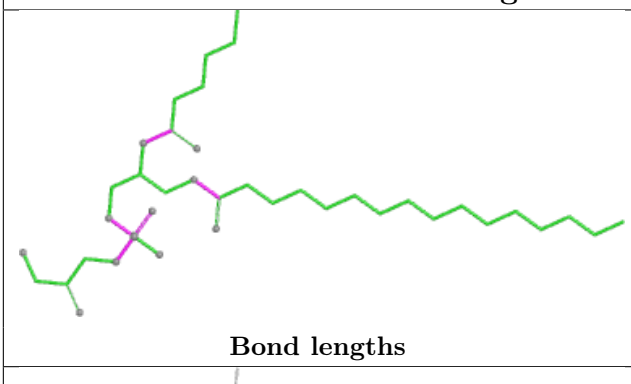


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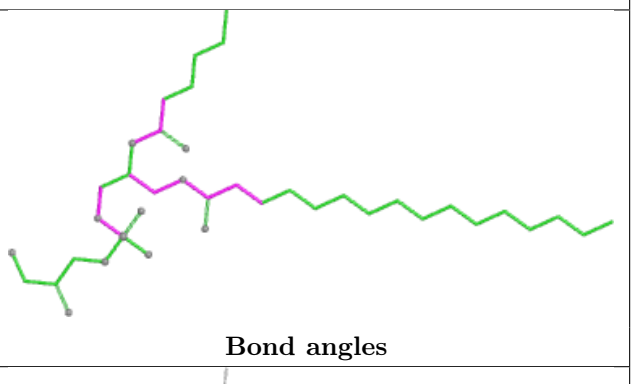


Rings

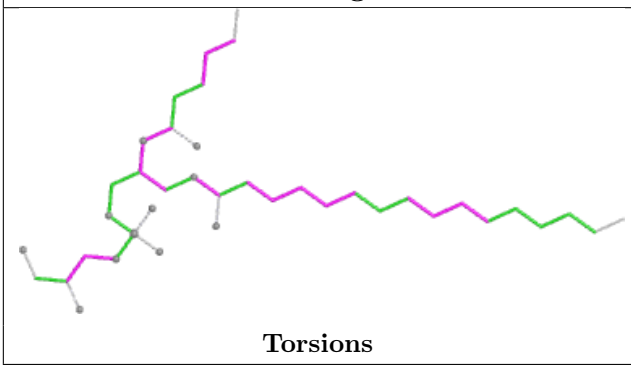
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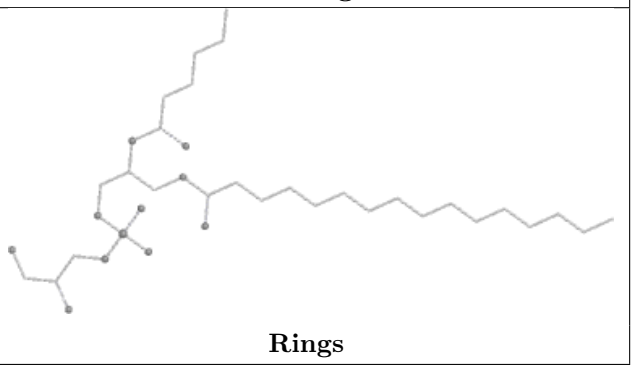
Bond lengths



Bond angles

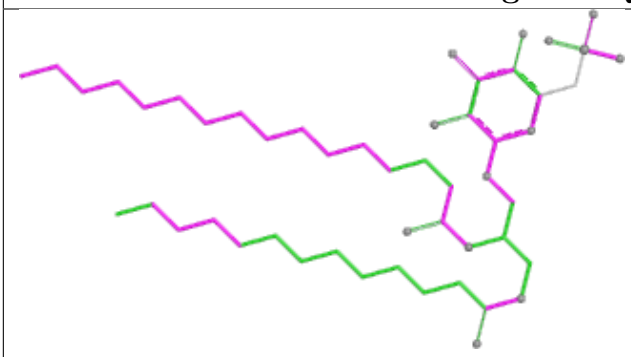


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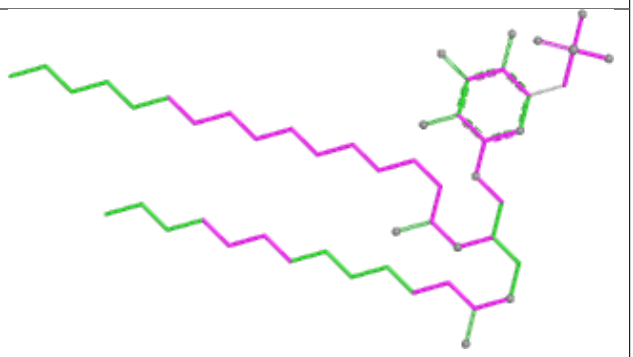


Rings

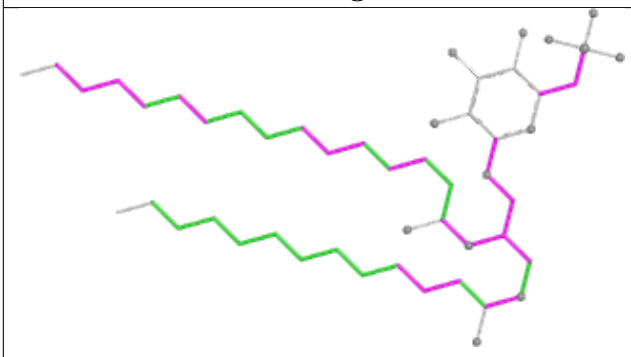
Ligand SQD BA 5414



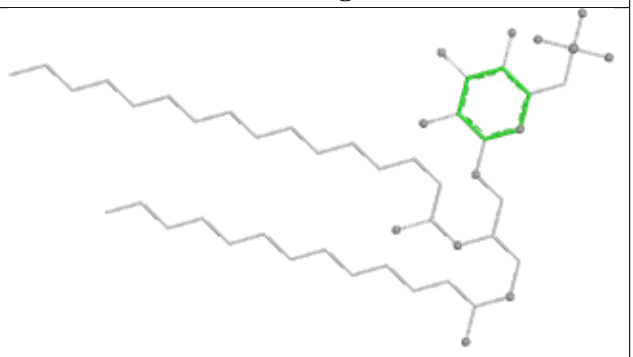
Bond lengths



Bond angles

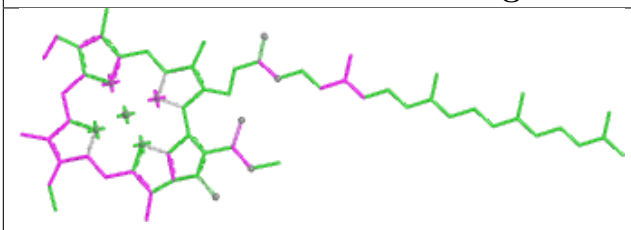


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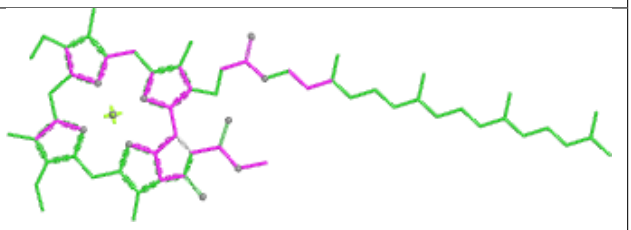


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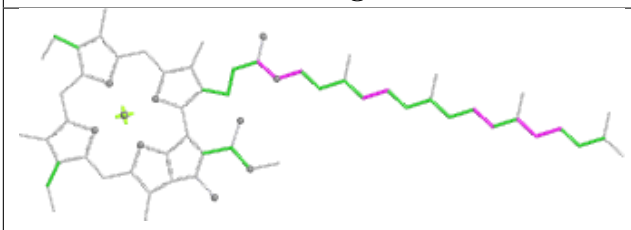
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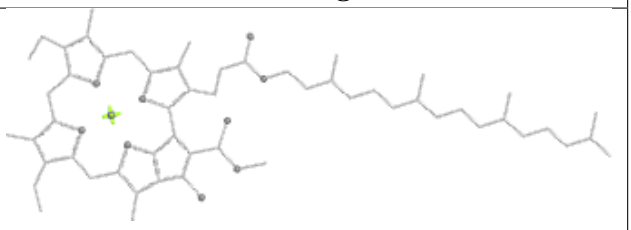
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Bond angles

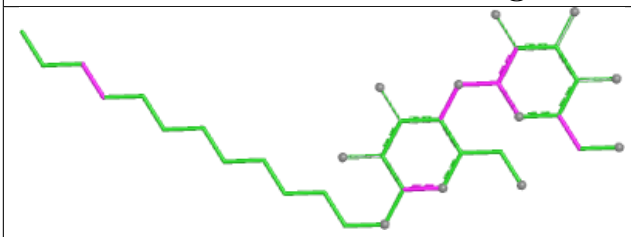


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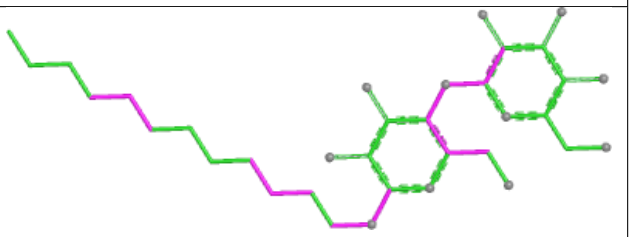


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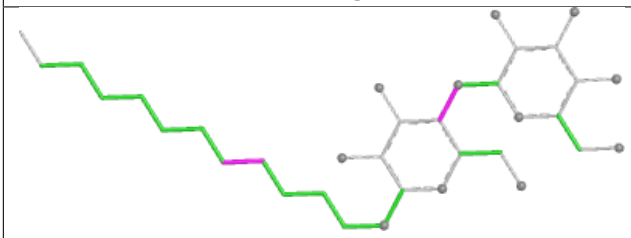
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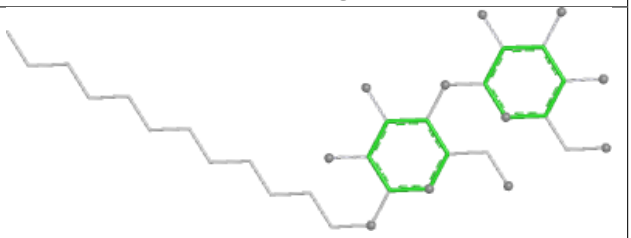
Bond lengths



Bond angles

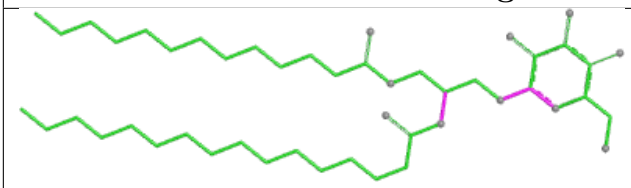


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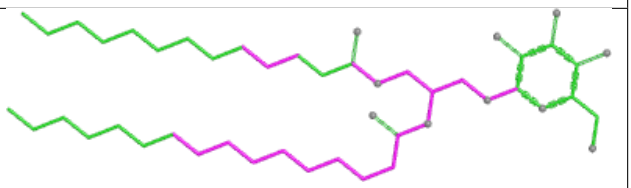


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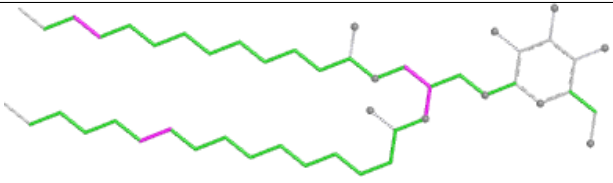
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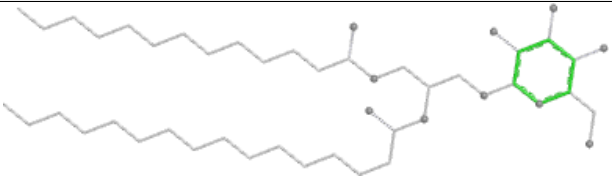
Bond lengths



Bond angles

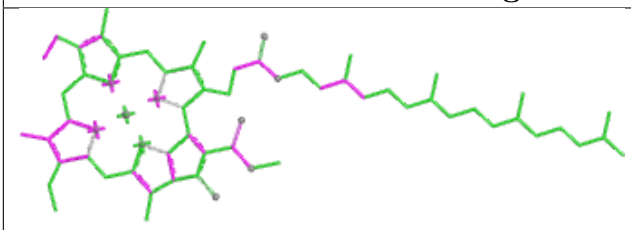


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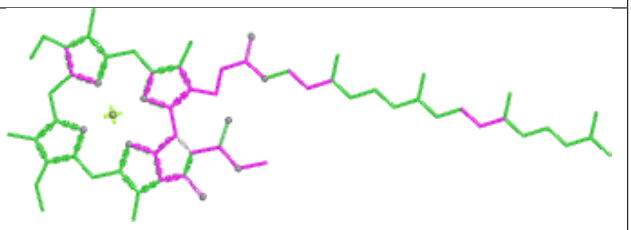


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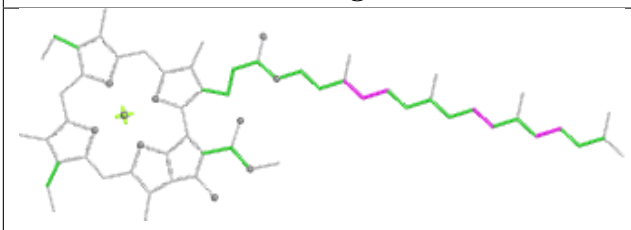
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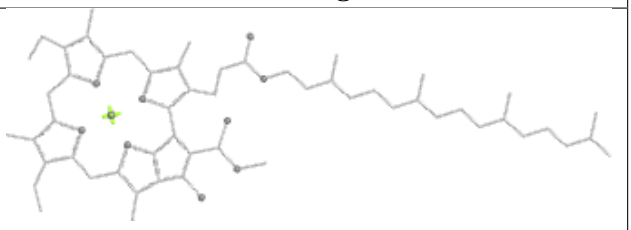
Bond lengths



Bond angles

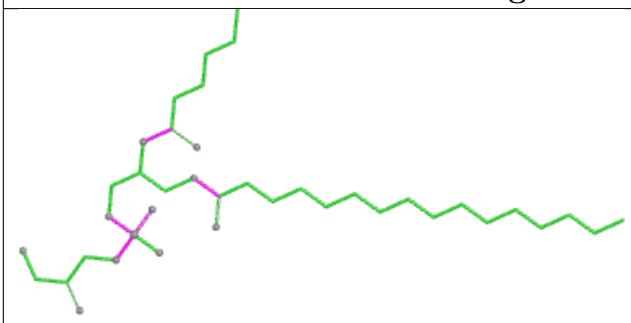


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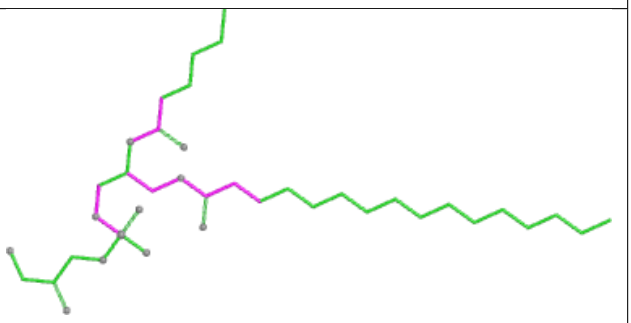


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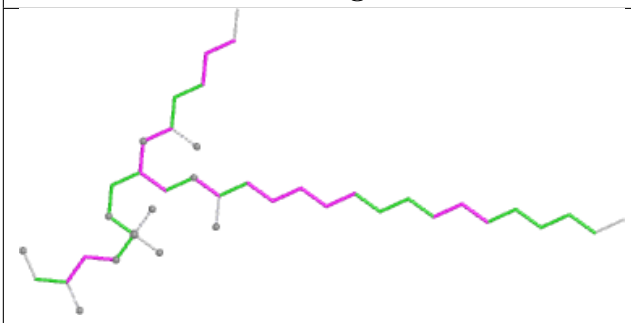
Ligand LHG AA 412



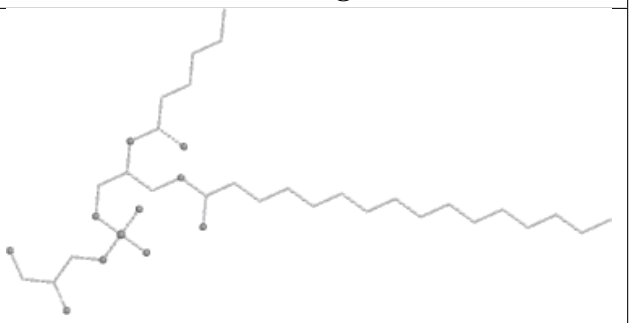
Bond lengths



Bond angles

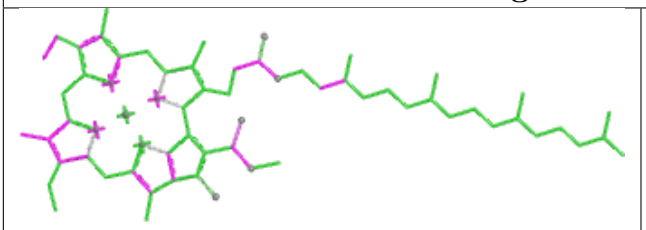


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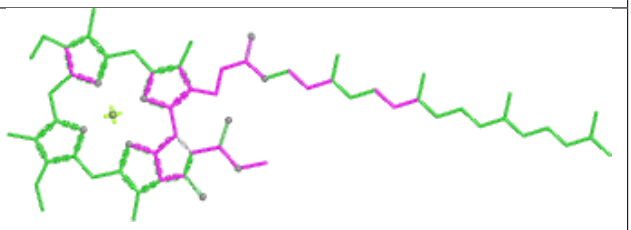


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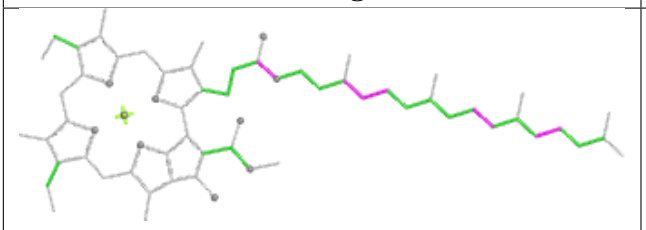
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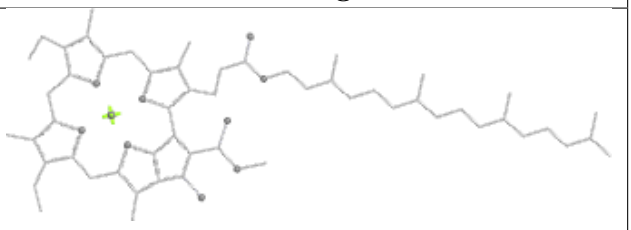
Bond lengths



Bond angles

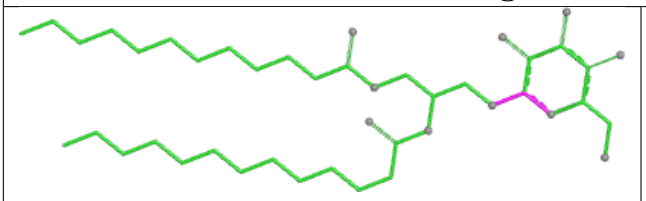


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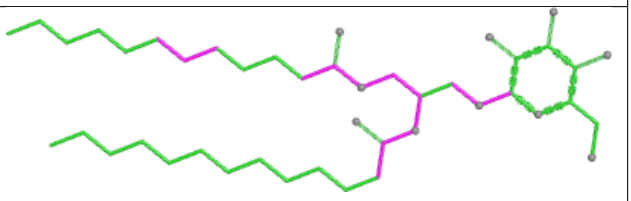


Rings

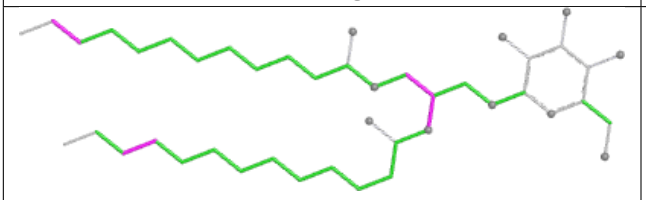
Ligand LMG BE 5101



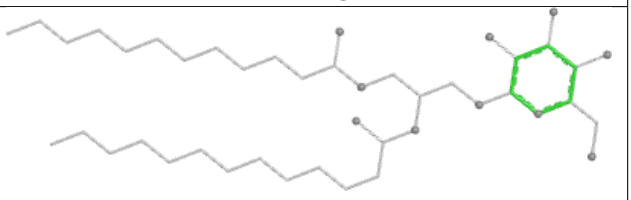
Bond lengths



Bond angles



Torsions

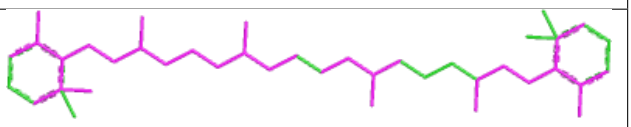


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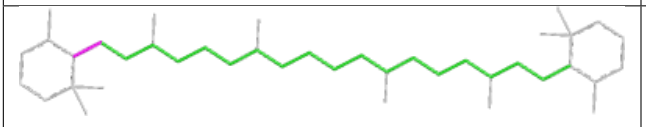
Ligand BCR AK 102



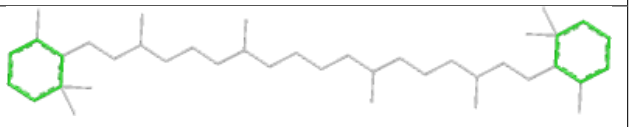
Bond lengths



Bond angles

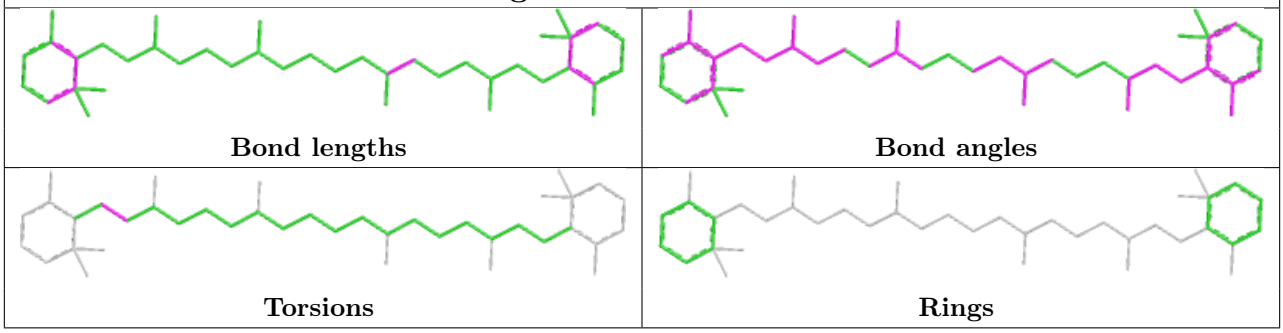


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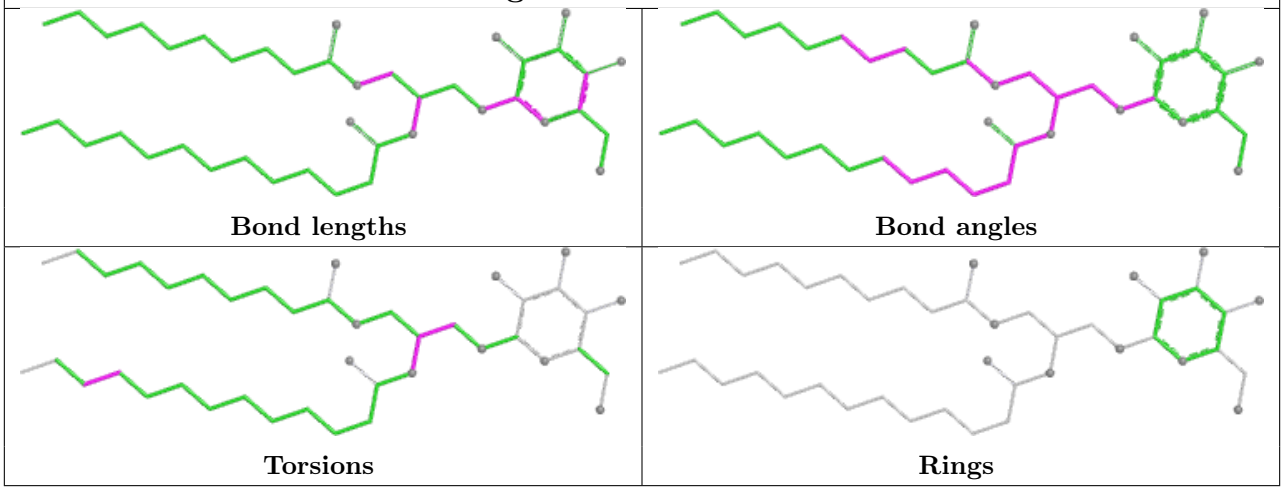


Rings

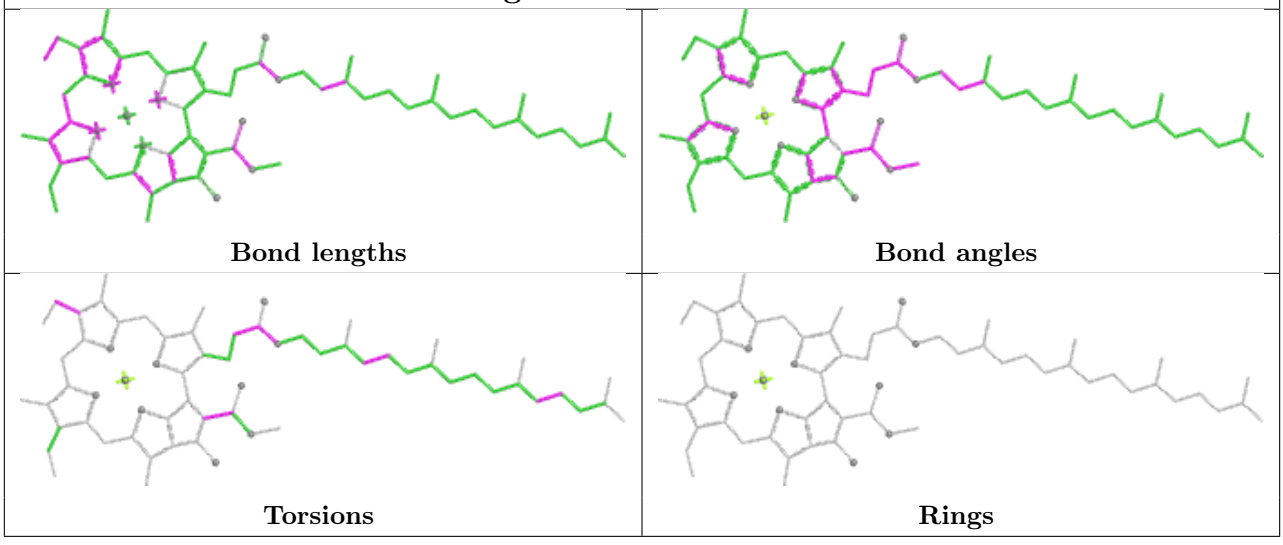
Ligand BCR AB 617



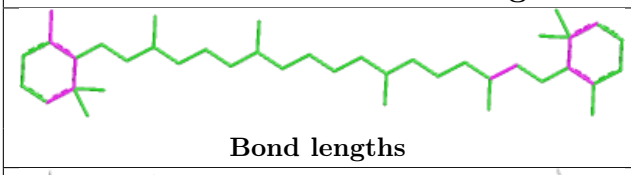
Ligand LMG AA 417



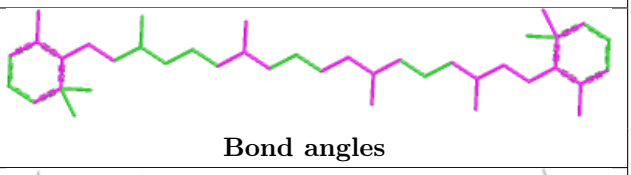
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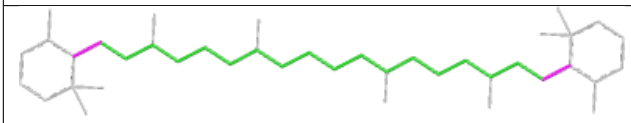
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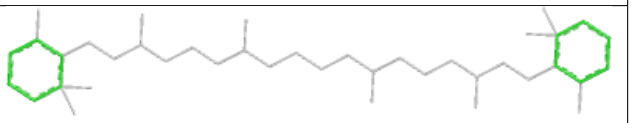
Bond lengths



Bond angles



Torsions

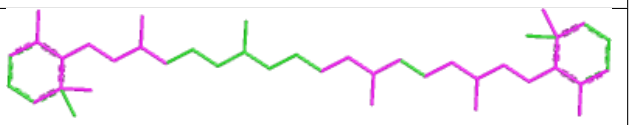


Rings

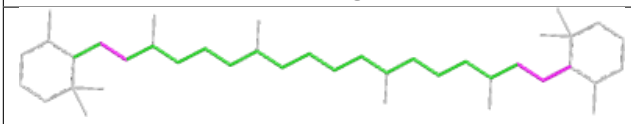
Ligand BCR AT 101



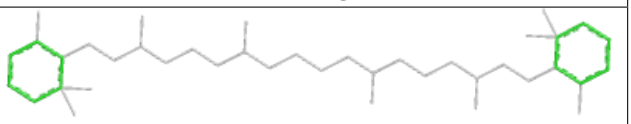
Bond lengths



Bond angles

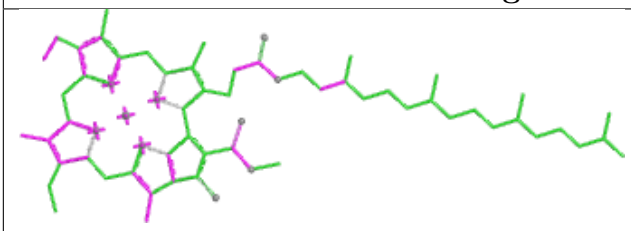


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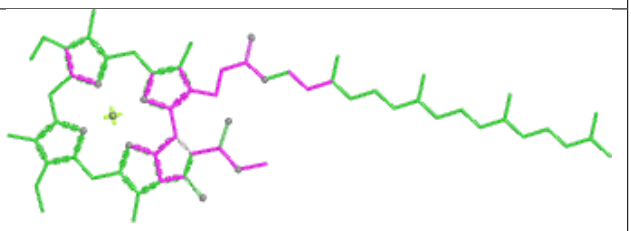


Rings

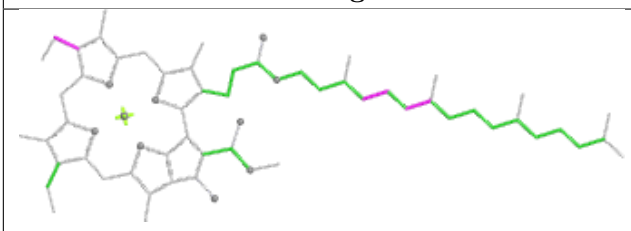
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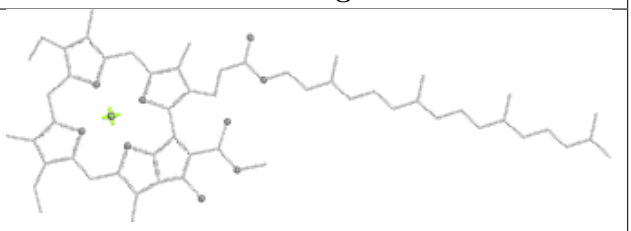
Bond lengths



Bond angles

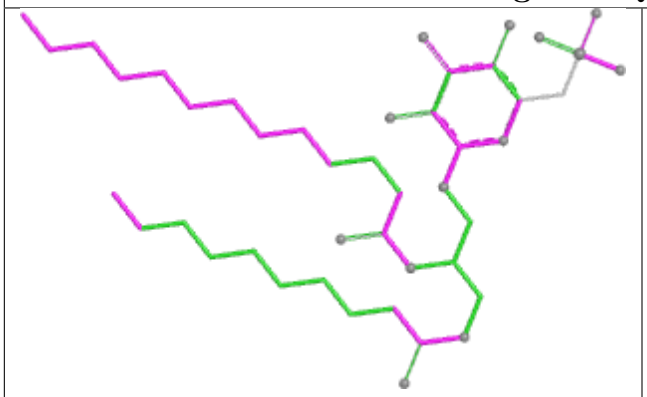


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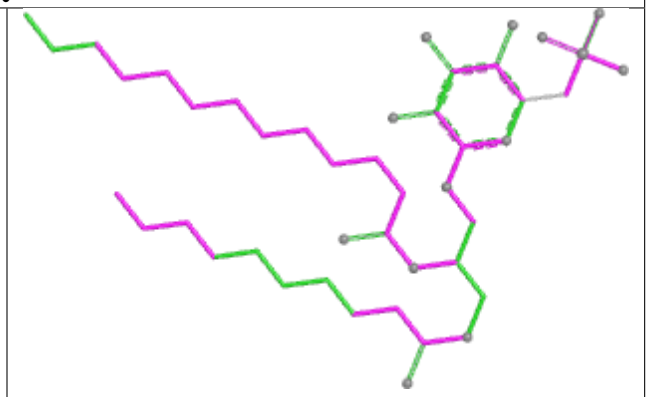


Rings

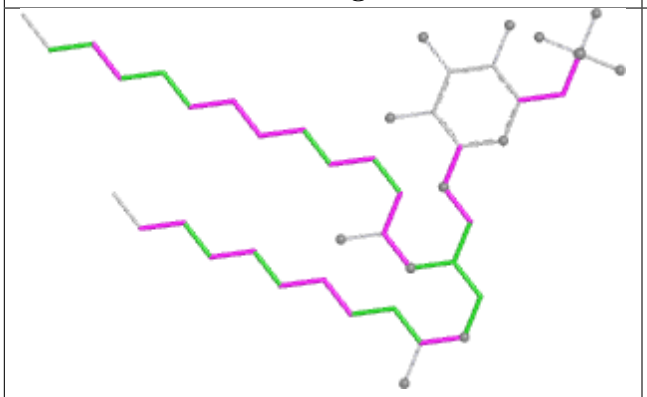
Ligand SQD AF 102



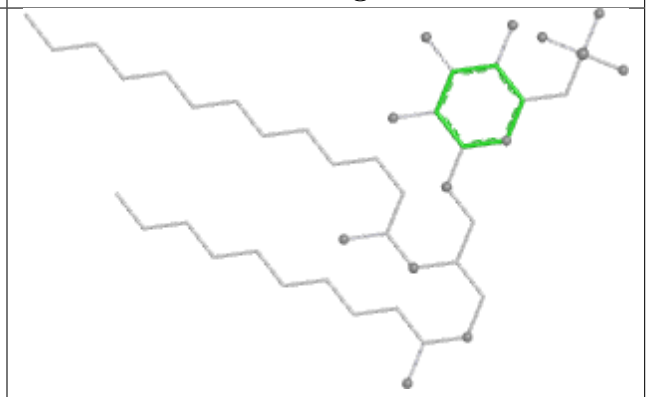
Bond lengths



Bond angles

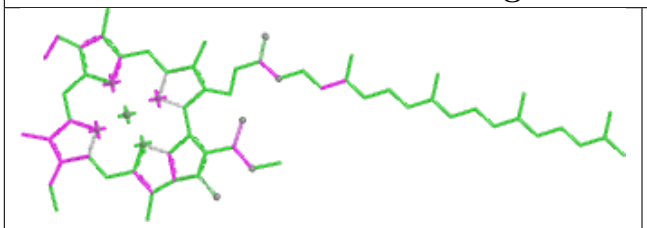


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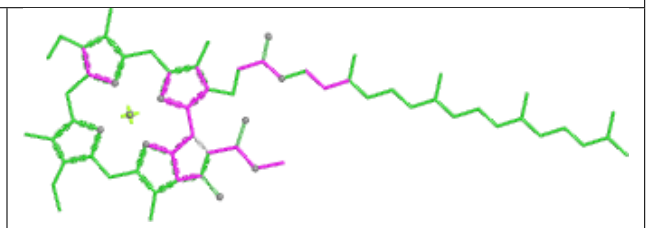


Rings

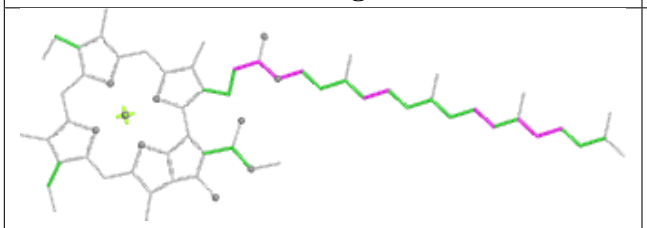
Ligand CLA BC 5512



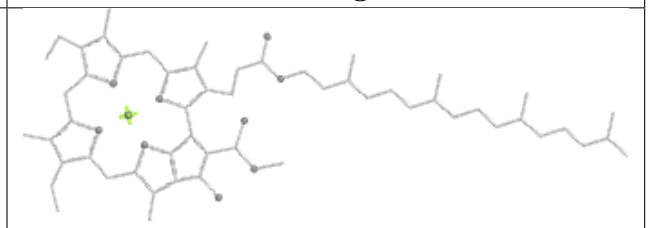
Bond lengths



Bond angles

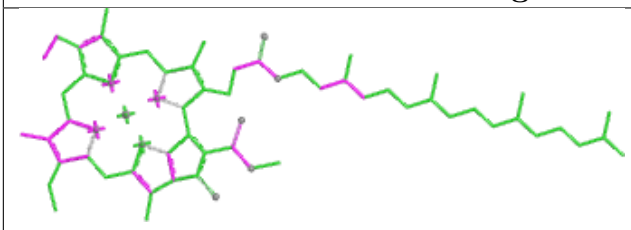


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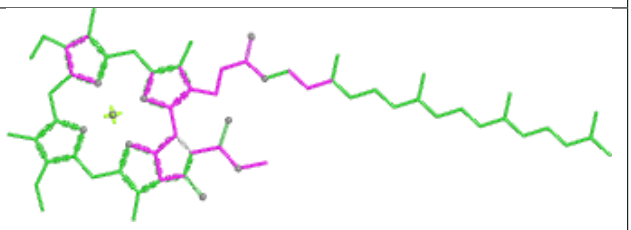


Rings

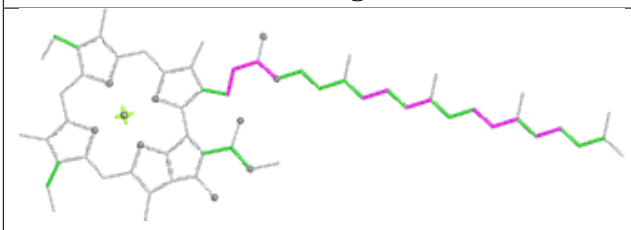
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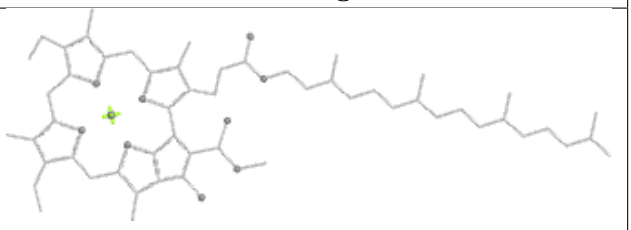
Bond lengths



Bond angles

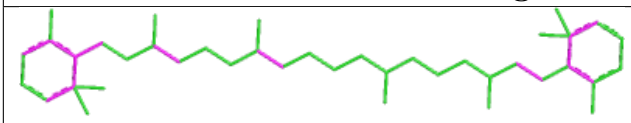


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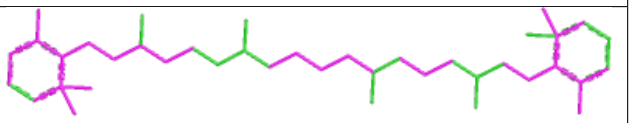


Rings

Ligand BCR AJ 101



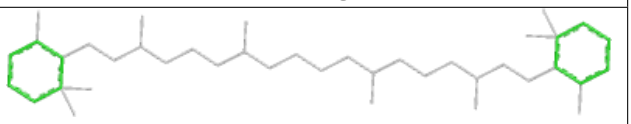
Bond lengths



Bond angles

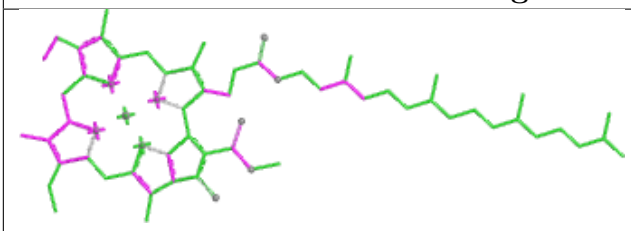


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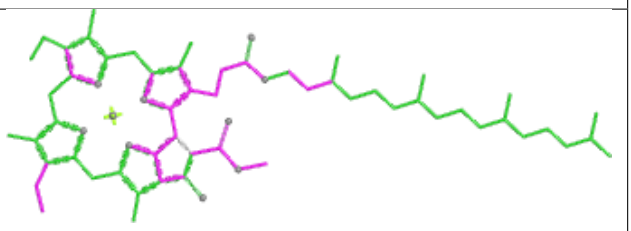


Rings

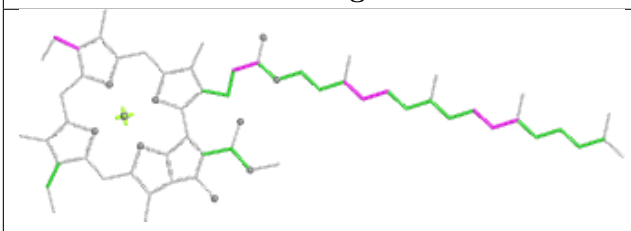
Ligand CLA AB 605



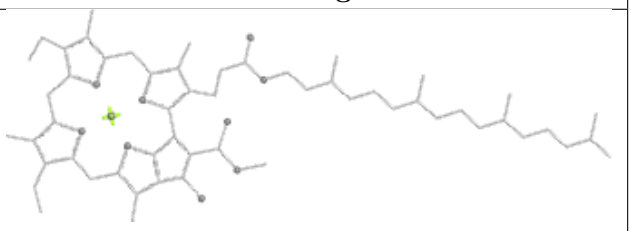
Bond lengths



Bond angles

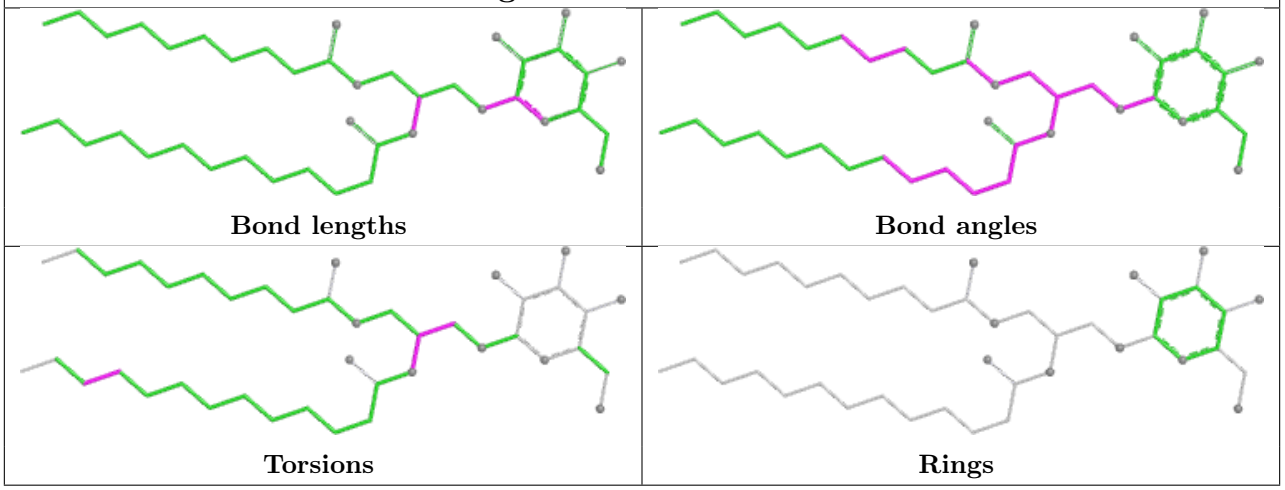


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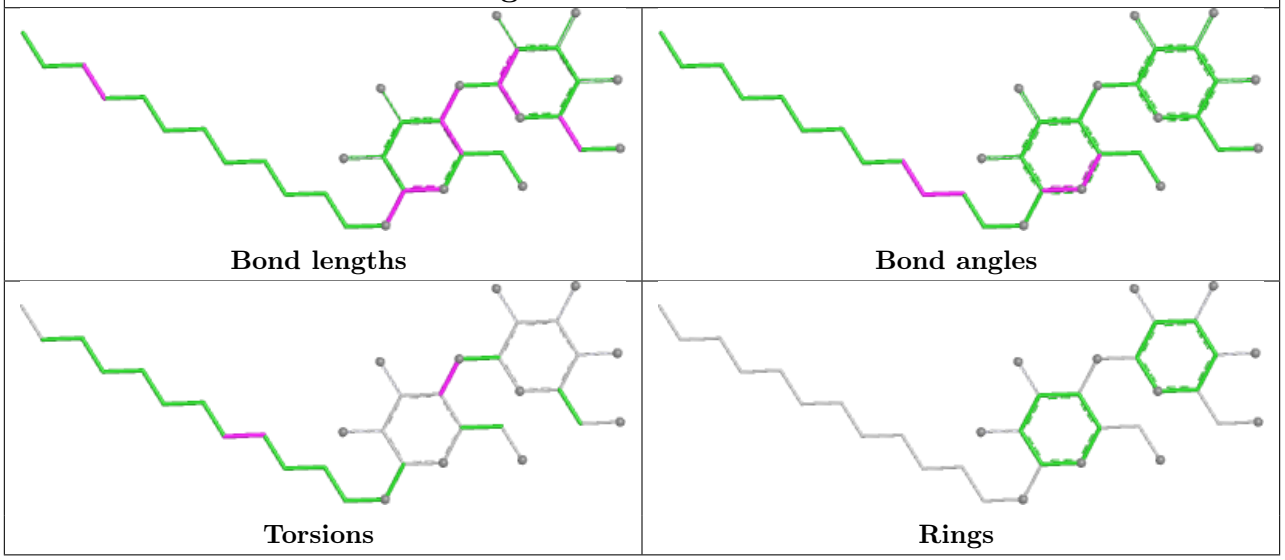


Rings

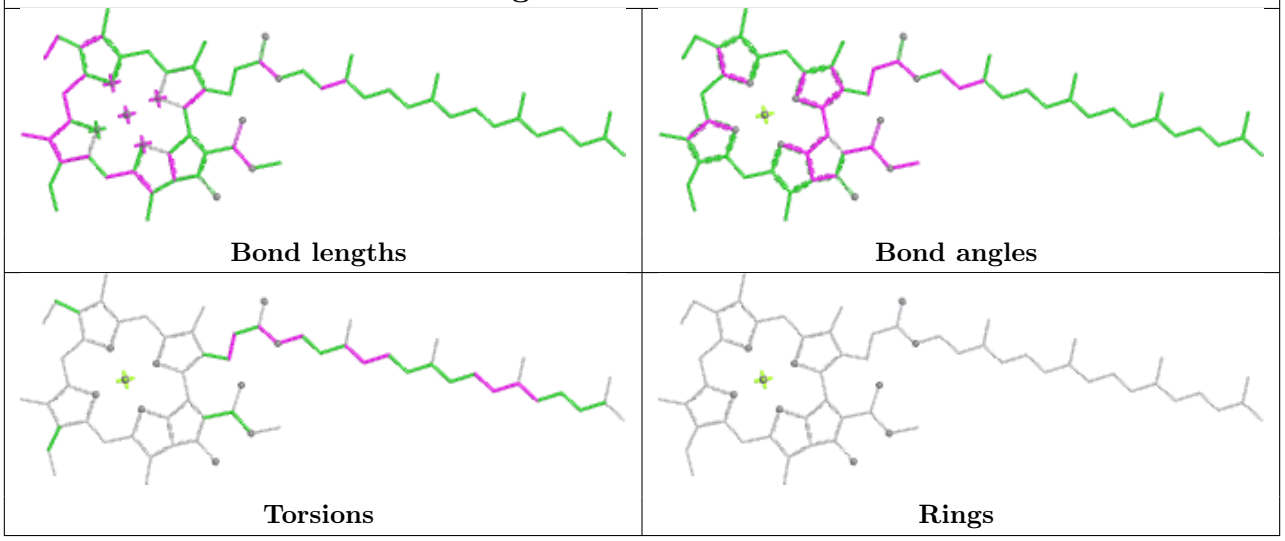
Ligand LMG BA 5402



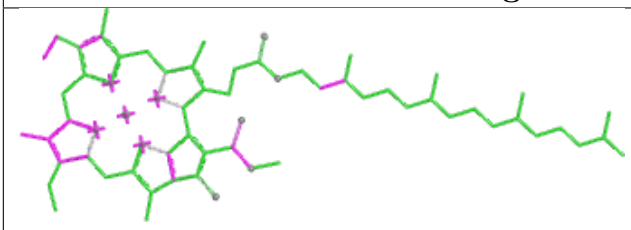
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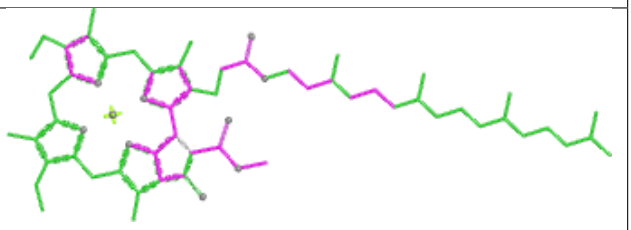
Ligand CLA AB 612



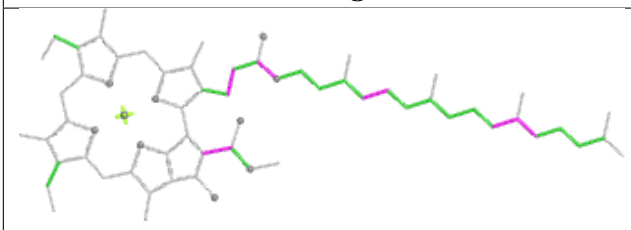
Ligand CLA BB 5614



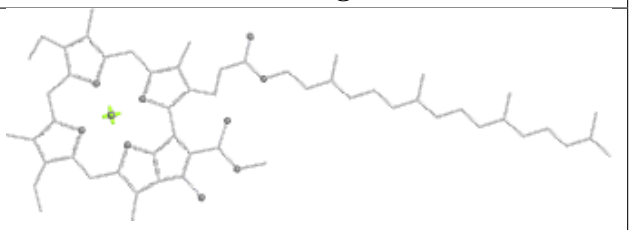
Bond lengths



Bond angles

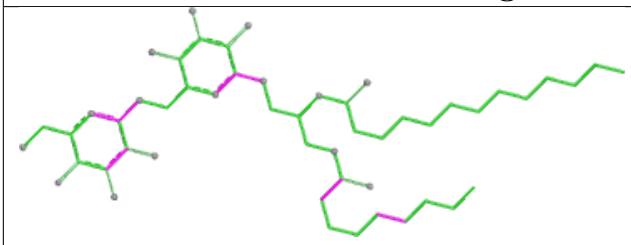


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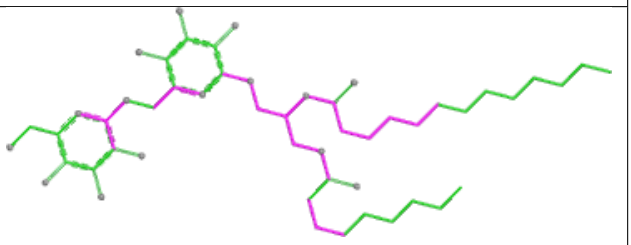


Rings

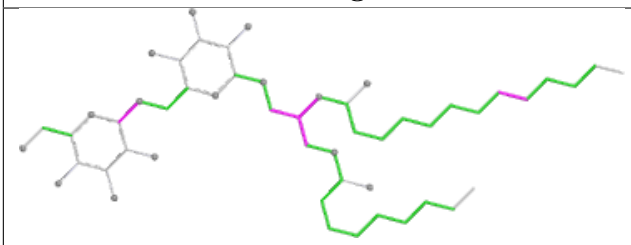
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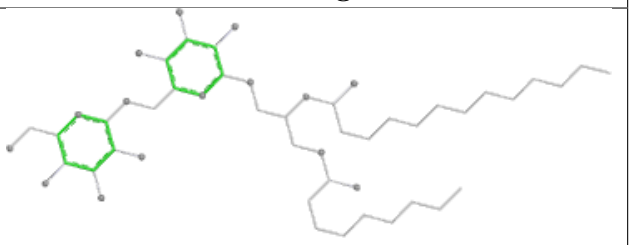
Bond lengths



Bond angles

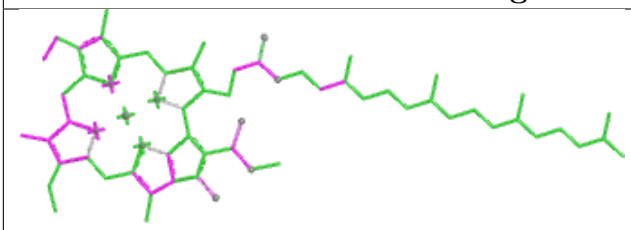


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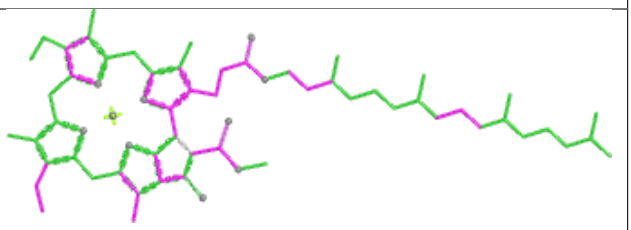


Rings

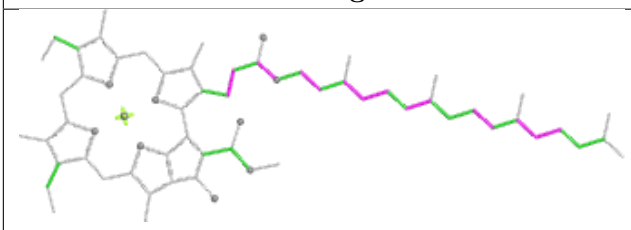
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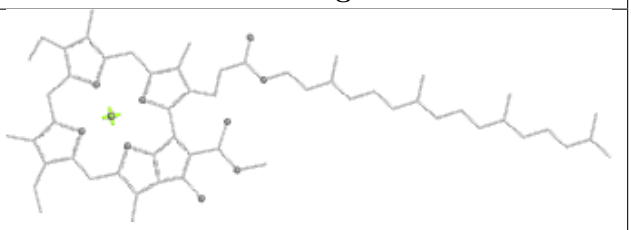
Bond lengths



Bond angles

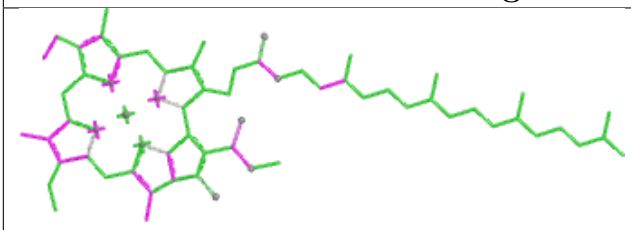


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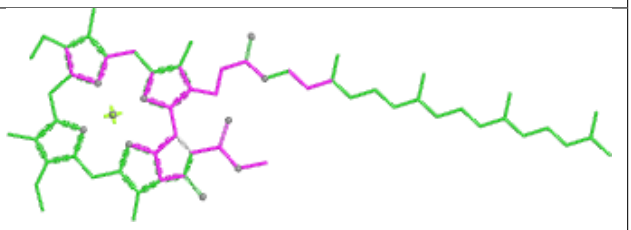


Rings

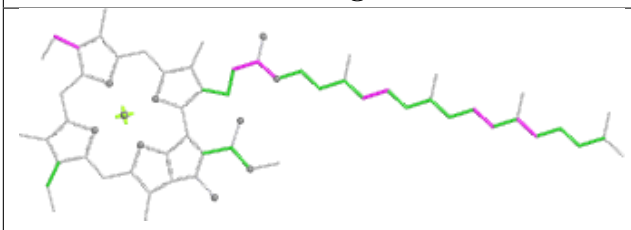
Ligand CLA BC 5502



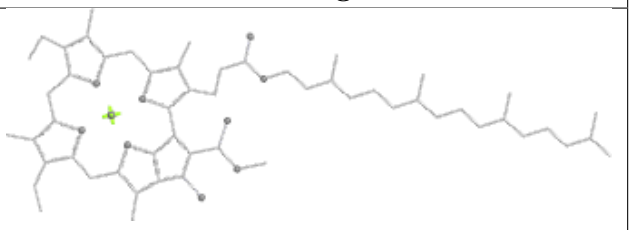
Bond lengths



Bond angles

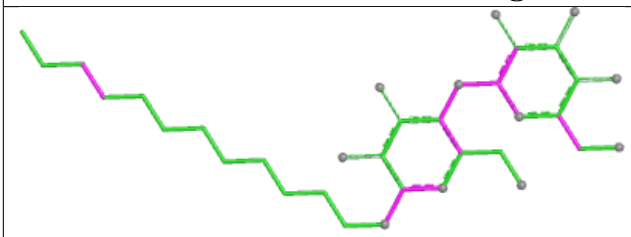


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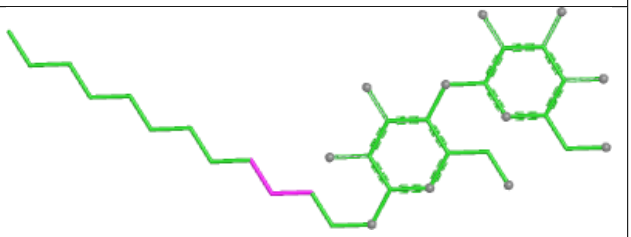


Rings

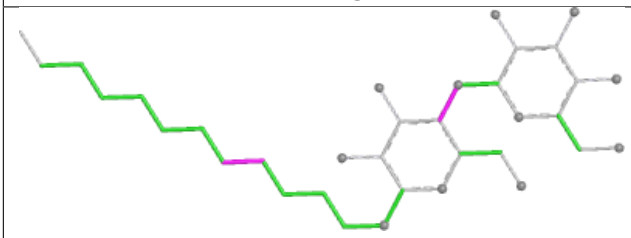
Ligand LMT AB 630



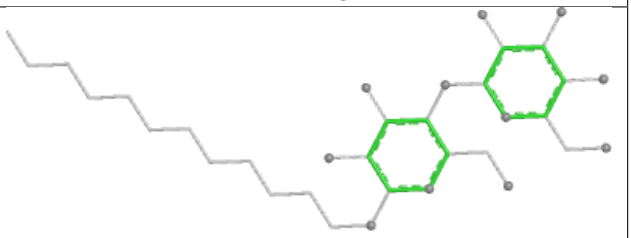
Bond lengths



Bond angles

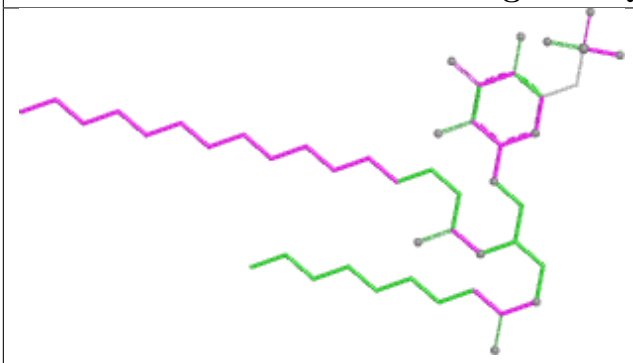


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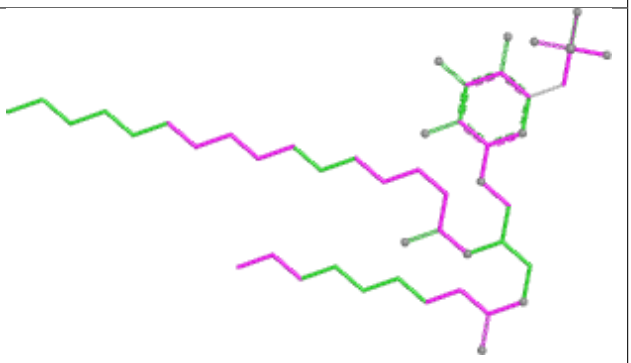


Rings

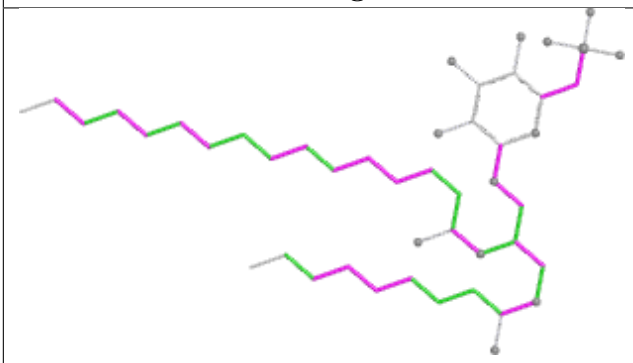
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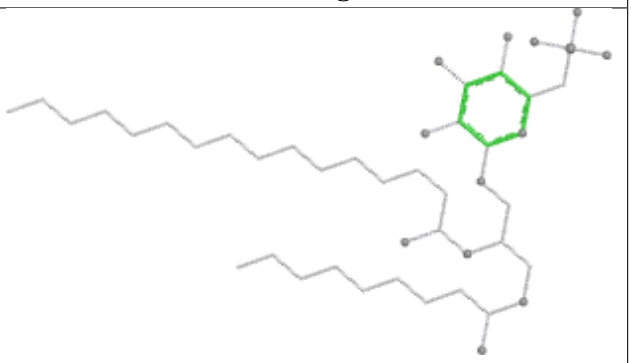
Bond lengths



Bond angles

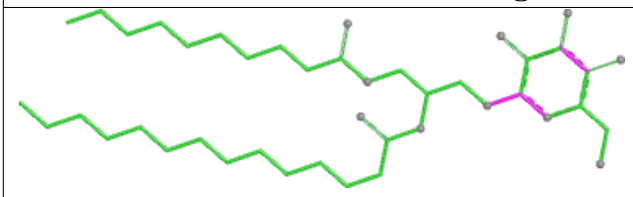


Torsions



Rings

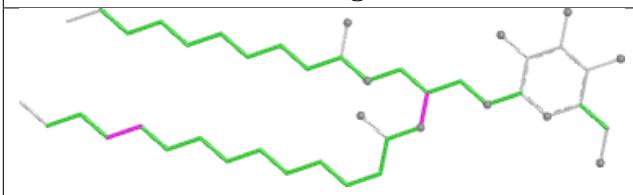
Ligand LMG AI 101



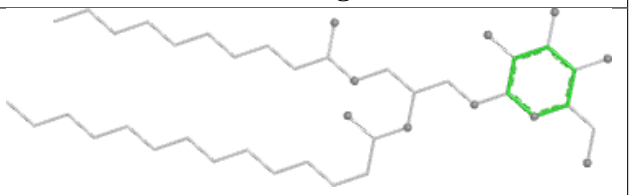
Bond lengths



Bond angles

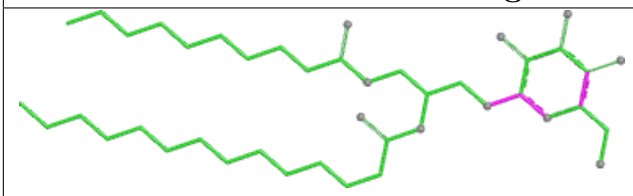


Torsions

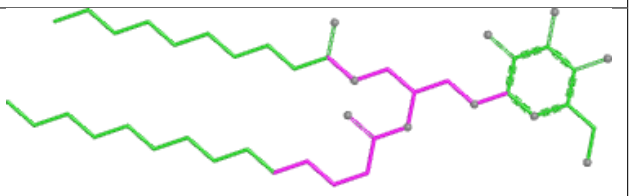


Rings

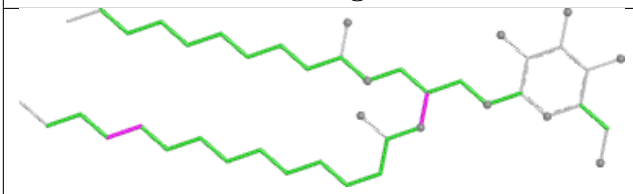
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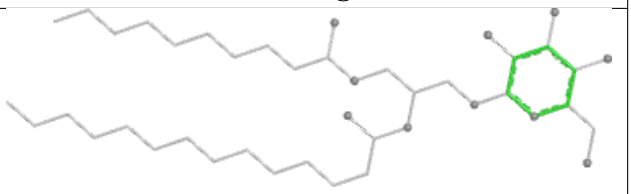
Bond lengths



Bond angles

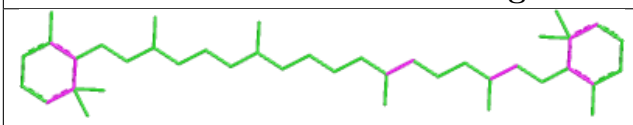


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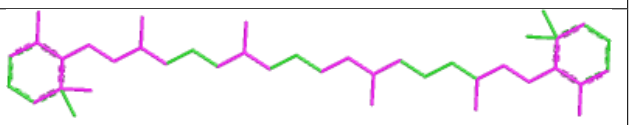


Rings

Ligand BCR AA 410



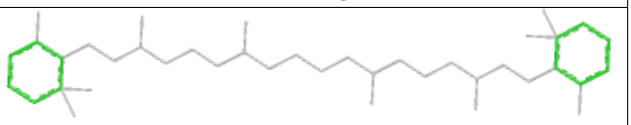
Bond lengths



Bond angles

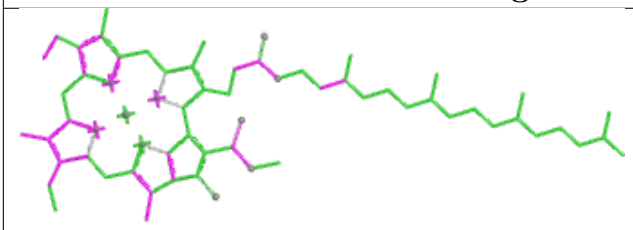


Torsions

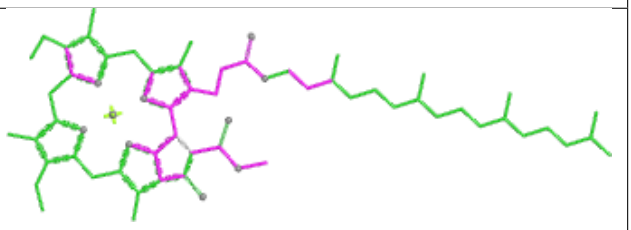


Rings

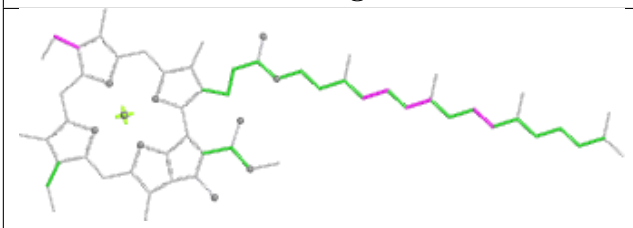
Ligand CLA AC 506



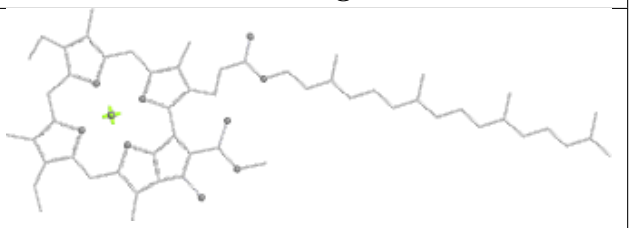
Bond lengths



Bond angles

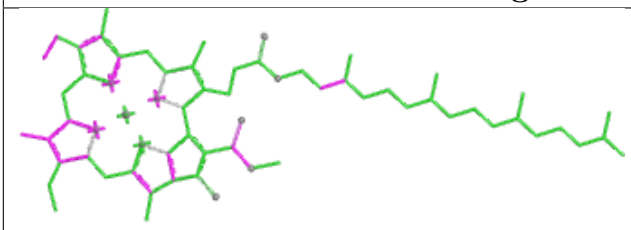


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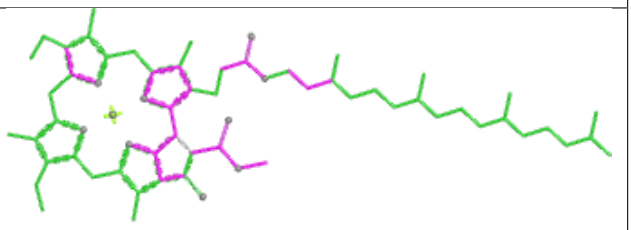


Rings

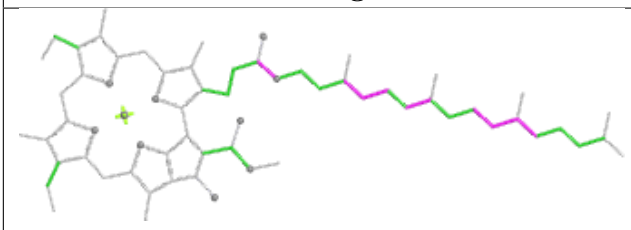
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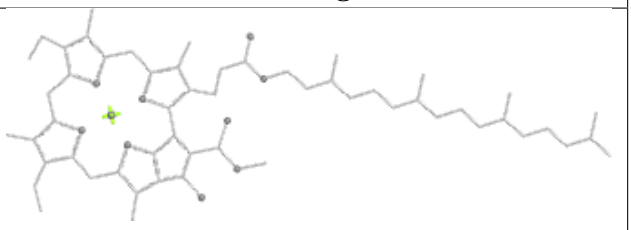
Bond lengths



Bond angles

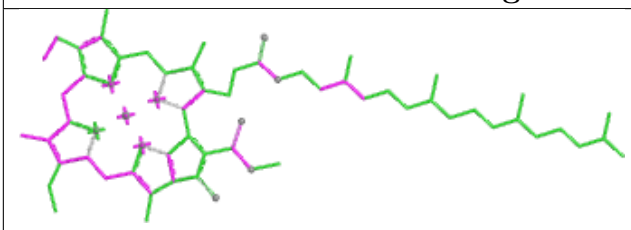


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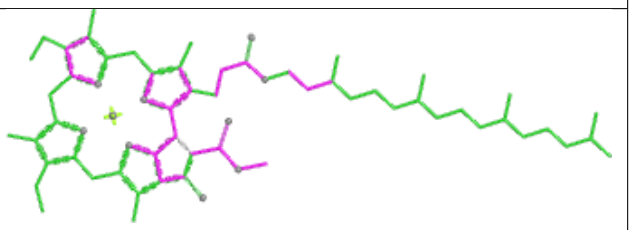


Rings

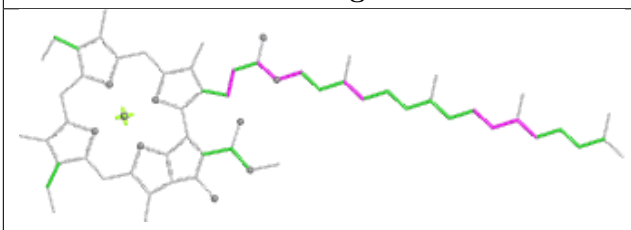
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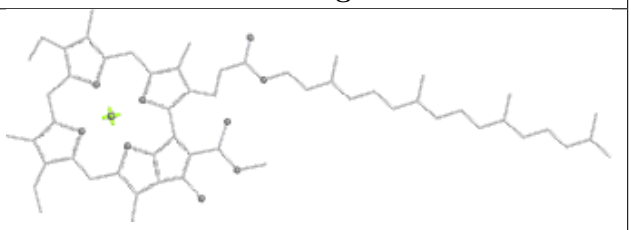
Bond lengths



Bond angles

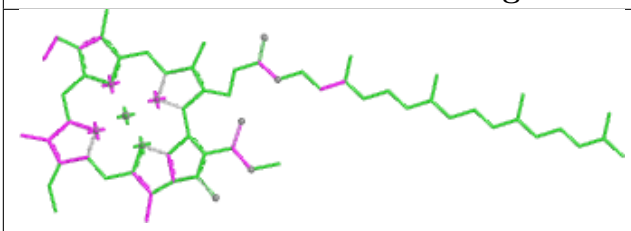


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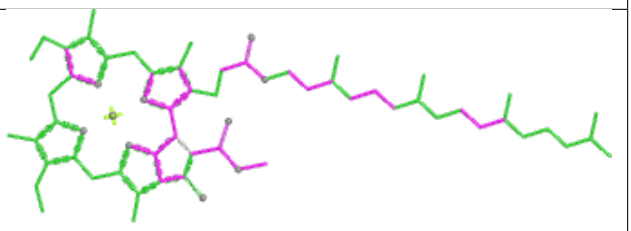


Rings

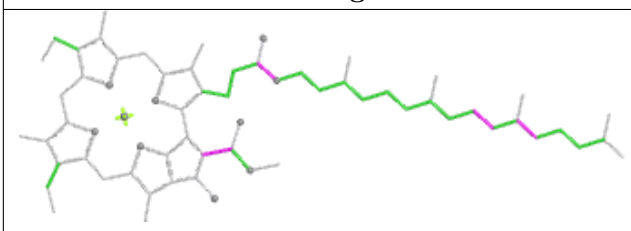
Ligand CLA BC 5507



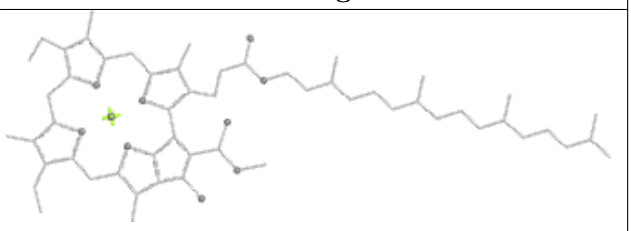
Bond lengths



Bond angles

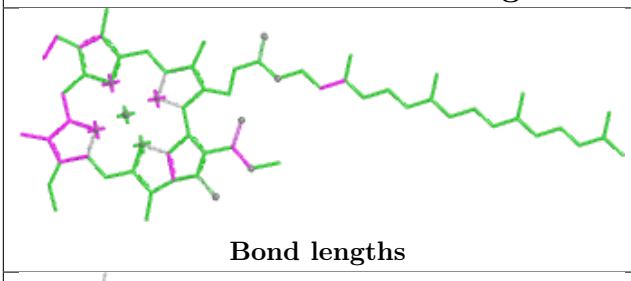


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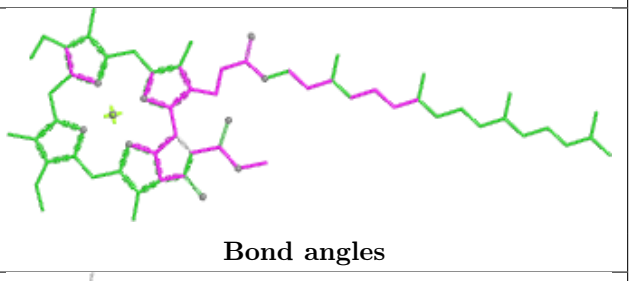


Rings

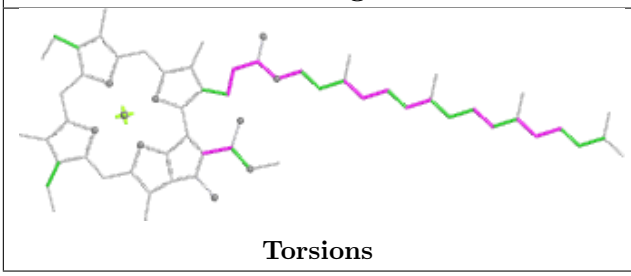
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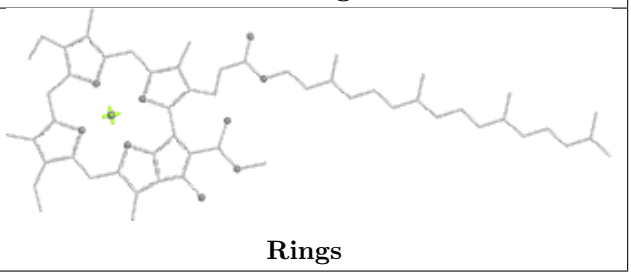
Bond lengths



Bond angles

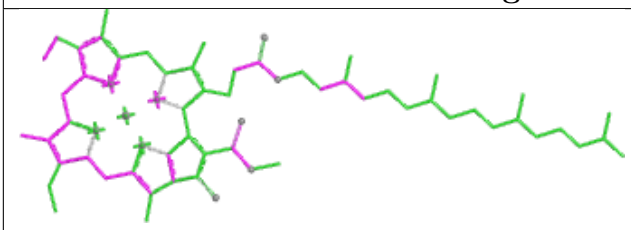


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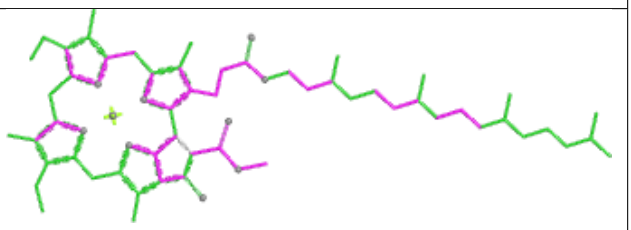


Rings

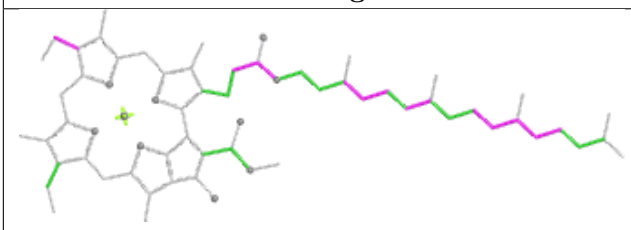
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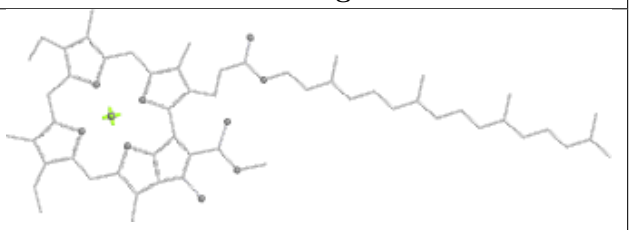
Bond lengths



Bond angles

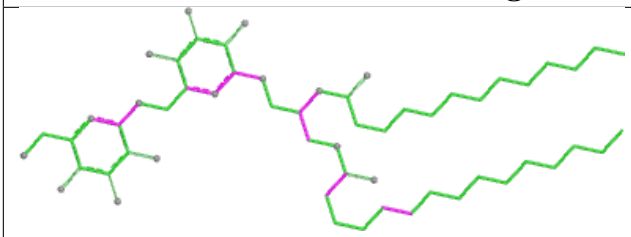


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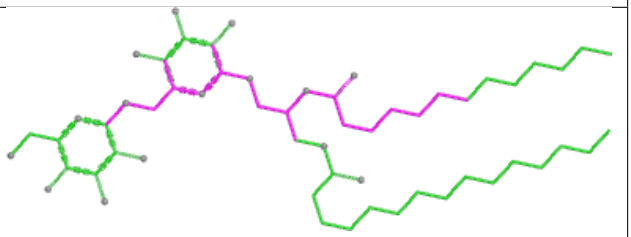


Rings

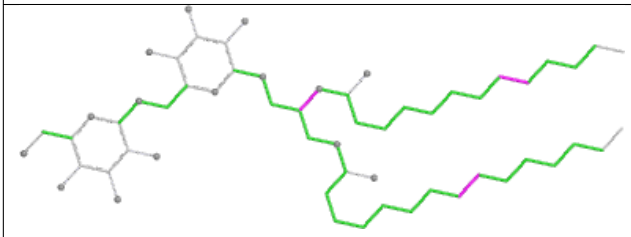
Ligand DGD AH 101



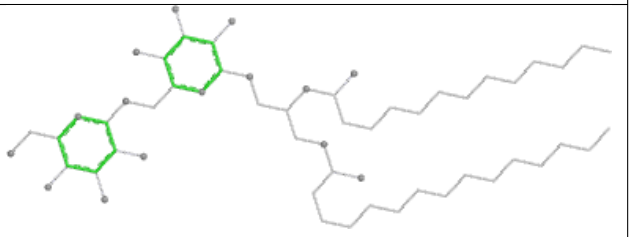
Bond lengths



Bond angles

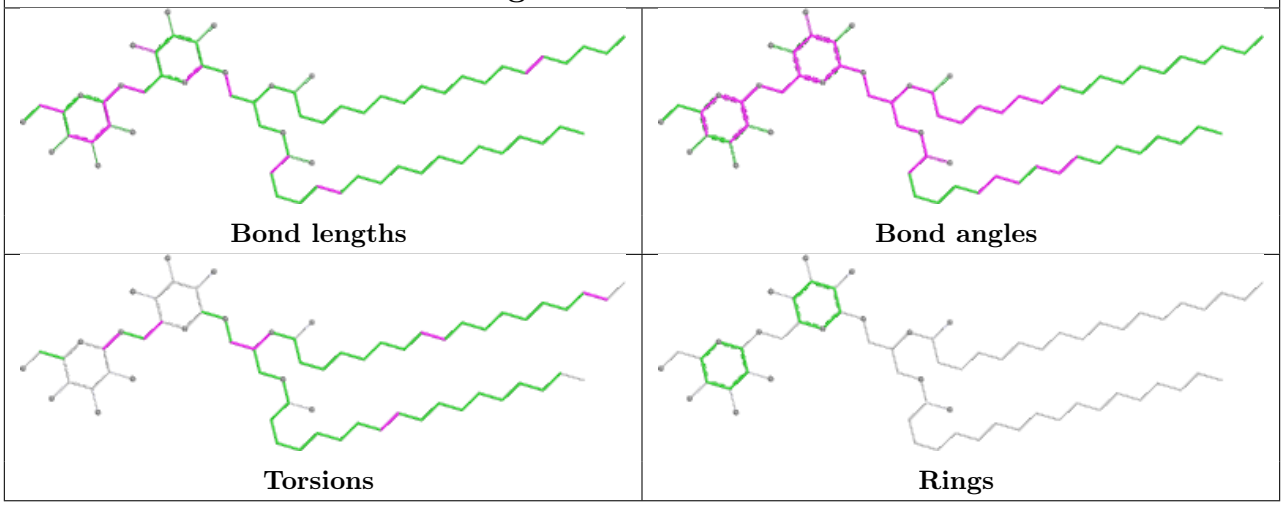


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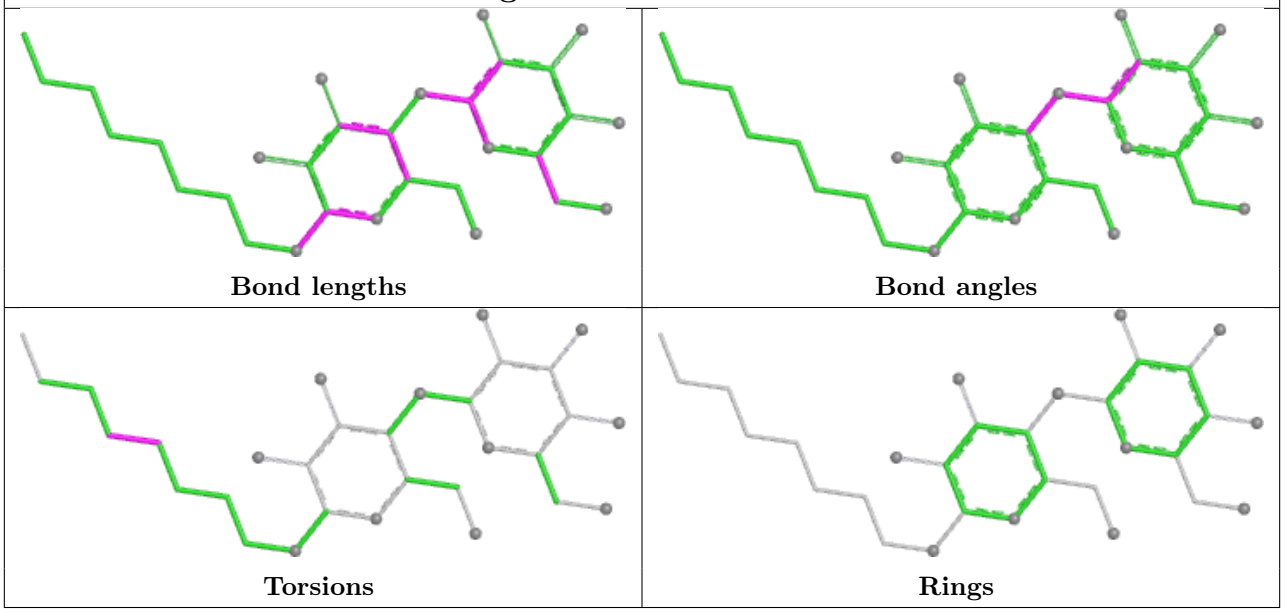


Rings

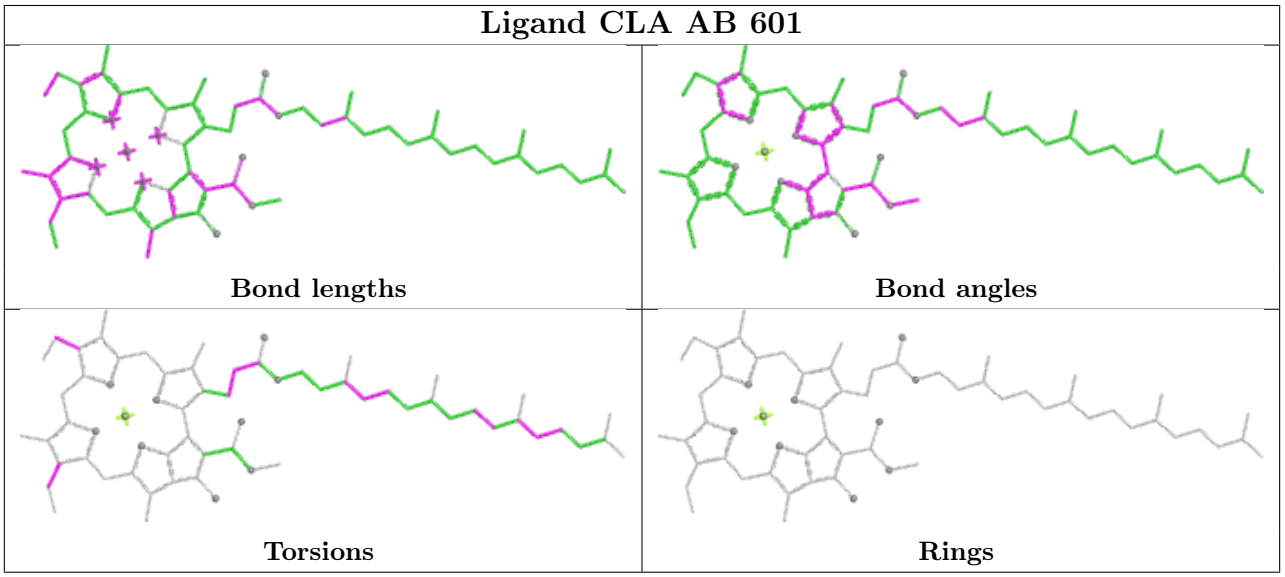
Ligand DGD AC 519



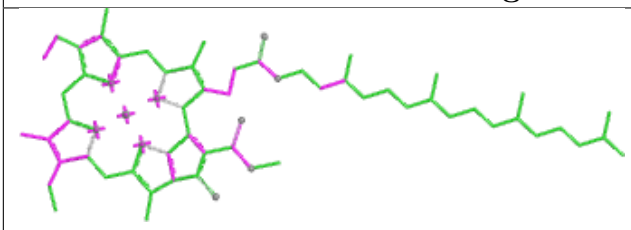
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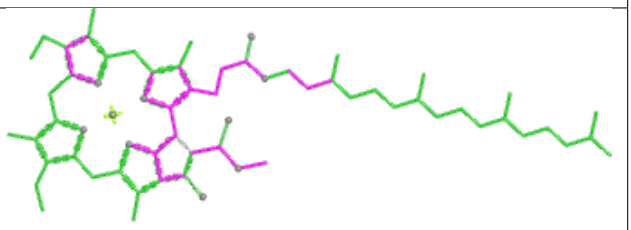
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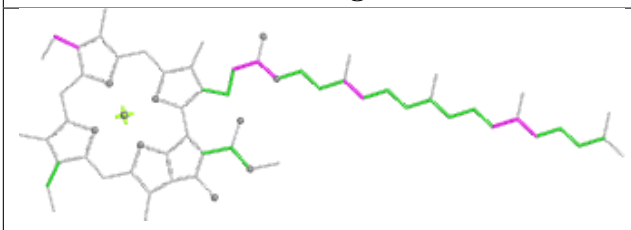
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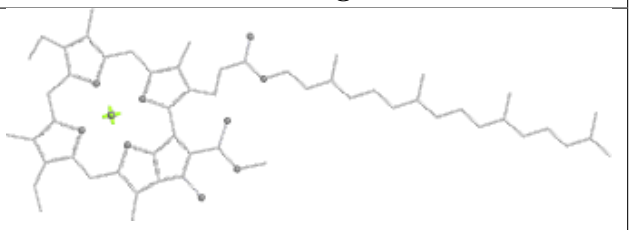
Bond lengths



Bond angles

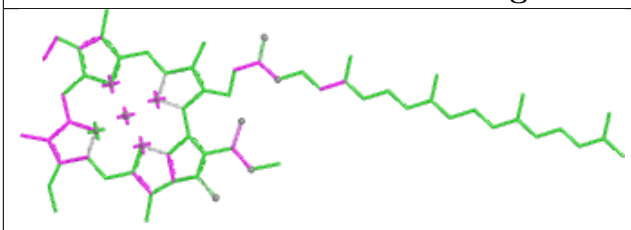


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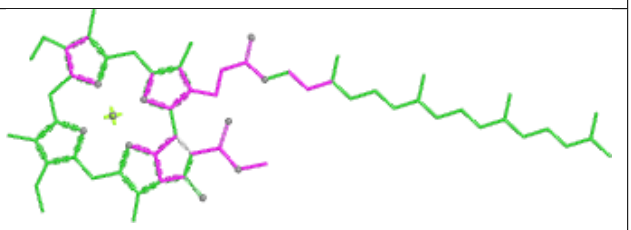


Rings

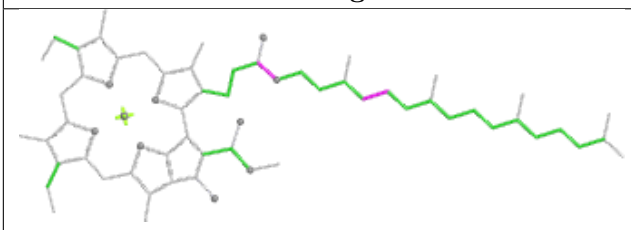
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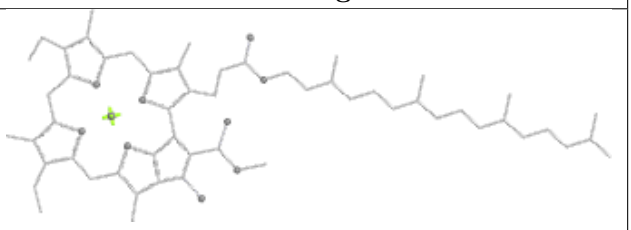
Bond lengths



Bond angles

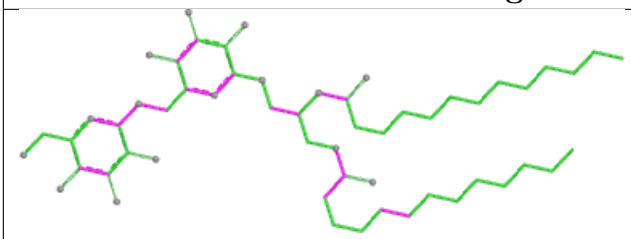


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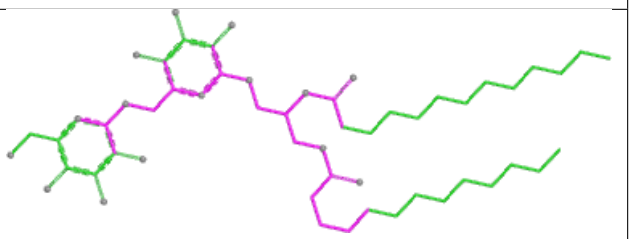


Rings

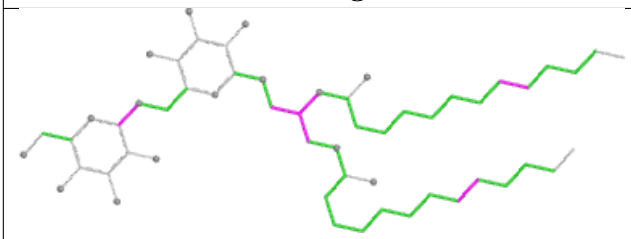
Ligand DGD AA 411



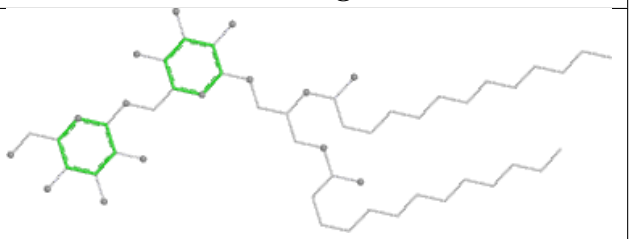
Bond lengths



Bond angles

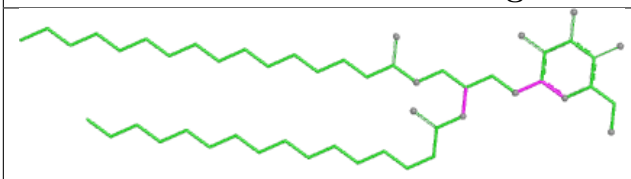


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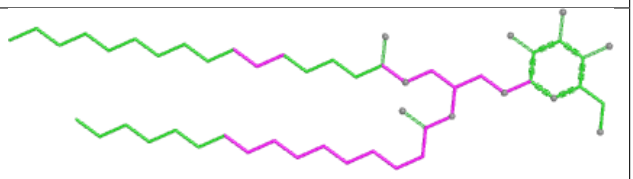


Rings

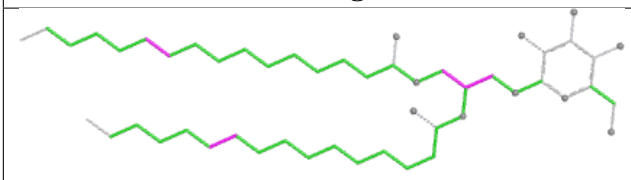
Ligand LMG AB 620



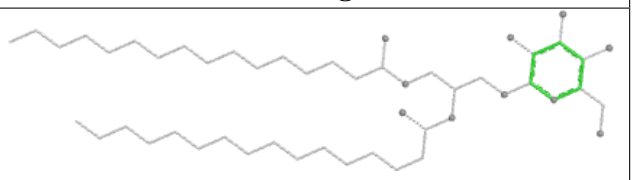
Bond lengths



Bond angles

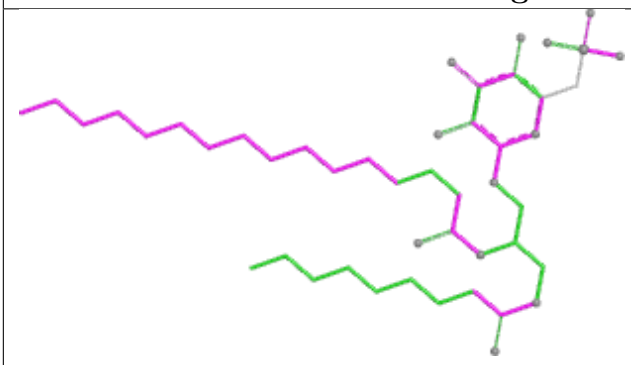


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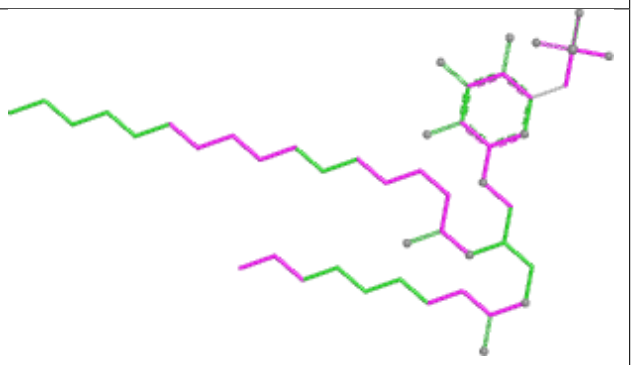


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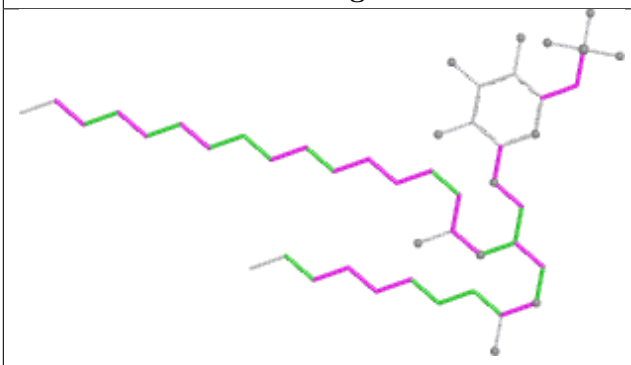
Ligand SQD AB 627



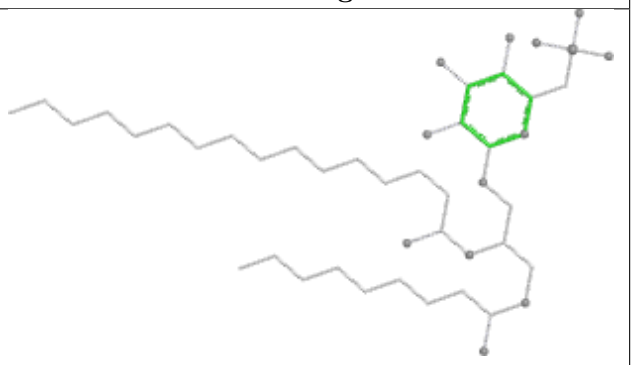
Bond lengths



Bond angles

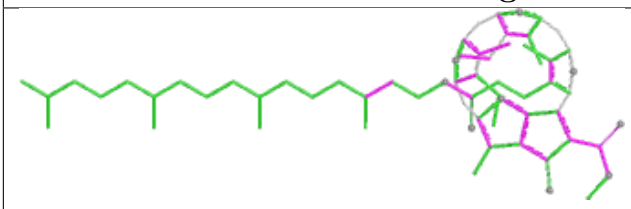


Torsions

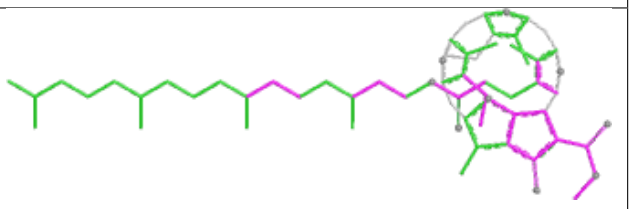


Rings

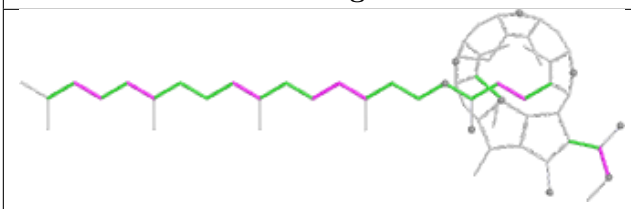
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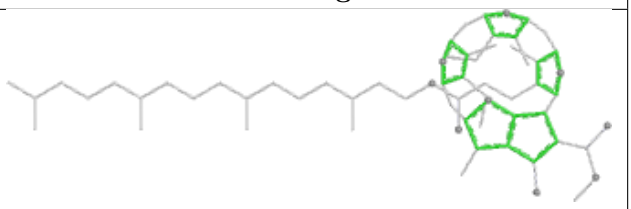
Bond lengths



Bond angles



Torsions

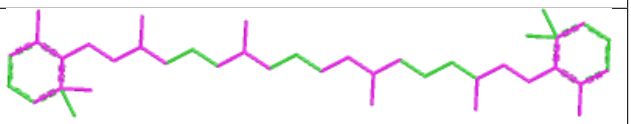


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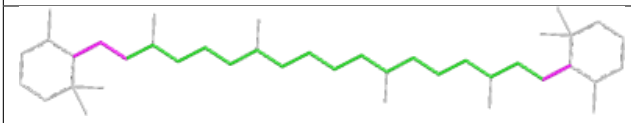
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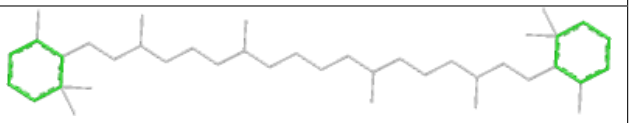
Bond lengths



Bond angles

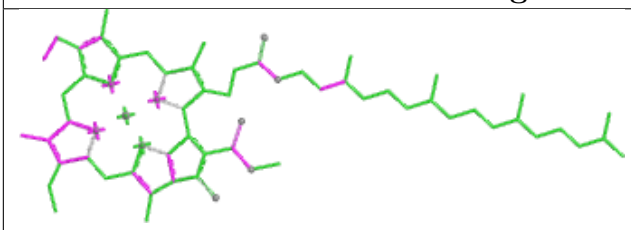


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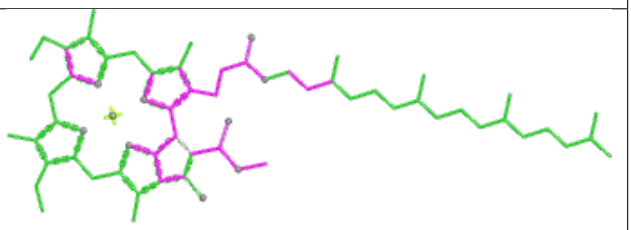


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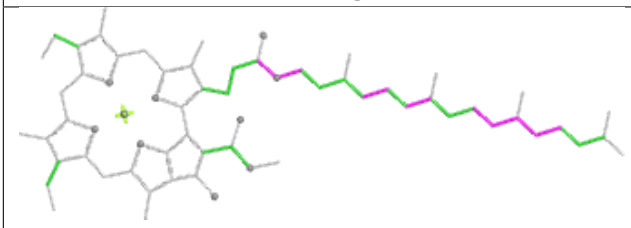
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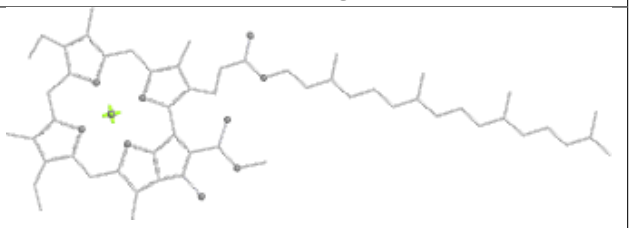
Bond lengths



Bond angles

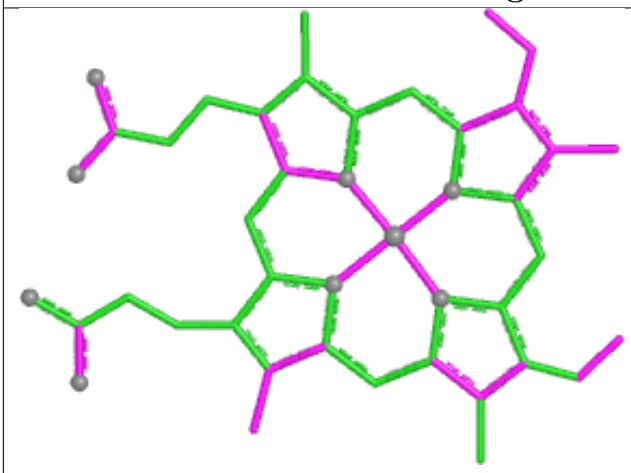


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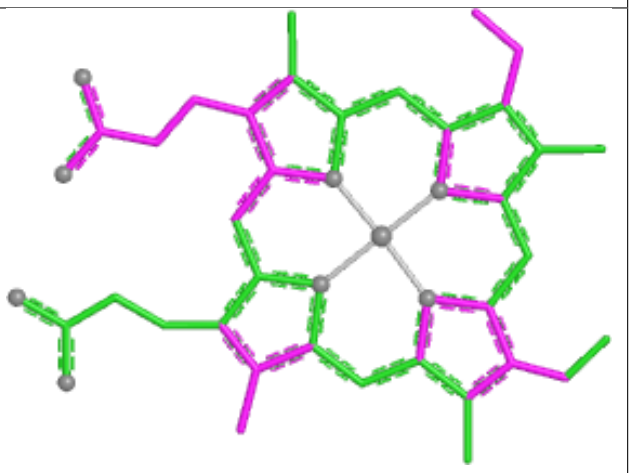


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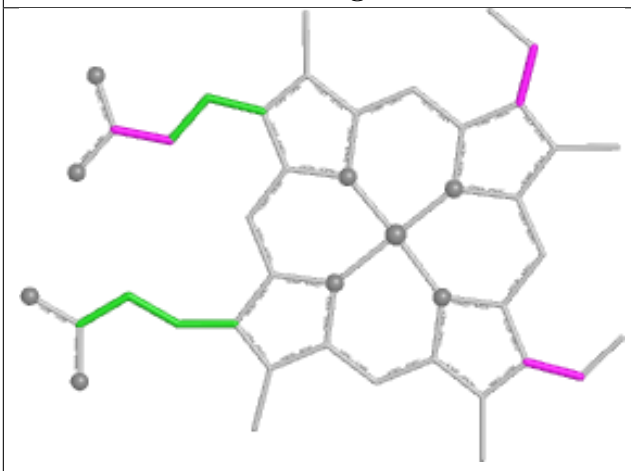
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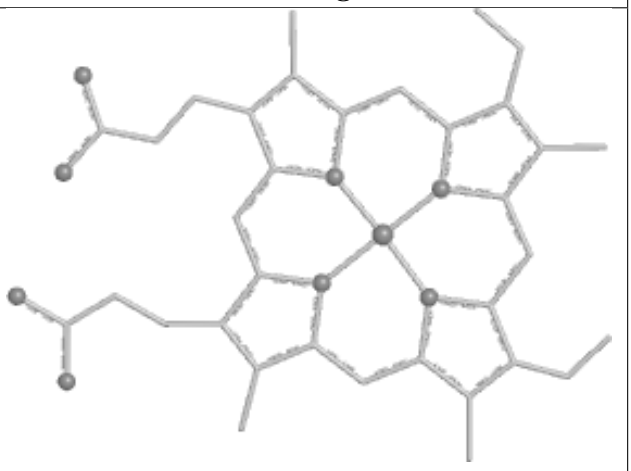
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Bond angles

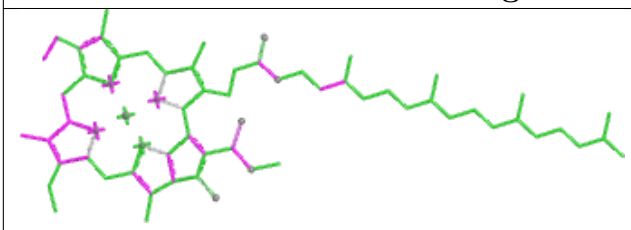


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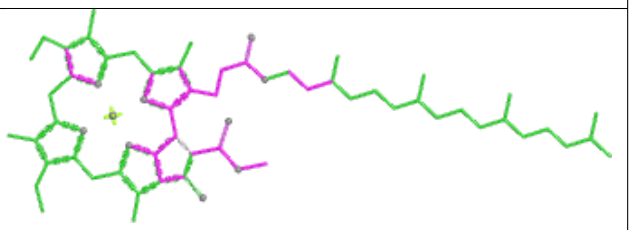


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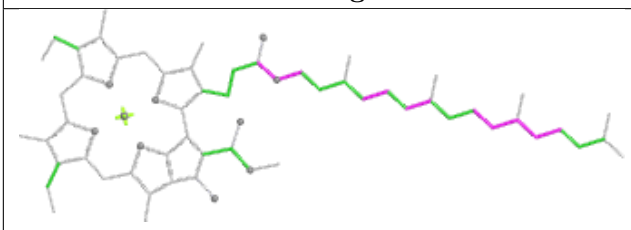
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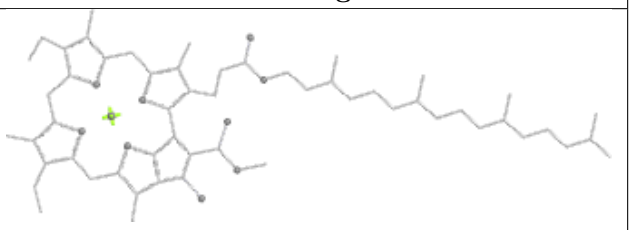
Bond lengths



Bond angles

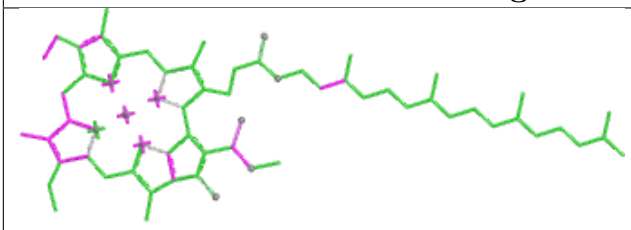


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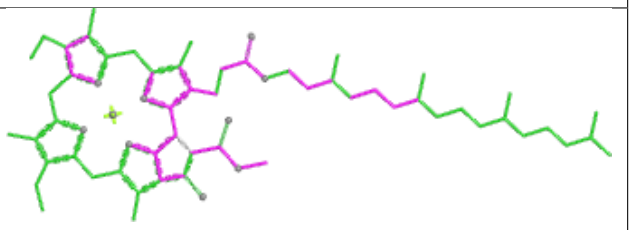


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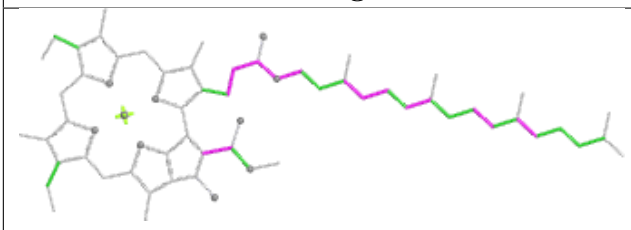
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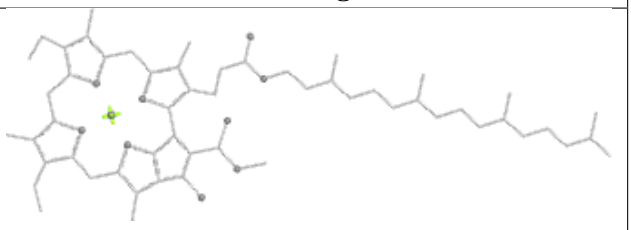
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Bond angles

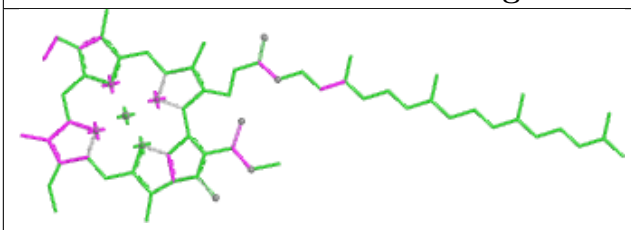


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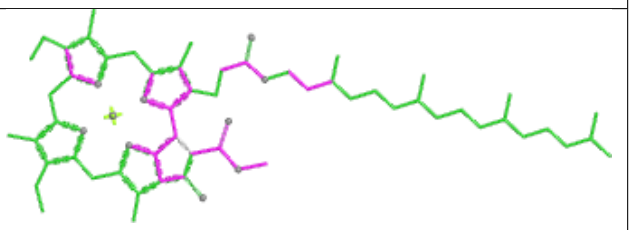


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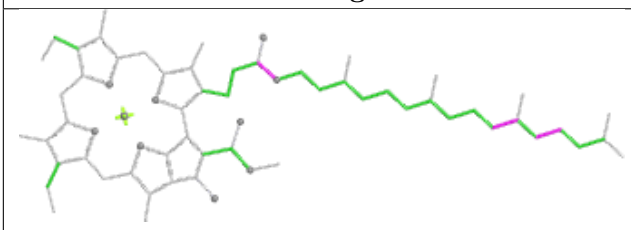
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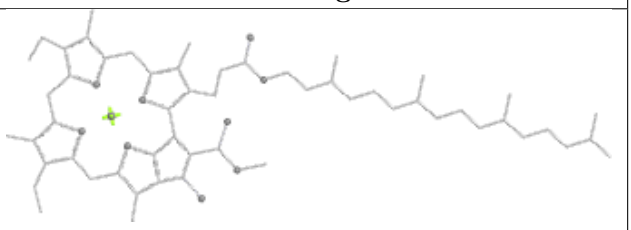
Bond lengths



Bond angles

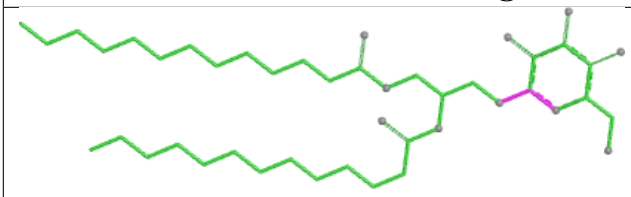


Torsions



Rings

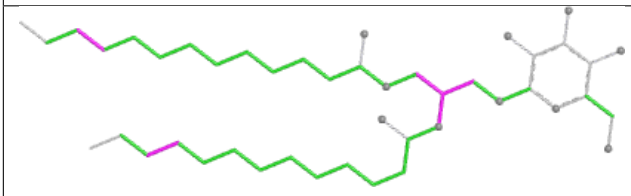
Ligand LMG BC 5521



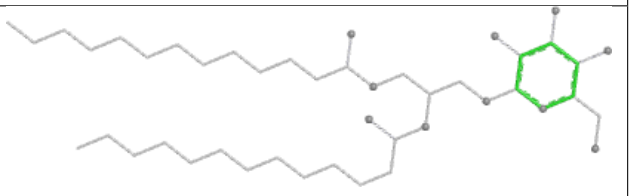
Bond lengths



Bond angles



Torsions

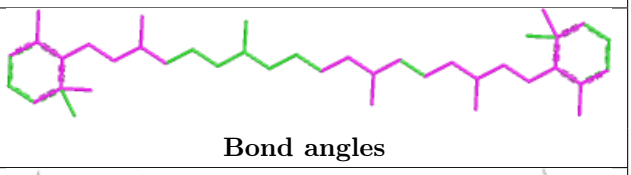


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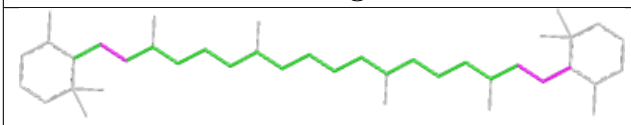
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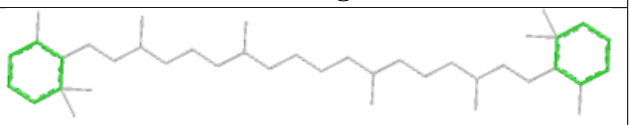
Bond lengths



Bond angles

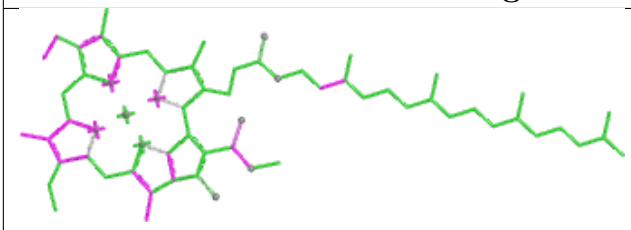


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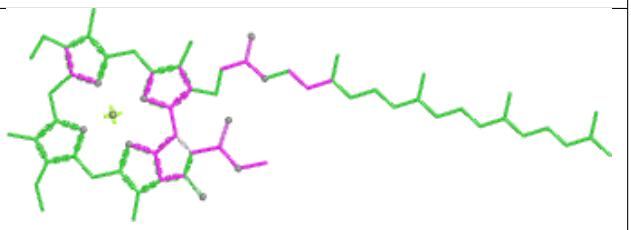


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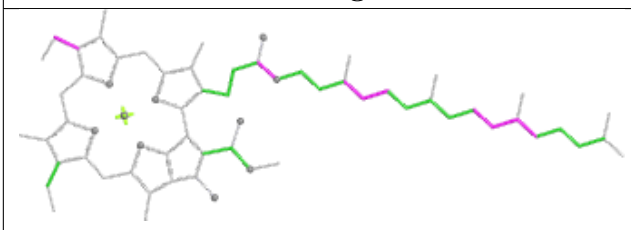
Ligand CLA BC 5510



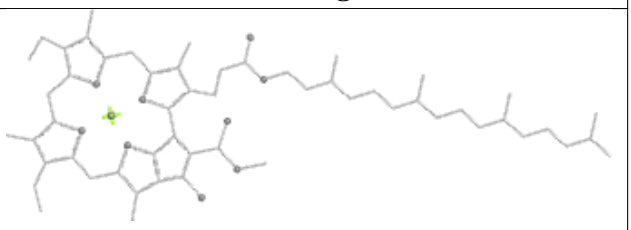
Bond lengths



Bond angles

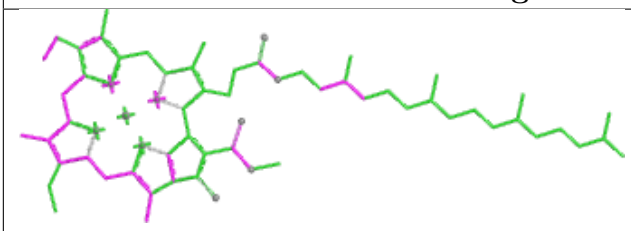


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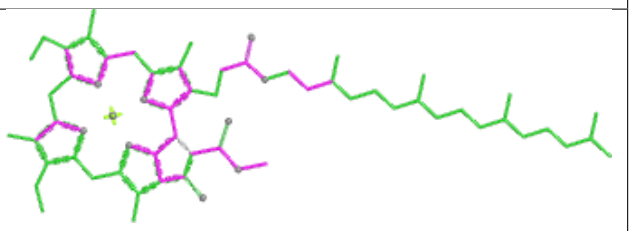


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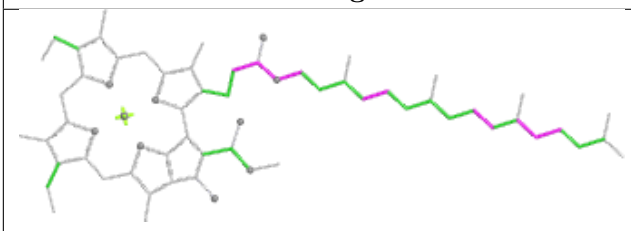
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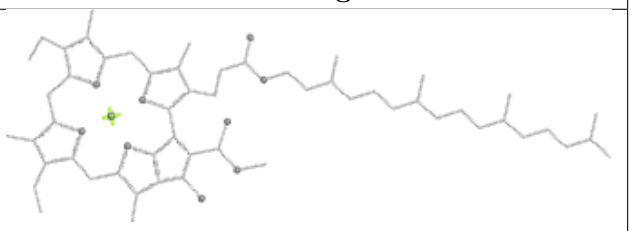
Bond lengths



Bond angles

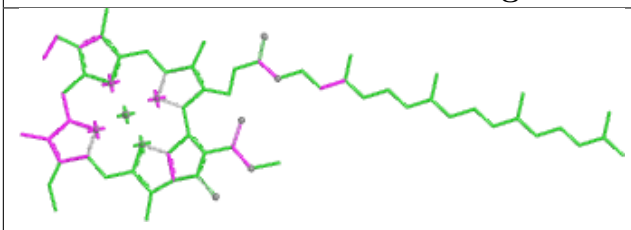


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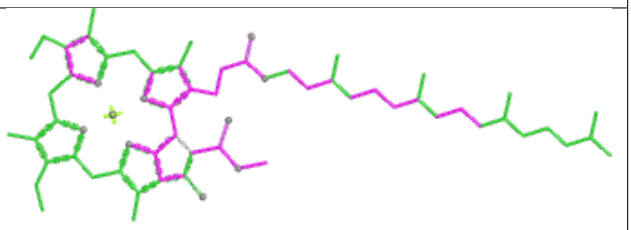


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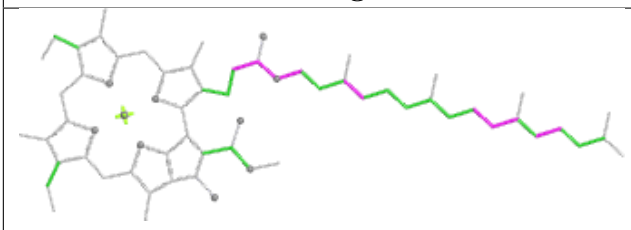
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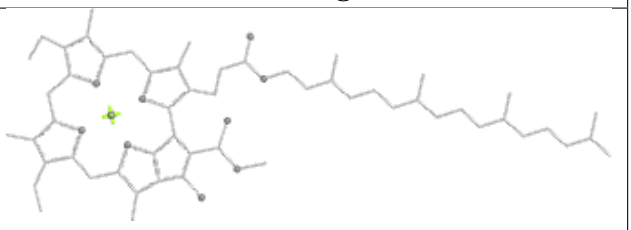
Bond lengths



Bond angles

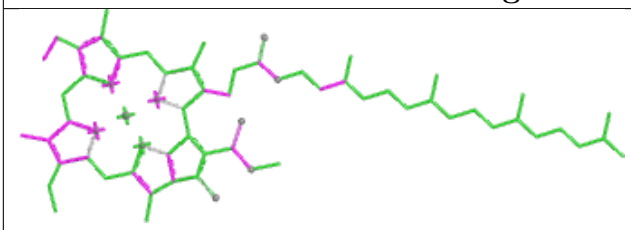


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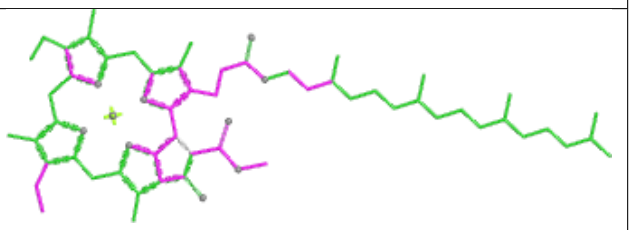


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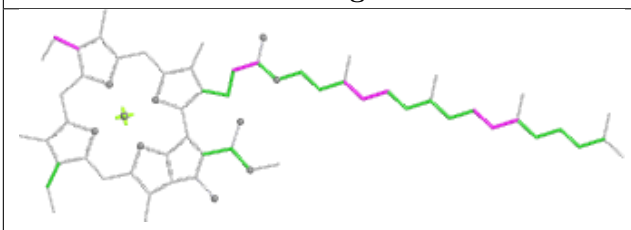
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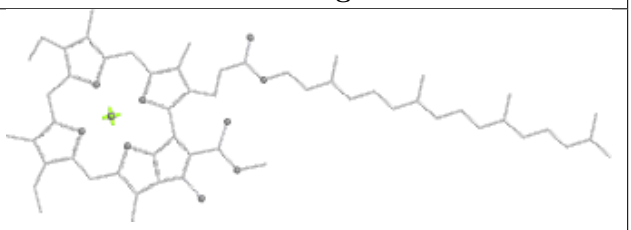
Bond lengths



Bond angles



Torsions

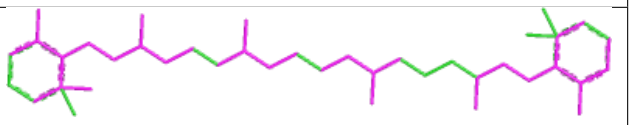


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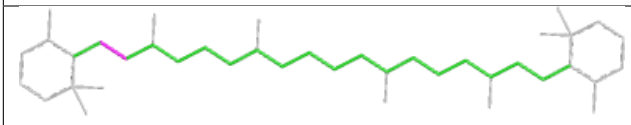
Ligand BCR AX 101



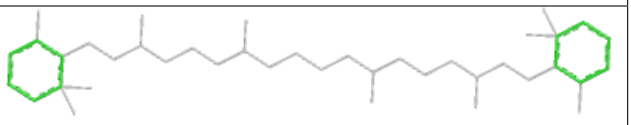
Bond lengths



Bond angles

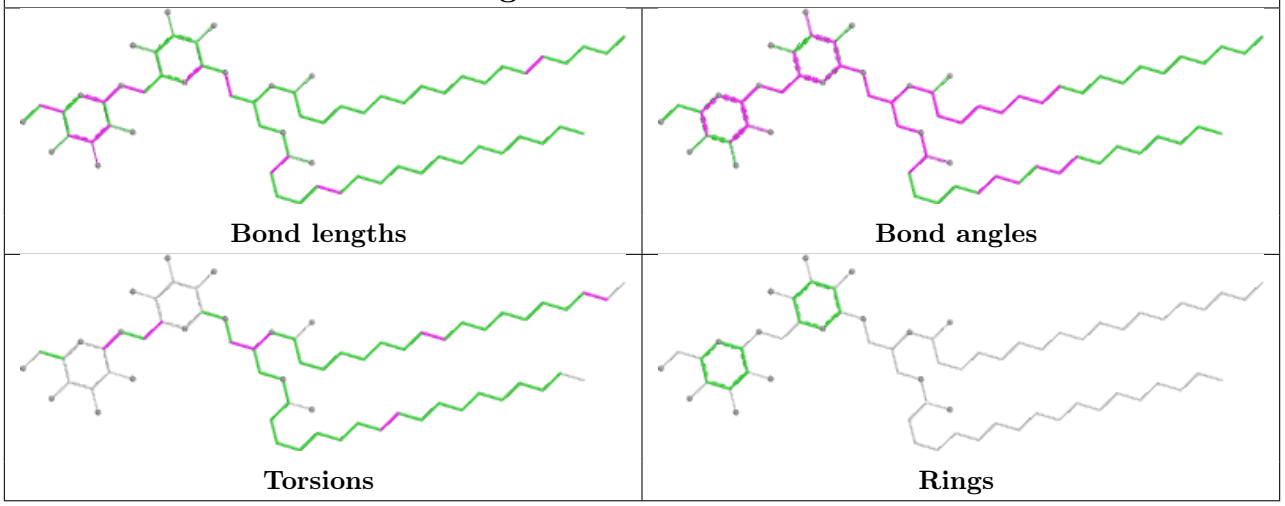


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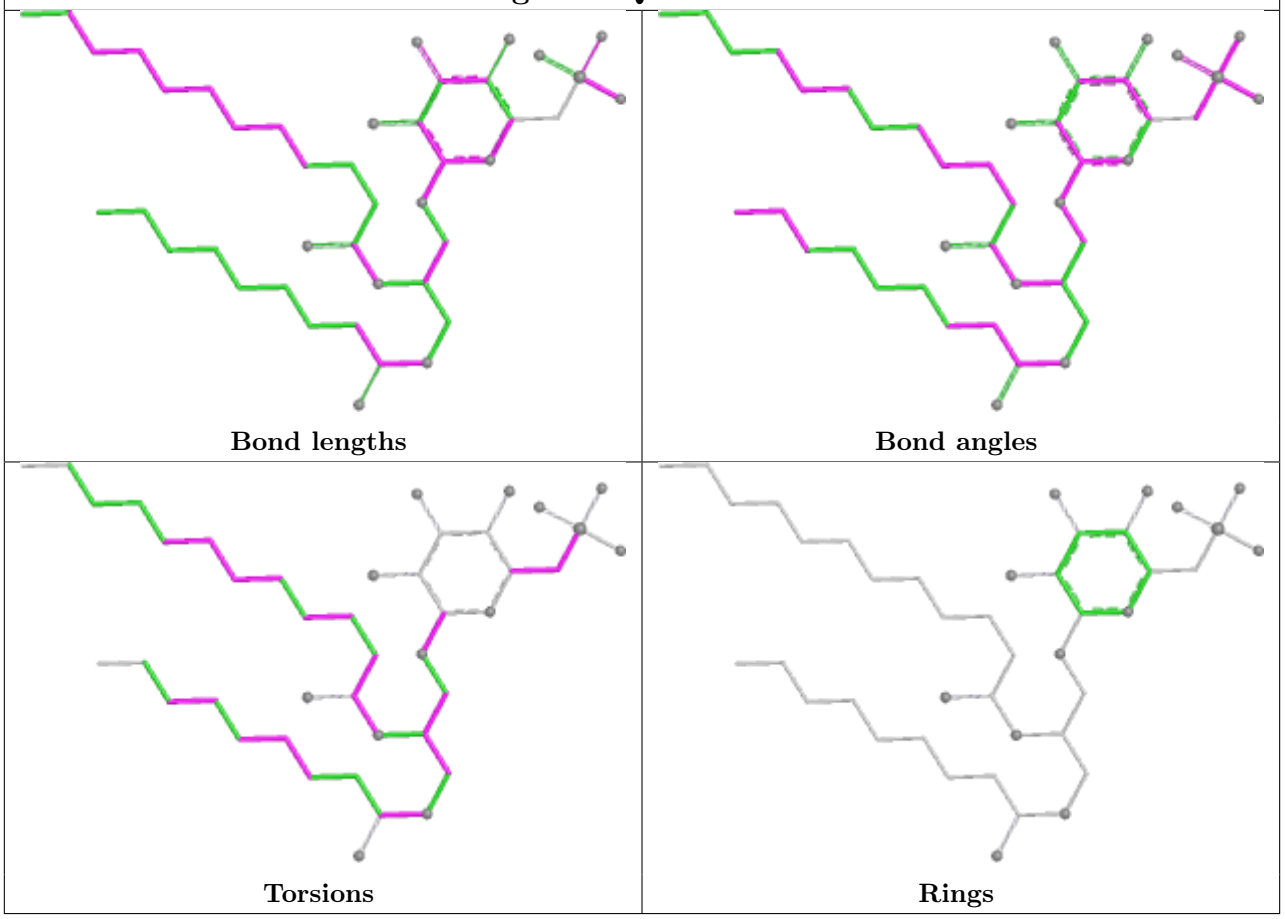


Rings

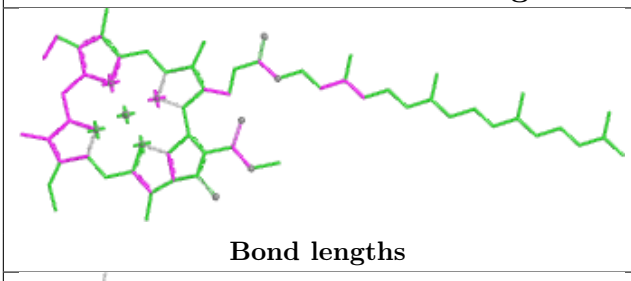
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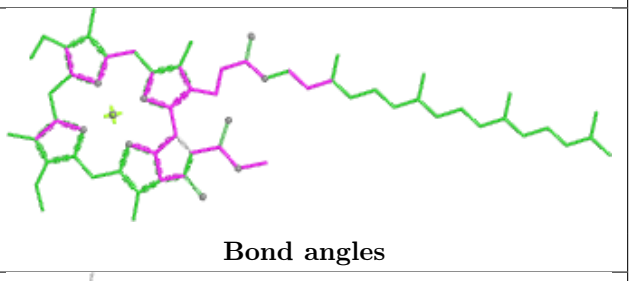
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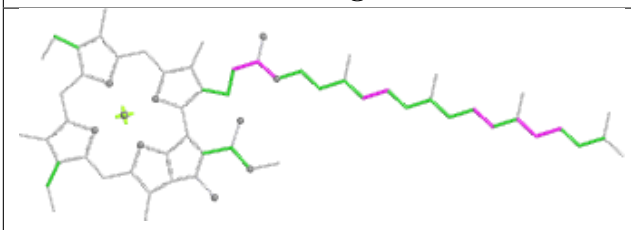
Ligand CLA AB 614



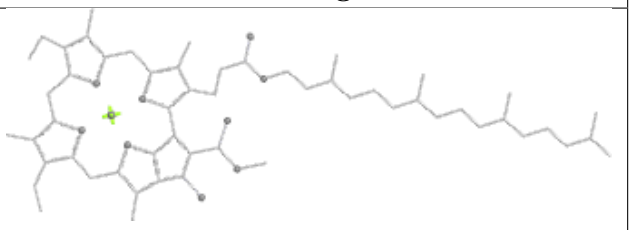
Bond lengths



Bond angles

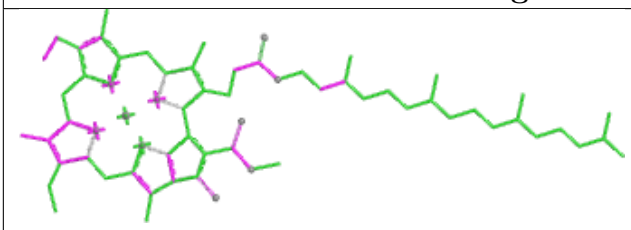


Torsions

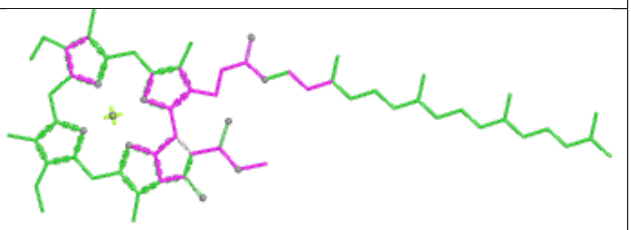


Rings

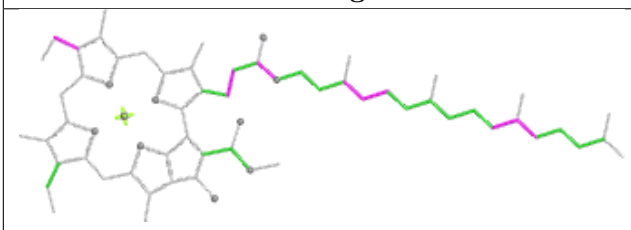
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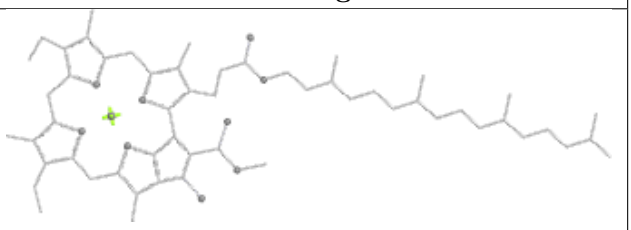
Bond lengths



Bond angles

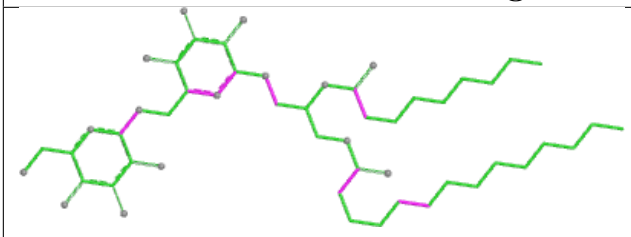


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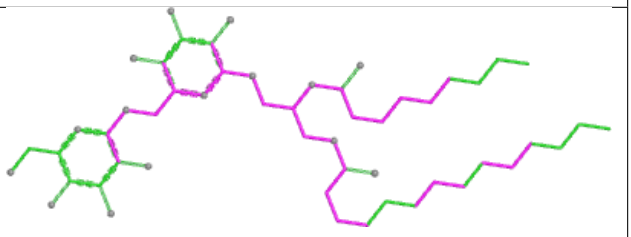


Rings

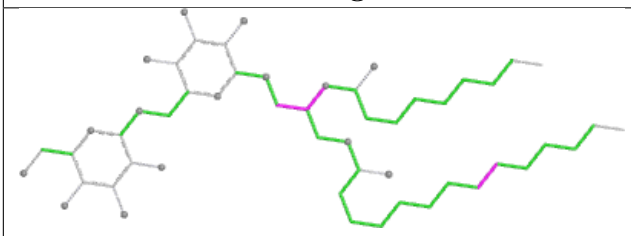
Ligand DGD AC 517



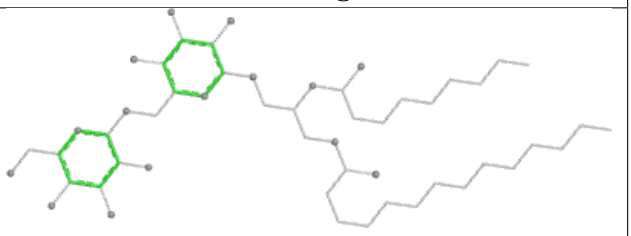
Bond lengths



Bond angles

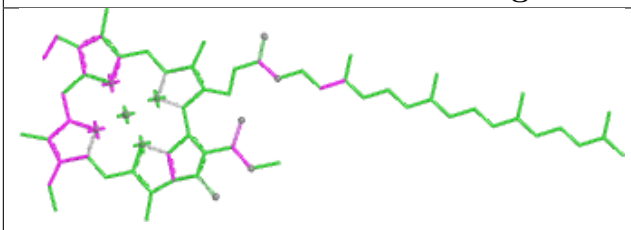


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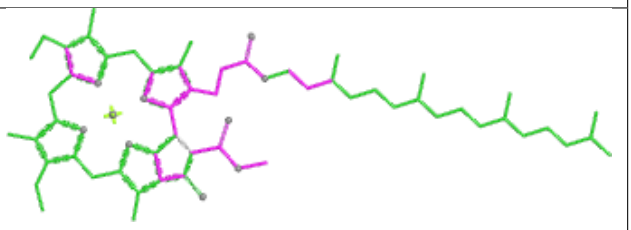


Rings

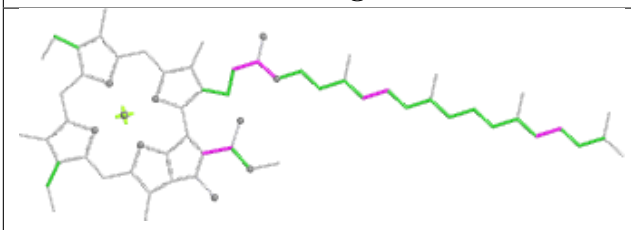
Ligand CLA AC 508



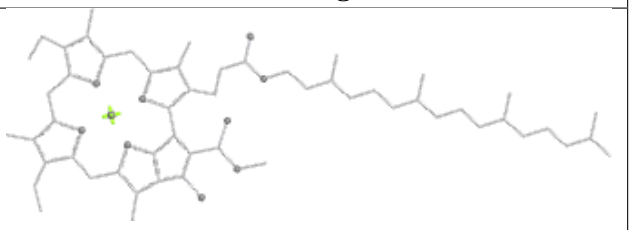
Bond lengths



Bond angles

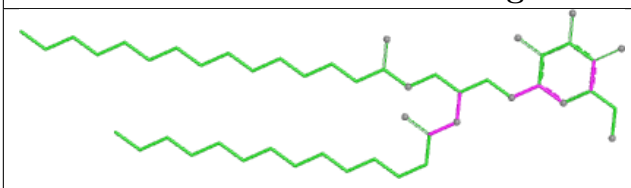


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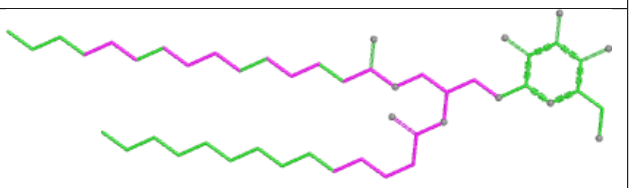


Rings

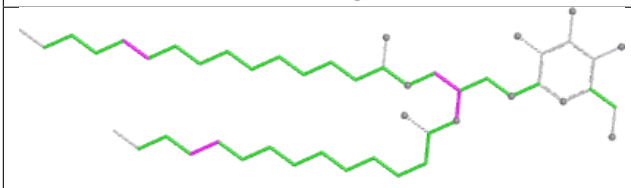
Ligand LMG AC 520



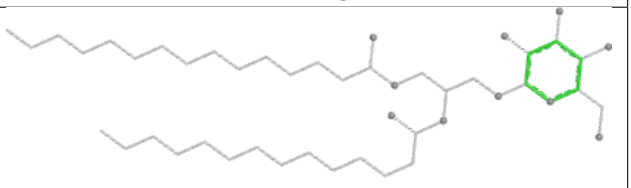
Bond lengths



Bond angles

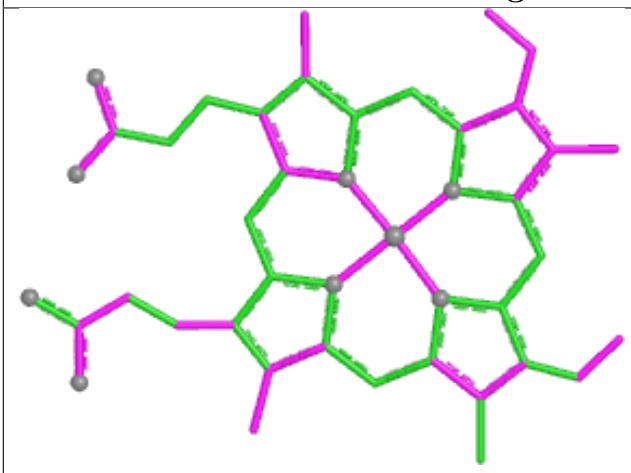


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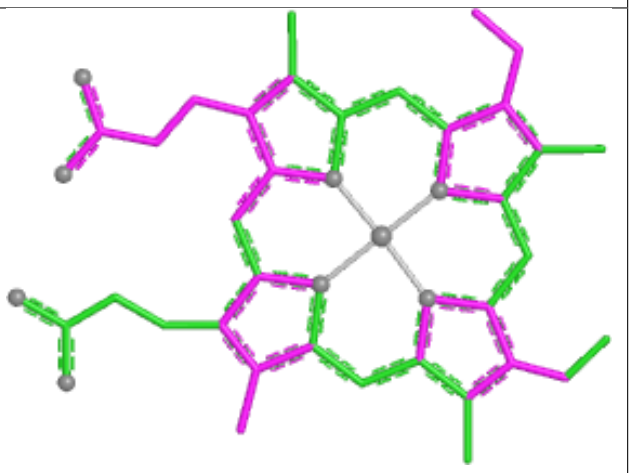


Rings

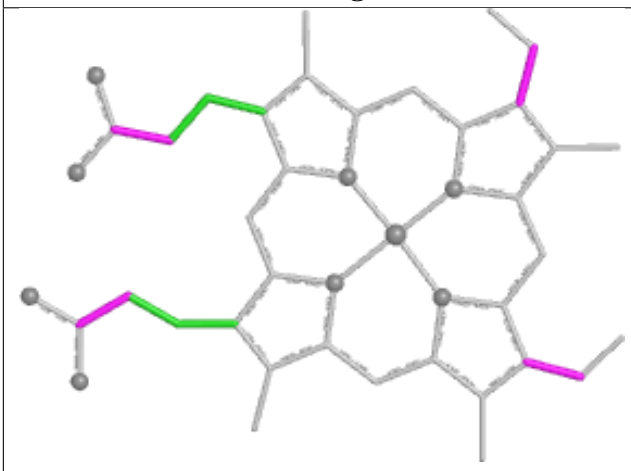
Ligand HEM AF 101



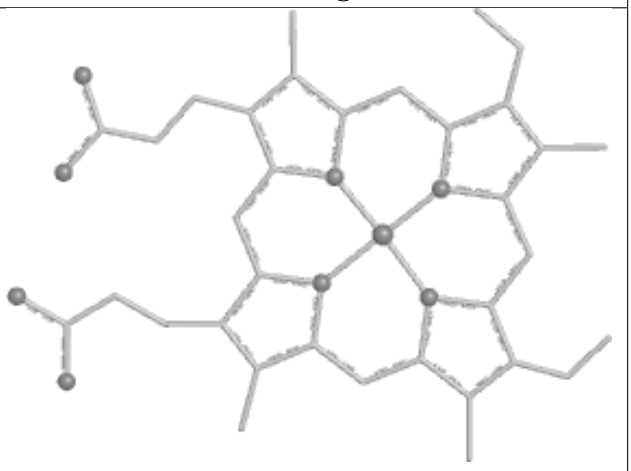
Bond lengths



Bond angles

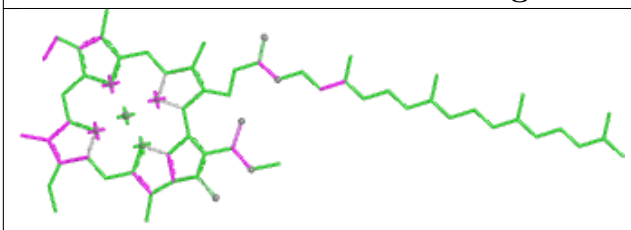


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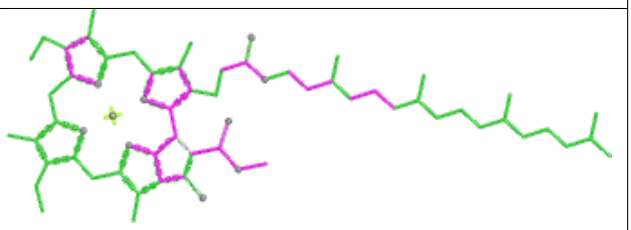


Rings

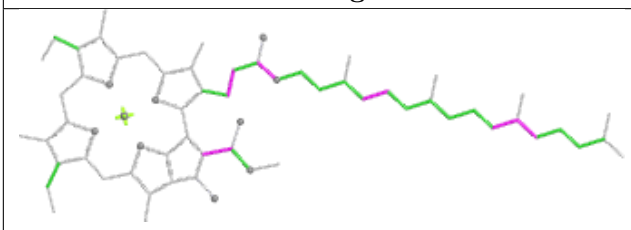
Ligand CLA AB 610



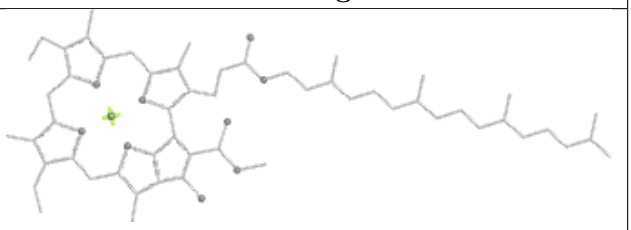
Bond lengths



Bond angles

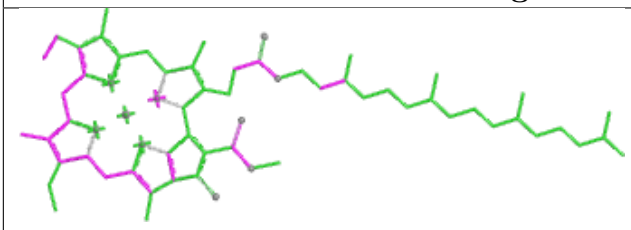


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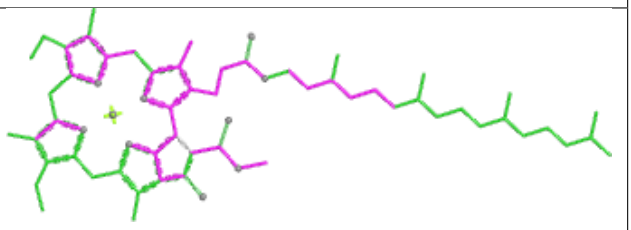


Rings

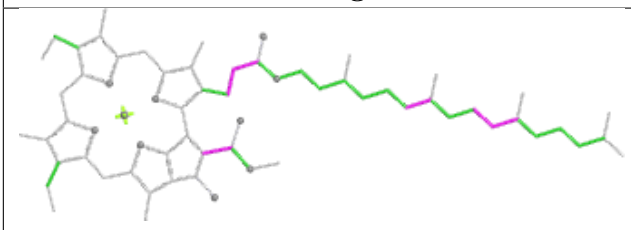
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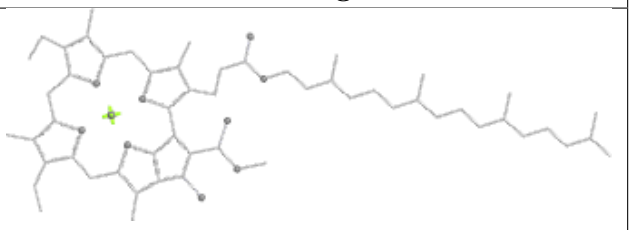
Bond lengths



Bond angles

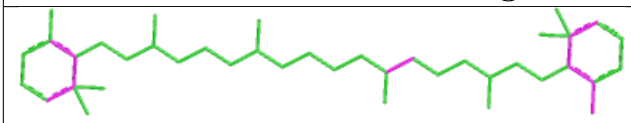


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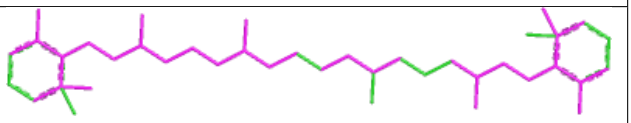


Rings

Ligand BCR BK 5102



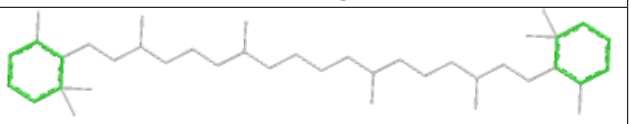
Bond lengths



Bond angles

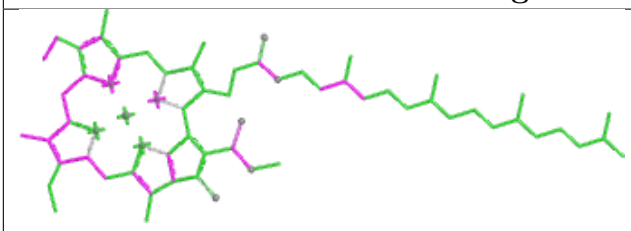


Torsions

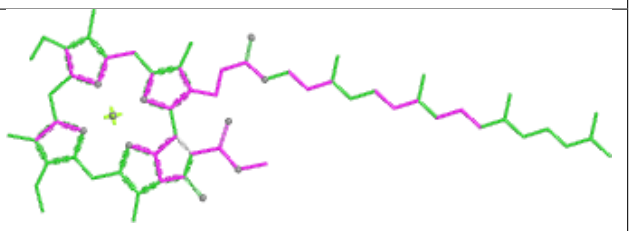


Rings

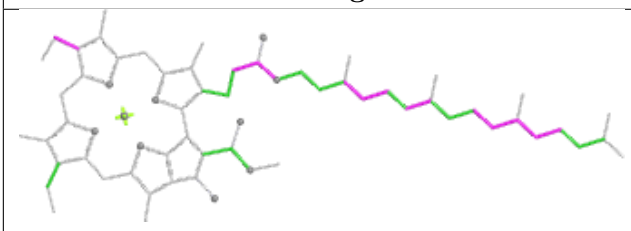
Ligand CLA AC 511



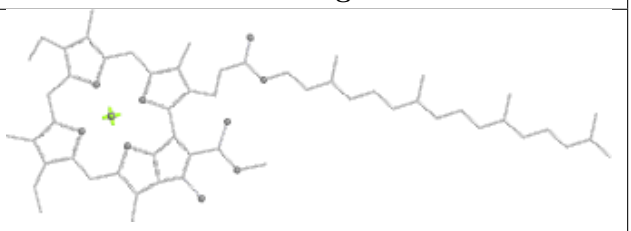
Bond lengths



Bond angles

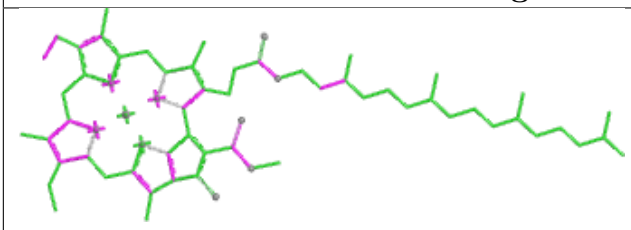


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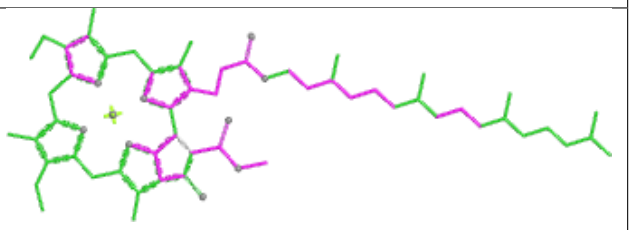


Rings

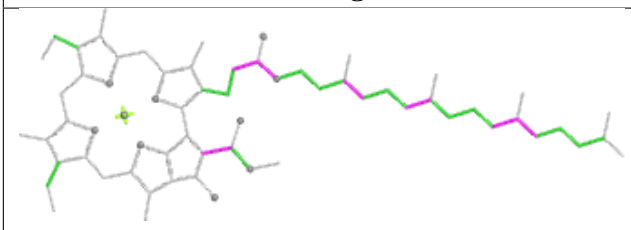
Ligand CLA AB 611



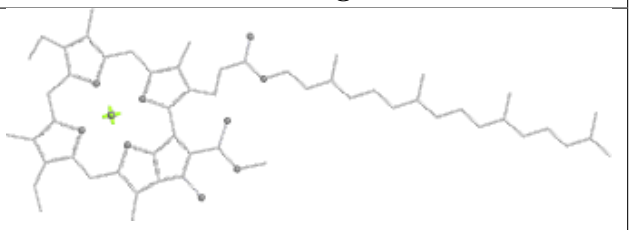
Bond lengths



Bond angles

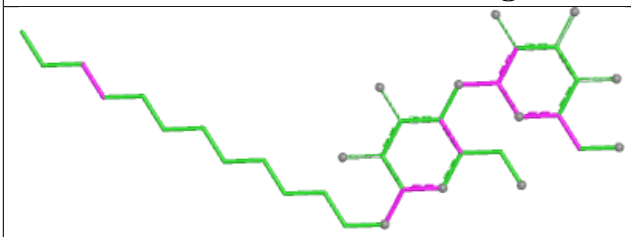


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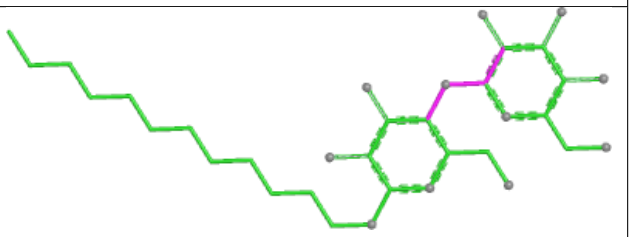


Rings

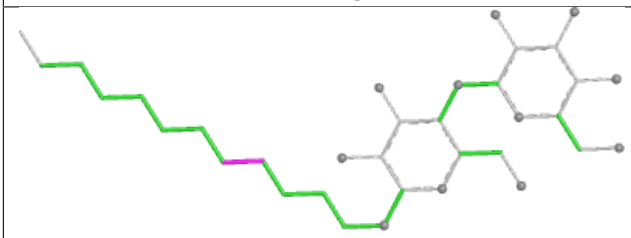
Ligand LMT BB 5626



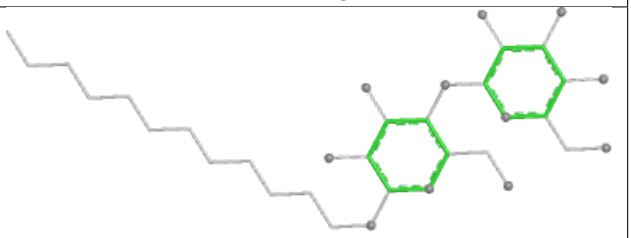
Bond lengths



Bond angles

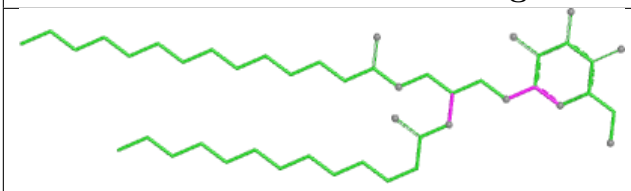


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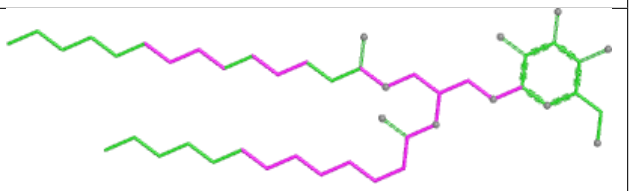


Rings

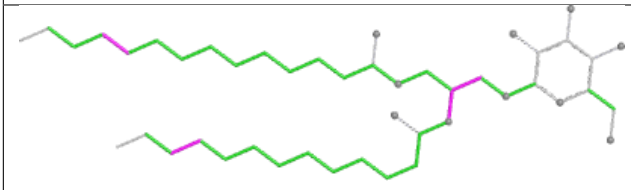
Ligand LMG AJ 102



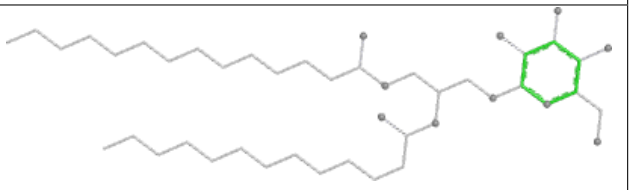
Bond lengths



Bond angles

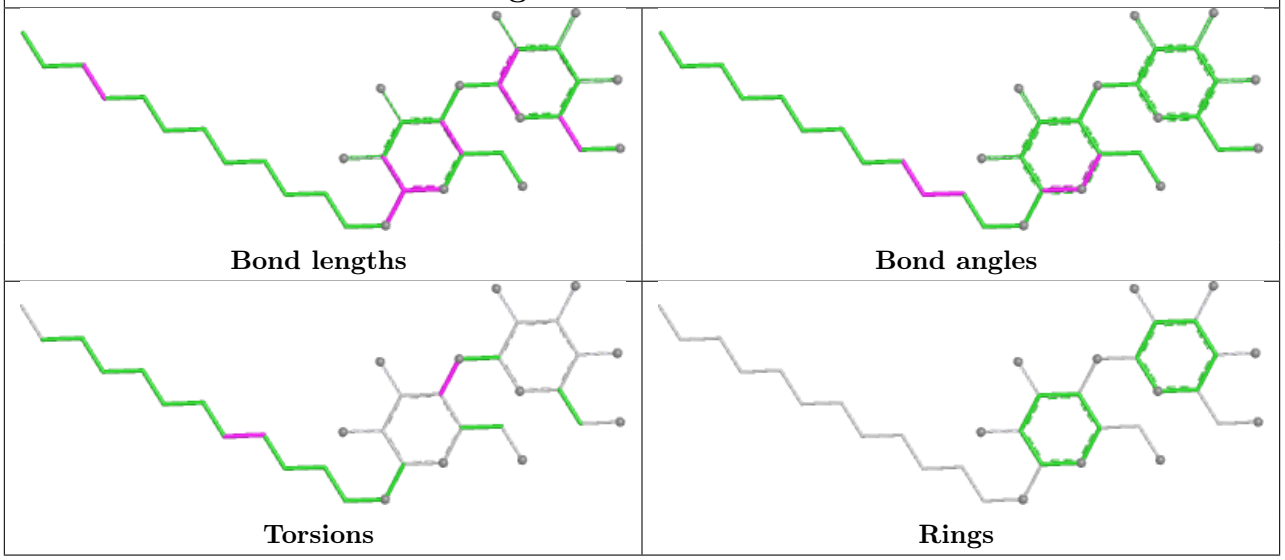


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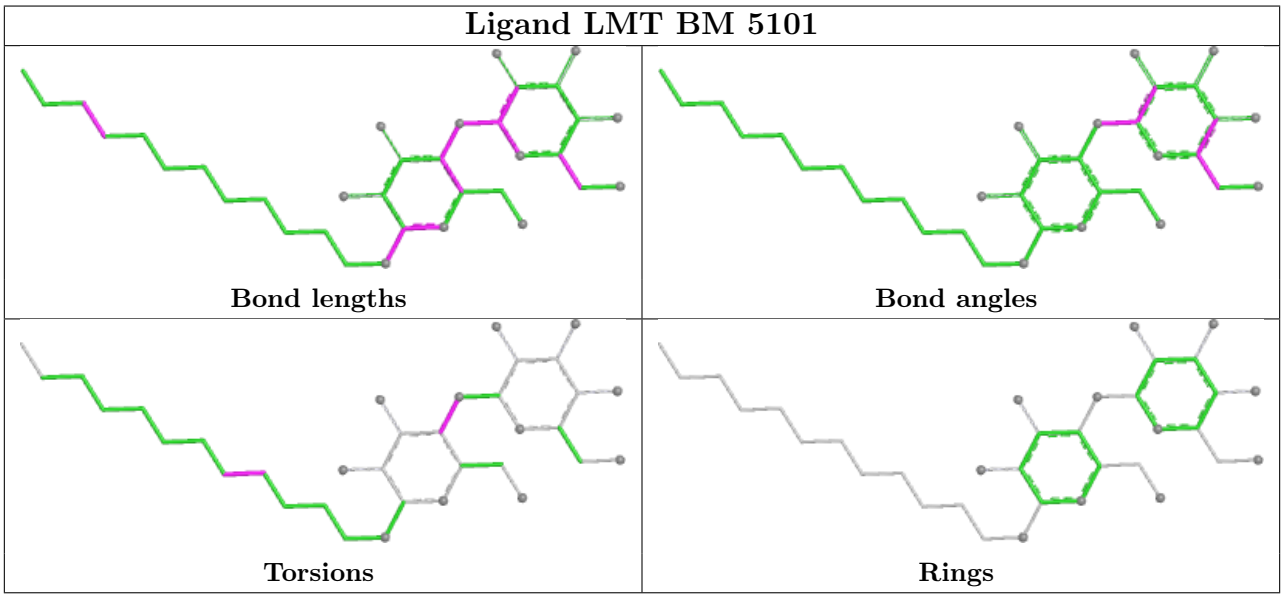


Rings

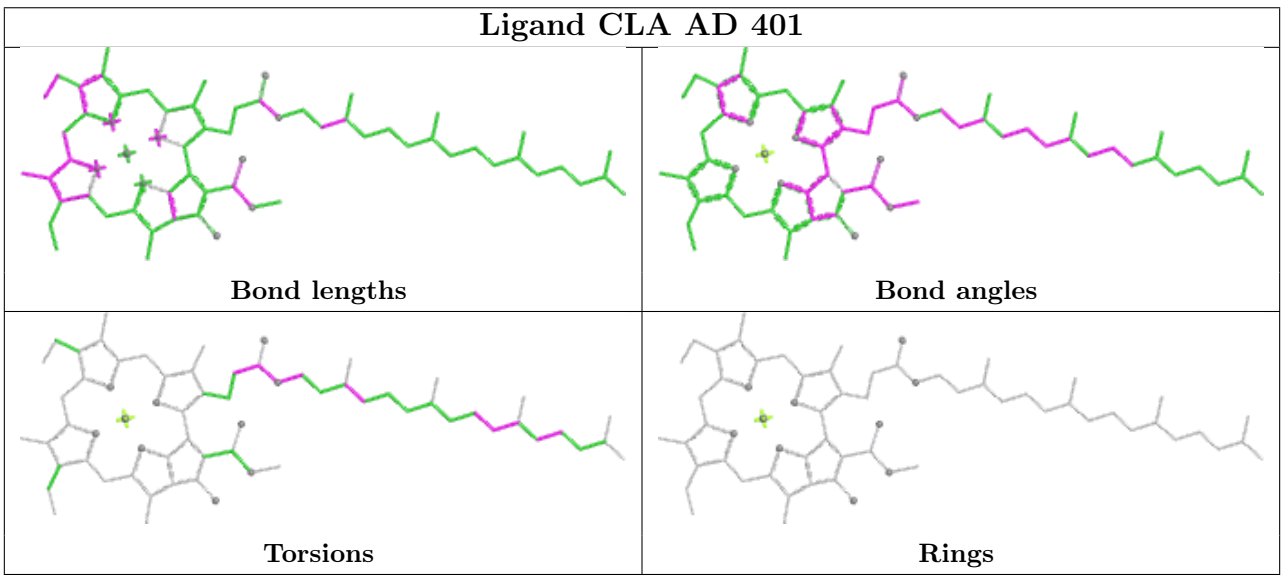
Ligand LMT AB 624



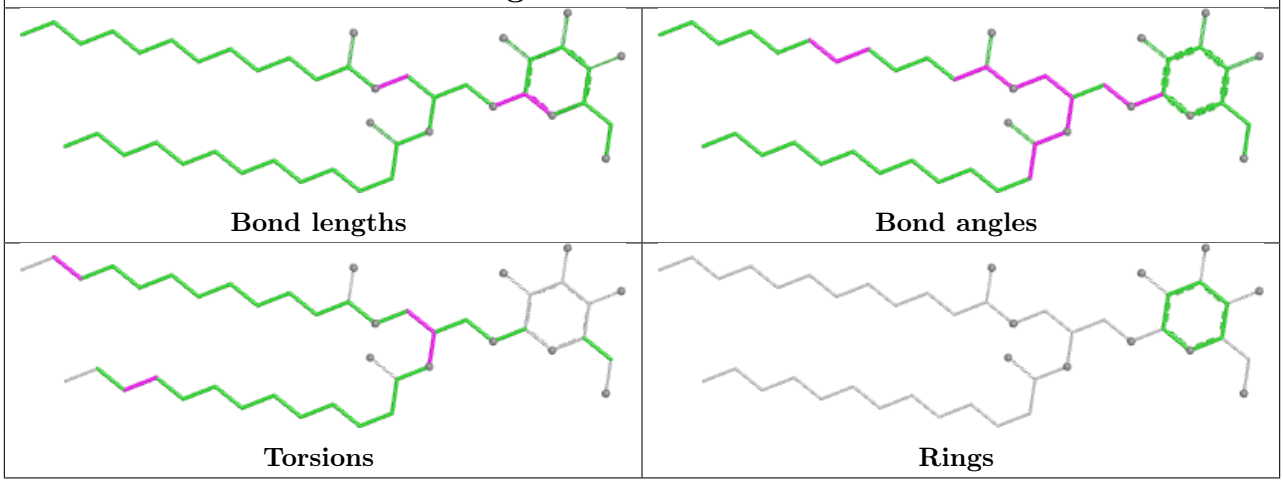
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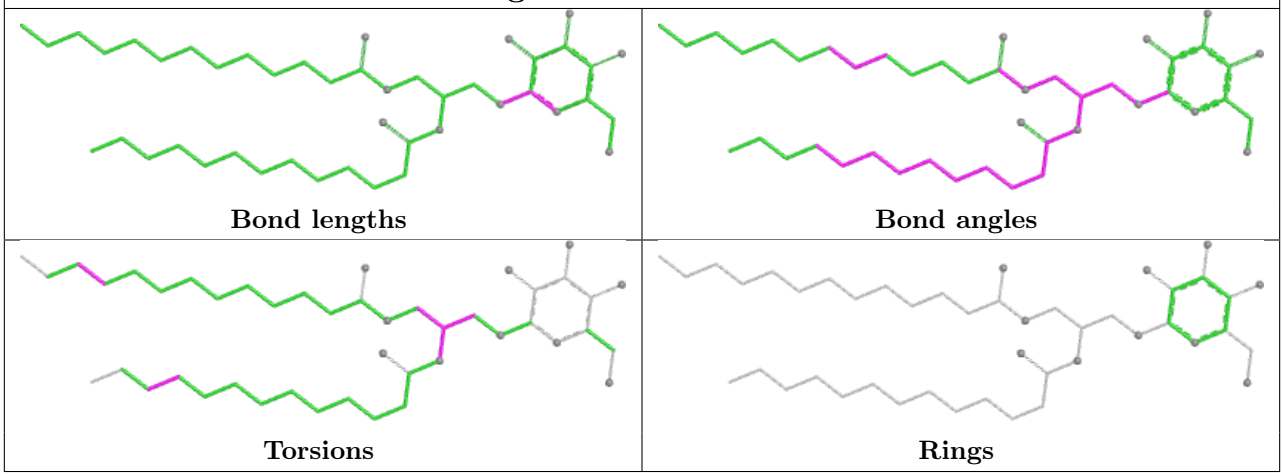
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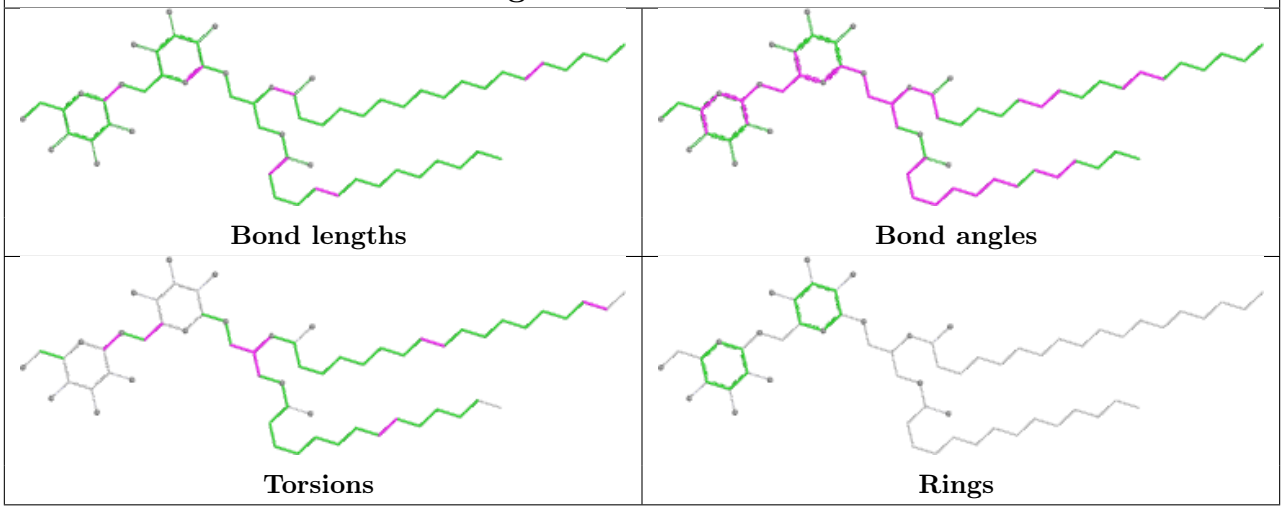
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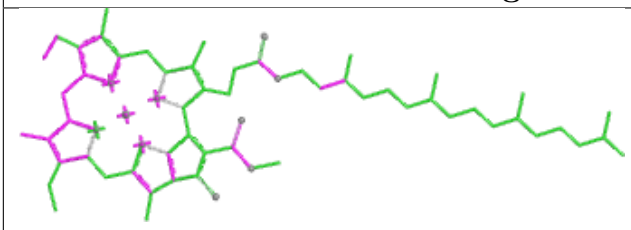
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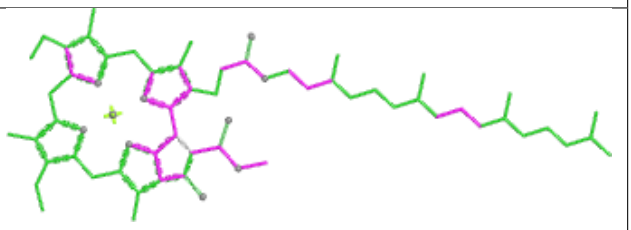
Ligand DGD AC 518



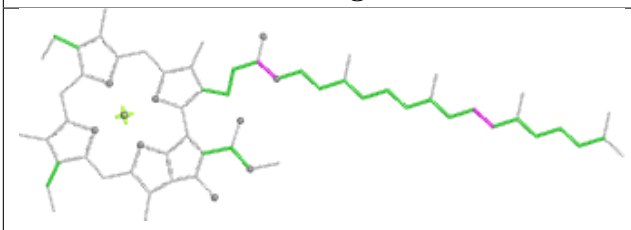
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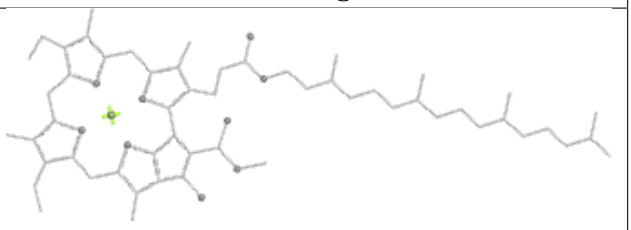
Bond lengths



Bond angles

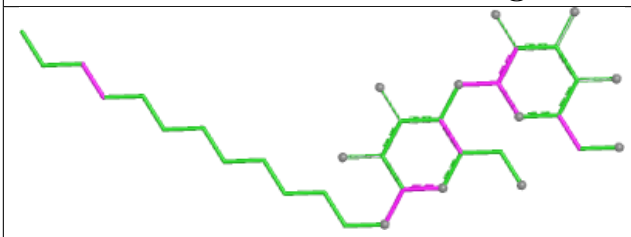


Torsions

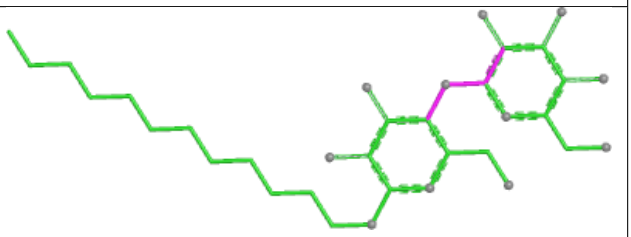


Rings

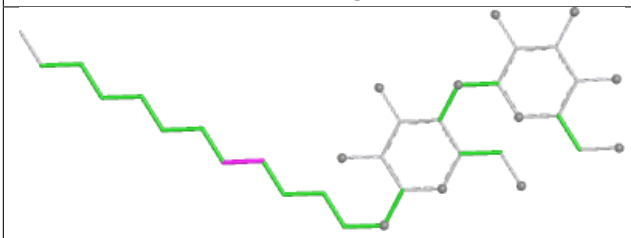
Ligand LMT AB 623



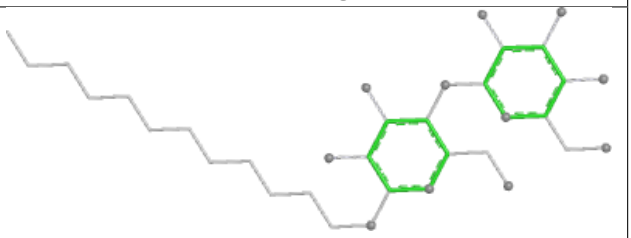
Bond lengths



Bond angles



Torsions

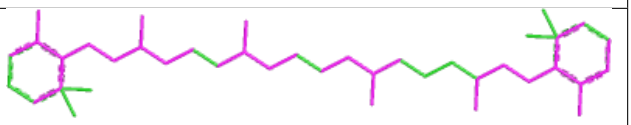


Rings

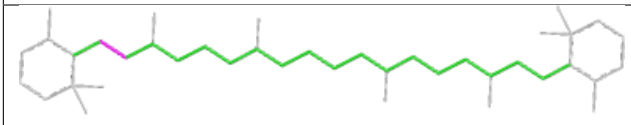
Ligand BCR BX 5101



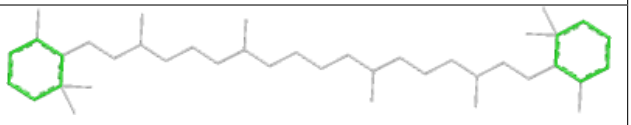
Bond lengths



Bond angles



Torsions

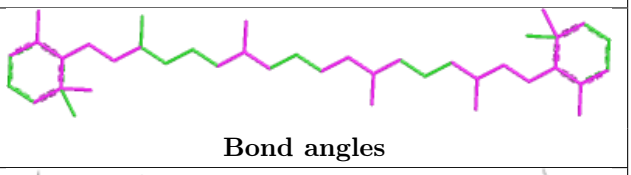


Rings

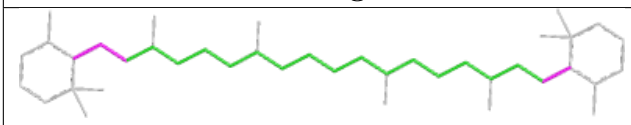
Ligand BCR AC 516



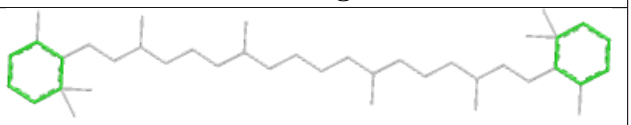
Bond lengths



Bond angles

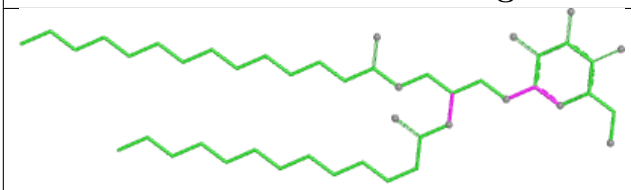


Torsions

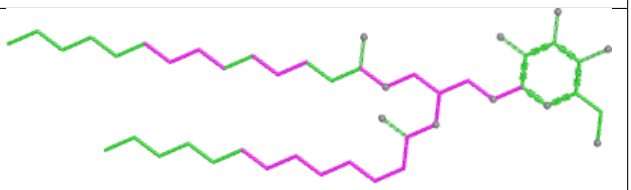


Rings

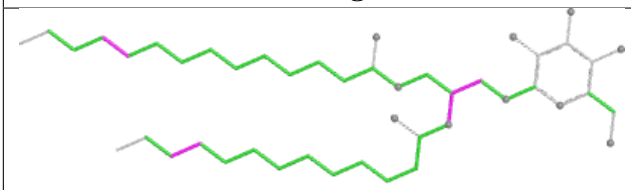
Ligand LMG BD 5408



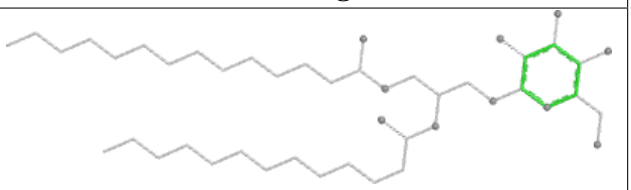
Bond lengths



Bond angles

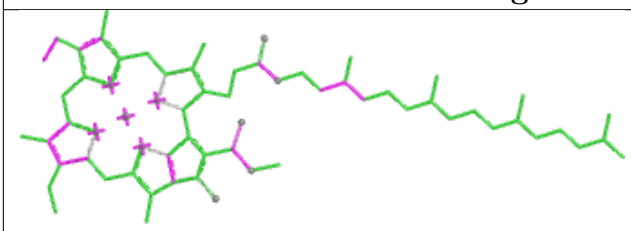


Torsions

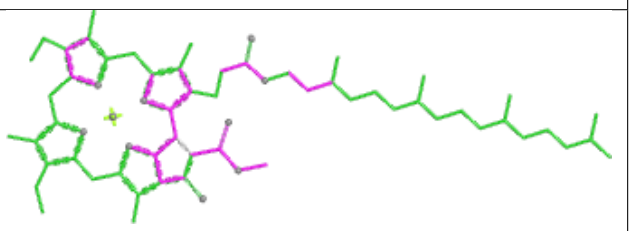


Rings

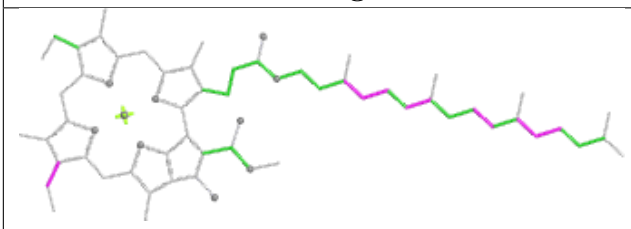
Ligand CLA AB 616



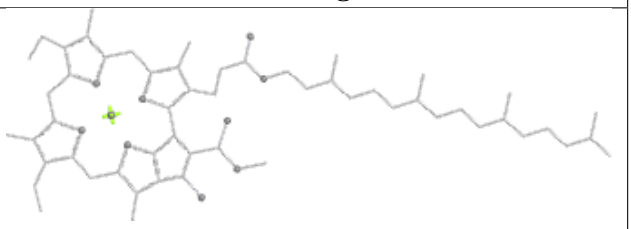
Bond lengths



Bond angles

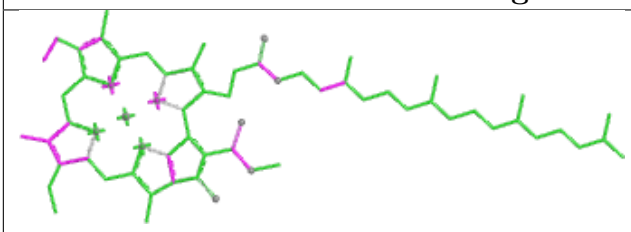


Torsions

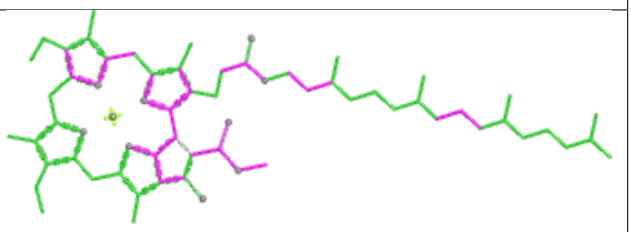


Rings

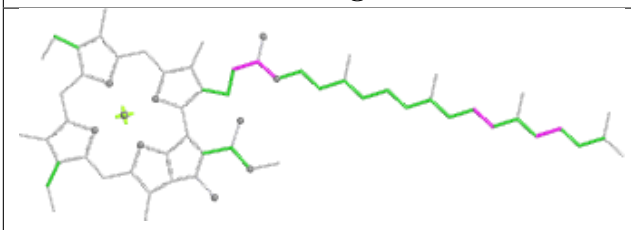
Ligand CLA AC 509



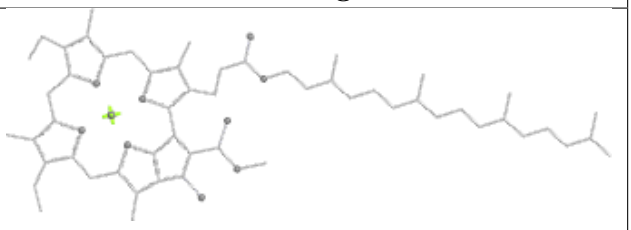
Bond lengths



Bond angles

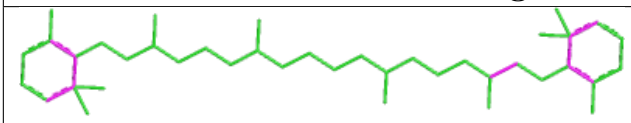


Torsions

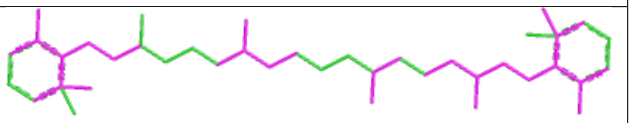


Rings

Ligand BCR AC 514



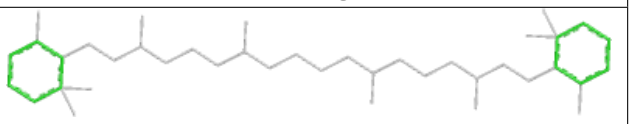
Bond lengths



Bond angles

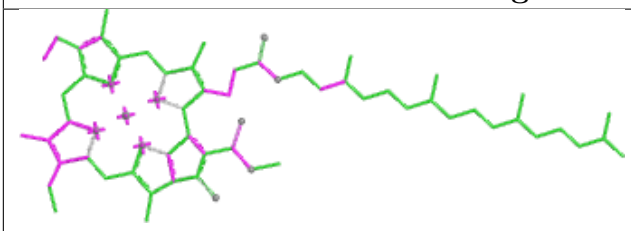


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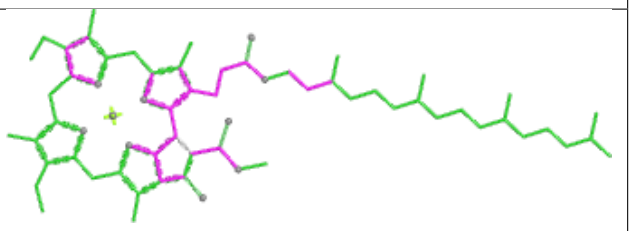


Rings

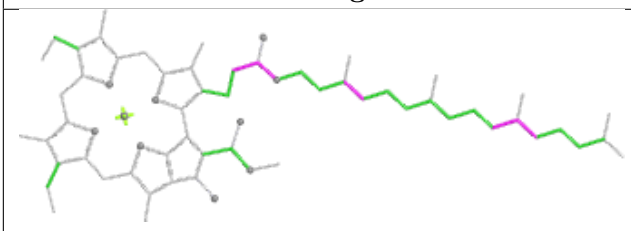
Ligand CLA AC 505



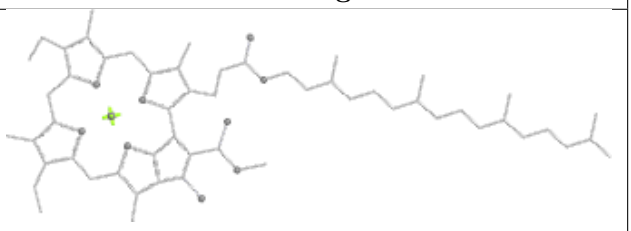
Bond lengths



Bond angles

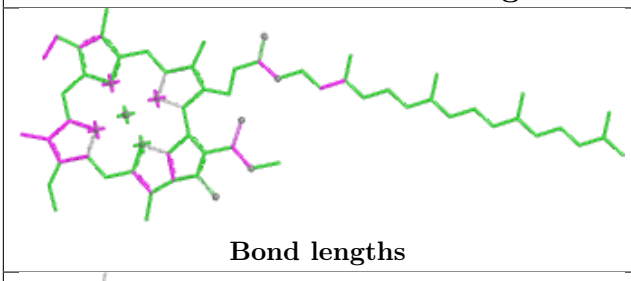


Torsions

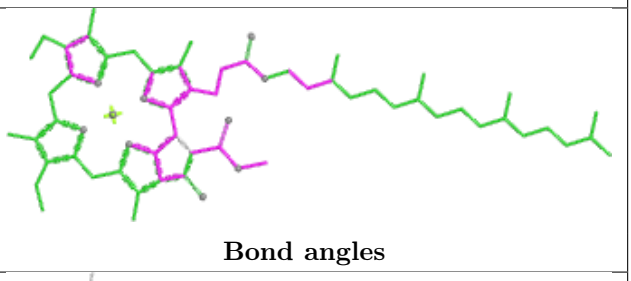


Rings

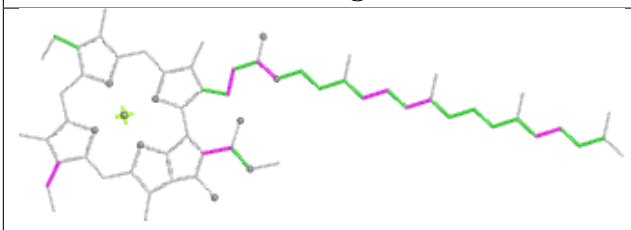
Ligand CLA BD 5405



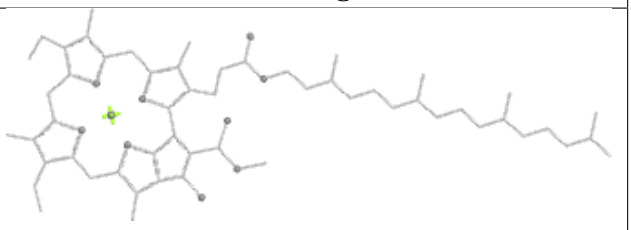
Bond lengths



Bond angles

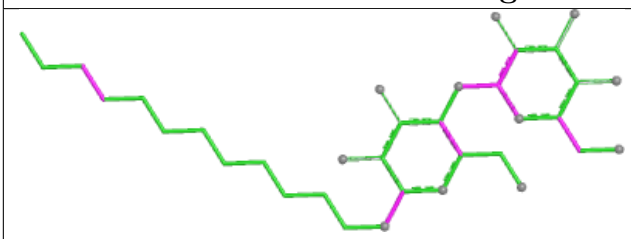


Torsions

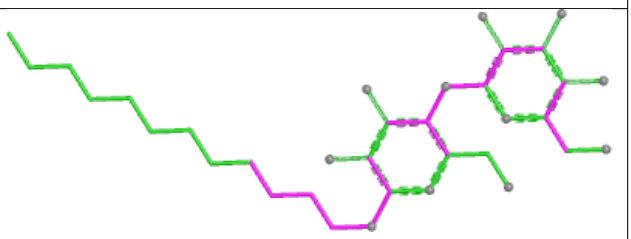


Rings

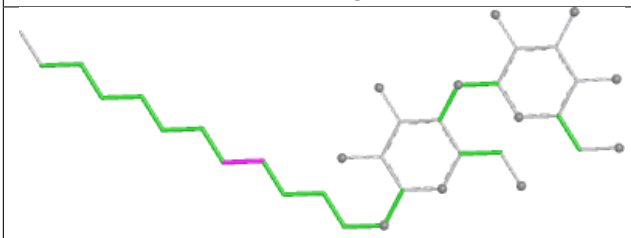
Ligand LMT BC 5522



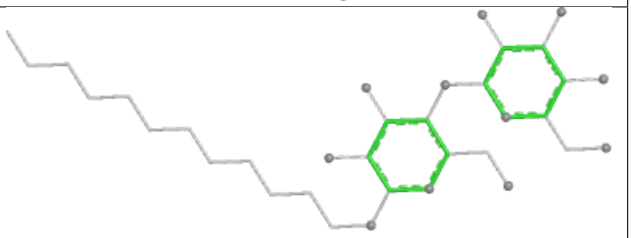
Bond lengths



Bond angles

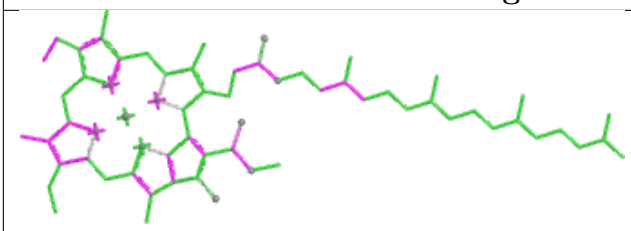


Torsions

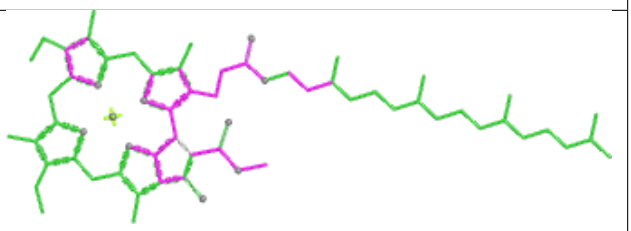


Rings

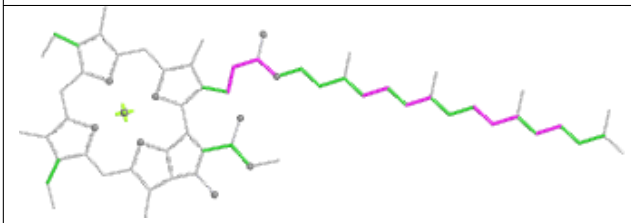
Ligand CLA BC 5501



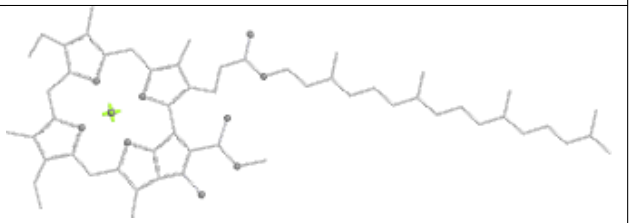
Bond lengths



Bond angles

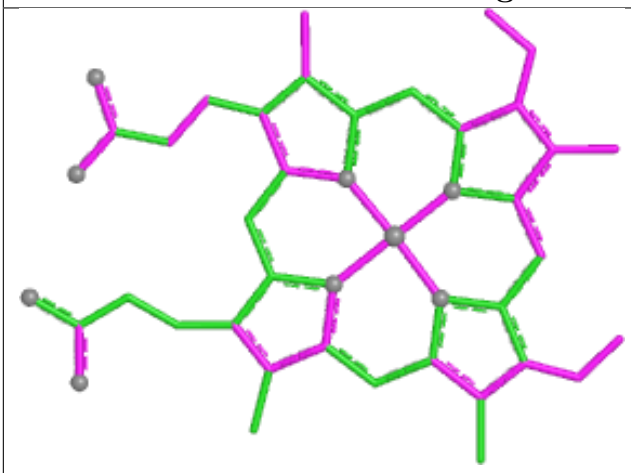


Torsions

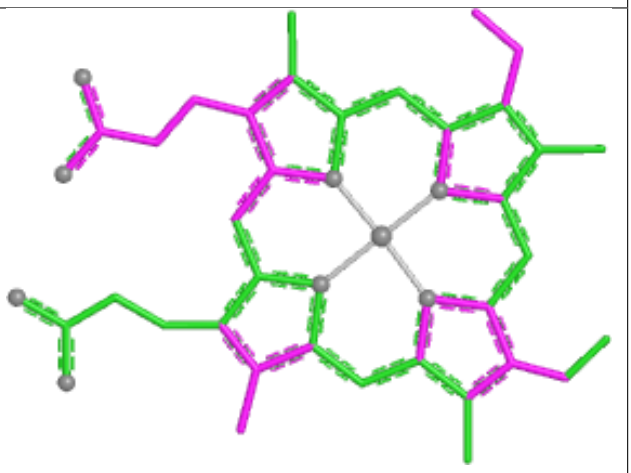


Rings

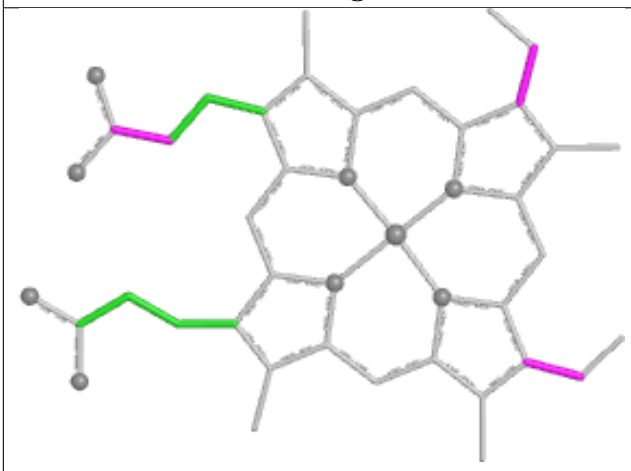
Ligand HEM BV 5201



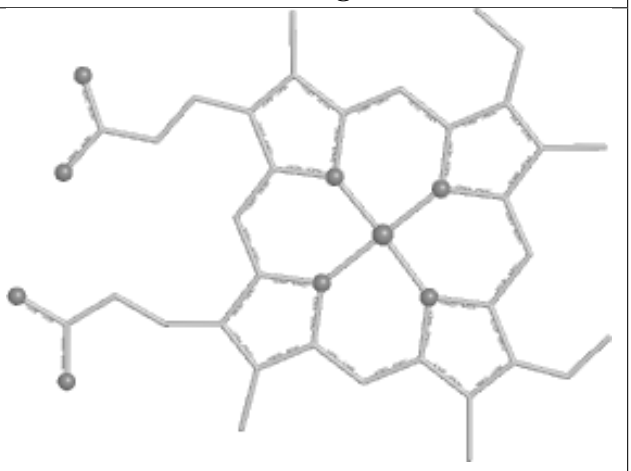
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	335/344 (97%)	-0.02	1 (0%) 90 81	82, 104, 147, 160	0
1	BA	335/344 (97%)	-0.05	0 100 100	86, 106, 148, 160	0
2	AB	490/510 (96%)	-0.18	3 (0%) 85 73	81, 103, 136, 152	0
2	BB	490/510 (96%)	-0.13	4 (0%) 82 67	81, 103, 137, 152	0
3	AC	447/461 (96%)	0.09	3 (0%) 84 69	88, 122, 148, 158	0
3	BC	447/461 (96%)	0.06	4 (0%) 81 64	91, 124, 149, 159	0
4	AD	341/352 (96%)	-0.07	2 (0%) 85 73	81, 105, 139, 153	0
4	BD	341/352 (96%)	-0.15	5 (1%) 72 52	84, 106, 140, 154	0
5	AE	82/84 (97%)	0.15	3 (3%) 45 28	104, 126, 151, 155	0
5	BE	82/84 (97%)	-0.09	0 100 100	106, 127, 152, 156	0
6	AF	35/45 (77%)	0.04	0 100 100	107, 122, 157, 160	0
6	BF	35/45 (77%)	0.16	0 100 100	110, 123, 157, 160	0
7	AH	65/66 (98%)	0.03	0 100 100	113, 124, 140, 147	0
7	BH	65/66 (98%)	-0.05	2 (3%) 51 32	114, 124, 140, 148	0
8	AI	35/38 (92%)	0.10	1 (2%) 53 35	108, 115, 141, 147	0
8	BI	35/38 (92%)	0.09	0 100 100	108, 116, 142, 147	0
9	AJ	38/40 (95%)	0.04	2 (5%) 32 20	109, 122, 157, 159	0
9	BJ	38/40 (95%)	-0.10	0 100 100	111, 125, 158, 159	0
10	AK	37/37 (100%)	-0.17	0 100 100	121, 135, 145, 147	0
10	BK	37/37 (100%)	-0.11	0 100 100	123, 136, 147, 148	0
11	AL	37/37 (100%)	-0.15	0 100 100	88, 104, 159, 160	0
11	BL	37/37 (100%)	0.02	2 (5%) 31 20	90, 104, 158, 160	0
12	AM	34/36 (94%)	-0.36	0 100 100	89, 99, 142, 153	0
12	BM	34/36 (94%)	-0.34	0 100 100	90, 99, 140, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AO	243/247 (98%)	0.04	0 100 100	83, 116, 148, 160	0
13	BO	243/247 (98%)	-0.11	3 (1%) 76 58	85, 117, 147, 160	0
14	AT	32/32 (100%)	-0.09	0 100 100	92, 106, 158, 160	0
14	BT	32/32 (100%)	-0.27	0 100 100	93, 106, 158, 160	0
15	AU	97/104 (93%)	-0.24	0 100 100	93, 105, 116, 125	0
15	BU	97/104 (93%)	-0.29	0 100 100	94, 106, 116, 127	0
16	AV	137/137 (100%)	-0.02	0 100 100	96, 112, 128, 132	0
16	BV	137/137 (100%)	-0.24	0 100 100	99, 114, 130, 134	0
17	Ay	28/46 (60%)	0.31	1 (3%) 46 28	141, 154, 160, 160	0
17	By	28/46 (60%)	0.33	0 100 100	143, 154, 160, 160	0
18	AX	37/41 (90%)	0.01	0 100 100	121, 129, 147, 150	0
18	BX	37/41 (90%)	-0.13	0 100 100	120, 130, 146, 149	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	-0.04	2 (3%) 50 31	134, 148, 160, 160	0
20	BZ	62/62 (100%)	0.36	1 (1%) 70 51	135, 150, 160, 160	0
All	All	5224/5494 (95%)	-0.06	39 (0%) 84 69	81, 113, 149, 160	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BH	5065	LEU	4.6
3	AC	260	ALA	4.5
2	BB	5491	VAL	3.3
9	AJ	15	THR	3.0
4	AD	241	GLU	2.9

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
31	LMG	AI	101	43/55	0.35	0.18	159,160,160,160	0
28	DGD	BE	5102	63/66	0.44	0.18	145,160,160,160	0
28	DGD	AE	101	63/66	0.47	0.19	146,160,160,160	0
29	LHG	BA	5415	37/49	0.48	0.17	151,160,160,160	0
31	LMG	BI	5101	43/55	0.49	0.13	160,160,160,160	0
28	DGD	AA	411	56/66	0.52	0.18	148,158,160,160	0
28	DGD	BA	5412	56/66	0.52	0.15	150,160,160,160	0
28	DGD	BB	5602	52/66	0.53	0.16	152,160,160,160	0
32	LMT	AB	623	35/35	0.53	0.15	135,160,160,160	0
28	DGD	AB	628	52/66	0.55	0.15	154,160,160,160	0
32	LMT	BI	5102	35/35	0.55	0.16	151,160,160,160	0
32	LMT	BB	5626	35/35	0.57	0.20	131,160,160,160	0
31	LMG	AA	414	44/55	0.57	0.15	140,160,160,160	0
30	SQD	BA	5401	54/54	0.58	0.14	136,160,160,160	0
31	LMG	BC	5521	45/55	0.60	0.13	154,160,160,160	0
27	BCR	BJ	5101	40/40	0.62	0.15	160,160,160,160	0
32	LMT	BB	5604	35/35	0.62	0.15	131,160,160,160	0
31	LMG	AC	520	48/55	0.63	0.17	136,157,160,160	0
31	LMG	BE	5101	44/55	0.64	0.16	140,160,160,160	0
32	LMT	BC	5522	35/35	0.64	0.11	157,160,160,160	0
30	SQD	BB	5625	43/54	0.64	0.13	132,148,160,160	0
37	CA	AF	103	1/1	0.64	0.08	150,150,150,150	0
32	LMT	AI	103	35/35	0.67	0.17	156,158,160,160	0
30	SQD	AB	622	43/54	0.68	0.13	133,149,160,160	0
30	SQD	BF	5102	45/54	0.68	0.13	154,160,160,160	0
30	SQD	AF	102	45/54	0.68	0.15	154,160,160,160	0
24	CLA	AB	601	65/65	0.68	0.17	146,159,160,160	0
31	LMG	AC	521	45/55	0.68	0.14	154,160,160,160	0
32	LMT	AB	624	35/35	0.68	0.14	156,160,160,160	0
32	LMT	AB	630	35/35	0.69	0.14	132,160,160,160	0
32	LMT	AI	102	35/35	0.69	0.14	149,158,160,160	0
32	LMT	BD	5411	31/35	0.69	0.16	140,152,160,160	0
31	LMG	BC	5520	48/55	0.69	0.15	138,159,160,160	0
30	SQD	BA	5414	51/54	0.69	0.14	145,150,160,160	0
28	DGD	BC	5518	62/66	0.70	0.17	147,156,160,160	0
27	BCR	AJ	101	40/40	0.70	0.20	158,160,160,160	0
32	LMT	BB	5603	35/35	0.70	0.17	132,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	CA	AO	301	1/1	0.70	0.07	152,152,152,152	0
31	LMG	BA	5402	42/55	0.71	0.20	144,157,160,160	0
31	LMG	AB	620	51/55	0.71	0.20	125,139,150,151	0
23	CL	AA	403[B]	1/1	0.72	0.33	108,108,108,108	1
32	LMT	AD	409	31/35	0.72	0.13	139,154,160,160	0
29	LHG	AA	415	37/49	0.72	0.14	149,160,160,160	0
23	CL	AA	403[A]	1/1	0.72	0.33	33,33,33,33	1
31	LMG	BL	5101	51/55	0.73	0.18	122,138,151,152	0
33	DMS	AV	202	4/4	0.73	0.22	148,148,148,149	0
28	DGD	BC	5519	66/66	0.74	0.16	112,121,158,159	0
24	CLA	BB	5605	65/65	0.74	0.20	146,159,160,160	0
32	LMT	AB	629	35/35	0.74	0.17	133,160,160,160	0
31	LMG	BD	5410	48/55	0.74	0.20	126,131,141,141	0
28	DGD	AC	518	62/66	0.75	0.16	146,155,160,160	0
28	DGD	AC	519	66/66	0.75	0.16	110,120,157,158	0
31	LMG	BD	5408	46/55	0.76	0.17	139,145,160,160	0
30	SQD	BB	5601	47/54	0.76	0.14	137,156,160,160	0
33	DMS	AU	201	4/4	0.76	0.23	160,160,160,160	0
30	SQD	AA	416	54/54	0.76	0.12	136,160,160,160	0
32	LMT	BB	5627	35/35	0.76	0.12	156,160,160,160	0
31	LMG	AM	101	42/55	0.76	0.17	136,158,160,160	0
31	LMG	AA	417	42/55	0.77	0.20	145,157,160,160	0
31	LMG	AB	621	49/55	0.77	0.17	145,150,157,160	0
24	CLA	BC	5513	65/65	0.78	0.14	158,160,160,160	0
33	DMS	BB	5629	4/4	0.78	0.18	125,126,127,127	0
31	LMG	AD	408	48/55	0.78	0.18	121,130,139,139	0
31	LMG	BM	5102	42/55	0.78	0.18	136,160,160,160	0
30	SQD	AA	413	51/54	0.79	0.12	143,150,160,160	0
32	LMT	AM	102	35/35	0.79	0.11	126,149,154,154	0
32	LMT	BM	5101	35/35	0.80	0.13	126,149,154,155	0
30	SQD	AB	627	47/54	0.80	0.12	138,157,160,160	0
27	BCR	BC	5516	40/40	0.80	0.14	136,140,145,145	0
27	BCR	BK	5102	40/40	0.81	0.16	136,140,152,152	0
24	CLA	AC	506	65/65	0.81	0.15	136,143,160,160	0
31	LMG	BB	5624	49/55	0.82	0.15	145,150,157,160	0
24	CLA	BC	5512	65/65	0.82	0.13	157,160,160,160	0
31	LMG	AJ	102	46/55	0.82	0.18	139,144,160,160	0
37	CA	BO	5301	1/1	0.82	0.10	160,160,160,160	0
24	CLA	BC	5511	65/65	0.83	0.16	154,158,159,160	0
33	DMS	BB	5628	4/4	0.83	0.14	156,157,157,157	0
27	BCR	AX	101	40/40	0.83	0.15	135,143,158,159	0
28	DGD	BC	5517	53/66	0.83	0.15	124,130,136,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	BCR	BT	5101	40/40	0.83	0.14	124,143,147,147	0
26	OEC	BA	5410	5/9	0.83	0.10	23,88,99,134	0
24	CLA	BD	5405	65/65	0.84	0.15	125,131,148,149	0
28	DGD	BH	5101	58/66	0.84	0.15	107,118,156,160	0
27	BCR	AC	515	40/40	0.84	0.14	149,152,155,155	0
28	DGD	AC	517	53/66	0.85	0.20	121,128,135,140	0
22	BCT	AA	402	4/4	0.85	0.10	135,136,137,137	0
27	BCR	BC	5515	40/40	0.85	0.13	150,152,155,156	0
24	CLA	BC	5505	65/65	0.85	0.14	123,148,152,153	0
31	LMG	AD	407	49/55	0.85	0.14	126,133,143,145	0
24	CLA	AD	404	65/65	0.85	0.14	126,130,148,149	0
27	BCR	AT	101	40/40	0.86	0.15	126,140,146,147	0
31	LMG	BD	5409	49/55	0.86	0.15	128,133,144,146	0
27	BCR	BX	5101	40/40	0.86	0.14	136,143,157,158	0
33	DMS	AB	625	4/4	0.86	0.14	156,157,157,157	0
33	DMS	AB	626	4/4	0.86	0.15	129,130,130,130	0
37	CA	BF	5103	1/1	0.86	0.07	146,146,146,146	0
24	CLA	BC	5503	65/65	0.86	0.15	137,147,148,152	0
27	BCR	BD	5407	40/40	0.87	0.12	112,127,132,132	0
24	CLA	BC	5504	65/65	0.87	0.12	132,135,160,160	0
24	CLA	AC	513	65/65	0.87	0.14	158,160,160,160	0
29	LHG	BA	5413	39/49	0.87	0.11	113,122,128,129	0
24	CLA	BC	5506	65/65	0.87	0.13	136,143,160,160	0
24	CLA	AB	608	65/65	0.87	0.15	123,127,135,140	0
24	CLA	AB	616	65/65	0.87	0.12	143,147,160,160	0
24	CLA	BB	5618	65/65	0.87	0.13	128,133,160,160	0
37	CA	BK	5101	1/1	0.87	0.09	145,145,145,145	0
24	CLA	AB	606	65/65	0.87	0.16	120,133,140,141	0
29	LHG	AA	412	39/49	0.88	0.13	110,118,128,132	0
28	DGD	AH	101	58/66	0.88	0.14	108,120,155,157	0
24	CLA	BA	5407	65/65	0.88	0.12	110,114,138,139	0
27	BCR	AB	617	40/40	0.88	0.10	112,121,125,125	0
27	BCR	AB	618	40/40	0.88	0.11	109,117,122,122	0
22	BCT	BA	5403	4/4	0.88	0.10	135,136,136,137	0
27	BCR	AD	406	40/40	0.88	0.13	110,126,131,131	0
24	CLA	AC	512	65/65	0.88	0.15	154,158,160,160	0
24	CLA	BB	5620	65/65	0.88	0.13	143,147,160,160	0
27	BCR	AB	619	40/40	0.89	0.12	111,117,131,131	0
24	CLA	AB	609	65/65	0.89	0.14	126,136,141,143	0
24	CLA	BB	5610	65/65	0.89	0.14	121,132,140,141	0
24	CLA	AA	407	65/65	0.89	0.12	93,101,150,151	0
24	CLA	AC	505	65/65	0.89	0.16	121,146,150,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	AA	406	65/65	0.89	0.15	105,112,138,139	0
27	BCR	BC	5514	40/40	0.89	0.12	123,126,129,129	0
24	CLA	BC	5501	65/65	0.90	0.13	134,137,141,144	0
27	BCR	AK	102	40/40	0.90	0.16	133,139,151,152	0
24	CLA	BB	5607	65/65	0.90	0.11	108,111,120,123	0
25	MST	BA	5409	16/16	0.90	0.12	124,129,131,132	0
27	BCR	BA	5411	40/40	0.90	0.12	94,122,132,132	0
27	BCR	BB	5623	40/40	0.90	0.14	111,116,131,131	0
24	CLA	AB	603	65/65	0.90	0.14	107,109,119,121	0
24	CLA	BB	5612	65/65	0.90	0.12	122,127,136,139	0
35	PL9	BD	5406	55/55	0.90	0.14	103,110,115,116	0
24	CLA	BB	5613	65/65	0.90	0.13	127,135,140,142	0
37	CA	AK	101	1/1	0.90	0.07	146,146,146,146	0
24	CLA	BC	5510	65/65	0.90	0.11	113,116,130,131	0
24	CLA	AC	504	65/65	0.90	0.14	129,134,160,160	0
27	BCR	AC	516	40/40	0.90	0.15	135,138,143,143	0
24	CLA	AB	614	65/65	0.90	0.13	129,133,160,160	0
24	CLA	AB	615	65/65	0.91	0.12	134,139,155,157	0
24	CLA	BC	5502	65/65	0.91	0.11	108,111,143,144	0
27	BCR	BB	5621	40/40	0.91	0.10	112,120,124,125	0
24	CLA	BC	5507	65/65	0.91	0.12	136,150,153,154	0
33	DMS	BV	5202	4/4	0.91	0.14	148,149,149,150	0
24	CLA	BC	5508	65/65	0.91	0.12	142,146,157,159	0
24	CLA	BB	5611	65/65	0.92	0.10	95,102,132,136	0
24	CLA	BC	5509	65/65	0.92	0.12	116,128,138,138	0
24	CLA	AB	611	65/65	0.92	0.12	99,113,116,122	0
24	CLA	AB	613	65/65	0.92	0.10	99,102,136,140	0
24	CLA	BB	5617	65/65	0.92	0.10	98,102,138,141	0
24	CLA	AB	604	65/65	0.92	0.10	96,104,125,127	0
27	BCR	BB	5622	40/40	0.92	0.10	110,117,120,121	0
24	CLA	BB	5619	65/65	0.92	0.12	135,137,155,157	0
24	CLA	BA	5406	65/65	0.92	0.11	89,94,108,112	0
33	DMS	BV	5203	4/4	0.92	0.16	160,160,160,160	0
34	PHO	BD	5404	64/64	0.92	0.13	123,125,129,130	0
24	CLA	AB	607	65/65	0.92	0.11	94,100,132,135	0
24	CLA	BA	5408	65/65	0.92	0.11	95,103,150,150	0
24	CLA	AC	507	65/65	0.92	0.14	137,149,152,153	0
24	CLA	BB	5606	65/65	0.92	0.13	124,127,130,131	0
24	CLA	AC	508	65/65	0.92	0.13	140,144,157,158	0
24	CLA	BB	5609	65/65	0.92	0.14	103,110,124,124	0
24	CLA	AC	510	65/65	0.92	0.11	110,113,129,130	0
24	CLA	AC	501	65/65	0.93	0.13	133,136,139,143	0

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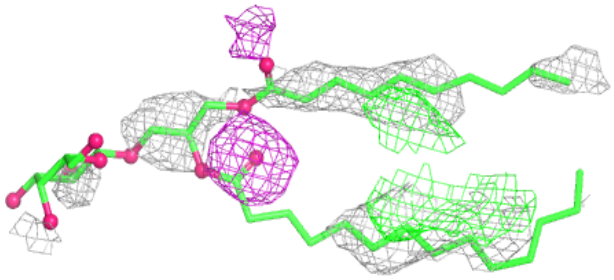
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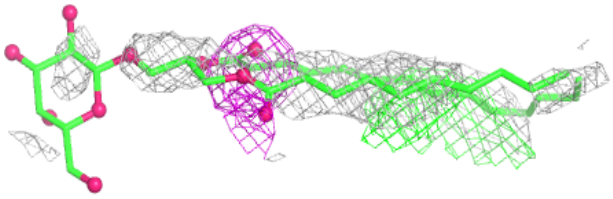
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	AC	503	65/65	0.93	0.16	137,144,147,152	0
34	PHO	AD	403	64/64	0.93	0.14	119,123,128,129	0
34	PHO	BD	5403	64/64	0.93	0.12	102,109,118,118	0
24	CLA	AA	405	65/65	0.93	0.11	88,93,108,111	0
35	PL9	AD	405	55/55	0.93	0.16	99,109,113,113	0
26	OEC	AA	409	5/9	0.93	0.10	82,83,90,110	0
36	HEM	AF	101	43/43	0.93	0.19	148,152,159,160	0
36	HEM	BF	5101	43/43	0.93	0.18	148,152,160,160	0
24	CLA	AC	511	65/65	0.93	0.16	152,155,157,158	0
27	BCR	AA	410	40/40	0.93	0.11	91,122,130,130	0
24	CLA	AB	602	65/65	0.93	0.12	124,127,129,132	0
24	CLA	AB	605	65/65	0.93	0.12	105,113,122,124	0
24	CLA	BB	5614	65/65	0.93	0.13	117,123,124,128	0
24	CLA	BB	5615	65/65	0.93	0.10	101,113,117,120	0
24	CLA	AD	401	65/65	0.94	0.13	93,100,115,119	0
24	CLA	AA	404	65/65	0.94	0.12	89,99,106,108	0
24	CLA	BA	5405	65/65	0.94	0.11	90,101,105,109	0
24	CLA	BD	5402	65/65	0.94	0.13	97,101,117,119	0
27	BCR	AC	514	40/40	0.94	0.12	120,123,127,128	0
24	CLA	AC	509	65/65	0.94	0.12	115,128,135,137	0
25	MST	AA	408	16/16	0.94	0.13	123,126,129,130	0
24	CLA	BB	5608	65/65	0.94	0.10	96,103,124,125	0
34	PHO	AD	402	64/64	0.94	0.12	99,109,116,117	0
24	CLA	AB	612	65/65	0.94	0.12	107,111,120,121	0
24	CLA	BB	5616	65/65	0.94	0.14	108,110,120,122	0
23	CL	BA	5404[A]	1/1	0.95	0.60	29,29,29,29	1
24	CLA	AB	610	65/65	0.95	0.12	117,121,123,127	0
23	CL	BA	5404[B]	1/1	0.95	0.60	115,115,115,115	1
24	CLA	AC	502	65/65	0.95	0.11	103,109,142,143	0
36	HEM	BV	5201	43/43	0.96	0.12	97,102,106,109	0
36	HEM	AV	201	43/43	0.98	0.13	94,100,102,103	0
21	FE2	AA	401	1/1	0.99	0.06	115,115,115,115	0
21	FE2	BD	5401	1/1	0.99	0.03	119,119,119,119	0

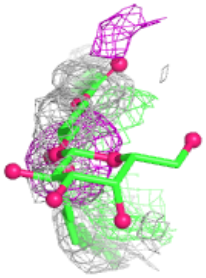
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMG AI 101:

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

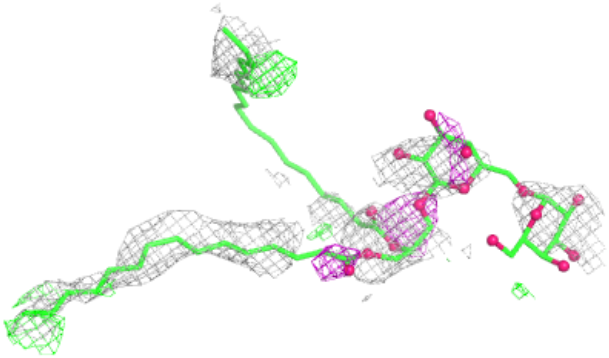


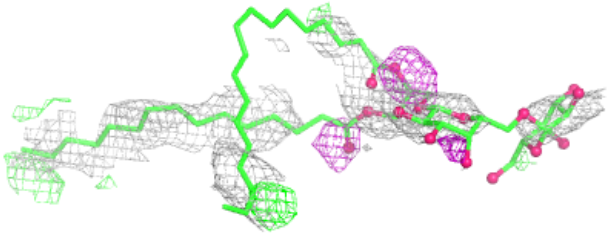


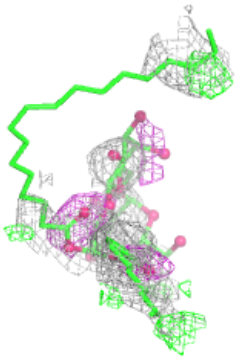


Electron density around DGD BE 5102:

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

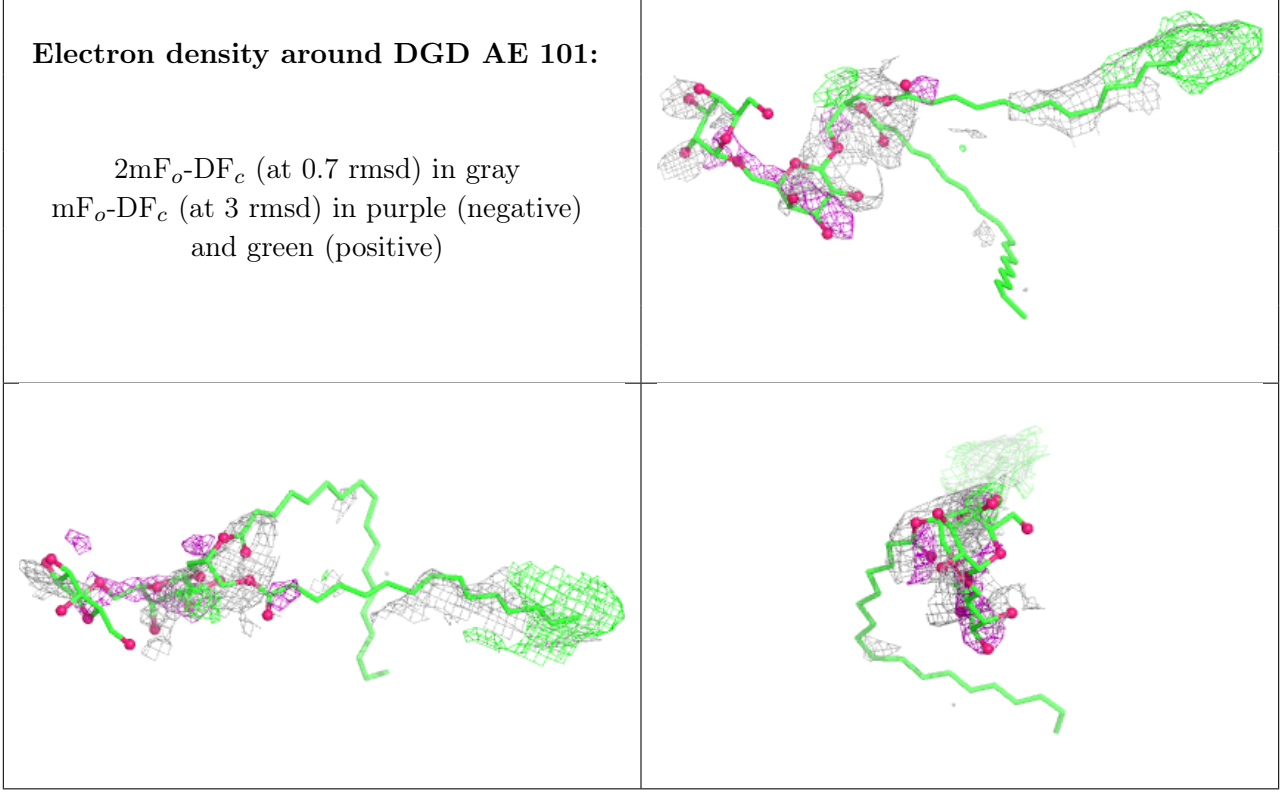






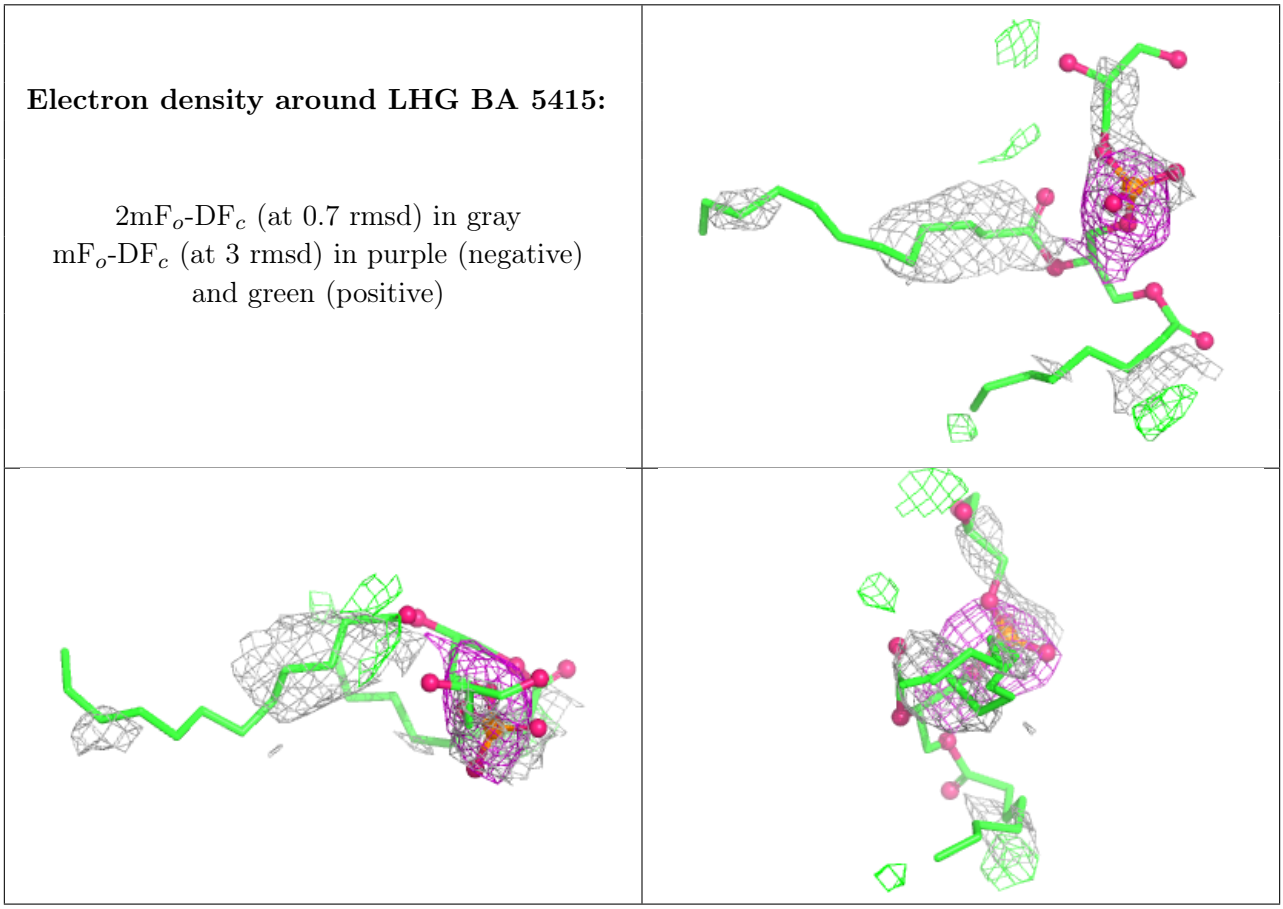
Electron density around DGD AE 101:

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



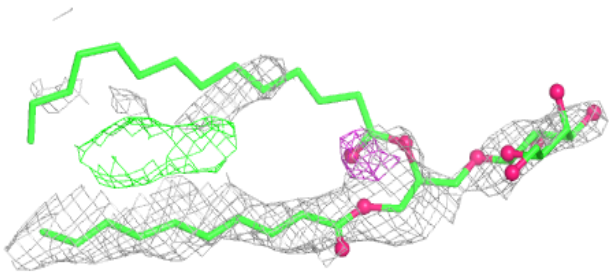
Electron density around LHG BA 5415:

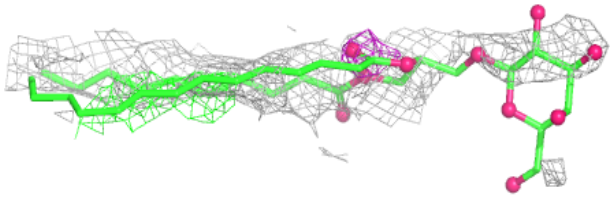
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

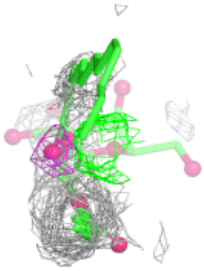


Electron density around LMG BI 5101:

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

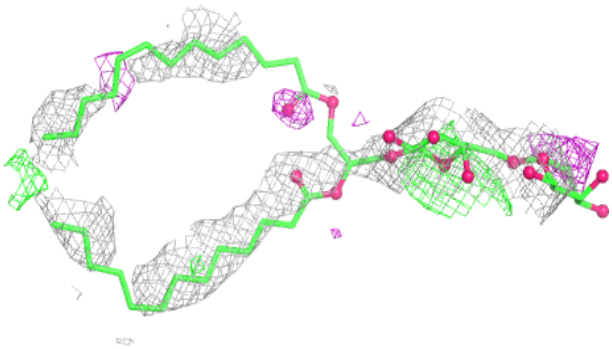


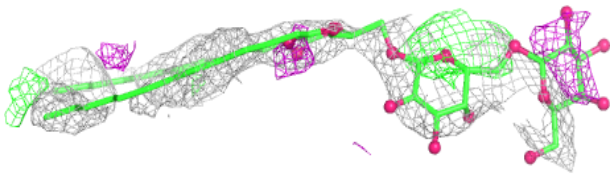


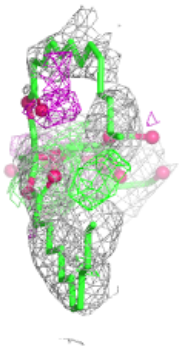


Electron density around DGD AA 411:

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

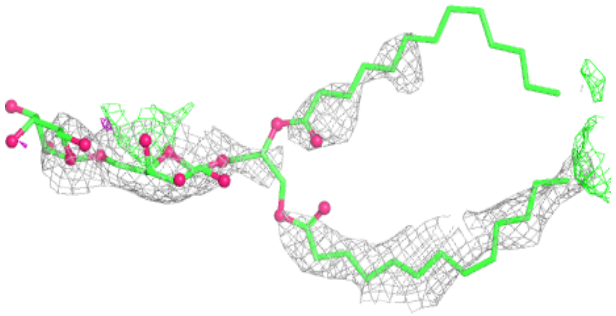


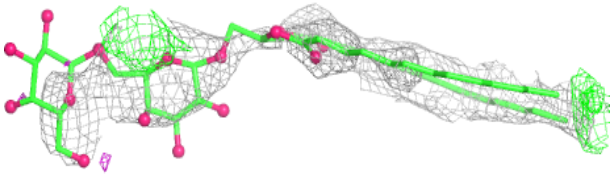


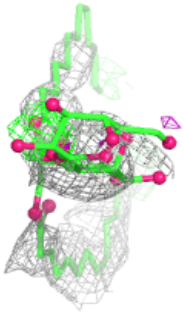


Electron density around DGD BA 5412:

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

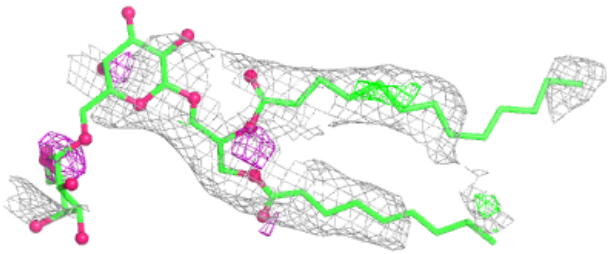


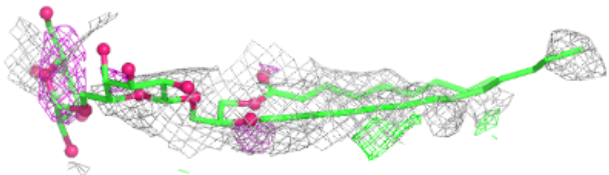




Electron density around DGD BB 5602:

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

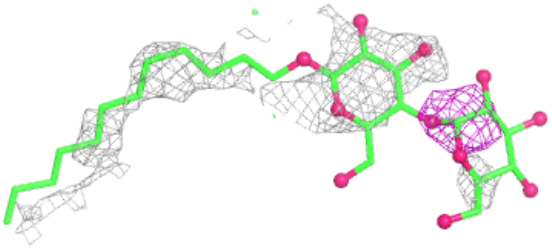


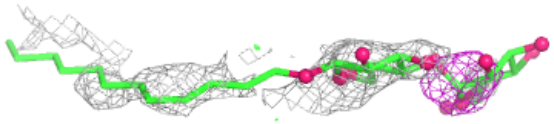


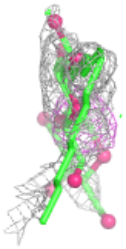


Electron density around LMT AB 623:

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

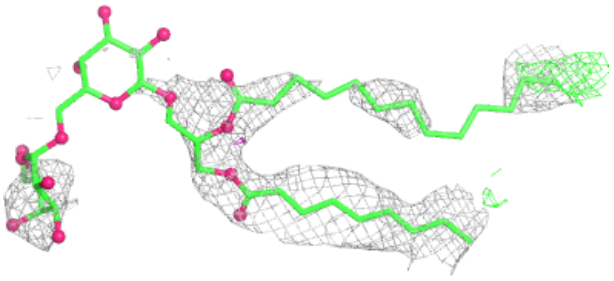


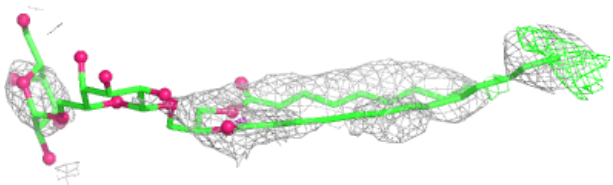


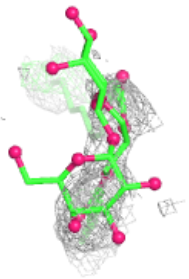


Electron density around DGD AB 628:

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

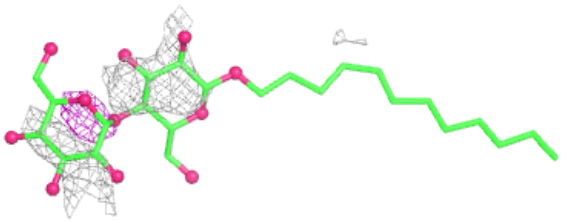






Electron density around LMT BI 5102:

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

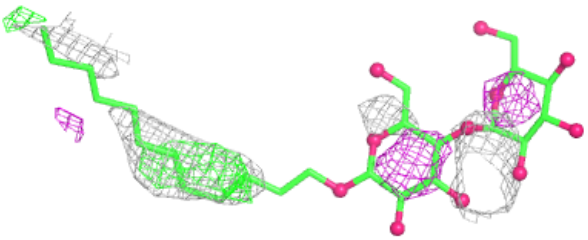


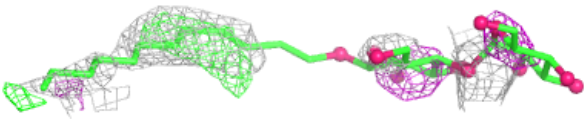


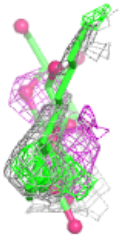


Electron density around LMT BB 5626:

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

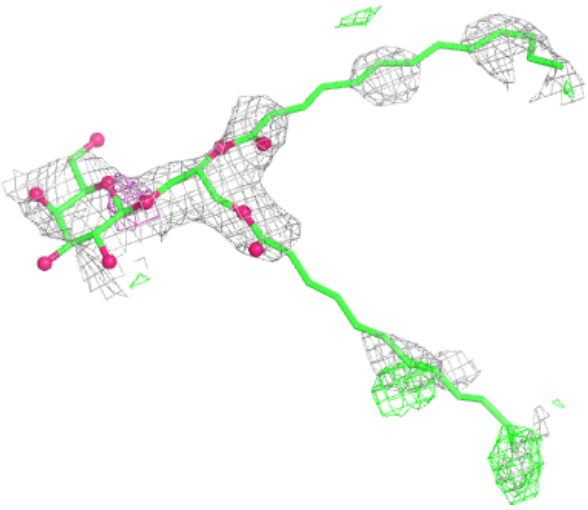


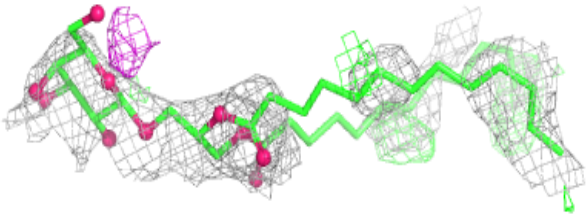


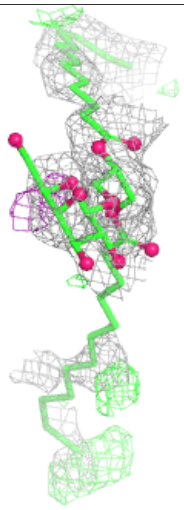


Electron density around LMG AA 414:

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

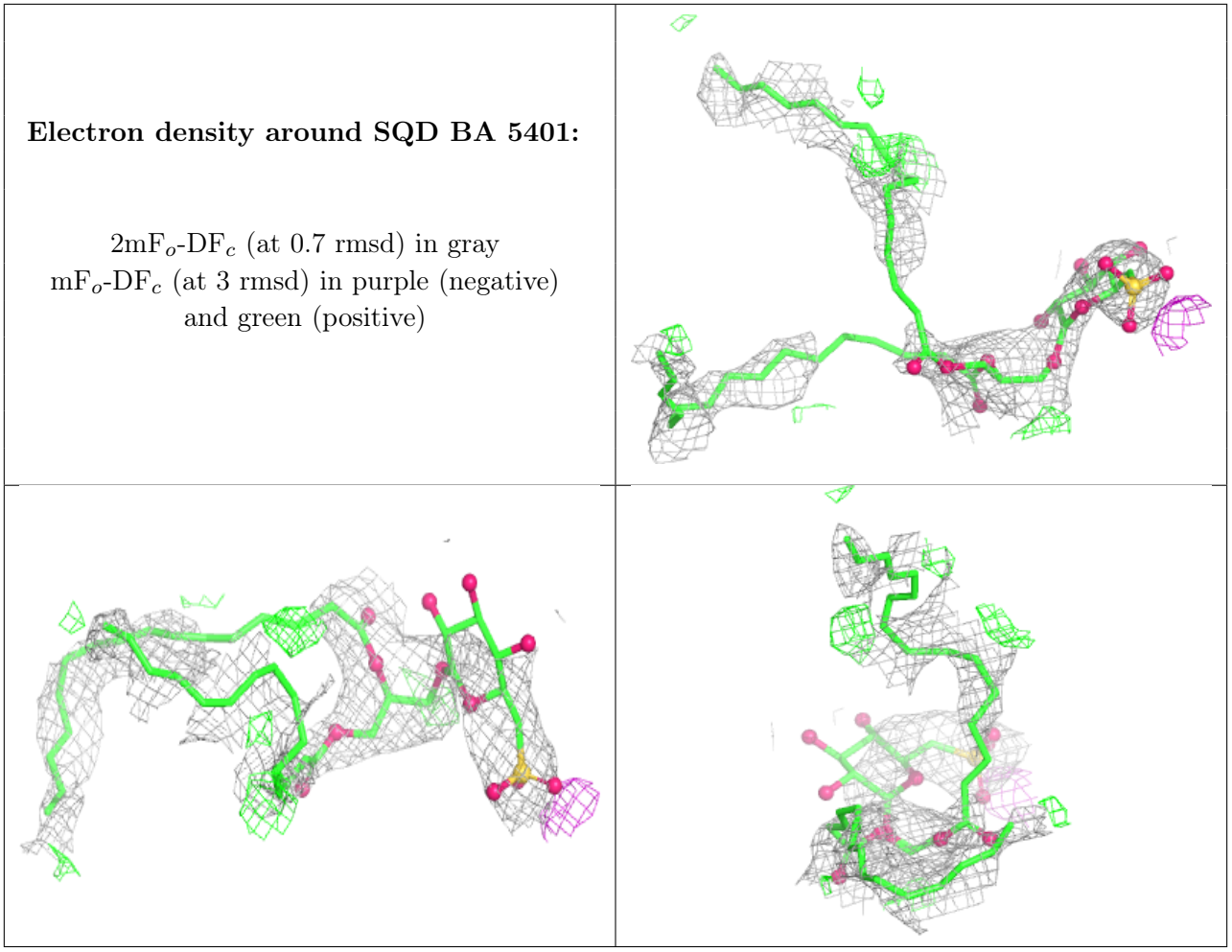






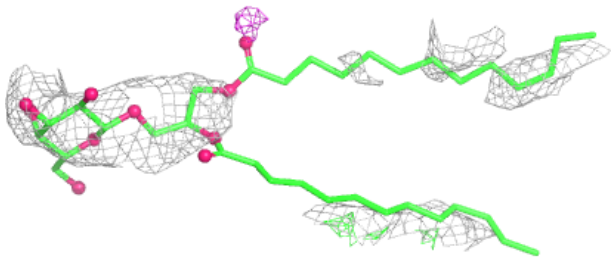
Electron density around SQD BA 5401:

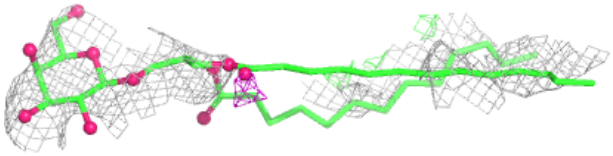
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

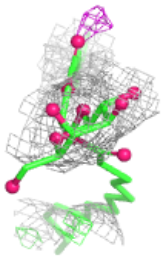


Electron density around LMG BC 5521:

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

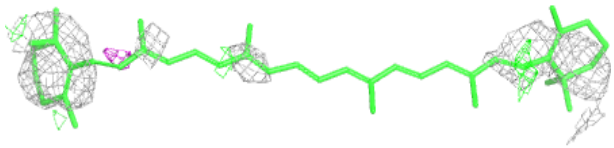


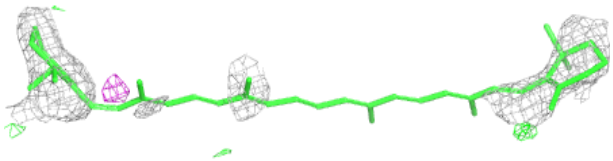


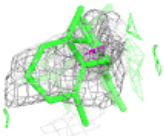


Electron density around BCR BJ 5101:

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

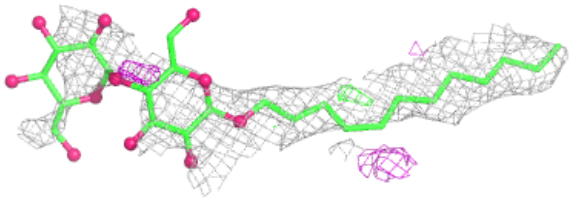


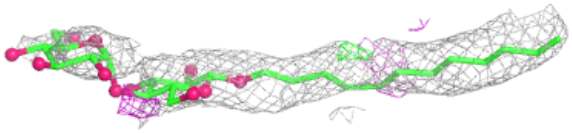




Electron density around LMT BB 5604:

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

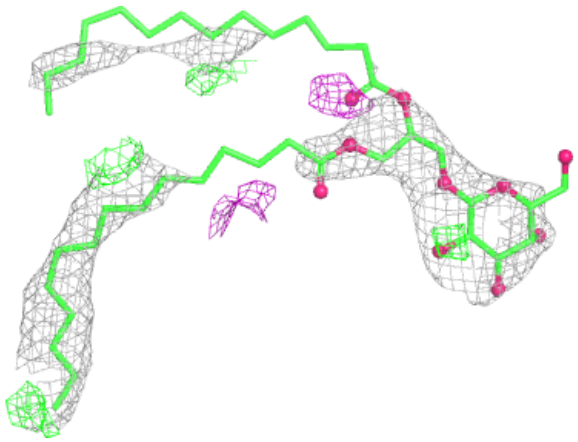


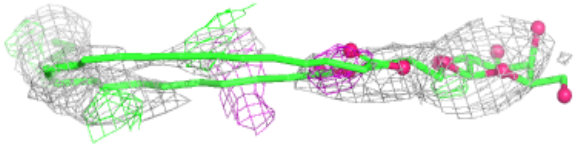


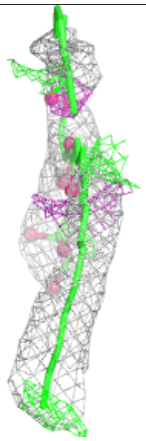


Electron density around LMG AC 520:

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

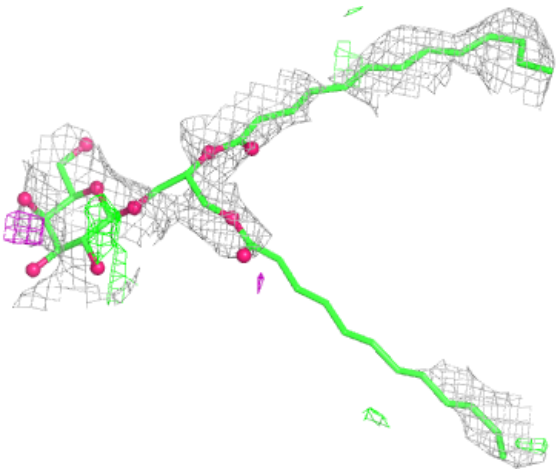


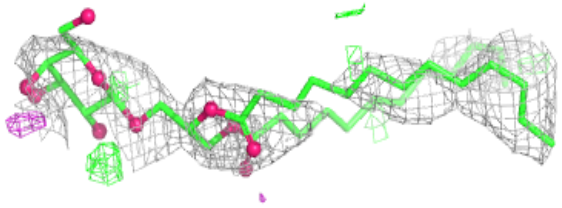


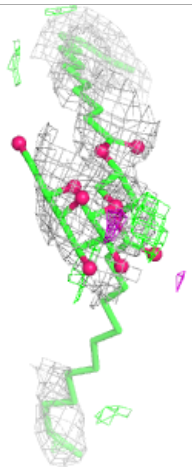


Electron density around LMG BE 5101:

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

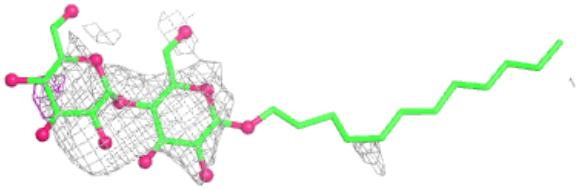


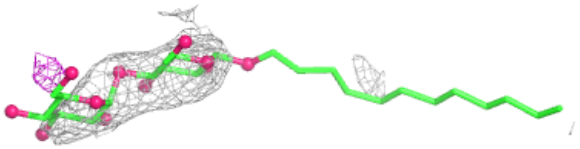


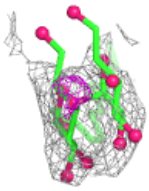


Electron density around LMT BC 5522:

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

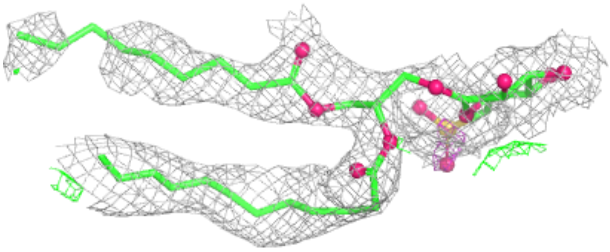


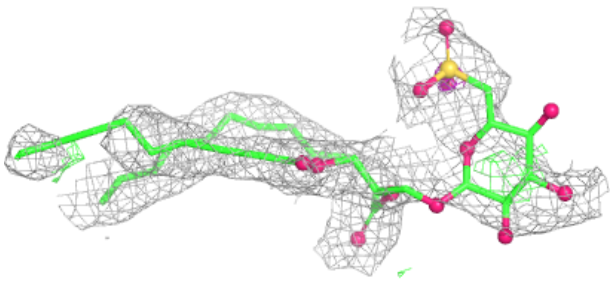


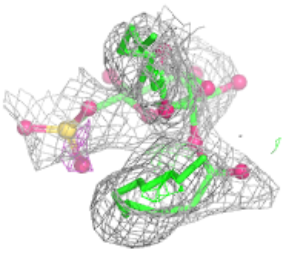


Electron density around SQD BB 5625:

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

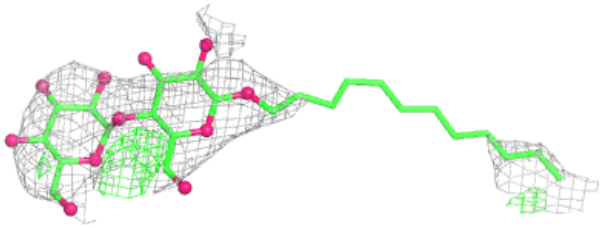


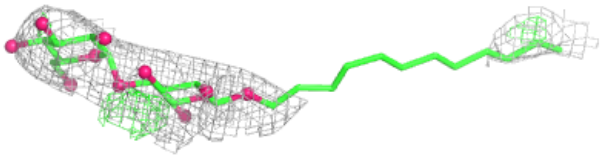


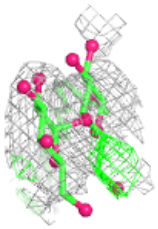


Electron density around LMT AI 103:

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

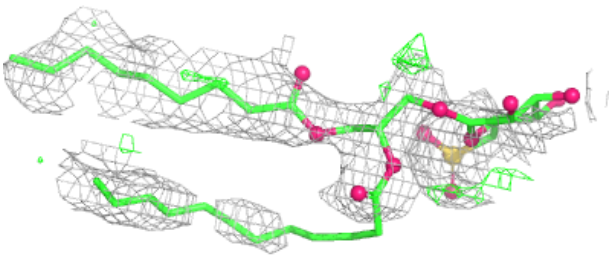


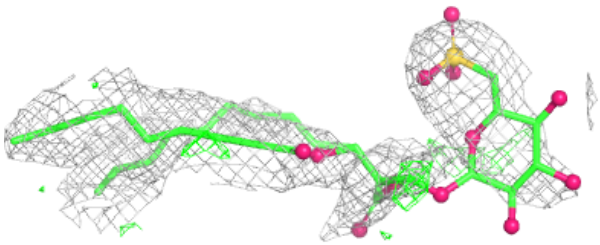


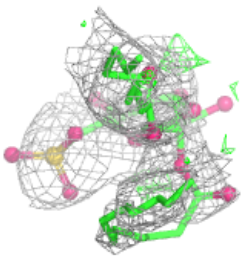


Electron density around SQD AB 622:

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

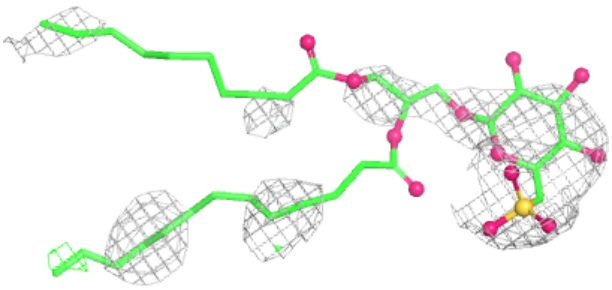


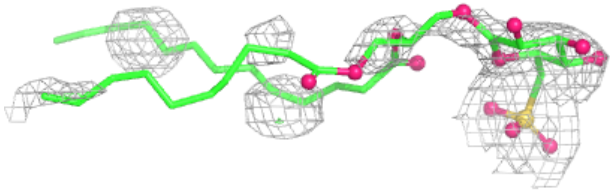


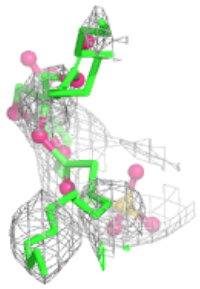


Electron density around SQD BF 5102:

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

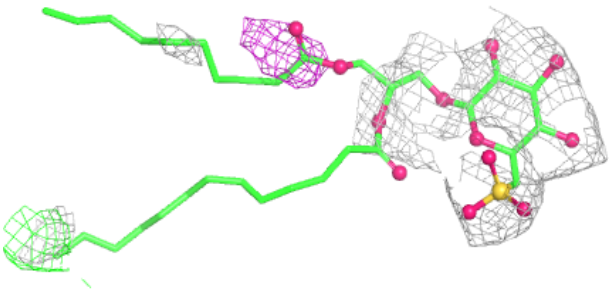


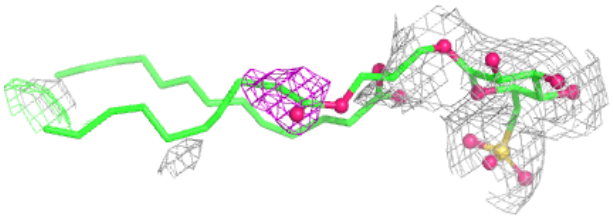


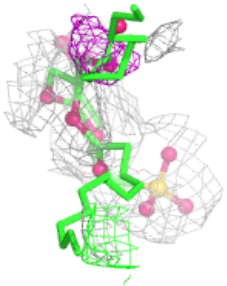


Electron density around SQD AF 102:

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

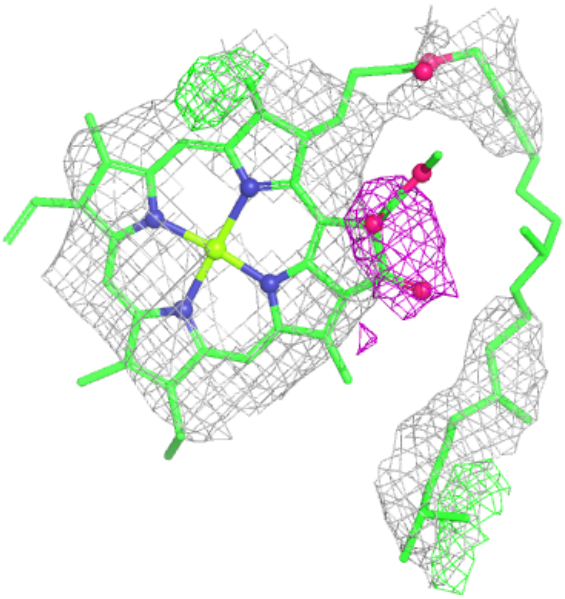


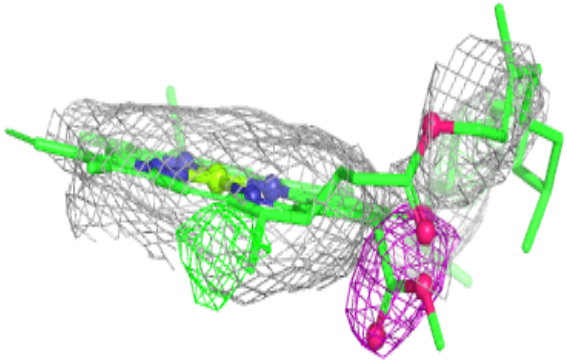


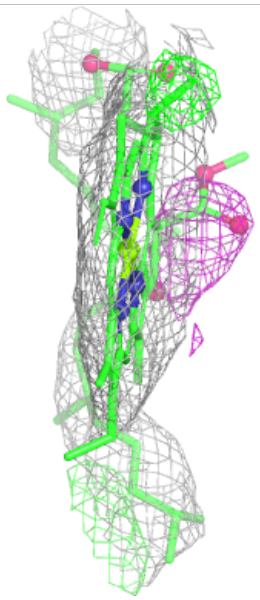


Electron density around CLA AB 601:

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

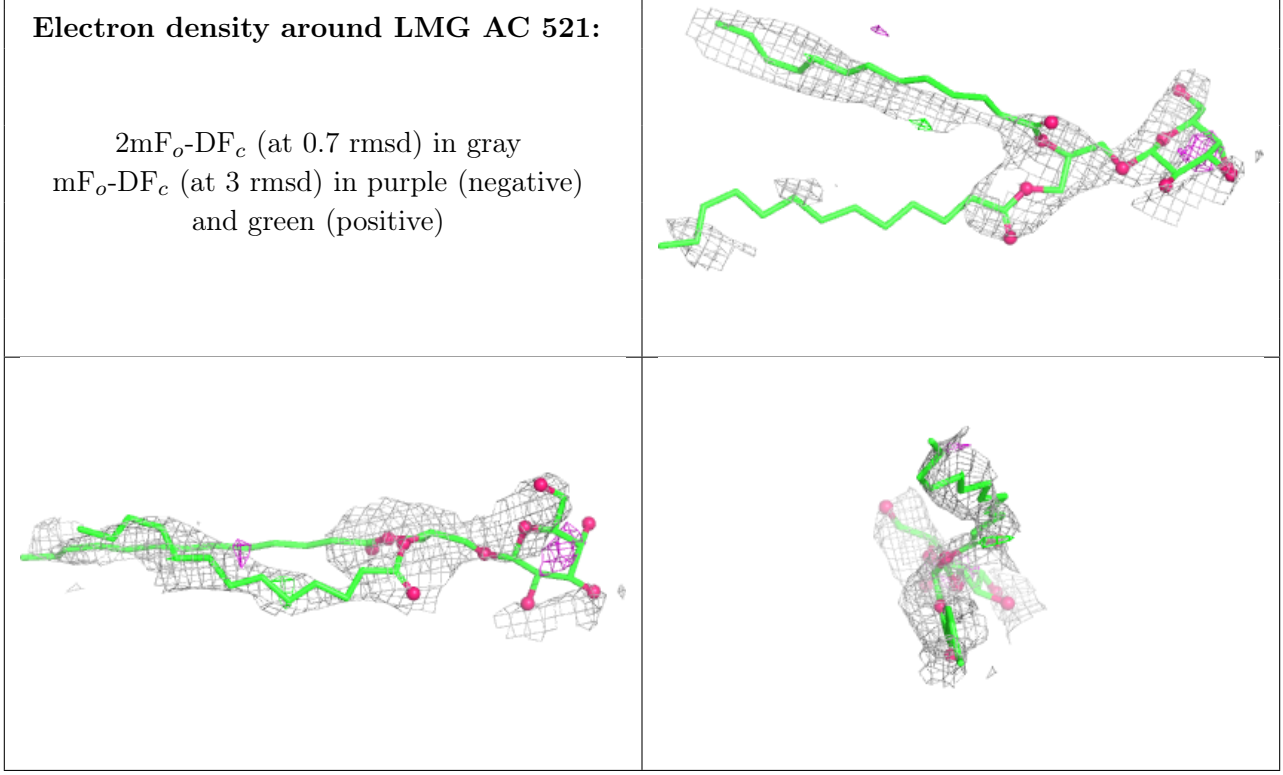






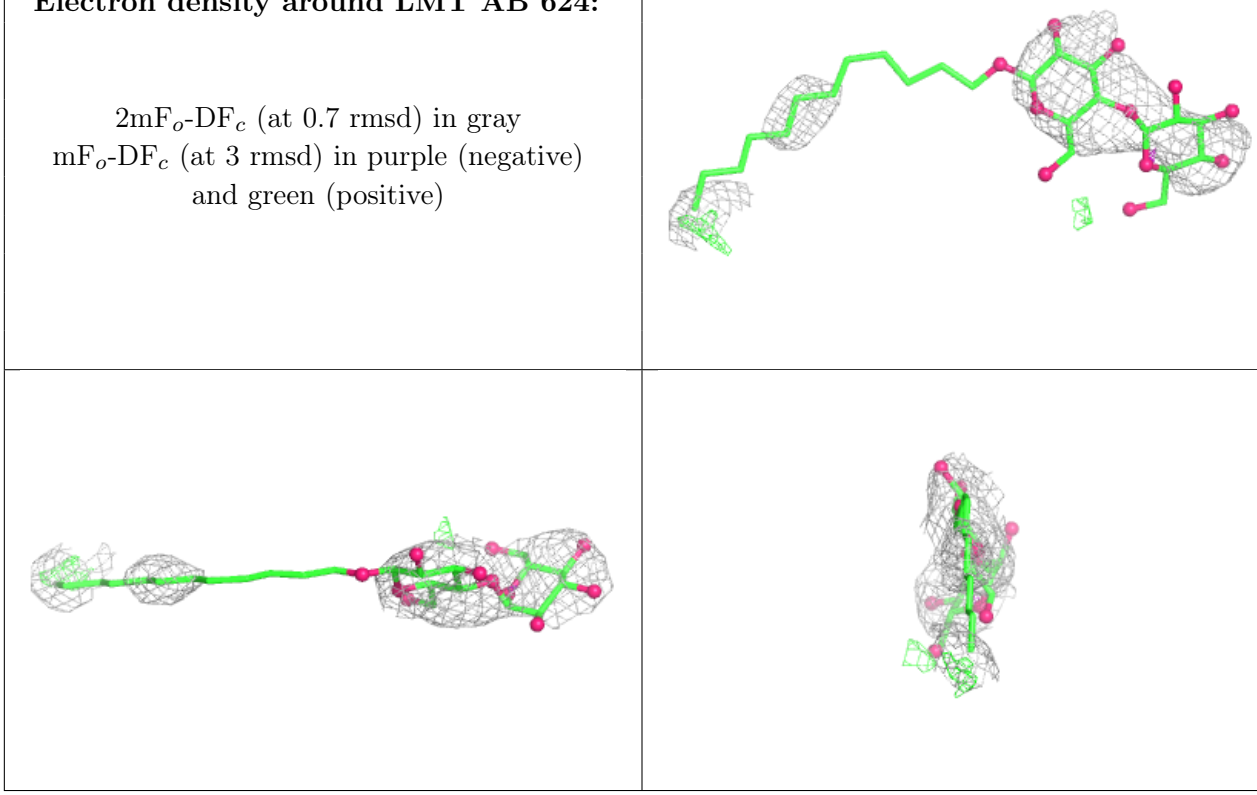
Electron density around LMG AC 521:

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



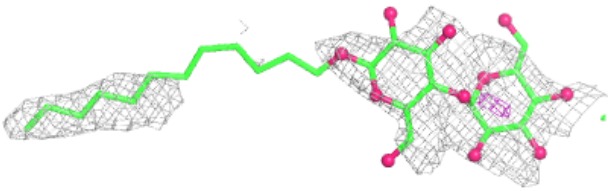
Electron density around LMT AB 624:

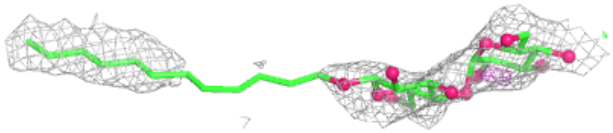
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

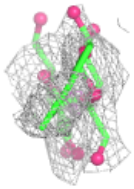


Electron density around LMT AB 630:

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

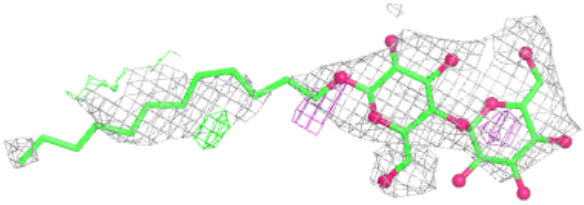


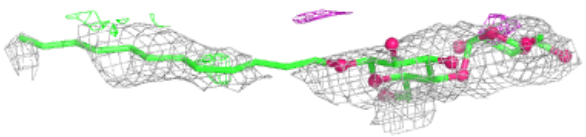


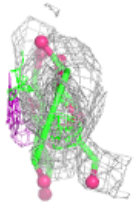


Electron density around LMT AI 102:

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

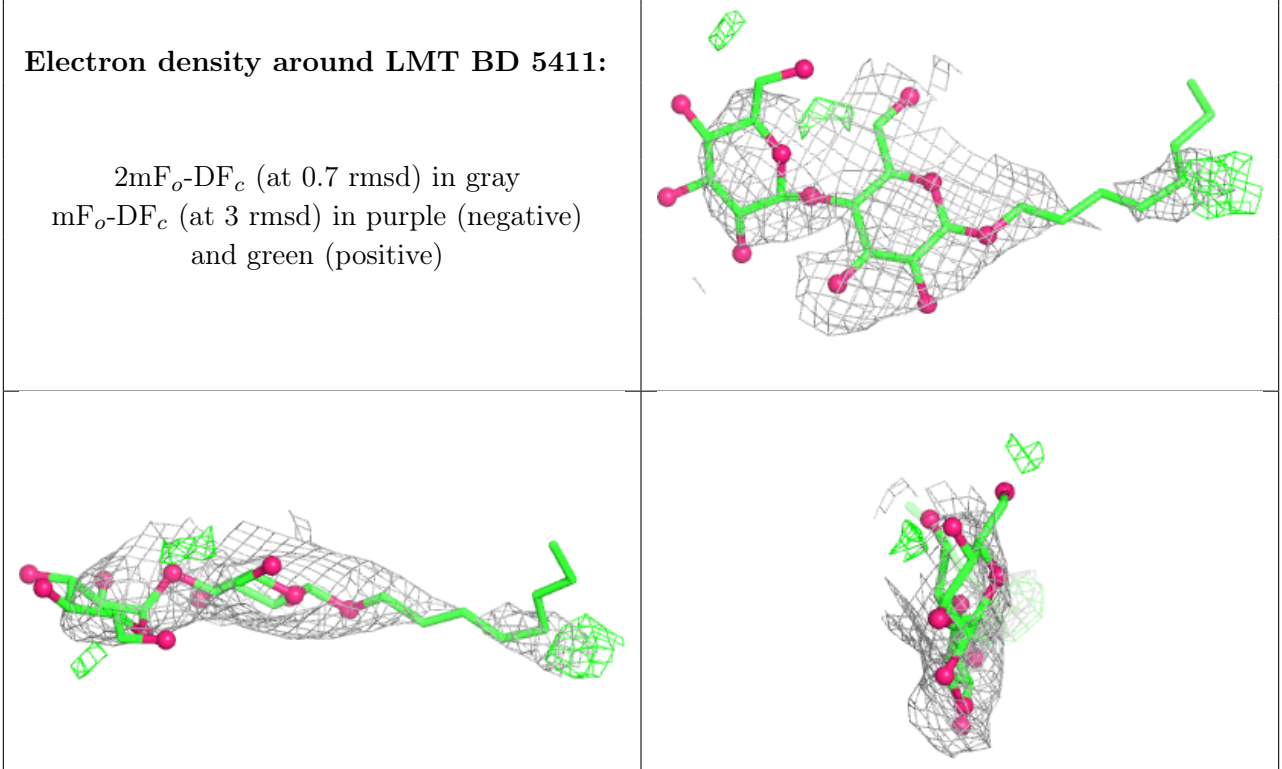






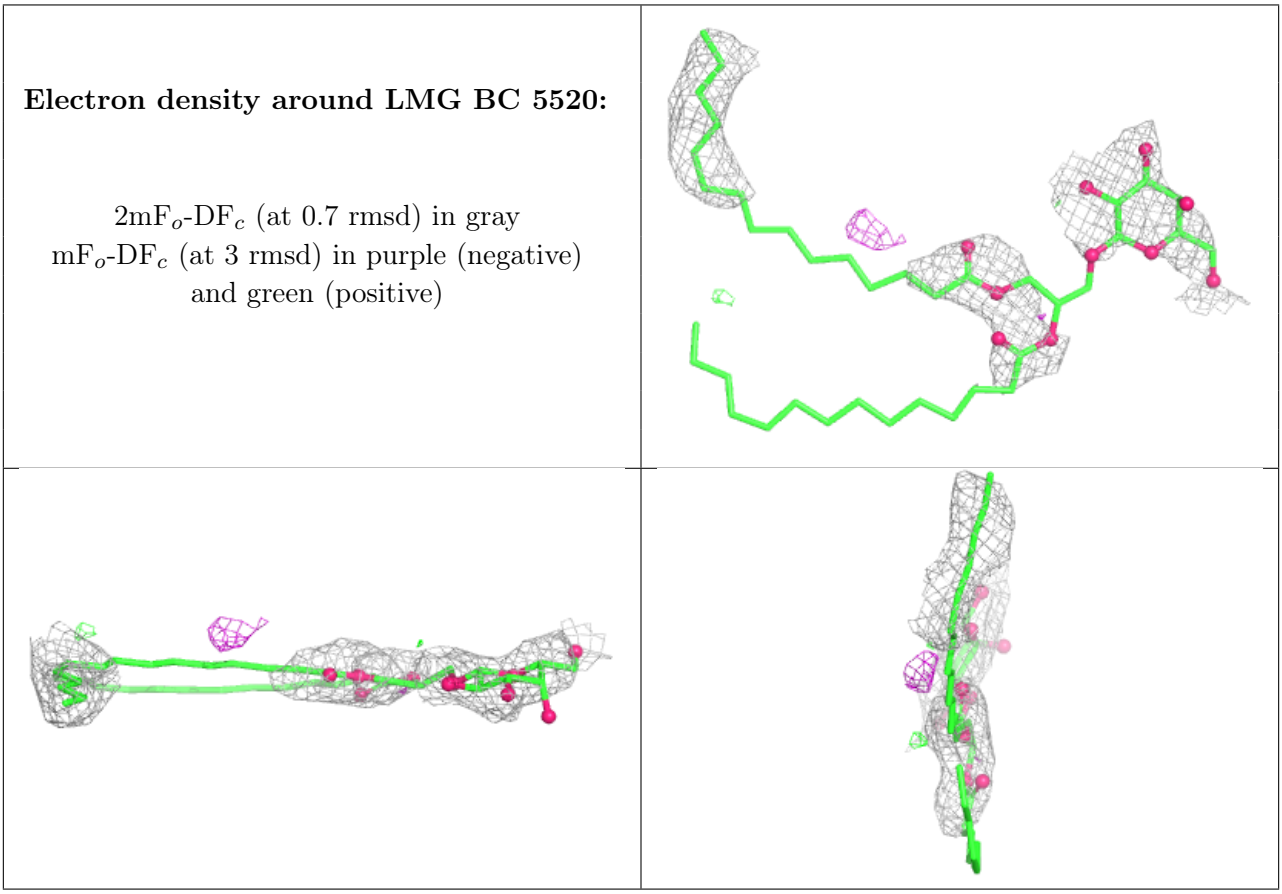
Electron density around LMT BD 5411:

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



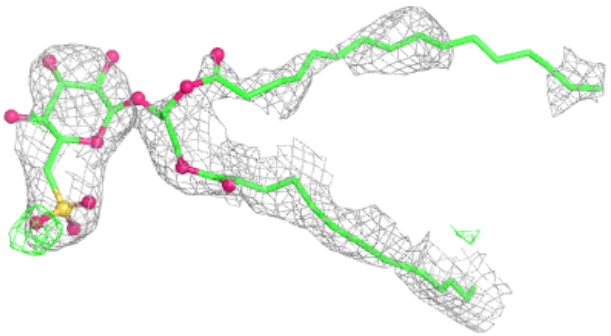
Electron density around LMG BC 5520:

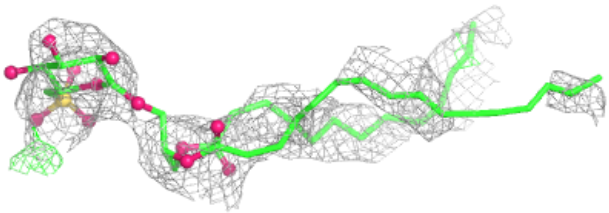
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

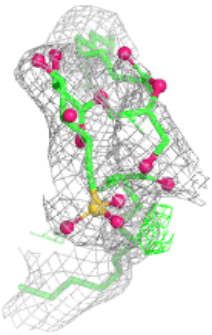


Electron density around SQD BA 5414:

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

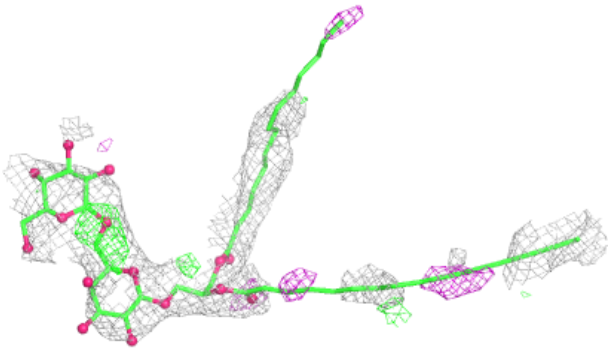


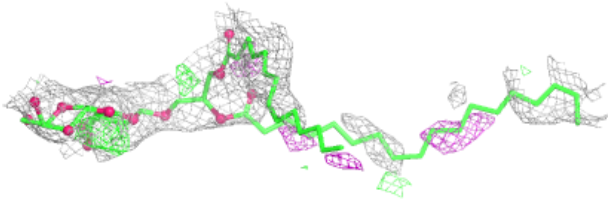


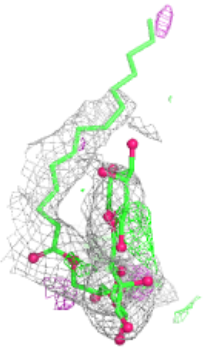


Electron density around DGD BC 5518:

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

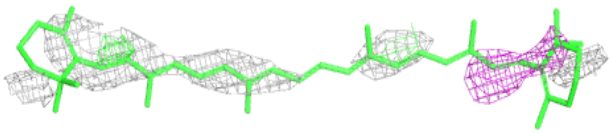


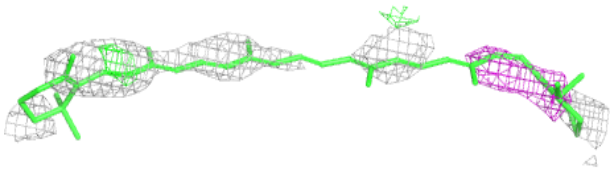


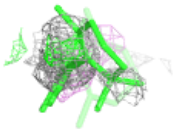


Electron density around BCR AJ 101:

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

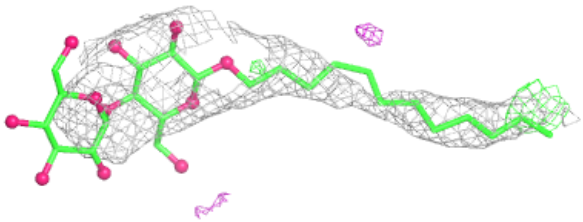


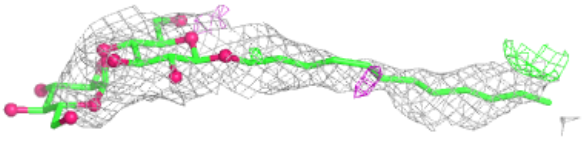


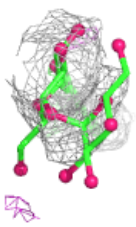


Electron density around LMT BB 5603:

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

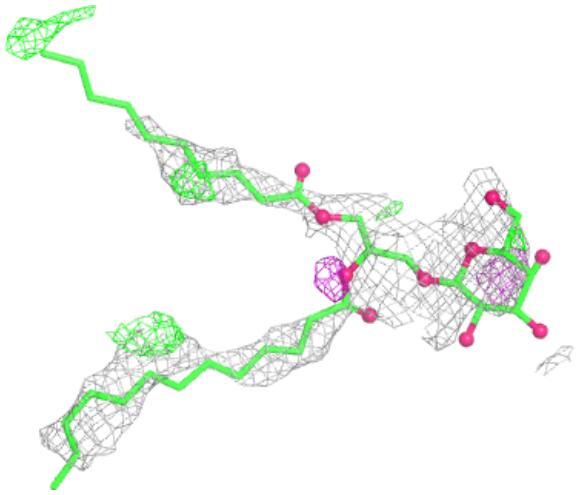


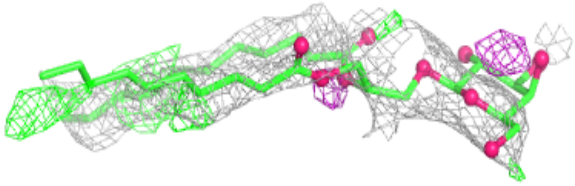


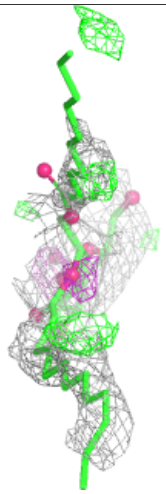


Electron density around LMG BA 5402:

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

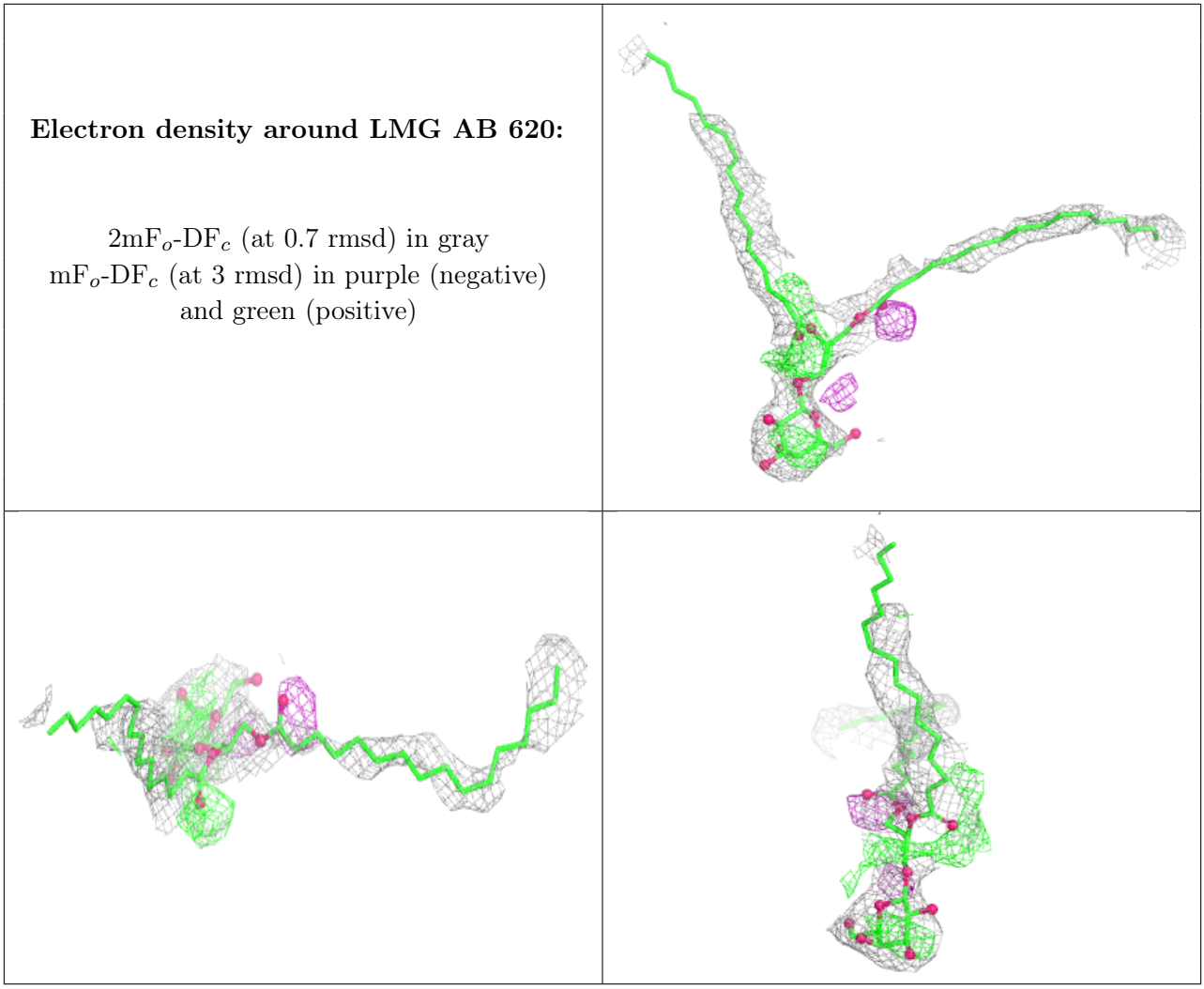






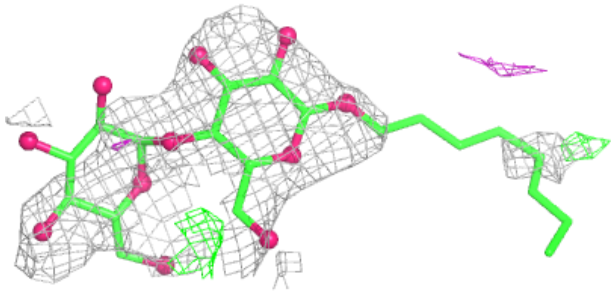
Electron density around LMG AB 620:

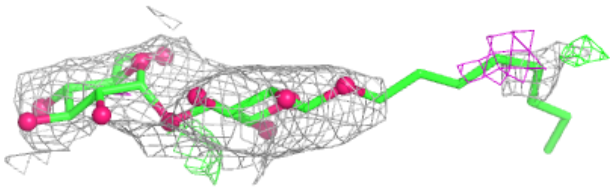
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

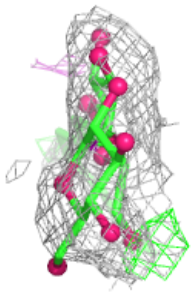


Electron density around LMT AD 409:

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

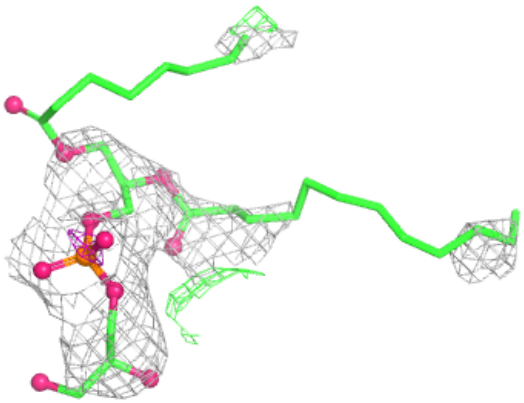


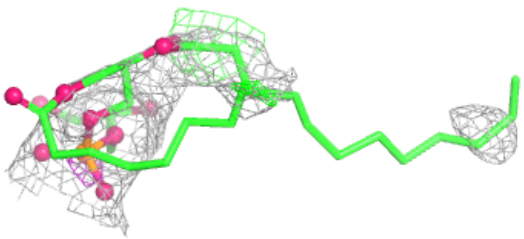


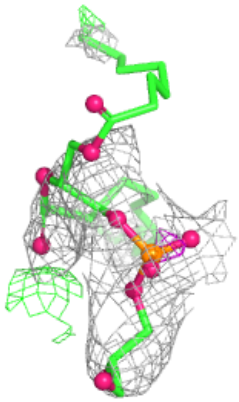


Electron density around LHG AA 415:

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

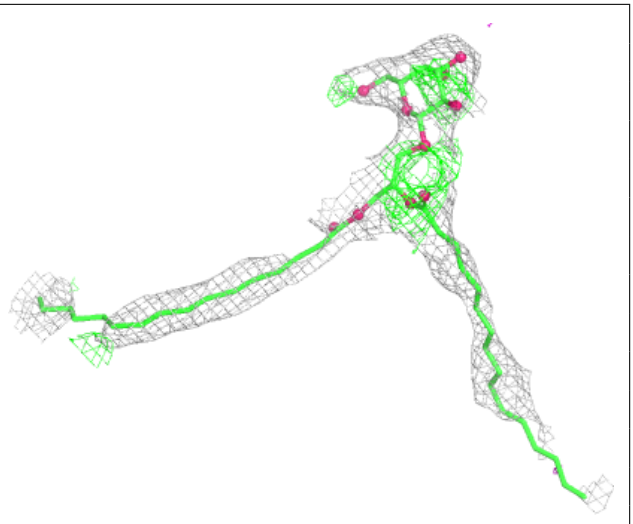


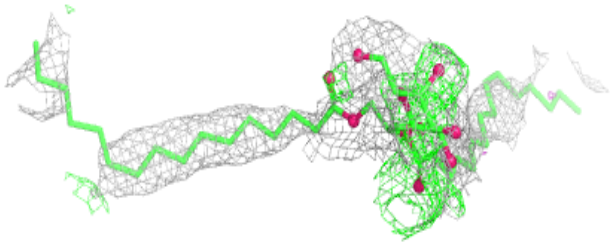




Electron density around LMG BL 5101:

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

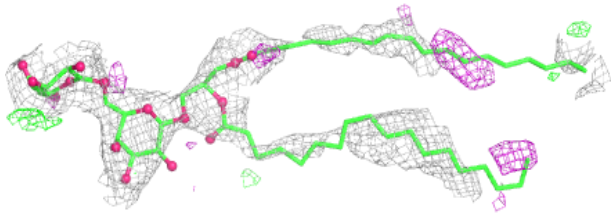


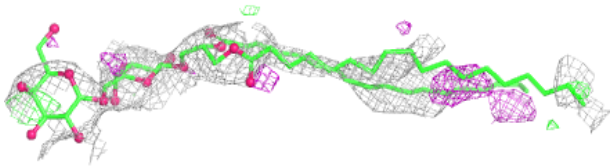


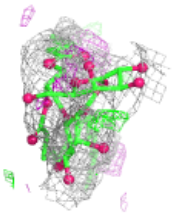


Electron density around DGD BC 5519:

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

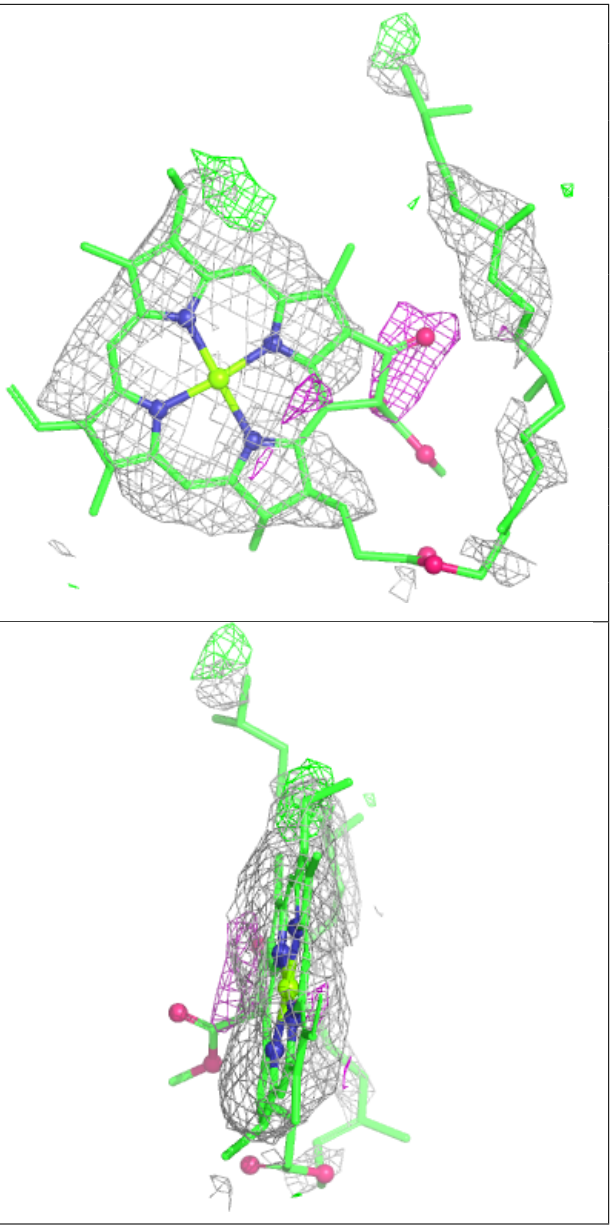






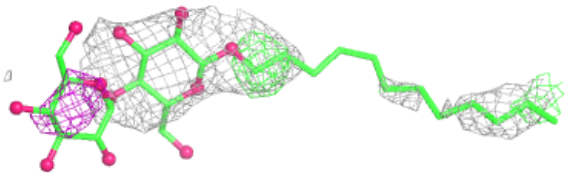
Electron density around CLA BB 5605:

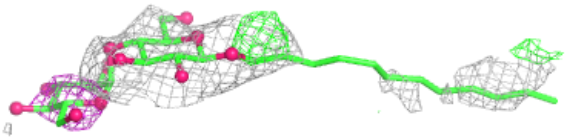
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

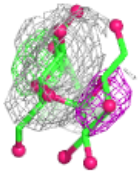


Electron density around LMT AB 629:

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

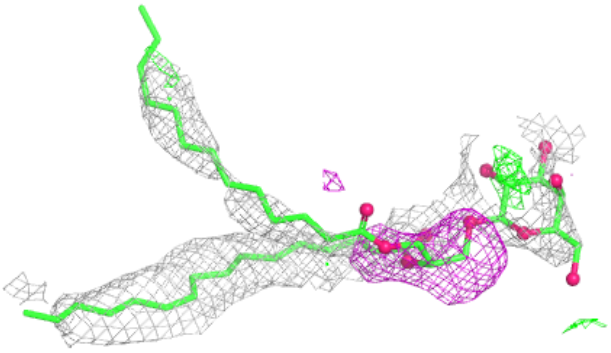


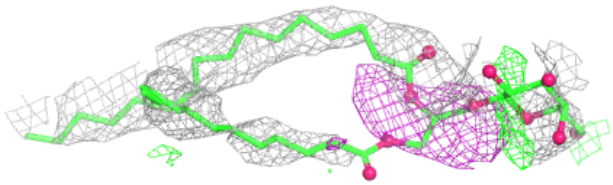


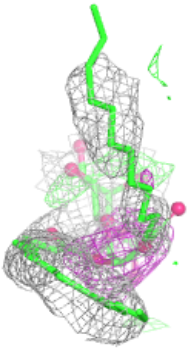


Electron density around LMG BD 5410:

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

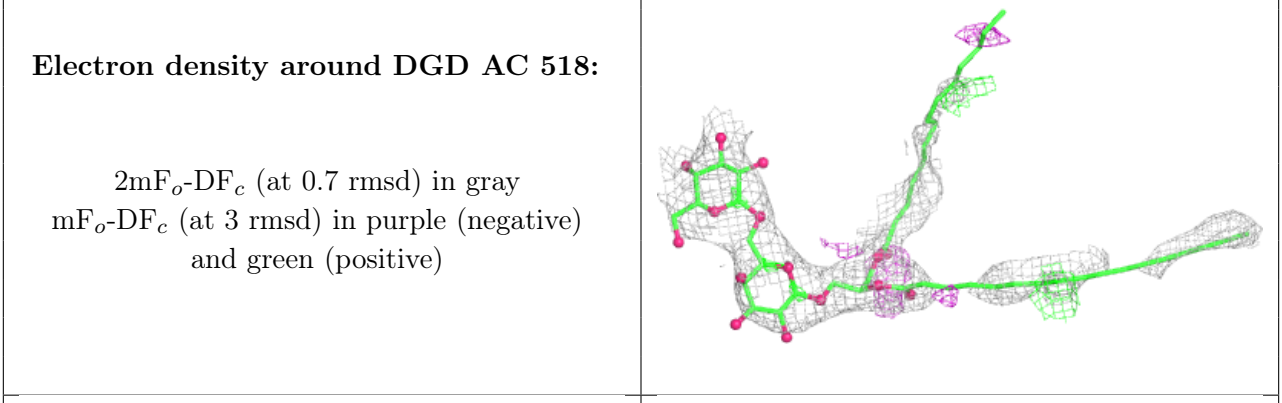






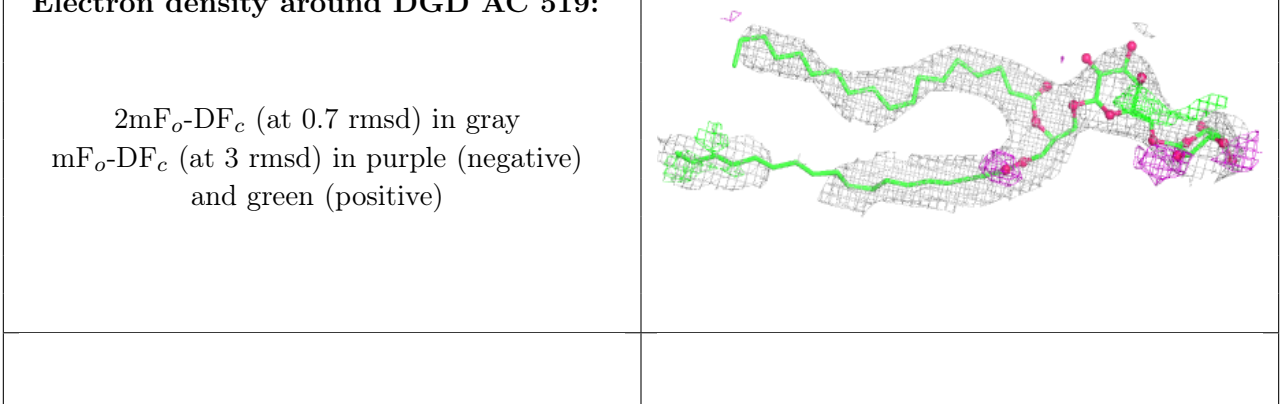
Electron density around DGD AC 518:

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



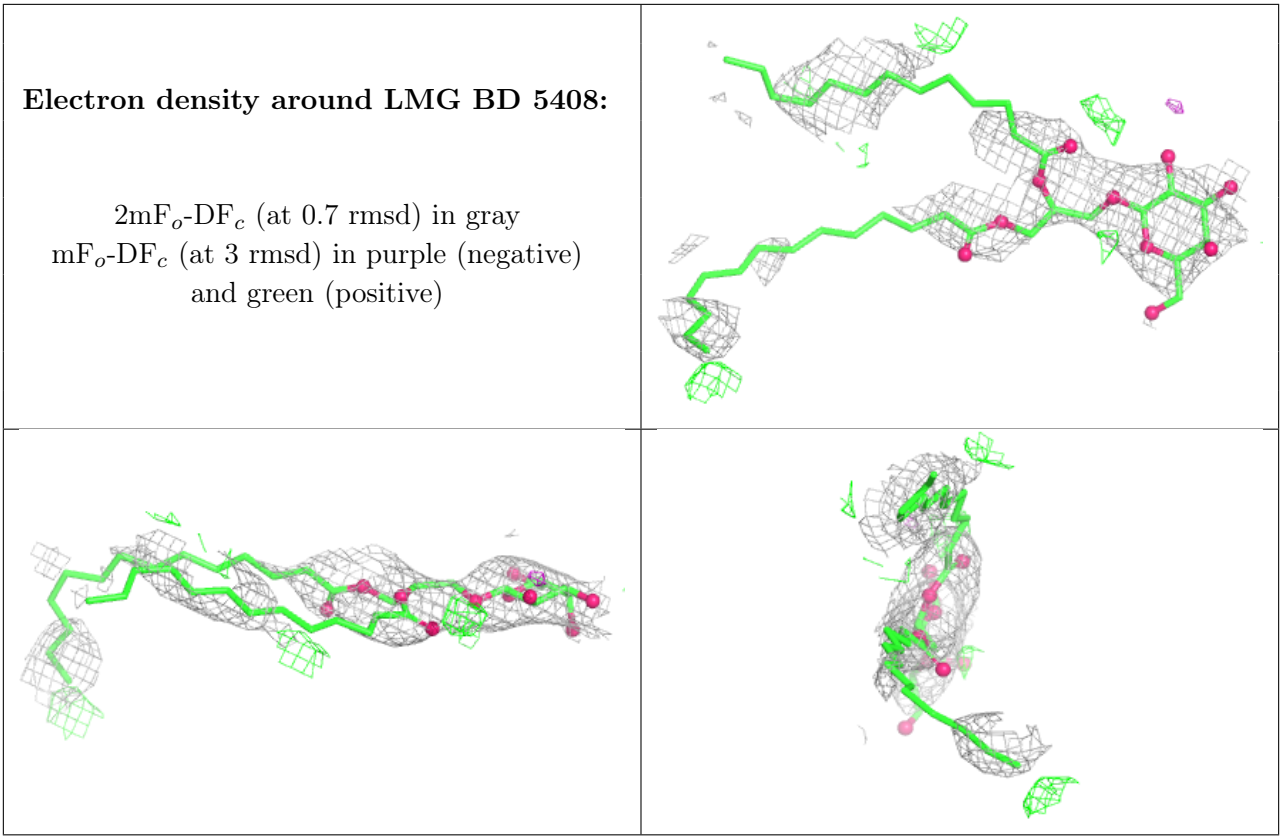
Electron density around DGD AC 519:

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



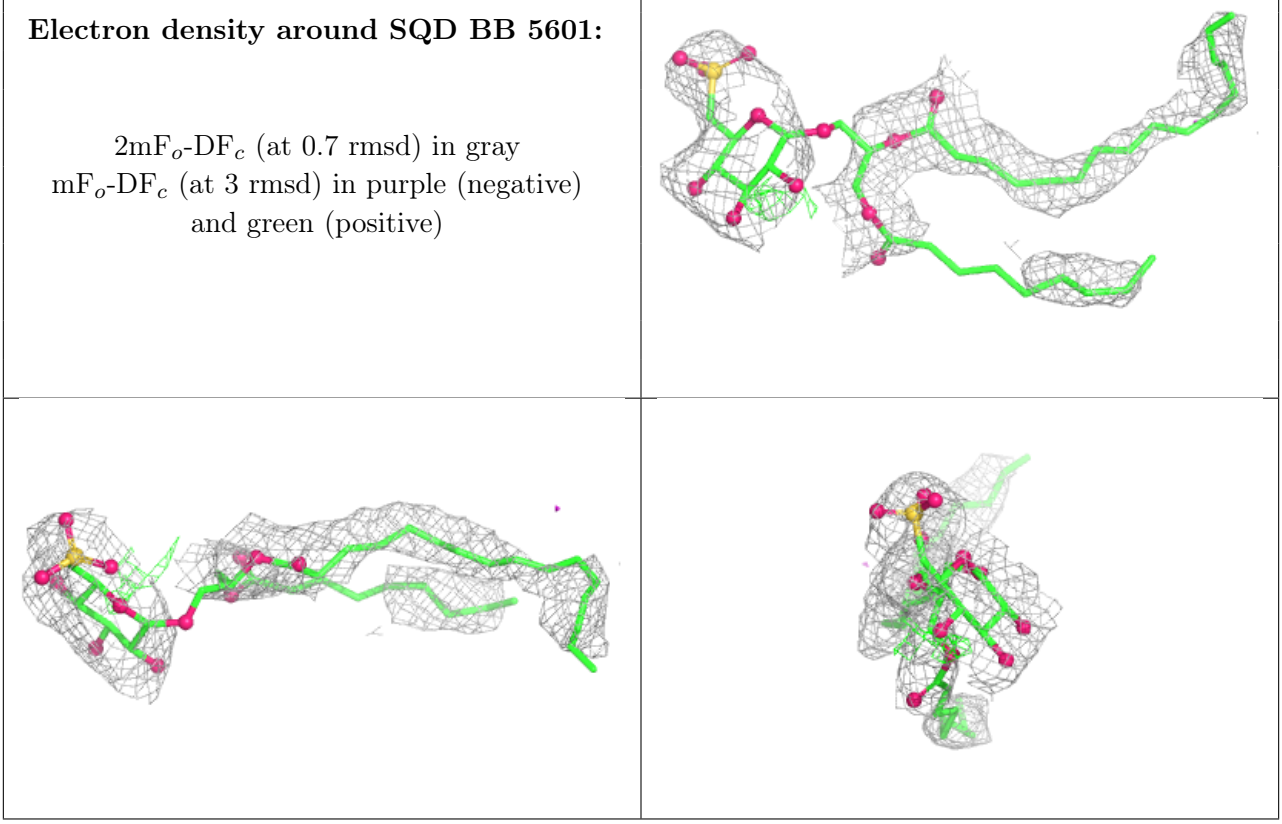
Electron density around LMG BD 5408:

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



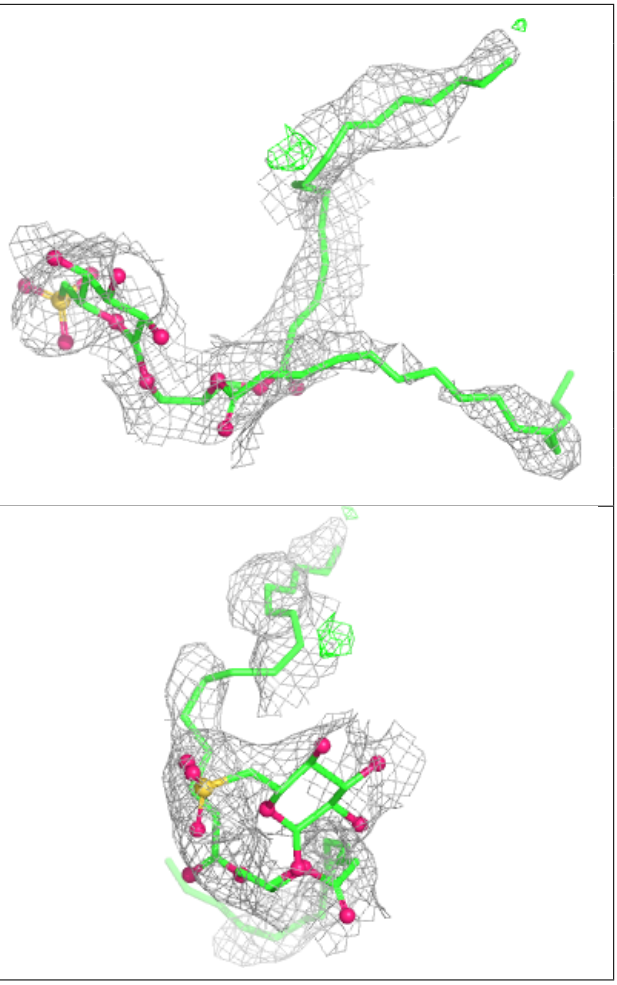
Electron density around SQD BB 5601:

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



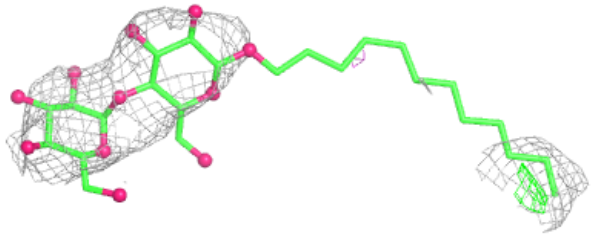
Electron density around SQD AA 416:

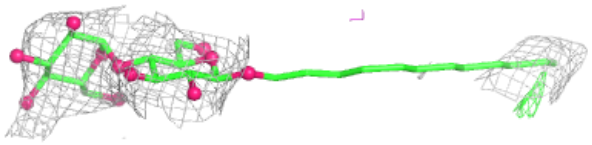
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

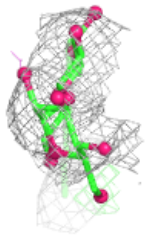


Electron density around LMT BB 5627:

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

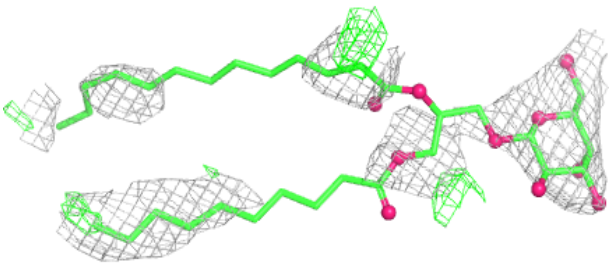


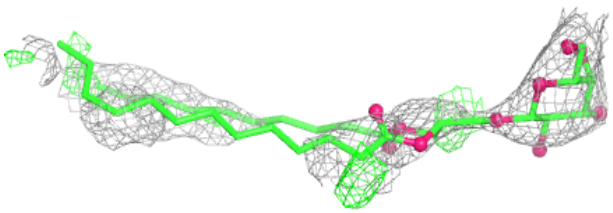


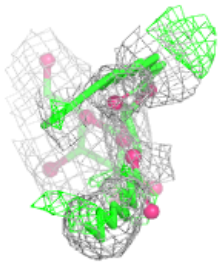


Electron density around LMG AM 101:

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

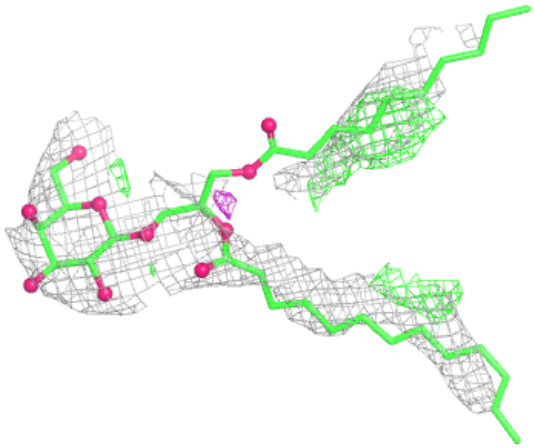


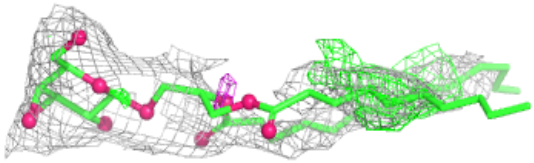


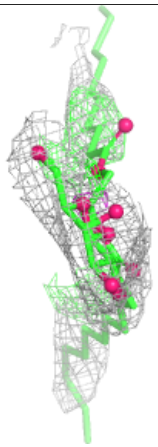


Electron density around LMG AA 417:

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

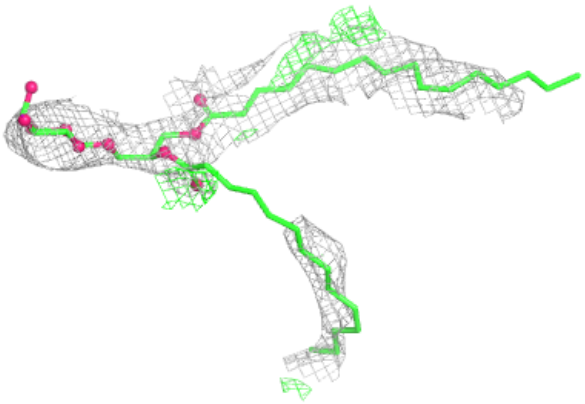


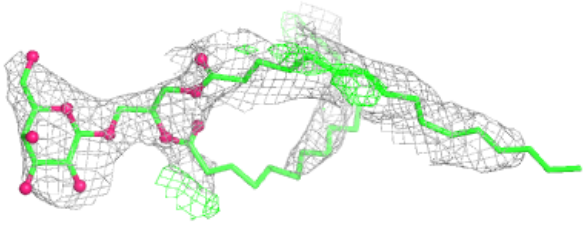


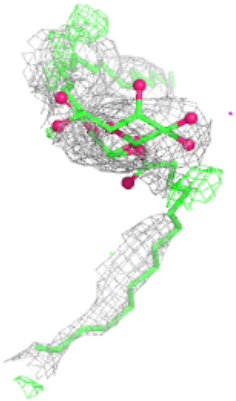


Electron density around LMG AB 621:

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

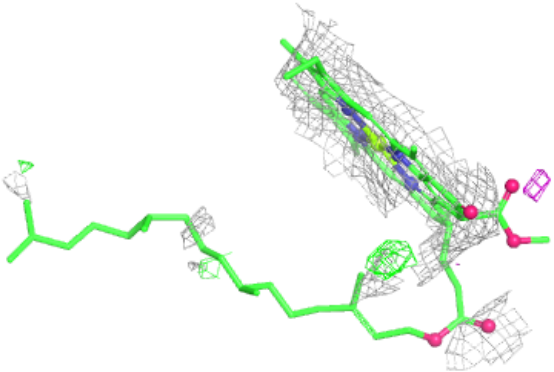


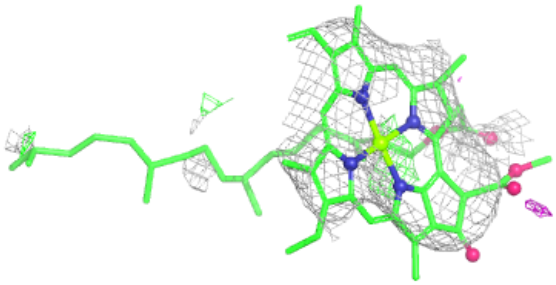




Electron density around CLA BC 5513:

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

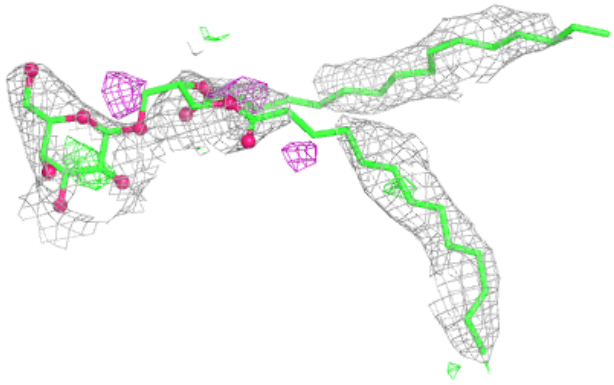


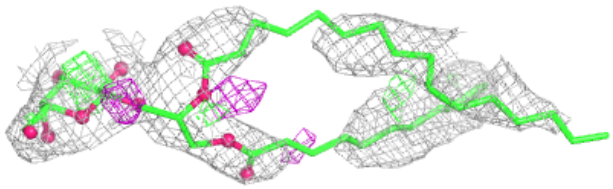


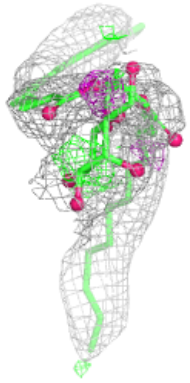


Electron density around LMG AD 408:

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

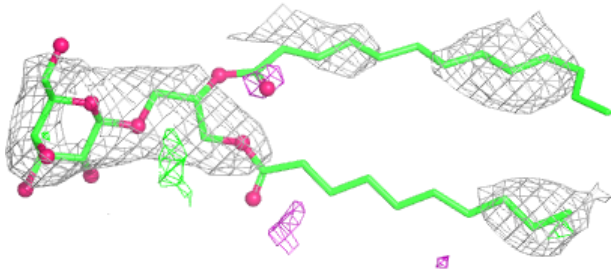


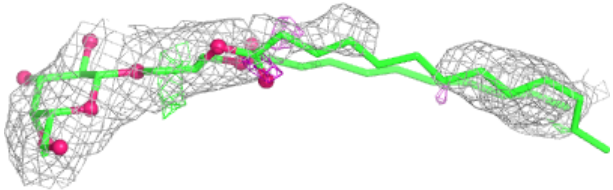


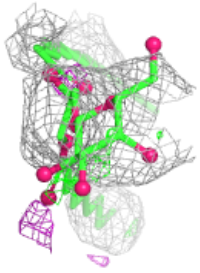


Electron density around LMG BM 5102:

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

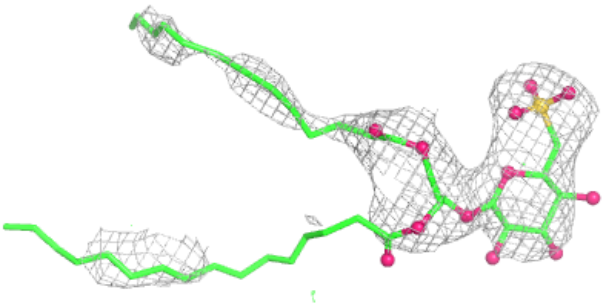


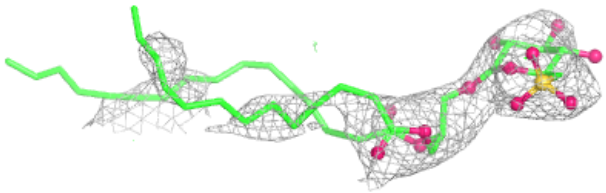


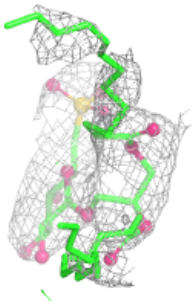


Electron density around SQD AA 413:

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

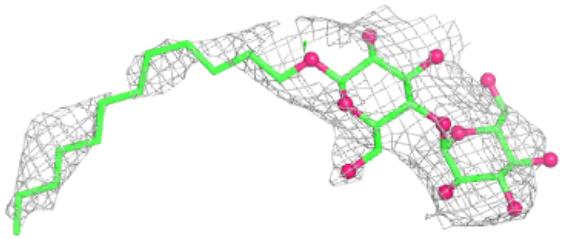


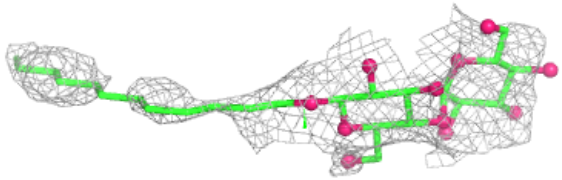


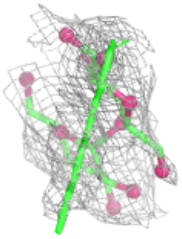


Electron density around LMT AM 102:

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

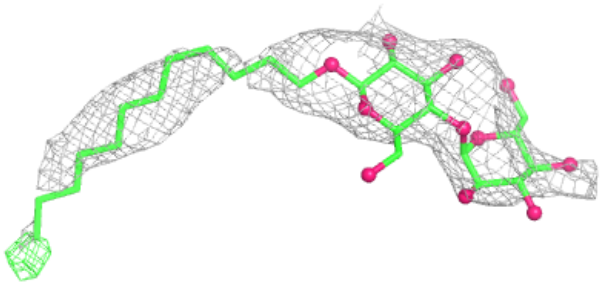


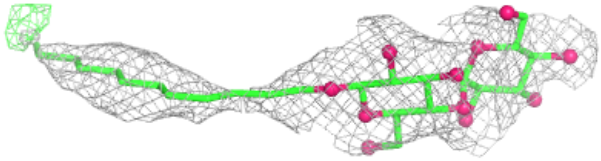


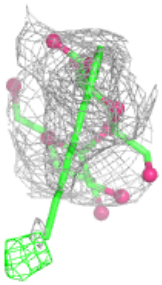


Electron density around LMT BM 5101:

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

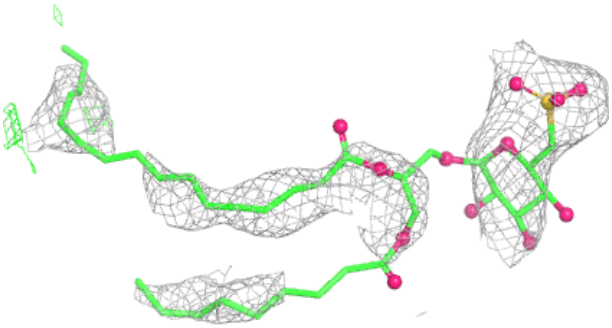


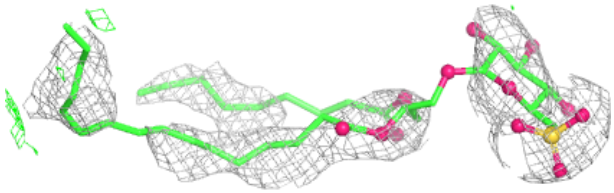


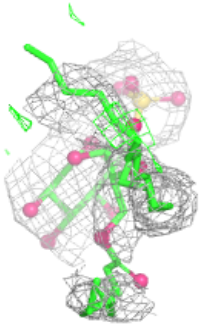


Electron density around SQD AB 627:

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

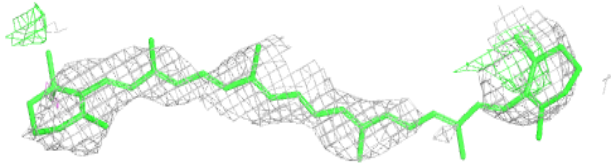


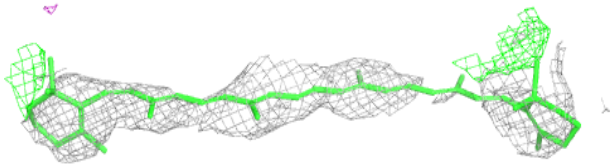


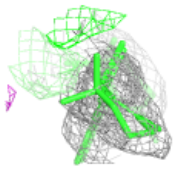


Electron density around BCR BC 5516:

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

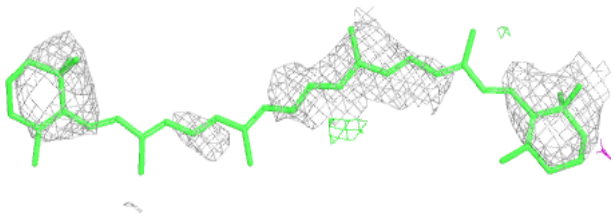


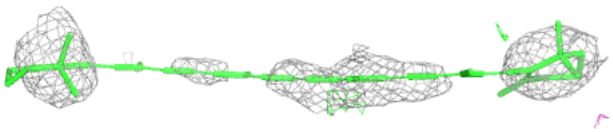


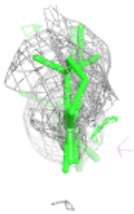


Electron density around BCR BK 5102:

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

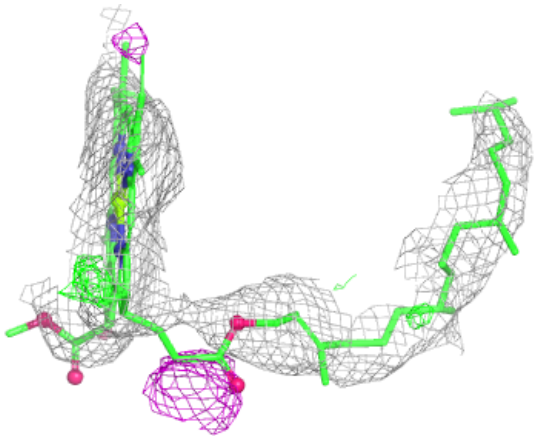


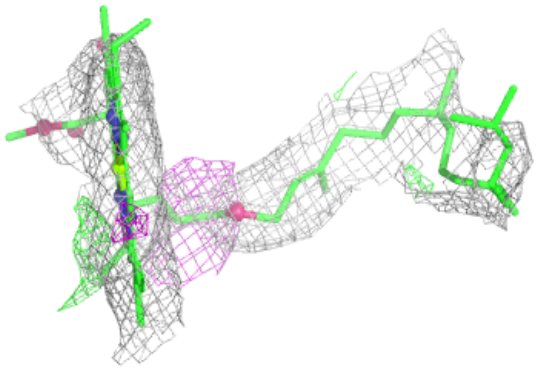


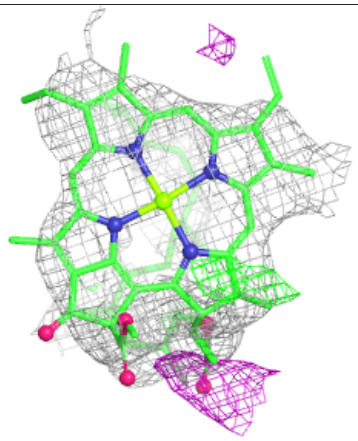


Electron density around CLA AC 506:

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

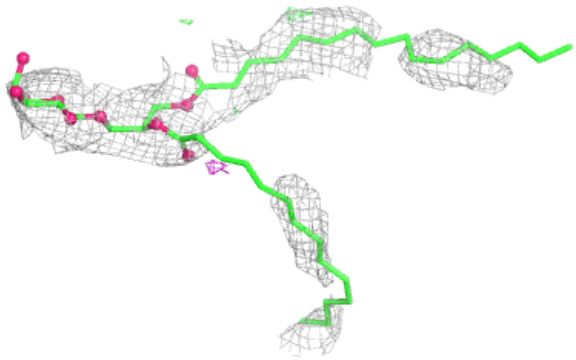


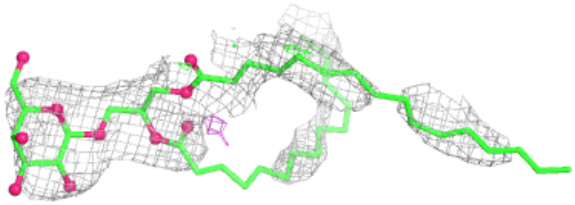


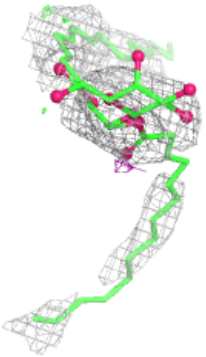


Electron density around LMG BB 5624:

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

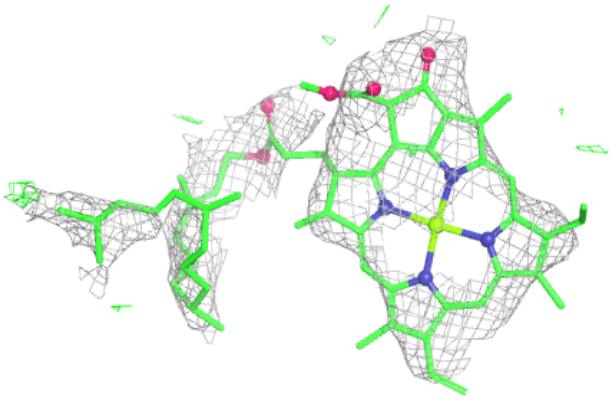


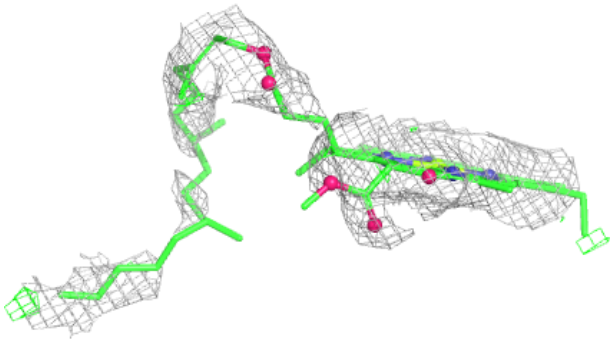


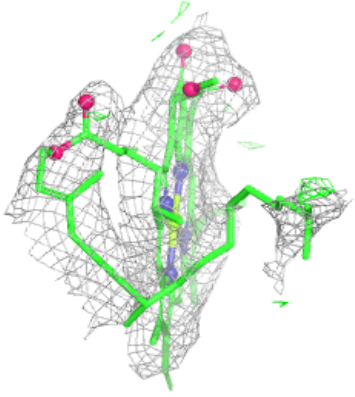


Electron density around CLA BC 5512:

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

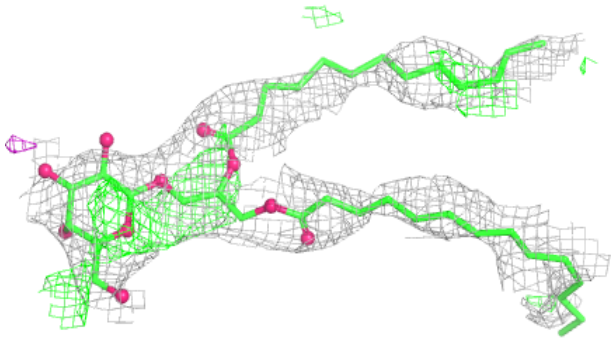


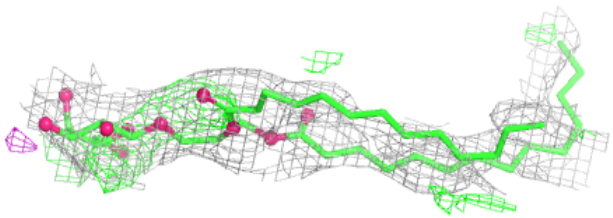


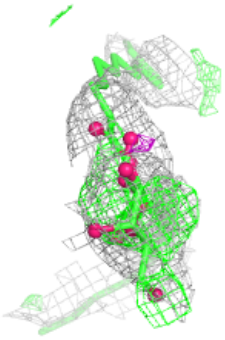


Electron density around LMG AJ 102:

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

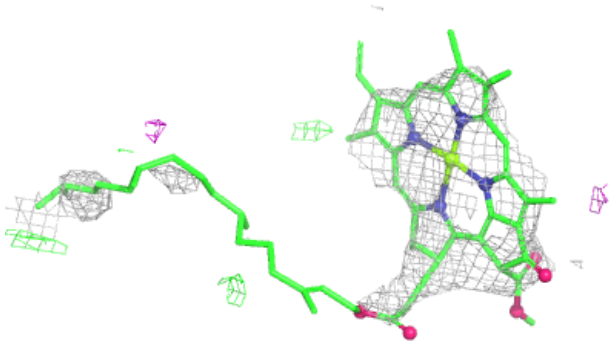


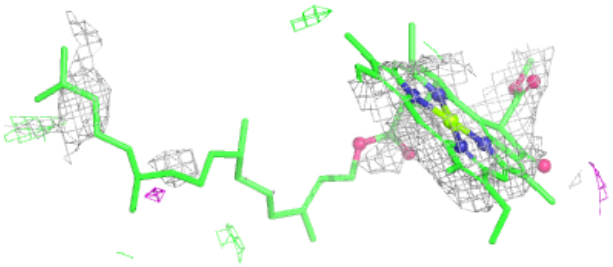


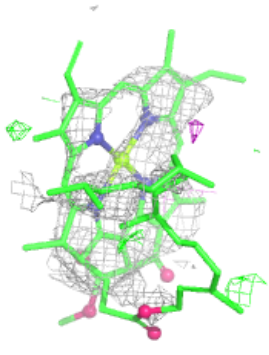


Electron density around CLA BC 5511:

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

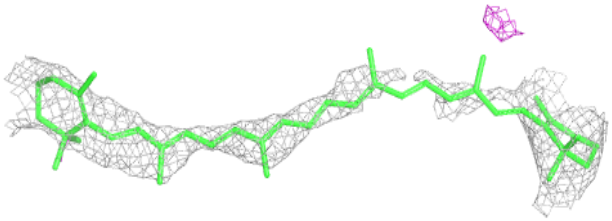


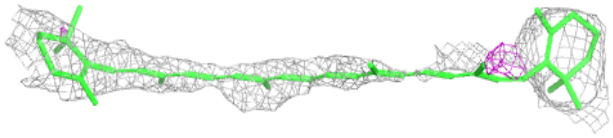


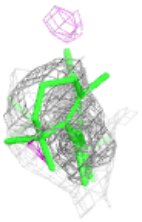


Electron density around BCR AX 101:

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

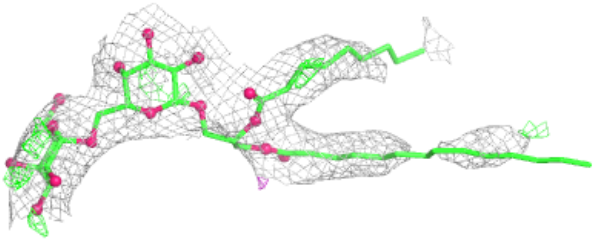


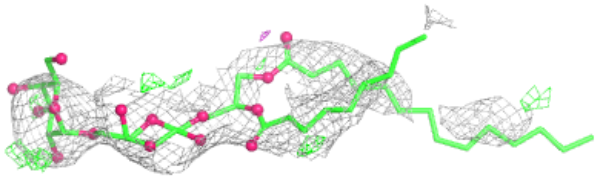


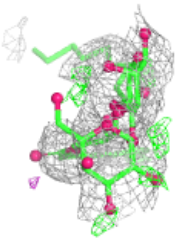


Electron density around DGD BC 5517:

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

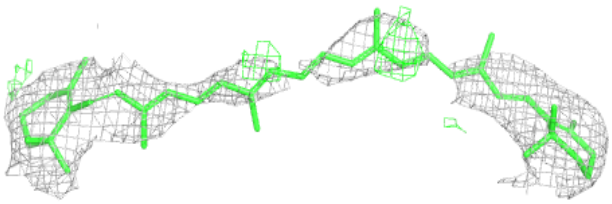




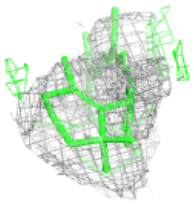


Electron density around BCR BT 5101:

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

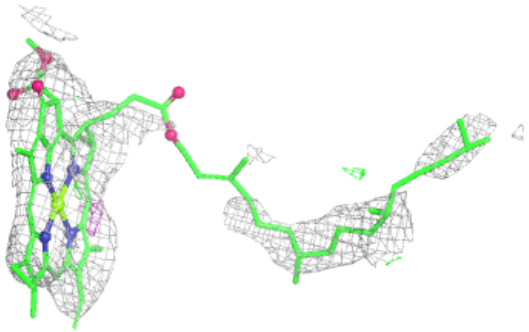


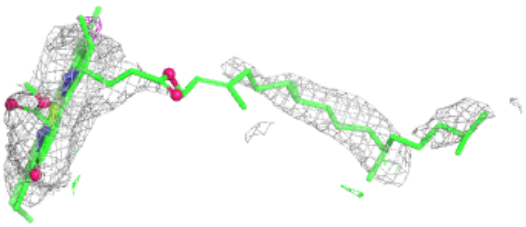


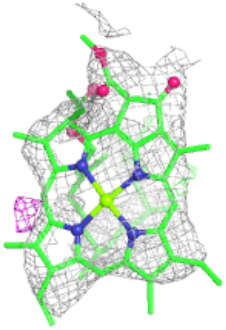


Electron density around CLA BD 5405:

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

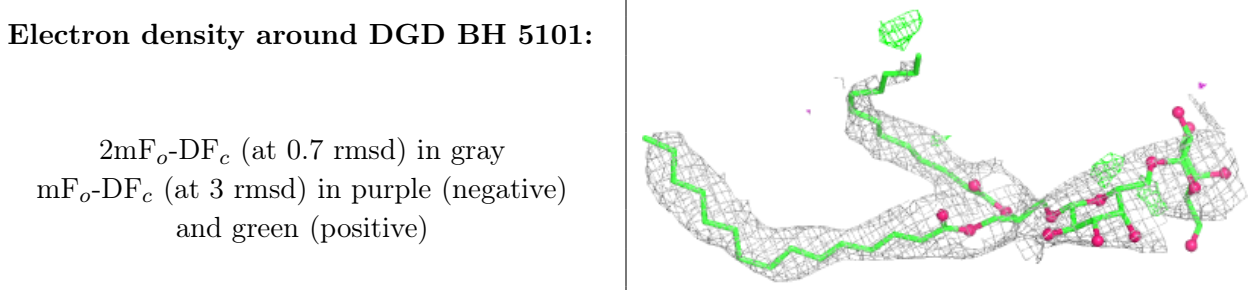


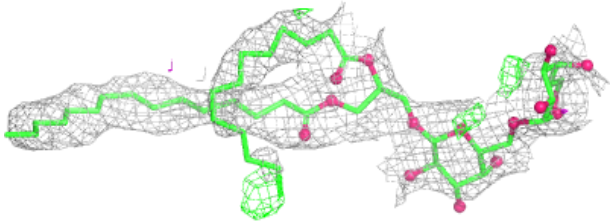


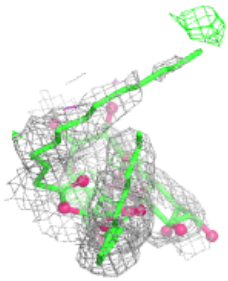


Electron density around DGD BH 5101:

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

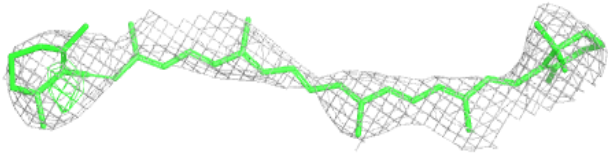


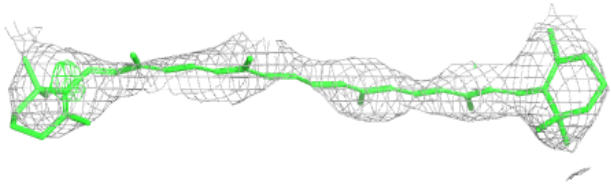


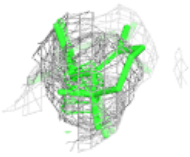


Electron density around BCR AC 515:

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

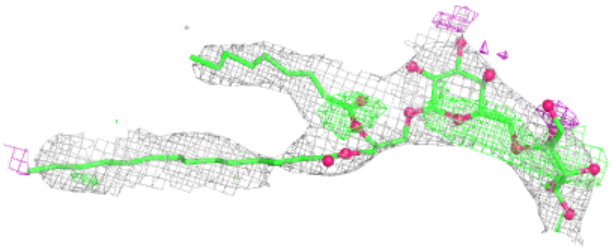


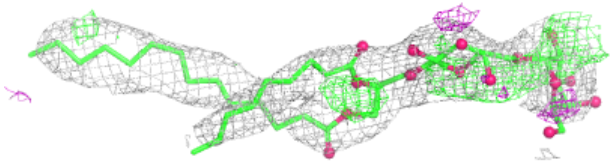


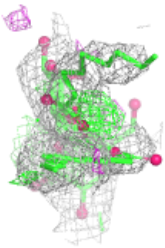


Electron density around DGD AC 517:

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

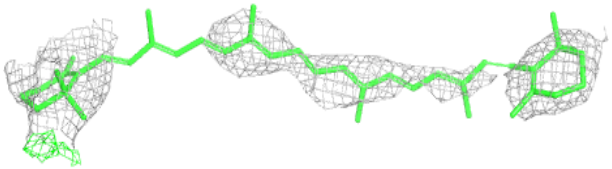


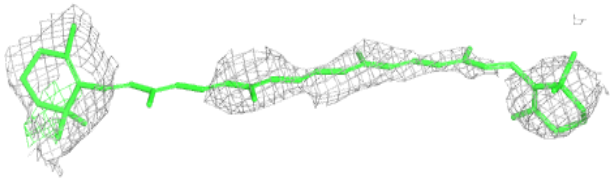


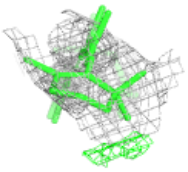


Electron density around BCR BC 5515:

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

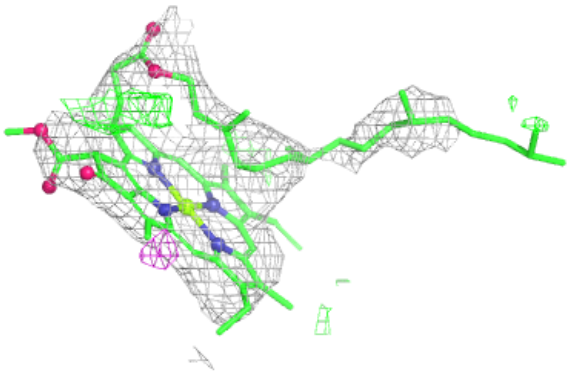


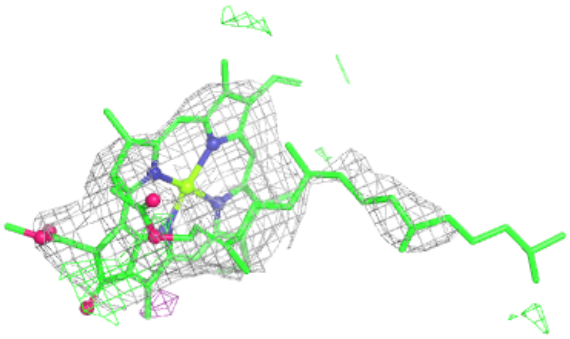


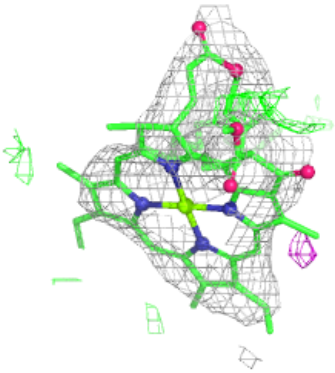


Electron density around CLA BC 5505:

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

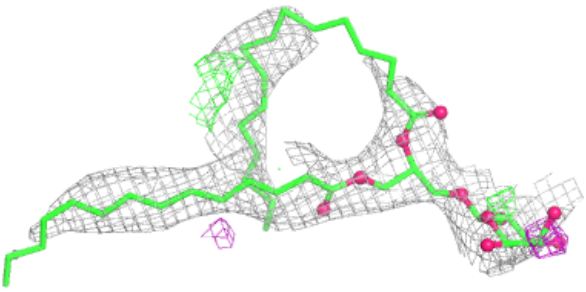


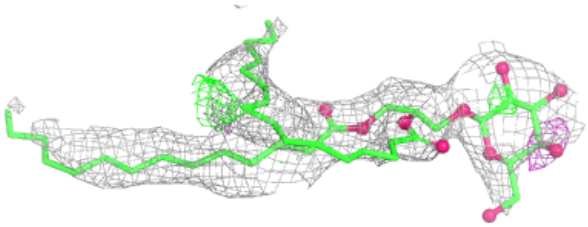


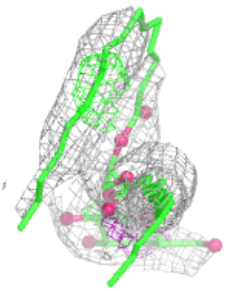


Electron density around LMG AD 407:

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

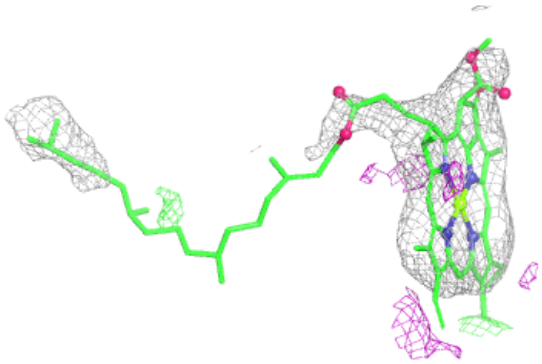


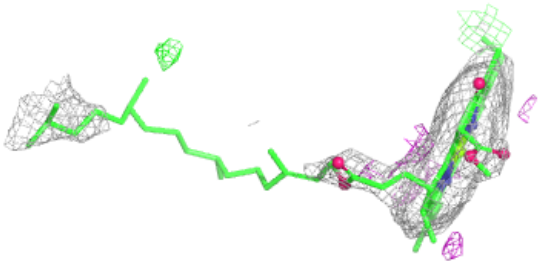


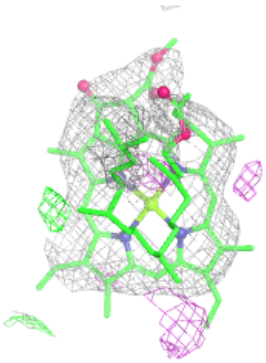


Electron density around CLA AD 404:

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

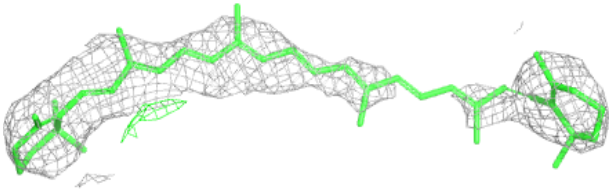


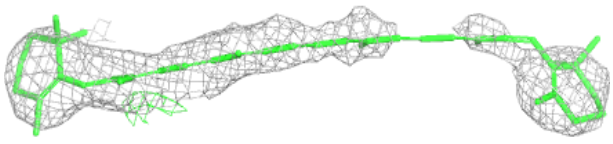


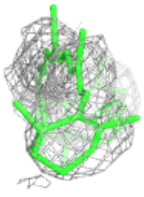


Electron density around BCR AT 101:

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

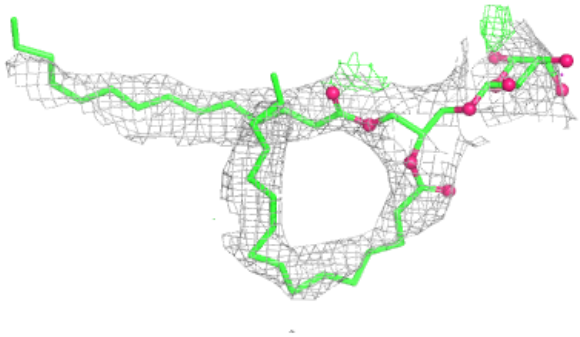


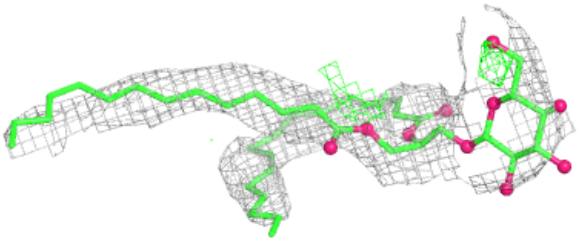


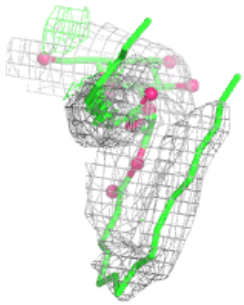


Electron density around LMG BD 5409:

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

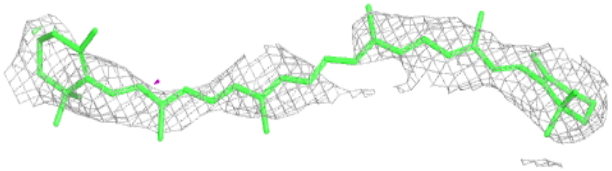


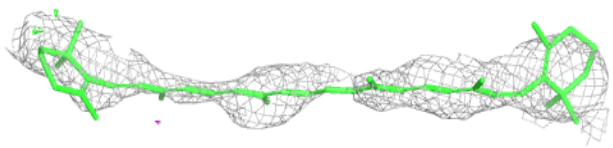


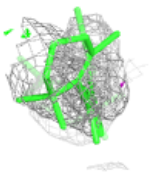


Electron density around BCR BX 5101:

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

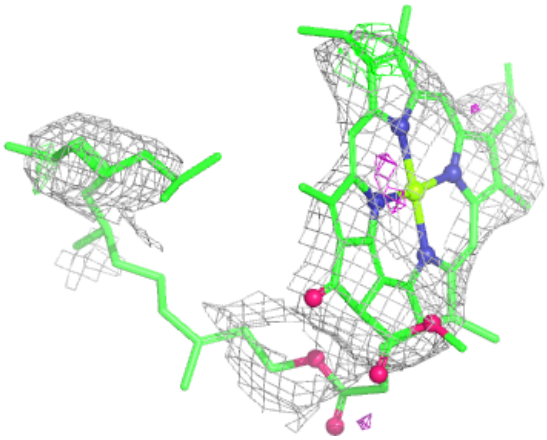


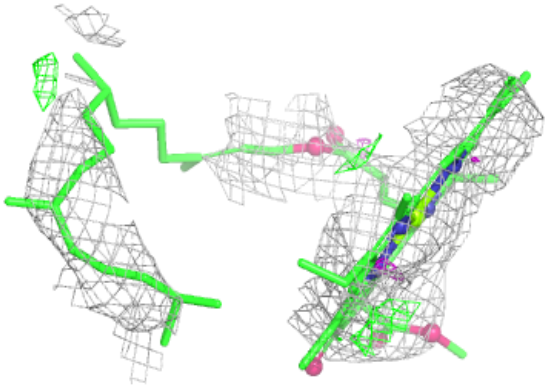


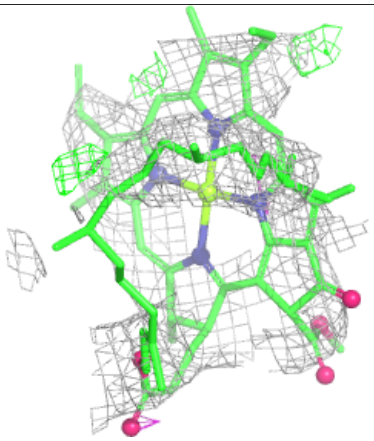


Electron density around CLA BC 5503:

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

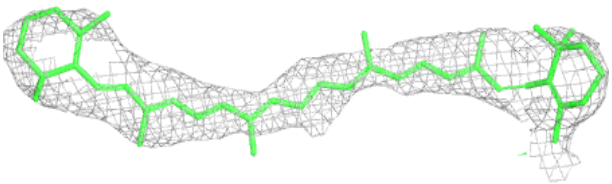


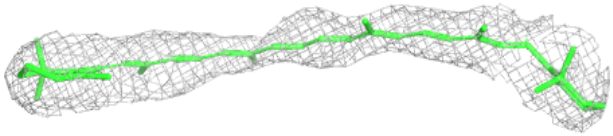


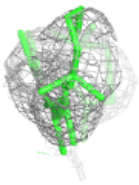


Electron density around BCR BD 5407:

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

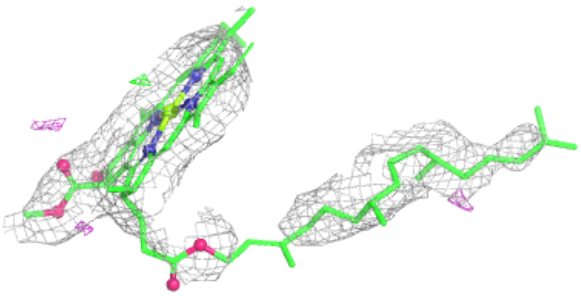


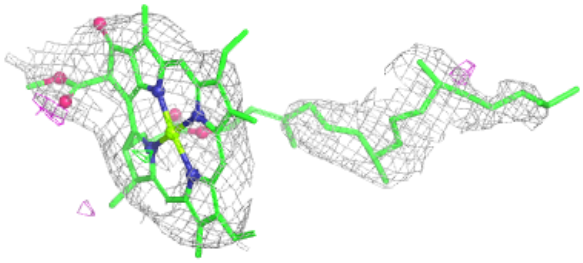


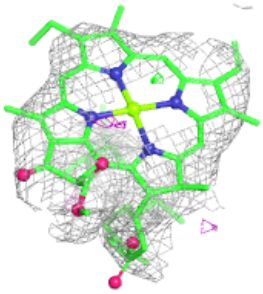


Electron density around CLA BC 5504:

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

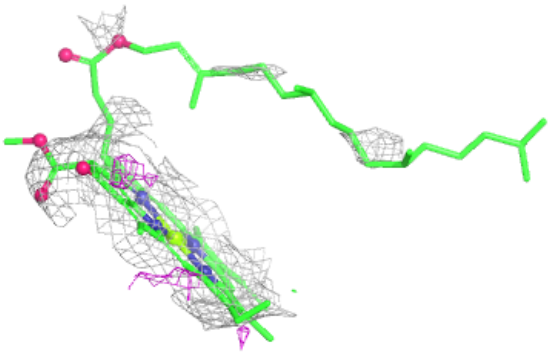


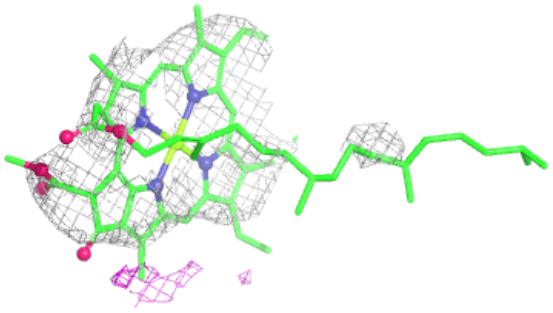


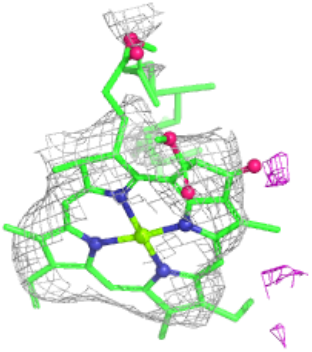


Electron density around CLA AC 513:

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

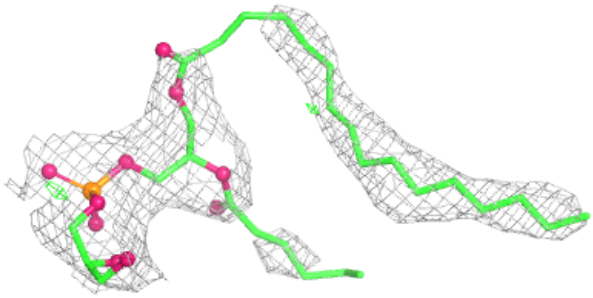


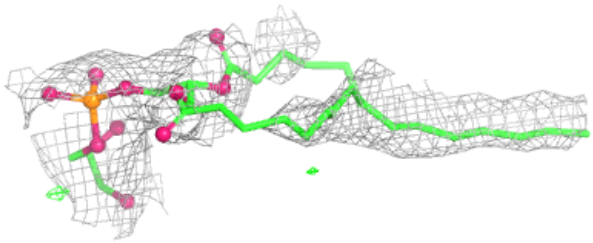


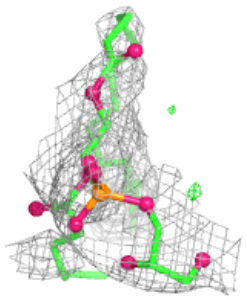


Electron density around LHG BA 5413:

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

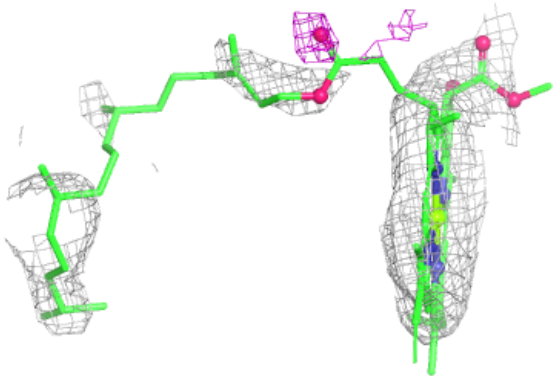


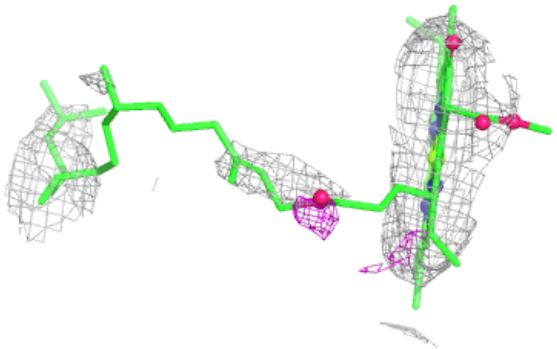


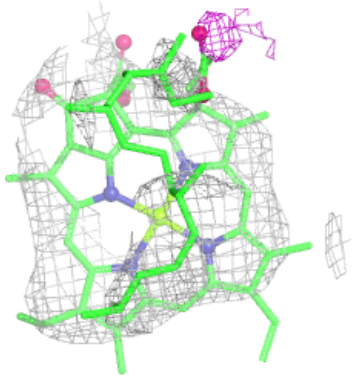


Electron density around CLA BC 5506:

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

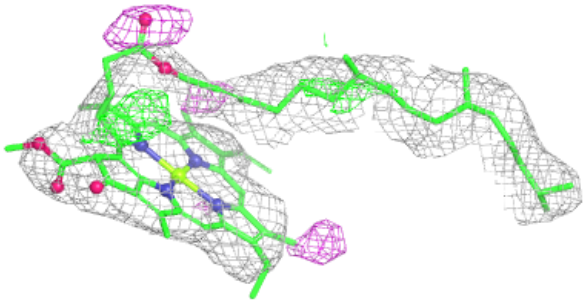


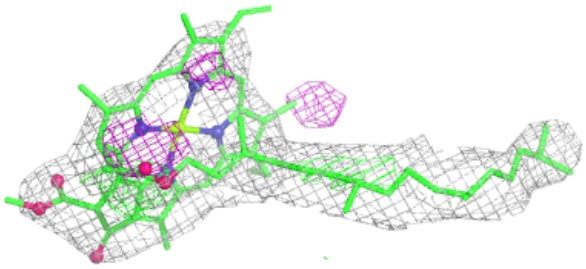


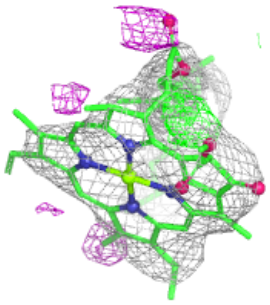


Electron density around CLA AB 608:

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

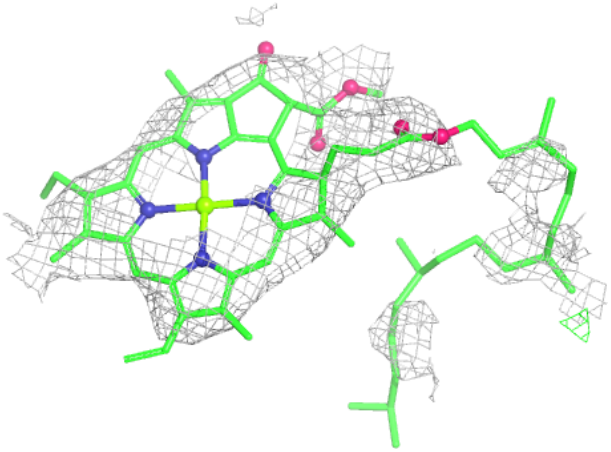


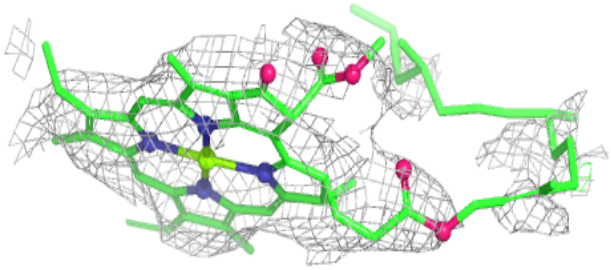


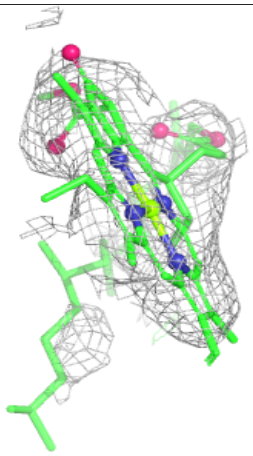


Electron density around CLA AB 616:

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

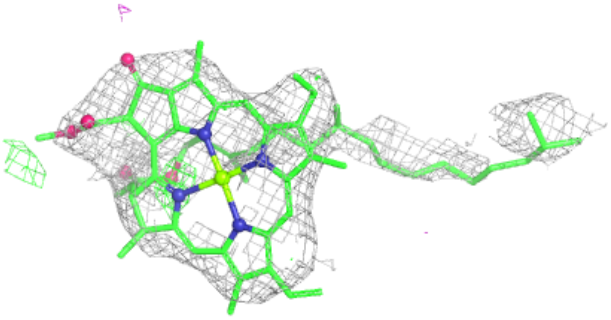


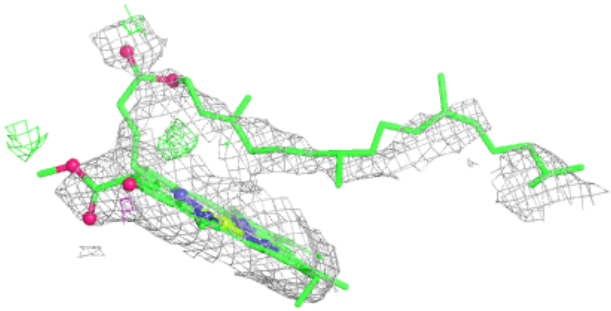


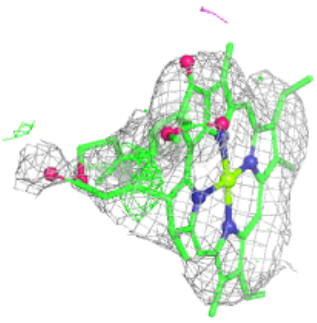


Electron density around CLA BB 5618:

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



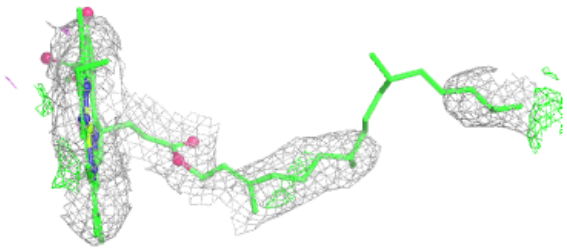


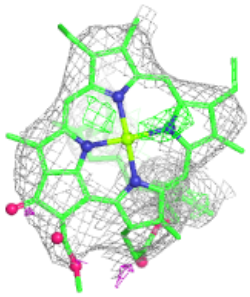


Electron density around CLA AB 606:

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



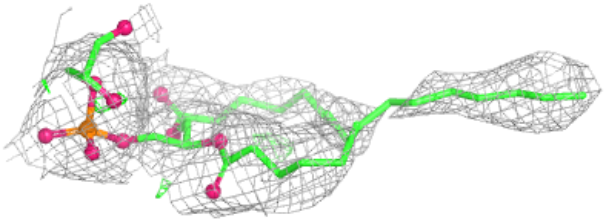


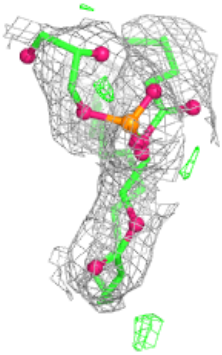


Electron density around LHG AA 412:

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

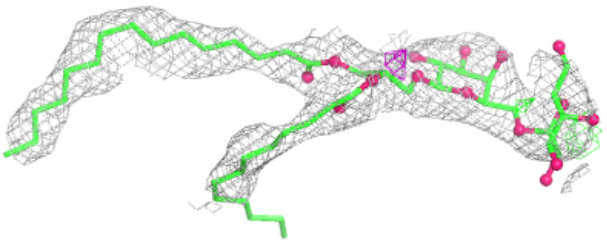


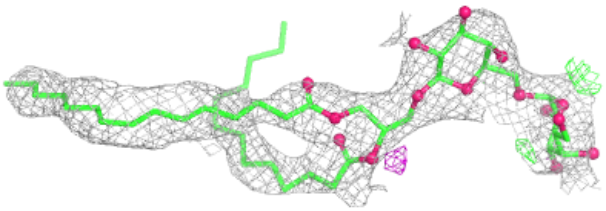


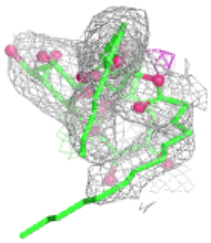


Electron density around DGD AH 101:

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

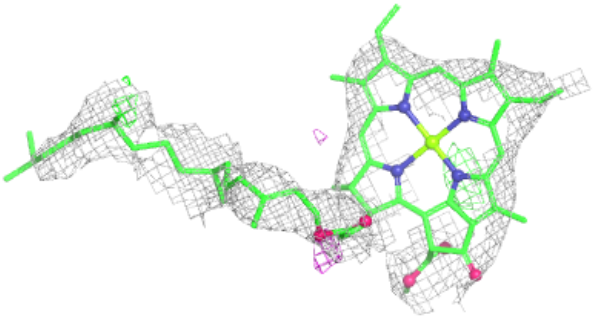


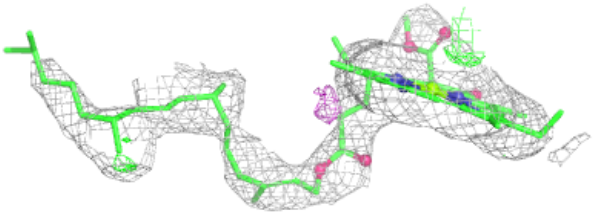


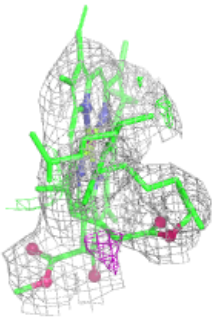


Electron density around CLA BA 5407:

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

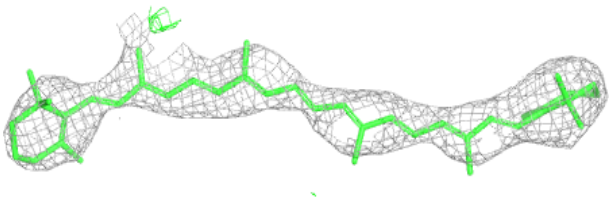


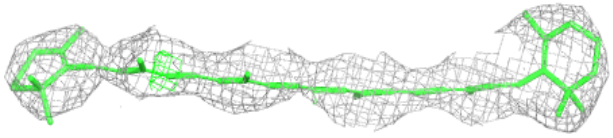


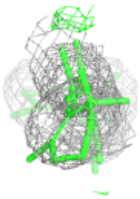


Electron density around BCR AB 617:

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

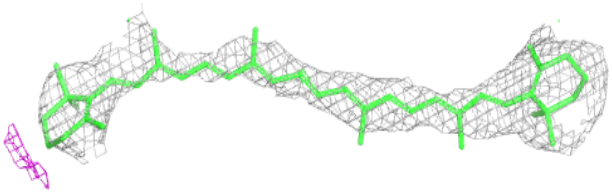


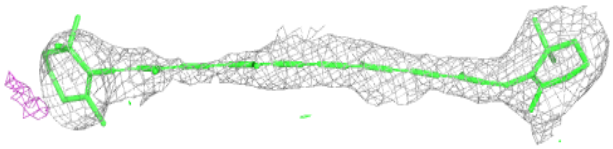


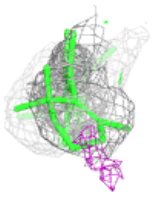


Electron density around BCR AB 618:

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

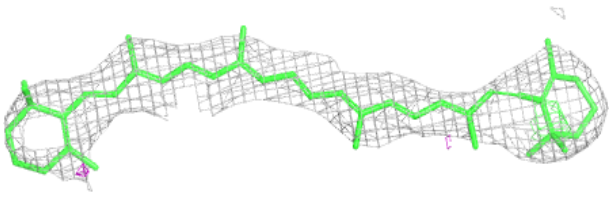


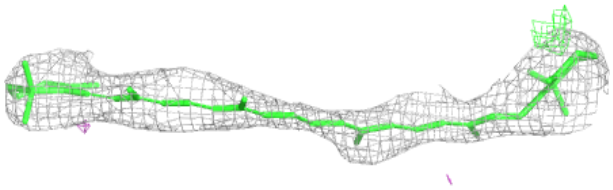


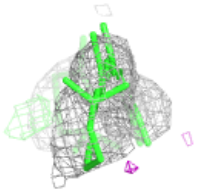


Electron density around BCR AD 406:

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

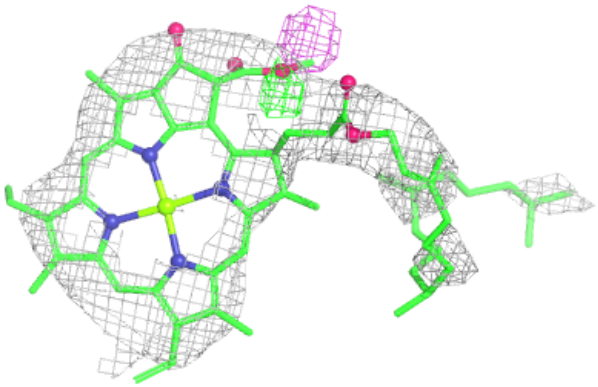


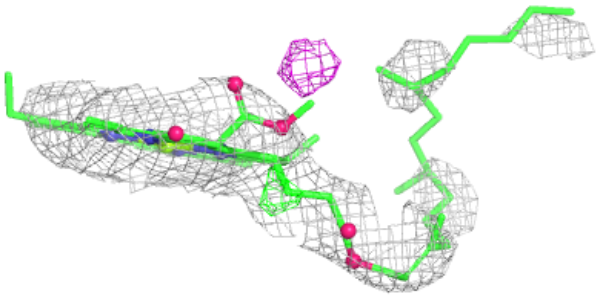


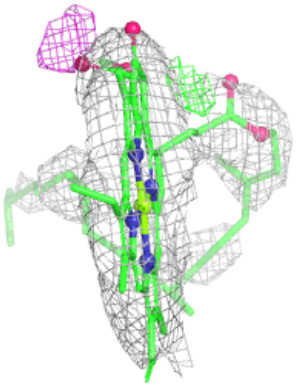


Electron density around CLA AC 512:

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

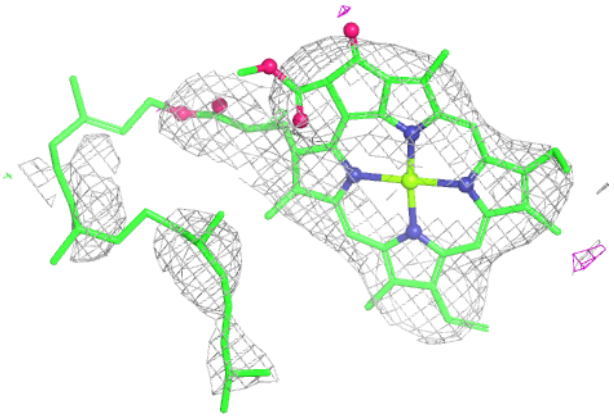


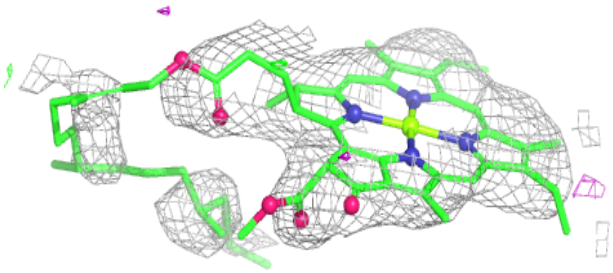




Electron density around CLA BB 5620:

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

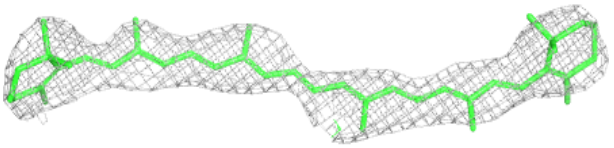


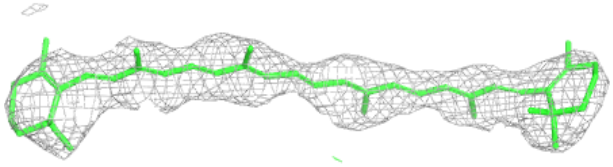


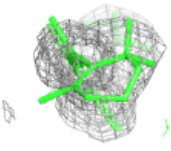


Electron density around BCR AB 619:

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

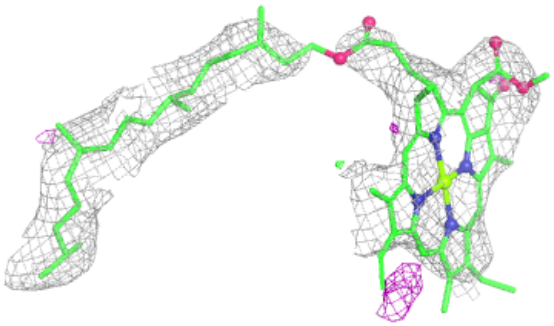


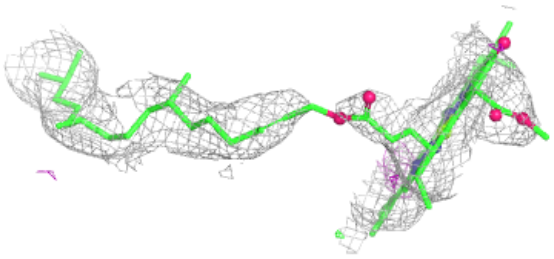


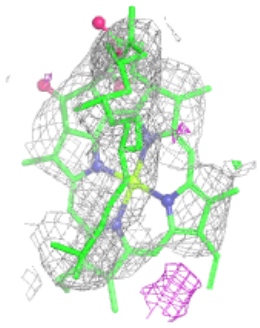


Electron density around CLA AB 609:

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

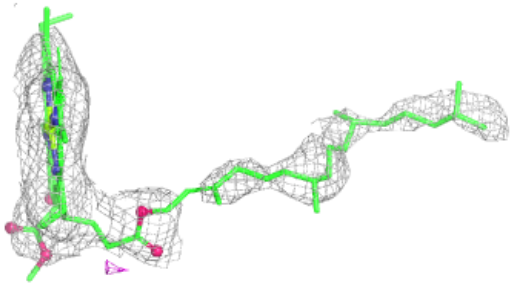


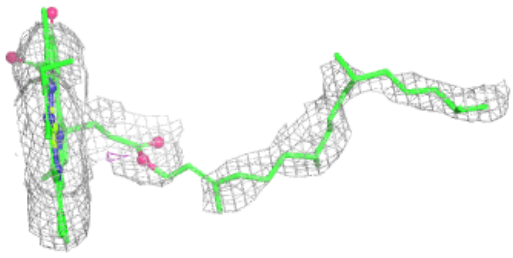


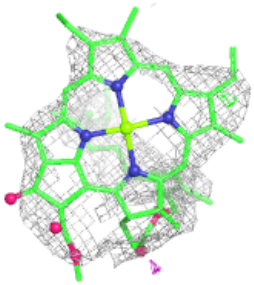


Electron density around CLA BB 5610:

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

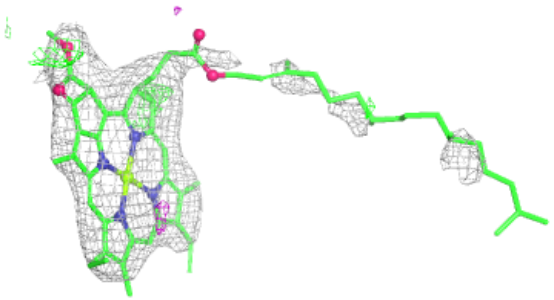


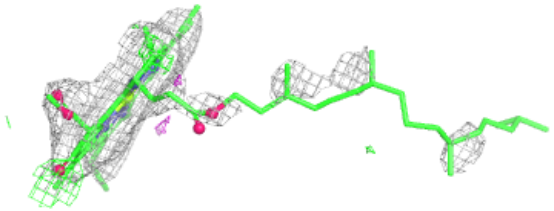


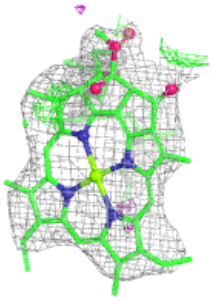


Electron density around CLA AA 407:

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

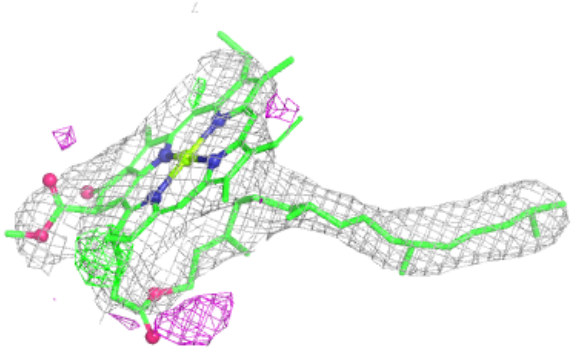


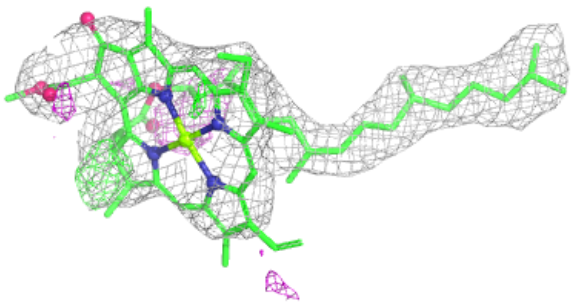


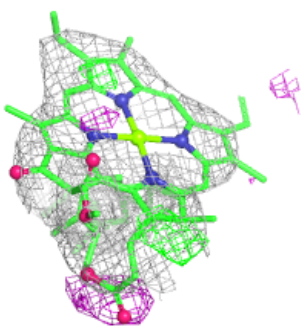


Electron density around CLA AC 505:

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

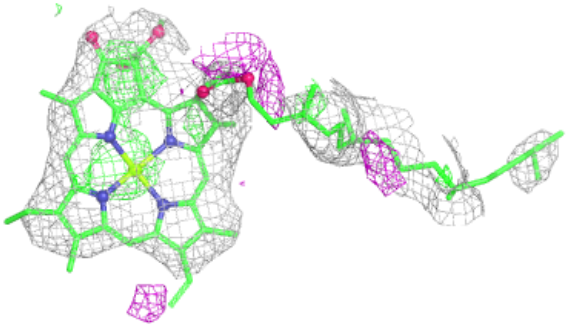


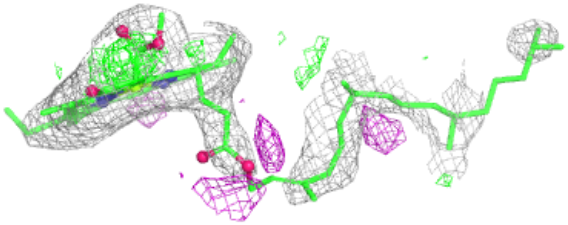


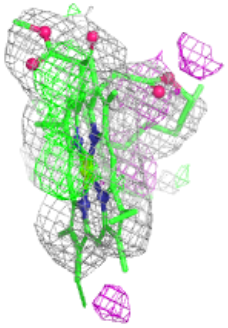


Electron density around CLA AA 406:

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

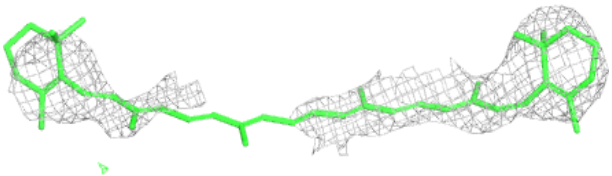


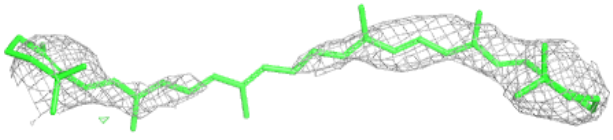


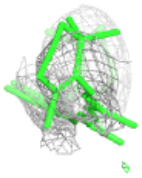


Electron density around BCR BC 5514:

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

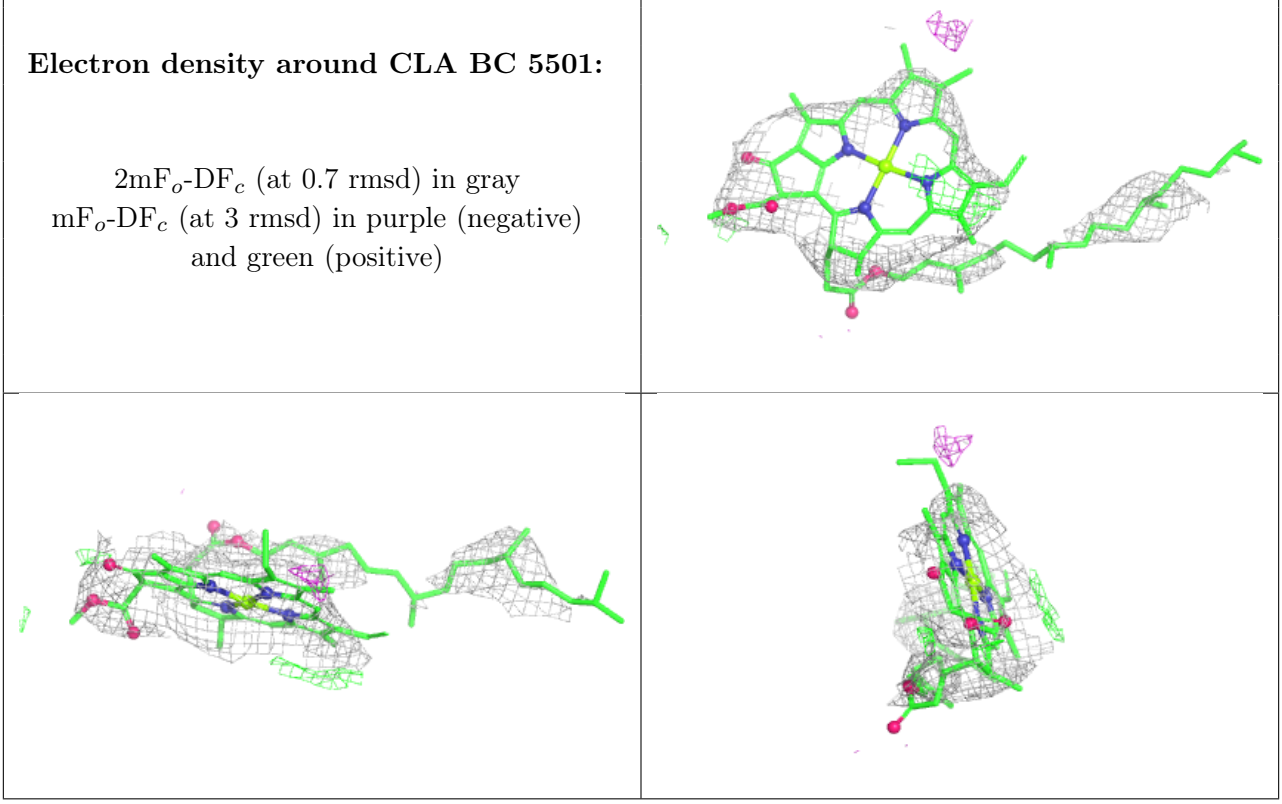






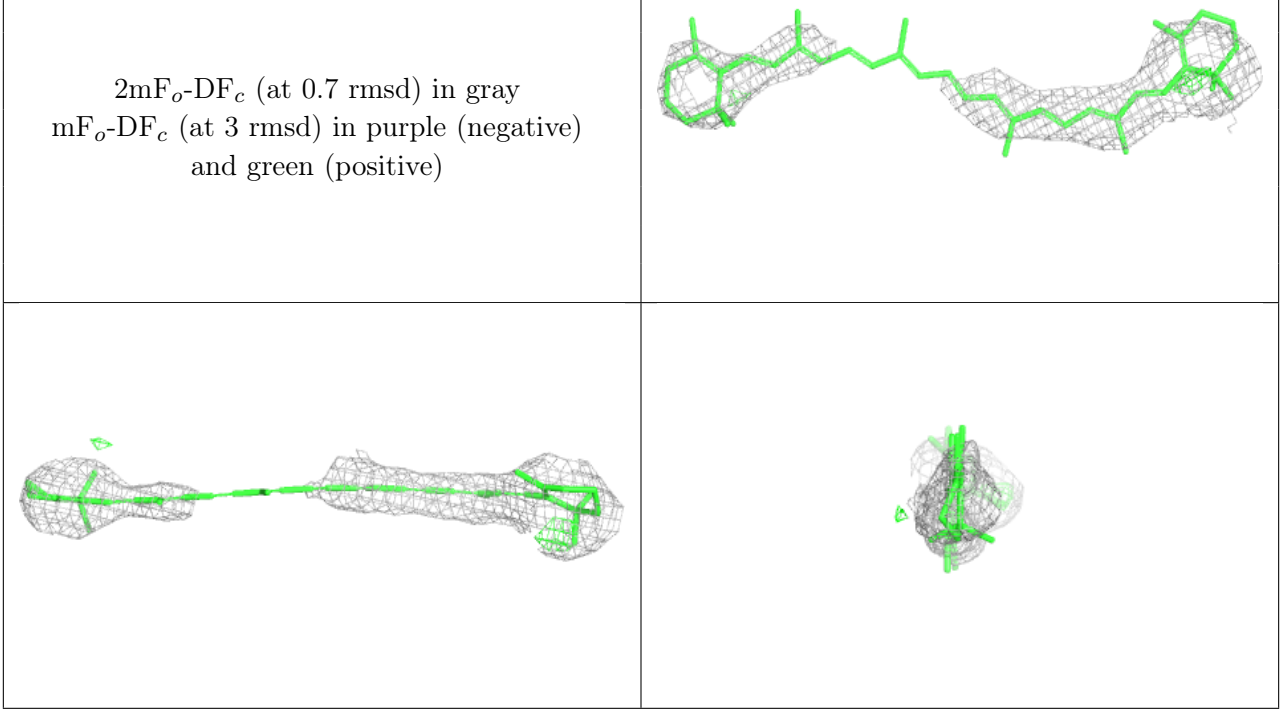
Electron density around CLA BC 5501:

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



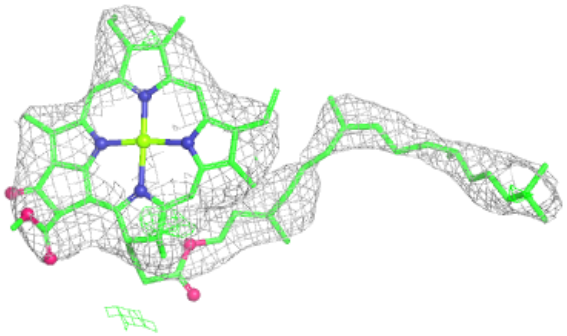
Electron density around BCR AK 102:

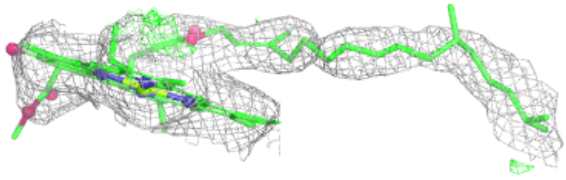
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

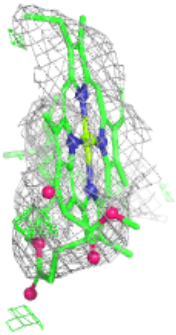


Electron density around CLA BB 5607:

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

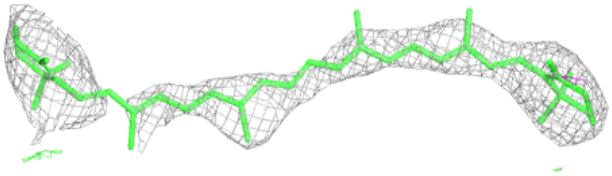


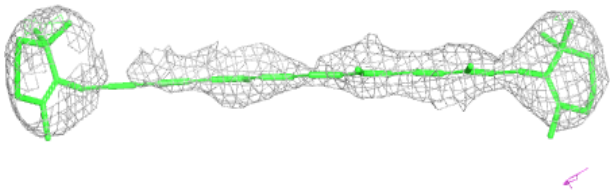


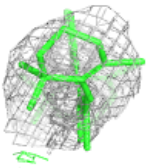


Electron density around BCR BA 5411:

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

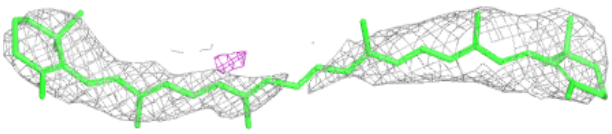


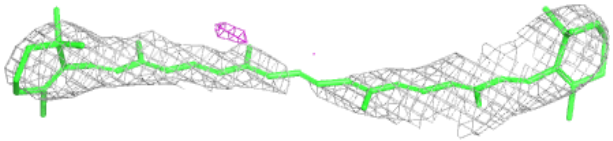


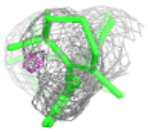


Electron density around BCR BB 5623:

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

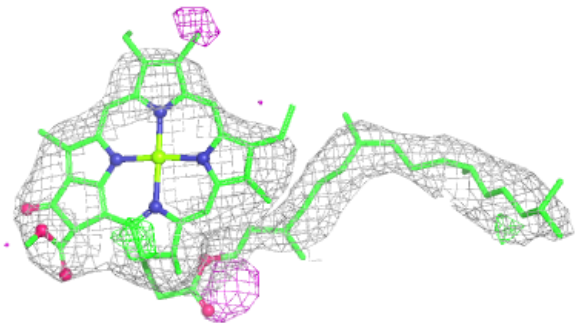


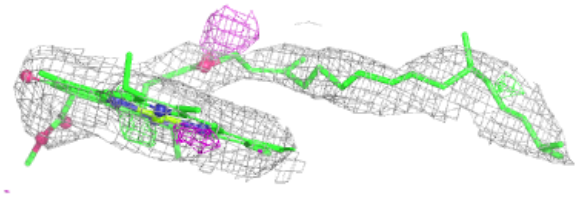


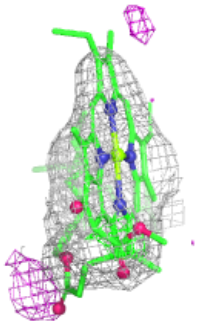


Electron density around CLA AB 603:

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

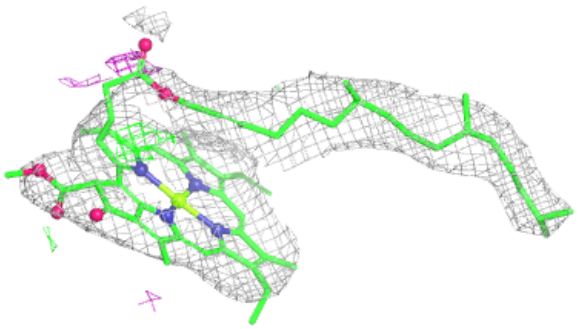


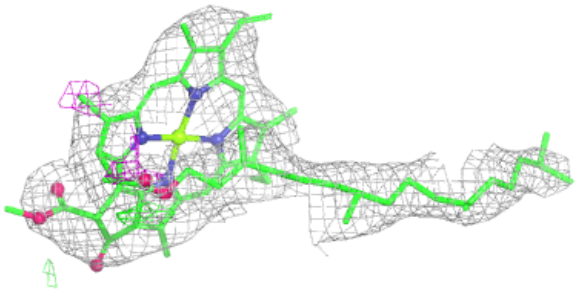


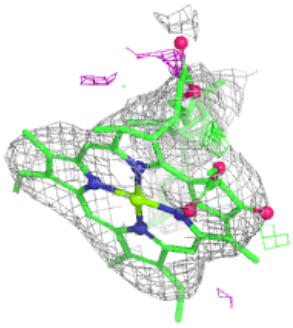


Electron density around CLA BB 5612:

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

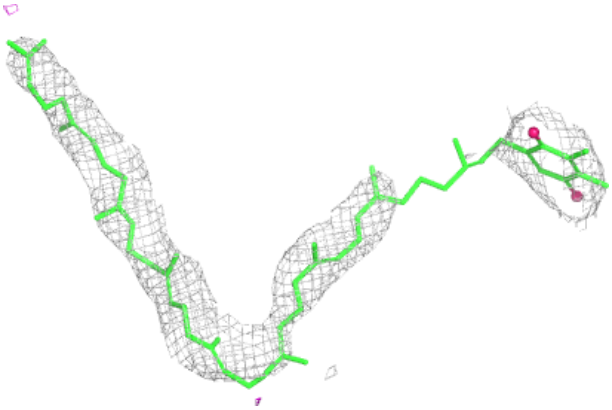


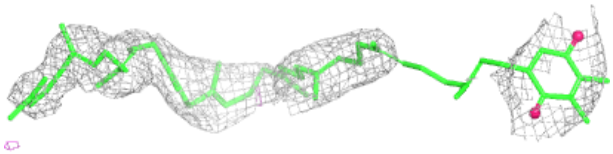




Electron density around PL9 BD 5406:

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

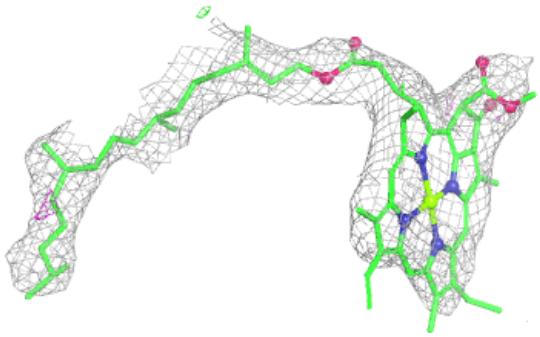


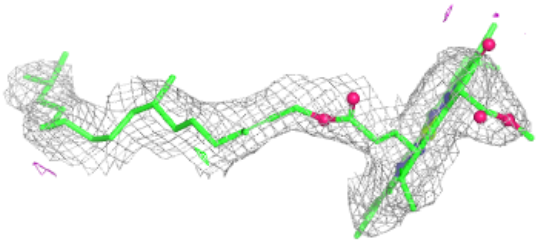


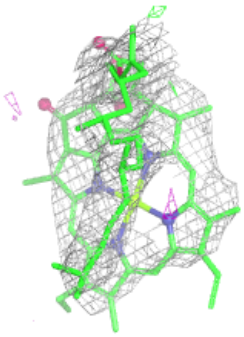


Electron density around CLA BB 5613:

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

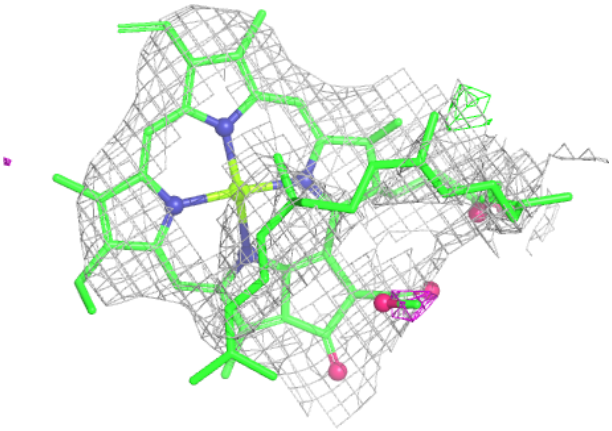


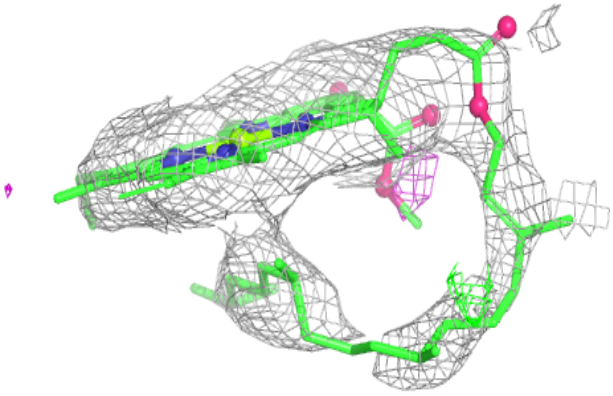


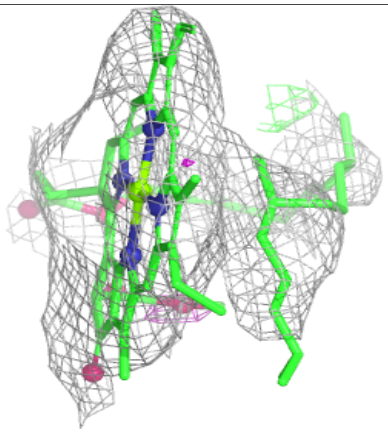


Electron density around CLA BC 5510:

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

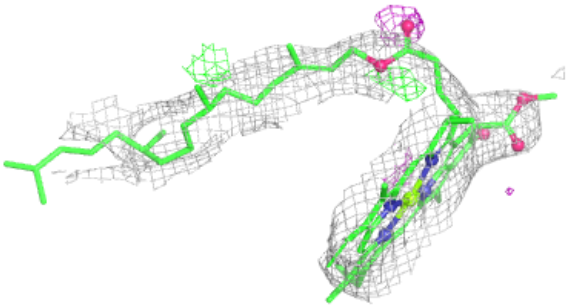


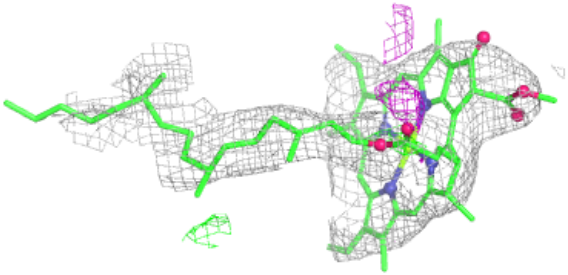


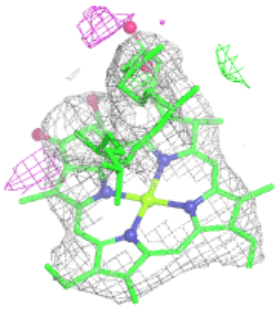


Electron density around CLA AC 504:

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

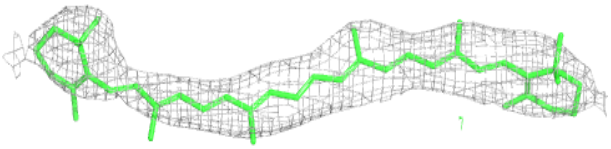


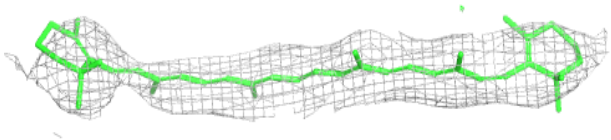




Electron density around BCR AC 516:

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

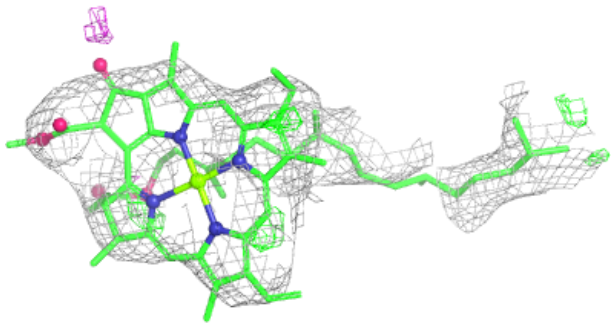


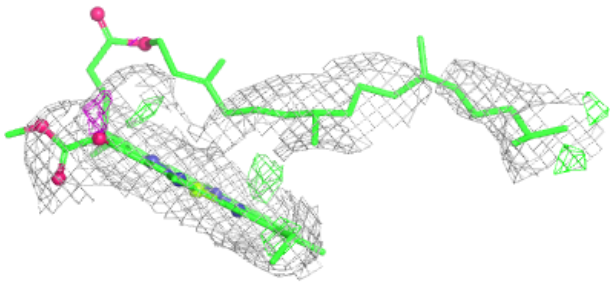


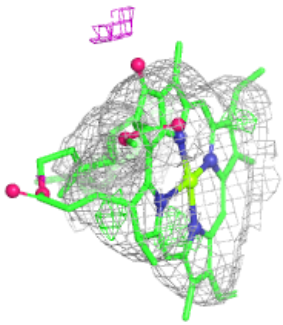


Electron density around CLA AB 614:

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

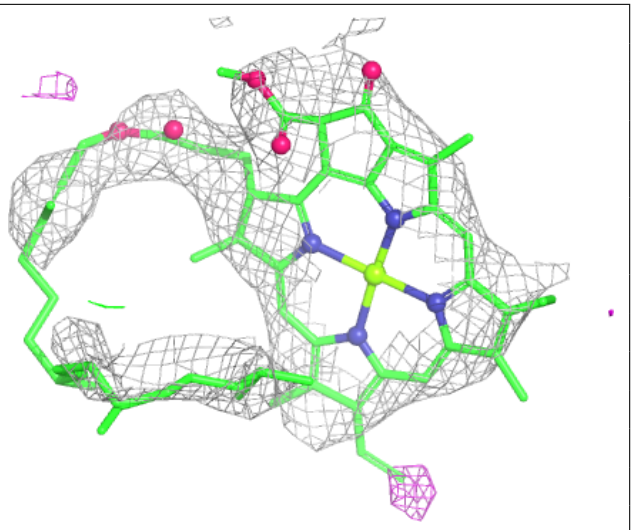


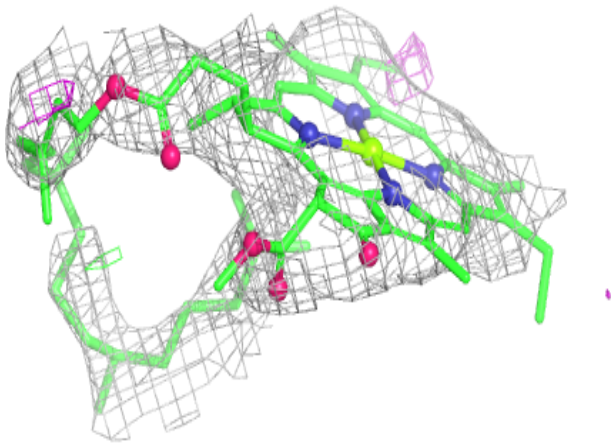


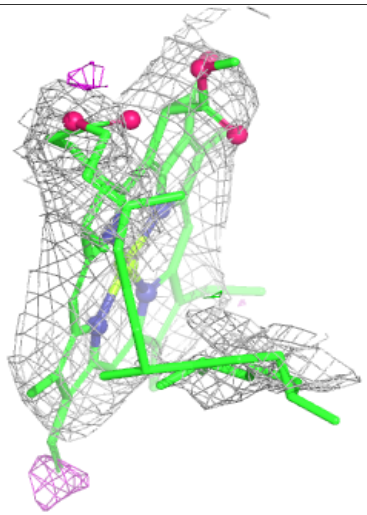


Electron density around CLA AB 615:

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

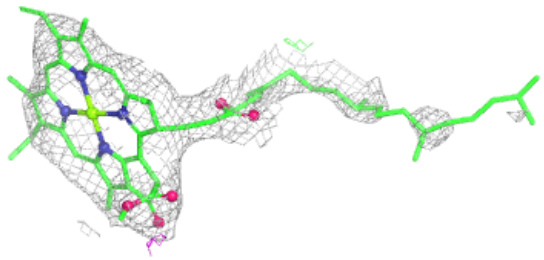


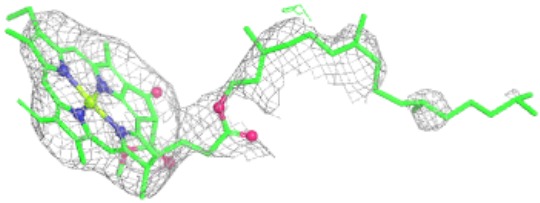


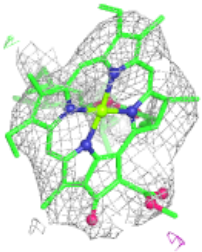


Electron density around CLA BC 5502:

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

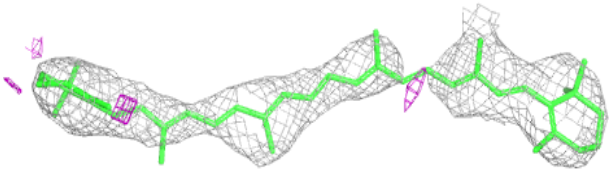


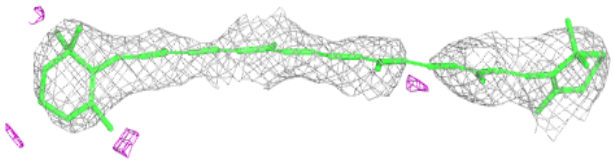


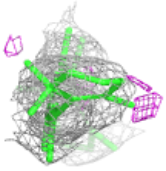


Electron density around BCR BB 5621:

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

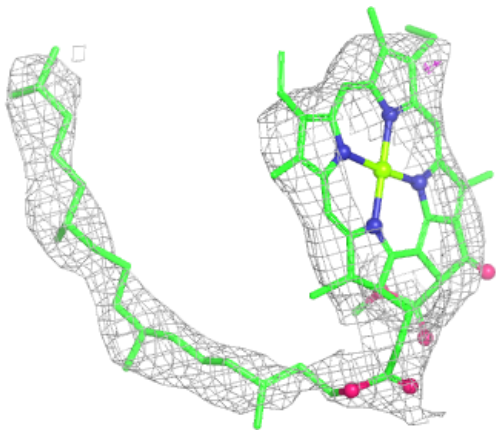


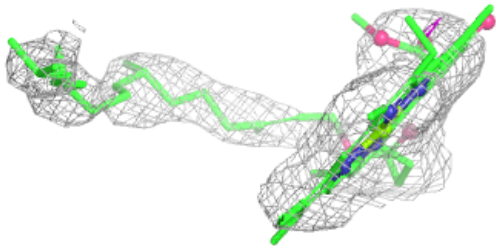


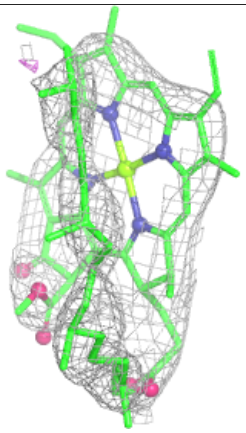


Electron density around CLA BC 5507:

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

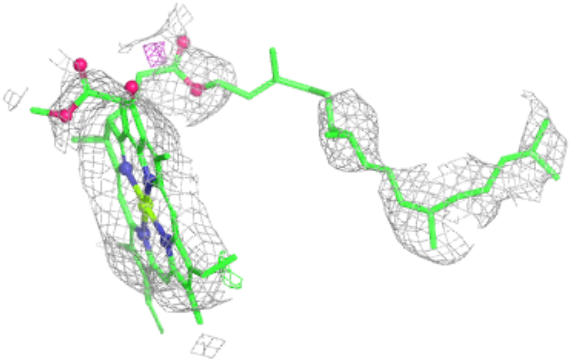


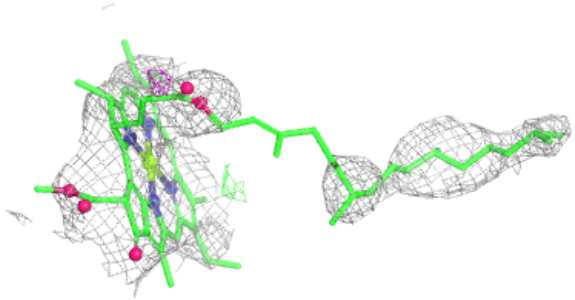


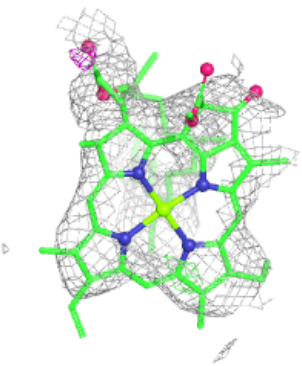


Electron density around CLA BC 5508:

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

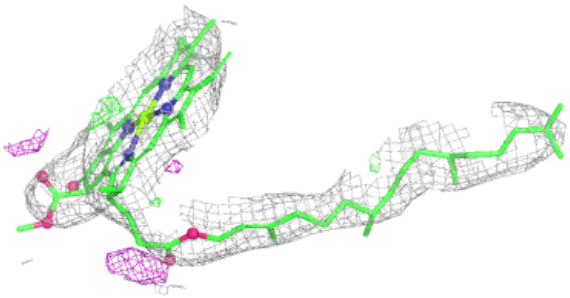


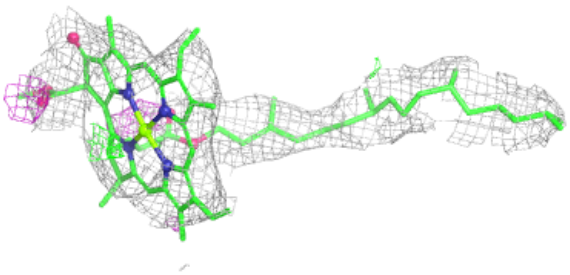


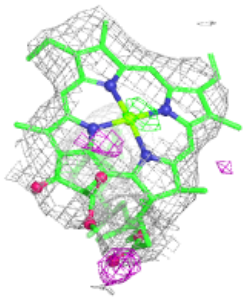


Electron density around CLA BB 5611:

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

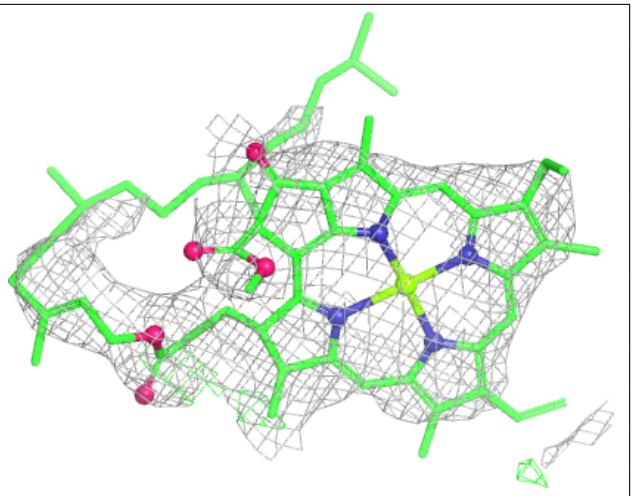


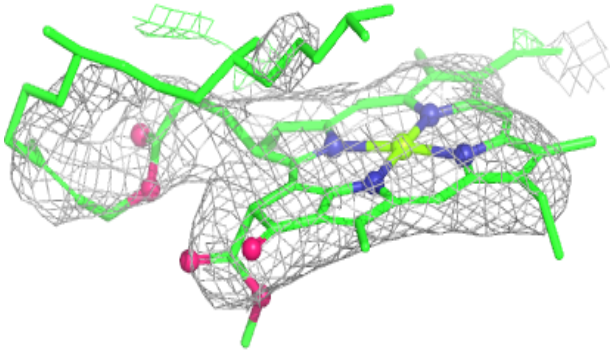


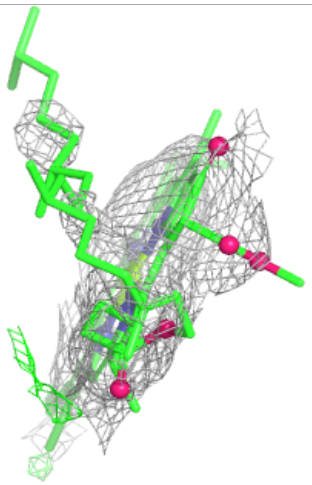


Electron density around CLA BC 5509:

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

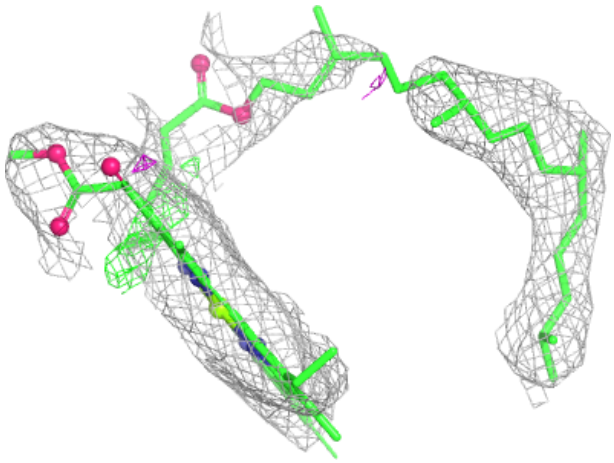


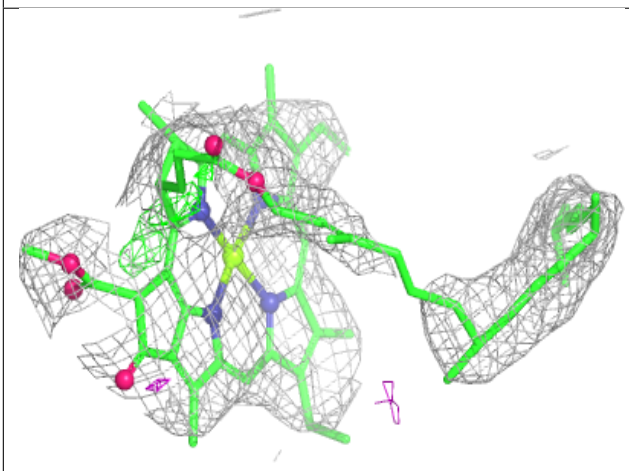


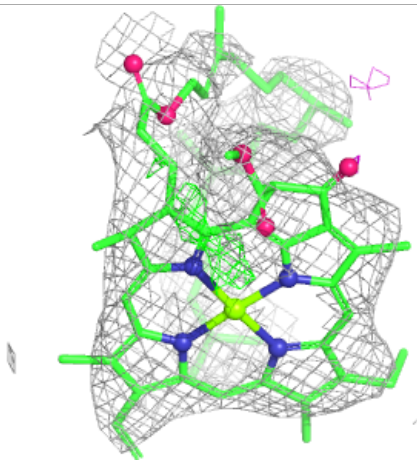


Electron density around CLA AB 611:

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

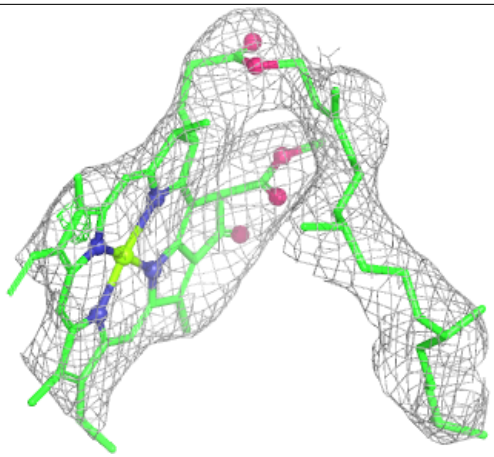


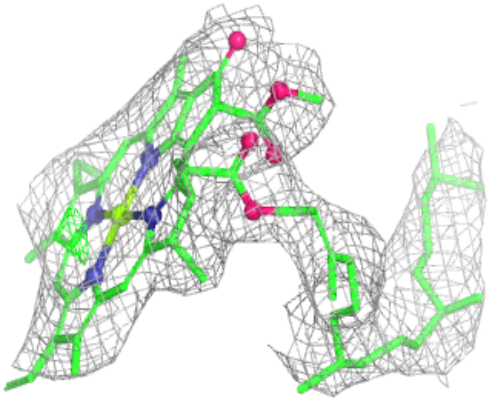


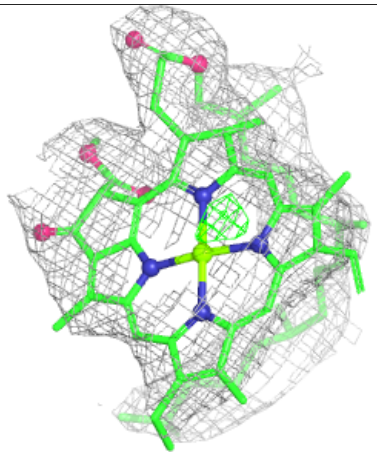


Electron density around CLA AB 613:

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

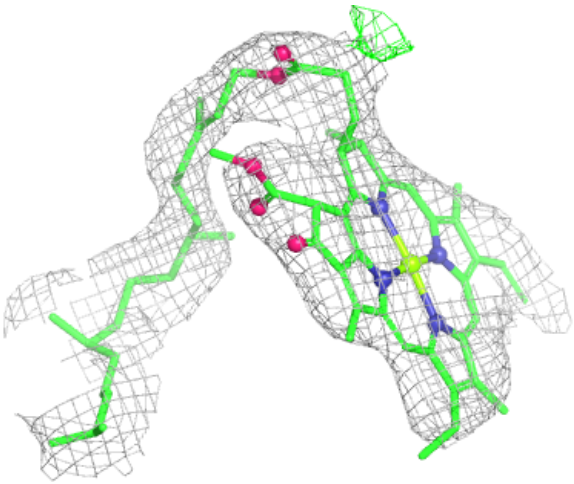


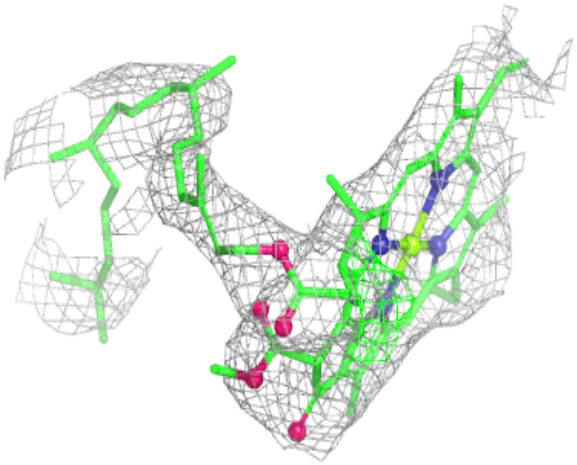


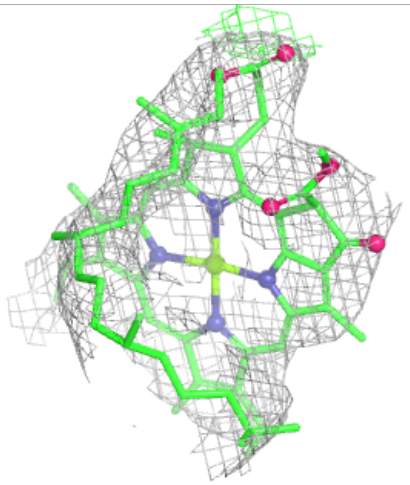


Electron density around CLA BB 5617:

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

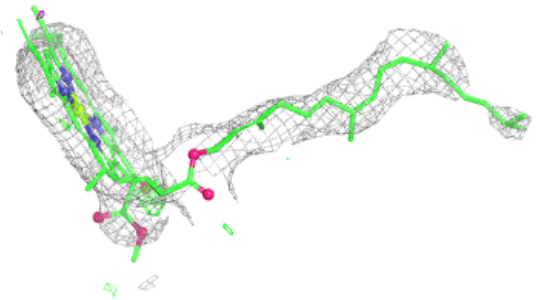


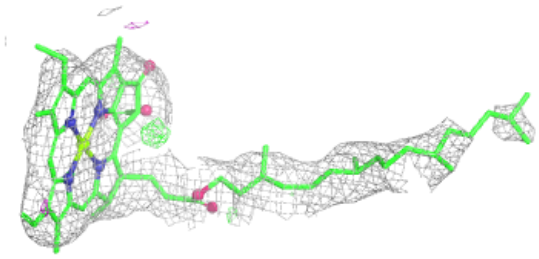


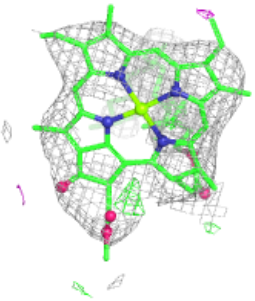


Electron density around CLA AB 604:

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

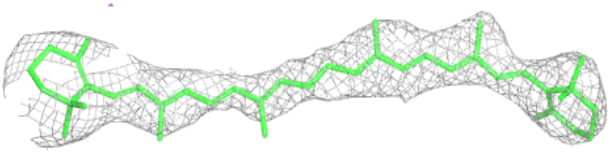


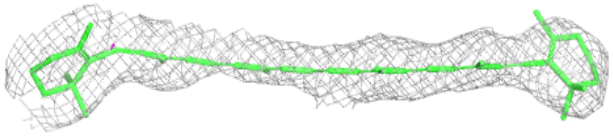


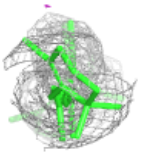


Electron density around BCR BB 5622:

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

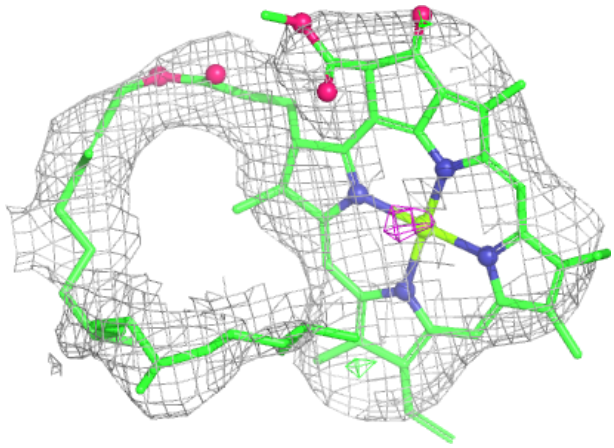


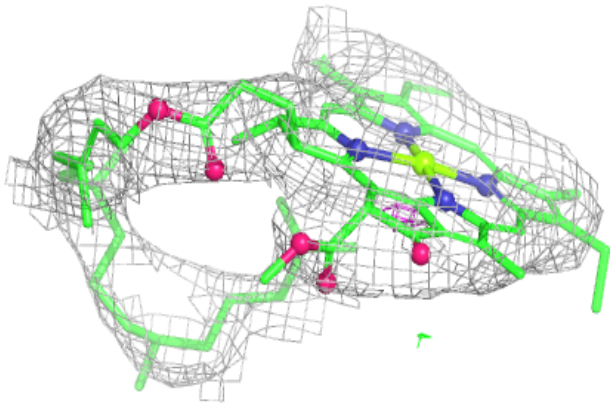




Electron density around CLA BB 5619:

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

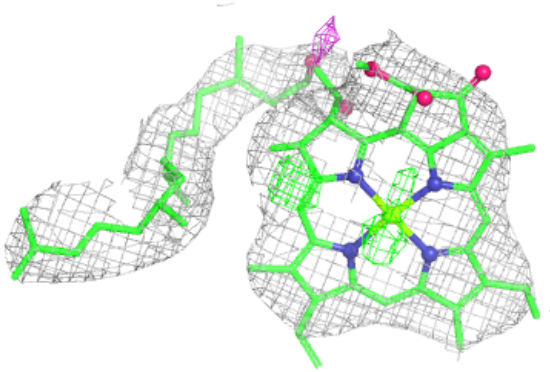


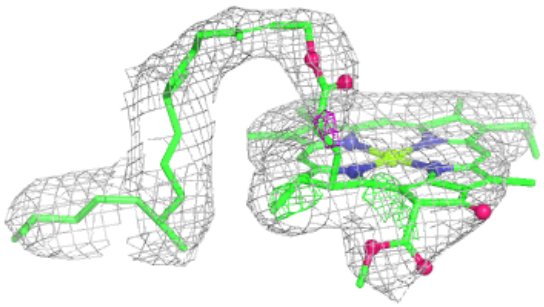


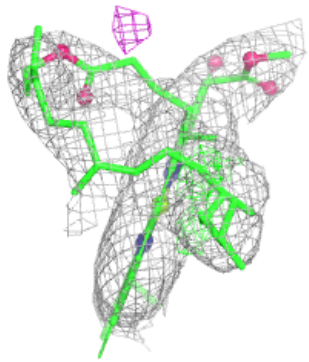


Electron density around CLA BA 5406:

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

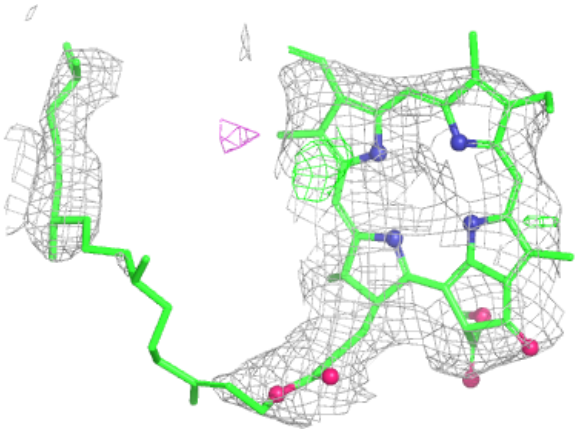


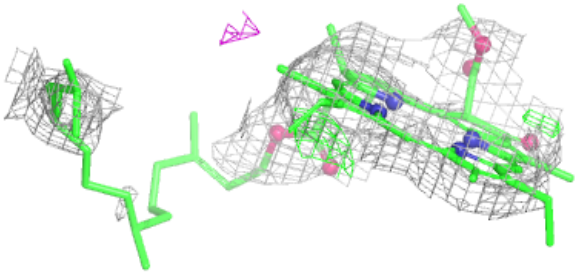




Electron density around PHO BD 5404:

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

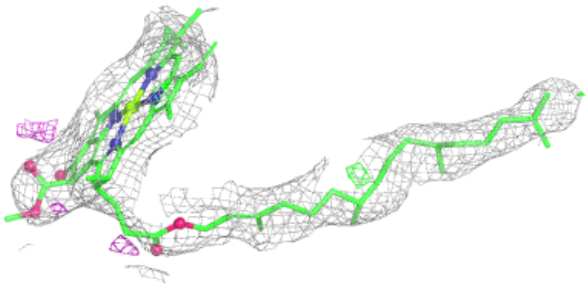


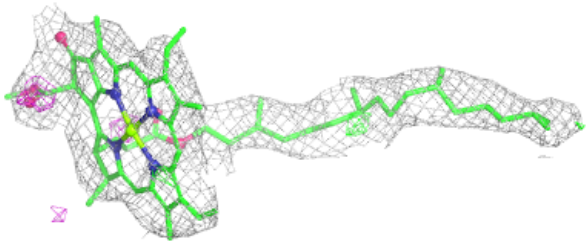


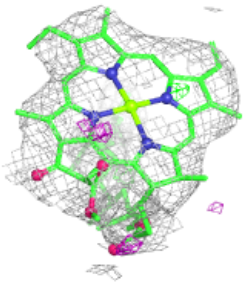


Electron density around CLA AB 607:

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

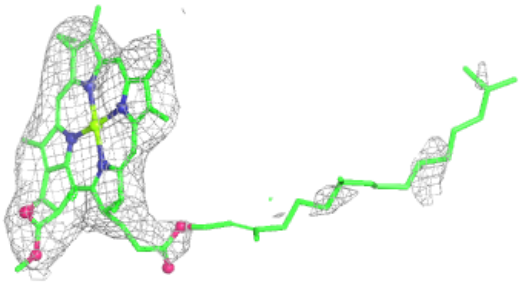


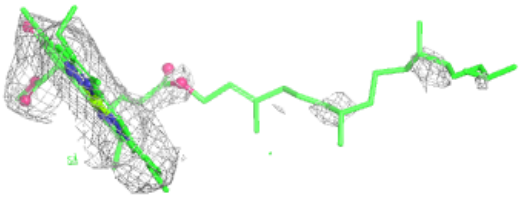


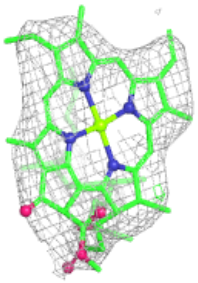


Electron density around CLA BA 5408:

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

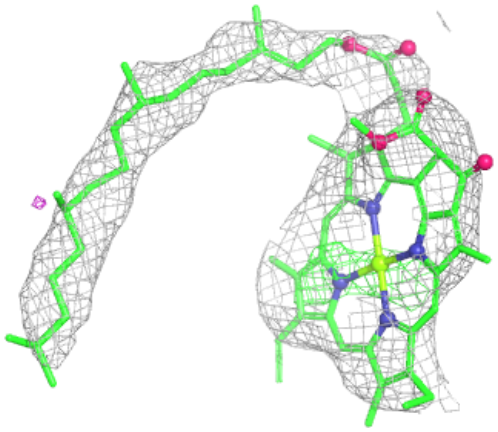


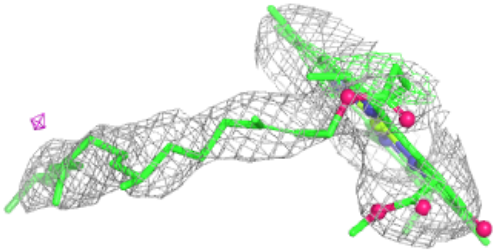


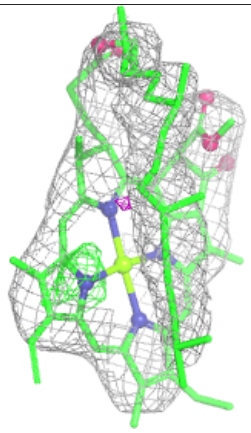


Electron density around CLA AC 507:

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

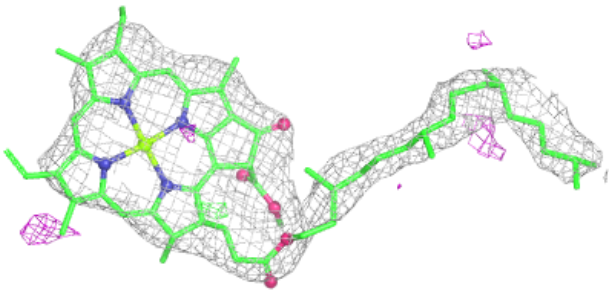


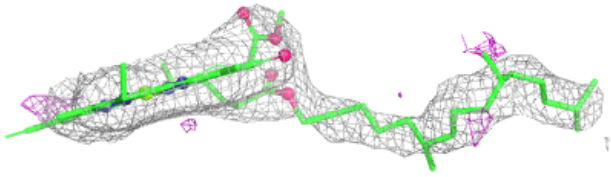


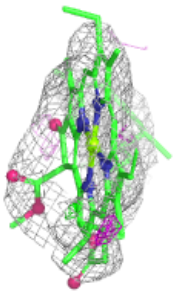


Electron density around CLA BB 5606:

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

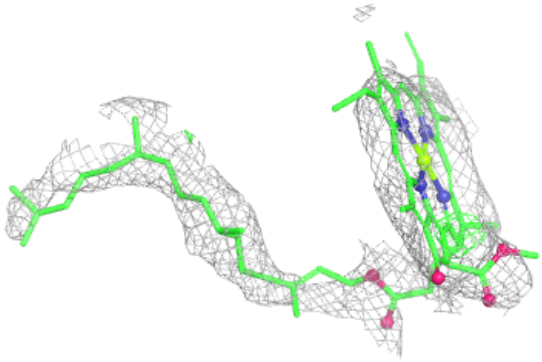


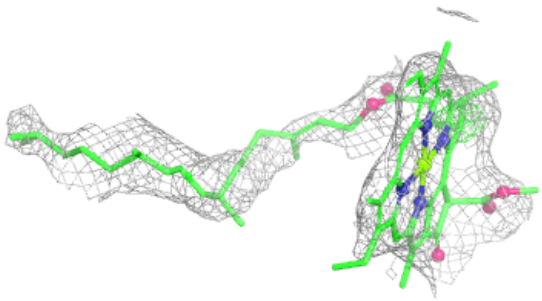


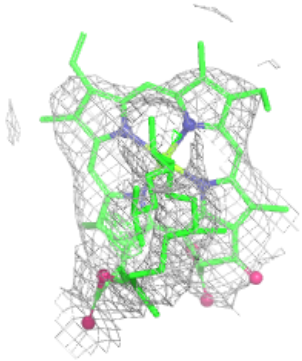


Electron density around CLA AC 508:

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

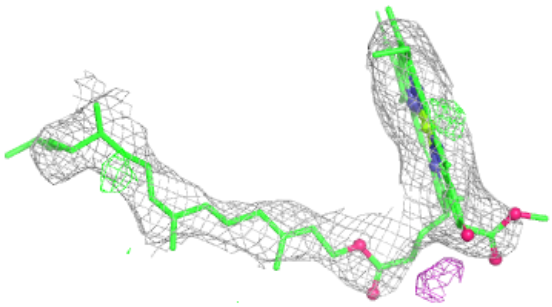


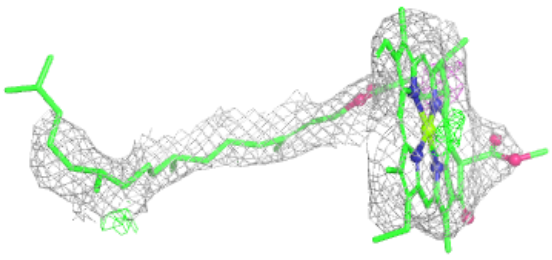


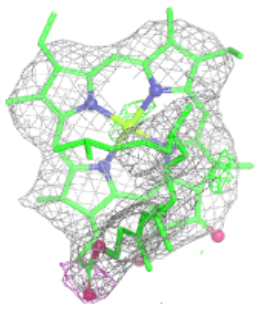


Electron density around CLA BB 5609:

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

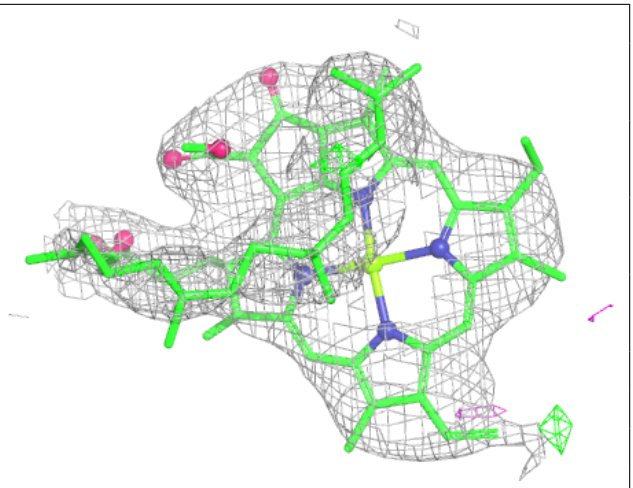




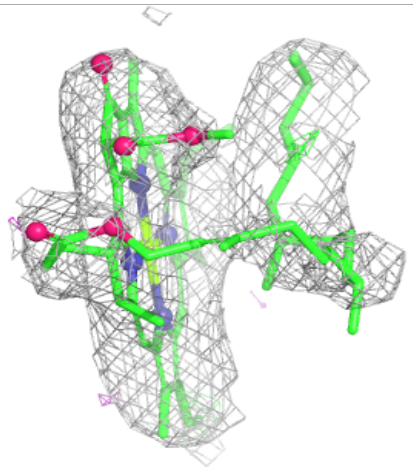


Electron density around CLA AC 510:

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

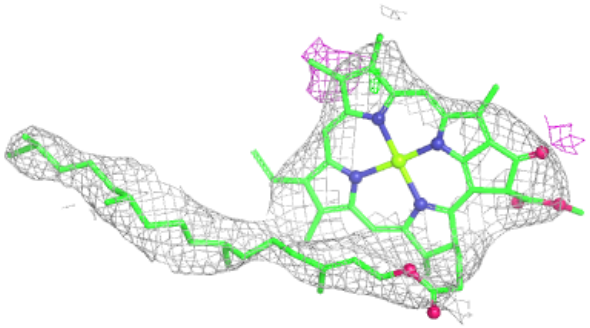


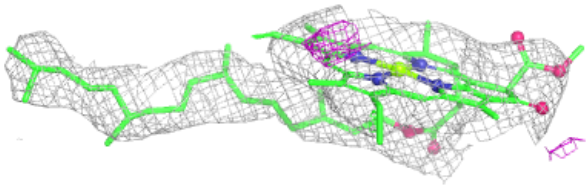


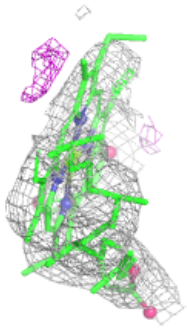


Electron density around CLA AC 501:

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

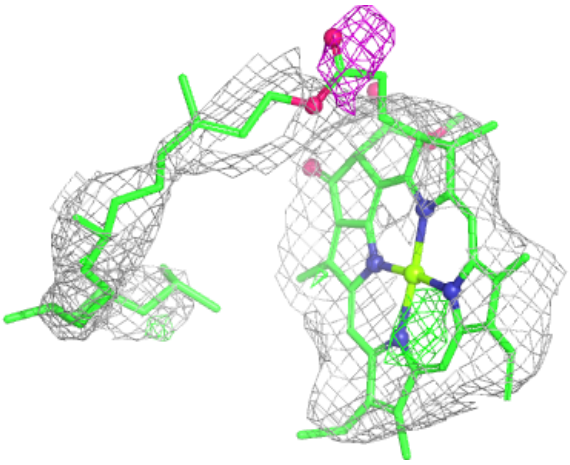


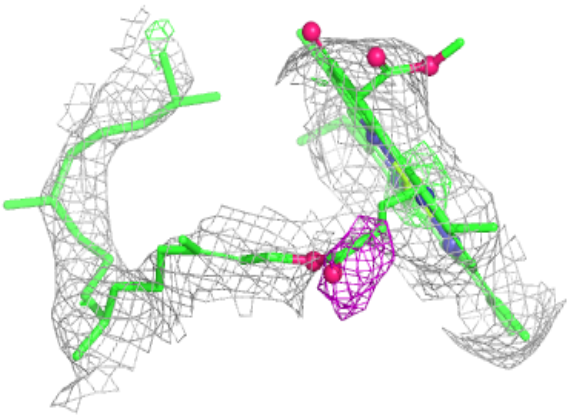


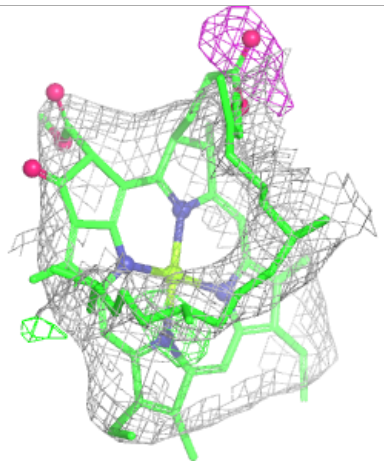


Electron density around CLA AC 503:

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

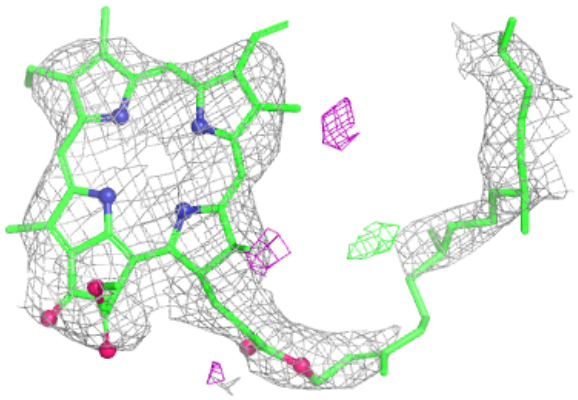


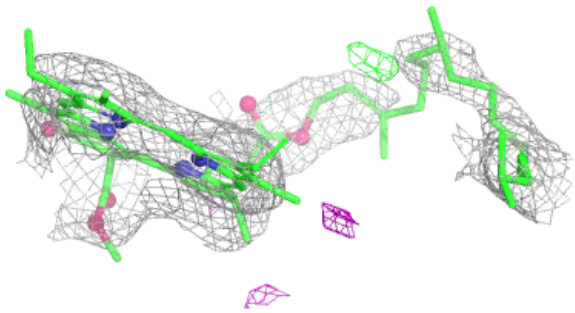


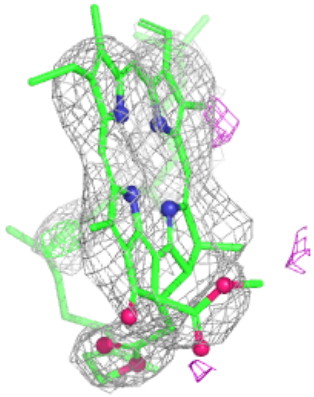


Electron density around PHO AD 403:

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

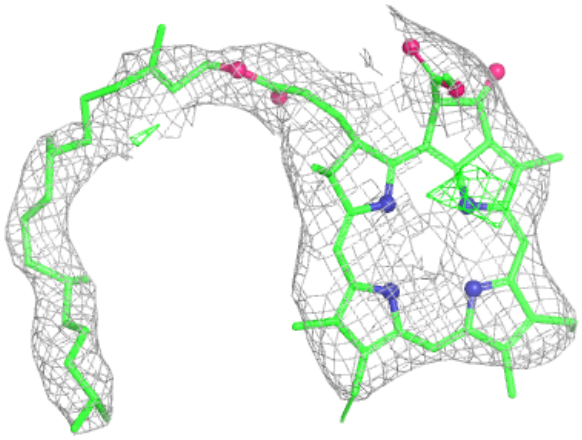


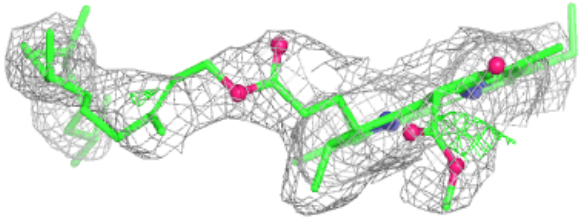


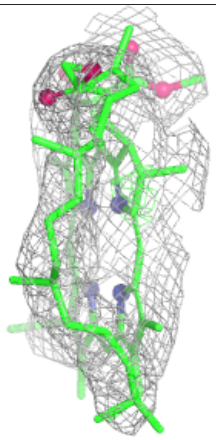


Electron density around PHO BD 5403:

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

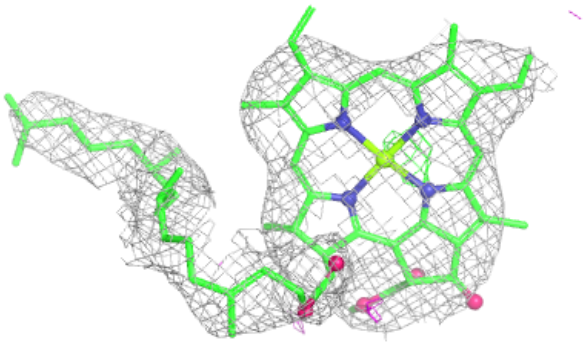


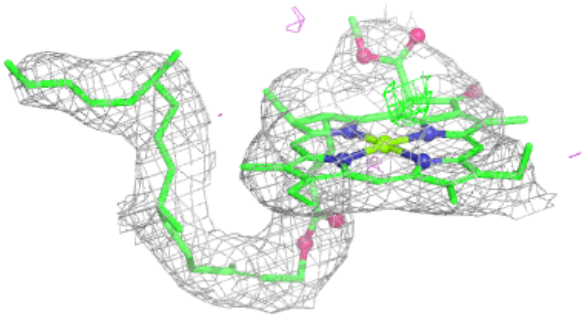


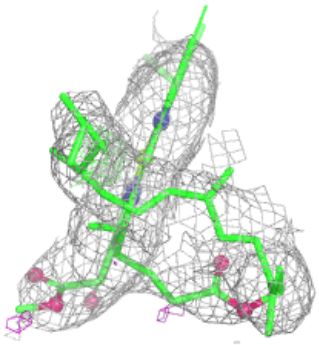


Electron density around CLA AA 405:

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

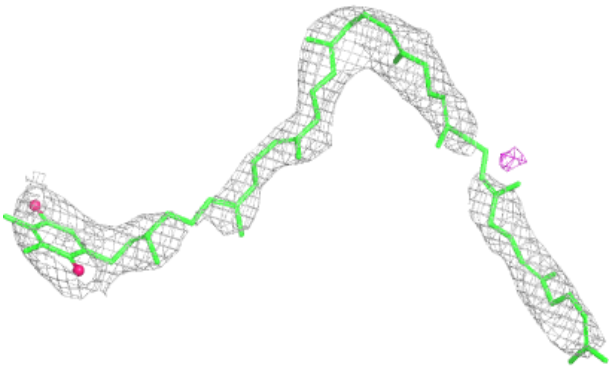


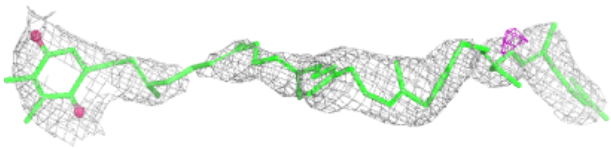




Electron density around PL9 AD 405:

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

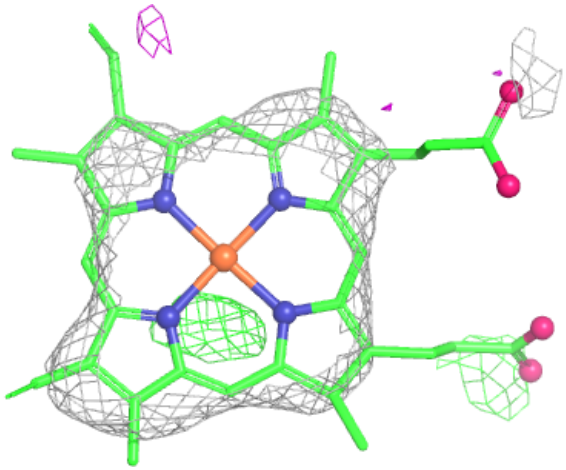


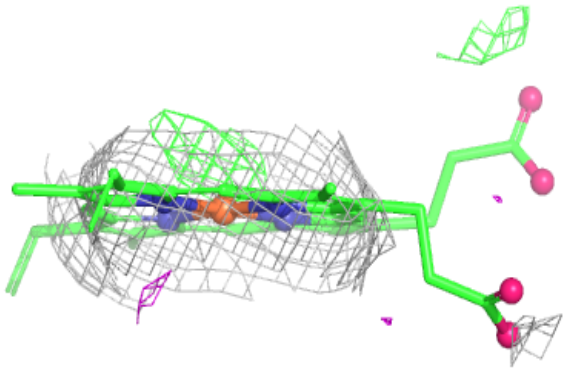


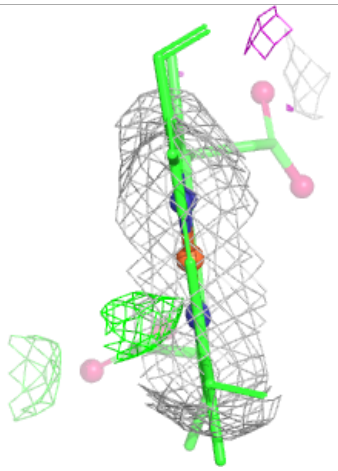


Electron density around HEM AF 101:

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

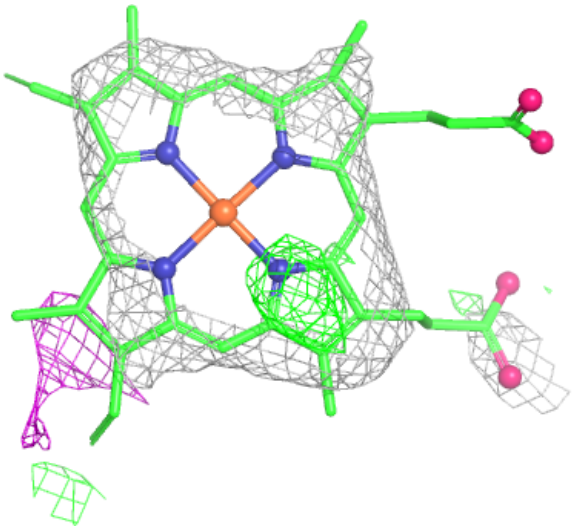


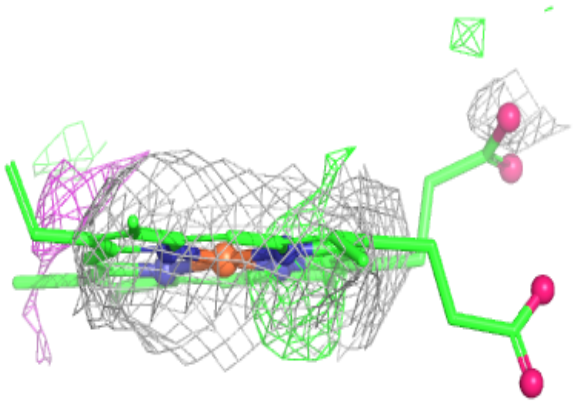


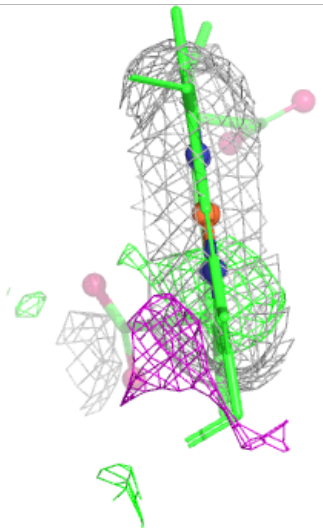


Electron density around HEM BF 5101:

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

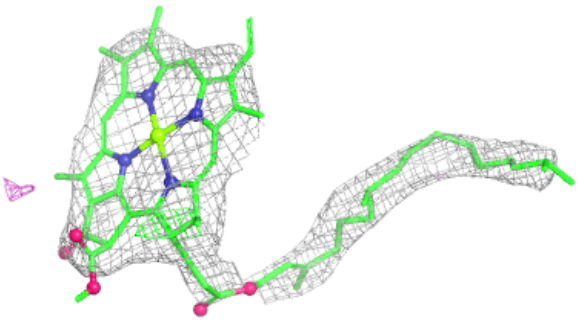


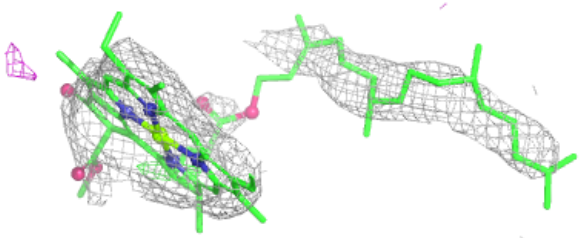


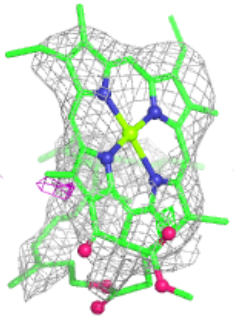


Electron density around CLA AC 511:

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

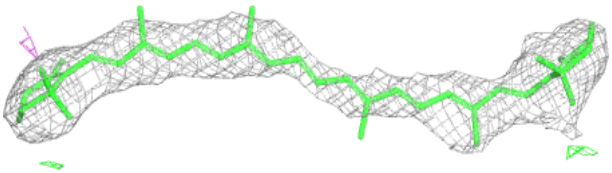


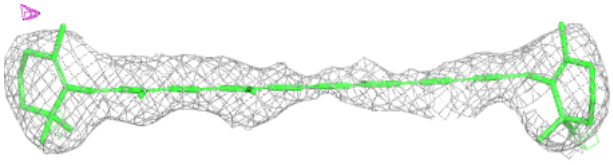


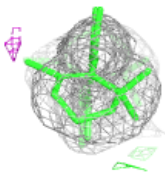


Electron density around BCR AA 410:

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

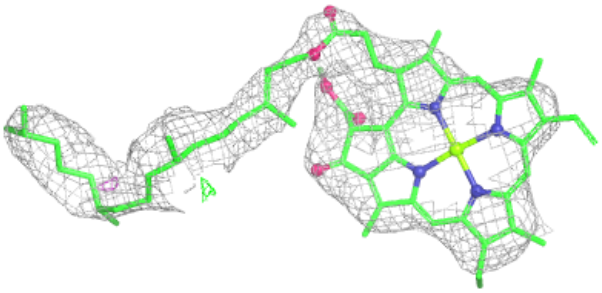


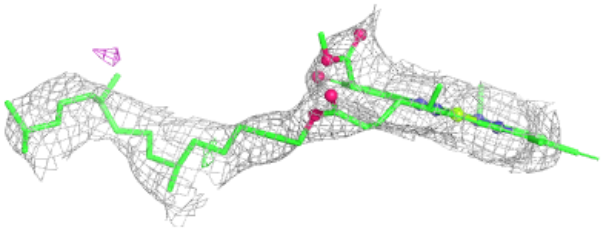


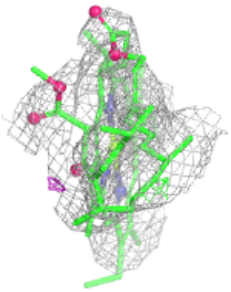


Electron density around CLA AB 602:

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

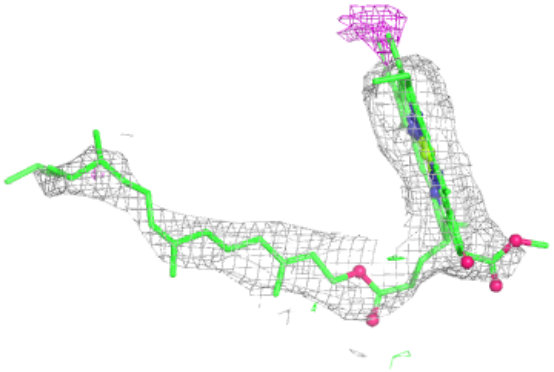


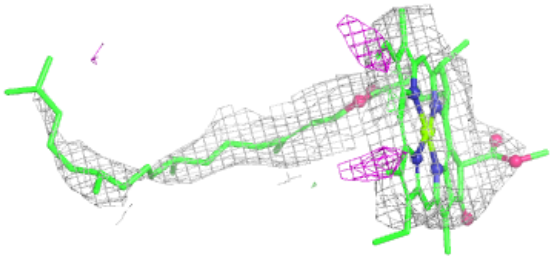


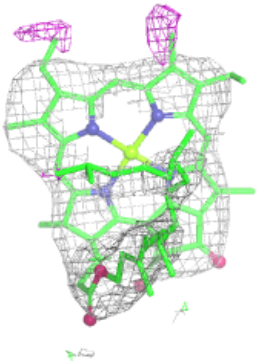


Electron density around CLA AB 605:

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

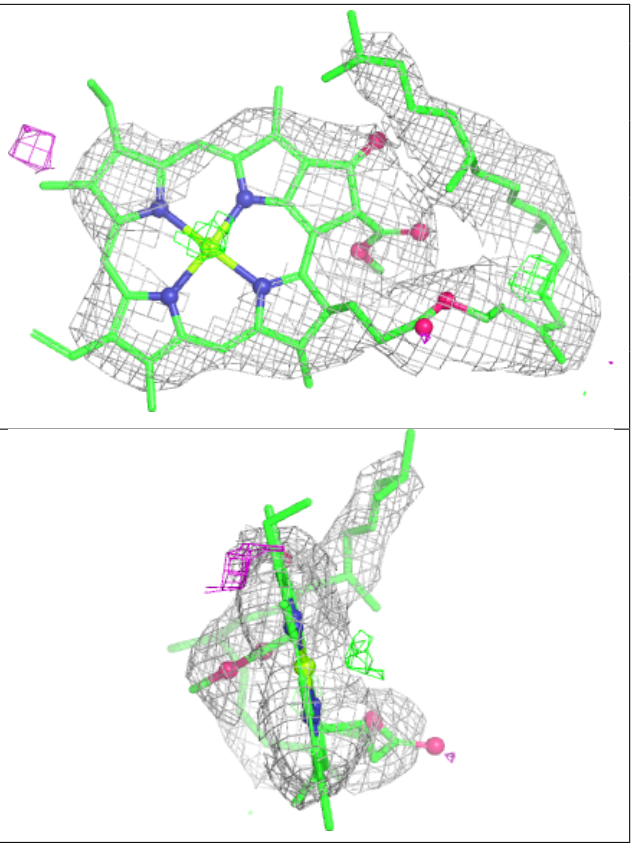


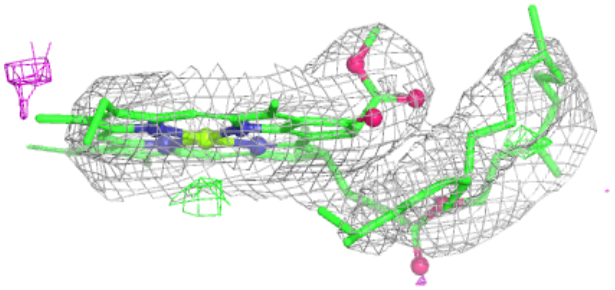




Electron density around CLA BB 5614:

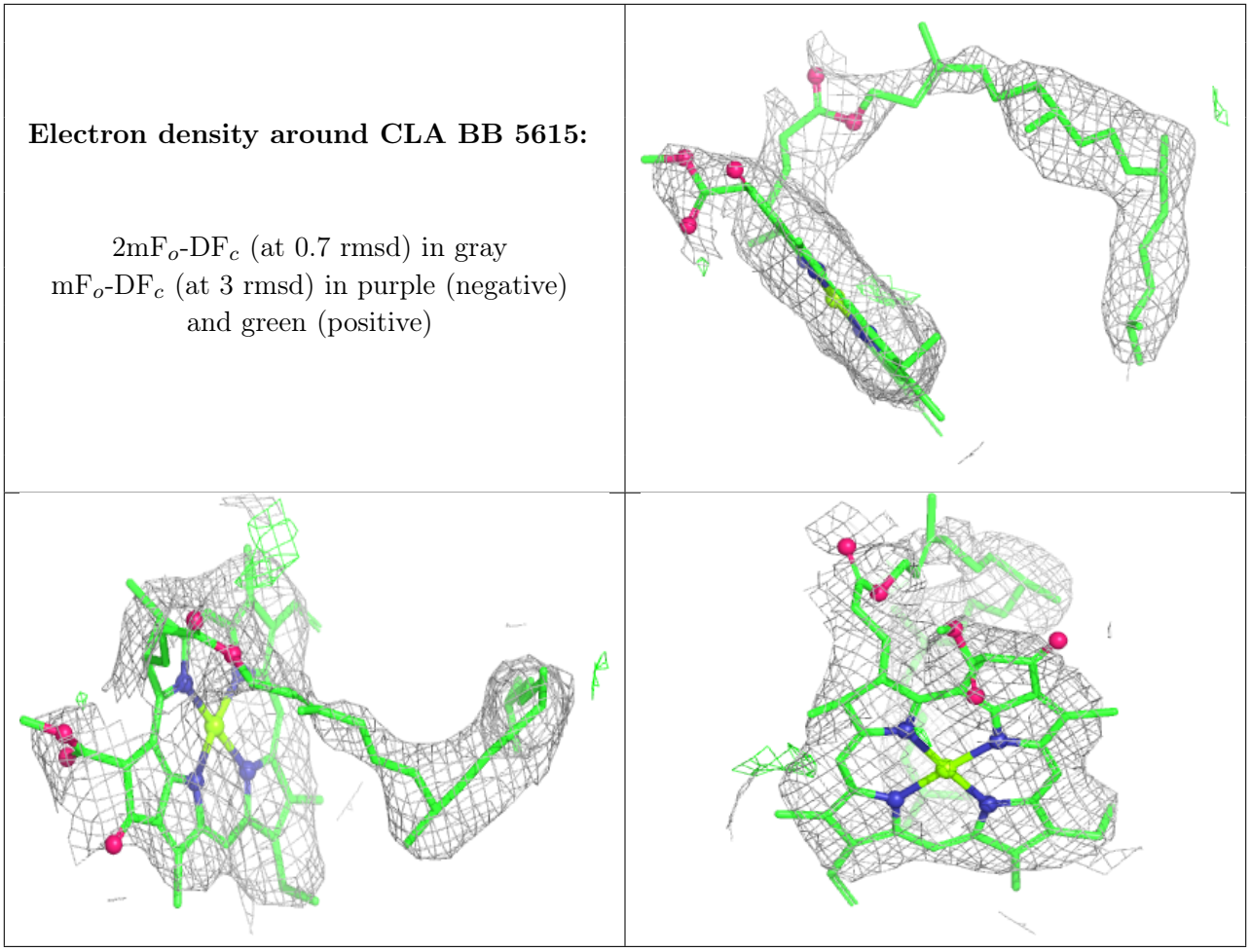
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





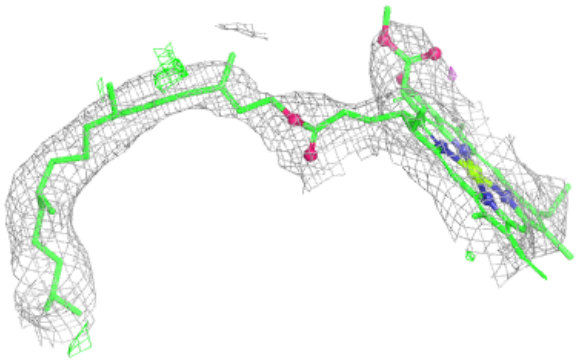
Electron density around CLA BB 5615:

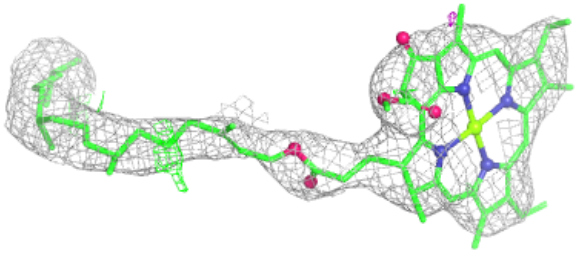
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA AD 401:

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

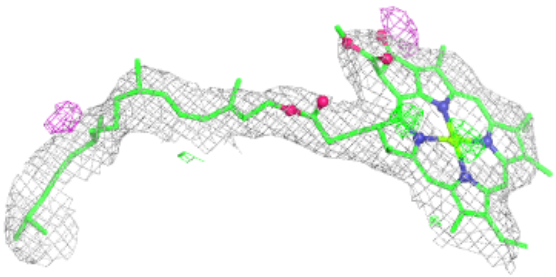


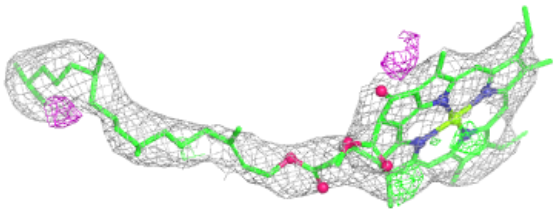


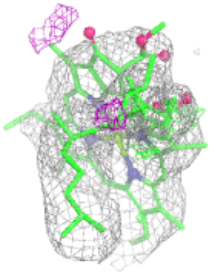


Electron density around CLA AA 404:

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

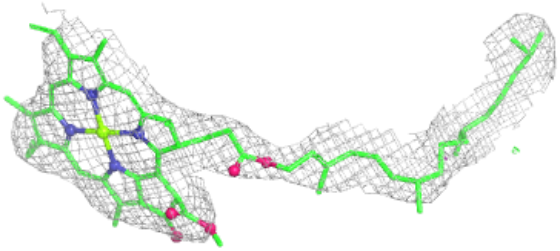


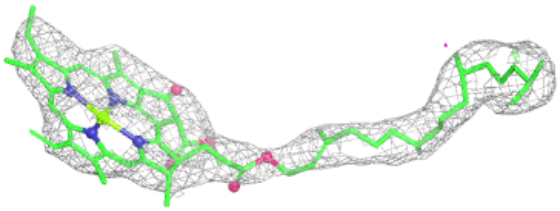


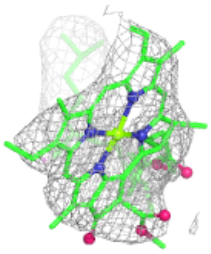


Electron density around CLA BA 5405:

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

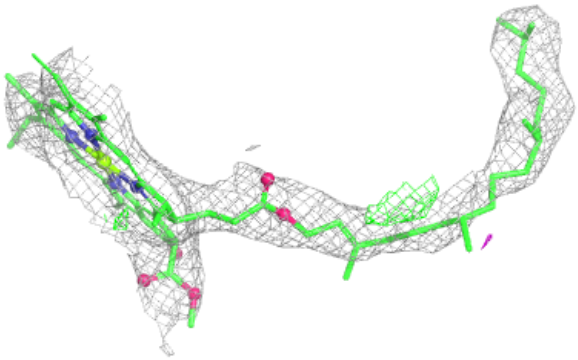


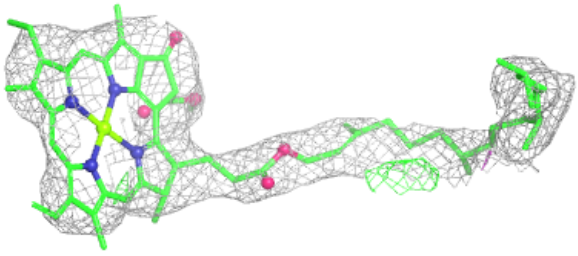


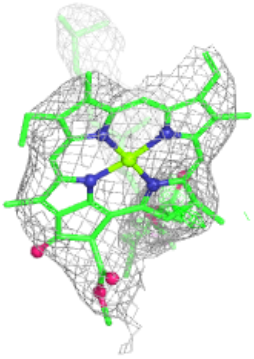


Electron density around CLA BD 5402:

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

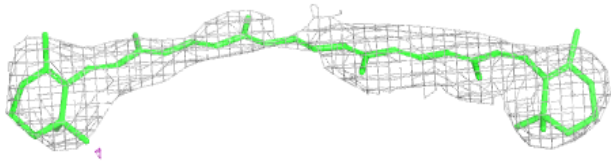




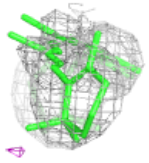


Electron density around BCR AC 514:

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

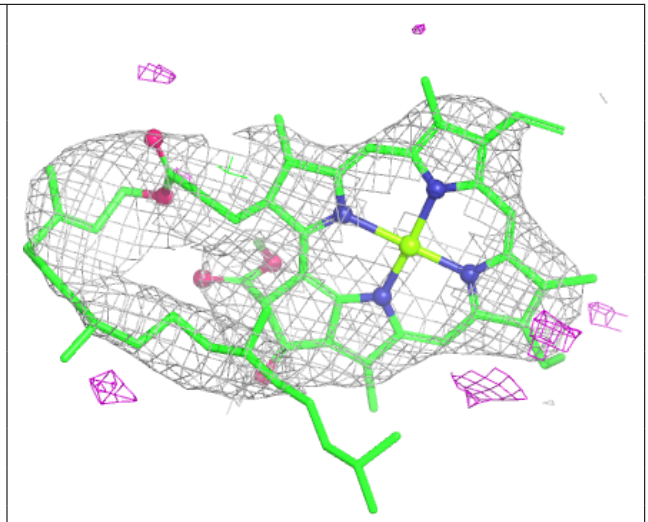


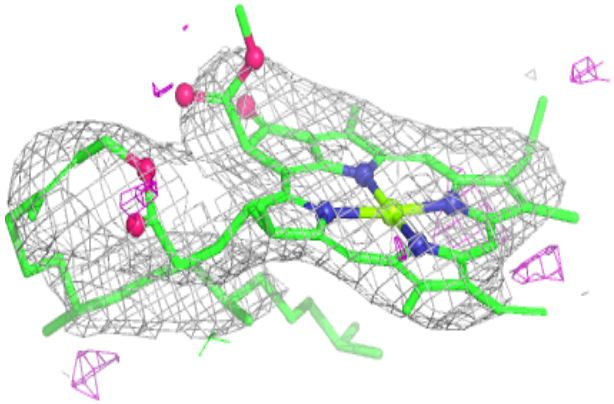


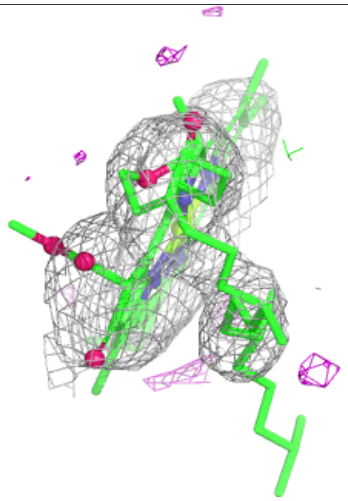


Electron density around CLA AC 509:

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

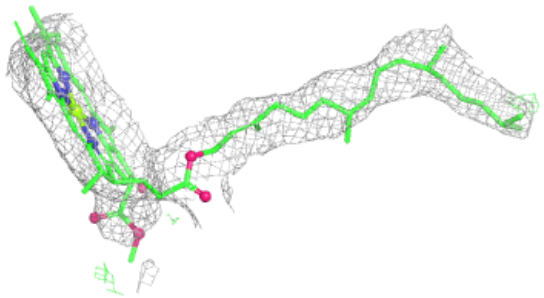


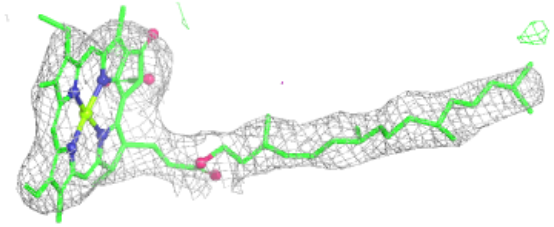


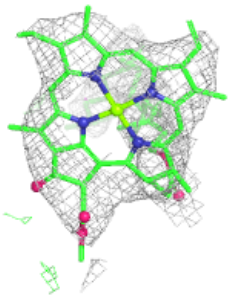


Electron density around CLA BB 5608:

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

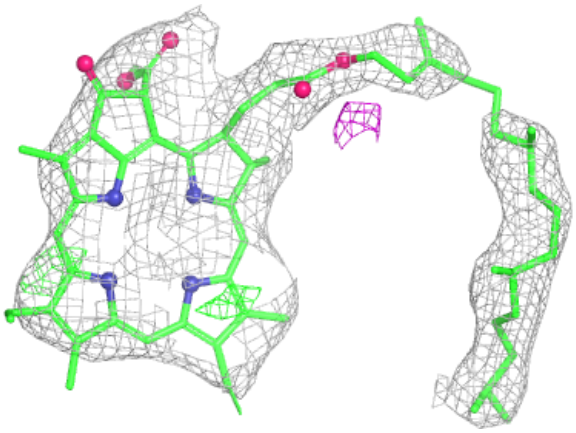


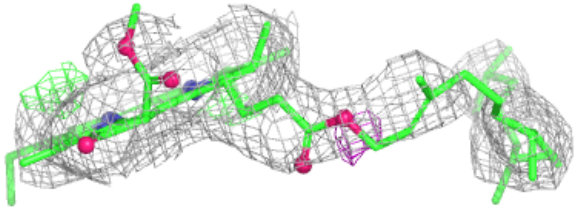


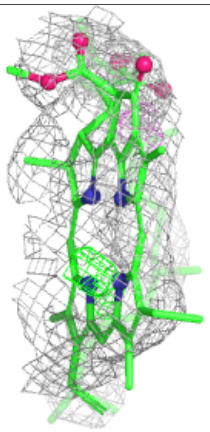


Electron density around PHO AD 402:

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

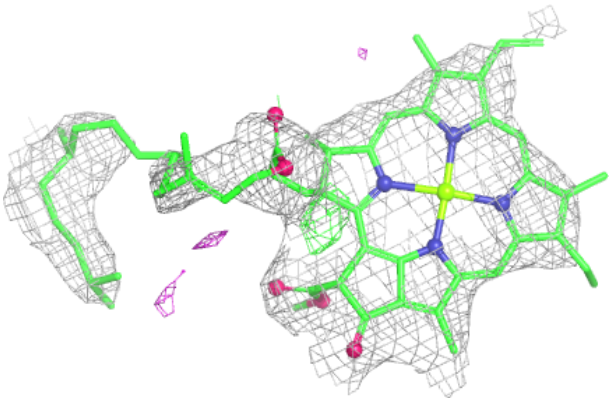


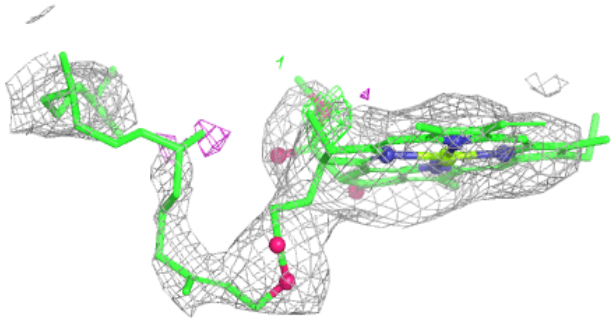


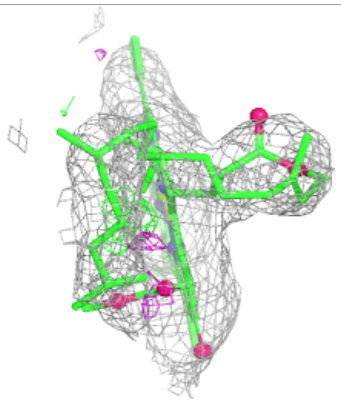


Electron density around CLA AB 612:

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

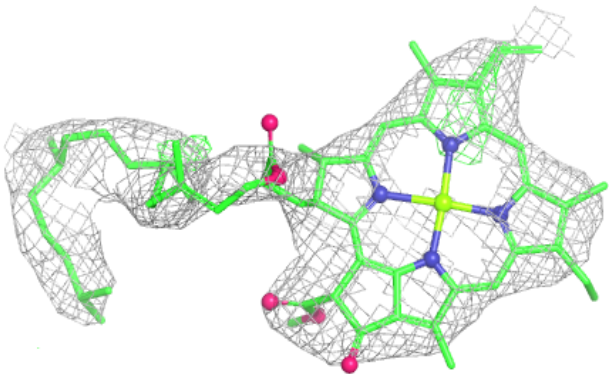


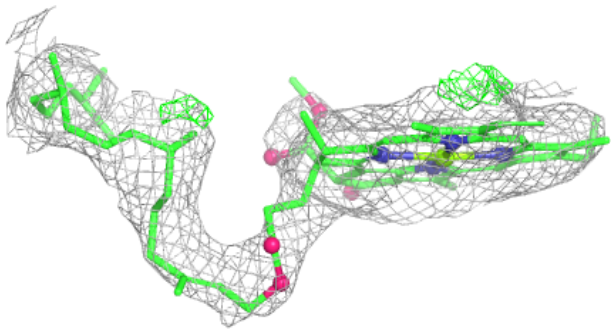


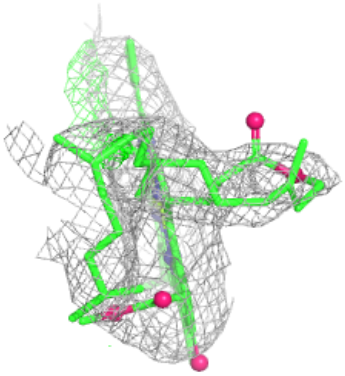


Electron density around CLA BB 5616:

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

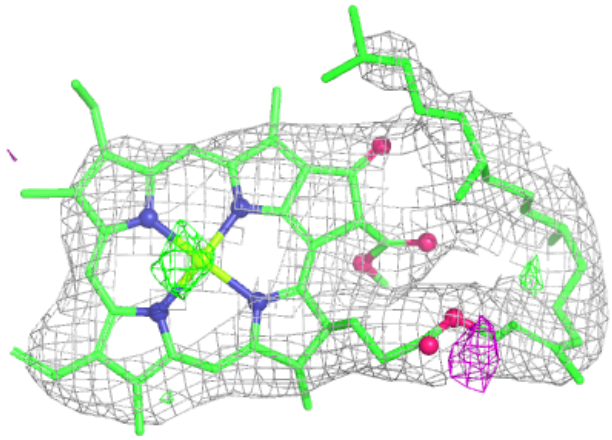


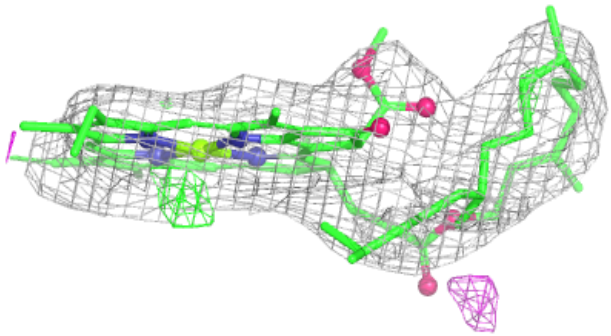




Electron density around CLA AB 610:

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

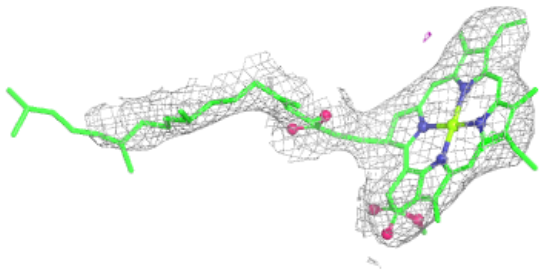


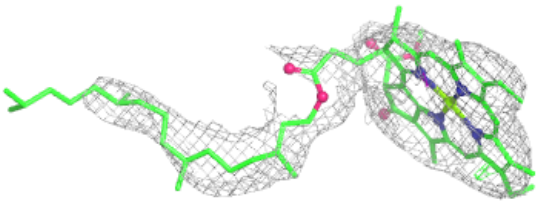


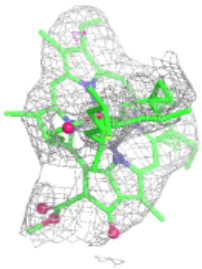


Electron density around CLA AC 502:

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

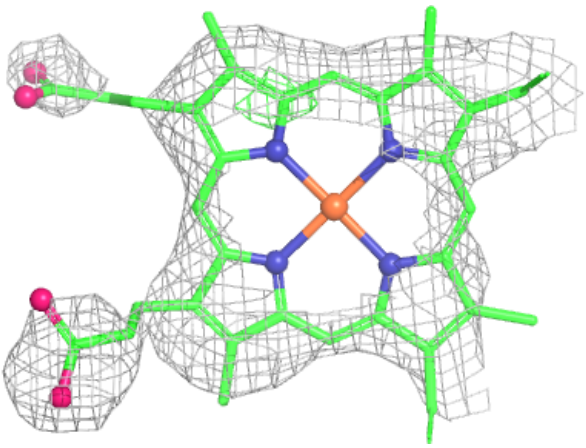


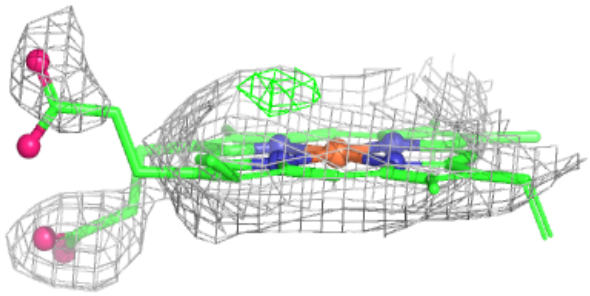


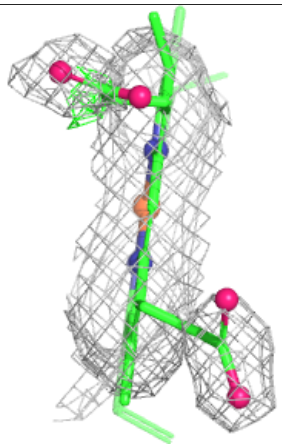


Electron density around HEM BV 5201:

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

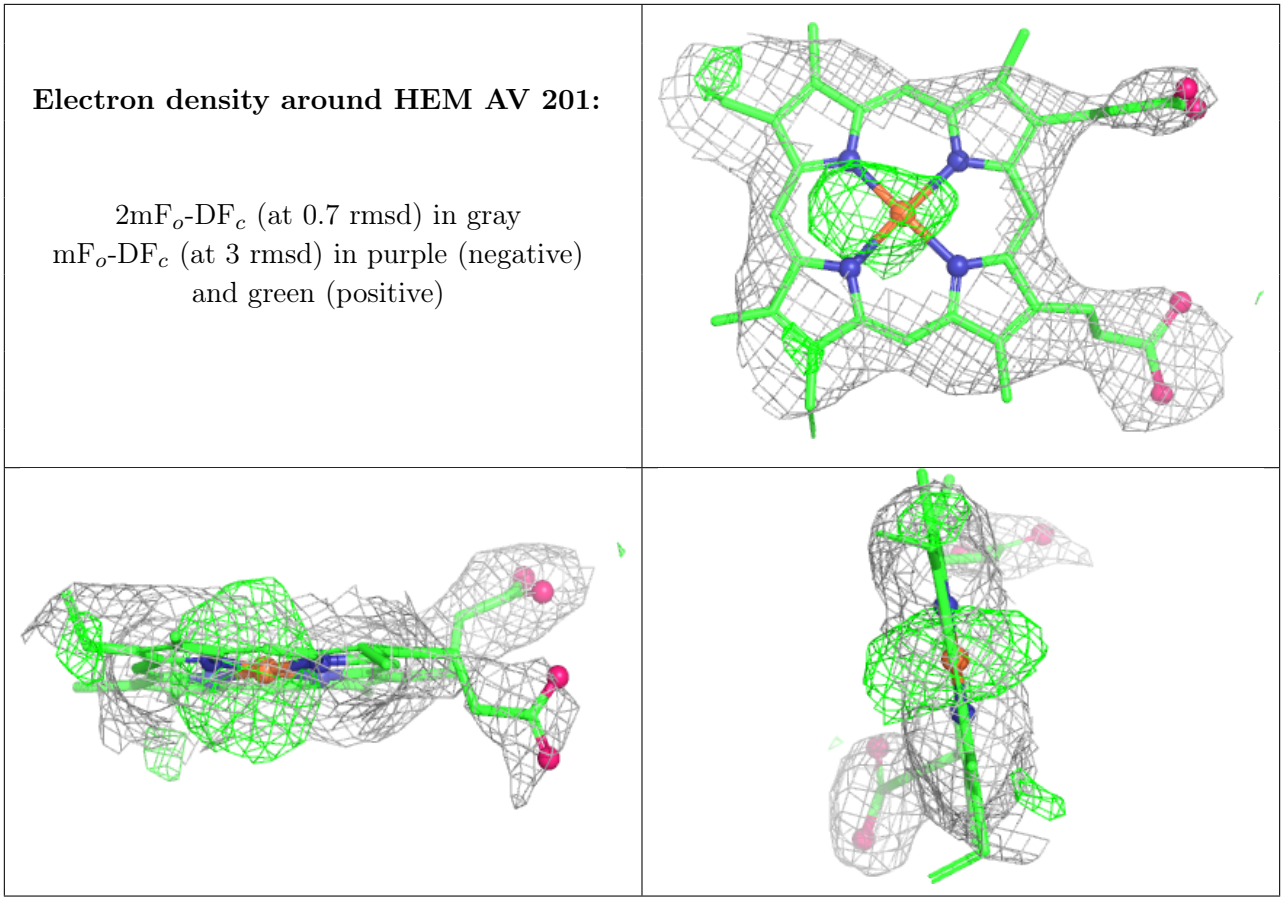






Electron density around HEM AV 201:

$2mF_o$-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.