



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 07:10 AM EDT

PDB ID : 3A0B / pdb_00003a0b
Title : Crystal structure of Br-substituted Photosystem II complex
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.
Deposited on : 2009-03-16
Resolution : 3.70 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 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

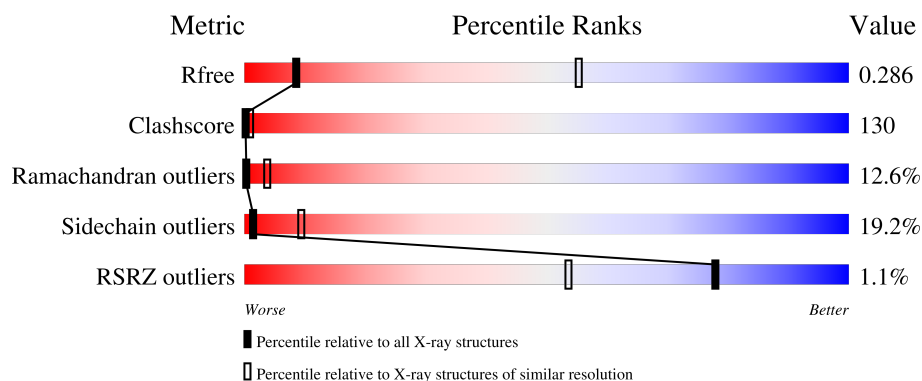
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	7% 60% 27% • •
1	a	344	7% 58% 28% 5% •
2	B	488	2% 14% 60% 22% • •
2	b	488	12% 58% 26% • •
3	C	447	14% 56% 28% •

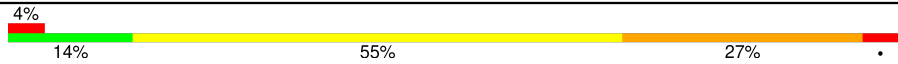
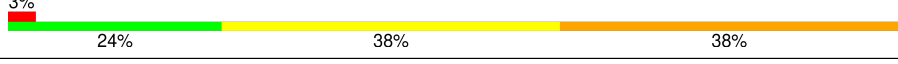
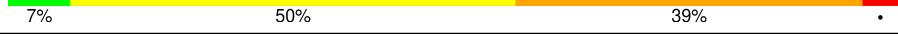
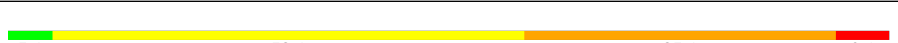
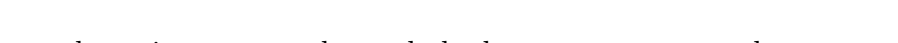
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Mol	Chain	Length	Quality of chain
3	c	447	
4	D	340	
4	d	340	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	64	
7	h	64	
8	I	35	
8	i	35	
9	J	40	
9	j	40	
10	K	36	
10	k	36	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	242	
13	o	242	
14	T	30	
14	t	30	
15	U	98	
15	u	98	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	34	
17	x	34	
18	Y	28	
18	y	28	
19	N	24	
19	n	24	
20	Z	62	
20	z	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
23	CLA	A	1003	-	-	X	-
23	CLA	A	1006	-	-	X	-
23	CLA	A	1007	X	-	-	-
23	CLA	B	1009	X	-	X	-
23	CLA	B	1010	-	-	X	-
23	CLA	B	1011	-	-	X	-
23	CLA	B	1012	-	-	X	-
23	CLA	B	1013	-	-	X	-
23	CLA	B	1014	X	-	X	-
23	CLA	B	1015	-	-	X	-
23	CLA	B	1016	-	-	X	-
23	CLA	B	1018	-	-	X	-
23	CLA	B	1019	X	-	X	-
23	CLA	B	1020	X	-	X	-
23	CLA	B	1021	X	-	X	-
23	CLA	B	1022	X	-	X	-
23	CLA	B	1023	X	-	X	-
23	CLA	B	1024	X	-	X	-
23	CLA	C	1025	X	-	X	-
23	CLA	C	1026	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	1027	X	-	X	-
23	CLA	C	1028	X	-	X	-
23	CLA	C	1029	X	-	X	-
23	CLA	C	1030	-	-	X	-
23	CLA	C	1031	X	-	X	-
23	CLA	C	1032	-	-	X	-
23	CLA	C	1033	X	-	X	-
23	CLA	C	1034	X	-	X	-
23	CLA	C	1036	X	-	X	-
23	CLA	C	1037	X	-	X	-
23	CLA	D	1005	X	-	X	-
23	CLA	D	1008	-	-	X	-
23	CLA	H	1017	X	-	X	-
23	CLA	a	6003	-	-	X	-
23	CLA	a	6006	-	-	X	-
23	CLA	a	6007	X	-	-	-
23	CLA	b	6009	X	-	X	-
23	CLA	b	6010	-	-	X	-
23	CLA	b	6011	-	-	X	-
23	CLA	b	6012	-	-	X	-
23	CLA	b	6013	-	-	X	-
23	CLA	b	6014	X	-	X	-
23	CLA	b	6015	-	-	X	-
23	CLA	b	6016	-	-	X	-
23	CLA	b	6017	X	-	X	-
23	CLA	b	6019	X	-	X	-
23	CLA	b	6020	X	-	X	-
23	CLA	b	6021	X	-	X	-
23	CLA	b	6022	X	-	X	-
23	CLA	b	6023	X	-	X	-
23	CLA	b	6024	X	-	X	-
23	CLA	c	6025	X	-	X	-
23	CLA	c	6026	X	-	X	-
23	CLA	c	6027	X	-	X	-
23	CLA	c	6028	X	-	X	-
23	CLA	c	6029	X	-	X	-
23	CLA	c	6030	-	-	X	-
23	CLA	c	6031	X	-	X	-
23	CLA	c	6032	-	-	X	-
23	CLA	c	6033	X	-	X	-
23	CLA	c	6034	X	-	X	-
23	CLA	c	6035	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	6036	X	-	X	-
23	CLA	c	6037	X	-	X	-
23	CLA	d	6005	X	-	X	-
23	CLA	d	6008	-	-	X	-
24	PHO	A	1038	X	-	X	-
24	PHO	A	1039	X	-	X	-
24	PHO	a	6039	X	-	X	-
24	PHO	d	6038	X	-	X	-
25	PQ9	D	1042	-	-	X	-
25	PQ9	d	6042	-	-	X	-
26	BCR	A	1044	-	-	X	-
26	BCR	B	1045	-	-	X	-
26	BCR	B	1047	-	-	X	-
26	BCR	B	1048	-	-	X	-
26	BCR	C	1054	-	-	X	-
26	BCR	D	1050	-	-	X	-
26	BCR	H	1049	-	-	X	-
26	BCR	K	1051	-	-	X	-
26	BCR	K	1052	-	-	X	-
26	BCR	T	6046	-	-	X	-
26	BCR	Z	1053	-	-	X	-
26	BCR	a	6044	-	-	X	-
26	BCR	b	6045	-	-	X	-
26	BCR	b	6047	-	-	X	-
26	BCR	b	6048	-	-	X	-
26	BCR	c	6054	-	-	X	-
26	BCR	d	6050	-	-	X	-
26	BCR	h	6049	-	-	X	-
26	BCR	k	6051	-	-	X	-
26	BCR	k	6052	-	-	X	-
26	BCR	t	1046	-	-	X	-
26	BCR	z	6053	-	-	X	-
27	LHG	A	1063	-	-	X	-
27	LHG	a	6063	-	-	X	-
28	BR	A	1065	-	-	X	-
29	MGE	B	1060	-	-	X	-
29	MGE	D	1062	-	-	X	-
29	MGE	J	1059	-	-	X	-
29	MGE	L	1061	-	-	X	-
29	MGE	b	6060	-	-	X	-
29	MGE	d	6059	-	-	X	-
29	MGE	d	6061	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MGE	d	6062	-	-	X	-
30	DGD	C	1055	-	-	X	-
30	DGD	C	1056	-	-	X	-
30	DGD	C	1057	-	-	X	-
30	DGD	H	1058	-	-	X	-
30	DGD	c	6055	-	-	X	-
30	DGD	c	6056	-	-	X	-
30	DGD	c	6057	-	-	X	-
30	DGD	h	6058	-	-	X	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 47988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	485	Total	C	N	O	S	0	0	0
			3816	2505	635	663	13			
2	b	485	Total	C	N	O	S	0	0	0
			3816	2505	635	663	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	13			
3	c	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	13			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			507	339	81	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			507	339	81	85	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			287	195	45	46	1			
8	i	35	Total	C	N	O	S	0	0	0
			287	195	45	46	1			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	36	Total	C	N	O	0	0	0
			278	195	38	45			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			278	195	38	45			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			283	187	42	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			283	187	42	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1841	1152	311	374	4			
13	o	242	Total	C	N	O	S	0	0	0
			1841	1152	311	374	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			257	180	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			257	180	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			783	496	130	157			
15	u	98	Total	C	N	O	0	0	0
			783	496	130	157			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

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

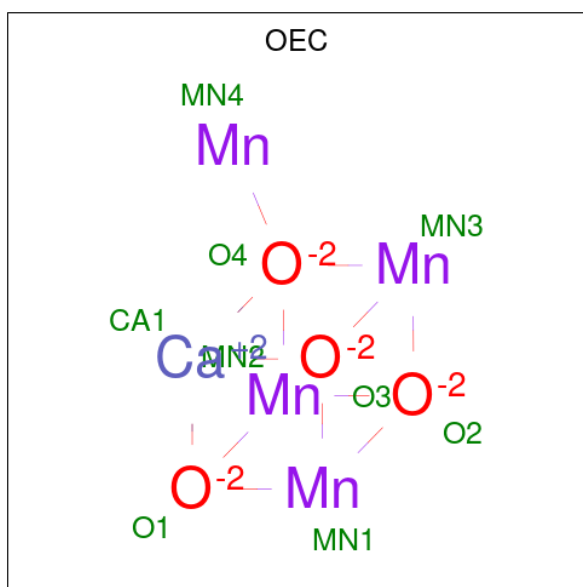
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	N	24	Total	C	N	O	0	0	0
			121	72	24	25			
19	n	24	Total	C	N	O	0	0	0
			121	72	24	25			

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

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

- Molecule 21 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).

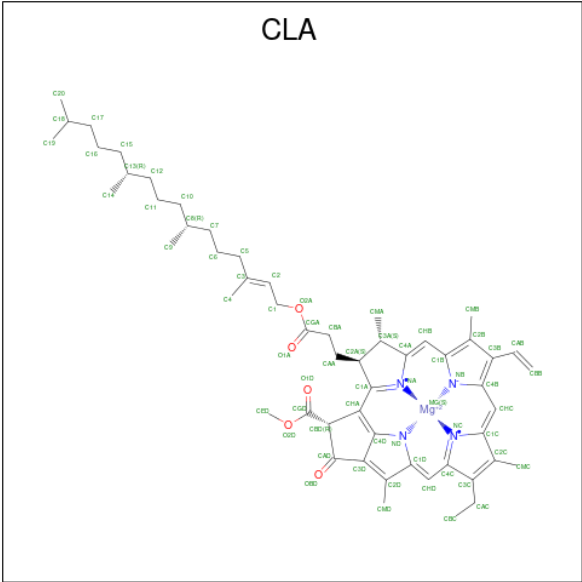


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total 5	Ca 1	Mn 4	0	0
21	a	1	Total 5	Ca 1	Mn 4	0	0

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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



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

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

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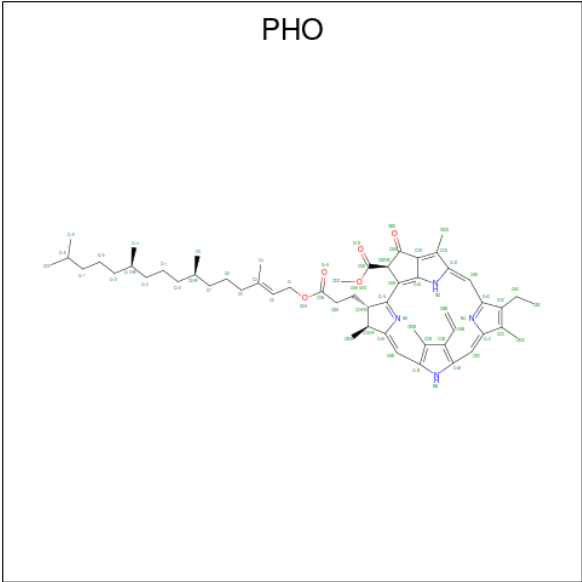
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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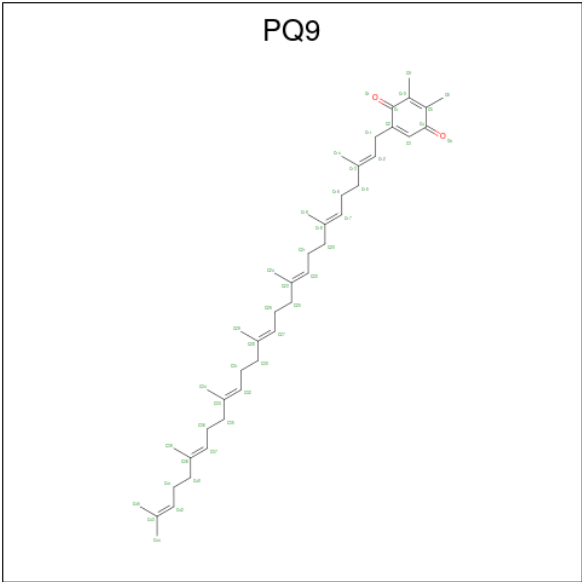
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

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



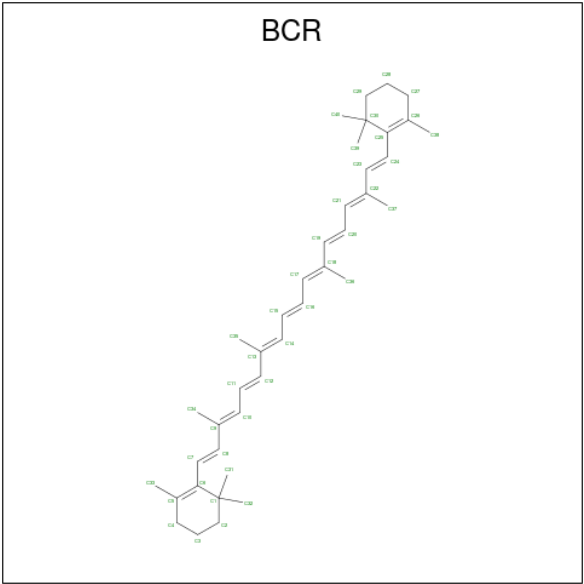
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C₄₃H₆₄O₂).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



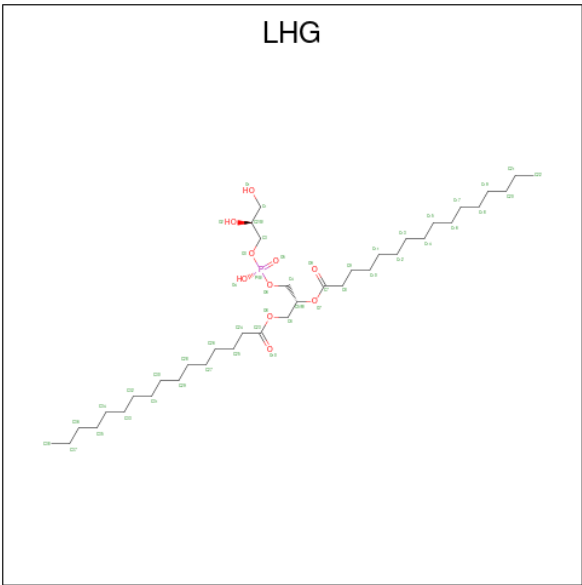
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	B	1	Total	C	0	0
			40	40		
26	C	1	Total	C	0	0
			40	40		
26	D	1	Total	C	0	0
			40	40		
26	H	1	Total	C	0	0
			40	40		
26	K	1	Total	C	0	0
			40	40		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Z	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	z	1	Total C 40 40	0	0

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

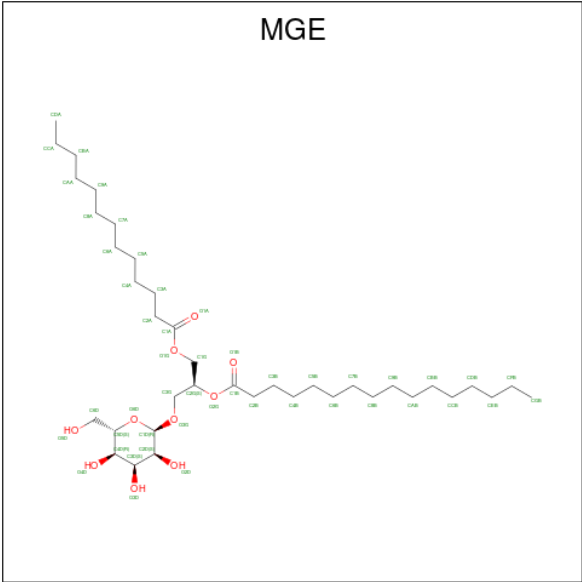


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 28 is BROMIDE ION (CCD ID: BR) (formula: Br).

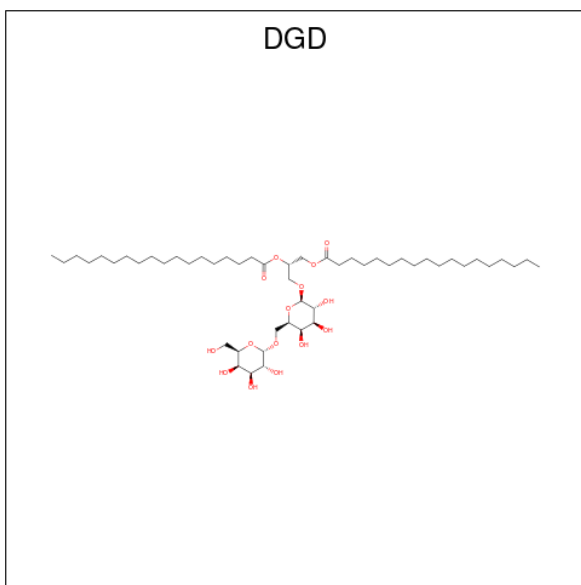
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	2	Total	Br	0	0
			2	2		
28	a	1	Total	Br	0	0
			1	1		
28	d	1	Total	Br	0	0
			1	1		

- Molecule 29 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀).



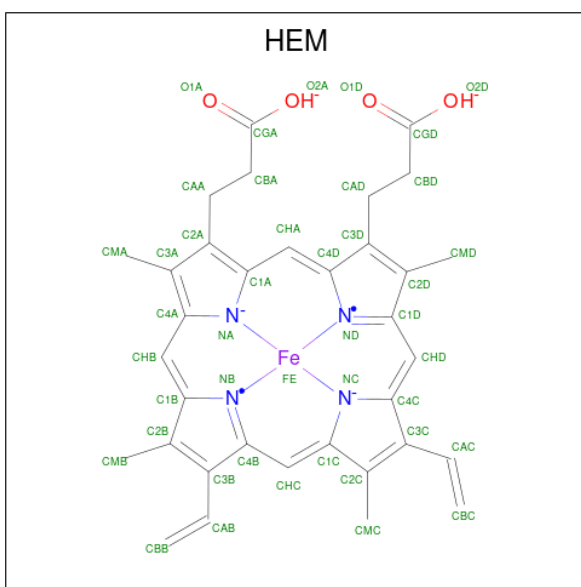
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	1	Total	C	O	0	0
			48	38	10		
29	D	1	Total	C	O	0	0
			48	38	10		
29	J	1	Total	C	O	0	0
			48	38	10		
29	L	1	Total	C	O	0	0
			48	38	10		
29	b	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total	C	O	0	0
			48	38	10		
29	d	1	Total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

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).

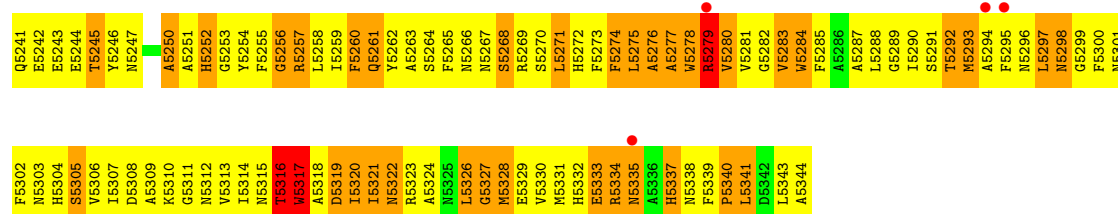


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	C	1	Total	C	O	0	0
			66	51	15		
30	H	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	c	1	Total	C	O	0	0
			66	51	15		
30	h	1	Total	C	O	0	0
			66	51	15		

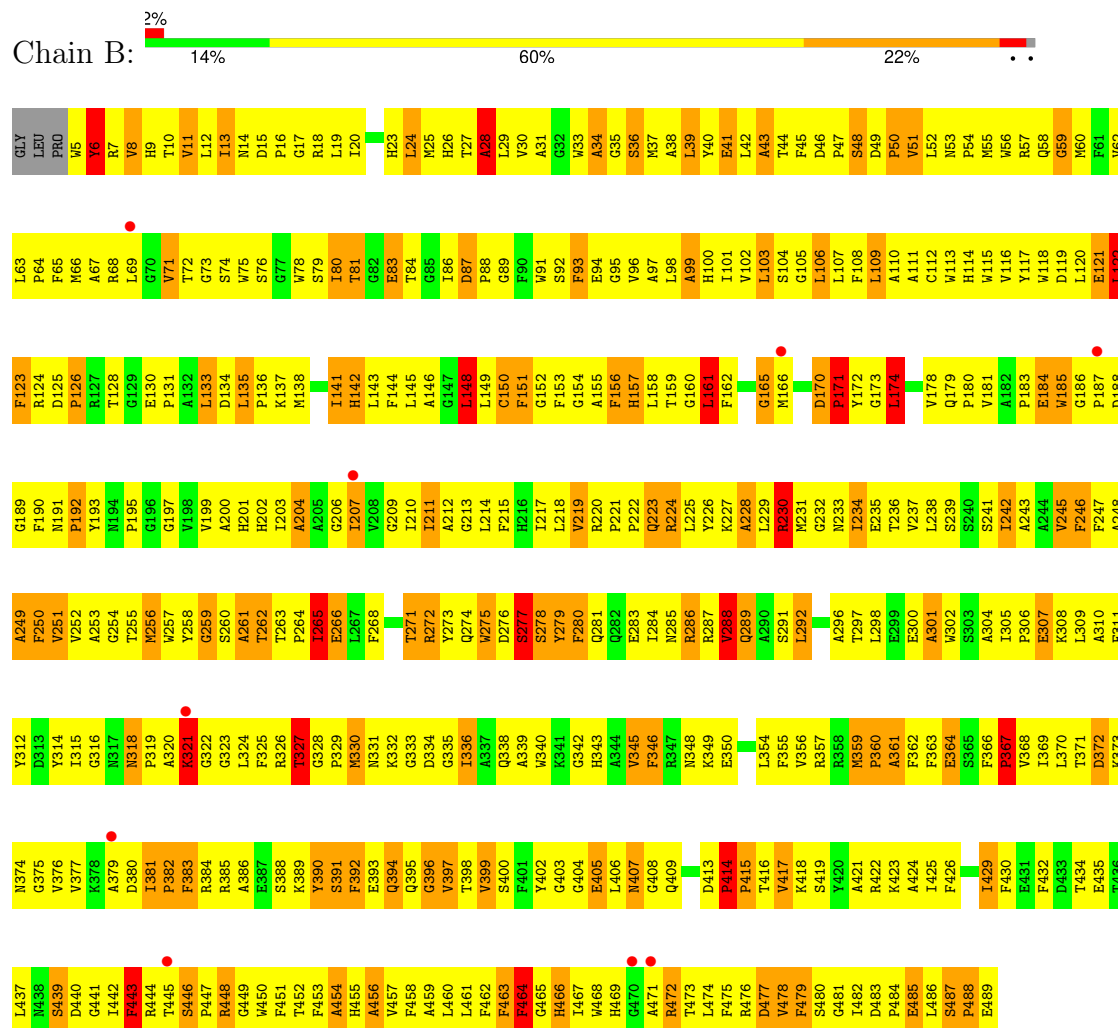
- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

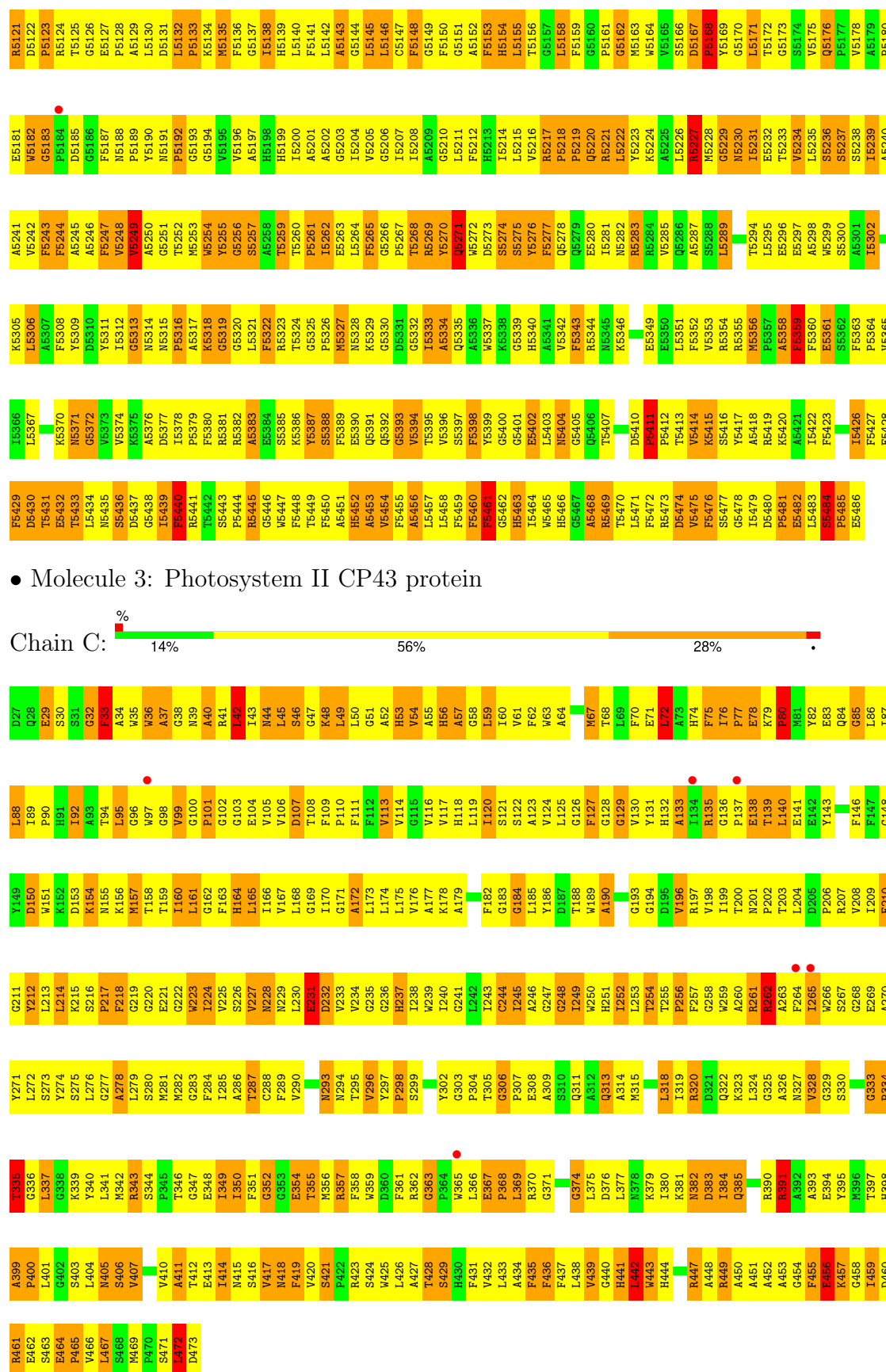


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
31	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

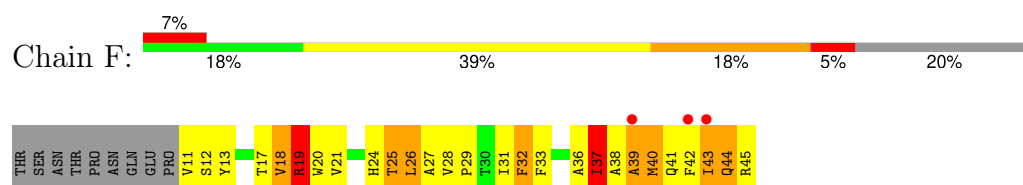


● Molecule 2: Photosystem II core light harvesting protein

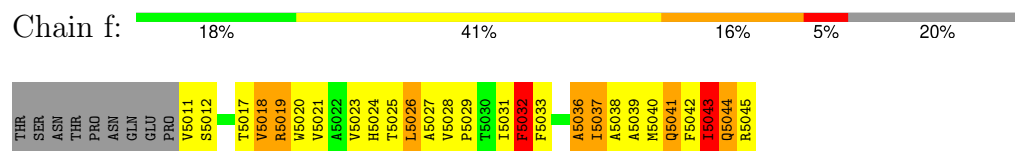




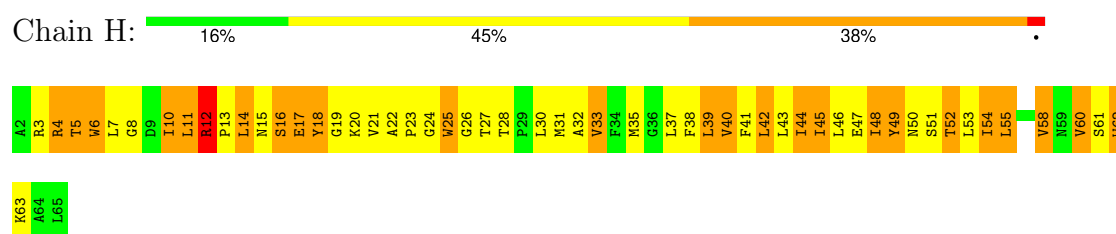




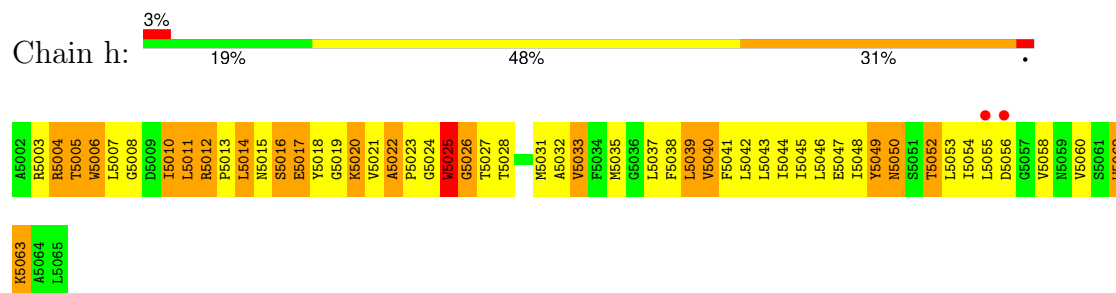
• Molecule 6: Cytochrome b559 subunit beta



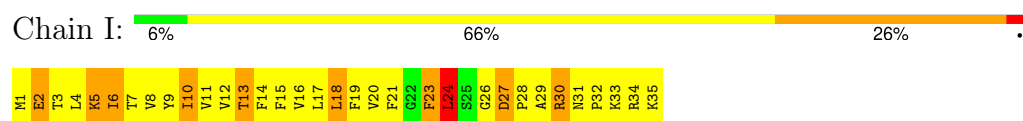
• Molecule 7: Photosystem II reaction center protein H



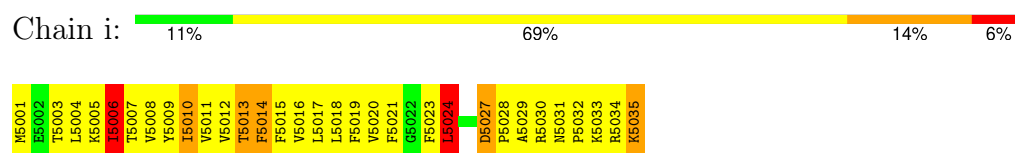
• Molecule 7: Photosystem II reaction center protein H



• Molecule 8: Photosystem II reaction center protein I



• Molecule 8: Photosystem II reaction center protein I

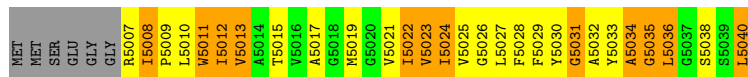


• Molecule 9: Photosystem II reaction center protein J

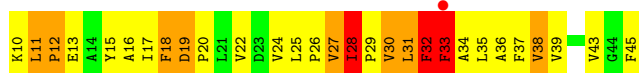
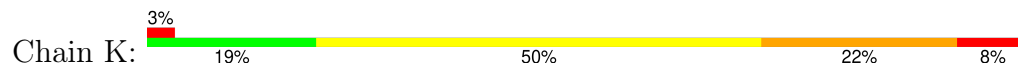




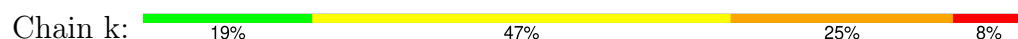
- Molecule 9: Photosystem II reaction center protein J



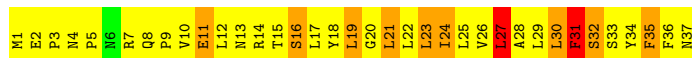
- Molecule 10: Photosystem II reaction center protein K



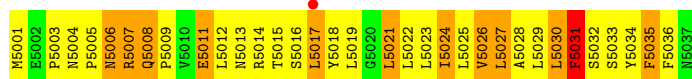
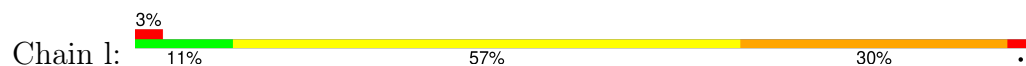
- Molecule 10: Photosystem II reaction center protein K



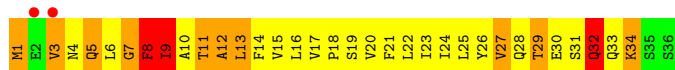
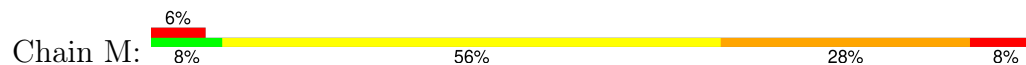
- Molecule 11: Photosystem II reaction center protein L



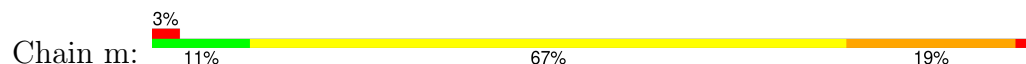
- Molecule 11: Photosystem II reaction center protein L

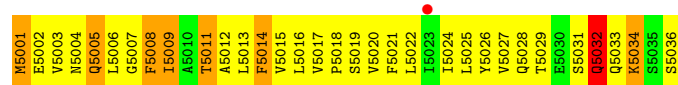


- Molecule 12: Photosystem II reaction center protein M

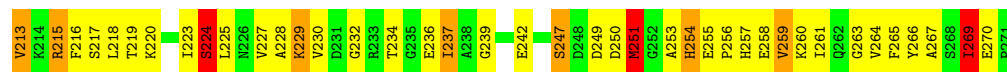
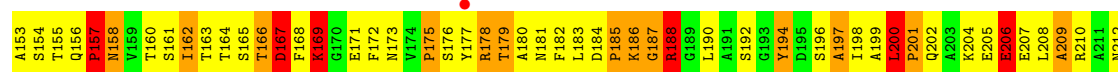
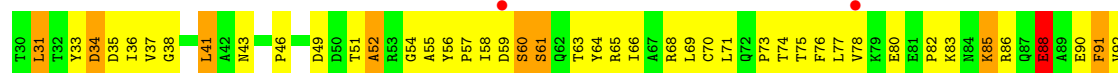


- Molecule 12: Photosystem II reaction center protein M

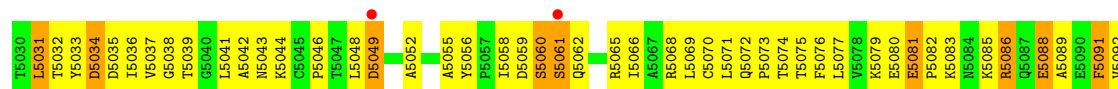




• Molecule 13: Photosystem II manganese-stabilizing polypeptide



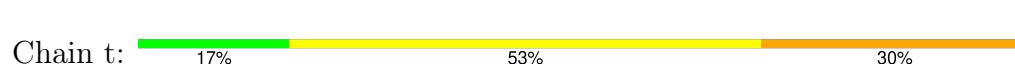
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



• Molecule 14: Photosystem II reaction center protein T



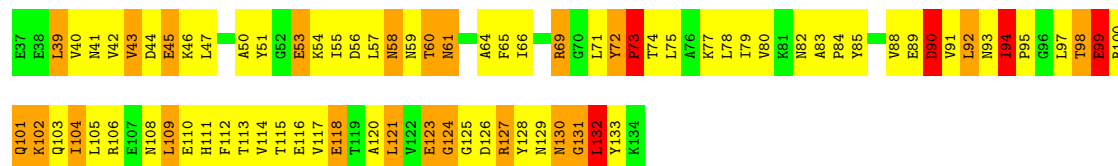
• Molecule 14: Photosystem II reaction center protein T





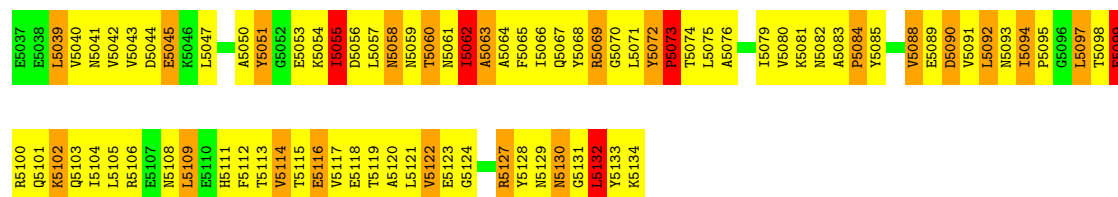
● Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 19% 53% 22% 5%



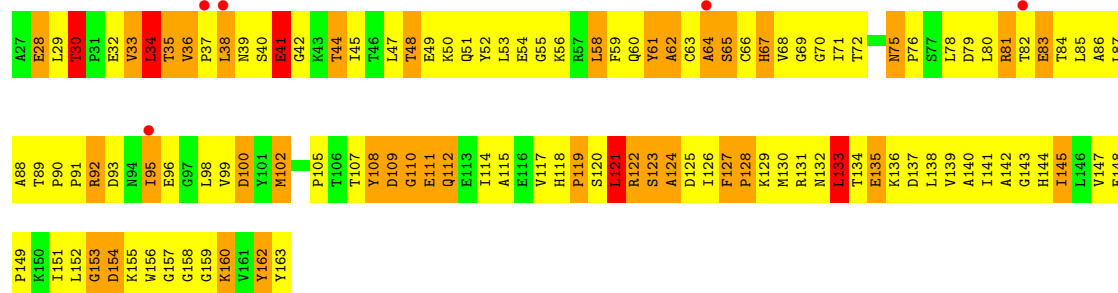
● Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 15% 58% 21% 5%



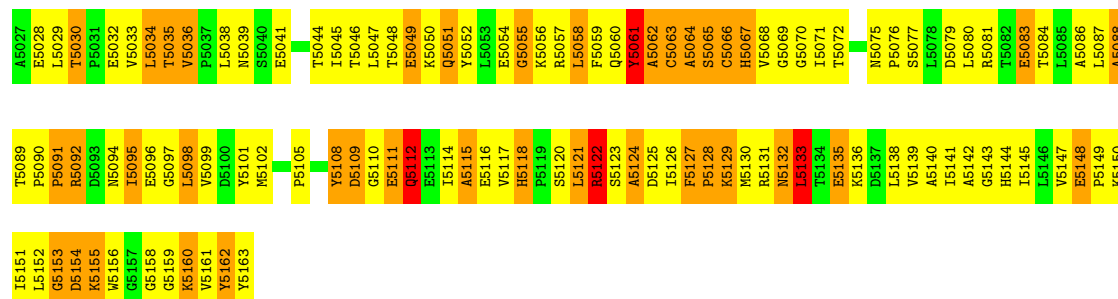
● Molecule 16: Cytochrome c-550

Chain V: 4% 14% 55% 27%

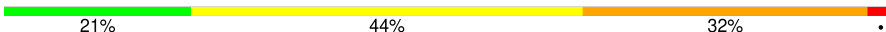


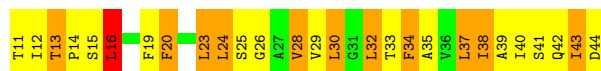
● Molecule 16: Cytochrome c-550

Chain v: 18% 52% 28%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  21% 44% 32% .

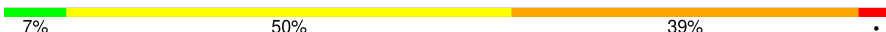


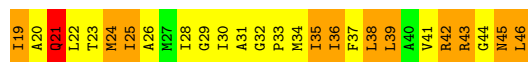
- Molecule 17: Photosystem II reaction center protein X

Chain x:  3% 24% 38% 35%

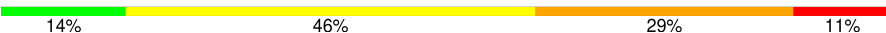


- Molecule 18: Photosystem II reaction center protein ycf12

Chain Y:  7% 50% 39% .



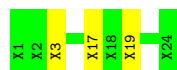
- Molecule 18: Photosystem II reaction center protein ycf12

Chain y:  14% 46% 29% 11%

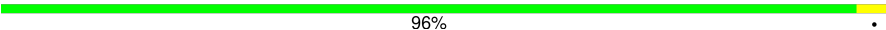


- Molecule 19: Photosystem II reaction center protein Y

Chain N:  88% 12%



- Molecule 19: Photosystem II reaction center protein Y

Chain n:  96%



- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  5% 53% 35% 7%



V5062

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.59Å 226.39Å 307.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.70 – 3.70 34.70 – 3.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (34.70-3.70) 85.7 (34.70-3.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.302 , 0.358 0.286 , 0.286	Depositor DCC
R_{free} test set	4216 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47988	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FE2, OEC, LHG, BR, DGD, CLA, BCR, PQ9, HEM, MGE, PHO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.65	0/2714	1.23	45/3699 (1.2%)
1	a	0.63	0/2714	1.24	43/3699 (1.2%)
2	B	0.64	2/3951 (0.1%)	1.24	40/5383 (0.7%)
2	b	0.66	1/3951 (0.0%)	1.25	58/5383 (1.1%)
3	C	0.60	0/3568	1.21	53/4858 (1.1%)
3	c	0.59	0/3568	1.15	33/4858 (0.7%)
4	D	0.61	0/2801	1.15	26/3818 (0.7%)
4	d	0.61	0/2801	1.21	34/3818 (0.9%)
5	E	0.55	0/685	1.19	9/933 (1.0%)
5	e	0.60	0/685	1.19	7/933 (0.8%)
6	F	0.69	0/291	1.34	7/397 (1.8%)
6	f	0.74	0/291	1.14	3/397 (0.8%)
7	H	0.63	1/520 (0.2%)	1.19	5/708 (0.7%)
7	h	0.64	0/520	1.26	9/708 (1.3%)
8	I	0.67	0/294	0.97	0/395
8	i	0.63	0/294	1.02	1/395 (0.3%)
9	J	0.57	0/255	1.14	3/346 (0.9%)
9	j	0.62	0/255	1.14	2/346 (0.6%)
10	K	0.76	0/287	1.34	4/394 (1.0%)
10	k	0.64	0/287	1.34	6/394 (1.5%)
11	L	0.60	0/311	1.25	6/422 (1.4%)
11	l	0.63	0/311	1.13	4/422 (0.9%)
12	M	0.73	0/287	1.10	3/388 (0.8%)
12	m	0.63	0/287	1.13	2/388 (0.5%)
13	O	0.62	0/1872	1.15	20/2539 (0.8%)
13	o	0.60	0/1872	1.09	9/2539 (0.4%)
14	T	0.70	0/266	1.28	3/359 (0.8%)
14	t	0.70	0/266	1.24	3/359 (0.8%)
15	U	0.60	0/794	1.13	7/1076 (0.7%)
15	u	0.60	0/794	1.21	9/1076 (0.8%)
16	V	0.65	0/1085	1.34	16/1473 (1.1%)
16	v	0.61	0/1085	1.31	14/1473 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	X	0.64	0/249	1.25	3/337 (0.9%)
17	x	0.68	0/249	1.07	0/337
18	Y	0.63	0/209	1.29	3/279 (1.1%)
18	y	0.66	0/209	1.39	3/279 (1.1%)
20	Z	0.61	0/490	1.23	9/669 (1.3%)
20	z	0.66	0/490	1.25	6/669 (0.9%)
All	All	0.63	4/41858 (0.0%)	1.21	508/56946 (0.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	5453	ALA	CA-C	-10.56	1.45	1.52
2	B	456	ALA	CA-C	-6.95	1.48	1.52
2	B	454	ALA	CA-CB	-6.88	1.43	1.53
7	H	54	ILE	CA-CB	5.26	1.59	1.53

The worst 5 of 508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	218	PHE	N-CA-C	14.16	122.34	108.75
2	B	232	GLY	N-CA-C	-13.18	99.00	114.69
2	b	5167	ASP	CA-C-N	12.99	136.07	119.84
2	b	5167	ASP	C-N-CA	12.99	136.07	119.84
2	B	466	HIS	N-CA-C	-12.56	97.06	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2630	0	2528	816	0
1	a	2630	0	2528	857	0
2	B	3816	0	3680	1011	0
2	b	3816	0	3680	1003	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3455	0	3376	834	0
3	c	3455	0	3376	863	0
4	D	2706	0	2608	803	0
4	d	2706	0	2608	803	0
5	E	666	0	651	156	0
5	e	666	0	651	127	0
6	F	282	0	291	74	0
6	f	282	0	291	67	0
7	H	507	0	529	135	0
7	h	507	0	529	129	0
8	I	287	0	308	81	0
8	i	287	0	305	59	0
9	J	249	0	262	65	0
9	j	249	0	262	36	0
10	K	278	0	289	118	0
10	k	278	0	289	124	0
11	L	304	0	316	106	0
11	l	304	0	313	132	0
12	M	283	0	297	107	0
12	m	283	0	294	118	0
13	O	1841	0	1799	298	0
13	o	1841	0	1799	322	0
14	T	257	0	262	92	0
14	t	257	0	259	82	0
15	U	783	0	779	156	0
15	u	783	0	779	146	0
16	V	1064	0	1072	198	0
16	v	1064	0	1072	183	0
17	X	246	0	269	47	0
17	x	246	0	269	51	0
18	Y	208	0	237	59	0
18	y	208	0	237	51	0
19	N	121	0	26	2	0
19	n	121	0	26	1	0
20	Z	479	0	516	130	0
20	z	479	0	513	134	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	195	0	216	169	0
23	B	975	0	1079	783	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	C	845	0	935	531	0
23	D	195	0	216	120	0
23	H	65	0	72	57	0
23	a	195	0	216	161	0
23	b	1040	0	1151	789	0
23	c	845	0	935	542	0
23	d	195	0	216	123	0
24	A	128	0	148	115	0
24	a	64	0	74	33	0
24	d	64	0	74	75	0
25	A	45	0	64	6	0
25	D	45	0	64	30	0
25	a	45	0	64	3	0
25	d	45	0	62	27	0
26	A	40	0	48	26	0
26	B	120	0	141	101	0
26	C	40	0	47	26	0
26	D	40	0	48	62	0
26	H	40	0	47	54	0
26	K	80	0	94	81	0
26	T	40	0	47	33	0
26	Z	40	0	48	41	0
26	a	40	0	48	25	0
26	b	120	0	141	102	0
26	c	40	0	47	22	0
26	d	40	0	48	58	0
26	h	40	0	47	47	0
26	k	80	0	94	81	0
26	t	40	0	47	24	0
26	z	40	0	48	40	0
27	A	49	0	74	60	0
27	a	49	0	74	53	0
28	A	2	0	0	4	0
28	a	1	0	0	1	0
28	d	1	0	0	1	0
29	B	48	0	72	46	0
29	D	48	0	72	24	0
29	J	48	0	72	32	0
29	L	48	0	72	33	0
29	b	48	0	72	52	0
29	d	144	0	216	96	0
30	C	198	0	288	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	H	66	0	96	32	0
30	c	198	0	288	136	0
30	h	66	0	96	35	0
31	E	43	0	30	10	0
31	V	43	0	30	10	0
31	e	43	0	30	11	0
31	v	43	0	30	11	0
All	All	47988	0	48413	12551	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 130.

The worst 5 of 12551 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:a:5300:PHE:CE2	3:c:5404:LEU:HD12	1.32	1.65
26:t:1046:BCR:H371	26:t:1046:BCR:C26	1.34	1.53
26:T:6046:BCR:H371	26:T:6046:BCR:C26	1.34	1.51
23:a:6006:CLA:H171	26:d:6050:BCR:C29	1.40	1.51
23:c:6032:CLA:H2A	23:c:6032:CLA:CED	1.41	1.50

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	210 (63%)	84 (25%)	39 (12%)	0	4
1	a	333/344 (97%)	214 (64%)	75 (22%)	44 (13%)	0	3
2	B	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0	4
2	b	483/488 (99%)	314 (65%)	109 (23%)	60 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	445/447 (100%)	306 (69%)	89 (20%)	50 (11%)	0	4
3	c	445/447 (100%)	316 (71%)	82 (18%)	47 (11%)	0	5
4	D	338/340 (99%)	199 (59%)	87 (26%)	52 (15%)	0	2
4	d	338/340 (99%)	214 (63%)	79 (23%)	45 (13%)	0	3
5	E	80/83 (96%)	44 (55%)	22 (28%)	14 (18%)	0	1
5	e	80/83 (96%)	51 (64%)	18 (22%)	11 (14%)	0	3
6	F	33/44 (75%)	26 (79%)	6 (18%)	1 (3%)	3	26
6	f	33/44 (75%)	26 (79%)	5 (15%)	2 (6%)	1	14
7	H	62/64 (97%)	39 (63%)	15 (24%)	8 (13%)	0	3
7	h	62/64 (97%)	38 (61%)	19 (31%)	5 (8%)	1	9
8	I	33/35 (94%)	19 (58%)	8 (24%)	6 (18%)	0	1
8	i	33/35 (94%)	24 (73%)	6 (18%)	3 (9%)	0	8
9	J	32/40 (80%)	26 (81%)	2 (6%)	4 (12%)	0	4
9	j	32/40 (80%)	26 (81%)	3 (9%)	3 (9%)	0	7
10	K	34/36 (94%)	22 (65%)	8 (24%)	4 (12%)	0	4
10	k	34/36 (94%)	23 (68%)	7 (21%)	4 (12%)	0	4
11	L	35/37 (95%)	20 (57%)	12 (34%)	3 (9%)	0	8
11	l	35/37 (95%)	22 (63%)	9 (26%)	4 (11%)	0	4
12	M	34/36 (94%)	19 (56%)	8 (24%)	7 (21%)	0	1
12	m	34/36 (94%)	24 (71%)	7 (21%)	3 (9%)	0	8
13	O	240/242 (99%)	155 (65%)	47 (20%)	38 (16%)	0	2
13	o	240/242 (99%)	163 (68%)	45 (19%)	32 (13%)	0	3
14	T	28/30 (93%)	18 (64%)	5 (18%)	5 (18%)	0	1
14	t	28/30 (93%)	20 (71%)	7 (25%)	1 (4%)	2	23
15	U	96/98 (98%)	56 (58%)	24 (25%)	16 (17%)	0	2
15	u	96/98 (98%)	55 (57%)	26 (27%)	15 (16%)	0	2
16	V	135/137 (98%)	91 (67%)	25 (18%)	19 (14%)	0	3
16	v	135/137 (98%)	90 (67%)	28 (21%)	17 (13%)	0	4
17	X	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	26
17	x	32/34 (94%)	29 (91%)	2 (6%)	1 (3%)	3	26
18	Y	26/28 (93%)	19 (73%)	5 (19%)	2 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	26/28 (93%)	19 (73%)	3 (12%)	4 (15%)	0	2
20	Z	60/62 (97%)	39 (65%)	10 (17%)	11 (18%)	0	1
20	z	60/62 (97%)	46 (77%)	8 (13%)	6 (10%)	0	6
All	All	5118/5250 (98%)	3365 (66%)	1106 (22%)	647 (13%)	0	4

5 of 647 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	Ile
1	A	75	ASN
1	A	79	THR
1	A	80	GLY
1	A	84	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/279 (97%)	219 (81%)	51 (19%)	1	10
1	a	270/279 (97%)	214 (79%)	56 (21%)	1	8
2	B	386/388 (100%)	323 (84%)	63 (16%)	2	14
2	b	386/388 (100%)	325 (84%)	61 (16%)	2	15
3	C	349/349 (100%)	287 (82%)	62 (18%)	2	12
3	c	349/349 (100%)	283 (81%)	66 (19%)	1	10
4	D	275/275 (100%)	220 (80%)	55 (20%)	1	9
4	d	275/275 (100%)	229 (83%)	46 (17%)	2	14
5	E	72/73 (99%)	58 (81%)	14 (19%)	1	9
5	e	72/73 (99%)	61 (85%)	11 (15%)	3	16
6	F	29/38 (76%)	21 (72%)	8 (28%)	0	3
6	f	29/38 (76%)	21 (72%)	8 (28%)	0	3
7	H	54/54 (100%)	38 (70%)	16 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	54/54 (100%)	42 (78%)	12 (22%)	1	7
8	I	32/32 (100%)	27 (84%)	5 (16%)	2	15
8	i	32/32 (100%)	27 (84%)	5 (16%)	2	15
9	J	24/28 (86%)	12 (50%)	12 (50%)	0	0
9	j	24/28 (86%)	14 (58%)	10 (42%)	0	0
10	K	29/29 (100%)	21 (72%)	8 (28%)	0	3
10	k	29/29 (100%)	23 (79%)	6 (21%)	1	8
11	L	35/35 (100%)	28 (80%)	7 (20%)	1	9
11	l	35/35 (100%)	29 (83%)	6 (17%)	2	13
12	M	33/33 (100%)	27 (82%)	6 (18%)	2	11
12	m	33/33 (100%)	28 (85%)	5 (15%)	3	16
13	O	200/206 (97%)	170 (85%)	30 (15%)	3	16
13	o	200/206 (97%)	163 (82%)	37 (18%)	1	10
14	T	27/27 (100%)	18 (67%)	9 (33%)	0	1
14	t	27/27 (100%)	20 (74%)	7 (26%)	0	4
15	U	85/85 (100%)	72 (85%)	13 (15%)	3	16
15	u	85/85 (100%)	72 (85%)	13 (15%)	3	16
16	V	117/117 (100%)	98 (84%)	19 (16%)	2	14
16	v	117/117 (100%)	97 (83%)	20 (17%)	2	13
17	X	27/27 (100%)	17 (63%)	10 (37%)	0	0
17	x	27/27 (100%)	15 (56%)	12 (44%)	0	0
18	Y	21/21 (100%)	13 (62%)	8 (38%)	0	0
18	y	21/21 (100%)	12 (57%)	9 (43%)	0	0
20	Z	52/52 (100%)	40 (77%)	12 (23%)	1	6
20	z	52/52 (100%)	37 (71%)	15 (29%)	0	2
All	All	4234/4296 (99%)	3421 (81%)	813 (19%)	1	9

5 of 813 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	5341	LEU
3	c	5382	ASN
20	z	5009	LEU

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Mol	Chain	Res	Type
2	b	5120	PHE
1	a	5337	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
4	d	5332	GLN
18	y	5003	GLN
5	e	5075	GLN
13	o	5150	ASN
10	K	40	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 130 ligands modelled in this entry, 6 are monoatomic - leaving 124 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	CLA	C	1033	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	6032	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	V	1041	16	50,50,50	1.88	8 (16%)	67,82,82	1.35	5 (7%)
23	CLA	d	6004	4	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
26	BCR	d	6050	-	41,41,41	3.94	16 (39%)	56,56,56	6.35	28 (50%)
23	CLA	C	1036	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	C	1054	-	41,41,41	4.00	17 (41%)	56,56,56	6.93	24 (42%)
23	CLA	b	6017	2	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
23	CLA	c	6034	-	69,73,73	1.90	16 (23%)	82,113,113	2.54	26 (31%)
26	BCR	b	6048	-	41,41,41	4.03	17 (41%)	56,56,56	6.42	22 (39%)
25	PQ9	a	6043	-	45,45,45	4.39	21 (46%)	56,57,57	4.90	20 (35%)
23	CLA	b	6023	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
24	PHO	A	1038	-	58,69,69	2.98	14 (24%)	55,99,99	3.43	20 (36%)
23	CLA	B	1011	2	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
24	PHO	A	1039	-	58,69,69	2.94	13 (22%)	55,99,99	3.52	19 (34%)
23	CLA	B	1015	-	69,73,73	1.95	20 (28%)	82,113,113	2.80	37 (45%)
23	CLA	d	6008	4	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
26	BCR	B	1045	-	41,41,41	4.01	17 (41%)	56,56,56	6.58	27 (48%)
23	CLA	C	1031	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	C	1034	-	69,73,73	1.97	17 (24%)	82,113,113	2.70	29 (35%)
23	CLA	D	1004	4	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
23	CLA	B	1012	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	b	6045	-	41,41,41	4.01	17 (41%)	56,56,56	6.58	26 (46%)
23	CLA	B	1018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6030	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	b	6014	-	69,73,73	1.89	19 (27%)	82,113,113	2.59	30 (36%)
23	CLA	b	6012	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	e	6040	6	50,50,50	1.88	8 (16%)	67,82,82	1.34	5 (7%)
23	CLA	d	6005	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
23	CLA	b	6021	2	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
26	BCR	b	6047	-	41,41,41	3.99	16 (39%)	56,56,56	7.22	26 (46%)
23	CLA	C	1037	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	k	6052	-	41,41,41	4.03	17 (41%)	56,56,56	5.22	21 (37%)
23	CLA	b	6018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	A	1044	-	41,41,41	3.84	16 (39%)	56,56,56	6.30	30 (53%)
23	CLA	B	1010	-	69,73,73	1.91	19 (27%)	82,113,113	2.73	31 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	1009	-	69,73,73	1.90	17 (24%)	82,113,113	2.44	28 (34%)
23	CLA	B	1020	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	z	6053	-	41,41,41	4.01	16 (39%)	56,56,56	6.64	26 (46%)
23	CLA	D	1008	4	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	H	1049	-	41,41,41	4.02	17 (41%)	56,56,56	6.31	21 (37%)
30	DGD	c	6055	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	H	1058	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	c	6029	3	69,73,73	1.91	18 (26%)	82,113,113	2.58	27 (32%)
23	CLA	a	6007	1	69,73,73	1.89	18 (26%)	82,113,113	2.53	30 (36%)
23	CLA	c	6033	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6031	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	A	1003	1	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	b	6013	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	A	1006	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
29	MGE	D	1062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
26	BCR	h	6049	-	41,41,41	4.02	17 (41%)	56,56,56	6.31	20 (35%)
23	CLA	B	1022	2	69,73,73	1.87	17 (24%)	82,113,113	2.60	31 (37%)
23	CLA	c	6037	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	MGE	d	6059	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
30	DGD	h	6058	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
26	BCR	t	1046	-	41,41,41	4.03	17 (41%)	56,56,56	6.58	24 (42%)
23	CLA	C	1028	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6035	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	MGE	b	6060	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	D	1005	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
26	BCR	K	1051	-	41,41,41	3.99	16 (39%)	56,56,56	6.52	29 (51%)
23	CLA	A	1007	-	69,73,73	1.89	18 (26%)	82,113,113	2.53	30 (36%)
23	CLA	b	6022	2	69,73,73	1.87	17 (24%)	82,113,113	2.60	31 (37%)
23	CLA	H	1017	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	v	6041	-	50,50,50	1.87	8 (16%)	67,82,82	1.34	5 (7%)
26	BCR	c	6054	-	41,41,41	4.00	17 (41%)	56,56,56	6.93	24 (42%)
23	CLA	B	1024	-	69,73,73	1.88	19 (27%)	82,113,113	2.67	34 (41%)
30	DGD	c	6056	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	C	1025	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	C	1026	-	69,73,73	1.85	18 (26%)	82,113,113	2.55	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	C	1055	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	C	1030	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	b	6024	-	69,73,73	1.89	19 (27%)	82,113,113	2.67	34 (41%)
23	CLA	B	1013	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	D	1050	-	41,41,41	3.94	16 (39%)	56,56,56	6.35	28 (50%)
23	CLA	b	6019	2	69,73,73	1.89	18 (26%)	82,113,113	2.65	36 (43%)
25	PQ9	D	1042	-	45,45,45	4.10	17 (37%)	56,57,57	5.08	25 (44%)
26	BCR	K	1052	-	41,41,41	4.02	17 (41%)	56,56,56	5.60	21 (37%)
25	PQ9	d	6042	-	45,45,45	4.12	15 (33%)	56,57,57	5.08	26 (46%)
26	BCR	B	1047	-	41,41,41	3.99	16 (39%)	56,56,56	7.22	26 (46%)
23	CLA	C	1032	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	a	6003	1	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	C	1035	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	E	1040	6	50,50,50	1.87	7 (14%)	67,82,82	1.34	5 (7%)
29	MGE	L	1061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	B	1023	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6027	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
30	DGD	C	1056	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
23	CLA	b	6016	2	69,73,73	1.94	16 (23%)	82,113,113	2.47	27 (32%)
29	MGE	B	1060	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
23	CLA	c	6025	3	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
23	CLA	b	6020	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	CLA	c	6028	-	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
23	CLA	c	6026	-	69,73,73	1.85	18 (26%)	82,113,113	2.55	29 (35%)
26	BCR	k	6051	-	41,41,41	3.99	16 (39%)	56,56,56	6.51	29 (51%)
30	DGD	C	1057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
30	DGD	c	6057	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
24	PHO	d	6038	-	58,69,69	2.98	14 (24%)	55,99,99	3.44	20 (36%)
23	CLA	a	6006	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	BCR	B	1048	-	41,41,41	4.03	17 (41%)	56,56,56	6.42	22 (39%)
23	CLA	C	1029	3	69,73,73	1.91	18 (26%)	82,113,113	2.58	27 (32%)
23	CLA	c	6036	3	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	MGE	d	6061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
29	MGE	d	6062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
26	BCR	T	6046	-	41,41,41	4.04	17 (41%)	56,56,56	7.68	28 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	a	6063	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)
29	MGE	J	1059	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
26	BCR	a	6044	-	41,41,41	3.84	16 (39%)	56,56,56	6.30	29 (51%)
26	BCR	Z	1053	-	41,41,41	4.01	16 (39%)	56,56,56	6.65	27 (48%)
23	CLA	b	6010	2	69,73,73	1.92	19 (27%)	82,113,113	2.74	31 (37%)
24	PHO	a	6039	-	58,69,69	2.94	13 (22%)	55,99,99	3.53	19 (34%)
23	CLA	B	1019	2	69,73,73	1.89	18 (26%)	82,113,113	2.65	36 (43%)
23	CLA	B	1016	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	PQ9	A	1043	-	45,45,45	4.25	17 (37%)	56,57,57	4.94	22 (39%)
23	CLA	b	6011	2	69,73,73	1.93	17 (24%)	82,113,113	2.48	28 (34%)
23	CLA	b	6015	-	69,73,73	1.95	19 (27%)	82,113,113	2.80	37 (45%)
23	CLA	B	1014	-	69,73,73	1.89	19 (27%)	82,113,113	2.59	29 (35%)
23	CLA	b	6009	-	69,73,73	1.91	18 (26%)	82,113,113	2.44	28 (34%)
23	CLA	C	1027	-	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
23	CLA	B	1021	2	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
27	LHG	A	1063	-	48,48,48	0.94	2 (4%)	51,54,54	1.05	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	1033	3	2/2/15/20	24/39/115/115	-
23	CLA	c	6032	-	-	16/39/115/115	-
31	HEM	V	1041	16	-	7/14/54/54	-
23	CLA	d	6004	4	-	16/39/115/115	-
26	BCR	d	6050	-	-	12/29/63/63	0/2/2/2
23	CLA	C	1036	3	2/2/15/20	25/39/115/115	-
26	BCR	C	1054	-	-	14/29/63/63	0/2/2/2
23	CLA	b	6017	2	1/1/15/20	21/39/115/115	-
23	CLA	c	6034	-	4/4/15/20	27/39/115/115	-
26	BCR	b	6048	-	-	17/29/63/63	0/2/2/2
25	PQ9	a	6043	-	-	10/41/61/61	0/1/1/1
23	CLA	b	6023	2	2/2/15/20	19/39/115/115	-
24	PHO	A	1038	-	2/2/17/22	19/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	1011	2	-	16/39/115/115	-
24	PHO	A	1039	-	1/1/17/22	19/37/103/103	0/5/6/6
23	CLA	B	1015	-	-	19/39/115/115	-
23	CLA	d	6008	4	-	22/39/115/115	-
26	BCR	B	1045	-	-	8/29/63/63	0/2/2/2
23	CLA	C	1031	3	3/3/15/20	14/39/115/115	-
23	CLA	C	1034	-	4/4/15/20	25/39/115/115	-
23	CLA	D	1004	4	-	16/39/115/115	-
23	CLA	B	1012	-	-	22/39/115/115	-
26	BCR	b	6045	-	-	8/29/63/63	0/2/2/2
23	CLA	B	1018	-	-	11/39/115/115	-
23	CLA	c	6030	3	-	16/39/115/115	-
23	CLA	b	6014	-	1/1/15/20	19/39/115/115	-
23	CLA	b	6012	-	-	23/39/115/115	-
31	HEM	e	6040	6	-	3/14/54/54	-
23	CLA	d	6005	-	1/1/15/20	17/39/115/115	-
23	CLA	b	6021	2	2/2/15/20	20/39/115/115	-
26	BCR	b	6047	-	-	15/29/63/63	0/2/2/2
23	CLA	C	1037	3	2/2/15/20	16/39/115/115	-
26	BCR	k	6052	-	-	20/29/63/63	0/2/2/2
23	CLA	b	6018	-	-	11/39/115/115	-
26	BCR	A	1044	-	-	10/29/63/63	0/2/2/2
23	CLA	B	1009	-	3/3/15/20	18/39/115/115	-
23	CLA	B	1010	-	-	15/39/115/115	-
23	CLA	B	1020	2	1/1/15/20	19/39/115/115	-
26	BCR	z	6053	-	-	13/29/63/63	0/2/2/2
23	CLA	D	1008	4	-	22/39/115/115	-
26	BCR	H	1049	-	-	15/29/63/63	0/2/2/2
30	DGD	c	6055	-	-	27/55/95/95	0/2/2/2
30	DGD	H	1058	-	-	36/55/95/95	0/2/2/2
23	CLA	c	6029	3	2/2/15/20	17/39/115/115	-
23	CLA	a	6007	1	1/1/15/20	22/39/115/115	-
23	CLA	c	6033	3	2/2/15/20	24/39/115/115	-
23	CLA	c	6031	3	3/3/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	1003	1	-	18/39/115/115	-
23	CLA	b	6013	2	-	17/39/115/115	-
23	CLA	A	1006	-	-	23/39/115/115	-
29	MGE	D	1062	-	-	24/43/63/63	0/1/1/1
26	BCR	h	6049	-	-	15/29/63/63	0/2/2/2
23	CLA	B	1022	2	2/2/15/20	16/39/115/115	-
23	CLA	c	6037	-	2/2/15/20	16/39/115/115	-
29	MGE	d	6059	-	-	23/43/63/63	0/1/1/1
30	DGD	h	6058	-	-	36/55/95/95	0/2/2/2
26	BCR	t	1046	-	-	14/29/63/63	0/2/2/2
23	CLA	C	1028	-	3/3/15/20	18/39/115/115	-
23	CLA	c	6035	-	-	21/39/115/115	-
29	MGE	b	6060	-	-	22/43/63/63	0/1/1/1
23	CLA	D	1005	-	1/1/15/20	17/39/115/115	-
26	BCR	K	1051	-	-	15/29/63/63	0/2/2/2
23	CLA	A	1007	-	1/1/15/20	22/39/115/115	-
23	CLA	b	6022	2	2/2/15/20	16/39/115/115	-
23	CLA	H	1017	2	1/1/15/20	21/39/115/115	-
31	HEM	v	6041	-	-	7/14/54/54	-
26	BCR	c	6054	-	-	14/29/63/63	0/2/2/2
23	CLA	B	1024	-	1/1/15/20	14/39/115/115	-
30	DGD	c	6056	-	-	31/55/95/95	0/2/2/2
23	CLA	C	1025	3	1/1/15/20	21/39/115/115	-
23	CLA	C	1026	-	1/1/15/20	16/39/115/115	-
30	DGD	C	1055	-	-	27/55/95/95	0/2/2/2
23	CLA	C	1030	3	-	16/39/115/115	-
23	CLA	b	6024	-	1/1/15/20	14/39/115/115	-
23	CLA	B	1013	-	-	17/39/115/115	-
26	BCR	D	1050	-	-	12/29/63/63	0/2/2/2
23	CLA	b	6019	2	2/2/15/20	23/39/115/115	-
25	PQ9	D	1042	-	-	7/41/61/61	0/1/1/1
26	BCR	K	1052	-	-	20/29/63/63	0/2/2/2
25	PQ9	d	6042	-	-	8/41/61/61	0/1/1/1
26	BCR	B	1047	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	1032	-	-	16/39/115/115	-
23	CLA	a	6003	1	-	18/39/115/115	-
23	CLA	C	1035	3	-	21/39/115/115	-
31	HEM	E	1040	6	-	3/14/54/54	-
29	MGE	L	1061	-	-	24/43/63/63	0/1/1/1
23	CLA	B	1023	-	2/2/15/20	19/39/115/115	-
23	CLA	c	6027	-	3/3/15/20	19/39/115/115	-
30	DGD	C	1056	-	-	31/55/95/95	0/2/2/2
23	CLA	b	6016	2	-	20/39/115/115	-
29	MGE	B	1060	-	-	24/43/63/63	0/1/1/1
23	CLA	c	6025	3	1/1/15/20	21/39/115/115	-
23	CLA	b	6020	2	1/1/15/20	19/39/115/115	-
23	CLA	c	6028	-	3/3/15/20	18/39/115/115	-
23	CLA	c	6026	-	1/1/15/20	16/39/115/115	-
26	BCR	k	6051	-	-	15/29/63/63	0/2/2/2
30	DGD	C	1057	-	-	19/55/95/95	0/2/2/2
30	DGD	c	6057	-	-	19/55/95/95	0/2/2/2
24	PHO	d	6038	-	2/2/17/22	19/37/103/103	0/5/6/6
23	CLA	a	6006	-	-	22/39/115/115	-
26	BCR	B	1048	-	-	17/29/63/63	0/2/2/2
23	CLA	C	1029	3	2/2/15/20	17/39/115/115	-
23	CLA	c	6036	3	2/2/15/20	25/39/115/115	-
29	MGE	d	6061	-	-	24/43/63/63	0/1/1/1
29	MGE	d	6062	-	-	24/43/63/63	0/1/1/1
26	BCR	T	6046	-	-	9/20/63/63	-
27	LHG	a	6063	-	-	26/53/53/53	-
29	MGE	J	1059	-	-	23/43/63/63	0/1/1/1
26	BCR	a	6044	-	-	10/29/63/63	0/2/2/2
26	BCR	Z	1053	-	-	13/29/63/63	0/2/2/2
23	CLA	b	6010	2	-	15/39/115/115	-
24	PHO	a	6039	-	1/1/17/22	19/37/103/103	0/5/6/6
23	CLA	B	1019	2	2/2/15/20	23/39/115/115	-
23	CLA	B	1016	2	-	20/39/115/115	-
25	PQ9	A	1043	-	-	11/41/61/61	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	6011	2	-	16/39/115/115	-
23	CLA	b	6015	-	-	19/39/115/115	-
23	CLA	B	1014	-	1/1/15/20	19/39/115/115	-
23	CLA	b	6009	-	3/3/15/20	18/39/115/115	-
23	CLA	C	1027	-	3/3/15/20	18/39/115/115	-
23	CLA	B	1021	2	2/2/15/20	20/39/115/115	-
27	LHG	A	1063	-	-	26/53/53/53	-

The worst 5 of 1717 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	6043	PQ9	C27-C28	15.14	1.67	1.33
24	A	1039	PHO	OBD-CAD	14.54	1.41	1.22
24	A	1038	PHO	OBD-CAD	14.53	1.41	1.22
24	a	6039	PHO	OBD-CAD	14.51	1.41	1.22
24	d	6038	PHO	OBD-CAD	14.50	1.41	1.22

The worst 5 of 2826 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	1047	BCR	C7-C8-C9	34.70	177.56	126.23
26	b	6047	BCR	C7-C8-C9	34.65	177.50	126.23
26	C	1054	BCR	C7-C8-C9	28.08	167.78	126.23
26	c	6054	BCR	C7-C8-C9	28.06	167.74	126.23
26	T	6046	BCR	C7-C8-C9	27.21	166.48	126.23

5 of 86 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	1007	CLA	C13
23	B	1009	CLA	C8
23	B	1009	CLA	C13
23	B	1009	CLA	CBD
23	B	1014	CLA	C3A

5 of 2210 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	1003	CLA	C14-C13-C15-C16
23	A	1006	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
23	A	1006	CLA	C3A-C2A-CAA-CBA
23	A	1006	CLA	C4C-C3C-CAC-CBC
23	A	1006	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

122 monomers are involved in 4438 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	1033	CLA	64	0
23	c	6032	CLA	59	0
31	V	1041	HEM	10	0
23	d	6004	CLA	20	0
26	d	6050	BCR	58	0
23	C	1036	CLA	49	0
26	C	1054	BCR	26	0
23	b	6017	CLA	56	0
23	c	6034	CLA	82	0
26	b	6048	BCR	40	0
25	a	6043	PQ9	3	0
23	b	6023	CLA	77	0
24	A	1038	PHO	81	0
23	B	1011	CLA	107	0
24	A	1039	PHO	34	0
23	B	1015	CLA	31	0
23	d	6008	CLA	35	0
26	B	1045	BCR	29	0
23	C	1031	CLA	63	0
23	C	1034	CLA	87	0
23	D	1004	CLA	19	0
23	B	1012	CLA	65	0
26	b	6045	BCR	29	0
23	B	1018	CLA	23	0
23	c	6030	CLA	29	0
23	b	6014	CLA	80	0
23	b	6012	CLA	58	0
31	e	6040	HEM	11	0
23	d	6005	CLA	69	0
23	b	6021	CLA	71	0
26	b	6047	BCR	38	0
23	C	1037	CLA	25	0
26	k	6052	BCR	43	0
23	b	6018	CLA	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	1044	BCR	26	0
23	B	1010	CLA	49	0
23	B	1009	CLA	49	0
23	B	1020	CLA	69	0
26	z	6053	BCR	40	0
23	D	1008	CLA	33	0
26	H	1049	BCR	54	0
30	c	6055	DGD	34	0
30	H	1058	DGD	32	0
23	c	6029	CLA	46	0
23	a	6007	CLA	19	0
23	c	6033	CLA	65	0
23	c	6031	CLA	69	0
23	A	1003	CLA	63	0
23	b	6013	CLA	85	0
23	A	1006	CLA	93	0
29	D	1062	MGE	24	0
26	h	6049	BCR	47	0
23	B	1022	CLA	70	0
23	c	6037	CLA	26	0
29	d	6059	MGE	33	0
30	h	6058	DGD	35	0
26	t	1046	BCR	24	0
23	C	1028	CLA	34	0
23	c	6035	CLA	32	0
29	b	6060	MGE	52	0
23	D	1005	CLA	69	0
26	K	1051	BCR	43	0
23	A	1007	CLA	20	0
23	b	6022	CLA	71	0
23	H	1017	CLA	57	0
31	v	6041	HEM	11	0
26	c	6054	BCR	22	0
23	B	1024	CLA	38	0
30	c	6056	DGD	53	0
23	C	1025	CLA	54	0
23	C	1026	CLA	33	0
30	C	1055	DGD	34	0
23	C	1030	CLA	29	0
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23	B	1013	CLA	84	0
26	D	1050	BCR	62	0

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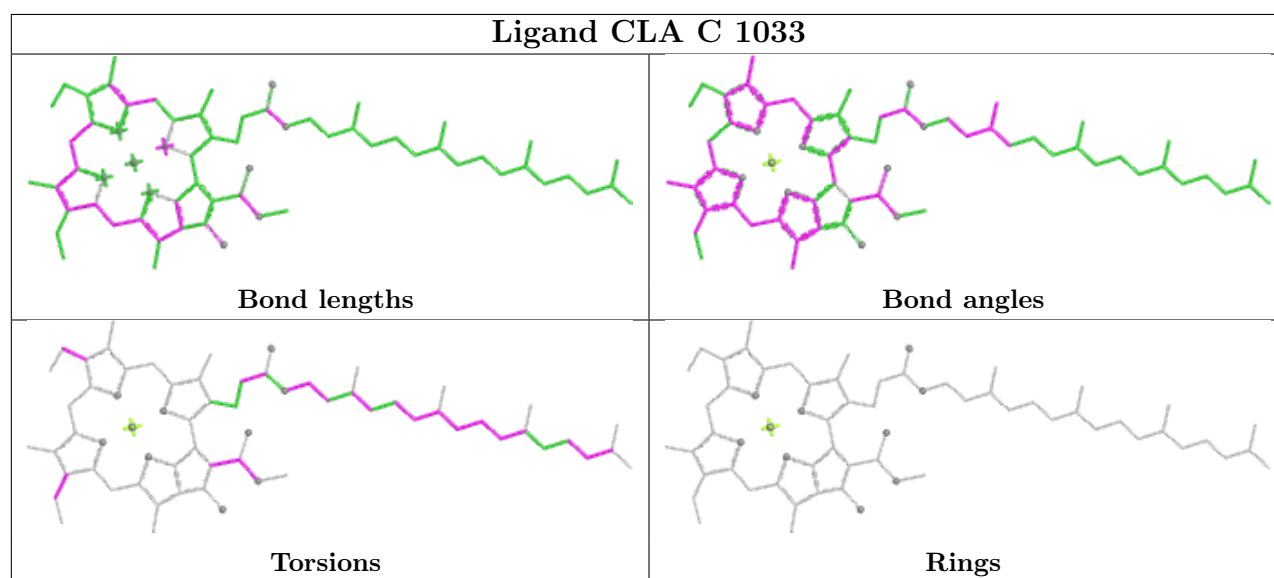
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26	K	1052	BCR	47	0
25	d	6042	PQ9	27	0
26	B	1047	BCR	39	0
23	C	1032	CLA	61	0
23	a	6003	CLA	72	0
23	C	1035	CLA	20	0
31	E	1040	HEM	10	0
29	L	1061	MGE	33	0
23	B	1023	CLA	80	0
23	c	6027	CLA	46	0
30	C	1056	DGD	57	0
23	b	6016	CLA	58	0
29	B	1060	MGE	46	0
23	c	6025	CLA	53	0
23	b	6020	CLA	71	0
23	c	6028	CLA	35	0
23	c	6026	CLA	31	0
26	k	6051	BCR	48	0
30	C	1057	DGD	61	0
30	c	6057	DGD	52	0
24	d	6038	PHO	75	0
23	a	6006	CLA	78	0
26	B	1048	BCR	38	0
23	C	1029	CLA	46	0
23	c	6036	CLA	51	0
29	d	6061	MGE	29	0
29	d	6062	MGE	35	0
26	T	6046	BCR	33	0
27	a	6063	LHG	53	0
29	J	1059	MGE	32	0
26	a	6044	BCR	25	0
26	Z	1053	BCR	41	0
23	b	6010	CLA	52	0
24	a	6039	PHO	33	0
23	B	1019	CLA	85	0
23	B	1016	CLA	62	0
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23	b	6011	CLA	109	0
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23	B	1014	CLA	84	0

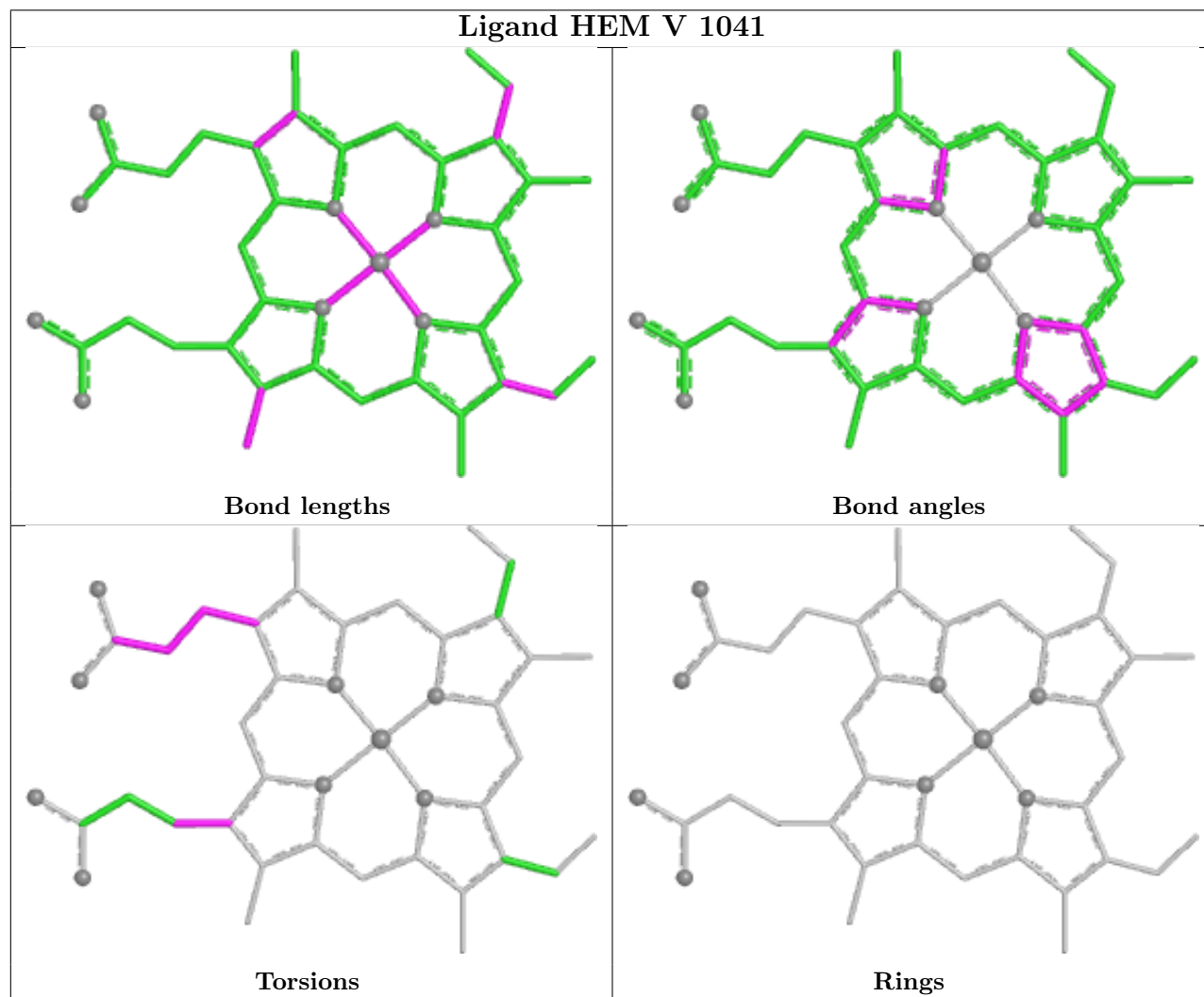
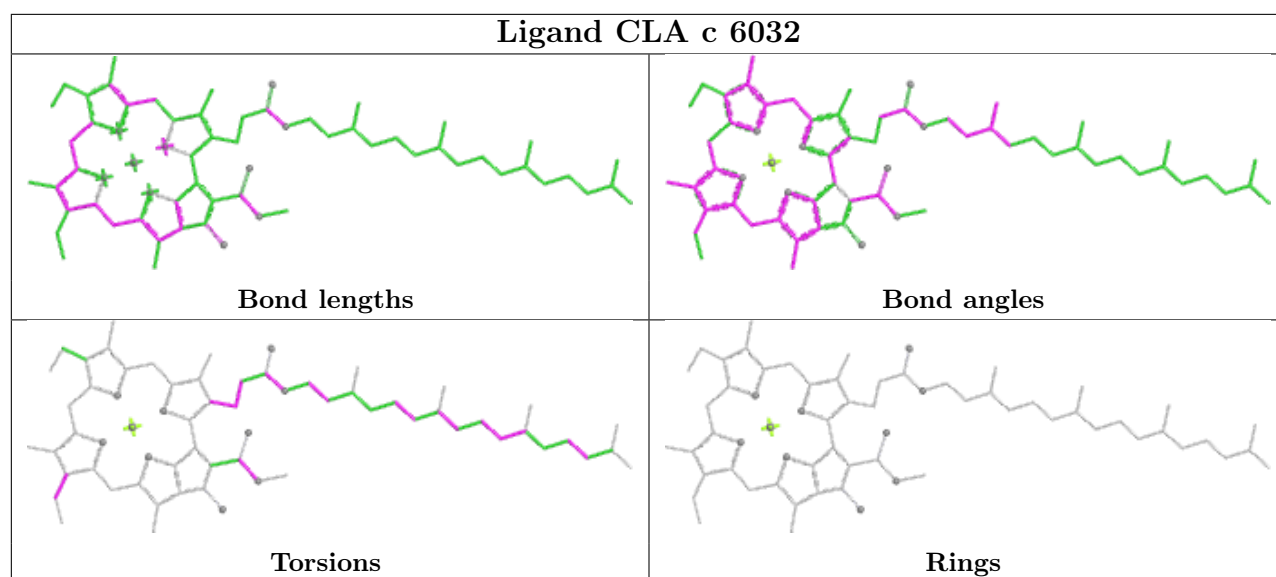
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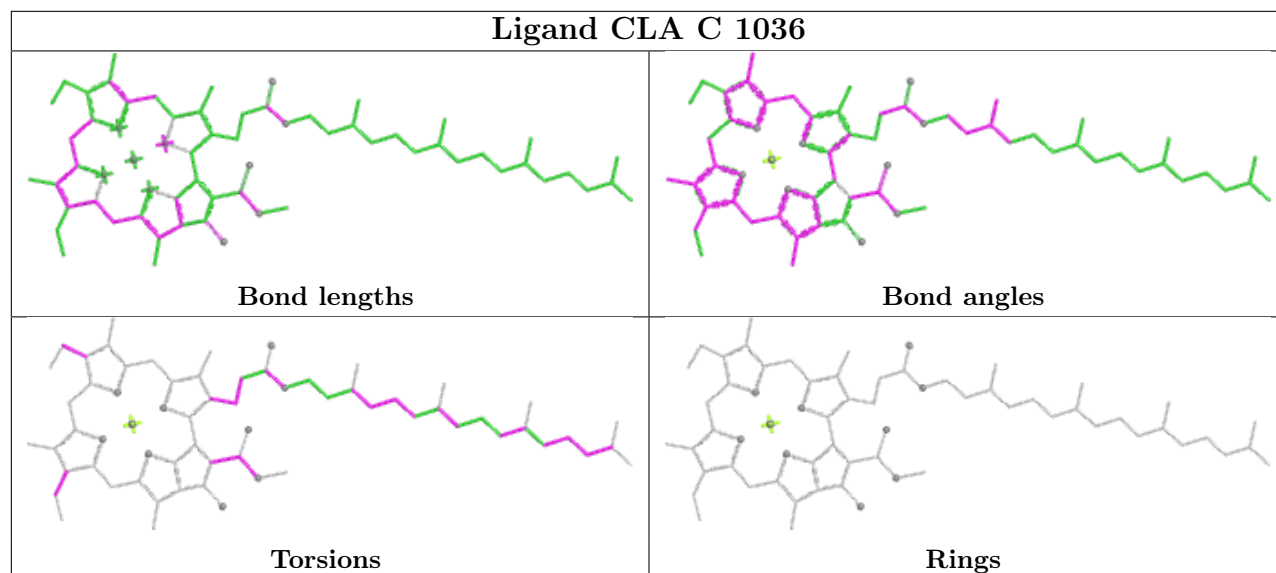
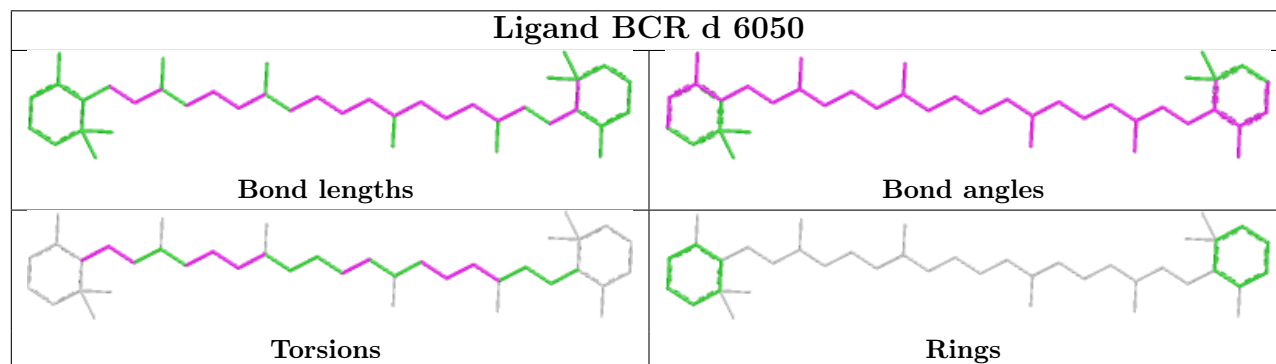
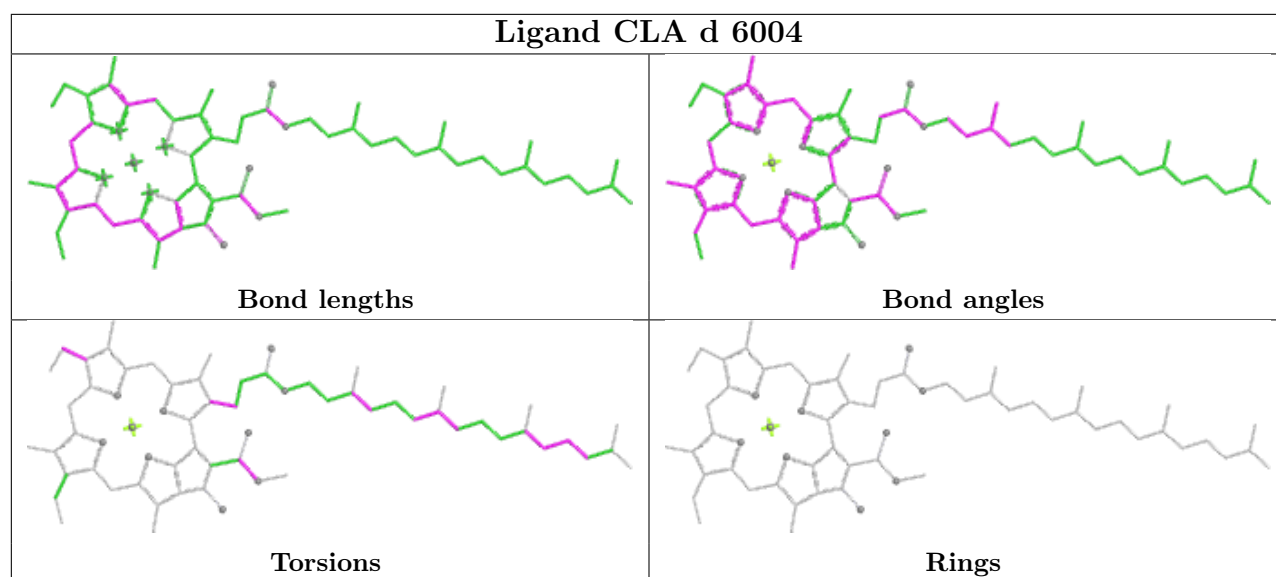
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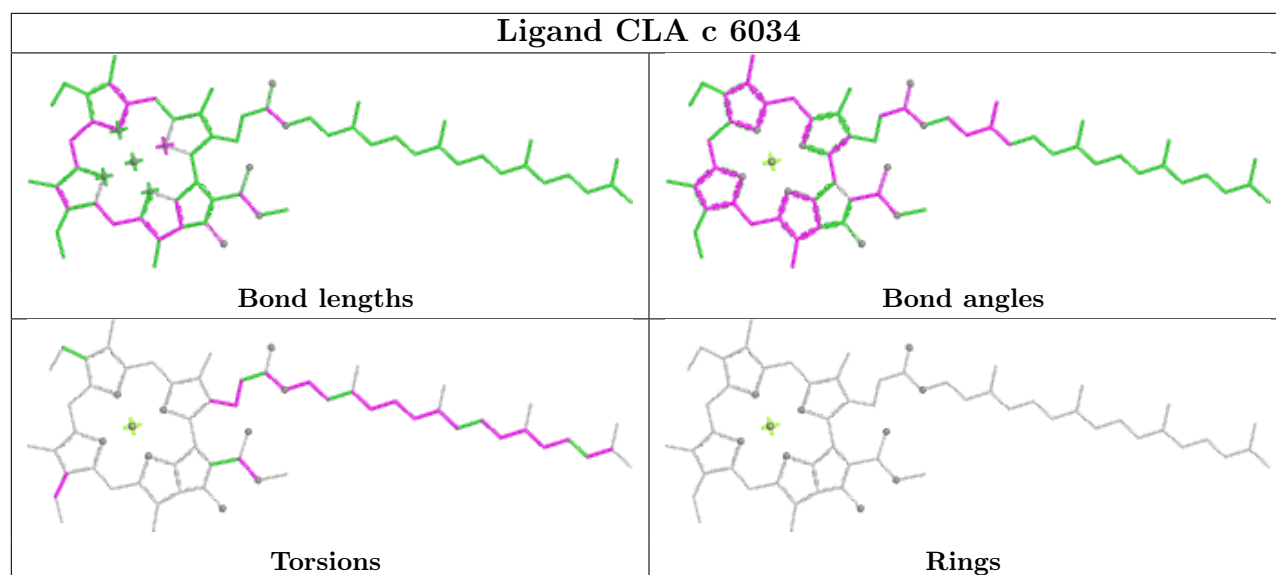
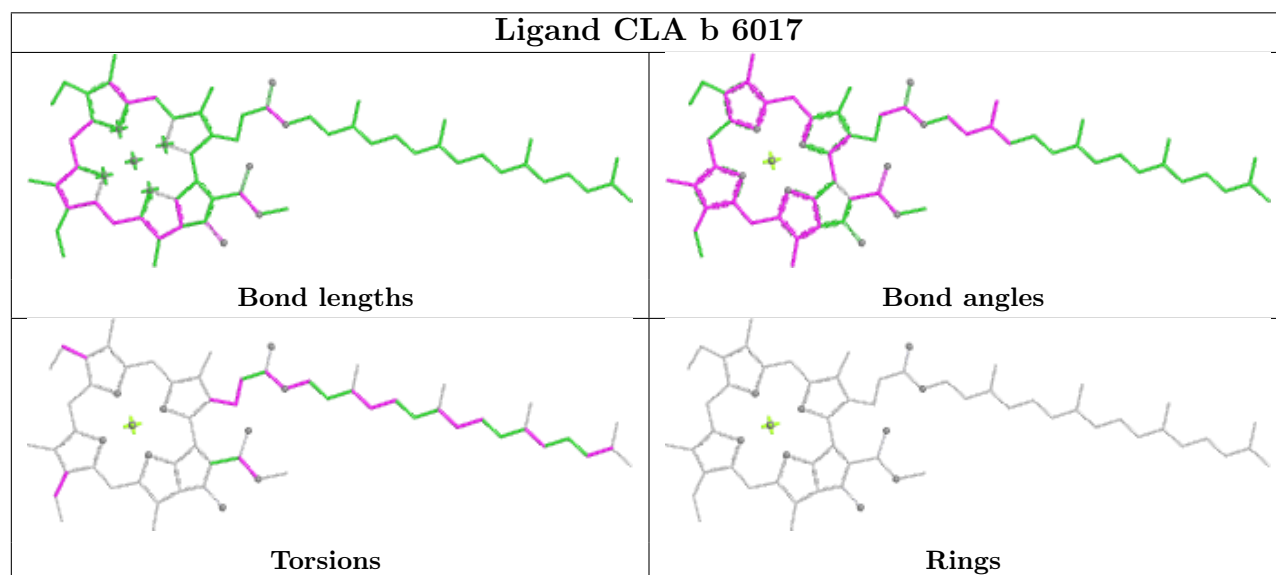
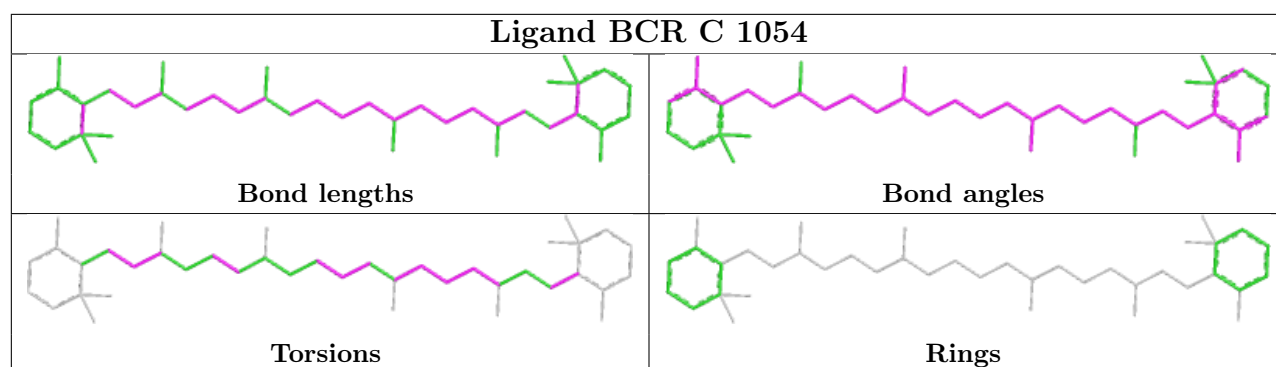
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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23	B	1021	CLA	75	0
27	A	1063	LHG	60	0

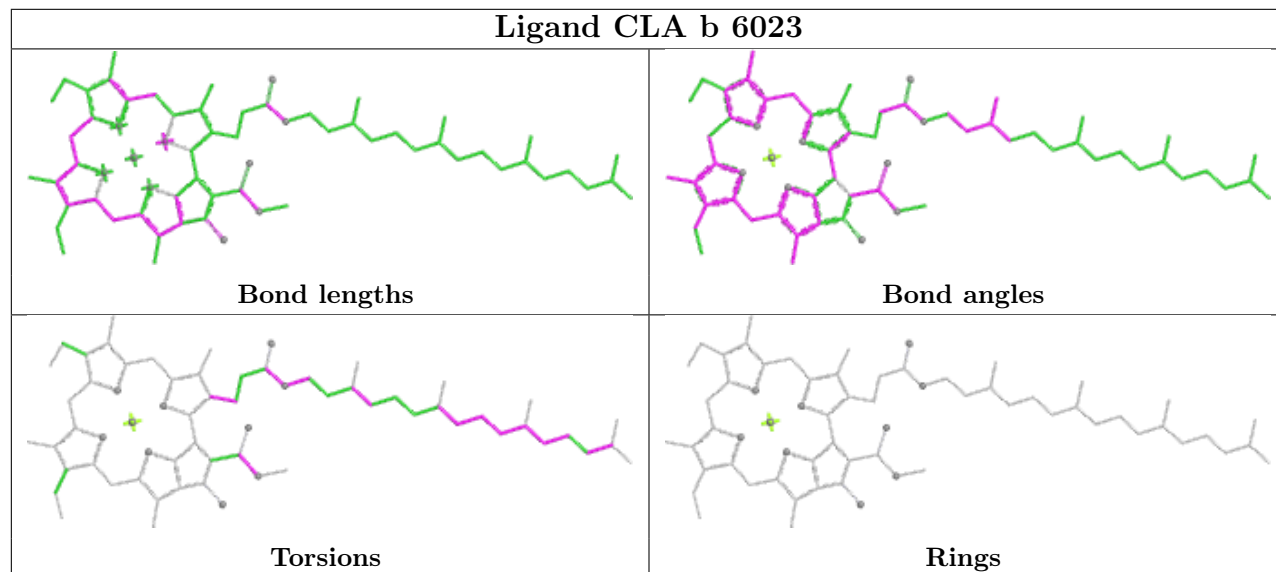
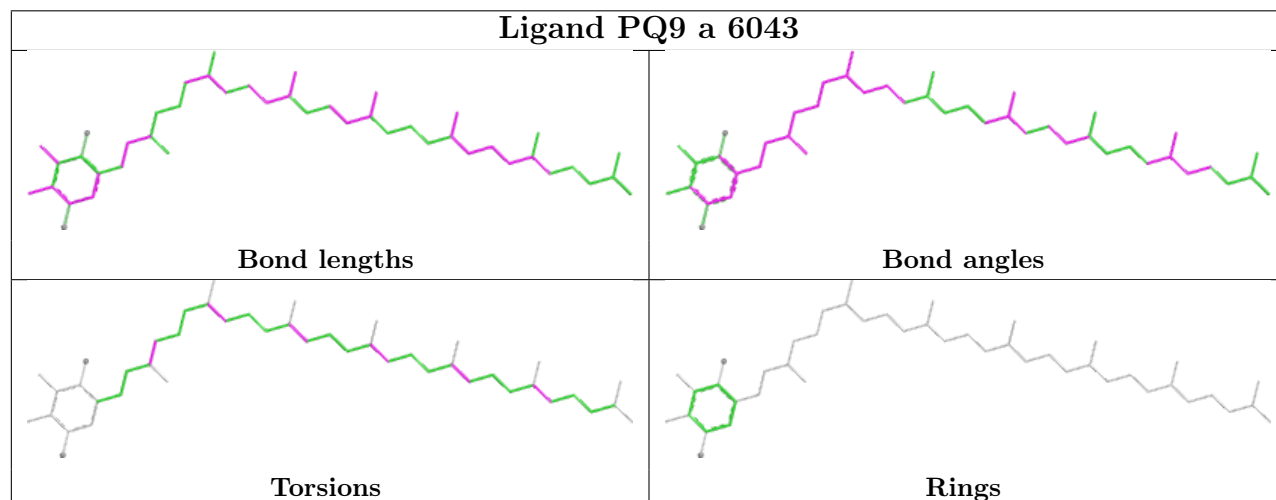
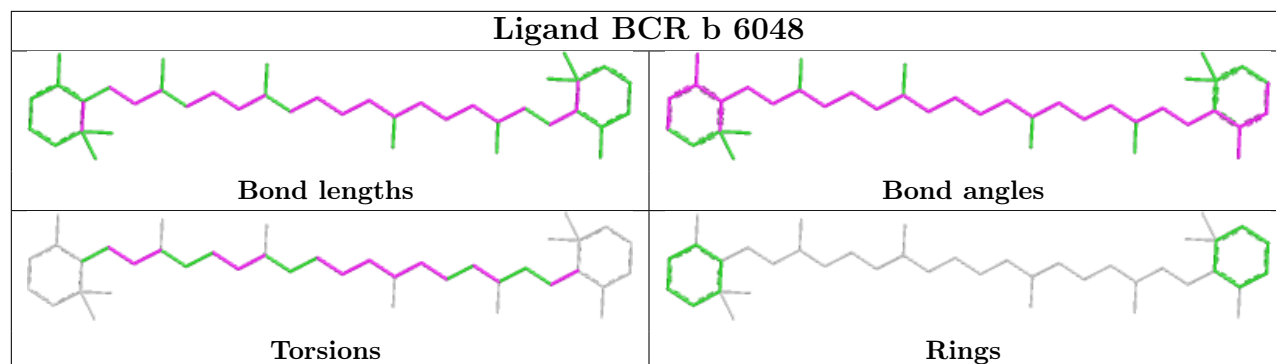
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



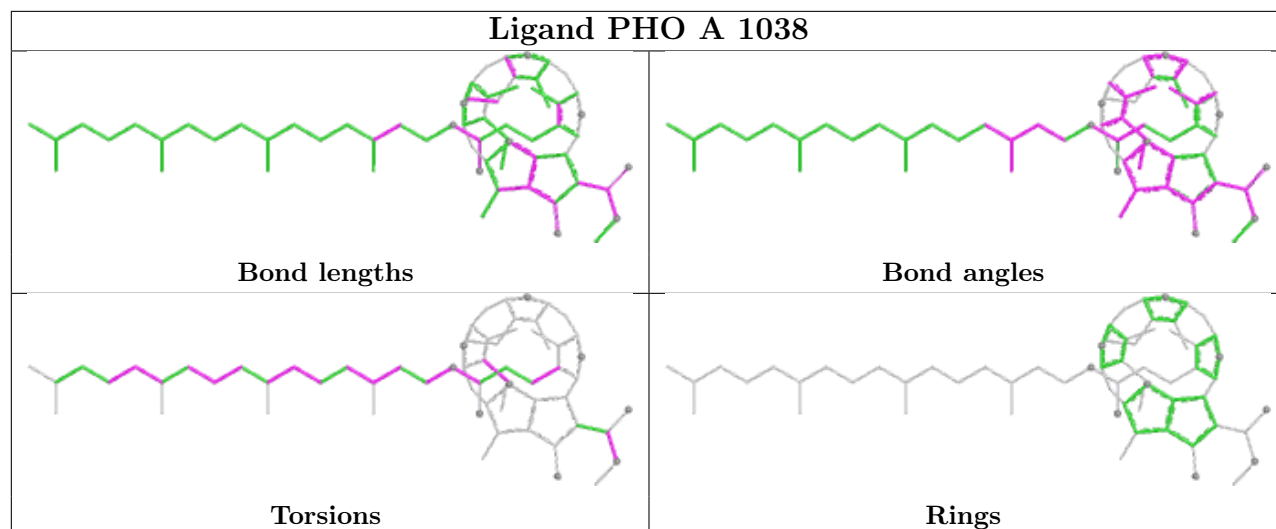




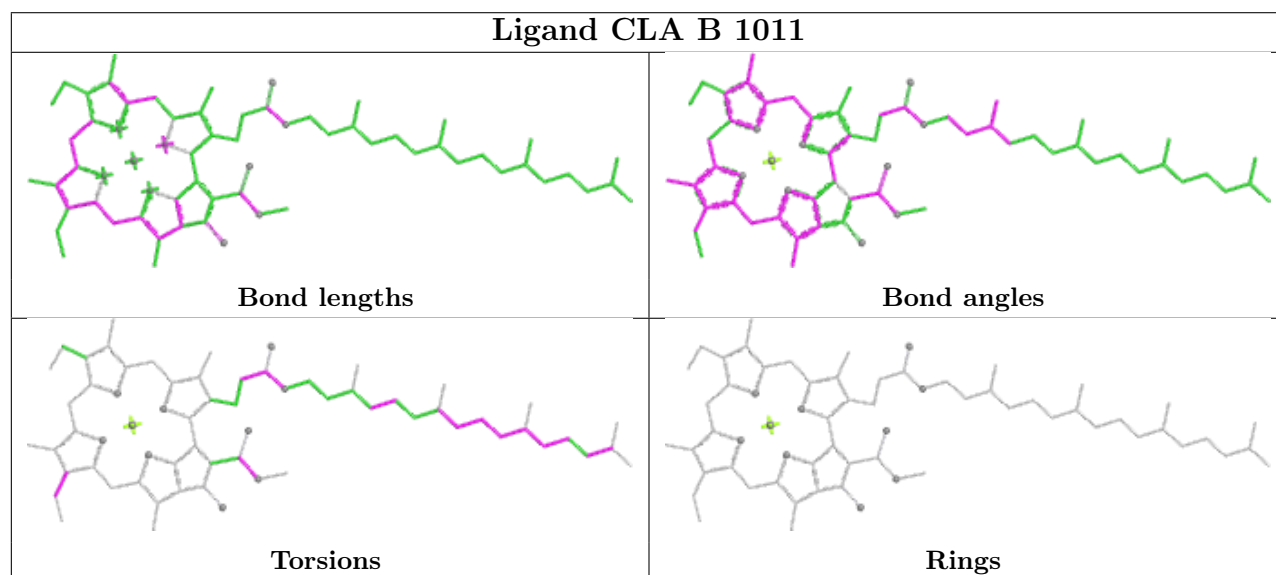




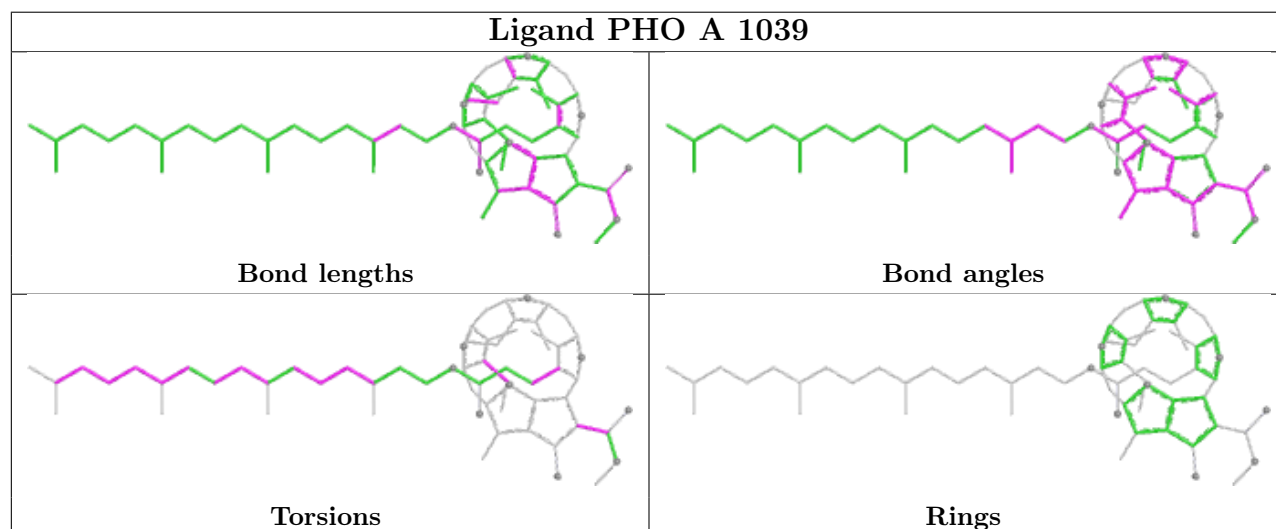
Ligand PHO A 1038

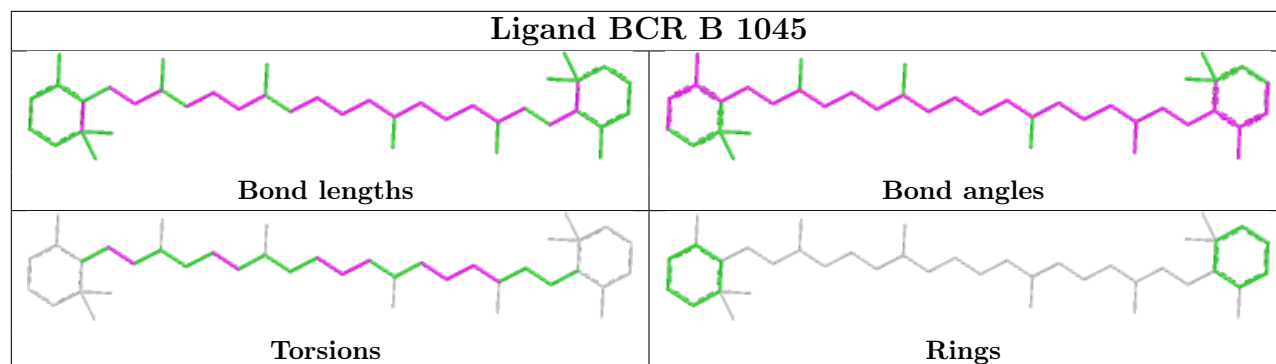
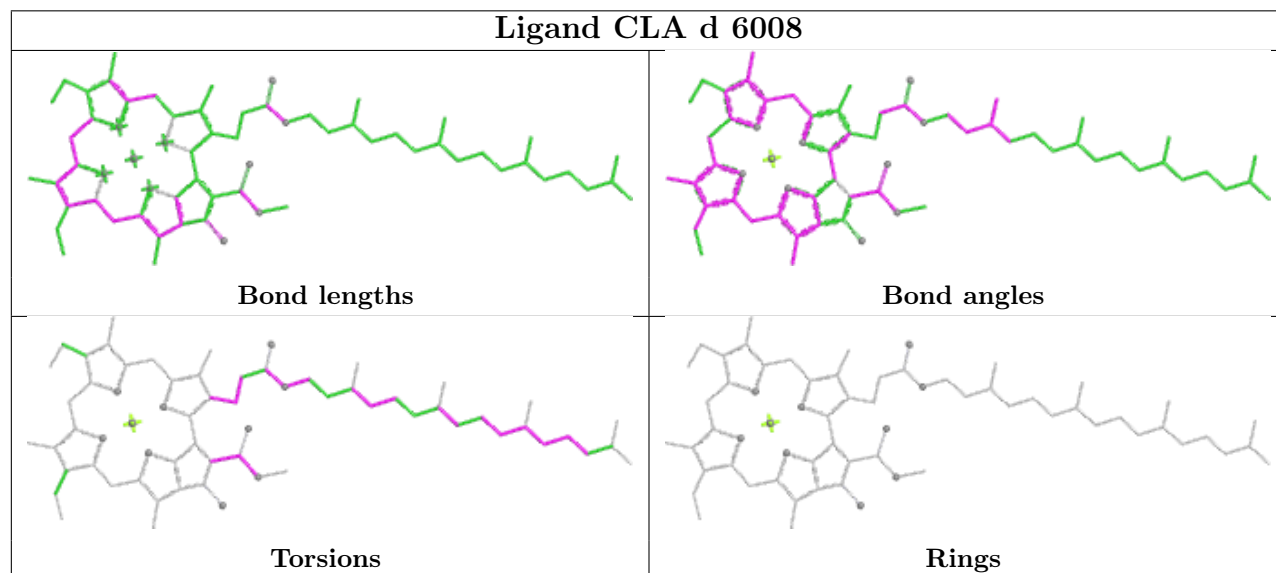
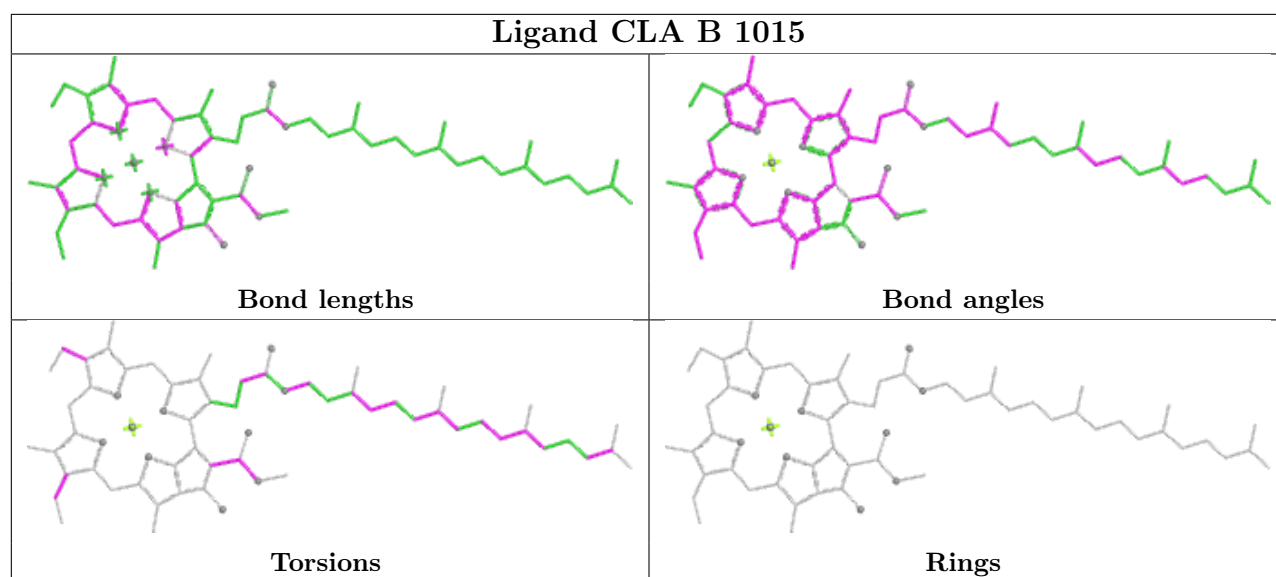


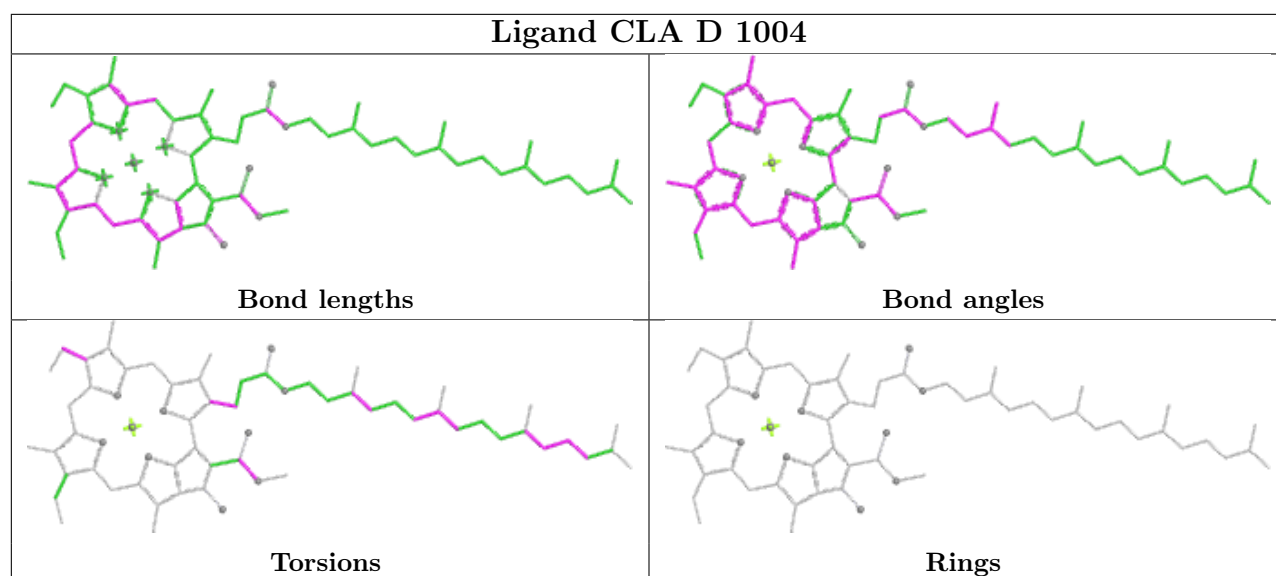
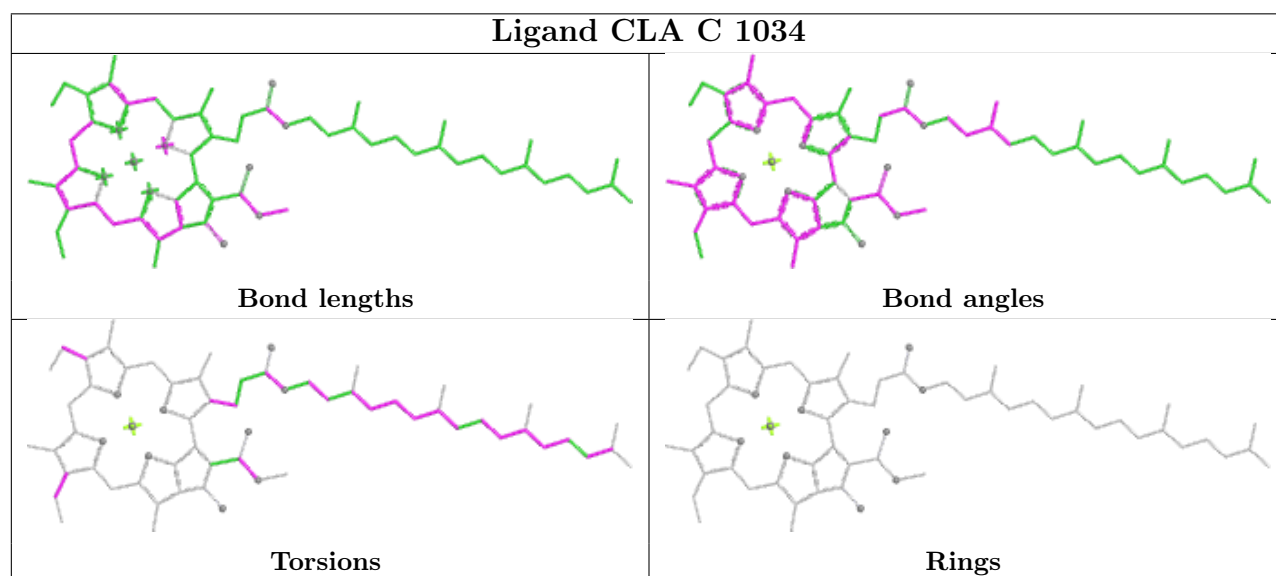
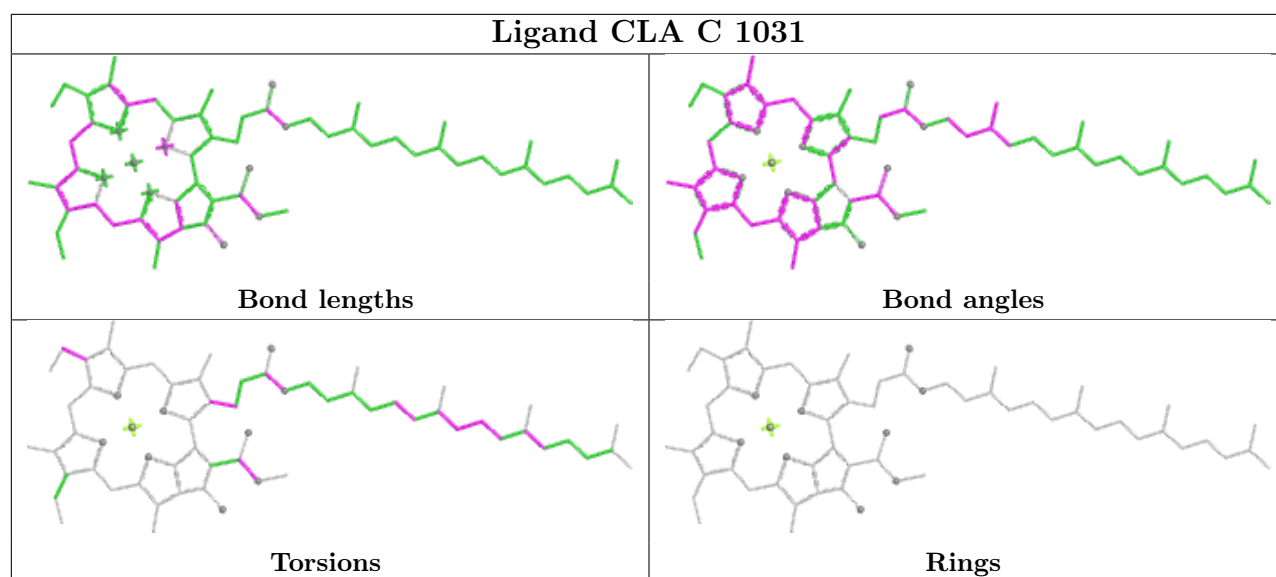
Ligand CLA B 1011

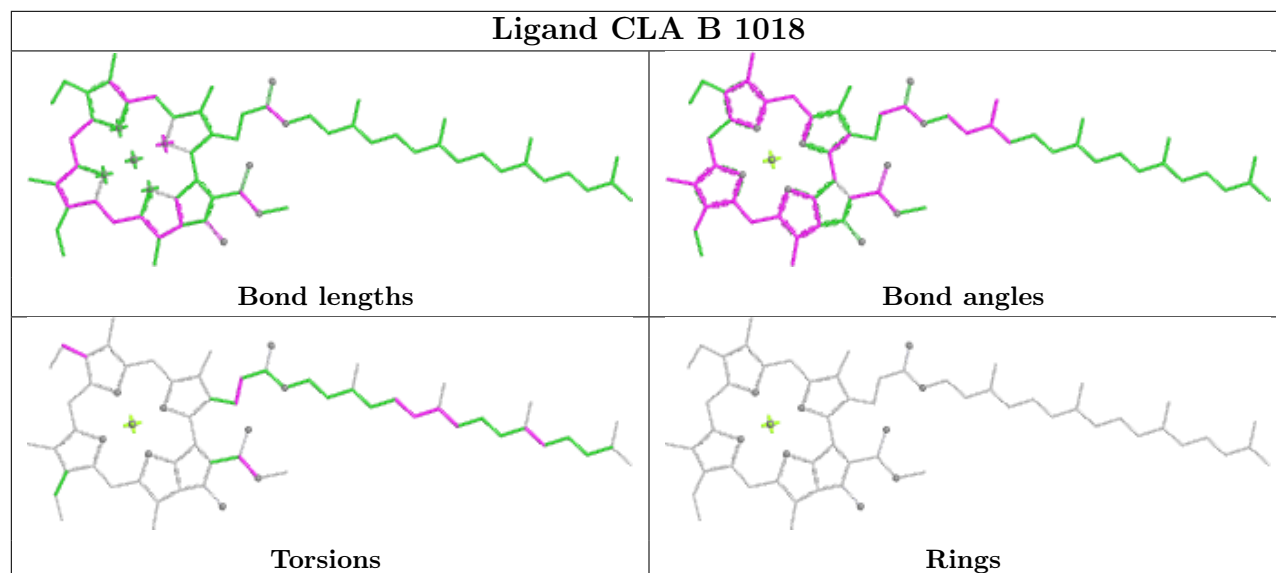
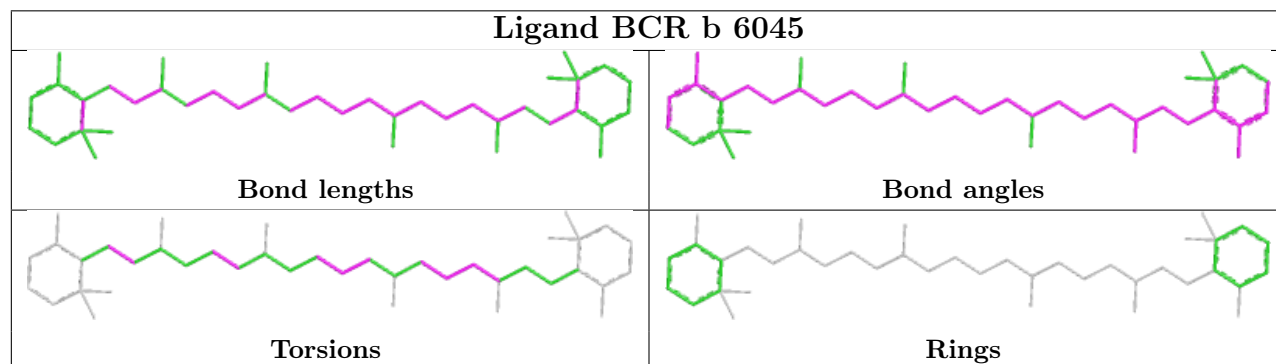
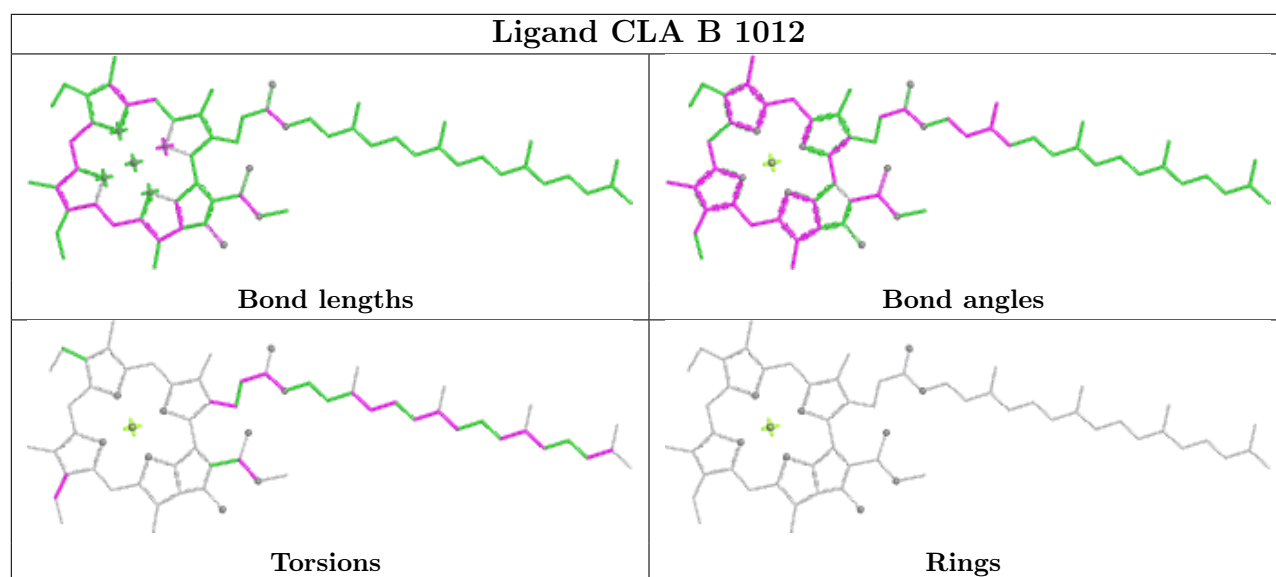


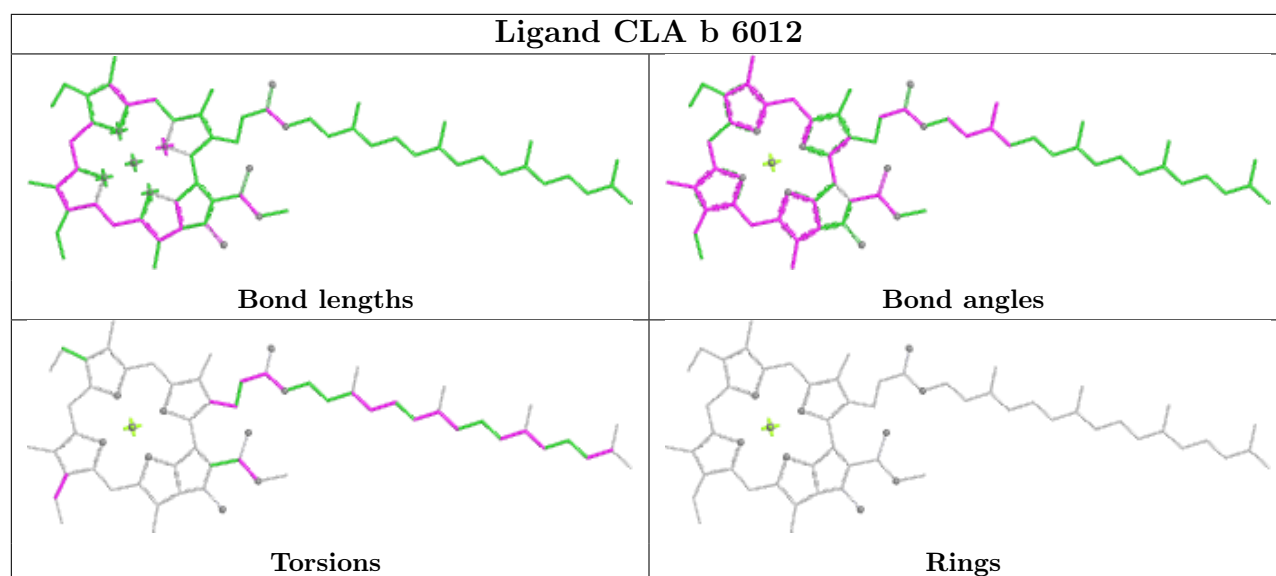
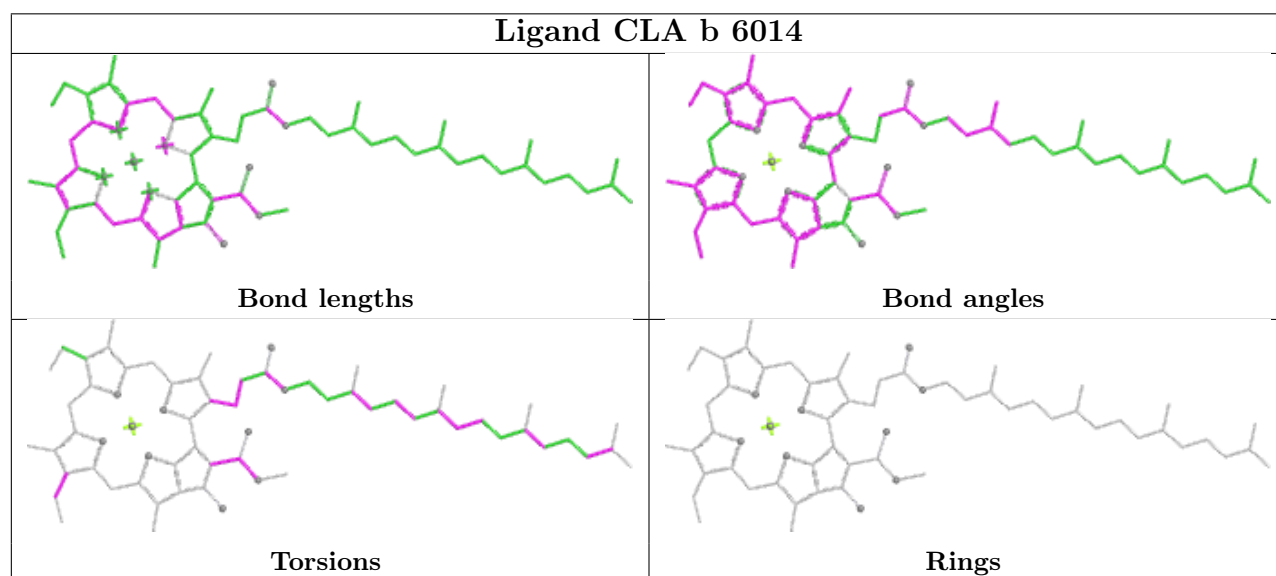
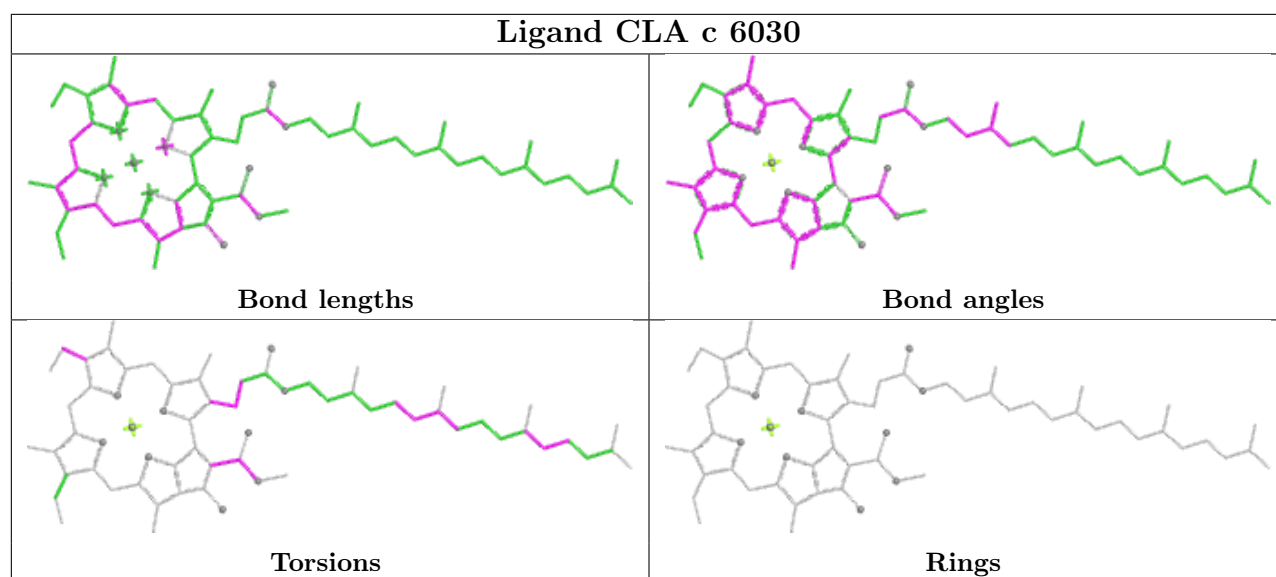
Ligand PHO A 1039



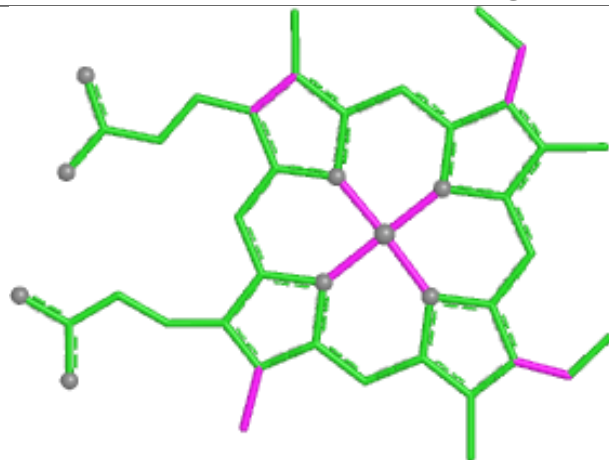




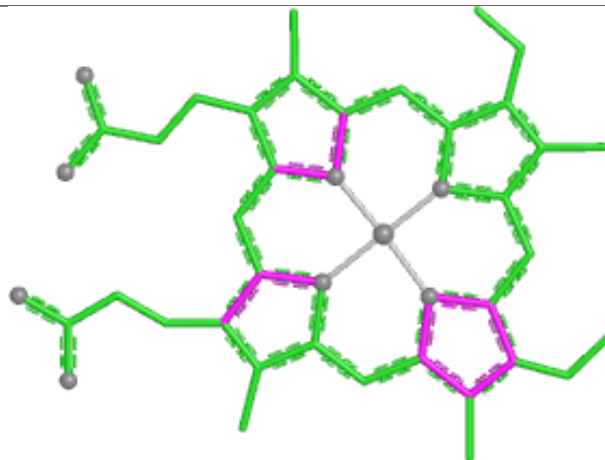




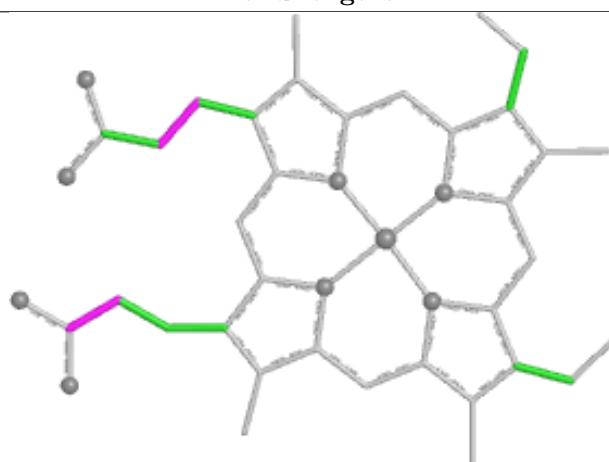
Ligand HEM e 6040



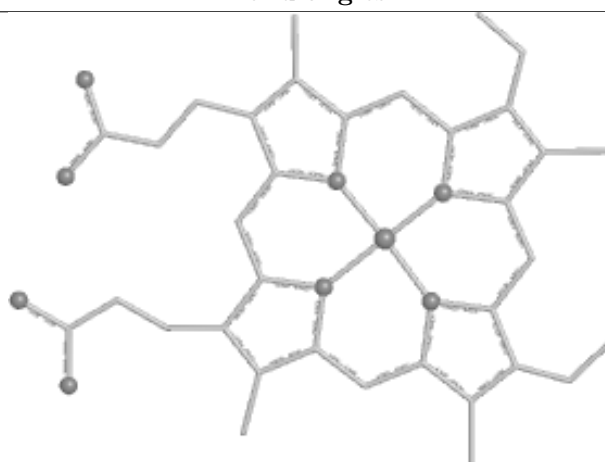
Bond lengths



Bond angles

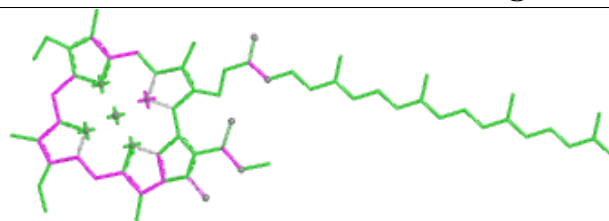


Torsions

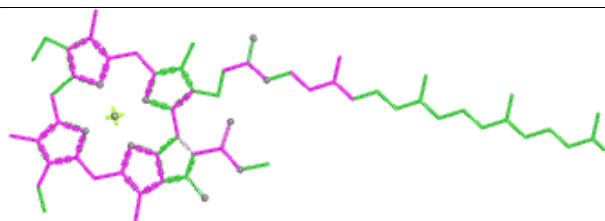


Rings

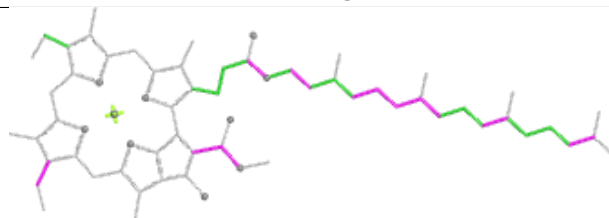
Ligand CLA d 6005



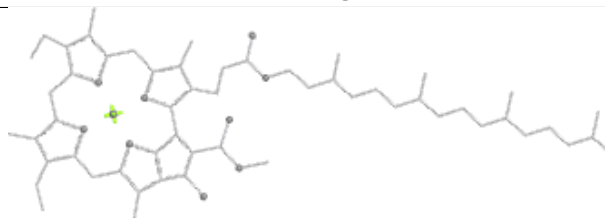
Bond lengths



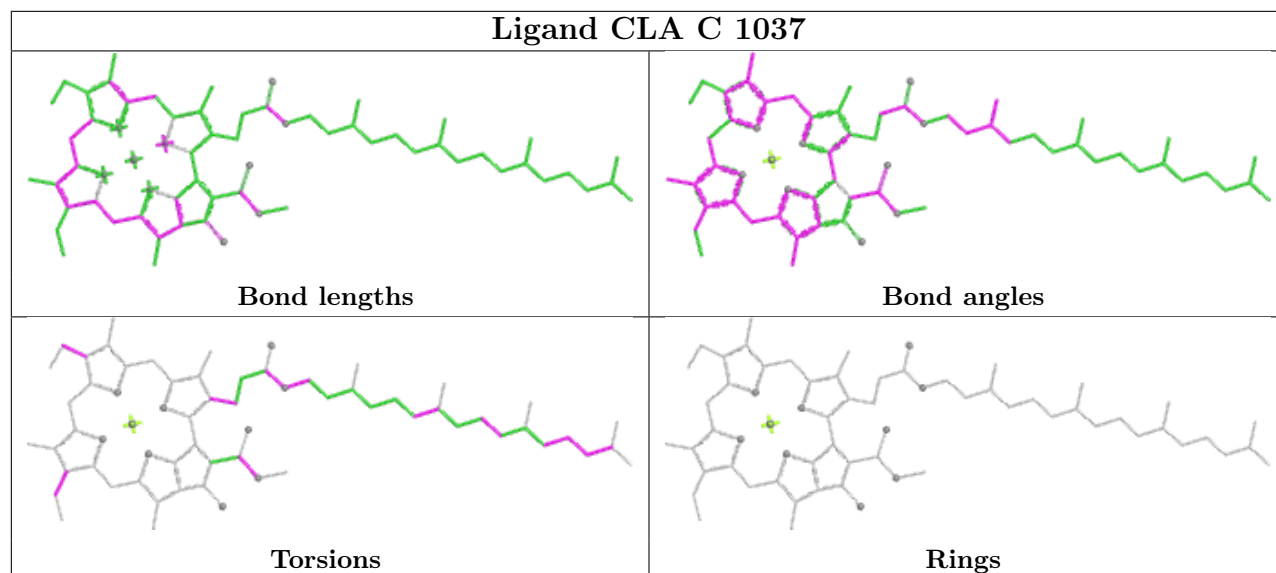
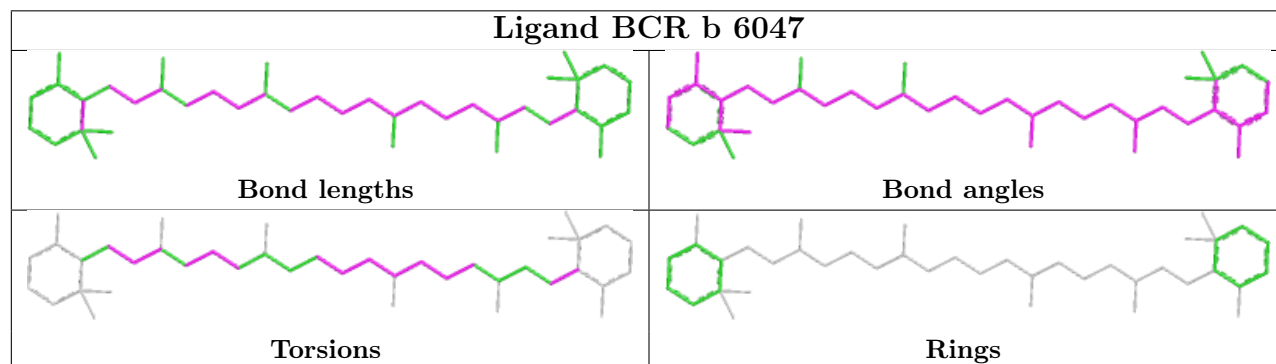
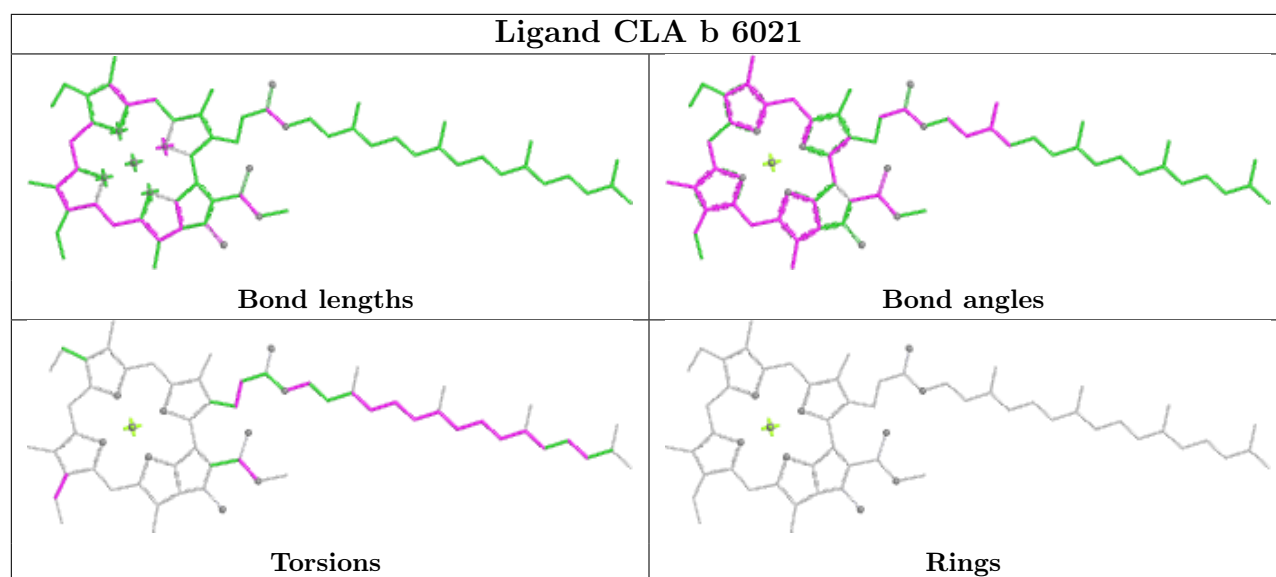
Bond angles

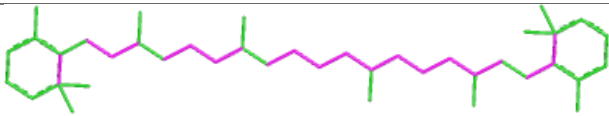
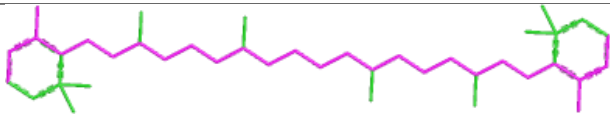
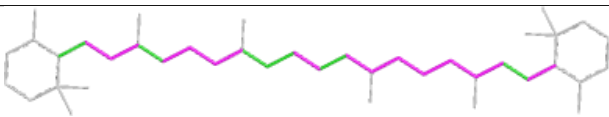
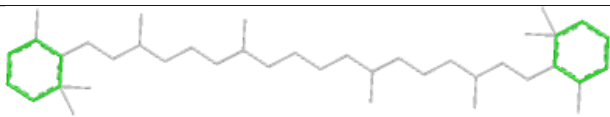


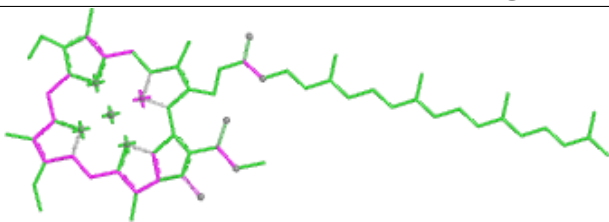
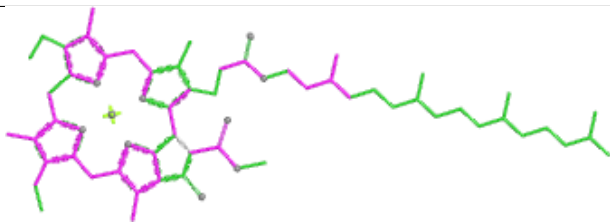
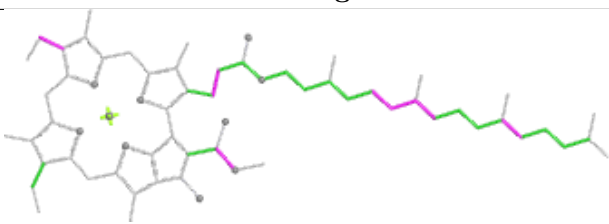
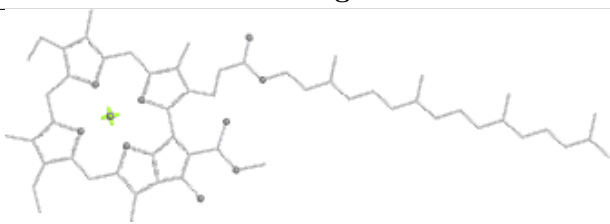
Torsions

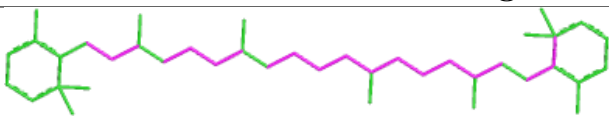
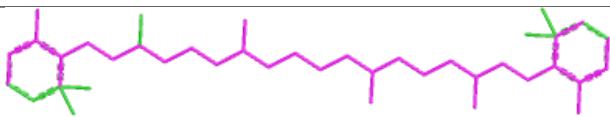
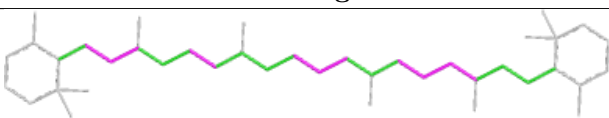
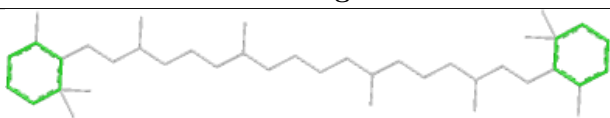


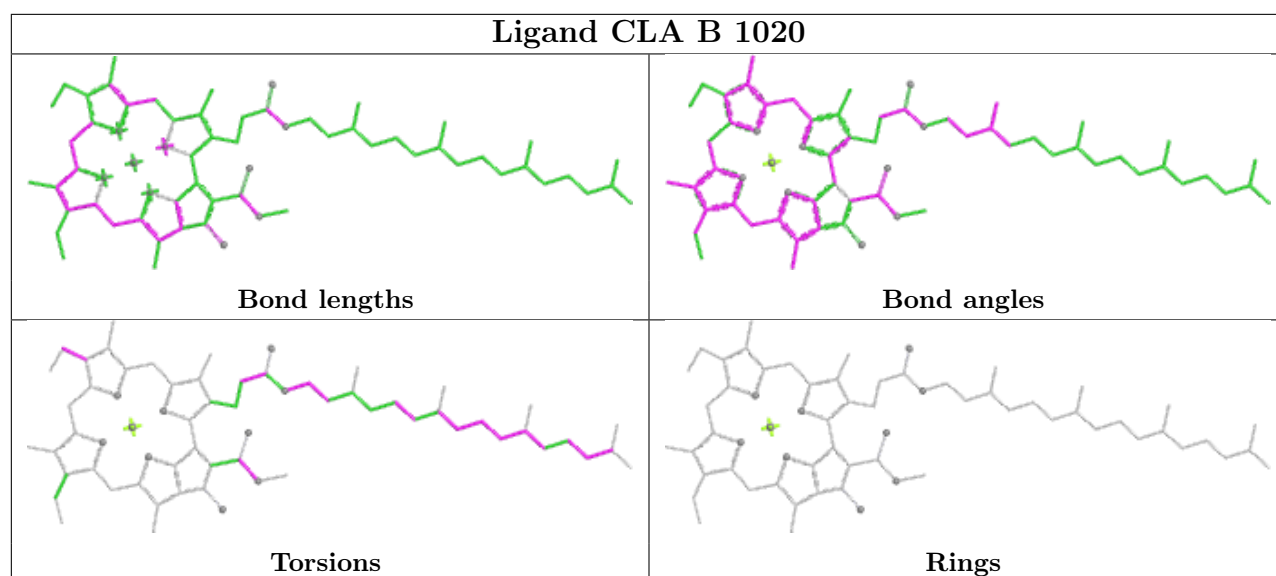
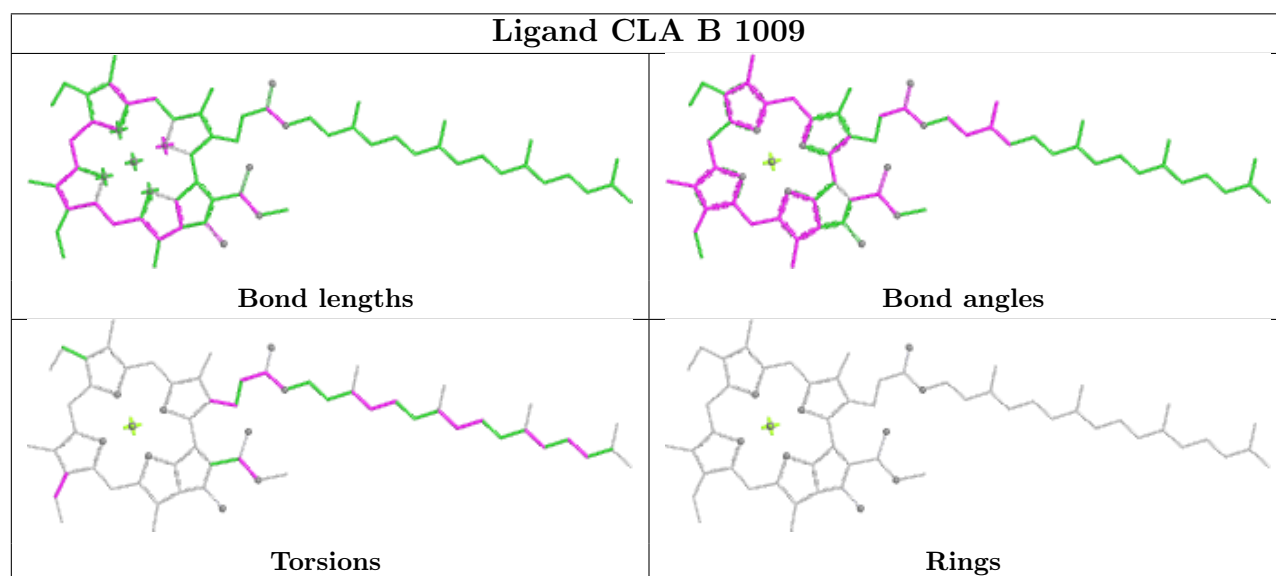
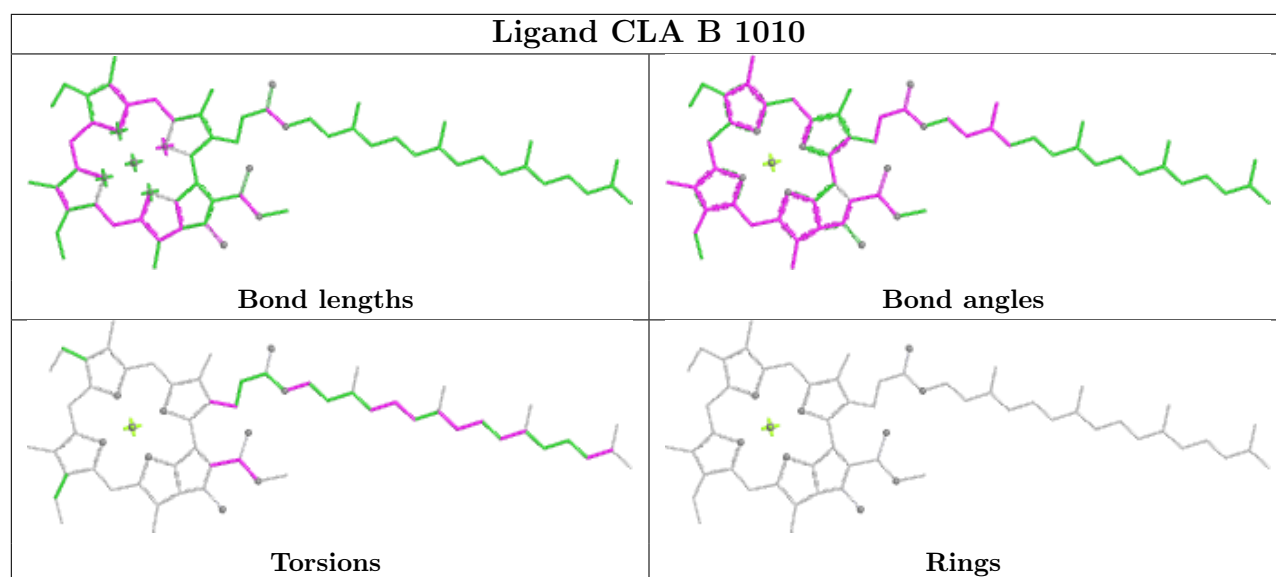
Rings

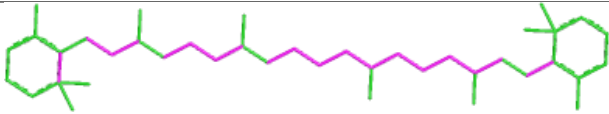
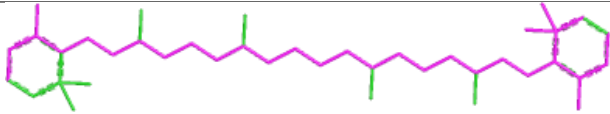
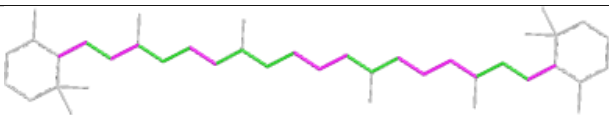
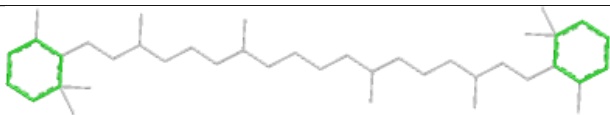


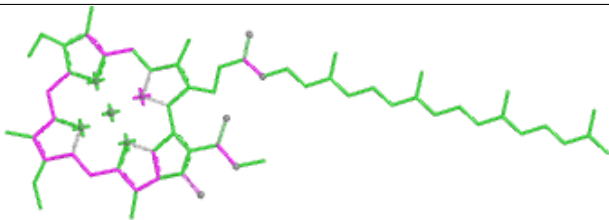
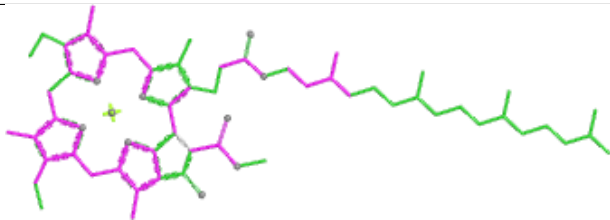
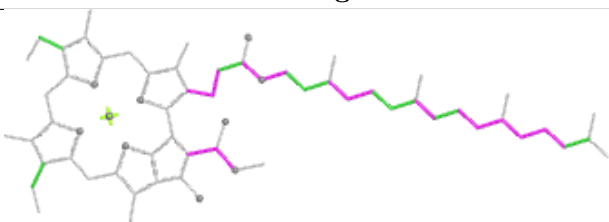
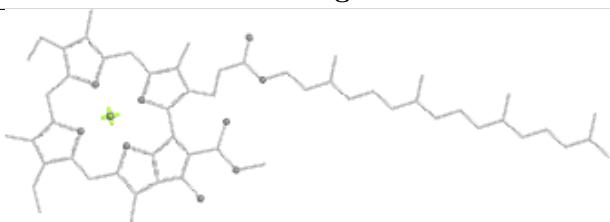
Ligand BCR k 6052	
	
Bond lengths	Bond angles
	
Torsions	Rings

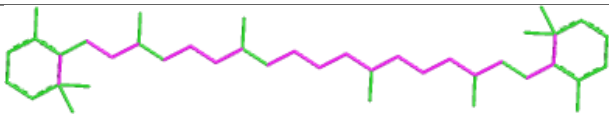
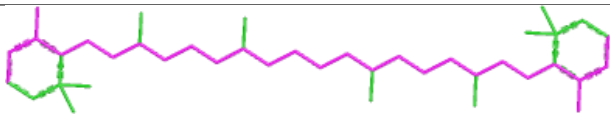
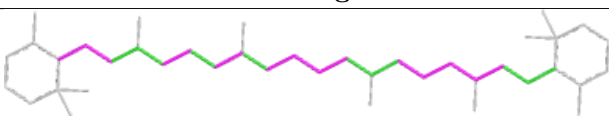
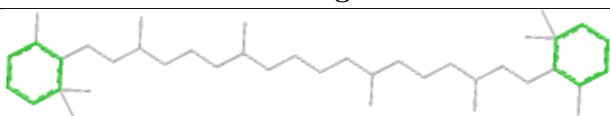
Ligand CLA b 6018	
	
Bond lengths	Bond angles
	
Torsions	Rings

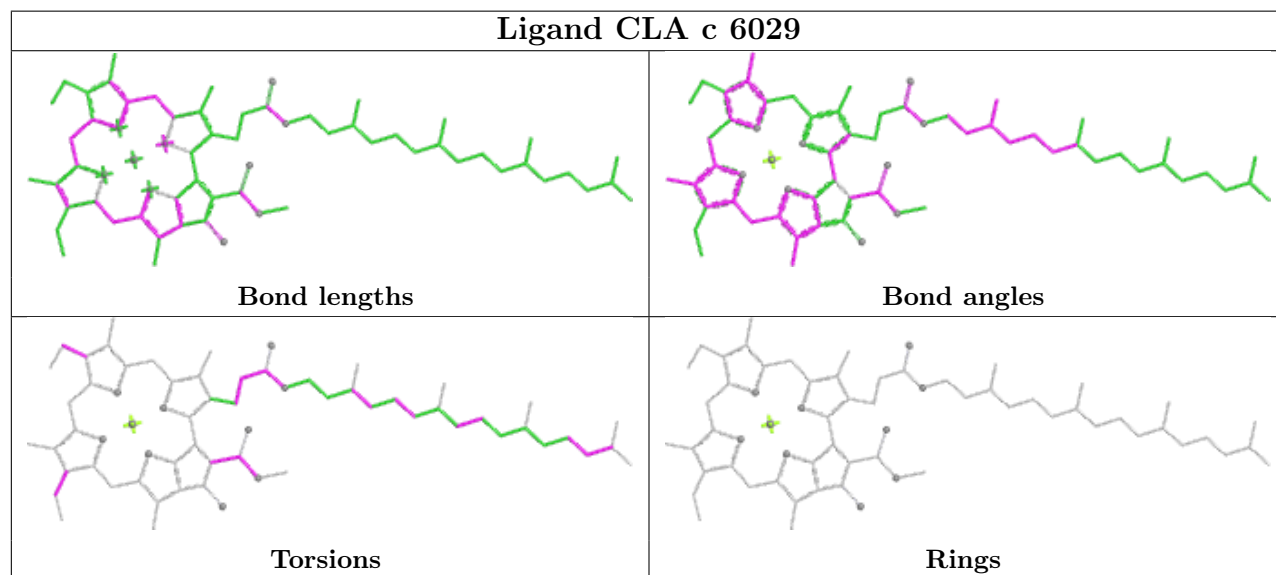
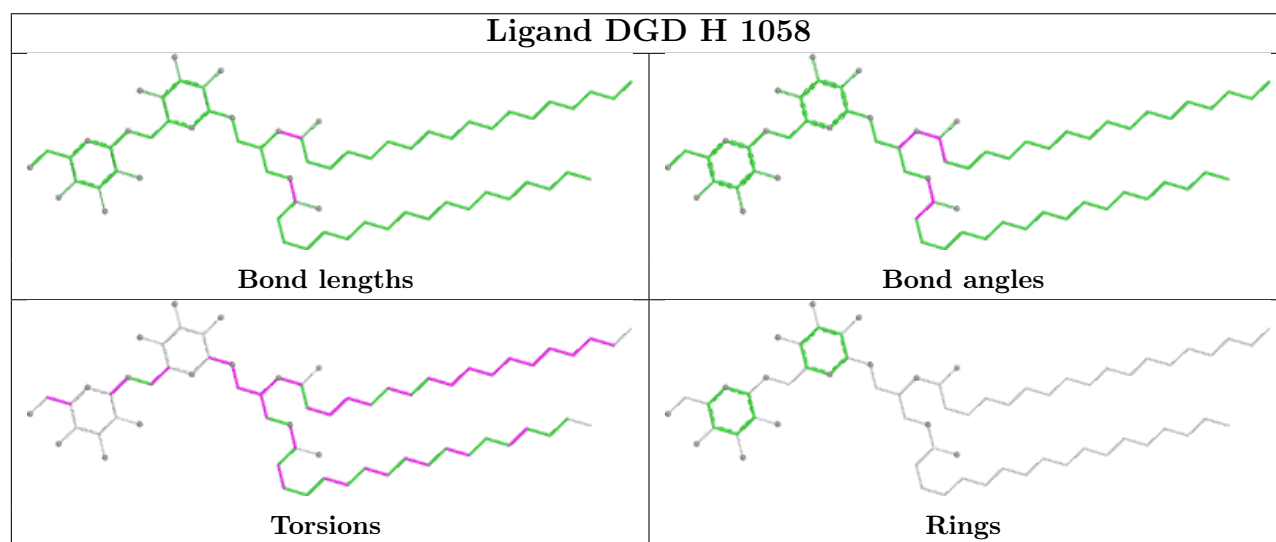
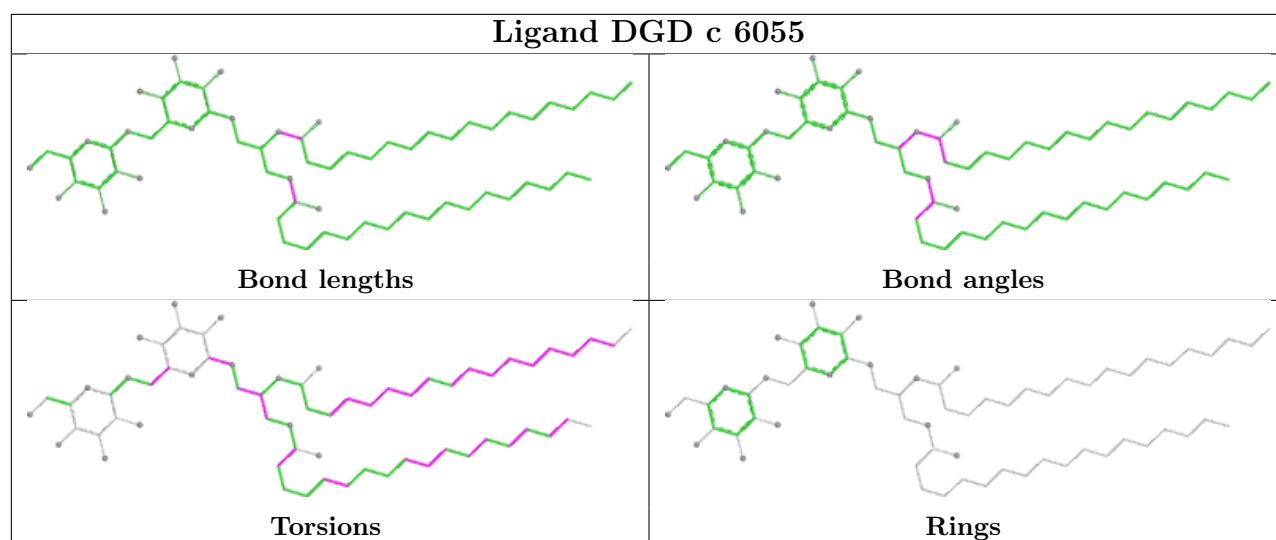
Ligand BCR A 1044	
	
Bond lengths	Bond angles
	
Torsions	Rings

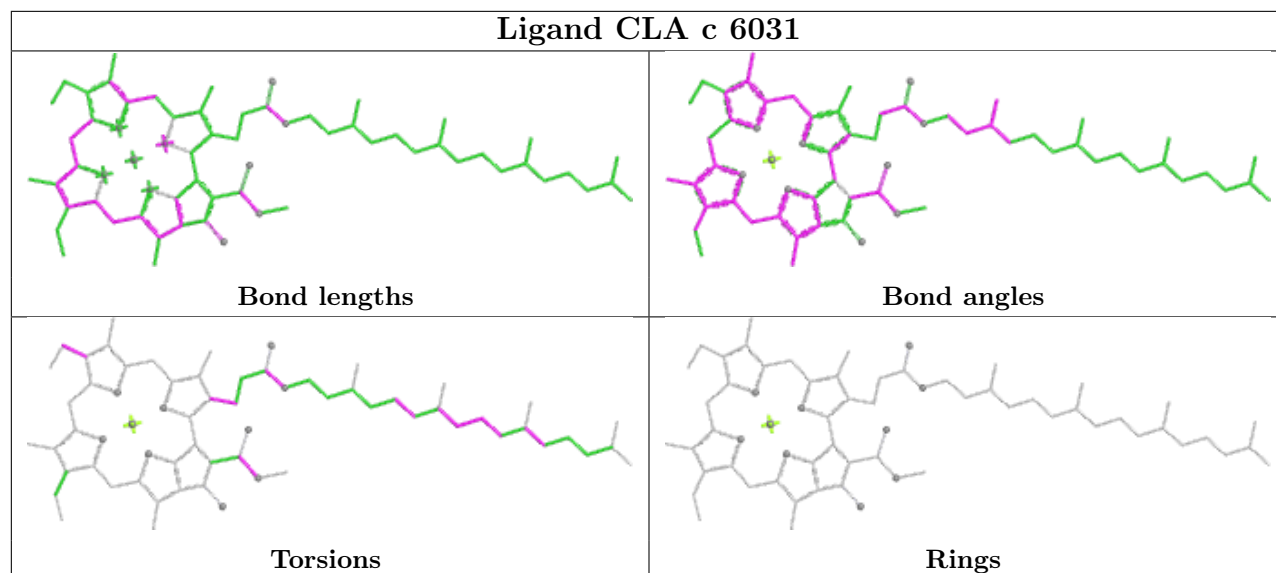
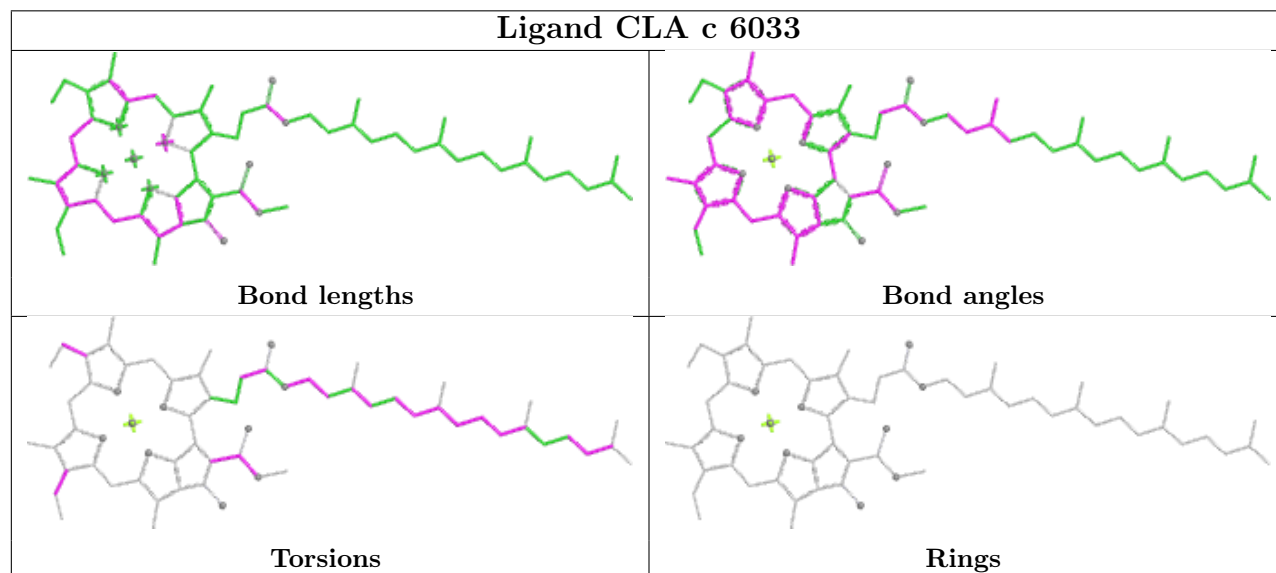
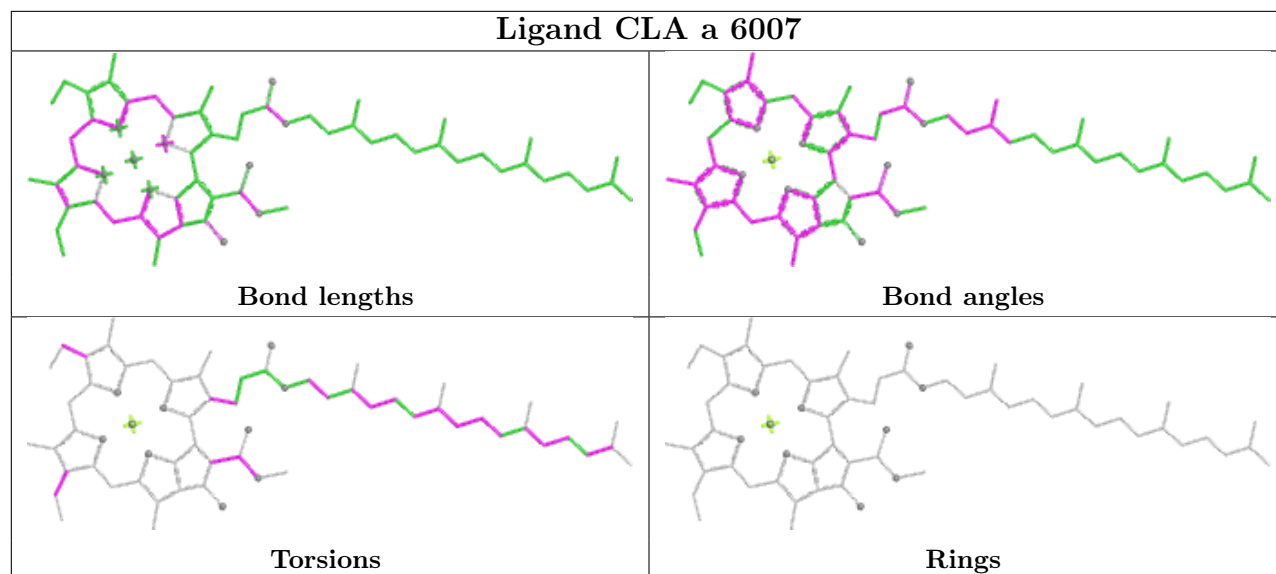


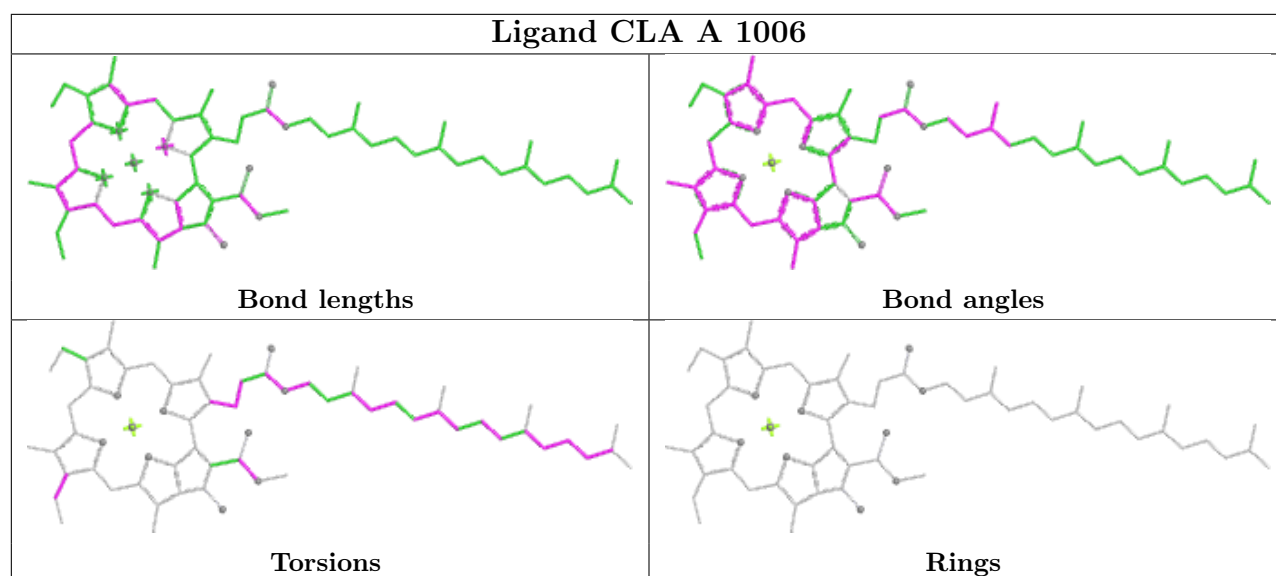
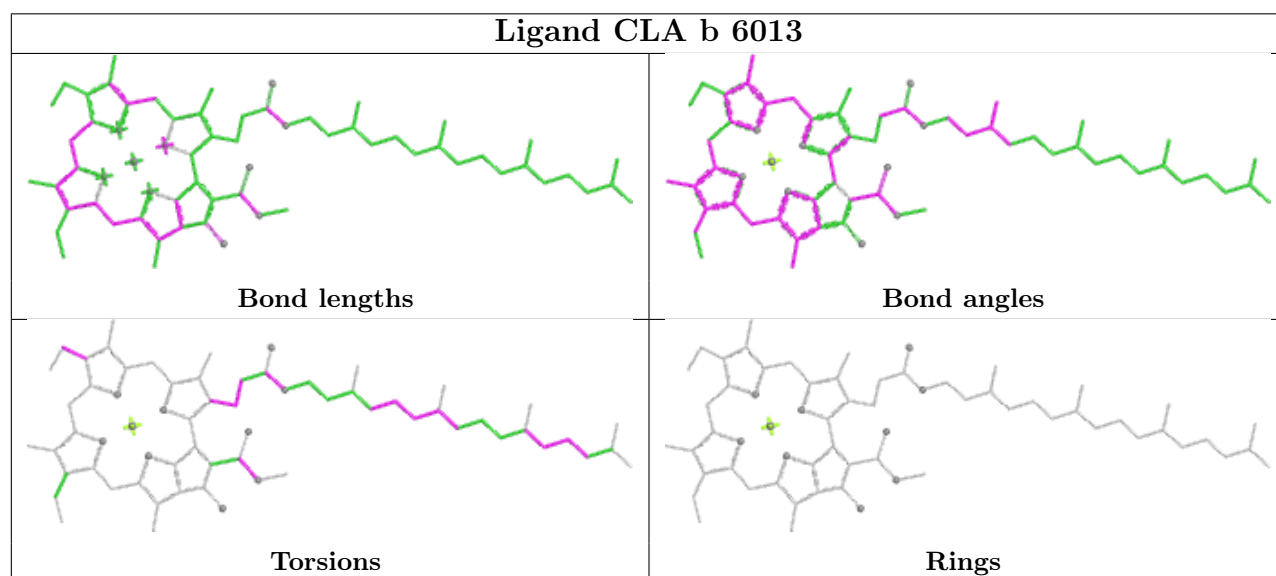
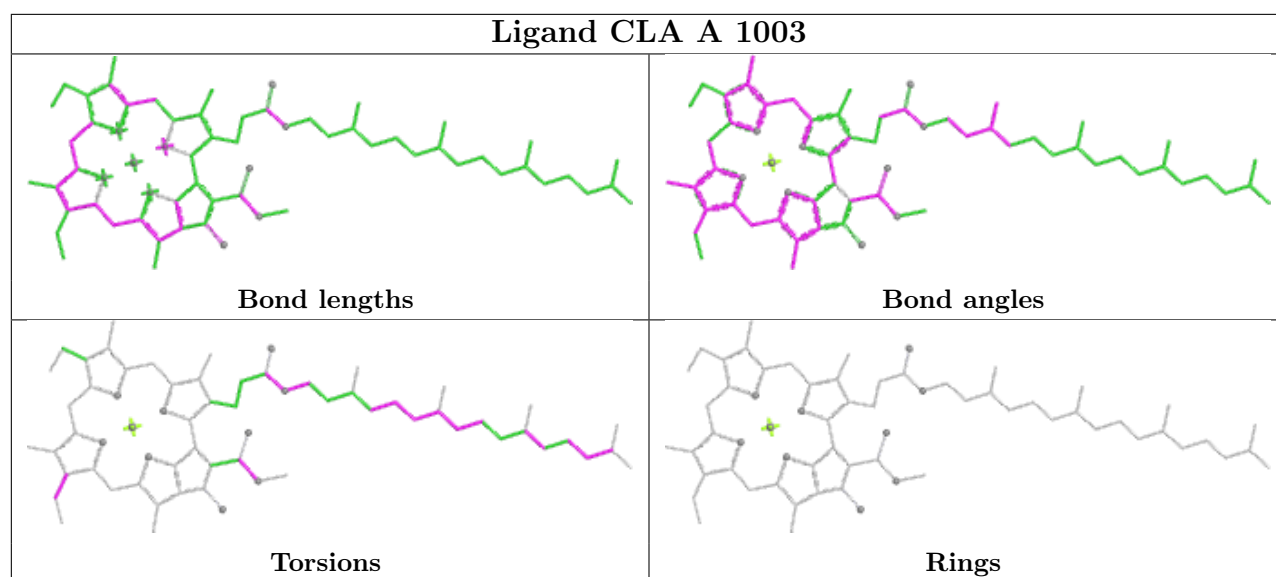
Ligand BCR z 6053	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA D 1008	
	
Bond lengths	Bond angles
	
Torsions	Rings

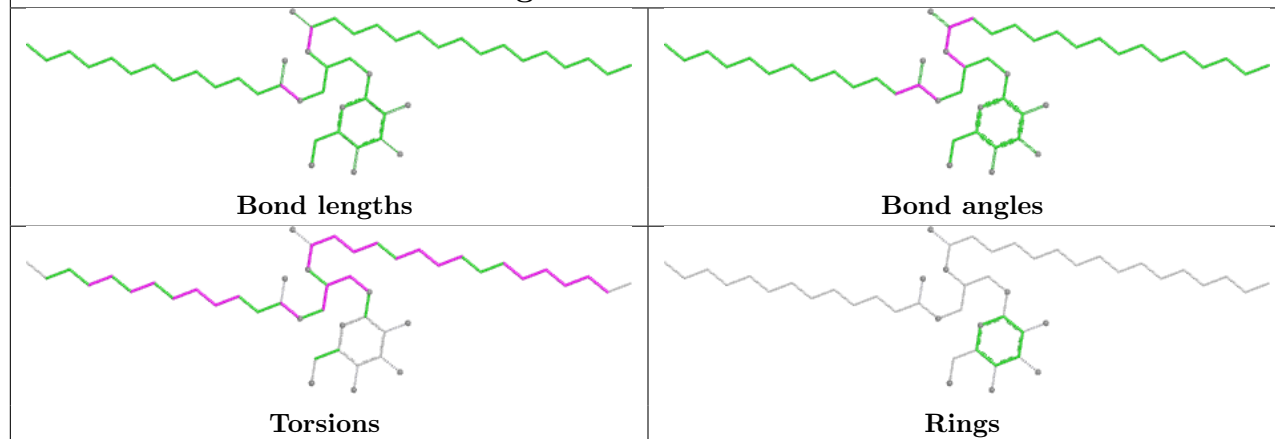
Ligand BCR H 1049	
	
Bond lengths	Bond angles
	
Torsions	Rings



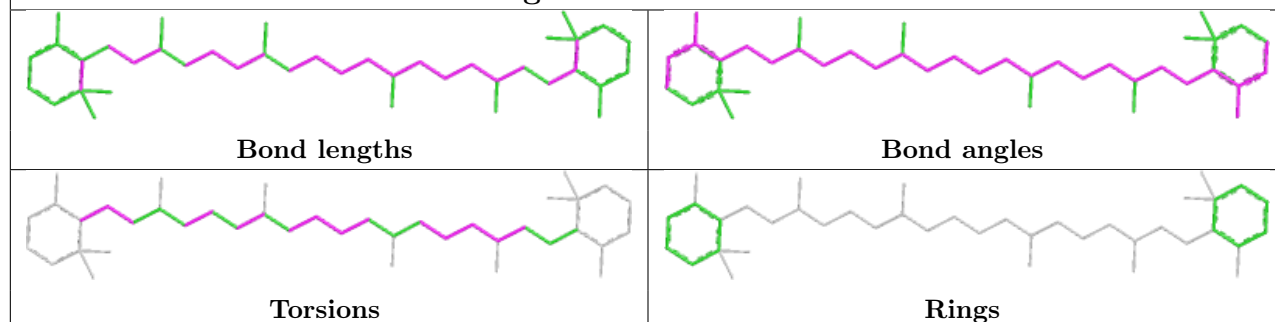




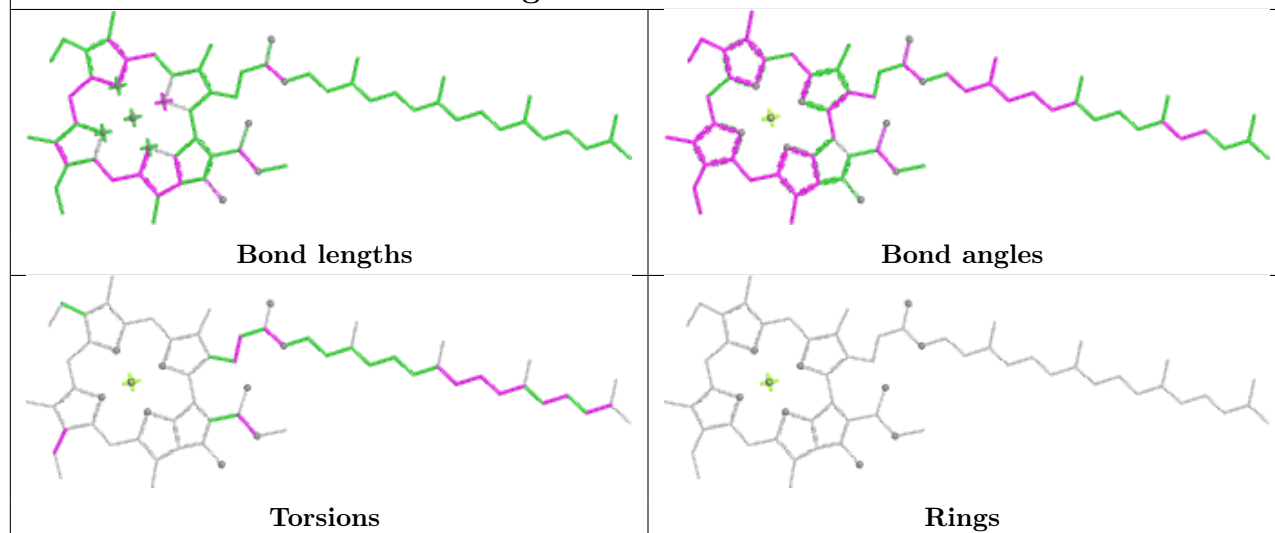
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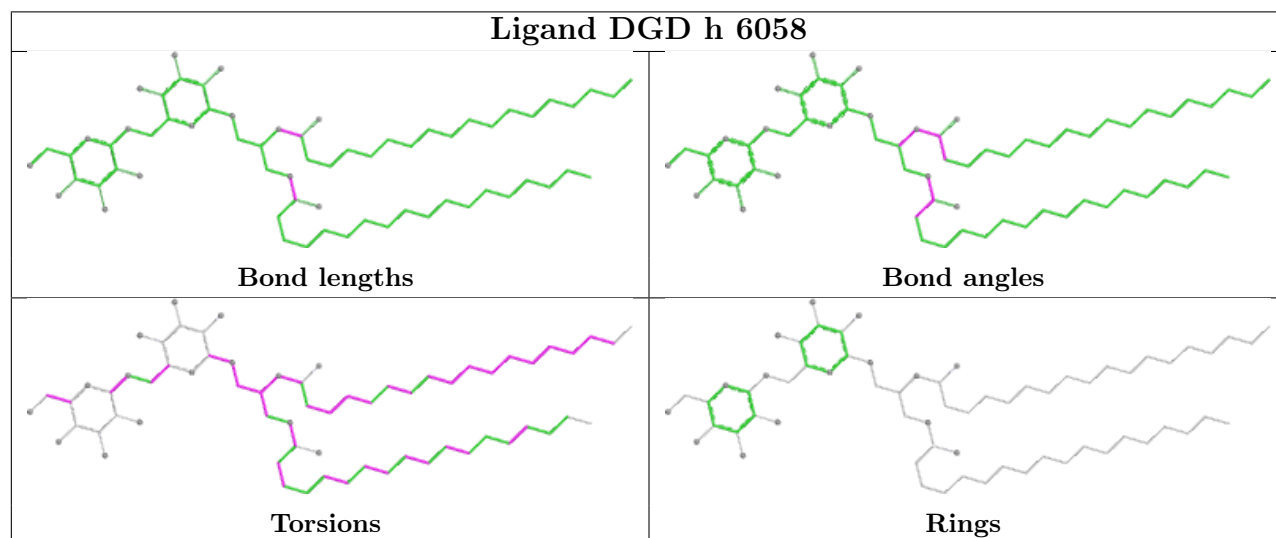
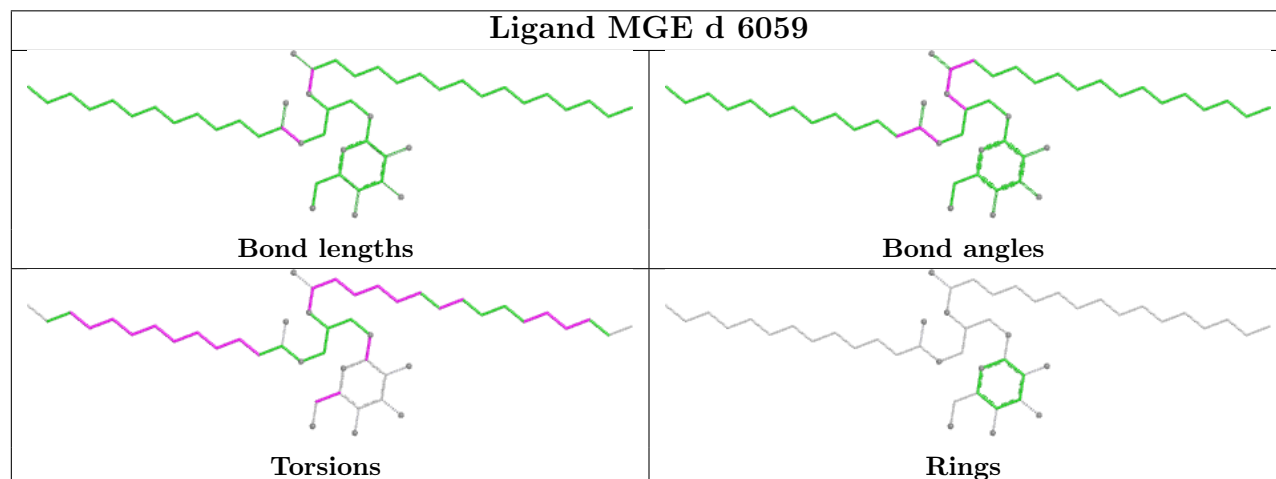
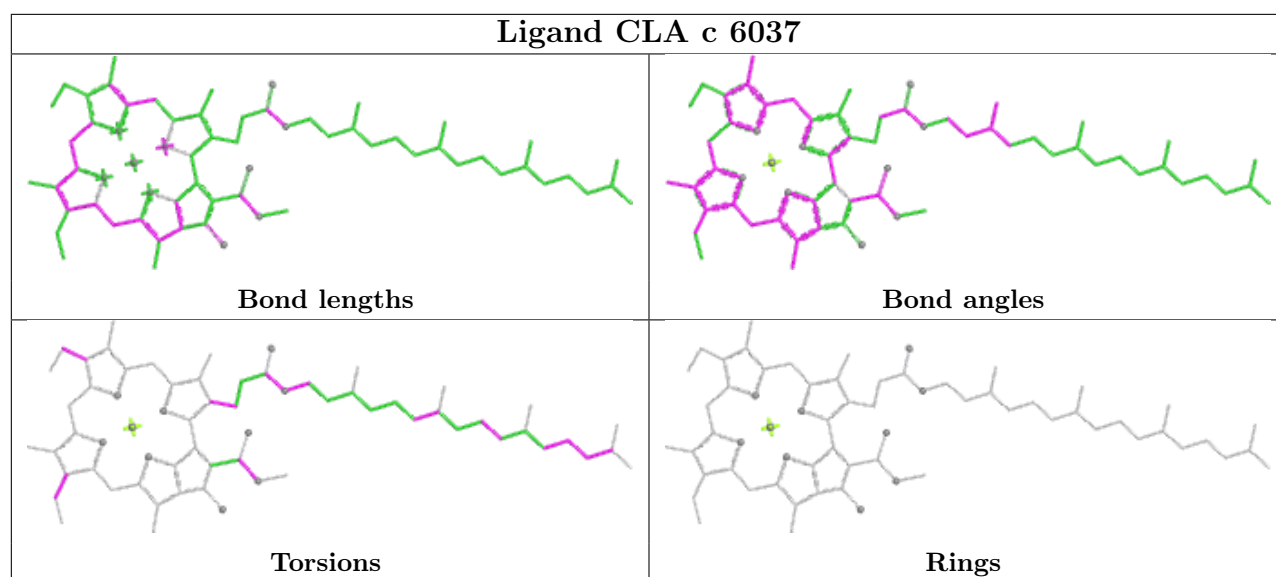


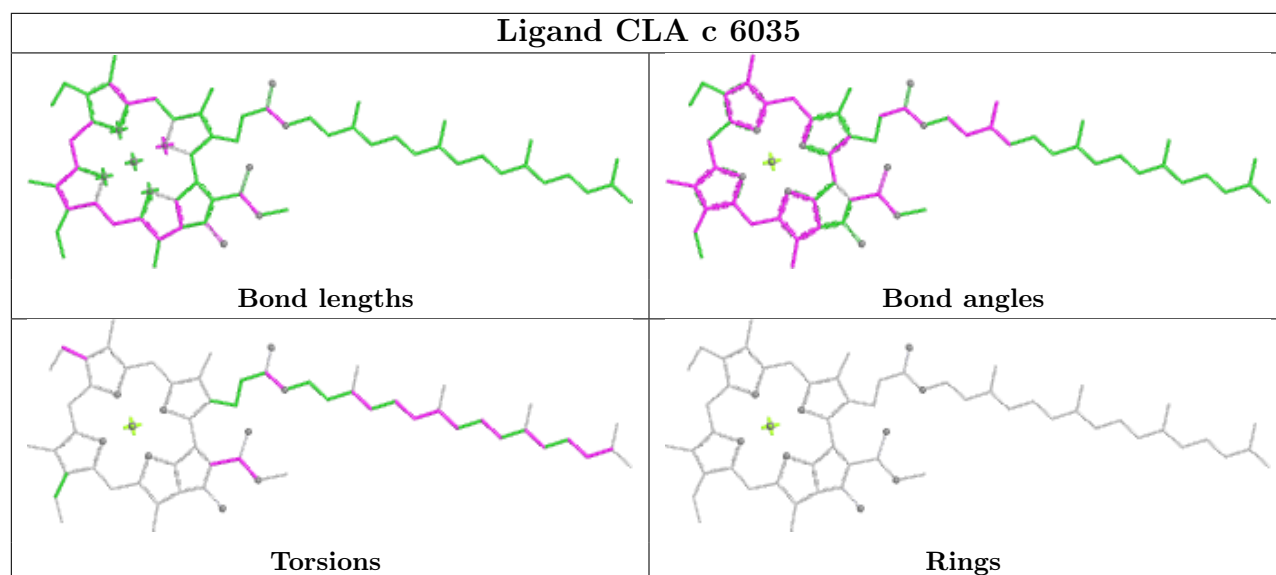
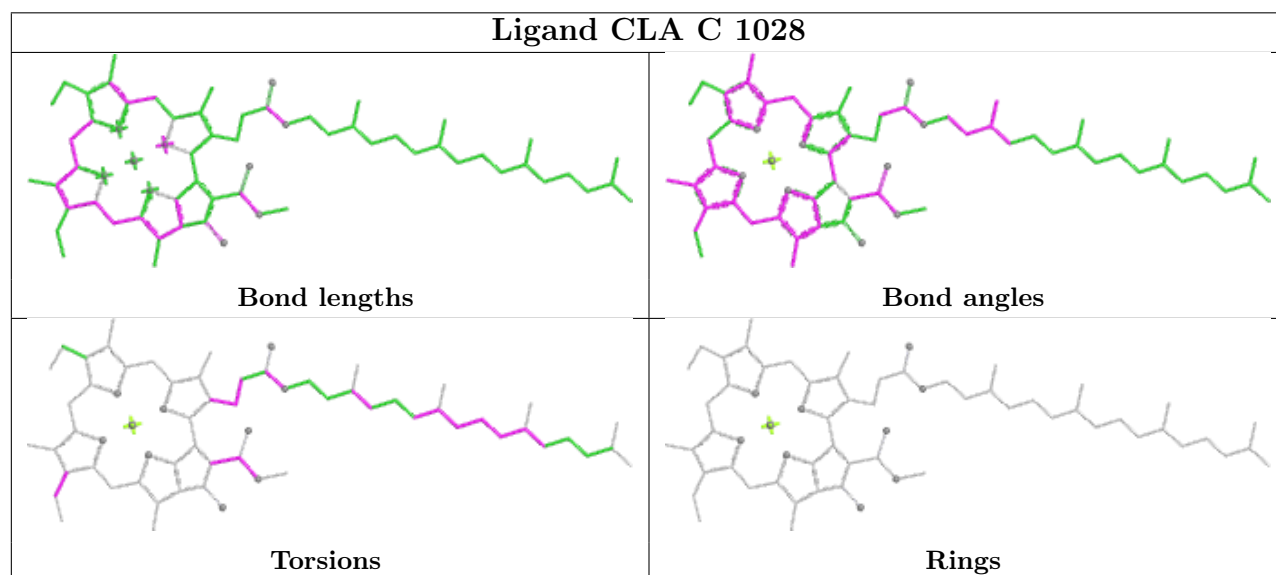
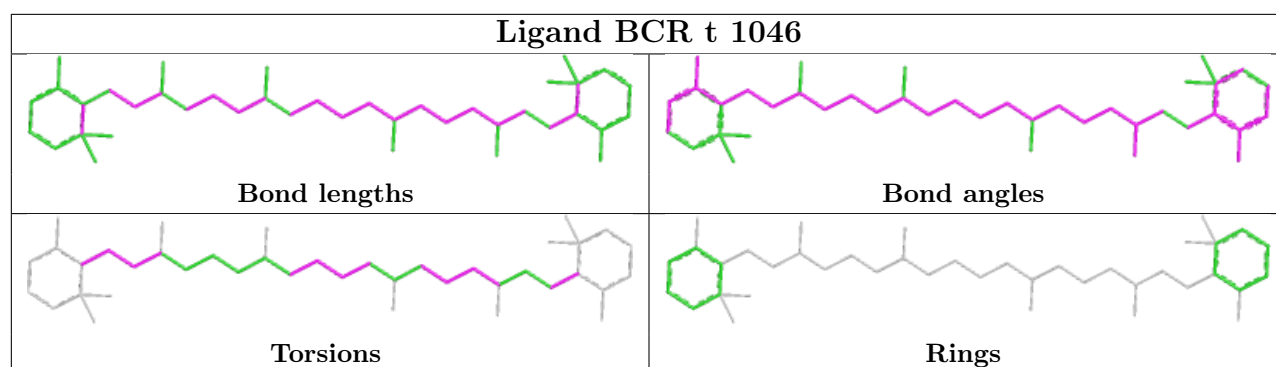
Ligand BCR h 6049

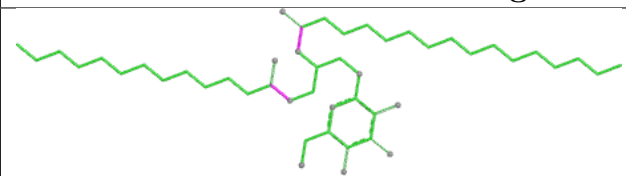
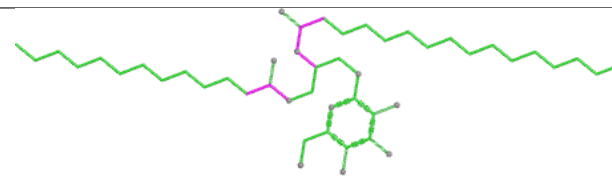
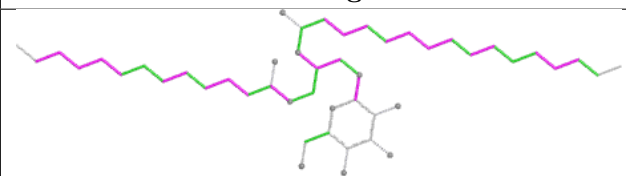
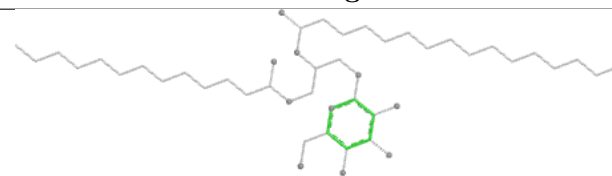


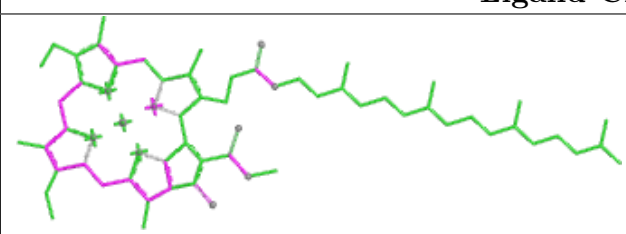
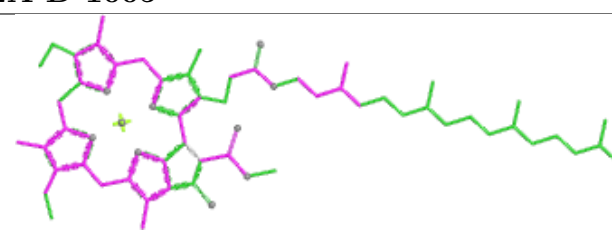
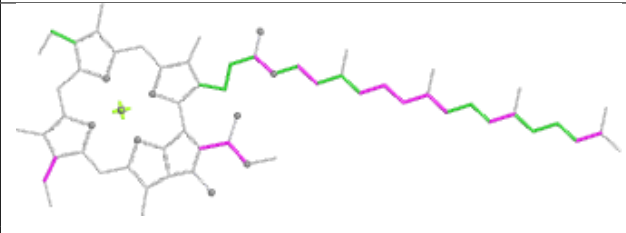
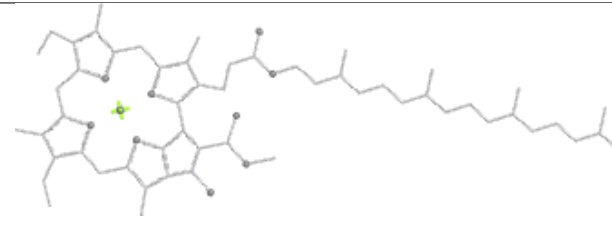
Ligand CLA B 1022

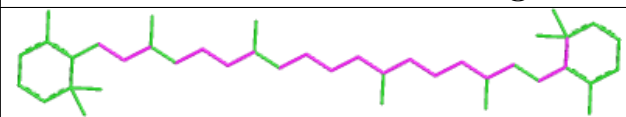
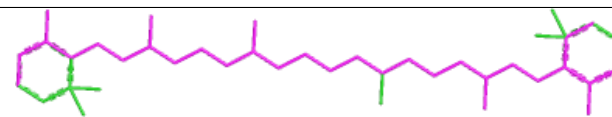
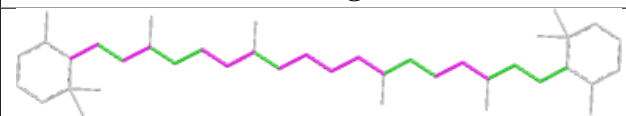
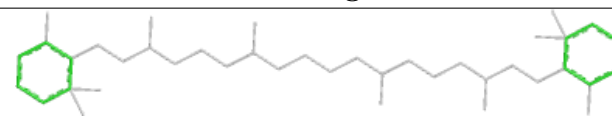


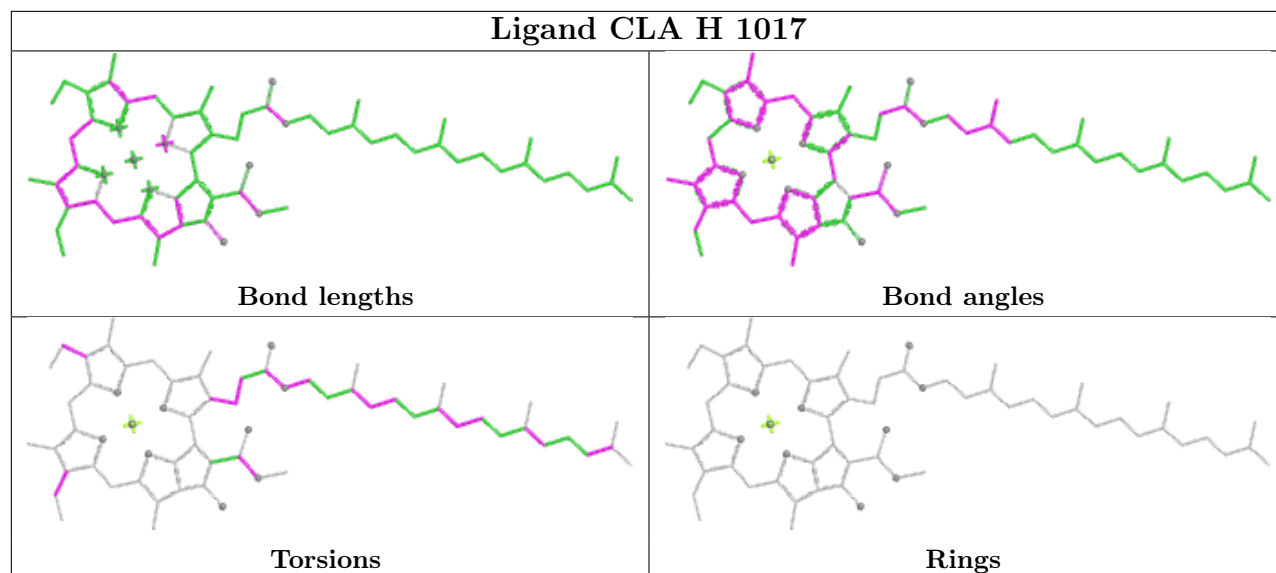
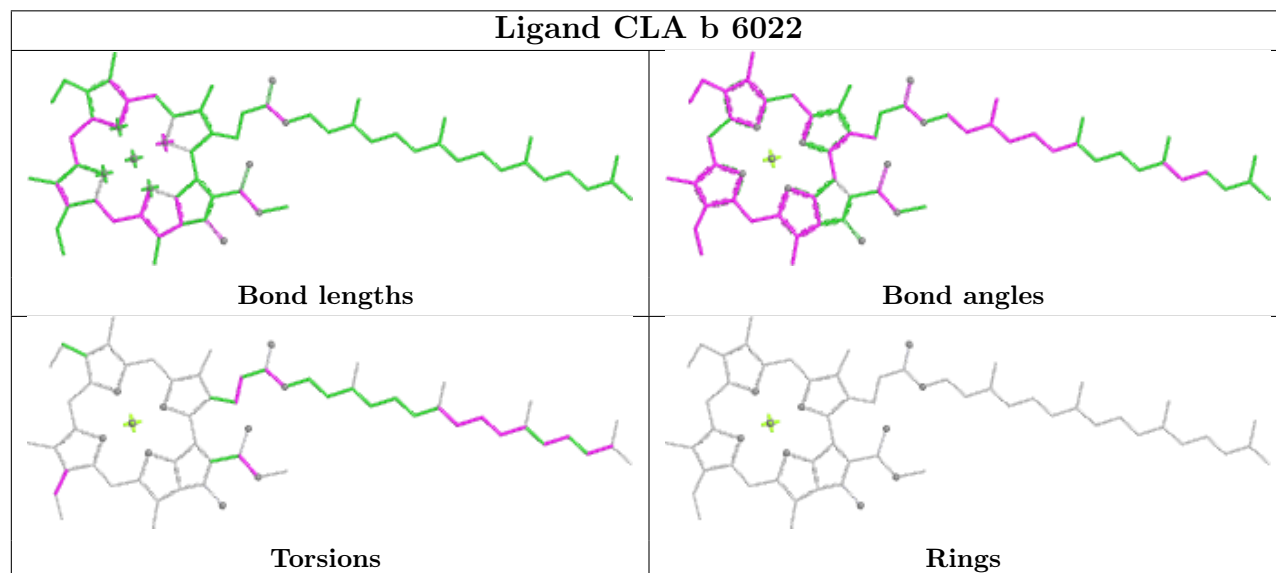
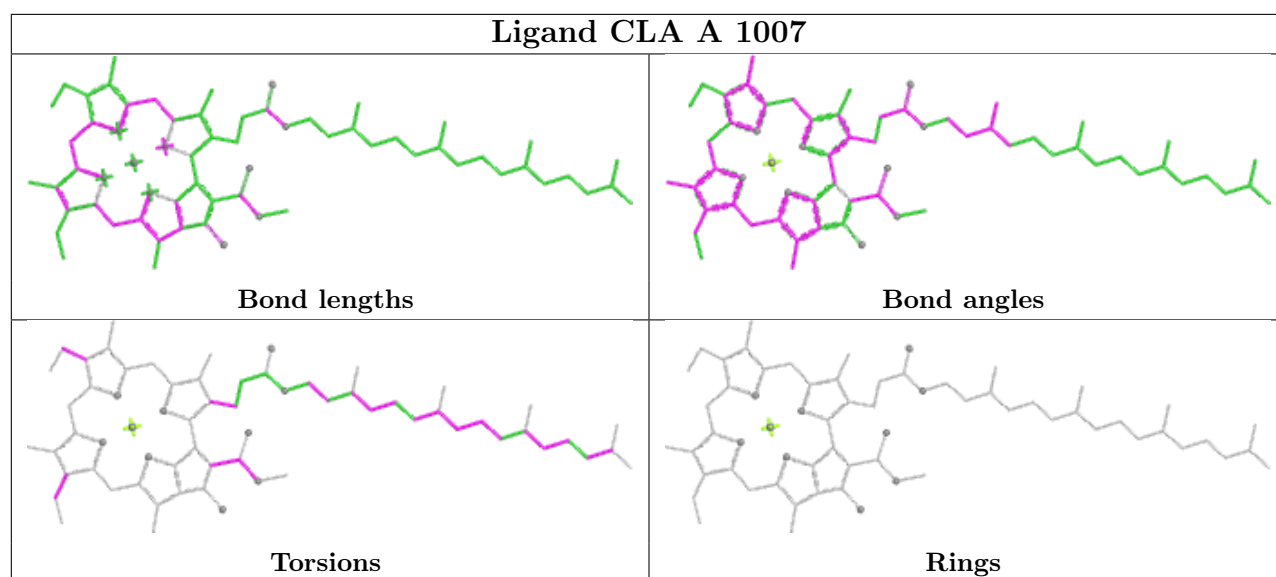




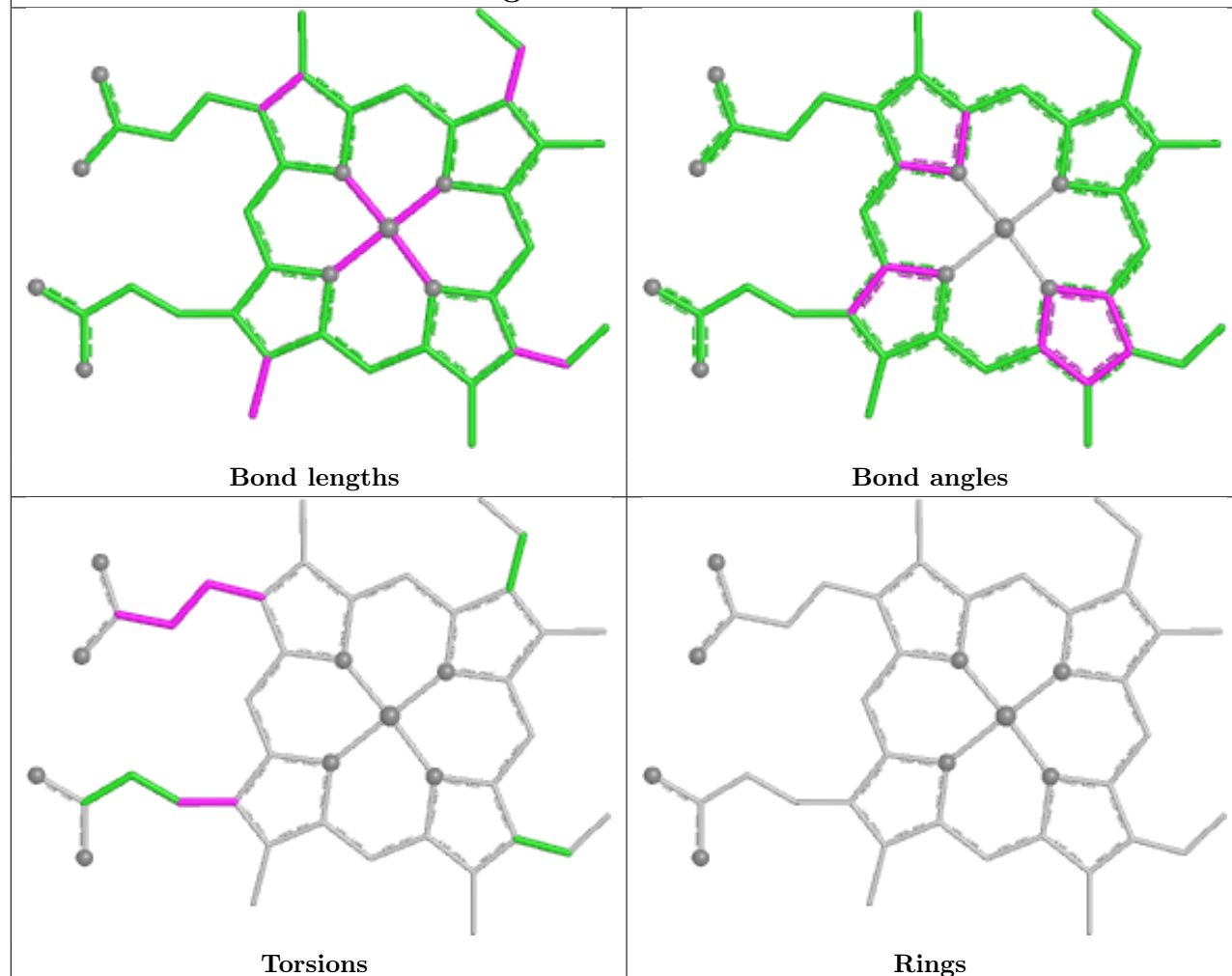
Ligand MGE b 6060	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA D 1005	
	
Bond lengths	Bond angles
	
Torsions	Rings

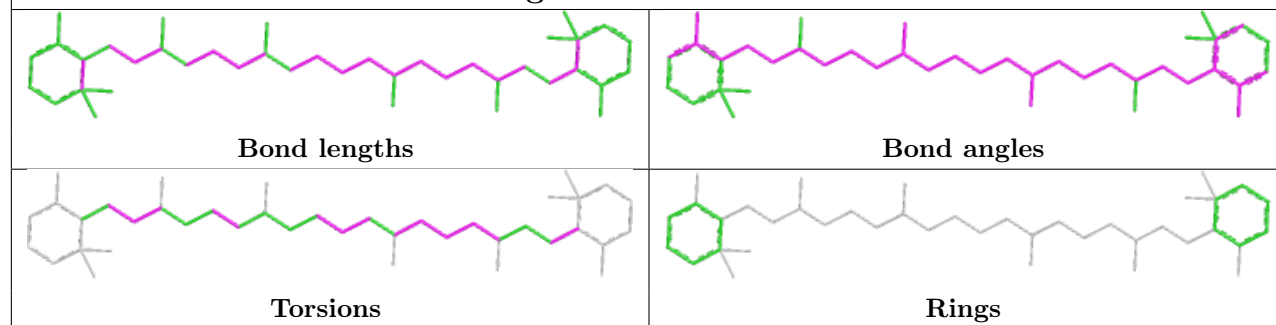
Ligand BCR K 1051	
	
Bond lengths	Bond angles
	
Torsions	Rings

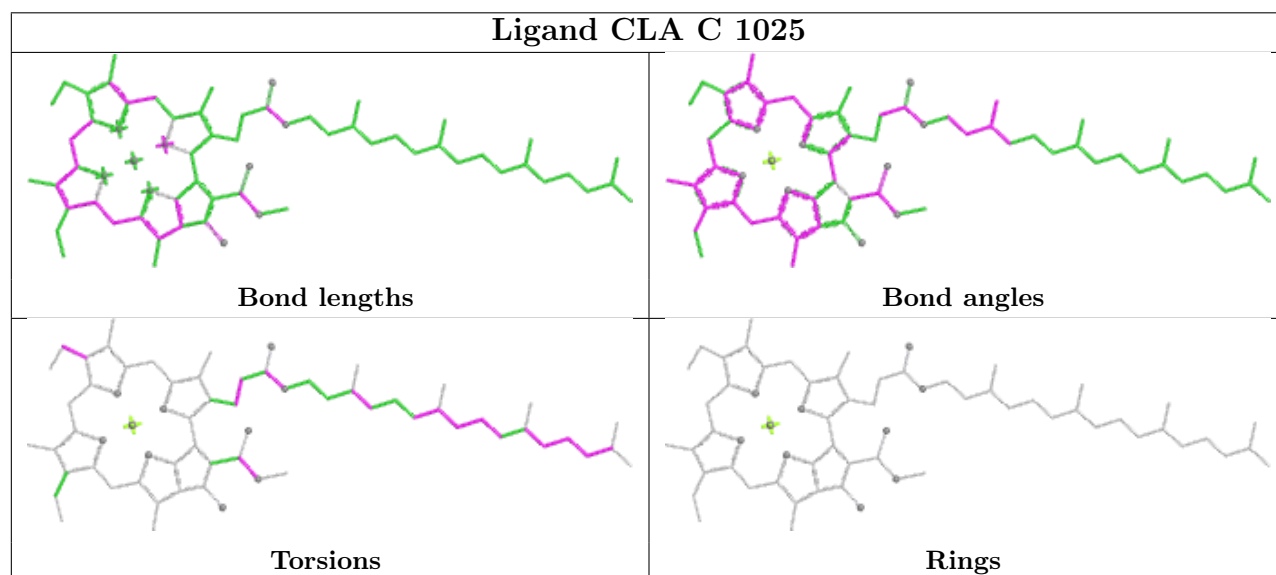
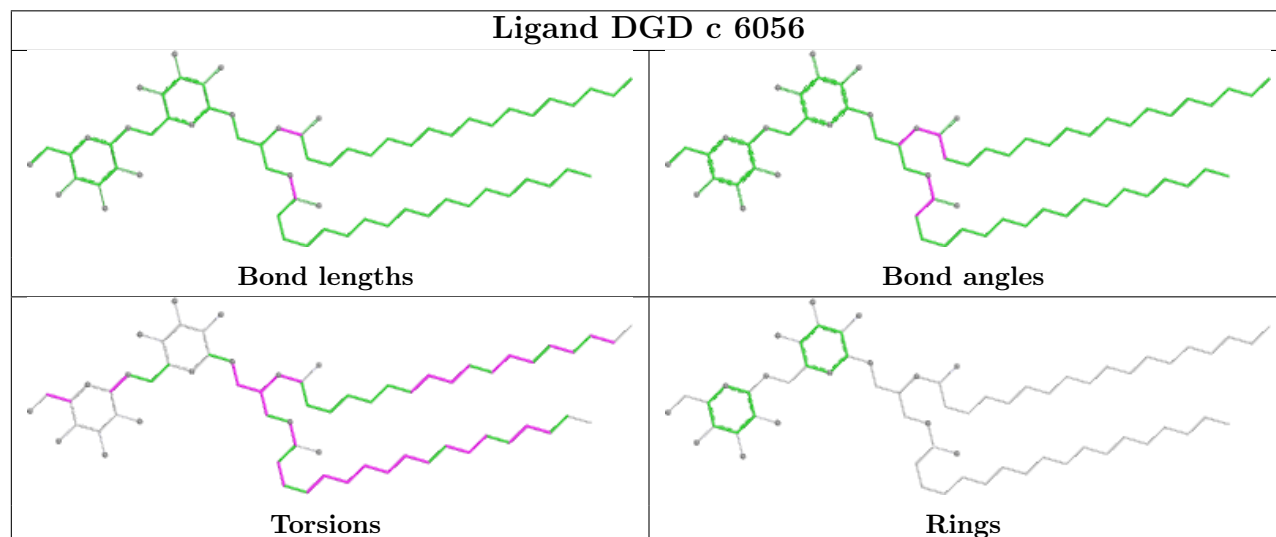
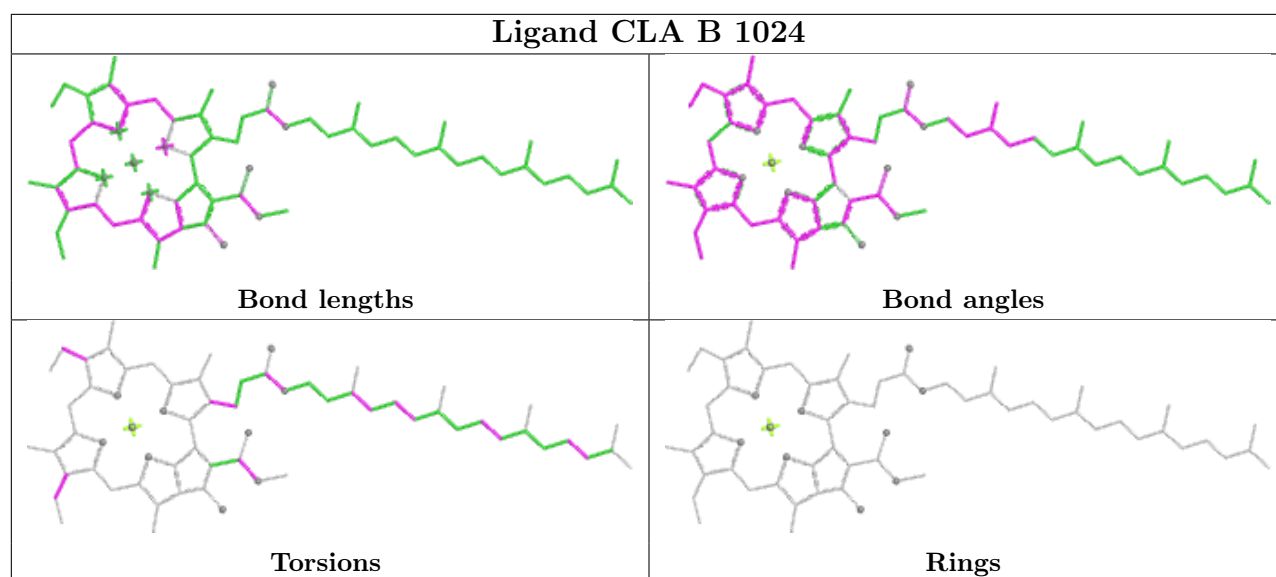


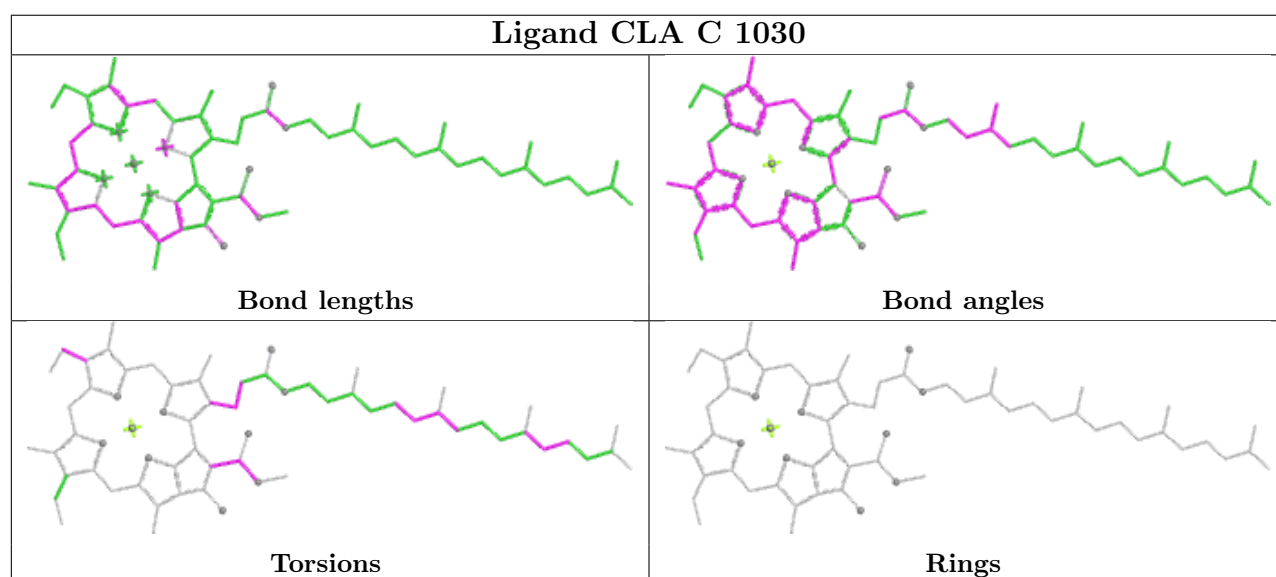
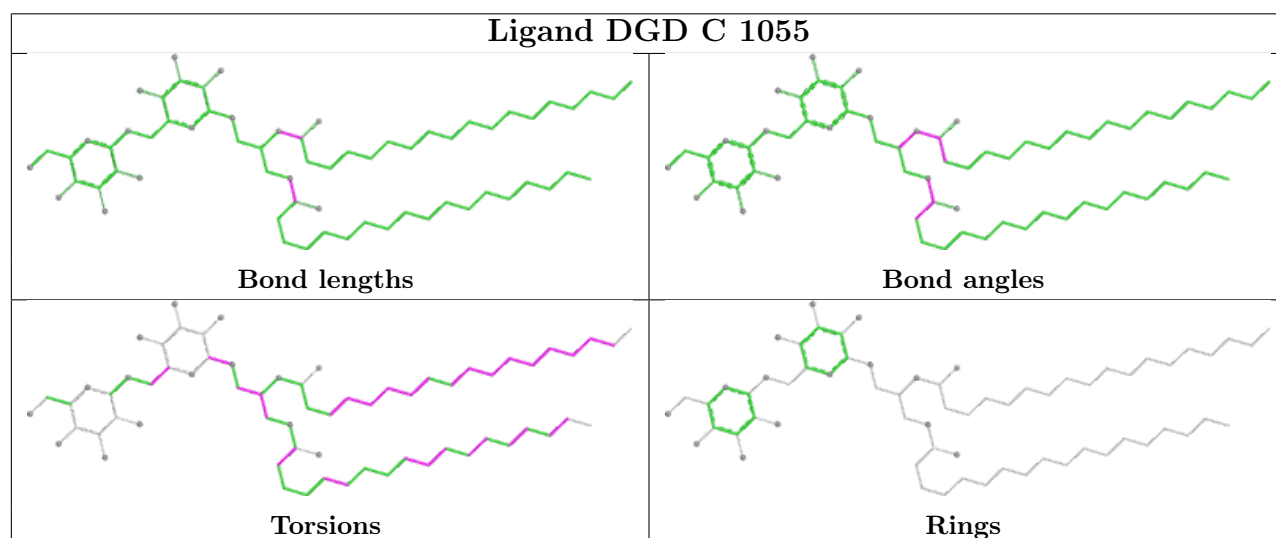
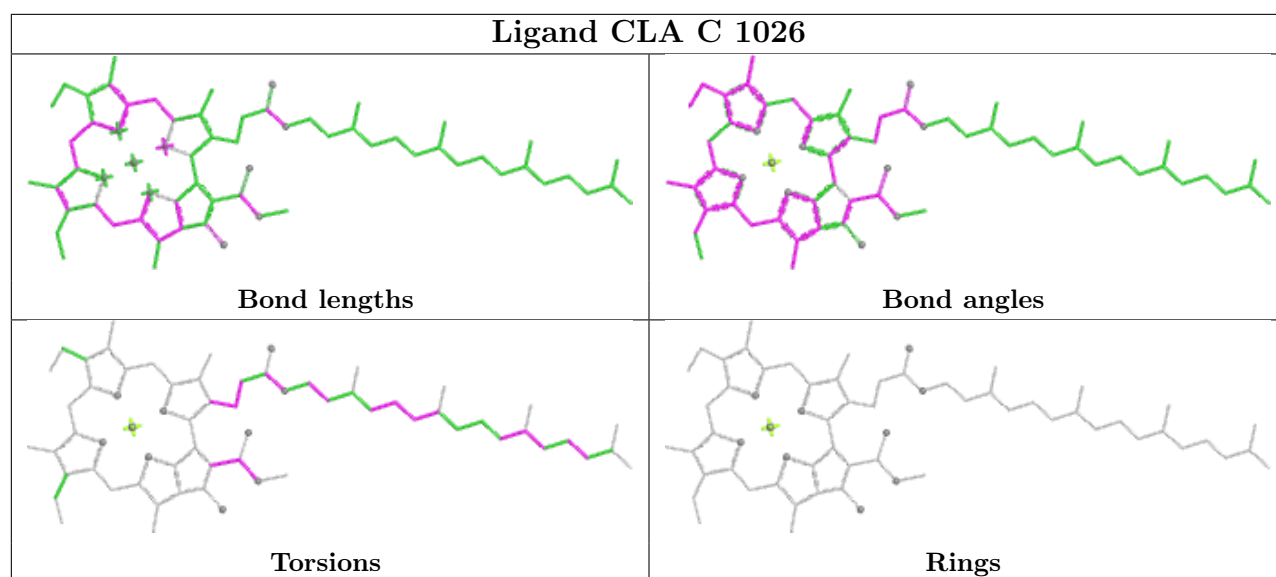
Ligand HEM v 6041

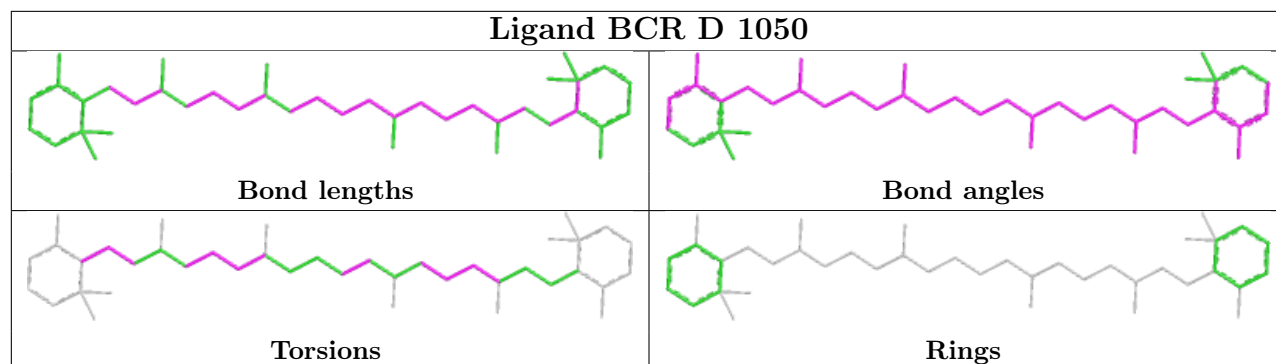
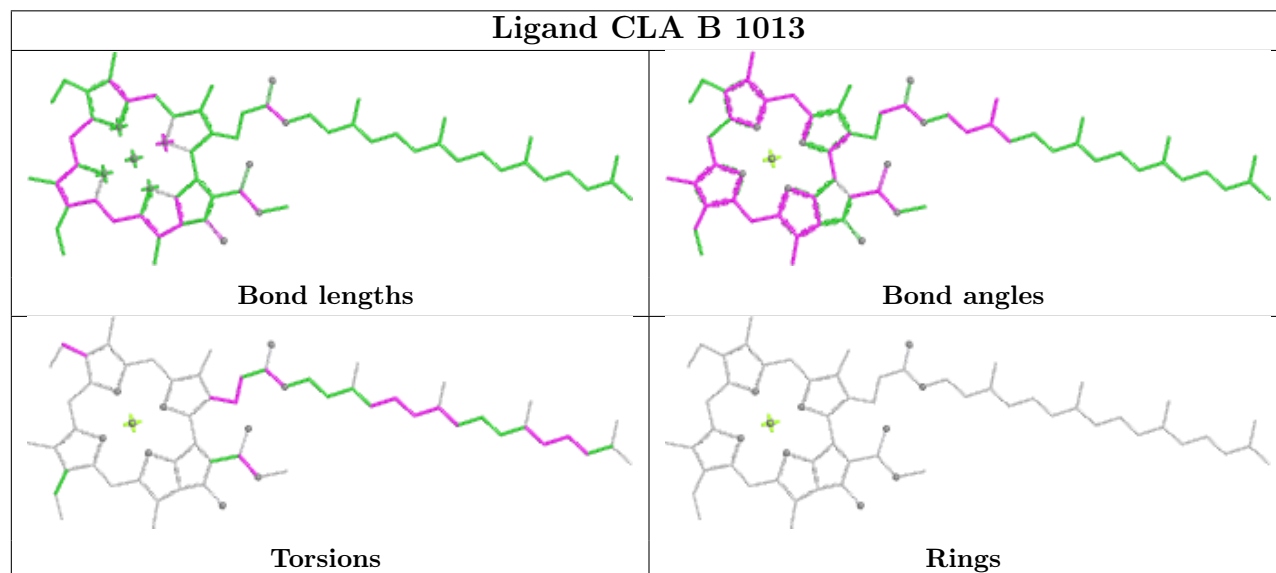
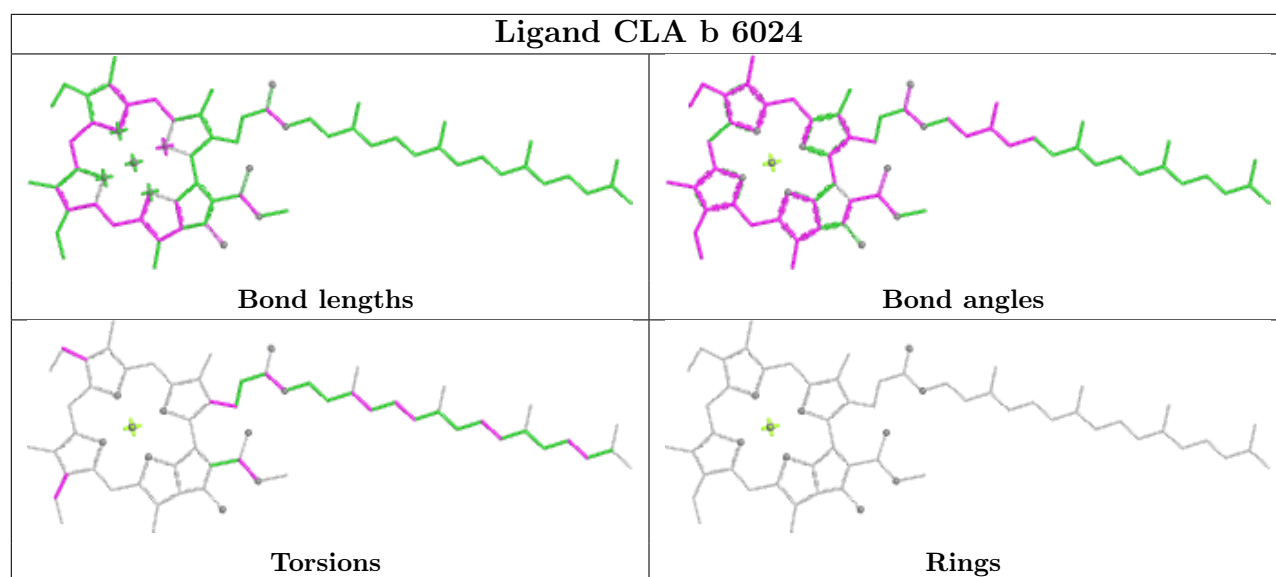


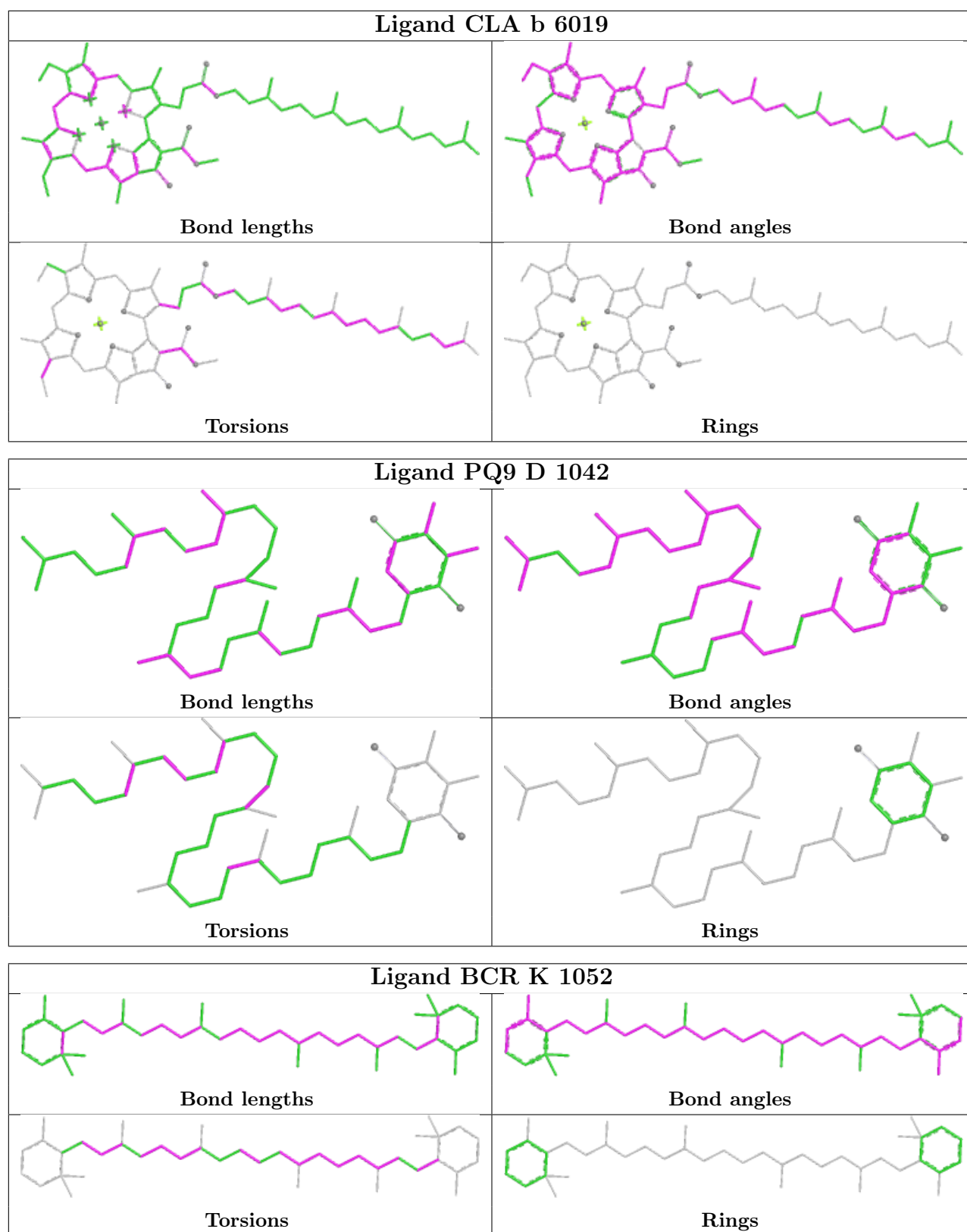
Ligand BCR c 6054

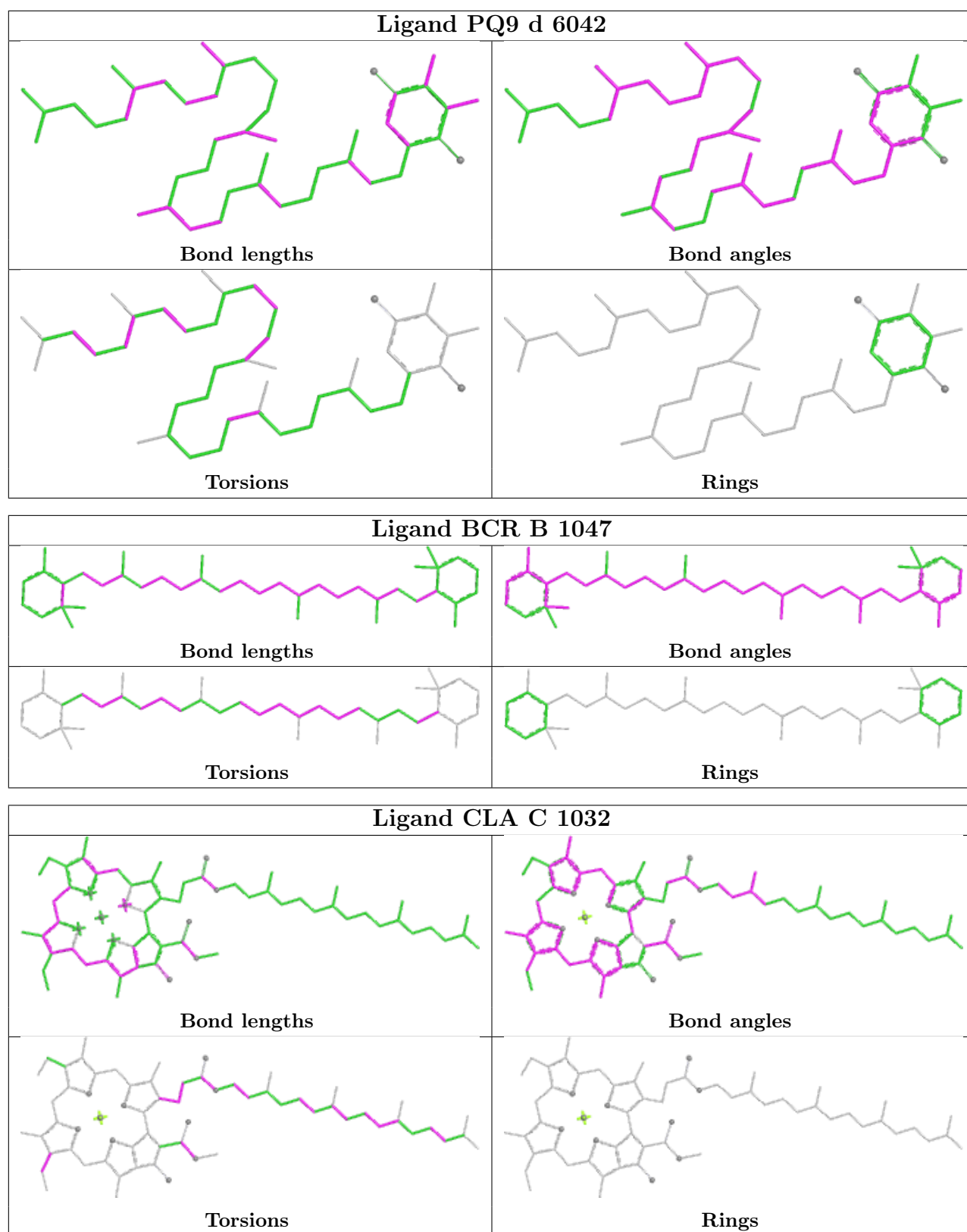


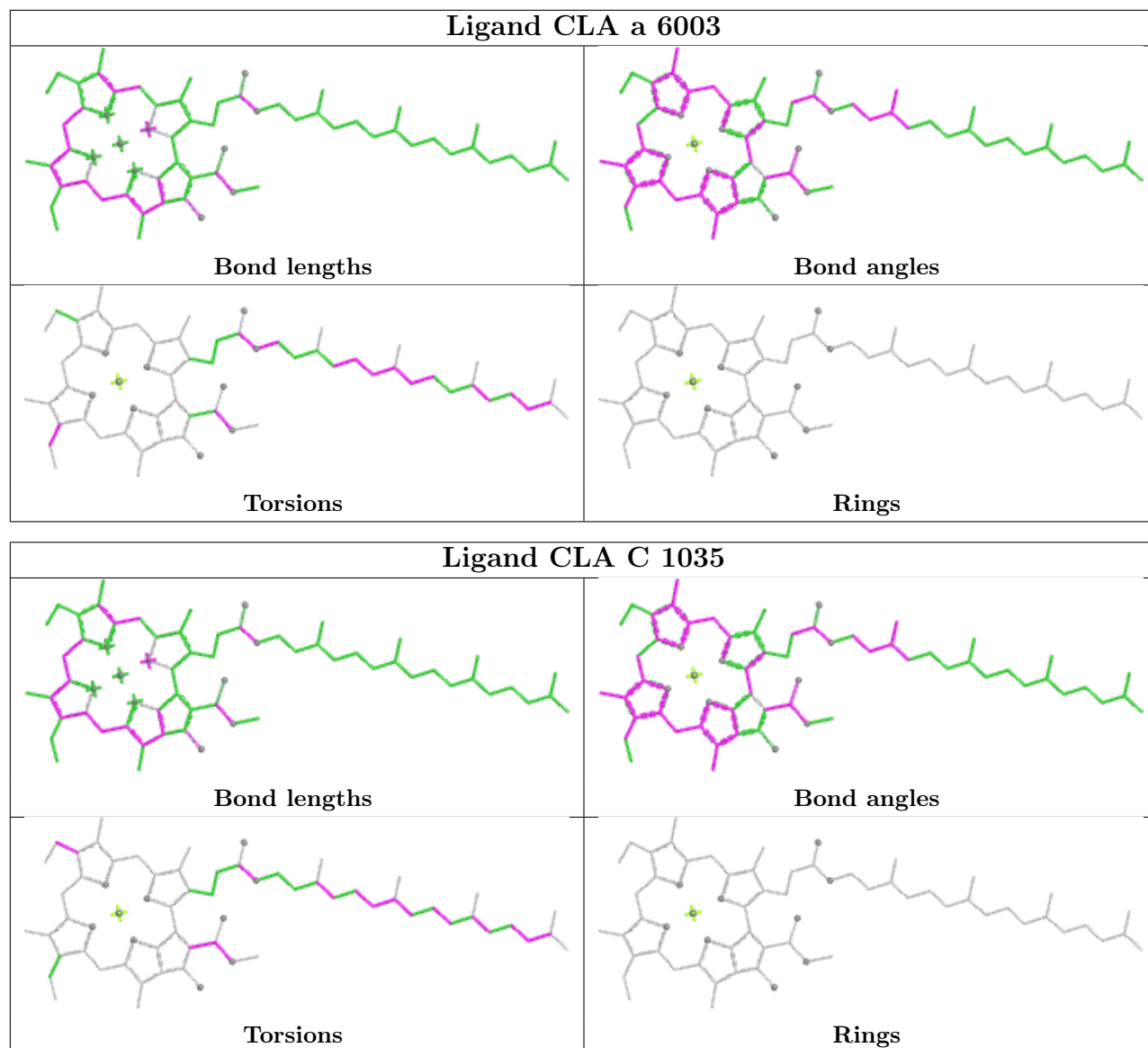




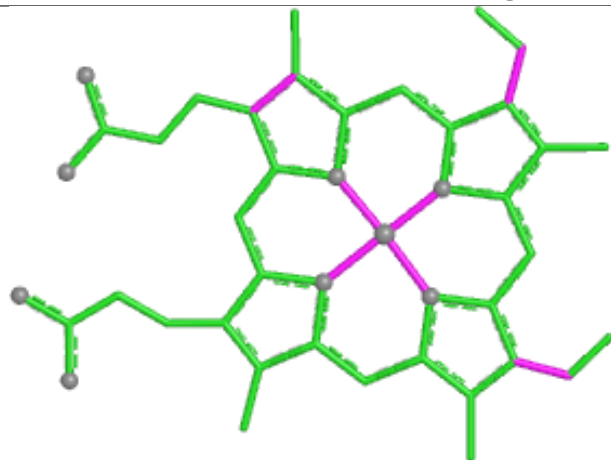




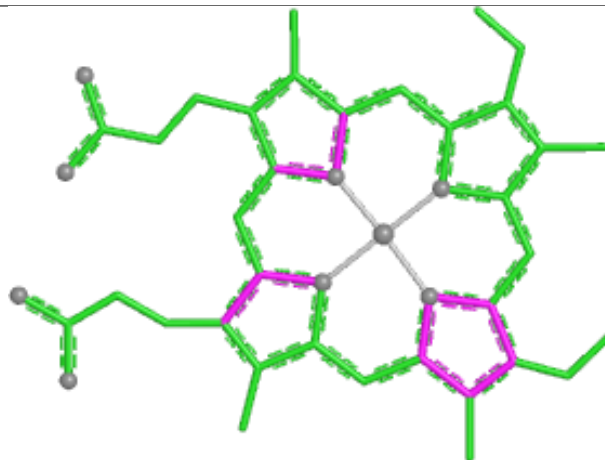




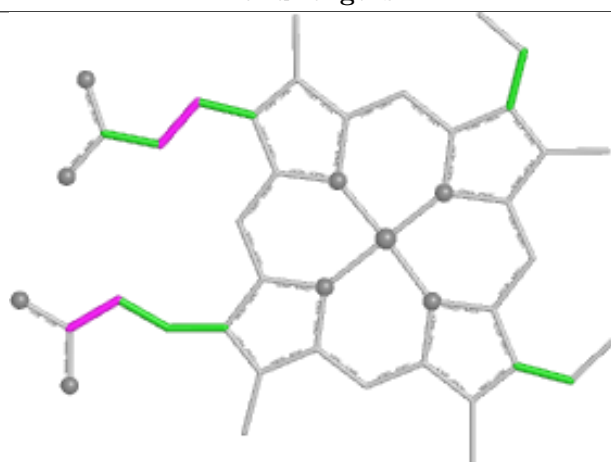
Ligand HEM E 1040



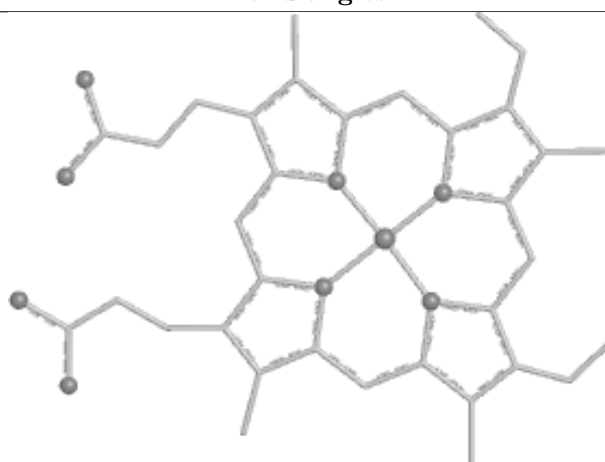
Bond lengths



Bond angles

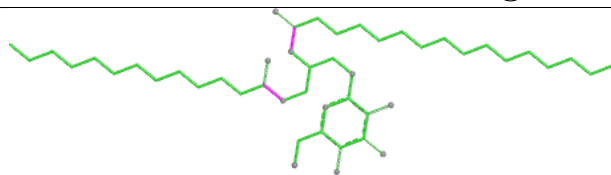


Torsions

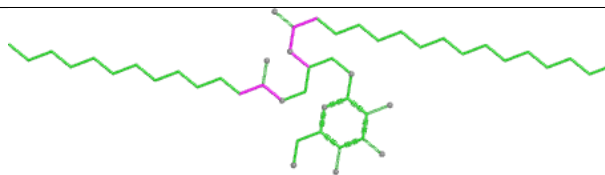


Rings

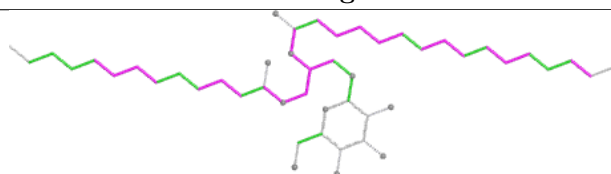
Ligand MGE L 1061



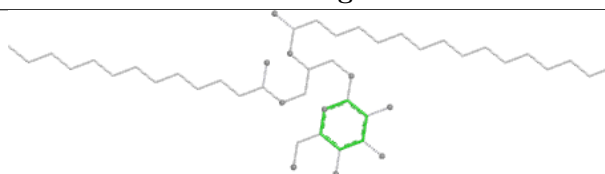
Bond lengths



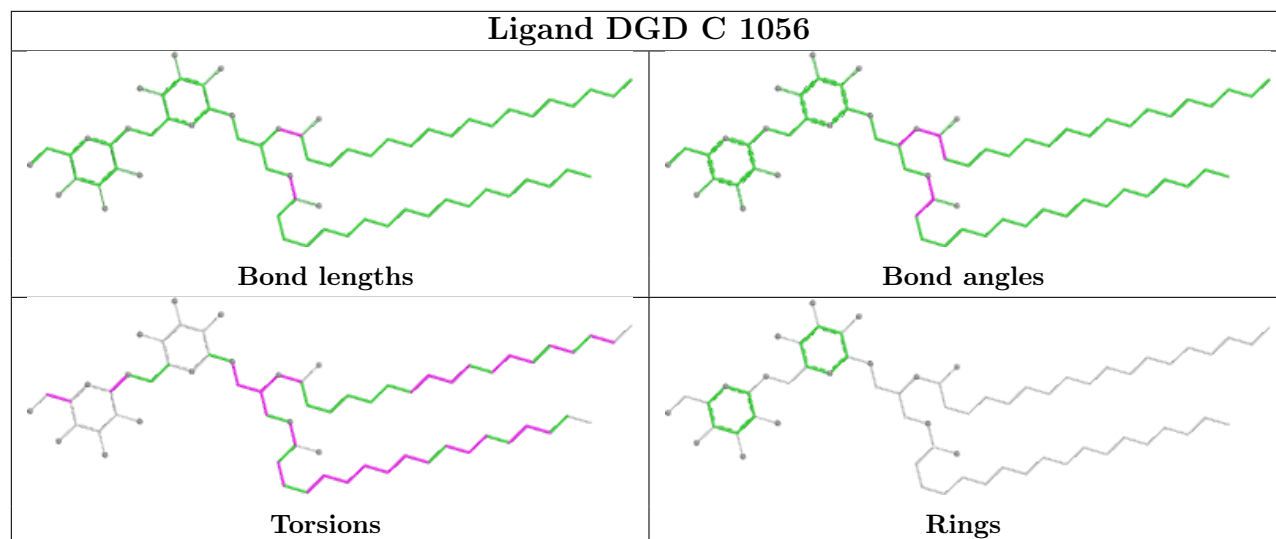
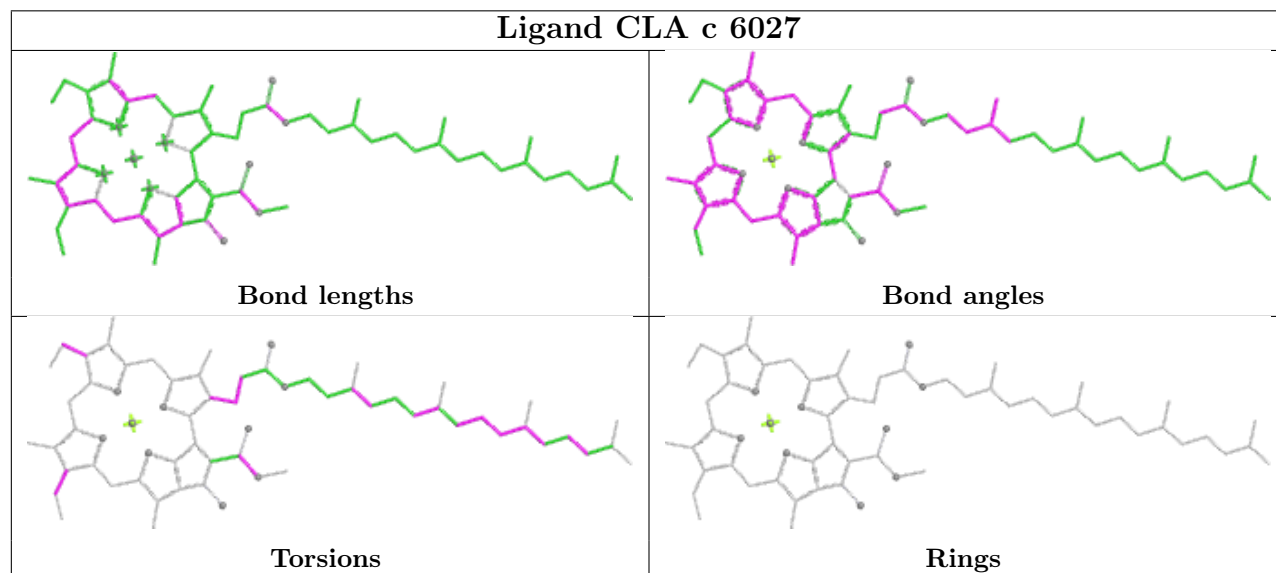
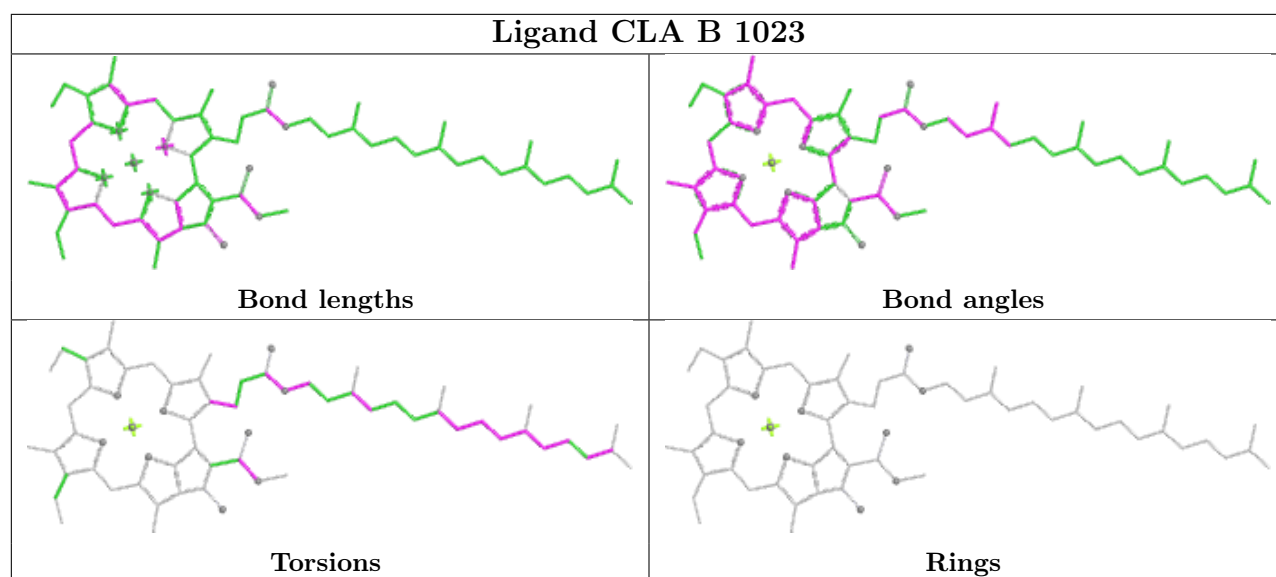
Bond angles

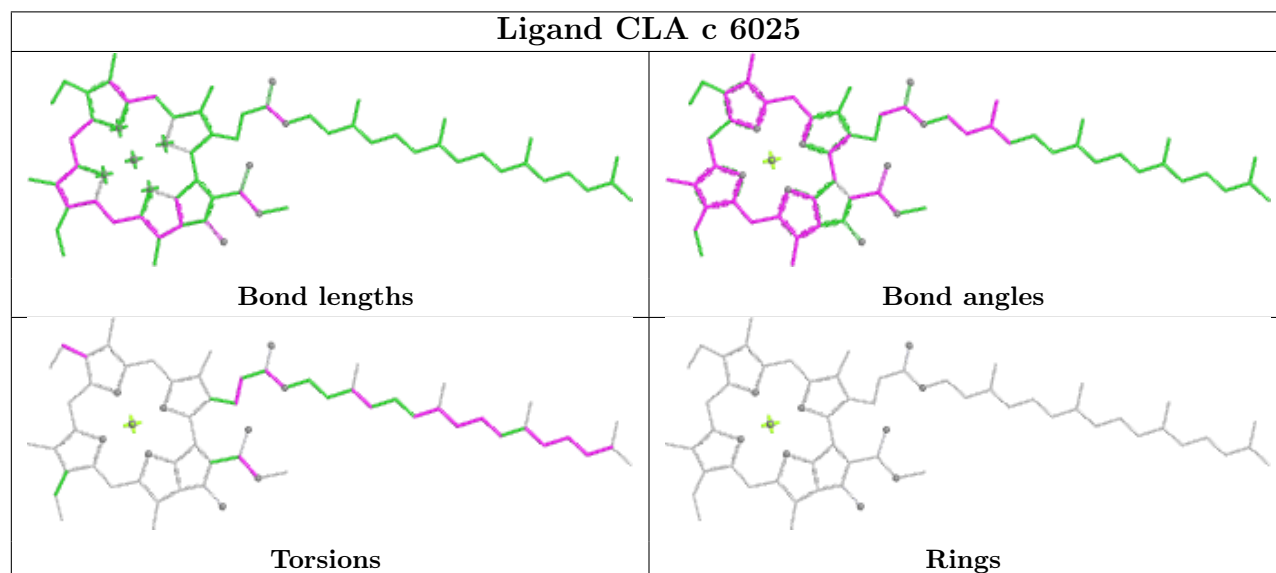
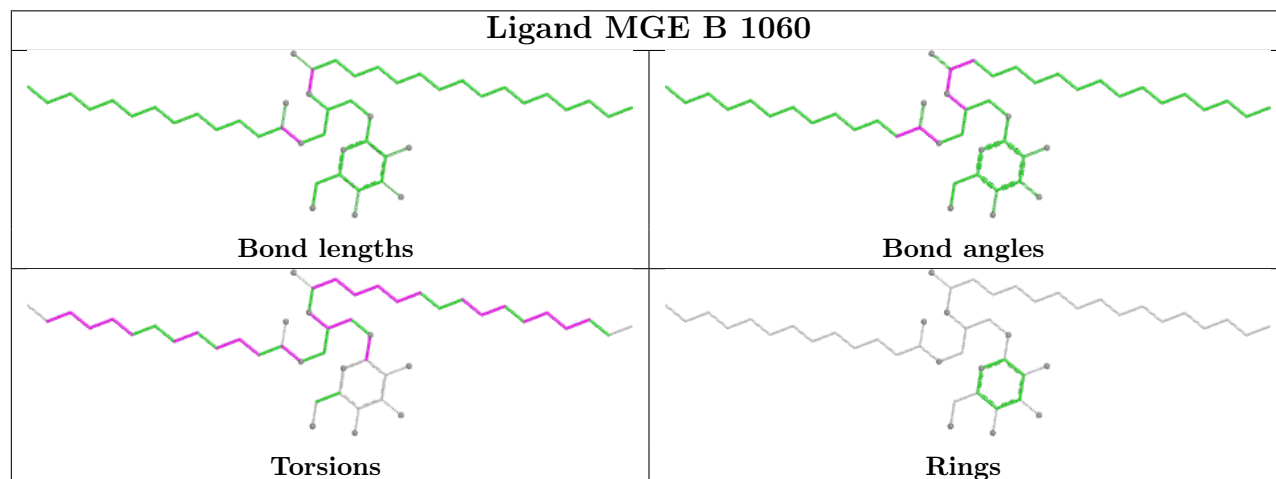
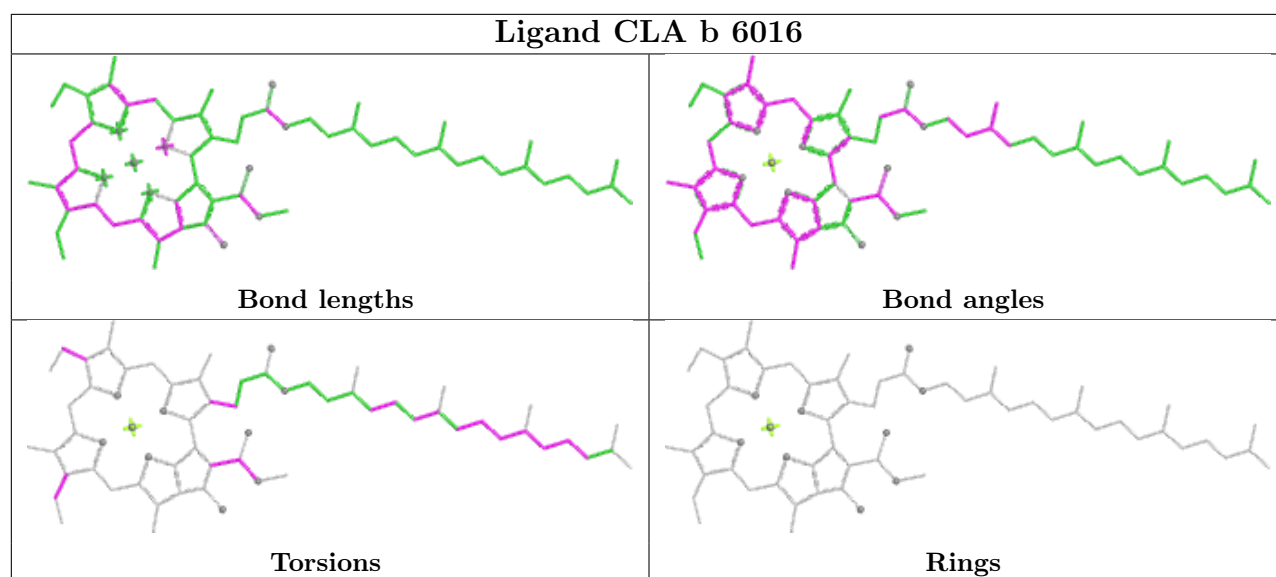


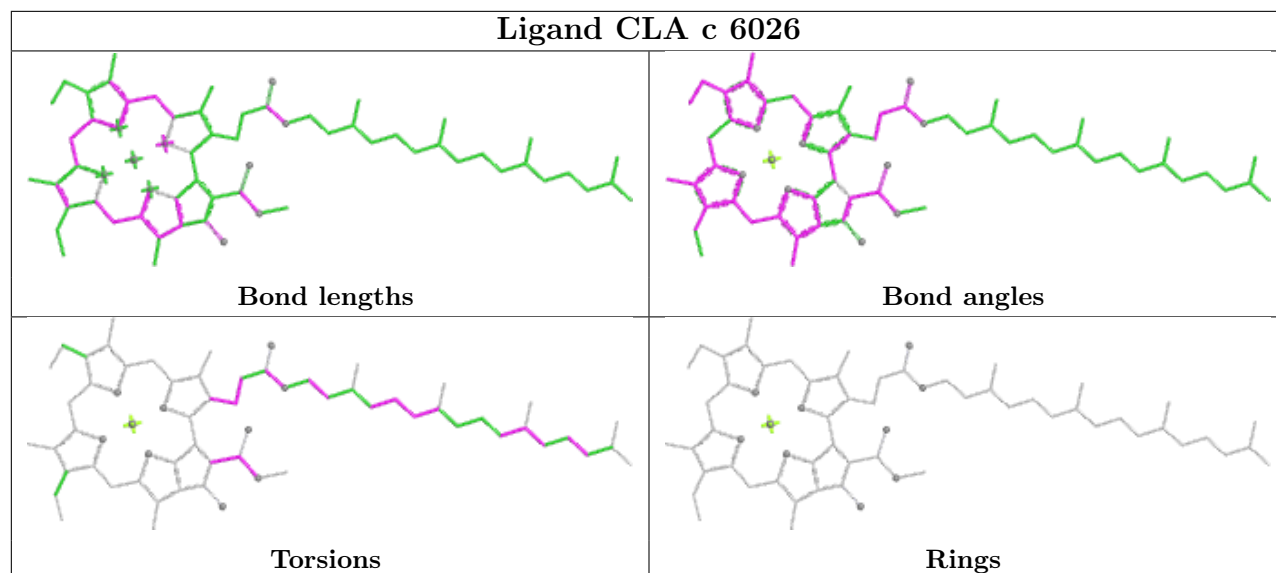
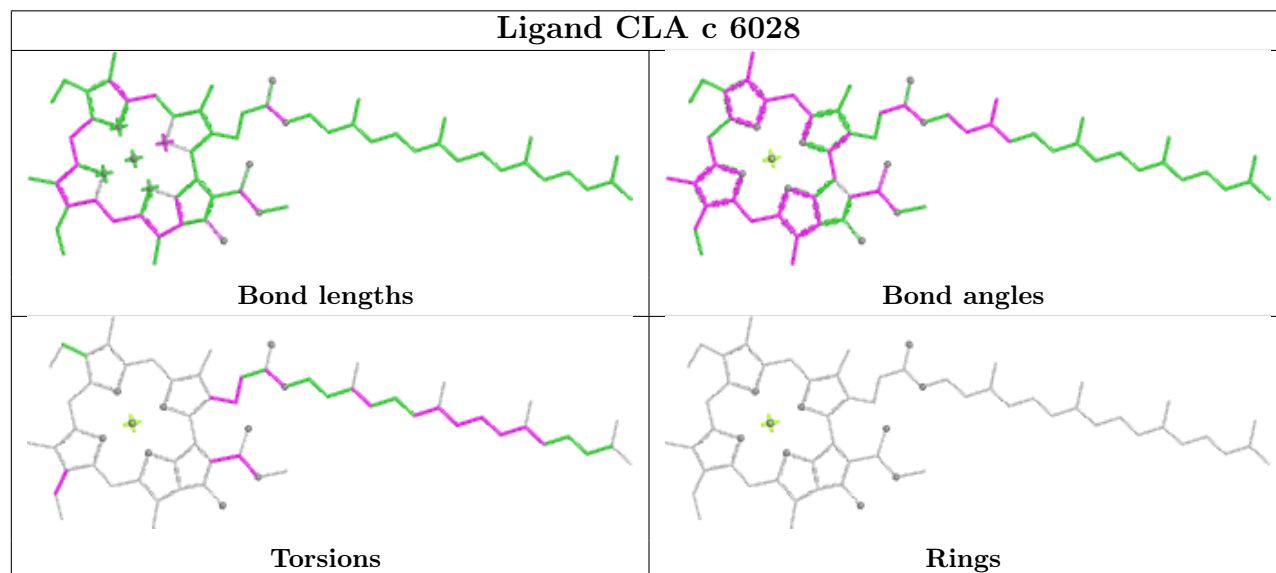
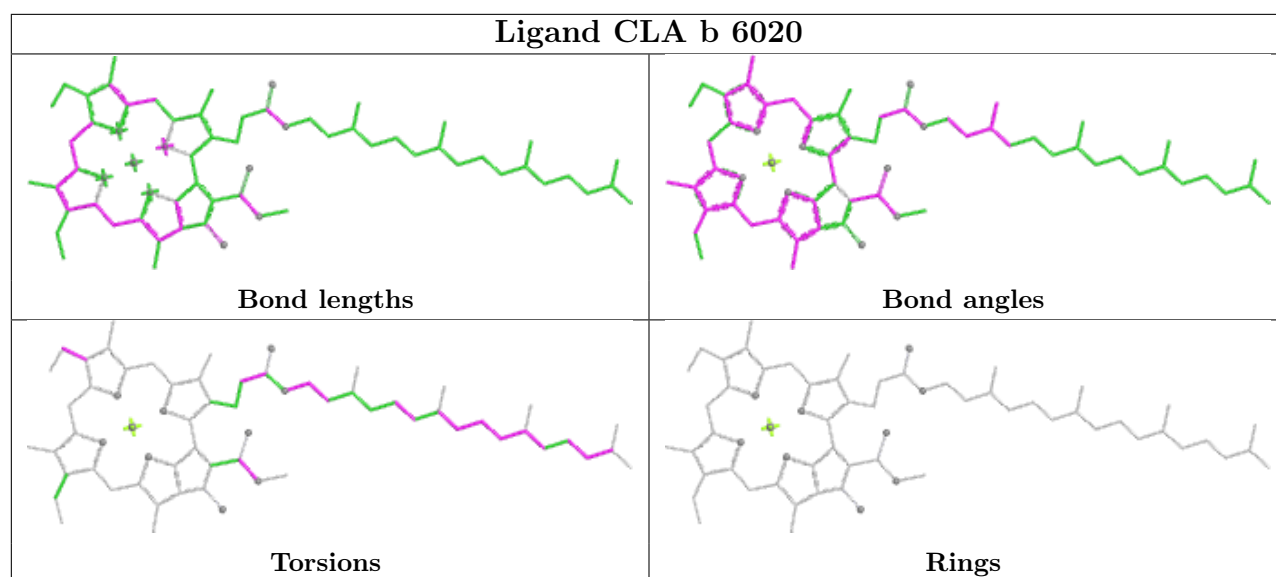
Torsions

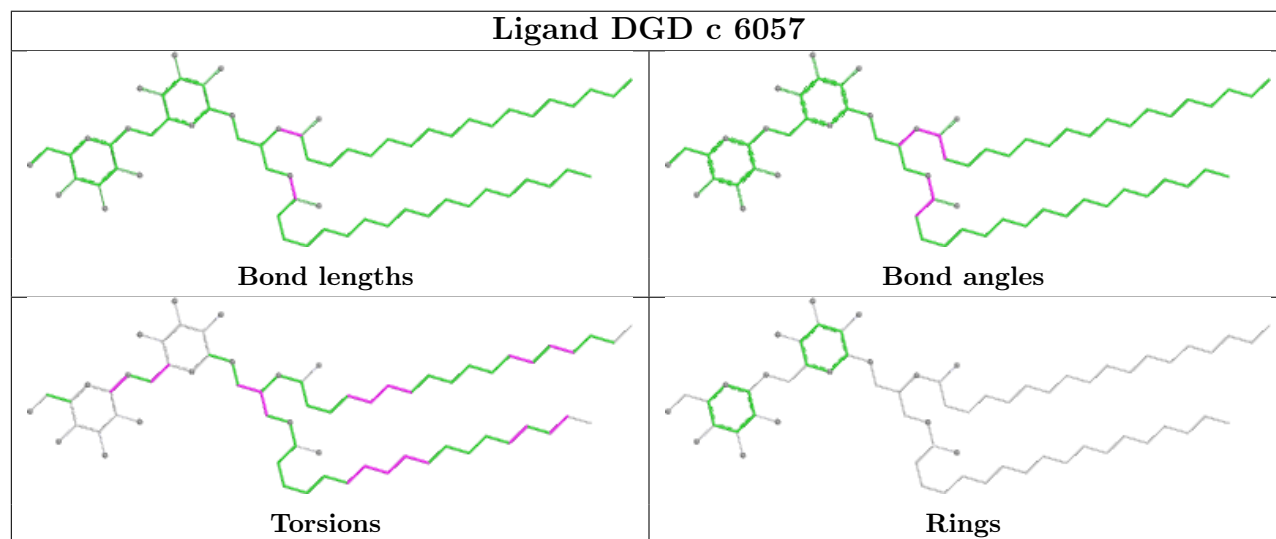
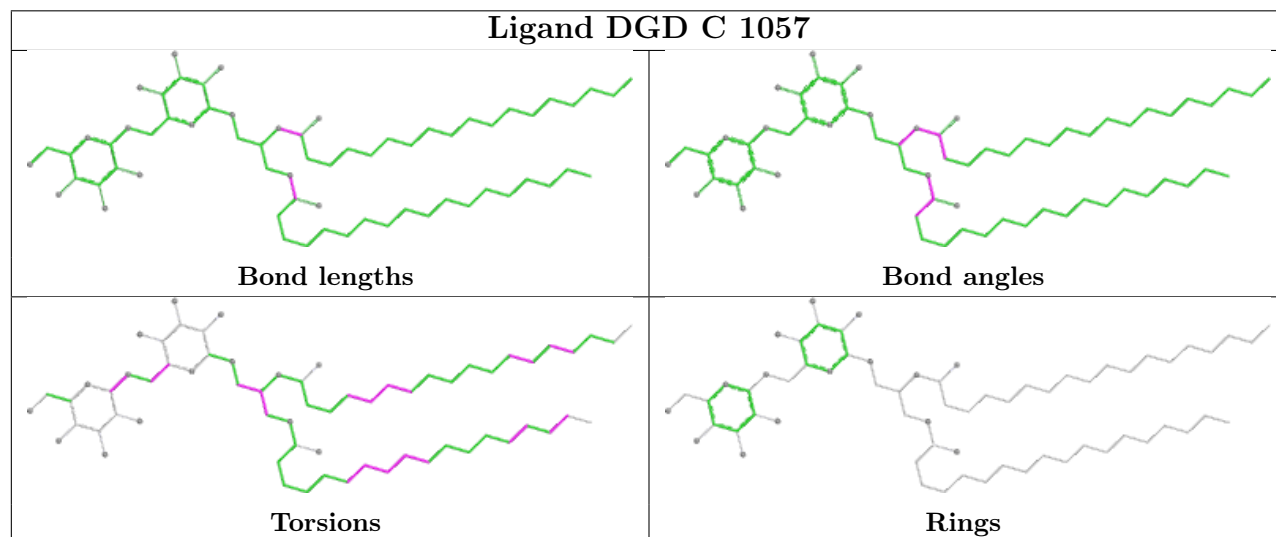
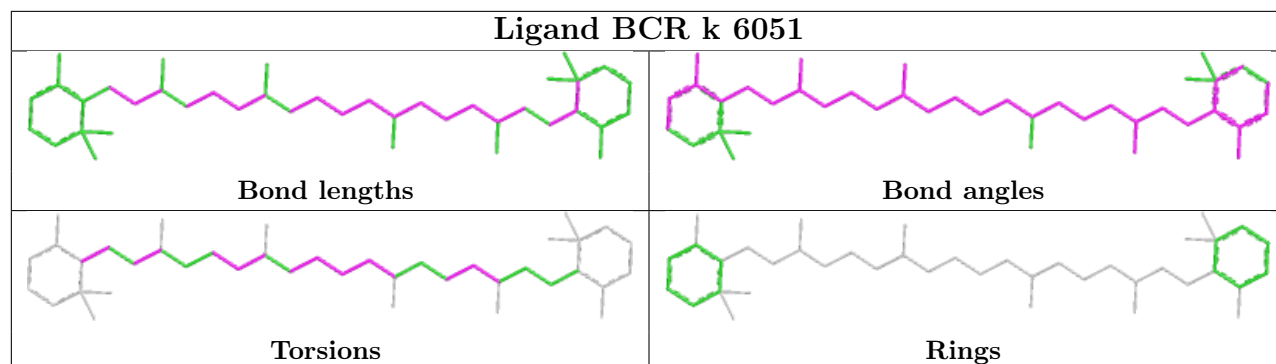


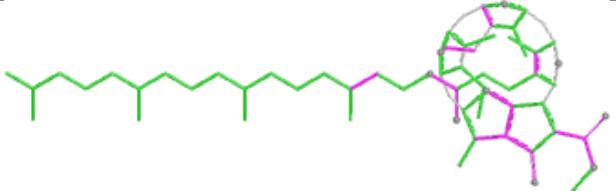
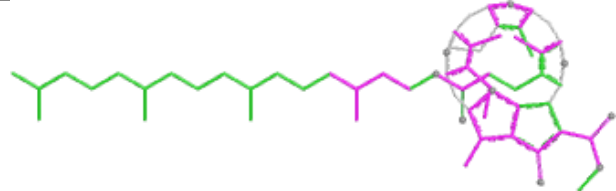
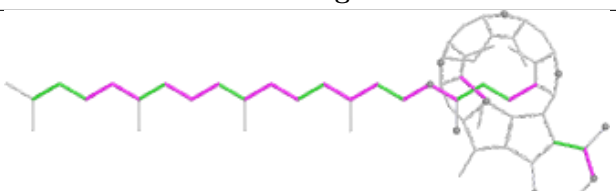
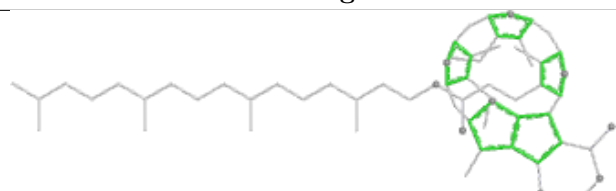
Rings

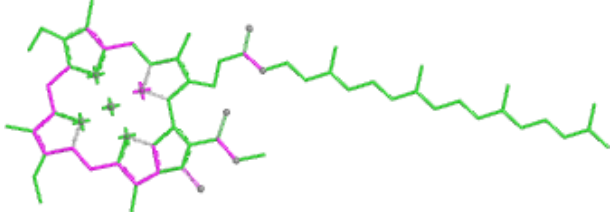
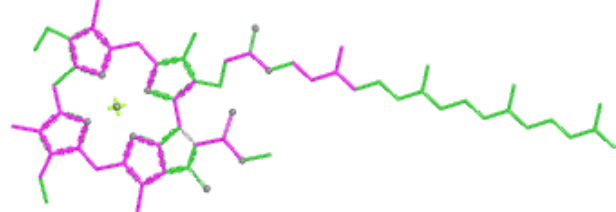
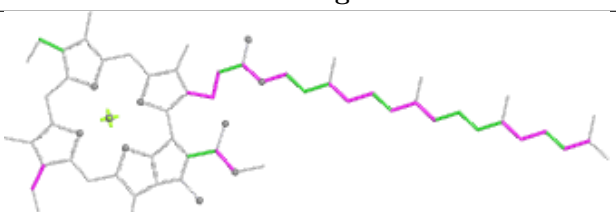
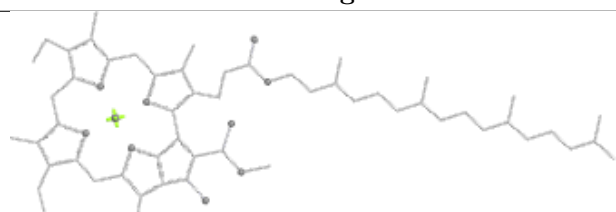


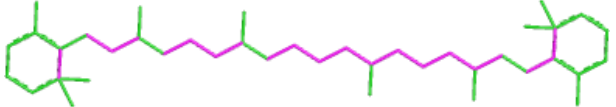
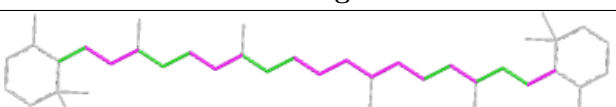
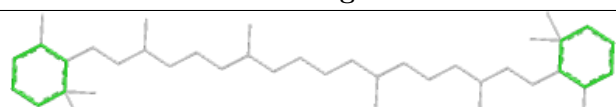


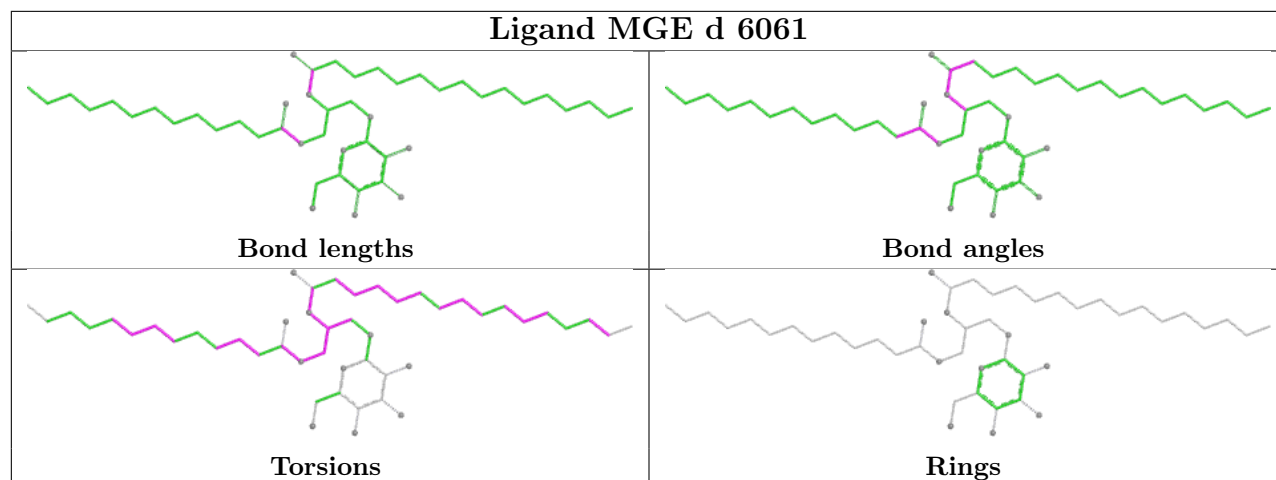
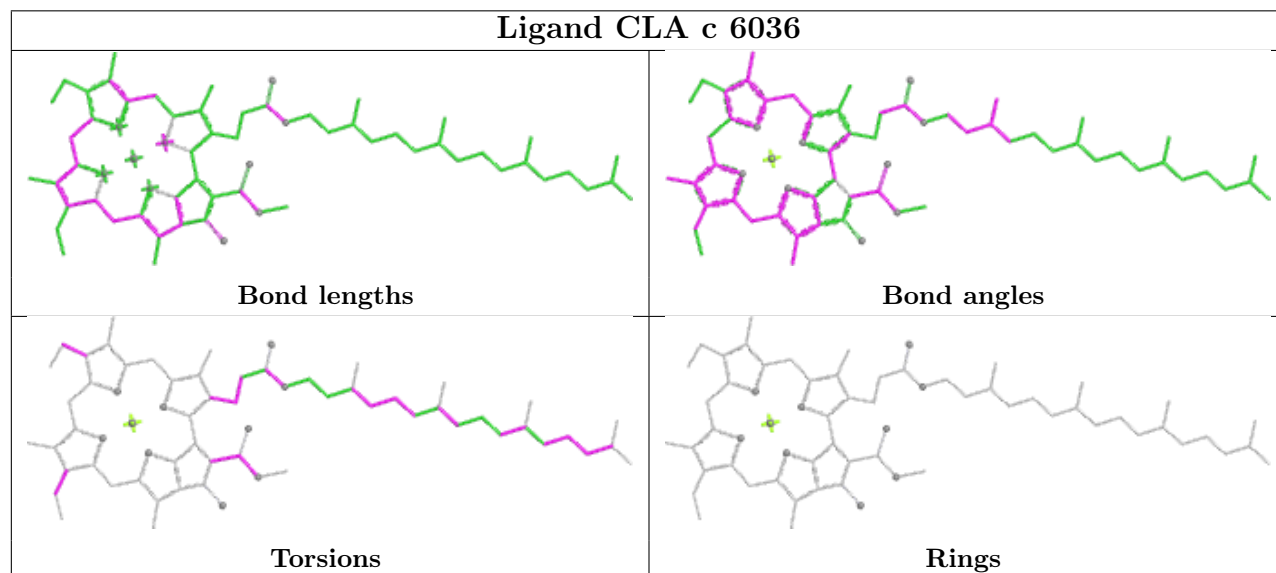
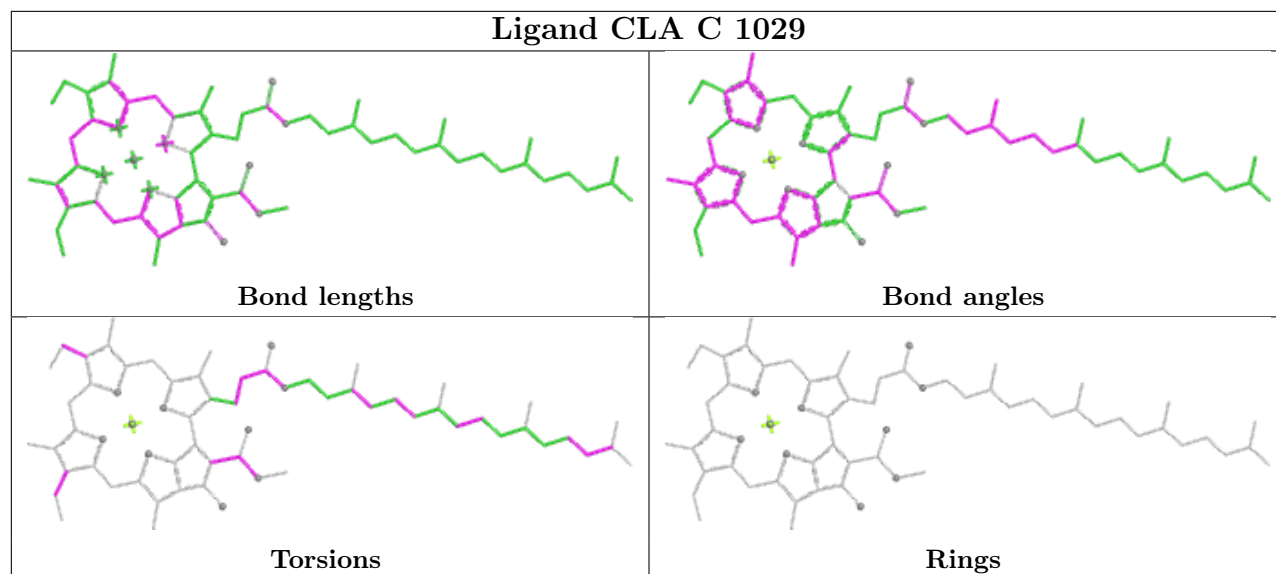


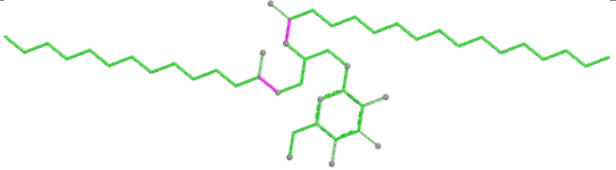
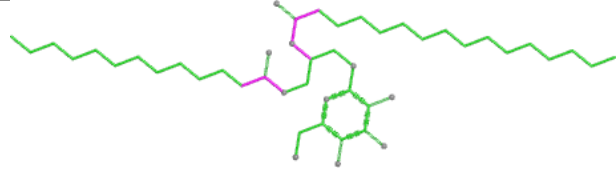
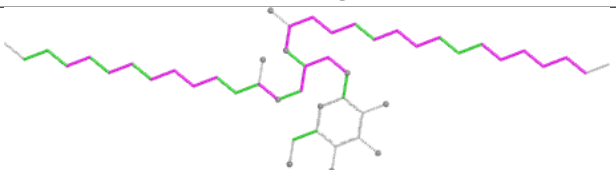
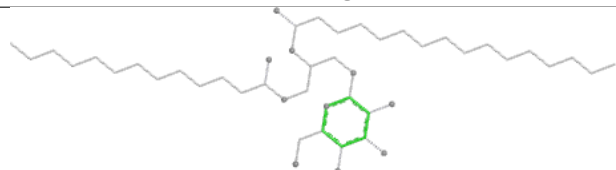
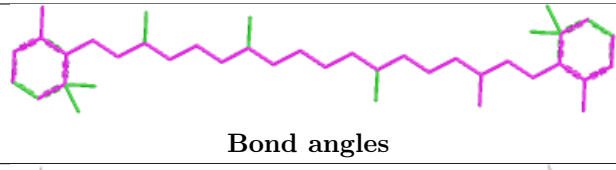


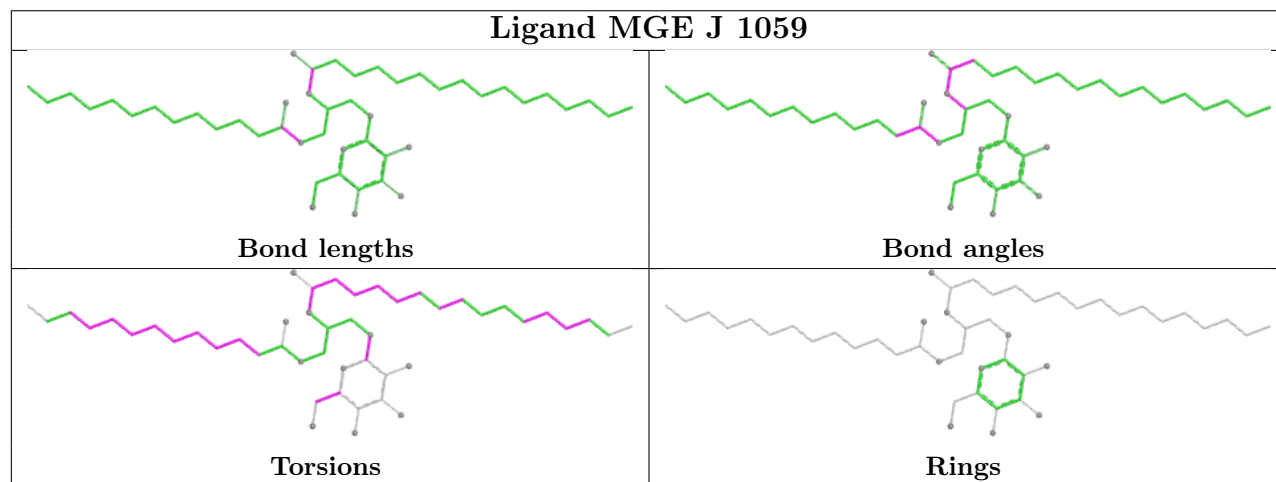
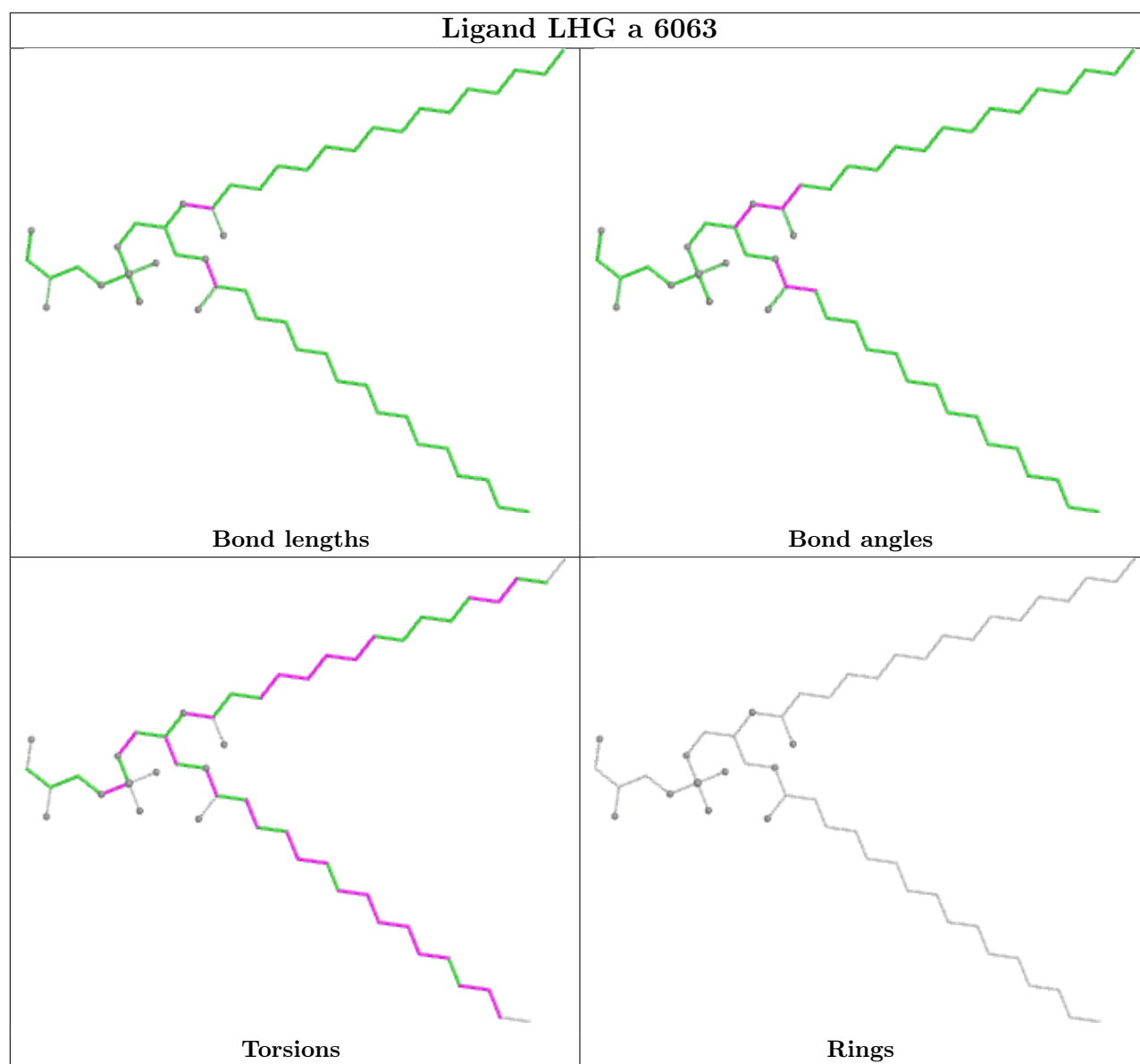
Ligand PHO d 6038	
	
Bond lengths	Bond angles
	
Torsions	Rings

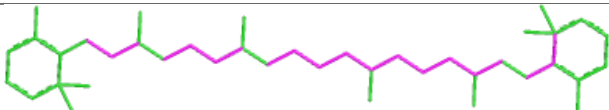
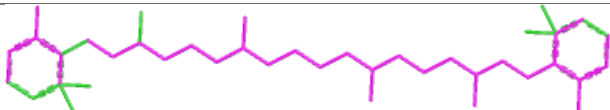
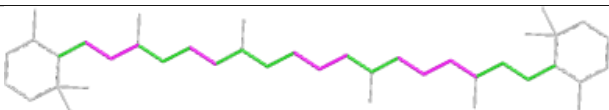
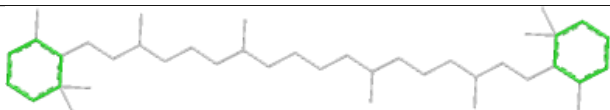
Ligand CLA a 6006	
	
Bond lengths	Bond angles
	
Torsions	Rings

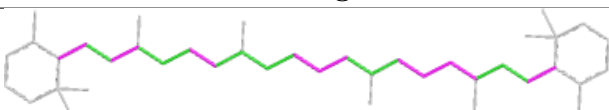
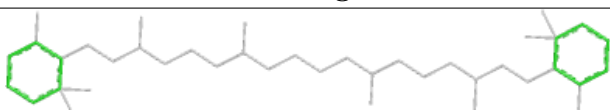
Ligand BCR B 1048	
	
Bond lengths	Bond angles
	
Torsions	Rings

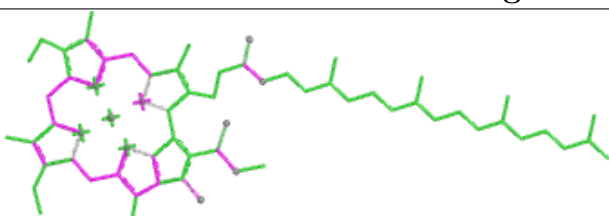
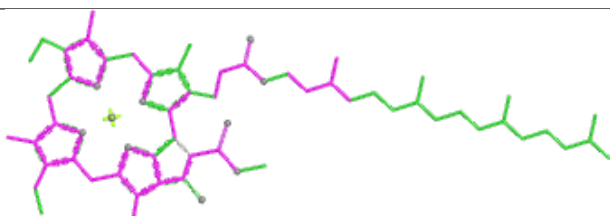
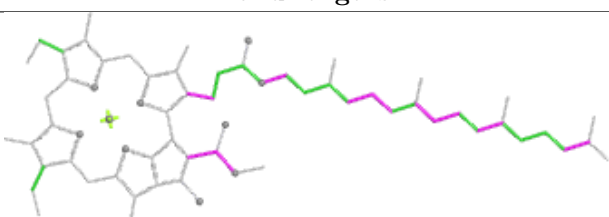
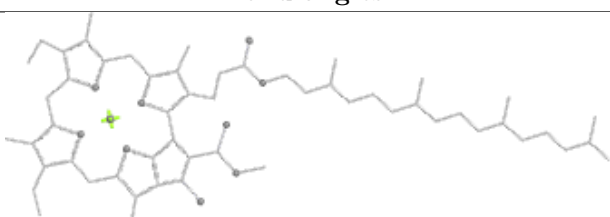


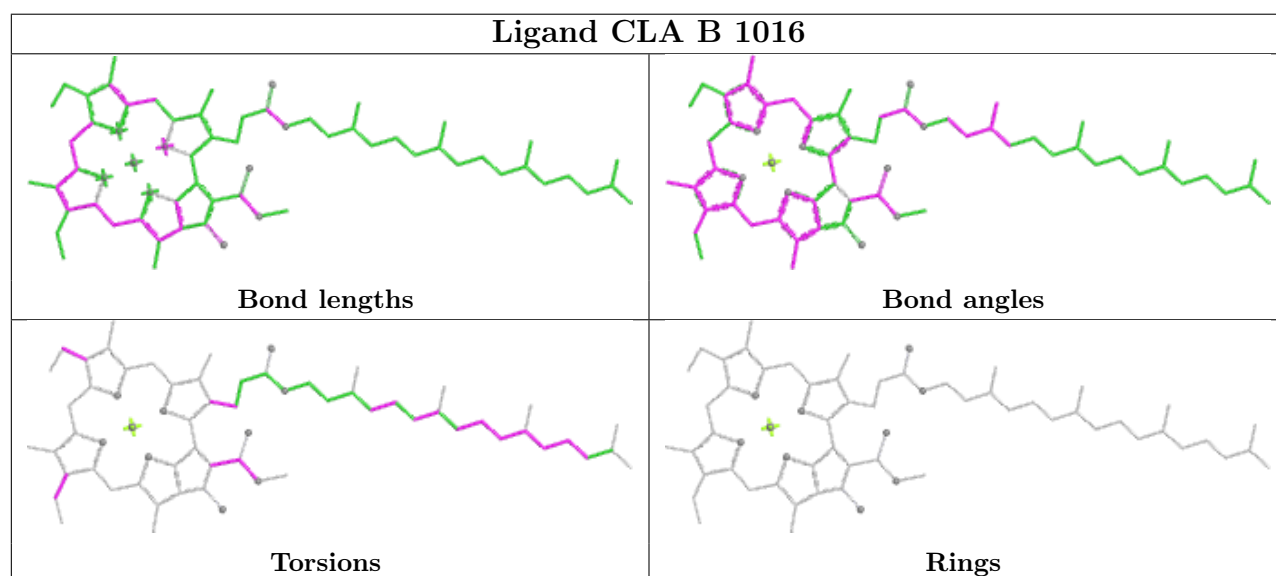
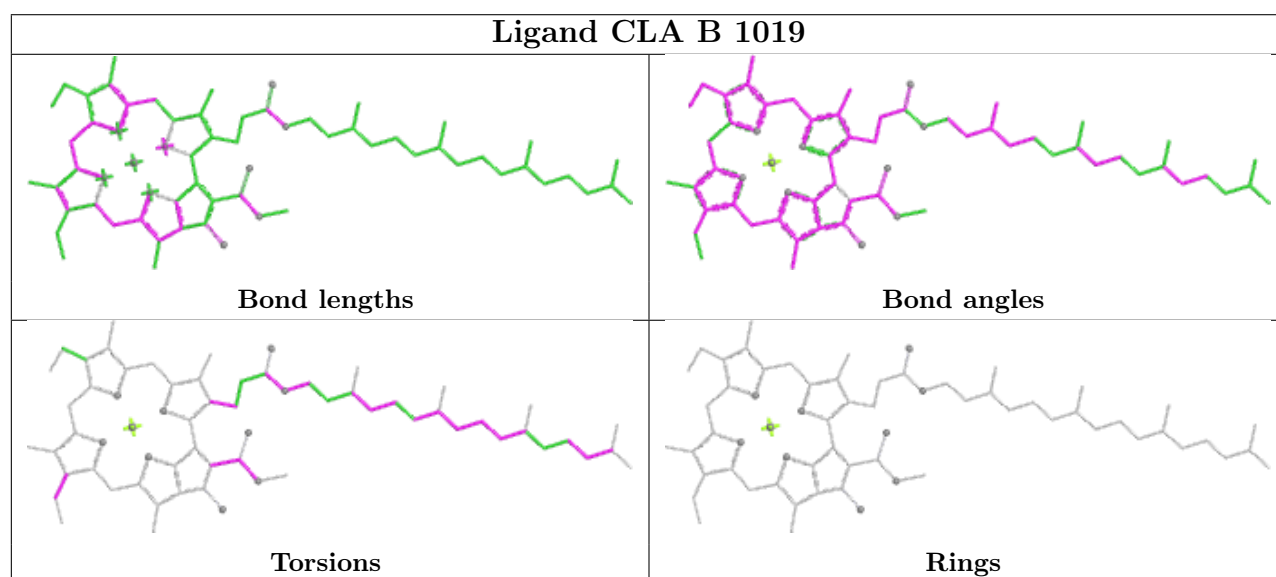
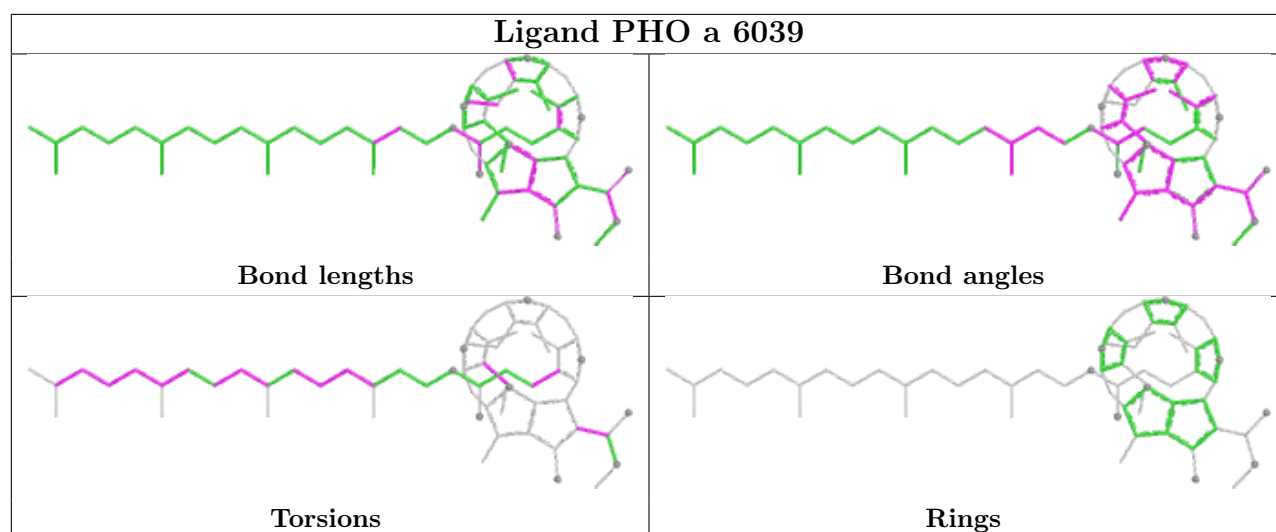
Ligand MGE d 6062	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR T 6046	
 Bond lengths	 Bond angles
 Torsions	 Rings

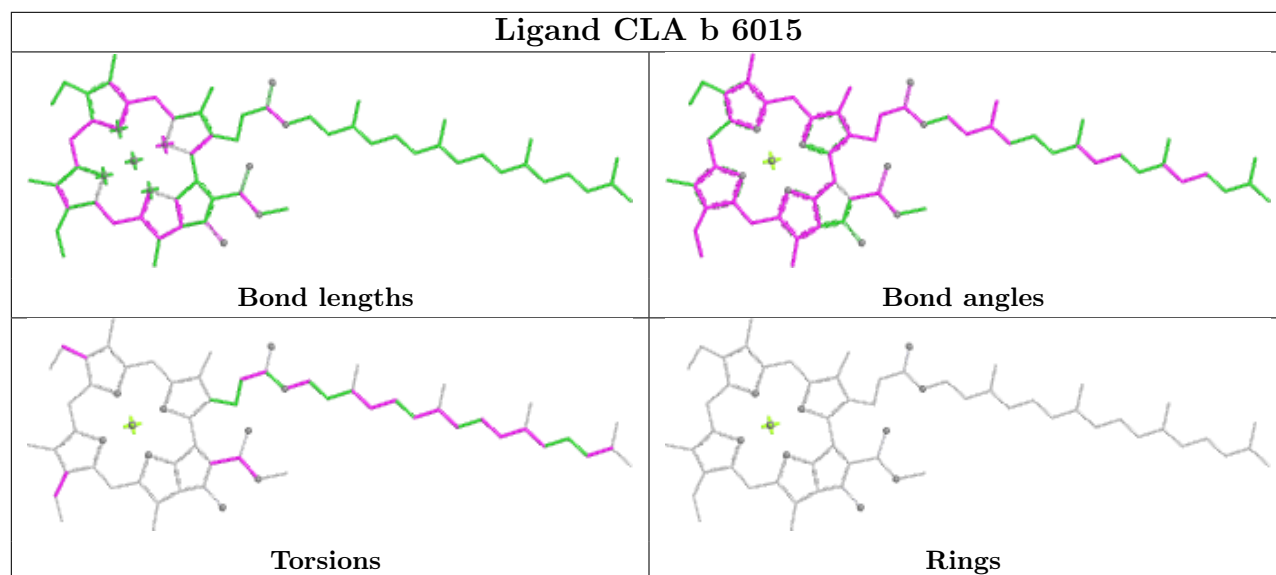
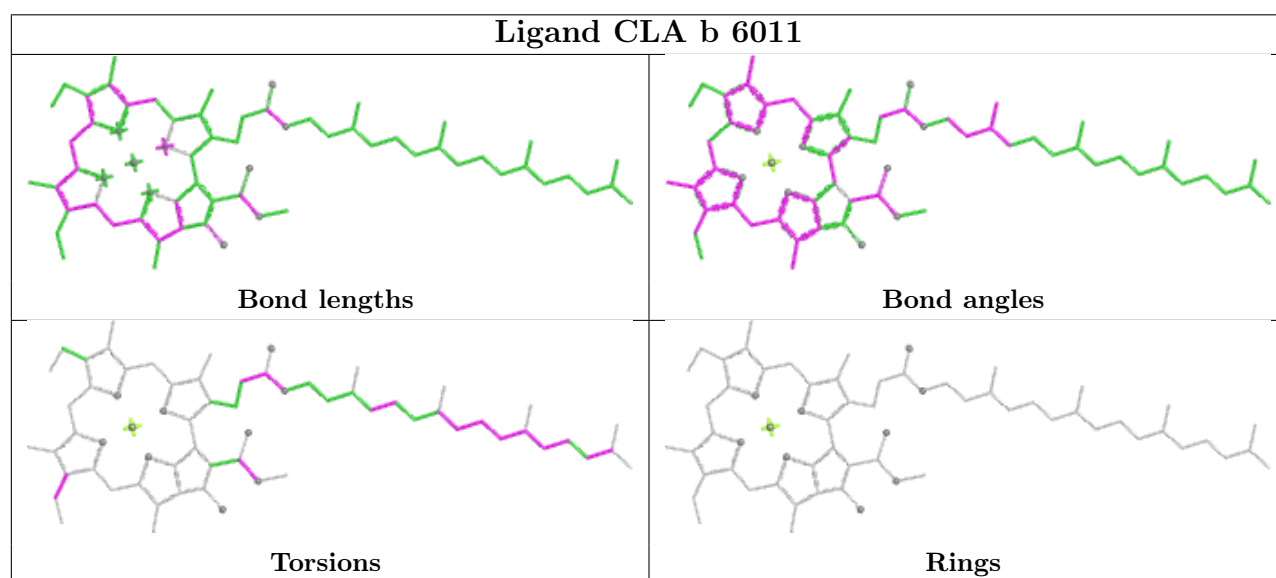
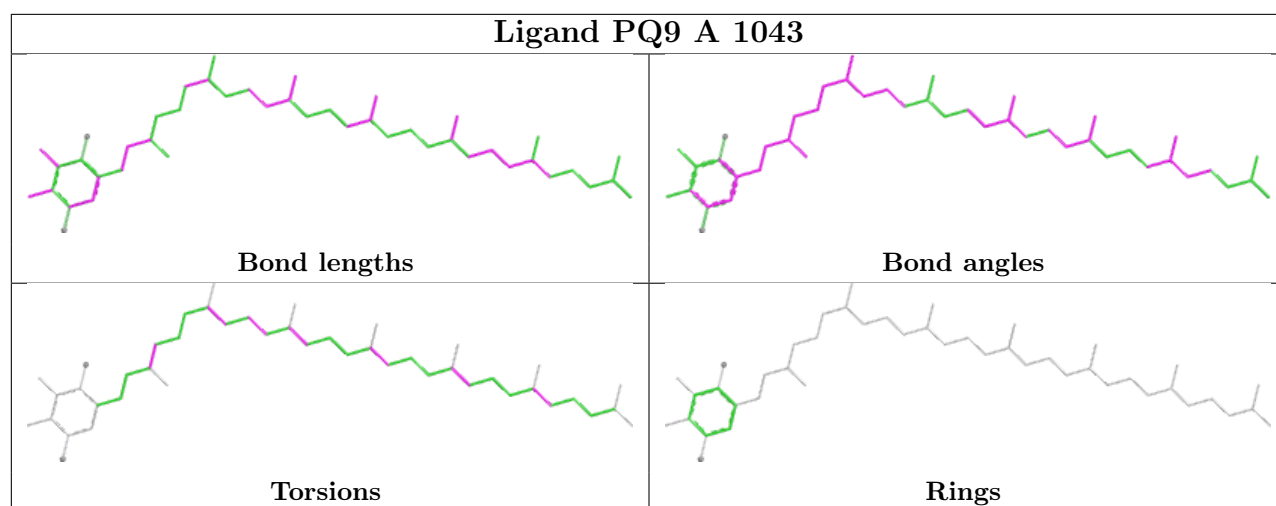


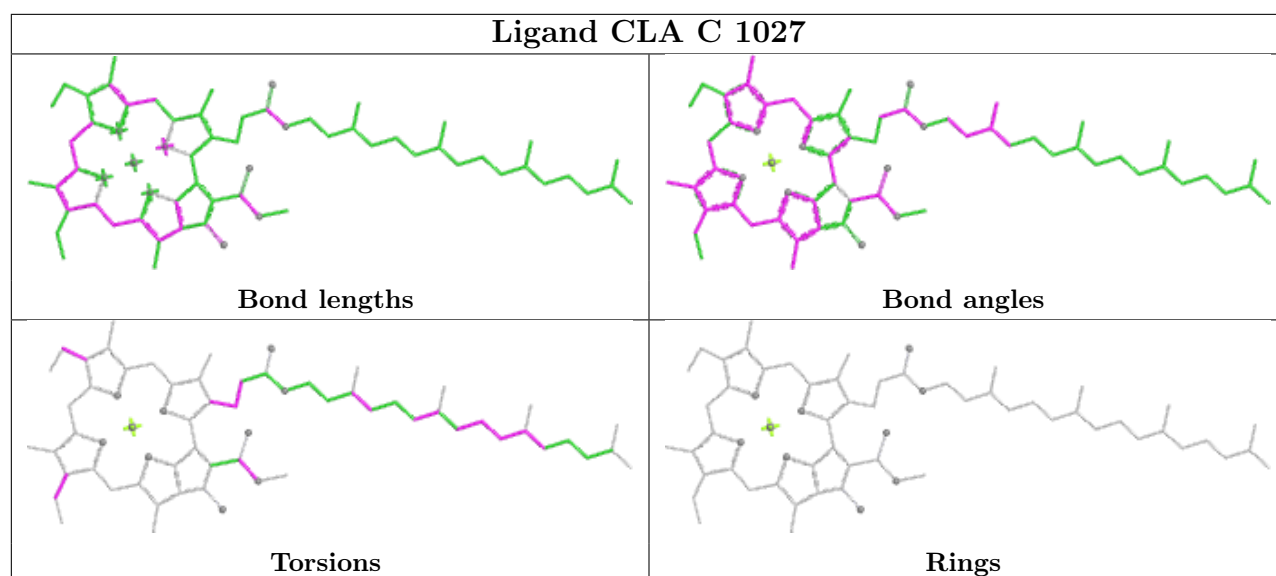
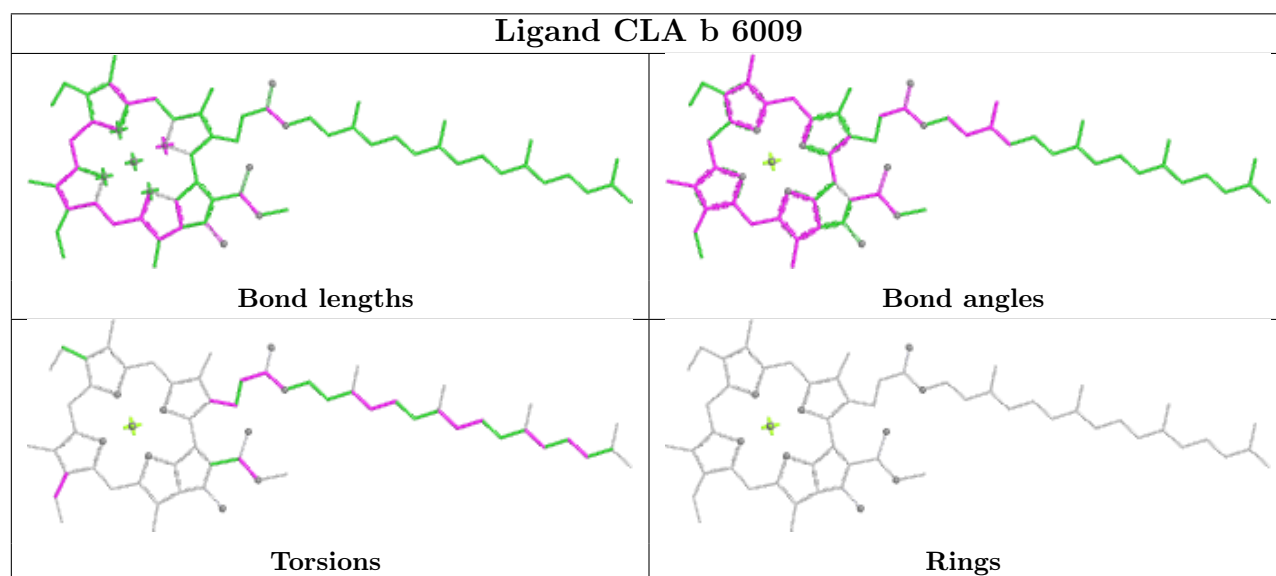
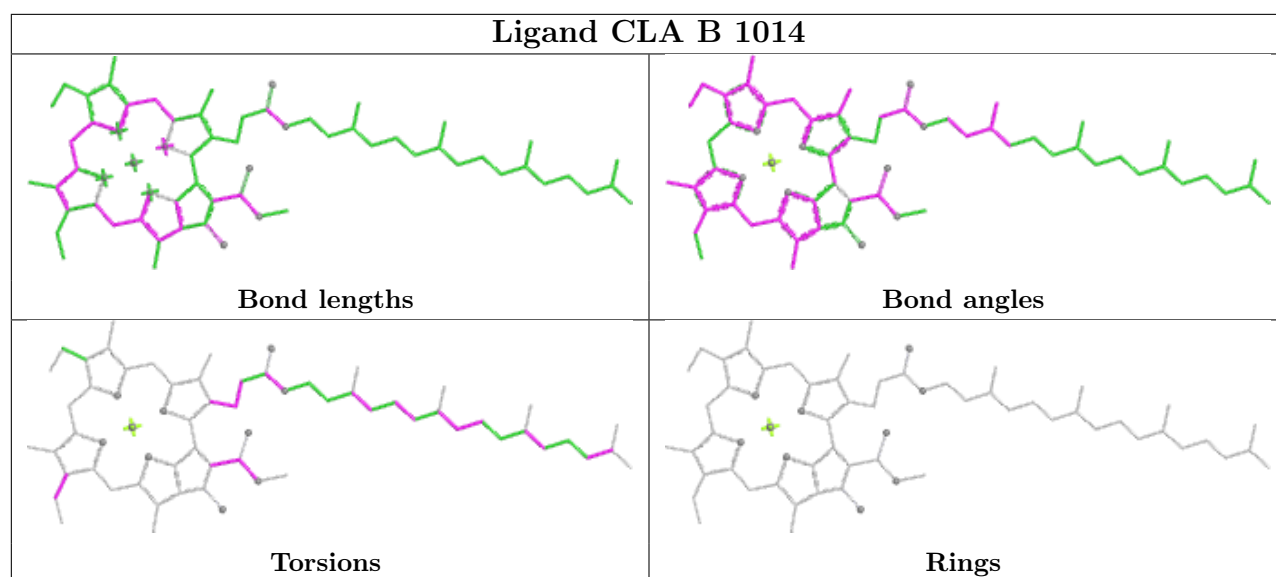
Ligand BCR a 6044	
	
Bond lengths	Bond angles
	
Torsions	Rings

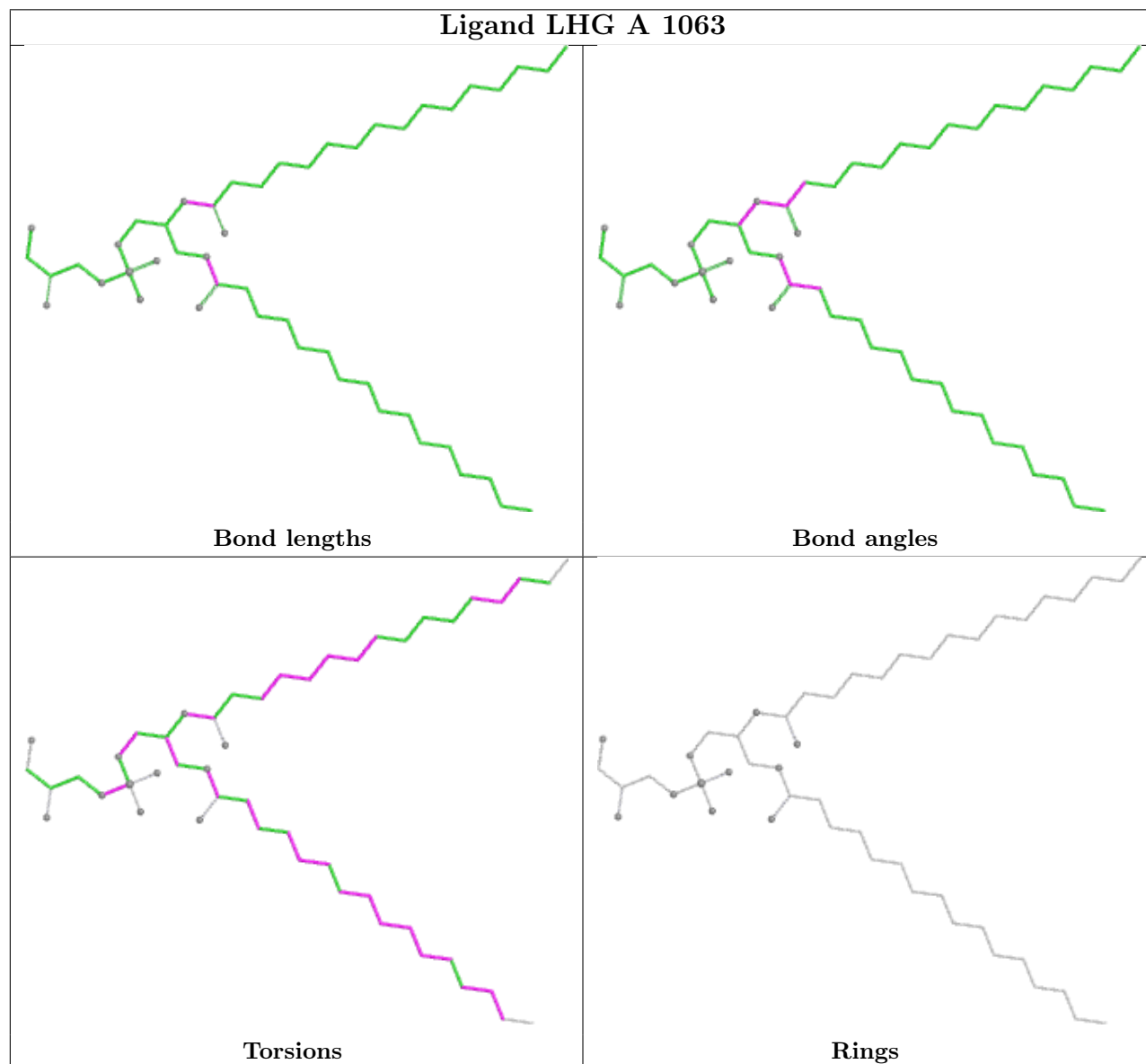
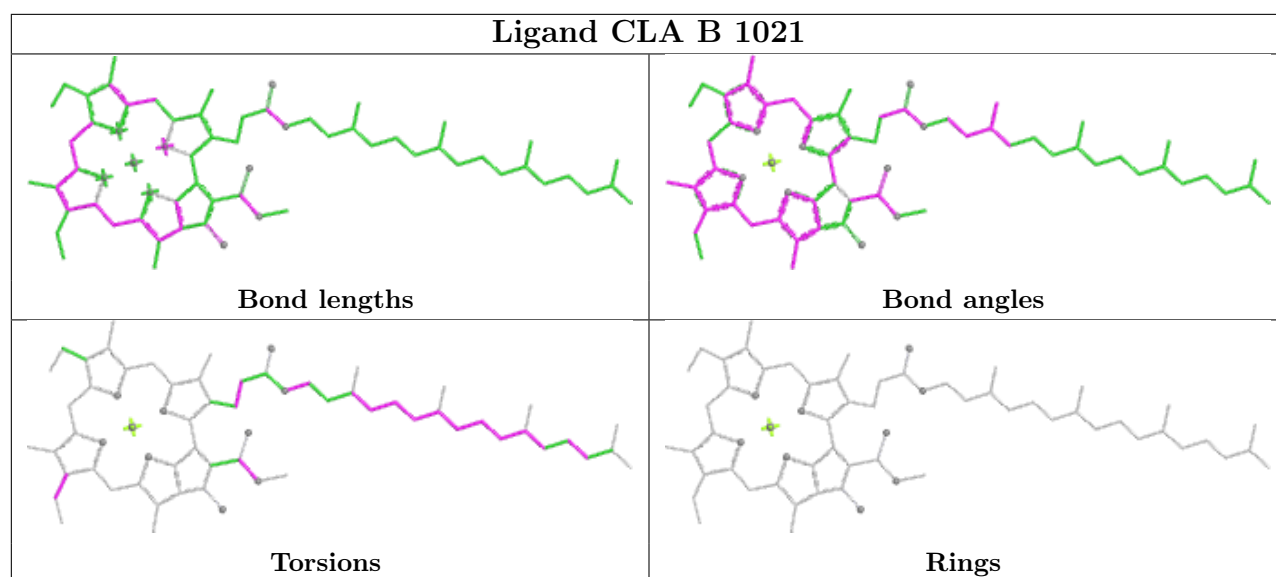
Ligand BCR Z 1053	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 6010	
	
Bond lengths	Bond angles
	
Torsions	Rings









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.23	3 (0%) 81 58	97, 127, 162, 173	0
1	a	335/344 (97%)	-0.13	5 (1%) 72 46	101, 131, 166, 178	0
2	B	485/488 (99%)	-0.25	9 (1%) 66 42	94, 130, 157, 181	0
2	b	485/488 (99%)	-0.29	1 (0%) 91 80	102, 129, 161, 183	0
3	C	447/447 (100%)	-0.17	6 (1%) 75 50	100, 143, 170, 185	0
3	c	447/447 (100%)	-0.16	3 (0%) 84 63	102, 150, 173, 187	0
4	D	340/340 (100%)	-0.24	3 (0%) 81 58	94, 127, 165, 187	0
4	d	340/340 (100%)	-0.16	5 (1%) 72 46	92, 133, 172, 191	0
5	E	82/83 (98%)	-0.29	1 (1%) 76 51	117, 156, 184, 186	0
5	e	82/83 (98%)	-0.10	1 (1%) 76 51	126, 160, 181, 186	0
6	F	35/44 (79%)	-0.04	3 (8%) 16 14	139, 147, 160, 163	0
6	f	35/44 (79%)	-0.28	0 100 100	143, 152, 160, 163	0
7	H	64/64 (100%)	-0.35	0 100 100	119, 143, 165, 170	0
7	h	64/64 (100%)	-0.26	2 (3%) 51 32	120, 143, 164, 169	0
8	I	35/35 (100%)	-0.49	0 100 100	127, 137, 166, 173	0
8	i	35/35 (100%)	-0.53	0 100 100	124, 141, 175, 176	0
9	J	34/40 (85%)	-0.16	0 100 100	127, 142, 165, 175	0
9	j	34/40 (85%)	-0.24	0 100 100	131, 146, 172, 174	0
10	K	36/36 (100%)	-0.29	1 (2%) 55 34	132, 145, 153, 155	0
10	k	36/36 (100%)	-0.09	0 100 100	140, 151, 162, 164	0
11	L	37/37 (100%)	-0.26	0 100 100	102, 123, 178, 184	0
11	l	37/37 (100%)	-0.32	1 (2%) 56 35	110, 130, 181, 188	0
12	M	36/36 (100%)	-0.13	2 (5%) 30 20	101, 119, 171, 174	0
12	m	36/36 (100%)	-0.26	1 (2%) 55 34	100, 121, 171, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/242 (100%)	-0.15	4 (1%) 69 43	108, 133, 165, 186	0
13	o	242/242 (100%)	-0.16	2 (0%) 82 60	114, 139, 164, 186	0
14	T	30/30 (100%)	-0.40	0 100 100	105, 124, 173, 178	0
14	t	30/30 (100%)	-0.38	0 100 100	101, 115, 173, 181	0
15	U	98/98 (100%)	-0.38	0 100 100	108, 123, 143, 158	0
15	u	98/98 (100%)	-0.34	0 100 100	112, 128, 143, 167	0
16	V	137/137 (100%)	-0.13	5 (3%) 46 29	104, 131, 160, 170	0
16	v	137/137 (100%)	-0.20	0 100 100	114, 145, 165, 176	0
17	X	34/34 (100%)	-0.11	0 100 100	148, 155, 164, 170	0
17	x	34/34 (100%)	-0.28	1 (2%) 53 33	151, 159, 169, 175	0
18	Y	28/28 (100%)	-0.18	0 100 100	164, 178, 189, 192	0
18	y	28/28 (100%)	0.06	0 100 100	170, 181, 191, 196	0
19	N	0/24	-	-	-	-
19	n	0/24	-	-	-	-
20	Z	62/62 (100%)	-0.16	0 100 100	138, 161, 180, 186	0
20	z	62/62 (100%)	-0.24	0 100 100	144, 164, 184, 187	0
All	All	5194/5298 (98%)	-0.21	59 (1%) 78 53	92, 136, 172, 196	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	39	ALA	5.8
1	a	5279	ARG	5.8
4	D	95	PRO	5.5
11	l	5017	LEU	4.5
1	A	279	ARG	4.4

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	LHG	a	6063	49/49	0.61	0.18	186,196,200,200	0
27	LHG	A	1063	49/49	0.62	0.19	181,187,194,195	0
23	CLA	C	1034	65/65	0.68	0.20	134,147,172,174	0
30	DGD	C	1057	66/66	0.69	0.18	125,140,187,193	0
26	BCR	z	6053	40/40	0.70	0.14	159,176,186,187	0
23	CLA	c	6034	65/65	0.70	0.18	87,162,181,181	0
23	CLA	c	6027	65/65	0.72	0.19	178,195,198,200	0
26	BCR	b	6047	40/40	0.72	0.17	114,127,145,147	0
23	CLA	c	6037	65/65	0.73	0.13	184,188,191,200	0
23	CLA	B	1009	65/65	0.73	0.15	119,178,184,185	0
26	BCR	B	1047	40/40	0.74	0.15	101,136,157,157	0
26	BCR	d	6050	40/40	0.74	0.15	149,160,166,167	0
23	CLA	b	6009	65/65	0.76	0.13	160,177,200,200	0
26	BCR	h	6049	40/40	0.76	0.17	156,175,191,192	0
23	CLA	C	1037	65/65	0.77	0.15	180,185,188,200	0
26	BCR	b	6045	40/40	0.78	0.17	145,156,167,168	0
29	MGE	d	6059	48/48	0.78	0.15	164,168,198,200	0
26	BCR	a	6044	40/40	0.78	0.21	154,160,163,166	0
26	BCR	A	1044	40/40	0.79	0.17	147,156,158,159	0
30	DGD	C	1056	66/66	0.79	0.16	155,171,183,188	0
26	BCR	D	1050	40/40	0.79	0.15	149,153,161,162	0
23	CLA	C	1032	65/65	0.80	0.19	153,166,174,176	0
26	BCR	b	6048	40/40	0.80	0.16	141,147,158,159	0
30	DGD	c	6057	66/66	0.80	0.13	128,149,183,184	0
23	CLA	B	1024	65/65	0.81	0.13	105,177,179,180	0
26	BCR	t	1046	40/40	0.82	0.14	144,156,163,163	0
23	CLA	c	6032	65/65	0.82	0.15	144,175,181,182	0
23	CLA	C	1025	65/65	0.82	0.20	131,170,180,200	0
30	DGD	c	6056	66/66	0.82	0.14	170,175,181,183	0
26	BCR	Z	1053	40/40	0.82	0.16	141,166,178,178	0
23	CLA	b	6024	65/65	0.83	0.14	172,183,186,187	0
29	MGE	d	6062	48/48	0.83	0.17	130,155,167,168	0
29	MGE	J	1059	48/48	0.83	0.12	152,158,185,186	0
23	CLA	b	6014	65/65	0.84	0.14	163,171,179,200	0
26	BCR	B	1045	40/40	0.84	0.16	146,156,169,170	0
23	CLA	C	1027	65/65	0.84	0.15	167,183,190,200	0
26	BCR	B	1048	40/40	0.84	0.14	148,155,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PHO	d	6038	64/64	0.84	0.17	136,147,150,150	0
26	BCR	T	6046	40/40	0.84	0.15	140,149,154,157	0
29	MGE	d	6061	48/48	0.85	0.19	141,152,165,169	0
23	CLA	c	6025	65/65	0.85	0.16	145,170,178,200	0
26	BCR	c	6054	40/40	0.85	0.18	174,177,183,183	0
23	CLA	d	6008	65/65	0.85	0.17	172,175,185,200	0
26	BCR	K	1051	40/40	0.85	0.23	175,179,182,183	0
23	CLA	c	6031	65/65	0.85	0.15	173,182,185,186	0
23	CLA	c	6033	65/65	0.86	0.16	84,142,180,180	0
25	PQ9	d	6042	45/45	0.86	0.25	137,146,167,168	0
23	CLA	B	1014	65/65	0.86	0.12	123,169,174,176	0
29	MGE	B	1060	48/48	0.86	0.18	151,170,182,184	0
23	CLA	c	6036	65/65	0.87	0.13	177,180,184,200	0
29	MGE	L	1061	48/48	0.87	0.20	141,144,154,155	0
29	MGE	b	6060	48/48	0.87	0.21	158,178,191,192	0
23	CLA	B	1022	65/65	0.87	0.12	135,155,159,161	0
26	BCR	k	6052	40/40	0.87	0.24	158,179,200,200	0
23	CLA	C	1033	65/65	0.87	0.14	117,131,162,164	0
23	CLA	b	6021	65/65	0.87	0.14	125,132,157,160	0
25	PQ9	A	1043	45/45	0.87	0.34	138,151,171,171	30
26	BCR	H	1049	40/40	0.87	0.16	155,162,188,188	0
23	CLA	c	6030	65/65	0.87	0.12	100,154,174,175	0
23	CLA	C	1028	65/65	0.88	0.14	141,154,159,168	0
23	CLA	c	6029	65/65	0.88	0.15	151,170,173,200	0
23	CLA	b	6022	65/65	0.88	0.10	133,148,156,157	0
23	CLA	b	6013	65/65	0.88	0.15	139,154,161,172	0
23	CLA	a	6003	65/65	0.88	0.18	121,130,145,193	0
23	CLA	b	6023	65/65	0.89	0.14	149,183,189,190	0
23	CLA	c	6035	65/65	0.89	0.18	170,173,177,200	0
23	CLA	C	1036	65/65	0.89	0.12	162,166,179,200	0
23	CLA	b	6011	65/65	0.89	0.14	156,159,165,170	0
26	BCR	K	1052	40/40	0.89	0.25	153,171,178,179	0
23	CLA	b	6012	65/65	0.89	0.17	146,153,159,198	0
24	PHO	A	1038	64/64	0.89	0.14	122,144,147,148	0
24	PHO	a	6039	64/64	0.89	0.15	151,165,169,170	0
23	CLA	c	6028	65/65	0.89	0.14	147,157,160,162	0
23	CLA	C	1029	65/65	0.89	0.13	146,156,159,200	0
25	PQ9	a	6043	45/45	0.89	0.31	135,149,185,185	30
23	CLA	C	1026	65/65	0.89	0.13	128,133,146,149	0
23	CLA	b	6015	65/65	0.89	0.15	137,149,155,164	0
30	DGD	c	6055	66/66	0.89	0.15	147,153,165,166	0
23	CLA	a	6006	65/65	0.89	0.11	140,145,197,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	a	6007	65/65	0.89	0.17	143,149,179,183	0
30	DGD	h	6058	66/66	0.89	0.19	140,153,163,170	0
31	HEM	e	6040	43/43	0.89	0.16	171,184,185,185	0
23	CLA	A	1007	65/65	0.90	0.13	137,141,171,183	0
23	CLA	B	1015	65/65	0.90	0.12	133,146,153,175	0
23	CLA	B	1016	65/65	0.90	0.12	87,143,150,150	0
23	CLA	A	1003	65/65	0.90	0.18	122,129,147,149	0
30	DGD	C	1055	66/66	0.90	0.19	131,140,147,152	0
23	CLA	D	1008	65/65	0.90	0.15	159,167,182,200	0
23	CLA	B	1023	65/65	0.90	0.15	155,179,185,200	0
30	DGD	H	1058	66/66	0.90	0.18	131,150,165,166	0
23	CLA	B	1013	65/65	0.90	0.14	131,157,165,168	0
23	CLA	d	6005	65/65	0.90	0.12	90,100,117,118	0
29	MGE	D	1062	48/48	0.90	0.17	129,148,165,165	0
23	CLA	b	6016	65/65	0.90	0.14	76,148,153,155	0
23	CLA	b	6020	65/65	0.90	0.17	75,148,170,173	0
23	CLA	B	1020	65/65	0.91	0.15	113,151,177,179	0
23	CLA	C	1030	65/65	0.91	0.11	92,145,175,176	0
23	CLA	C	1031	65/65	0.91	0.17	164,170,179,200	0
23	CLA	A	1006	65/65	0.91	0.14	119,124,190,192	0
31	HEM	E	1040	43/43	0.91	0.21	141,181,194,198	0
26	BCR	C	1054	40/40	0.91	0.15	158,165,169,170	0
23	CLA	b	6018	65/65	0.92	0.15	142,154,162,165	0
23	CLA	b	6019	65/65	0.92	0.10	124,150,155,193	0
23	CLA	B	1021	65/65	0.92	0.10	104,129,142,146	0
23	CLA	H	1017	65/65	0.92	0.12	116,169,174,200	0
23	CLA	B	1012	65/65	0.92	0.14	148,152,159,176	0
24	PHO	A	1039	64/64	0.92	0.13	149,151,160,161	0
23	CLA	C	1035	65/65	0.92	0.18	155,167,173,200	0
23	CLA	B	1019	65/65	0.92	0.09	121,156,158,200	0
23	CLA	B	1010	65/65	0.92	0.15	115,164,166,169	0
26	BCR	k	6051	40/40	0.92	0.15	187,193,197,197	0
23	CLA	c	6026	65/65	0.92	0.11	140,144,157,170	0
23	CLA	D	1004	65/65	0.93	0.16	101,131,139,142	0
23	CLA	D	1005	65/65	0.93	0.10	101,108,116,157	0
23	CLA	b	6017	65/65	0.93	0.12	118,165,168,200	0
23	CLA	B	1011	65/65	0.93	0.13	144,159,161,166	0
28	BR	a	6065	1/1	0.93	0.09	164,164,164,164	0
28	BR	d	6064	1/1	0.93	0.07	130,130,130,130	0
25	PQ9	D	1042	45/45	0.94	0.18	131,145,154,155	0
23	CLA	d	6004	65/65	0.94	0.14	111,128,134,134	0
23	CLA	B	1018	65/65	0.94	0.13	111,158,165,168	0

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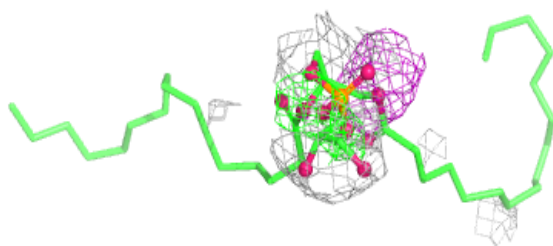
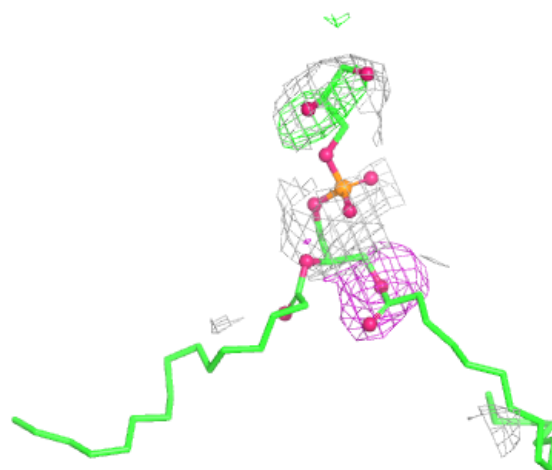
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	BR	A	1064	1/1	0.94	0.10	113,113,113,113	0
23	CLA	b	6010	65/65	0.95	0.12	93,165,169,170	0
22	FE2	a	6002	1/1	0.95	0.04	149,149,149,149	0
28	BR	A	1065	1/1	0.96	0.06	158,158,158,158	0
31	HEM	v	6041	43/43	0.96	0.14	99,135,139,140	0
22	FE2	A	1002	1/1	0.97	0.09	125,125,125,125	0
31	HEM	V	1041	43/43	0.97	0.16	81,131,132,133	0
21	OEC	a	6001	5/9	0.98	0.11	87,94,106,107	0
21	OEC	A	1001	5/9	0.99	0.09	79,94,115,119	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.

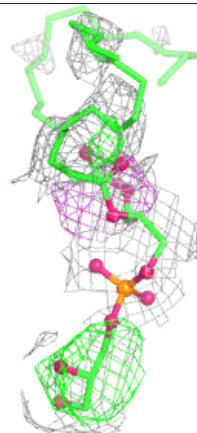
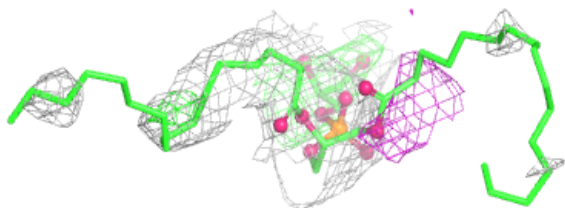
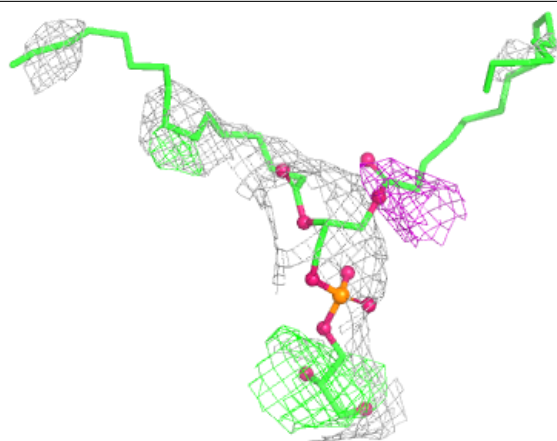
Electron density around LHG a 6063:

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



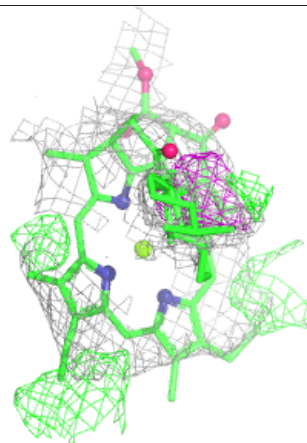
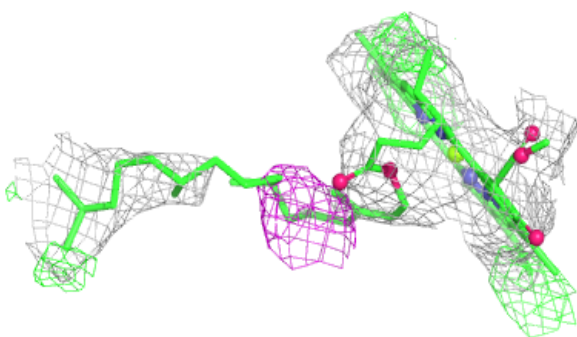
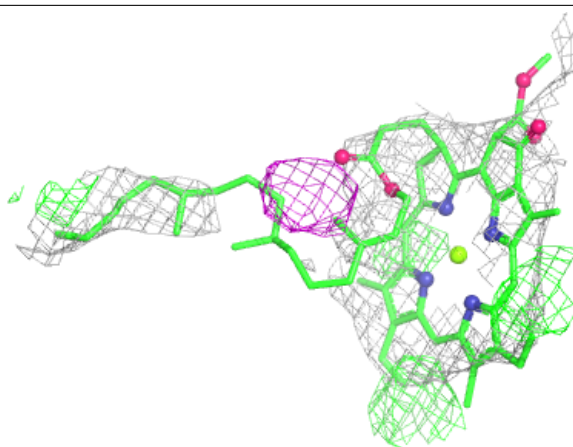
Electron density around LHG A 1063:

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

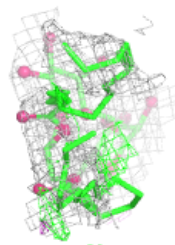
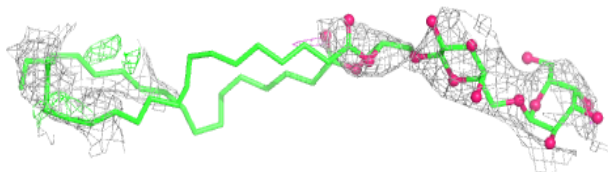
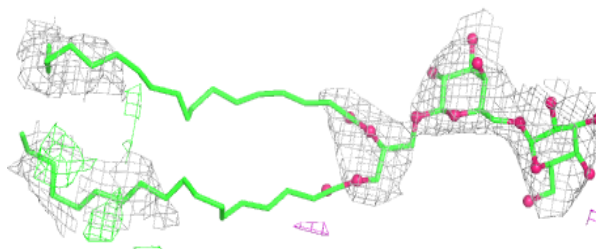


Electron density around CLA C 1034:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

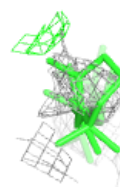
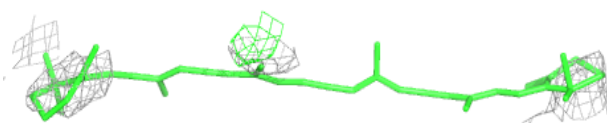
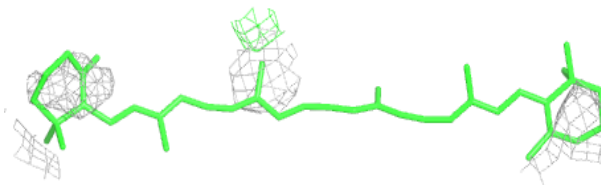
**Electron density around DGD C 1057:**

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

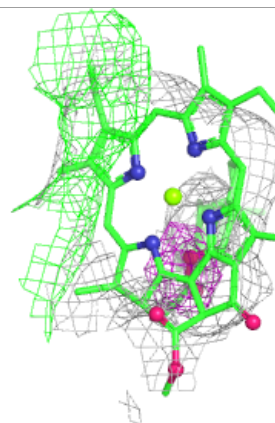
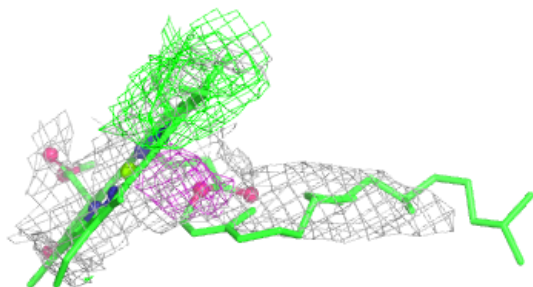
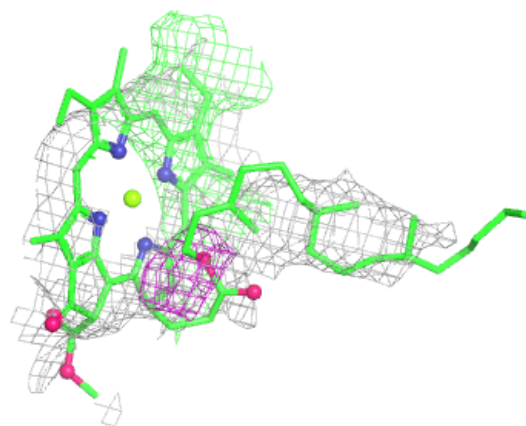


Electron density around BCR z 6053:

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

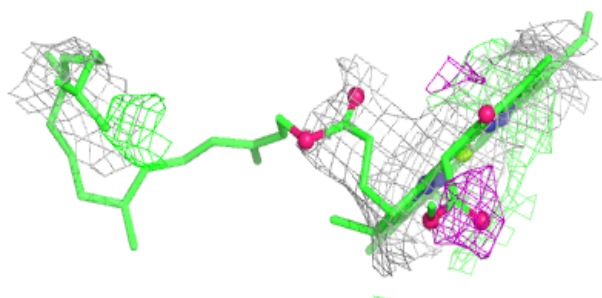
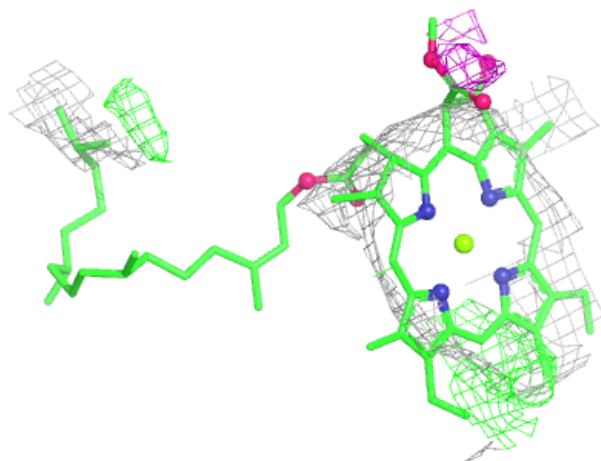
**Electron density around CLA c 6034:**

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



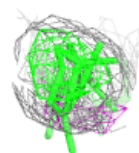
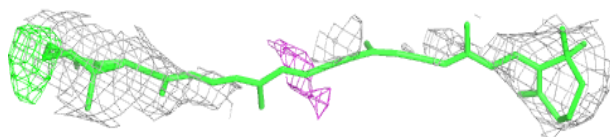
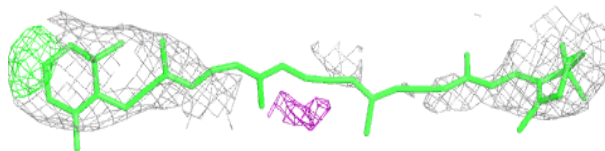
Electron density around CLA c 6027:

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



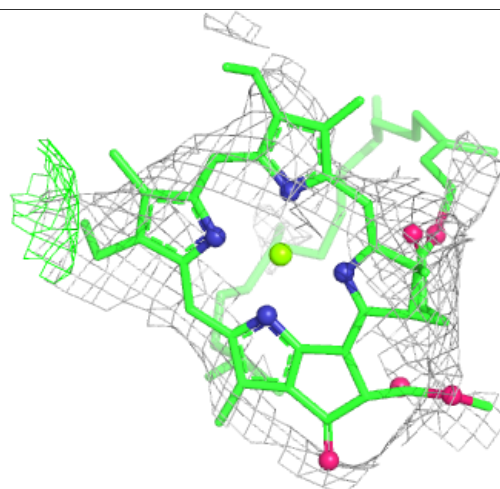
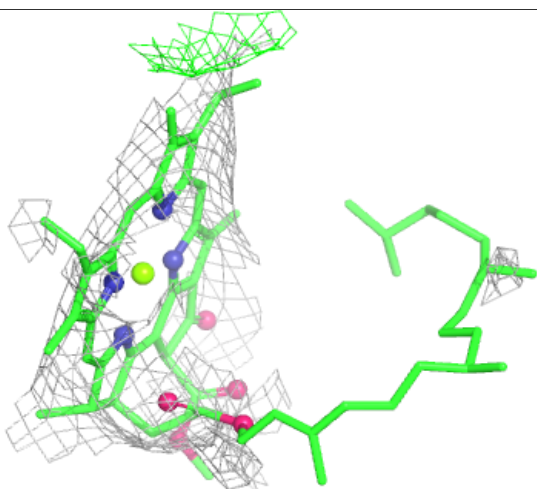
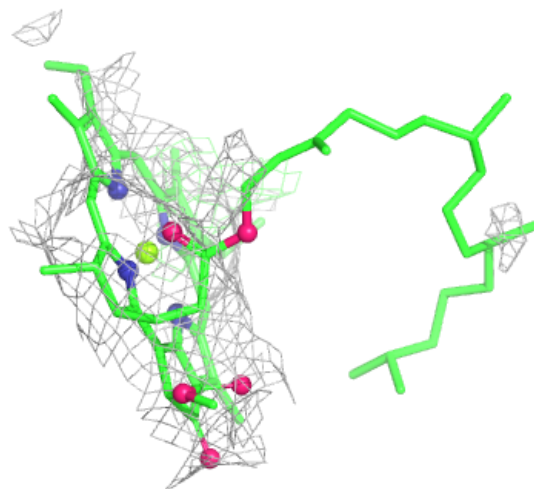
Electron density around BCR b 6047:

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



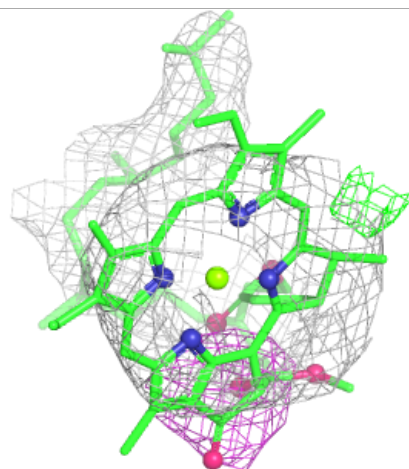
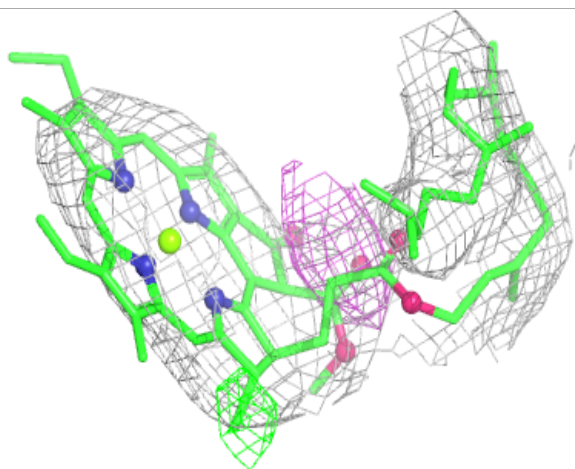
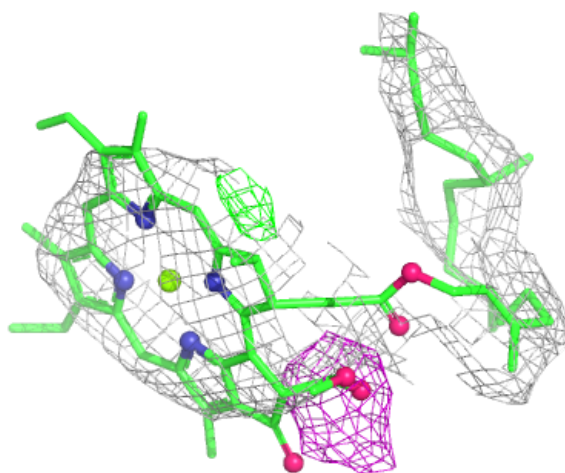
Electron density around CLA c 6037:

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



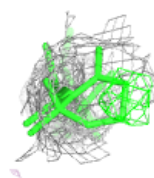
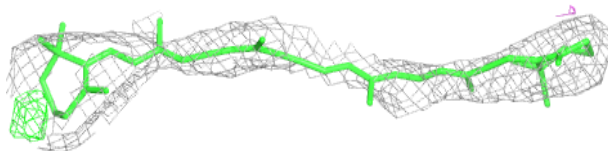
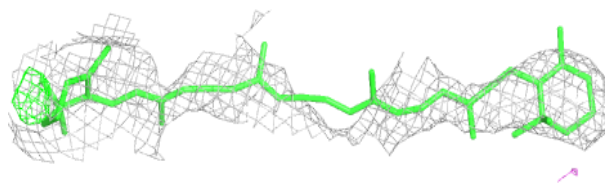
Electron density around CLA B 1009:

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

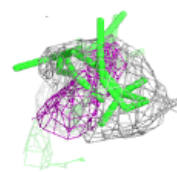
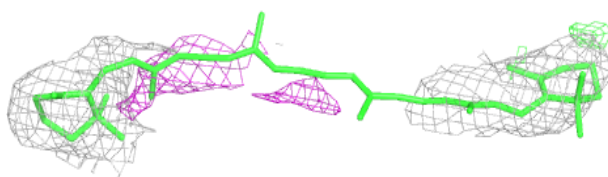
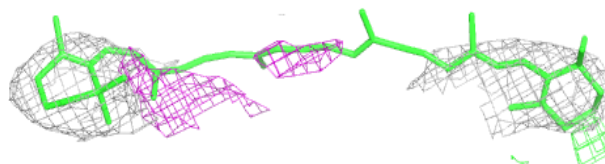


Electron density around BCR B 1047:

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

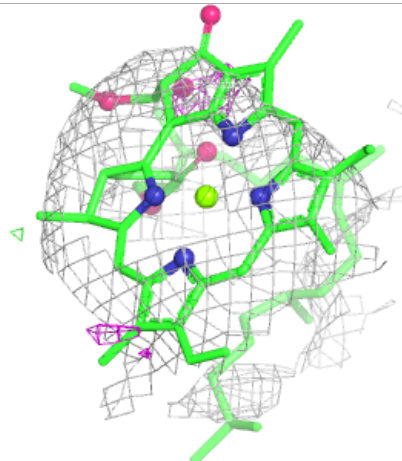
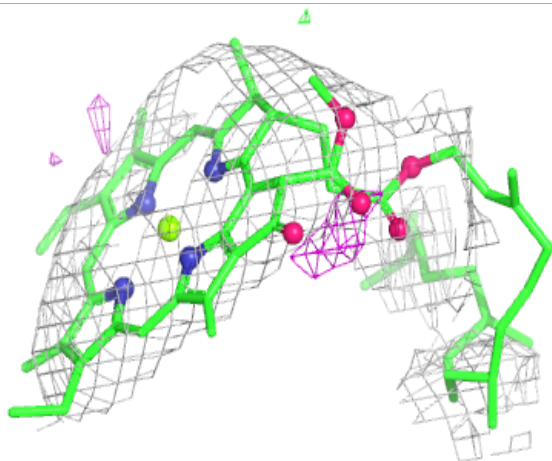
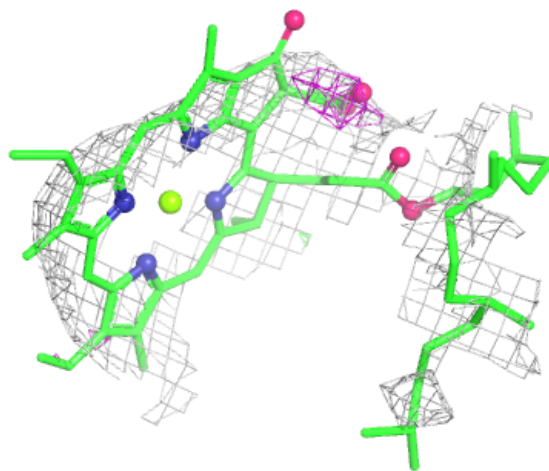
**Electron density around BCR d 6050:**

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



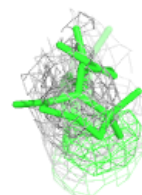
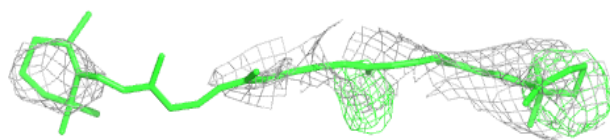
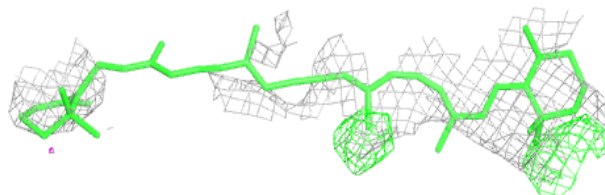
Electron density around CLA b 6009:

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

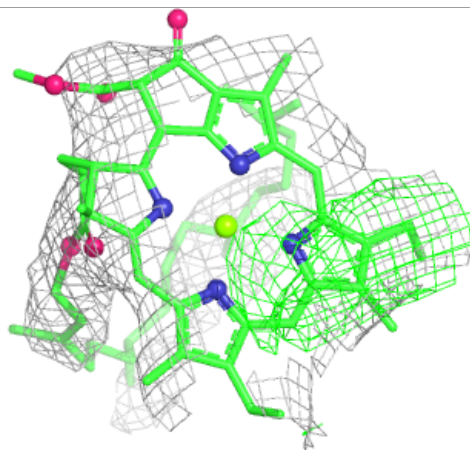
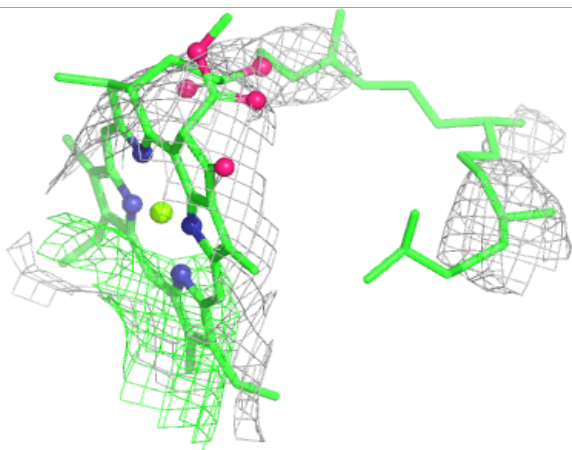
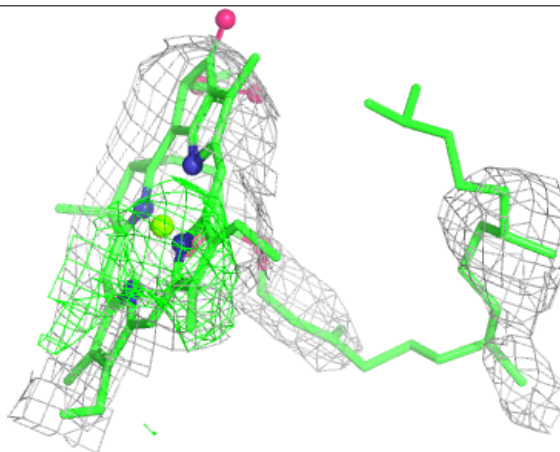


Electron density around BCR h 6049:

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

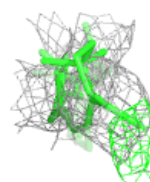
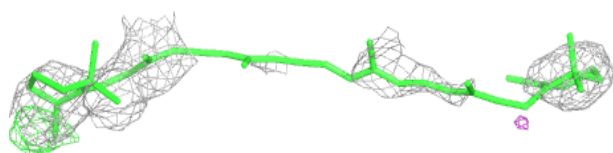
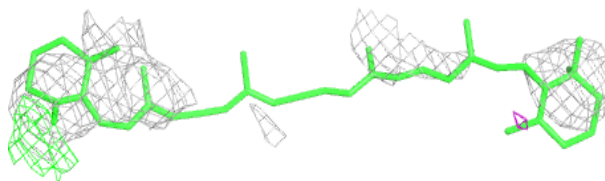
**Electron density around CLA C 1037:**

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

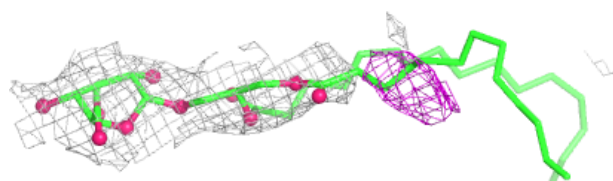
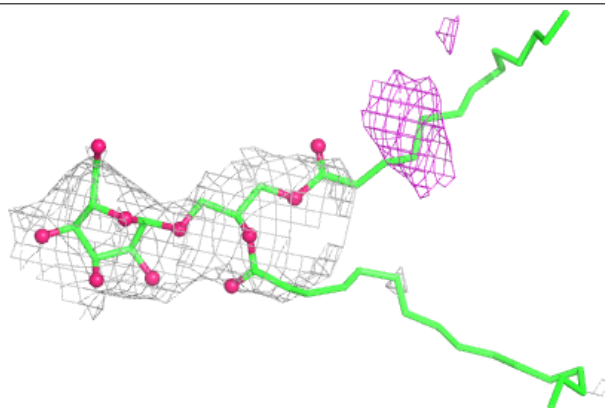


Electron density around BCR b 6045:

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

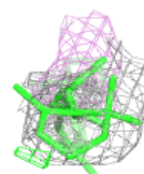
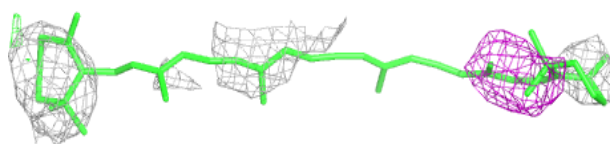
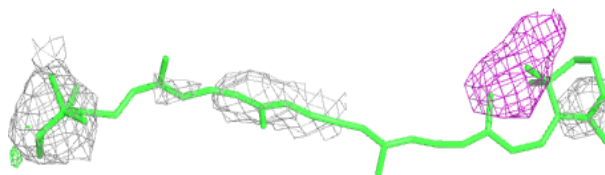
**Electron density around MGE d 6059:**

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

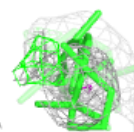
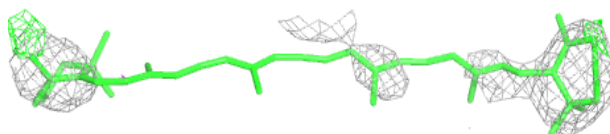
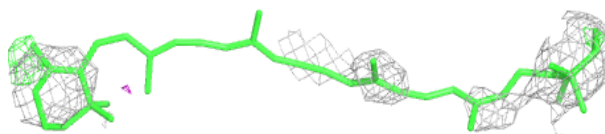


Electron density around BCR a 6044:

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

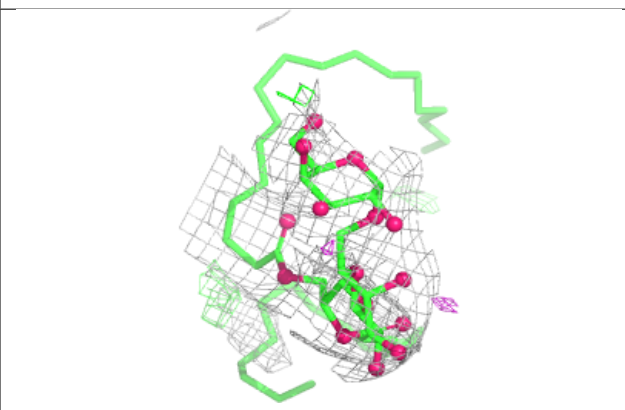
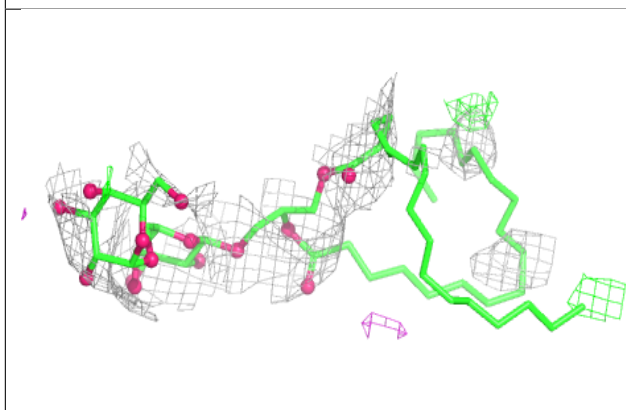
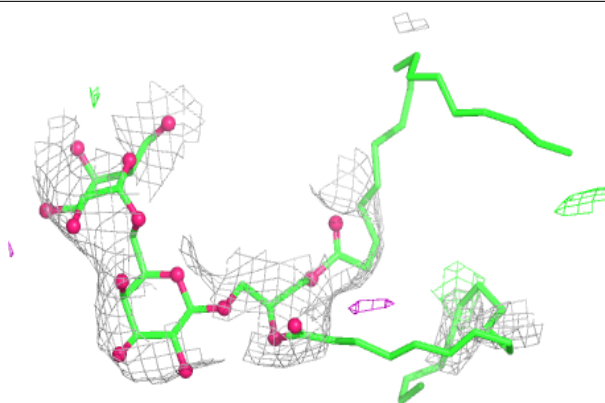
**Electron density around BCR A 1044:**

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

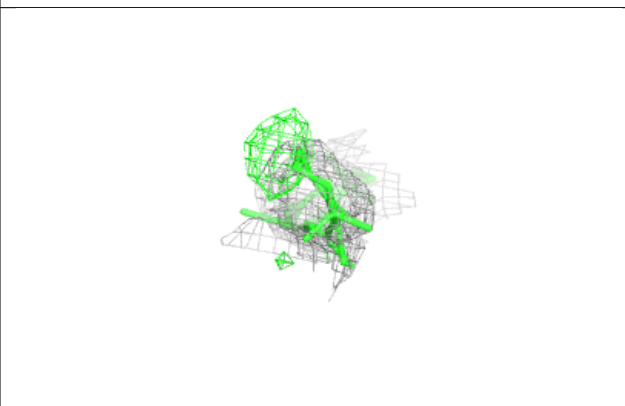
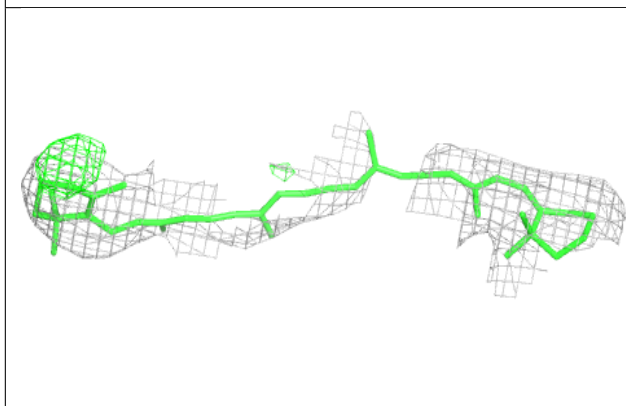


Electron density around DGD C 1056:

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

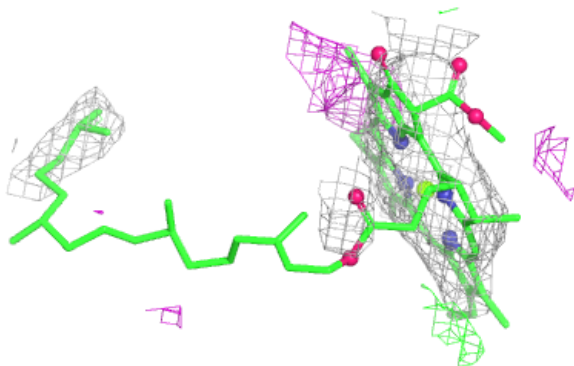
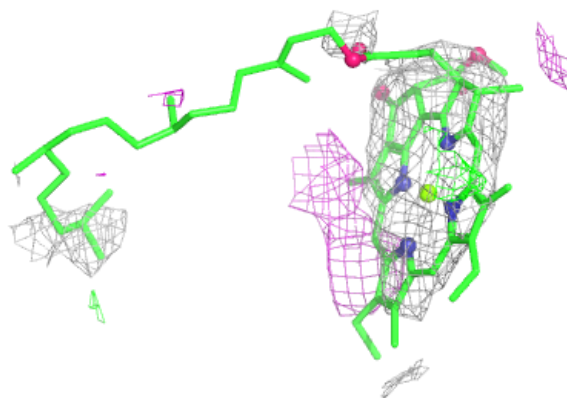
**Electron density around BCR D 1050:**

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

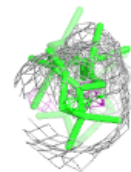
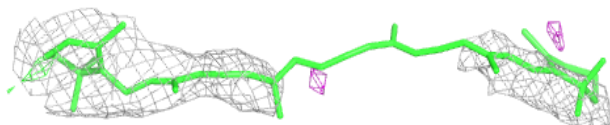
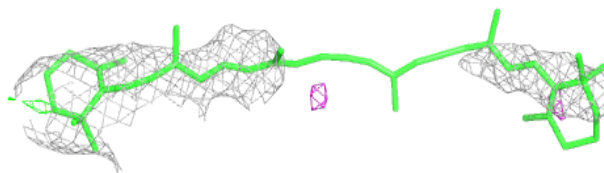


Electron density around CLA C 1032:

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

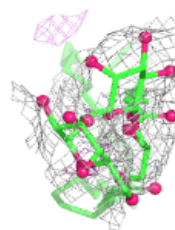
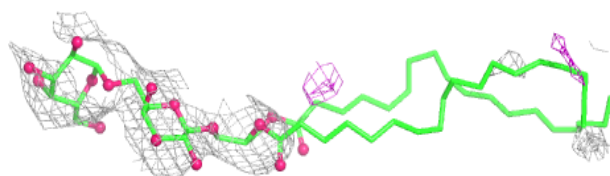
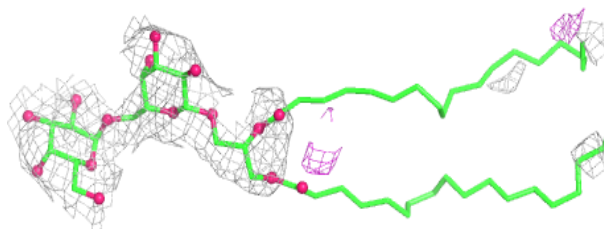
**Electron density around BCR b 6048:**

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



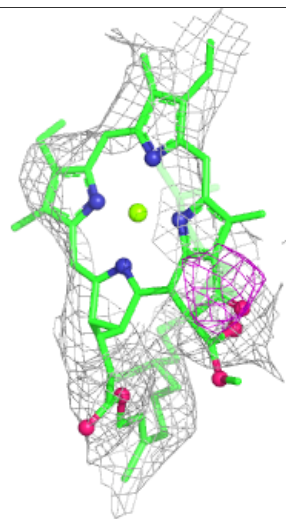
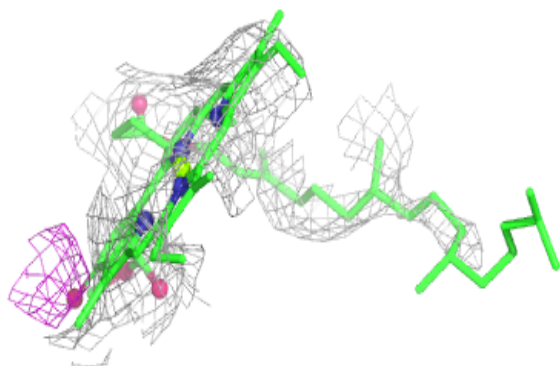
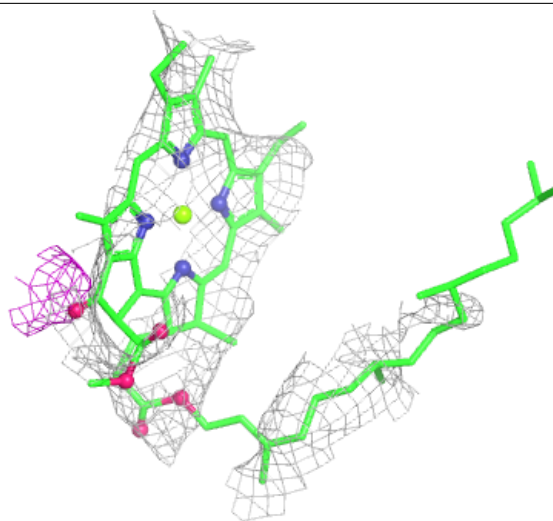
Electron density around DGD c 6057:

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



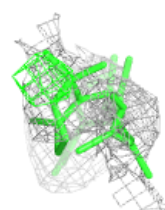
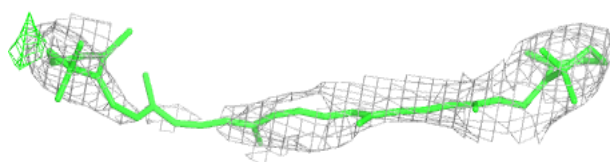
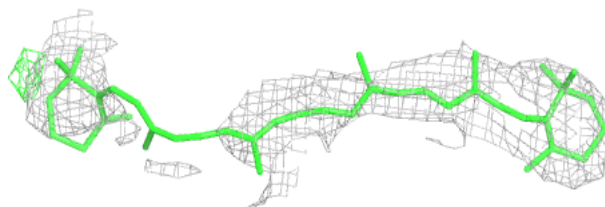
Electron density around CLA B 1024:

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

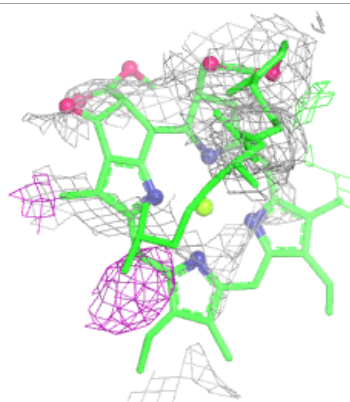
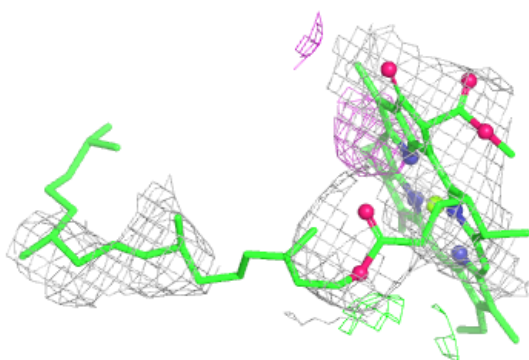
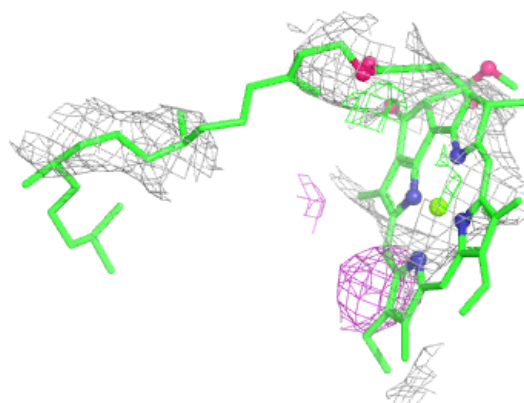


Electron density around BCR t 1046:

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

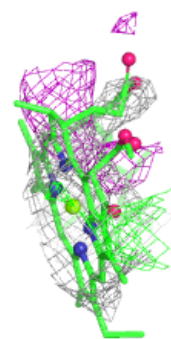
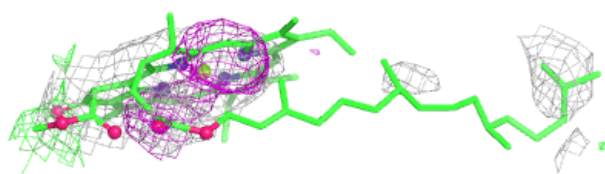
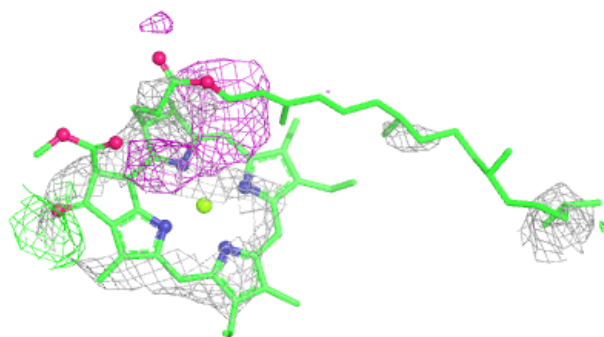
**Electron density around CLA c 6032:**

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

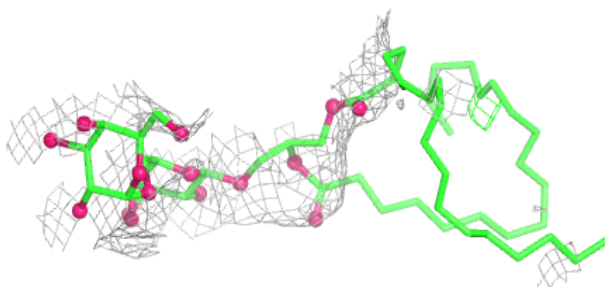
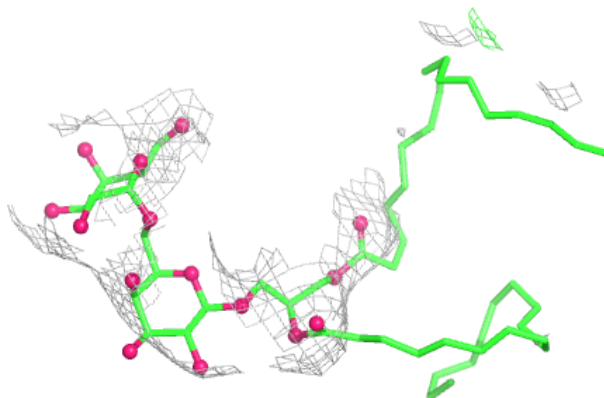


Electron density around CLA C 1025:

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

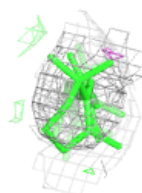
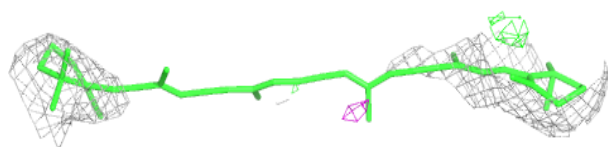
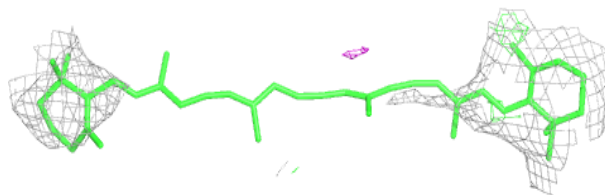
**Electron density around DGD c 6056:**

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



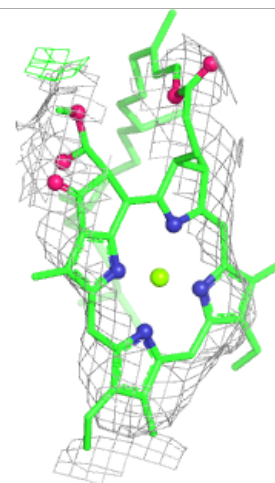
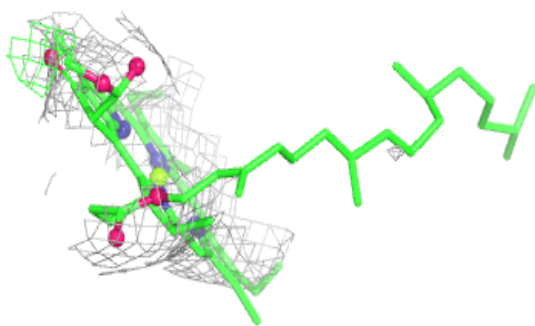
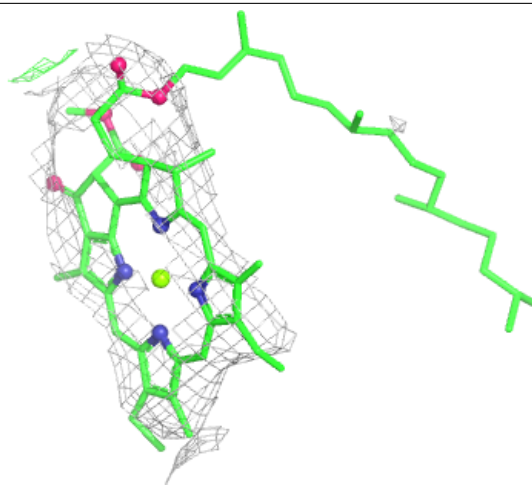
Electron density around BCR Z 1053:

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



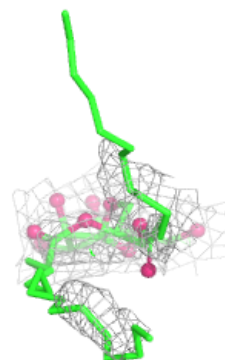
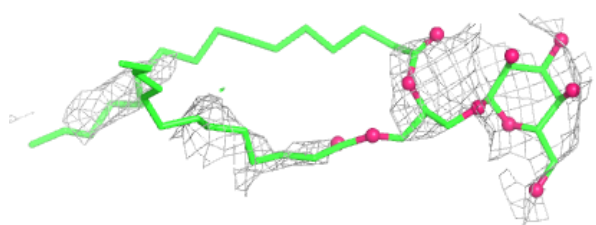
Electron density around CLA b 6024:

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

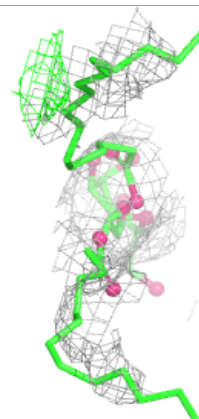
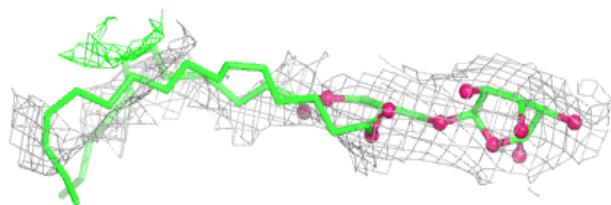
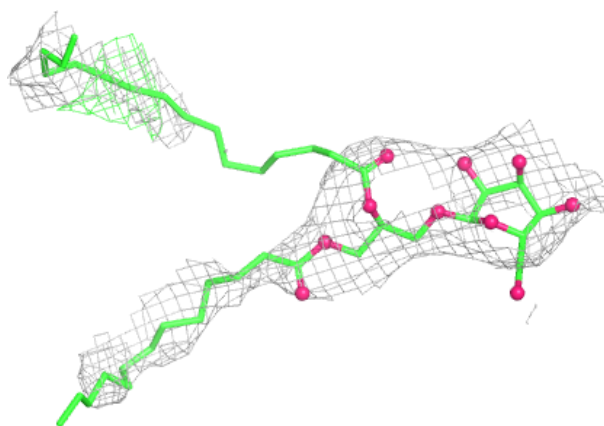


Electron density around MGE d 6062:

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

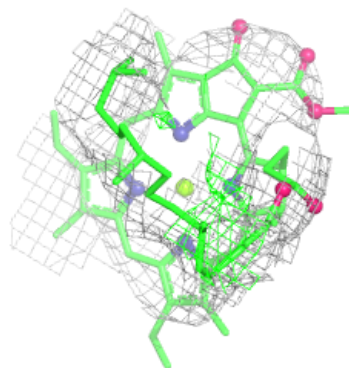
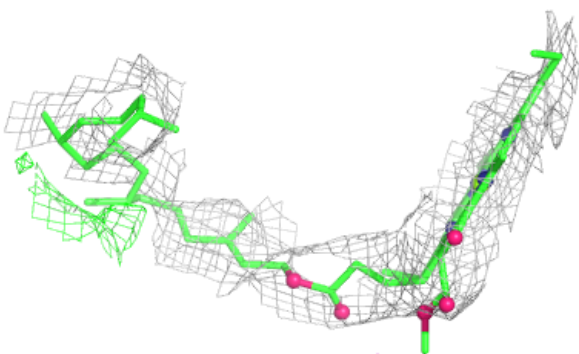
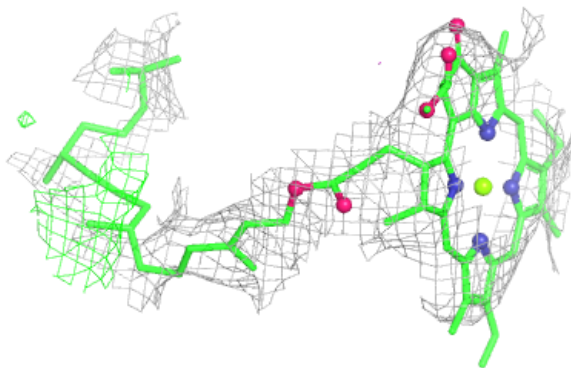
**Electron density around MGE J 1059:**

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

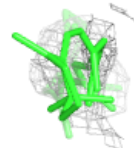
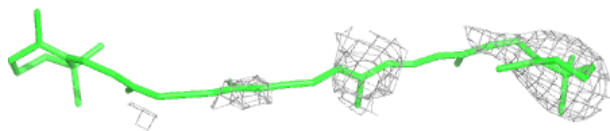
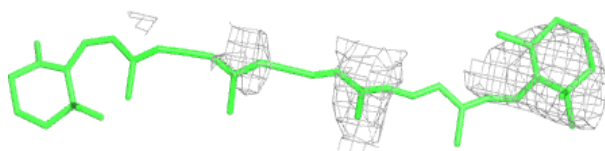


Electron density around CLA b 6014:

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

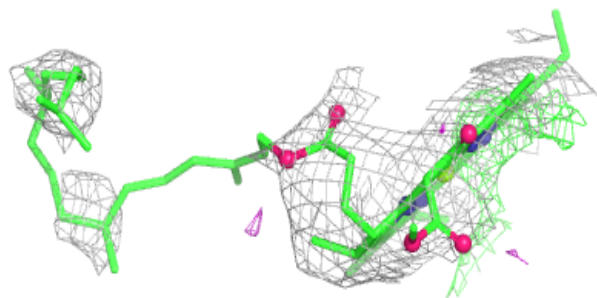
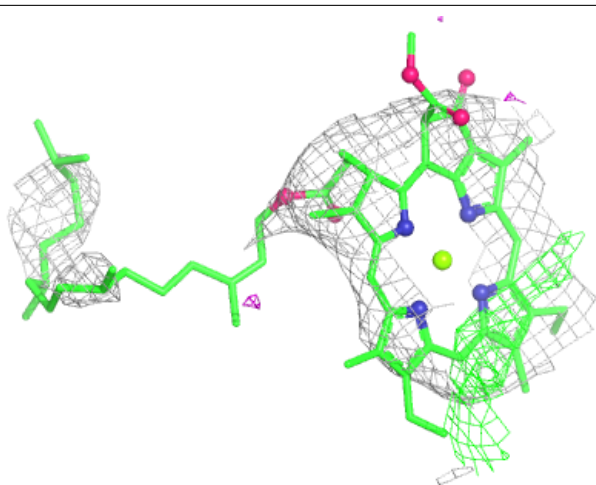
**Electron density around BCR B 1045:**

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



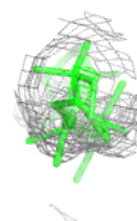
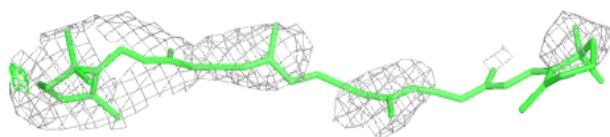
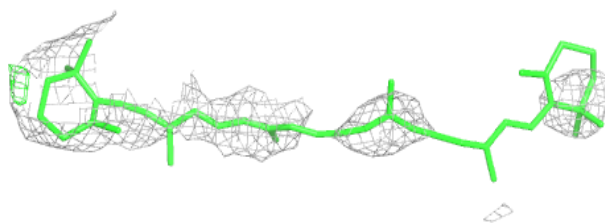
Electron density around CLA C 1027:

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



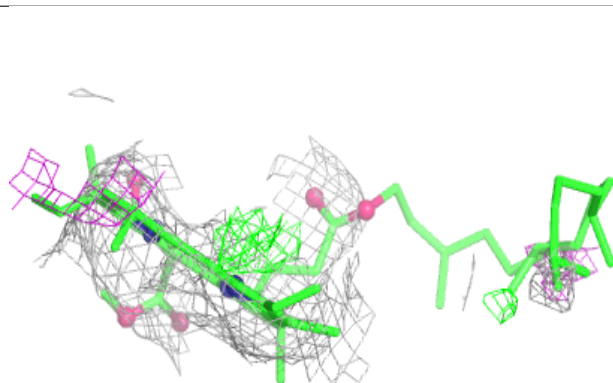
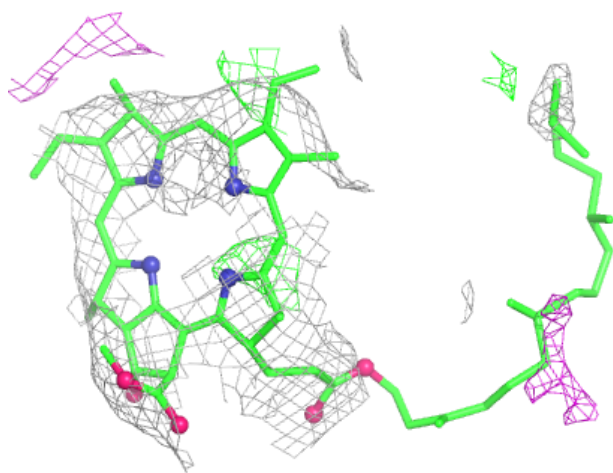
Electron density around BCR B 1048:

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



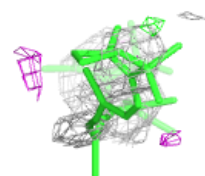
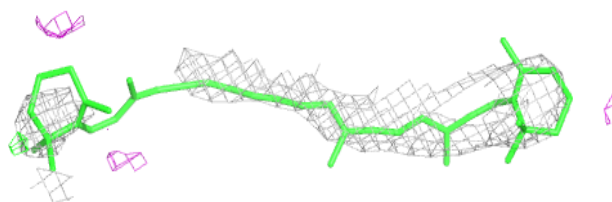
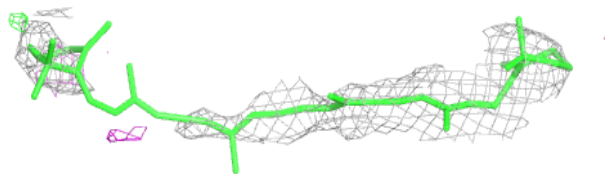
Electron density around PHO d 6038:

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



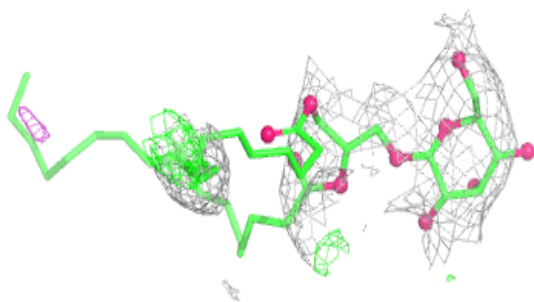
Electron density around BCR T 6046:

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



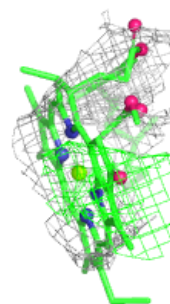
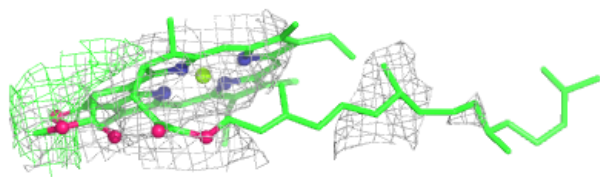
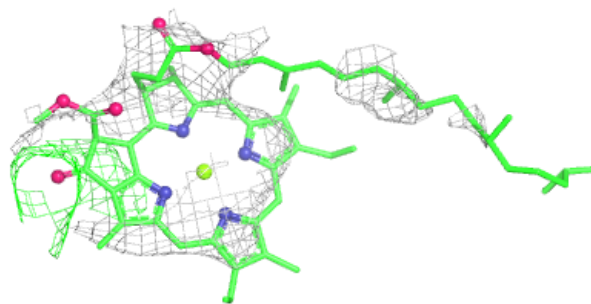
Electron density around MGE d 6061:

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

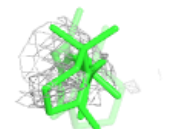
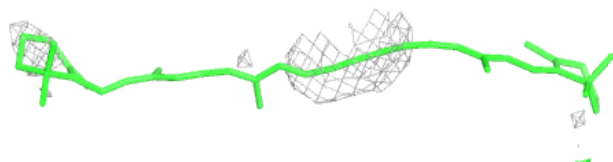
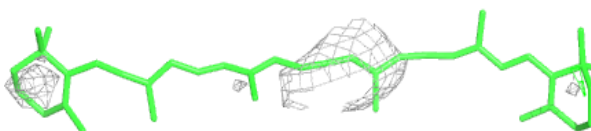


Electron density around CLA c 6025:

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

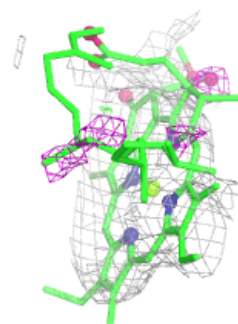
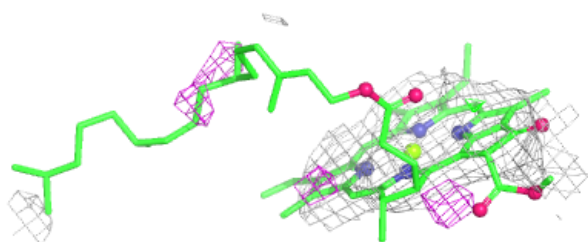
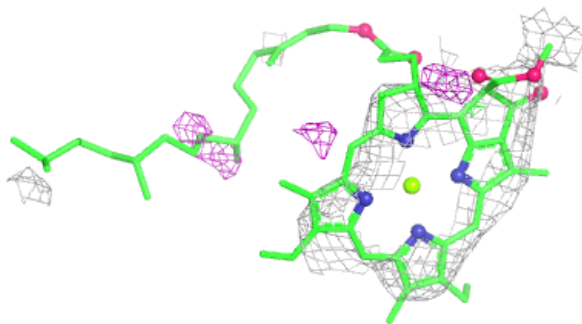
**Electron density around BCR c 6054:**

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

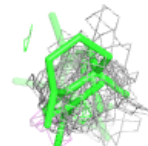
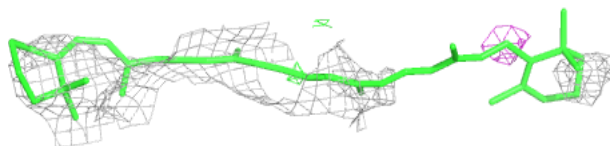
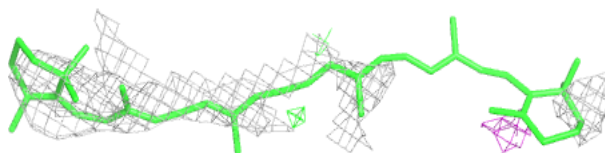


Electron density around CLA d 6008:

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

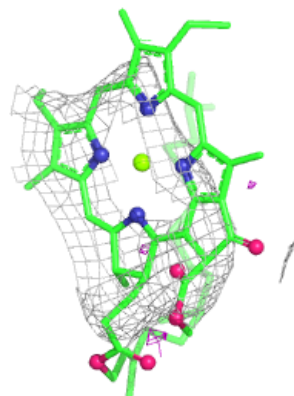
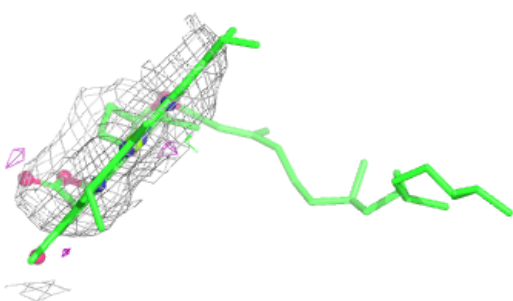
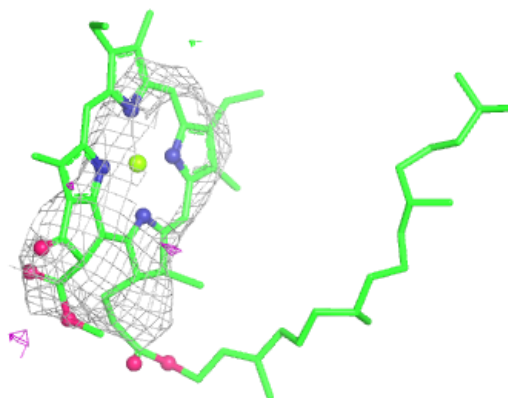
**Electron density around BCR K 1051:**

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



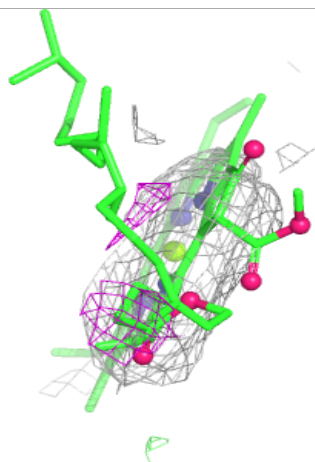
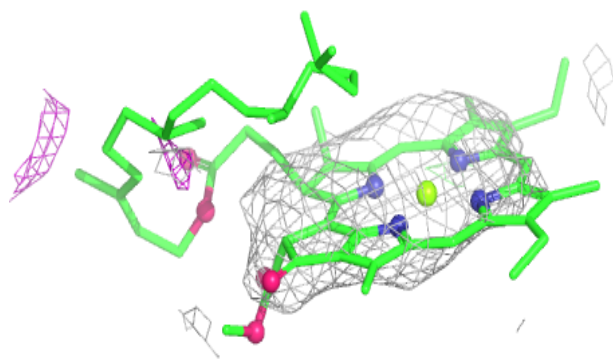
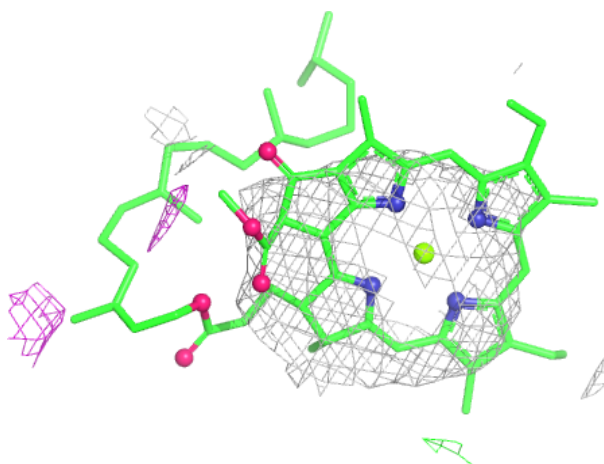
Electron density around CLA c 6031:

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



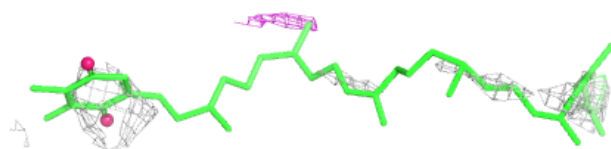
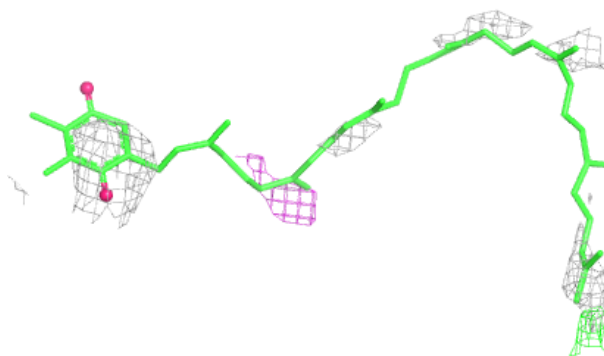
Electron density around CLA c 6033:

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

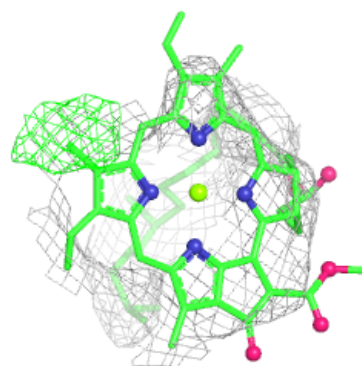
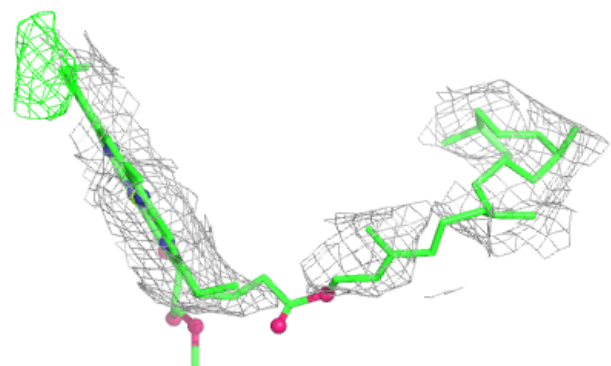
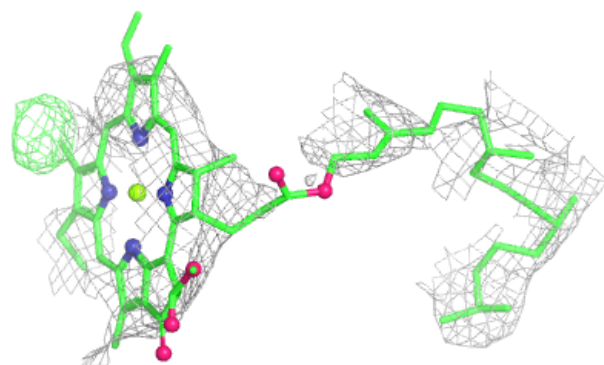


Electron density around PQ9 d 6042:

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

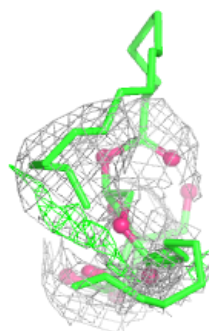
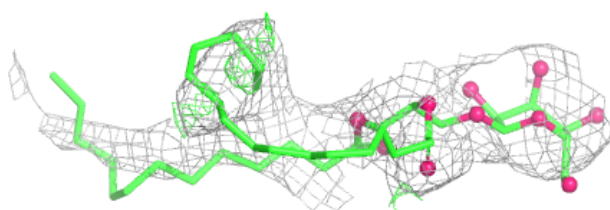
**Electron density around CLA B 1014:**

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

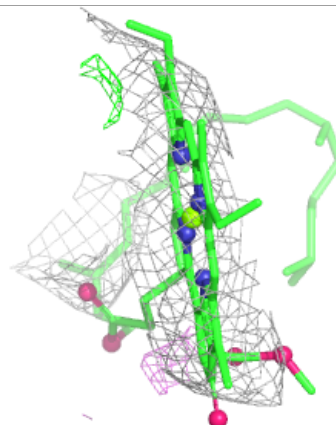
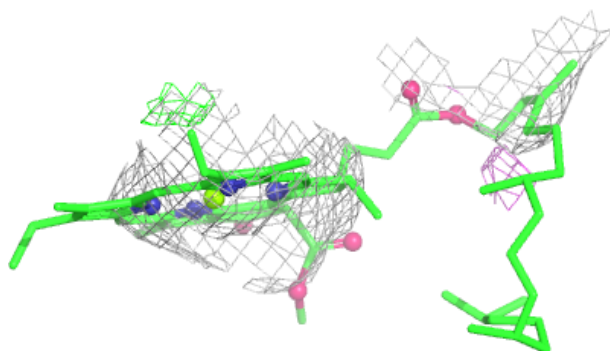
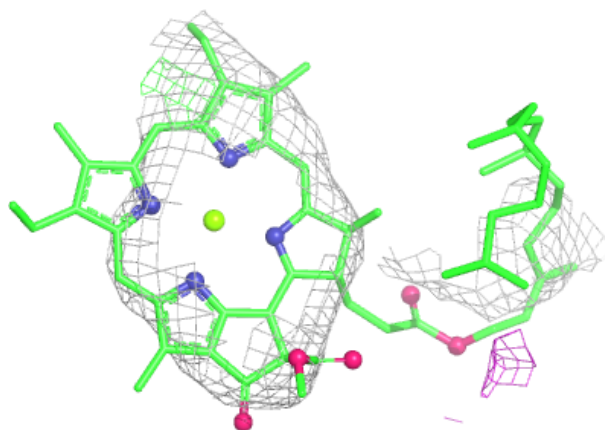


Electron density around MGE B 1060:

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

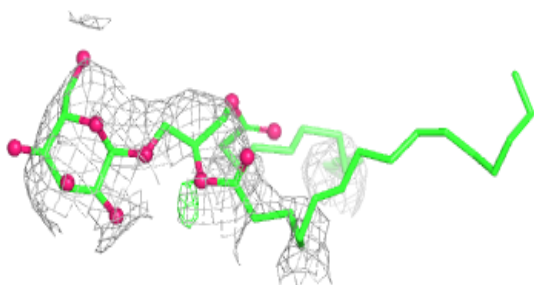
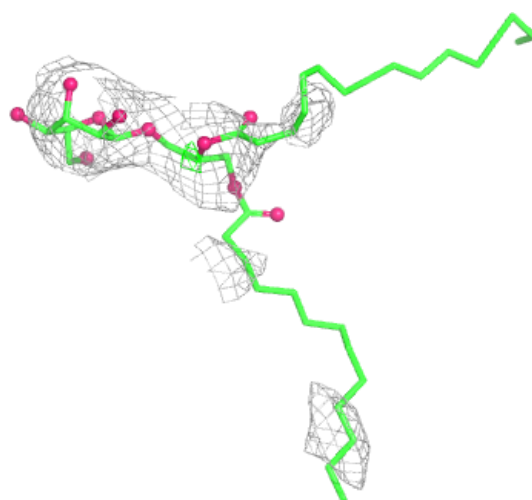
**Electron density around CLA c 6036:**

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



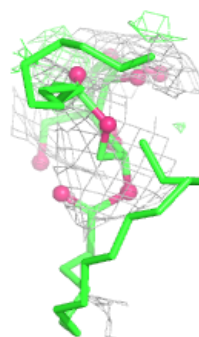
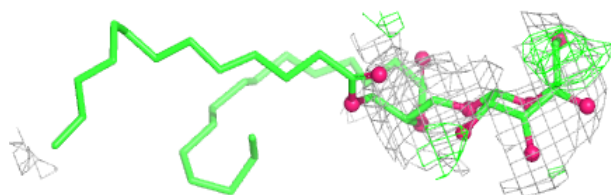
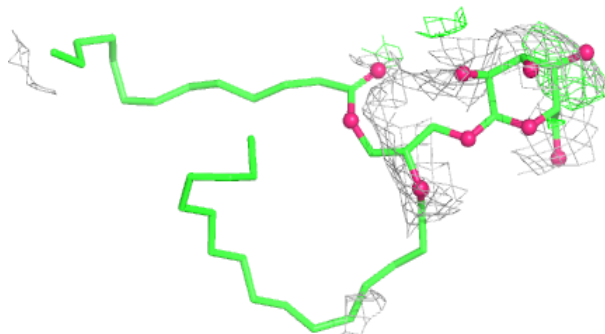
Electron density around MGE L 1061:

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



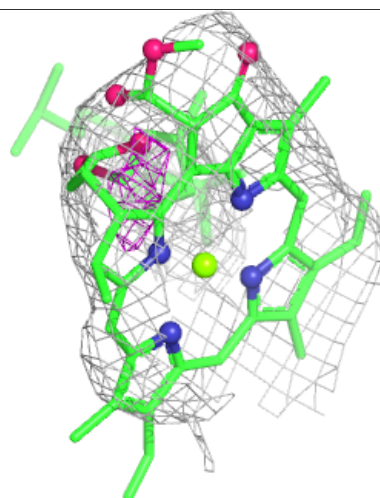
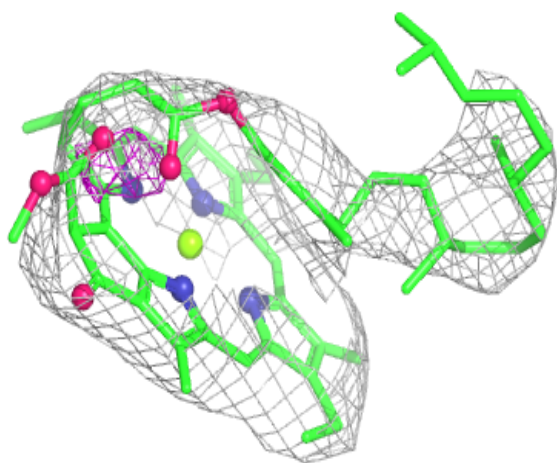
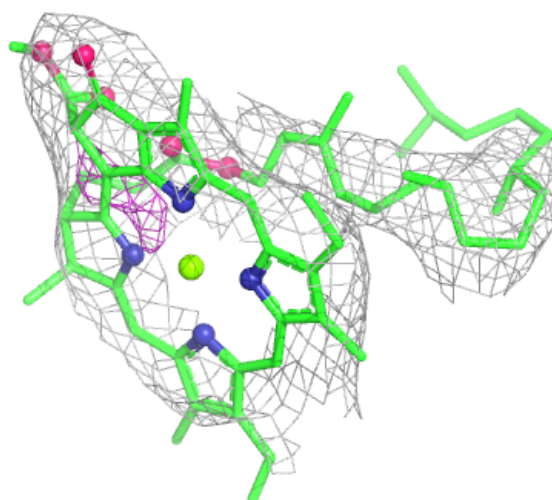
Electron density around MGE b 6060:

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



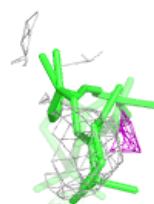
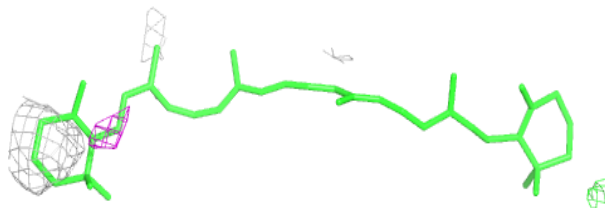
Electron density around CLA B 1022:

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

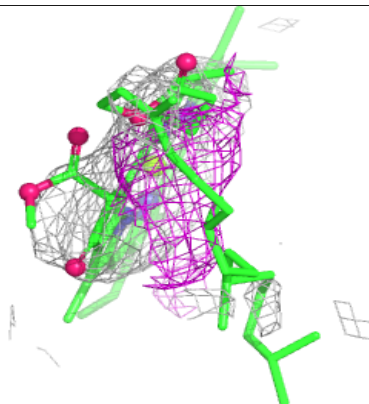
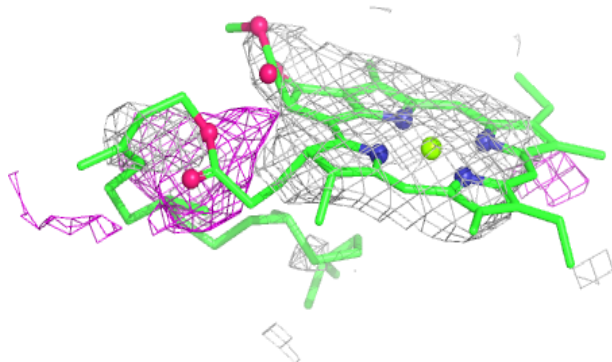
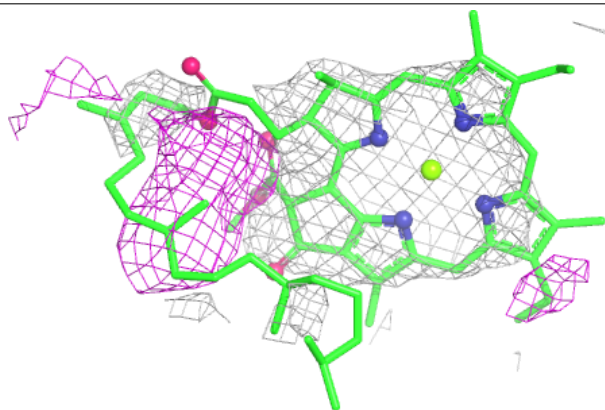


Electron density around BCR k 6052:

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

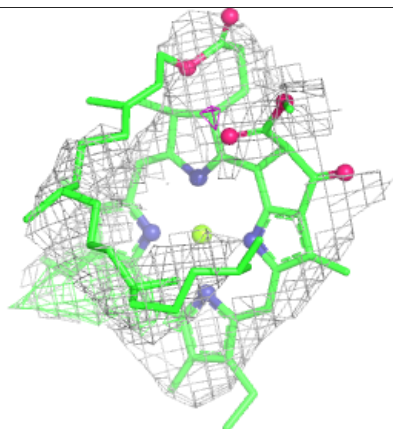
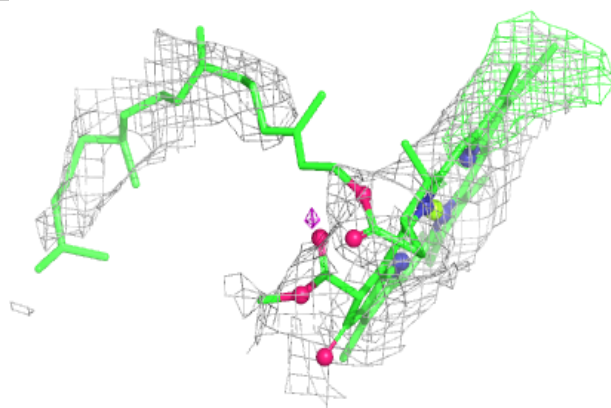
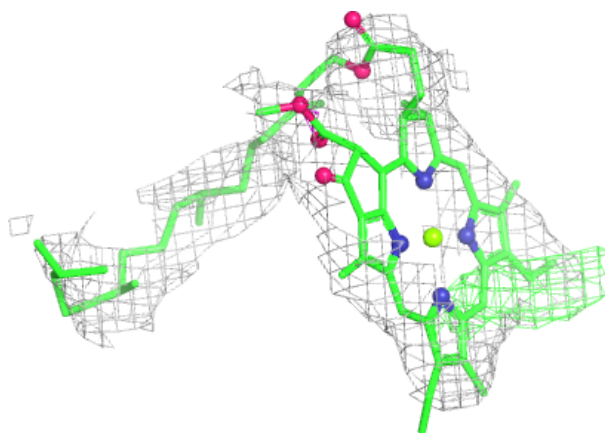
**Electron density around CLA C 1033:**

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

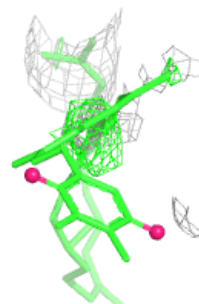
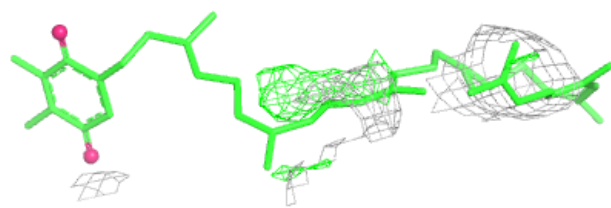
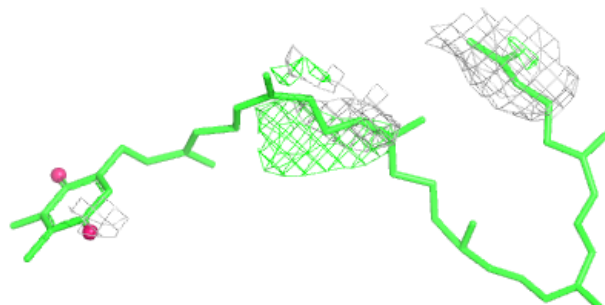


Electron density around CLA b 6021:

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

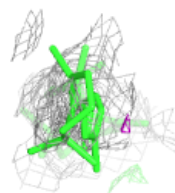
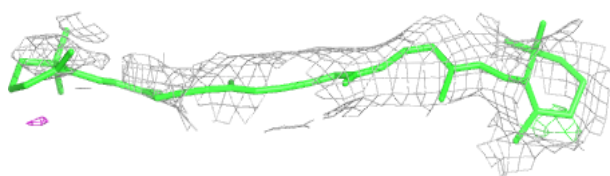
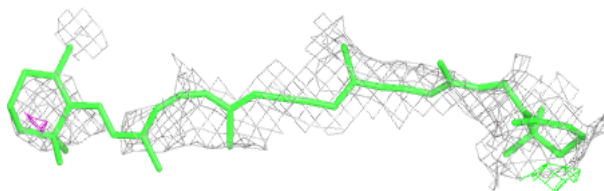
**Electron density around PQ9 A 1043:**

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

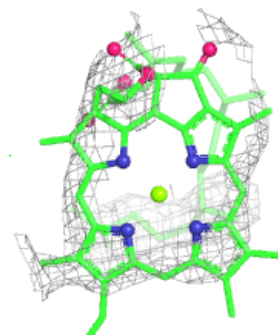
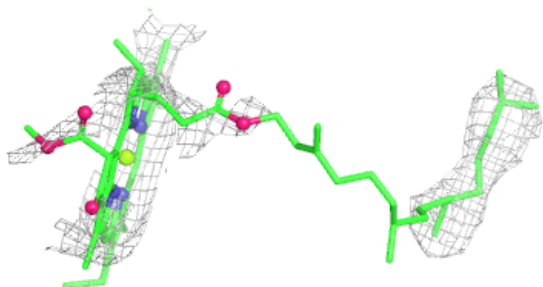
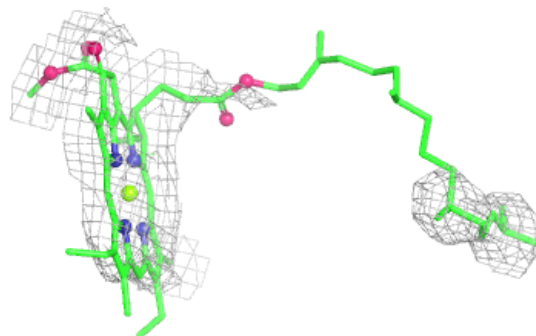


Electron density around BCR H 1049:

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

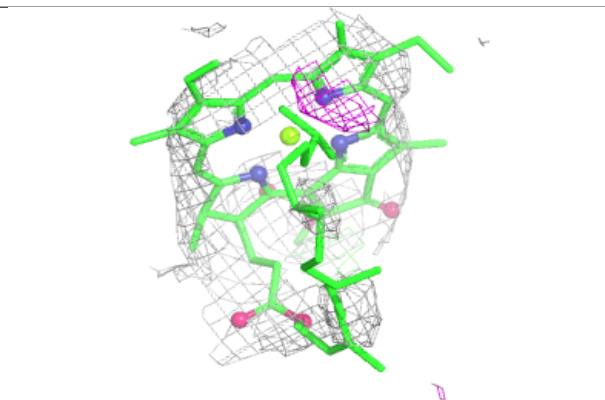
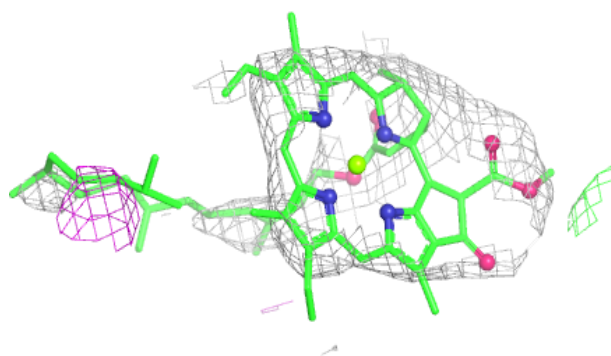
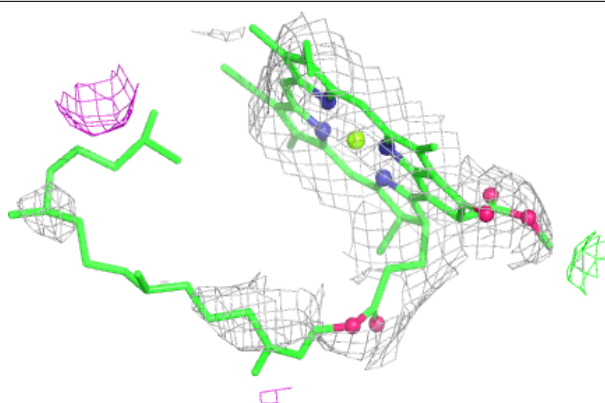
**Electron density around CLA c 6030:**

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

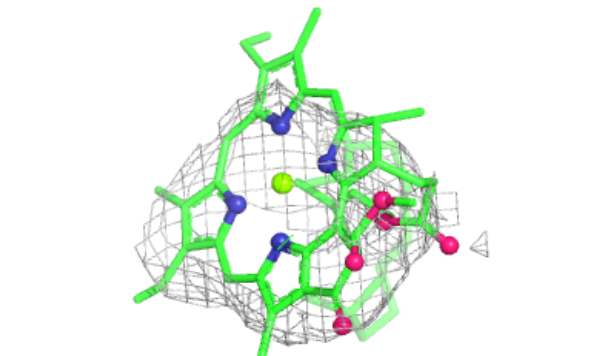
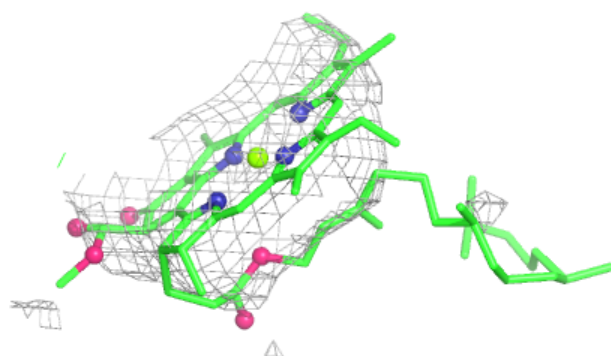
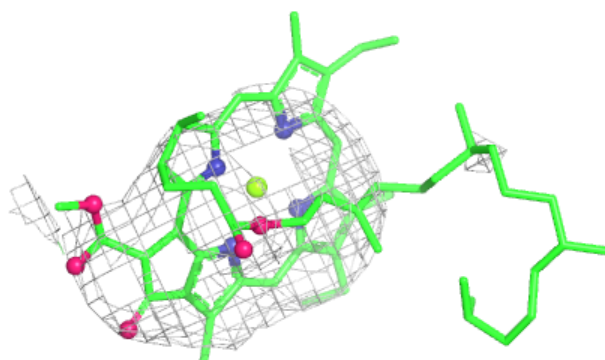


Electron density around CLA C 1028:

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

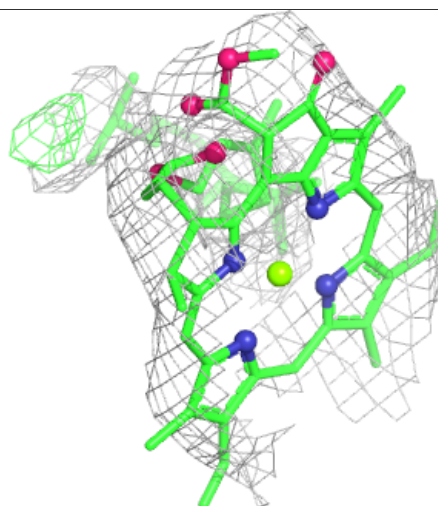
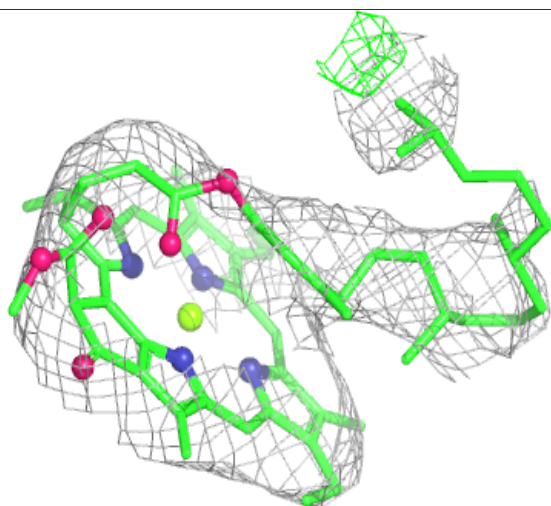
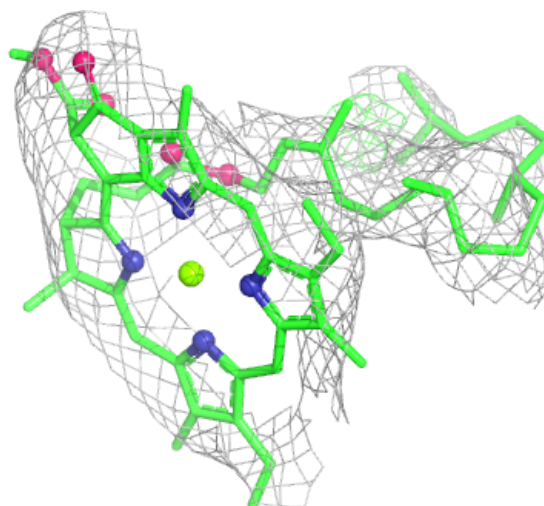
**Electron density around CLA c 6029:**

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



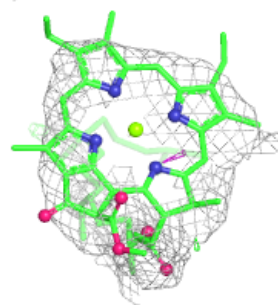
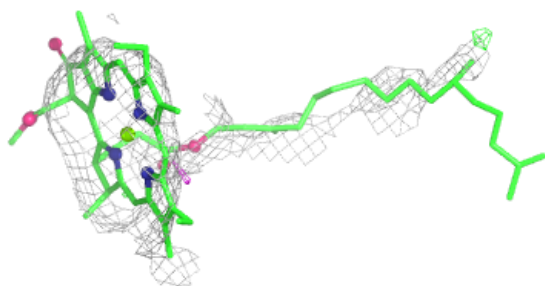
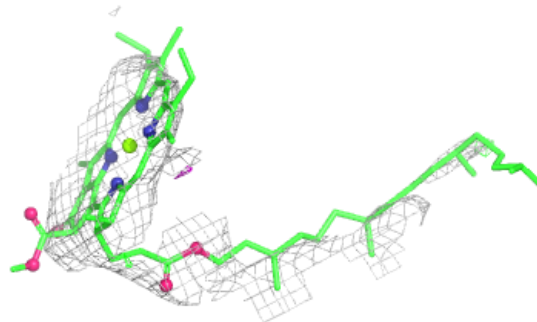
Electron density around CLA b 6022:

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

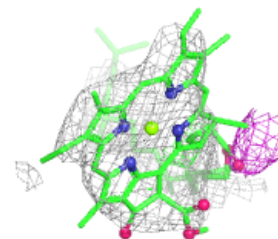
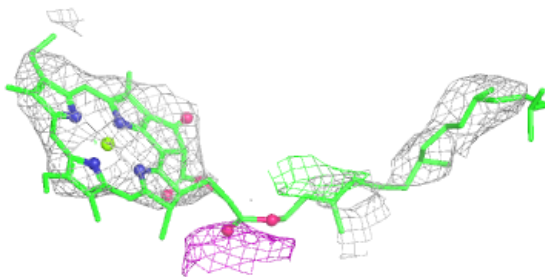
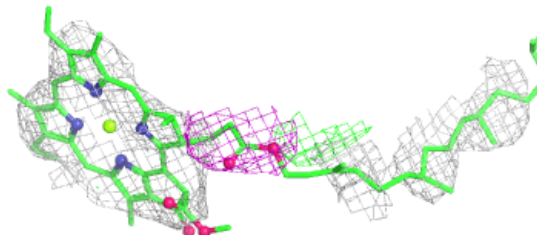


Electron density around CLA b 6013:

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

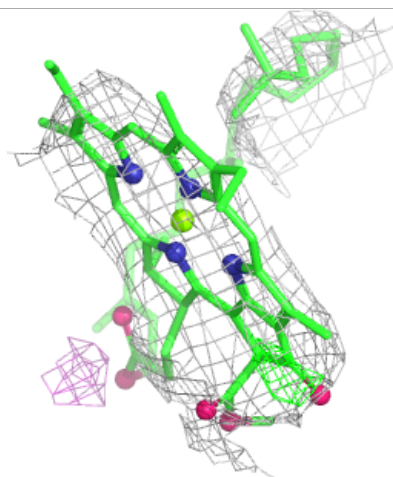
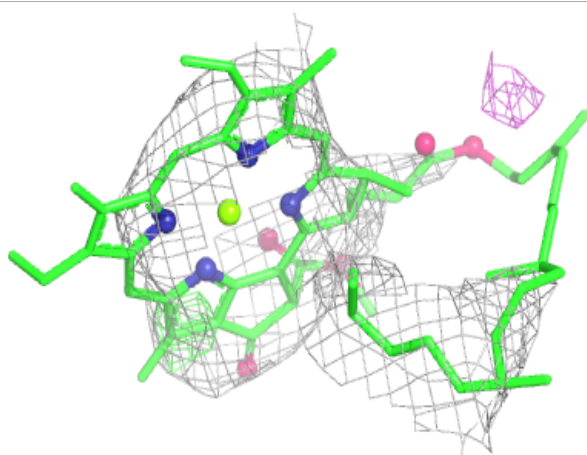
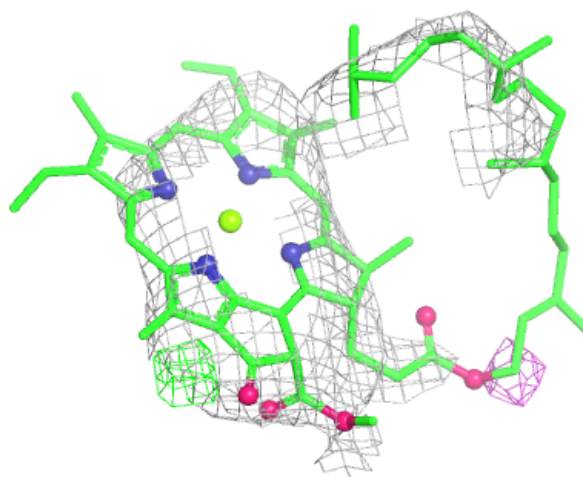
**Electron density around CLA a 6003:**

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



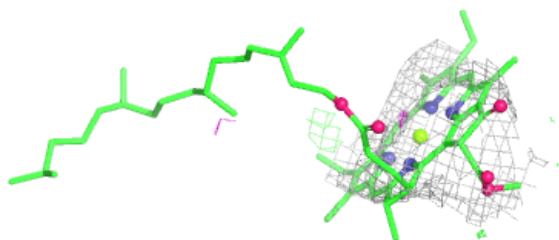
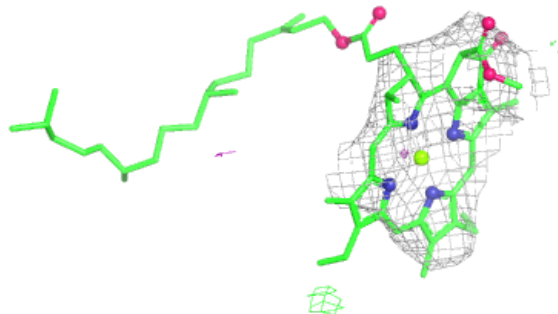
Electron density around CLA b 6023:

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



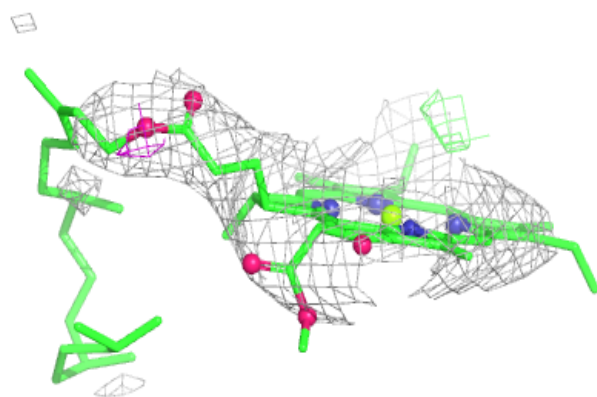
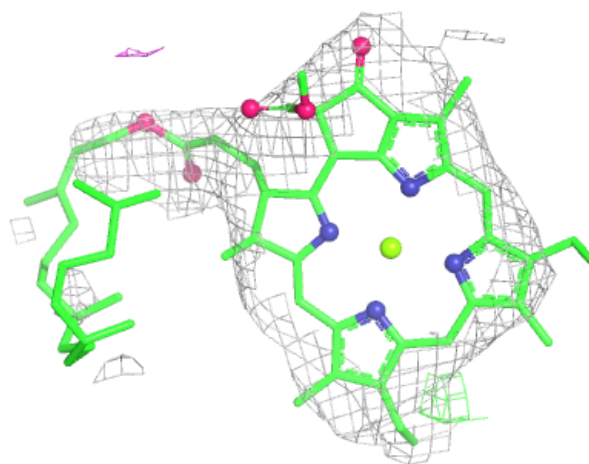
Electron density around CLA c 6035:

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



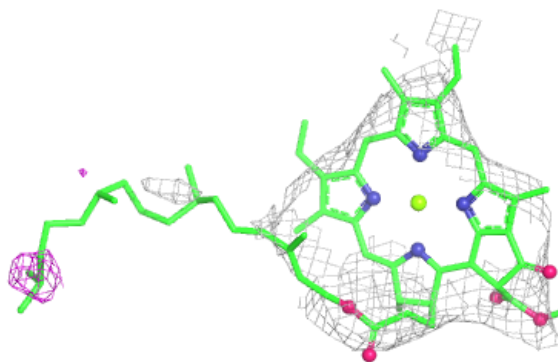
Electron density around CLA C 1036:

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

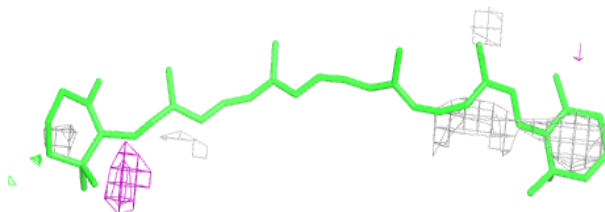


Electron density around CLA b 6011:

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

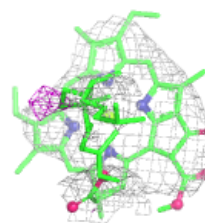
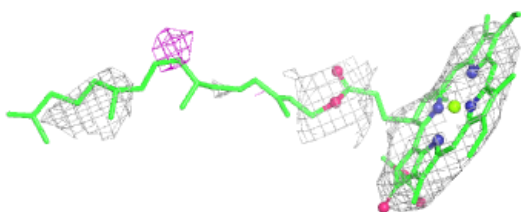
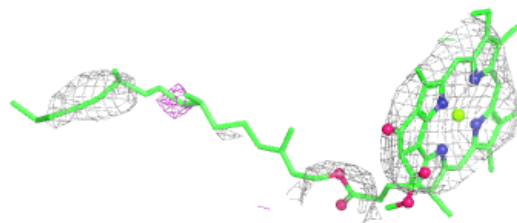
**Electron density around BCR K 1052:**

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

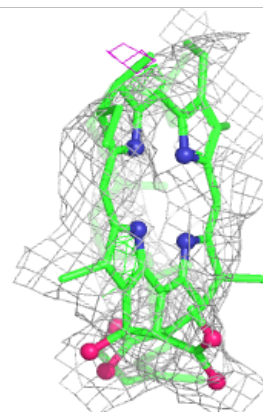
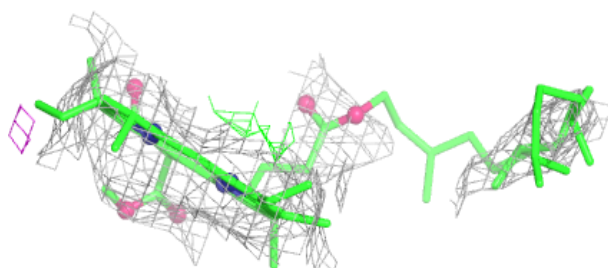
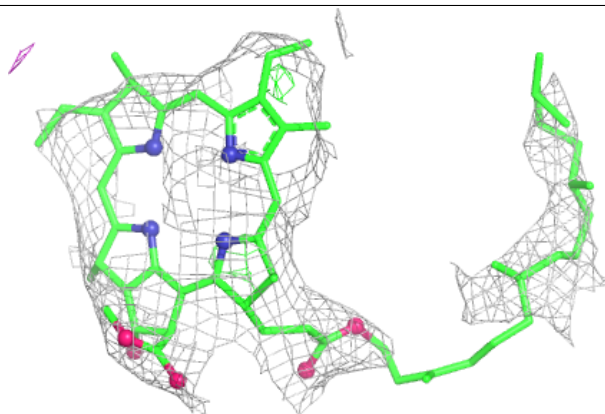


Electron density around CLA b 6012:

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

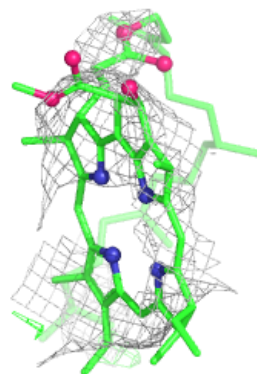
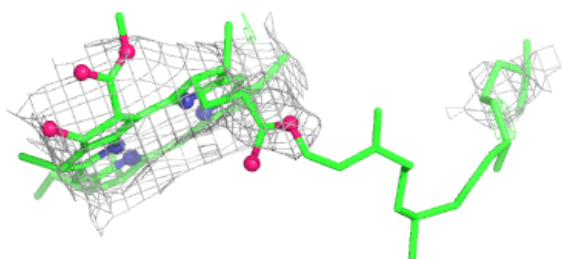
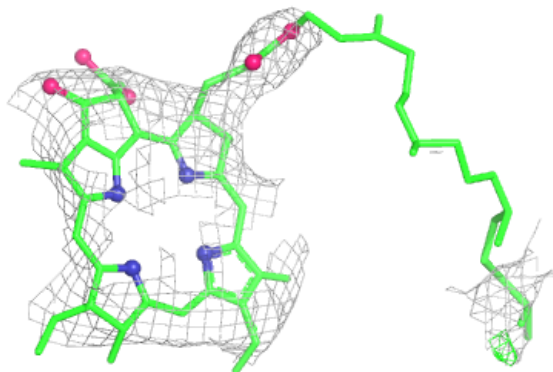
**Electron density around PHO A 1038:**

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

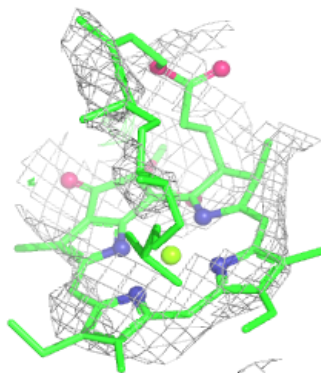
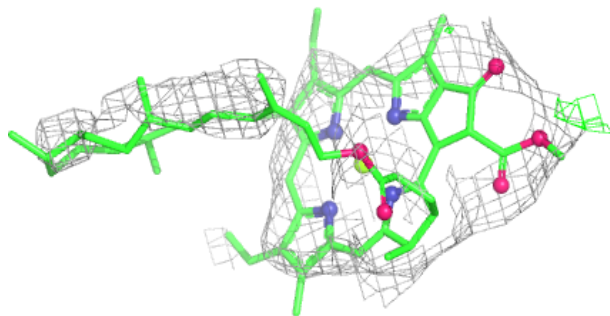
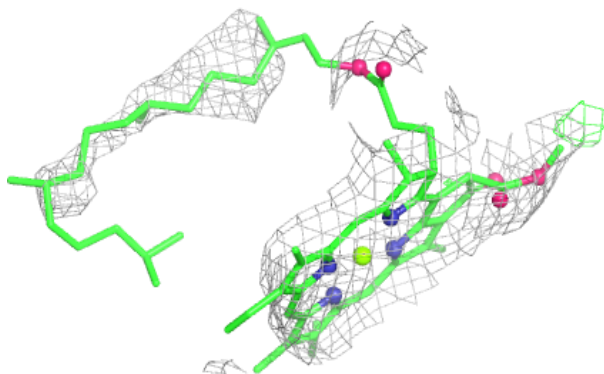


Electron density around PHO a 6039:

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

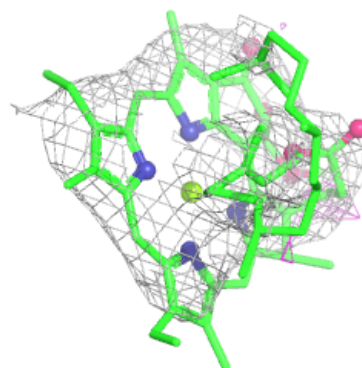
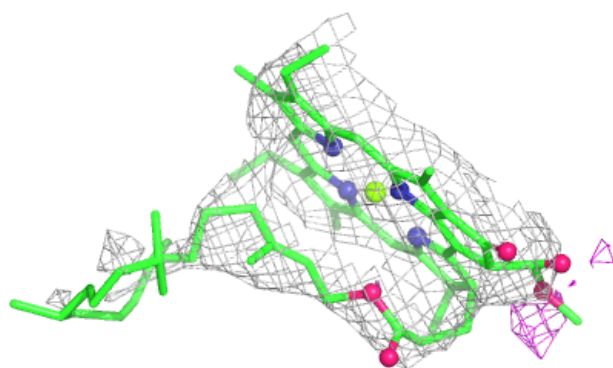
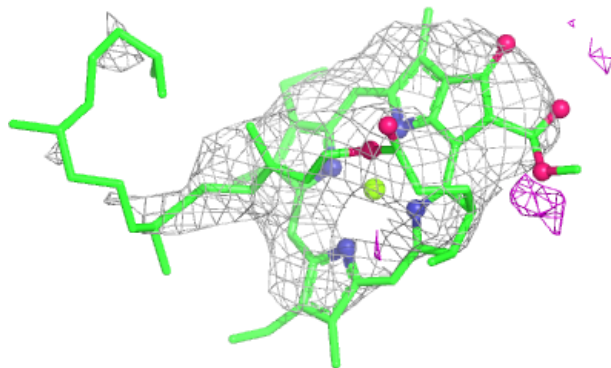
**Electron density around CLA c 6028:**

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

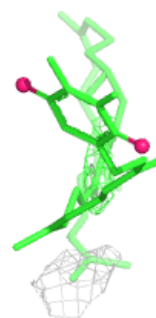
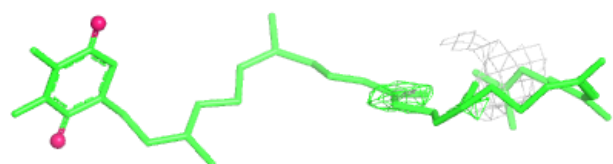
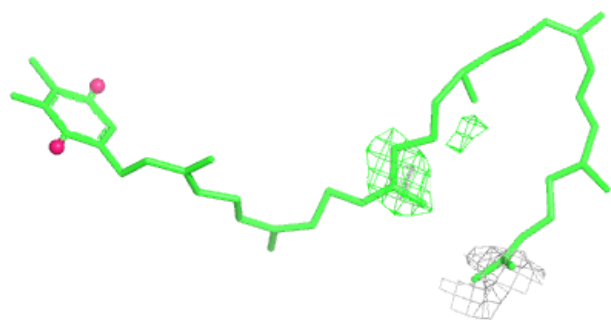


Electron density around CLA C 1029:

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

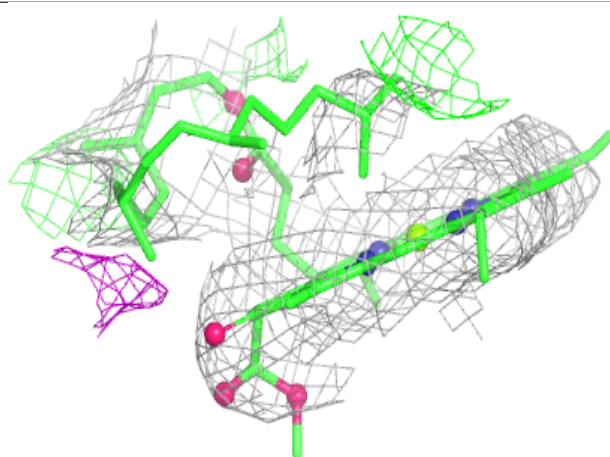
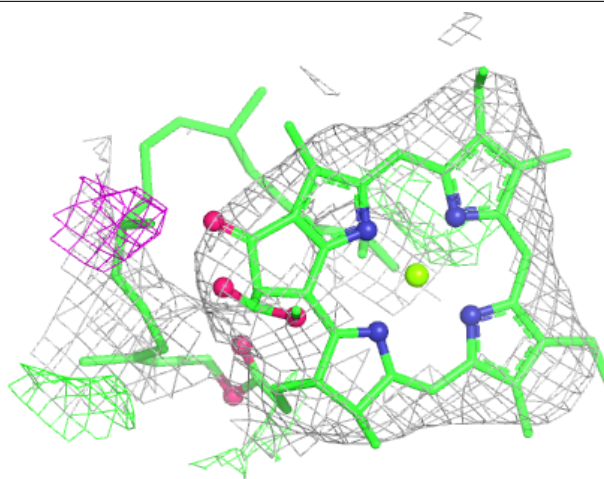
**Electron density around PQ9 a 6043:**

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



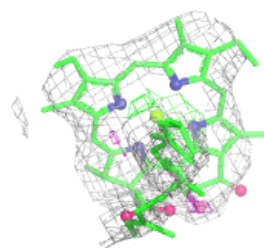
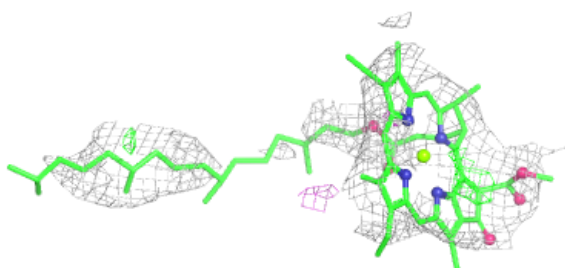
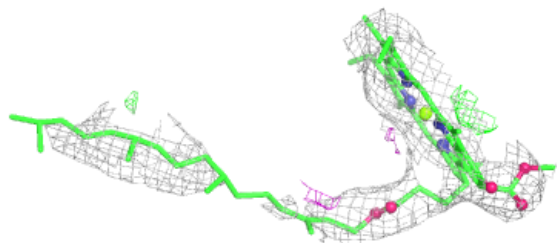
Electron density around CLA C 1026:

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

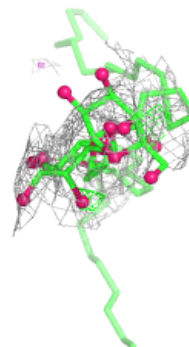
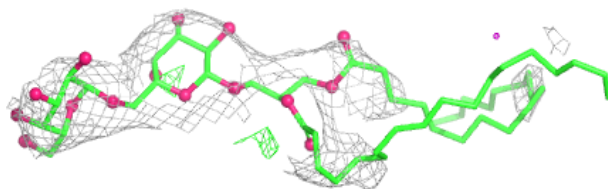


Electron density around CLA b 6015:

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

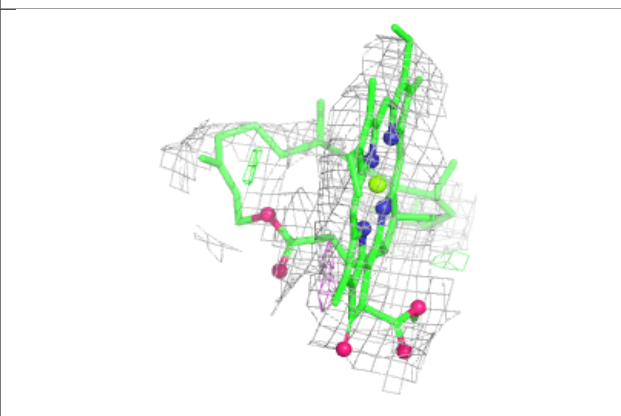
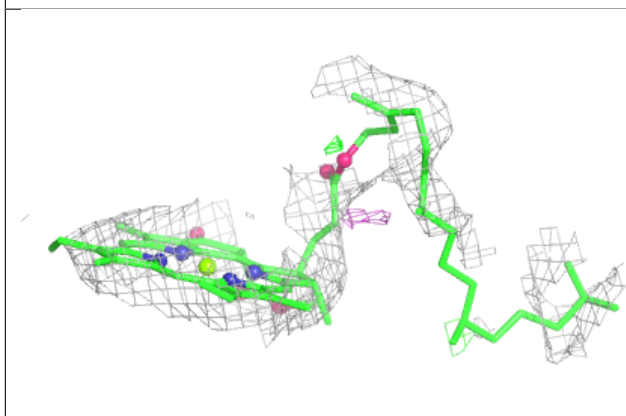
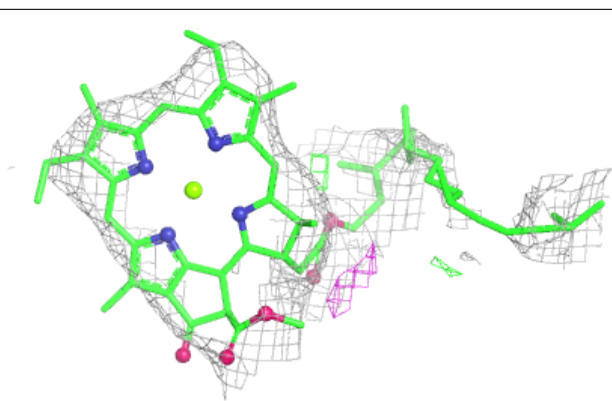
**Electron density around DGD c 6055:**

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

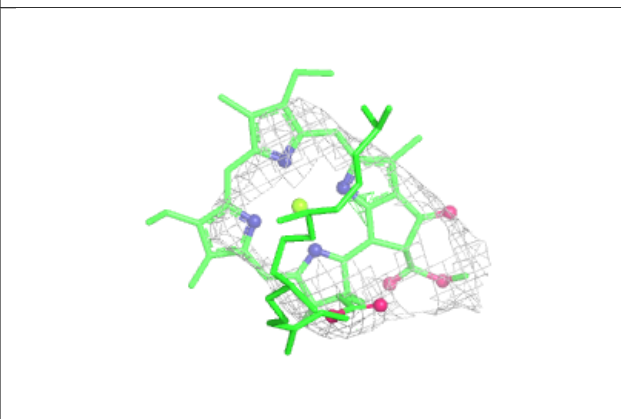
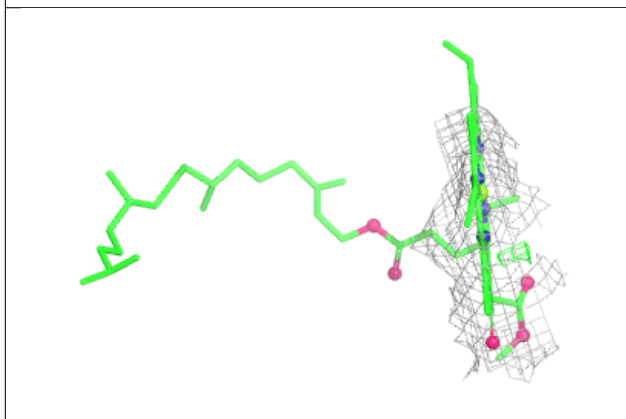
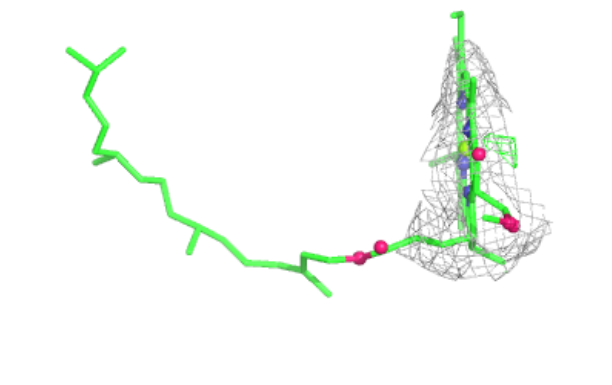


Electron density around CLA a 6006:

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

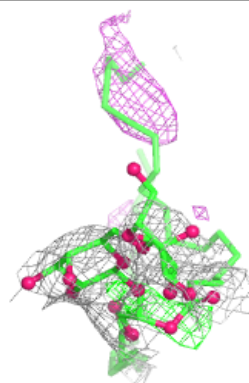
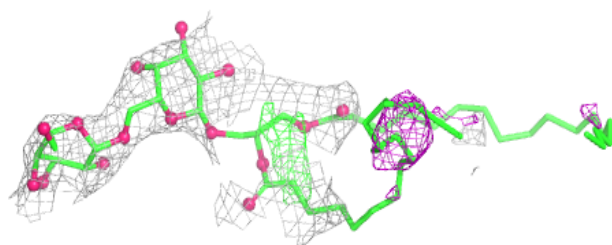
**Electron density around CLA a 6007:**

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



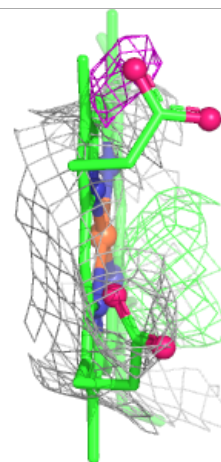
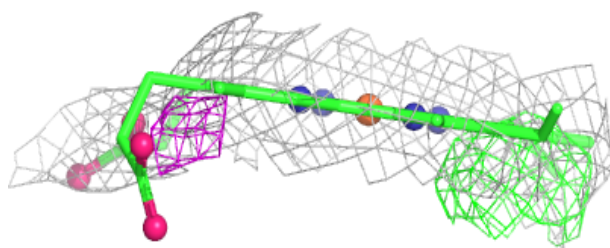
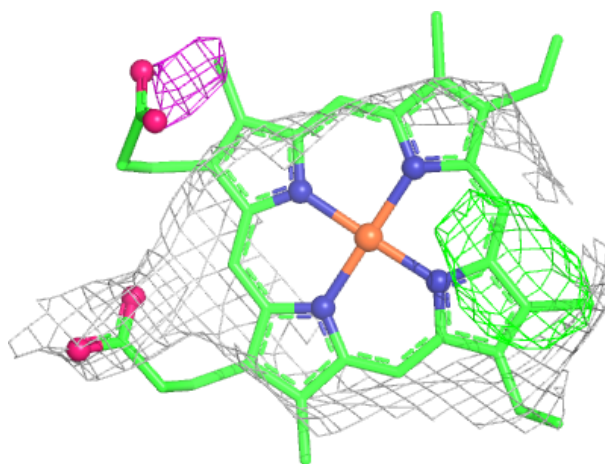
Electron density around DGD h 6058:

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



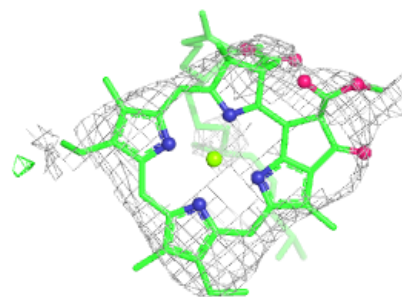
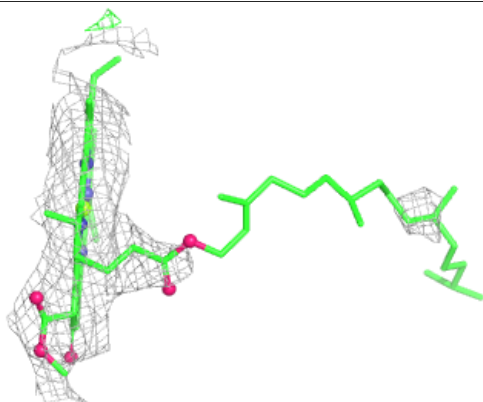
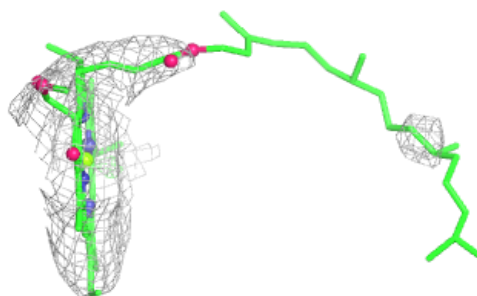
Electron density around HEM e 6040:

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

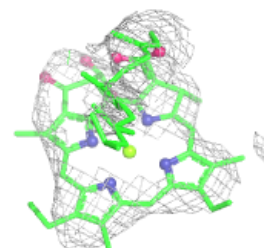
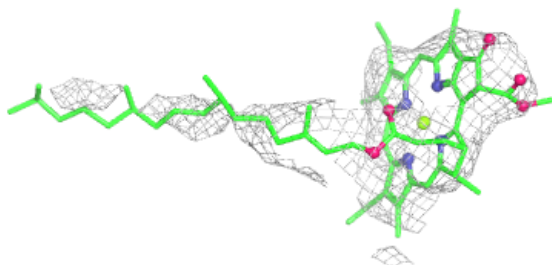
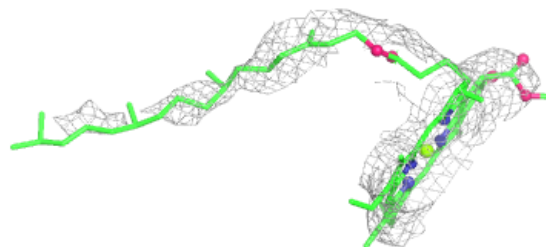


Electron density around CLA A 1007:

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

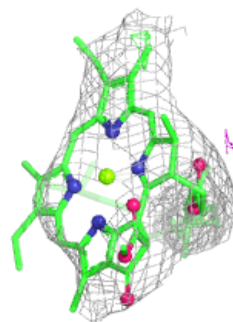
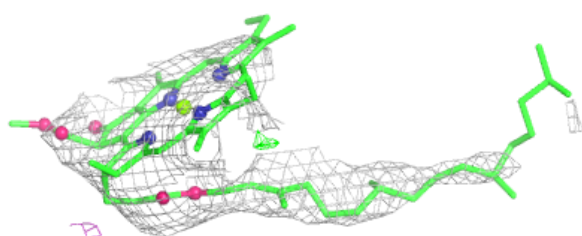
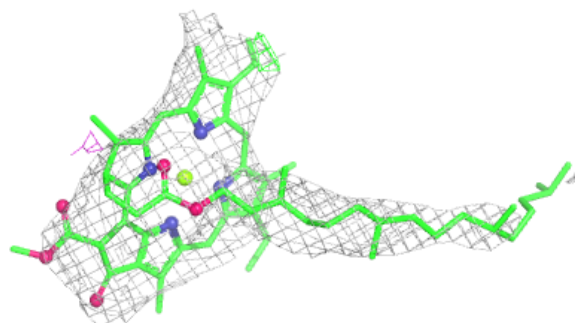
**Electron density around CLA B 1015:**

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

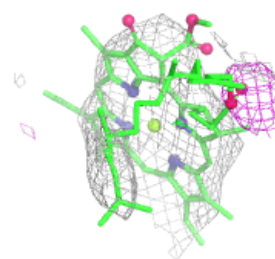
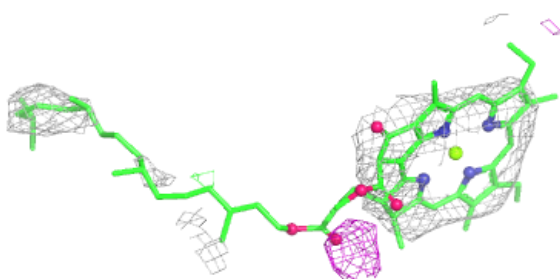
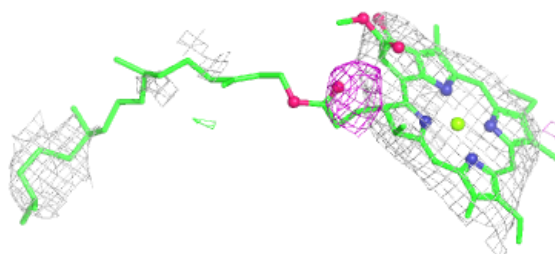


Electron density around CLA B 1016:

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

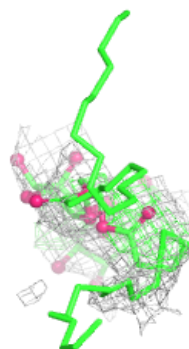
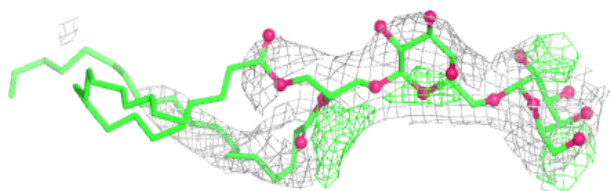
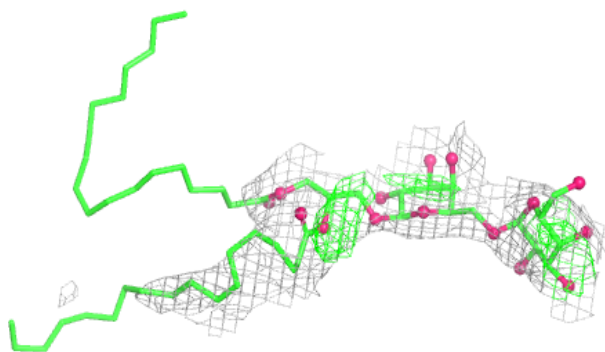
**Electron density around CLA A 1003:**

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

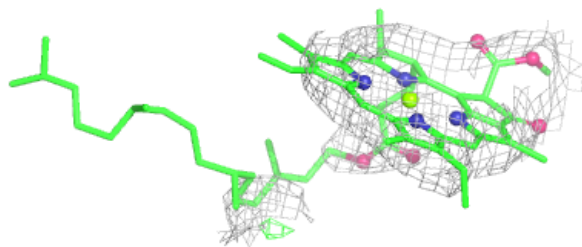
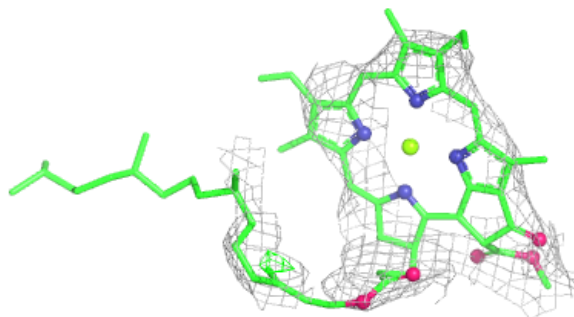


Electron density around DGD C 1055:

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

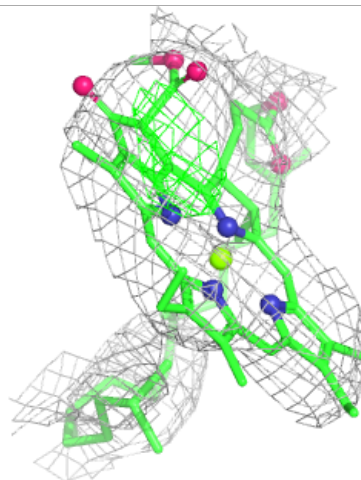
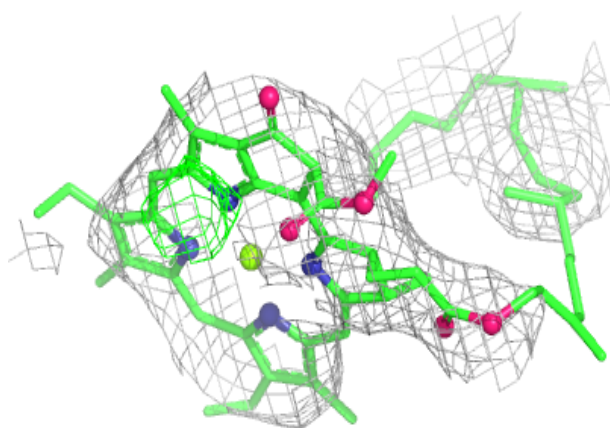
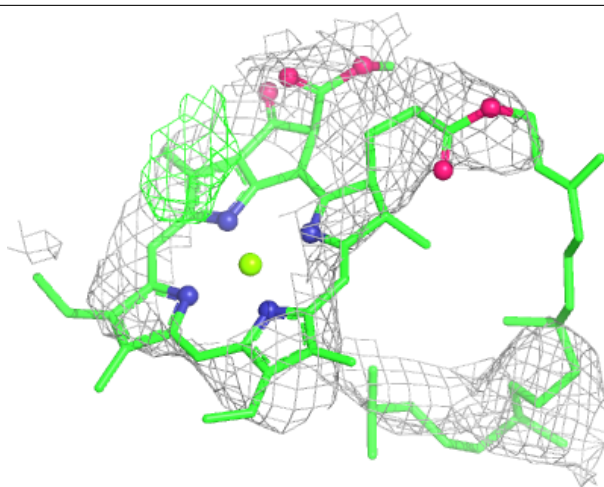
**Electron density around CLA D 1008:**

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



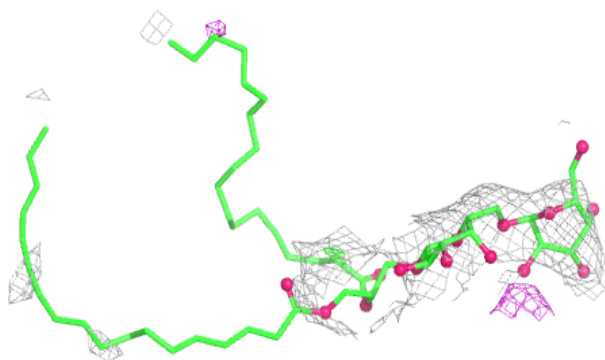
Electron density around CLA B 1023:

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

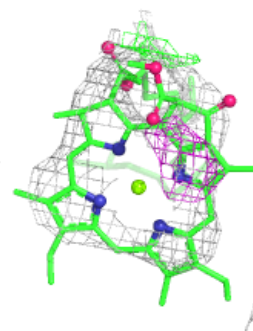
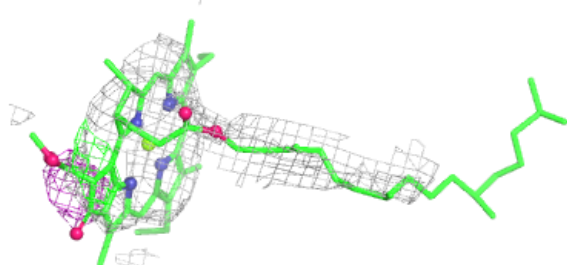
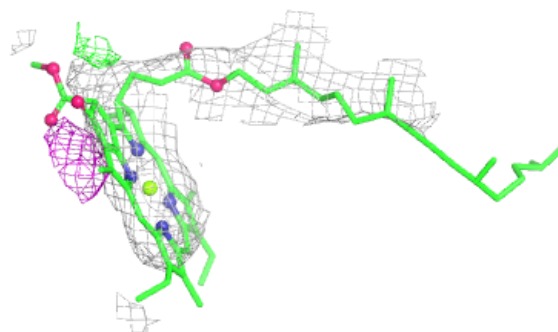


Electron density around DGD H 1058:

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

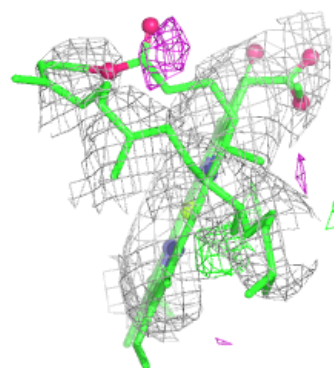
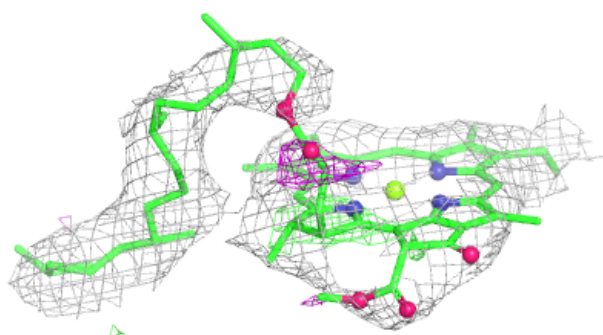
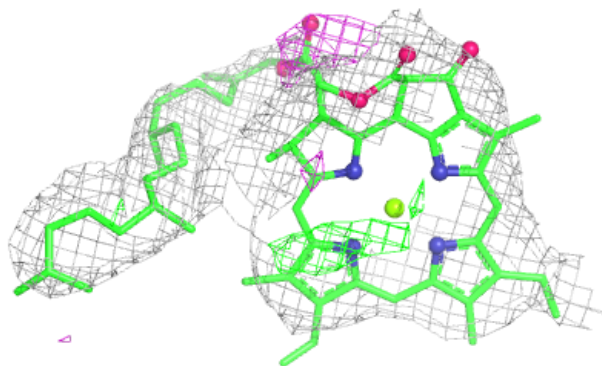
**Electron density around CLA B 1013:**

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

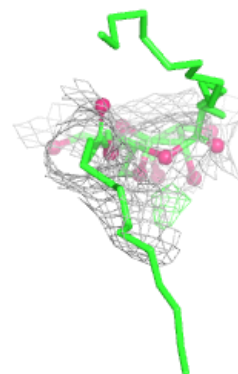
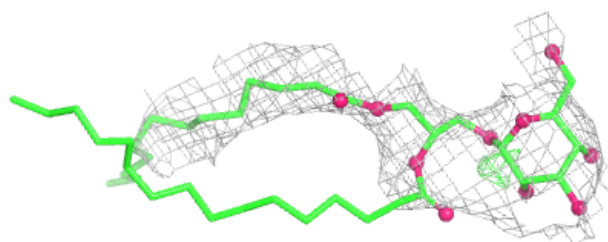
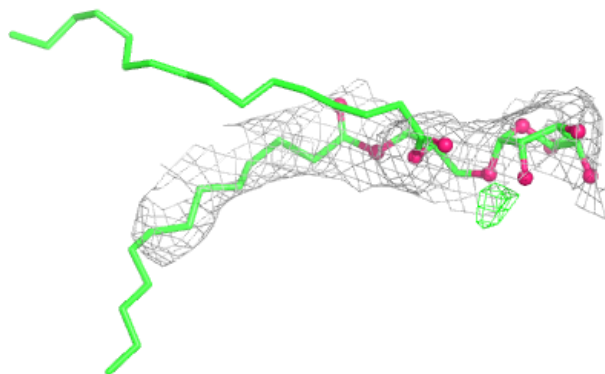


Electron density around CLA d 6005:

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

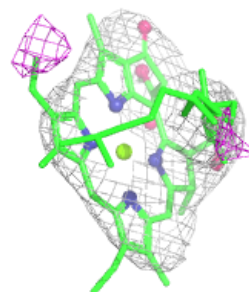
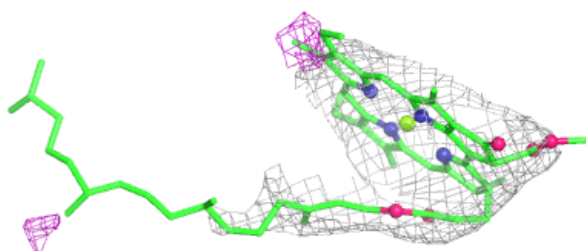
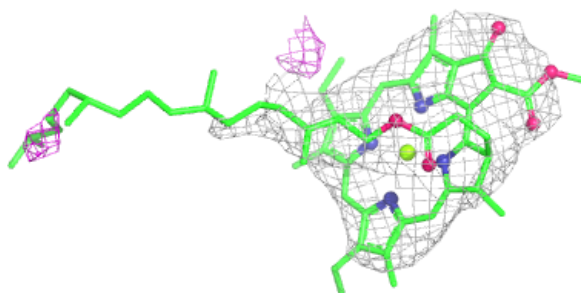
**Electron density around MGE D 1062:**

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

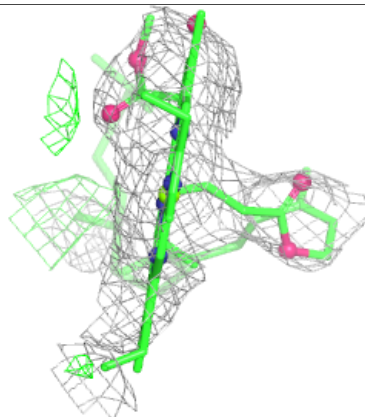
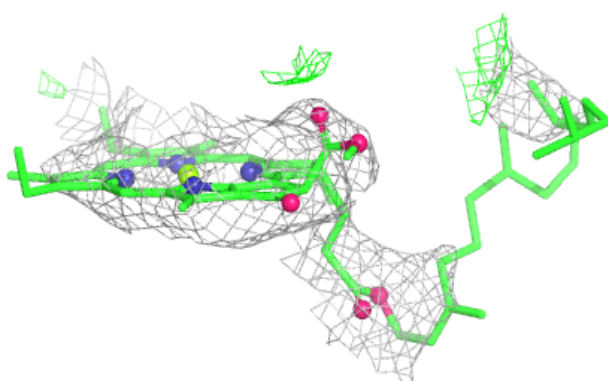
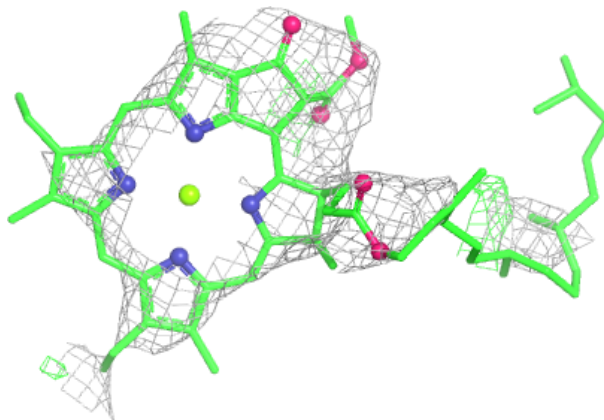


Electron density around CLA b 6016:

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

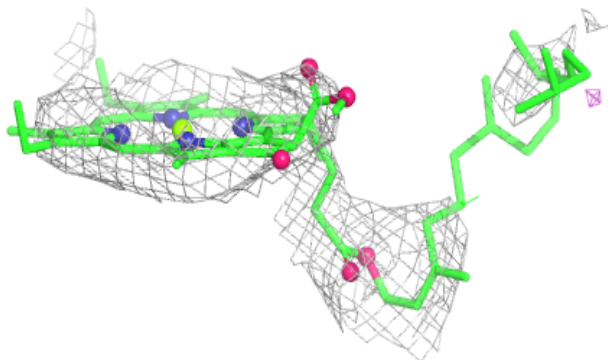
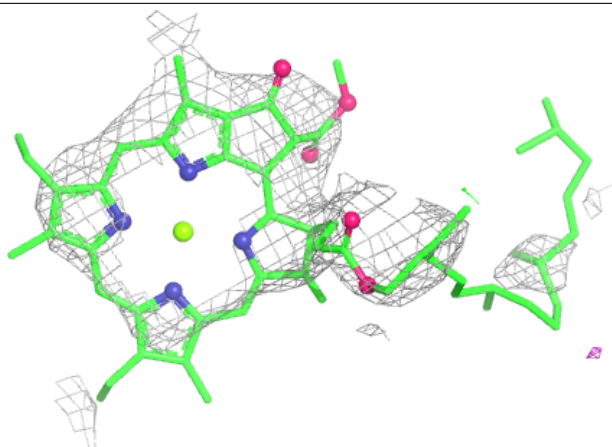
**Electron density around CLA b 6020:**

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



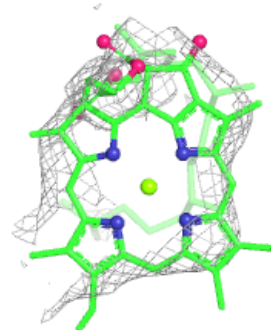
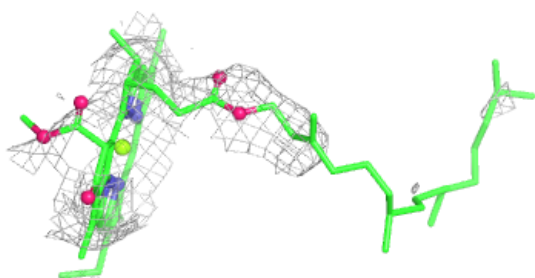
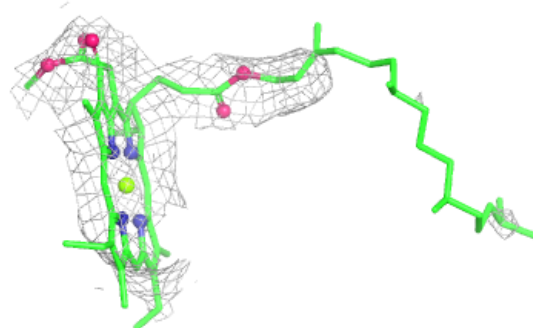
Electron density around CLA B 1020:

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

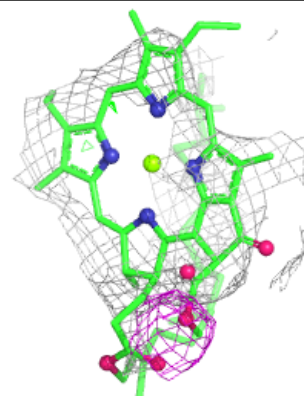
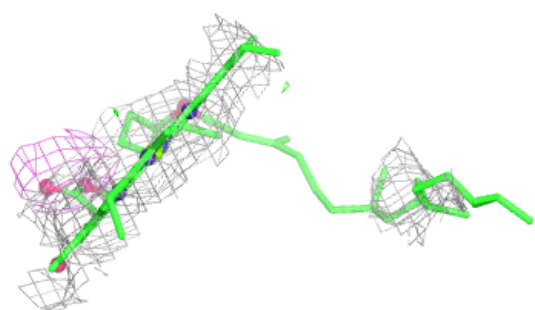
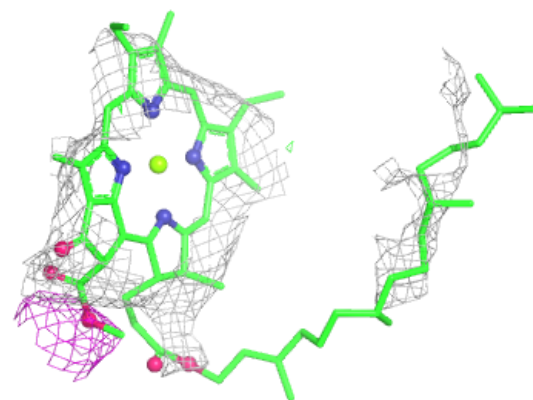


Electron density around CLA C 1030:

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

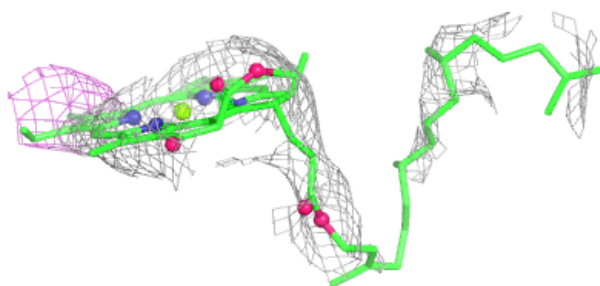
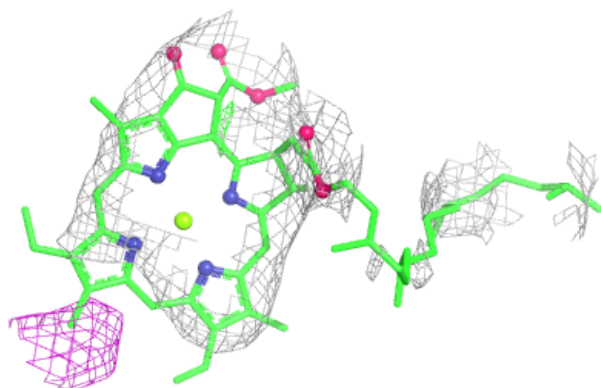
**Electron density around CLA C 1031:**

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



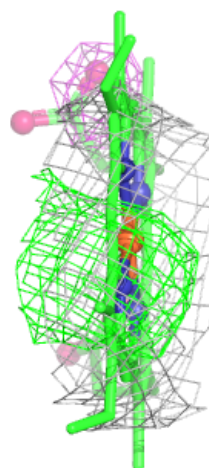
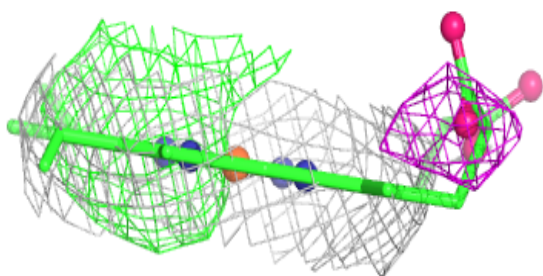
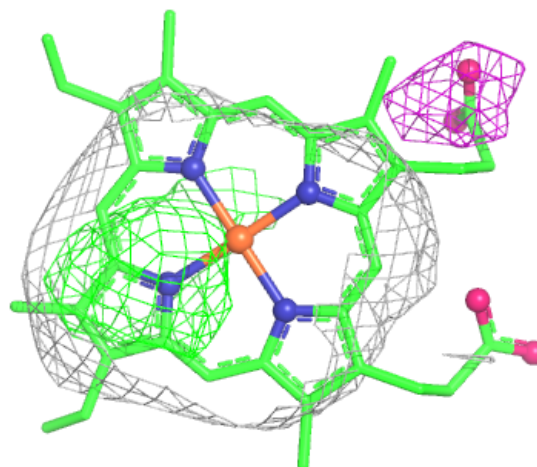
Electron density around CLA A 1006:

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



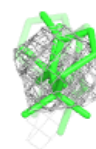
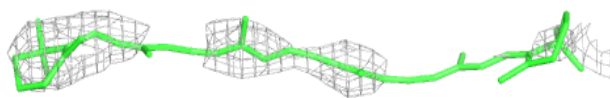
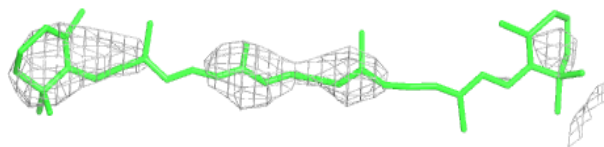
Electron density around HEM E 1040:

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



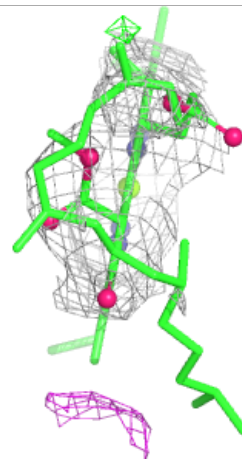
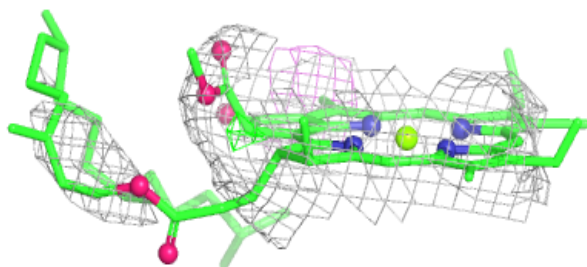
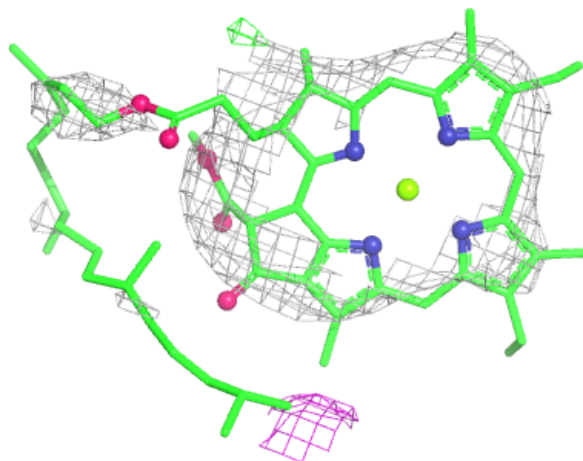
Electron density around BCR C 1054:

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



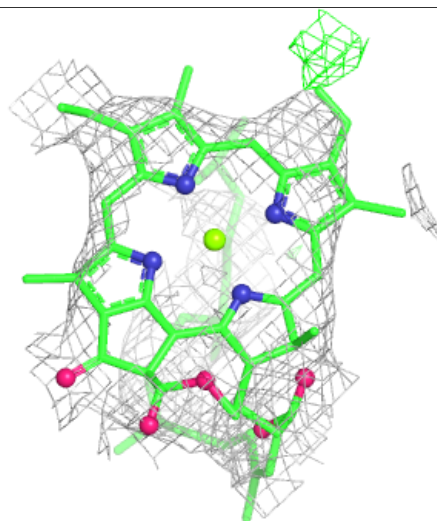
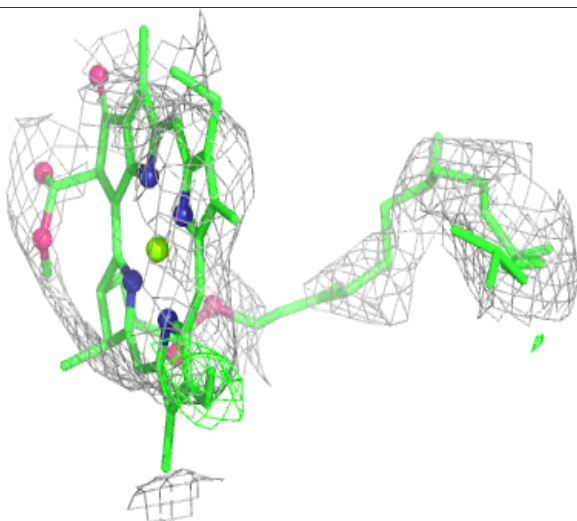
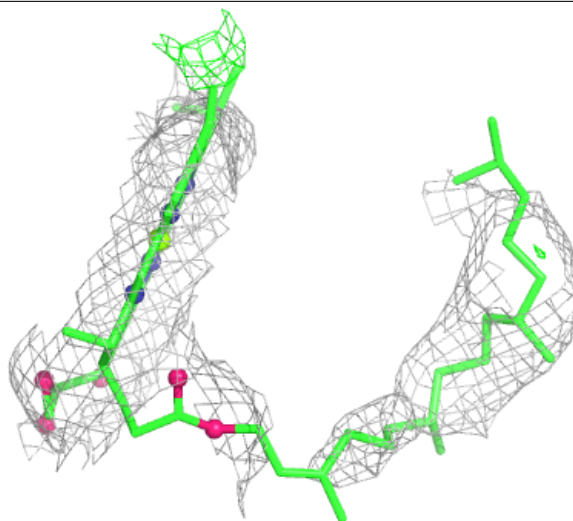
Electron density around CLA b 6018:

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



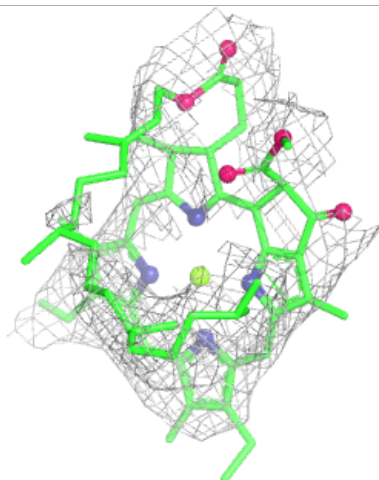
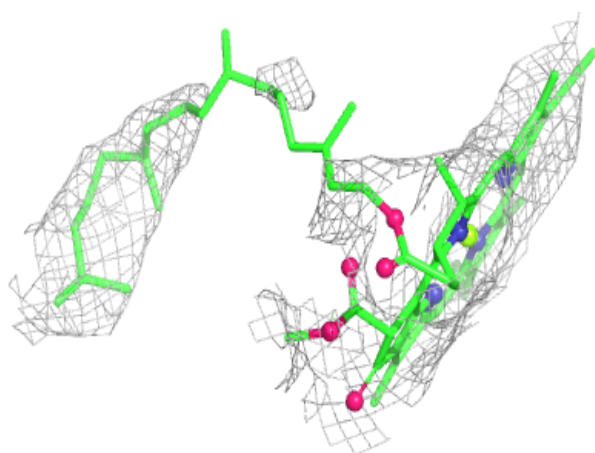
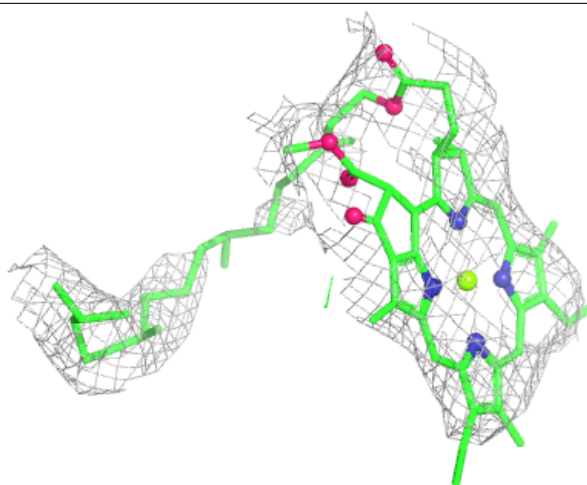
Electron density around CLA b 6019:

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



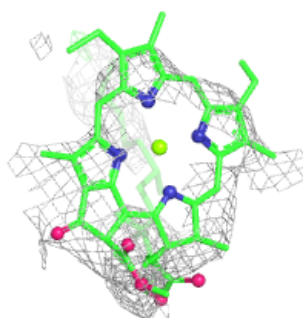
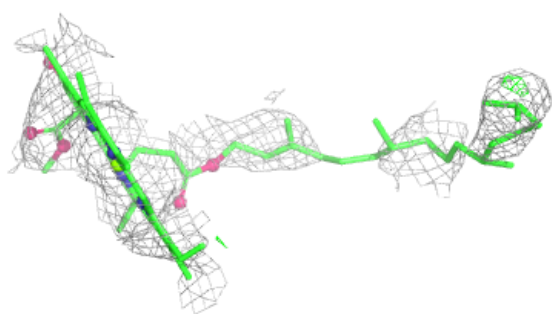
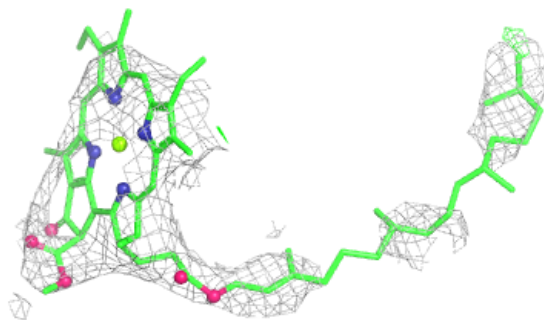
Electron density around CLA B 1021:

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

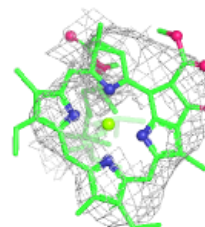
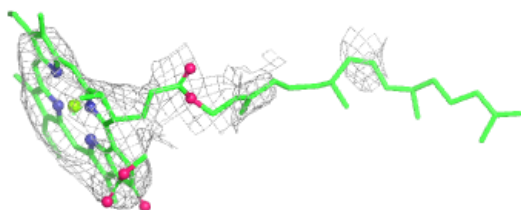
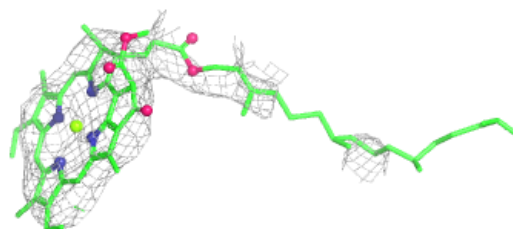


Electron density around CLA H 1017:

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

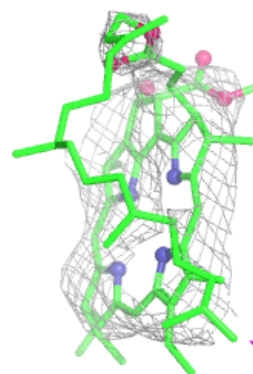
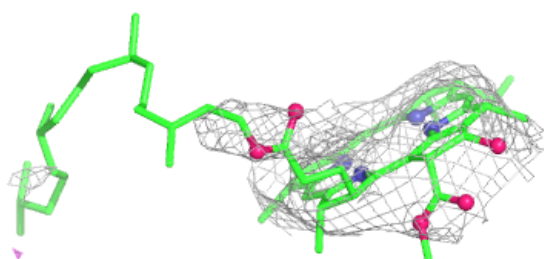
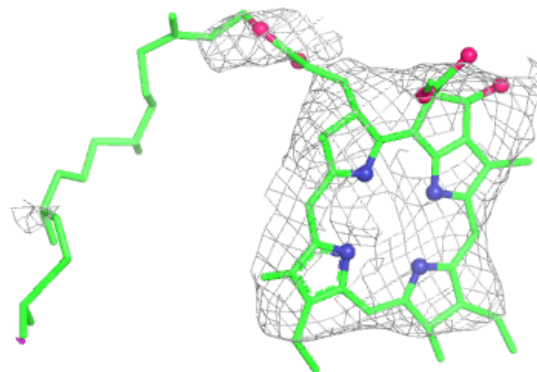
**Electron density around CLA B 1012:**

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

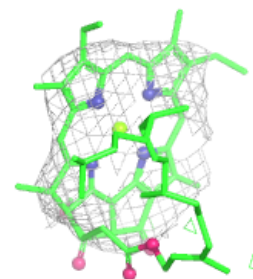
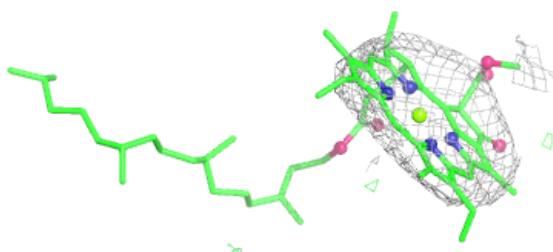
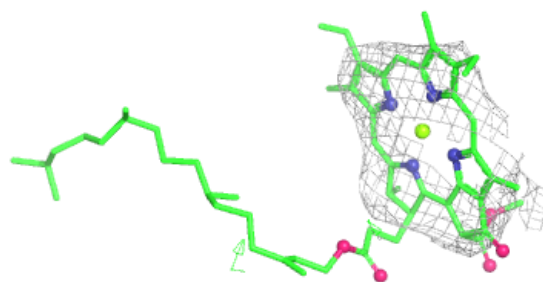


Electron density around PHO A 1039:

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

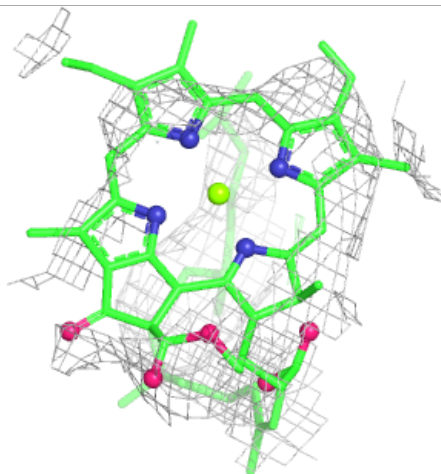
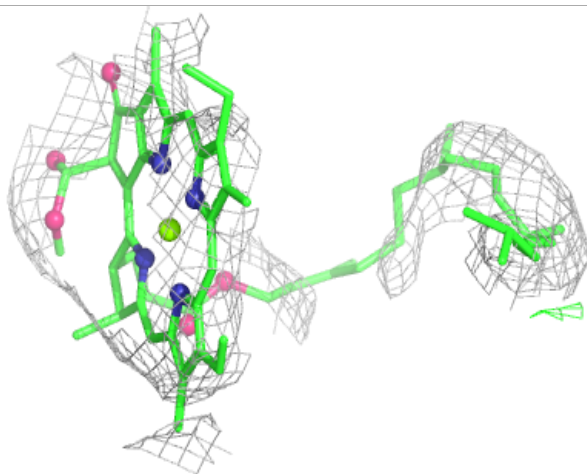
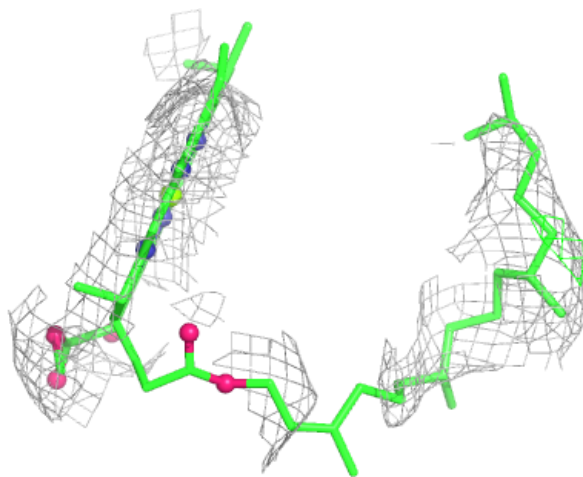
**Electron density around CLA C 1035:**

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



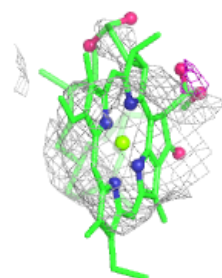
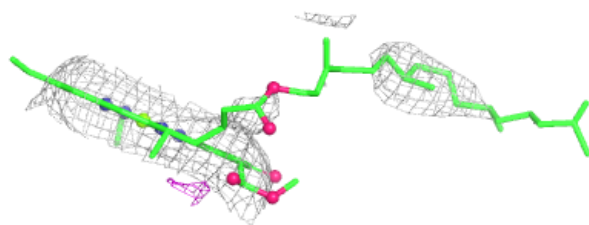
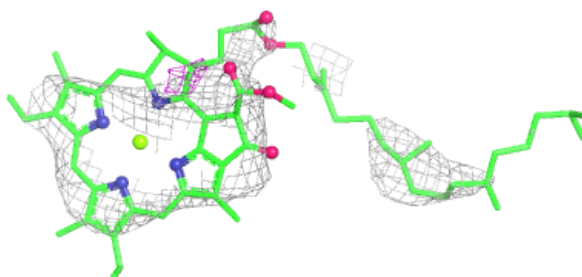
Electron density around CLA B 1019:

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

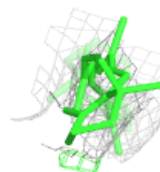
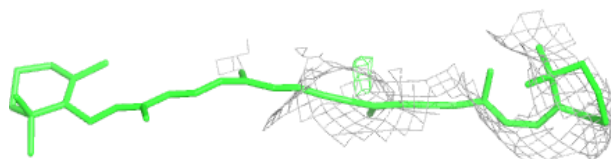
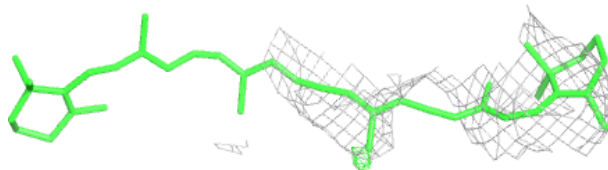


Electron density around CLA B 1010:

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

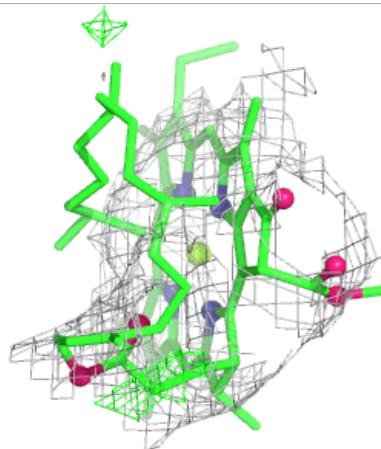
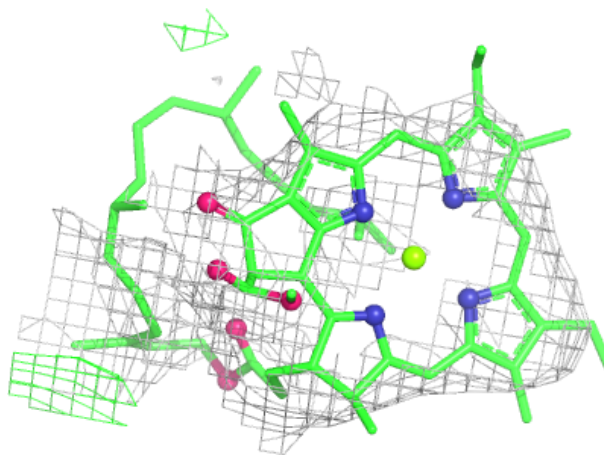
**Electron density around BCR k 6051:**

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



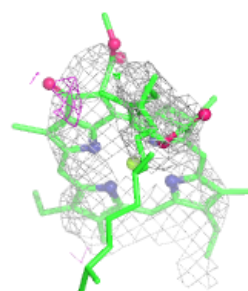
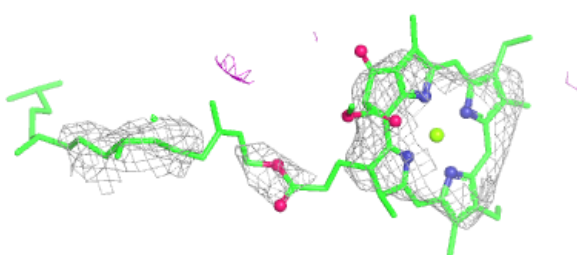
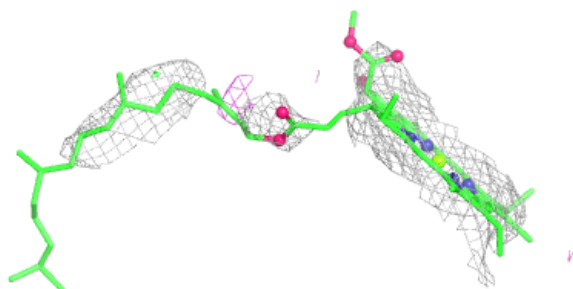
Electron density around CLA c 6026:

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

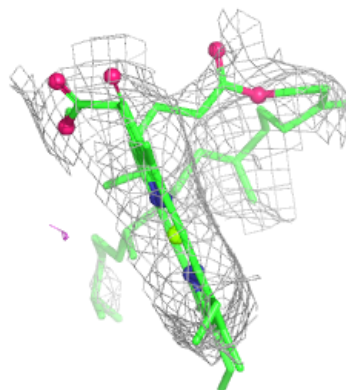
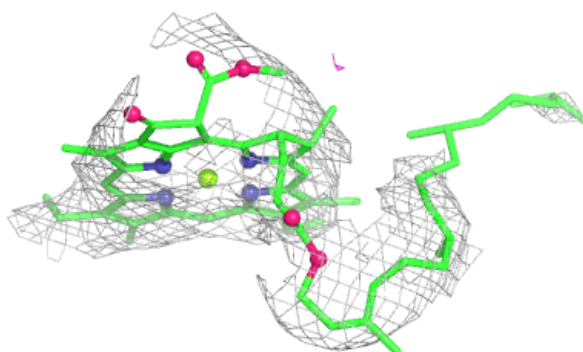
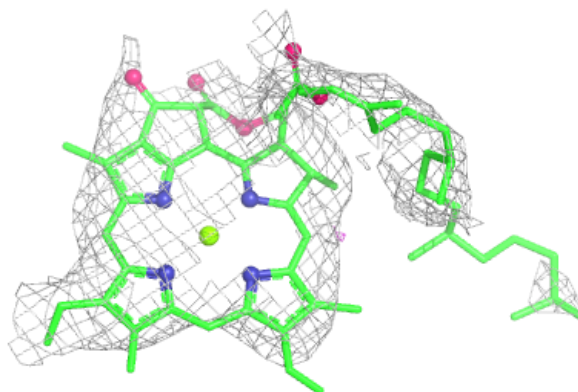


Electron density around CLA D 1004:

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

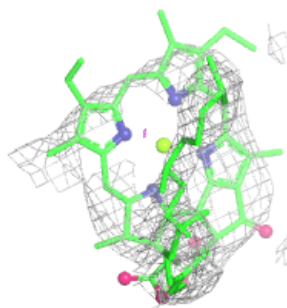
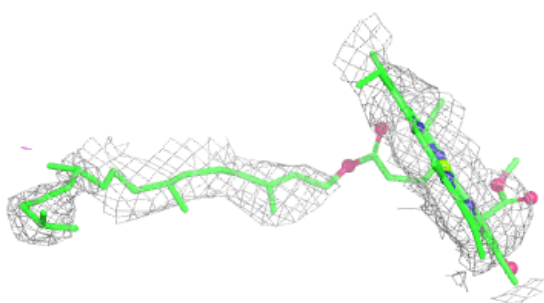
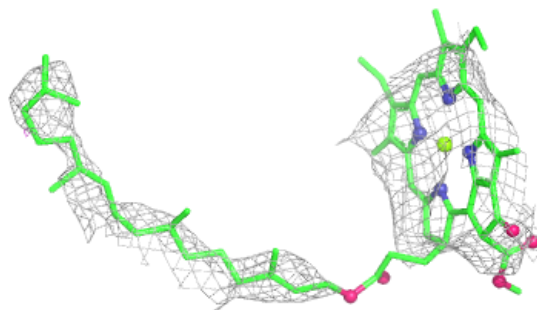
**Electron density around CLA D 1005:**

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

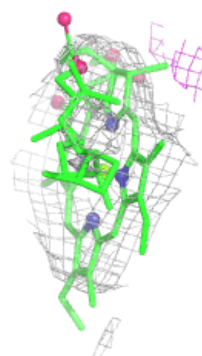
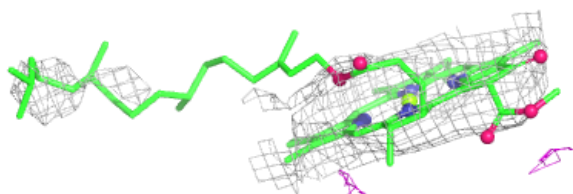
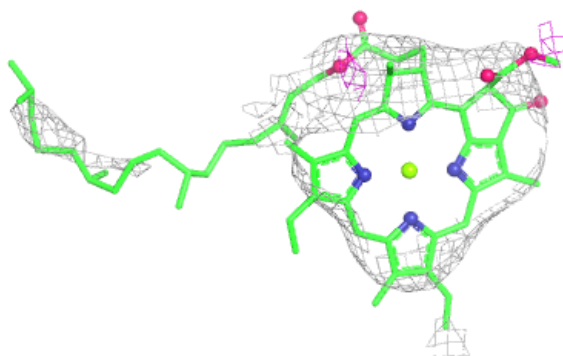


Electron density around CLA b 6017:

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

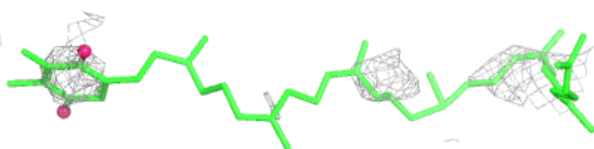
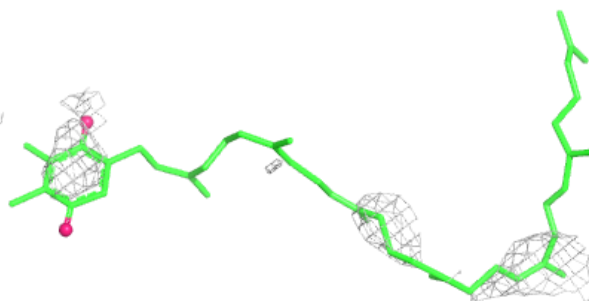
**Electron density around CLA B 1011:**

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

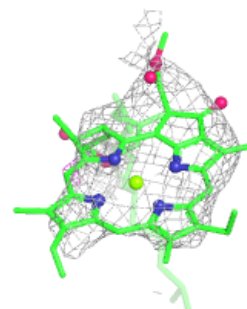
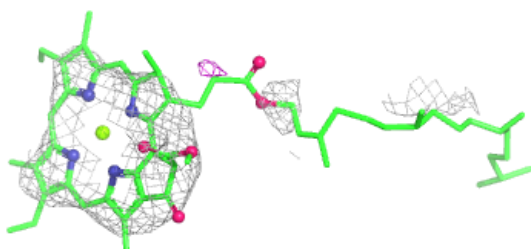
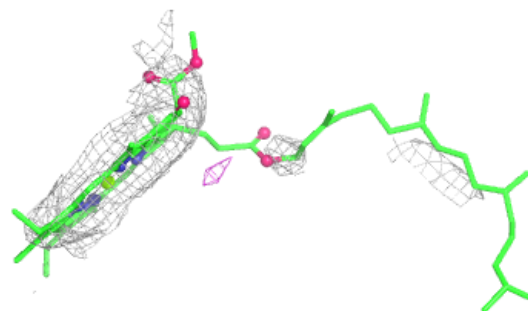


Electron density around PQ9 D 1042:

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

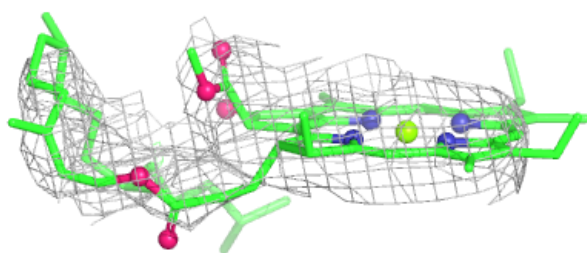
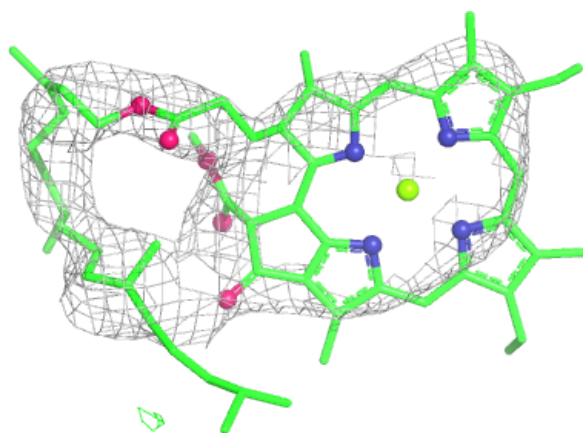
**Electron density around CLA d 6004:**

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

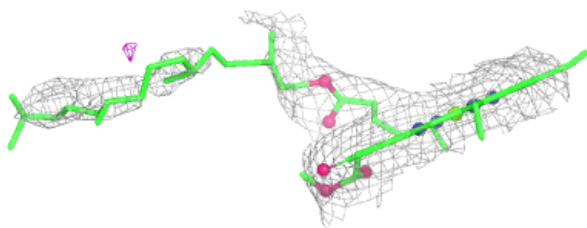
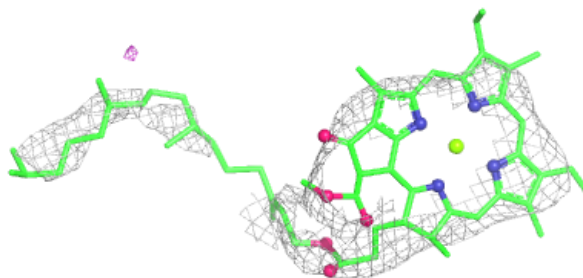


Electron density around CLA B 1018:

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

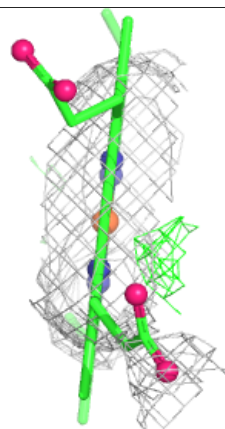
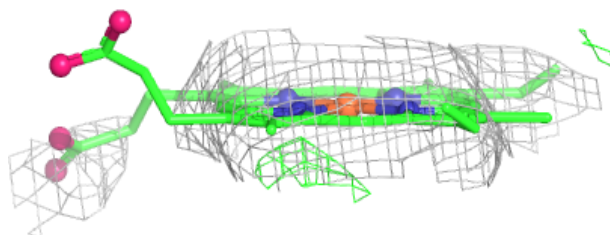
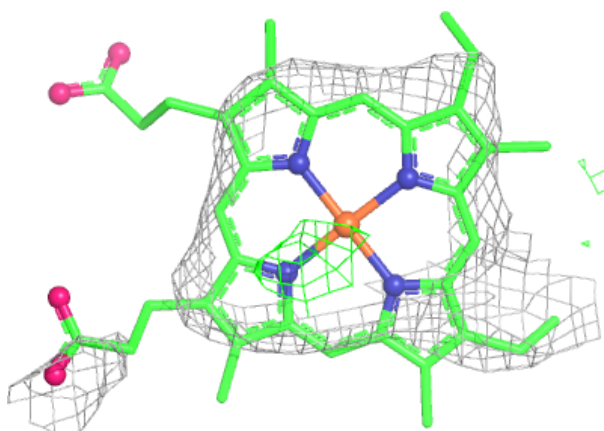
**Electron density around CLA b 6010:**

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



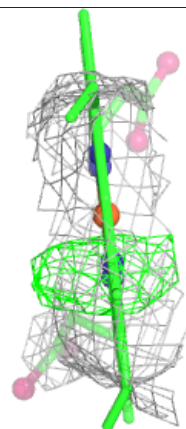
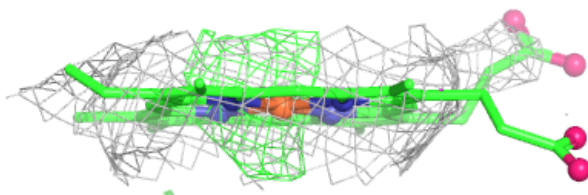
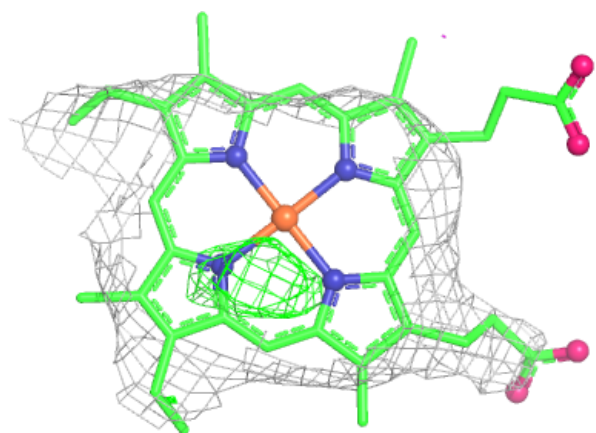
Electron density around HEM v 6041:

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



Electron density around HEM V 1041:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.