



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:13 PM UTC

PDB ID : 3A0H / pdb_00003a0h
Title : Crystal structure of I-substituted Photosystem II complex
Authors : Kawakami, K.; Umena, Y.; Kamiya, N.; Shen, J.-R.
Deposited on : 2009-03-17
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

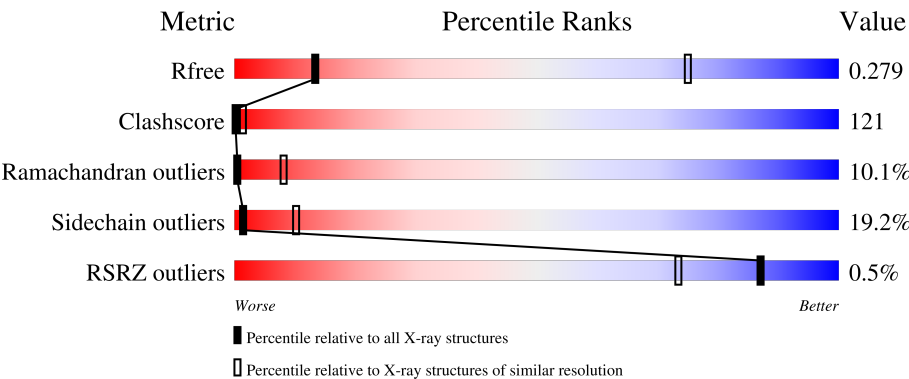
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 Å.

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



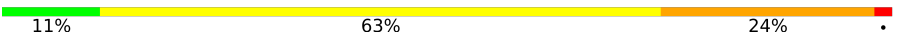
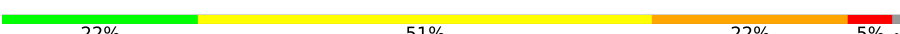
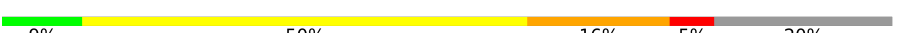
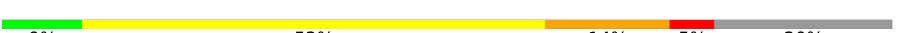
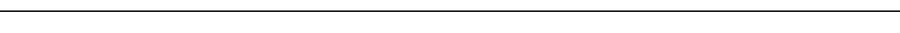
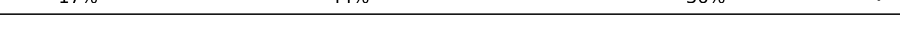
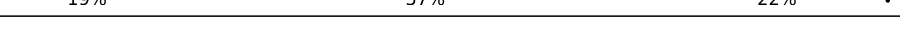
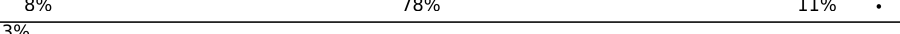
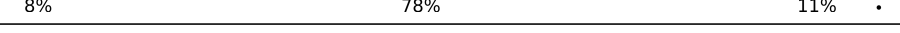
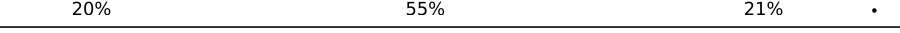
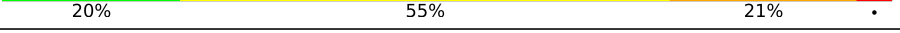
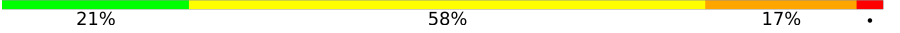
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	11%56%26%.
1	a	344	11%56%26%.
2	B	488	17%56%24%.
2	b	488	17%56%24%.
3	C	447	14%59%23%.

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	6035	X	-	X	-
22	CLA	c	6036	X	-	X	-
22	CLA	c	6037	X	-	X	-
22	CLA	d	6004	X	-	X	-
22	CLA	d	6005	X	-	X	-
22	CLA	d	6008	X	-	X	-
22	CLA	h	6017	X	-	X	-
22	CLA	k	6034	X	-	X	-
23	PHO	A	1038	X	-	X	-
23	PHO	D	1039	X	-	X	-
23	PHO	a	6038	X	-	X	-
23	PHO	d	6039	X	-	X	-
24	PQ9	A	1043	-	-	X	-
24	PQ9	D	1042	-	-	X	-
24	PQ9	a	6043	-	-	X	-
24	PQ9	d	6042	-	-	X	-
25	BCR	A	1044	-	-	X	-
25	BCR	B	1045	-	-	X	-
25	BCR	B	1047	-	-	X	-
25	BCR	B	1048	-	-	X	-
25	BCR	C	1052	-	-	X	-
25	BCR	C	1054	-	-	X	-
25	BCR	D	1050	-	-	X	-
25	BCR	H	1049	-	-	X	-
25	BCR	K	1051	-	-	X	-
25	BCR	T	6046	-	-	X	-
25	BCR	T	6048	-	-	X	-
25	BCR	a	6044	-	-	X	-
25	BCR	b	6045	-	-	X	-
25	BCR	b	6047	-	-	X	-
25	BCR	c	6054	-	-	X	-
25	BCR	d	6050	-	-	X	-
25	BCR	h	6049	-	-	X	-
25	BCR	k	6051	-	-	X	-
25	BCR	k	6052	-	-	X	-
25	BCR	t	1046	-	-	X	-
26	LHG	A	1063	-	-	X	-
26	LHG	a	6063	-	-	X	-
27	IOD	B	1067	-	-	X	X
27	IOD	D	1064	-	-	X	-
27	IOD	D	1068	-	-	X	X
27	IOD	T	1066	-	-	X	-

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

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 48060 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	13			
2	b	488	Total	C	N	O	S	0	0	0
			3835	2518	638	666	13			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	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
			1860	1162	314	380	4			
13	o	242	Total	C	N	O	S	0	0	0
			1860	1162	314	380	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			

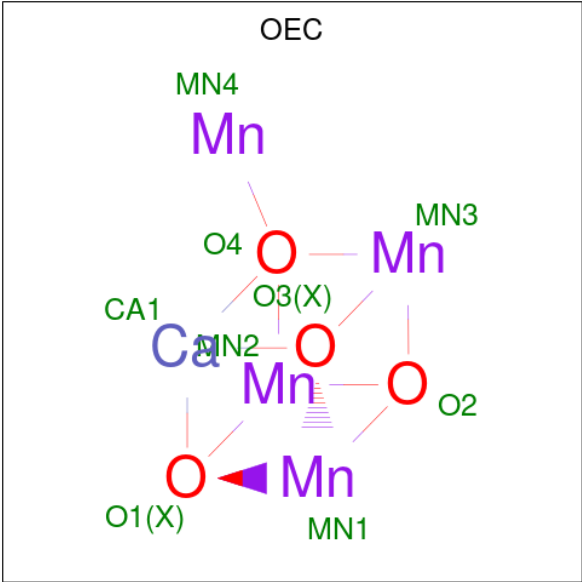
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

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

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

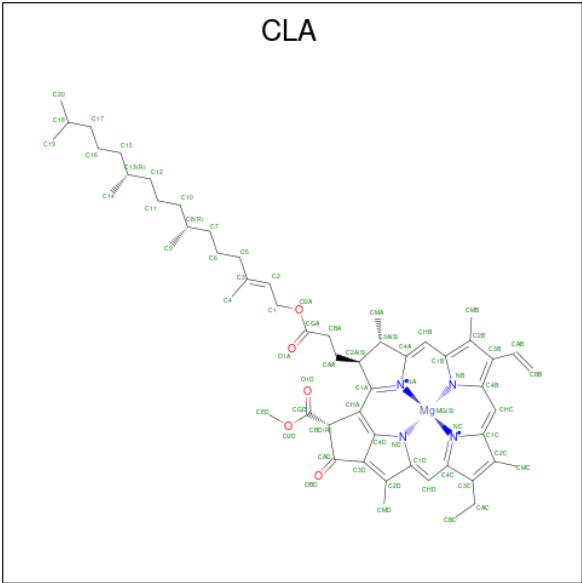
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

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



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

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



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

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

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

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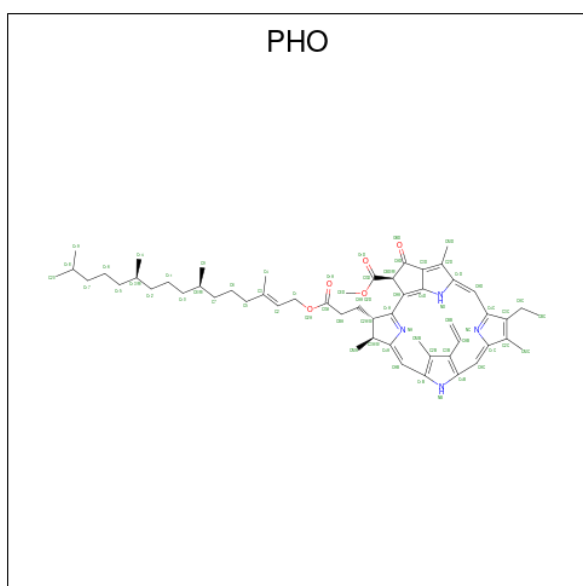
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N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

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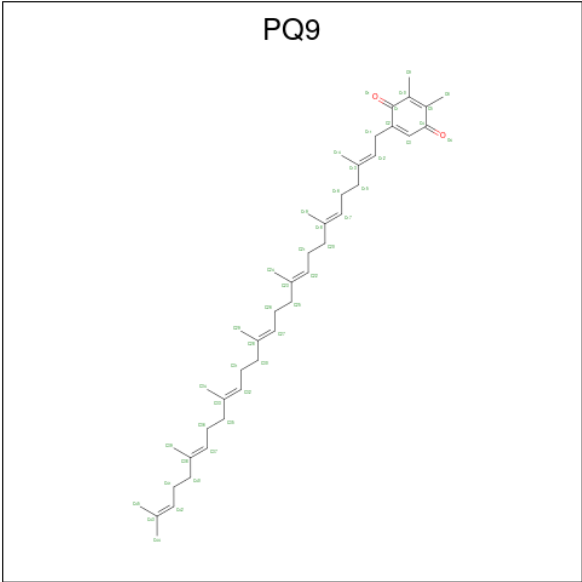
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	h	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	k	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



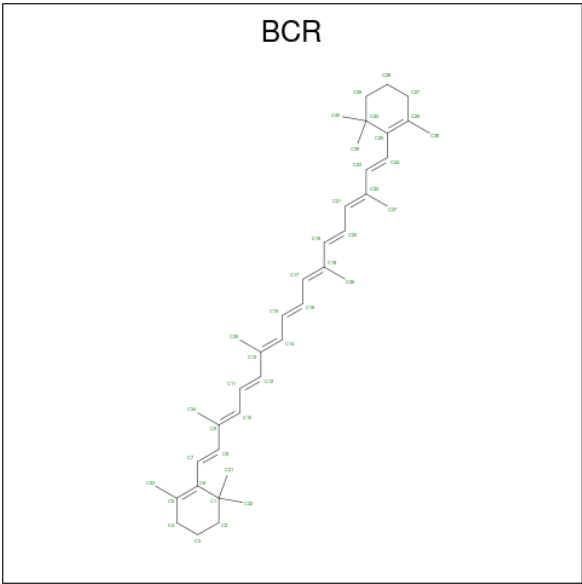
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



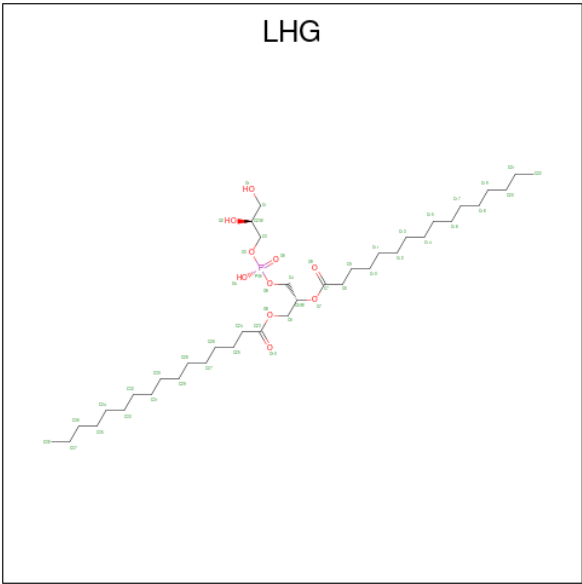
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			45	43	2		
24	D	1	Total	C	O	0	0
			45	43	2		
24	a	1	Total	C	O	0	0
			45	43	2		
24	d	1	Total	C	O	0	0
			45	43	2		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).

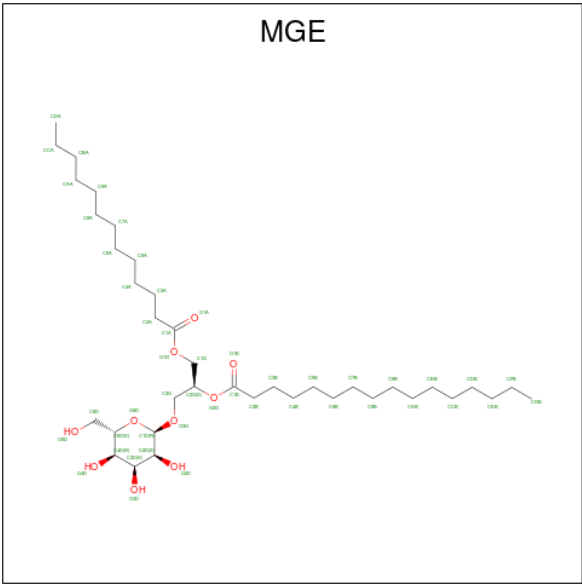


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			49	38	10	1		
26	a	1	Total	C	O	P	0	0
			49	38	10	1		

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

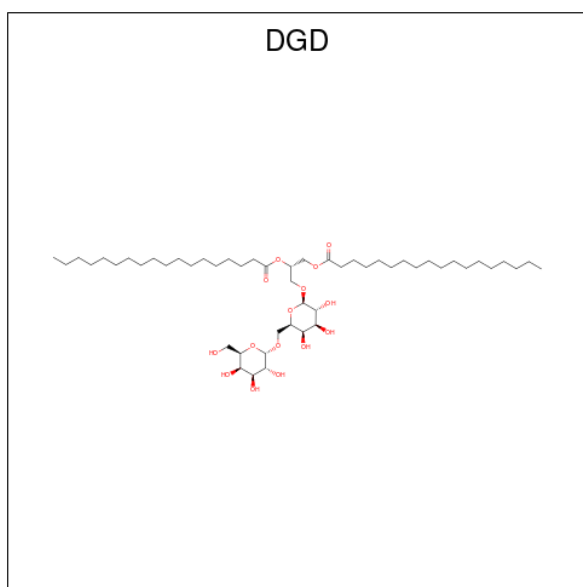
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	1	Total	I	0	0
			1	1		
27	B	1	Total	I	0	0
			1	1		
27	D	2	Total	I	0	0
			2	2		
27	T	1	Total	I	0	0
			1	1		
27	a	1	Total	I	0	0
			1	1		
27	b	1	Total	I	0	0
			1	1		
27	d	2	Total	I	0	0
			2	2		
27	t	1	Total	I	0	0
			1	1		

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀).



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

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).

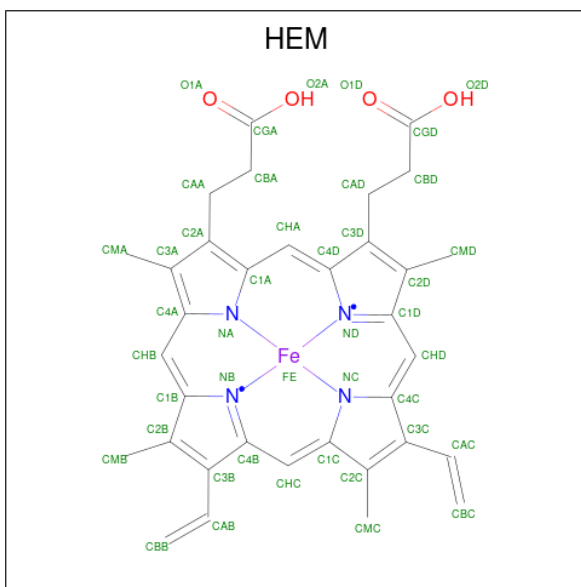


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	B	1	Total	C	O	0	0
			66	51	15		
29	C	1	Total	C	O	0	0
			66	51	15		
29	C	1	Total	C	O	0	0
			66	51	15		
29	C	1	Total	C	O	0	0
			66	51	15		
29	b	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total	C	O	0	0
			66	51	15		
29	c	1	Total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

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

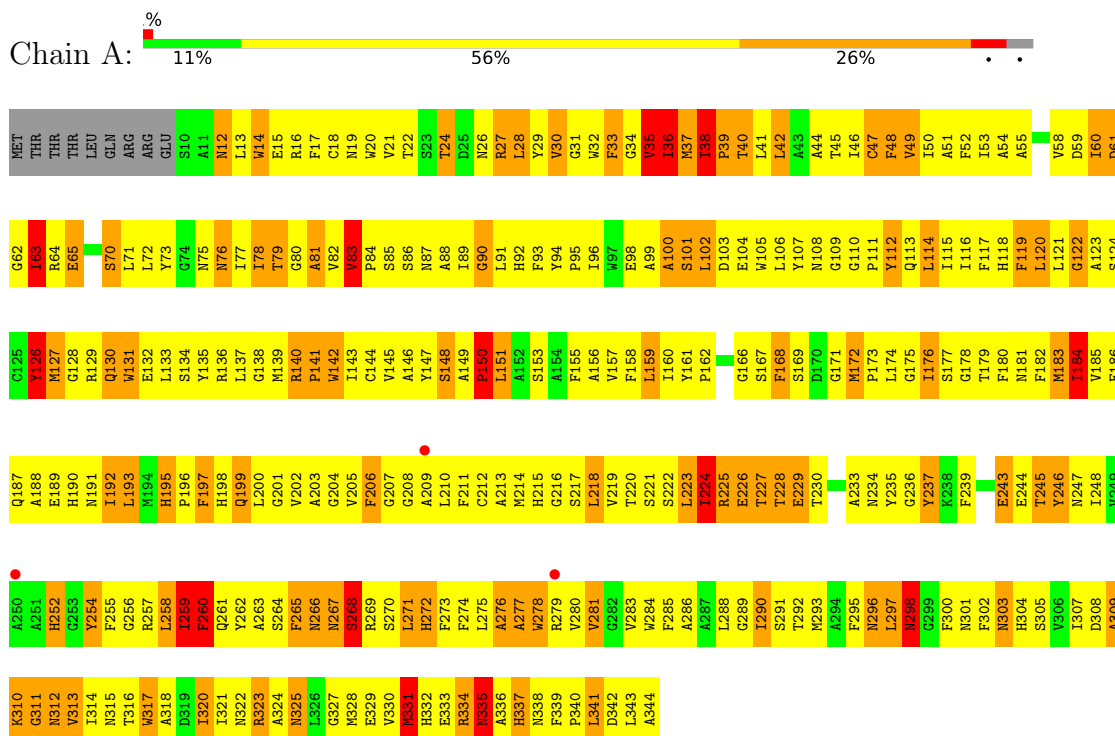


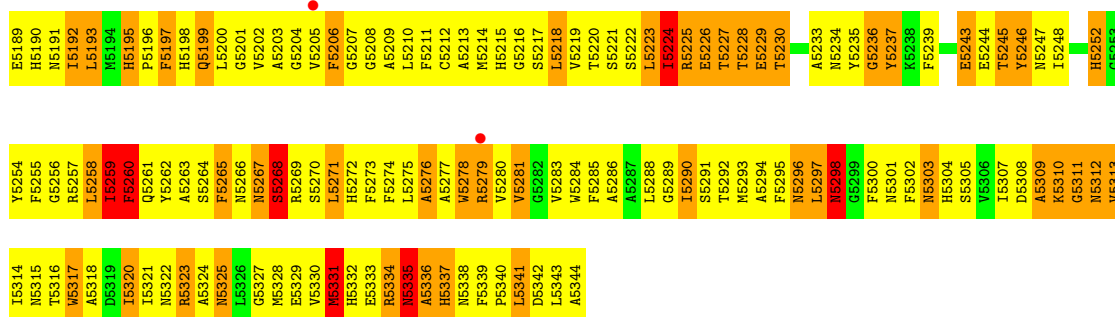
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
31	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	f	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
31	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

3 Residue-property plots

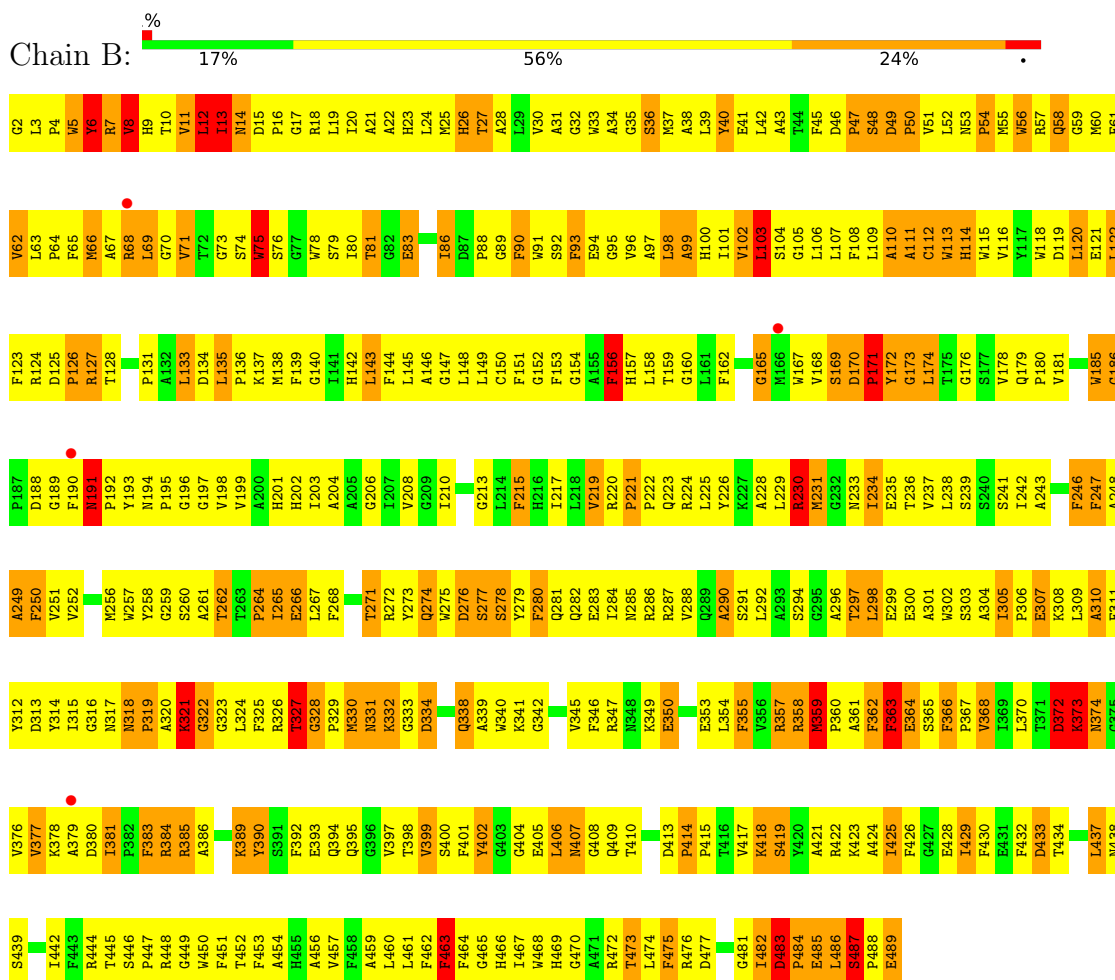
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Photosystem Q(B) protein

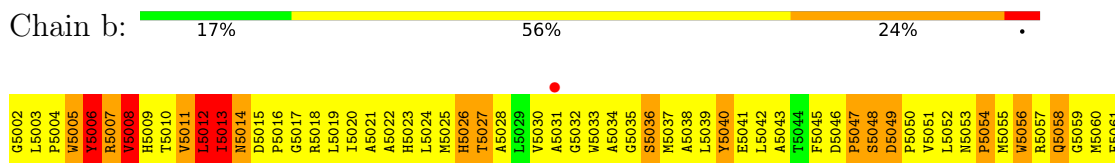




• Molecule 2: Photosystem II core light harvesting protein

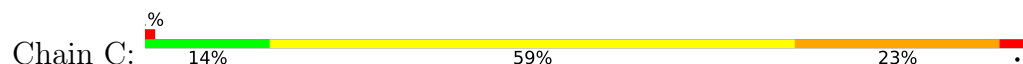


• Molecule 2: Photosystem II core light harvesting protein



V5062	F5123	P5187	F5250	Y5312	V5376	S5439
L5063	R5124	D5188	V5251	D5313	V5377	
P5064	D5125	G5189	F5252	Y5314	V5378	
F5065	F5126	G5190		I5315	A5379	I5442
	F5127	M5191	M5256	G5316	D5380	F5443
A5067	R5128	N5192	W5257	N5317	I5381	T5445
R5068		Y5193	Y5258	N5318	P5382	T5446
L5069	P5131	N5194	G5259	P5319	F5383	P5447
G5070	A5132	P5195	S5260	A5320	R5448	R5449
	L5133	G5196	S5261	K5321	R5384	G5449
T5072	D5134	G5197	T5262	G5322	A5386	W5450
G5073	L5135	V5198	T5263	G5323	K5389	F5451
S5074	P5136	V5199	P5264	L5324	T5452	T5453
W5075	K5137	A5200	I5265	F5325	F5454	F5455
G5077	M5138	H5201	E5266	R5326	S5391	H5456
S5078	P5139	H5202	E5267	T5327	F5392	H5457
W5079	L5140	I5203	F5268	G5328	E5393	A5458
T5080	L5141	A5204	G5269	P5329	O5394	A5459
T5081	H5142	A5205	P5270	M5330	O5395	F5463
G5082	L5143	G5206	T5271	N5331	G5396	A5464
E5083	A5146	V5208	R5272	K5332	V5397	G5465
	G5147	G5209	Y5273	G5333	T5398	H5466
		I5210	Q5274	D5334	V5399	W5468
D5086	L5148		W5275		S5400	A5469
D5087	L5149		D5276	Q5338	F5401	G5470
P5088	C5150		S5277	A5339	Y5402	A5471
G5089	F5151		F5278	W5340	G5403	R5472
F5090	G5152		Y5279	K5341	I5407	L5473
W5091	G5153		F5280	G5342	E5408	F5474
S5092	F5154		Q5281		Q5409	D5477
F5093	G5155		Q5282	V5345	W5407	V5478
E5094	F5156		E5283	F5346	G5408	A5479
G5095	R5157		I5284	R5347	Q5410	
A5097	L5158		R5285	N5348	T5410	
L5098	T5159		R5287	K5349		
A5099	G5160		V5288	E5350	D5413	
H5100	F5162				P5414	
I5101			Q5289	E5353	P5415	
V5102			A5290	L5354	T5416	
S5103	G5165		S5291	F5355	V5417	
G5105	M5166		L5229	V5356	K5418	
L5106	W5167		A5228	R5357	S5419	
L5107	V5168		M5230	R5358	Y5420	
F5108	S5169		G5232	M5359	A5421	
L5109	D5170		N5233	P5360	R5422	
	P5171		I5234	A5361	K5423	
A5110	Y5172		E5235	F5362	A5424	
A5111	G5173		E5299	E5363	I5425	
C5112	L5174		F5300	E5364	F5426	
W5113	T5175		A5301	S5365	G5427	
C5114	G5176		W5302	F5366	E5428	
W5115	S5239		S5303	P5367	I5429	
V5116	S5240		A5304	V5368	F5430	
V5117	S5241		I5305	I5369	E5431	
V5118	Q5179		P5306	L5370	F5432	
W5119	P5180		F5307	T5371	D5433	
L5120	V5181		K5308	D5372	T5434	
E5121			L5309	K5373	L5437	
L5122	G5186		A5248	S5374	N5438	
			F5311	G5375		

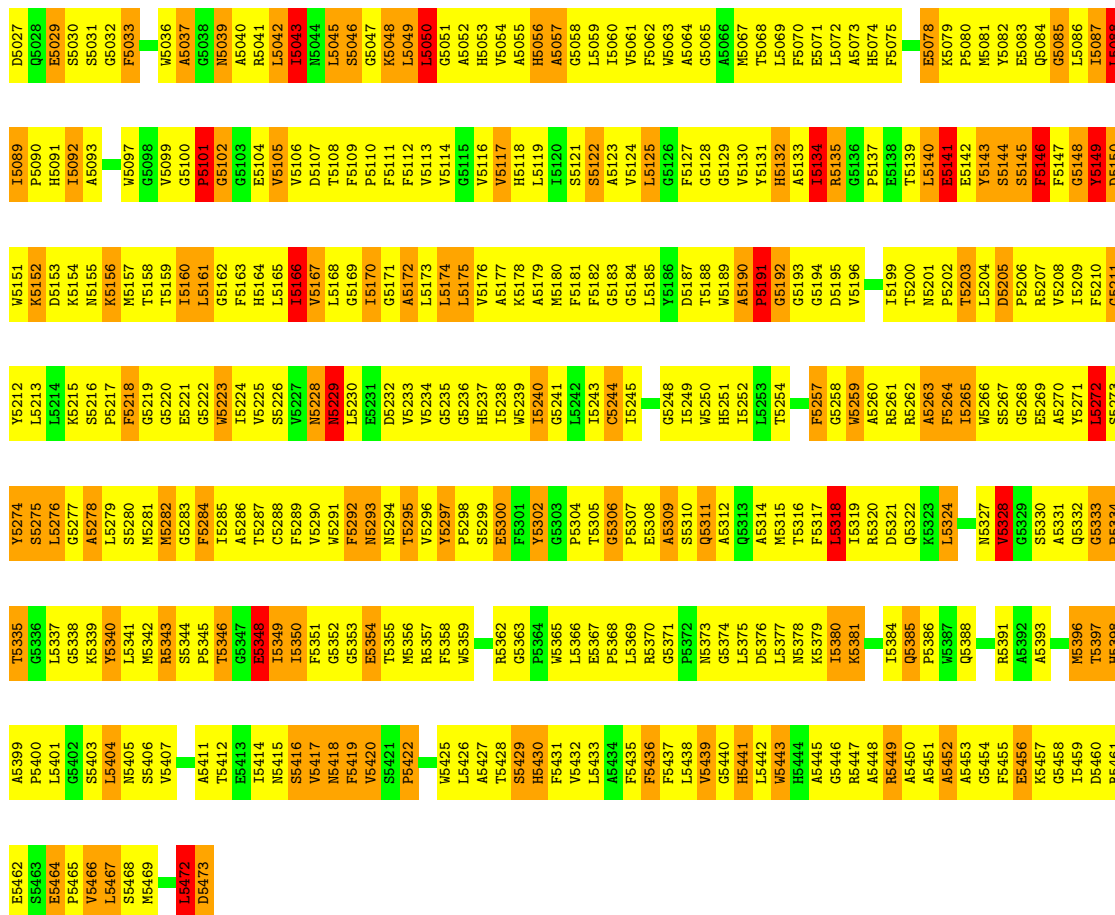
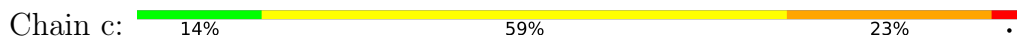
• Molecule 3: Photosystem II CP43 protein



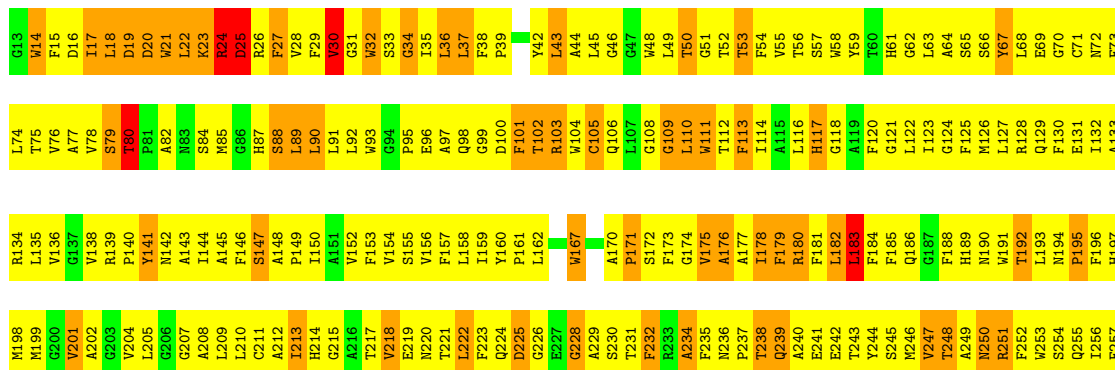
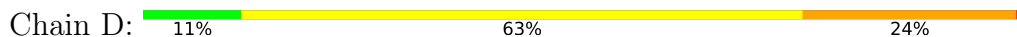
D27	I89	W151	Y212	Y274	T335	A399
Q28	P90	K152	L213	S275	G336	P400
E29	H91	D153	L214	L276	L337	L401
S30	I92	K154	K215	G277	G338	G402
A93	A93	N155	S216	A278	K339	S403
G32	K97	K156	P217	L279	K340	L404
F33	G98	M157	F218	S280	L341	N405
	W99	T158	G219	M281	M342	N406
W36	G100	L159	G220	M282	R343	N407
G38	P101	I160	E221	G283	P344	G408
G37	F102	L161	G222	F284	P345	G409
N39	G103	G162	W223	L285	T346	V410
A40	G104	F163	L224	A286	G347	A411
R41	E104	H164	V225	T287	E348	T412
L42	V105	L165	S226	C288	I349	E413
L43	V106	I166	V227	F289	I350	E414
N44	D107	V167	N228	W290	F351	N415
L45	T108	L168	N229	W291	G352	S416
S46	F109	G169	L230	F292	G353	V417
G47	P110	I170	E231	N293	E354	N418
K48	F111	G171	D232	N294	T355	F419
L49	F112	A172	V233	M295	M356	V420
L50	V113	L173	V234	V296	R357	S421
G51	V114	L174	G235	Y297	F358	P422
A52	G115	L175	G236	P298	W359	
H53	V116	V176	H237	S299		W425
V54	V117	A177	L238	E300	R362	L426
A55	H118	K178	W239	F301	G363	A427
H56	L119	A179	Y302	W302	P364	T428
A57	N120	M180	G241	G303	W365	S429
G58	S121	F181	L242	P304	L366	H430
L59	S122	F182	L243	T305	E367	F431
L60	A123	G183	G244	G306	P368	V432
V61	V124	G184	L245	P307	L369	L433
F62	L125	L185		E308	R370	A434
W63	G126	Y186	G248	A309	G371	F435
A64	F127	D187	L249	S310	P372	F436
G65	G128	T188	V250	Q311	N373	F437
A66	G129	W189	H251	A312	G374	L438
M67	V130	A190	L252	Q313	L375	A439
T68	Y131	P191	L253	A314	D376	G440
L69	H132	G192	T254	M315	L377	H441
F70	A133	G193		T316	K378	L442
E71	I134	G194	F257	F317	K379	W443
L72	R135	D195	G258	L318	I380	H444
H74	P137	V196	W259	I319	A445	A446
F75	G136	T199	A260	R320	G446	R447
	E138	N201	R261	D321	Q384	A448
E78	T139	L200	A262	Q322	Q385	R449
K79	L140	N201	L263	K323	P386	A450
P80	E141	P202	F264	L324	W387	A451
E142	E142	T203	I265		Q388	A452
Y143	Y143	L204	W266	N327		A453
Y82	S144	D205	S267	V328	R391	A454
E83	S145	P206	G268	G329	G454	A455
O84	F146	R207	E269	S330	A393	F456
G85	F147	V208	A270	A331	E456	
L86	G148	T209	L271	Q332	K457	G458
L87	Y149	G210	L272	G333	T397	I459
L88	D150	G211	S273	P334		

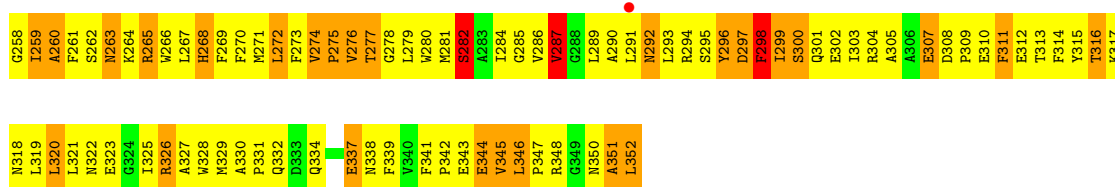


• Molecule 3: Photosystem II CP43 protein



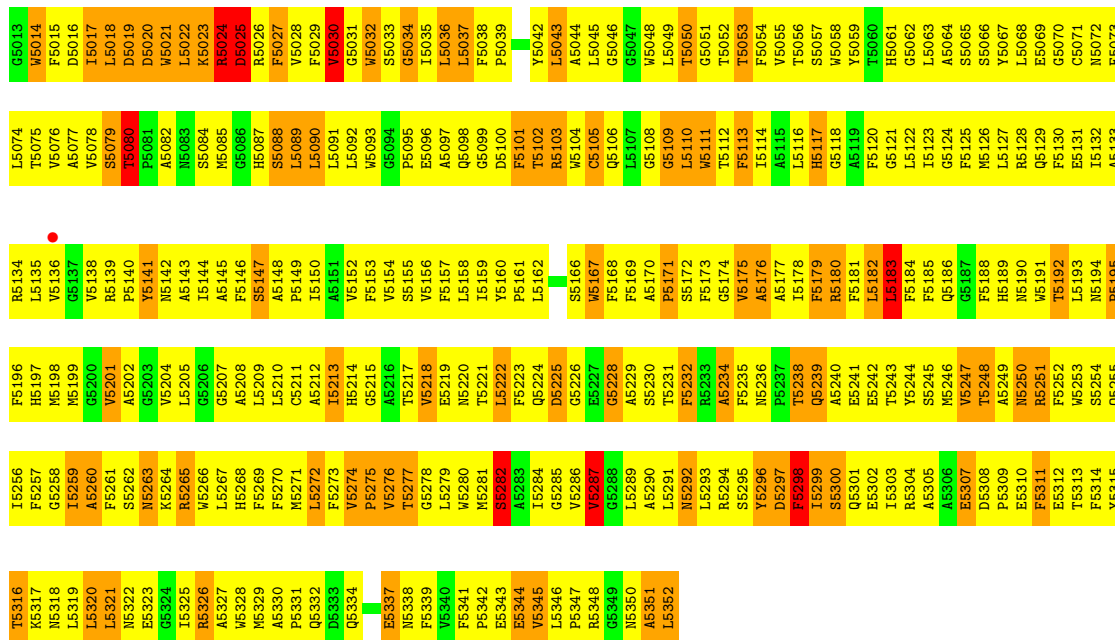
• Molecule 4: Photosystem II D2 protein





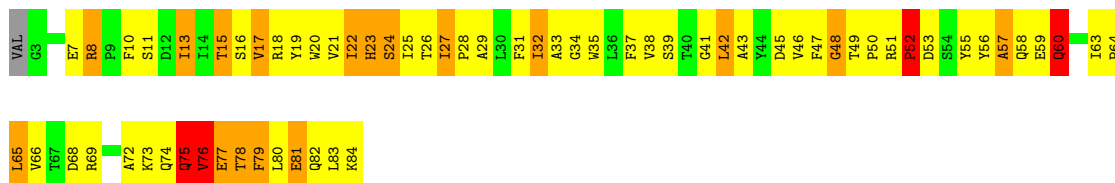
• Molecule 4: Photosystem II D2 protein

Chain d: 10% 64% 23%



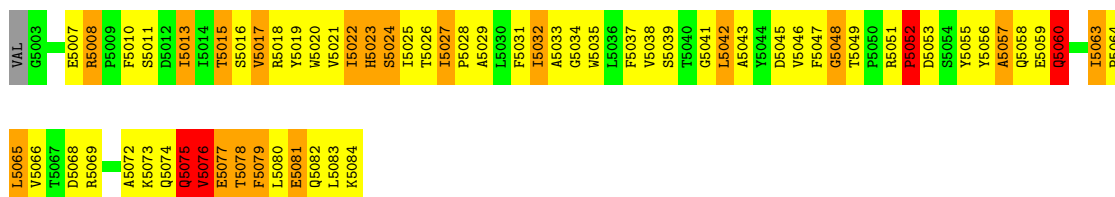
• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 20% 53% 20% 5%

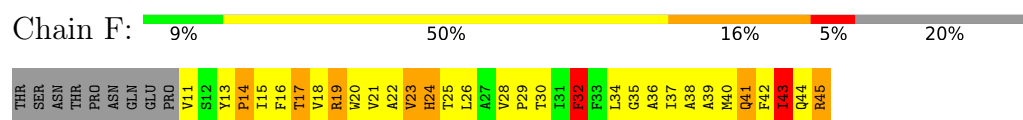


• Molecule 5: Cytochrome b559 subunit alpha

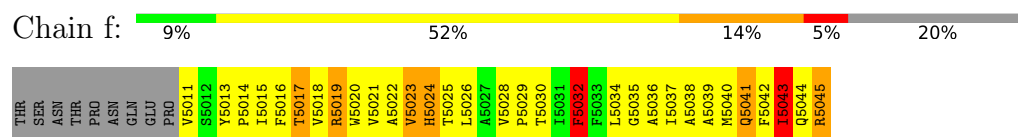
Chain e: 22% 51% 22% 5%



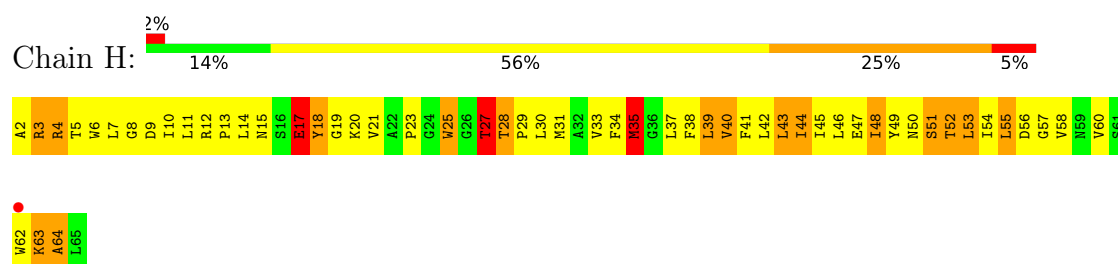
- Molecule 6: Cytochrome b559 subunit beta



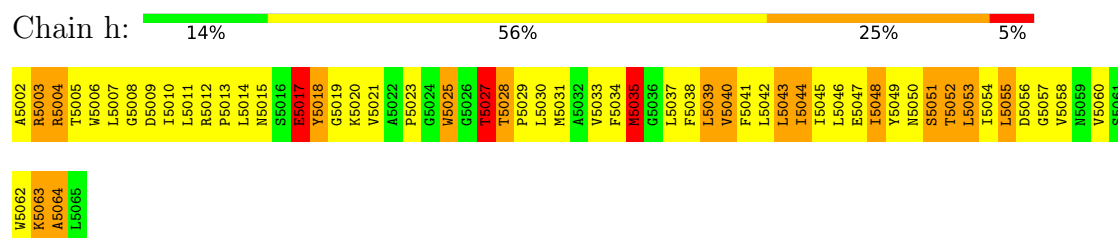
- Molecule 6: Cytochrome b559 subunit beta



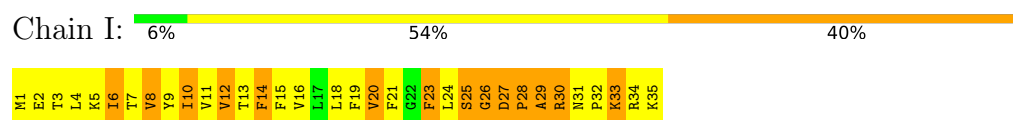
- Molecule 7: Photosystem II reaction center protein H



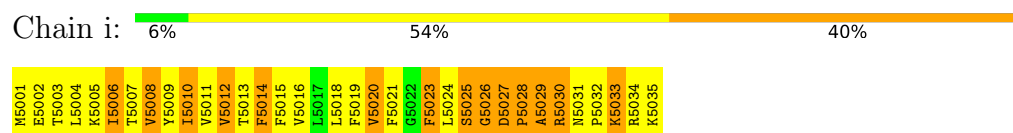
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

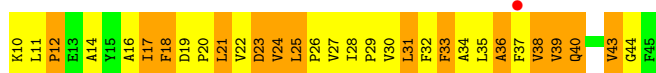
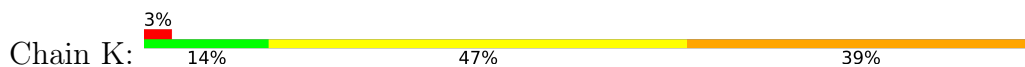




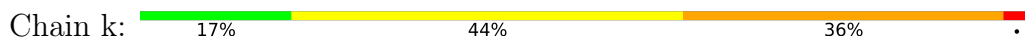
• Molecule 9: Photosystem II reaction center protein J



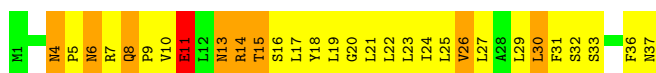
• Molecule 10: Photosystem II reaction center protein K



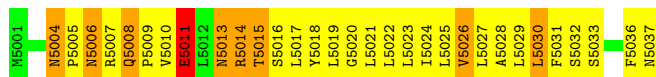
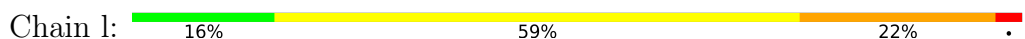
• Molecule 10: Photosystem II reaction center protein K



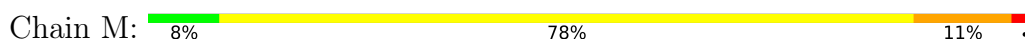
• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



• Molecule 12: Photosystem II reaction center protein M



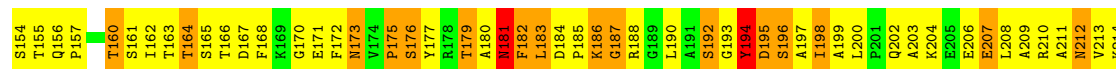
• Molecule 12: Photosystem II reaction center protein M





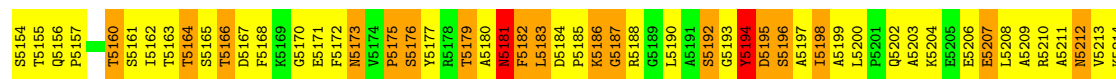
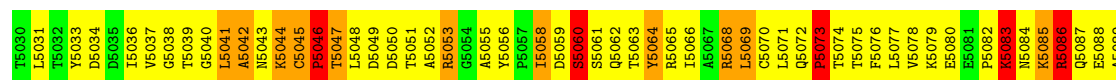
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 20% 55% 21%



• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 20% 55% 21%



• Molecule 14: Photosystem II reaction center protein T

Chain T: 10% 67% 20%

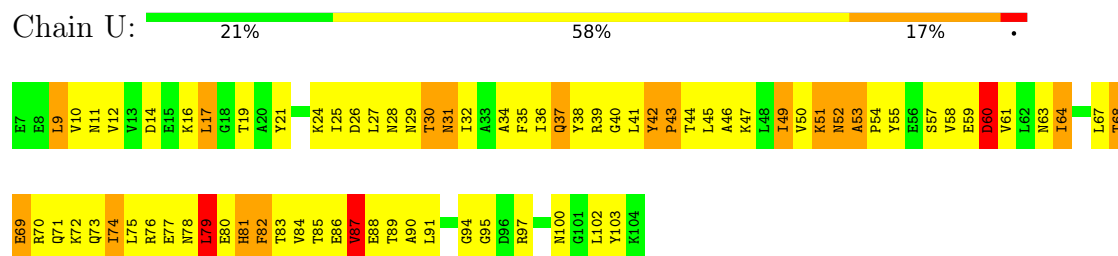


• Molecule 14: Photosystem II reaction center protein T

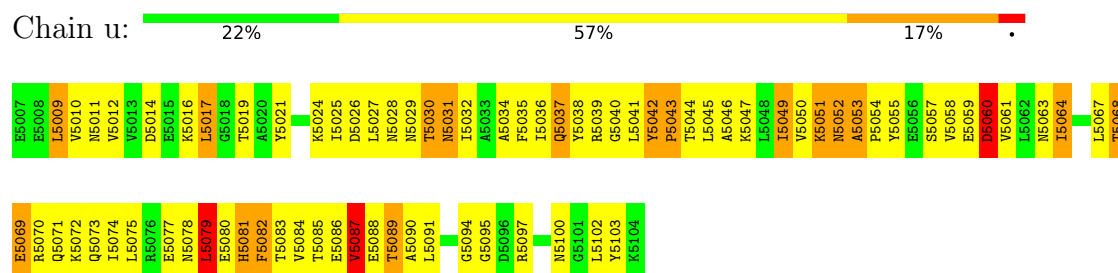
Chain t: 13% 63% 17% 7%



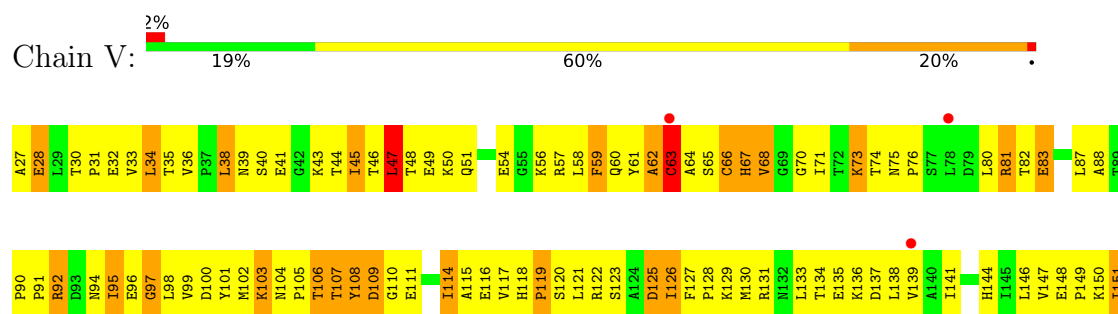
• Molecule 15: Photosystem II 12 kDa extrinsic protein



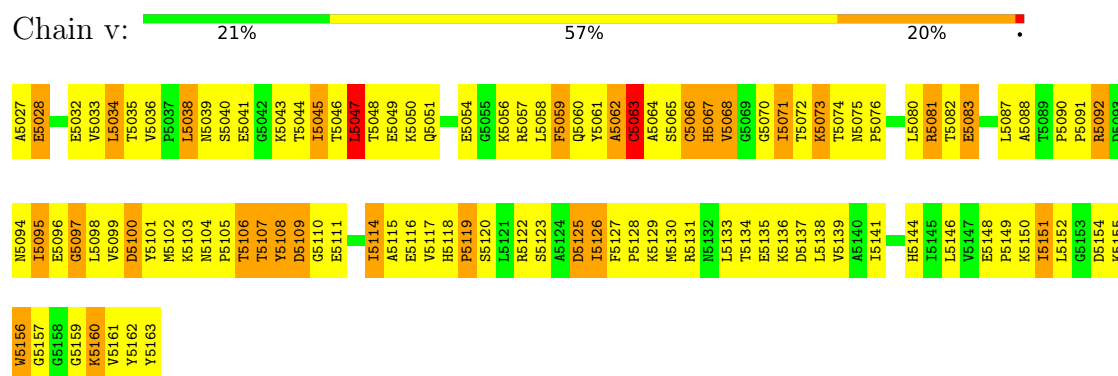
• Molecule 15: Photosystem II 12 kDa extrinsic protein



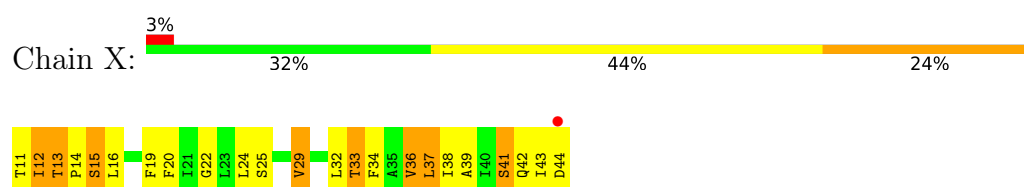
• Molecule 16: Cytochrome c-550



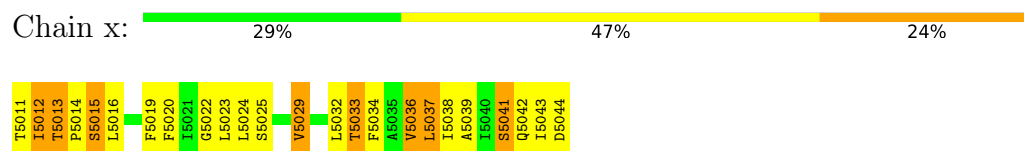
• Molecule 16: Cytochrome c-550



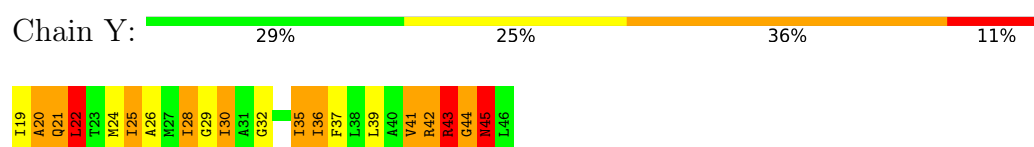
• Molecule 17: Photosystem II reaction center protein X



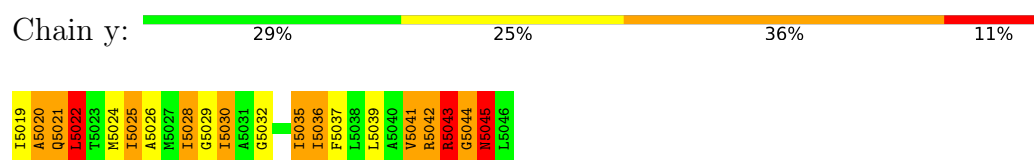
- Molecule 17: Photosystem II reaction center protein X



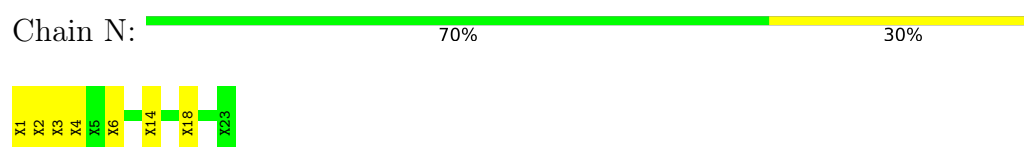
- Molecule 18: Photosystem II reaction center protein ycf12



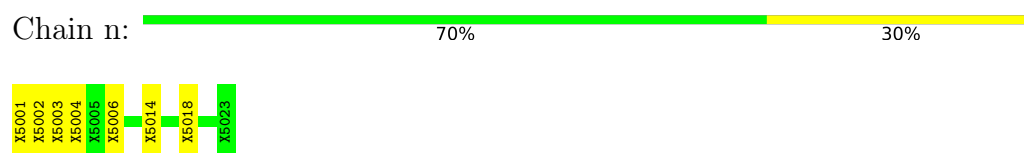
- Molecule 18: Photosystem II reaction center protein ycf12



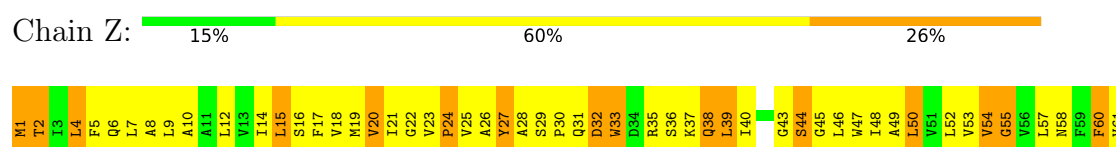
- Molecule 19: Photosystem II reaction center protein Y



- Molecule 19: Photosystem II reaction center protein Y

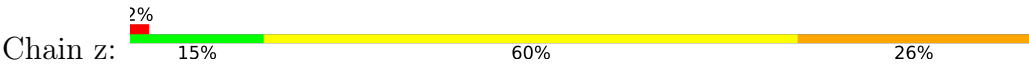


- Molecule 20: Photosystem II reaction center protein Z



V62

• Molecule 20: Photosystem II reaction center protein Z



V5061
V5062

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	128.50Å 224.70Å 304.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 20.00 – 4.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-4.00) 93.9 (20.00-4.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 4.07Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.290 , 0.326 0.278 , 0.279	Depositor DCC
R_{free} test set	3592 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	148.7	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	48060	wwPDB-VP
Average B, all atoms (Å ²)	165.0	wwPDB-VP

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

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: IOD, HEM, DGD, FE2, CLA, PQ9, LHG, MGE, BCR, OEC, 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	0.66	0/2714	1.19	38/3699 (1.0%)
1	a	0.66	0/2714	1.19	37/3699 (1.0%)
2	B	0.68	0/3971	1.27	59/5411 (1.1%)
2	b	0.68	0/3971	1.27	59/5411 (1.1%)
3	C	0.62	1/3568 (0.0%)	1.28	52/4858 (1.1%)
3	c	0.63	1/3568 (0.0%)	1.28	52/4858 (1.1%)
4	D	0.65	0/2801	1.22	34/3818 (0.9%)
4	d	0.65	0/2801	1.22	33/3818 (0.9%)
5	E	0.66	0/685	1.32	7/933 (0.8%)
5	e	0.66	0/685	1.32	7/933 (0.8%)
6	F	0.69	0/291	1.07	1/397 (0.3%)
6	f	0.69	0/291	1.07	1/397 (0.3%)
7	H	0.70	1/520 (0.2%)	1.27	8/708 (1.1%)
7	h	0.70	1/520 (0.2%)	1.27	8/708 (1.1%)
8	I	0.80	0/294	1.07	2/395 (0.5%)
8	i	0.80	0/294	1.07	2/395 (0.5%)
9	J	0.78	0/255	1.22	2/346 (0.6%)
9	j	0.78	0/255	1.22	2/346 (0.6%)
10	K	0.66	0/287	1.25	2/394 (0.5%)
10	k	0.66	0/287	1.27	3/394 (0.8%)
11	L	0.69	0/311	1.12	3/422 (0.7%)
11	l	0.69	0/311	1.11	3/422 (0.7%)
12	M	0.70	0/287	1.10	3/388 (0.8%)
12	m	0.70	0/287	1.09	3/388 (0.8%)
13	O	0.66	0/1891	1.24	23/2564 (0.9%)
13	o	0.66	0/1891	1.24	23/2564 (0.9%)
14	T	0.77	0/266	1.47	7/359 (1.9%)
14	t	0.74	0/266	1.45	7/359 (1.9%)
15	U	0.60	0/794	1.19	8/1076 (0.7%)
15	u	0.59	0/794	1.18	8/1076 (0.7%)
16	V	0.58	0/1085	1.18	13/1473 (0.9%)
16	v	0.58	0/1085	1.18	13/1473 (0.9%)

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

All (4) bond length outliers are listed below:

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

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

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2630	0	2528	776	0
1	a	2630	0	2528	771	0
2	B	3835	0	3700	851	0
2	b	3835	0	3700	836	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3455	0	3376	877	0
3	c	3455	0	3376	878	0
4	D	2706	0	2607	782	0
4	d	2706	0	2608	777	0
5	E	666	0	651	111	0
5	e	666	0	651	112	0
6	F	282	0	291	84	0
6	f	282	0	291	83	0
7	H	507	0	529	146	0
7	h	507	0	529	155	0
8	I	287	0	308	65	0
8	i	287	0	305	64	0
9	J	249	0	262	64	0
9	j	249	0	262	63	0
10	K	278	0	289	88	0
10	k	278	0	289	118	0
11	L	304	0	316	82	0
11	l	304	0	313	87	0
12	M	283	0	297	81	0
12	m	283	0	294	82	0
13	O	1860	0	1833	325	0
13	o	1860	0	1833	334	0
14	T	257	0	261	60	0
14	t	257	0	259	61	0
15	U	783	0	779	143	0
15	u	783	0	779	148	0
16	V	1064	0	1072	218	0
16	v	1064	0	1072	209	0
17	X	246	0	269	39	0
17	x	246	0	269	36	0
18	Y	208	0	237	77	0
18	y	208	0	237	76	0
19	N	116	0	26	5	0
19	n	116	0	26	5	0
20	Z	479	0	516	74	0
20	z	479	0	513	74	0
21	A	5	0	0	0	0
21	a	5	0	0	0	0
22	A	195	0	216	133	0
22	B	975	0	1080	648	0
22	C	780	0	864	478	0
22	D	195	0	216	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	65	0	72	46	0
22	K	65	0	72	89	0
22	a	195	0	216	135	0
22	b	975	0	1080	640	0
22	c	780	0	864	473	0
22	d	195	0	216	149	0
22	h	65	0	72	47	0
22	k	65	0	72	93	0
23	A	64	0	74	63	0
23	D	64	0	74	51	0
23	a	64	0	74	63	0
23	d	64	0	74	52	0
24	A	45	0	64	36	0
24	D	45	0	64	56	0
24	a	45	0	64	35	0
24	d	45	0	64	55	0
25	A	40	0	47	25	0
25	B	120	0	142	86	0
25	C	80	0	96	76	0
25	D	40	0	48	40	0
25	H	40	0	48	34	0
25	K	40	0	47	27	0
25	T	80	0	95	67	0
25	Z	40	0	47	17	0
25	a	40	0	47	26	0
25	b	80	0	95	62	0
25	c	40	0	48	36	0
25	d	40	0	48	39	0
25	h	40	0	48	34	0
25	k	80	0	95	74	0
25	t	40	0	48	44	0
25	z	40	0	47	19	0
26	A	49	0	74	36	0
26	a	49	0	74	36	0
27	A	1	0	0	1	0
27	B	1	0	0	3	0
27	D	2	0	0	10	0
27	T	1	0	0	2	0
27	a	1	0	0	0	0
27	b	1	0	0	0	0
27	d	2	0	0	10	0
27	t	1	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	48	0	72	39	0
28	D	96	0	144	66	0
28	L	48	0	72	29	0
28	b	48	0	72	38	0
28	d	96	0	144	67	0
28	l	48	0	72	27	0
29	B	66	0	96	32	0
29	C	198	0	288	118	0
29	b	66	0	96	34	0
29	c	198	0	288	121	0
30	D	1	0	0	0	0
30	a	1	0	0	0	0
31	F	43	0	30	17	0
31	V	43	0	30	12	0
31	f	43	0	30	17	0
31	v	43	0	30	10	0
All	All	48060	0	48531	11727	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 121.

The worst 5 of 11727 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:5169:PHE:HB3	27:d:6068:IOD:I	1.69	1.61
14:t:5012:CYS:SG	27:t:6066:IOD:I	1.65	1.58
25:k:6052:BCR:H371	25:k:6052:BCR:C26	1.34	1.56
22:B:1011:CLA:HED2	22:B:1012:CLA:CED	1.31	1.53
22:b:6011:CLA:HED2	22:b:6012:CLA:CED	1.31	1.53

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	219 (66%)	75 (22%)	39 (12%)	0	5
1	a	333/344 (97%)	216 (65%)	76 (23%)	41 (12%)	0	4
2	B	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	7
2	b	486/488 (100%)	350 (72%)	86 (18%)	50 (10%)	0	7
3	C	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	12
3	c	445/447 (100%)	330 (74%)	80 (18%)	35 (8%)	1	12
4	D	338/340 (99%)	222 (66%)	78 (23%)	38 (11%)	0	6
4	d	338/340 (99%)	224 (66%)	77 (23%)	37 (11%)	0	7
5	E	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0	5
5	e	80/83 (96%)	54 (68%)	17 (21%)	9 (11%)	0	5
6	F	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	4
6	f	33/44 (75%)	20 (61%)	9 (27%)	4 (12%)	0	4
7	H	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	4
7	h	62/64 (97%)	42 (68%)	12 (19%)	8 (13%)	0	4
8	I	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0	2
8	i	33/35 (94%)	21 (64%)	6 (18%)	6 (18%)	0	2
9	J	32/40 (80%)	29 (91%)	0	3 (9%)	0	10
9	j	32/40 (80%)	29 (91%)	0	3 (9%)	0	10
10	K	34/36 (94%)	23 (68%)	5 (15%)	6 (18%)	0	2
10	k	34/36 (94%)	17 (50%)	8 (24%)	9 (26%)	0	0
11	L	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	1	17
11	l	35/37 (95%)	25 (71%)	8 (23%)	2 (6%)	1	17
12	M	34/36 (94%)	23 (68%)	11 (32%)	0	100	100
12	m	34/36 (94%)	23 (68%)	11 (32%)	0	100	100
13	O	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0	5
13	o	240/242 (99%)	172 (72%)	41 (17%)	27 (11%)	0	5
14	T	28/30 (93%)	22 (79%)	5 (18%)	1 (4%)	2	23
14	t	28/30 (93%)	22 (79%)	4 (14%)	2 (7%)	1	14
15	U	96/98 (98%)	70 (73%)	17 (18%)	9 (9%)	0	10
15	u	96/98 (98%)	70 (73%)	18 (19%)	8 (8%)	0	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	V	135/137 (98%)	100 (74%)	25 (18%)	10 (7%)	1	13
16	v	135/137 (98%)	99 (73%)	26 (19%)	10 (7%)	1	13
17	X	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
17	x	32/34 (94%)	29 (91%)	3 (9%)	0	100	100
18	Y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0	2
18	y	26/28 (93%)	20 (77%)	1 (4%)	5 (19%)	0	2
20	Z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	15
20	z	60/62 (97%)	44 (73%)	12 (20%)	4 (7%)	1	15
All	All	5124/5250 (98%)	3622 (71%)	986 (19%)	516 (10%)	0	8

5 of 516 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/73 (99%)	57 (79%)	15 (21%)	1	7
5	e	72/73 (99%)	57 (79%)	15 (21%)	1	7
6	F	29/38 (76%)	22 (76%)	7 (24%)	1	5
6	f	29/38 (76%)	22 (76%)	7 (24%)	1	5
7	H	54/54 (100%)	45 (83%)	9 (17%)	2	13
7	h	54/54 (100%)	45 (83%)	9 (17%)	2	13
8	I	32/32 (100%)	24 (75%)	8 (25%)	0	4
8	i	32/32 (100%)	24 (75%)	8 (25%)	0	4
9	J	24/28 (86%)	18 (75%)	6 (25%)	0	4
9	j	24/28 (86%)	18 (75%)	6 (25%)	0	4
10	K	29/29 (100%)	21 (72%)	8 (28%)	0	3
10	k	29/29 (100%)	23 (79%)	6 (21%)	1	7
11	L	35/35 (100%)	29 (83%)	6 (17%)	2	13
11	l	35/35 (100%)	29 (83%)	6 (17%)	2	13
12	M	33/33 (100%)	28 (85%)	5 (15%)	3	15
12	m	33/33 (100%)	28 (85%)	5 (15%)	3	15
13	O	206/206 (100%)	170 (82%)	36 (18%)	2	13
13	o	206/206 (100%)	170 (82%)	36 (18%)	2	13
14	T	27/27 (100%)	24 (89%)	3 (11%)	6	23
14	t	27/27 (100%)	24 (89%)	3 (11%)	6	23
15	U	85/85 (100%)	74 (87%)	11 (13%)	4	19
15	u	85/85 (100%)	75 (88%)	10 (12%)	5	21
16	V	117/117 (100%)	96 (82%)	21 (18%)	2	12
16	v	117/117 (100%)	97 (83%)	20 (17%)	2	13
17	X	27/27 (100%)	16 (59%)	11 (41%)	0	0
17	x	27/27 (100%)	16 (59%)	11 (41%)	0	0
18	Y	21/21 (100%)	11 (52%)	10 (48%)	0	0
18	y	21/21 (100%)	11 (52%)	10 (48%)	0	0
20	Z	52/52 (100%)	41 (79%)	11 (21%)	1	7
20	z	52/52 (100%)	41 (79%)	11 (21%)	1	7
All	All	4250/4296 (99%)	3434 (81%)	816 (19%)	1	10

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

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

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

Mol	Chain	Res	Type
1	a	5267	ASN
3	c	5294	ASN
20	z	5006	GLN
1	a	5312	ASN
2	b	5274	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 136 ligands modelled in this entry, 12 are monoatomic - leaving 124 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	6003	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
23	PHO	a	6038	-	58,69,69	2.94	13 (22%)	55,99,99	3.53	19 (34%)
22	CLA	B	1013	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
24	PQ9	D	1042	-	45,45,45	0.68	2 (4%)	56,57,57	1.79	17 (30%)
22	CLA	c	6026	-	69,73,73	1.93	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	A	1006	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
29	DGD	c	6056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6014	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
31	HEM	v	6041	16	50,50,50	1.88	8 (16%)	67,82,82	1.36	5 (7%)
25	BCR	t	1046	-	41,41,41	3.96	17 (41%)	56,56,56	6.06	26 (46%)
22	CLA	a	6006	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
23	PHO	A	1038	-	58,69,69	2.94	13 (22%)	55,99,99	3.53	19 (34%)
22	CLA	D	1005	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
28	MGE	D	1062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
25	BCR	b	6045	-	41,41,41	4.02	17 (41%)	56,56,56	6.17	20 (35%)
25	BCR	k	6052	-	41,41,41	4.02	17 (41%)	56,56,56	6.97	24 (42%)
22	CLA	B	1020	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	D	1008	-	69,73,73	1.92	17 (24%)	82,113,113	2.48	29 (35%)
22	CLA	B	1015	-	69,73,73	1.93	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	C	1031	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1016	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	C	1032	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	k	6034	-	69,73,73	1.93	16 (23%)	82,113,113	2.49	28 (34%)
25	BCR	C	1052	-	41,41,41	4.02	17 (41%)	56,56,56	6.97	24 (42%)
22	CLA	B	1018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1021	2	69,73,73	1.92	16 (23%)	82,113,113	2.49	30 (36%)
26	LHG	A	1063	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
22	CLA	b	6024	-	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
22	CLA	b	6011	-	69,73,73	1.92	17 (24%)	82,113,113	2.48	30 (36%)
22	CLA	d	6004	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	K	1051	-	41,41,41	4.03	17 (41%)	56,56,56	4.97	20 (35%)
25	BCR	T	6048	-	41,41,41	4.01	17 (41%)	56,56,56	6.30	27 (48%)
22	CLA	c	6030	-	69,73,73	1.91	17 (24%)	82,113,113	2.48	29 (35%)
22	CLA	A	1003	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	b	6019	-	69,73,73	1.93	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
28	MGE	d	6062	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	b	6012	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	B	1014	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	c	6028	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
22	CLA	C	1033	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	h	6017	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	C	1027	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	b	6010	2	69,73,73	1.91	16 (23%)	82,113,113	2.49	29 (35%)
25	BCR	a	6044	-	41,41,41	3.92	16 (39%)	56,56,56	7.23	28 (50%)
22	CLA	B	1023	-	69,73,73	1.91	16 (23%)	82,113,113	2.48	29 (35%)
22	CLA	d	6008	-	69,73,73	1.92	18 (26%)	82,113,113	2.48	29 (35%)
25	BCR	Z	1053	-	41,41,41	4.03	17 (41%)	56,56,56	6.02	21 (37%)
29	DGD	B	1058	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	c	6033	-	69,73,73	1.94	16 (23%)	82,113,113	2.47	28 (34%)
25	BCR	D	1050	-	41,41,41	4.02	17 (41%)	56,56,56	5.17	22 (39%)
25	BCR	B	1048	-	41,41,41	4.01	17 (41%)	56,56,56	6.30	27 (48%)
22	CLA	c	6032	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	28 (34%)
22	CLA	D	1004	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	a	6007	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	C	1025	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	f	6040	5	50,50,50	1.87	9 (18%)	67,82,82	1.34	5 (7%)
22	CLA	B	1010	2	69,73,73	1.92	16 (23%)	82,113,113	2.49	29 (35%)
22	CLA	K	1034	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
29	DGD	C	1056	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
24	PQ9	d	6042	-	45,45,45	0.68	2 (4%)	56,57,57	1.79	17 (30%)
22	CLA	c	6027	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	b	6023	-	69,73,73	1.91	16 (23%)	82,113,113	2.48	29 (35%)
22	CLA	C	1036	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	C	1028	-	69,73,73	1.93	16 (23%)	82,113,113	2.47	27 (32%)
22	CLA	b	6022	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	d	6005	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	B	1011	-	69,73,73	1.92	16 (23%)	82,113,113	2.47	30 (36%)
22	CLA	C	1029	-	69,73,73	1.91	17 (24%)	82,113,113	2.48	29 (35%)
25	BCR	A	1044	-	41,41,41	3.93	16 (39%)	56,56,56	7.23	28 (50%)
22	CLA	C	1030	-	69,73,73	1.91	17 (24%)	82,113,113	2.48	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	1035	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	b	6047	-	41,41,41	4.02	17 (41%)	56,56,56	5.46	27 (48%)
23	PHO	d	6039	-	58,69,69	2.94	13 (22%)	55,99,99	3.52	19 (34%)
22	CLA	c	6037	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	c	6025	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
26	LHG	a	6063	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
25	BCR	k	6051	-	41,41,41	4.03	17 (41%)	56,56,56	4.97	20 (35%)
31	HEM	V	1041	16	50,50,50	1.88	8 (16%)	67,82,82	1.35	5 (7%)
22	CLA	b	6013	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	B	1045	-	41,41,41	4.02	17 (41%)	56,56,56	6.17	21 (37%)
22	CLA	b	6021	2	69,73,73	1.92	16 (23%)	82,113,113	2.49	30 (36%)
22	CLA	b	6018	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	A	1007	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
22	CLA	B	1012	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	b	6015	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	C	1037	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	B	1024	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
28	MGE	b	6060	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	B	1019	-	69,73,73	1.93	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	B	1047	-	41,41,41	4.01	17 (41%)	56,56,56	5.46	26 (46%)
29	DGD	c	6055	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
25	BCR	T	6046	-	41,41,41	3.96	17 (41%)	56,56,56	6.06	26 (46%)
22	CLA	b	6009	-	69,73,73	1.91	15 (21%)	82,113,113	2.47	29 (35%)
25	BCR	h	6049	-	41,41,41	4.02	17 (41%)	56,56,56	5.30	20 (35%)
25	BCR	H	1049	-	41,41,41	4.02	16 (39%)	56,56,56	5.30	20 (35%)
28	MGE	L	1061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
29	DGD	c	6057	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
28	MGE	B	1060	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
22	CLA	c	6031	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
25	BCR	c	6054	-	41,41,41	4.02	16 (39%)	56,56,56	5.43	21 (37%)
25	BCR	C	1054	-	41,41,41	4.02	16 (39%)	56,56,56	5.42	21 (37%)
29	DGD	b	6058	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	H	1017	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
29	DGD	C	1055	-	67,67,67	0.86	2 (2%)	81,81,81	0.91	3 (3%)
22	CLA	b	6020	-	69,73,73	1.94	15 (21%)	82,113,113	2.49	28 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	MGE	d	6059	-	48,48,48	0.97	2 (4%)	56,56,56	1.01	3 (5%)
22	CLA	c	6036	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	b	6016	-	69,73,73	1.93	15 (21%)	82,113,113	2.48	28 (34%)
28	MGE	D	1059	-	48,48,48	0.97	2 (4%)	56,56,56	1.02	3 (5%)
25	BCR	z	6053	-	41,41,41	4.03	17 (41%)	56,56,56	6.02	22 (39%)
28	MGE	l	6061	-	48,48,48	0.96	2 (4%)	56,56,56	1.02	3 (5%)
29	DGD	C	1057	-	67,67,67	0.85	2 (2%)	81,81,81	0.91	3 (3%)
24	PQ9	A	1043	-	45,45,45	0.68	2 (4%)	56,57,57	1.79	17 (30%)
22	CLA	B	1009	-	69,73,73	1.92	15 (21%)	82,113,113	2.47	29 (35%)
25	BCR	d	6050	-	41,41,41	4.02	17 (41%)	56,56,56	5.17	21 (37%)
22	CLA	B	1022	-	69,73,73	1.94	16 (23%)	82,113,113	2.48	28 (34%)
31	HEM	F	1040	5	50,50,50	1.87	8 (16%)	67,82,82	1.34	5 (7%)
22	CLA	C	1026	-	69,73,73	1.94	15 (21%)	82,113,113	2.48	28 (34%)
22	CLA	c	6035	-	69,73,73	1.94	16 (23%)	82,113,113	2.49	28 (34%)
23	PHO	D	1039	-	58,69,69	2.94	13 (22%)	55,99,99	3.52	19 (34%)
24	PQ9	a	6043	-	45,45,45	0.69	2 (4%)	56,57,57	1.79	17 (30%)
22	CLA	c	6029	-	69,73,73	1.91	16 (23%)	82,113,113	2.48	29 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	6003	-	2/2/15/20	23/39/115/115	-
23	PHO	a	6038	-	1/1/17/22	18/37/103/103	0/5/6/6
22	CLA	B	1013	-	2/2/15/20	24/39/115/115	-
24	PQ9	D	1042	-	-	11/41/61/61	0/1/1/1
22	CLA	c	6026	-	1/1/15/20	18/39/115/115	-
22	CLA	A	1006	-	2/2/15/20	19/39/115/115	-
29	DGD	c	6056	-	-	32/55/95/95	0/2/2/2
22	CLA	b	6014	-	2/2/15/20	18/39/115/115	-
31	HEM	v	6041	16	-	5/14/54/54	-
25	BCR	t	1046	-	-	11/29/63/63	0/2/2/2
22	CLA	a	6006	-	2/2/15/20	19/39/115/115	-
23	PHO	A	1038	-	1/1/17/22	18/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	1005	-	2/2/15/20	20/39/115/115	-
28	MGE	D	1062	-	-	24/43/63/63	0/1/1/1
25	BCR	b	6045	-	-	20/29/63/63	0/2/2/2
25	BCR	k	6052	-	-	13/29/63/63	0/2/2/2
22	CLA	B	1020	-	3/3/15/20	18/39/115/115	-
22	CLA	D	1008	-	3/3/15/20	15/39/115/115	-
22	CLA	B	1015	-	2/2/15/20	18/39/115/115	-
22	CLA	C	1031	-	2/2/15/20	14/39/115/115	-
22	CLA	B	1016	-	1/1/15/20	20/39/115/115	-
22	CLA	C	1032	-	3/3/15/20	19/39/115/115	-
22	CLA	k	6034	-	5/5/15/20	24/39/115/115	-
25	BCR	C	1052	-	-	13/29/63/63	0/2/2/2
22	CLA	B	1018	-	2/2/15/20	23/39/115/115	-
22	CLA	B	1021	2	2/2/15/20	24/39/115/115	-
26	LHG	A	1063	-	-	27/53/53/53	-
22	CLA	b	6024	-	1/1/15/20	17/39/115/115	-
22	CLA	b	6011	-	3/3/15/20	21/39/115/115	-
22	CLA	d	6004	-	2/2/15/20	12/39/115/115	-
25	BCR	K	1051	-	-	15/29/63/63	0/2/2/2
25	BCR	T	6048	-	-	10/29/63/63	0/2/2/2
22	CLA	c	6030	-	2/2/15/20	18/39/115/115	-
22	CLA	A	1003	-	2/2/15/20	23/39/115/115	-
22	CLA	b	6019	-	2/2/15/20	19/39/115/115	-
28	MGE	d	6062	-	-	24/43/63/63	0/1/1/1
22	CLA	b	6012	-	2/2/15/20	18/39/115/115	-
22	CLA	B	1014	-	2/2/15/20	18/39/115/115	-
22	CLA	c	6028	-	2/2/15/20	24/39/115/115	-
22	CLA	C	1033	-	2/2/15/20	16/39/115/115	-
22	CLA	h	6017	-	2/2/15/20	24/39/115/115	-
22	CLA	C	1027	-	3/3/15/20	18/39/115/115	-
22	CLA	b	6010	2	2/2/15/20	15/39/115/115	-
25	BCR	a	6044	-	-	12/29/63/63	0/2/2/2
22	CLA	B	1023	-	3/3/15/20	16/39/115/115	-
22	CLA	d	6008	-	3/3/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	Z	1053	-	-	15/29/63/63	0/2/2/2
29	DGD	B	1058	-	-	32/55/95/95	0/2/2/2
22	CLA	c	6033	-	2/2/15/20	16/39/115/115	-
25	BCR	D	1050	-	-	21/29/63/63	0/2/2/2
25	BCR	B	1048	-	-	10/29/63/63	0/2/2/2
22	CLA	c	6032	-	3/3/15/20	19/39/115/115	-
22	CLA	D	1004	-	2/2/15/20	12/39/115/115	-
22	CLA	a	6007	-	1/1/15/20	25/39/115/115	-
22	CLA	C	1025	-	2/2/15/20	17/39/115/115	-
31	HEM	f	6040	5	-	10/14/54/54	-
22	CLA	B	1010	2	2/2/15/20	15/39/115/115	-
22	CLA	K	1034	-	5/5/15/20	24/39/115/115	-
29	DGD	C	1056	-	-	32/55/95/95	0/2/2/2
24	PQ9	d	6042	-	-	11/41/61/61	0/1/1/1
22	CLA	c	6027	-	3/3/15/20	18/39/115/115	-
22	CLA	b	6023	-	3/3/15/20	16/39/115/115	-
22	CLA	C	1036	-	2/2/15/20	23/39/115/115	-
22	CLA	C	1028	-	2/2/15/20	24/39/115/115	-
22	CLA	b	6022	-	3/3/15/20	20/39/115/115	-
22	CLA	d	6005	-	2/2/15/20	20/39/115/115	-
22	CLA	B	1011	-	3/3/15/20	21/39/115/115	-
22	CLA	C	1029	-	3/3/15/20	15/39/115/115	-
25	BCR	A	1044	-	-	12/29/63/63	0/2/2/2
22	CLA	C	1030	-	2/2/15/20	18/39/115/115	-
22	CLA	C	1035	-	2/2/15/20	14/39/115/115	-
25	BCR	b	6047	-	-	17/29/63/63	0/2/2/2
23	PHO	d	6039	-	3/3/17/22	16/37/103/103	0/5/6/6
22	CLA	c	6037	-	2/2/15/20	16/39/115/115	-
22	CLA	c	6025	-	2/2/15/20	17/39/115/115	-
26	LHG	a	6063	-	-	28/53/53/53	-
25	BCR	k	6051	-	-	15/29/63/63	0/2/2/2
31	HEM	V	1041	16	-	6/14/54/54	-
22	CLA	b	6013	-	2/2/15/20	24/39/115/115	-
25	BCR	B	1045	-	-	20/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	6021	2	2/2/15/20	24/39/115/115	-
22	CLA	b	6018	-	2/2/15/20	23/39/115/115	-
22	CLA	A	1007	-	1/1/15/20	25/39/115/115	-
22	CLA	B	1012	-	2/2/15/20	18/39/115/115	-
22	CLA	b	6015	-	2/2/15/20	18/39/115/115	-
22	CLA	C	1037	-	2/2/15/20	16/39/115/115	-
22	CLA	B	1024	-	1/1/15/20	17/39/115/115	-
28	MGE	b	6060	-	-	31/43/63/63	0/1/1/1
22	CLA	B	1019	-	2/2/15/20	19/39/115/115	-
25	BCR	B	1047	-	-	17/29/63/63	0/2/2/2
29	DGD	c	6055	-	-	33/55/95/95	0/2/2/2
25	BCR	T	6046	-	-	11/29/63/63	0/2/2/2
22	CLA	b	6009	-	2/2/15/20	17/39/115/115	-
25	BCR	h	6049	-	-	13/29/63/63	0/2/2/2
25	BCR	H	1049	-	-	13/29/63/63	0/2/2/2
28	MGE	L	1061	-	-	26/43/63/63	0/1/1/1
29	DGD	c	6057	-	-	32/55/95/95	0/2/2/2
28	MGE	B	1060	-	-	31/43/63/63	0/1/1/1
22	CLA	c	6031	-	2/2/15/20	14/39/115/115	-
25	BCR	c	6054	-	-	14/29/63/63	0/2/2/2
25	BCR	C	1054	-	-	14/29/63/63	0/2/2/2
29	DGD	b	6058	-	-	32/55/95/95	0/2/2/2
22	CLA	H	1017	-	2/2/15/20	24/39/115/115	-
29	DGD	C	1055	-	-	33/55/95/95	0/2/2/2
22	CLA	b	6020	-	3/3/15/20	18/39/115/115	-
28	MGE	d	6059	-	-	23/43/63/63	0/1/1/1
22	CLA	c	6036	-	2/2/15/20	23/39/115/115	-
22	CLA	b	6016	-	1/1/15/20	20/39/115/115	-
28	MGE	D	1059	-	-	23/43/63/63	0/1/1/1
25	BCR	z	6053	-	-	15/29/63/63	0/2/2/2
28	MGE	l	6061	-	-	26/43/63/63	0/1/1/1
29	DGD	C	1057	-	-	32/55/95/95	0/2/2/2
24	PQ9	A	1043	-	-	16/41/61/61	0/1/1/1
22	CLA	B	1009	-	2/2/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	d	6050	-	-	21/29/63/63	0/2/2/2
22	CLA	B	1022	-	3/3/15/20	20/39/115/115	-
31	HEM	F	1040	5	-	10/14/54/54	-
22	CLA	C	1026	-	1/1/15/20	18/39/115/115	-
22	CLA	c	6035	-	2/2/15/20	14/39/115/115	-
23	PHO	D	1039	-	3/3/17/22	16/37/103/103	0/5/6/6
24	PQ9	a	6043	-	-	16/41/61/61	0/1/1/1
22	CLA	c	6029	-	3/3/15/20	15/39/115/115	-

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

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

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

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

5 of 162 chirality outliers are listed below:

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

5 of 2320 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
22	A	1003	CLA	C2B-C3B-CAB-CBB
22	A	1003	CLA	C4B-C3B-CAB-CBB
22	A	1003	CLA	CBD-CGD-O2D-CED
22	A	1003	CLA	O1D-CGD-O2D-CED

There are no ring outliers.

122 monomers are involved in 4181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	a	6003	CLA	51	0
23	a	6038	PHO	63	0
22	B	1013	CLA	65	0
24	D	1042	PQ9	56	0
22	c	6026	CLA	28	0
22	A	1006	CLA	44	0
29	c	6056	DGD	59	0
22	b	6014	CLA	41	0
31	v	6041	HEM	10	0
25	t	1046	BCR	44	0
22	a	6006	CLA	47	0
23	A	1038	PHO	63	0
22	D	1005	CLA	58	0
28	D	1062	MGE	21	0
25	b	6045	BCR	21	0
25	k	6052	BCR	51	0
22	B	1020	CLA	52	0
22	D	1008	CLA	48	0
22	B	1015	CLA	47	0
22	C	1031	CLA	63	0
22	B	1016	CLA	46	0
22	C	1032	CLA	42	0
22	k	6034	CLA	93	0
25	C	1052	BCR	38	0
22	B	1018	CLA	34	0
22	B	1021	CLA	60	0
26	A	1063	LHG	36	0
22	b	6024	CLA	45	0
22	b	6011	CLA	87	0
22	d	6004	CLA	52	0
25	K	1051	BCR	27	0
25	T	6048	BCR	23	0
22	c	6030	CLA	37	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1003	CLA	51	0
22	b	6019	CLA	37	0
28	d	6062	MGE	21	0
22	b	6012	CLA	61	0
22	B	1014	CLA	44	0
22	c	6028	CLA	37	0
22	C	1033	CLA	66	0
22	h	6017	CLA	47	0
22	C	1027	CLA	35	0
22	b	6010	CLA	37	0
25	a	6044	BCR	26	0
22	B	1023	CLA	68	0
22	d	6008	CLA	46	0
25	Z	1053	BCR	17	0
29	B	1058	DGD	32	0
22	c	6033	CLA	68	0
25	D	1050	BCR	40	0
25	B	1048	BCR	23	0
22	c	6032	CLA	39	0
22	D	1004	CLA	51	0
22	a	6007	CLA	38	0
22	C	1025	CLA	64	0
31	f	6040	HEM	17	0
22	B	1010	CLA	38	0
22	K	1034	CLA	89	0
29	C	1056	DGD	55	0
24	d	6042	PQ9	55	0
22	c	6027	CLA	37	0
22	b	6023	CLA	67	0
22	C	1036	CLA	22	0
22	C	1028	CLA	37	0
22	b	6022	CLA	76	0
22	d	6005	CLA	57	0
22	B	1011	CLA	86	0
22	C	1029	CLA	62	0
25	A	1044	BCR	25	0
22	C	1030	CLA	37	0
22	C	1035	CLA	53	0
25	b	6047	BCR	42	0
23	d	6039	PHO	52	0
22	c	6037	CLA	21	0
22	c	6025	CLA	65	0

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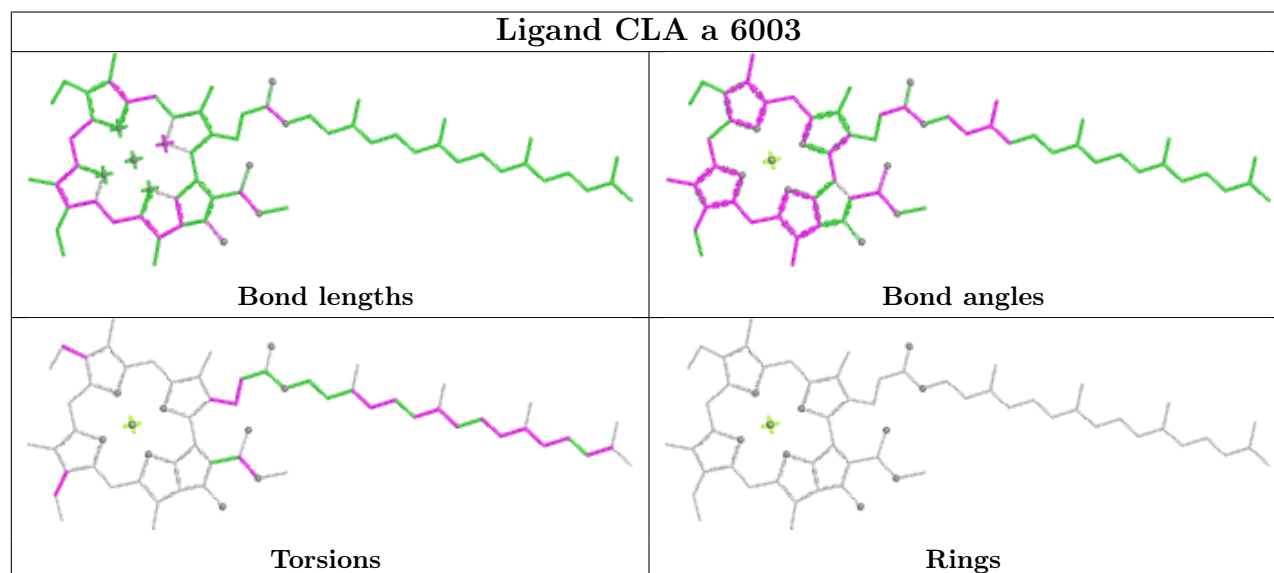
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	a	6063	LHG	36	0
25	k	6051	BCR	26	0
31	V	1041	HEM	12	0
22	b	6013	CLA	63	0
25	B	1045	BCR	21	0
22	b	6021	CLA	57	0
22	b	6018	CLA	35	0
22	A	1007	CLA	39	0
22	B	1012	CLA	61	0
22	b	6015	CLA	46	0
22	C	1037	CLA	21	0
22	B	1024	CLA	45	0
28	b	6060	MGE	38	0
22	B	1019	CLA	40	0
25	B	1047	BCR	43	0
29	c	6055	DGD	25	0
25	T	6046	BCR	44	0
22	b	6009	CLA	62	0
25	h	6049	BCR	34	0
25	H	1049	BCR	34	0
28	L	1061	MGE	29	0
29	c	6057	DGD	41	0
28	B	1060	MGE	39	0
22	c	6031	CLA	61	0
25	c	6054	BCR	36	0
25	C	1054	BCR	38	0
29	b	6058	DGD	34	0
22	H	1017	CLA	46	0
29	C	1055	DGD	26	0
22	b	6020	CLA	52	0
28	d	6059	MGE	46	0
22	c	6036	CLA	21	0
22	b	6016	CLA	43	0
28	D	1059	MGE	45	0
25	z	6053	BCR	19	0
28	l	6061	MGE	27	0
29	C	1057	DGD	41	0
24	A	1043	PQ9	36	0
22	B	1009	CLA	59	0
25	d	6050	BCR	39	0
22	B	1022	CLA	74	0
31	F	1040	HEM	17	0

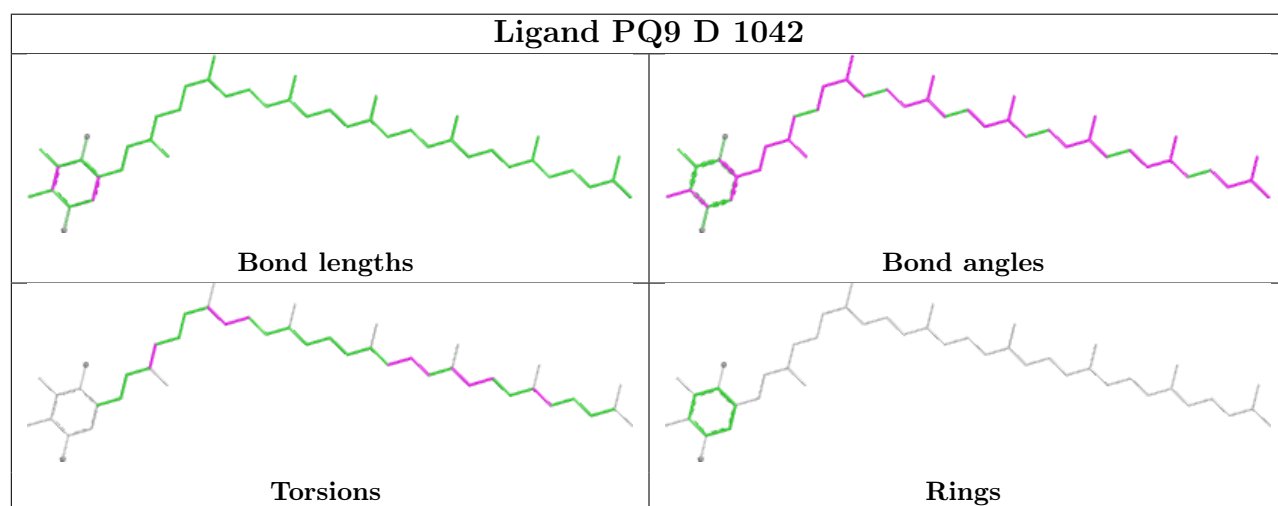
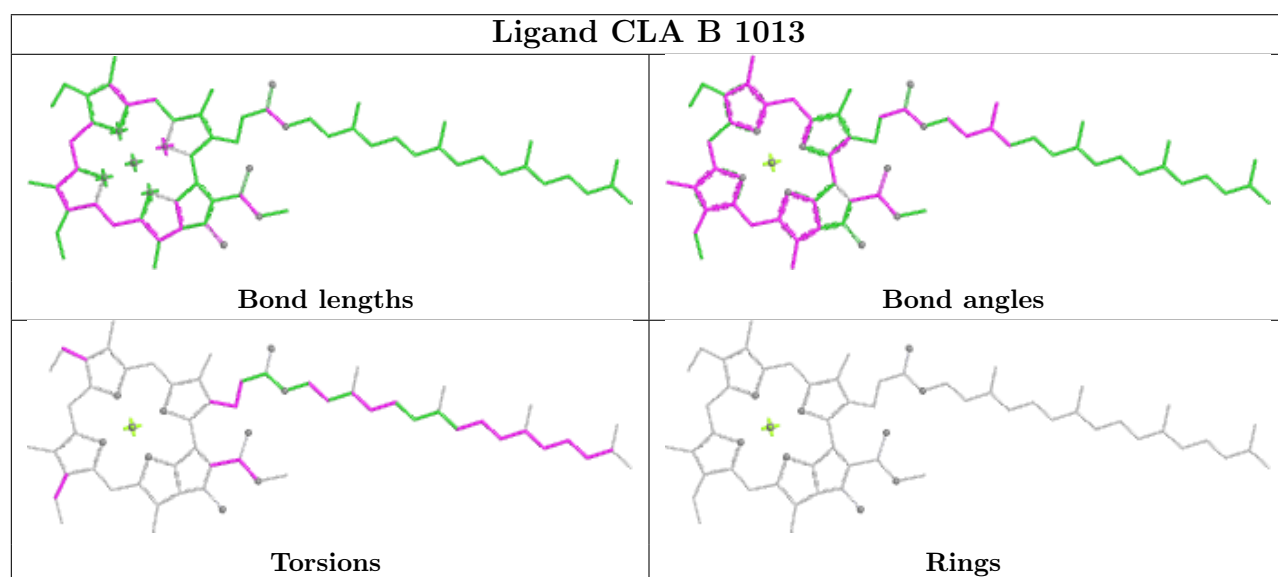
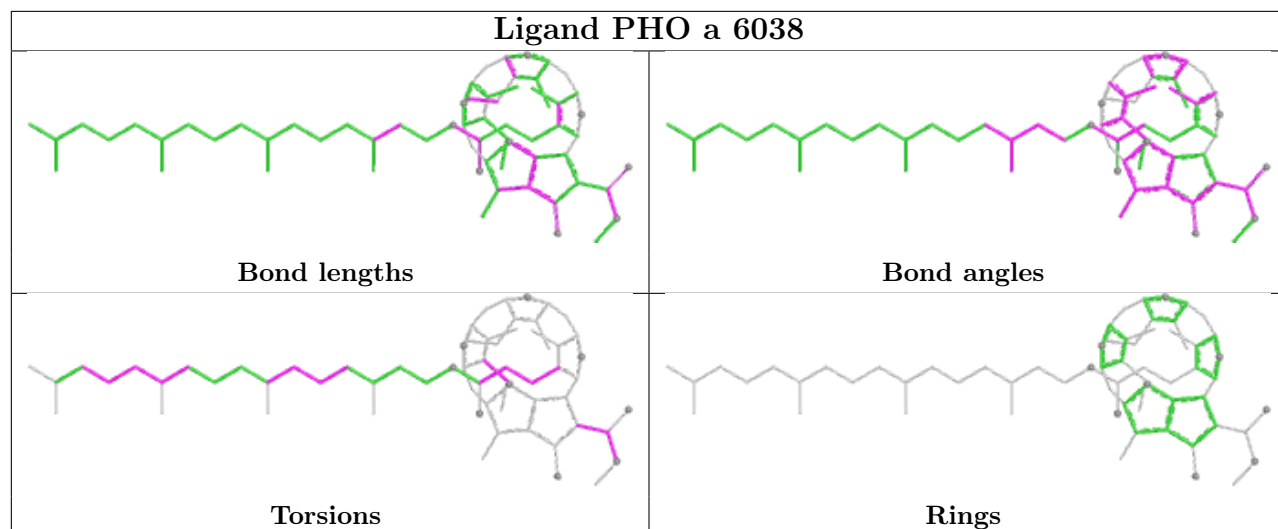
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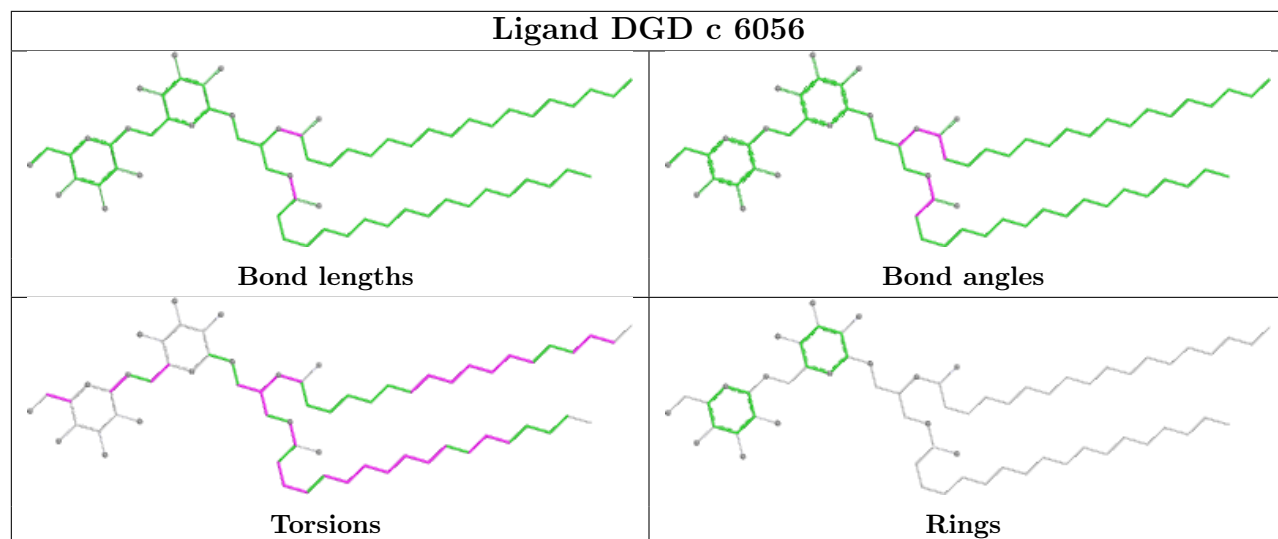
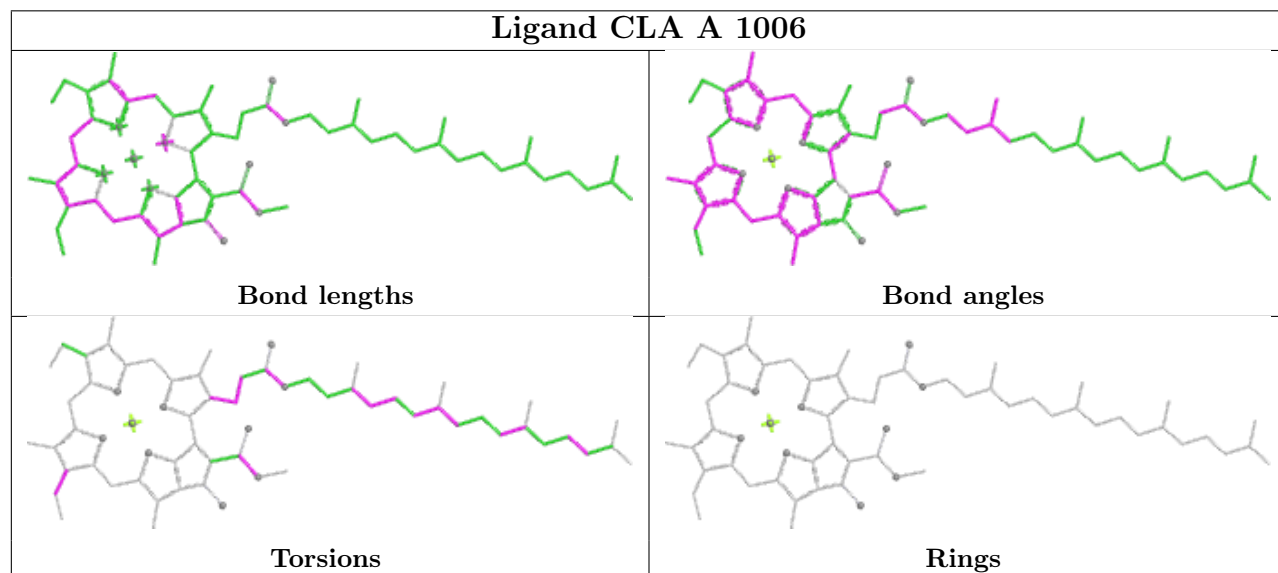
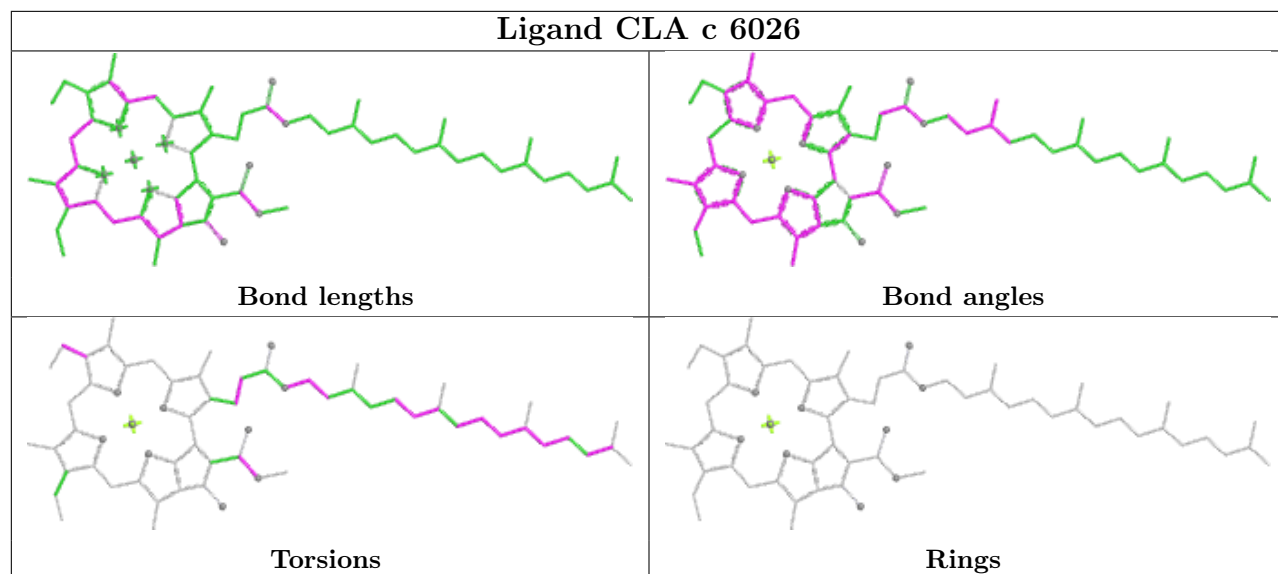
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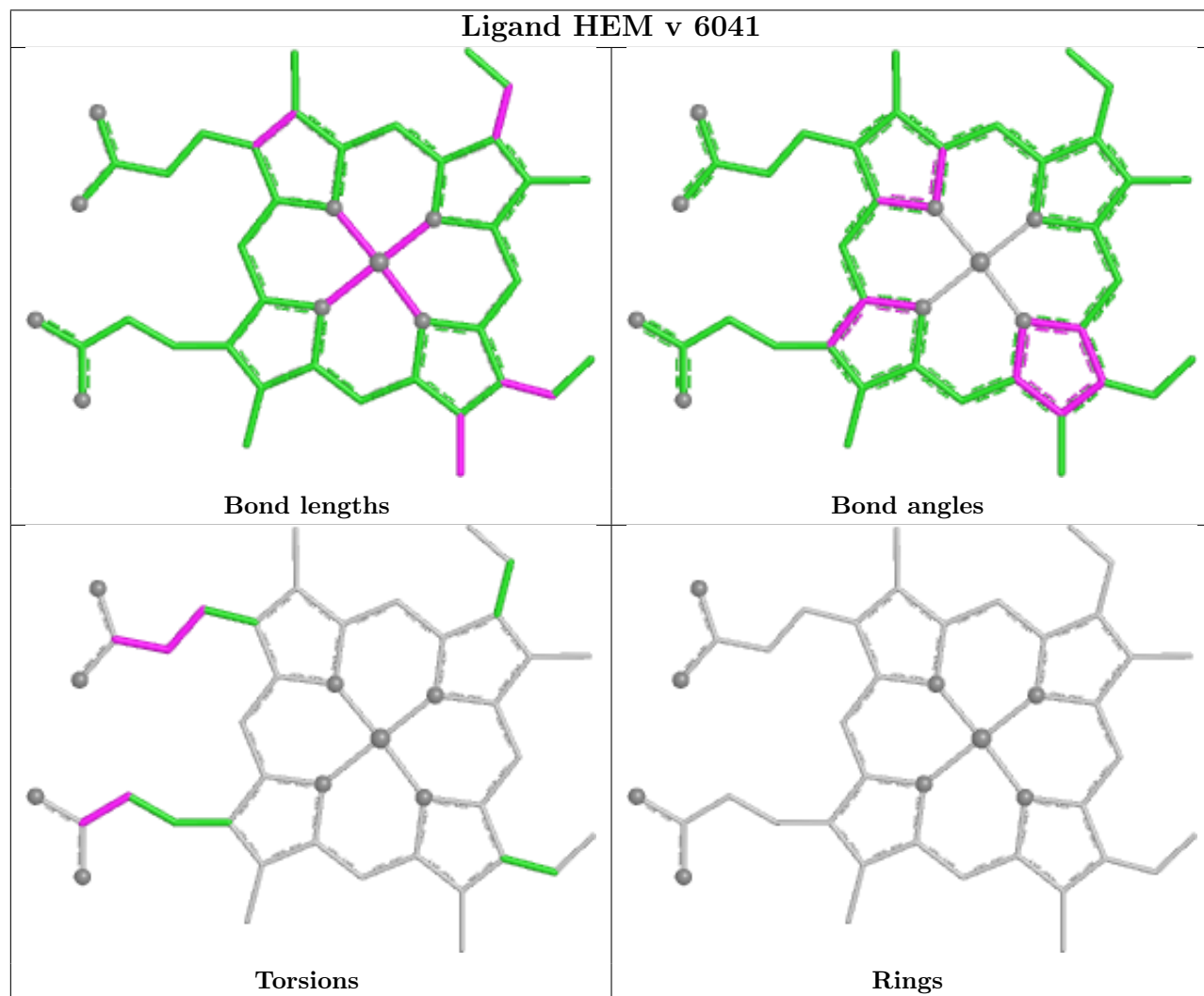
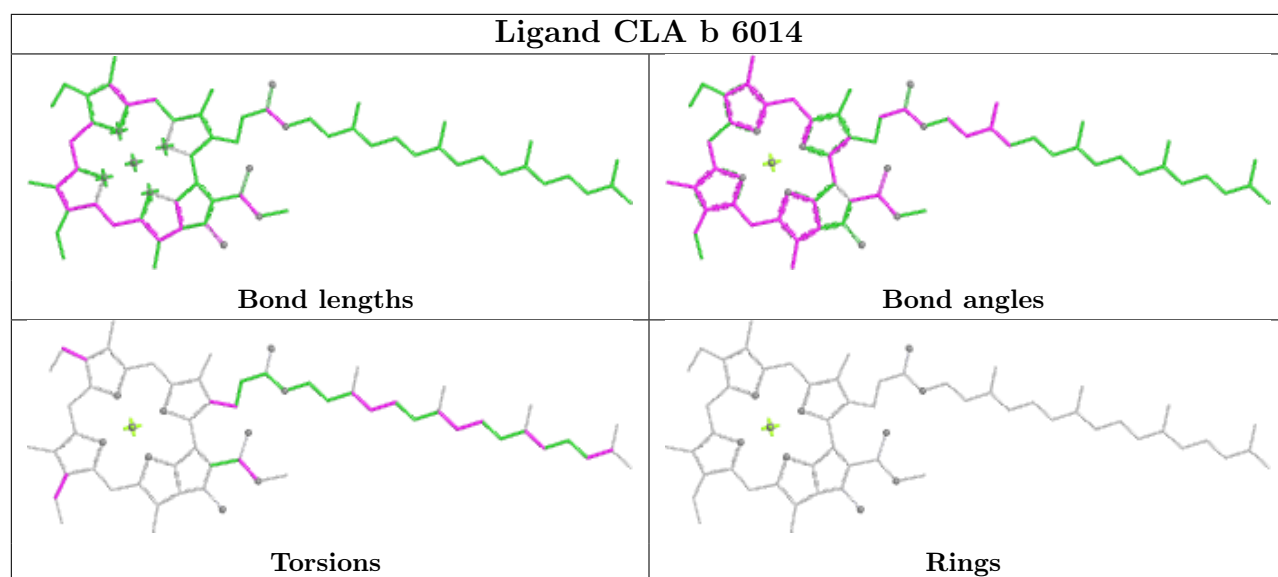
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	1026	CLA	27	0
22	c	6035	CLA	49	0
23	D	1039	PHO	51	0
24	a	6043	PQ9	35	0
22	c	6029	CLA	59	0

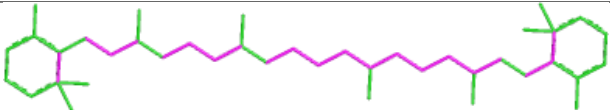
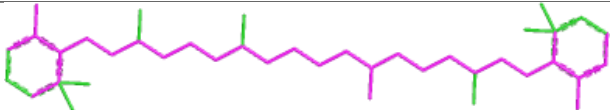
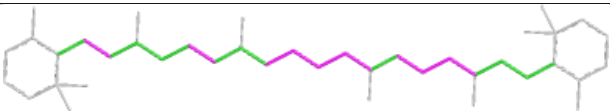
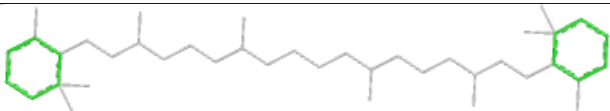
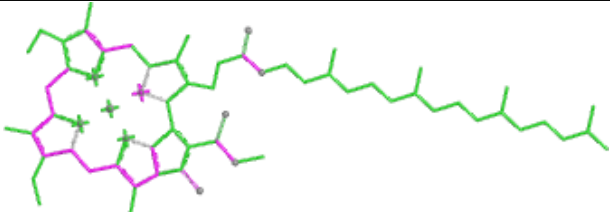
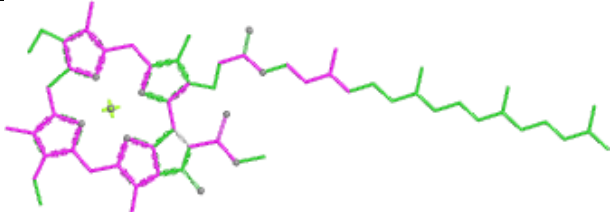
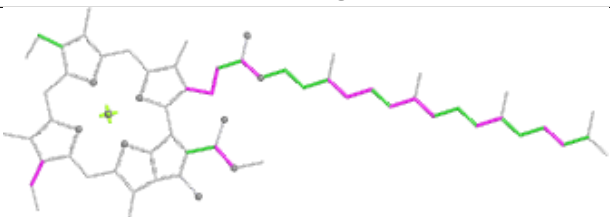
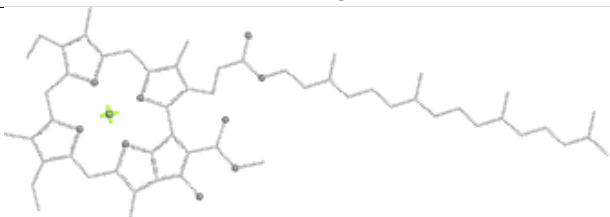
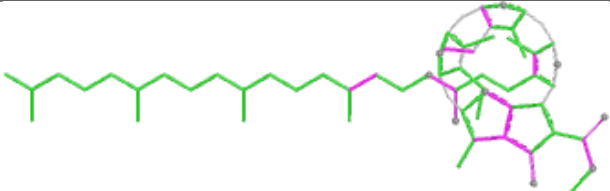
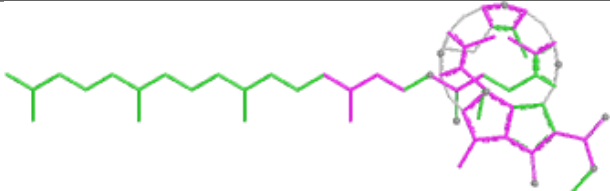
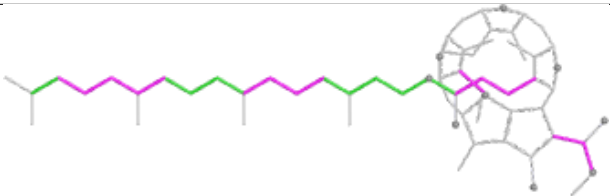
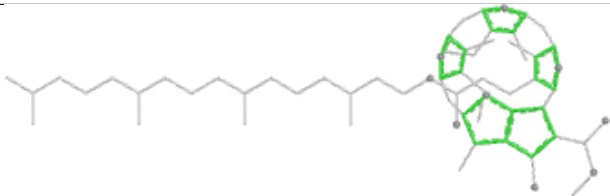
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

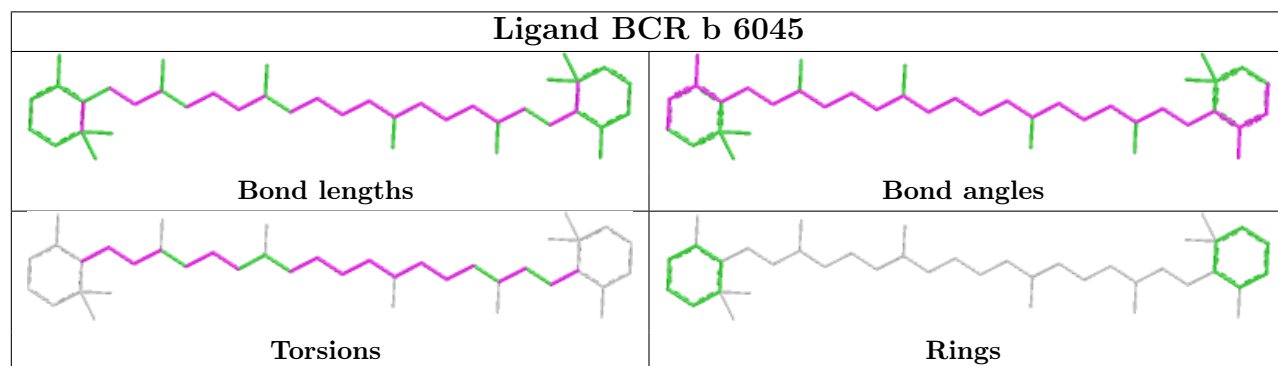
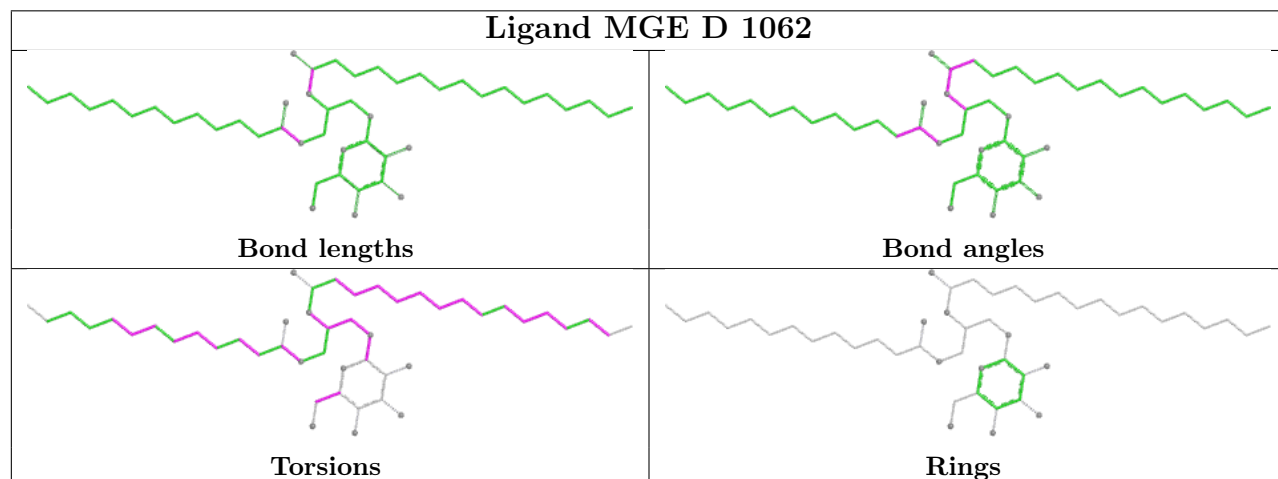
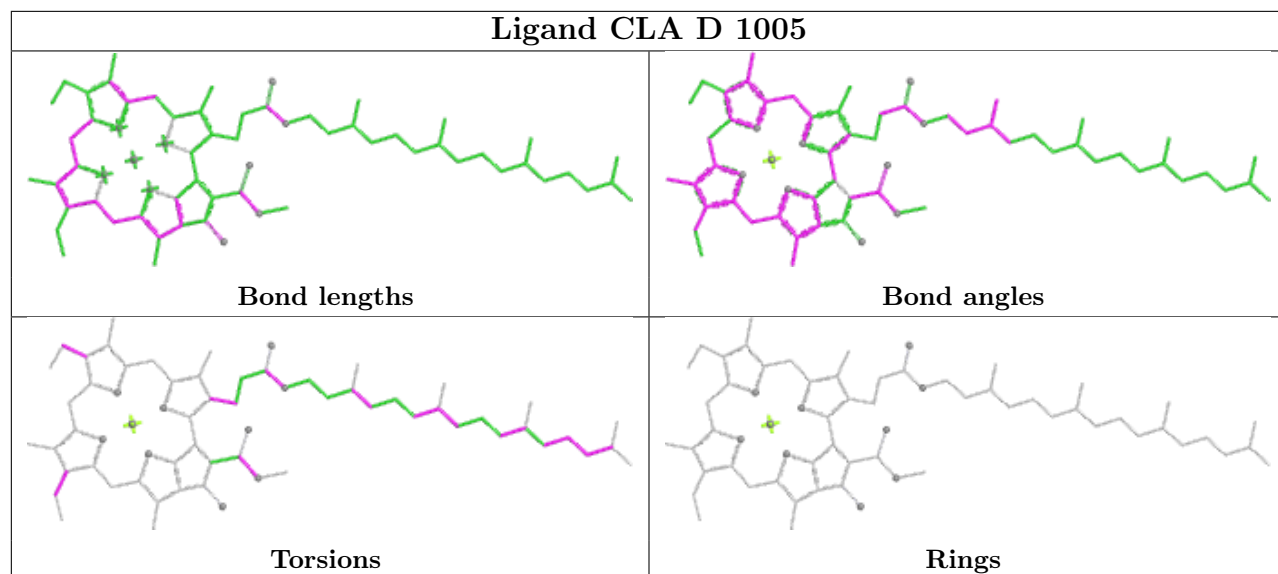


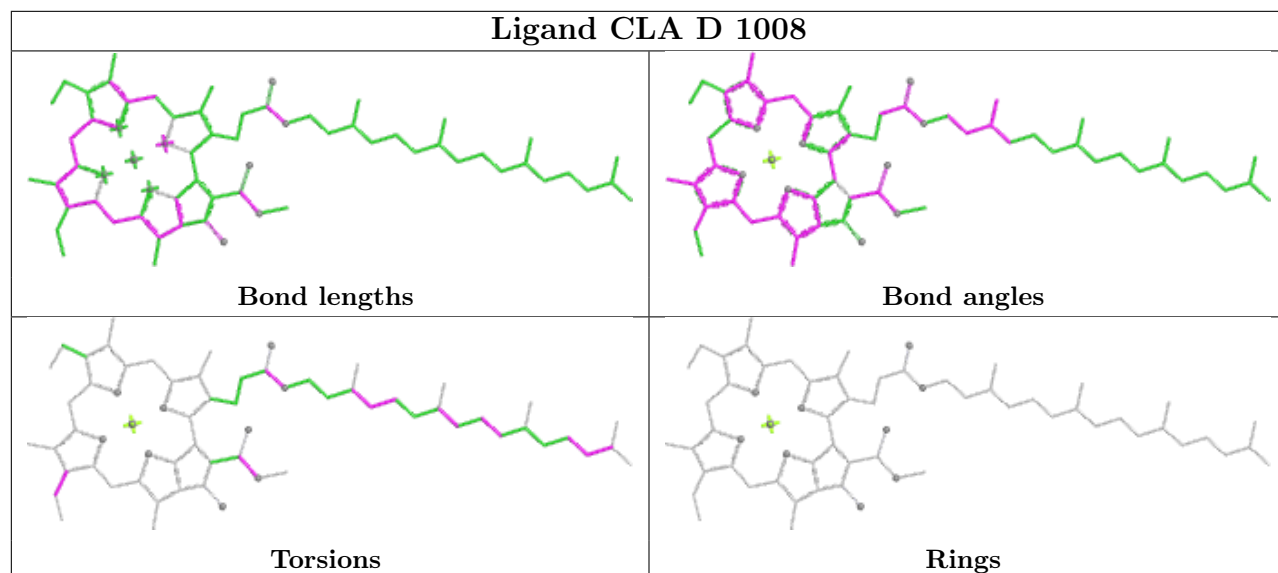
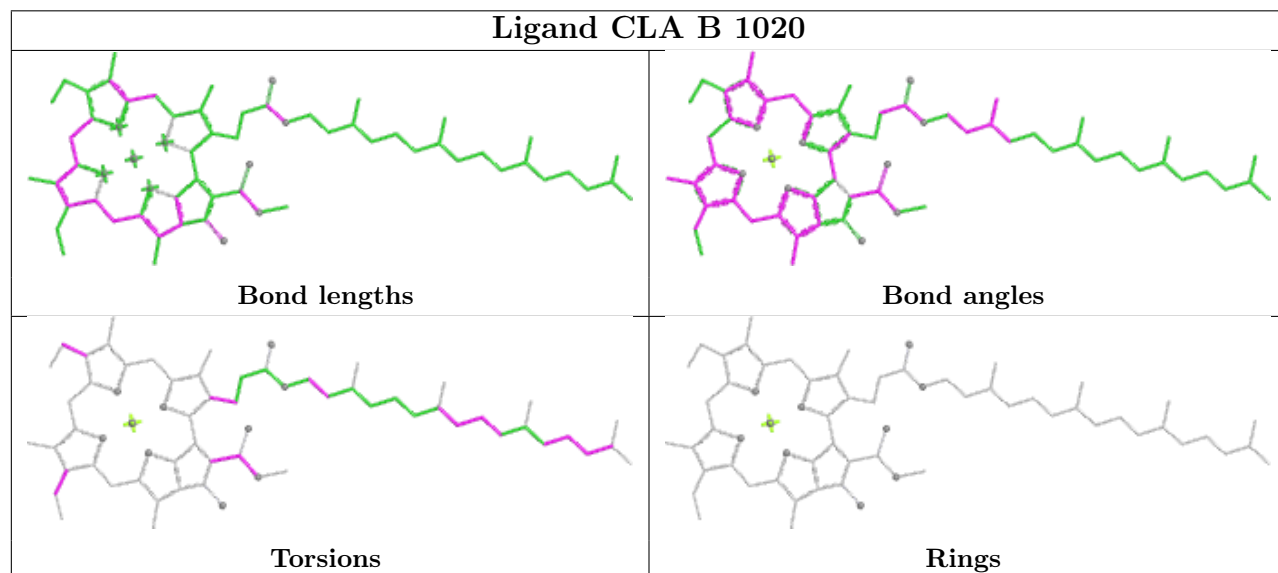
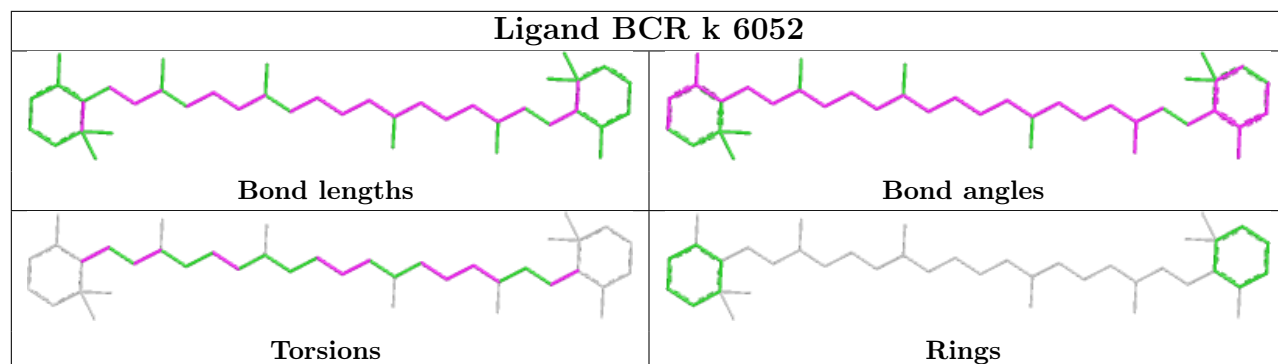


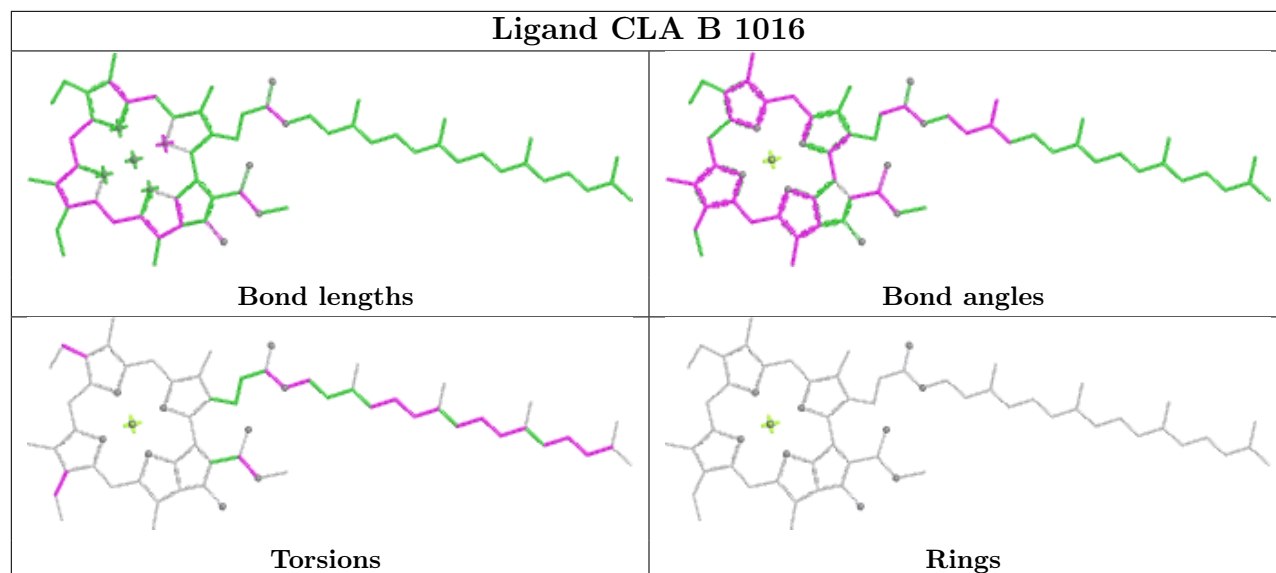
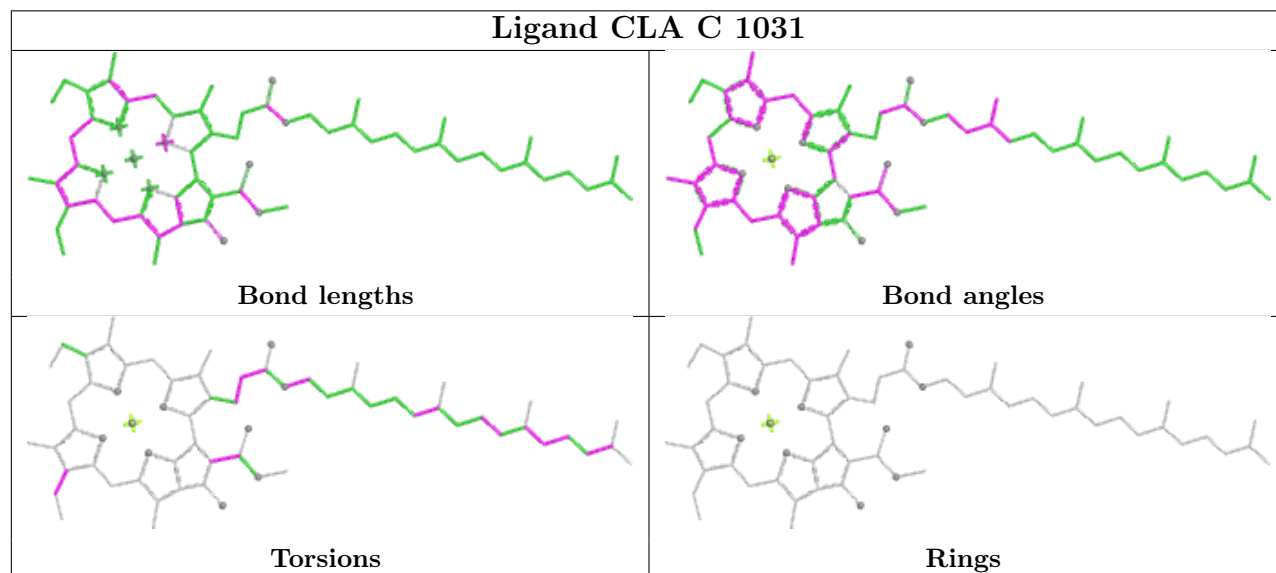
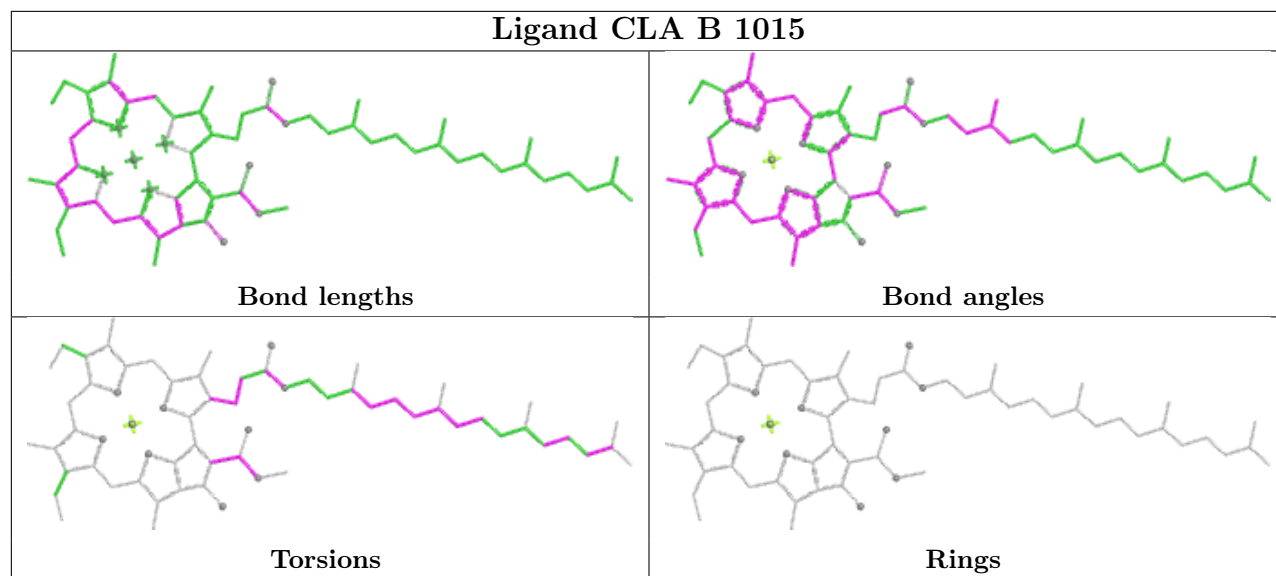


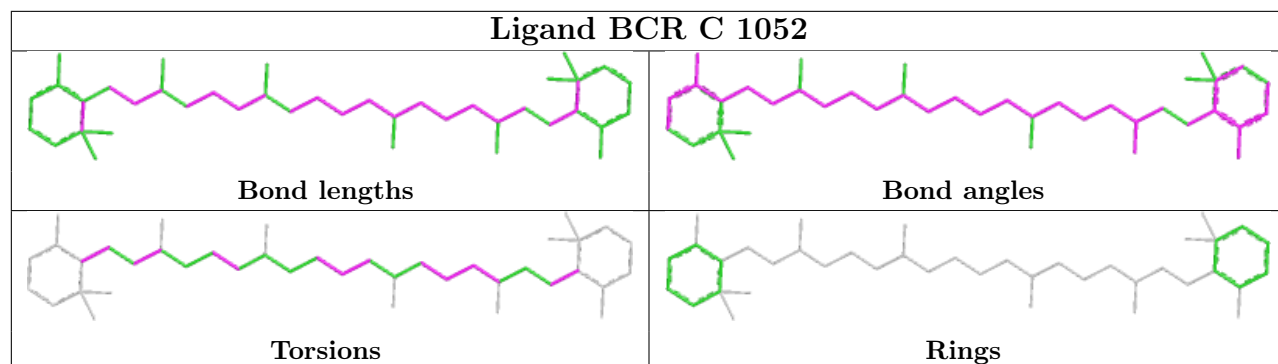
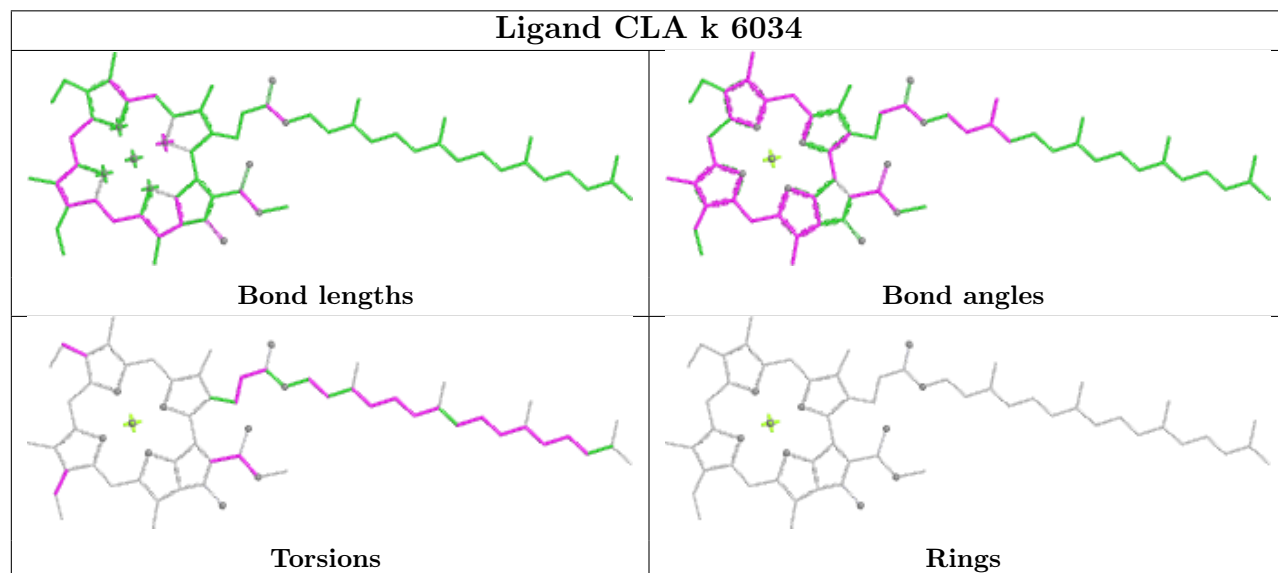
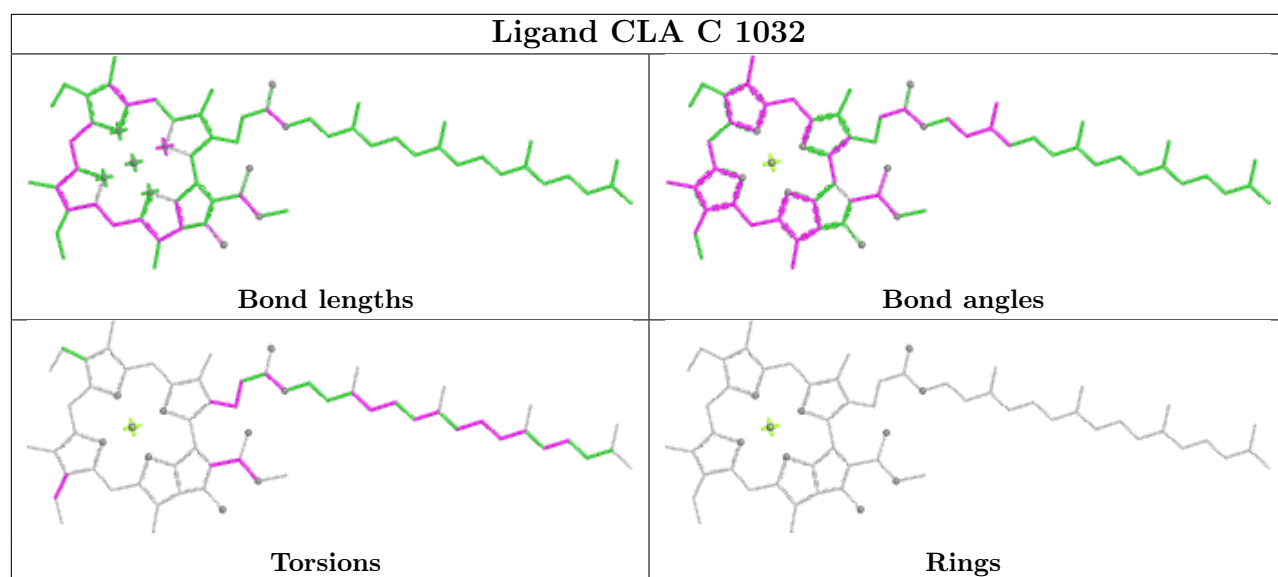


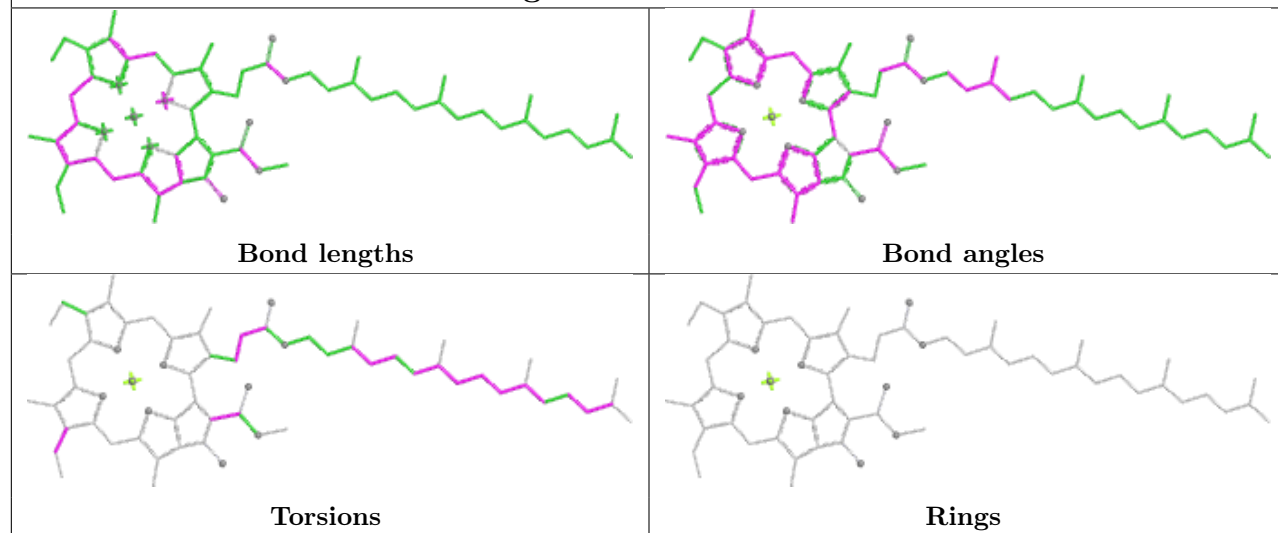
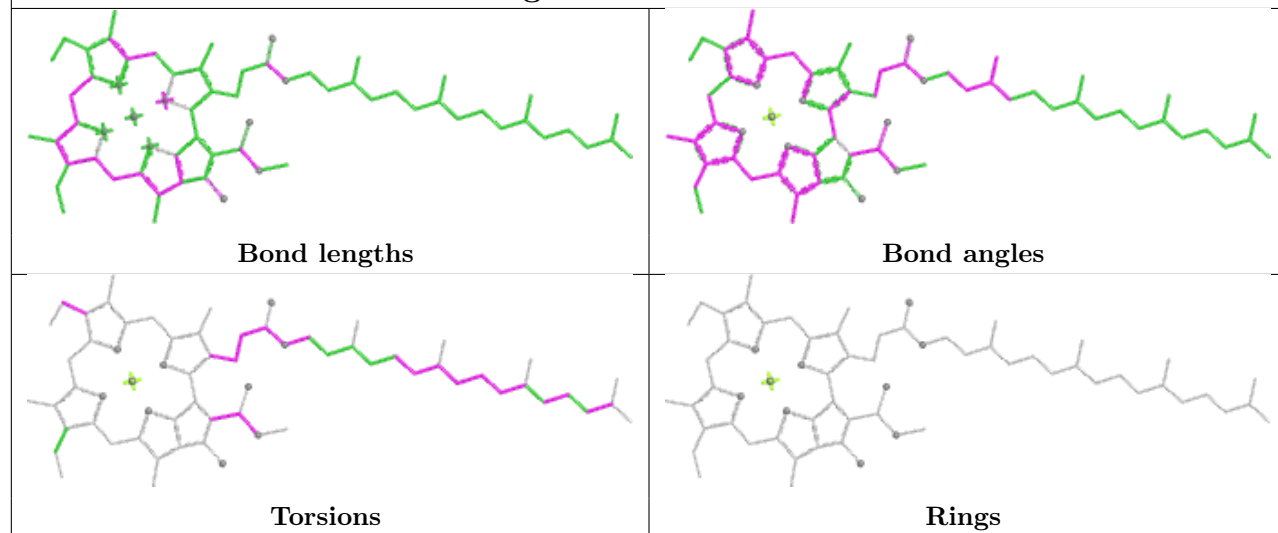
Ligand BCR t 1046	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 6006	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO A 1038	
 Bond lengths	 Bond angles
 Torsions	 Rings

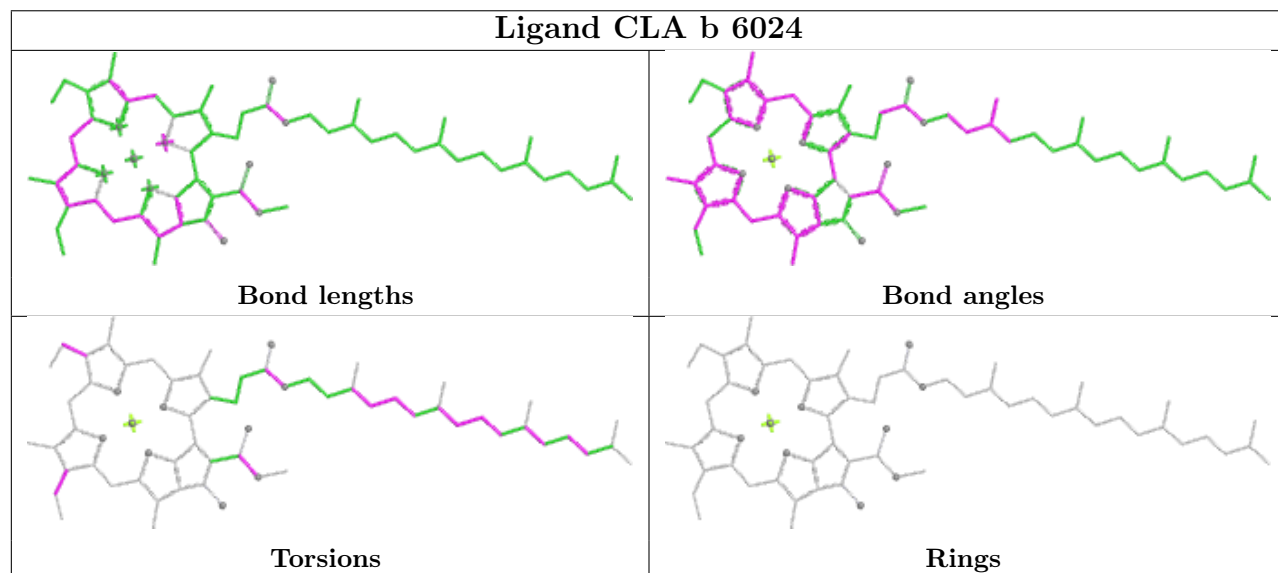
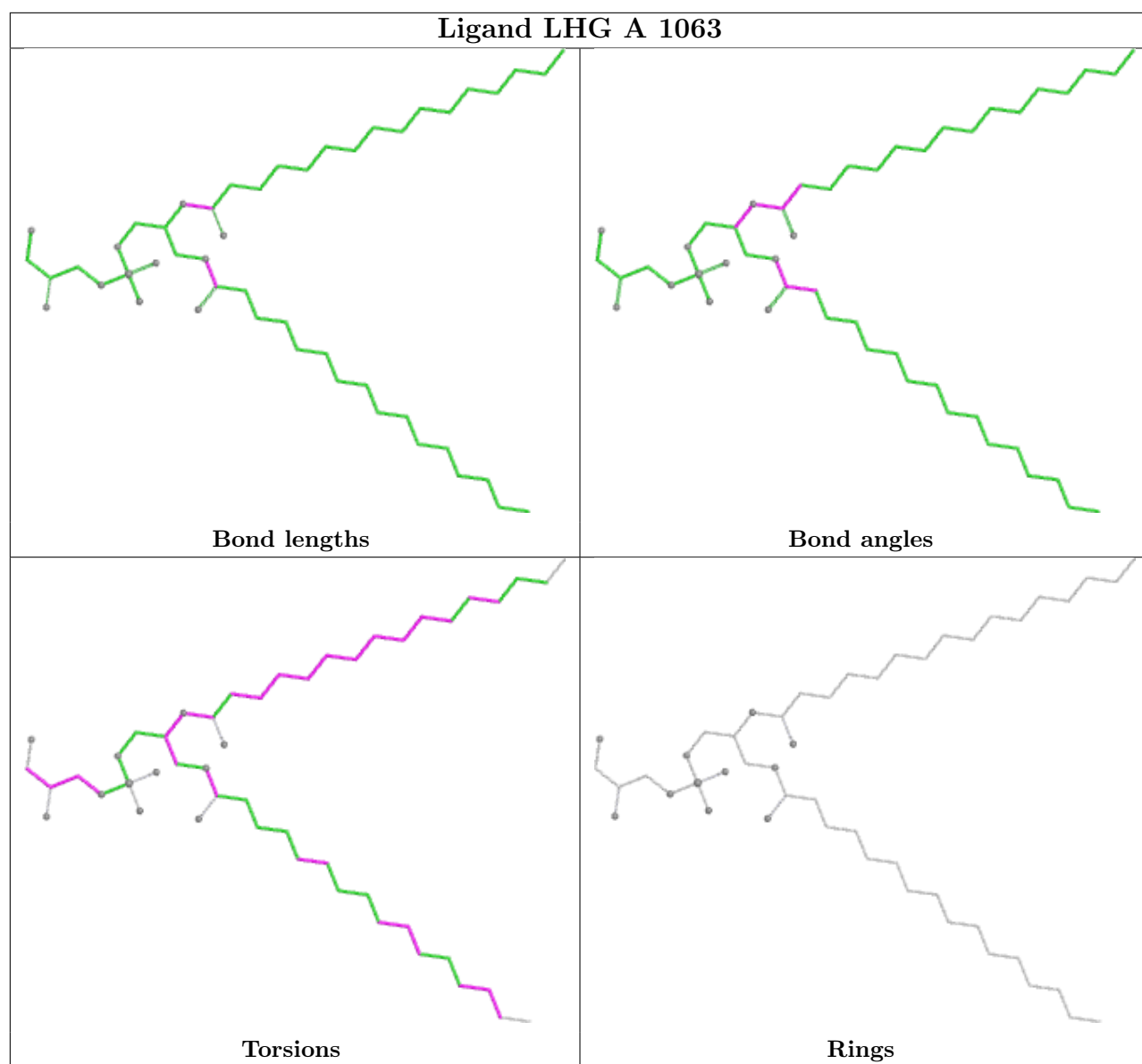


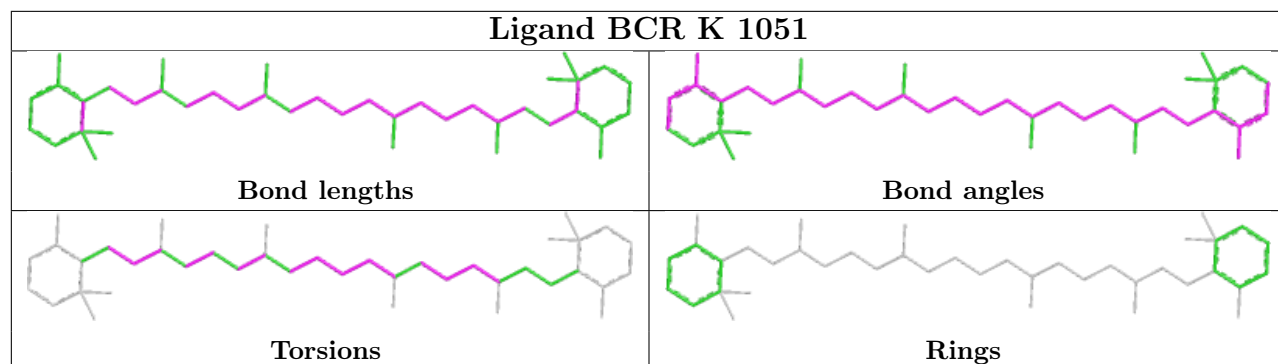
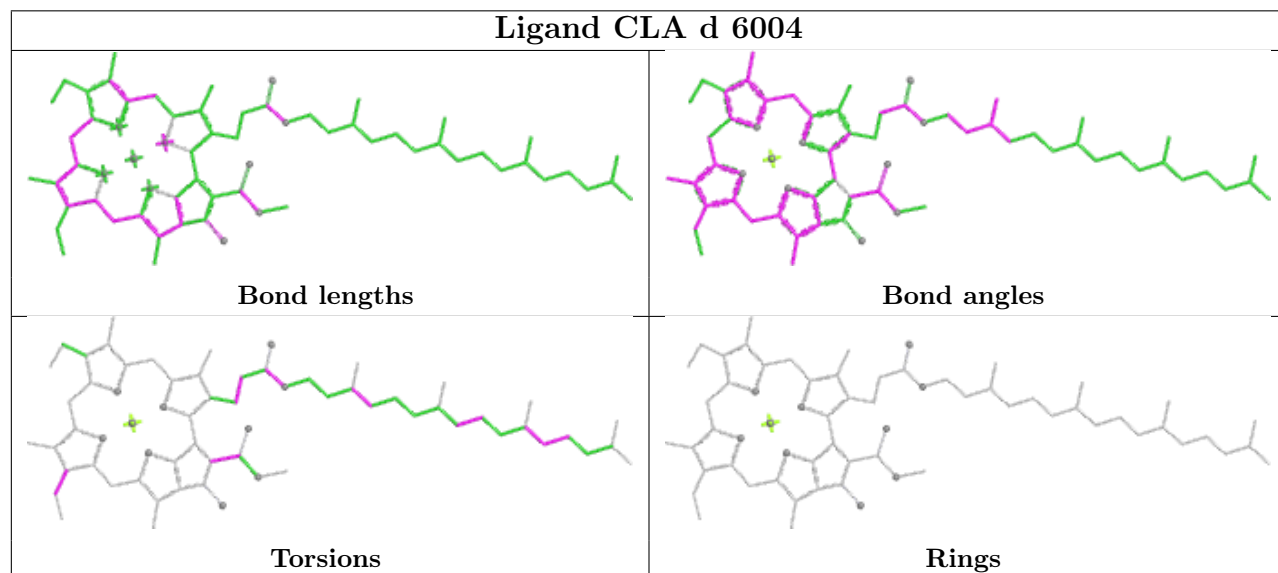
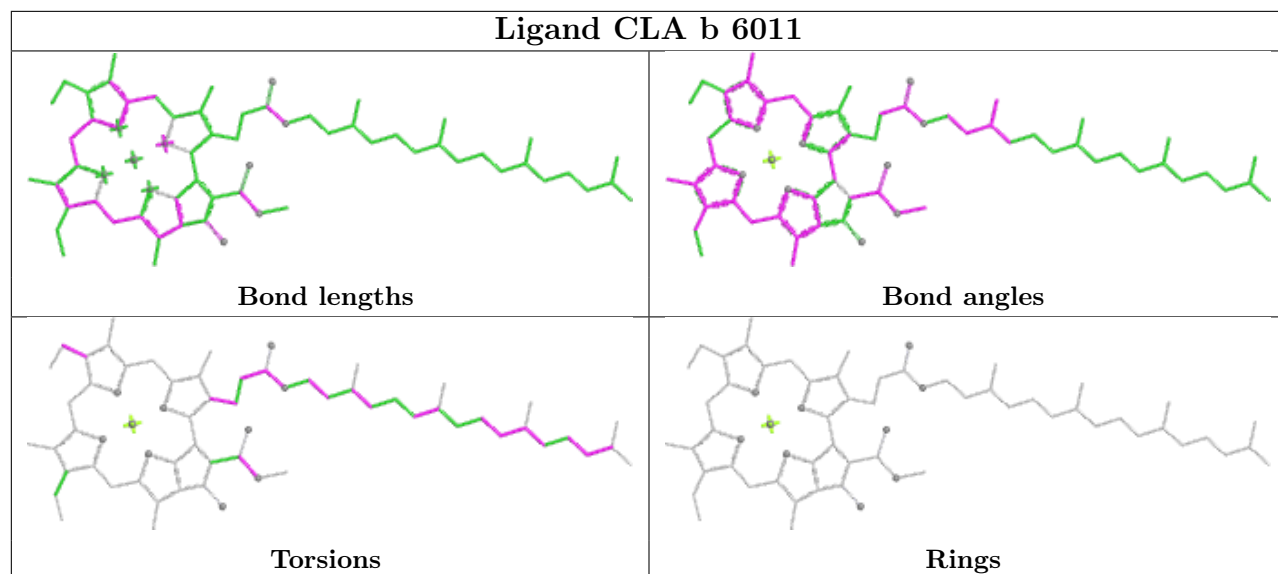


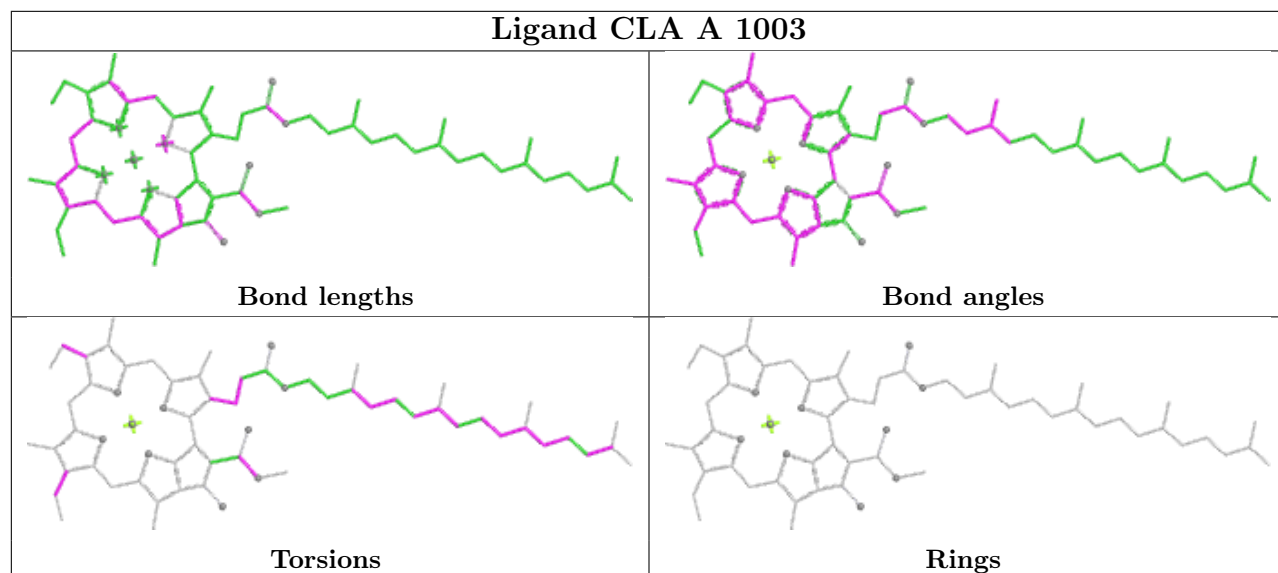
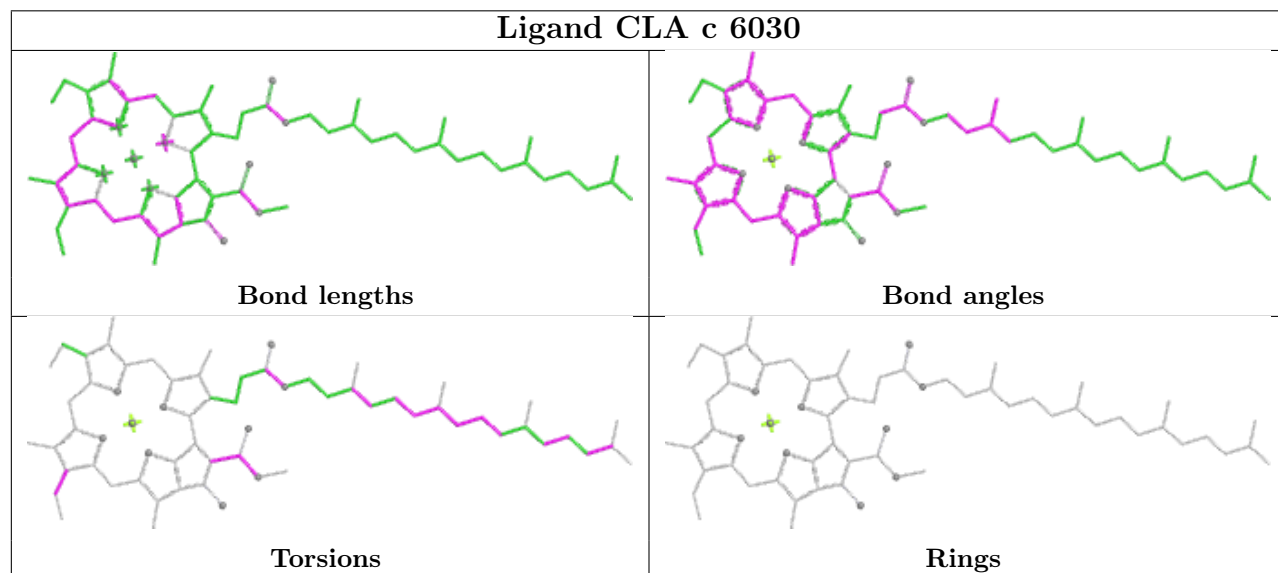
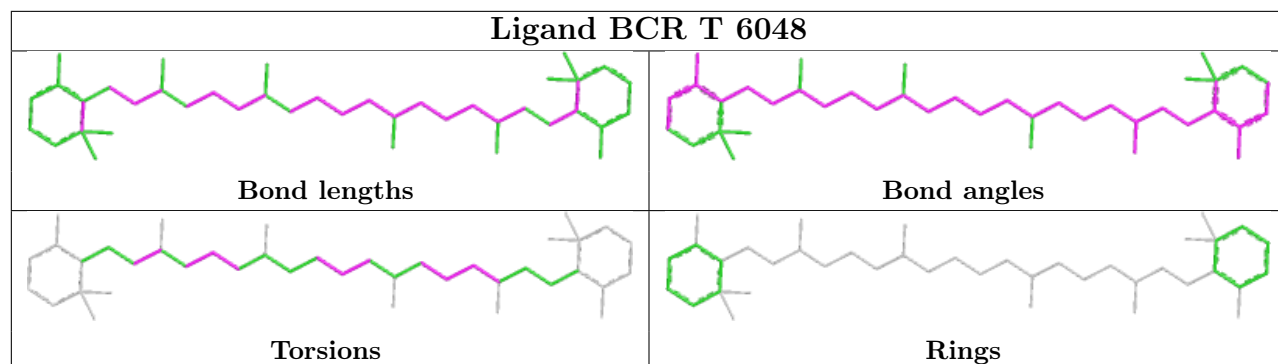


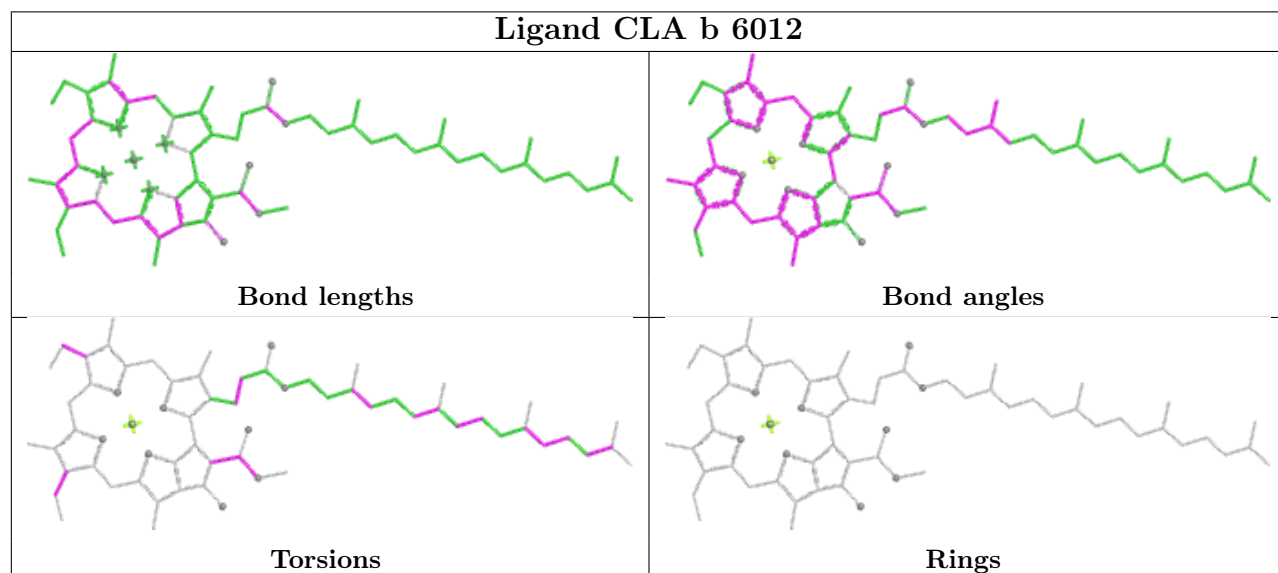
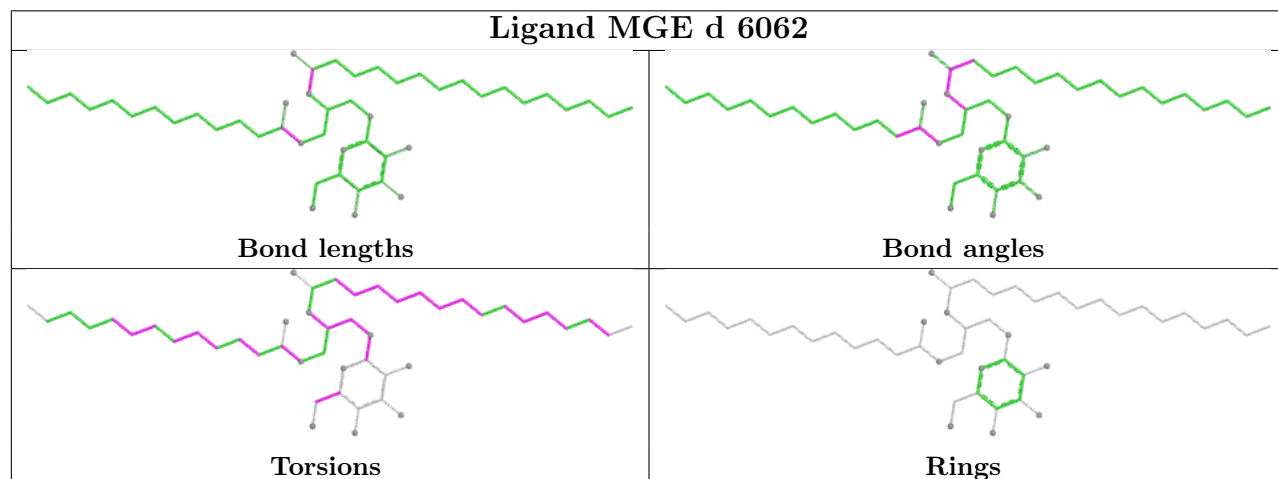
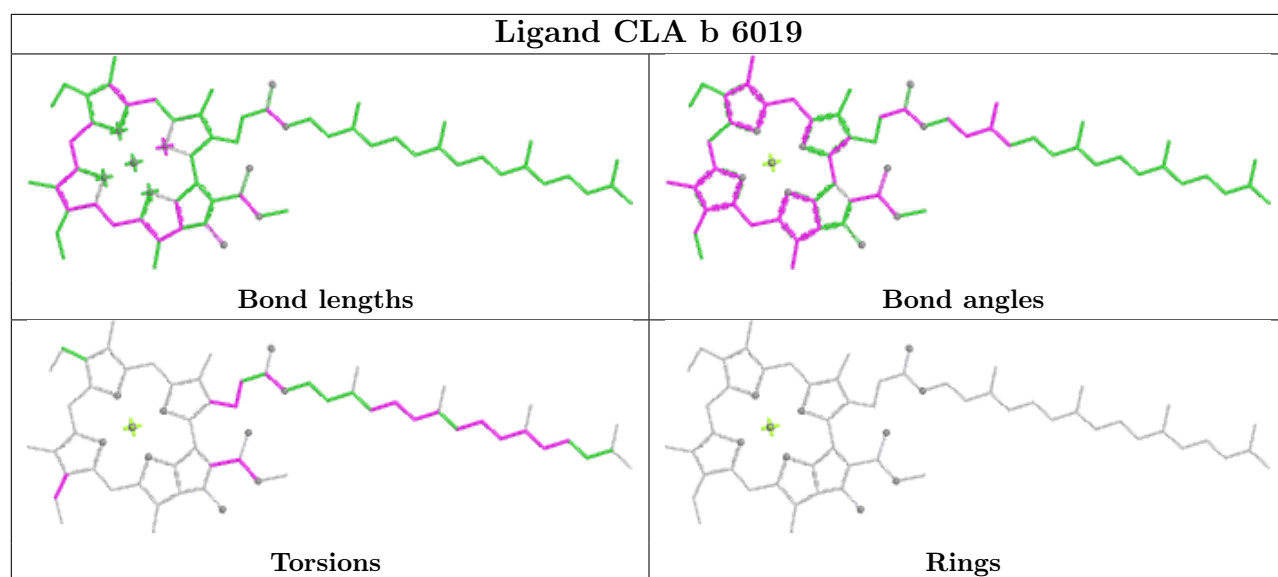


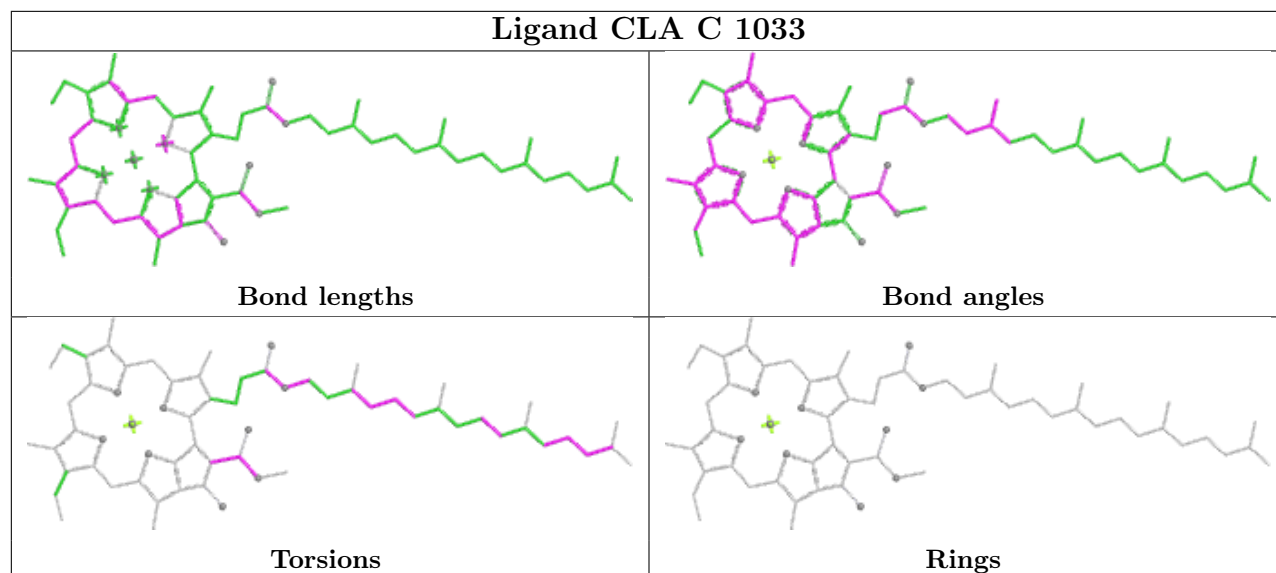
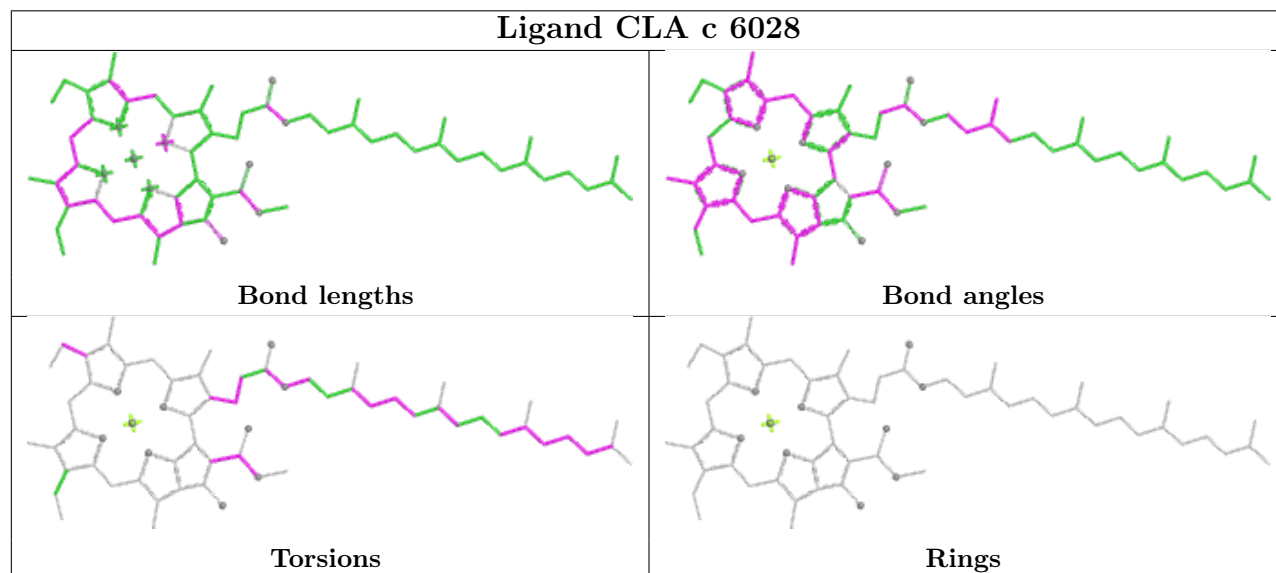
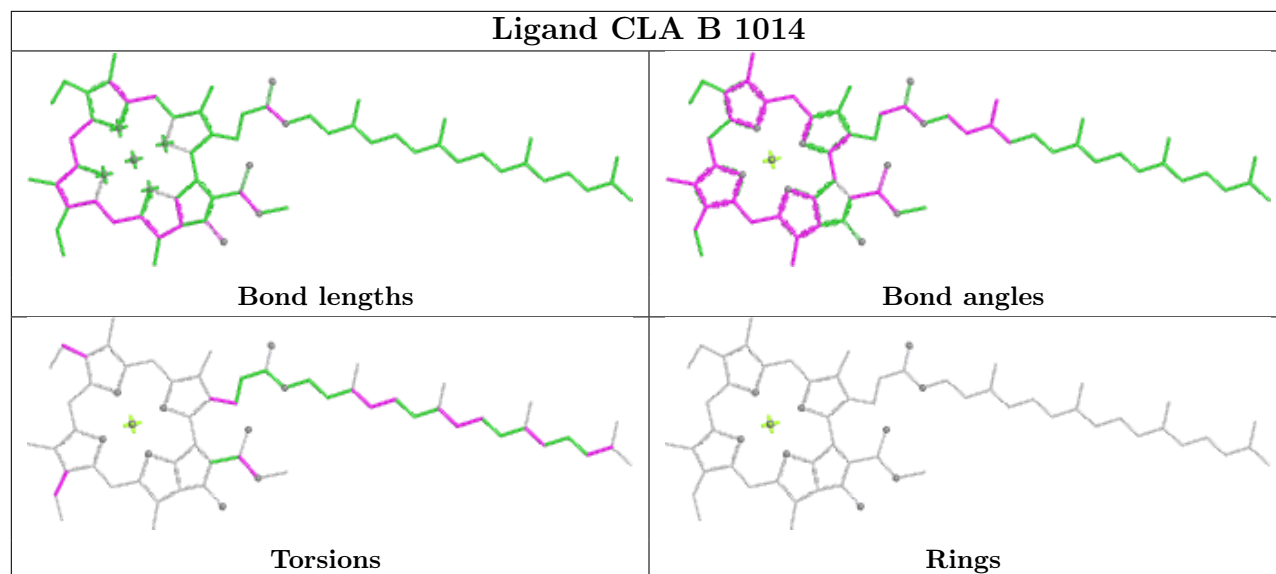
Ligand CLA B 1018**Ligand CLA B 1021**

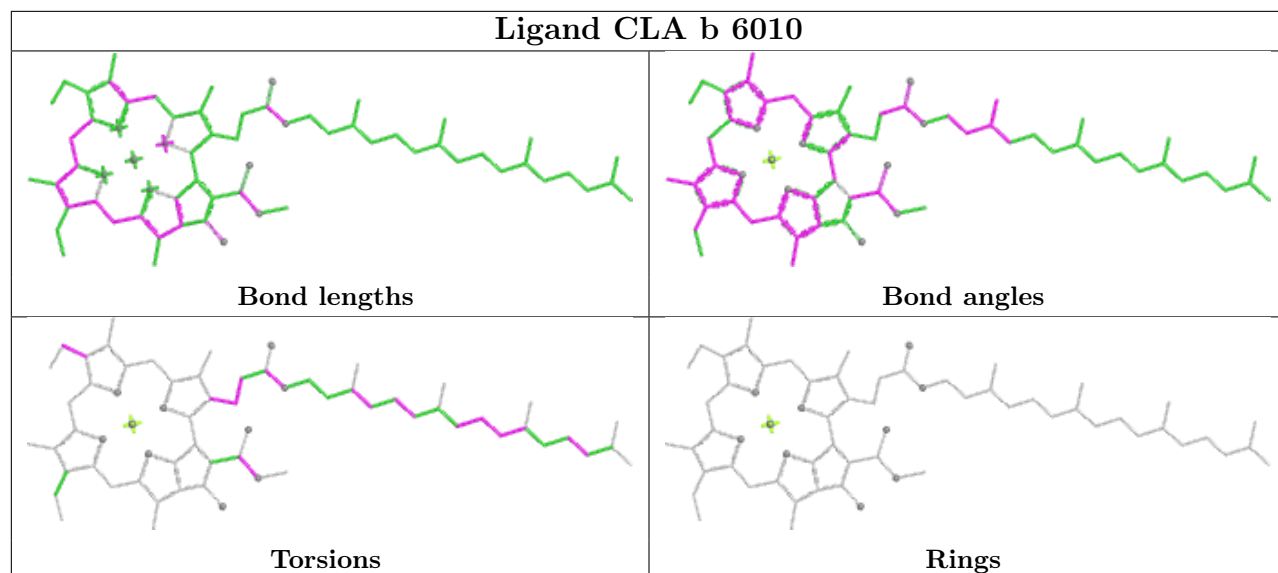
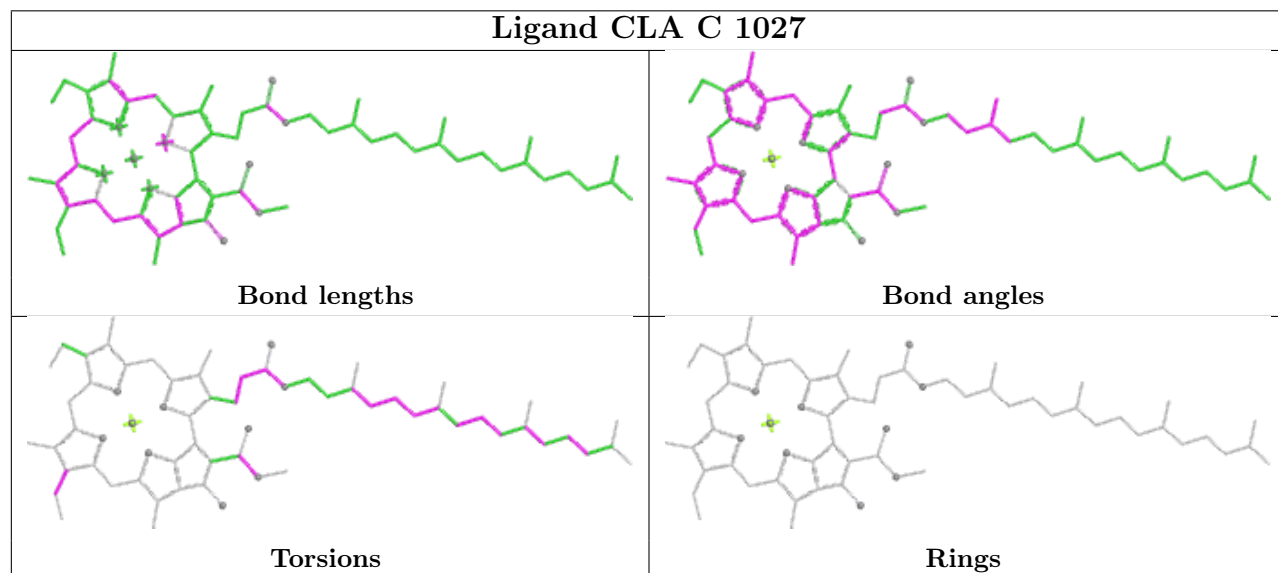
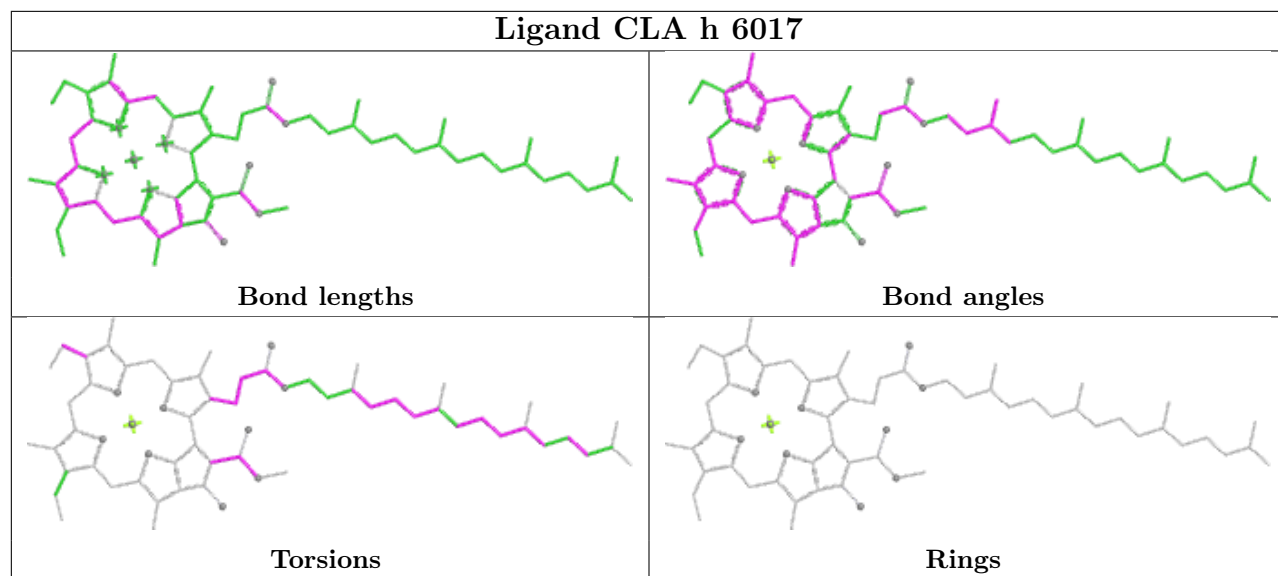


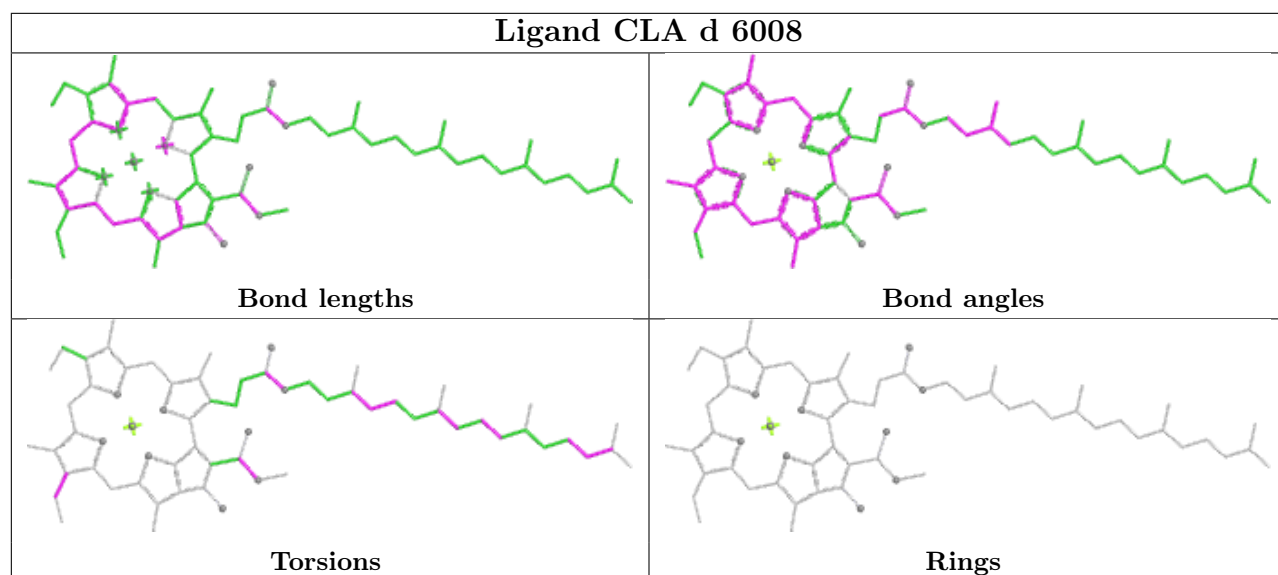
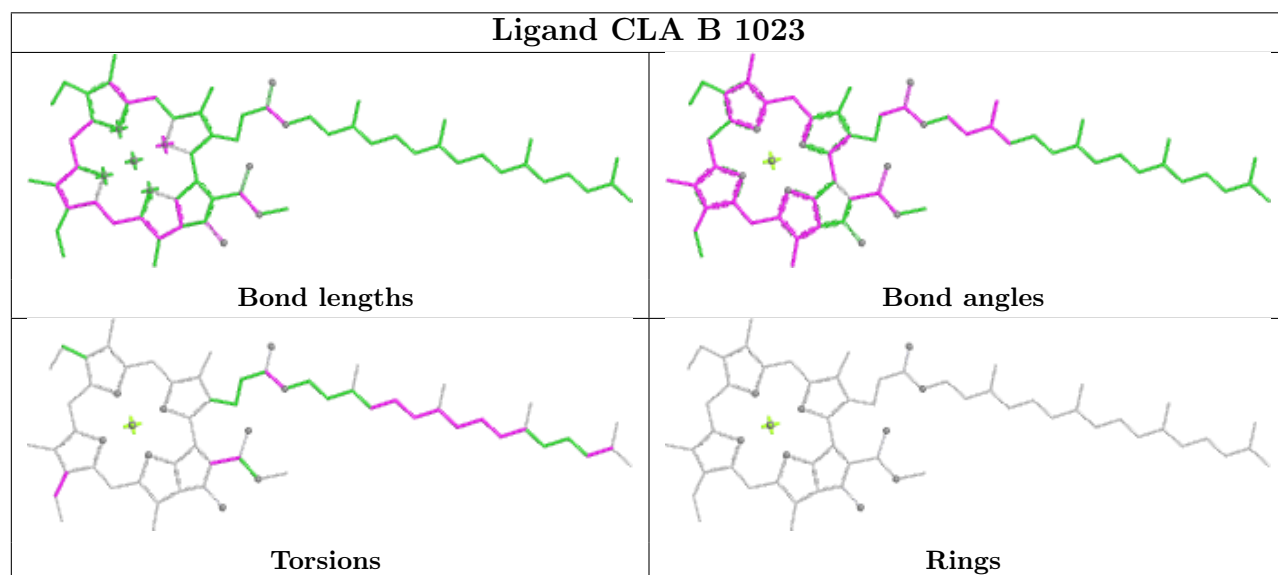
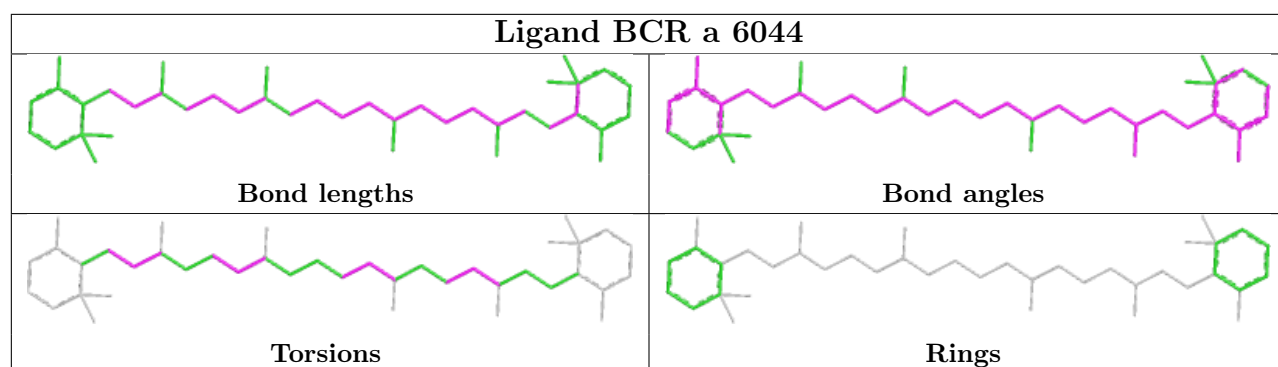


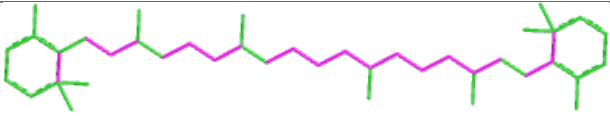
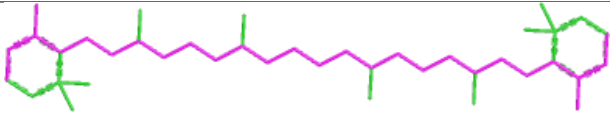
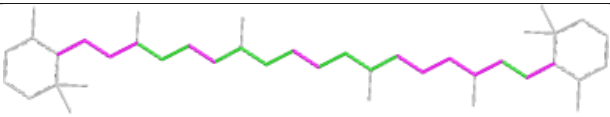
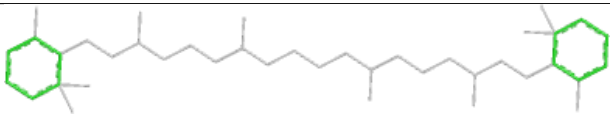
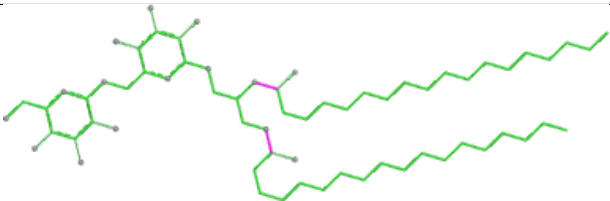
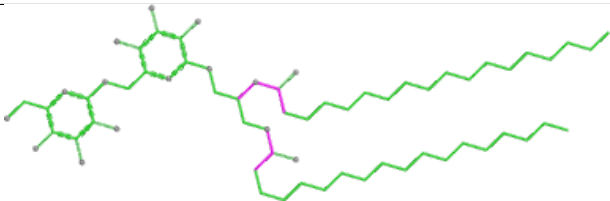
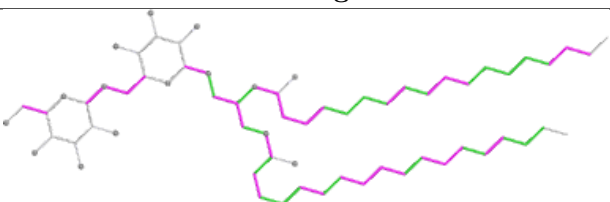
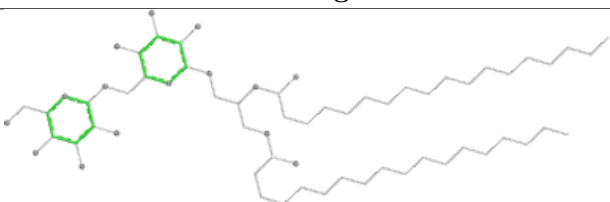
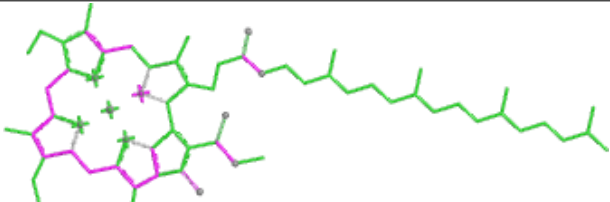
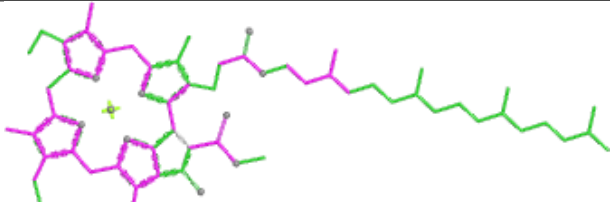
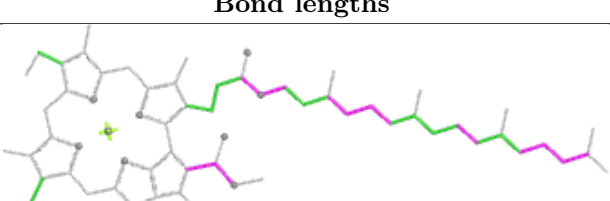
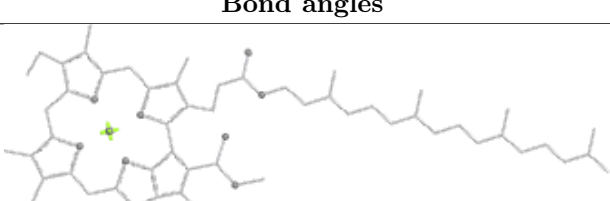


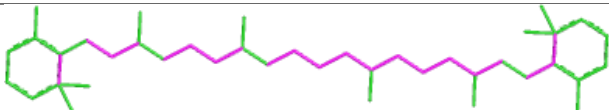
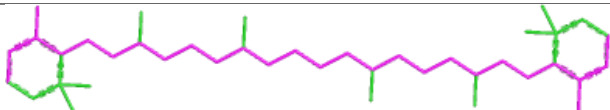
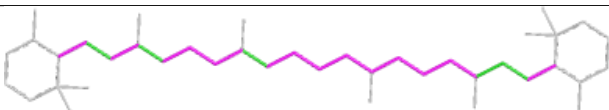
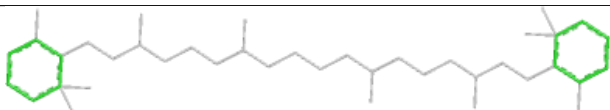


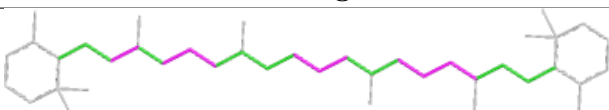
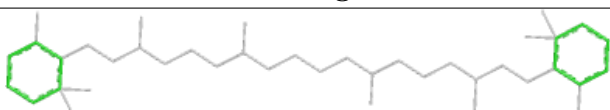


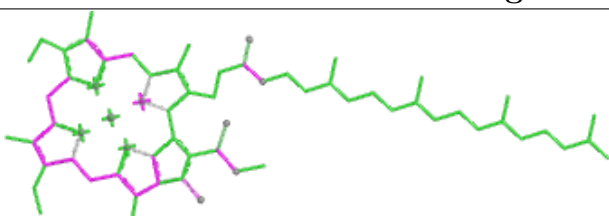
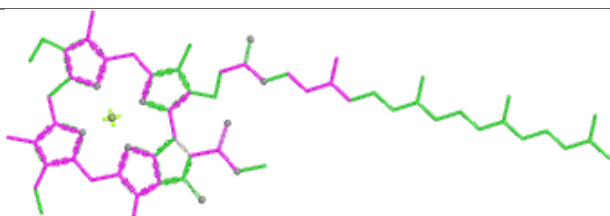
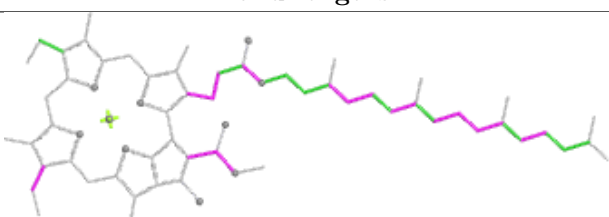
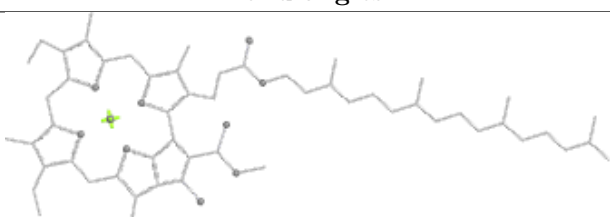


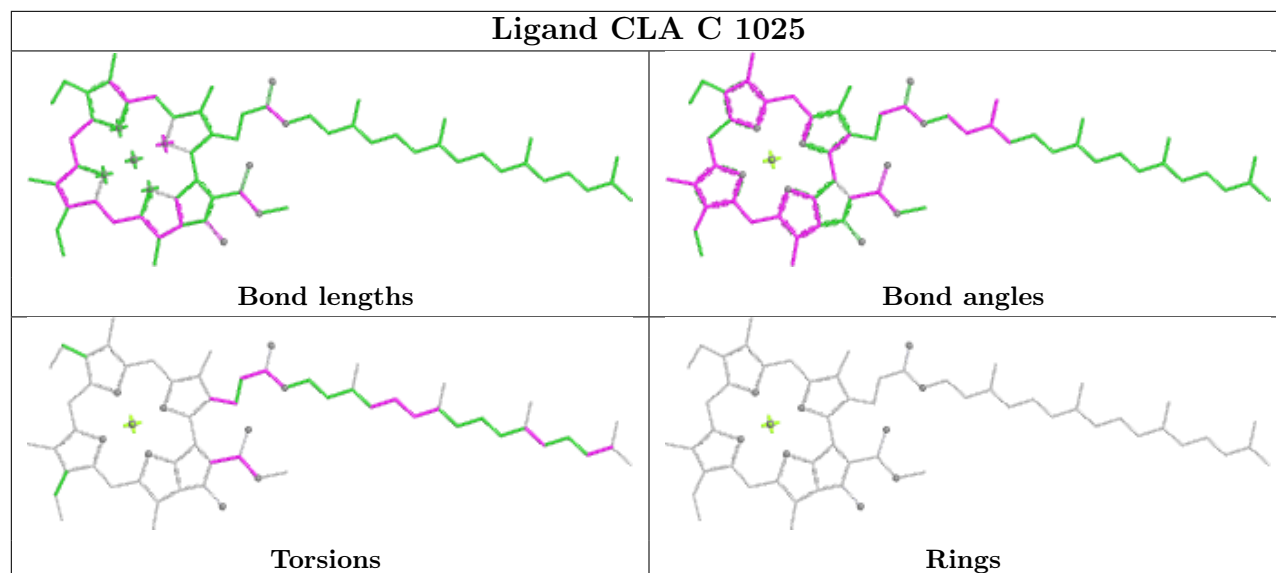
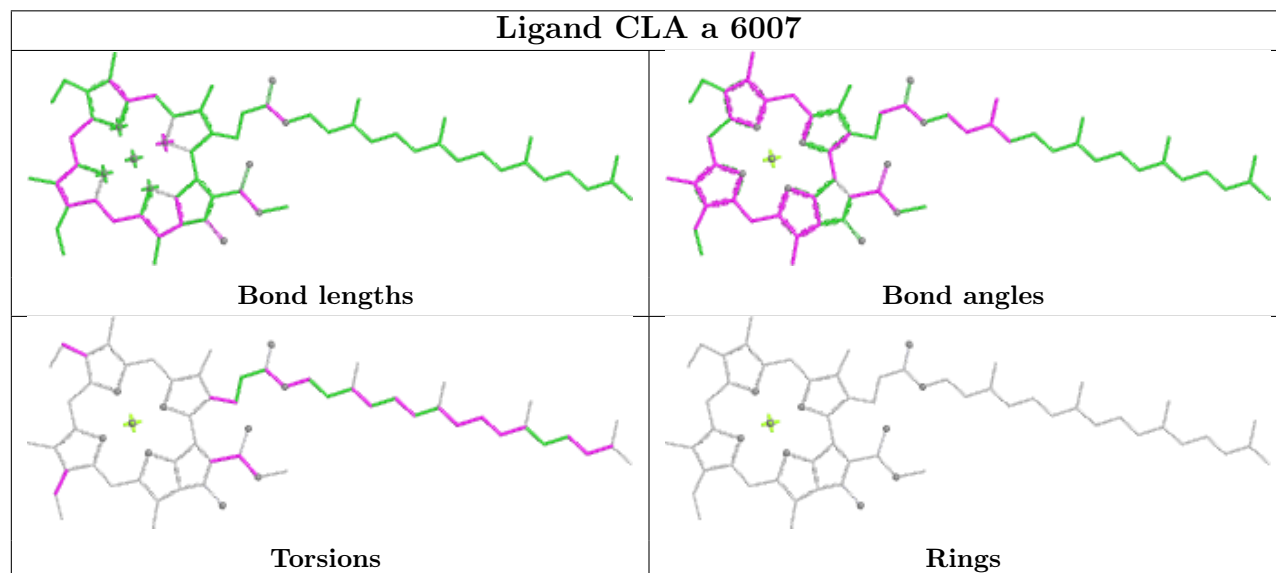
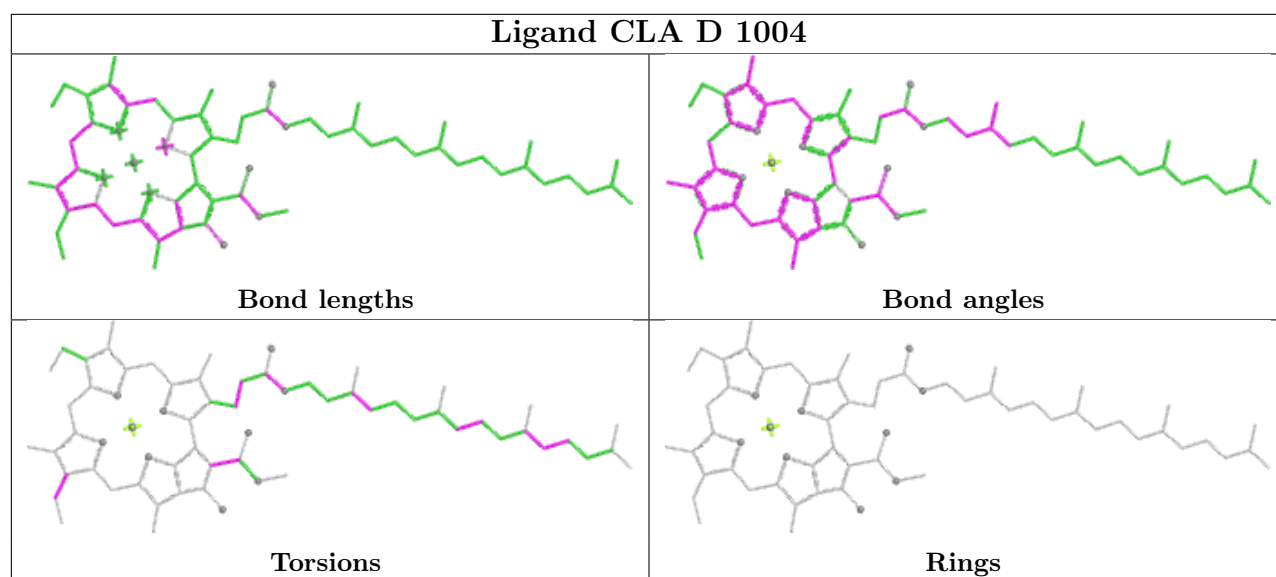


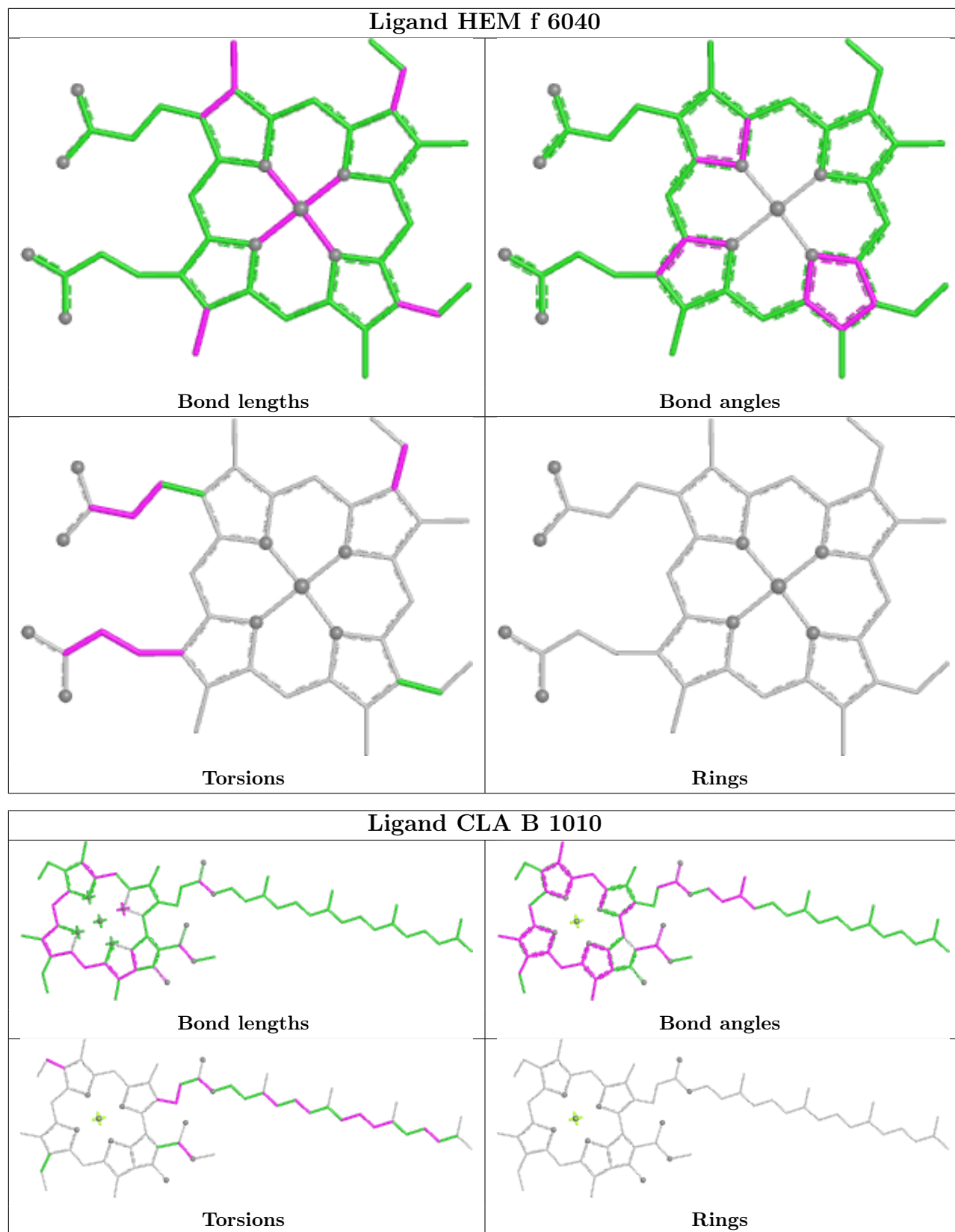
Ligand BCR Z 1053	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand DGD B 1058	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA c 6033	
 Bond lengths	 Bond angles
 Torsions	 Rings

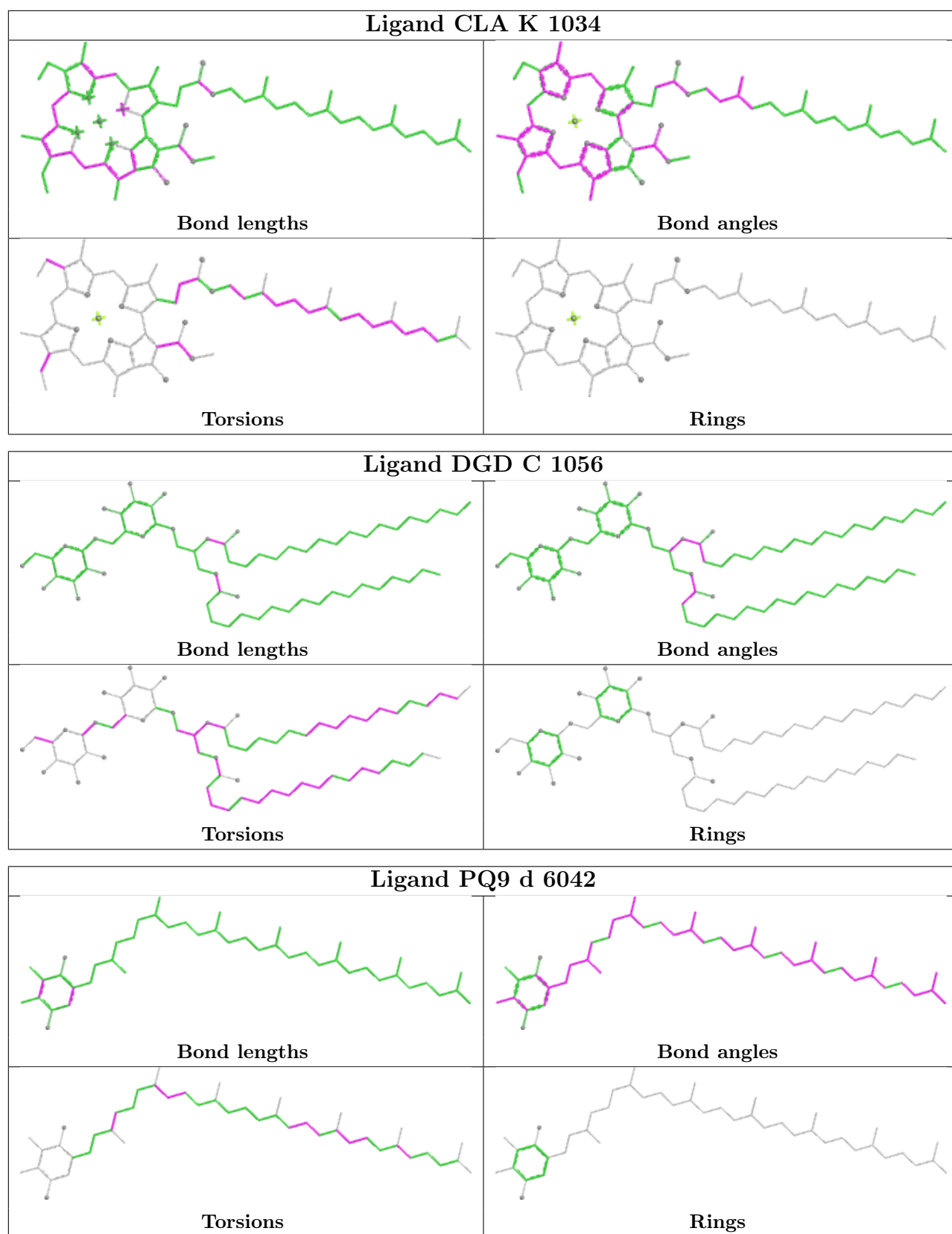
Ligand BCR D 1050	
	
Bond lengths	Bond angles
	
Torsions	Rings

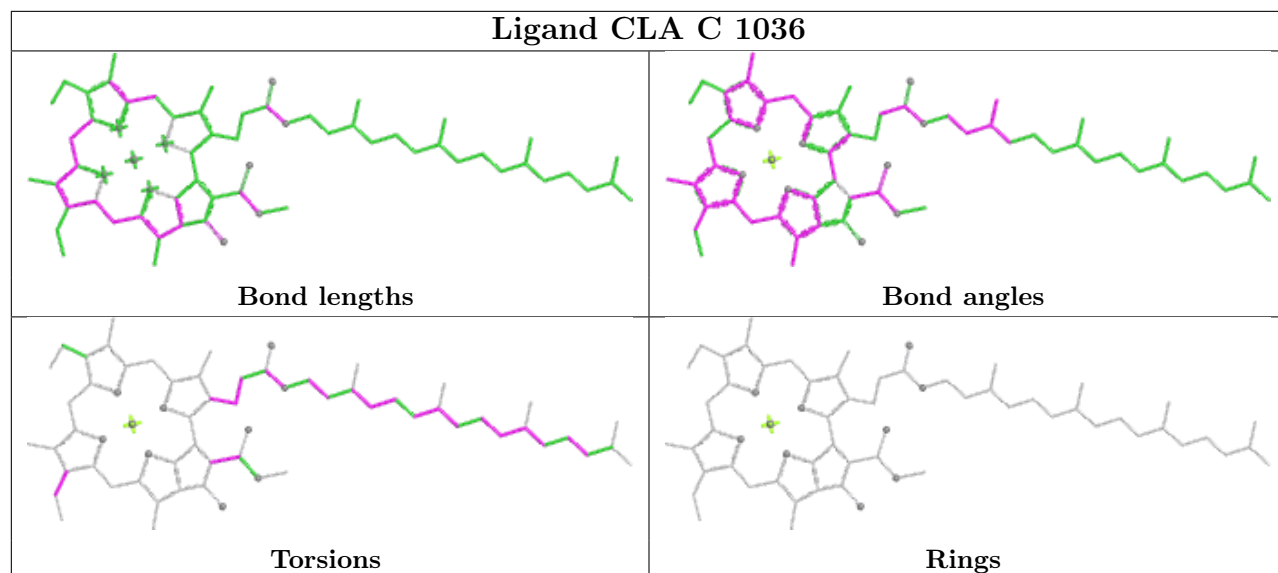
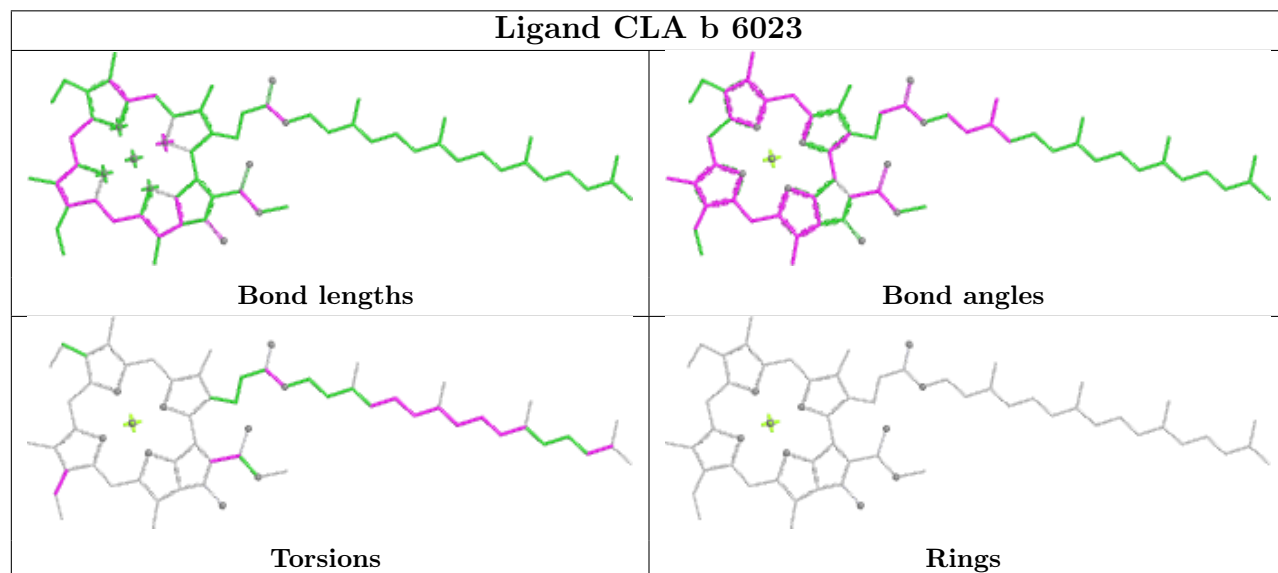
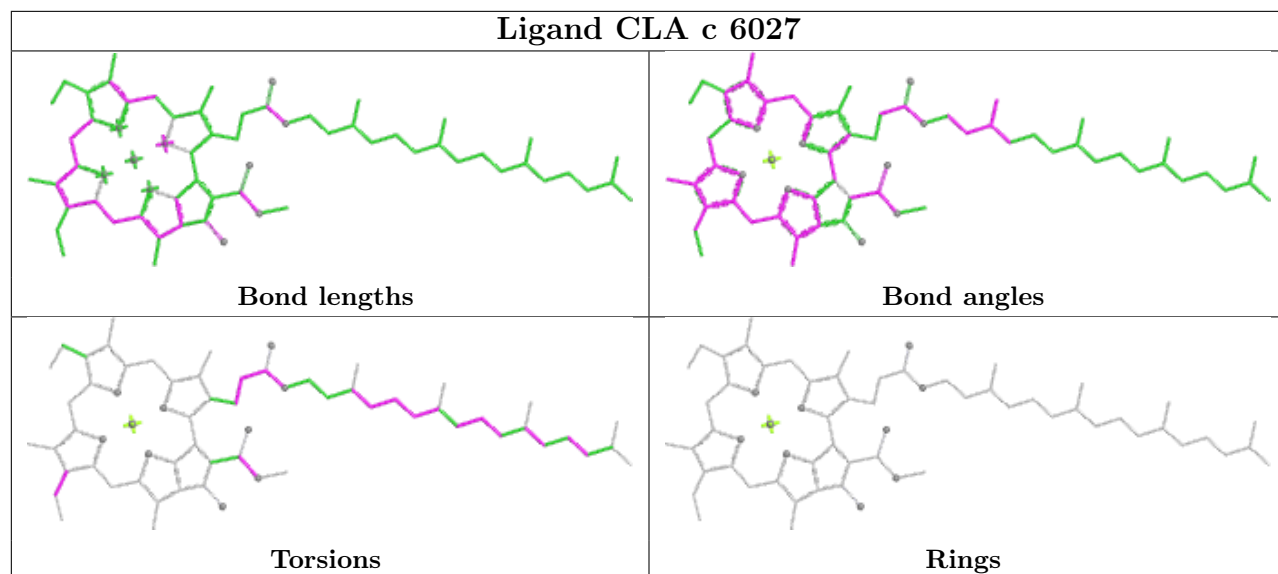
Ligand BCR B 1048	
	
Bond lengths	Bond angles
	
Torsions	Rings

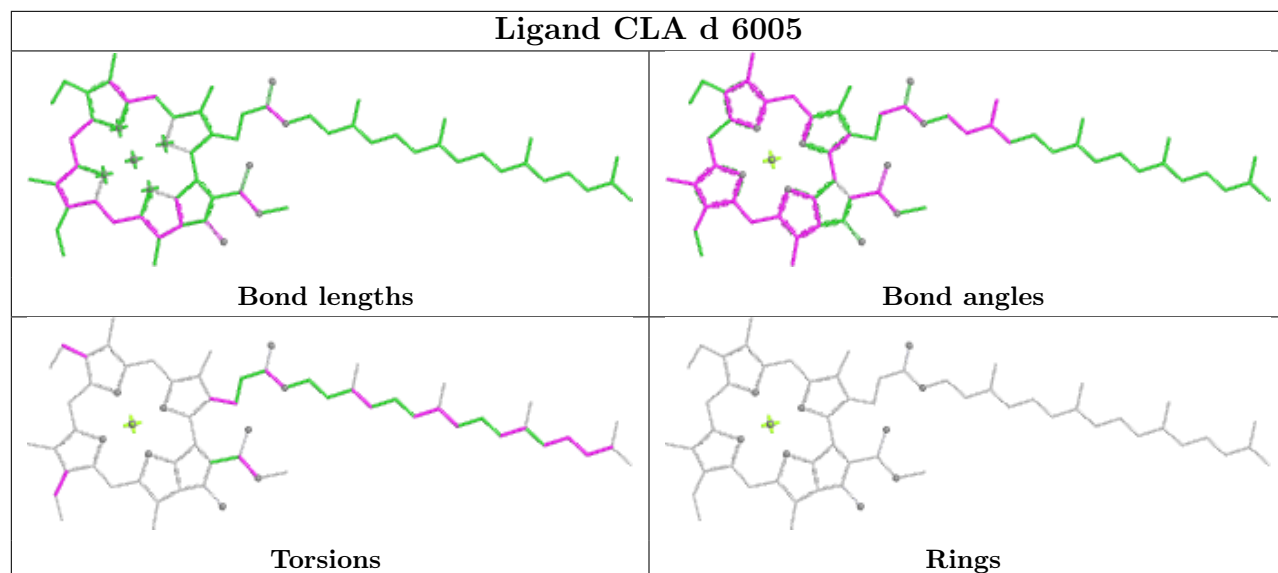
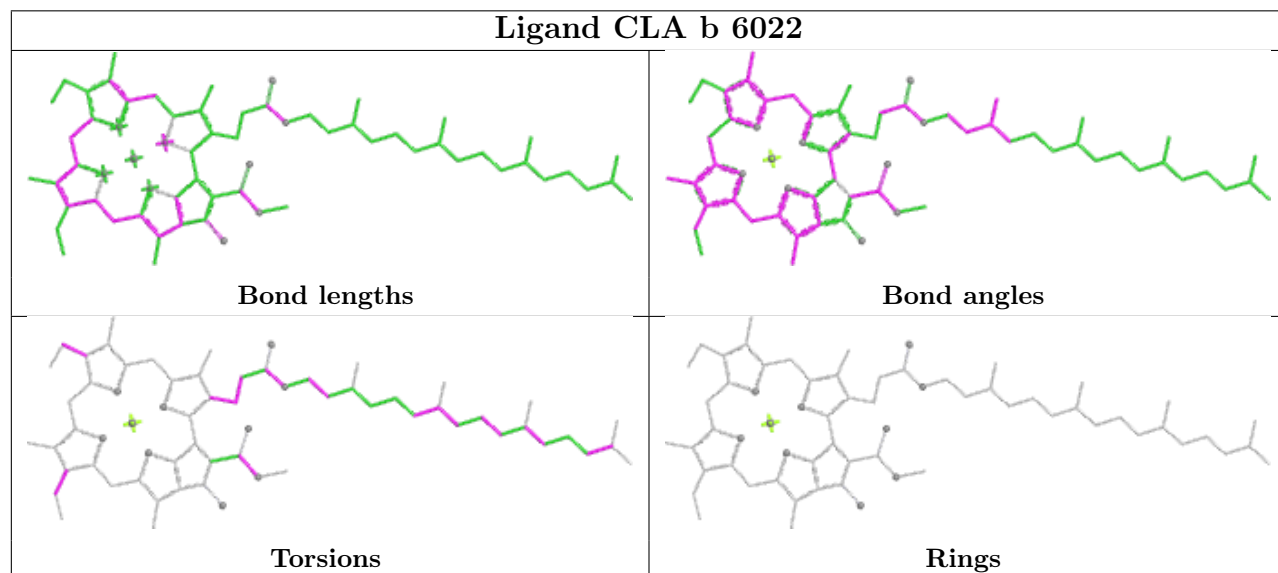
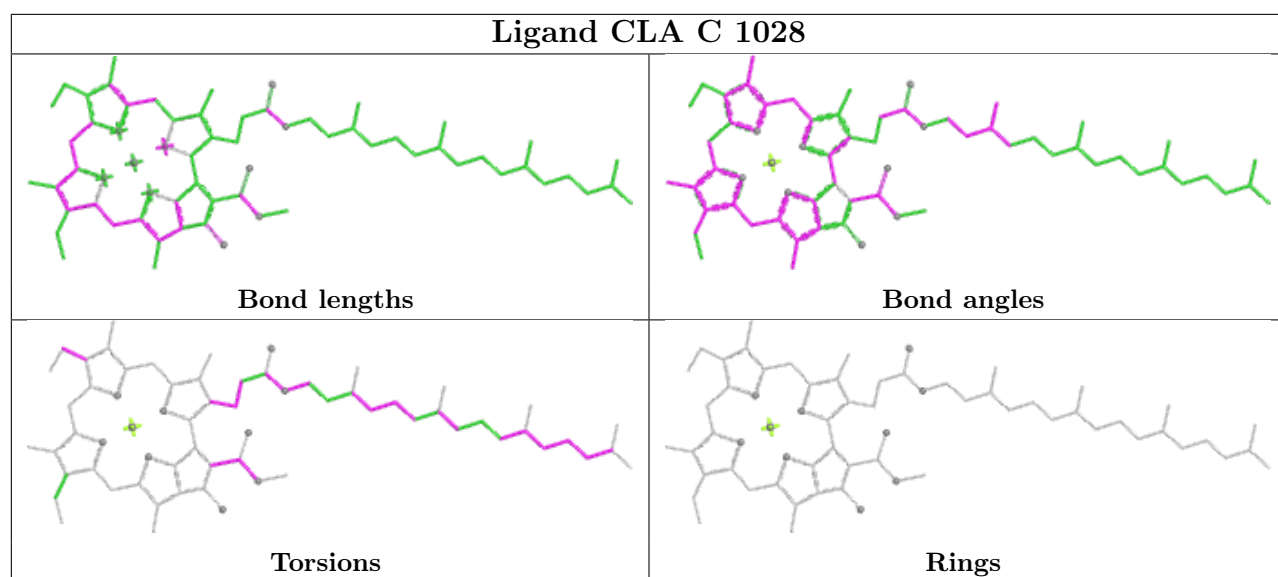
Ligand CLA c 6032	
	
Bond lengths	Bond angles
	
Torsions	Rings

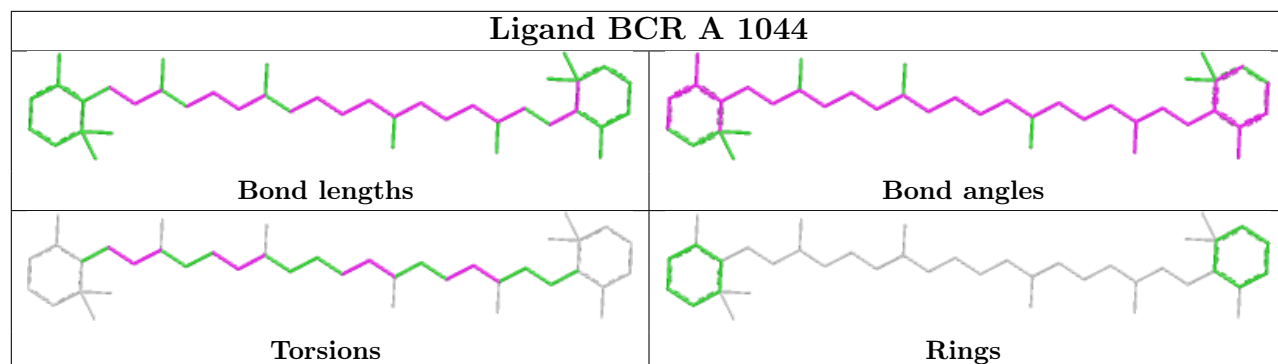
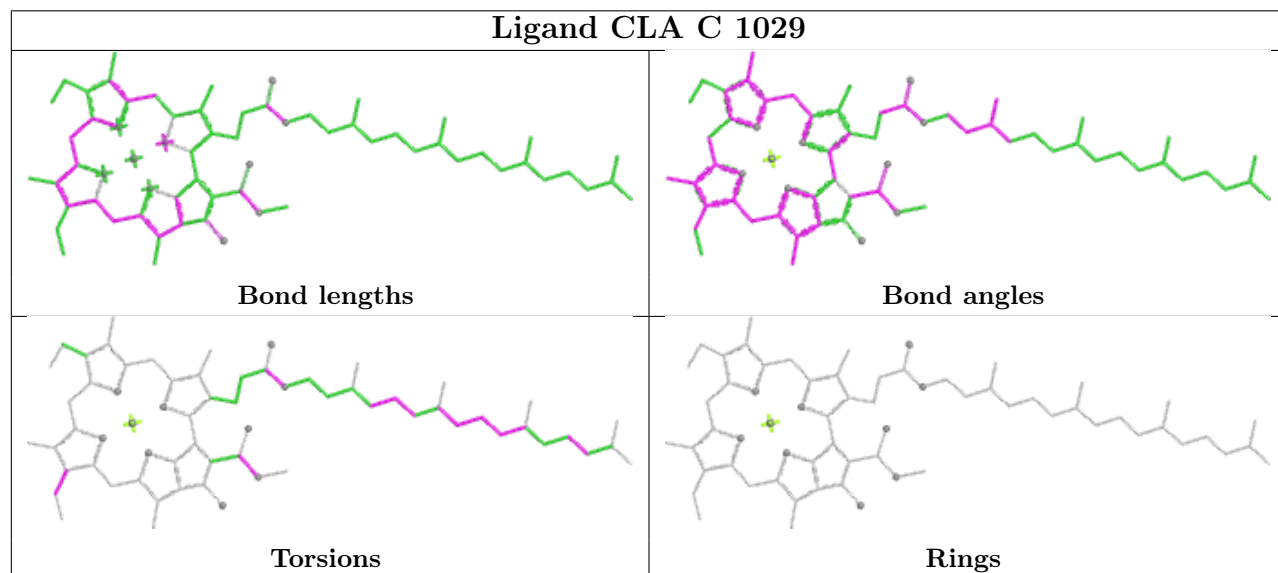
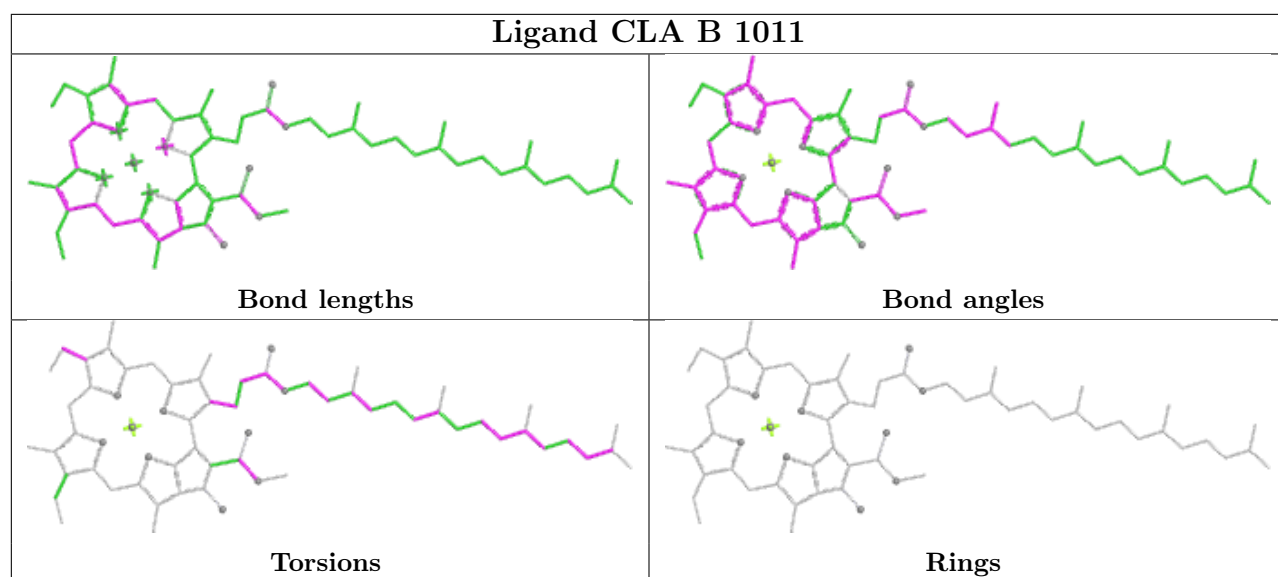


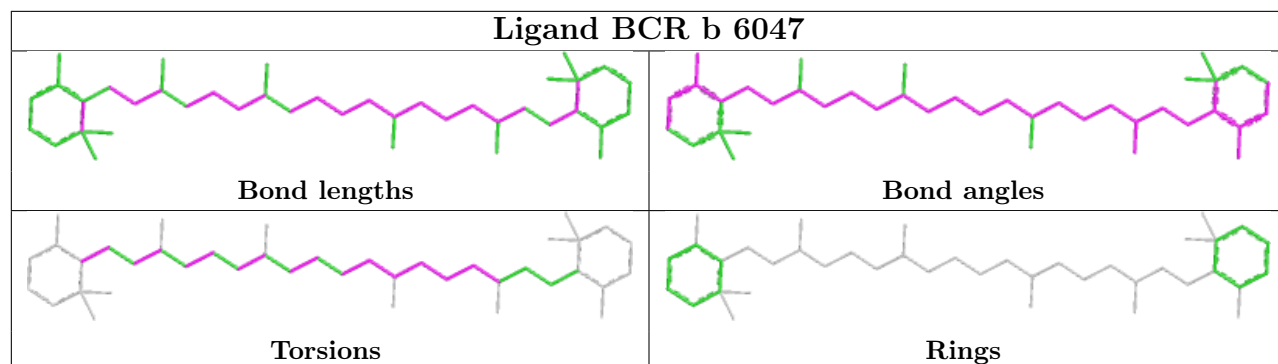
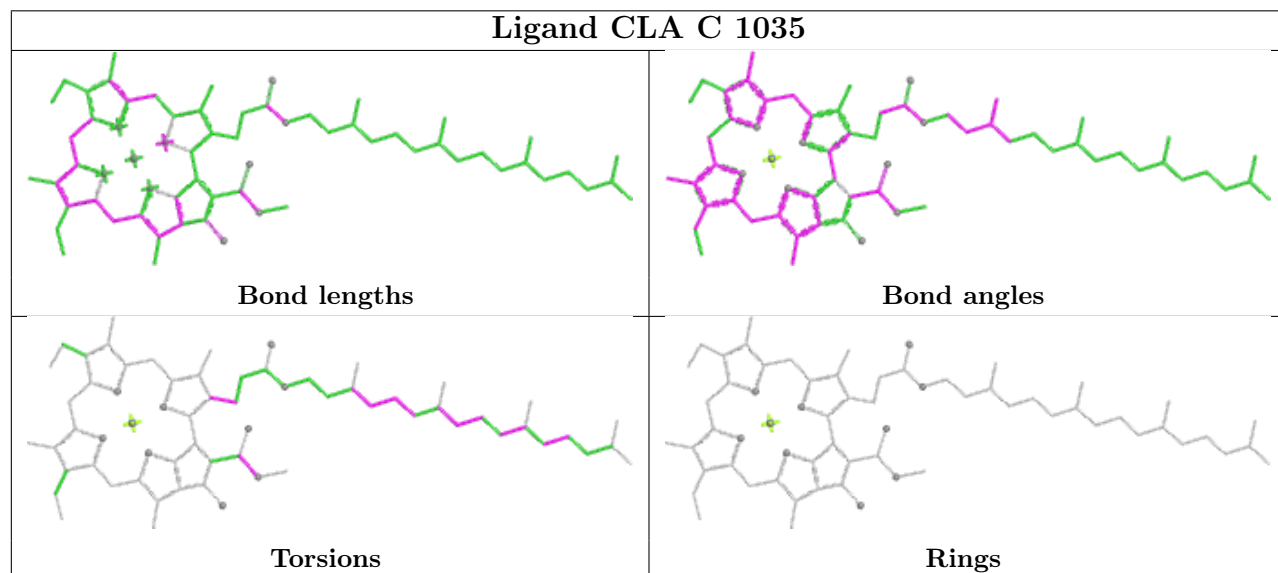
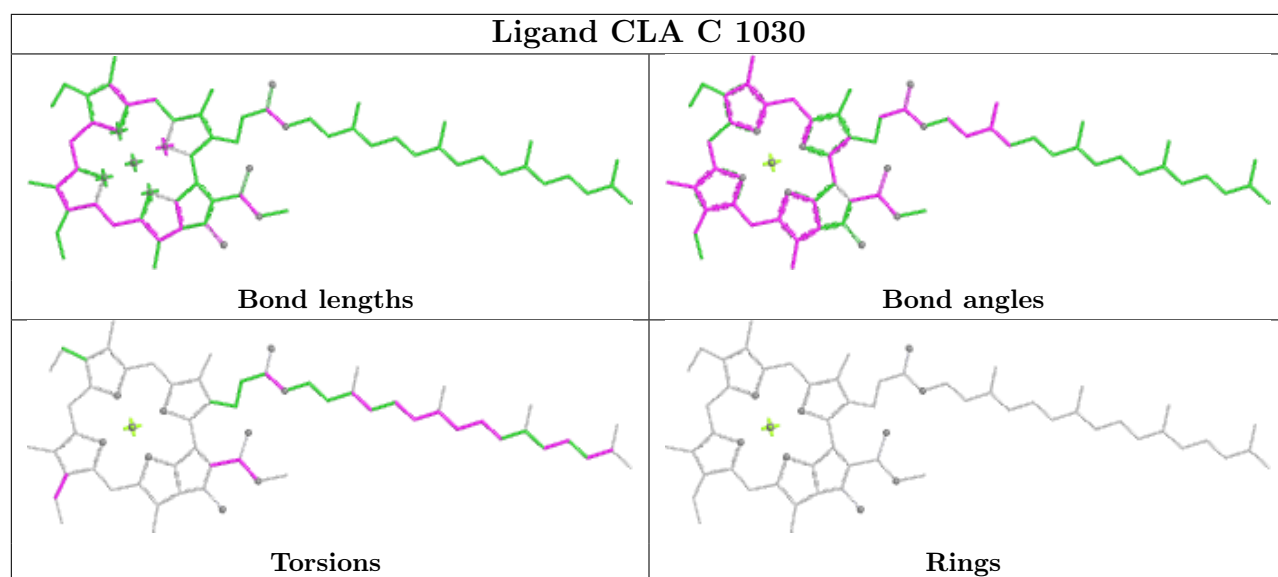


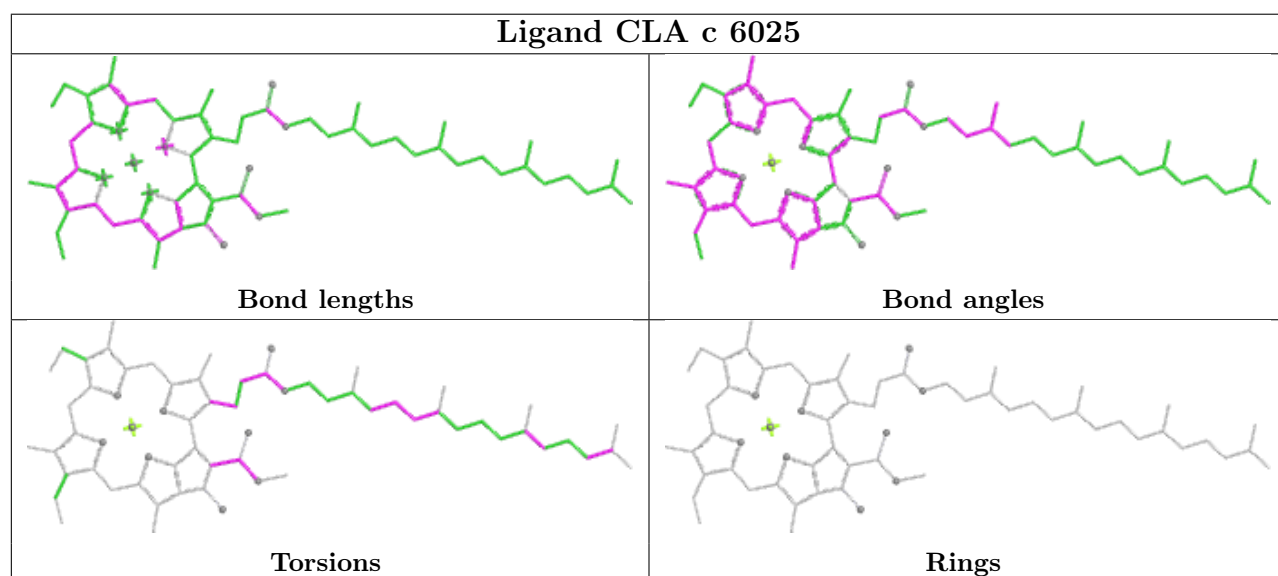
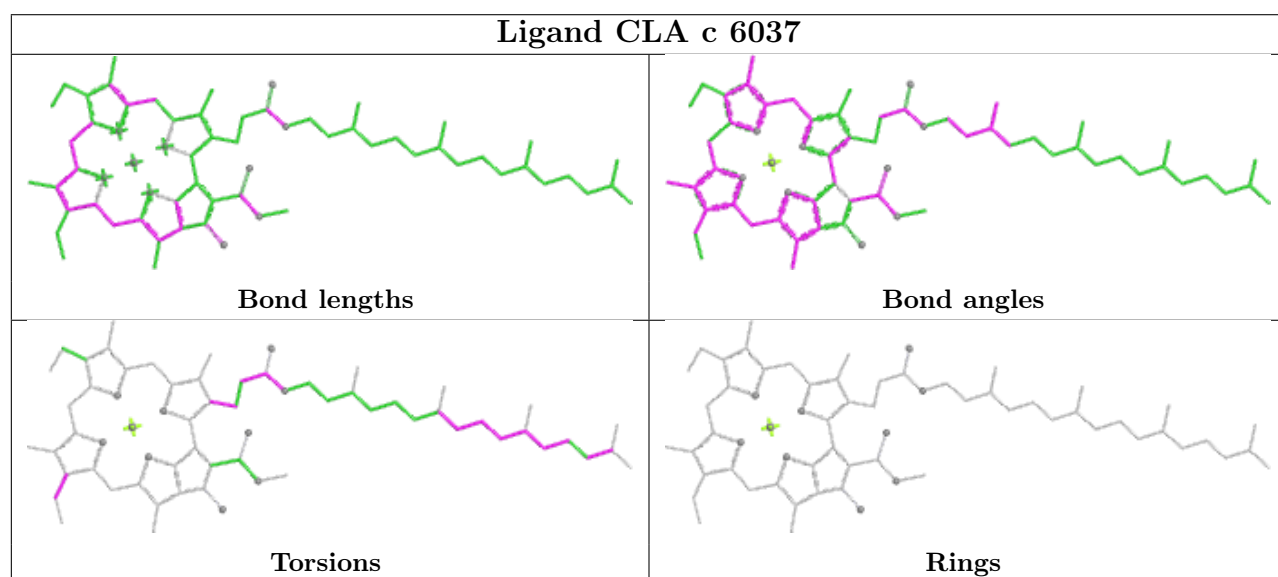
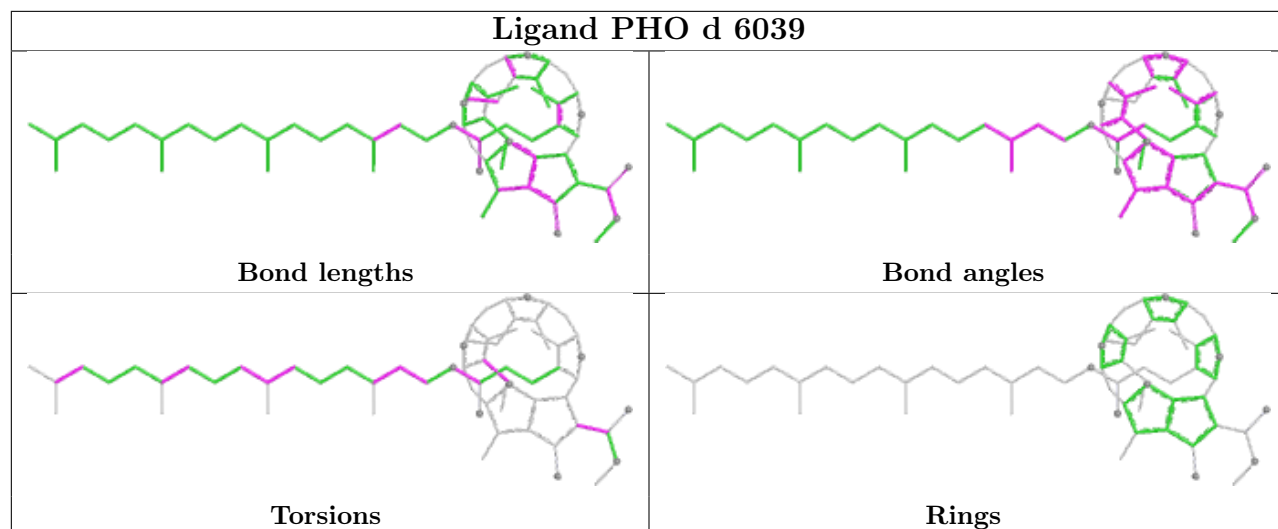


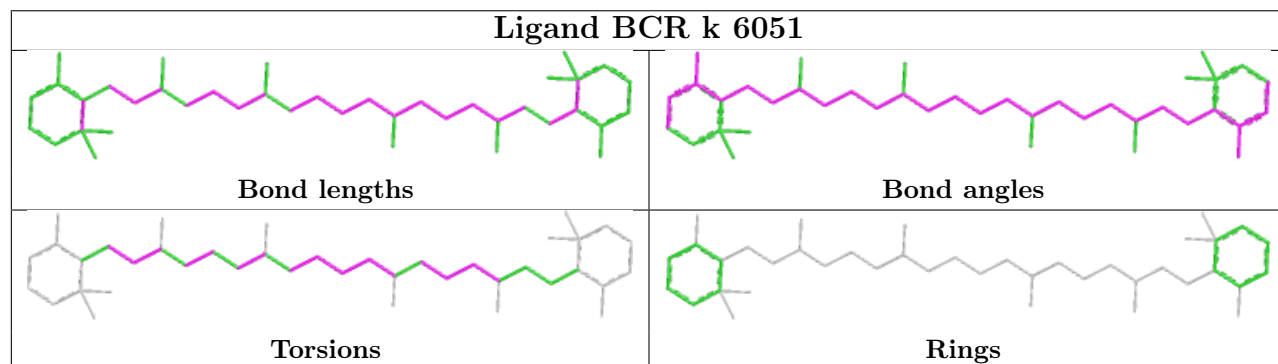
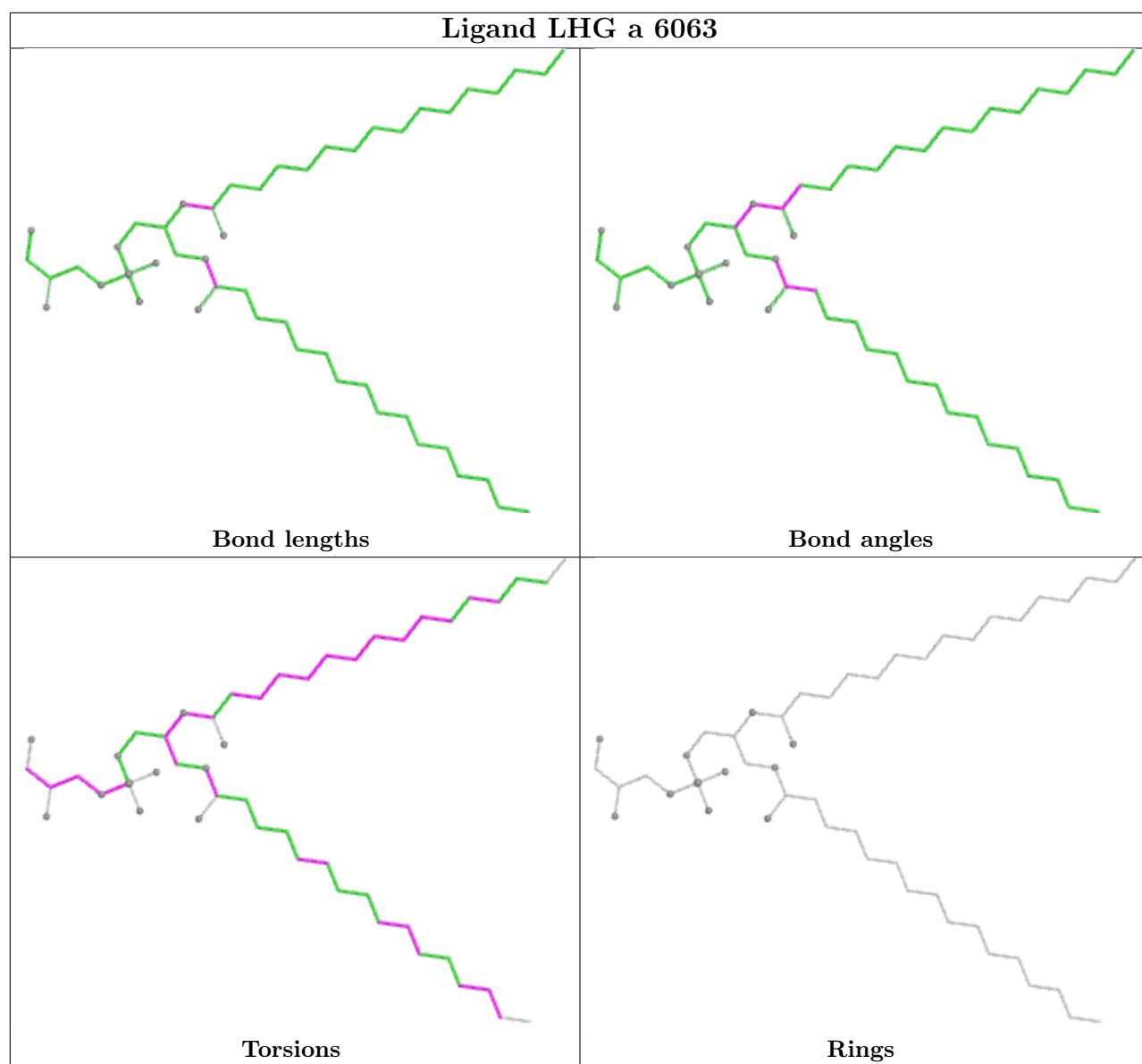




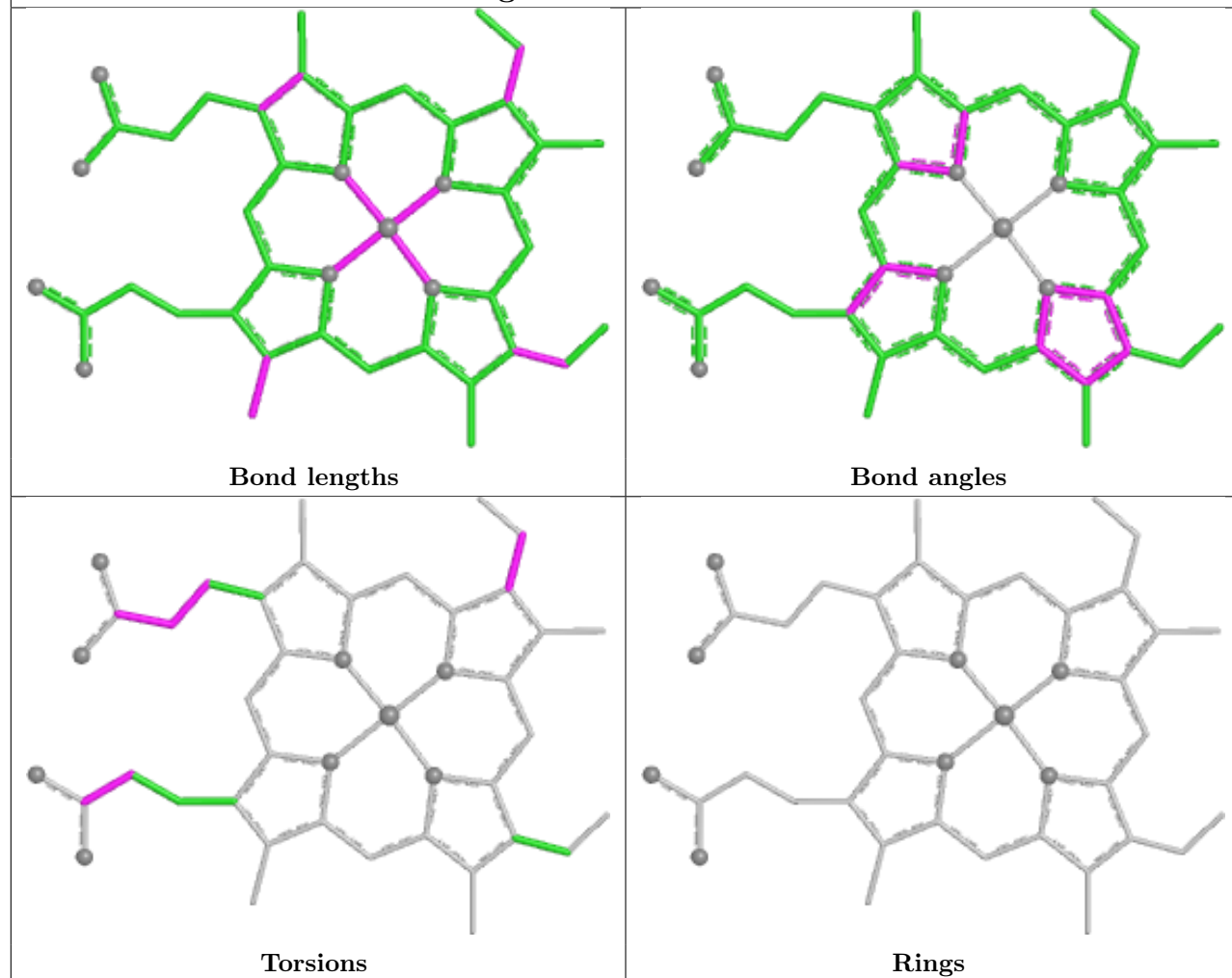




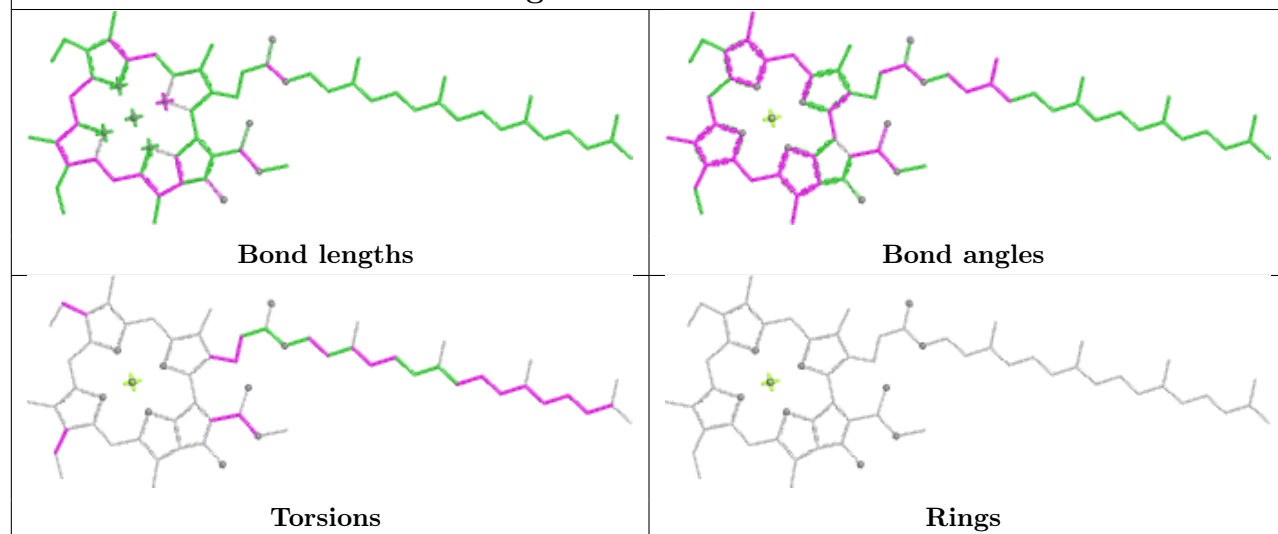


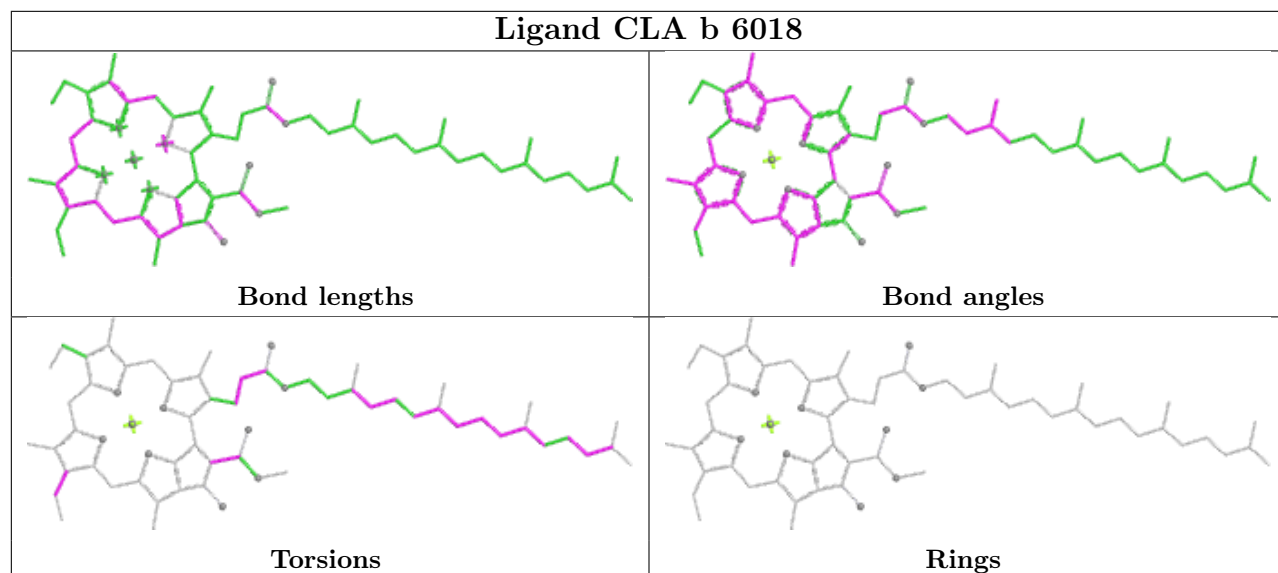
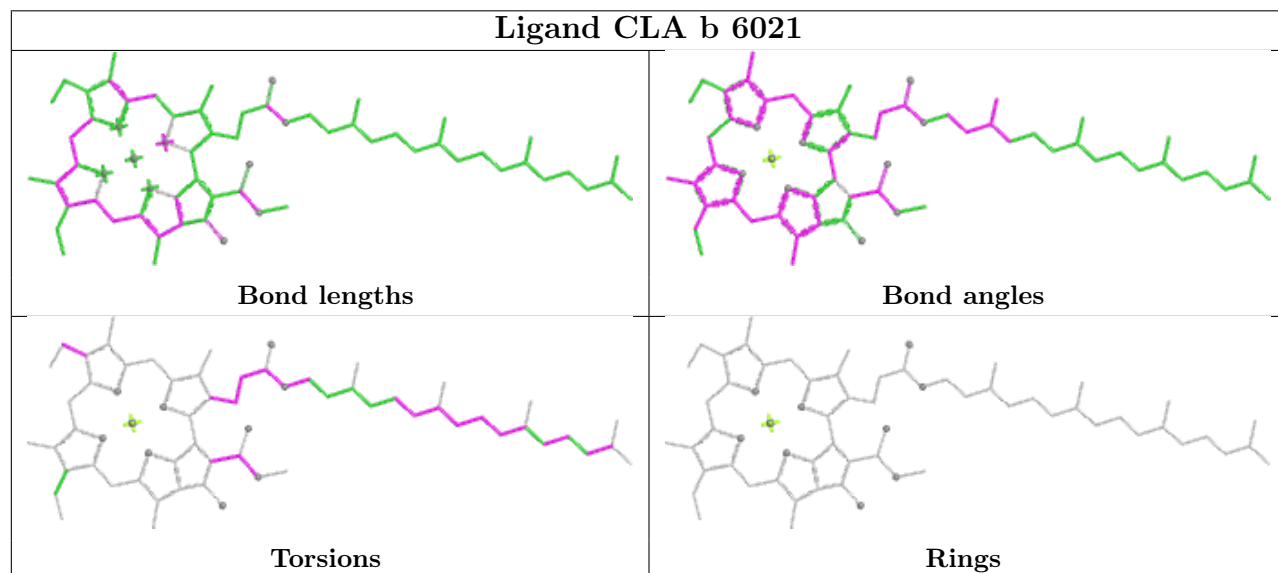
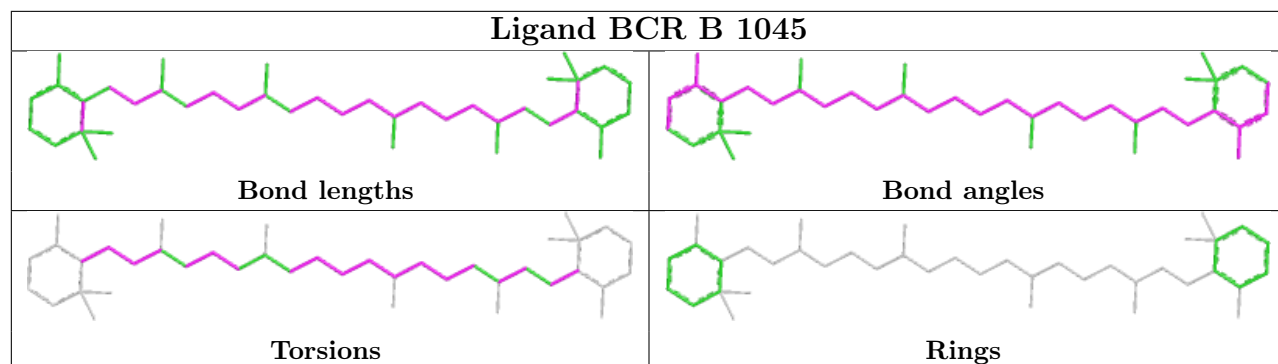


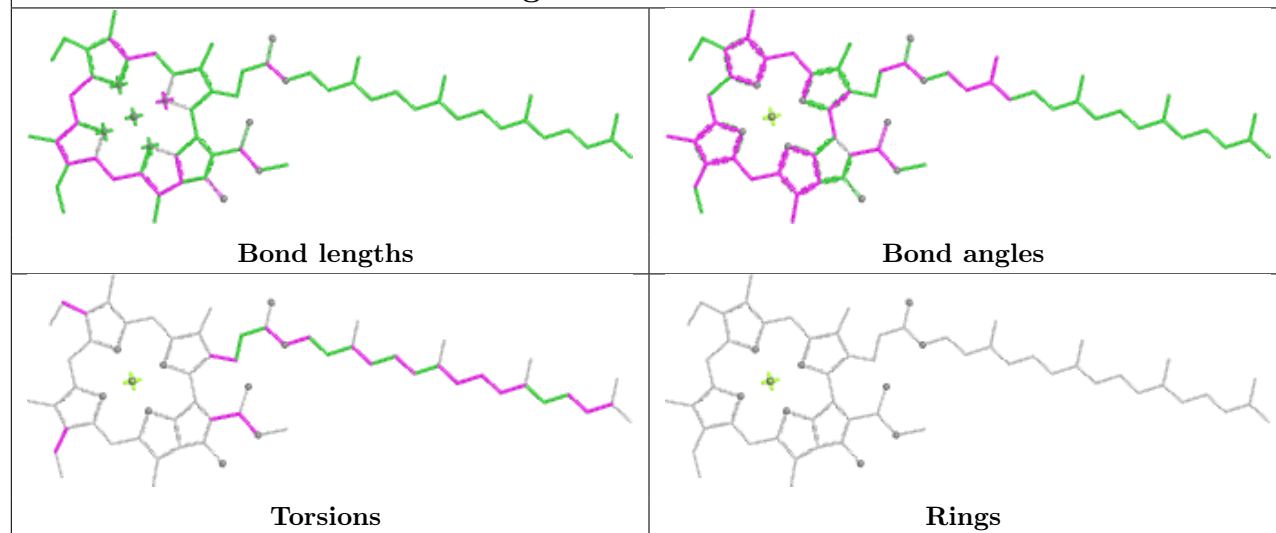
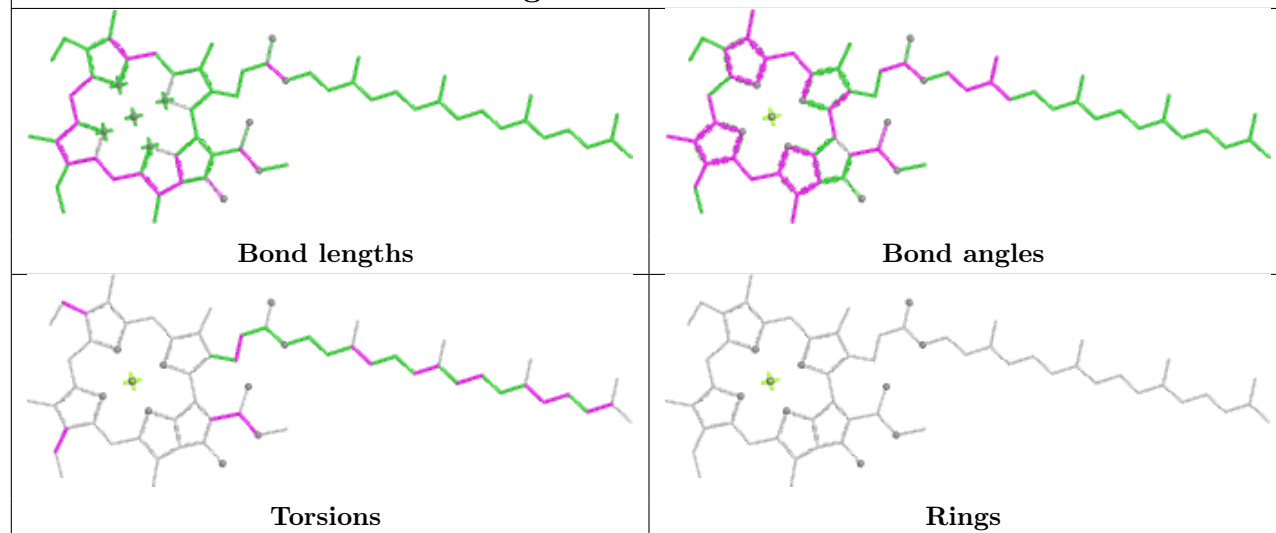
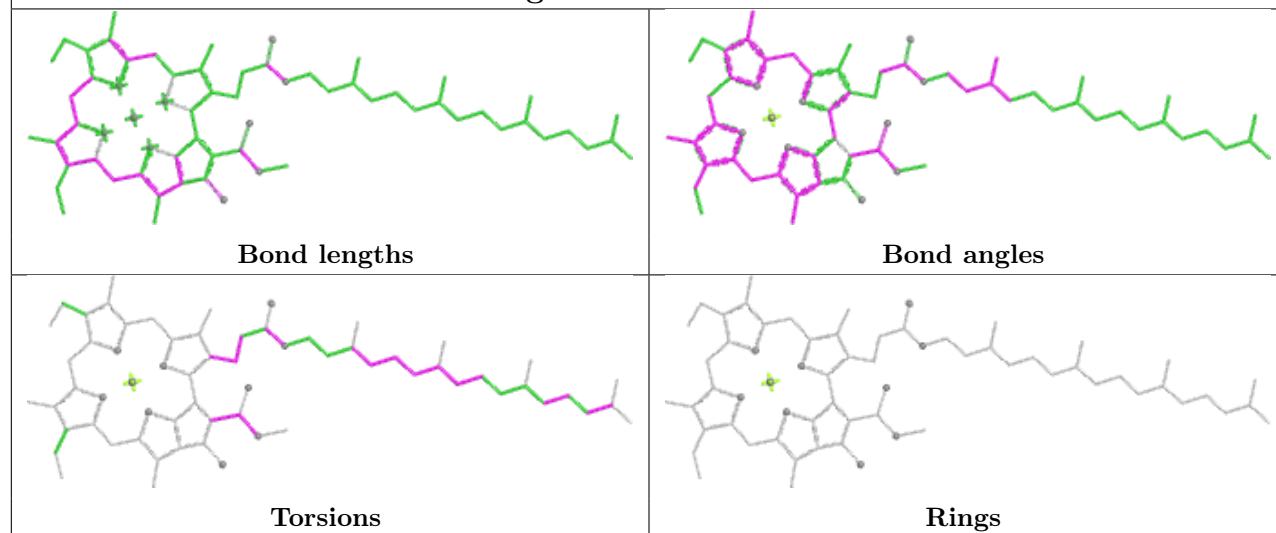
Ligand HEM V 1041

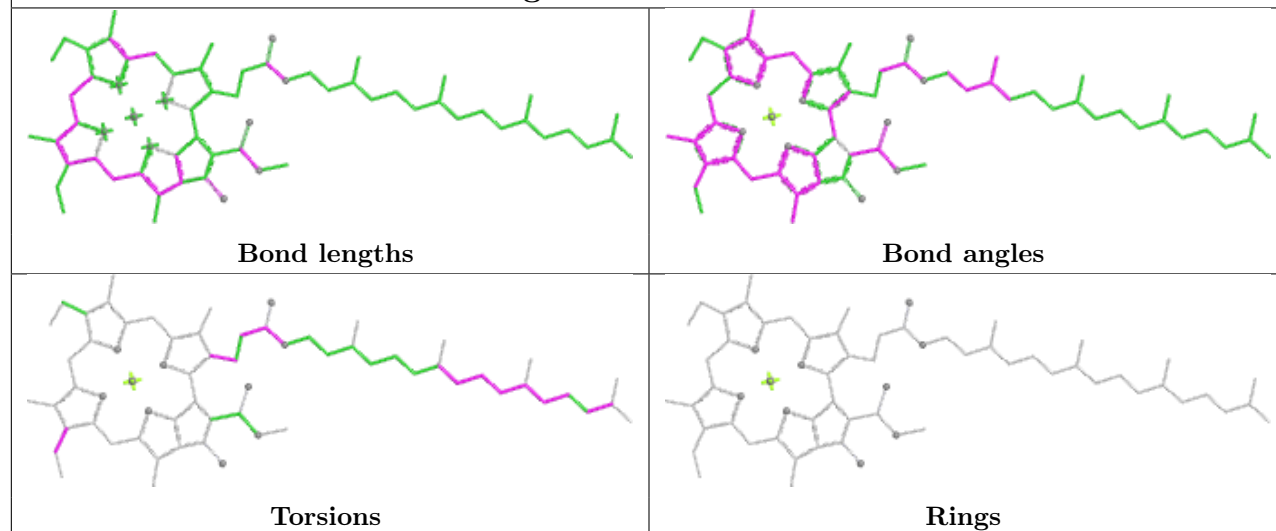
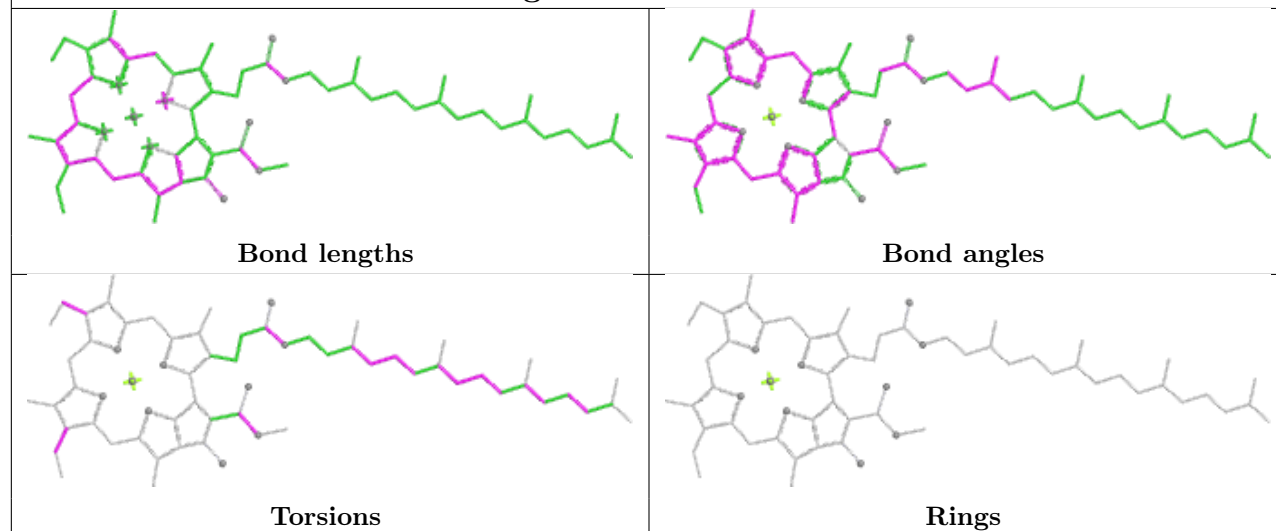
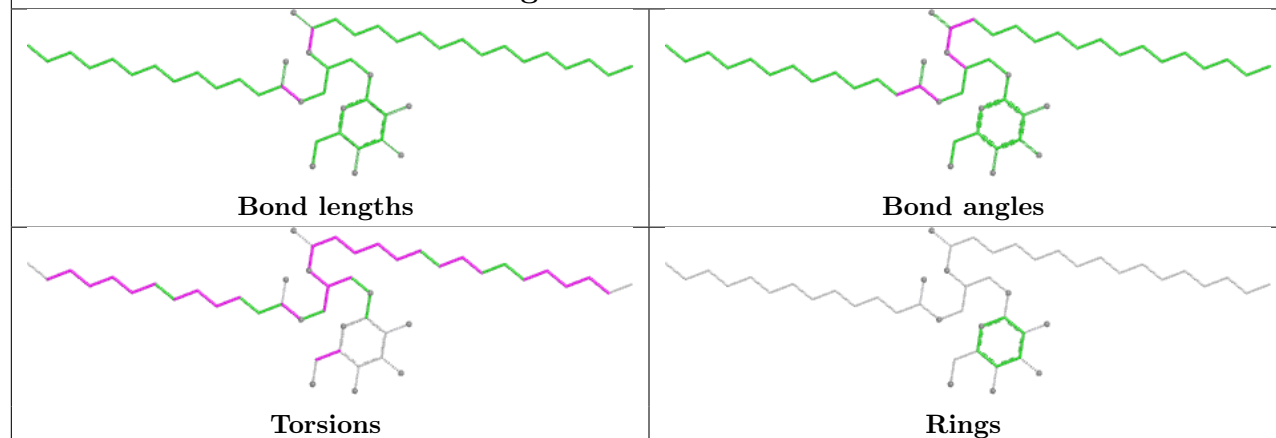


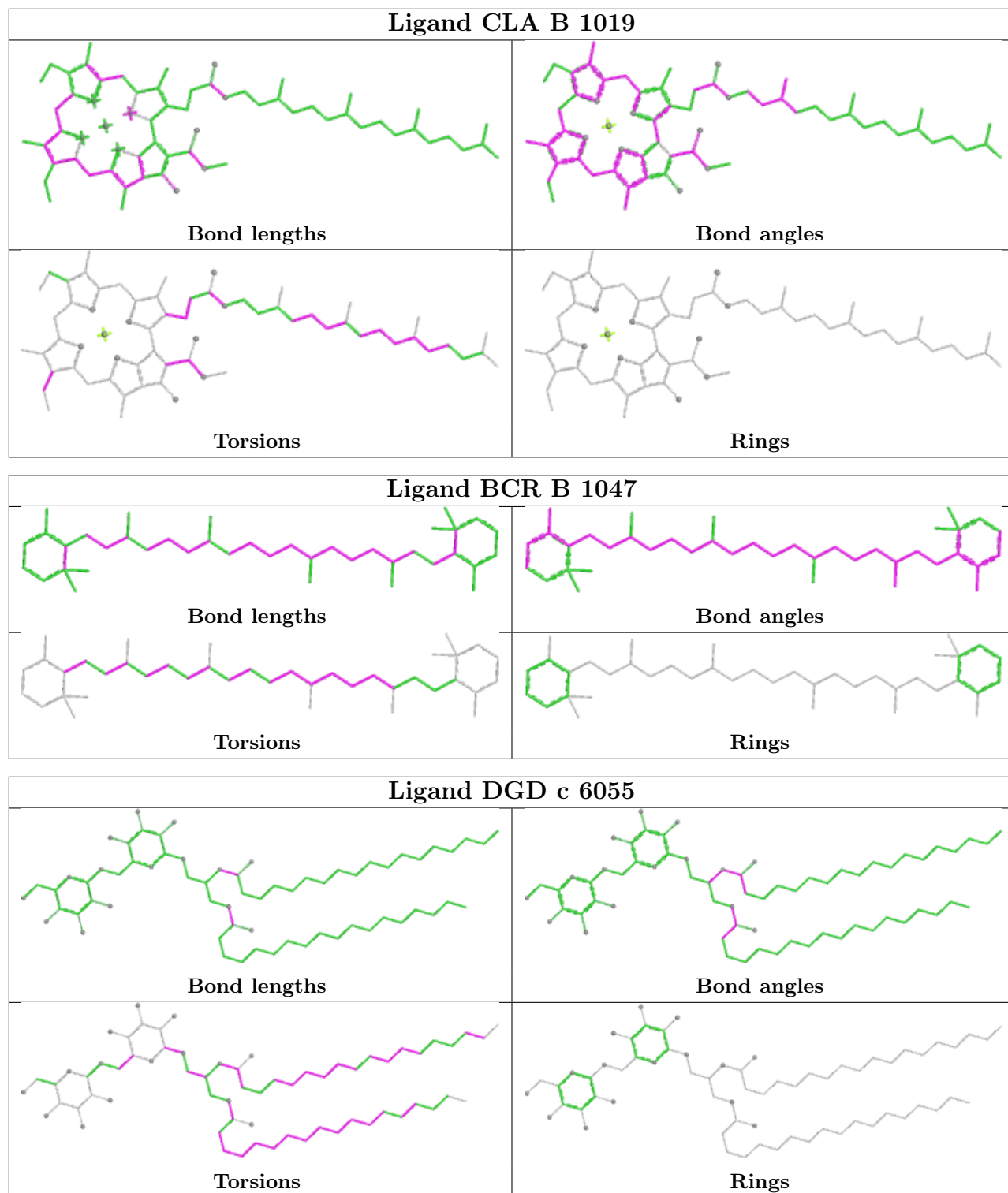
Ligand CLA b 6013

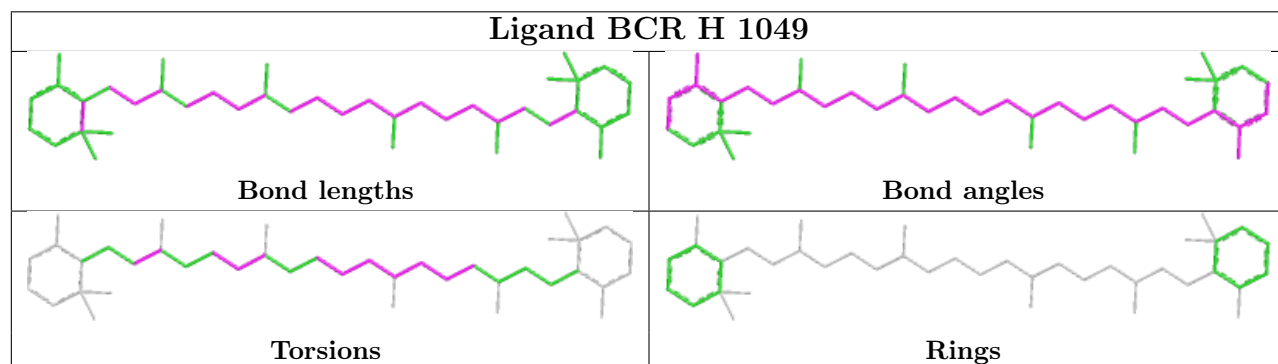
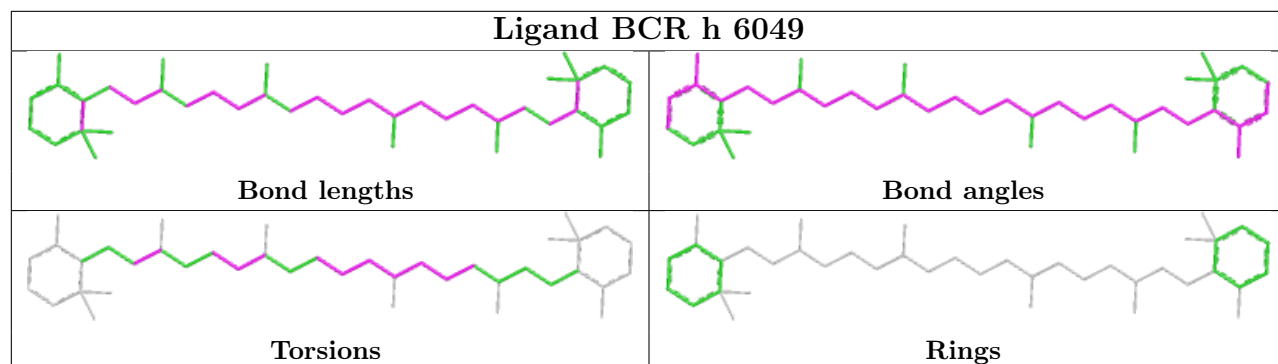
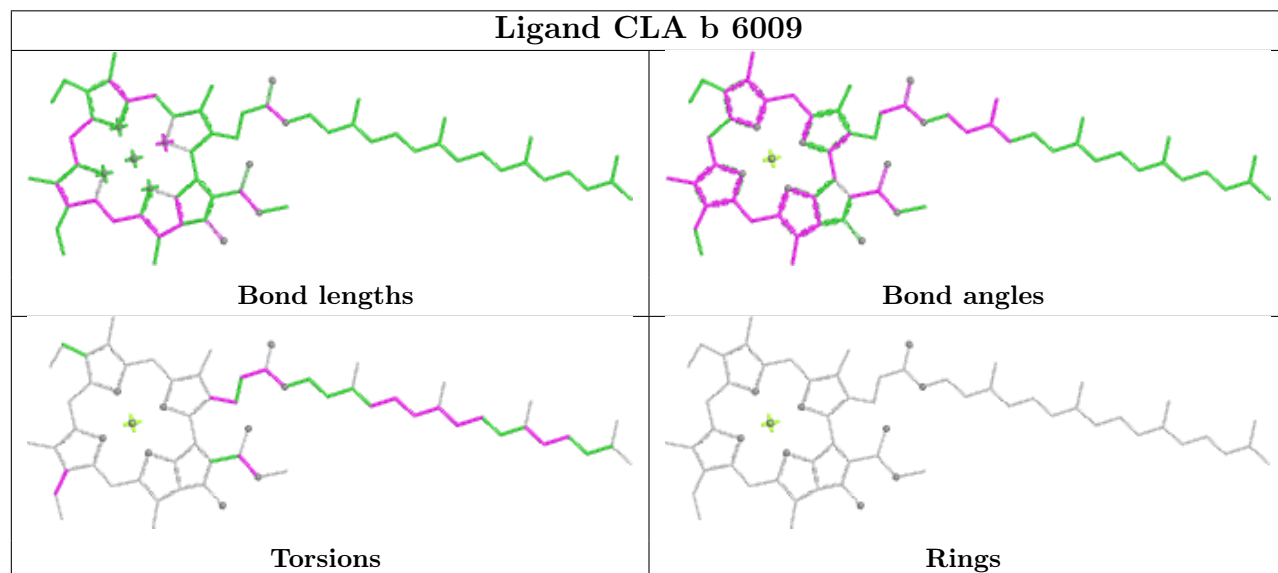
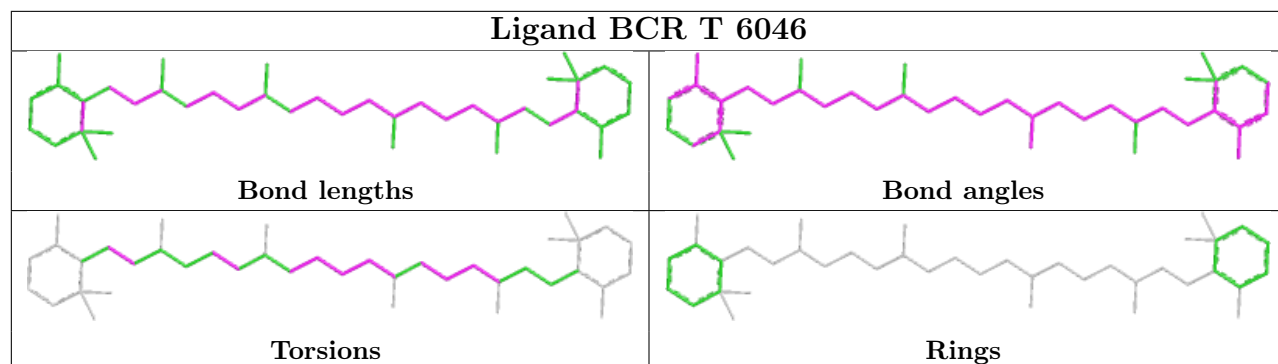




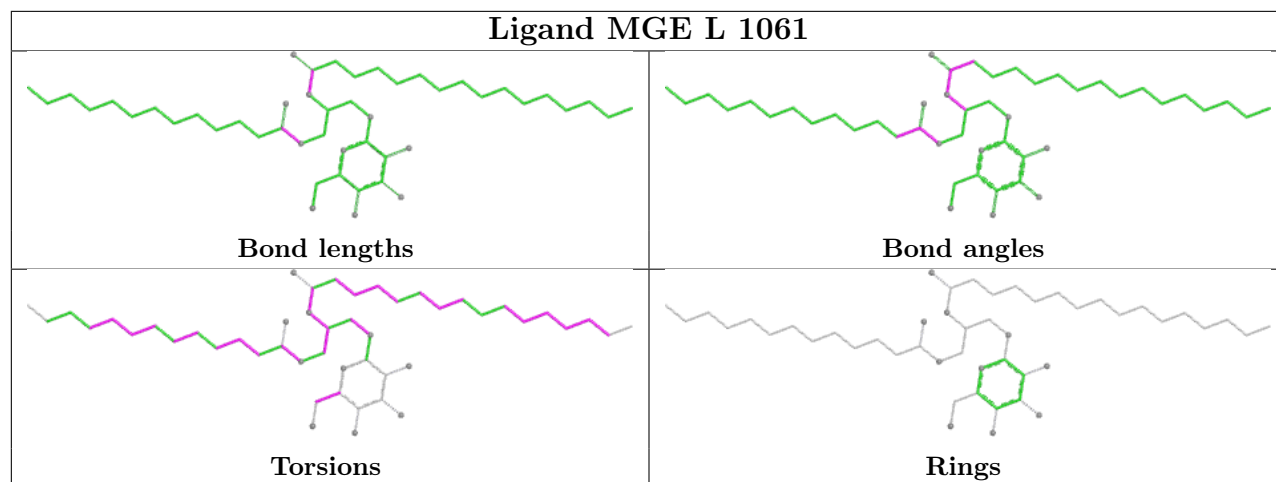
Ligand CLA A 1007**Ligand CLA B 1012****Ligand CLA b 6015**

Ligand CLA C 1037**Ligand CLA B 1024****Ligand MGE b 6060**

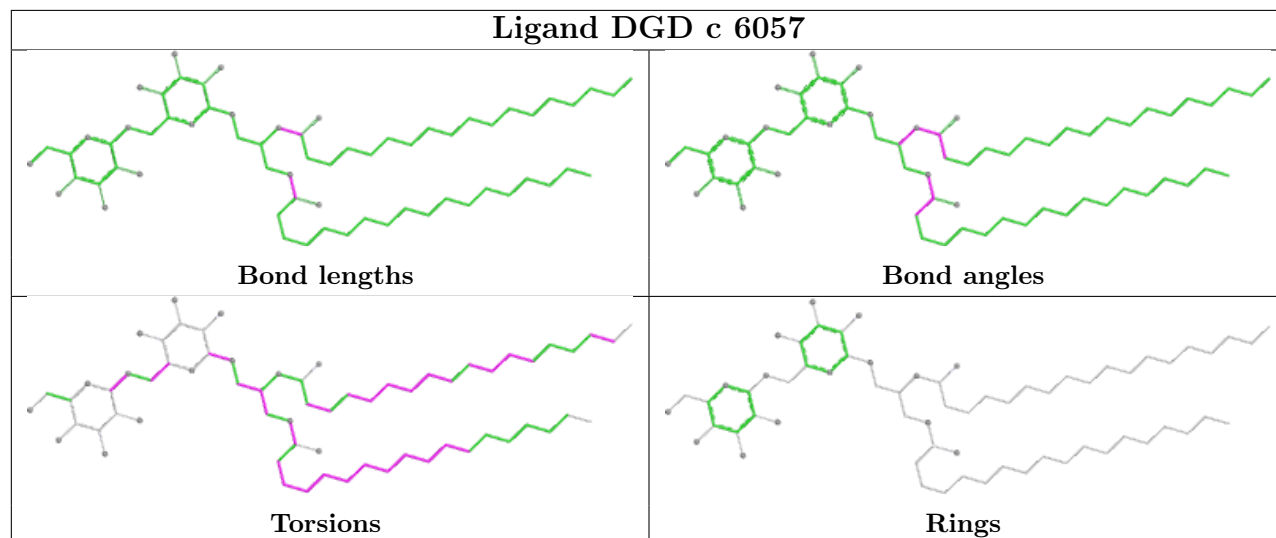




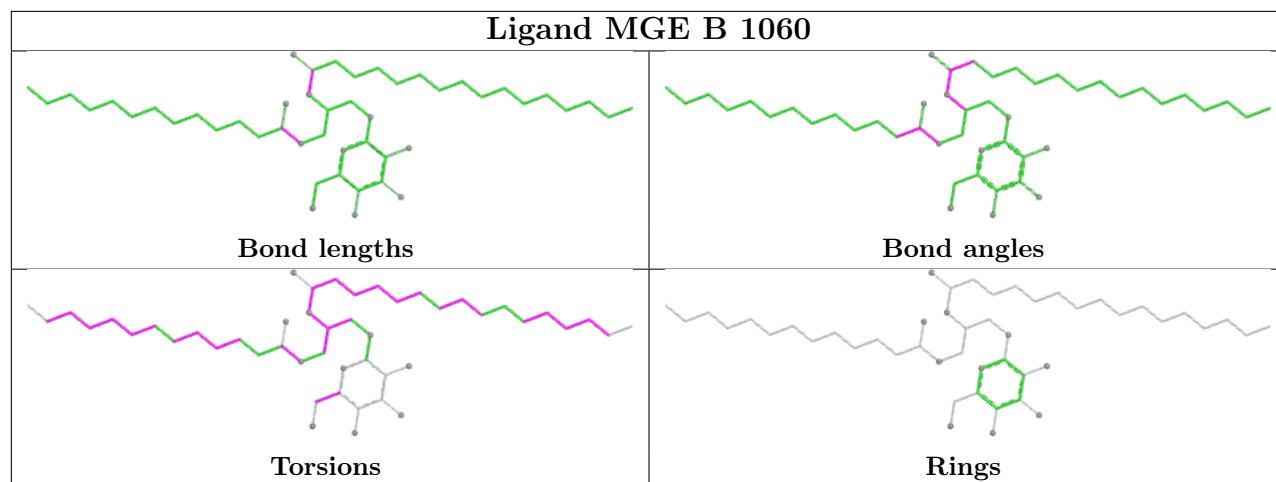
Ligand MGE L 1061

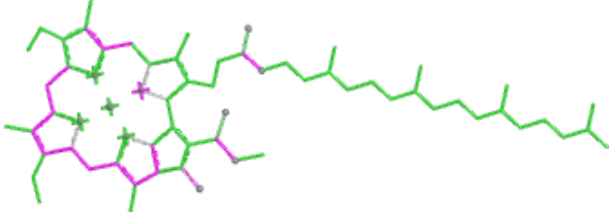
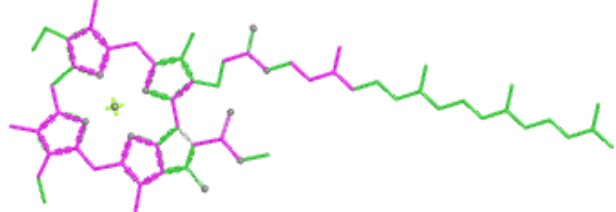
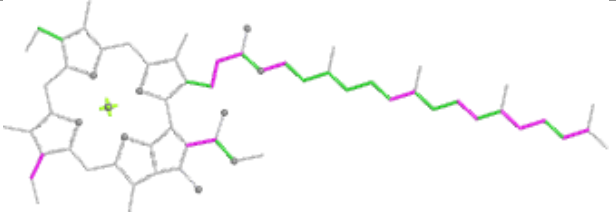
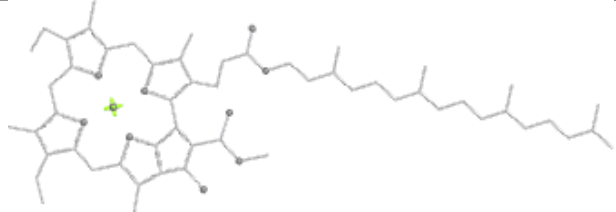
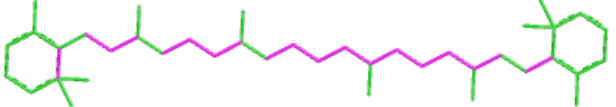
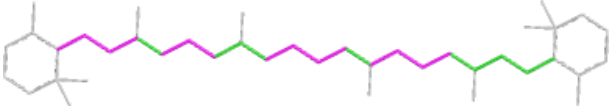
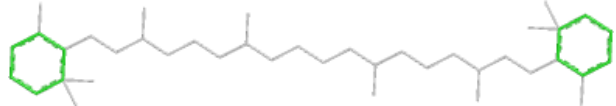
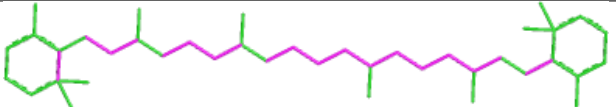
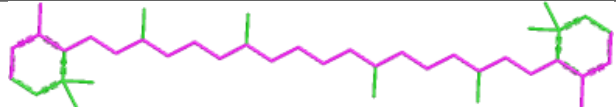
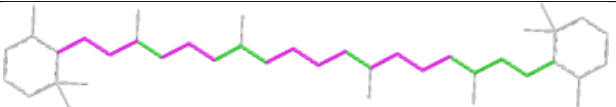
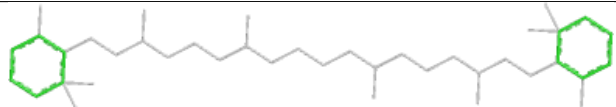


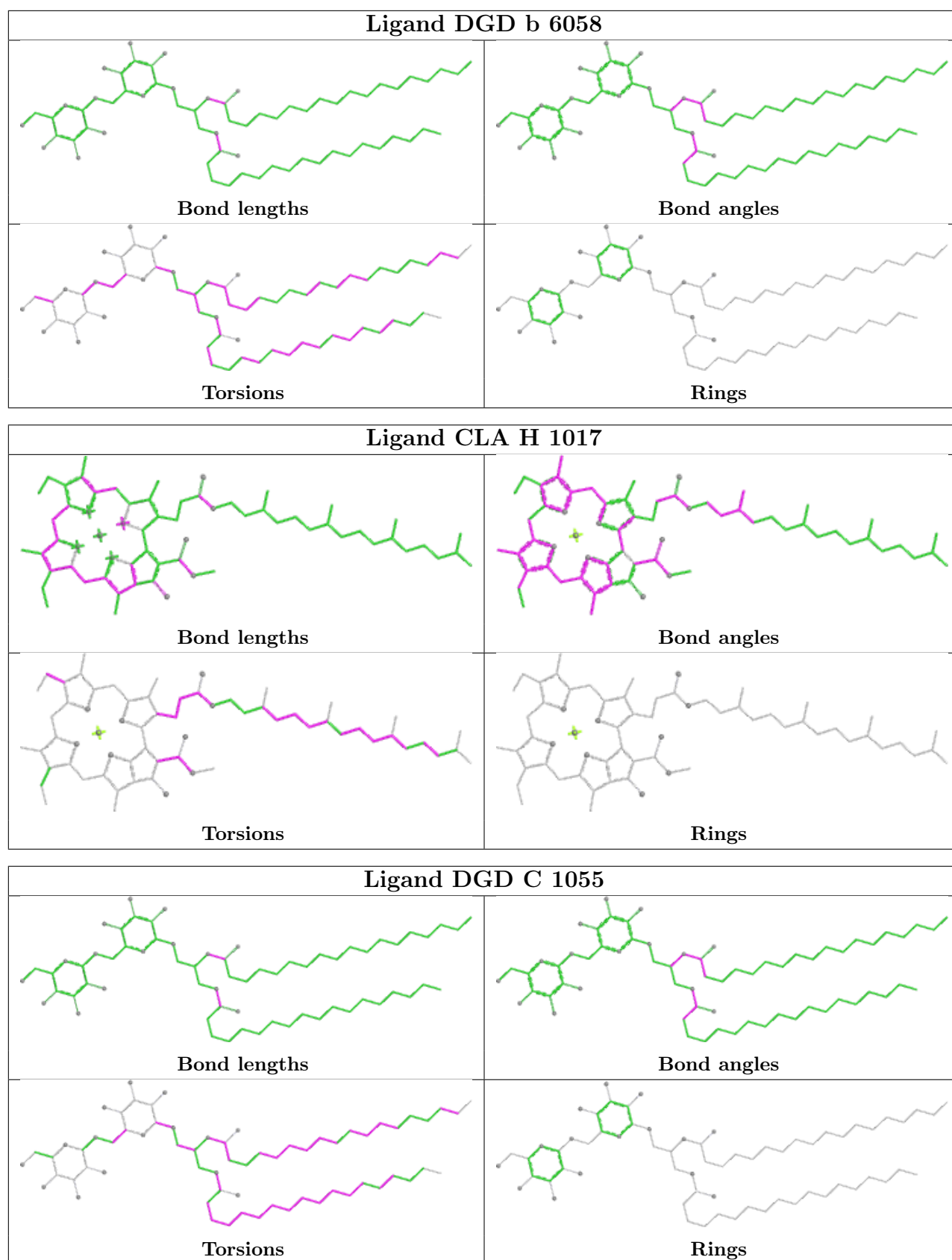
Ligand DGD c 6057

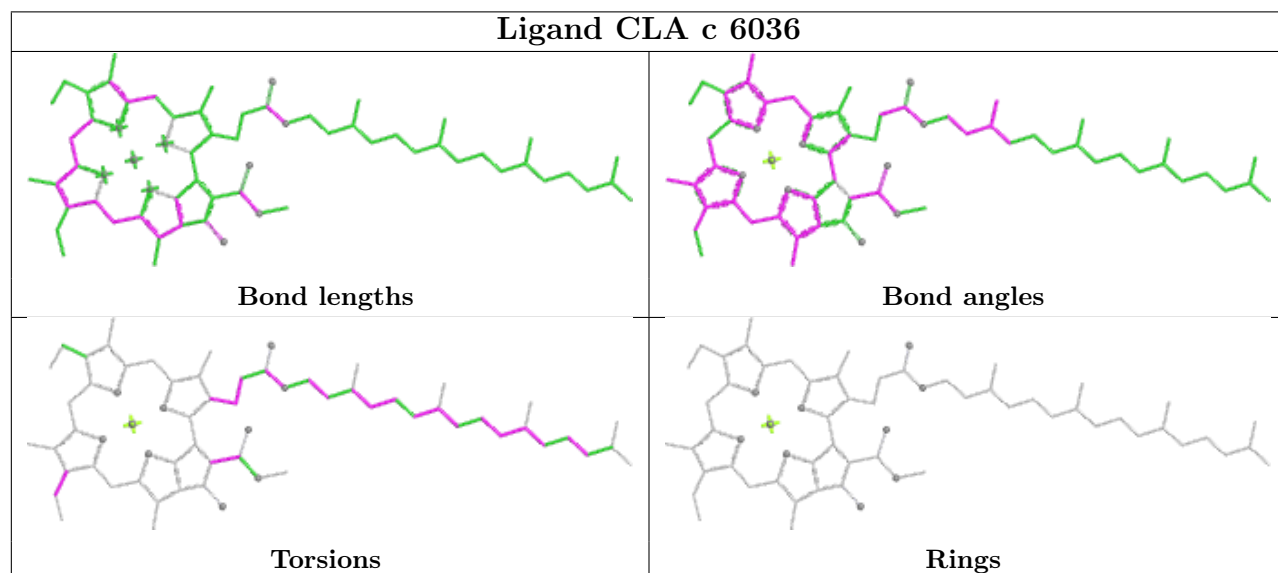
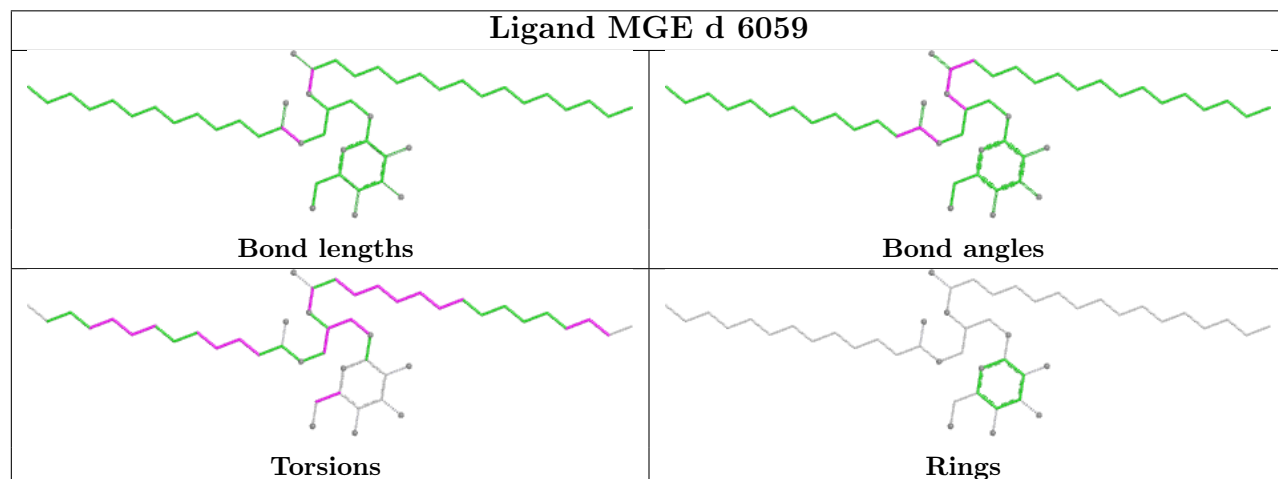
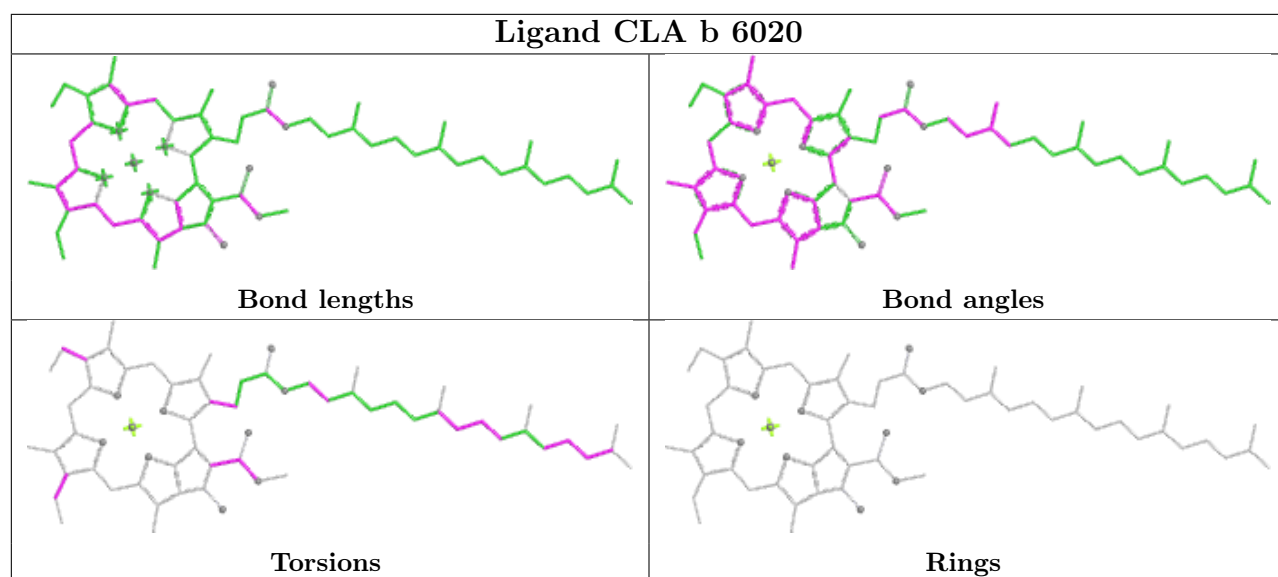


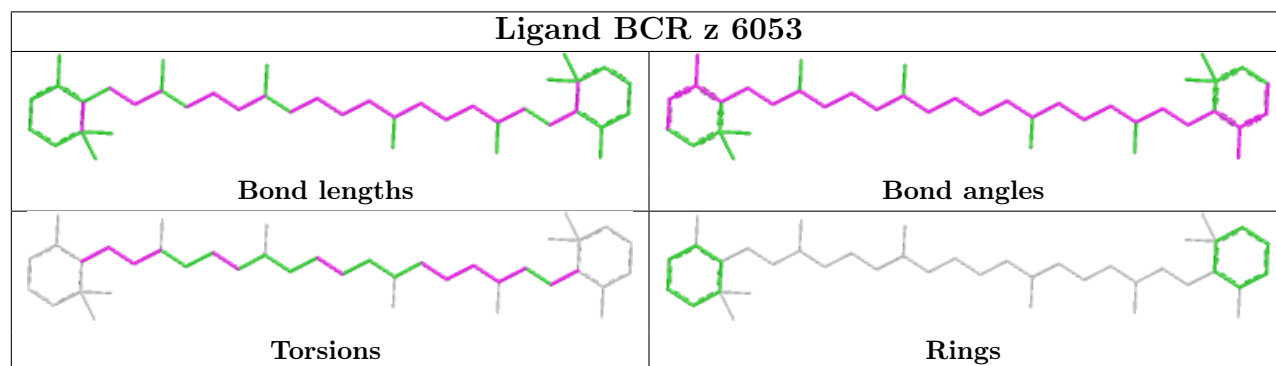
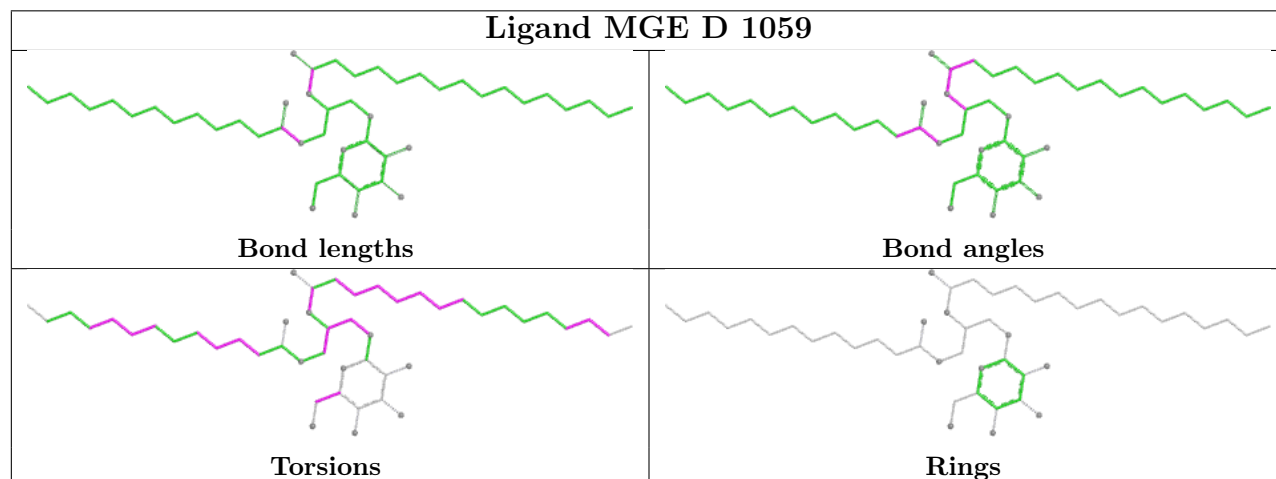
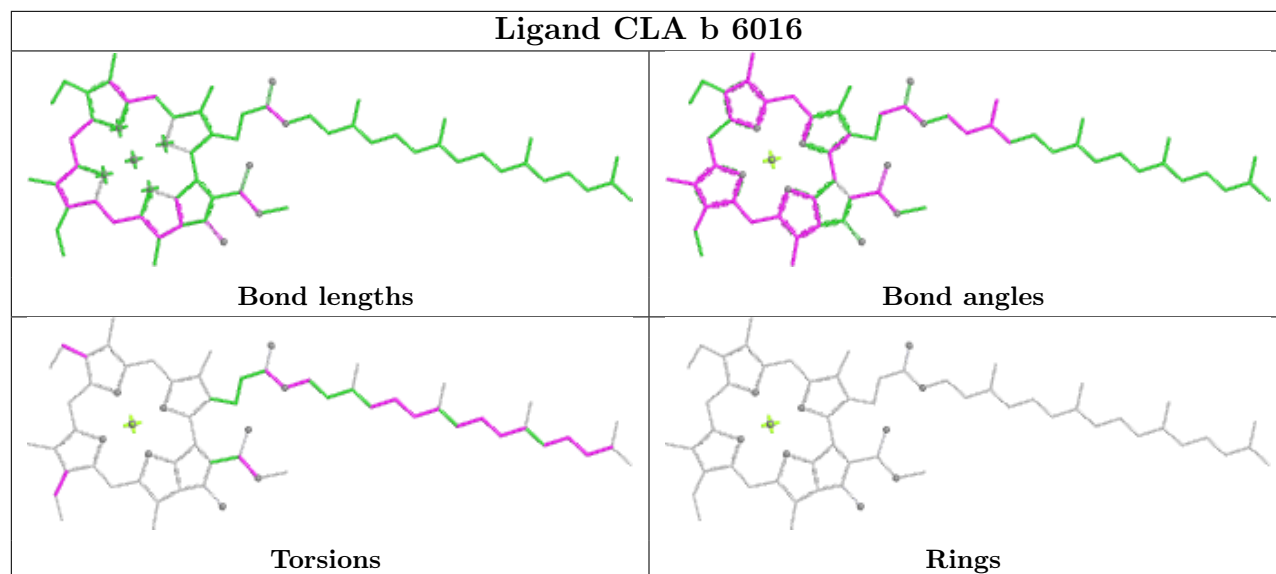
Ligand MGE B 1060

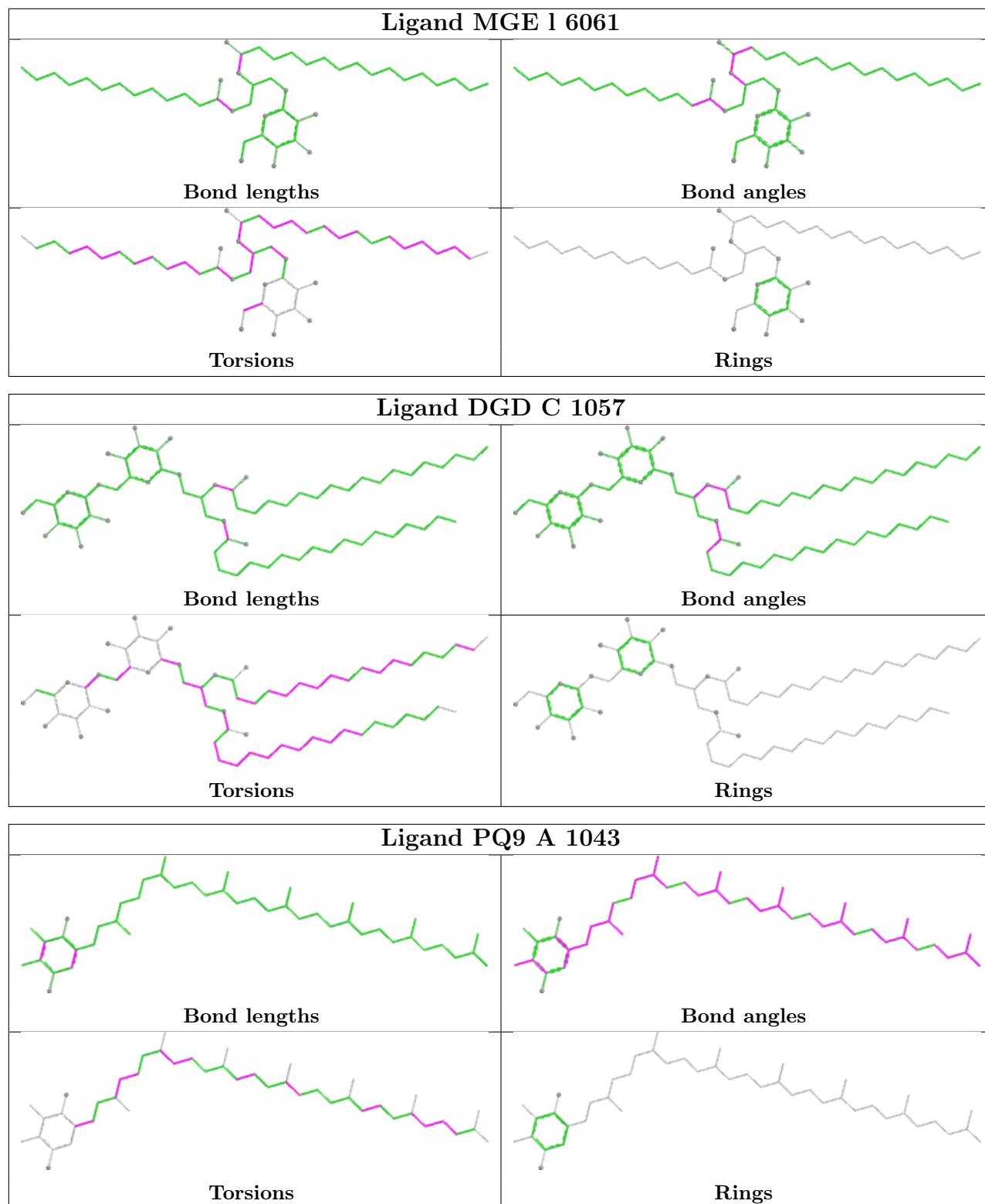


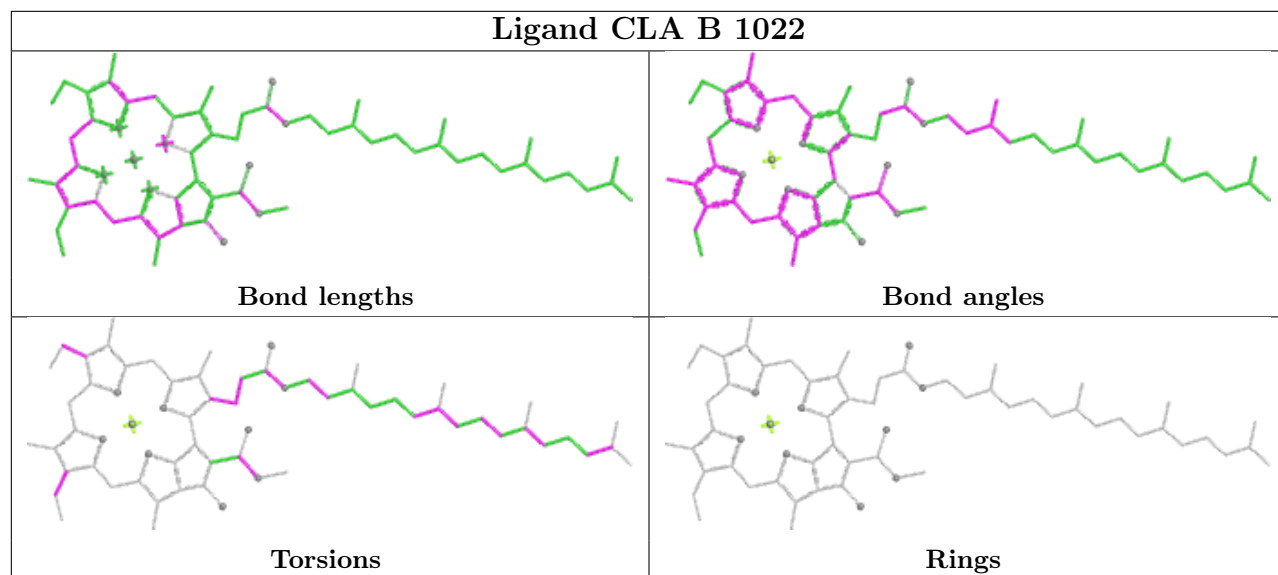
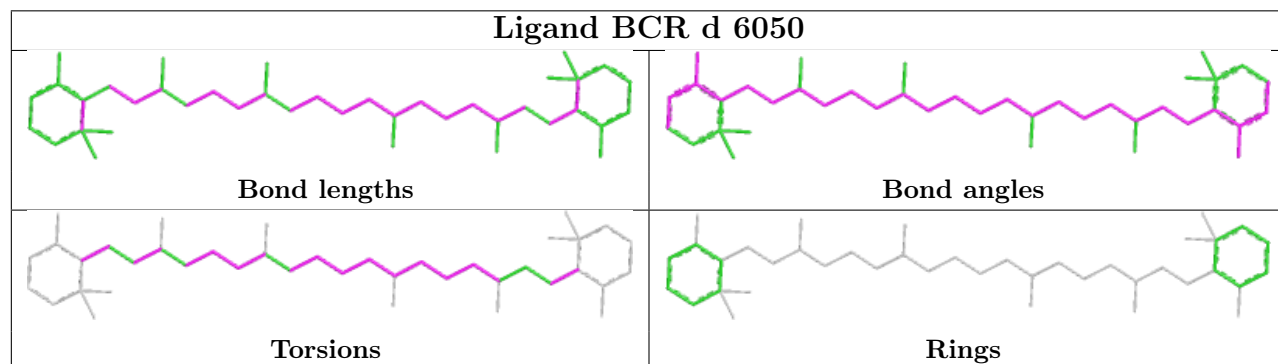
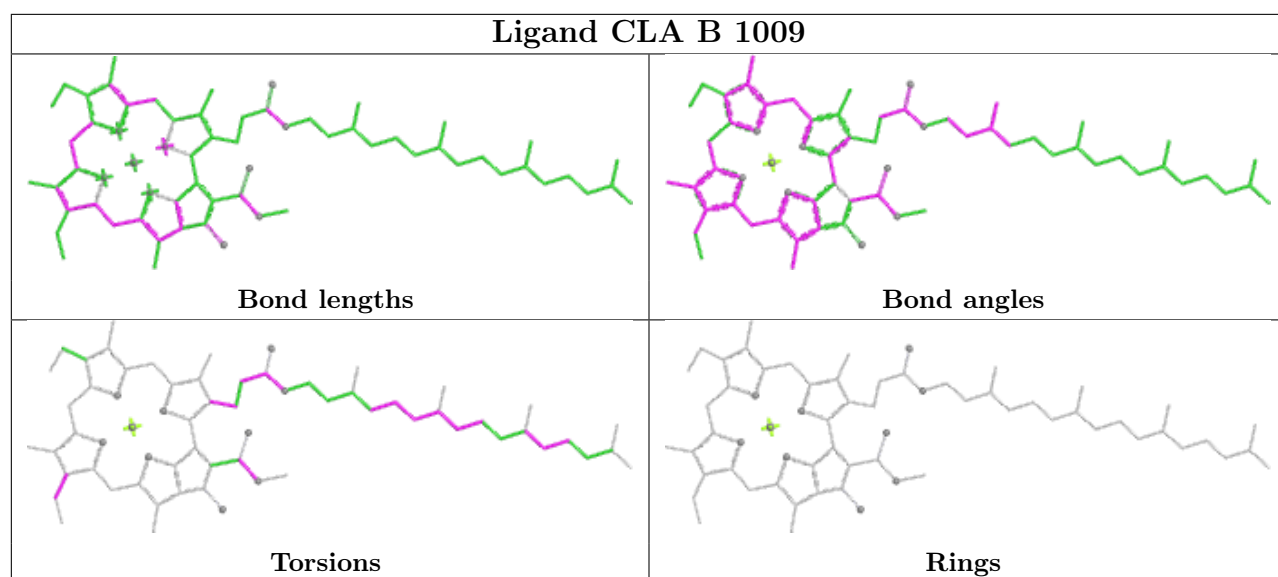
Ligand CLA c 6031	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR c 6054	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 1054	
 Bond lengths	 Bond angles
 Torsions	 Rings



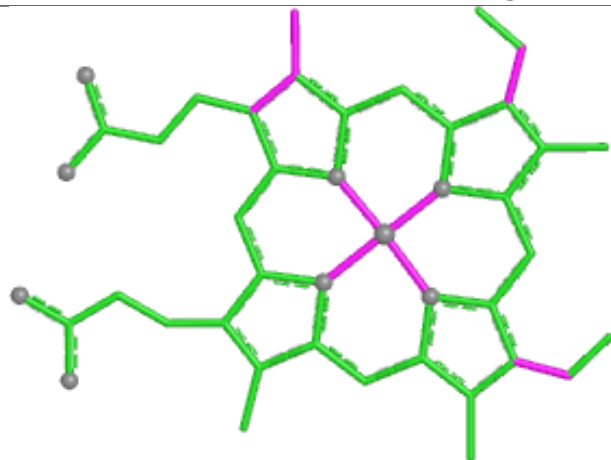




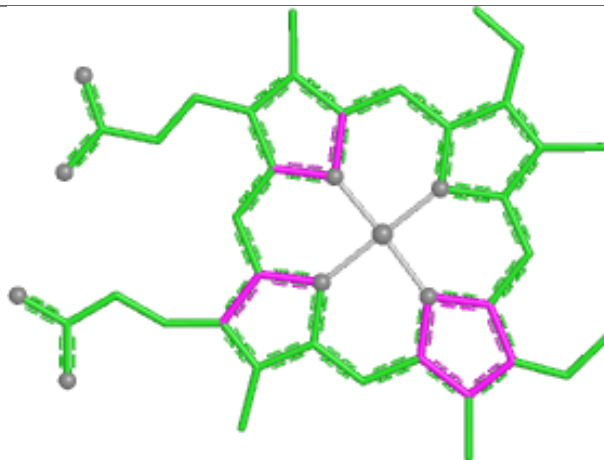




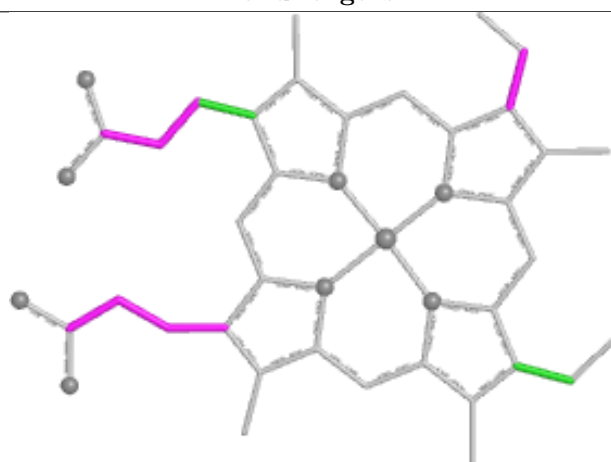
Ligand HEM F 1040



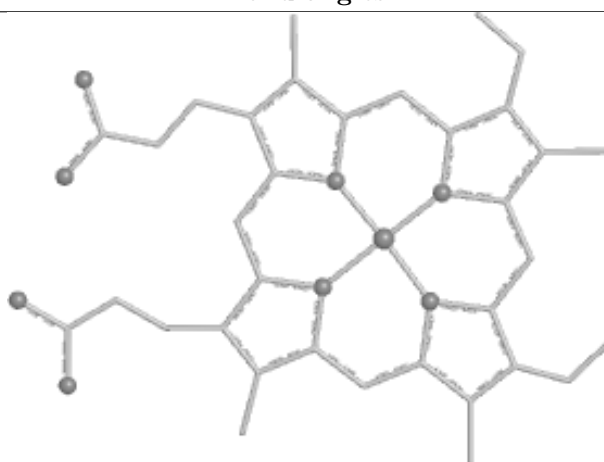
Bond lengths



Bond angles

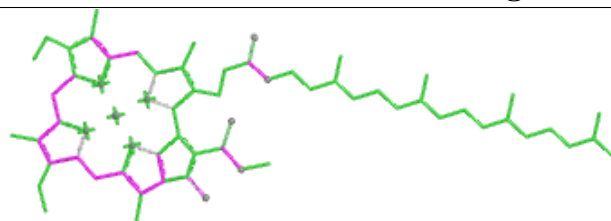


Torsions

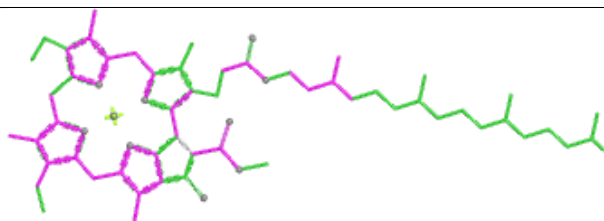


Rings

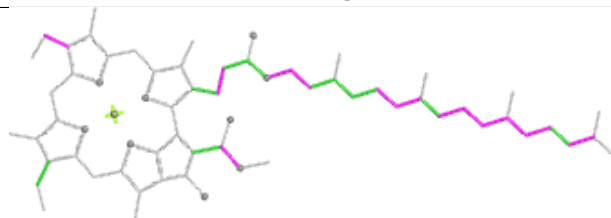
Ligand CLA C 1026



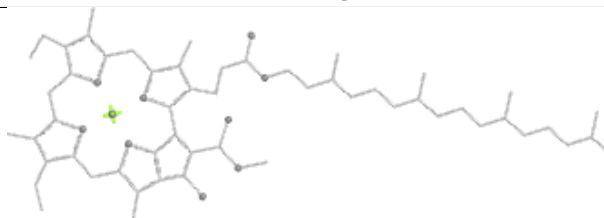
Bond lengths



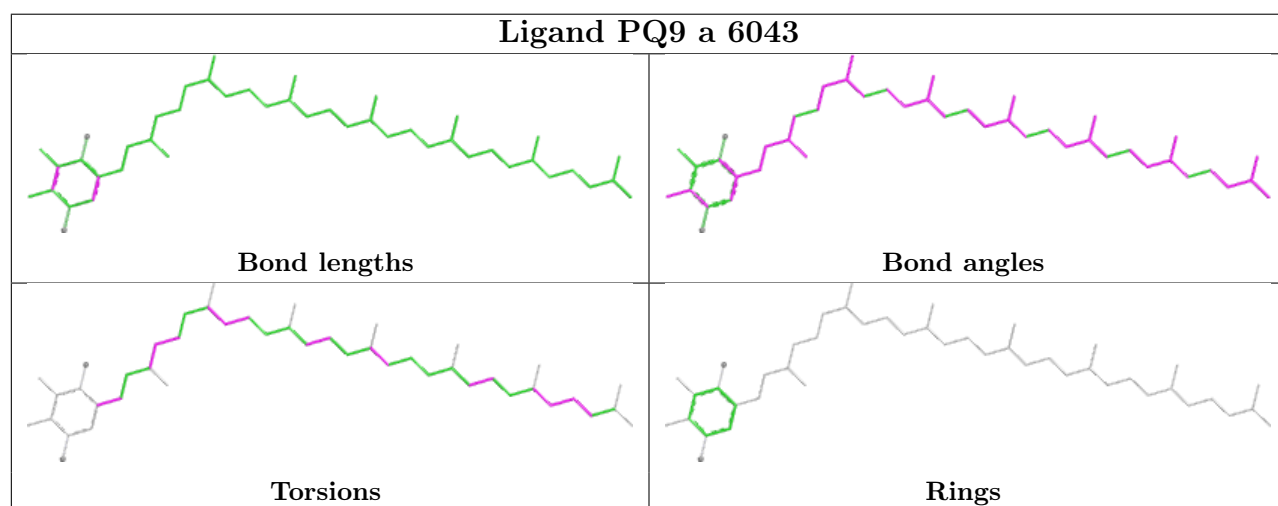
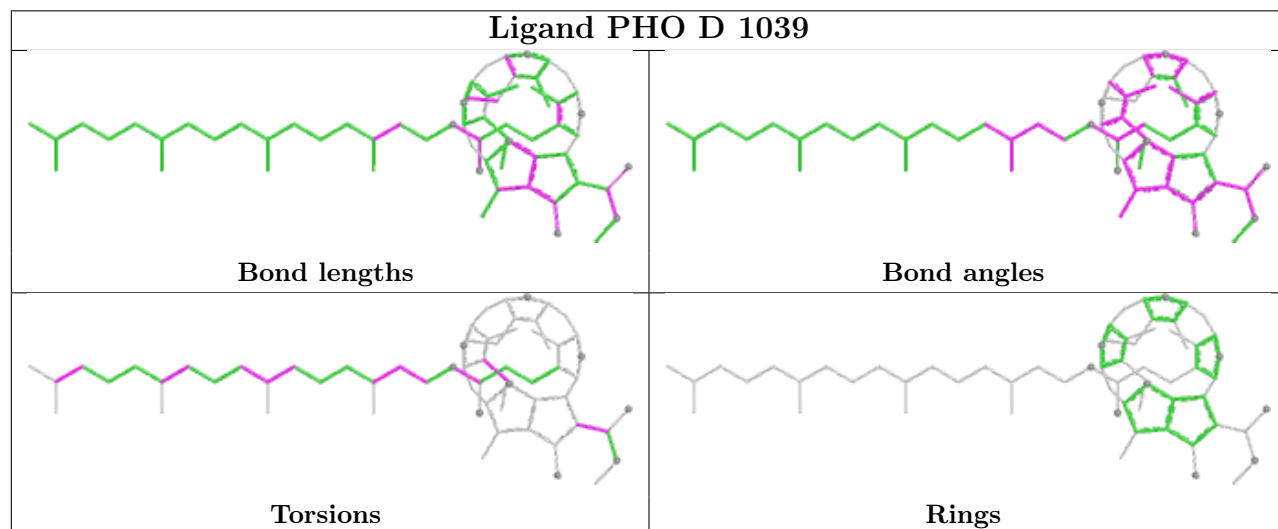
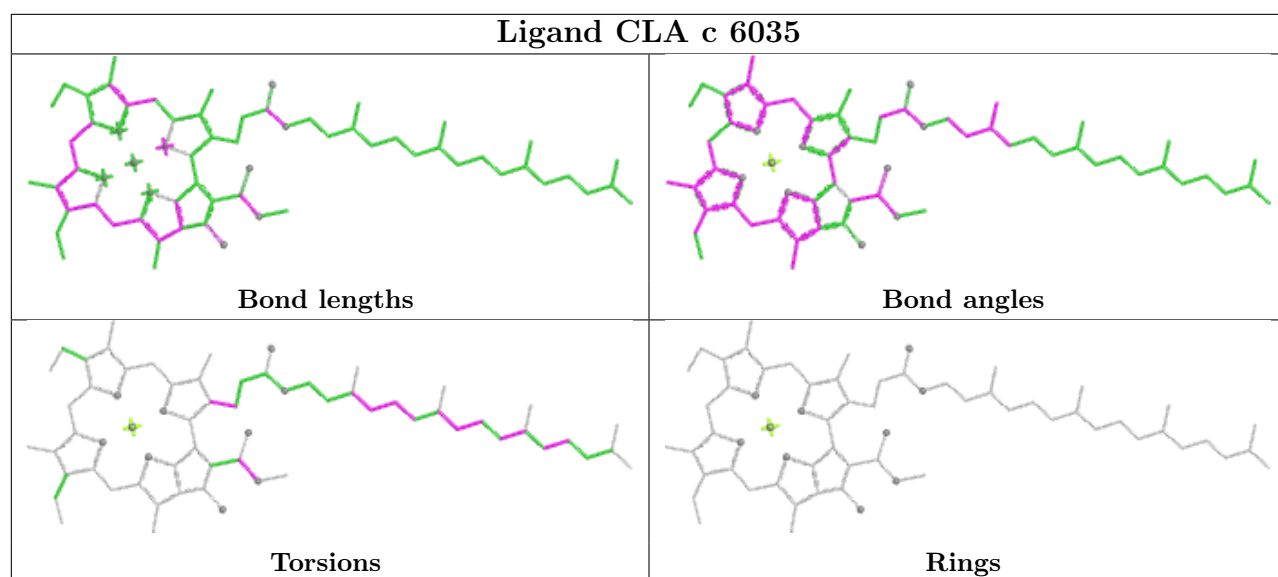
Bond angles

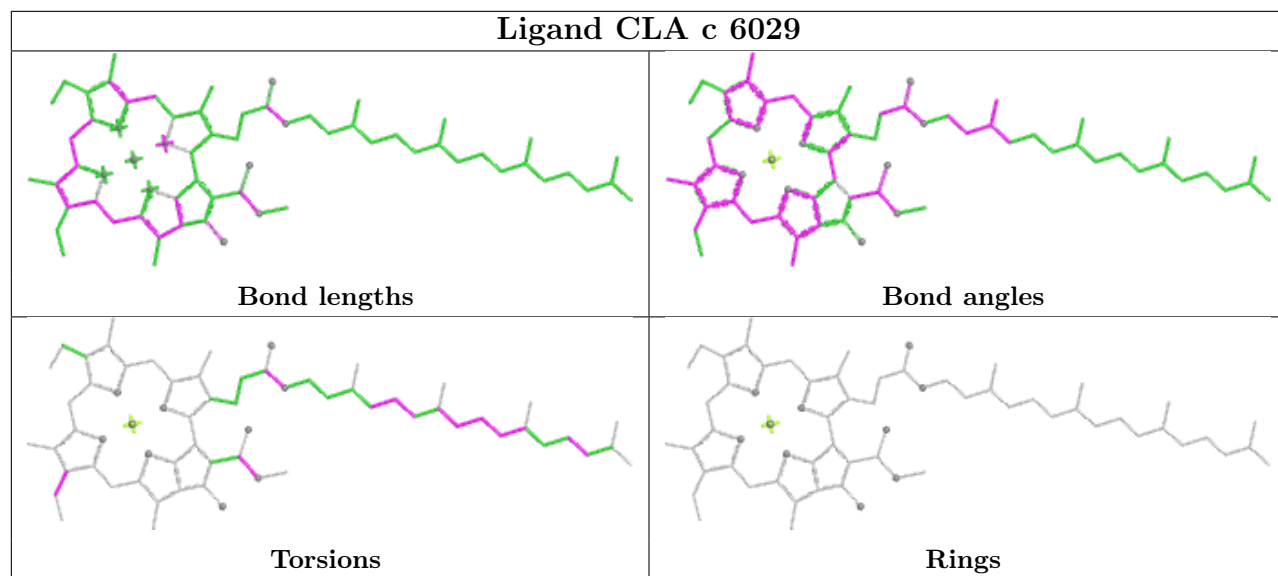


Torsions



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%)	-0.18	3 (0%) 81 64	135, 156, 186, 200	0
1	a	335/344 (97%)	-0.30	2 (0%) 85 71	135, 156, 186, 200	0
2	B	488/488 (100%)	-0.28	4 (0%) 82 65	133, 156, 180, 191	0
2	b	488/488 (100%)	-0.29	2 (0%) 88 75	133, 156, 180, 191	0
3	C	447/447 (100%)	-0.24	5 (1%) 78 60	138, 165, 181, 193	0
3	c	447/447 (100%)	-0.27	0 100 100	138, 165, 181, 193	0
4	D	340/340 (100%)	-0.24	1 (0%) 90 78	134, 156, 179, 192	0
4	d	340/340 (100%)	-0.28	1 (0%) 90 78	134, 156, 179, 192	0
5	E	82/83 (98%)	-0.35	0 100 100	153, 172, 191, 198	0
5	e	82/83 (98%)	-0.41	0 100 100	153, 172, 191, 198	0
6	F	35/44 (79%)	-0.47	0 100 100	153, 167, 187, 191	0
6	f	35/44 (79%)	-0.32	0 100 100	153, 167, 187, 191	0
7	H	64/64 (100%)	-0.36	1 (1%) 70 52	154, 163, 175, 185	0
7	h	64/64 (100%)	-0.38	0 100 100	154, 163, 175, 185	0
8	I	35/35 (100%)	-0.38	0 100 100	152, 169, 196, 201	0
8	i	35/35 (100%)	-0.18	0 100 100	152, 169, 196, 201	0
9	J	34/40 (85%)	-0.57	0 100 100	155, 162, 184, 192	0
9	j	34/40 (85%)	-0.45	0 100 100	155, 162, 184, 192	0
10	K	36/36 (100%)	-0.19	1 (2%) 55 40	144, 168, 182, 185	0
10	k	36/36 (100%)	-0.16	0 100 100	156, 170, 182, 192	0
11	L	37/37 (100%)	-0.43	0 100 100	138, 160, 191, 197	0
11	l	37/37 (100%)	-0.38	0 100 100	138, 160, 191, 197	0
12	M	36/36 (100%)	-0.23	0 100 100	131, 146, 188, 194	0
12	m	36/36 (100%)	-0.29	1 (2%) 55 40	131, 146, 188, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/242 (100%)	-0.38	0 100 100	139, 160, 181, 187	0
13	o	242/242 (100%)	-0.38	0 100 100	139, 160, 181, 187	0
14	T	30/30 (100%)	-0.58	0 100 100	124, 143, 186, 191	0
14	t	30/30 (100%)	-0.39	0 100 100	131, 143, 186, 191	0
15	U	98/98 (100%)	-0.46	0 100 100	139, 155, 165, 173	0
15	u	98/98 (100%)	-0.52	0 100 100	139, 155, 165, 173	0
16	V	137/137 (100%)	-0.17	3 (2%) 62 46	144, 162, 173, 178	0
16	v	137/137 (100%)	-0.33	0 100 100	144, 162, 173, 178	0
17	X	34/34 (100%)	-0.25	1 (2%) 53 39	173, 181, 198, 201	0
17	x	34/34 (100%)	-0.39	0 100 100	173, 181, 198, 201	0
18	Y	28/28 (100%)	-0.18	0 100 100	187, 199, 208, 210	0
18	y	28/28 (100%)	-0.27	0 100 100	187, 199, 208, 210	0
19	N	0/23	-	-	-	-
19	n	0/23	-	-	-	-
20	Z	62/62 (100%)	-0.45	0 100 100	159, 173, 188, 196	0
20	z	62/62 (100%)	-0.33	1 (1%) 70 52	159, 173, 188, 196	0
All	All	5200/5296 (98%)	-0.30	26 (0%) 87 73	124, 161, 185, 210	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	ARG	6.3
1	a	5279	ARG	6.1
3	C	44	ASN	3.9
2	B	166	MET	3.2
3	C	45	LEU	3.1

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

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

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

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

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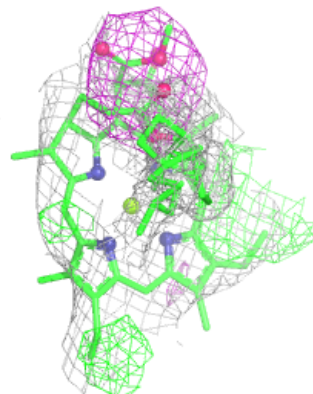
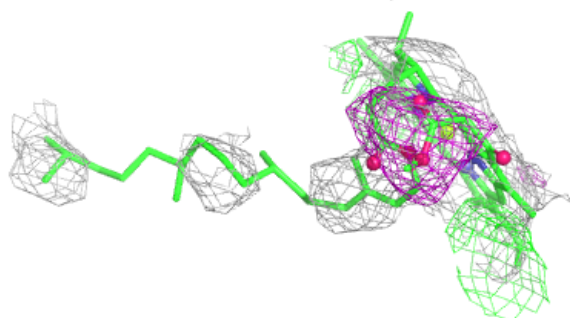
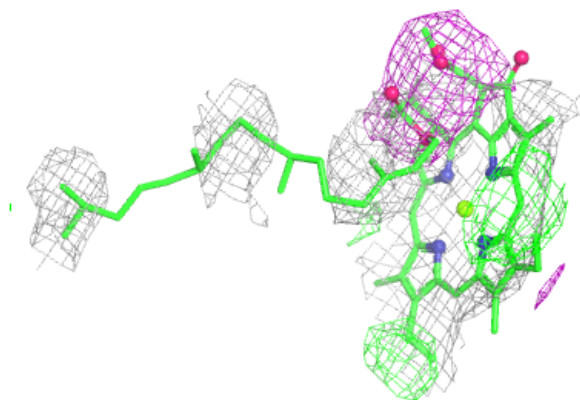
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	6023	65/65	0.93	0.11	174,179,181,191	0
22	CLA	b	6013	65/65	0.94	0.17	146,173,183,184	0
22	CLA	B	1018	65/65	0.94	0.13	172,186,191,192	0
31	HEM	V	1041	43/43	0.94	0.23	131,181,185,187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

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

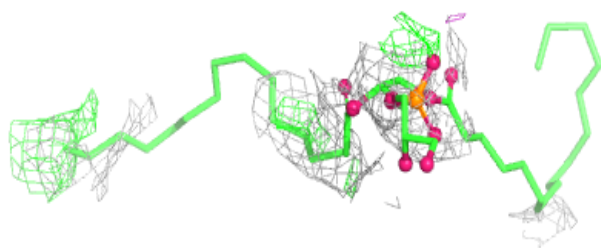
Electron density around CLA K 1034:

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



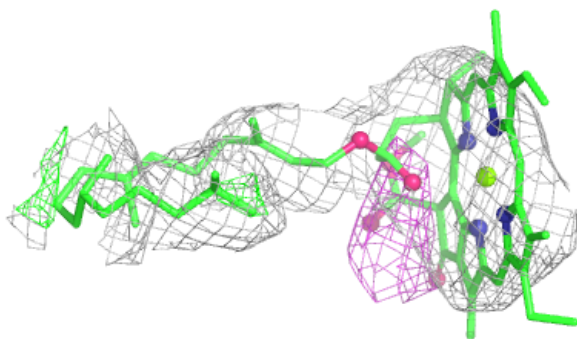
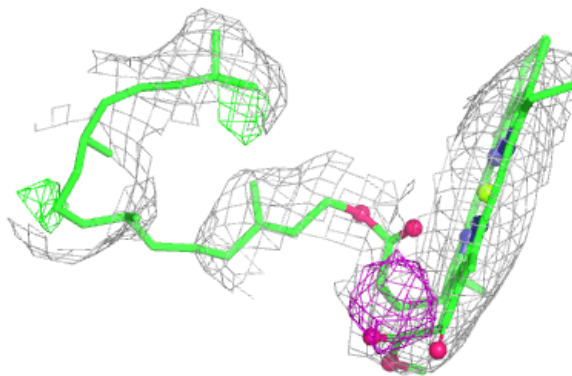
Electron density around LHG a 6063:

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



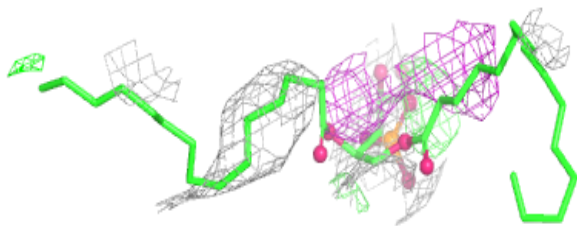
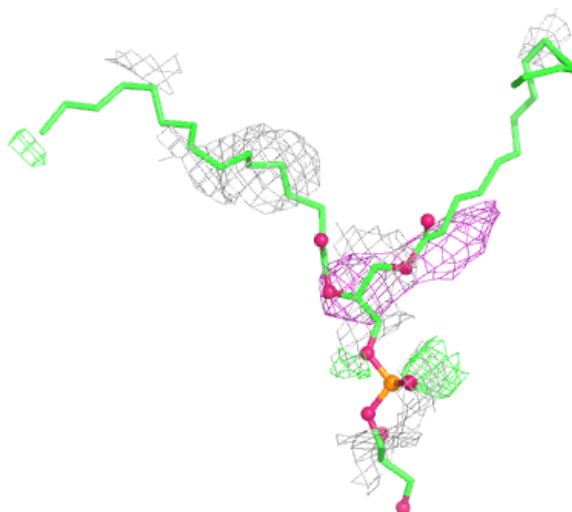
Electron density around CLA B 1009:

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



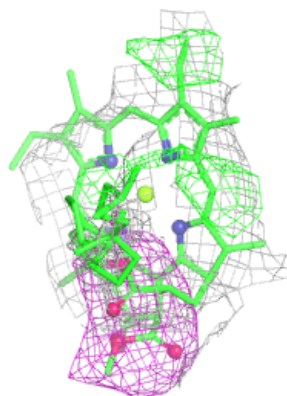
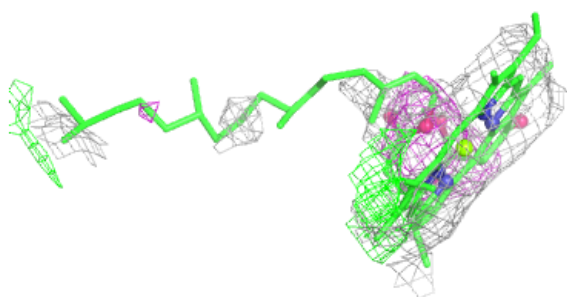
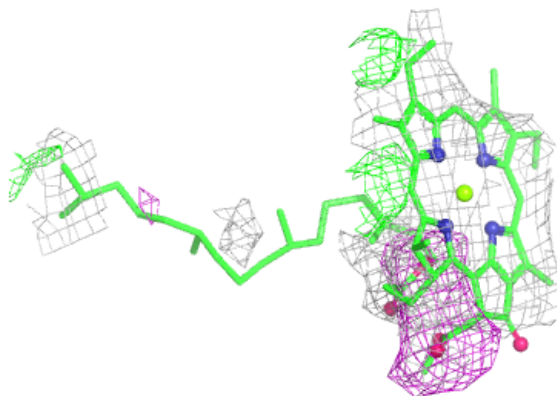
Electron density around LHG A 1063:

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

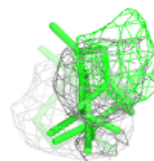
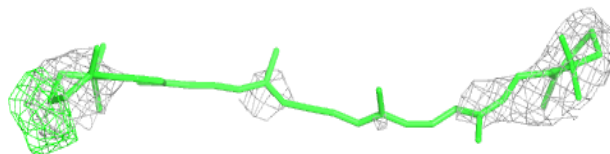
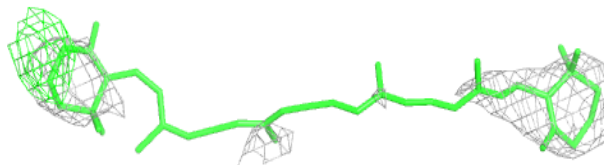


Electron density around CLA k 6034:

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

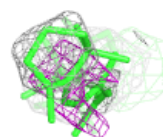
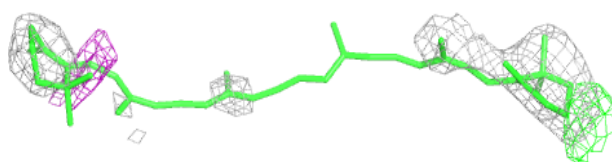
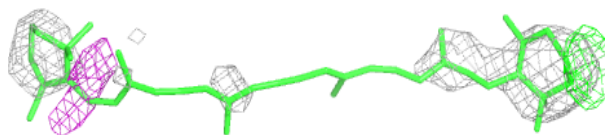
**Electron density around BCR T 6048:**

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

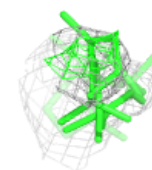
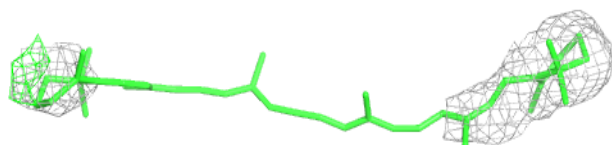
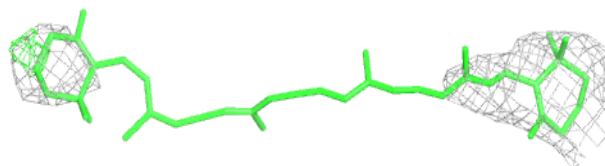


Electron density around BCR A 1044:

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

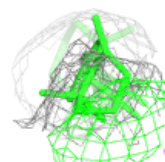
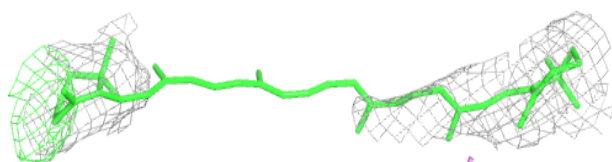
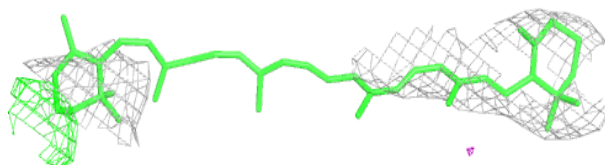
**Electron density around BCR B 1048:**

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

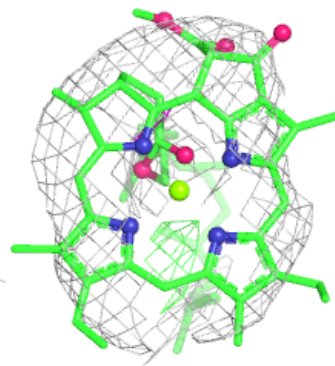
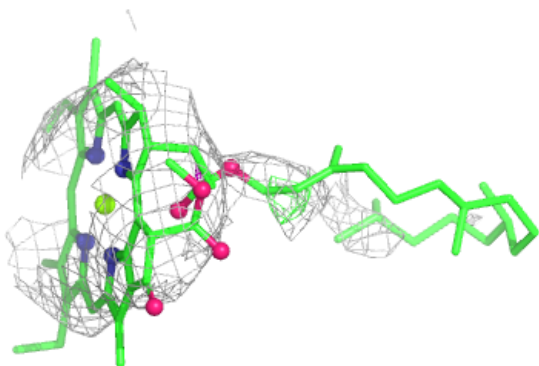
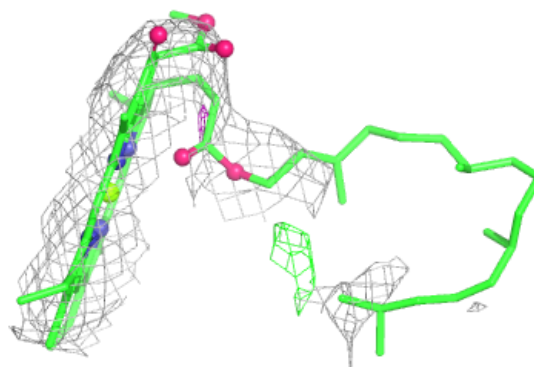


Electron density around BCR b 6047:

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

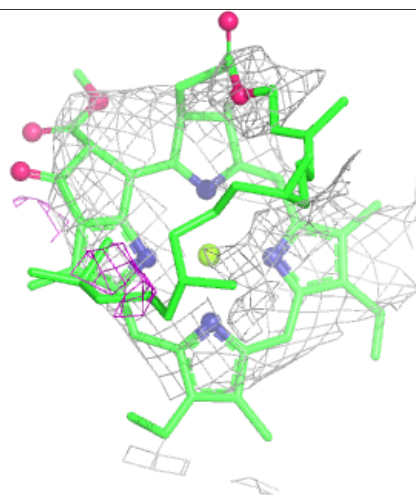
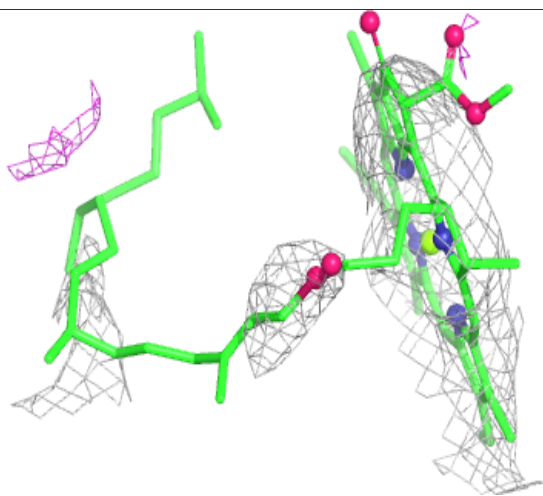
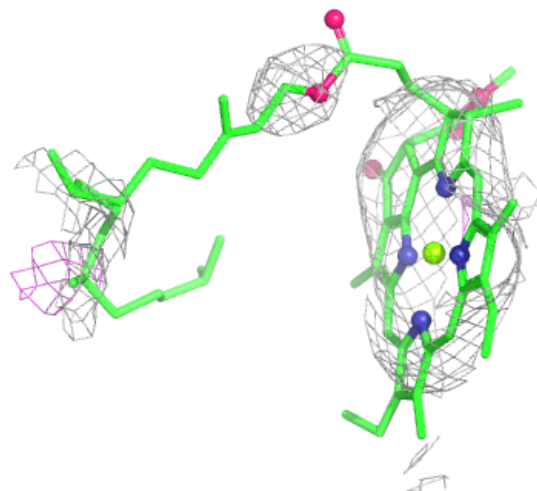
**Electron density around CLA b 6009:**

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



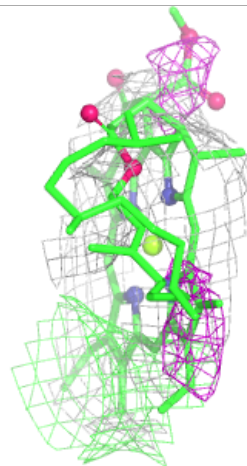
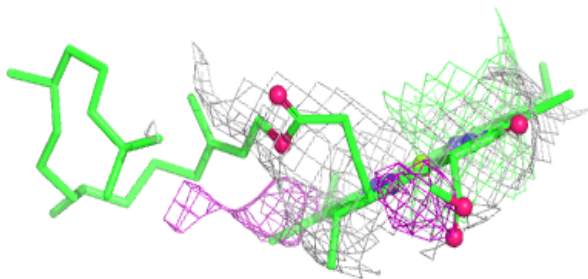
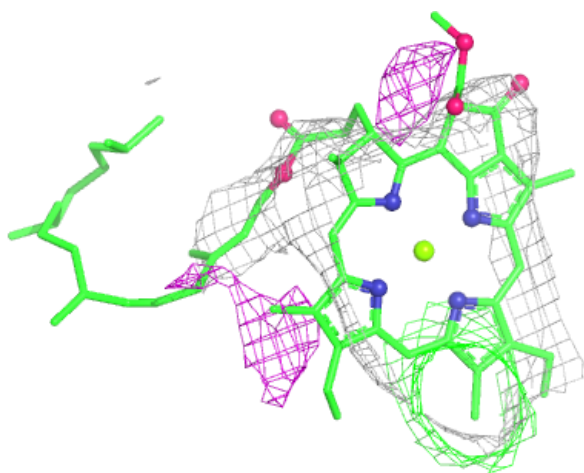
Electron density around CLA c 6037:

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



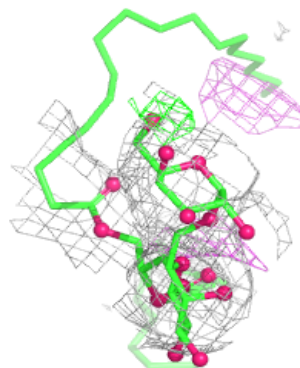
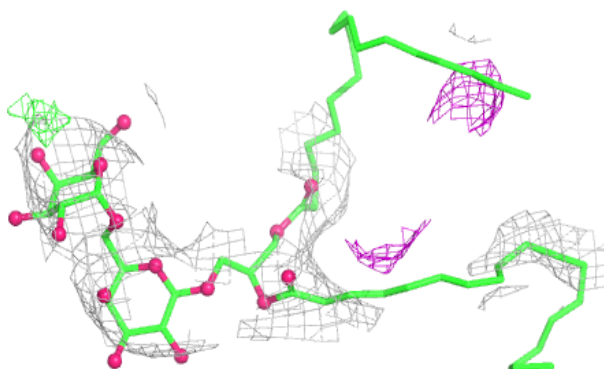
Electron density around CLA c 6027:

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

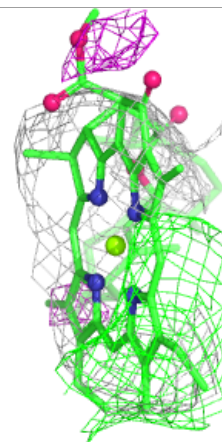
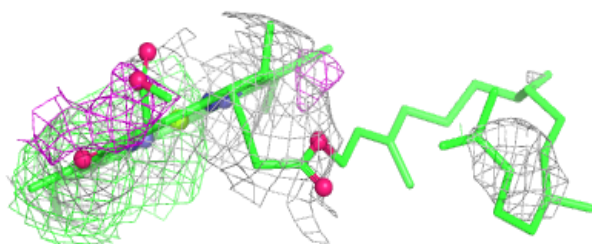
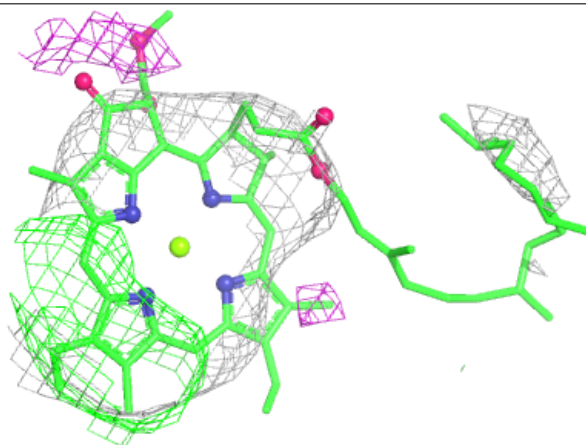


Electron density around DGD C 1056:

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

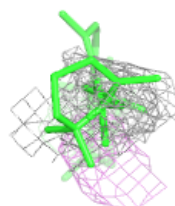
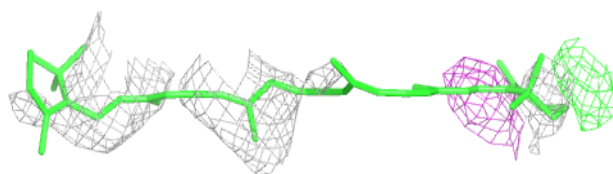
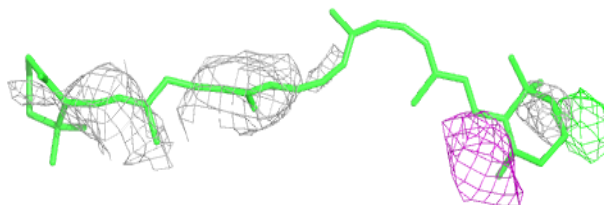
**Electron density around CLA C 1027:**

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

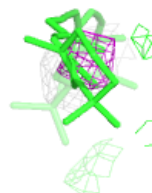
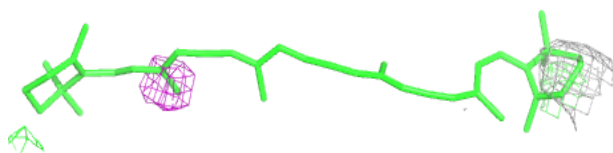
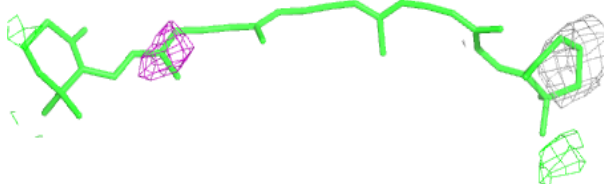


Electron density around BCR c 6054:

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

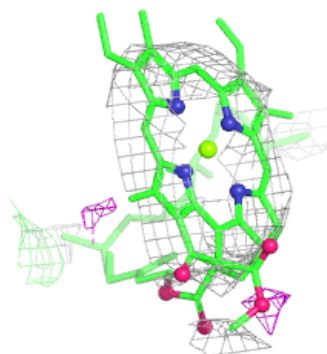
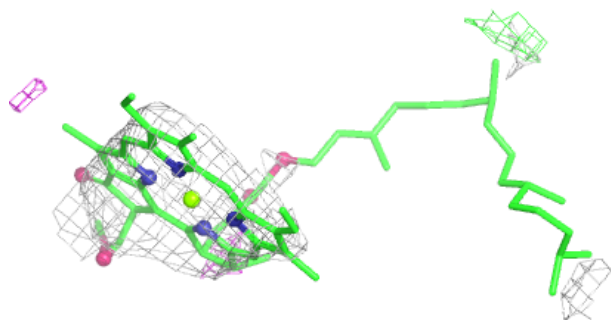
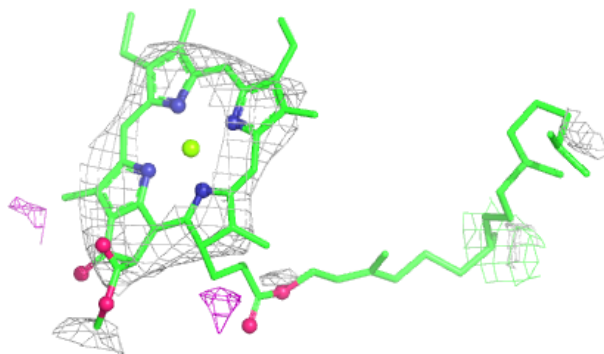
**Electron density around BCR k 6052:**

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

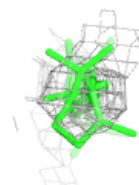
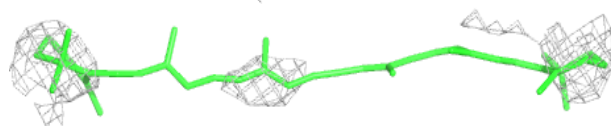
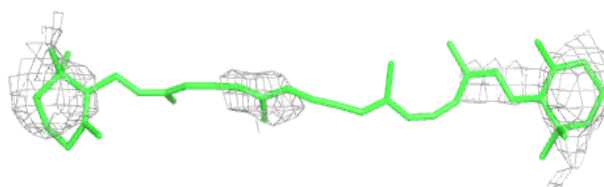


Electron density around CLA d 6008:

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

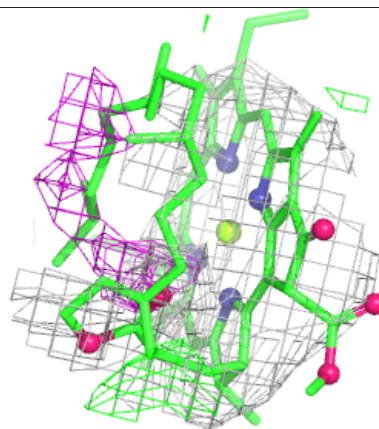
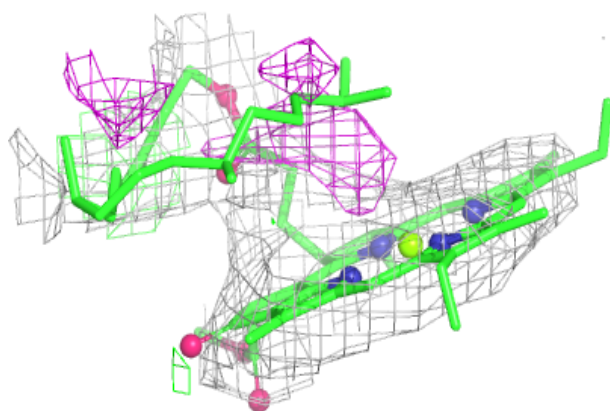
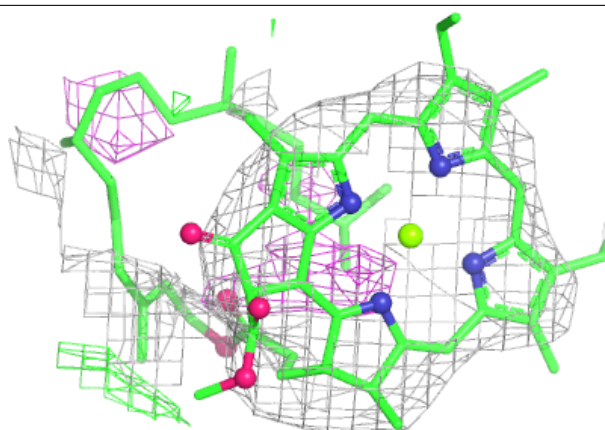
**Electron density around BCR Z 1053:**

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

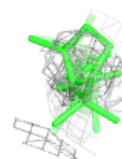
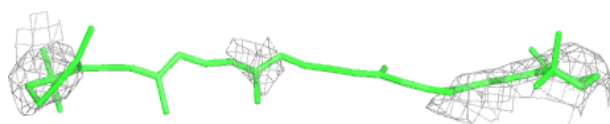
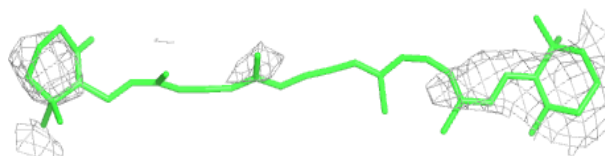


Electron density around CLA c 6026:

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

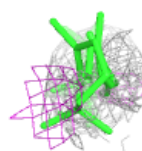
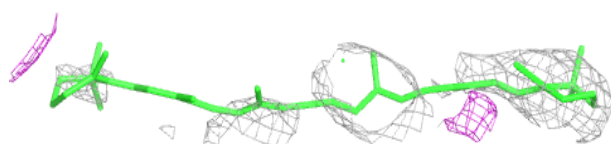
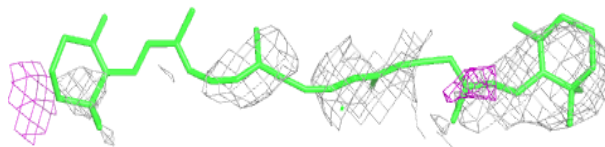
**Electron density around BCR z 6053:**

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

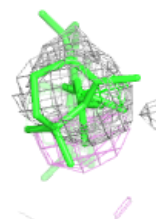
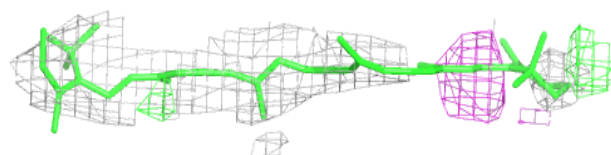


Electron density around BCR b 6045:

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

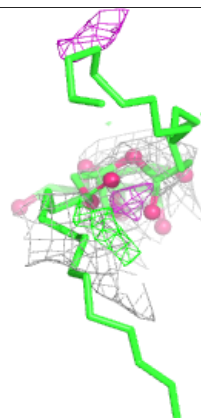
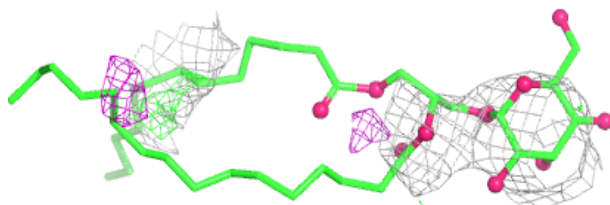
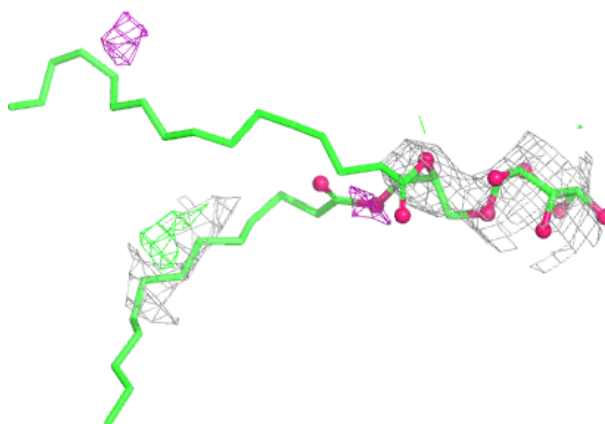
**Electron density around BCR C 1054:**

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

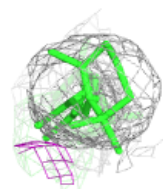
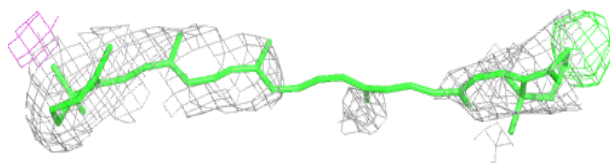
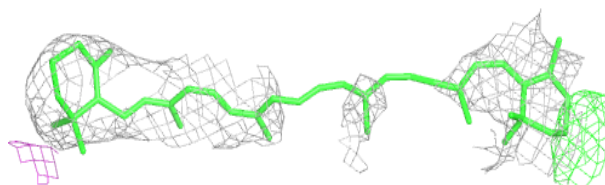


Electron density around MGE d 6062:

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

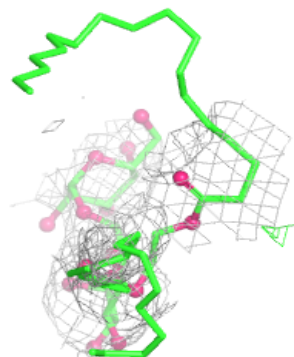
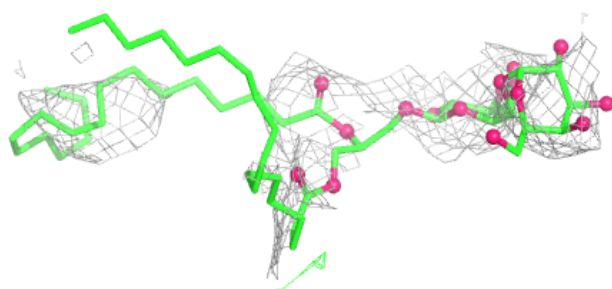
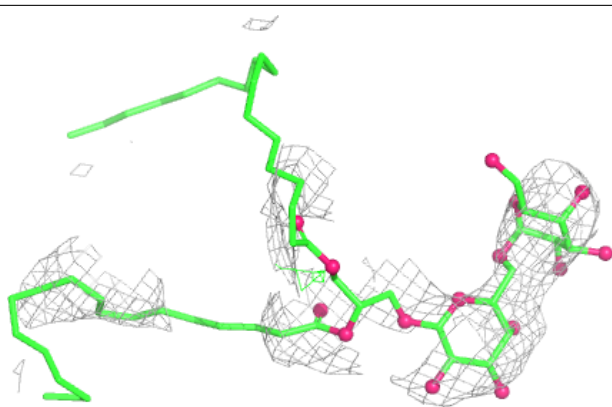
**Electron density around BCR B 1047:**

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

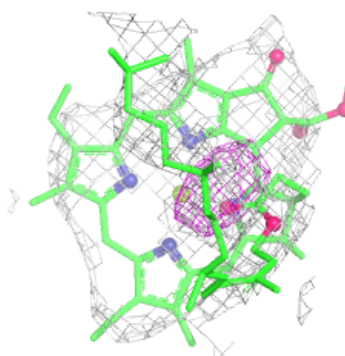
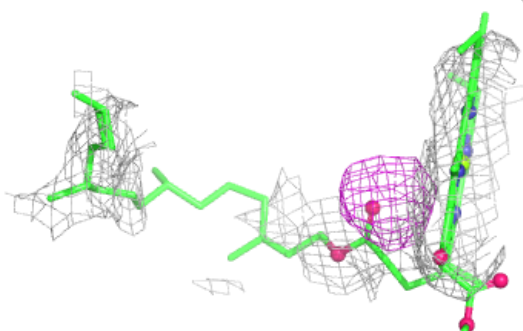
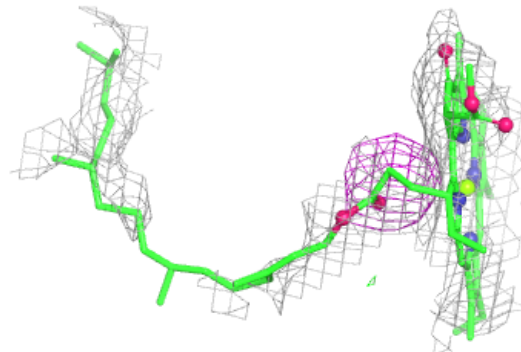


Electron density around DGD c 6056:

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

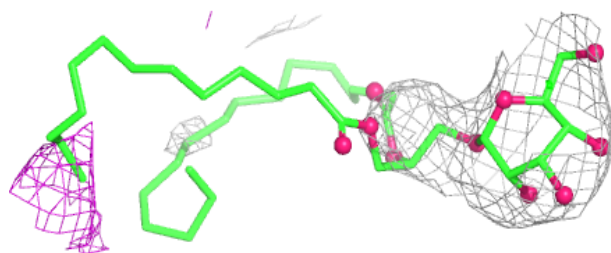
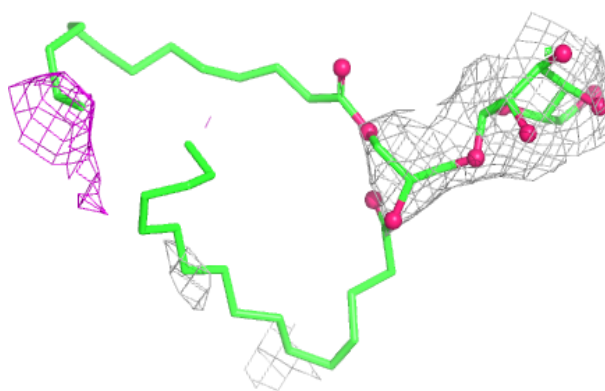
**Electron density around CLA b 6014:**

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

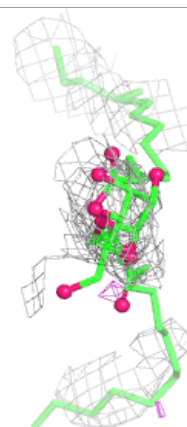
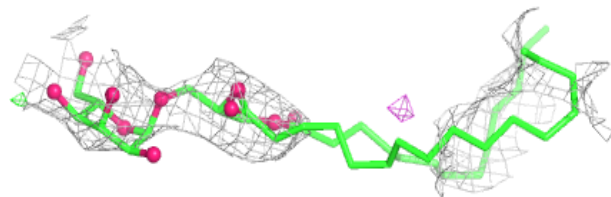
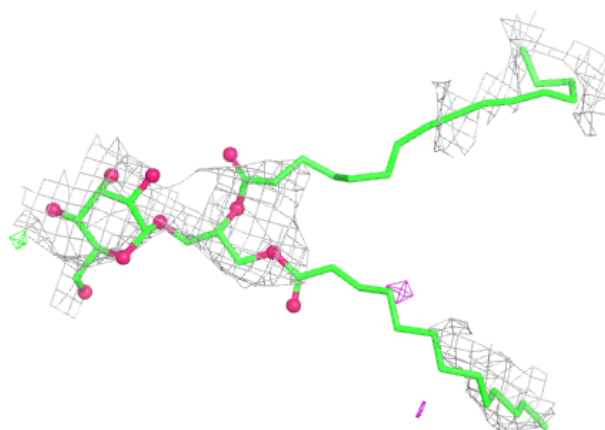


Electron density around MGE B 1060:

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

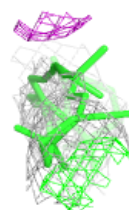
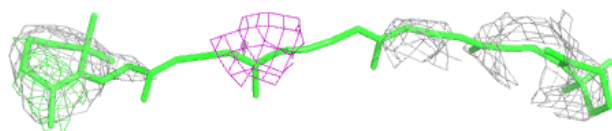
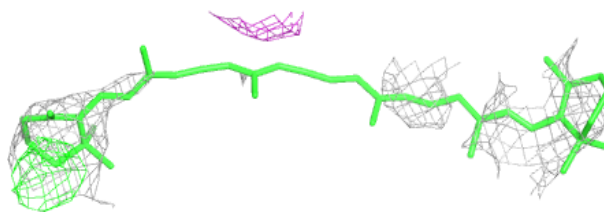
**Electron density around MGE D 1059:**

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



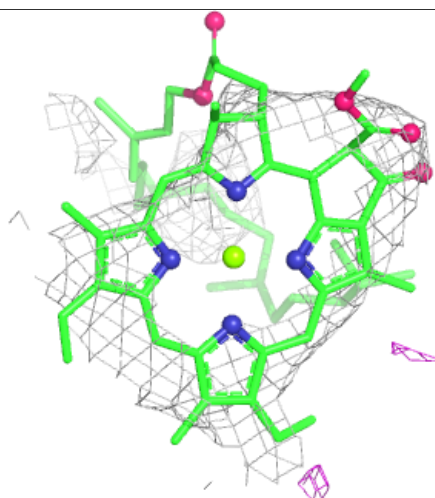
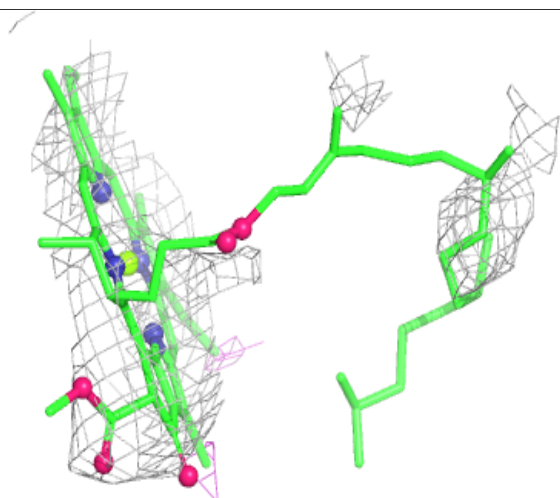
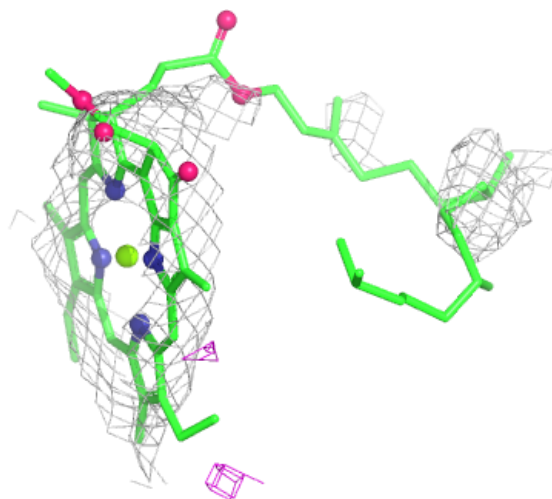
Electron density around BCR T 6046:

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



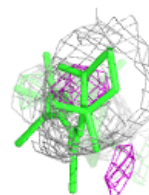
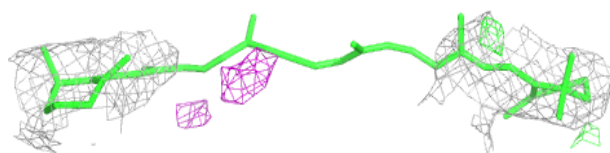
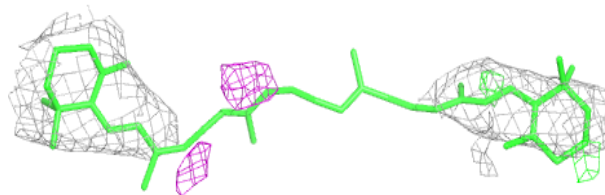
Electron density around CLA C 1037:

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

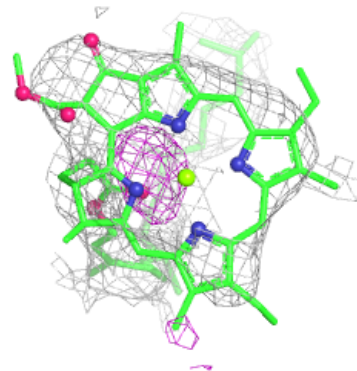
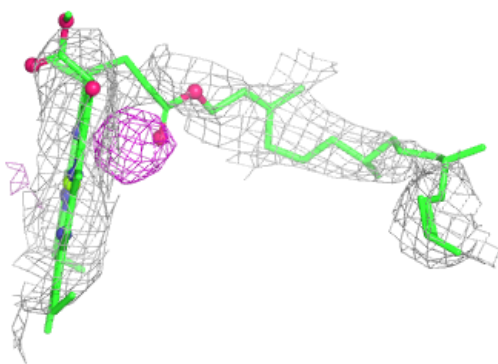
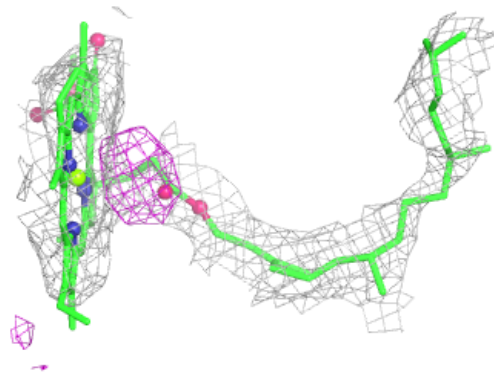


Electron density around BCR d 6050:

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

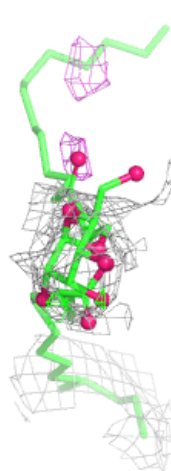
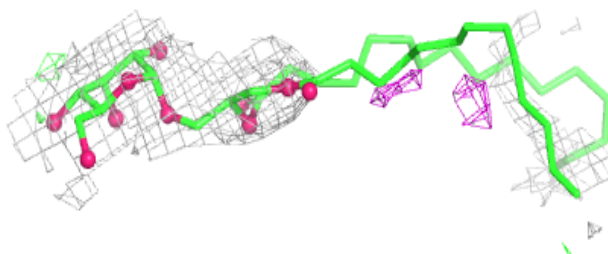
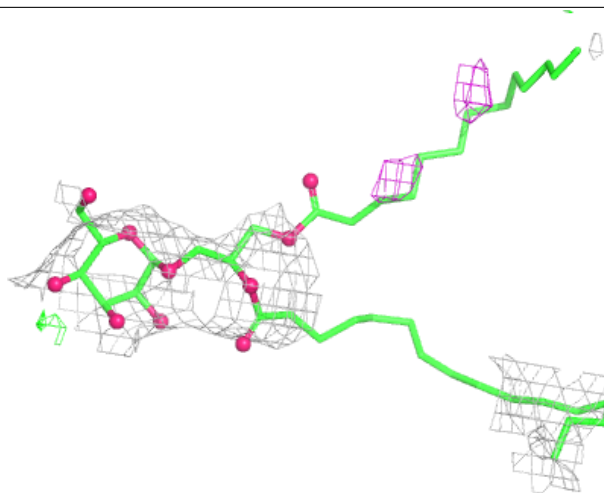
**Electron density around CLA B 1014:**

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



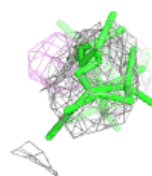
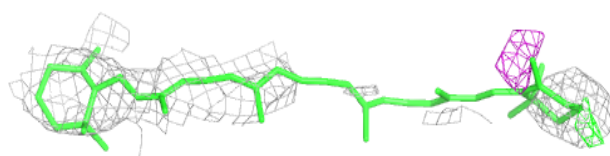
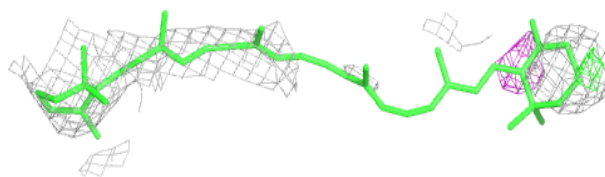
Electron density around MGE d 6059:

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

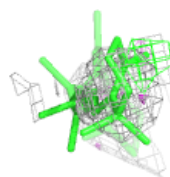
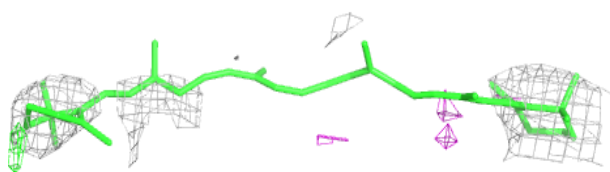
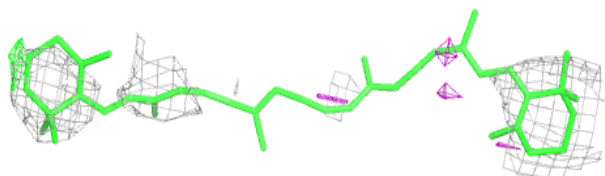


Electron density around BCR h 6049:

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

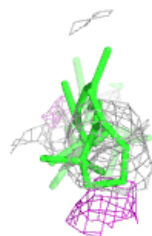
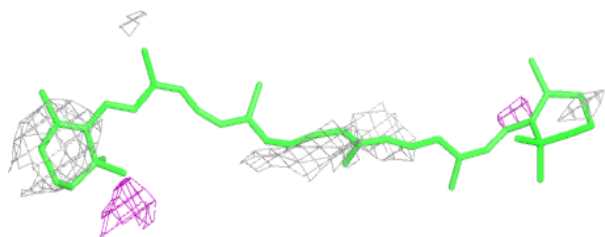
**Electron density around BCR D 1050:**

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

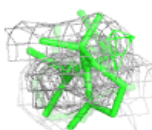
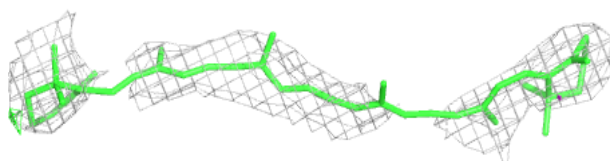
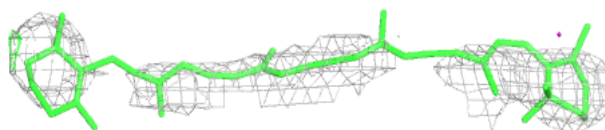


Electron density around BCR K 1051:

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

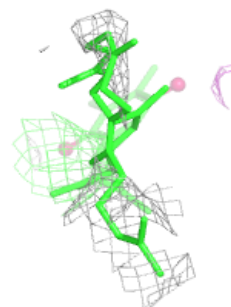
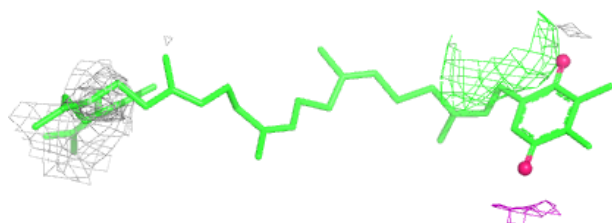
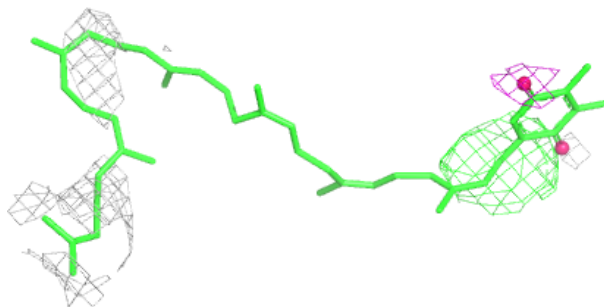
**Electron density around BCR a 6044:**

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



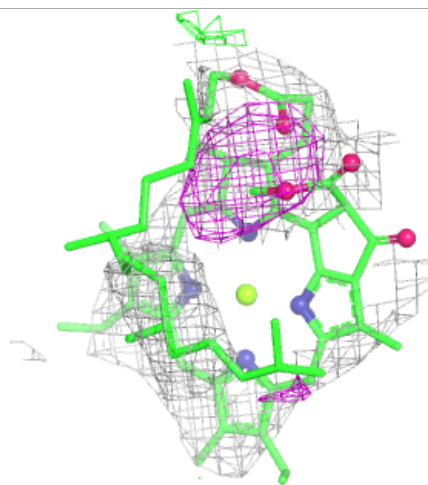
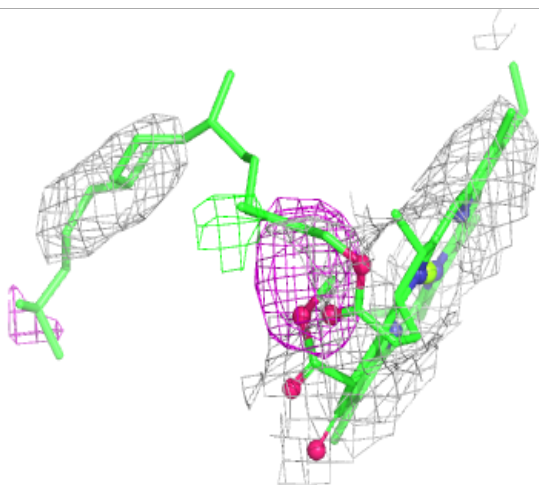
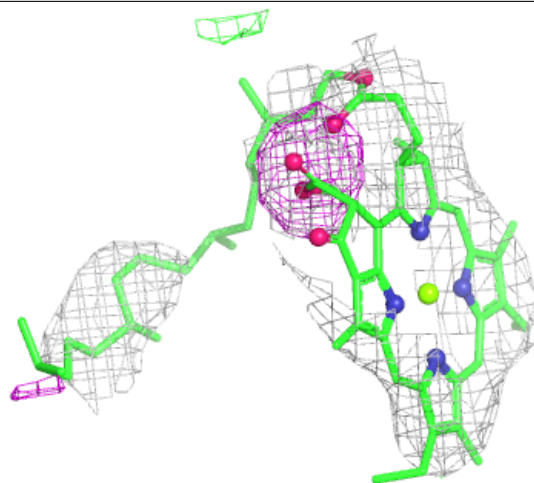
Electron density around PQ9 A 1043:

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



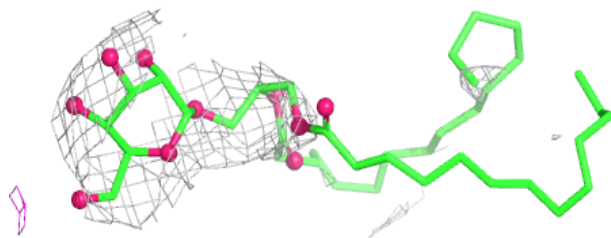
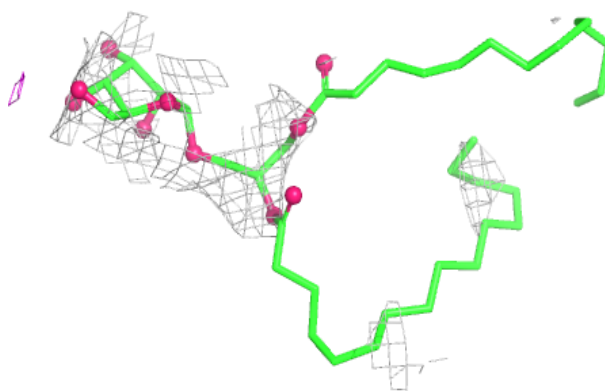
Electron density around CLA b 6021:

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

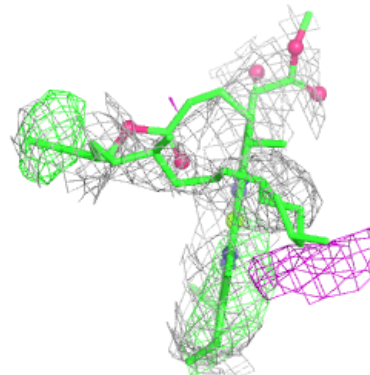
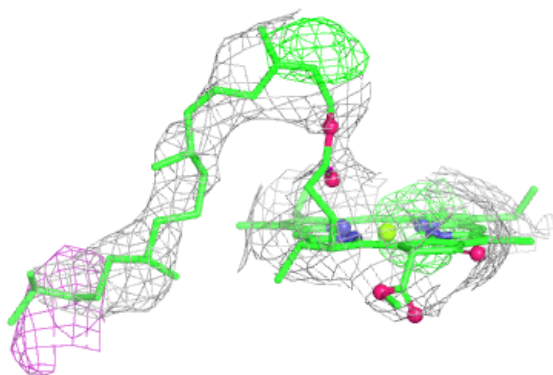
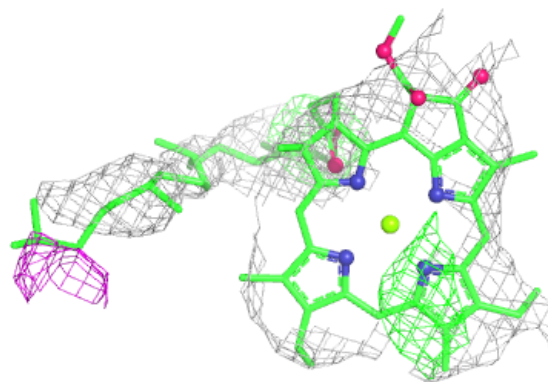


Electron density around MGE b 6060:

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

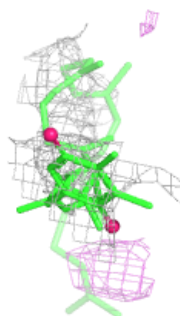
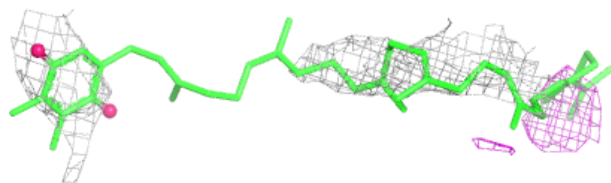
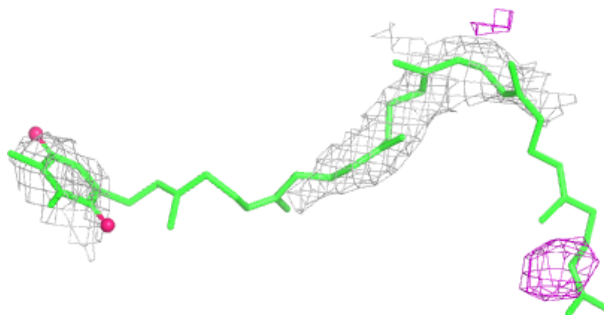
**Electron density around CLA d 6005:**

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



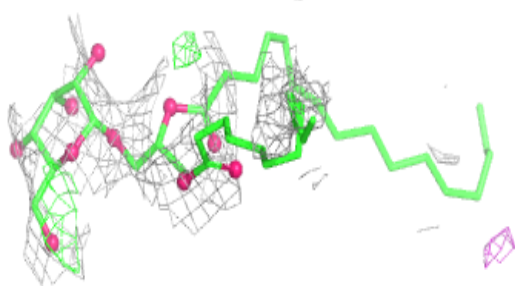
Electron density around PQ9 d 6042:

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



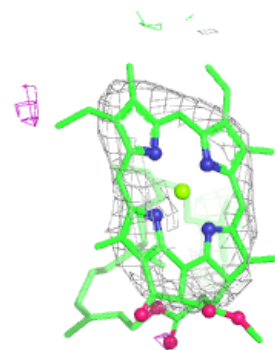
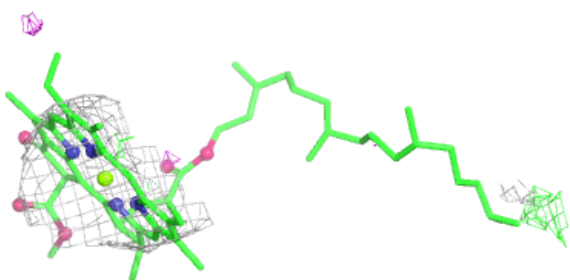
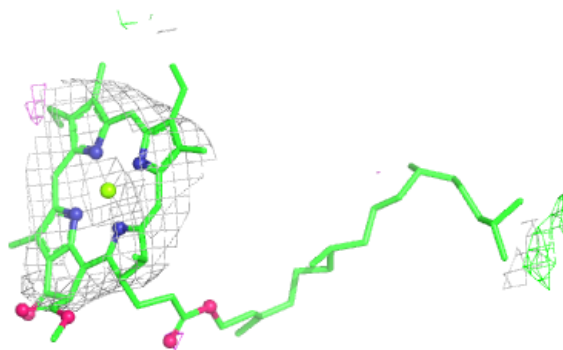
Electron density around MGE 1 6061:

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

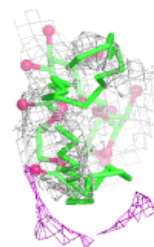
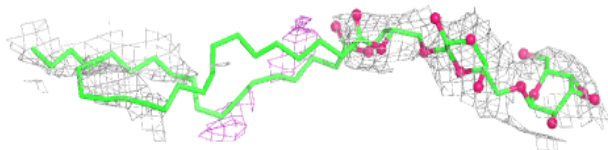


Electron density around CLA c 6035:

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

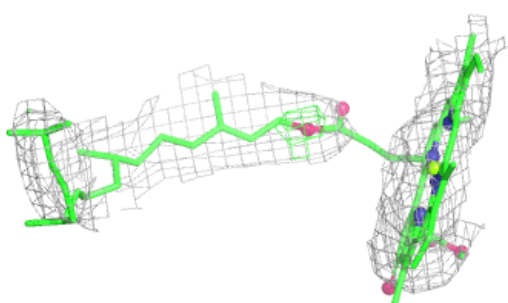
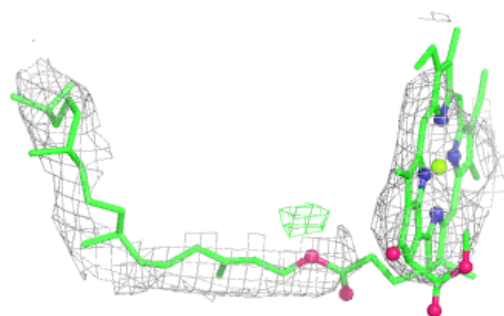
**Electron density around DGD C 1057:**

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

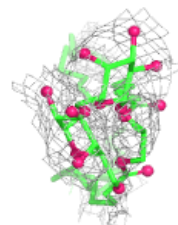
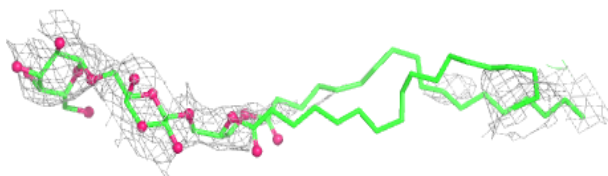


Electron density around CLA C 1030:

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

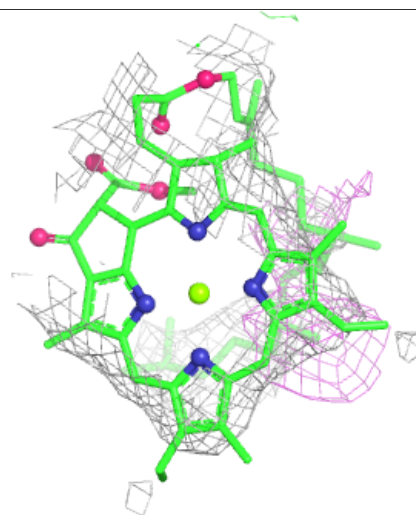
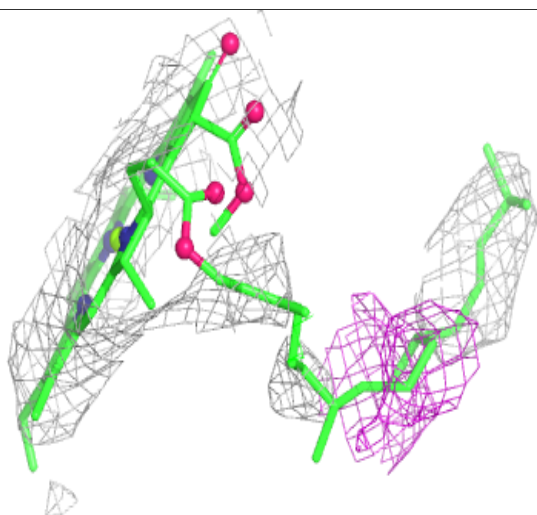
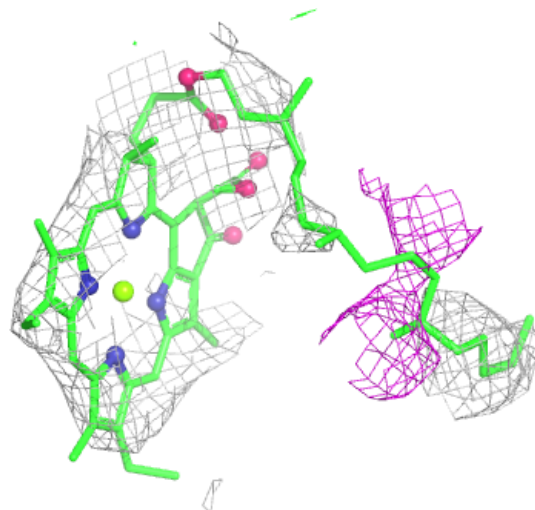
**Electron density around DGD c 6057:**

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



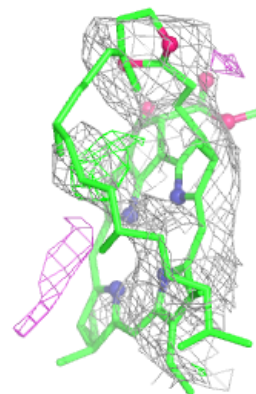
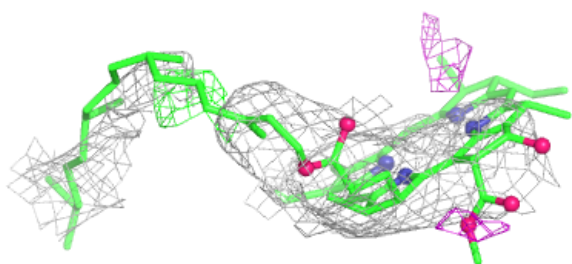
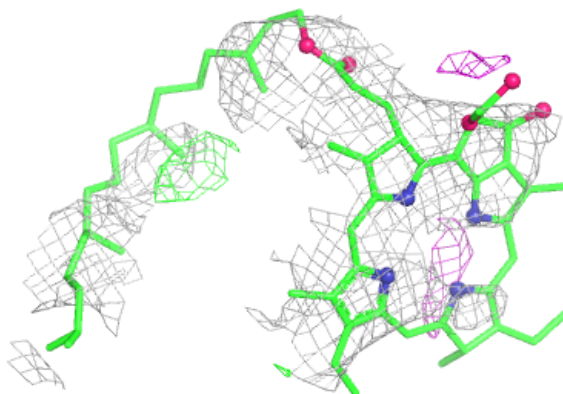
Electron density around CLA B 1021:

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

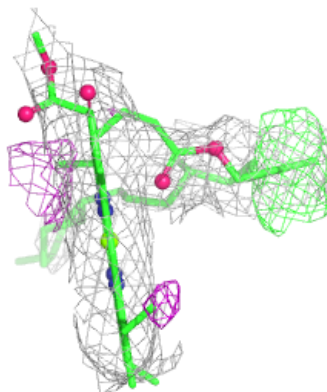
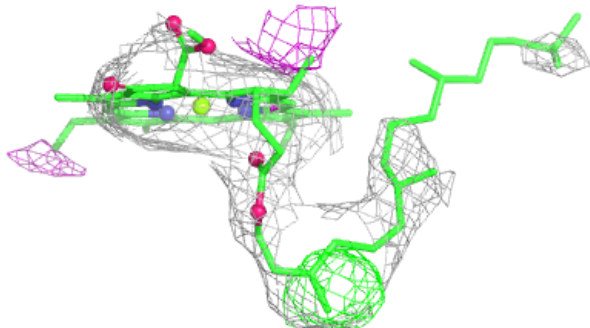
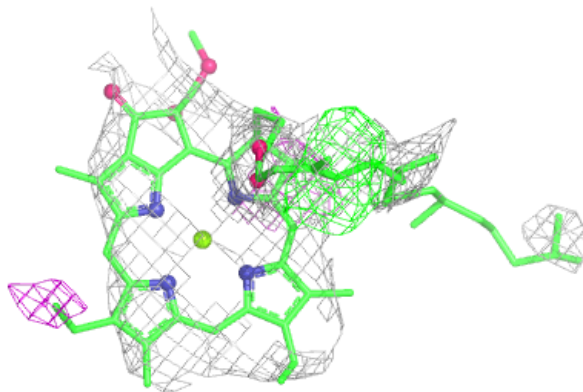


Electron density around PHO D 1039:

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

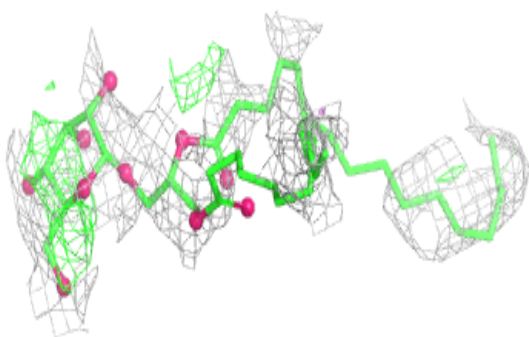
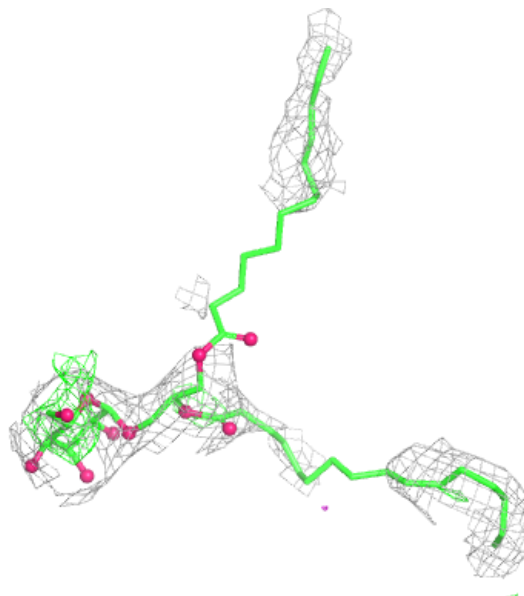
**Electron density around CLA D 1005:**

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



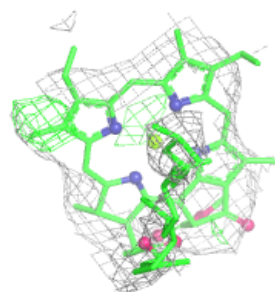
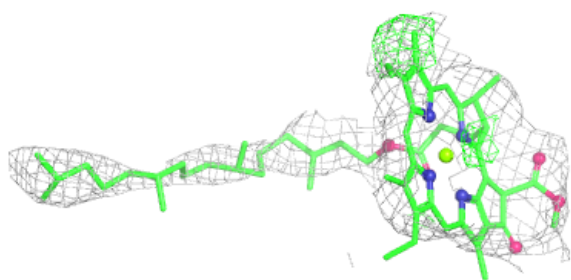
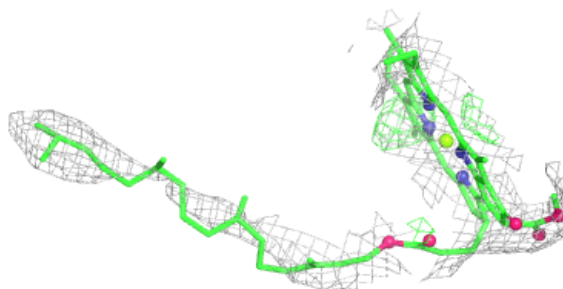
Electron density around MGE L 1061:

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

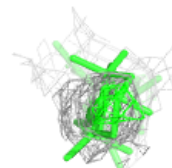
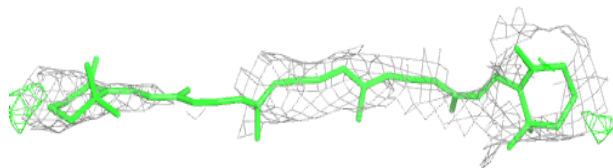
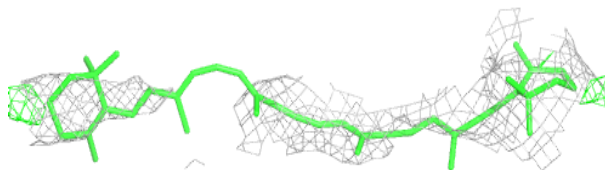


Electron density around CLA b 6015:

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

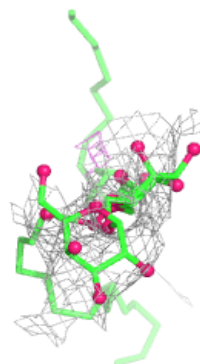
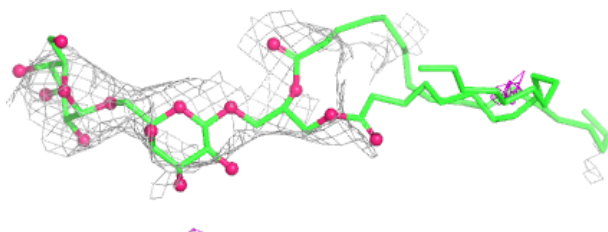
**Electron density around BCR H 1049:**

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

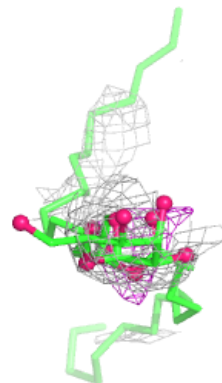
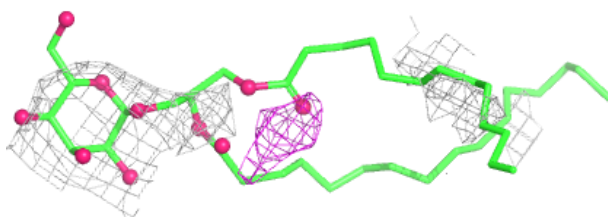
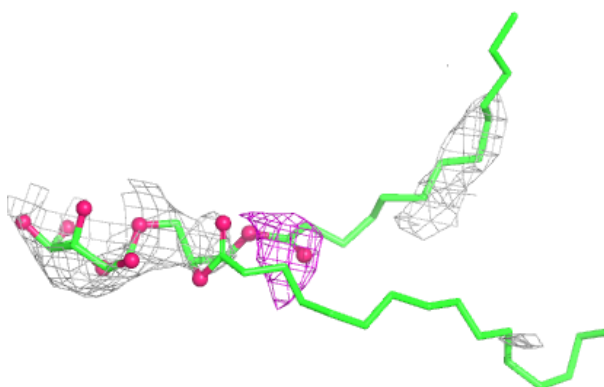


Electron density around DGD c 6055:

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

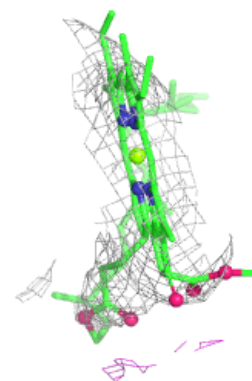
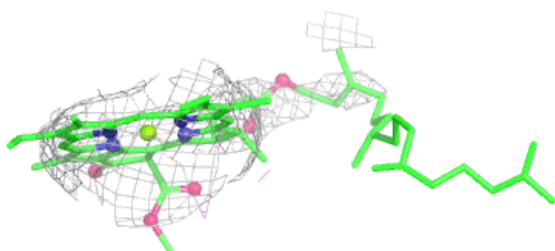
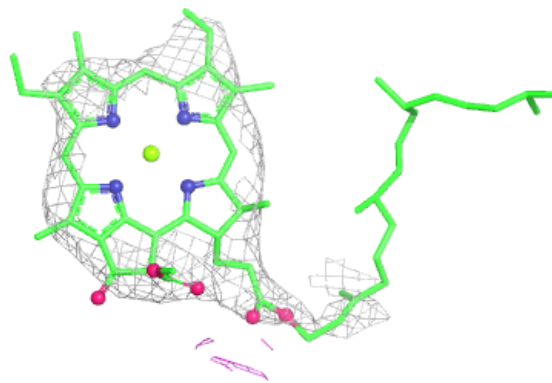
**Electron density around MGE D 1062:**

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

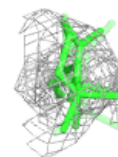
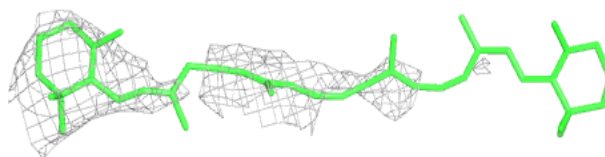


Electron density around CLA C 1036:

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

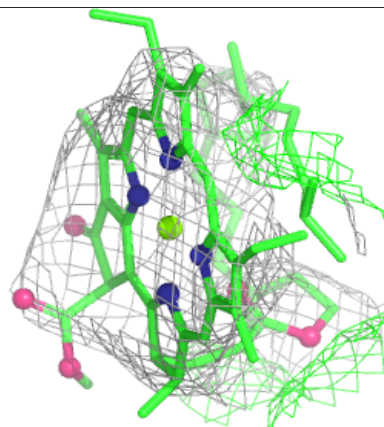
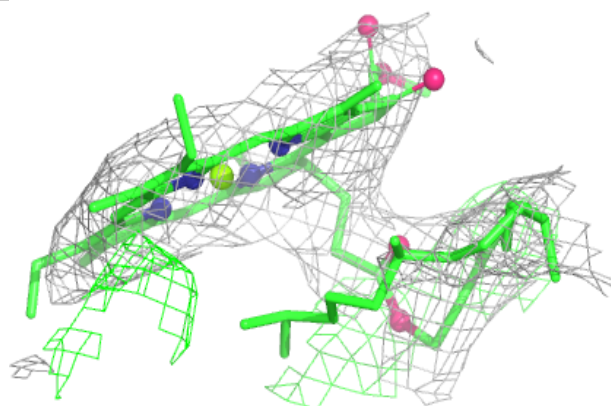
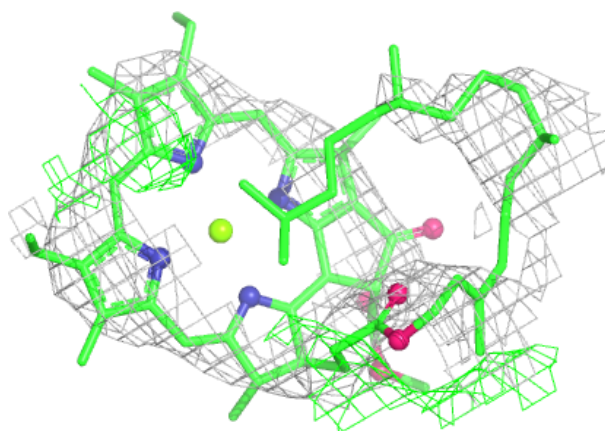
**Electron density around BCR B 1045:**

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

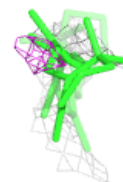
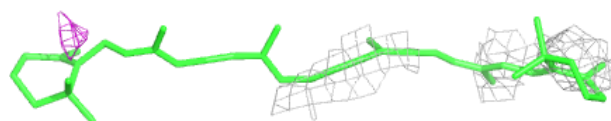
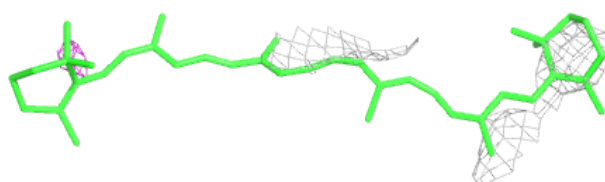


Electron density around CLA C 1026:

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

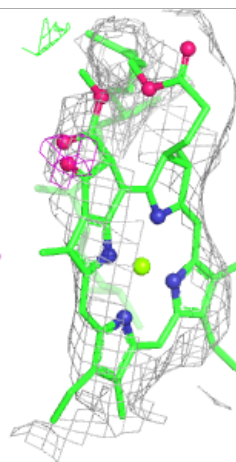
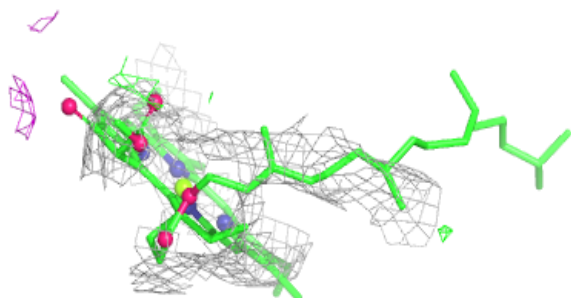
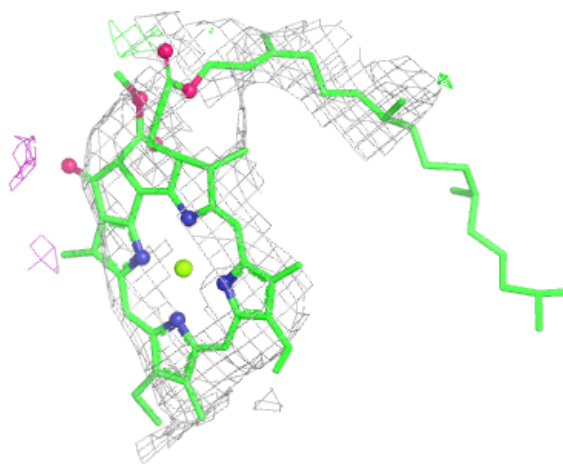
**Electron density around BCR k 6051:**

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



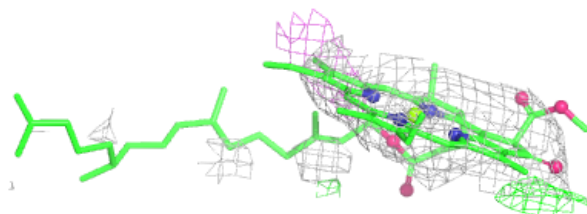
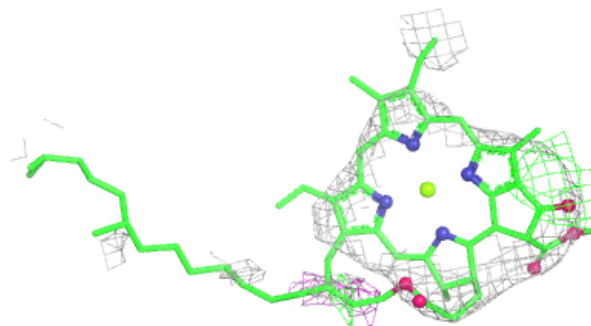
Electron density around CLA b 6024:

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

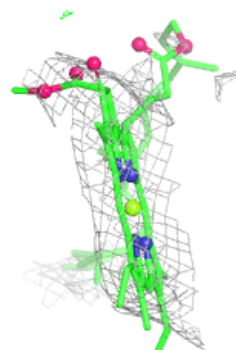
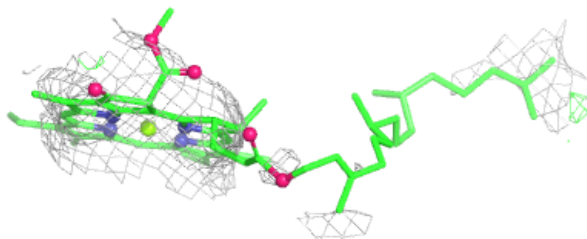
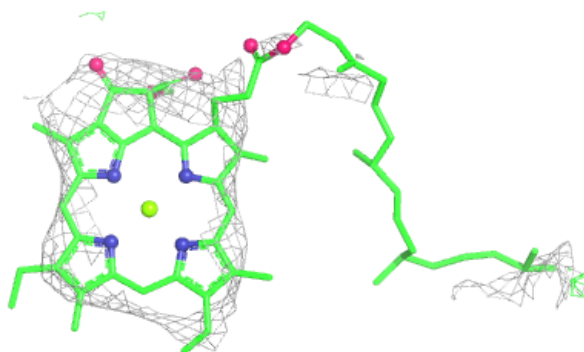


Electron density around CLA c 6025:

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

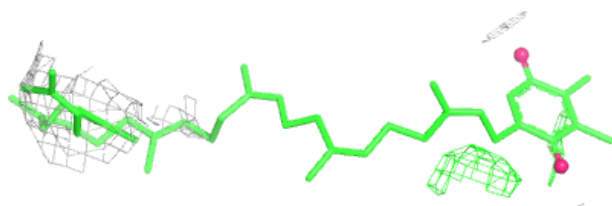
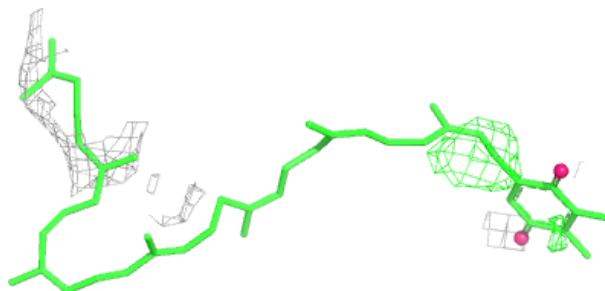
**Electron density around CLA c 6036:**

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

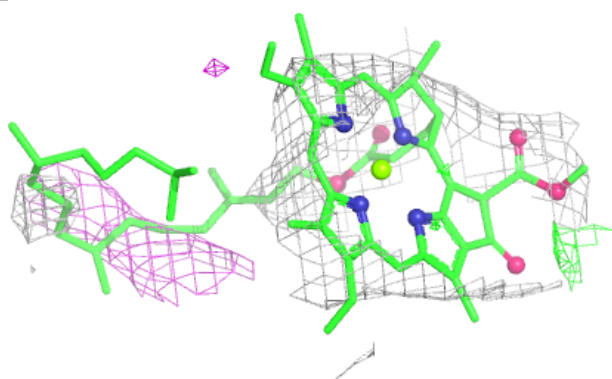
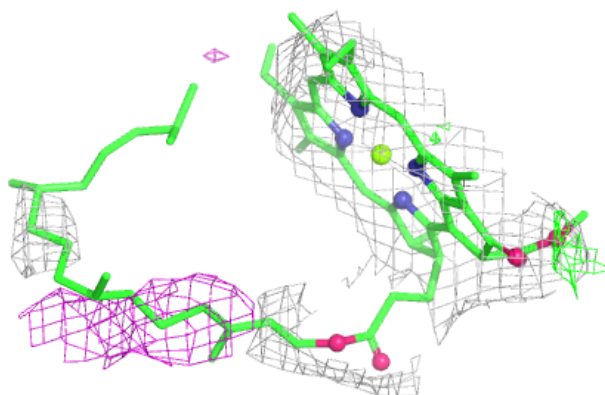


Electron density around PQ9 a 6043:

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

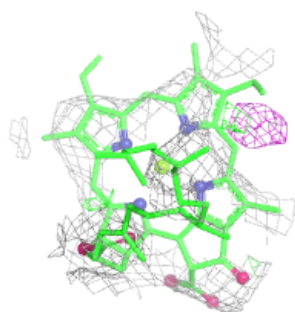
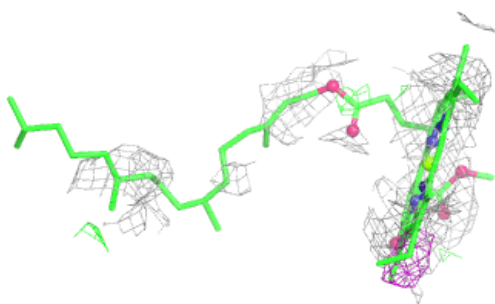
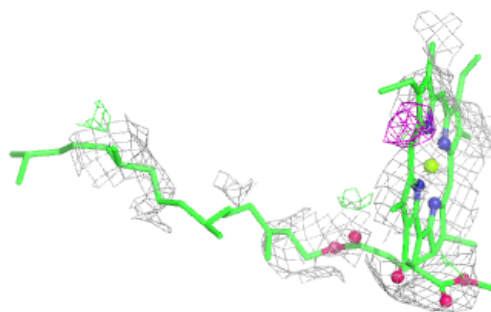
**Electron density around CLA C 1028:**

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



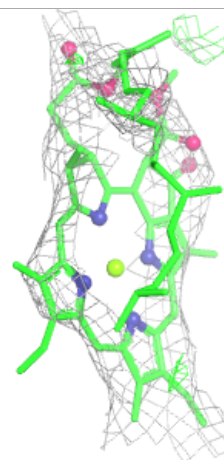
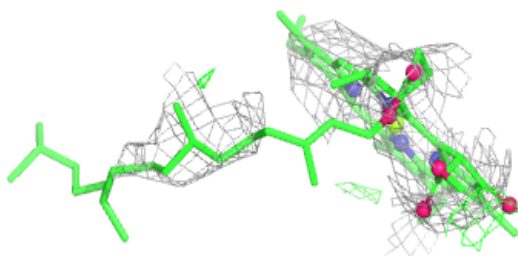
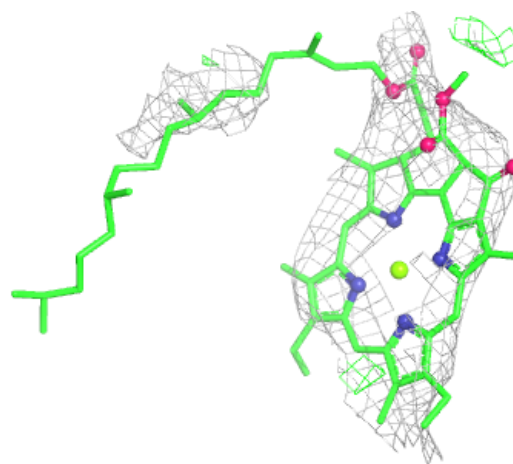
Electron density around CLA c 6032:

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



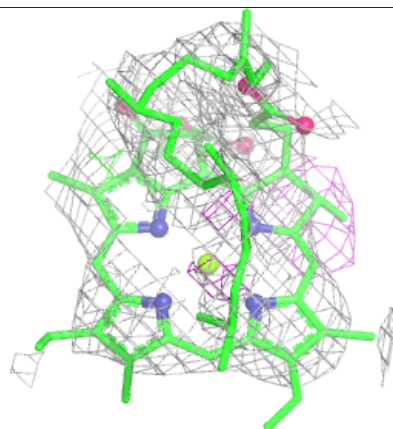
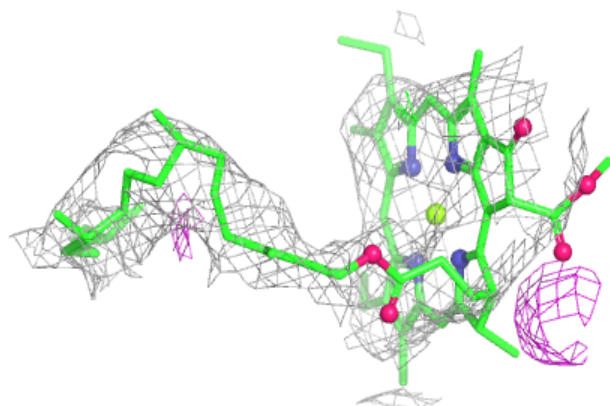
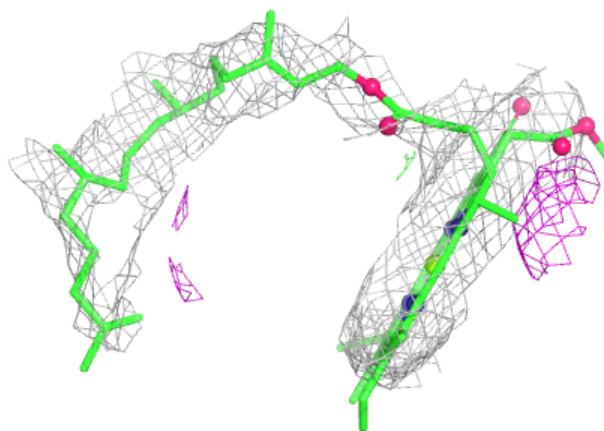
Electron density around CLA B 1024:

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

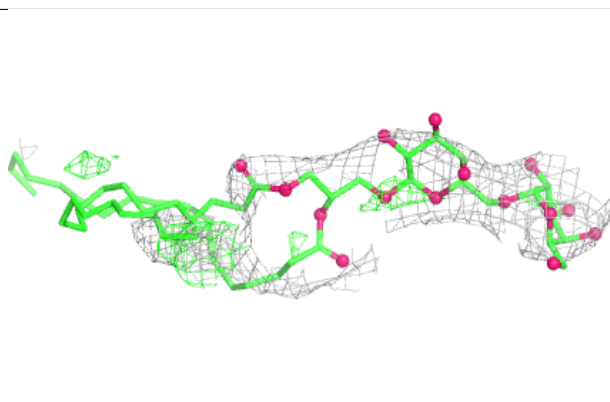
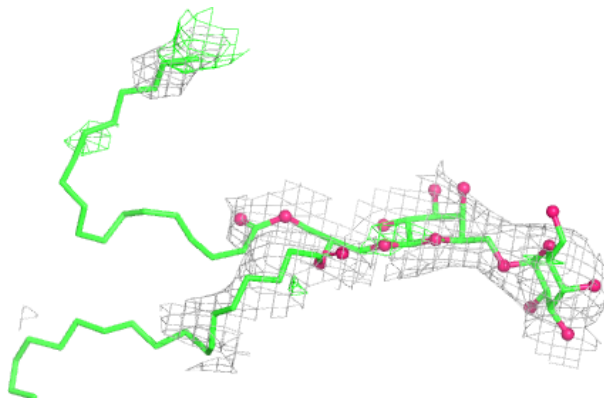


Electron density around CLA b 6019:

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

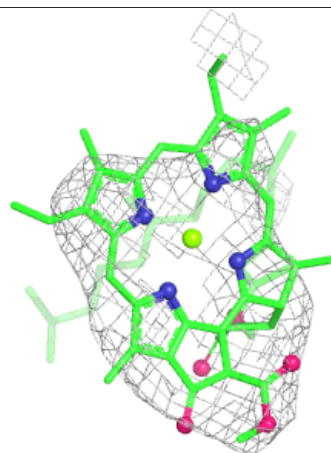
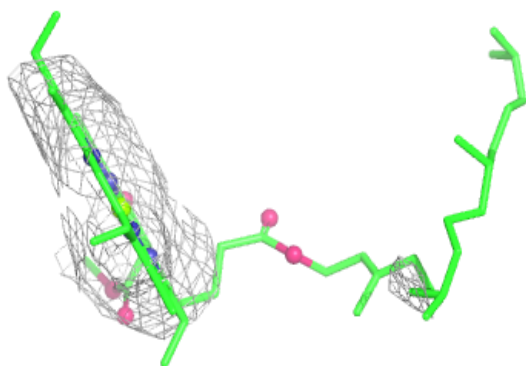
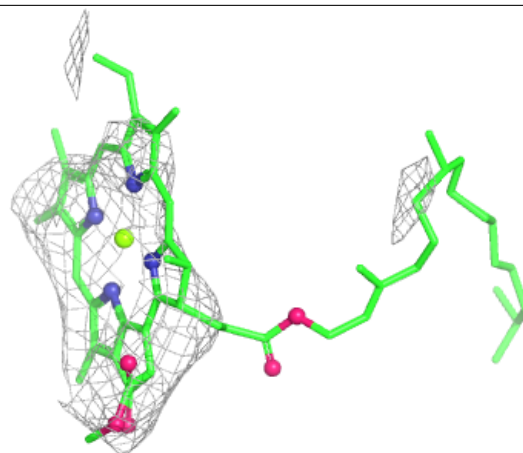
**Electron density around DGD C 1055:**

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

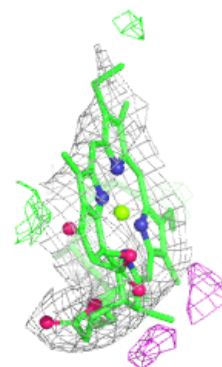
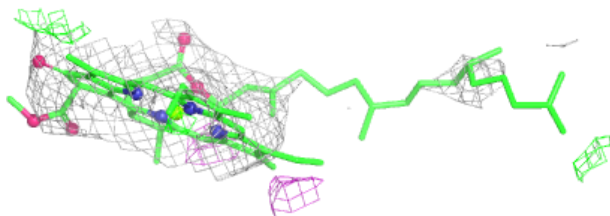
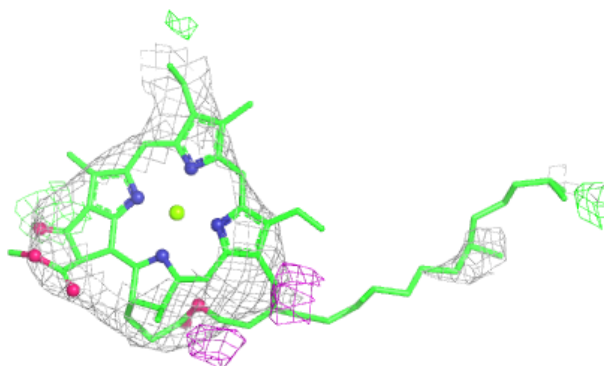


Electron density around CLA a 6007:

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

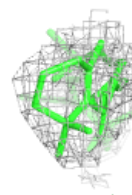
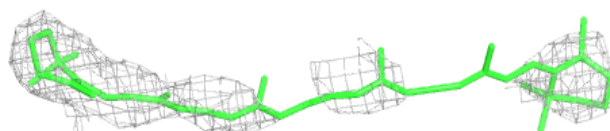
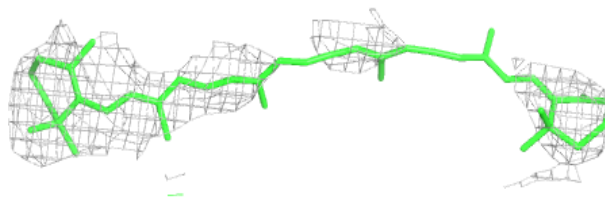
**Electron density around CLA C 1025:**

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

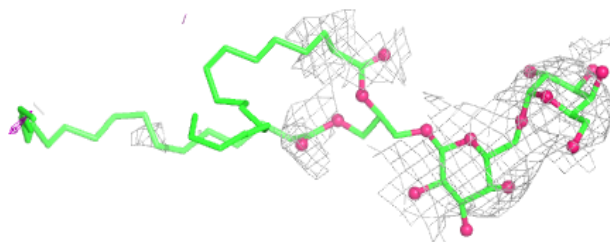


Electron density around BCR t 1046:

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

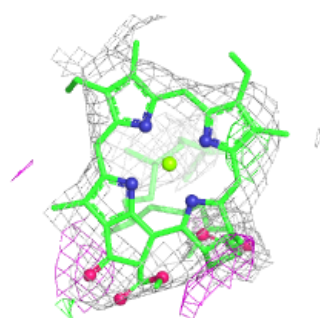
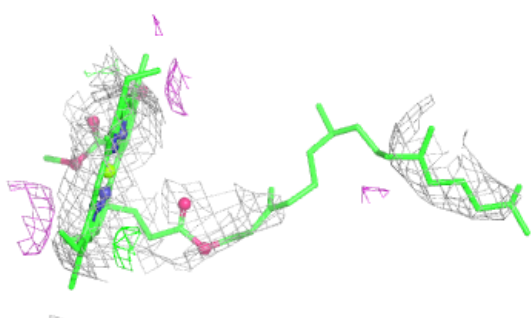
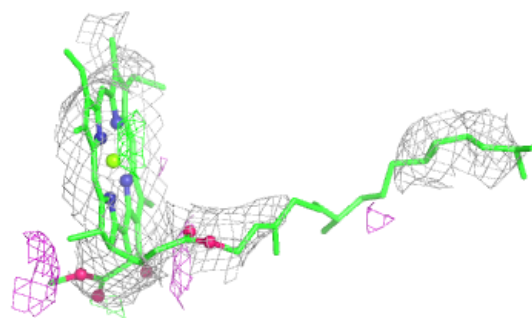
**Electron density around DGD B 1058:**

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

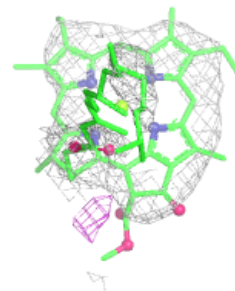
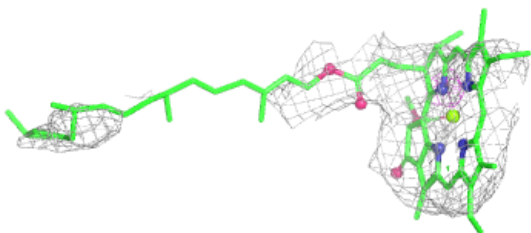
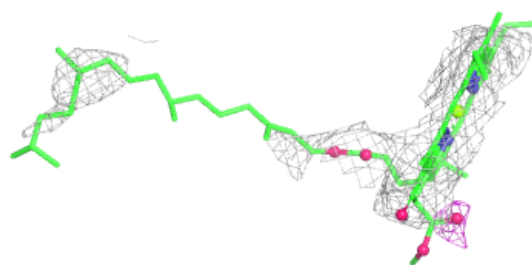


Electron density around CLA C 1032:

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

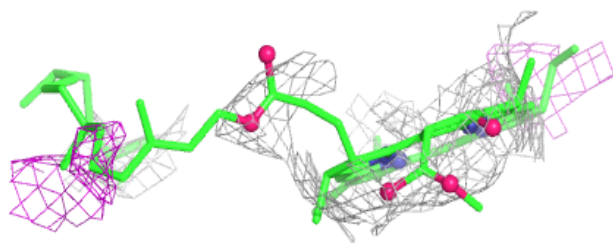
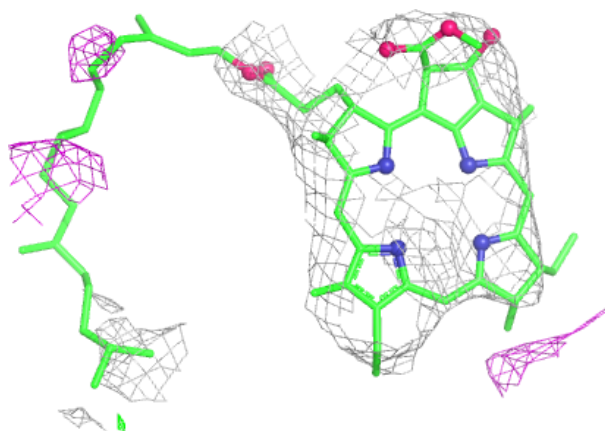
**Electron density around CLA b 6012:**

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

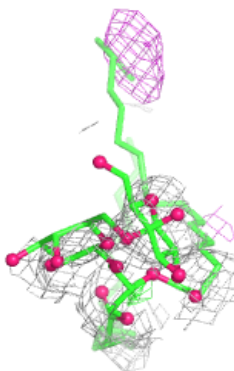
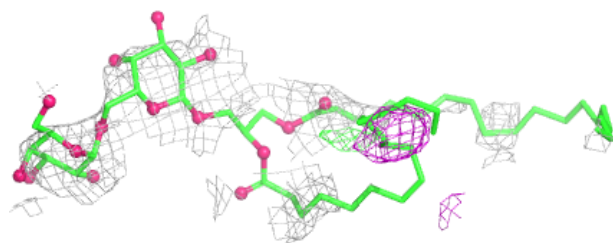
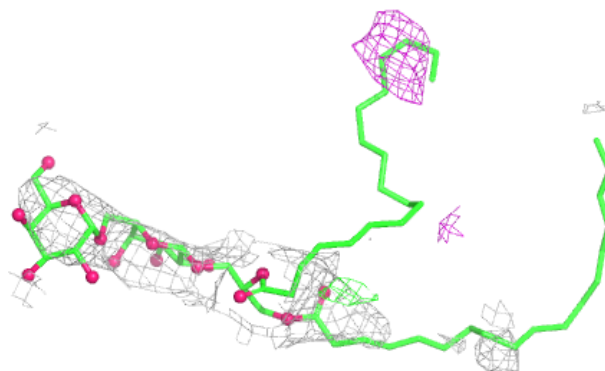


Electron density around PHO a 6038:

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

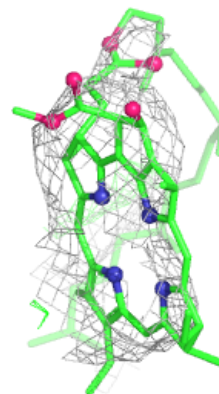
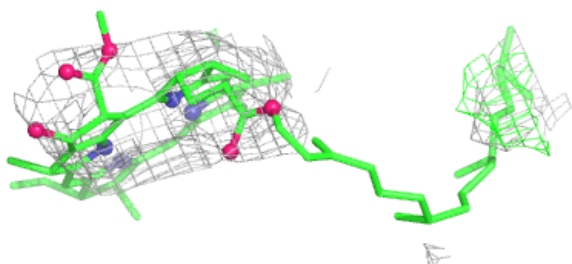
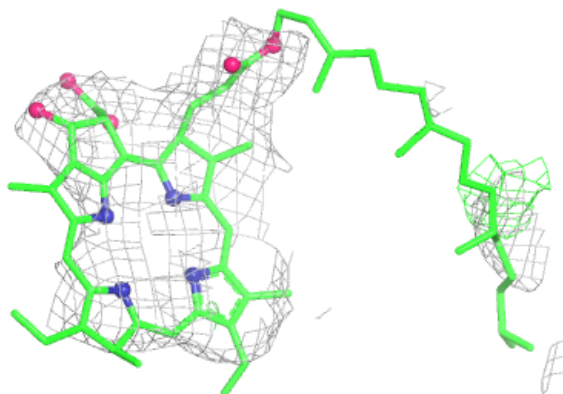
**Electron density around DGD b 6058:**

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

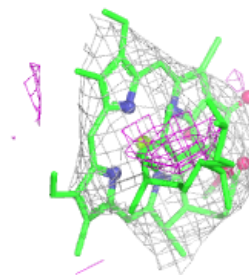
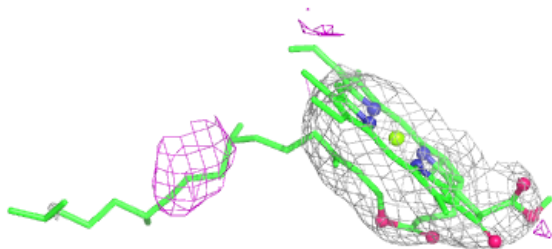
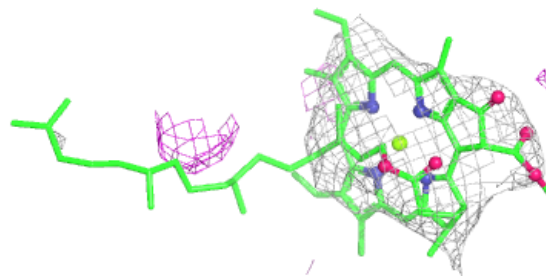


Electron density around PHO d 6039:

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

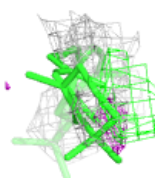
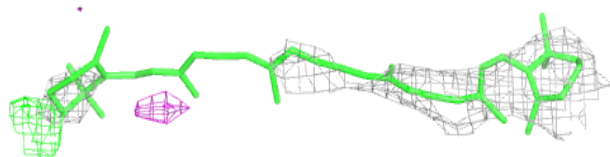
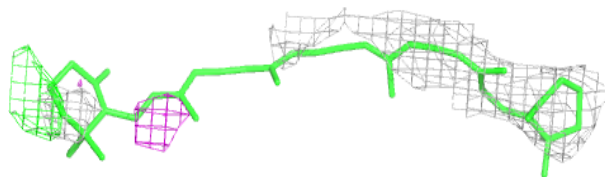
**Electron density around CLA C 1029:**

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

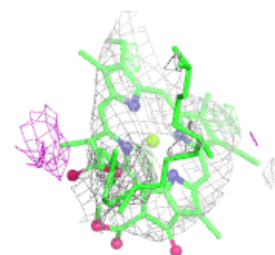
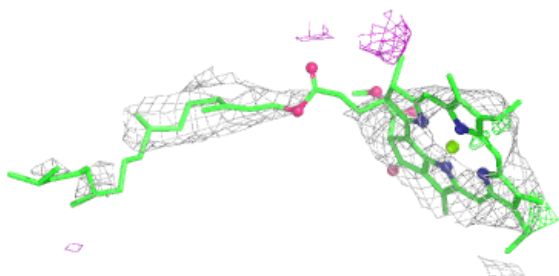
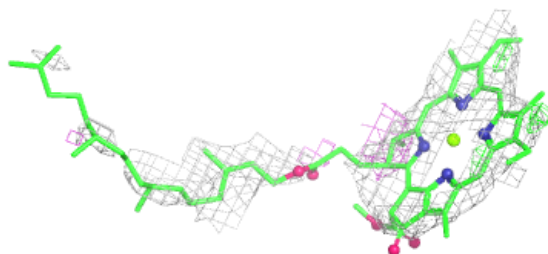


Electron density around BCR C 1052:

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

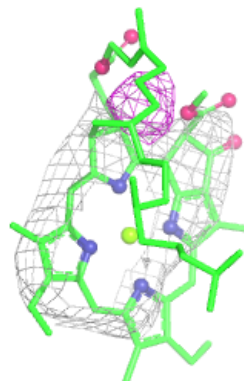
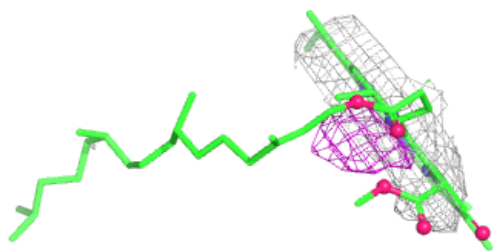
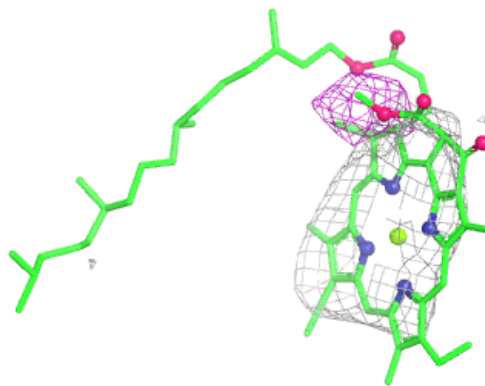
**Electron density around CLA a 6003:**

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



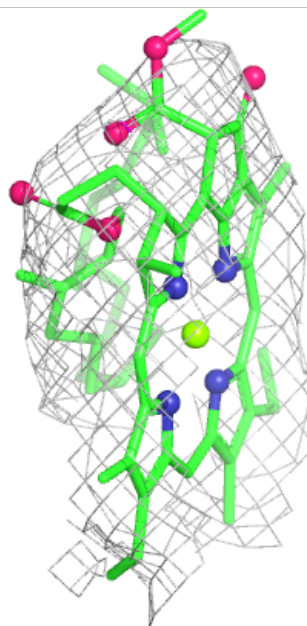
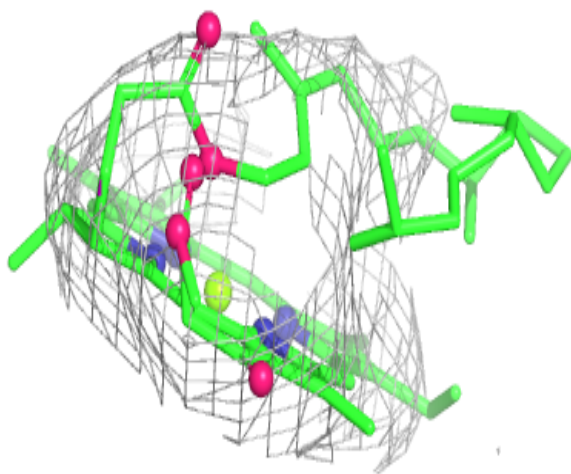
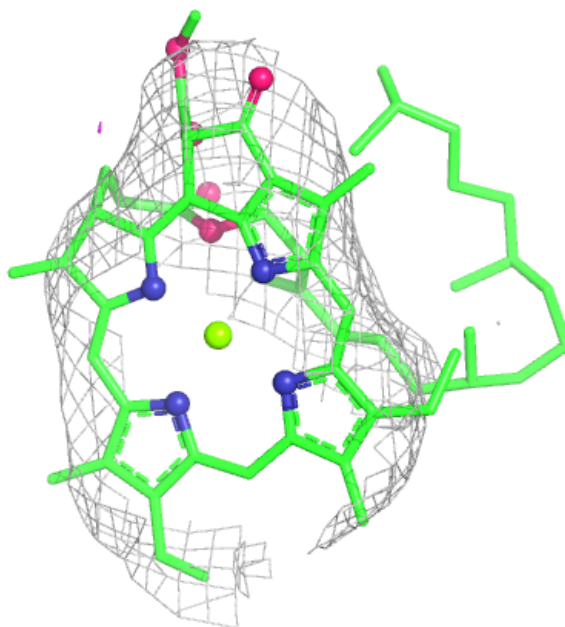
Electron density around CLA c 6031:

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



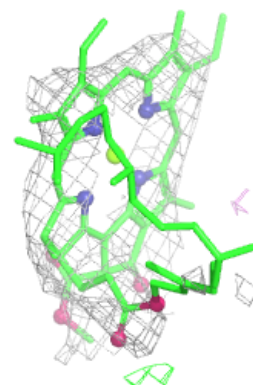
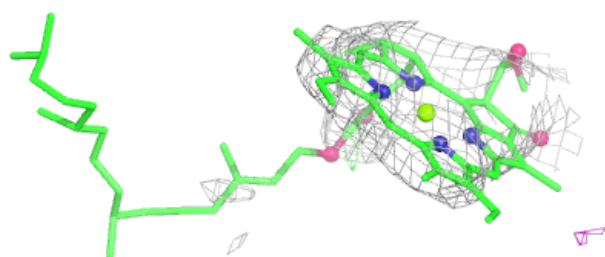
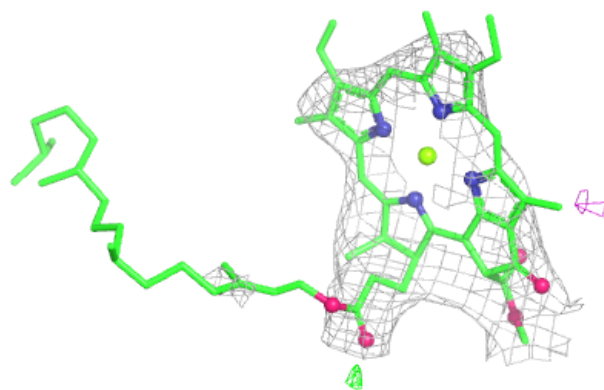
Electron density around CLA b 6022:

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

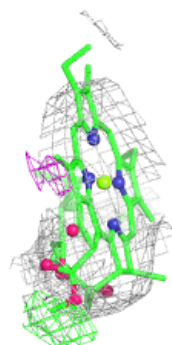
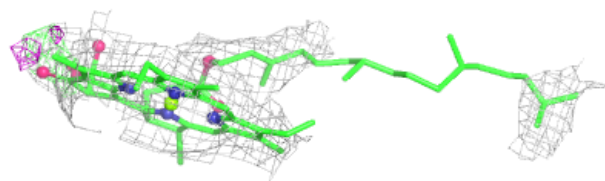
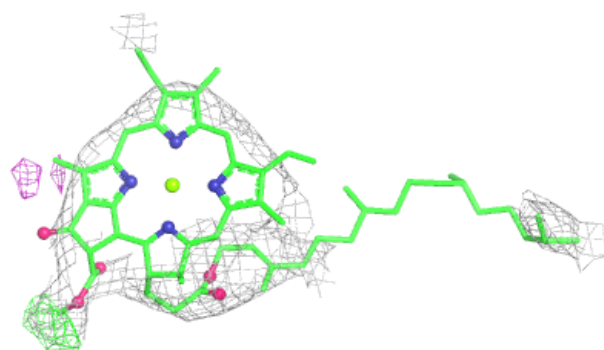


Electron density around CLA D 1008:

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

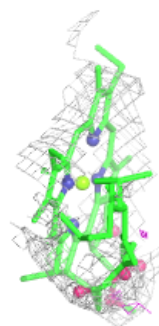
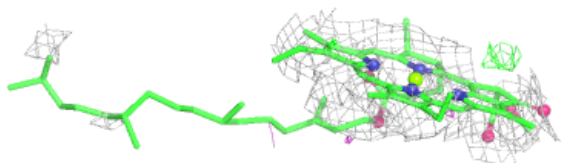
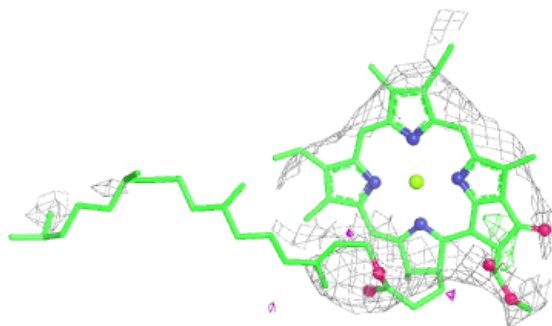
**Electron density around CLA B 1011:**

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



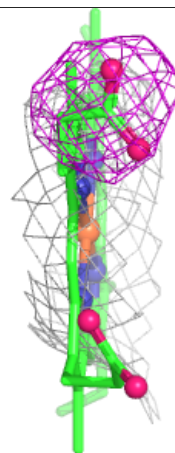
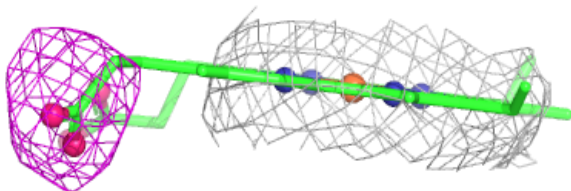
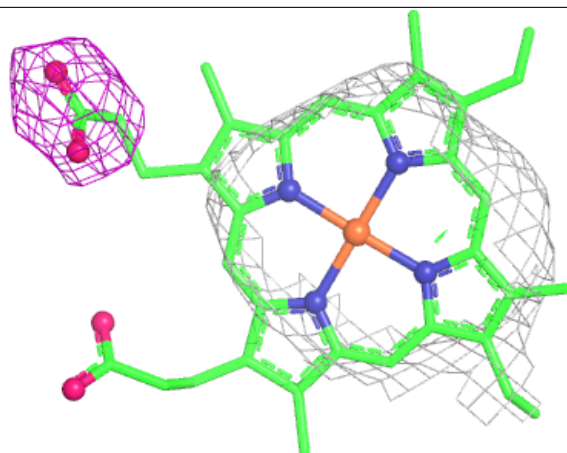
Electron density around CLA b 6011:

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

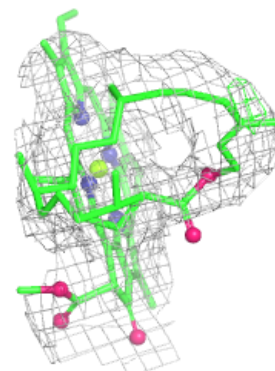
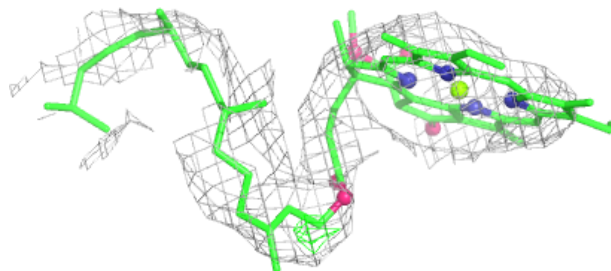
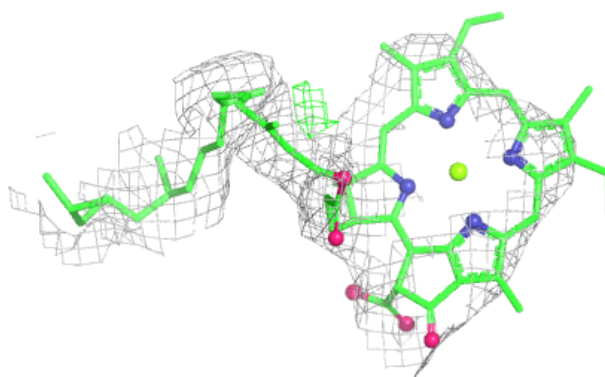


Electron density around HEM f 6040:

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

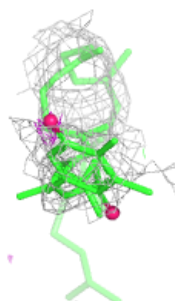
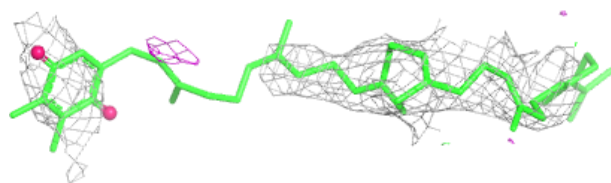
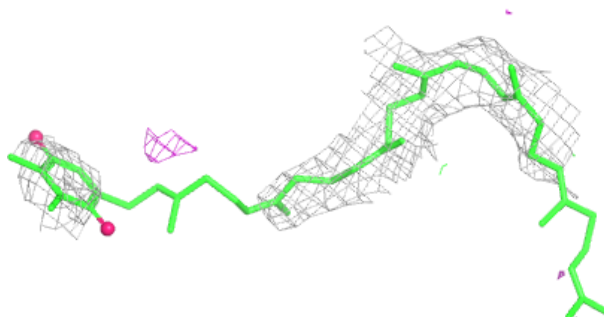
**Electron density around CLA a 6006:**

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

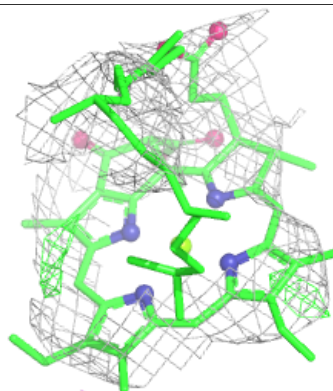
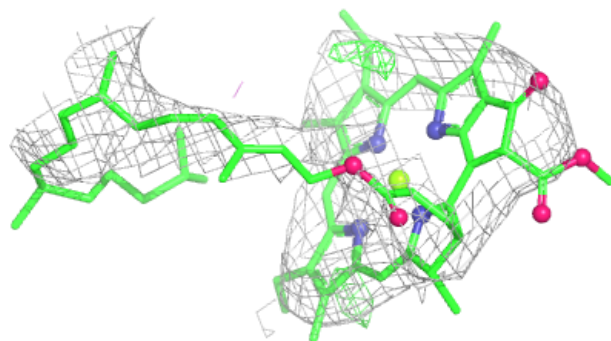
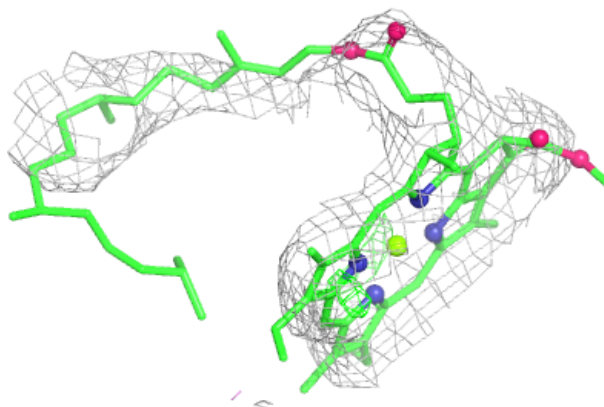


Electron density around PQ9 D 1042:

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

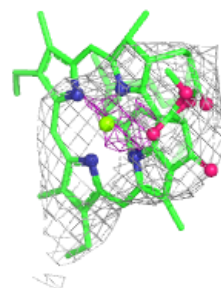
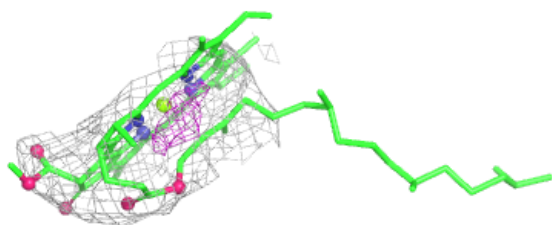
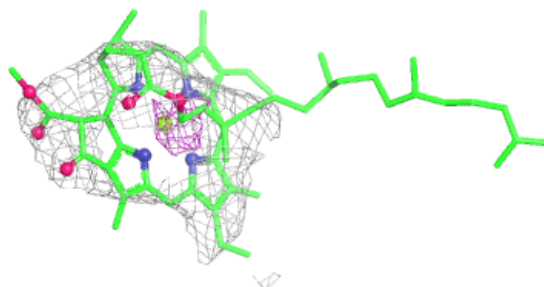
**Electron density around CLA c 6028:**

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

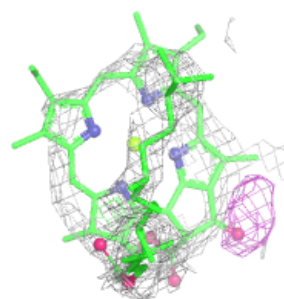
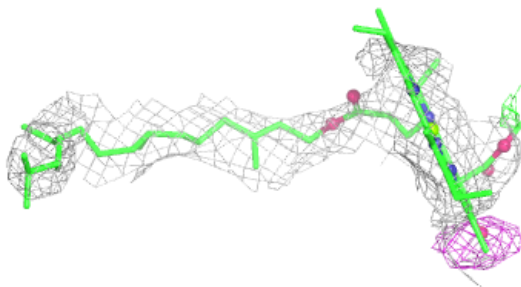
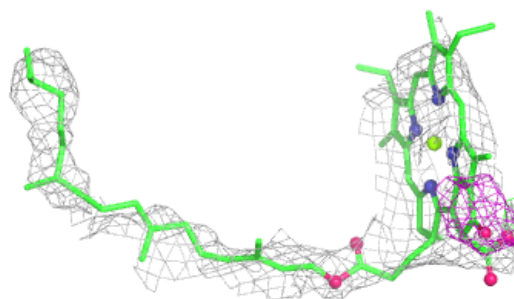


Electron density around CLA c 6029:

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

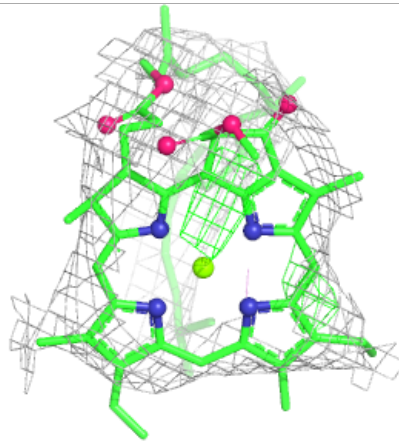
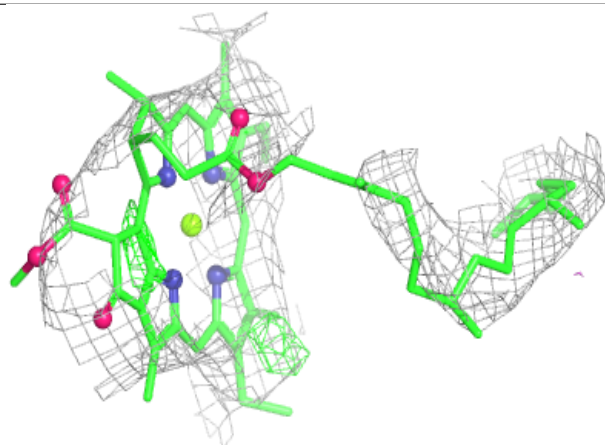
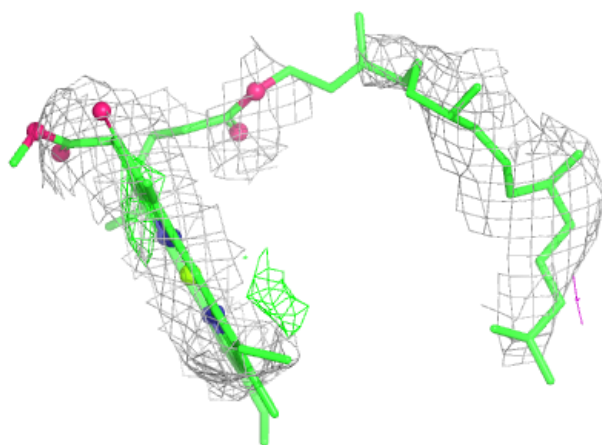
**Electron density around CLA h 6017:**

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



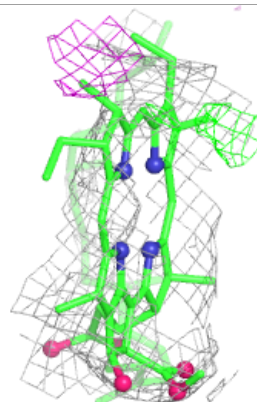
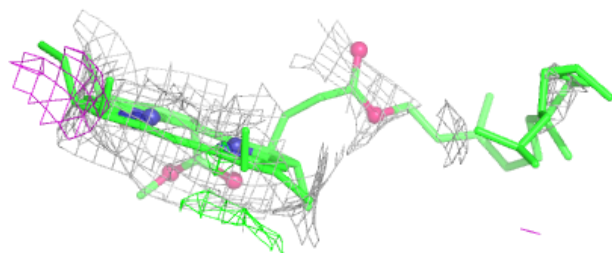
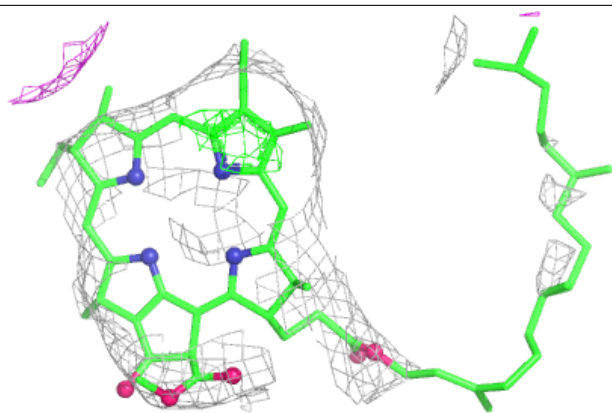
Electron density around CLA B 1019:

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

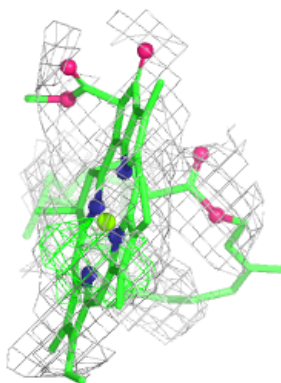
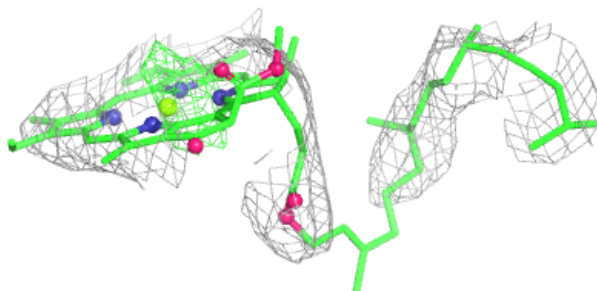
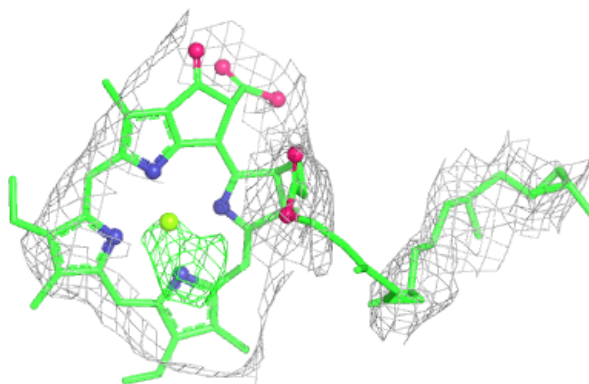


Electron density around PHO A 1038:

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

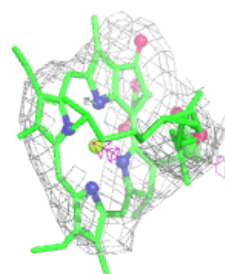
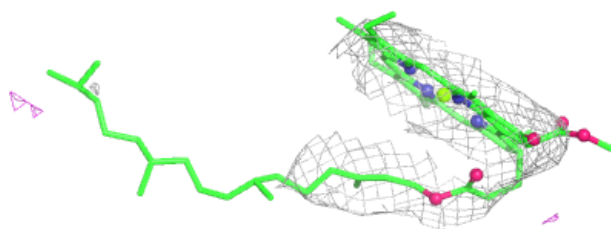
**Electron density around CLA A 1006:**

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

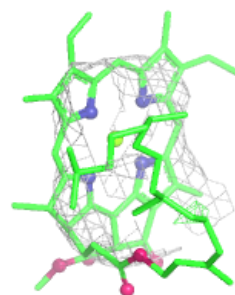
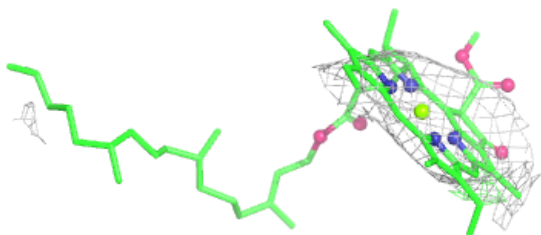


Electron density around CLA b 6016:

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

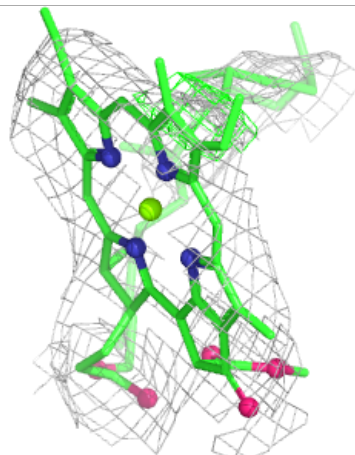
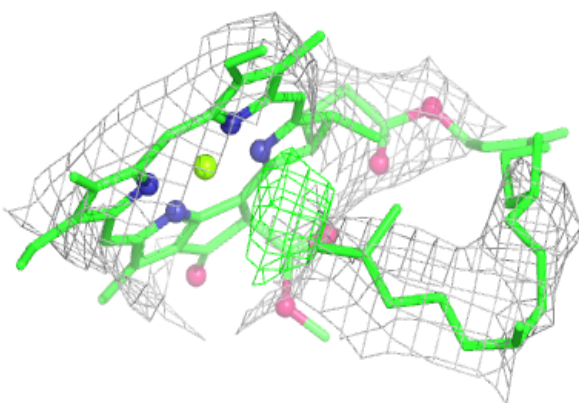
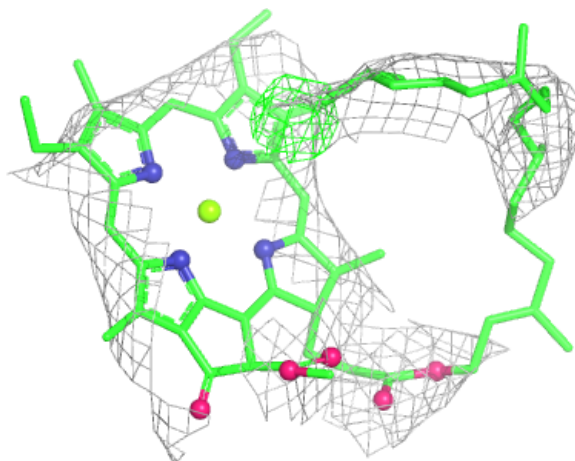
**Electron density around CLA C 1035:**

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



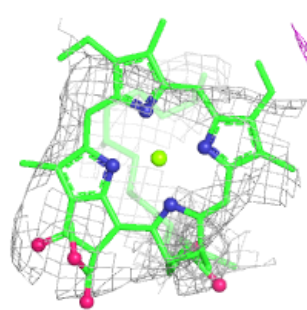
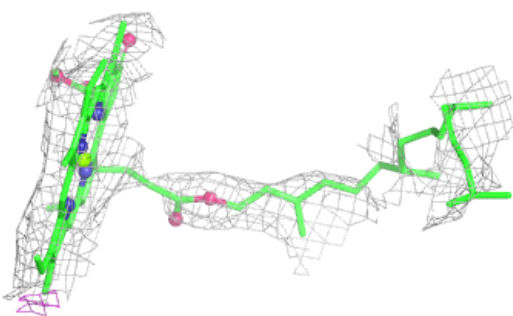
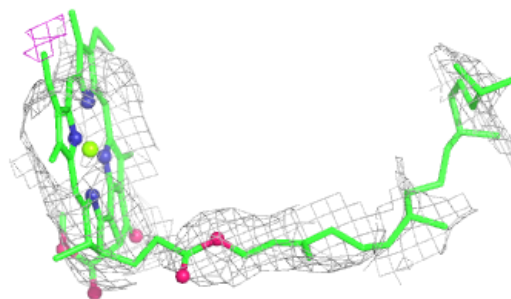
Electron density around CLA B 1023:

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

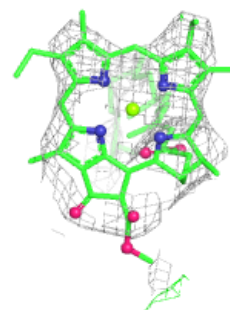
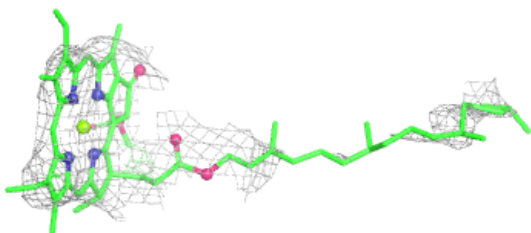
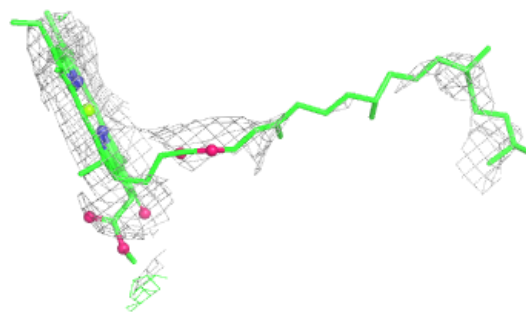


Electron density around CLA c 6030:

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

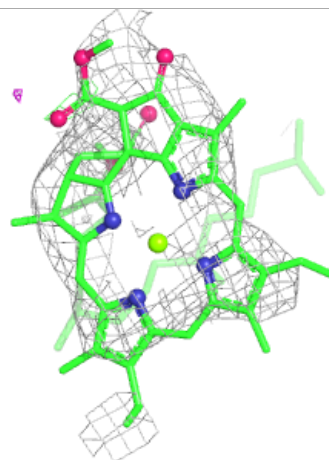
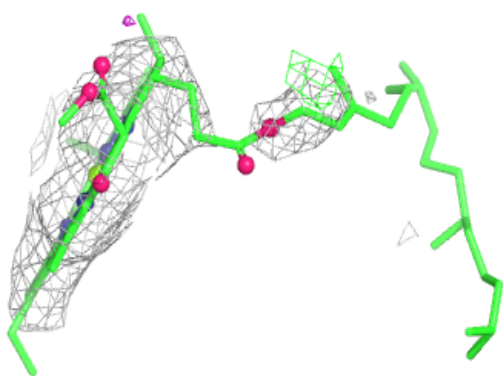
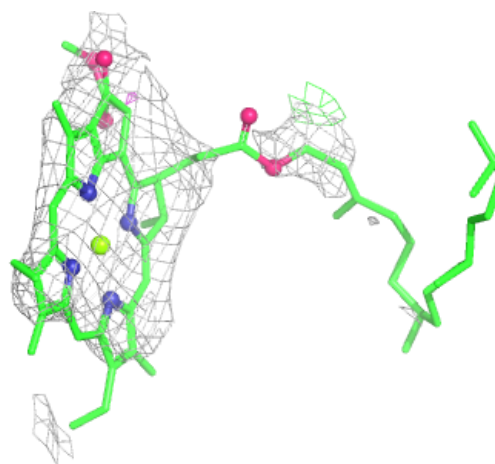
**Electron density around CLA B 1012:**

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



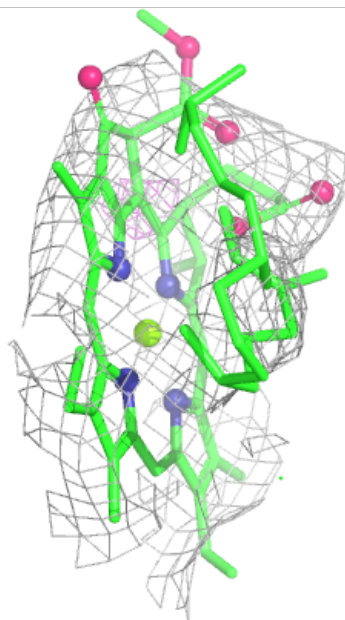
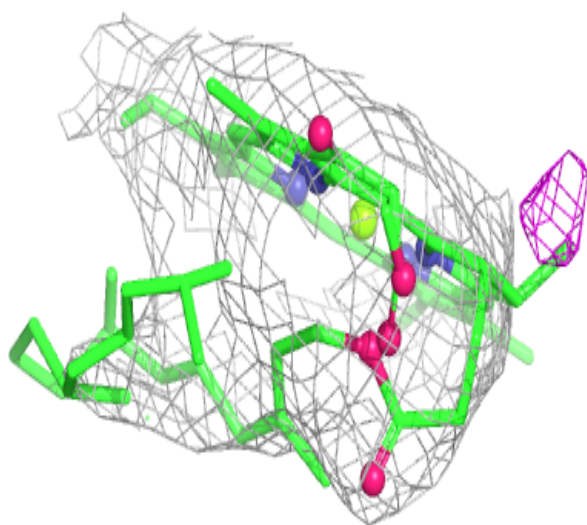
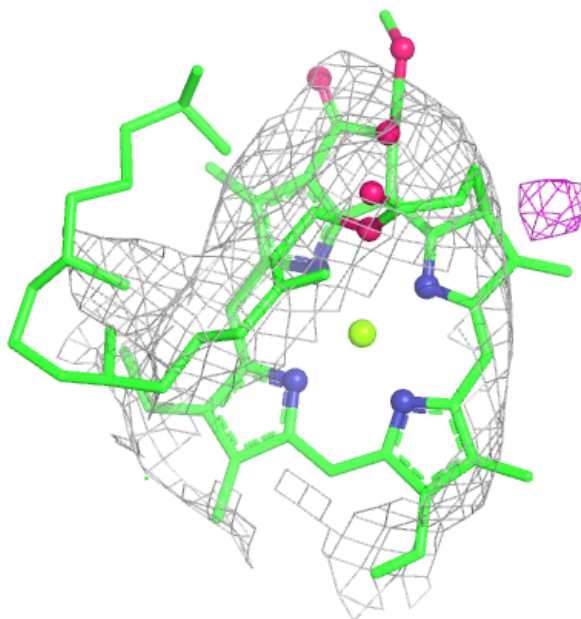
Electron density around CLA A 1007:

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



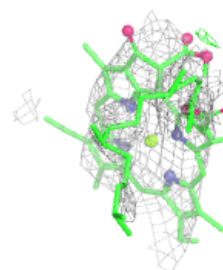
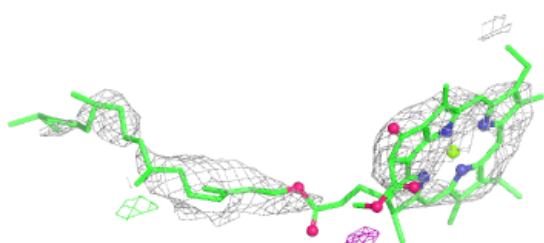
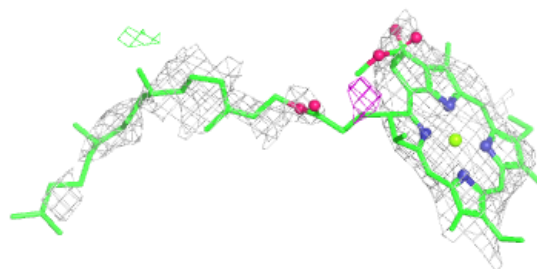
Electron density around CLA B 1022:

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

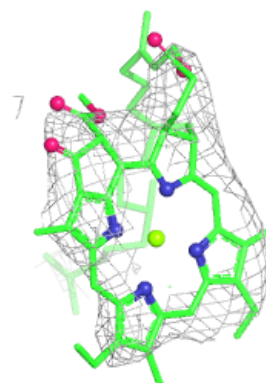
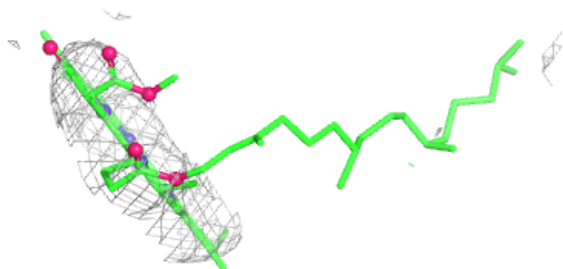
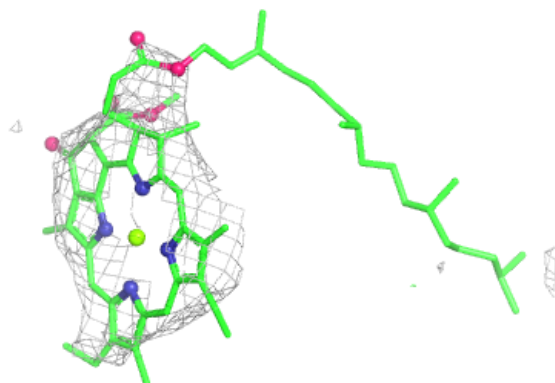


Electron density around CLA A 1003:

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

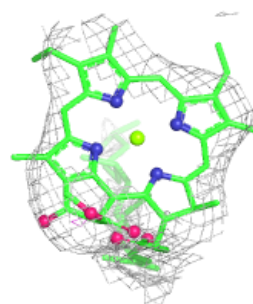
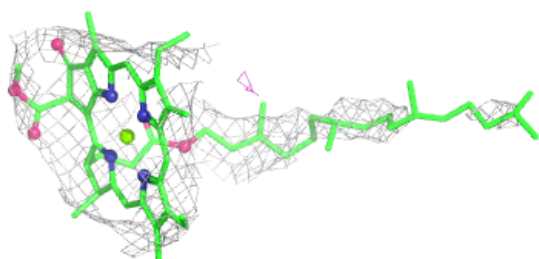
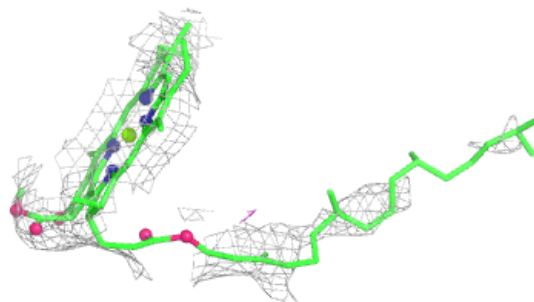
**Electron density around CLA C 1031:**

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

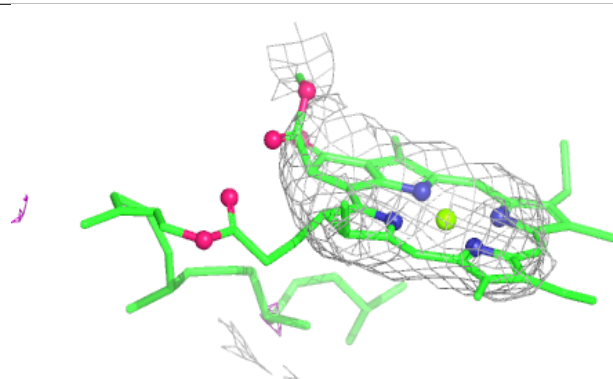
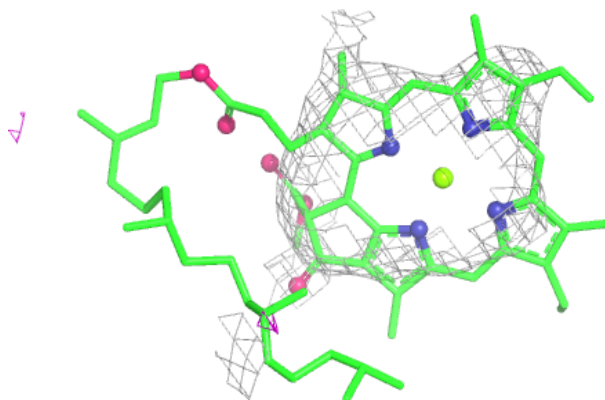


Electron density around CLA B 1015:

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

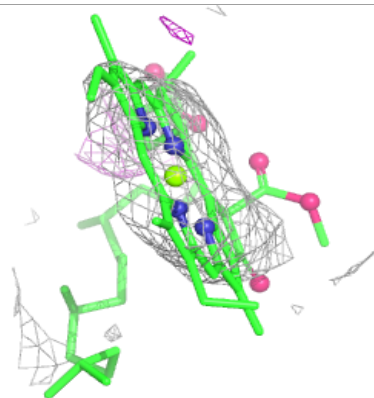
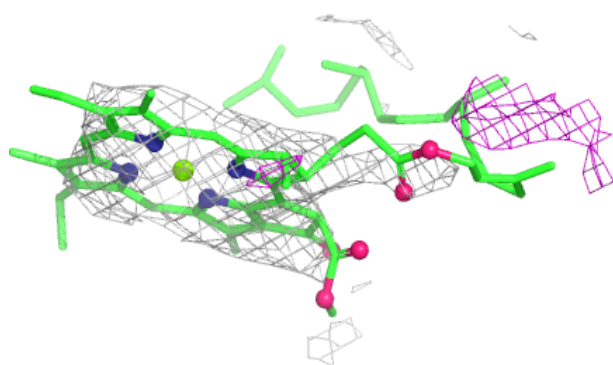
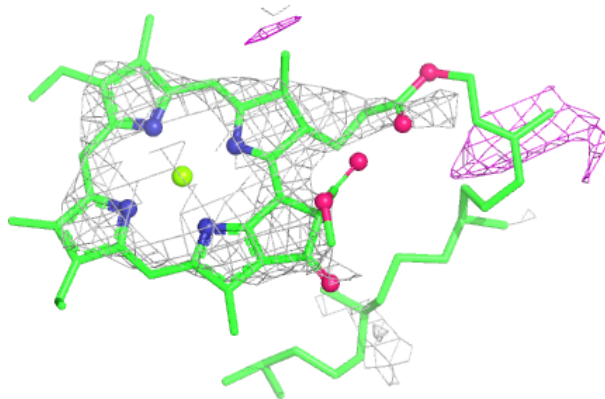
**Electron density around CLA c 6033:**

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

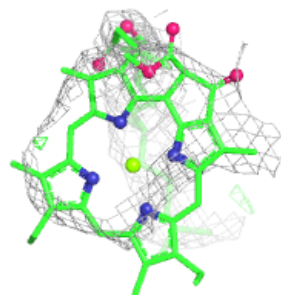
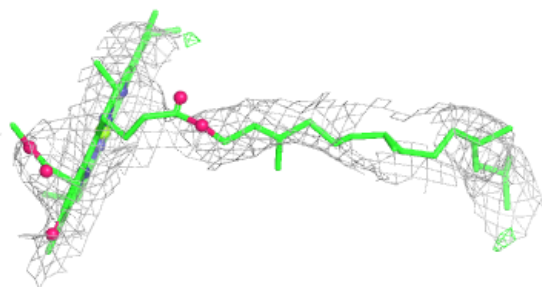


Electron density around CLA C 1033:

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

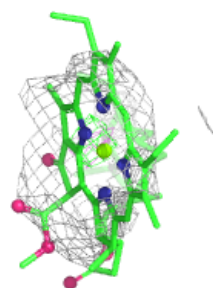
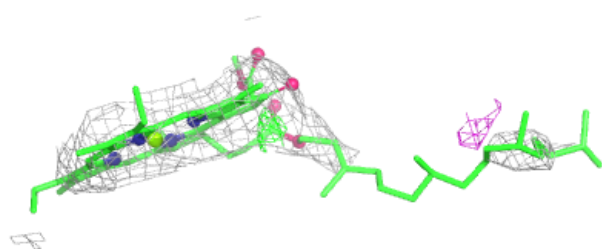
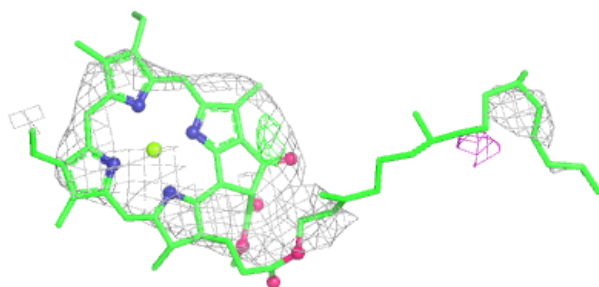
**Electron density around CLA H 1017:**

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



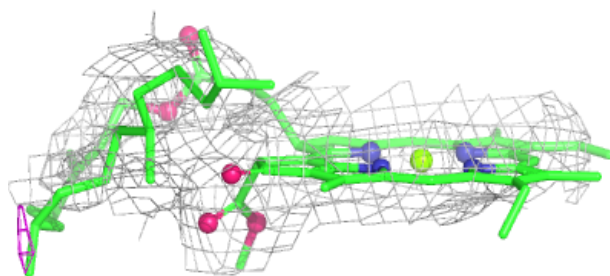
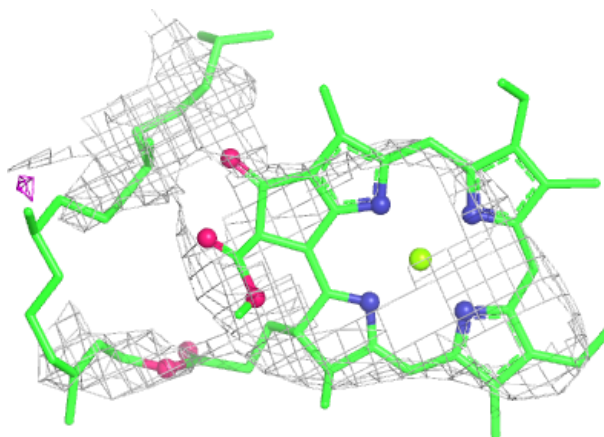
Electron density around CLA B 1010:

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



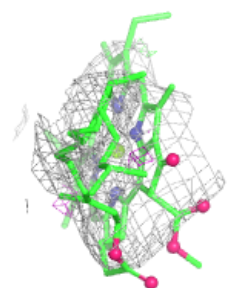
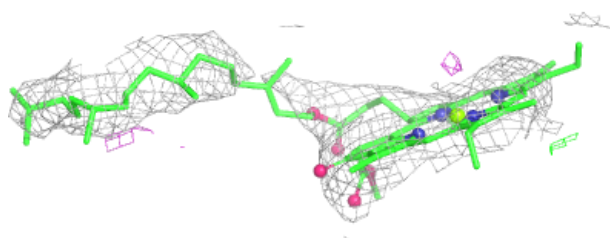
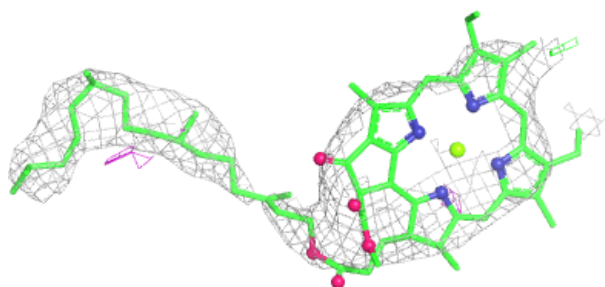
Electron density around CLA b 6018:

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

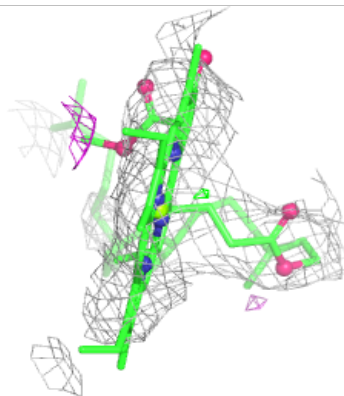
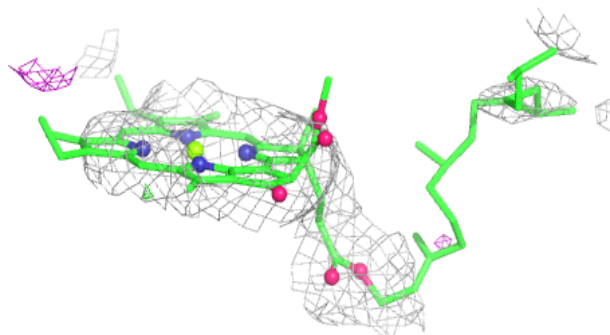
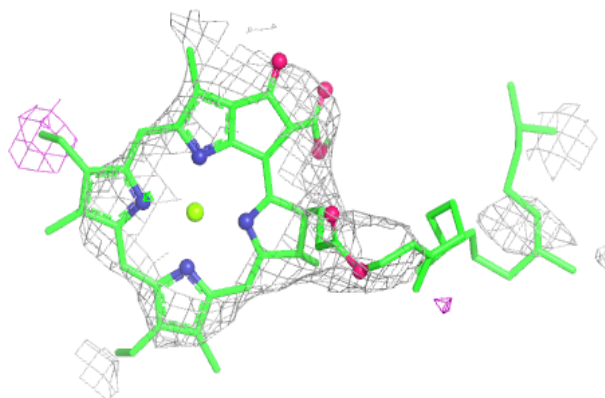


Electron density around CLA b 6010:

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

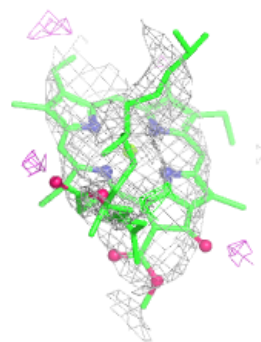
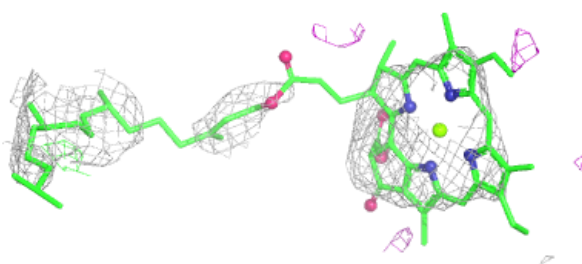
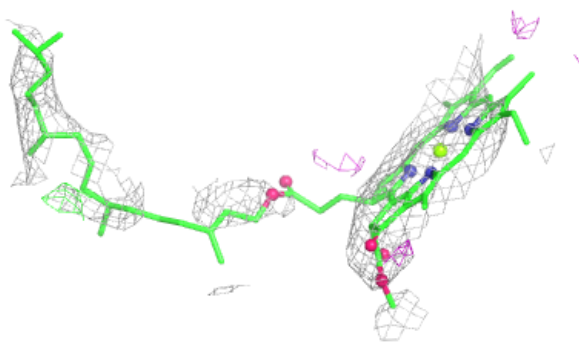
**Electron density around CLA b 6020:**

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

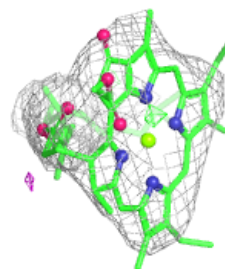
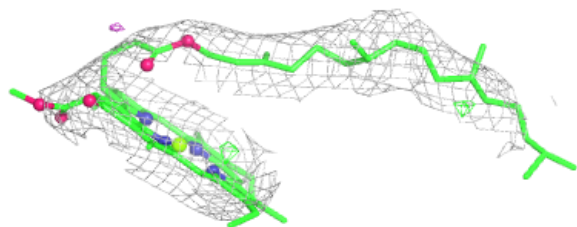
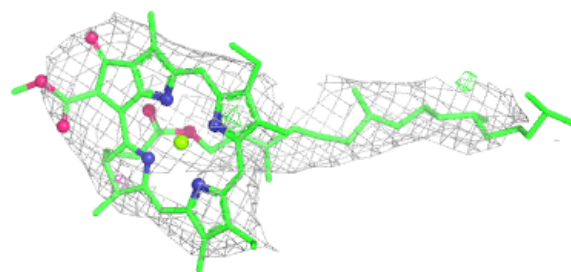


Electron density around CLA D 1004:

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

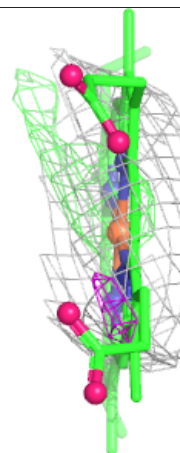
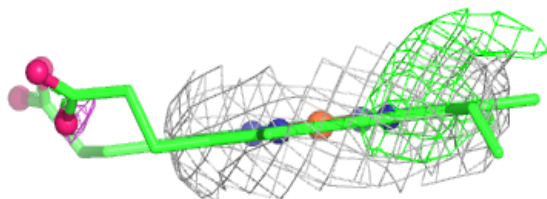
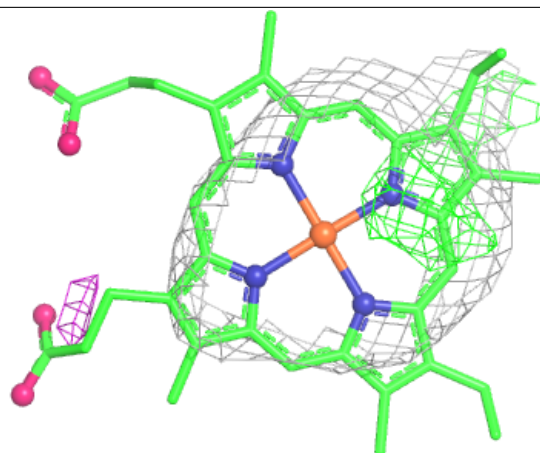
**Electron density around CLA B 1016:**

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



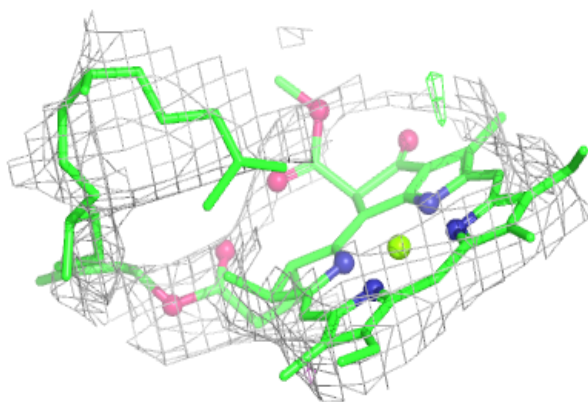
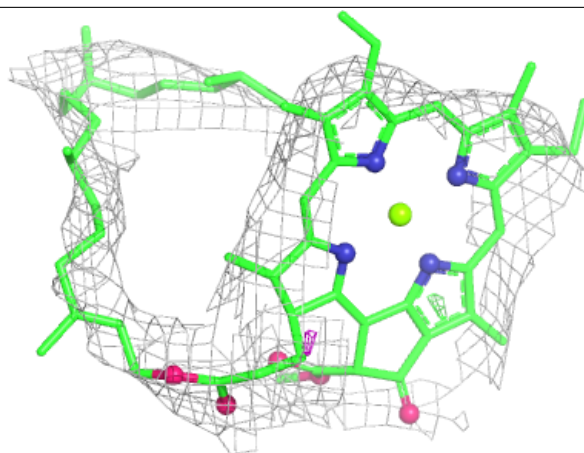
Electron density around HEM F 1040:

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



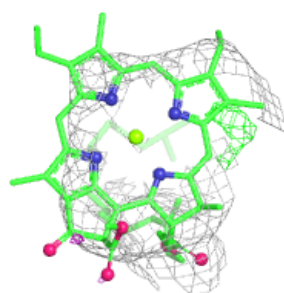
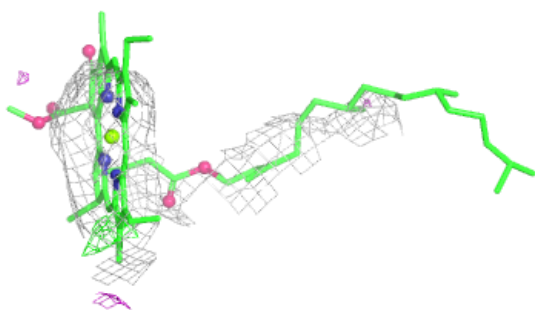
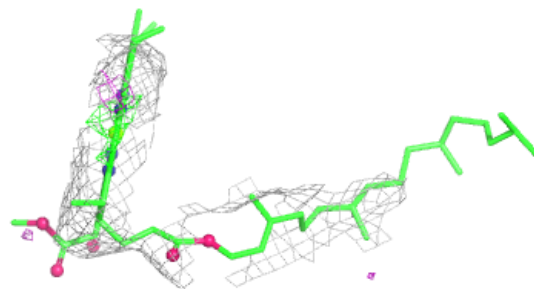
Electron density around CLA b 6023:

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

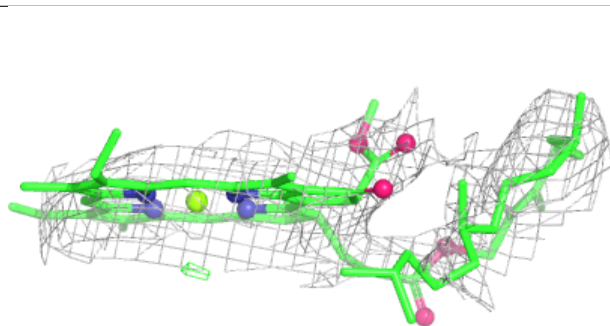
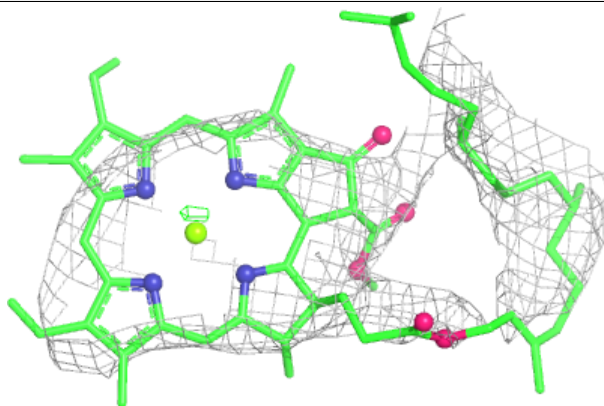


Electron density around CLA b 6013:

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

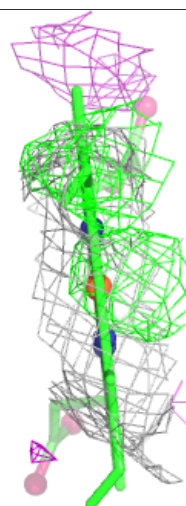
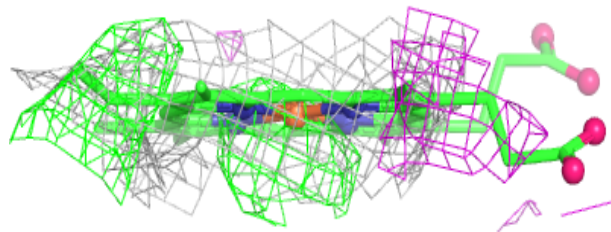
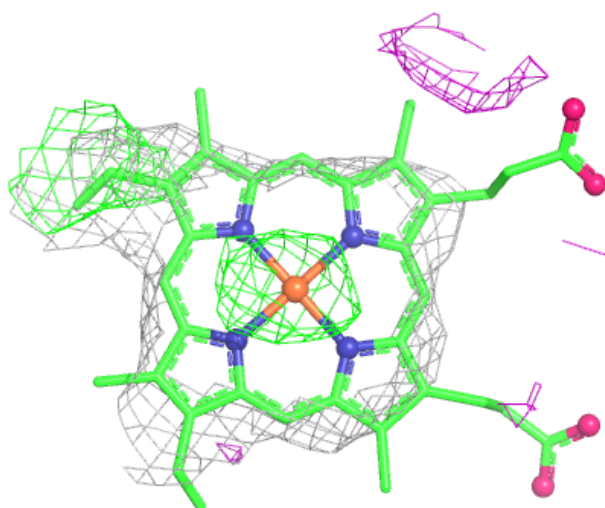
**Electron density around CLA B 1018:**

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



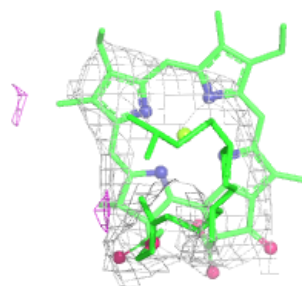
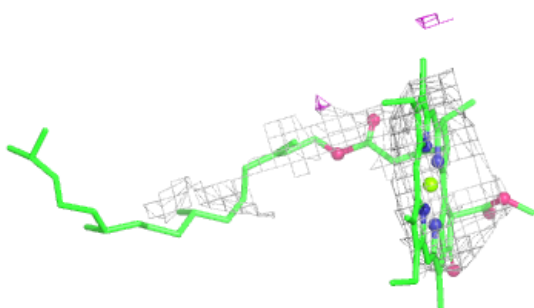
Electron density around HEM V 1041:

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



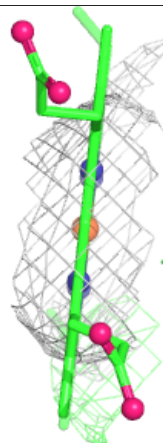
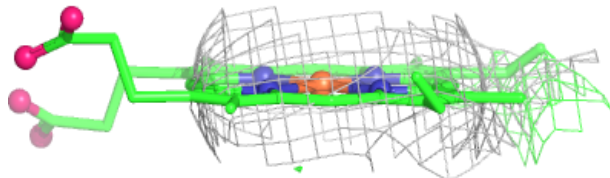
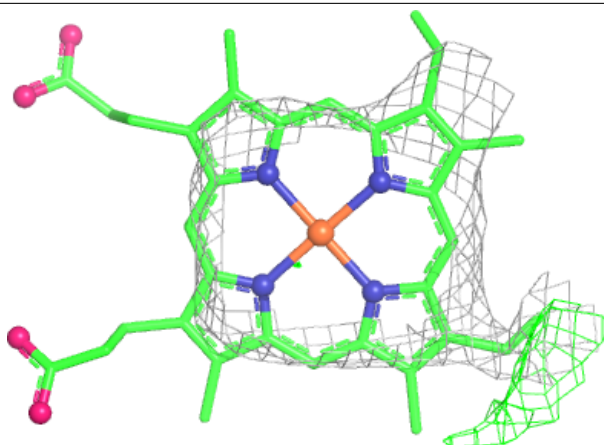
Electron density around CLA B 1013:

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



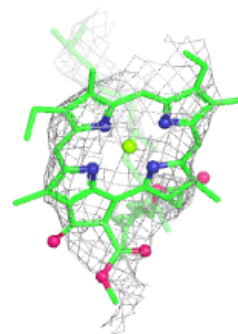
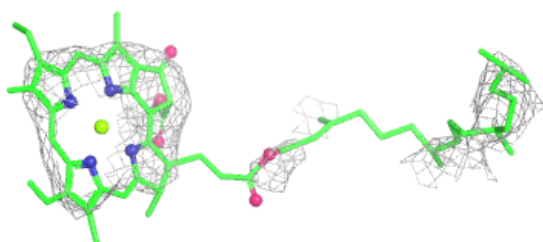
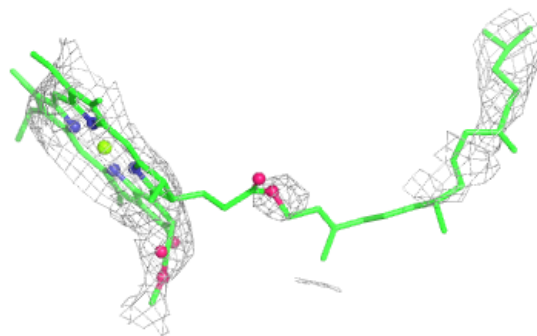
Electron density around HEM v 6041:

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

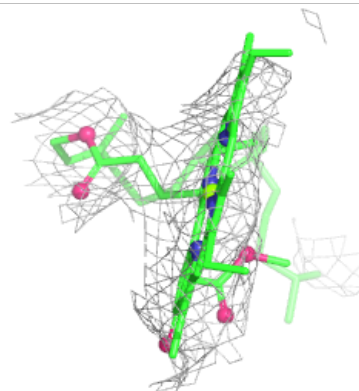
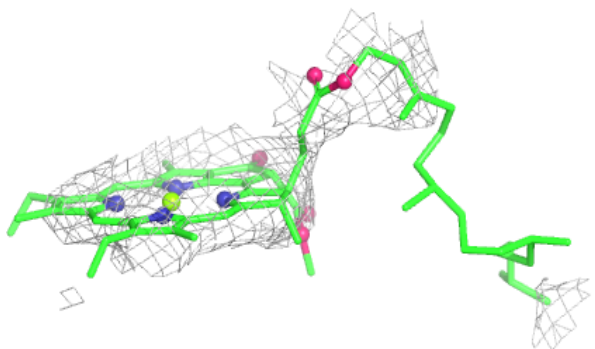
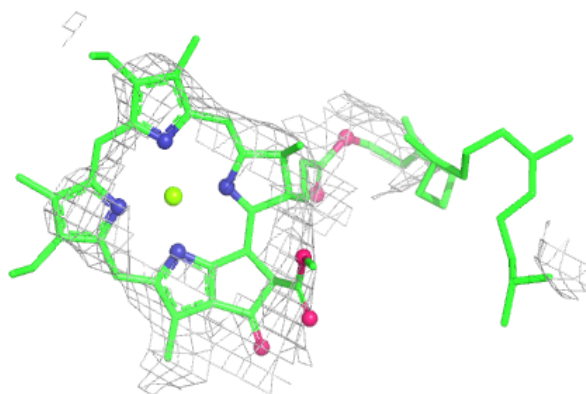


Electron density around CLA d 6004:

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

**Electron density around CLA B 1020:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.