



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2021 – 03:03 AM BST

PDB ID : 6ZXS
Title : Cold grown Pea Photosystem I
Authors : Caspy, I.; Borovikova-Sheinker, A.; Subramanyam, R.; Nelson, N.
Deposited on : 2020-07-30
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

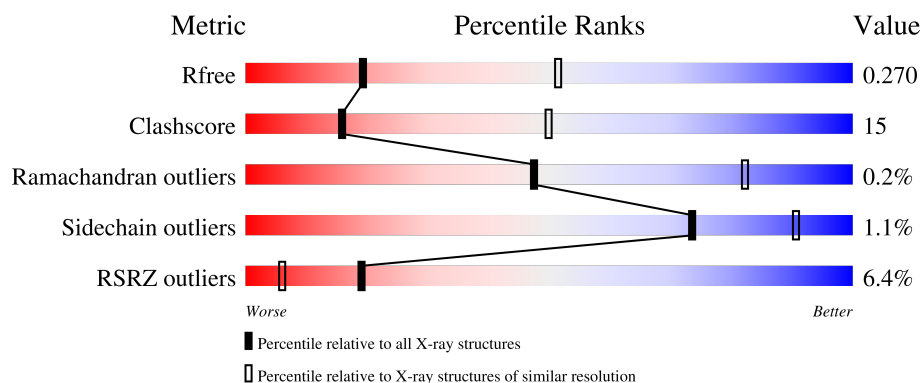
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	743	<div> <div>3%</div> <div>77%</div> <div>23%</div> </div>
2	B	733	<div> <div>3%</div> <div>76%</div> <div>24%</div> </div>
3	C	80	<div> <div>5%</div> <div>85%</div> <div>15%</div> </div>
4	D	143	<div> <div>8%</div> <div>78%</div> <div>22%</div> </div>
5	E	66	<div> <div>17%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	154	
7	G	97	
8	H	88	
9	I	30	
10	J	42	
11	K	80	
12	L	157	
13	1	193	
14	2	208	
15	3	221	
16	4	198	

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
17	CL0	A	801	X	-	-	-
18	CLA	1	5006	X	-	-	-
18	CLA	1	5007	X	-	-	-
18	CLA	1	5008	X	-	-	-
18	CLA	1	5009	X	-	-	-
18	CLA	1	5010	X	-	-	-
18	CLA	1	5011	X	-	-	-
18	CLA	1	5012	X	-	-	-
18	CLA	1	5013	X	-	-	-
18	CLA	1	5015	X	-	-	-
18	CLA	1	5017	X	-	-	-
18	CLA	1	5018	X	-	-	-
18	CLA	2	306	X	-	-	-
18	CLA	2	307	X	-	-	-
18	CLA	2	308	X	-	-	-
18	CLA	2	309	X	-	-	-
18	CLA	2	310	X	-	-	-
18	CLA	2	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	2	312	X	-	-	-
18	CLA	2	313	X	-	-	-
18	CLA	2	317	X	-	-	-
18	CLA	2	326	X	-	-	-
18	CLA	3	301	X	-	-	-
18	CLA	3	307	X	-	-	-
18	CLA	3	308	X	-	-	-
18	CLA	3	309	X	-	-	-
18	CLA	3	311	X	-	-	-
18	CLA	3	314	X	-	-	-
18	CLA	3	315	X	-	-	-
18	CLA	3	317	X	-	-	-
18	CLA	3	318	X	-	-	-
18	CLA	3	319	X	-	-	-
18	CLA	4	305	X	-	-	-
18	CLA	4	306	X	-	-	-
18	CLA	4	307	X	-	-	-
18	CLA	4	308	X	-	-	-
18	CLA	4	309	X	-	-	-
18	CLA	4	310	X	-	-	-
18	CLA	4	311	X	-	-	-
18	CLA	4	312	X	-	-	-
18	CLA	4	315	X	-	-	-
18	CLA	A	802	X	-	-	-
18	CLA	A	803	X	-	-	-
18	CLA	A	804	X	-	-	-
18	CLA	A	805	X	-	-	-
18	CLA	A	806	X	-	-	-
18	CLA	A	807	X	-	-	-
18	CLA	A	808	X	-	-	-
18	CLA	A	809	X	-	-	-
18	CLA	A	810	X	-	-	-
18	CLA	A	811	X	-	-	-
18	CLA	A	812	X	-	-	-
18	CLA	A	813	X	-	-	-
18	CLA	A	814	X	-	-	-
18	CLA	A	815	X	-	-	-
18	CLA	A	816	X	-	-	-
18	CLA	A	817	X	-	-	-
18	CLA	A	818	X	-	-	-
18	CLA	A	819	X	-	-	-
18	CLA	A	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	A	821	X	-	-	-
18	CLA	A	822	X	-	-	-
18	CLA	A	823	X	-	-	-
18	CLA	A	824	X	-	-	-
18	CLA	A	825	X	-	-	-
18	CLA	A	826	X	-	-	-
18	CLA	A	827	X	-	-	-
18	CLA	A	828	X	-	-	-
18	CLA	A	829	X	-	-	-
18	CLA	A	830	X	-	-	-
18	CLA	A	831	X	-	-	-
18	CLA	A	832	X	-	-	-
18	CLA	A	833	X	-	-	-
18	CLA	A	834	X	-	-	-
18	CLA	A	835	X	-	-	-
18	CLA	A	836	X	-	-	-
18	CLA	A	837	X	-	-	-
18	CLA	A	838	X	-	-	-
18	CLA	A	839	X	-	-	-
18	CLA	A	840	X	-	-	-
18	CLA	A	852	X	-	-	-
18	CLA	A	853	X	-	-	-
18	CLA	B	801	X	-	-	-
18	CLA	B	803	X	-	-	-
18	CLA	B	804	X	-	-	-
18	CLA	B	805	X	-	-	-
18	CLA	B	806	X	-	-	-
18	CLA	B	807	X	-	-	-
18	CLA	B	808	X	-	-	-
18	CLA	B	809	X	-	-	-
18	CLA	B	810	X	-	-	-
18	CLA	B	811	X	-	-	-
18	CLA	B	812	X	-	-	-
18	CLA	B	813	X	-	-	-
18	CLA	B	814	X	-	-	-
18	CLA	B	815	X	-	-	-
18	CLA	B	816	X	-	-	-
18	CLA	B	817	X	-	-	-
18	CLA	B	818	X	-	-	-
18	CLA	B	819	X	-	-	-
18	CLA	B	820	X	-	-	-
18	CLA	B	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	B	822	X	-	-	-
18	CLA	B	823	X	-	-	-
18	CLA	B	824	X	-	-	-
18	CLA	B	825	X	-	-	-
18	CLA	B	826	X	-	-	-
18	CLA	B	827	X	-	-	-
18	CLA	B	828	X	-	-	-
18	CLA	B	829	X	-	-	-
18	CLA	B	830	X	-	-	-
18	CLA	B	831	X	-	-	-
18	CLA	B	832	X	-	-	-
18	CLA	B	833	X	-	-	-
18	CLA	B	834	X	-	-	-
18	CLA	B	835	X	-	-	-
18	CLA	B	836	X	-	-	-
18	CLA	B	837	X	-	-	-
18	CLA	B	838	X	-	-	-
18	CLA	B	839	X	-	-	-
18	CLA	B	840	X	-	-	-
18	CLA	B	841	X	-	-	-
18	CLA	F	301	X	-	-	-
18	CLA	F	302	X	-	-	-
18	CLA	F	303	X	-	-	-
18	CLA	G	1601	X	-	-	-
18	CLA	G	1602	X	-	-	-
18	CLA	G	1603	X	-	-	-
18	CLA	H	1701	X	-	-	-
18	CLA	J	1101	X	-	-	-
18	CLA	J	1103	X	-	-	-
18	CLA	K	1401	X	-	-	-
18	CLA	K	1402	X	-	-	-
18	CLA	K	1403	X	-	-	-
18	CLA	K	1404	X	-	-	X
18	CLA	L	301	X	-	-	-
18	CLA	L	304	X	-	-	-
18	CLA	L	305	X	-	-	-
18	CLA	L	306	X	-	-	-
21	BCR	1	5005	-	-	-	X
21	BCR	2	305	-	-	-	X
21	BCR	3	306	-	-	-	X
21	BCR	B	845	-	-	-	X
21	BCR	K	1405	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	BCR	L	302	-	-	-	X
22	LHG	B	849	-	-	-	X
23	LMT	A	850	-	-	-	X
23	LMT	B	852	-	-	-	X
23	LMT	G	1606	-	-	-	X
23	LMT	J	1107	-	-	-	X
24	LMG	1	5020	-	-	-	X
24	LMG	2	301	-	-	-	X
24	LMG	4	320	-	-	-	X
24	LMG	A	851	-	-	-	X
25	GOL	4	321	-	-	-	X
26	DGD	1	5002	-	-	-	X
29	LUT	1	5004	X	-	-	-
29	LUT	2	303	X	-	-	-
29	LUT	3	304	X	-	-	-
29	LUT	J	1105	X	-	-	-
30	CHL	1	5014	X	-	-	-
30	CHL	1	5016	X	-	-	-
30	CHL	2	314	X	-	-	-
30	CHL	2	315	X	-	-	-
30	CHL	2	316	X	-	-	-
30	CHL	2	318	X	-	-	-
30	CHL	2	319	X	-	-	-
30	CHL	3	310	X	-	-	-
30	CHL	3	312	X	-	-	-
30	CHL	3	313	X	-	-	-
30	CHL	3	316	X	-	-	-
30	CHL	4	302	X	-	-	-
30	CHL	4	313	X	-	-	-
30	CHL	4	314	X	-	-	-
30	CHL	4	316	X	-	-	-
30	CHL	4	317	X	-	-	-
30	CHL	4	318	X	-	-	-
31	XAT	2	304	X	-	-	-
31	XAT	4	304	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 37423 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 I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	743	Total	C	N	O	S	0	0	0
			5858	3839	998	1003	18			

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	733	Total	C	N	O	S	0	0	0
			5857	3848	998	997	14			

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	0	0
			1132	731	194	204	3			

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	66	Total	C	N	O	0	0	0
			528	336	93	99			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	154	Total	C	N	O	S	0	0	0
			1206	782	207	215	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	80	ALA	SER	conflict	UNP A0A0M3KL12
F	87	ASP	GLU	conflict	UNP A0A0M3KL12
F	108	LEU	ILE	conflict	UNP A0A0M3KL12
F	111	PRO	ALA	conflict	UNP A0A0M3KL12
F	134	GLY	ALA	conflict	UNP A0A0M3KL12
F	188	ASP	GLU	conflict	UNP A0A0M3KL12
F	204	THR	SER	conflict	UNP A0A0M3KL12
F	205	GLY	ARG	conflict	UNP A0A0M3KL12

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	97	Total	C	N	O	0	0	0
			757	492	125	140			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	88	Total	C	N	O	0	0	0
			673	442	106	125			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	60	LEU	ILE	conflict	UNP A0A0M3KL10
H	79	ASN	SER	conflict	UNP A0A0M3KL10
H	80	SER	PRO	conflict	UNP A0A0M3KL10
H	116	ALA	THR	conflict	UNP A0A0M3KL10
H	126	LYS	VAL	conflict	UNP A0A0M3KL10
H	134	GLN	LYS	conflict	UNP A0A0M3KL10
H	139	LEU	-	insertion	UNP A0A0M3KL10
H	?	-	LYS	deletion	UNP A0A0M3KL10

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	30	Total	C	N	O	S	0	0	0
			232	159	37	35	1			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	42	Total	C	N	O	S	0	0	0
			338	231	51	55	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	PHE	LEU	conflict	UNP D5MAL3

- Molecule 11 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	80	Total	C	N	O	S	0	0	0
			558	353	98	104	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	86	ALA	VAL	conflict	UNP E1C9L3

- Molecule 12 is a protein called PsaL domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	157	Total	C	N	O	S	0	0	0
			1174	772	189	212	1			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	57	VAL	ILE	conflict	UNP E1C9L1
L	79	VAL	ILE	conflict	UNP E1C9L1
L	88	GLY	ALA	conflict	UNP E1C9L1
L	94	ASN	SER	conflict	UNP E1C9L1
L	108	PHE	TYR	conflict	UNP E1C9L1
L	143	ILE	LEU	conflict	UNP E1C9L1
L	157	ASP	ALA	conflict	UNP E1C9L1
L	172	GLN	GLU	conflict	UNP E1C9L1
L	201	PHE	TYR	conflict	UNP E1C9L1

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1	193	Total	C	N	O	S	0	0	0
			1508	982	252	269	5			

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	2	208	Total	C	N	O	S	0	0	0
			1620	1059	265	292	4			

- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	3	221	Total	C	N	O	S	0	0	0
			1706	1118	278	305	5			

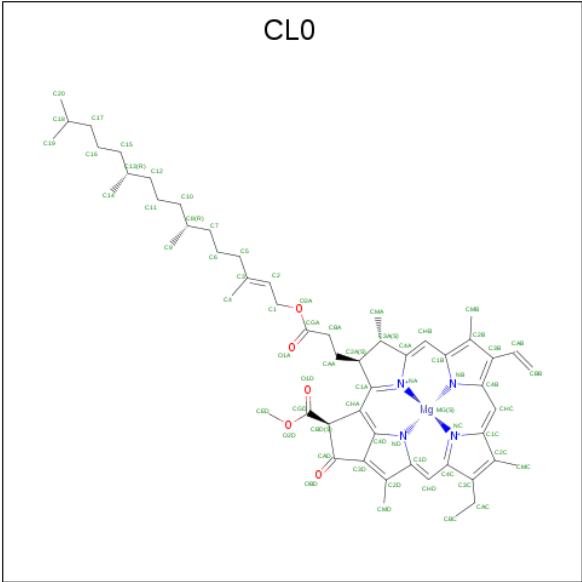
- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	4	198	Total	C	N	O	S	0	0	0
			1559	1022	253	281	3			

There are 3 discrepancies between the modelled and reference sequences:

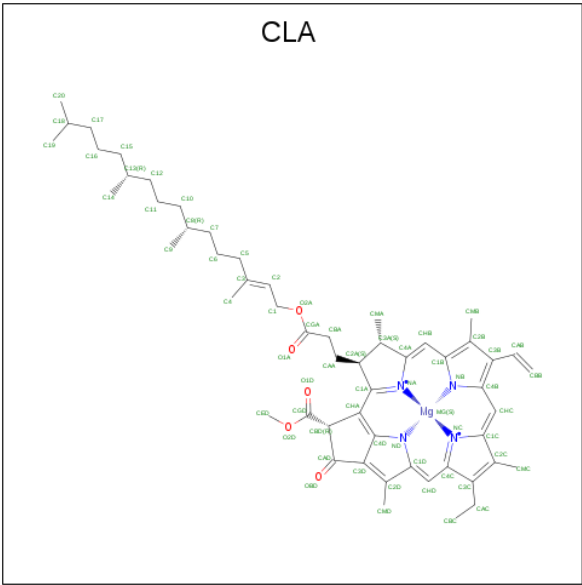
Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 17 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 18 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	A	1	Total 51	C 41	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 58	C 48	Mg 1	N 4	O 5	0	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	F	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
18	G	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
18	G	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
18	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	H	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

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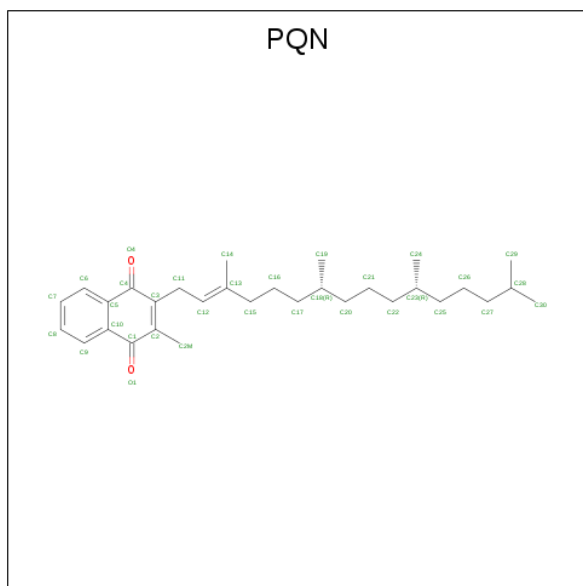
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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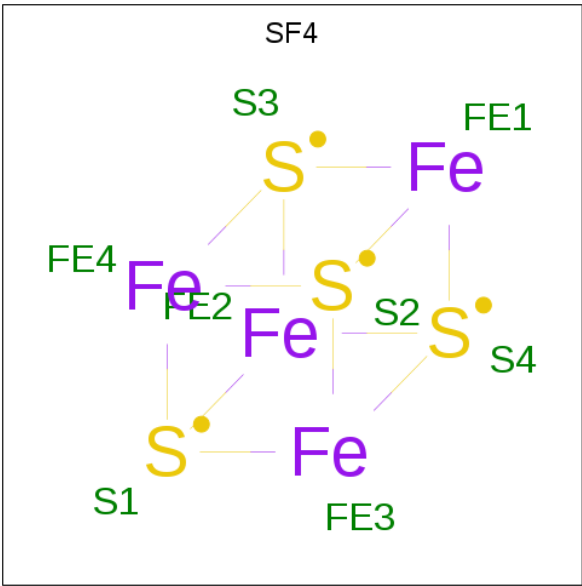
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 19 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



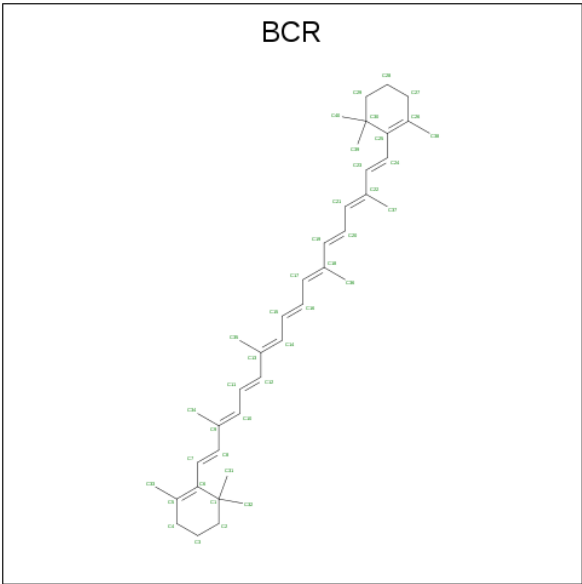
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			33	31	2		
19	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 20 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	Fe	S	0	0
			8	4	4		
20	C	1	Total	Fe	S	0	0
			8	4	4		
20	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



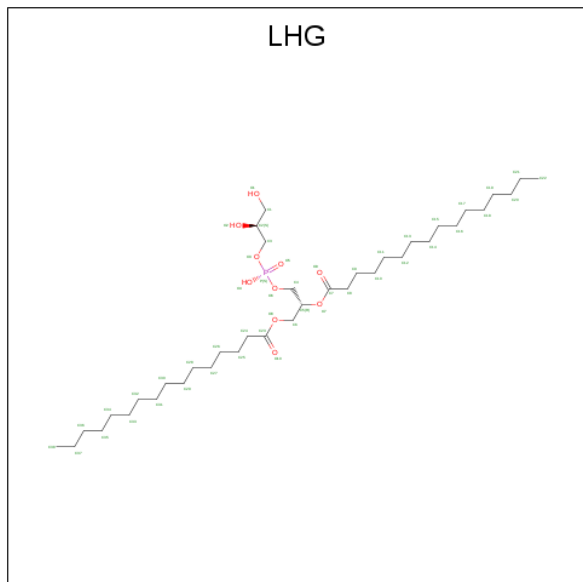
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	A	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	B	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	F	1	Total C 40 40	0	0
21	G	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	I	1	Total C 40 40	0	0
21	J	1	Total C 40 40	0	0
21	K	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0
21	L	1	Total C 40 40	0	0

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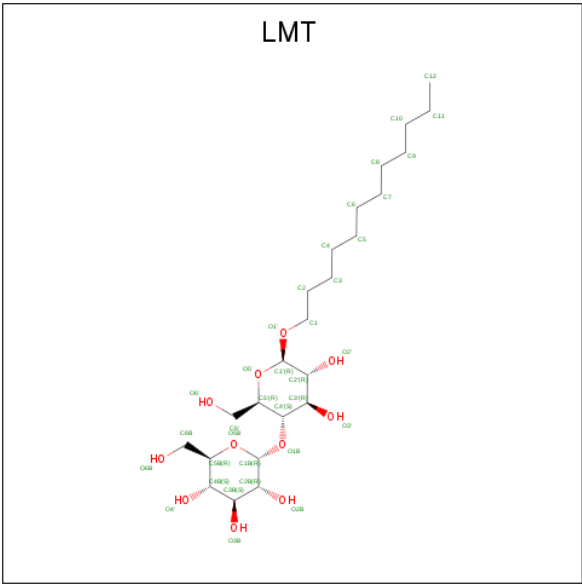
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	1	1	Total C 40 40	0	0
21	2	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	3	1	Total C 40 40	0	0
21	4	1	Total C 40 40	0	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



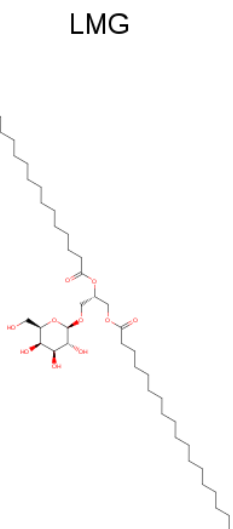
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C O P 49 38 10 1	0	0
22	A	1	Total C O P 40 29 10 1	0	0
22	B	1	Total C O P 21 10 10 1	0	0
22	B	1	Total C O P 49 38 10 1	0	0
22	1	1	Total C O P 49 38 10 1	0	0
22	2	1	Total C O P 35 24 10 1	0	0

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			35	24	11		
23	B	1	Total	C	O	0	0
			35	24	11		
23	B	1	Total	C	O	0	0
			32	21	11		
23	B	1	Total	C	O	0	0
			31	20	11		
23	G	1	Total	C	O	0	0
			35	24	11		
23	G	1	Total	C	O	0	0
			31	20	11		
23	J	1	Total	C	O	0	0
			25	14	11		
23	2	1	Total	C	O	0	0
			35	24	11		
23	4	1	Total	C	O	0	0
			35	24	11		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).

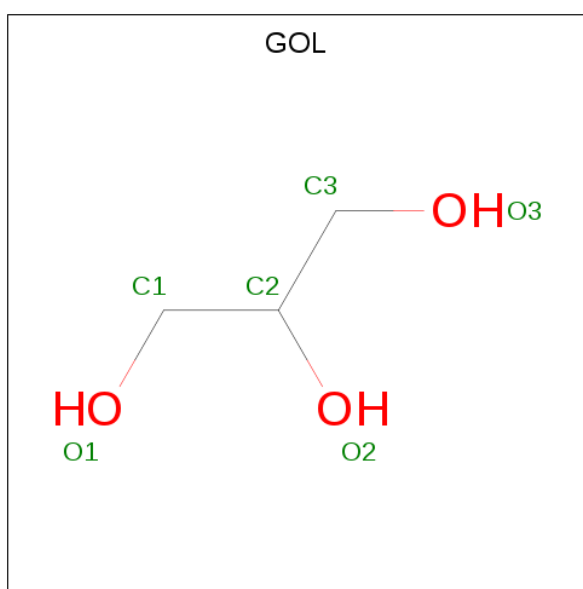


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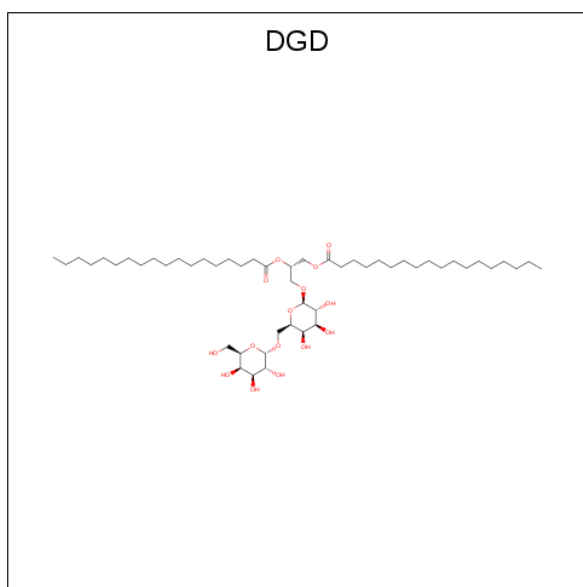
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	2	1	Total	C	O	0	0
			36	26	10		
24	2	1	Total	C	O	0	0
			13	7	6		
24	2	1	Total	C	O	0	0
			13	7	6		
24	4	1	Total	C	O	0	0
			13	7	6		

- Molecule 25 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			6	3	3		
25	4	1	Total	C	O	0	0
			6	3	3		

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

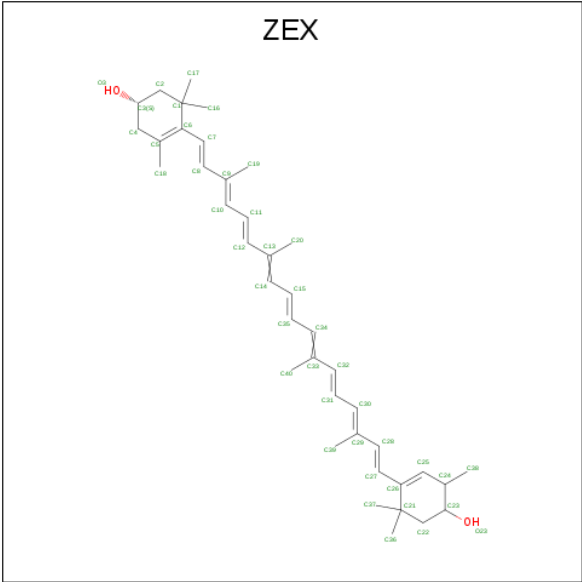


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total	C	O	0	0
			61	46	15		
26	F	1	Total	C	O	0	0
			57	42	15		
26	J	1	Total	C	O	0	0
			58	43	15		
26	1	1	Total	C	O	0	0
			35	26	9		
26	2	1	Total	C	O	0	0
			51	36	15		

- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca).

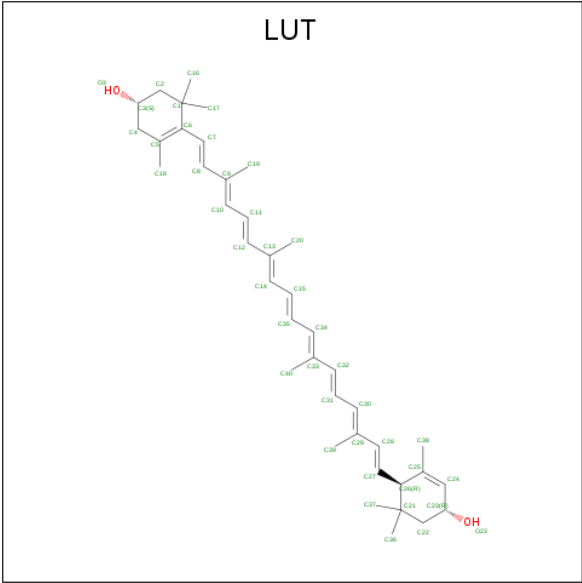
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	B	1	Total	Ca	0	0
			1	1		
27	3	1	Total	Ca	0	0
			1	1		

- Molecule 28 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	F	1	Total	C	O	0	0
			42	40	2		

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



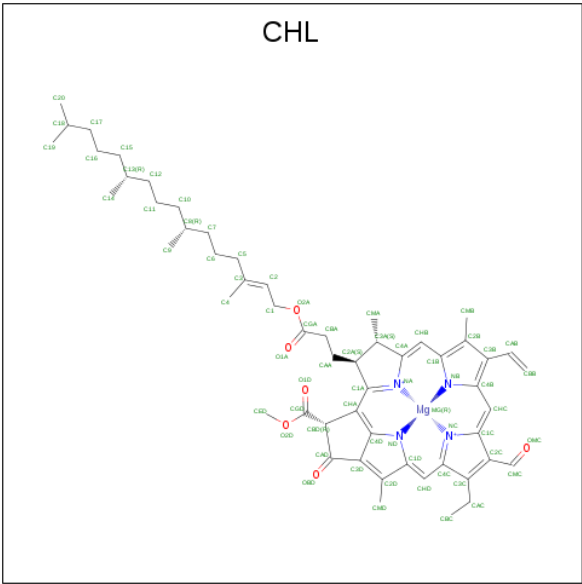
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	J	1	Total	C	O	0	0
			42	40	2		
29	1	1	Total	C	O	0	0
			42	40	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	1	1	Total	C	O	0	0
			42	40	2		
29	2	1	Total	C	O	0	0
			42	40	2		
29	3	1	Total	C	O	0	0
			42	40	2		
29	3	1	Total	C	O	0	0
			42	40	2		
29	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 30 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



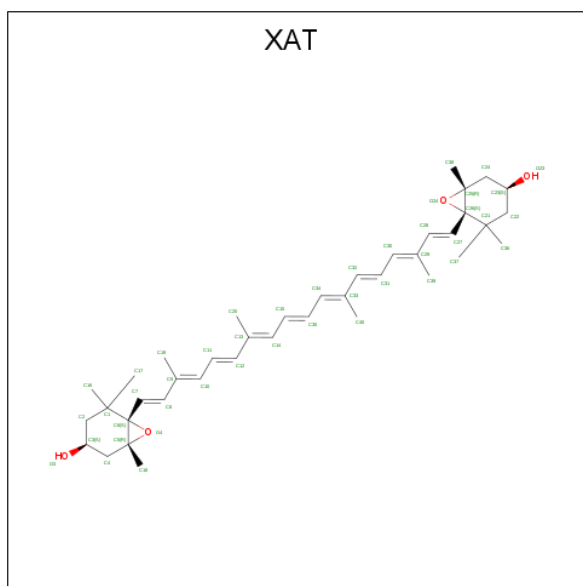
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	1	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
30	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	2	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			61	50	1	4	6		
30	4	1	Total	C	Mg	N	O	0	0
			43	34	1	4	4		
30	4	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).

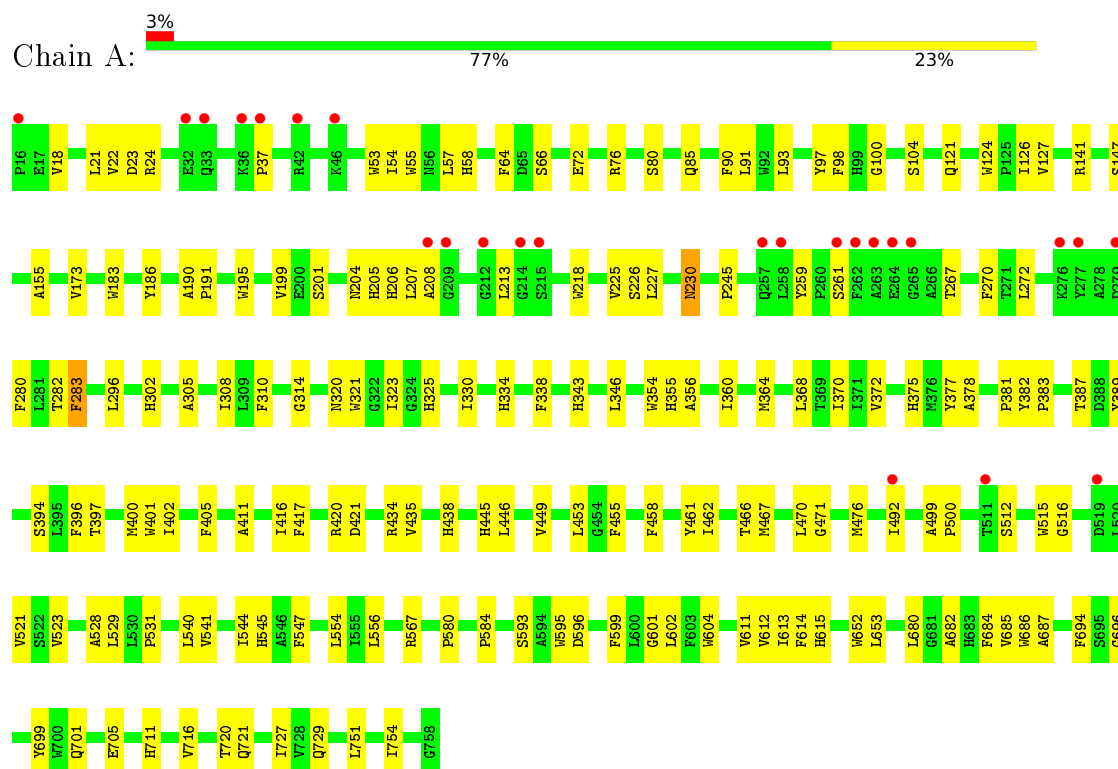


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	2	1	Total	C	O	0	0
			44	40	4		
31	4	1	Total	C	O	0	0
			44	40	4		

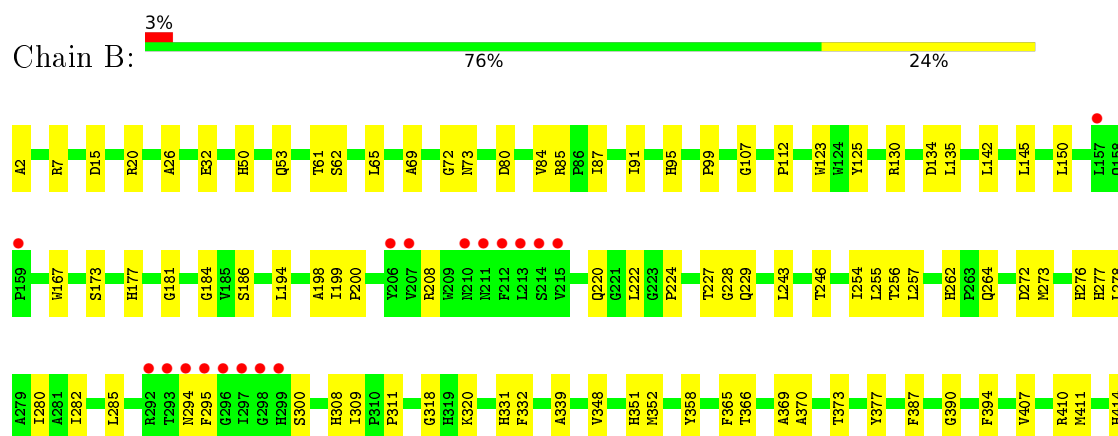
3 Residue-property plots

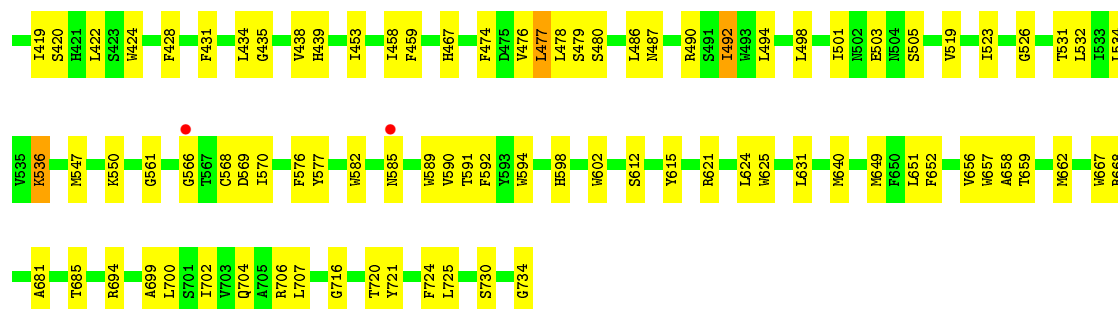
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 I P700 chlorophyll a apoprotein A1

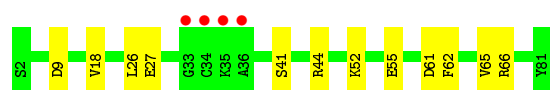
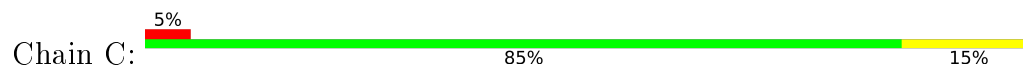


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

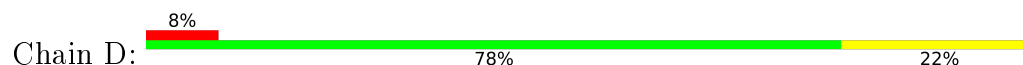




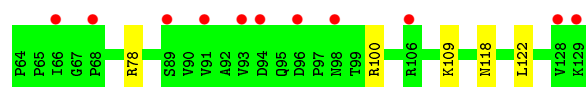
• Molecule 3: Photosystem I iron-sulfur center



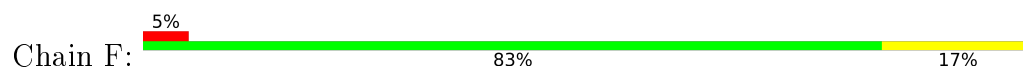
• Molecule 4: PsaD



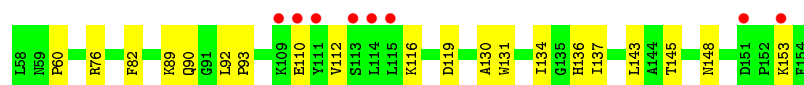
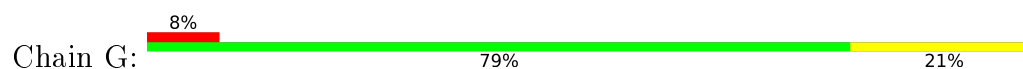
• Molecule 5: PsaE



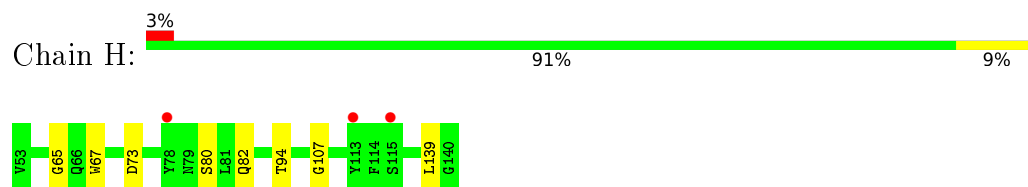
• Molecule 6: Photosystem I reaction center subunit III



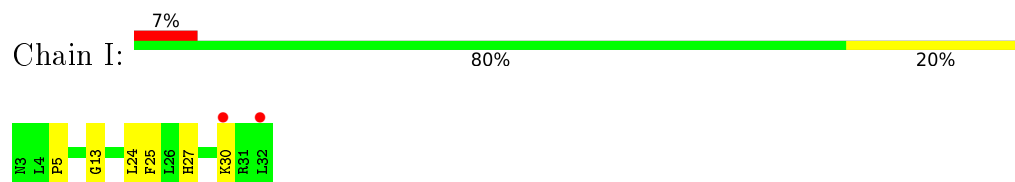
• Molecule 7: PsaG



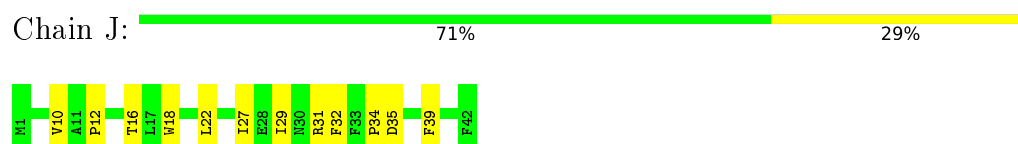
- Molecule 8: Photosystem I reaction center subunit VI



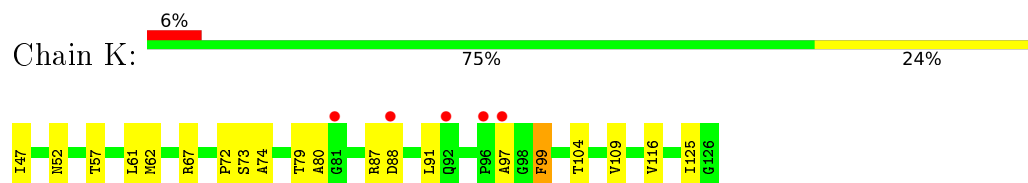
- Molecule 9: Photosystem I reaction center subunit VIII



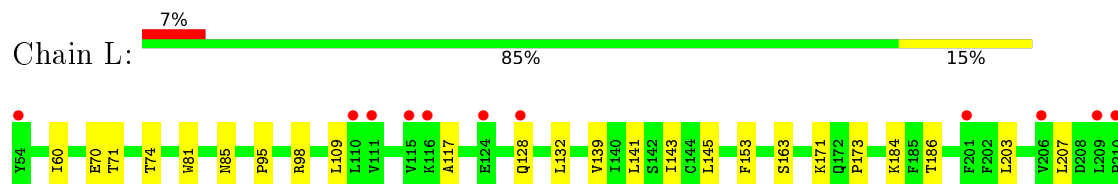
- Molecule 10: Photosystem I reaction center subunit IX



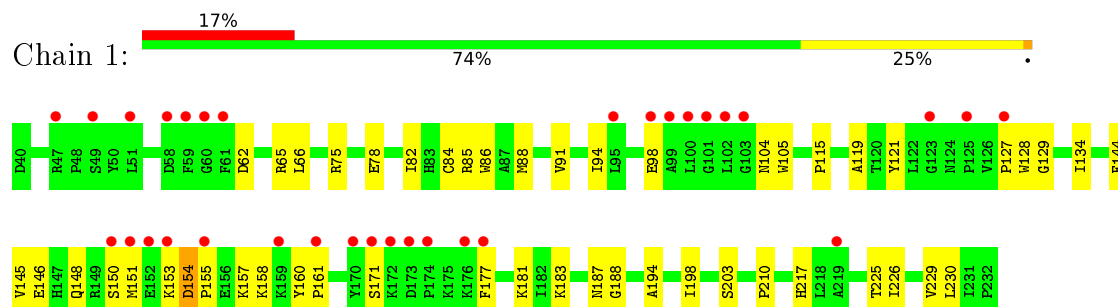
- Molecule 11: Photosystem I reaction center subunit X psaK



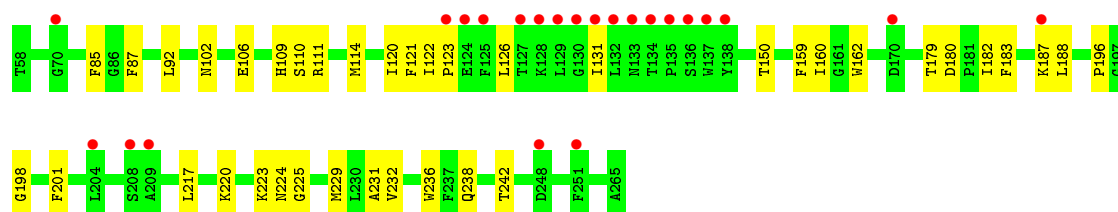
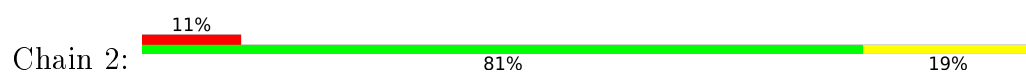
- Molecule 12: PsaL domain-containing protein



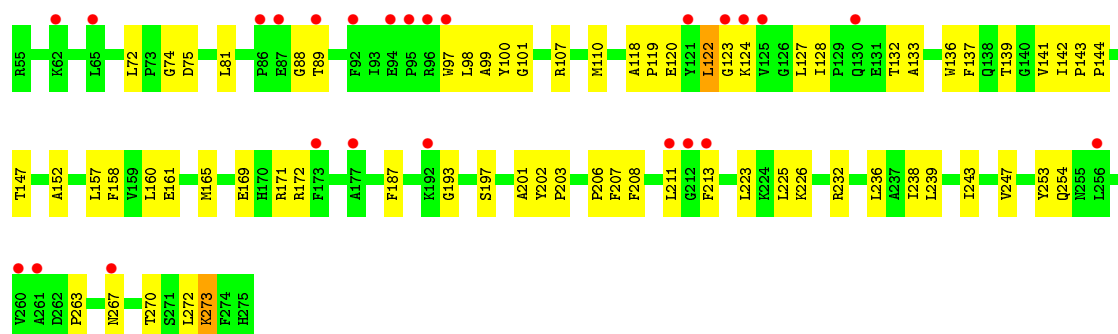
- Molecule 13: Lhca1



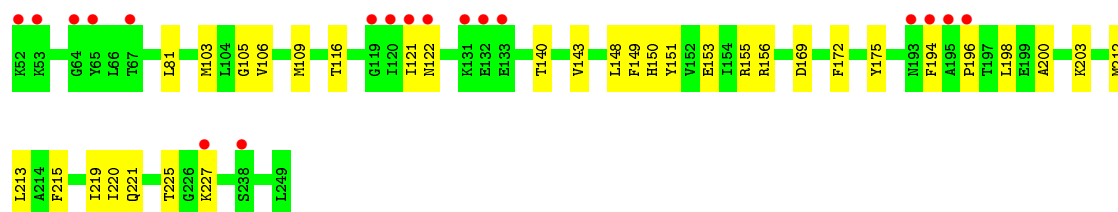
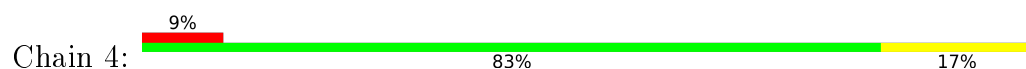
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	190.20Å 201.79Å 213.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.63 – 3.00 49.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.63-3.00) 91.7 (49.63-3.00)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.239 , 0.270 0.239 , 0.270	Depositor DCC
R_{free} test set	3139 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	37423	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: LHG, ZEX, LUT, BCR, CLA, CA, LMG, XAT, PQN, CL0, DGD, SF4, CHL, LMT, GOL

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	0.25	0/6057	0.40	0/8264
2	B	0.24	0/6069	0.39	0/8286
3	C	0.24	0/625	0.44	0/846
4	D	0.24	0/1163	0.43	0/1572
5	E	0.24	0/540	0.40	0/734
6	F	0.24	0/1234	0.38	0/1670
7	G	0.24	0/776	0.37	0/1054
8	H	0.25	0/693	0.40	0/942
9	I	0.25	0/238	0.38	0/324
10	J	0.26	0/349	0.39	0/476
11	K	0.24	0/564	0.47	0/763
12	L	0.25	0/1207	0.41	0/1651
13	1	0.24	0/1558	0.38	0/2125
14	2	0.24	0/1679	0.39	0/2302
15	3	0.25	0/1760	0.40	0/2390
16	4	0.24	0/1608	0.37	0/2191
All	All	0.25	0/26120	0.40	0/35590

There are no bond length outliers.

There are no bond angle outliers.

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	5858	0	5717	154	0
2	B	5857	0	5653	141	0
3	C	612	0	591	11	0
4	D	1132	0	1141	16	0
5	E	528	0	528	6	0
6	F	1206	0	1231	20	0
7	G	757	0	743	16	0
8	H	673	0	667	7	0
9	I	232	0	253	5	0
10	J	338	0	345	13	0
11	K	558	0	587	17	0
12	L	1174	0	1183	18	0
13	1	1508	0	1489	45	0
14	2	1620	0	1554	35	0
15	3	1706	0	1659	59	0
16	4	1559	0	1524	28	0
17	A	65	0	72	9	0
18	1	608	0	562	43	0
18	2	572	0	538	41	0
18	3	531	0	456	33	0
18	4	516	0	488	22	0
18	A	2543	0	2661	237	0
18	B	2480	0	2602	214	0
18	F	195	0	215	16	0
18	G	166	0	152	6	0
18	H	60	0	59	8	0
18	J	115	0	110	9	0
18	K	199	0	158	15	0
18	L	215	0	183	7	0
19	A	33	0	46	4	0
19	B	33	0	46	2	0
20	A	8	0	0	0	0
20	C	16	0	0	1	0
21	1	40	0	53	3	0
21	2	40	0	53	11	0
21	3	80	0	106	6	0
21	4	40	0	52	6	0
21	A	240	0	317	38	0
21	B	240	0	317	29	0
21	F	80	0	105	11	0
21	G	40	0	53	4	0
21	I	80	0	105	4	0
21	J	40	0	53	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	K	40	0	53	2	0
21	L	120	0	159	8	0
22	1	49	0	74	3	0
22	2	35	0	40	1	0
22	A	89	0	127	16	0
22	B	70	0	86	8	0
23	2	35	0	46	1	0
23	4	35	0	46	0	0
23	A	35	0	45	0	0
23	B	98	0	118	5	0
23	G	66	0	80	3	0
23	J	25	0	22	0	0
24	1	95	0	136	10	0
24	2	113	0	106	5	0
24	4	13	0	11	0	0
24	A	50	0	73	5	0
24	B	81	0	87	2	0
24	F	117	0	147	5	0
24	G	25	0	20	1	0
24	J	30	0	30	0	0
25	4	6	0	8	0	0
25	A	6	0	8	1	0
26	1	35	0	39	0	0
26	2	51	0	60	5	0
26	B	61	0	83	8	0
26	F	57	0	75	0	0
26	J	58	0	77	4	0
27	3	1	0	0	0	0
27	B	1	0	0	0	0
28	F	42	0	56	3	0
29	1	84	0	110	15	0
29	2	42	0	55	6	0
29	3	84	0	110	12	0
29	4	42	0	55	2	0
29	J	42	0	55	9	0
30	1	108	0	87	14	0
30	2	272	0	224	18	0
30	3	215	0	172	24	0
30	4	314	0	243	19	0
31	2	44	0	56	7	0
31	4	44	0	56	6	0
All	All	37423	0	37562	1094	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 15.

The worst 5 of 1094 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)
11:K:61:LEU:HB3	18:K:1403:CLA:HAB	1.45	0.97
31:2:304:XAT:H8	18:2:311:CLA:HBB1	1.50	0.94
1:A:401:TRP:CD1	18:A:826:CLA:HAB	2.10	0.87
18:B:807:CLA:H152	18:B:829:CLA:HBB2	1.58	0.85
21:2:305:BCR:H333	18:4:311:CLA:HMC3	1.58	0.84

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	741/743 (100%)	700 (94%)	40 (5%)	1 (0%)	51	85
2	B	731/733 (100%)	707 (97%)	23 (3%)	1 (0%)	51	85
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	22	60
5	E	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
6	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
9	I	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
10	J	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
11	K	78/80 (98%)	70 (90%)	8 (10%)	0	100	100
12	L	155/157 (99%)	147 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	1	191/193 (99%)	181 (95%)	7 (4%)	3 (2%)	9	40
14	2	206/208 (99%)	189 (92%)	17 (8%)	0	100	100
15	3	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
16	4	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
All	All	3201/3233 (99%)	3034 (95%)	161 (5%)	6 (0%)	47	82

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	161	PRO
1	A	720	THR
2	B	492	ILE
13	1	115	PRO
13	1	154	ASP

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	604/604 (100%)	599 (99%)	5 (1%)	81	93
2	B	598/598 (100%)	588 (98%)	10 (2%)	60	85
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	122/122 (100%)	120 (98%)	2 (2%)	62	86
5	E	58/58 (100%)	58 (100%)	0	100	100
6	F	125/126 (99%)	125 (100%)	0	100	100
7	G	82/82 (100%)	82 (100%)	0	100	100
8	H	71/71 (100%)	71 (100%)	0	100	100
9	I	26/26 (100%)	26 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	58/58 (100%)	56 (97%)	2 (3%)	37	72
12	L	124/124 (100%)	121 (98%)	3 (2%)	49	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1	158/158 (100%)	158 (100%)	0	100	100
14	2	167/167 (100%)	166 (99%)	1 (1%)	86	95
15	3	171/172 (99%)	166 (97%)	5 (3%)	42	76
16	4	164/164 (100%)	164 (100%)	0	100	100
All	All	2632/2634 (100%)	2604 (99%)	28 (1%)	73	90

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	702	ILE
15	3	273	LYS
11	K	52	ASN
15	3	122	LEU
4	D	190	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 240 ligands modelled in this entry, 2 are monoatomic - leaving 238 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$
21	BCR	L	303	-	41,41,41	1.86	4 (9%)	56,56,56	4.36	15 (26%)
26	DGD	F	309	-	58,58,67	1.04	4 (6%)	72,72,81	1.07	3 (4%)
18	CLA	J	1103	-	41,58,73	1.55	7 (17%)	37,95,113	2.31	10 (27%)
18	CLA	A	806	-	51,68,73	1.38	7 (13%)	49,107,113	1.99	8 (16%)
24	LMG	J	1102	-	30,30,55	0.54	0	38,38,63	1.13	3 (7%)
18	CLA	B	812	-	51,68,73	1.38	6 (11%)	49,107,113	1.91	8 (16%)
23	LMT	B	852	-	36,36,36	1.14	5 (13%)	47,47,47	1.07	2 (4%)
18	CLA	B	834	-	51,68,73	1.36	5 (9%)	49,107,113	1.97	9 (18%)
18	CLA	3	308	-	43,60,73	1.50	7 (16%)	39,97,113	2.23	9 (23%)
21	BCR	B	845	-	41,41,41	1.83	4 (9%)	56,56,56	4.09	20 (35%)
18	CLA	2	313	-	41,58,73	1.54	7 (17%)	37,95,113	2.35	10 (27%)
18	CLA	A	830	-	56,73,73	1.32	6 (10%)	55,113,113	1.85	7 (12%)
18	CLA	A	822	-	56,73,73	1.33	7 (12%)	55,113,113	1.84	8 (14%)
18	CLA	B	830	-	56,73,73	1.28	6 (10%)	55,113,113	2.03	12 (21%)
22	LHG	B	849	-	48,48,48	0.39	0	51,54,54	1.02	2 (3%)
21	BCR	L	307	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	15 (26%)
30	CHL	2	316	-	42,56,74	1.02	3 (7%)	42,92,114	1.38	11 (26%)
18	CLA	A	819	-	56,73,73	1.27	4 (7%)	55,113,113	1.78	9 (16%)
18	CLA	A	833	1	46,63,73	1.47	7 (15%)	43,101,113	2.10	9 (20%)
21	BCR	B	846	-	41,41,41	1.85	4 (9%)	56,56,56	4.23	15 (26%)
18	CLA	A	836	-	56,73,73	1.32	7 (12%)	55,113,113	1.88	8 (14%)
18	CLA	3	307	-	46,63,73	1.44	7 (15%)	43,101,113	2.11	11 (25%)
24	LMG	B	851	-	33,33,55	0.58	0	41,41,63	1.44	8 (19%)
18	CLA	3	319	-	51,68,73	1.39	7 (13%)	49,107,113	1.97	7 (14%)
30	CHL	4	317	-	37,51,74	1.03	3 (8%)	36,86,114	1.50	9 (25%)
18	CLA	3	315	15	56,73,73	1.30	6 (10%)	55,113,113	1.87	8 (14%)
30	CHL	2	314	14	60,74,74	0.83	3 (5%)	64,114,114	1.21	10 (15%)
18	CLA	L	304	12	41,58,73	1.51	6 (14%)	37,95,113	2.34	9 (24%)
21	BCR	4	301	-	41,41,41	1.85	4 (9%)	56,56,56	4.29	17 (30%)
29	LUT	1	5003	-	42,43,43	2.40	1 (2%)	51,60,60	1.95	14 (27%)
18	CLA	B	839	-	56,73,73	1.31	7 (12%)	55,113,113	1.93	9 (16%)
18	CLA	B	801	-	56,73,73	1.33	7 (12%)	55,113,113	2.08	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	821	-	37,54,73	1.59	7 (18%)	32,90,113	2.23	5 (15%)
18	CLA	B	813	-	37,54,73	1.58	5 (13%)	32,90,113	2.24	7 (21%)
24	LMG	F	307	-	36,36,55	0.73	1 (2%)	44,44,63	1.04	2 (4%)
18	CLA	B	833	-	49,66,73	1.39	7 (14%)	46,104,113	2.19	9 (19%)
18	CLA	B	814	-	56,73,73	1.30	6 (10%)	55,113,113	2.00	9 (16%)
29	LUT	J	1105	-	42,43,43	2.36	1 (2%)	51,60,60	2.17	12 (23%)
31	XAT	4	304	-	39,47,47	0.69	1 (2%)	54,74,74	1.92	12 (22%)
21	BCR	A	843	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	19 (33%)
18	CLA	A	807	1	56,73,73	1.29	6 (10%)	55,113,113	2.00	9 (16%)
18	CLA	B	837	-	56,73,73	1.29	7 (12%)	55,113,113	1.98	8 (14%)
30	CHL	2	319	-	50,64,74	0.89	2 (4%)	52,102,114	1.32	12 (23%)
18	CLA	B	840	-	56,73,73	1.30	7 (12%)	55,113,113	1.93	10 (18%)
18	CLA	2	307	14	43,60,73	1.51	7 (16%)	39,97,113	2.22	9 (23%)
18	CLA	2	311	-	41,58,73	1.50	7 (17%)	37,95,113	2.31	8 (21%)
17	CL0	A	801	-	59,73,73	2.33	15 (25%)	67,113,113	2.21	13 (19%)
30	CHL	4	314	16	45,59,74	1.00	3 (6%)	46,96,114	1.43	10 (21%)
26	DGD	2	327	-	52,52,67	0.92	3 (5%)	66,66,81	1.09	5 (7%)
18	CLA	B	804	-	56,73,73	1.29	6 (10%)	55,113,113	1.90	9 (16%)
18	CLA	A	820	-	51,68,73	1.37	7 (13%)	49,107,113	1.96	7 (14%)
23	LMT	G	1606	-	32,32,36	1.22	5 (15%)	43,43,47	1.00	1 (2%)
22	LHG	A	849	18	39,39,48	0.42	0	42,45,54	1.25	3 (7%)
30	CHL	3	316	15	41,55,74	1.03	3 (7%)	41,91,114	1.47	10 (24%)
24	LMG	B	854	-	13,13,55	0.55	0	18,18,63	0.73	0
30	CHL	4	313	-	41,55,74	0.99	3 (7%)	41,91,114	1.44	11 (26%)
18	CLA	B	824	-	46,63,73	1.45	7 (15%)	43,101,113	2.01	8 (18%)
18	CLA	F	301	-	56,73,73	1.30	5 (8%)	55,113,113	1.90	10 (18%)
18	CLA	A	826	-	56,73,73	1.32	6 (10%)	55,113,113	1.86	8 (14%)
24	LMG	A	851	-	50,50,55	1.05	5 (10%)	58,58,63	1.05	3 (5%)
24	LMG	F	306	-	47,47,55	0.97	3 (6%)	55,55,63	1.11	4 (7%)
30	CHL	3	312	-	45,59,74	0.89	2 (4%)	46,96,114	1.50	12 (26%)
18	CLA	B	828	-	56,73,73	1.31	6 (10%)	55,113,113	1.95	10 (18%)
18	CLA	A	835	-	56,73,73	1.31	7 (12%)	55,113,113	1.92	7 (12%)
18	CLA	K	1401	-	33,53,73	1.67	5 (15%)	27,89,113	2.36	8 (29%)
18	CLA	A	828	-	56,73,73	1.26	6 (10%)	55,113,113	2.10	11 (20%)
24	LMG	2	302	-	13,13,55	0.57	0	18,18,63	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	2	318	-	37,54,74	1.02	3 (8%)	36,90,114	1.45	9 (25%)
30	CHL	3	310	-	60,74,74	0.80	3 (5%)	64,114,114	1.32	10 (15%)
21	BCR	I	101	-	41,41,41	1.87	4 (9%)	56,56,56	4.29	19 (33%)
18	CLA	B	819	-	56,73,73	1.29	7 (12%)	55,113,113	2.02	9 (16%)
18	CLA	A	805	-	56,73,73	1.29	4 (7%)	55,113,113	1.89	11 (20%)
18	CLA	A	823	-	56,73,73	1.31	5 (8%)	55,113,113	2.03	10 (18%)
18	CLA	4	309	-	51,68,73	1.37	7 (13%)	49,107,113	2.01	8 (16%)
18	CLA	1	5010	-	56,73,73	1.28	5 (8%)	55,113,113	2.00	12 (21%)
18	CLA	1	5009	-	56,73,73	1.31	6 (10%)	55,113,113	1.94	9 (16%)
18	CLA	A	827	-	56,73,73	1.29	6 (10%)	55,113,113	1.95	8 (14%)
18	CLA	B	827	-	56,73,73	1.30	5 (8%)	55,113,113	2.07	12 (21%)
18	CLA	A	838	-	56,73,73	1.30	5 (8%)	55,113,113	1.90	10 (18%)
24	LMG	2	301	-	13,13,55	0.57	0	18,18,63	0.58	0
19	PQN	A	841	-	34,34,34	0.42	0	42,45,45	1.12	3 (7%)
24	LMG	4	320	-	13,13,55	0.55	0	18,18,63	0.67	0
18	CLA	3	311	-	46,63,73	1.43	5 (10%)	43,101,113	2.13	10 (23%)
30	CHL	1	5014	-	41,55,74	0.96	2 (4%)	41,91,114	1.41	11 (26%)
18	CLA	A	808	1	56,73,73	1.30	5 (8%)	55,113,113	1.95	11 (20%)
18	CLA	G	1601	-	46,63,73	1.42	5 (10%)	43,101,113	2.14	11 (25%)
18	CLA	2	326	14,16	41,58,73	1.55	6 (14%)	37,95,113	2.23	8 (21%)
18	CLA	L	301	-	46,63,73	1.42	5 (10%)	43,101,113	2.16	10 (23%)
26	DGD	J	1106	-	59,59,67	1.07	5 (8%)	73,73,81	1.20	5 (6%)
18	CLA	B	841	22	56,73,73	1.30	6 (10%)	55,113,113	1.90	9 (16%)
18	CLA	2	306	-	51,68,73	1.35	6 (11%)	49,107,113	2.04	9 (18%)
30	CHL	1	5016	-	55,69,74	0.85	2 (3%)	58,108,114	1.34	13 (22%)
21	BCR	J	1104	-	41,41,41	1.83	4 (9%)	56,56,56	4.28	15 (26%)
18	CLA	A	810	1	56,73,73	1.32	7 (12%)	55,113,113	1.86	6 (10%)
18	CLA	A	809	-	41,58,73	1.53	6 (14%)	37,95,113	2.20	7 (18%)
18	CLA	A	821	-	51,68,73	1.36	6 (11%)	49,107,113	2.06	9 (18%)
18	CLA	B	807	2	56,73,73	1.29	6 (10%)	55,113,113	1.90	6 (10%)
18	CLA	B	815	-	56,73,73	1.28	5 (8%)	55,113,113	2.05	11 (20%)
20	SF4	A	842	2,1	0,12,12	0.00	-	-	-	-
18	CLA	3	318	-	37,54,73	1.58	6 (16%)	32,90,113	2.18	8 (25%)
18	CLA	3	314	-	39,56,73	1.59	7 (17%)	34,92,113	2.24	6 (17%)
18	CLA	B	817	-	51,68,73	1.38	7 (13%)	49,107,113	2.00	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	1	5008	-	46,63,73	1.45	7 (15%)	43,101,113	2.17	7 (16%)
26	DGD	B	855	-	62,62,67	1.11	6 (9%)	76,76,81	0.98	3 (3%)
18	CLA	G	1603	-	56,73,73	1.31	7 (12%)	55,113,113	1.90	8 (14%)
18	CLA	2	312	22	51,68,73	1.36	5 (9%)	49,107,113	2.08	11 (22%)
18	CLA	A	831	-	56,73,73	1.32	7 (12%)	55,113,113	1.93	9 (16%)
29	LUT	2	303	-	42,43,43	2.33	1 (2%)	51,60,60	2.01	17 (33%)
24	LMG	2	324	-	13,13,55	0.57	0	18,18,63	0.67	0
23	LMT	G	1605	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	1 (2%)
18	CLA	4	312	-	37,54,73	1.61	7 (18%)	32,90,113	2.17	6 (18%)
21	BCR	1	5005	-	41,41,41	1.85	4 (9%)	56,56,56	4.35	16 (28%)
18	CLA	A	852	-	56,73,73	1.33	6 (10%)	55,113,113	1.94	10 (18%)
21	BCR	B	802	-	41,41,41	1.88	4 (9%)	56,56,56	4.72	18 (32%)
18	CLA	A	802	-	56,73,73	1.27	6 (10%)	55,113,113	1.85	9 (16%)
18	CLA	2	310	-	56,73,73	1.25	5 (8%)	55,113,113	2.20	12 (21%)
18	CLA	B	806	-	56,73,73	1.30	7 (12%)	55,113,113	1.98	8 (14%)
18	CLA	4	307	-	56,73,73	1.31	7 (12%)	55,113,113	1.92	7 (12%)
21	BCR	K	1405	-	41,41,41	1.86	4 (9%)	56,56,56	4.28	18 (32%)
18	CLA	1	5006	13	56,73,73	1.32	7 (12%)	55,113,113	1.88	10 (18%)
18	CLA	4	315	-	56,73,73	1.31	7 (12%)	55,113,113	1.96	10 (18%)
21	BCR	A	846	-	41,41,41	1.85	4 (9%)	56,56,56	4.25	15 (26%)
18	CLA	1	5013	-	37,54,73	1.61	7 (18%)	32,90,113	2.25	4 (12%)
18	CLA	A	832	-	56,73,73	1.32	6 (10%)	55,113,113	1.82	8 (14%)
18	CLA	L	306	-	41,58,73	1.53	7 (17%)	37,95,113	2.27	9 (24%)
30	CHL	3	313	-	45,59,74	0.93	2 (4%)	46,96,114	1.42	10 (21%)
18	CLA	B	822	-	56,73,73	1.32	7 (12%)	55,113,113	1.92	8 (14%)
18	CLA	3	317	-	41,58,73	1.50	6 (14%)	37,95,113	2.46	9 (24%)
23	LMT	B	853	-	33,33,36	1.22	6 (18%)	44,44,47	1.12	3 (6%)
18	CLA	B	829	-	56,73,73	1.29	5 (8%)	55,113,113	1.91	10 (18%)
22	LHG	1	5019	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
22	LHG	A	848	-	48,48,48	0.38	0	51,54,54	1.04	3 (5%)
26	DGD	1	5002	-	35,35,67	0.95	2 (5%)	43,43,81	1.10	3 (6%)
18	CLA	1	5012	-	37,54,73	1.62	7 (18%)	32,90,113	2.16	6 (18%)
31	XAT	2	304	-	39,47,47	0.68	1 (2%)	54,74,74	1.82	13 (24%)
28	ZEX	F	310	-	42,43,43	0.80	0	55,60,60	1.90	12 (21%)
18	CLA	B	809	-	56,73,73	1.31	7 (12%)	55,113,113	1.88	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMT	2	325	-	36,36,36	1.16	5 (13%)	47,47,47	1.09	3 (6%)
24	LMG	G	1607	-	25,25,55	0.68	1 (4%)	33,33,63	1.36	5 (15%)
24	LMG	2	323	-	13,13,55	0.62	0	18,18,63	0.93	1 (5%)
21	BCR	2	305	-	41,41,41	1.87	4 (9%)	56,56,56	4.93	27 (48%)
21	BCR	A	844	-	41,41,41	1.82	4 (9%)	56,56,56	4.29	16 (28%)
23	LMT	B	856	-	32,32,36	1.22	6 (18%)	43,43,47	1.03	3 (6%)
29	LUT	3	303	-	42,43,43	2.38	1 (2%)	51,60,60	1.96	16 (31%)
22	LHG	2	320	18	34,34,48	0.45	0	37,40,54	1.14	3 (8%)
18	CLA	A	840	22	51,68,73	1.36	5 (9%)	49,107,113	2.06	10 (20%)
21	BCR	3	305	-	41,41,41	1.84	4 (9%)	56,56,56	4.34	15 (26%)
18	CLA	B	836	-	46,63,73	1.45	6 (13%)	43,101,113	2.15	11 (25%)
23	LMT	J	1107	-	26,26,36	1.33	5 (19%)	37,37,47	1.06	2 (5%)
18	CLA	A	825	-	56,73,73	1.29	5 (8%)	55,113,113	2.04	11 (20%)
18	CLA	1	5017	-	33,53,73	1.69	7 (21%)	27,89,113	2.34	5 (18%)
30	CHL	4	316	-	55,69,74	0.91	3 (5%)	58,108,114	1.26	12 (20%)
18	CLA	B	826	-	56,73,73	1.28	5 (8%)	55,113,113	2.05	9 (16%)
21	BCR	A	855	-	41,41,41	1.85	4 (9%)	56,56,56	4.39	17 (30%)
21	BCR	A	847	-	41,41,41	1.83	4 (9%)	56,56,56	4.32	20 (35%)
18	CLA	A	818	-	41,58,73	1.52	7 (17%)	37,95,113	2.31	8 (21%)
18	CLA	B	818	-	56,73,73	1.31	7 (12%)	55,113,113	1.83	9 (16%)
18	CLA	B	811	-	56,73,73	1.31	6 (10%)	55,113,113	1.88	9 (16%)
18	CLA	1	5007	13	37,54,73	1.59	6 (16%)	32,90,113	2.16	5 (15%)
18	CLA	A	837	-	56,73,73	1.30	6 (10%)	55,113,113	1.93	9 (16%)
18	CLA	B	825	-	56,73,73	1.29	5 (8%)	55,113,113	2.07	10 (18%)
21	BCR	F	304	-	41,41,41	1.84	4 (9%)	56,56,56	4.33	17 (30%)
19	PQN	B	842	-	34,34,34	0.40	0	42,45,45	1.08	3 (7%)
18	CLA	4	306	16	41,58,73	1.55	7 (17%)	37,95,113	2.37	9 (24%)
23	LMT	4	319	-	36,36,36	1.14	5 (13%)	47,47,47	0.97	2 (4%)
18	CLA	F	303	6	56,73,73	1.32	7 (12%)	55,113,113	1.84	9 (16%)
18	CLA	1	5011	-	41,58,73	1.52	7 (17%)	37,95,113	2.29	9 (24%)
18	CLA	1	5015	-	56,73,73	1.31	7 (12%)	55,113,113	1.90	7 (12%)
18	CLA	2	317	-	46,63,73	1.43	6 (13%)	43,101,113	2.11	9 (20%)
21	BCR	A	845	-	41,41,41	1.84	4 (9%)	56,56,56	4.31	19 (33%)
24	LMG	B	850	-	35,35,55	0.72	1 (2%)	43,43,63	1.14	3 (6%)
18	CLA	K	1403	-	39,56,73	1.58	7 (17%)	34,92,113	2.33	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	838	-	41,58,73	1.52	7 (17%)	37,95,113	2.30	9 (24%)
18	CLA	B	820	-	56,73,73	1.31	6 (10%)	55,113,113	1.83	8 (14%)
20	SF4	C	102	3	0,12,12	0.00	-	-		
24	LMG	1	5001	-	49,49,55	1.02	5 (10%)	57,57,63	1.12	4 (7%)
30	CHL	4	318	-	50,64,74	0.89	2 (4%)	52,102,114	1.32	12 (23%)
18	CLA	A	853	-	56,73,73	1.30	6 (10%)	55,113,113	1.98	7 (12%)
18	CLA	B	808	-	56,73,73	1.31	7 (12%)	55,113,113	1.87	7 (12%)
25	GOL	4	321	-	5,5,5	0.55	0	5,5,5	0.26	0
18	CLA	F	302	-	56,73,73	1.31	6 (10%)	55,113,113	1.91	11 (20%)
30	CHL	2	315	-	50,64,74	0.82	2 (4%)	52,102,114	1.34	11 (21%)
29	LUT	4	303	-	42,43,43	2.38	1 (2%)	51,60,60	1.90	13 (25%)
21	BCR	F	305	-	41,41,41	1.84	4 (9%)	56,56,56	4.44	20 (35%)
18	CLA	4	308	-	51,68,73	1.36	6 (11%)	49,107,113	2.09	10 (20%)
18	CLA	A	839	-	56,73,73	1.32	7 (12%)	55,113,113	1.84	8 (14%)
24	LMG	1	5020	-	46,46,55	0.93	3 (6%)	54,54,63	1.07	3 (5%)
18	CLA	3	309	-	46,63,73	1.46	7 (15%)	43,101,113	2.26	10 (23%)
18	CLA	B	816	-	46,63,73	1.42	5 (10%)	43,101,113	2.30	12 (27%)
18	CLA	K	1402	-	51,68,73	1.40	7 (13%)	49,107,113	1.95	8 (16%)
18	CLA	B	831	-	56,73,73	1.30	6 (10%)	55,113,113	1.97	9 (16%)
18	CLA	4	305	-	51,68,73	1.36	6 (11%)	49,107,113	2.00	11 (22%)
18	CLA	A	834	-	42,59,73	1.49	5 (11%)	38,96,113	2.30	10 (26%)
18	CLA	A	811	-	46,63,73	1.44	7 (15%)	43,101,113	2.14	10 (23%)
18	CLA	H	1701	-	51,68,73	1.38	7 (13%)	49,107,113	2.01	8 (16%)
18	CLA	A	814	-	37,54,73	1.62	6 (16%)	32,90,113	2.13	5 (15%)
18	CLA	A	813	-	56,73,73	1.30	6 (10%)	55,113,113	2.03	12 (21%)
18	CLA	A	817	-	56,73,73	1.30	6 (10%)	55,113,113	1.89	9 (16%)
29	LUT	1	5004	-	42,43,43	2.38	1 (2%)	51,60,60	2.05	15 (29%)
24	LMG	2	321	-	25,25,55	0.56	0	33,33,63	1.19	3 (9%)
18	CLA	J	1101	-	56,73,73	1.29	6 (10%)	55,113,113	2.00	12 (21%)
25	GOL	A	854	-	5,5,5	0.55	0	5,5,5	0.27	0
21	BCR	I	102	-	41,41,41	1.85	4 (9%)	56,56,56	4.26	15 (26%)
18	CLA	G	1602	7	37,54,73	1.58	5 (13%)	32,90,113	2.25	8 (25%)
18	CLA	4	311	-	51,68,73	1.38	7 (13%)	49,107,113	2.00	7 (14%)
18	CLA	B	805	-	56,73,73	1.29	5 (8%)	55,113,113	1.92	10 (18%)
18	CLA	B	803	-	56,73,73	1.27	4 (7%)	55,113,113	1.91	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	4	302	13	50,64,74	0.89	3 (6%)	52,102,114	1.34	11 (21%)
18	CLA	A	804	-	56,73,73	1.29	7 (12%)	55,113,113	2.00	9 (16%)
18	CLA	B	832	-	51,68,73	1.36	5 (9%)	49,107,113	2.06	12 (24%)
18	CLA	1	5018	13	51,68,73	1.38	7 (13%)	49,107,113	1.98	9 (18%)
18	CLA	B	810	2	56,73,73	1.30	6 (10%)	55,113,113	1.88	8 (14%)
18	CLA	A	812	-	56,73,73	1.26	5 (8%)	55,113,113	1.98	11 (20%)
18	CLA	A	815	-	56,73,73	1.29	7 (12%)	55,113,113	1.90	7 (12%)
18	CLA	K	1404	-	37,54,73	1.62	7 (18%)	32,90,113	2.15	6 (18%)
18	CLA	A	803	-	56,73,73	1.31	7 (12%)	55,113,113	1.94	9 (16%)
18	CLA	4	310	-	41,58,73	1.51	6 (14%)	37,95,113	2.27	9 (24%)
18	CLA	A	829	-	56,73,73	1.31	6 (10%)	55,113,113	1.98	11 (20%)
24	LMG	F	308	-	34,34,55	0.50	0	42,42,63	1.09	2 (4%)
21	BCR	3	306	-	41,41,41	1.89	4 (9%)	56,56,56	4.07	18 (32%)
18	CLA	A	824	-	46,63,73	1.45	7 (15%)	43,101,113	2.08	8 (18%)
22	LHG	B	848	18	20,20,48	0.58	0	23,26,54	1.51	2 (8%)
18	CLA	B	835	-	46,63,73	1.45	7 (15%)	43,101,113	2.14	10 (23%)
21	BCR	B	843	-	41,41,41	1.90	4 (9%)	56,56,56	4.66	21 (37%)
20	SF4	C	101	3	0,12,12	0.00	-	-	-	-
18	CLA	2	308	-	56,73,73	1.32	7 (12%)	55,113,113	2.01	7 (12%)
18	CLA	2	309	14	56,73,73	1.31	6 (10%)	55,113,113	1.95	8 (14%)
21	BCR	L	302	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	21 (37%)
18	CLA	B	823	-	56,73,73	1.32	7 (12%)	55,113,113	1.90	9 (16%)
18	CLA	L	305	-	51,68,73	1.37	6 (11%)	49,107,113	2.04	7 (14%)
21	BCR	G	1604	-	41,41,41	1.85	4 (9%)	56,56,56	4.35	15 (26%)
21	BCR	B	844	-	41,41,41	1.85	4 (9%)	56,56,56	4.35	17 (30%)
18	CLA	A	816	-	47,64,73	1.43	7 (14%)	44,102,113	2.11	9 (20%)
21	BCR	B	847	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	14 (25%)
23	LMT	A	850	-	36,36,36	1.12	5 (13%)	47,47,47	1.15	1 (2%)
29	LUT	3	304	-	42,43,43	2.35	1 (2%)	51,60,60	1.99	13 (25%)
18	CLA	3	301	-	33,53,73	1.69	6 (18%)	27,89,113	2.26	5 (18%)
24	LMG	2	322	-	36,36,55	0.64	1 (2%)	44,44,63	1.06	2 (4%)

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
21	BCR	L	303	-	-	12/29/63/63	0/2/2/2
26	DGD	F	309	-	-	18/46/86/95	0/2/2/2
18	CLA	J	1103	-	1/1/12/20	7/19/97/115	-
18	CLA	A	806	-	1/1/14/20	16/31/109/115	-
24	LMG	J	1102	-	-	5/25/45/70	0/1/1/1
18	CLA	B	812	-	1/1/14/20	10/31/109/115	-
23	LMT	B	852	-	-	13/21/61/61	0/2/2/2
18	CLA	B	834	-	1/1/14/20	12/31/109/115	-
18	CLA	3	308	-	1/1/12/20	8/22/100/115	-
21	BCR	B	845	-	-	14/29/63/63	0/2/2/2
18	CLA	2	313	-	1/1/12/20	10/19/97/115	-
18	CLA	A	830	-	1/1/15/20	11/37/115/115	-
18	CLA	A	822	-	1/1/15/20	16/37/115/115	-
18	CLA	B	830	-	1/1/15/20	16/37/115/115	-
30	CHL	2	316	-	3/3/16/26	0/18/116/137	-
21	BCR	L	307	-	-	14/29/63/63	0/2/2/2
22	LHG	B	849	-	-	36/53/53/53	-
18	CLA	A	819	-	1/1/15/20	20/37/115/115	-
18	CLA	A	833	1	1/1/13/20	9/25/103/115	-
21	BCR	B	846	-	-	8/29/63/63	0/2/2/2
18	CLA	A	836	-	1/1/15/20	17/37/115/115	-
18	CLA	3	307	-	1/1/13/20	11/25/103/115	-
24	LMG	B	851	-	-	10/28/48/70	0/1/1/1
18	CLA	3	319	-	1/1/14/20	18/31/109/115	-
30	CHL	4	317	-	3/3/15/26	2/12/110/137	-
18	CLA	3	315	15	1/1/15/20	23/37/115/115	-
30	CHL	2	314	14	4/4/20/26	10/39/137/137	-
18	CLA	L	304	12	1/1/12/20	7/19/97/115	-
21	BCR	4	301	-	-	13/29/63/63	0/2/2/2
29	LUT	1	5003	-	-	6/29/67/67	0/2/2/2
18	CLA	B	839	-	1/1/15/20	17/37/115/115	-
18	CLA	B	801	-	1/1/15/20	17/37/115/115	-
18	CLA	B	821	-	1/1/11/20	7/15/93/115	-
18	CLA	B	813	-	1/1/11/20	3/15/93/115	-
24	LMG	F	307	-	-	10/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	833	-	1/1/13/20	14/29/107/115	-
18	CLA	B	814	-	1/1/15/20	15/37/115/115	-
29	LUT	J	1105	-	1/1/12/27	4/29/67/67	0/2/2/2
31	XAT	4	304	-	1/1/12/26	0/31/93/93	0/4/4/4
21	BCR	A	843	-	-	15/29/63/63	0/2/2/2
18	CLA	A	807	1	1/1/15/20	17/37/115/115	-
18	CLA	B	837	-	1/1/15/20	21/37/115/115	-
30	CHL	2	319	-	4/4/18/26	8/27/125/137	-
18	CLA	B	840	-	1/1/15/20	20/37/115/115	-
18	CLA	2	307	14	1/1/12/20	8/22/100/115	-
18	CLA	2	311	-	1/1/12/20	9/19/97/115	-
17	CL0	A	801	-	3/3/20/25	7/37/135/135	-
30	CHL	4	314	16	3/3/17/26	0/21/119/137	-
26	DGD	2	327	-	-	14/40/80/95	0/2/2/2
18	CLA	B	804	-	1/1/15/20	16/37/115/115	-
18	CLA	A	820	-	1/1/14/20	15/31/109/115	-
23	LMT	G	1606	-	-	13/17/57/61	0/2/2/2
22	LHG	A	849	18	-	23/44/44/53	-
30	CHL	3	316	15	3/3/16/26	5/17/115/137	-
30	CHL	4	313	-	3/3/16/26	3/17/115/137	-
24	LMG	B	854	-	-	1/4/24/70	0/1/1/1
18	CLA	B	824	-	1/1/13/20	13/25/103/115	-
18	CLA	F	301	-	1/1/15/20	18/37/115/115	-
18	CLA	A	826	-	1/1/15/20	22/37/115/115	-
24	LMG	A	851	-	-	19/45/65/70	0/1/1/1
24	LMG	F	306	-	-	6/42/62/70	0/1/1/1
30	CHL	3	312	-	3/3/17/26	2/21/119/137	-
18	CLA	B	828	-	1/1/15/20	22/37/115/115	-
18	CLA	A	835	-	1/1/15/20	12/37/115/115	-
18	CLA	K	1401	-	1/1/11/20	2/11/91/115	-
18	CLA	A	828	-	1/1/15/20	15/37/115/115	-
30	CHL	2	318	-	3/3/16/26	2/13/113/137	-
30	CHL	3	310	-	4/4/20/26	10/39/137/137	-
24	LMG	2	302	-	-	0/4/24/70	0/1/1/1
21	BCR	I	101	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	819	-	1/1/15/20	18/37/115/115	-
18	CLA	A	805	-	1/1/15/20	20/37/115/115	-
18	CLA	A	823	-	1/1/15/20	18/37/115/115	-
18	CLA	4	309	-	1/1/14/20	12/31/109/115	-
18	CLA	1	5010	-	1/1/15/20	13/37/115/115	-
18	CLA	1	5009	-	1/1/15/20	15/37/115/115	-
18	CLA	A	827	-	1/1/15/20	17/37/115/115	-
18	CLA	B	827	-	1/1/15/20	12/37/115/115	-
18	CLA	A	838	-	1/1/15/20	16/37/115/115	-
30	CHL	1	5014	-	3/3/16/26	1/17/115/137	-
19	PQN	A	841	-	-	6/23/43/43	0/2/2/2
24	LMG	2	301	-	-	3/4/24/70	0/1/1/1
18	CLA	3	311	-	1/1/13/20	7/25/103/115	-
24	LMG	4	320	-	-	0/4/24/70	0/1/1/1
18	CLA	A	808	1	1/1/15/20	19/37/115/115	-
18	CLA	G	1601	-	1/1/13/20	8/25/103/115	-
18	CLA	2	326	14,16	1/1/12/20	11/19/97/115	-
18	CLA	L	301	-	1/1/13/20	12/25/103/115	-
26	DGD	J	1106	-	-	14/47/87/95	0/2/2/2
18	CLA	B	841	22	1/1/15/20	17/37/115/115	-
18	CLA	2	306	-	1/1/14/20	9/31/109/115	-
30	CHL	1	5016	-	4/4/19/26	7/33/131/137	-
21	BCR	J	1104	-	-	15/29/63/63	0/2/2/2
18	CLA	A	810	1	1/1/15/20	19/37/115/115	-
18	CLA	A	809	-	1/1/12/20	8/19/97/115	-
18	CLA	A	821	-	1/1/14/20	10/31/109/115	-
18	CLA	B	807	2	1/1/15/20	15/37/115/115	-
18	CLA	B	815	-	1/1/15/20	16/37/115/115	-
20	SF4	A	842	2,1	-	-	0/6/5/5
18	CLA	3	318	-	1/1/11/20	8/15/93/115	-
18	CLA	3	314	-	1/1/11/20	5/17/95/115	-
18	CLA	B	817	-	1/1/14/20	11/31/109/115	-
18	CLA	1	5008	-	1/1/13/20	9/25/103/115	-
26	DGD	B	855	-	-	19/50/90/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	G	1603	-	1/1/15/20	17/37/115/115	-
18	CLA	2	312	22	1/1/14/20	20/31/109/115	-
18	CLA	A	831	-	1/1/15/20	21/37/115/115	-
29	LUT	2	303	-	1/1/12/27	3/29/67/67	0/2/2/2
24	LMG	2	324	-	-	4/4/24/70	0/1/1/1
23	LMT	G	1605	-	-	10/21/61/61	0/2/2/2
18	CLA	4	312	-	1/1/11/20	7/15/93/115	-
21	BCR	1	5005	-	-	10/29/63/63	0/2/2/2
18	CLA	A	852	-	1/1/15/20	13/37/115/115	-
21	BCR	B	802	-	-	7/29/63/63	0/2/2/2
18	CLA	A	802	-	1/1/15/20	22/37/115/115	-
18	CLA	2	310	-	1/1/15/20	15/37/115/115	-
18	CLA	B	806	-	1/1/15/20	17/37/115/115	-
18	CLA	4	307	-	1/1/15/20	13/37/115/115	-
21	BCR	K	1405	-	-	13/29/63/63	0/2/2/2
18	CLA	1	5006	13	1/1/15/20	16/37/115/115	-
18	CLA	4	315	-	1/1/15/20	21/37/115/115	-
21	BCR	A	846	-	-	14/29/63/63	0/2/2/2
18	CLA	1	5013	-	1/1/11/20	6/15/93/115	-
18	CLA	A	832	-	1/1/15/20	18/37/115/115	-
18	CLA	L	306	-	1/1/12/20	8/19/97/115	-
30	CHL	3	313	-	3/3/17/26	4/21/119/137	-
18	CLA	B	822	-	1/1/15/20	18/37/115/115	-
18	CLA	3	317	-	1/1/12/20	10/19/97/115	-
23	LMT	B	853	-	-	9/18/58/61	0/2/2/2
18	CLA	B	829	-	1/1/15/20	20/37/115/115	-
22	LHG	1	5019	-	-	23/53/53/53	-
22	LHG	A	848	-	-	31/53/53/53	-
26	DGD	1	5002	-	-	11/29/49/95	0/1/1/2
18	CLA	1	5012	-	1/1/11/20	7/15/93/115	-
31	XAT	2	304	-	1/1/12/26	4/31/93/93	0/4/4/4
28	ZEX	F	310	-	-	3/29/67/67	0/2/2/2
18	CLA	B	809	-	1/1/15/20	9/37/115/115	-
23	LMT	2	325	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	G	1607	-	-	9/20/40/70	0/1/1/1
24	LMG	2	323	-	-	0/4/24/70	0/1/1/1
21	BCR	2	305	-	-	10/29/63/63	0/2/2/2
21	BCR	A	844	-	-	10/29/63/63	0/2/2/2
23	LMT	B	856	-	-	3/17/57/61	0/2/2/2
29	LUT	3	303	-	-	3/29/67/67	0/2/2/2
22	LHG	2	320	18	-	18/39/39/53	-
18	CLA	A	840	22	1/1/14/20	14/31/109/115	-
21	BCR	3	305	-	-	12/29/63/63	0/2/2/2
18	CLA	B	836	-	1/1/13/20	9/25/103/115	-
23	LMT	J	1107	-	-	5/11/51/61	0/2/2/2
18	CLA	A	825	-	1/1/15/20	16/37/115/115	-
18	CLA	1	5017	-	1/1/11/20	5/11/91/115	-
30	CHL	4	316	-	4/4/19/26	8/33/131/137	-
18	CLA	B	826	-	1/1/15/20	19/37/115/115	-
21	BCR	A	855	-	-	9/29/63/63	0/2/2/2
21	BCR	A	847	-	-	14/29/63/63	0/2/2/2
18	CLA	A	818	-	1/1/12/20	8/19/97/115	-
18	CLA	B	818	-	1/1/15/20	14/37/115/115	-
18	CLA	B	811	-	1/1/15/20	16/37/115/115	-
18	CLA	1	5007	13	1/1/11/20	7/15/93/115	-
18	CLA	A	837	-	1/1/15/20	9/37/115/115	-
18	CLA	B	825	-	1/1/15/20	13/37/115/115	-
21	BCR	F	304	-	-	10/29/63/63	0/2/2/2
19	PQN	B	842	-	-	9/23/43/43	0/2/2/2
18	CLA	4	306	16	1/1/12/20	7/19/97/115	-
23	LMT	4	319	-	-	4/21/61/61	0/2/2/2
18	CLA	F	303	6	1/1/15/20	21/37/115/115	-
18	CLA	1	5011	-	1/1/12/20	7/19/97/115	-
18	CLA	1	5015	-	1/1/15/20	16/37/115/115	-
18	CLA	2	317	-	1/1/13/20	10/25/103/115	-
21	BCR	A	845	-	-	12/29/63/63	0/2/2/2
24	LMG	B	850	-	-	9/30/50/70	0/1/1/1
18	CLA	K	1403	-	1/1/11/20	9/17/95/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	838	-	1/1/12/20	5/19/97/115	-
18	CLA	B	820	-	1/1/15/20	13/37/115/115	-
30	CHL	4	318	-	4/4/18/26	4/27/125/137	-
24	LMG	1	5001	-	-	15/44/64/70	0/1/1/1
20	SF4	C	102	3	-	-	0/6/5/5
18	CLA	A	853	-	1/1/15/20	17/37/115/115	-
18	CLA	B	808	-	1/1/15/20	15/37/115/115	-
25	GOL	4	321	-	-	0/4/4/4	-
18	CLA	F	302	-	1/1/15/20	19/37/115/115	-
30	CHL	2	315	-	4/4/18/26	8/27/125/137	-
29	LUT	4	303	-	-	4/29/67/67	0/2/2/2
21	BCR	F	305	-	-	14/29/63/63	0/2/2/2
18	CLA	4	308	-	1/1/14/20	19/31/109/115	-
18	CLA	A	839	-	1/1/15/20	5/37/115/115	-
24	LMG	1	5020	-	-	10/41/61/70	0/1/1/1
18	CLA	3	309	-	1/1/13/20	13/25/103/115	-
18	CLA	B	816	-	1/1/13/20	6/25/103/115	-
18	CLA	K	1402	-	1/1/14/20	20/31/109/115	-
18	CLA	B	831	-	1/1/15/20	14/37/115/115	-
18	CLA	4	305	-	1/1/14/20	9/31/109/115	-
18	CLA	A	834	-	1/1/12/20	9/21/99/115	-
18	CLA	A	811	-	1/1/13/20	7/25/103/115	-
18	CLA	H	1701	-	1/1/14/20	13/31/109/115	-
18	CLA	A	814	-	1/1/11/20	9/15/93/115	-
18	CLA	A	813	-	1/1/15/20	15/37/115/115	-
18	CLA	A	817	-	1/1/15/20	18/37/115/115	-
29	LUT	1	5004	-	1/1/12/27	4/29/67/67	0/2/2/2
24	LMG	2	321	-	-	5/20/40/70	0/1/1/1
18	CLA	J	1101	-	1/1/15/20	15/37/115/115	-
25	GOL	A	854	-	-	2/4/4/4	-
21	BCR	I	102	-	-	16/29/63/63	0/2/2/2
18	CLA	G	1602	7	1/1/11/20	6/15/93/115	-
18	CLA	4	311	-	1/1/14/20	14/31/109/115	-
18	CLA	B	805	-	1/1/15/20	22/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	803	-	1/1/15/20	11/37/115/115	-
30	CHL	4	302	13	4/4/18/26	8/27/125/137	-
18	CLA	A	804	-	1/1/15/20	27/37/115/115	-
18	CLA	B	832	-	1/1/14/20	21/31/109/115	-
18	CLA	1	5018	13	1/1/14/20	18/31/109/115	-
18	CLA	B	810	2	1/1/15/20	14/37/115/115	-
18	CLA	A	812	-	1/1/15/20	18/37/115/115	-
18	CLA	A	815	-	1/1/15/20	13/37/115/115	-
18	CLA	K	1404	-	1/1/11/20	8/15/93/115	-
18	CLA	A	803	-	1/1/15/20	19/37/115/115	-
18	CLA	4	310	-	1/1/12/20	11/19/97/115	-
18	CLA	A	829	-	1/1/15/20	16/37/115/115	-
24	LMG	F	308	-	-	12/29/49/70	0/1/1/1
21	BCR	3	306	-	-	14/29/63/63	0/2/2/2
18	CLA	A	824	-	1/1/13/20	13/25/103/115	-
22	LHG	B	848	18	-	10/23/23/53	-
18	CLA	B	835	-	1/1/13/20	9/25/103/115	-
21	BCR	B	843	-	-	10/29/63/63	0/2/2/2
20	SF4	C	101	3	-	-	0/6/5/5
18	CLA	2	308	-	1/1/15/20	15/37/115/115	-
18	CLA	2	309	14	1/1/15/20	20/37/115/115	-
21	BCR	L	302	-	-	12/29/63/63	0/2/2/2
18	CLA	B	823	-	1/1/15/20	16/37/115/115	-
18	CLA	L	305	-	1/1/14/20	18/31/109/115	-
21	BCR	G	1604	-	-	8/29/63/63	0/2/2/2
21	BCR	B	844	-	-	10/29/63/63	0/2/2/2
18	CLA	A	816	-	1/1/13/20	16/27/105/115	-
21	BCR	B	847	-	-	15/29/63/63	0/2/2/2
23	LMT	A	850	-	-	11/21/61/61	0/2/2/2
29	LUT	3	304	-	1/1/12/27	9/29/67/67	0/2/2/2
18	CLA	3	301	-	1/1/11/20	4/11/91/115	-
24	LMG	2	322	-	-	17/31/51/70	0/1/1/1

The worst 5 of 1123 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	5003	LUT	C24-C25	14.73	1.51	1.33
29	4	303	LUT	C24-C25	14.64	1.51	1.33
29	3	303	LUT	C24-C25	14.60	1.51	1.33
29	1	5004	LUT	C24-C25	14.58	1.51	1.33
29	J	1105	LUT	C24-C25	14.44	1.51	1.33

The worst 5 of 2124 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	101	BCR	C10-C11-C12	18.19	180.00	123.22
21	G	1604	BCR	C10-C11-C12	17.83	178.87	123.22
21	K	1405	BCR	C10-C11-C12	17.69	178.43	123.22
21	F	304	BCR	C10-C11-C12	17.57	178.06	123.22
21	A	855	BCR	C10-C11-C12	17.55	177.97	123.22

5 of 206 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	801	CL0	NC
17	A	801	CL0	ND
17	A	801	CL0	NA
18	A	802	CLA	ND
18	A	803	CLA	ND

5 of 2767 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	802	CLA	C2-C1-O2A-CGA
18	A	802	CLA	CHA-CBD-CGD-O1D
18	A	802	CLA	CHA-CBD-CGD-O2D
18	A	802	CLA	C2-C3-C5-C6
18	A	802	CLA	C4-C3-C5-C6

There are no ring outliers.

221 monomers are involved in 828 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	L	303	BCR	3	0
18	J	1103	CLA	1	0
18	A	806	CLA	6	0
18	B	812	CLA	7	0
23	B	852	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	B	834	CLA	5	0
18	3	308	CLA	1	0
21	B	845	BCR	9	0
18	2	313	CLA	4	0
18	A	830	CLA	3	0
18	A	822	CLA	17	0
18	B	830	CLA	6	0
22	B	849	LHG	4	0
21	L	307	BCR	3	0
30	2	316	CHL	4	0
18	A	819	CLA	13	0
18	A	833	CLA	6	0
21	B	846	BCR	3	0
18	A	836	CLA	5	0
18	3	307	CLA	10	0
18	3	319	CLA	5	0
30	4	317	CHL	3	0
18	3	315	CLA	3	0
30	2	314	CHL	5	0
18	L	304	CLA	4	0
21	4	301	BCR	6	0
29	1	5003	LUT	8	0
18	B	839	CLA	7	0
18	B	801	CLA	11	0
18	B	821	CLA	2	0
18	B	813	CLA	4	0
24	F	307	LMG	1	0
18	B	833	CLA	7	0
18	B	814	CLA	5	0
29	J	1105	LUT	9	0
31	4	304	XAT	6	0
21	A	843	BCR	6	0
18	A	807	CLA	7	0
18	B	837	CLA	7	0
30	2	319	CHL	1	0
18	B	840	CLA	4	0
18	2	307	CLA	4	0
18	2	311	CLA	1	0
17	A	801	CL0	9	0
30	4	314	CHL	2	0
26	2	327	DGD	5	0
18	B	804	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	820	CLA	3	0
23	G	1606	LMT	1	0
22	A	849	LHG	8	0
30	3	316	CHL	7	0
30	4	313	CHL	1	0
18	B	824	CLA	7	0
18	F	301	CLA	4	0
18	A	826	CLA	9	0
24	A	851	LMG	5	0
24	F	306	LMG	4	0
30	3	312	CHL	7	0
18	B	828	CLA	9	0
18	A	835	CLA	6	0
18	K	1401	CLA	2	0
18	A	828	CLA	11	0
24	2	302	LMG	1	0
30	2	318	CHL	4	0
30	3	310	CHL	9	0
21	I	101	BCR	2	0
18	B	819	CLA	5	0
18	A	805	CLA	6	0
18	A	823	CLA	11	0
18	4	309	CLA	3	0
18	1	5010	CLA	8	0
18	1	5009	CLA	6	0
18	A	827	CLA	4	0
18	B	827	CLA	5	0
18	A	838	CLA	5	0
24	2	301	LMG	1	0
19	A	841	PQN	4	0
18	3	311	CLA	4	0
30	1	5014	CHL	6	0
18	A	808	CLA	9	0
18	G	1601	CLA	1	0
18	2	326	CLA	4	0
18	L	301	CLA	1	0
26	J	1106	DGD	4	0
18	B	841	CLA	12	0
18	2	306	CLA	6	0
30	1	5016	CHL	8	0
21	J	1104	BCR	4	0
18	A	810	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	809	CLA	3	0
18	A	821	CLA	3	0
18	B	807	CLA	5	0
18	B	815	CLA	5	0
18	3	318	CLA	3	0
18	3	314	CLA	3	0
18	1	5008	CLA	2	0
26	B	855	DGD	8	0
18	G	1603	CLA	4	0
18	2	312	CLA	7	0
18	A	831	CLA	5	0
29	2	303	LUT	6	0
23	G	1605	LMT	2	0
21	1	5005	BCR	3	0
18	A	852	CLA	9	0
21	B	802	BCR	4	0
18	A	802	CLA	11	0
18	2	310	CLA	6	0
18	B	806	CLA	10	0
18	4	307	CLA	2	0
21	K	1405	BCR	2	0
18	1	5006	CLA	11	0
18	4	315	CLA	5	0
21	A	846	BCR	8	0
18	1	5013	CLA	2	0
18	A	832	CLA	7	0
18	L	306	CLA	1	0
30	3	313	CHL	1	0
18	B	822	CLA	5	0
18	3	317	CLA	8	0
23	B	853	LMT	2	0
18	B	829	CLA	7	0
22	1	5019	LHG	3	0
22	A	848	LHG	8	0
18	1	5012	CLA	3	0
31	2	304	XAT	7	0
28	F	310	ZEX	3	0
18	B	809	CLA	4	0
23	2	325	LMT	1	0
24	G	1607	LMG	1	0
21	2	305	BCR	11	0
21	A	844	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	856	LMT	2	0
29	3	303	LUT	3	0
22	2	320	LHG	1	0
18	A	840	CLA	9	0
21	3	305	BCR	3	0
18	B	836	CLA	7	0
18	A	825	CLA	7	0
18	1	5017	CLA	5	0
30	4	316	CHL	4	0
18	B	826	CLA	11	0
21	A	855	BCR	6	0
21	A	847	BCR	7	0
18	A	818	CLA	1	0
18	B	818	CLA	10	0
18	B	811	CLA	7	0
18	1	5007	CLA	1	0
18	A	837	CLA	8	0
18	B	825	CLA	8	0
21	F	304	BCR	5	0
19	B	842	PQN	2	0
18	4	306	CLA	1	0
18	F	303	CLA	8	0
18	1	5011	CLA	2	0
18	1	5015	CLA	3	0
18	2	317	CLA	4	0
21	A	845	BCR	8	0
24	B	850	LMG	2	0
18	K	1403	CLA	5	0
18	B	838	CLA	6	0
18	B	820	CLA	5	0
20	C	102	SF4	1	0
24	1	5001	LMG	8	0
30	4	318	CHL	4	0
18	A	853	CLA	8	0
18	B	808	CLA	5	0
18	F	302	CLA	4	0
30	2	315	CHL	6	0
29	4	303	LUT	2	0
21	F	305	BCR	6	0
18	4	308	CLA	3	0
18	A	839	CLA	6	0
24	1	5020	LMG	2	0

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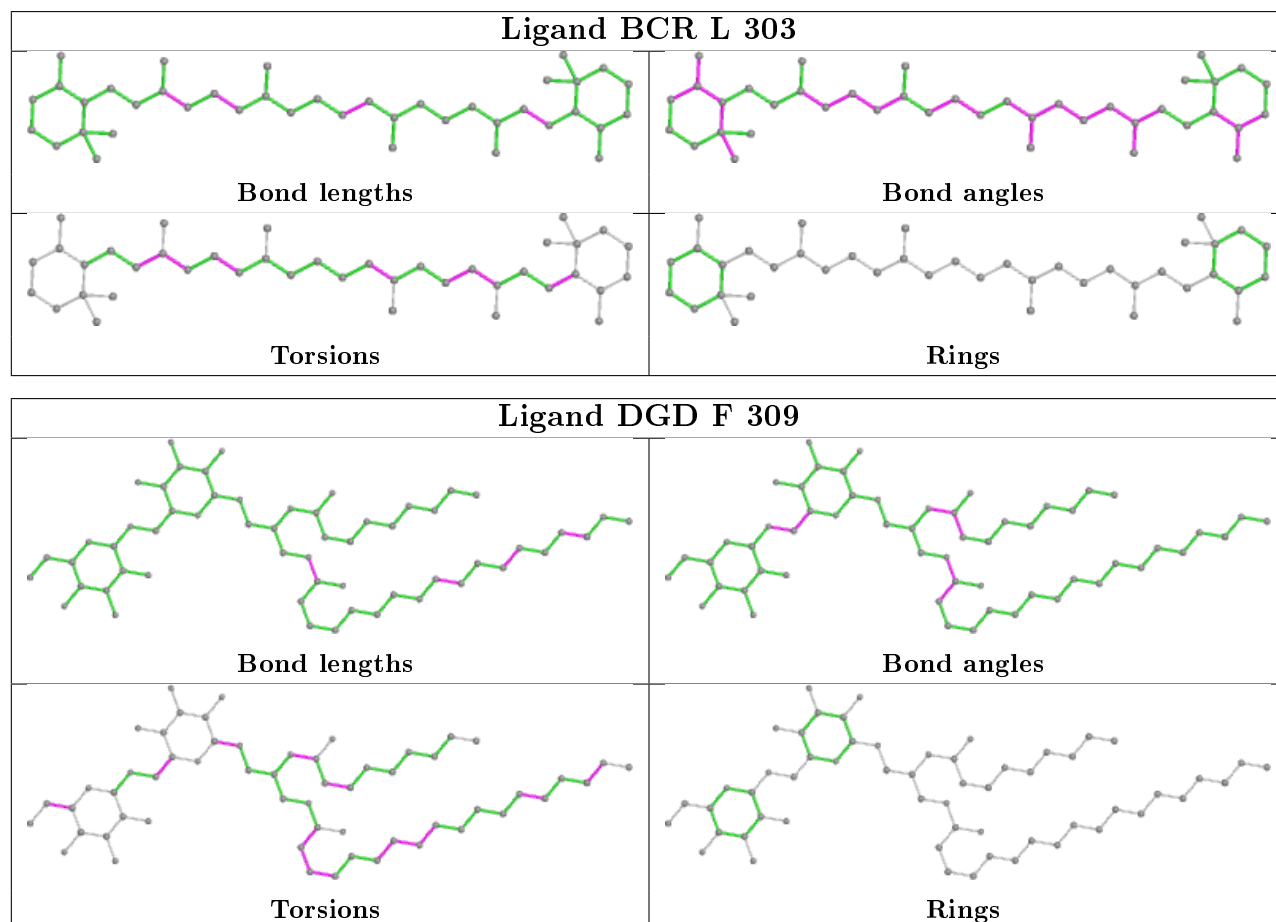
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	3	309	CLA	3	0
18	B	816	CLA	5	0
18	K	1402	CLA	6	0
18	B	831	CLA	6	0
18	4	305	CLA	4	0
18	A	834	CLA	3	0
18	A	811	CLA	13	0
18	H	1701	CLA	8	0
18	A	814	CLA	1	0
18	A	813	CLA	7	0
18	A	817	CLA	6	0
29	1	5004	LUT	7	0
24	2	321	LMG	2	0
18	J	1101	CLA	8	0
25	A	854	GOL	1	0
21	I	102	BCR	2	0
18	G	1602	CLA	1	0
18	4	311	CLA	3	0
18	B	805	CLA	8	0
18	B	803	CLA	9	0
30	4	302	CHL	5	0
18	A	804	CLA	7	0
18	B	832	CLA	1	0
18	1	5018	CLA	3	0
18	B	810	CLA	6	0
18	A	812	CLA	6	0
18	A	815	CLA	3	0
18	K	1404	CLA	2	0
18	A	803	CLA	10	0
18	4	310	CLA	3	0
18	A	829	CLA	6	0
21	3	306	BCR	3	0
18	A	824	CLA	6	0
22	B	848	LHG	4	0
18	B	835	CLA	5	0
21	B	843	BCR	8	0
18	2	308	CLA	4	0
18	2	309	CLA	7	0
21	L	302	BCR	2	0
18	B	823	CLA	8	0
18	L	305	CLA	1	0
21	G	1604	BCR	4	0

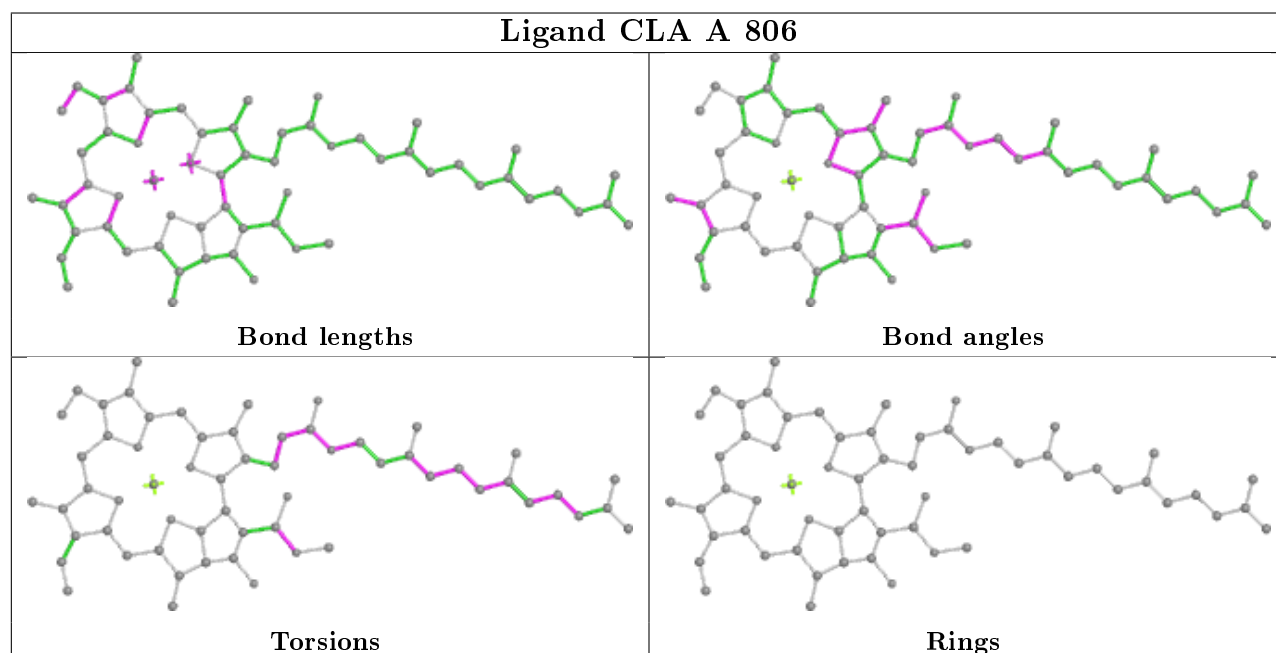
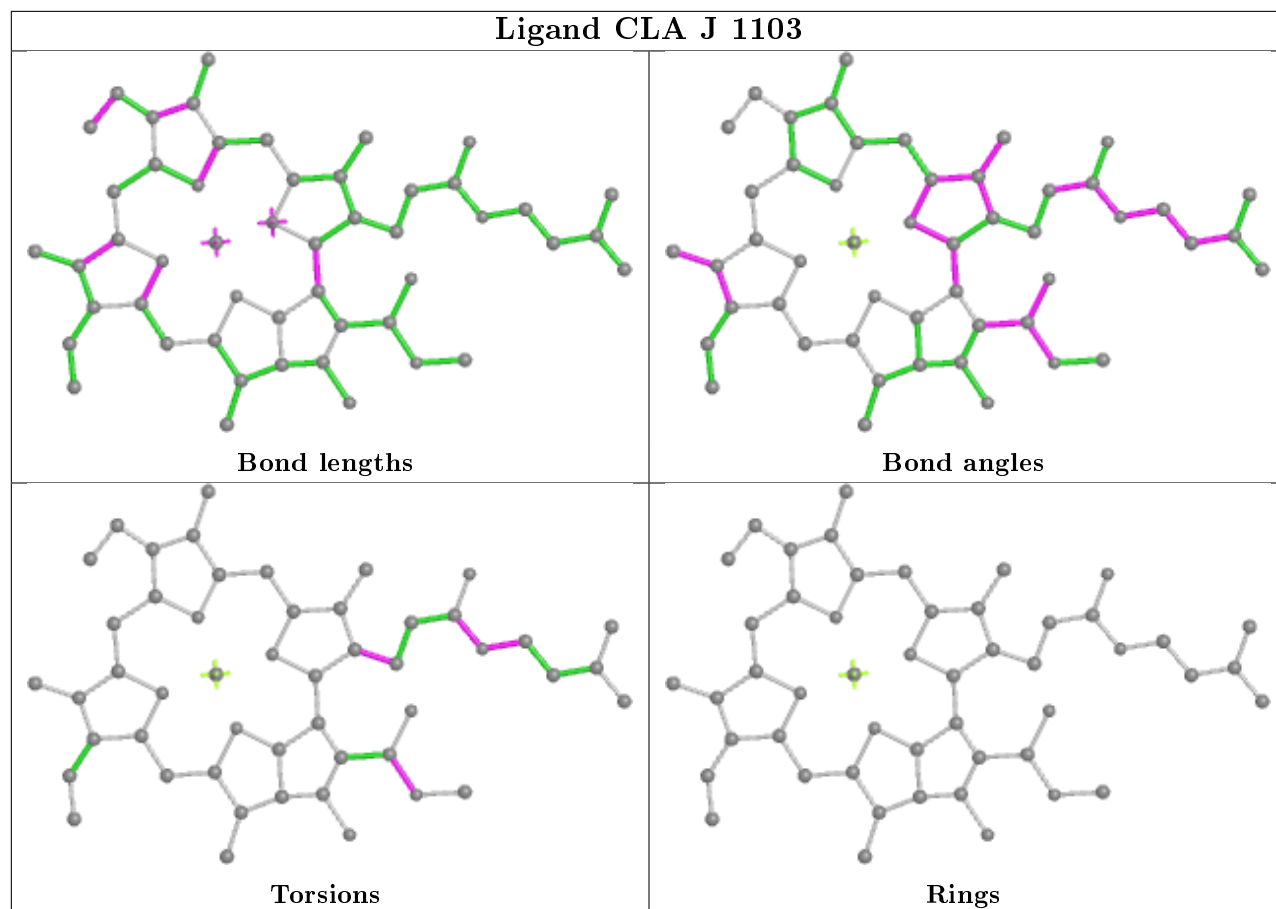
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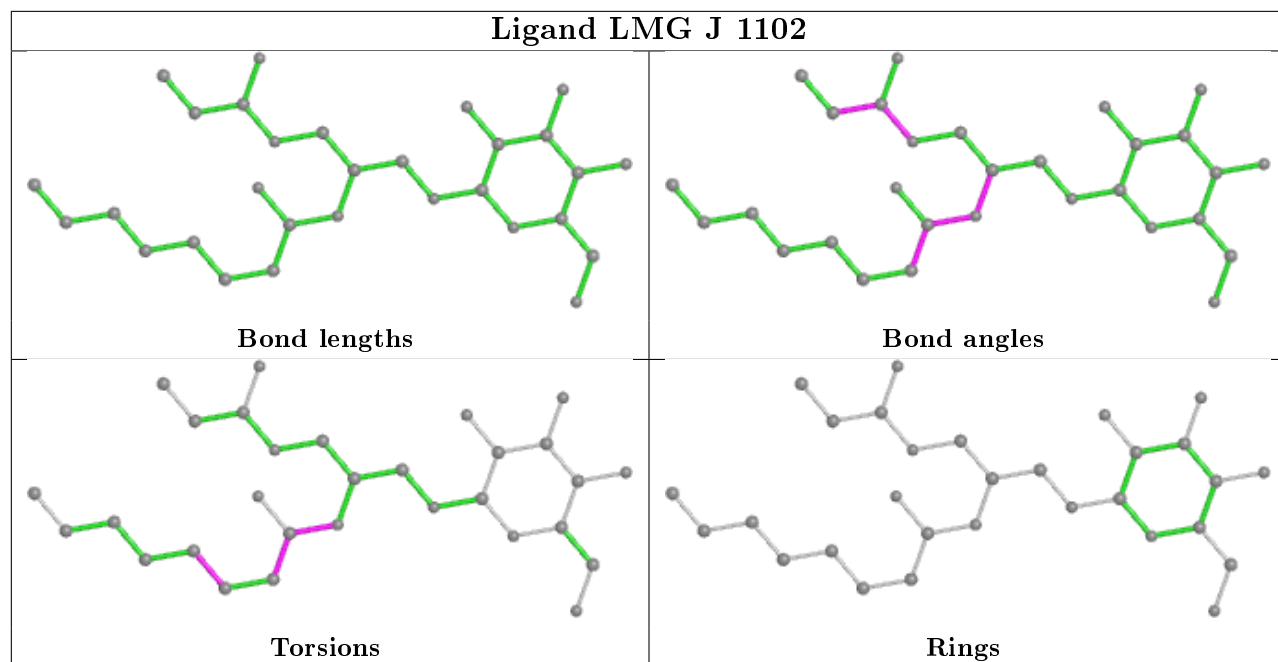
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	844	BCR	5	0
18	A	816	CLA	9	0
21	B	847	BCR	2	0
29	3	304	LUT	9	0
18	3	301	CLA	1	0
24	2	322	LMG	2	0

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.

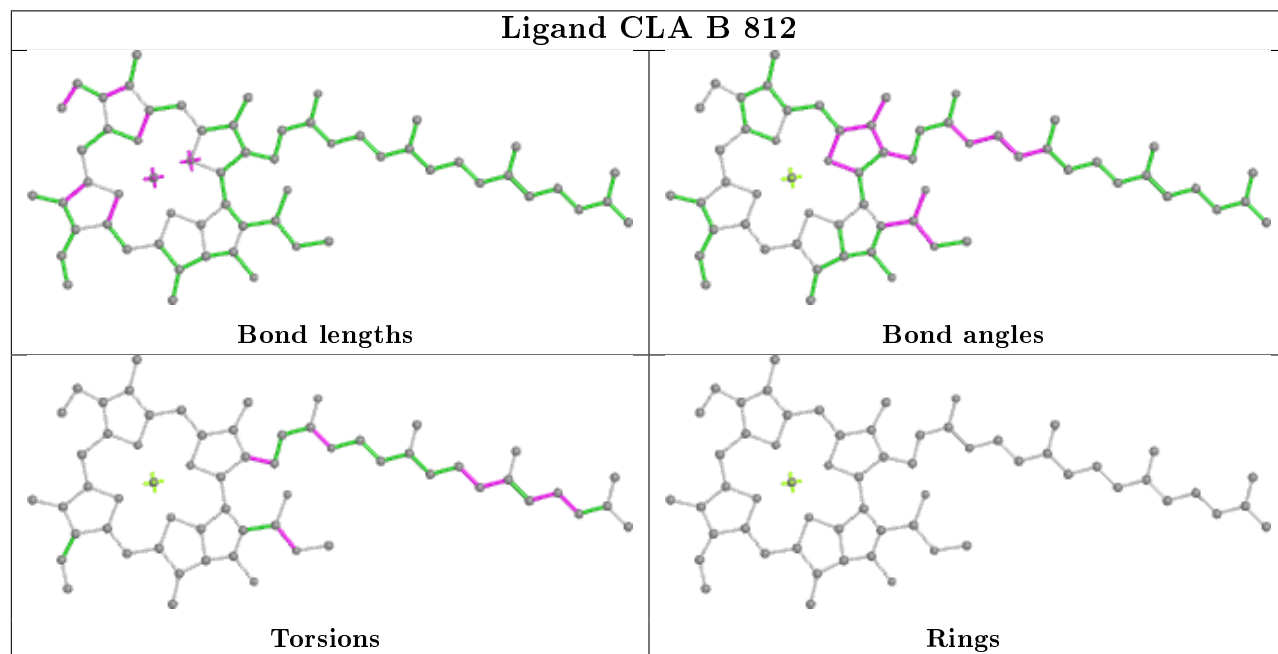


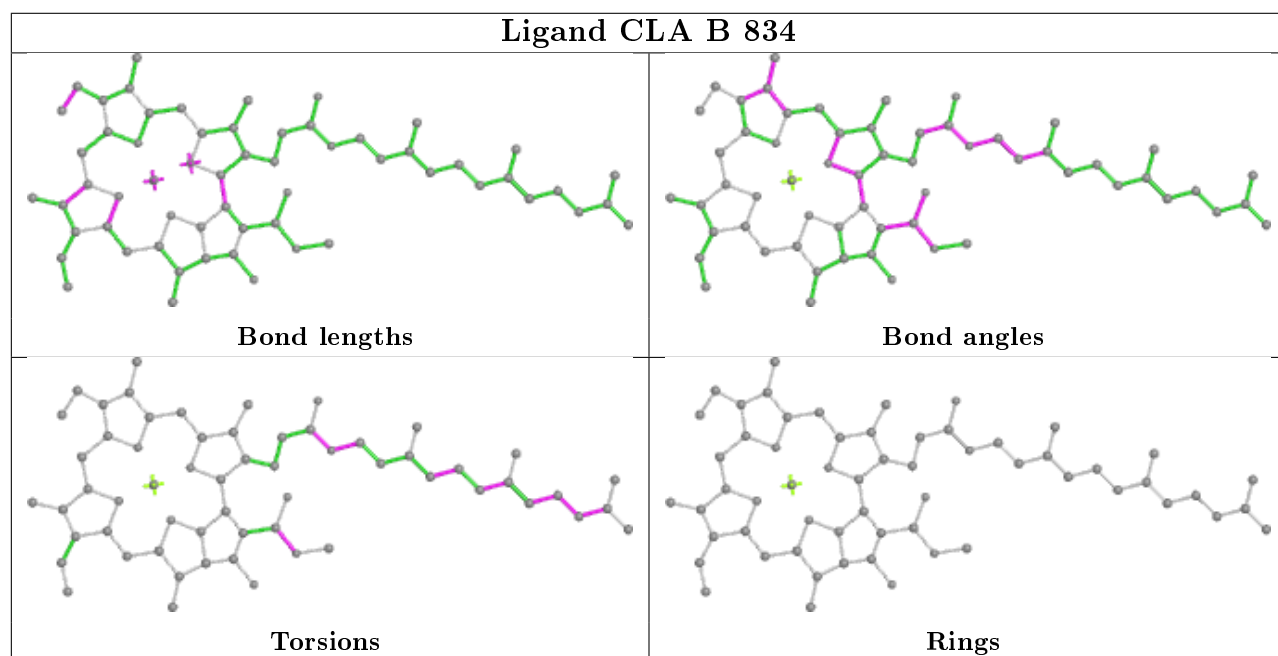
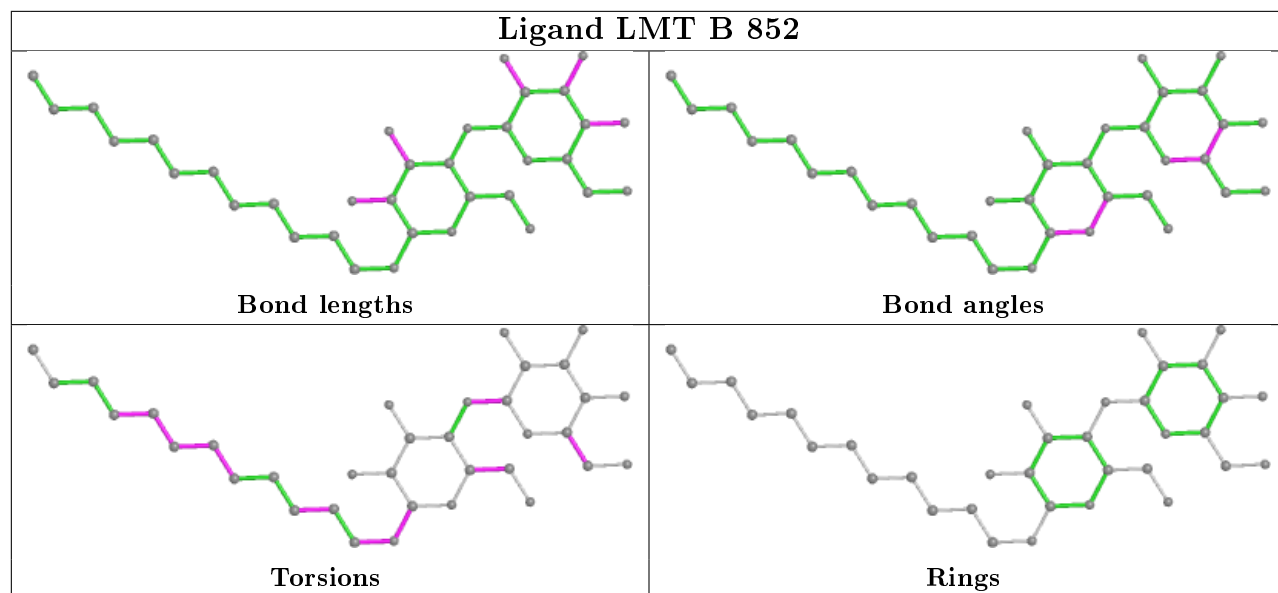


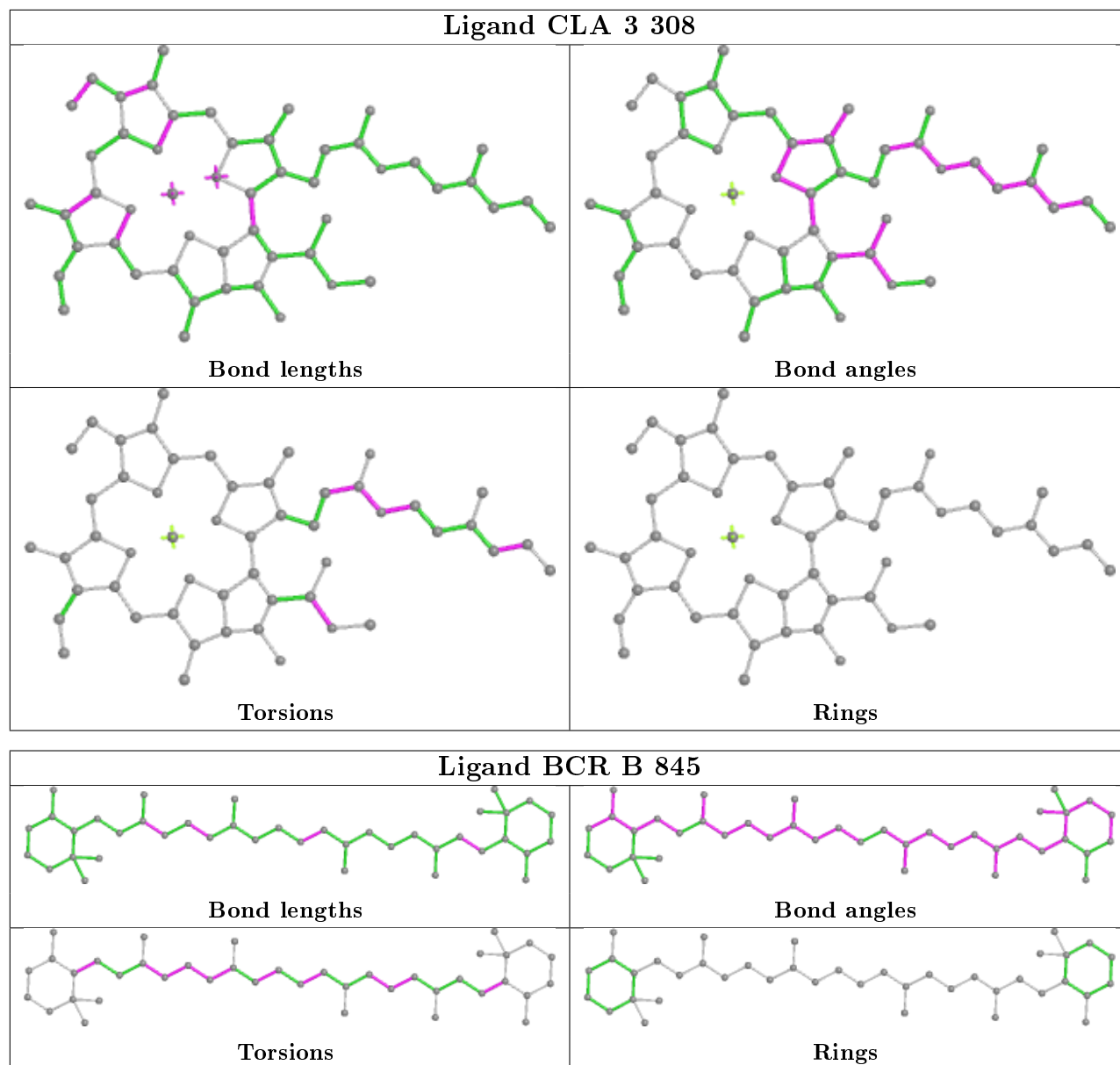
Ligand LMG J 1102



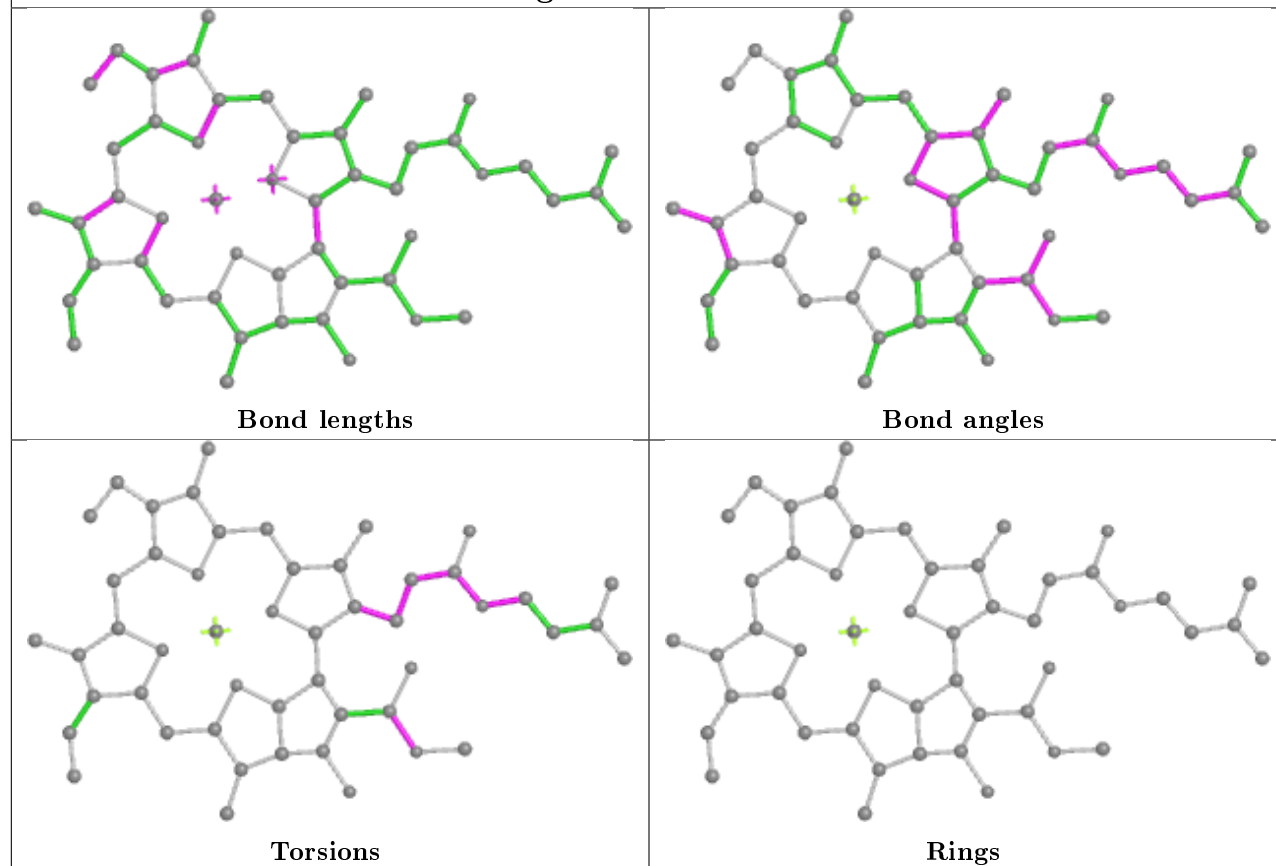
Ligand CLA B 812



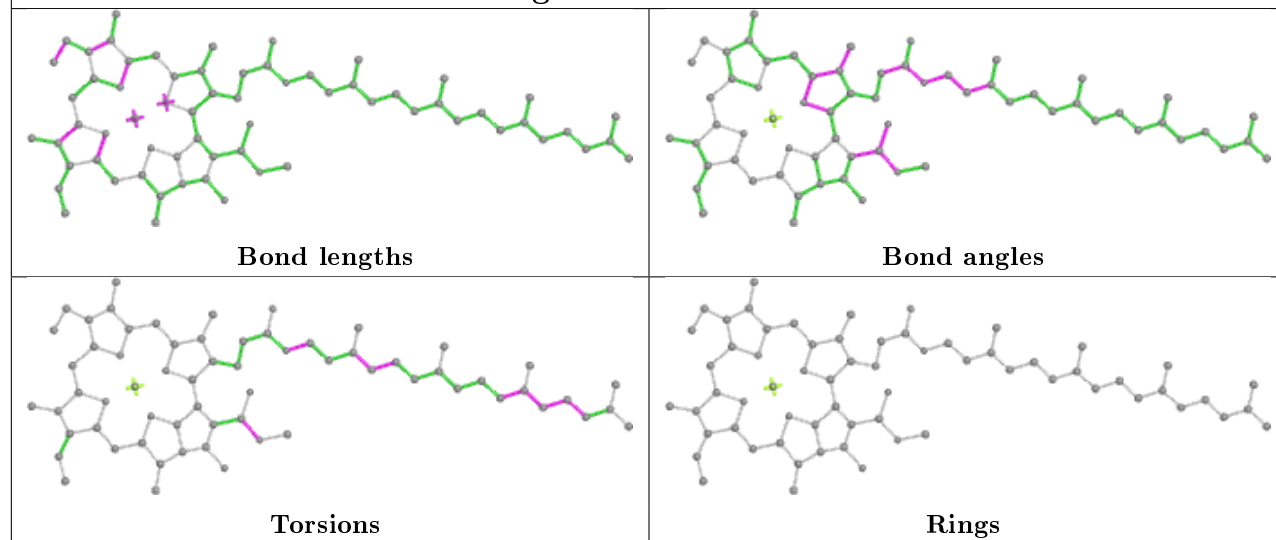


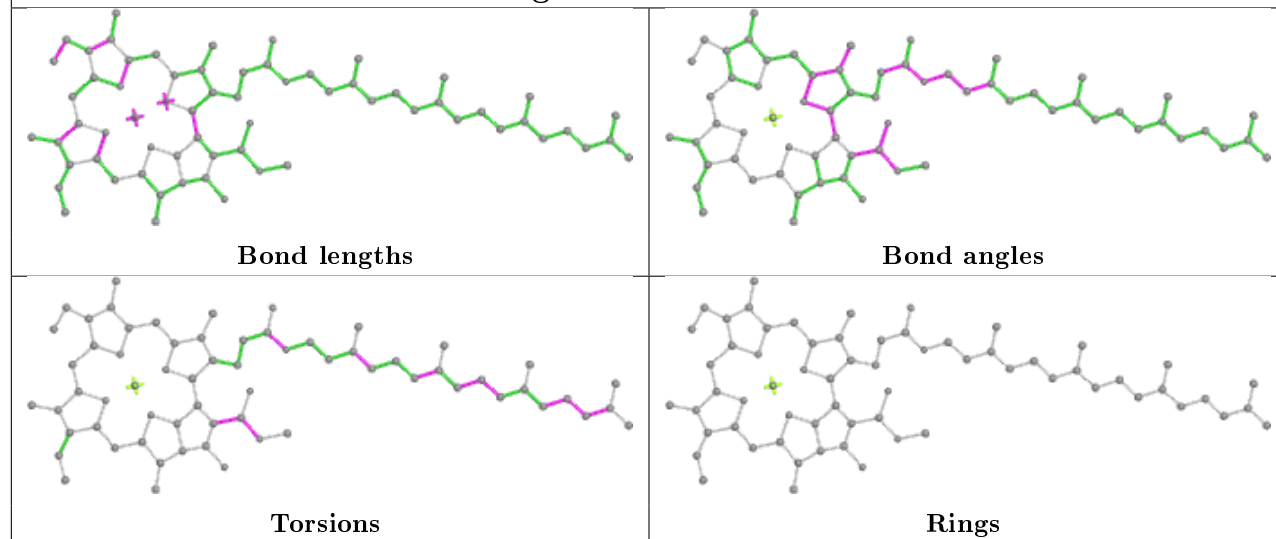
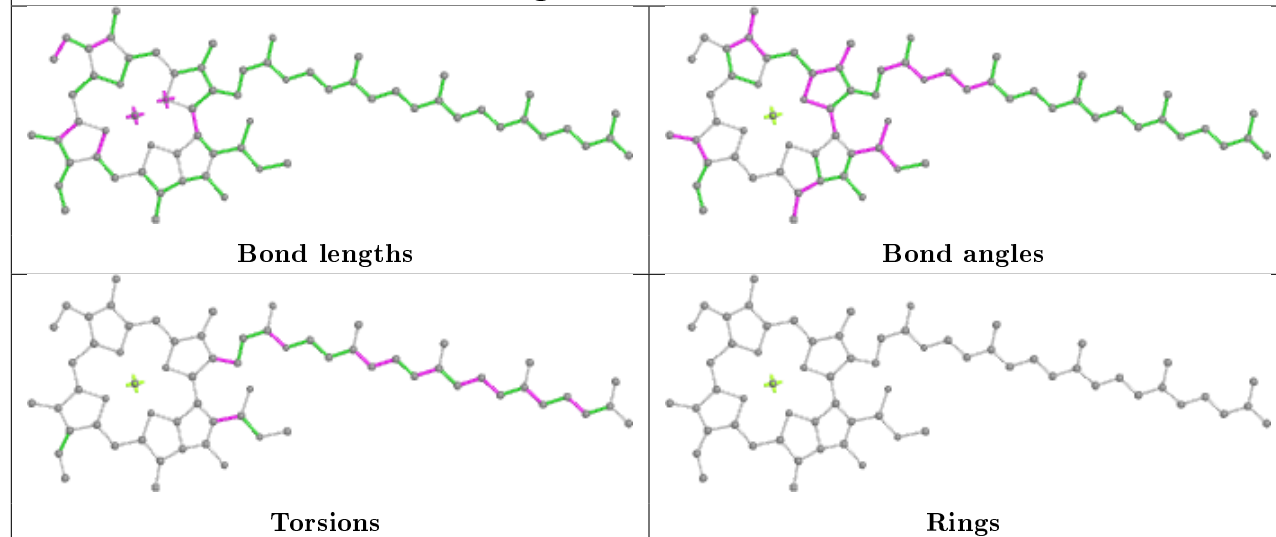


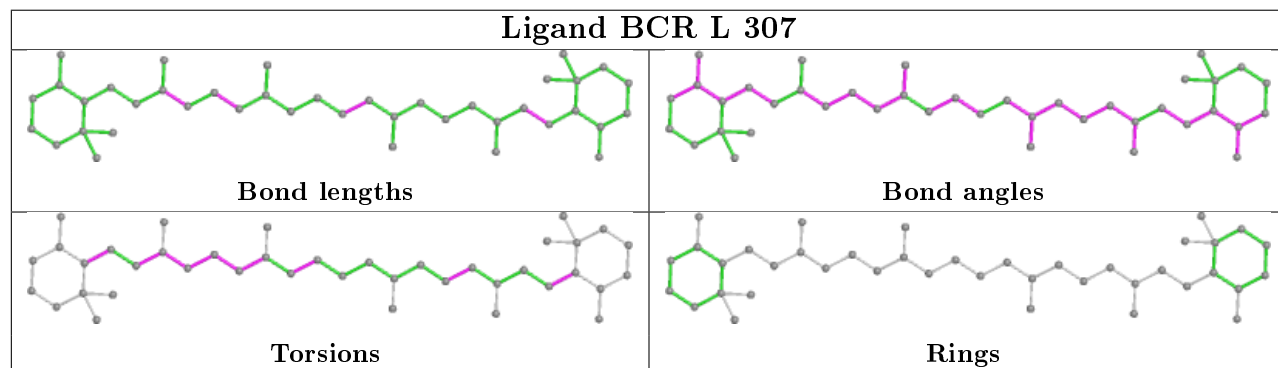
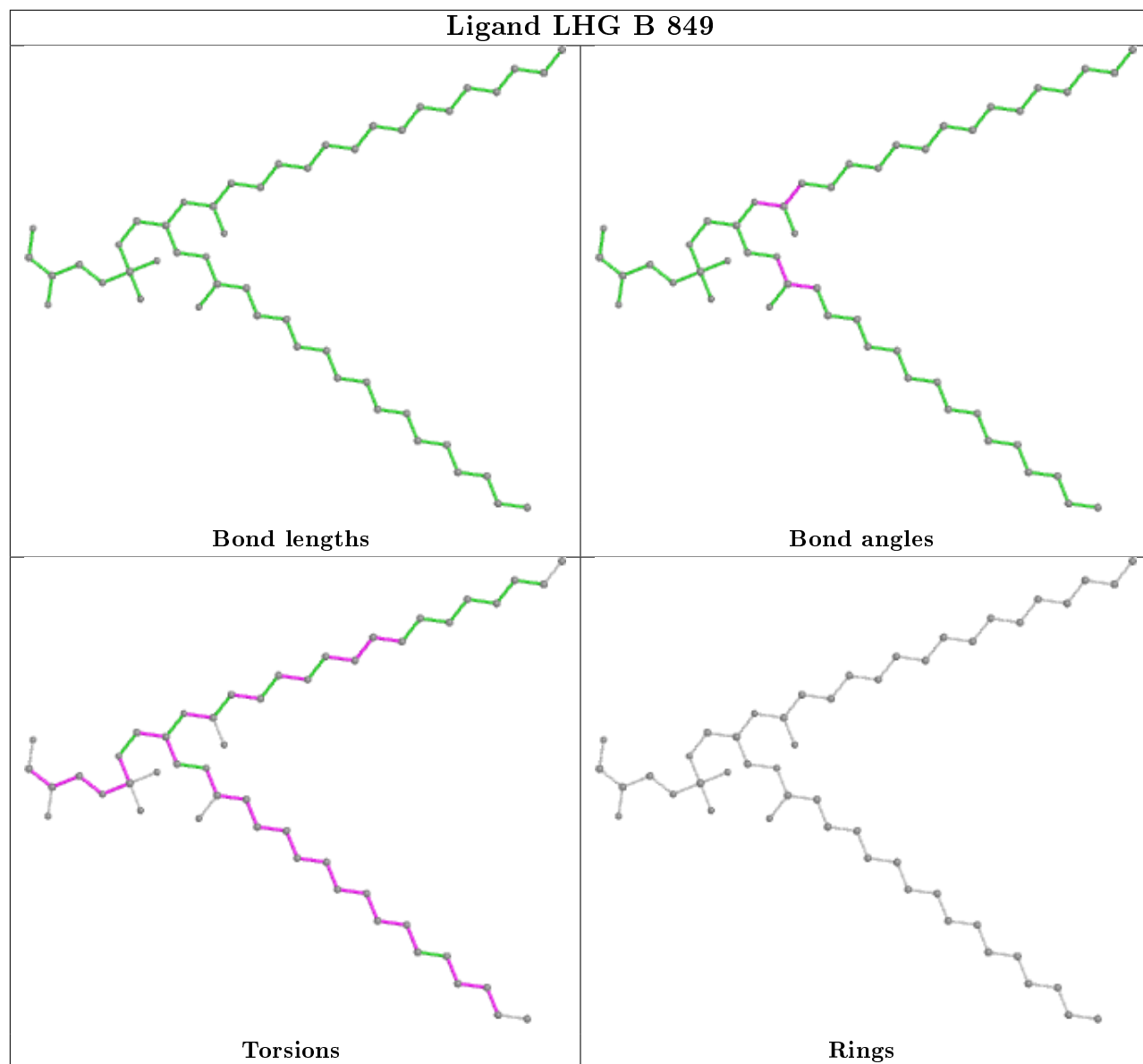
Ligand CLA 2 313



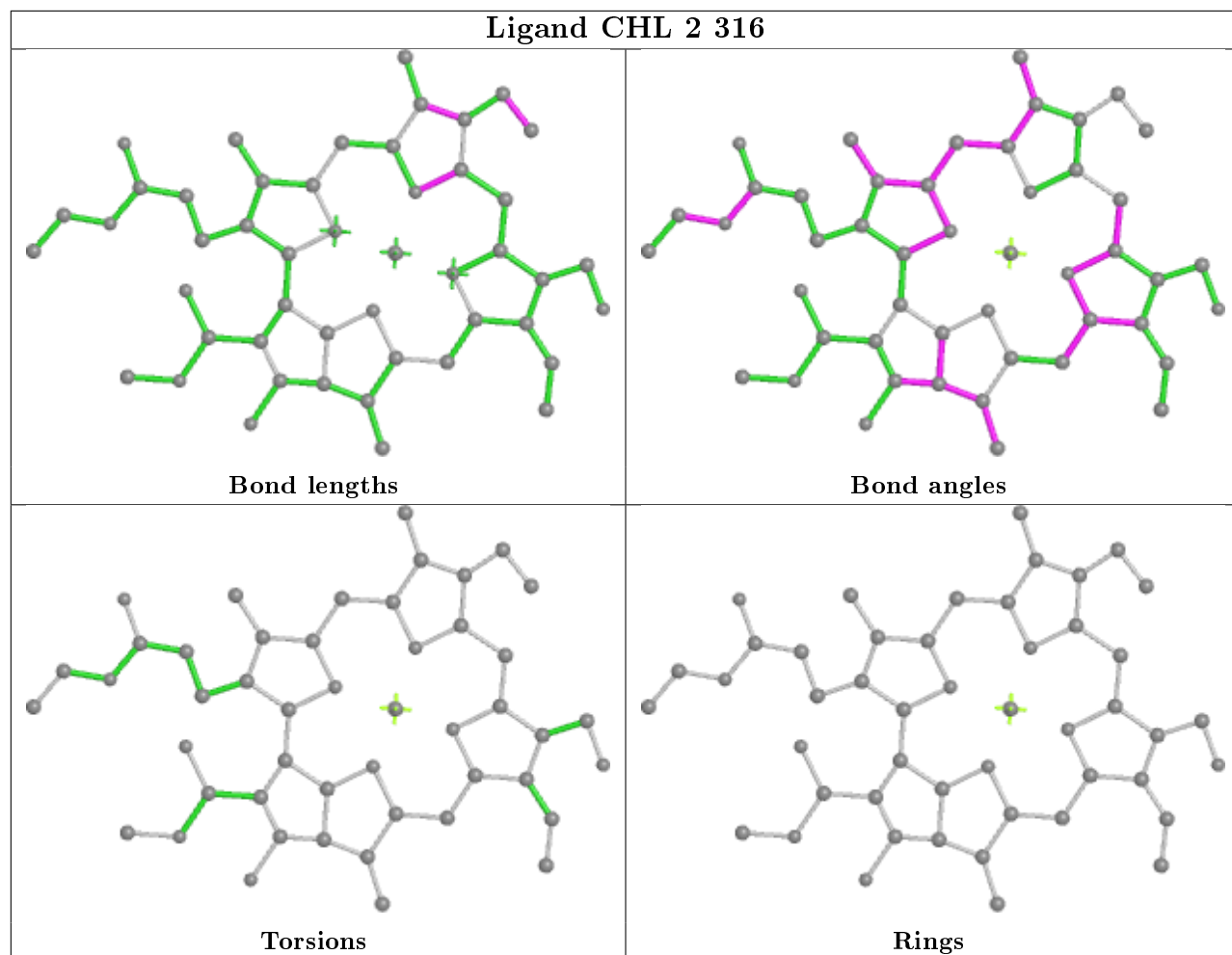
Ligand CLA A 830



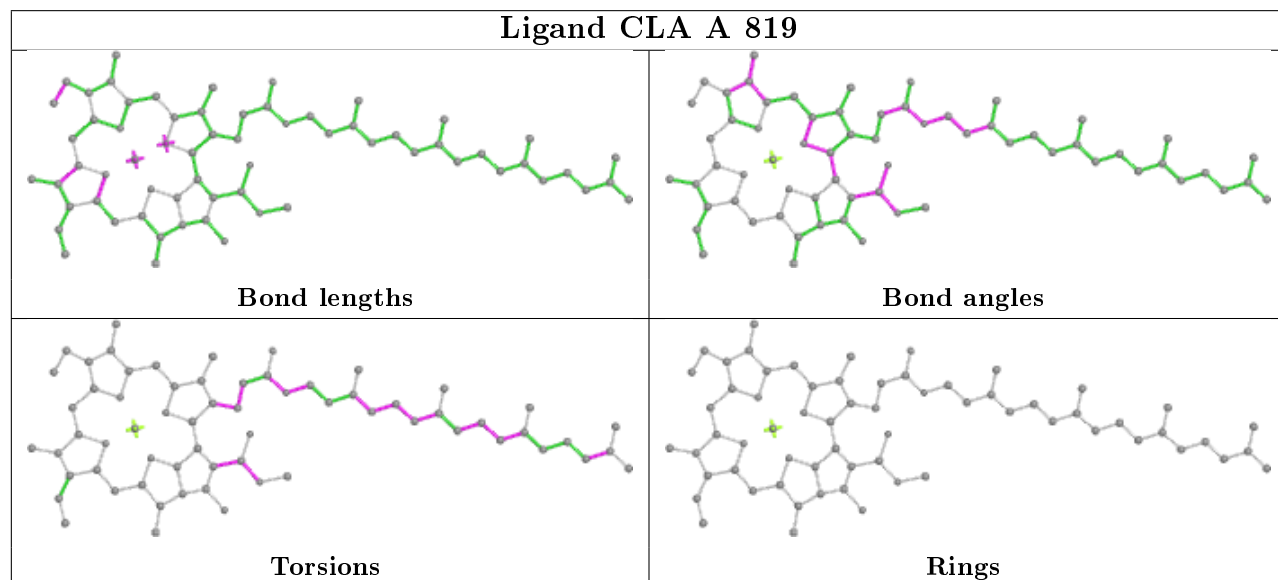
Ligand CLA A 822**Ligand CLA B 830**

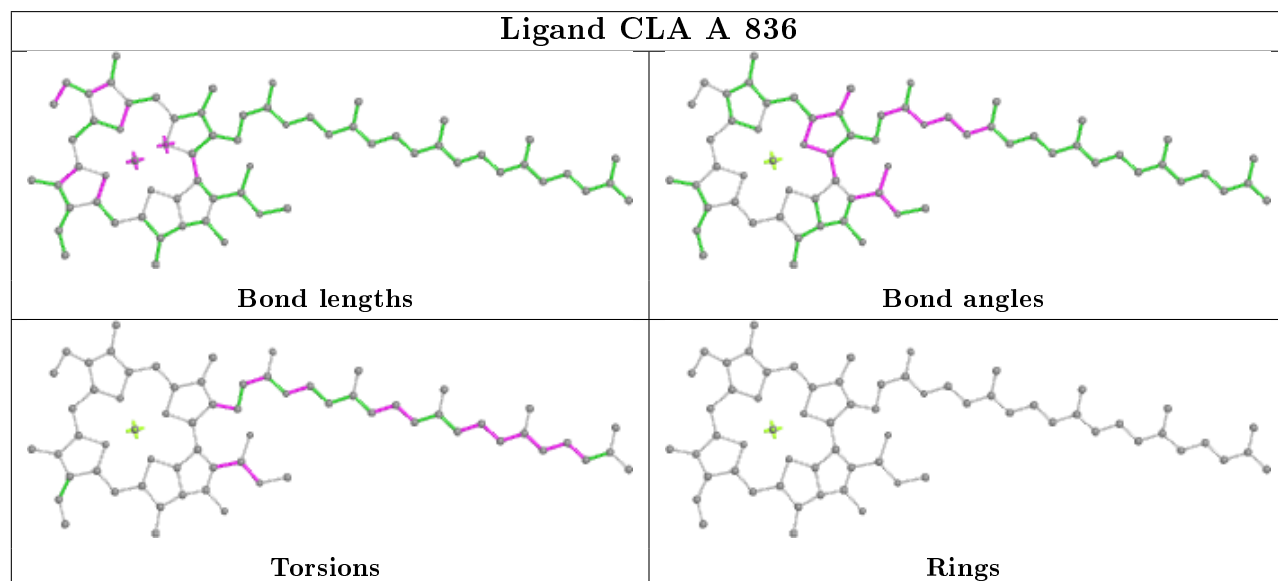
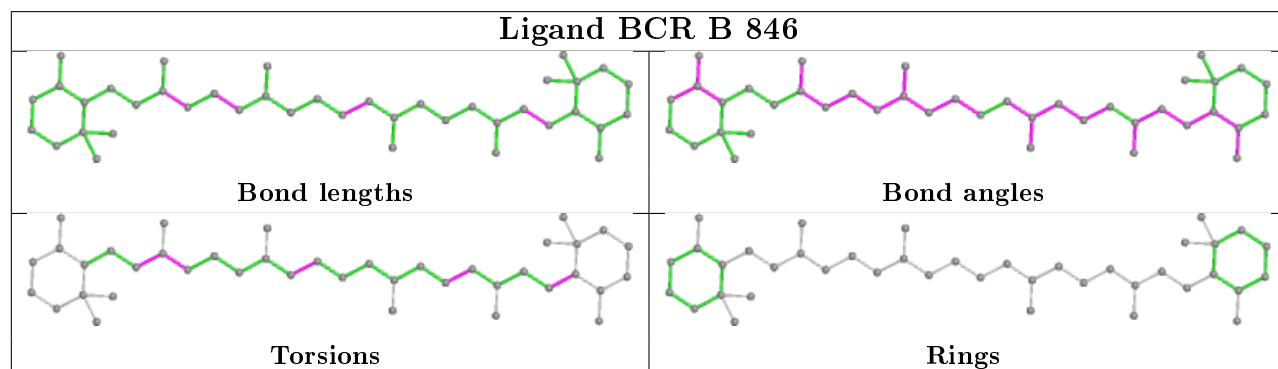
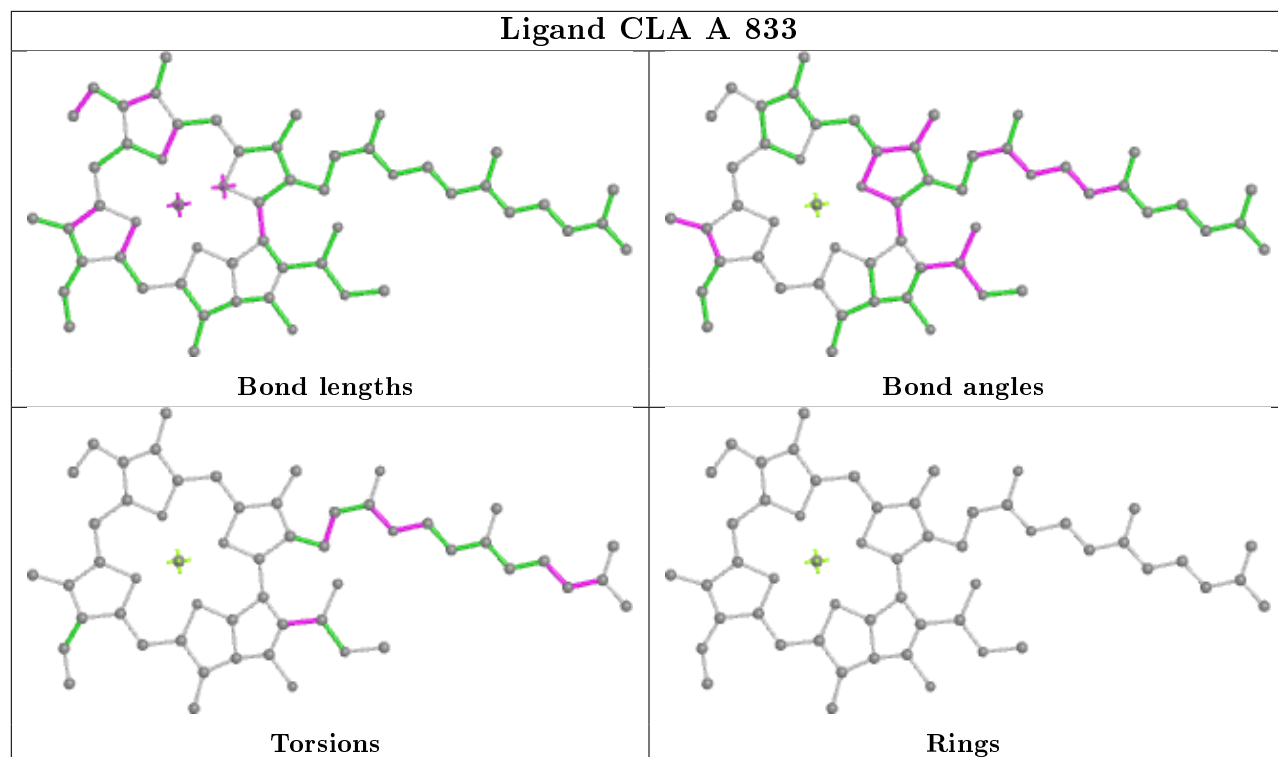


Ligand CHL 2 316

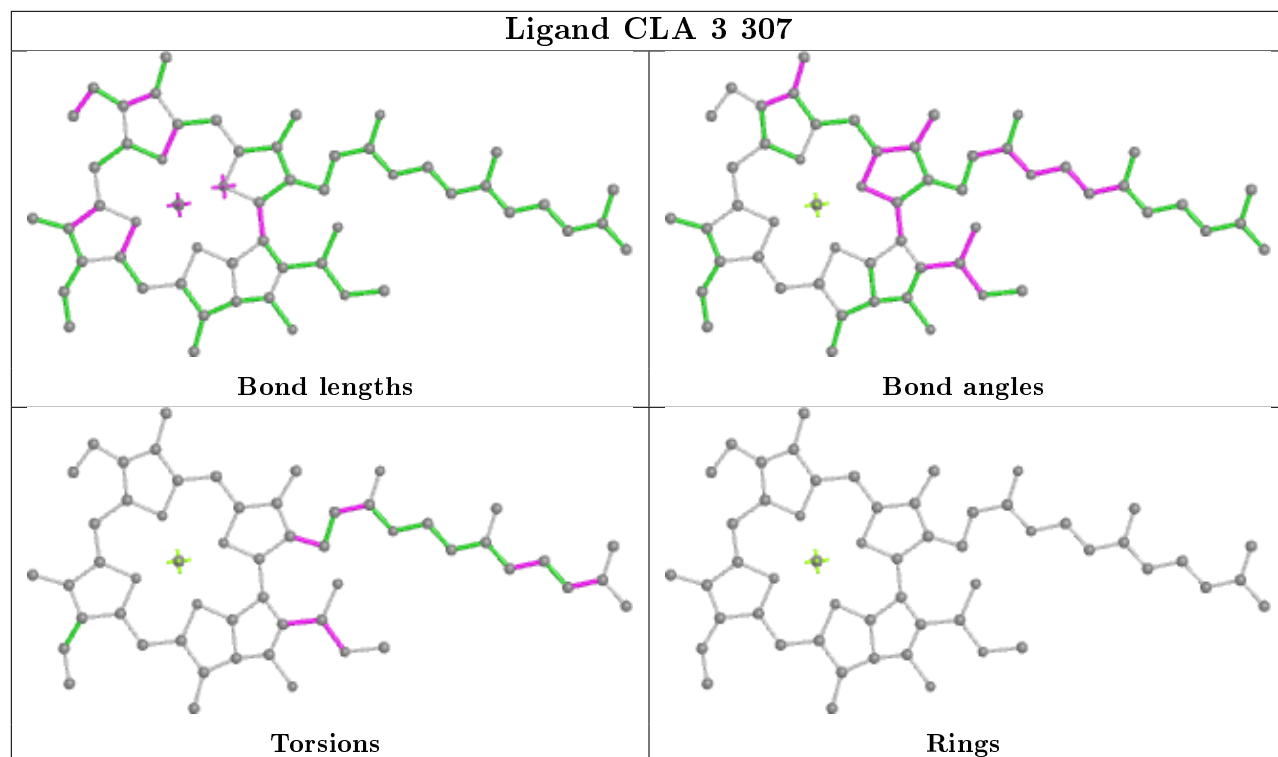


Ligand CLA A 819

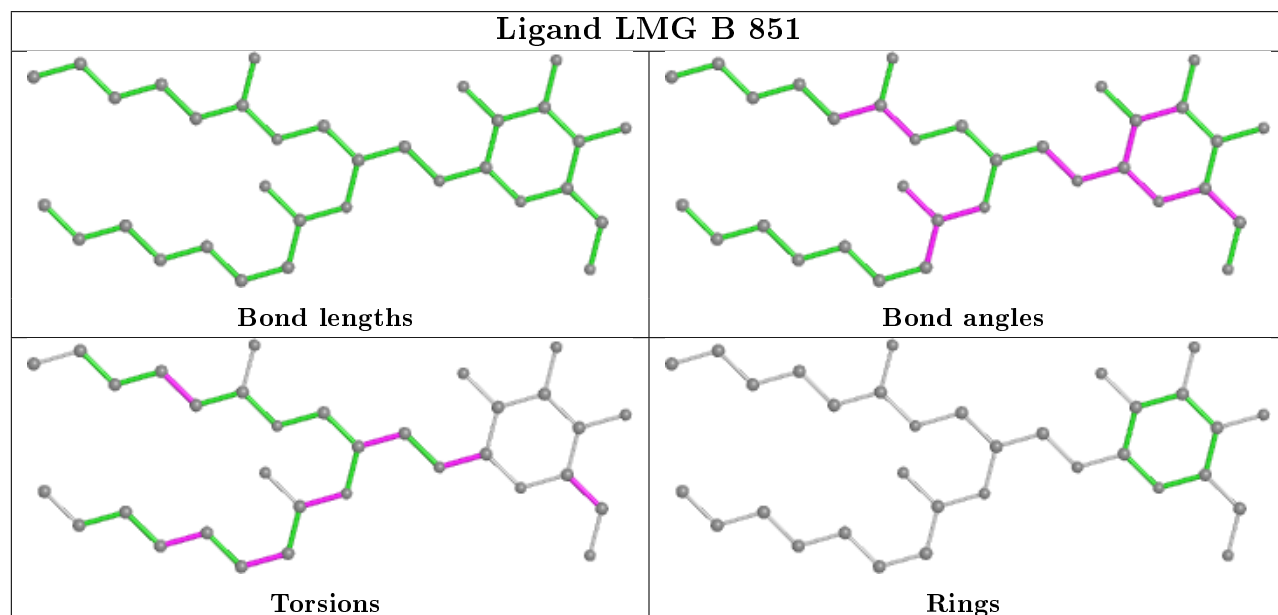




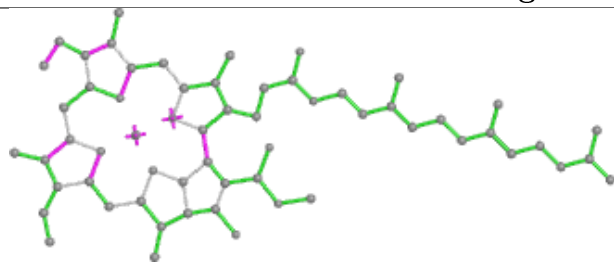
Ligand CLA 3 307



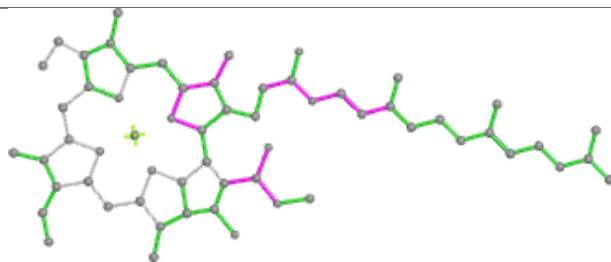
Ligand LMG B 851



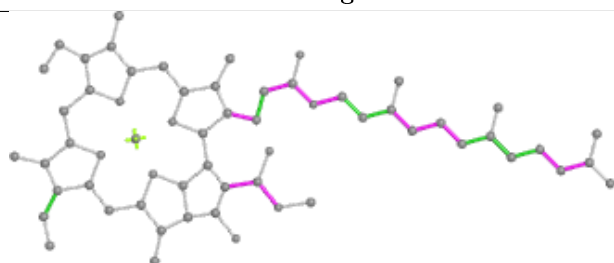
Ligand CLA 3 319



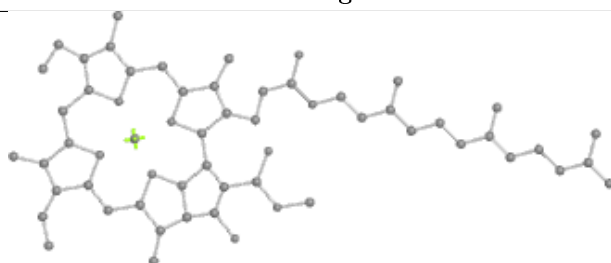
Bond lengths



Bond angles

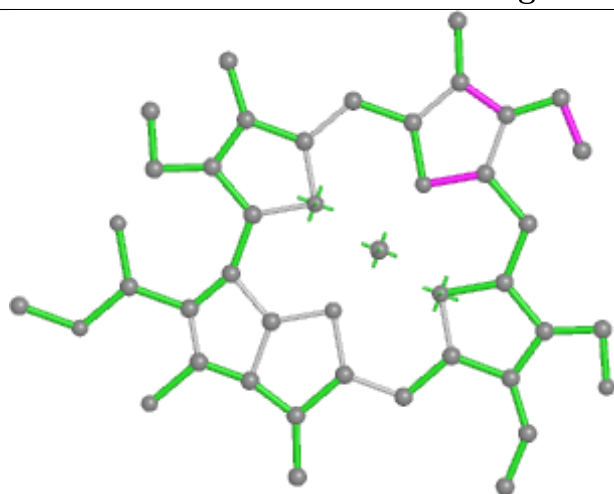


Torsions

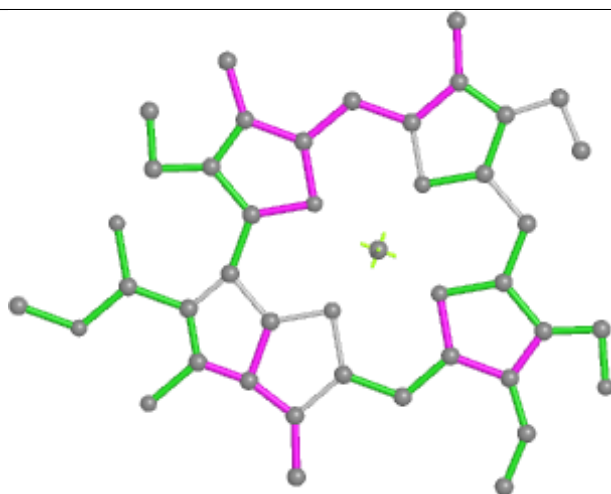


Rings

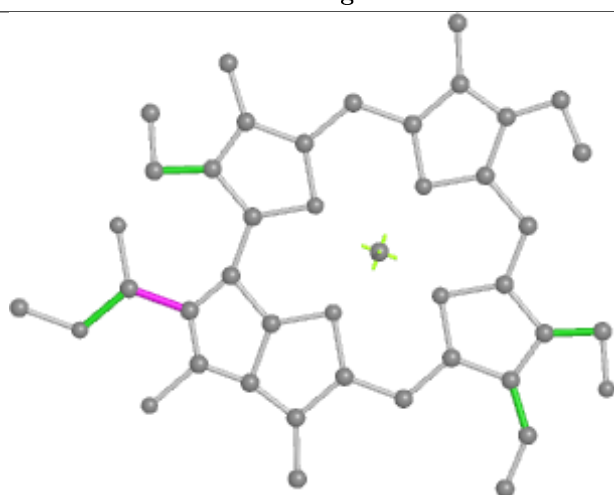
Ligand CHL 4 317



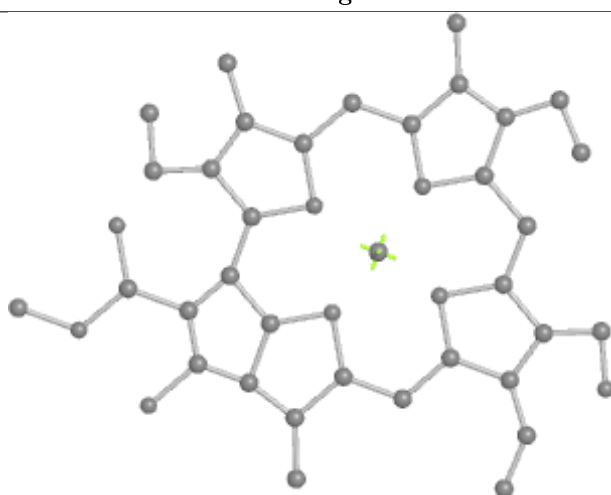
Bond lengths



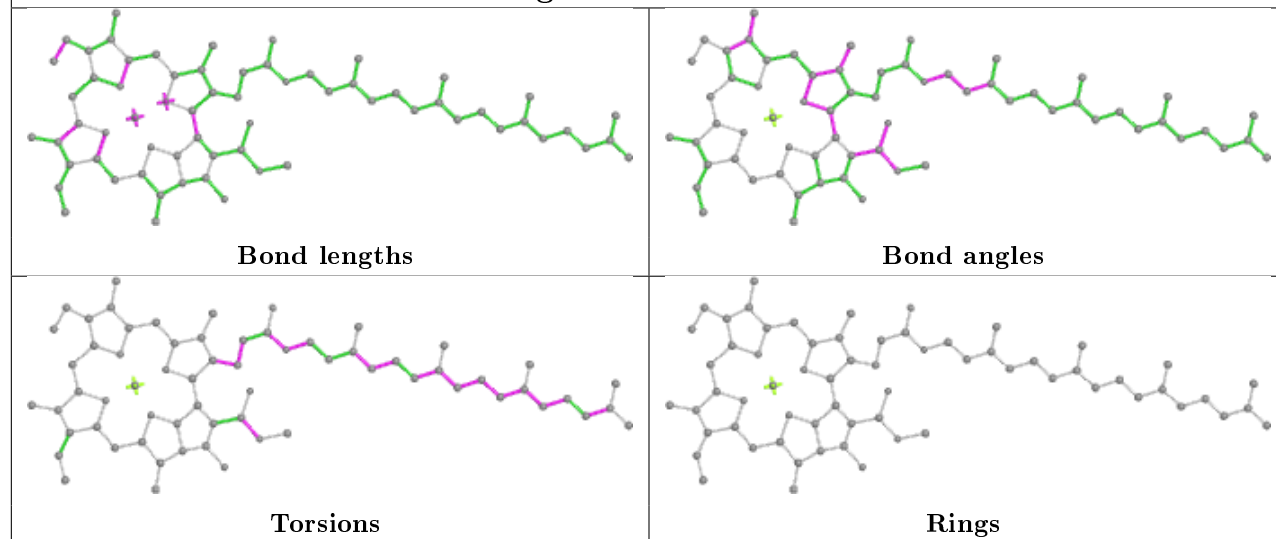
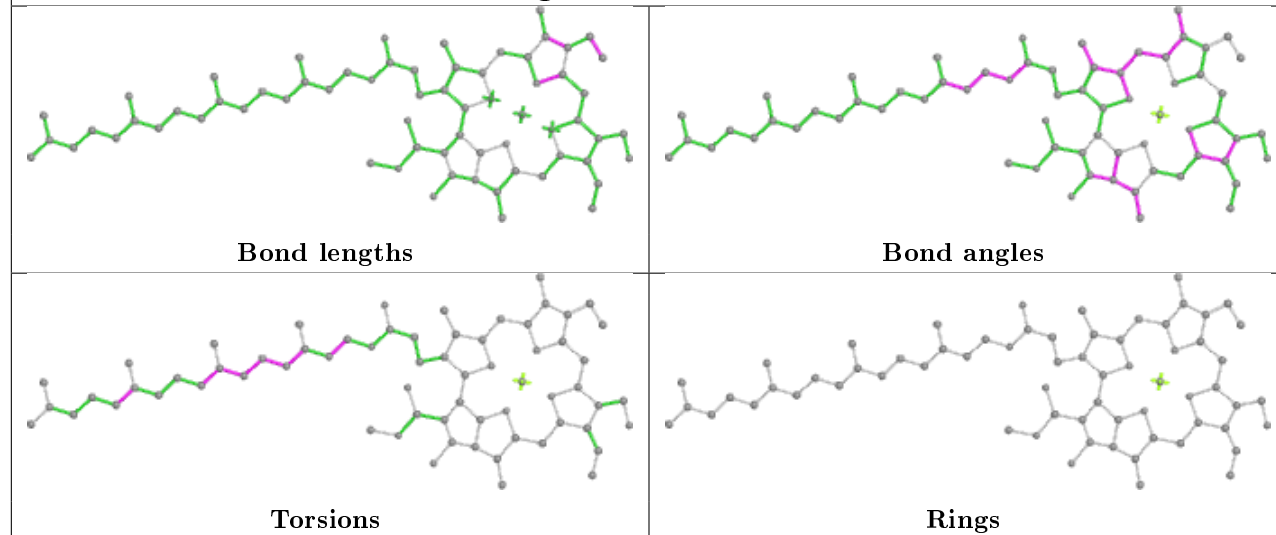
Bond angles

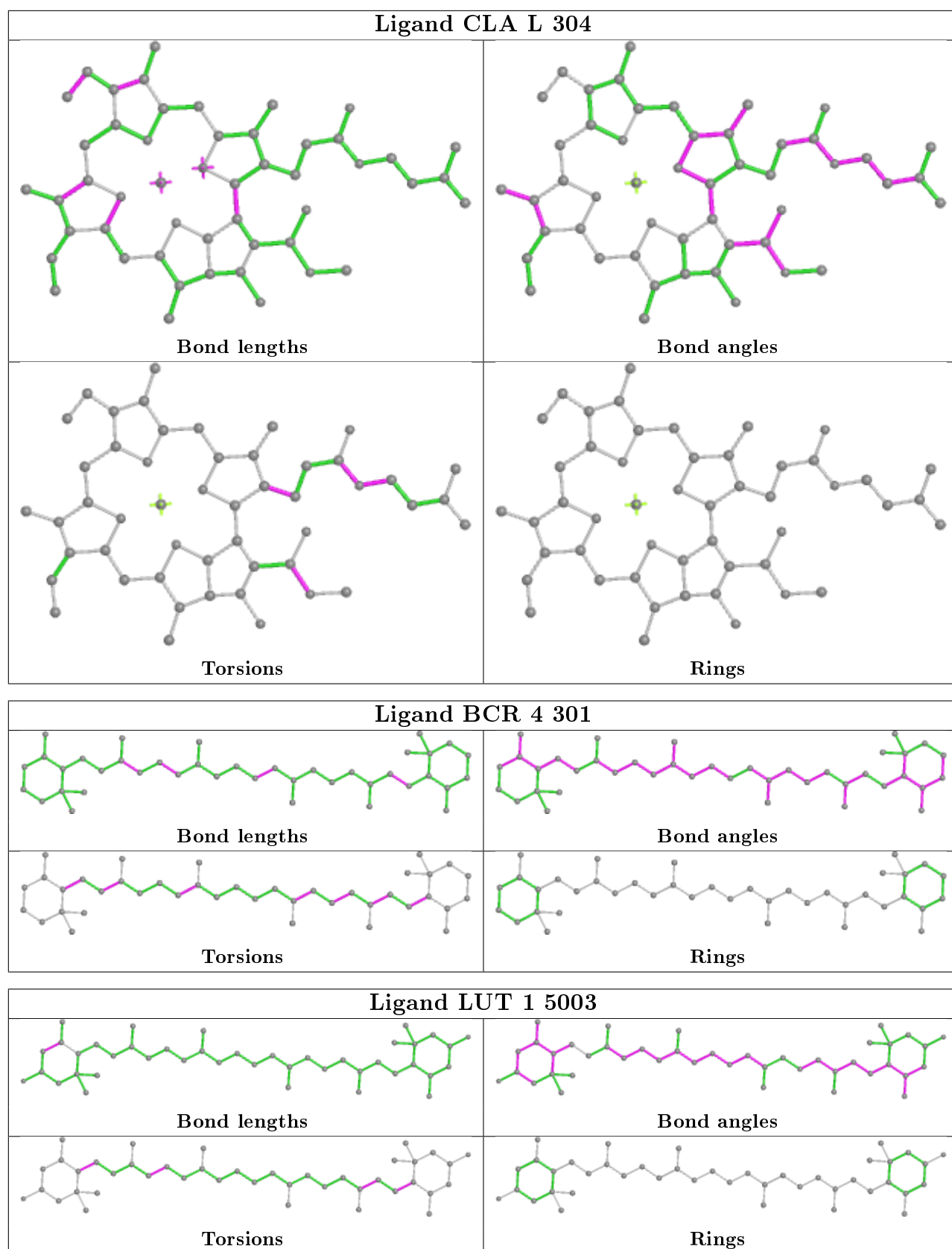


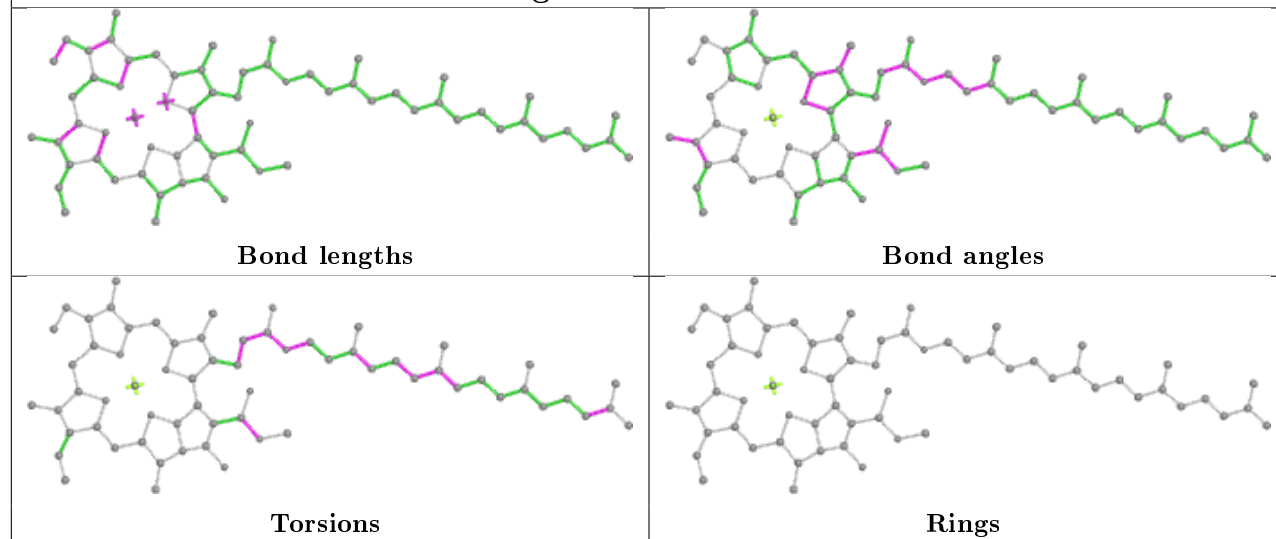
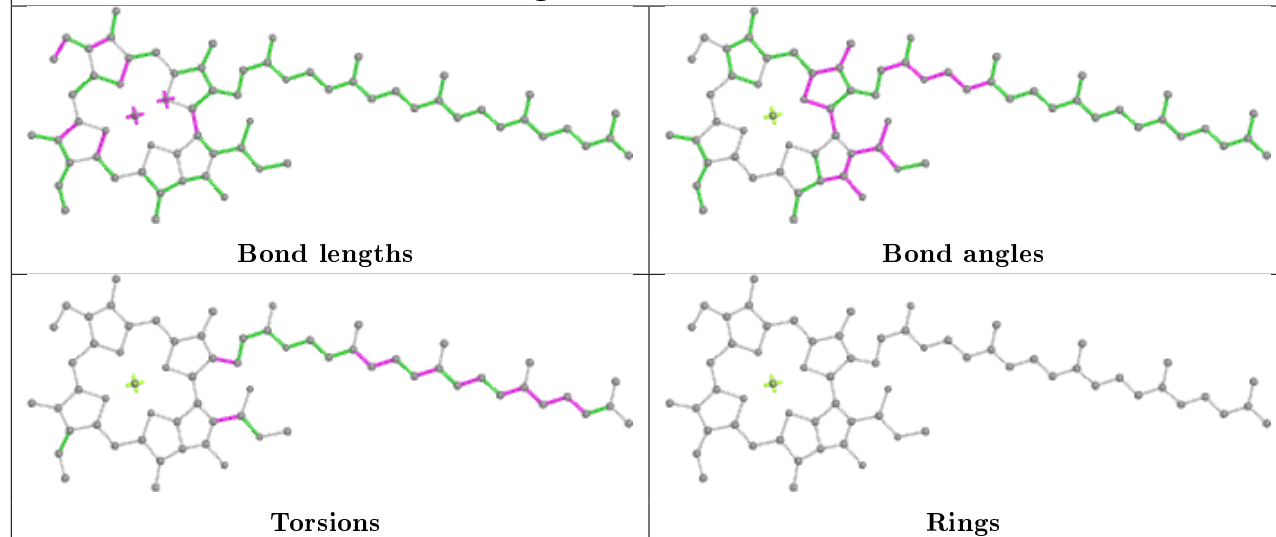
Torsions



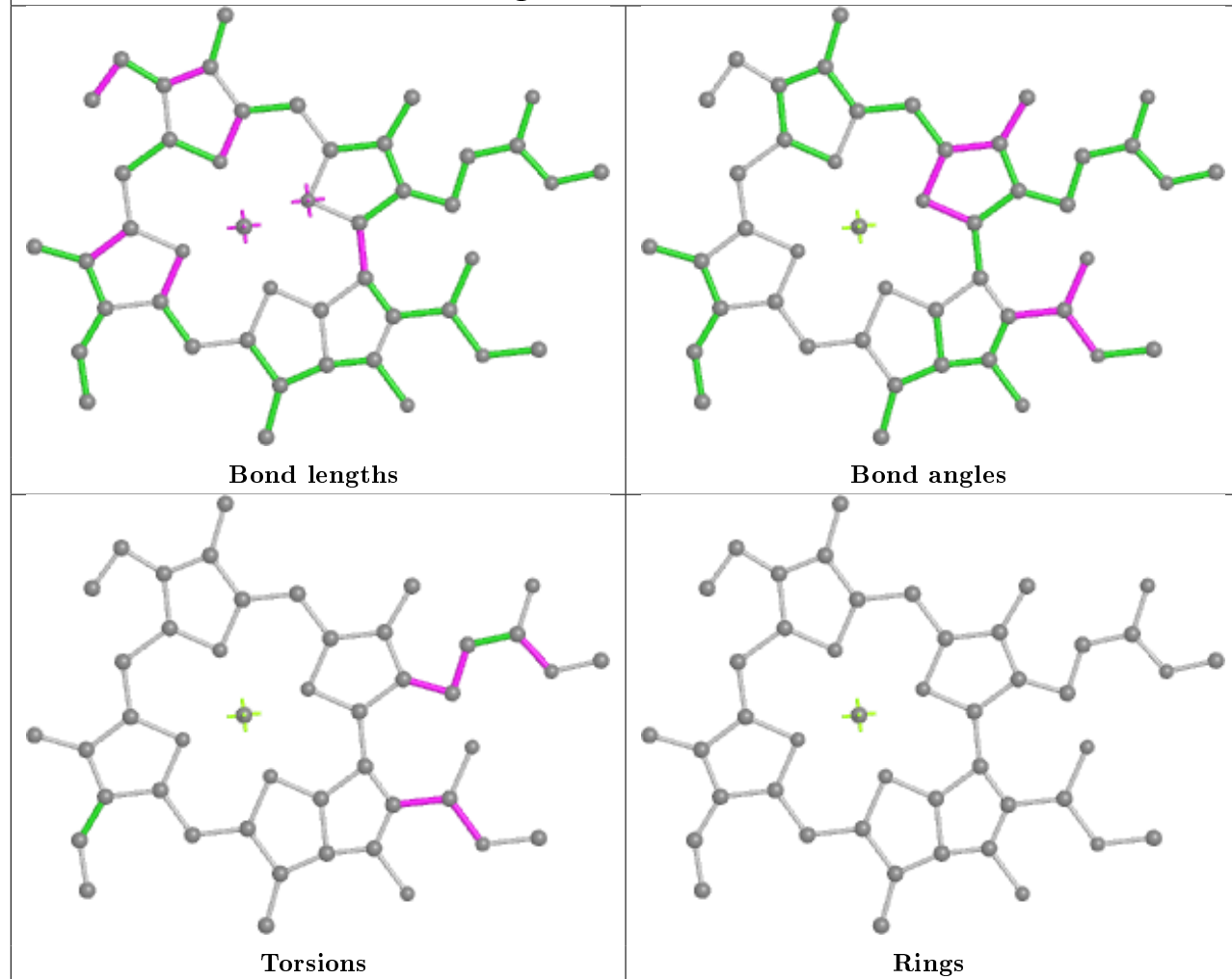
Rings

Ligand CLA 3 315**Ligand CHL 2 314**

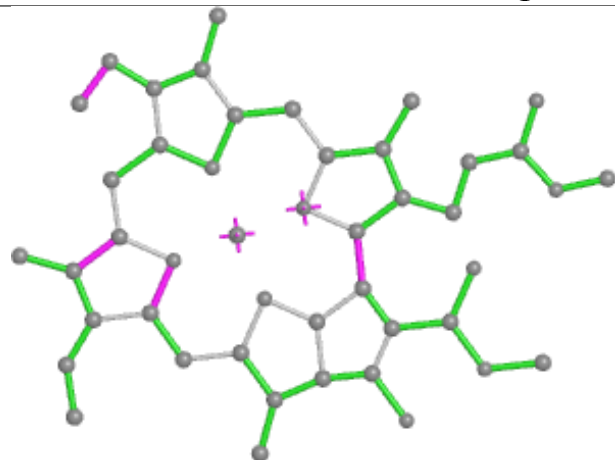


Ligand CLA B 839**Ligand CLA B 801**

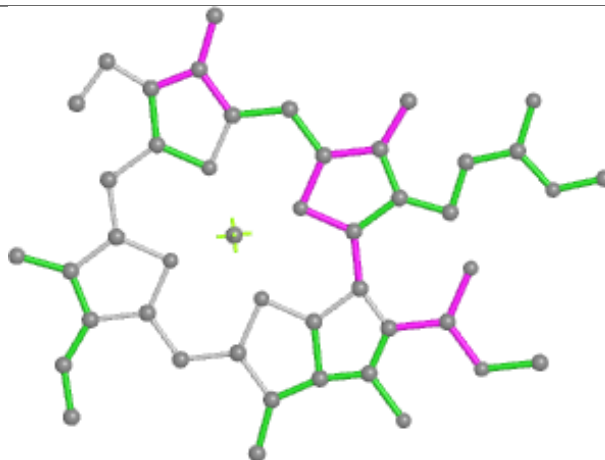
Ligand CLA B 821



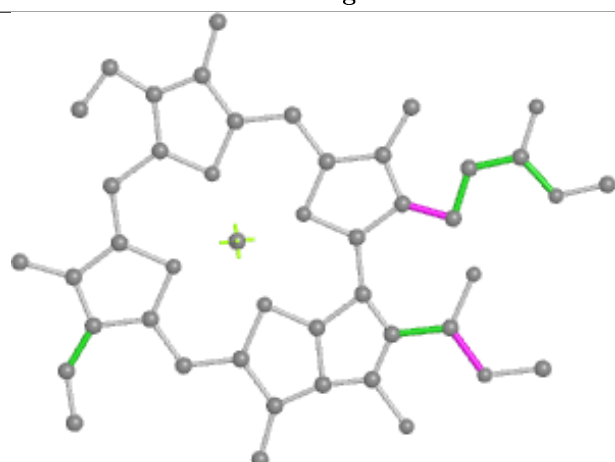
Ligand CLA B 813



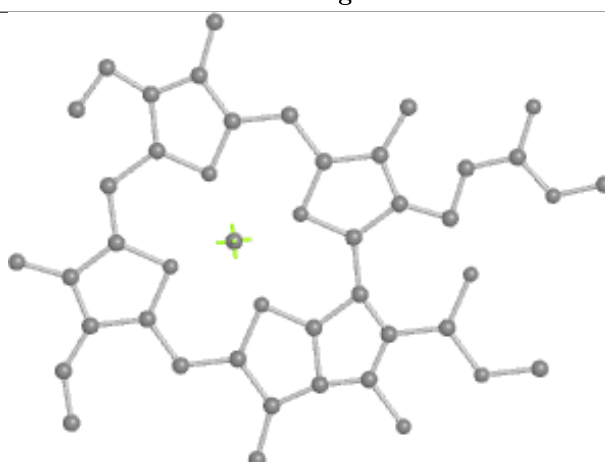
Bond lengths



Bond angles

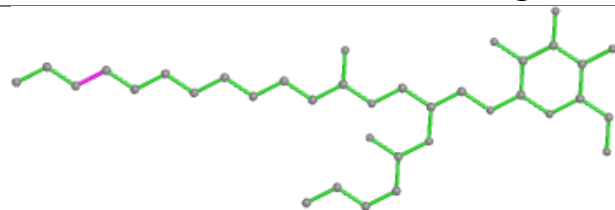


Torsions

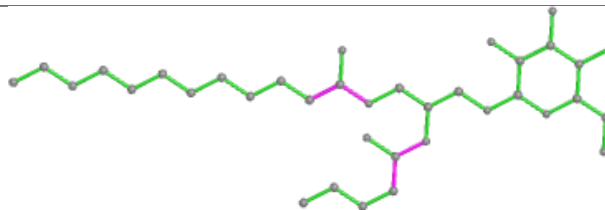


Rings

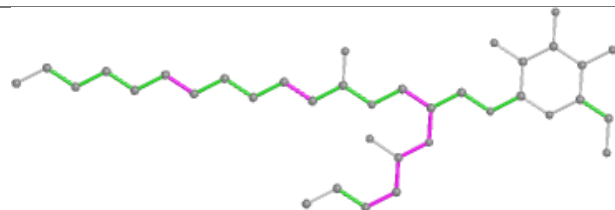
Ligand LMG F 307



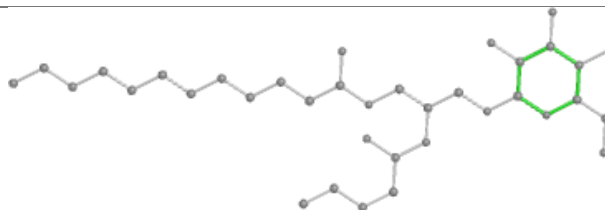
Bond lengths



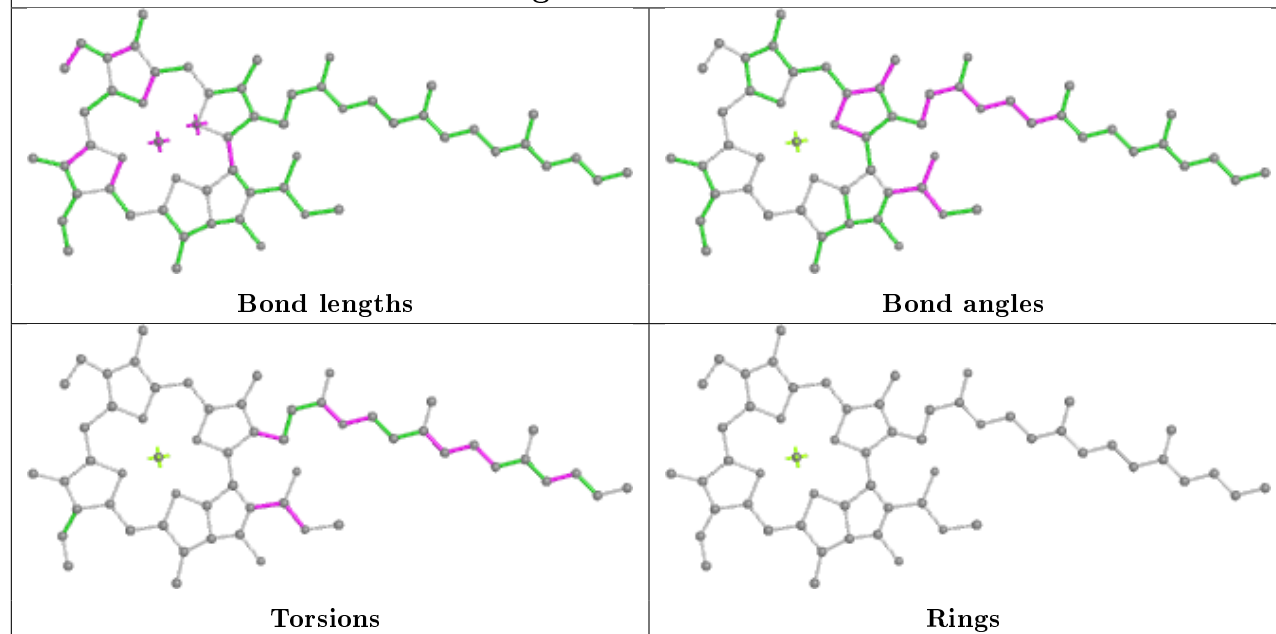
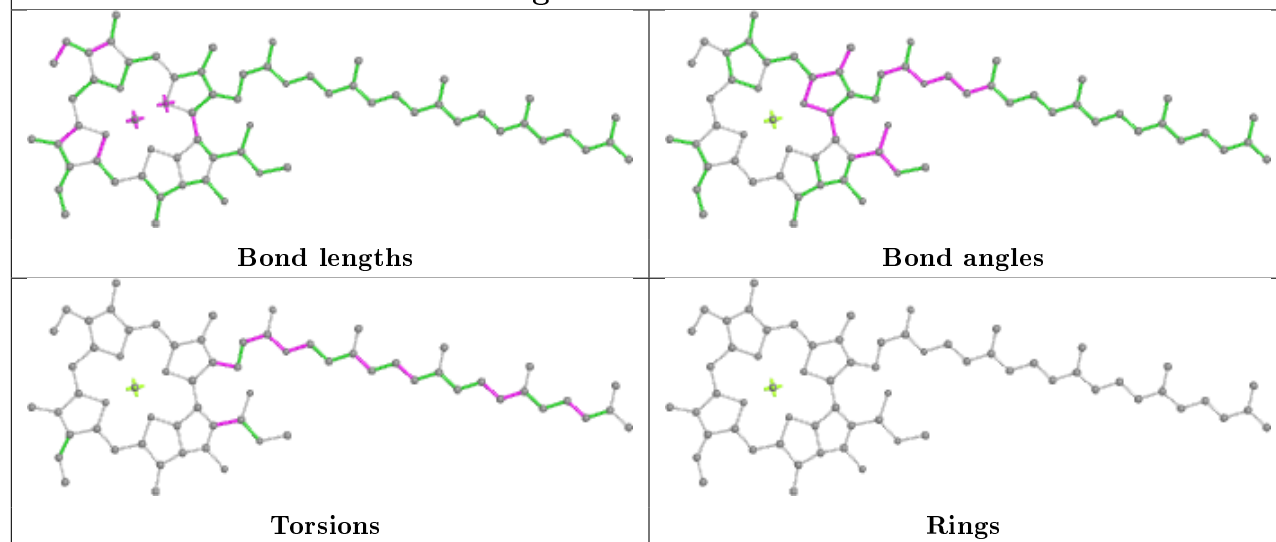
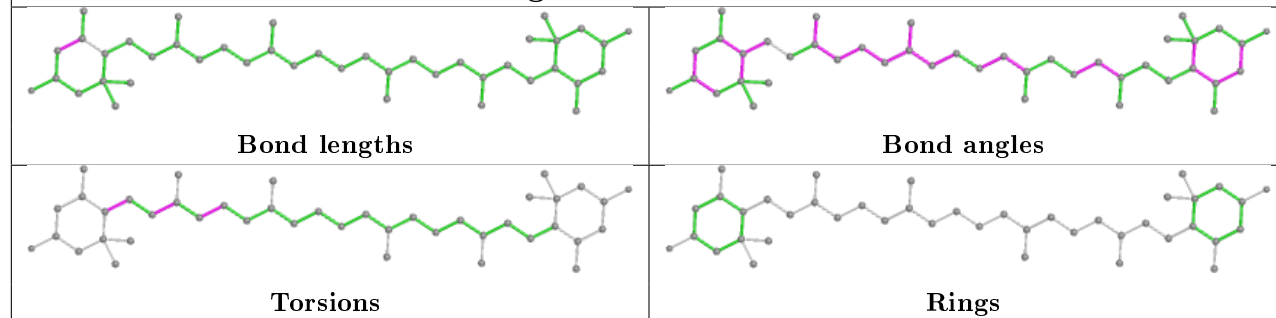
Bond angles

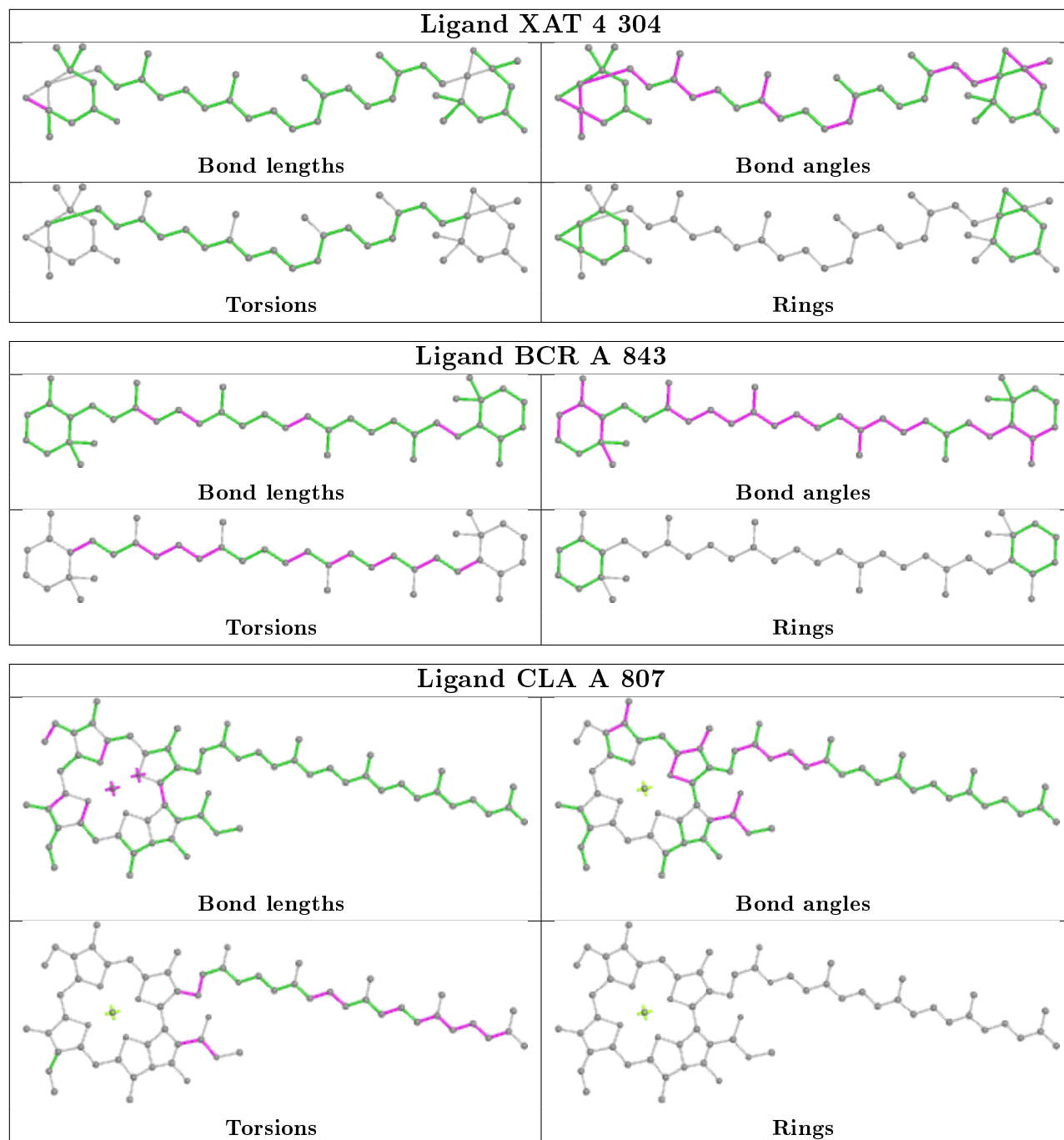


Torsions

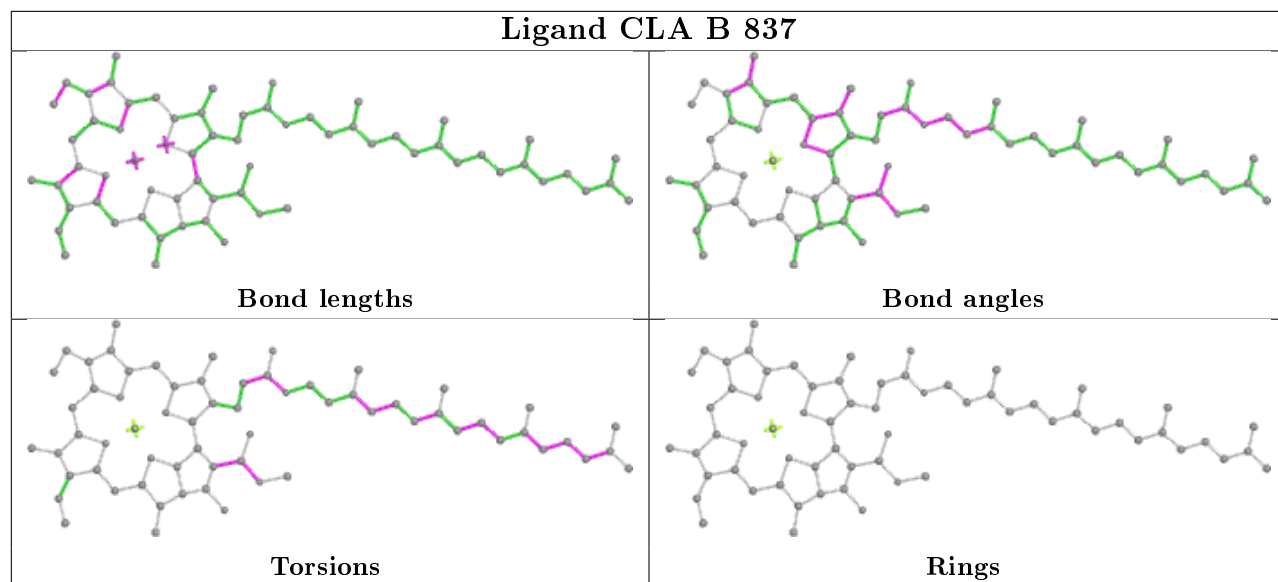


Rings

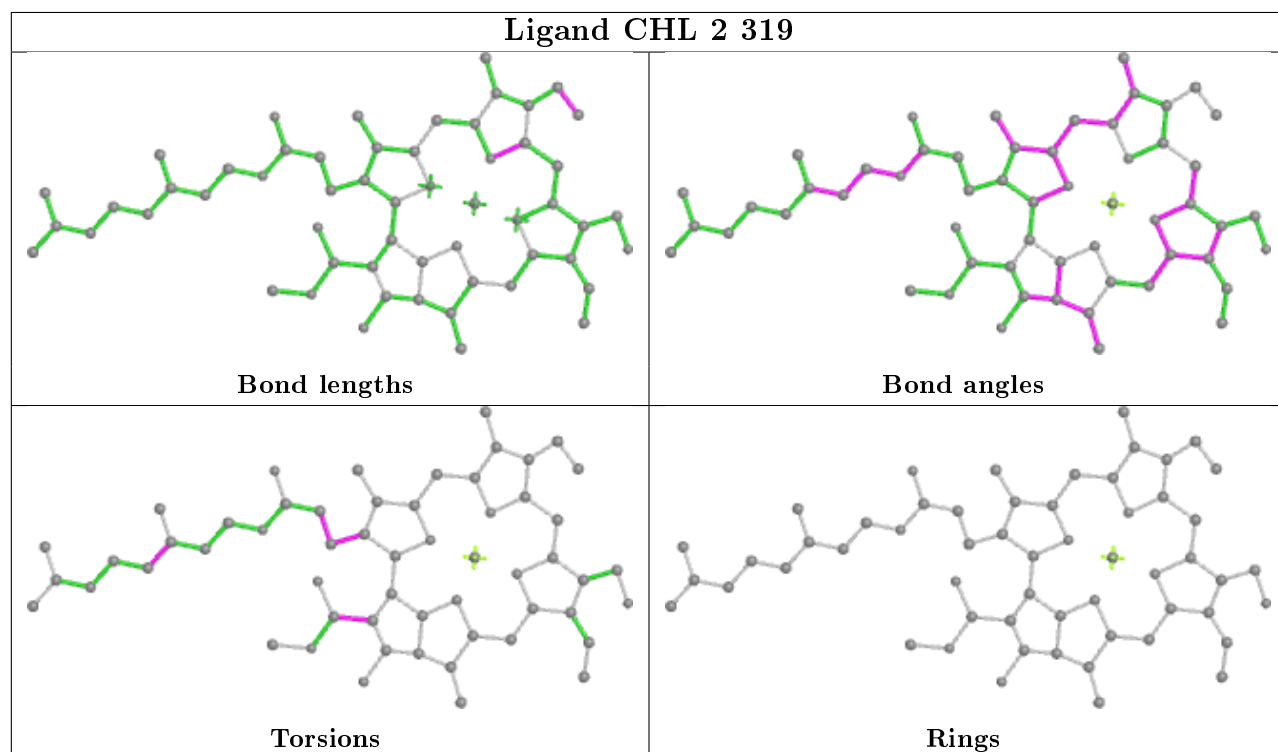
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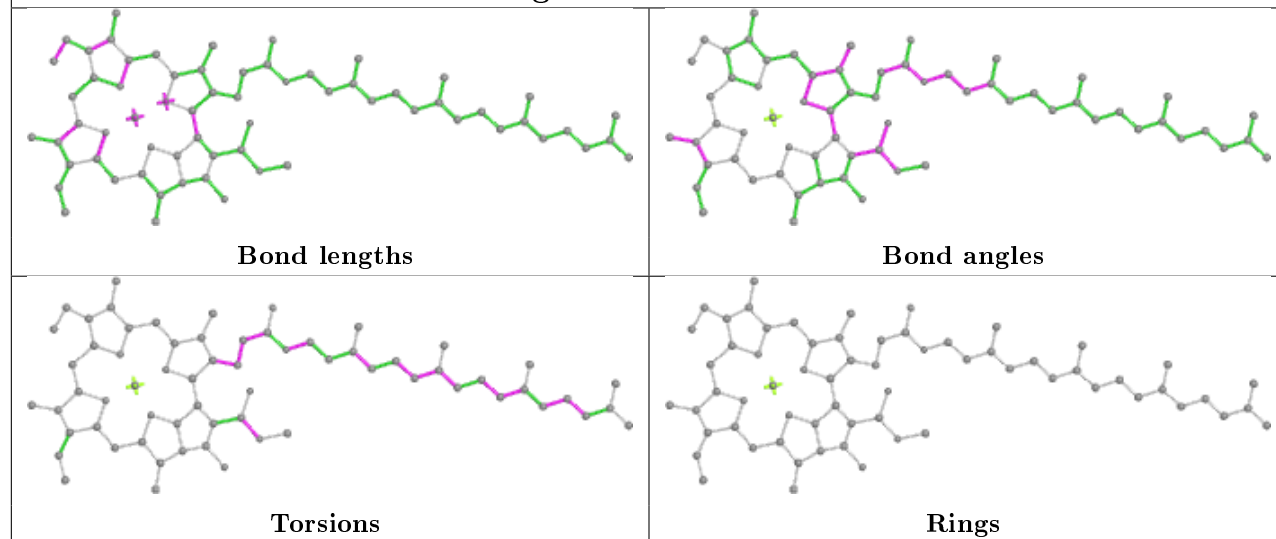
Ligand CLA B 837



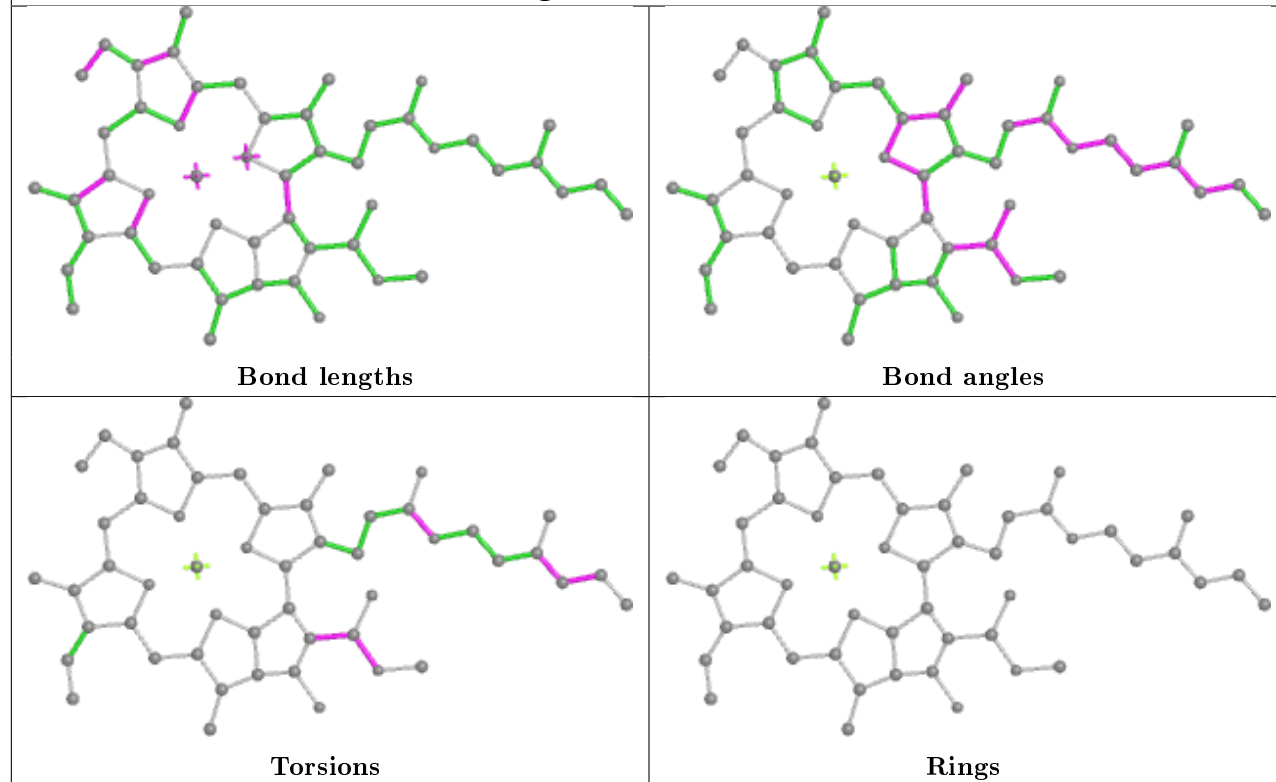
Ligand CHL 2 319



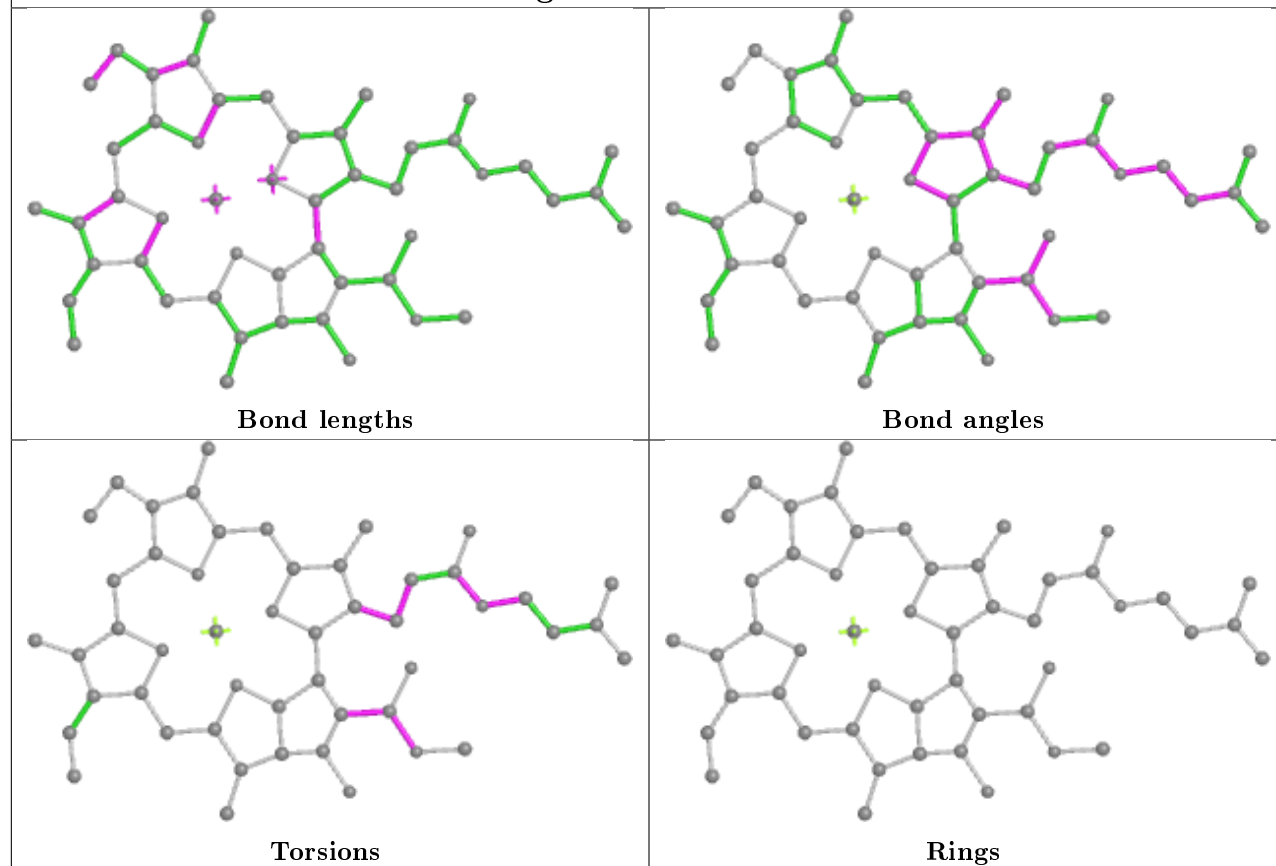
Ligand CLA B 840



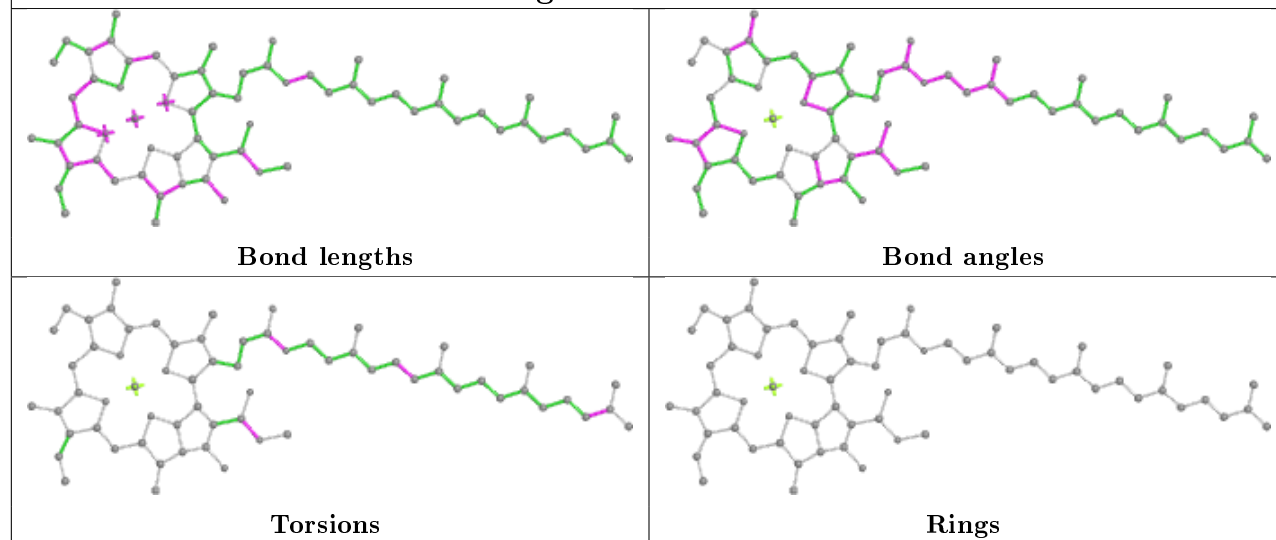
Ligand CLA 2 307



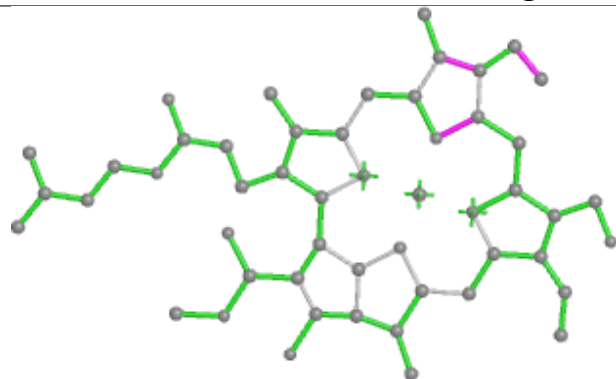
Ligand CLA 2 311



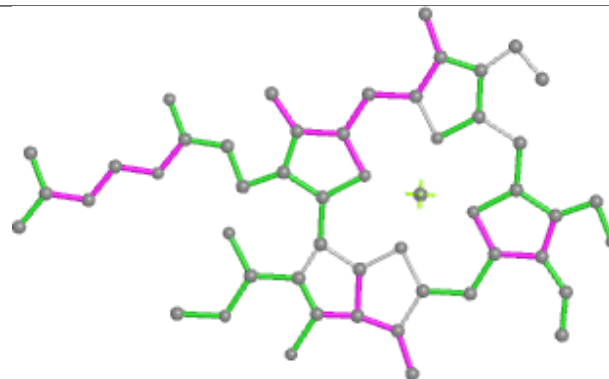
Ligand CL0 A 801



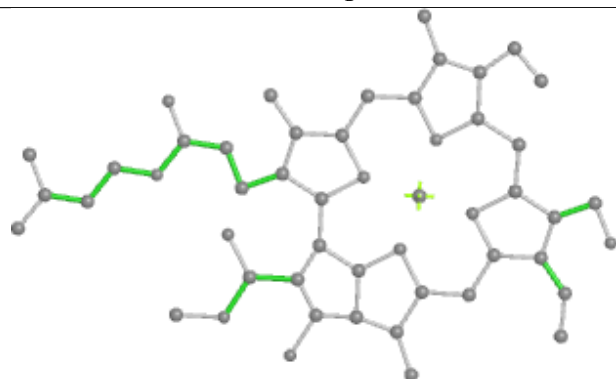
Ligand CHL 4 314



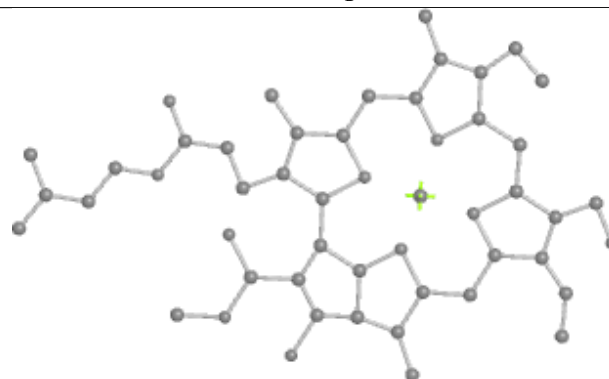
Bond lengths



Bond angles

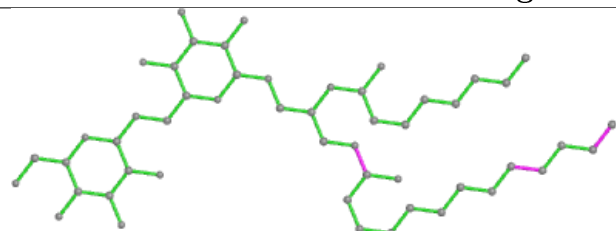


Torsions

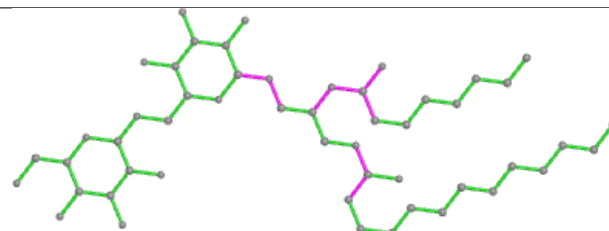


Rings

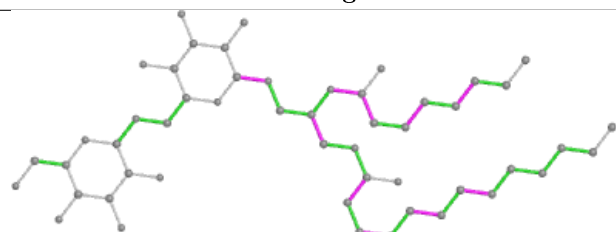
Ligand DGD 2 327



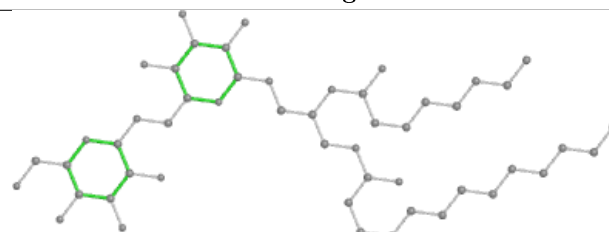
Bond lengths



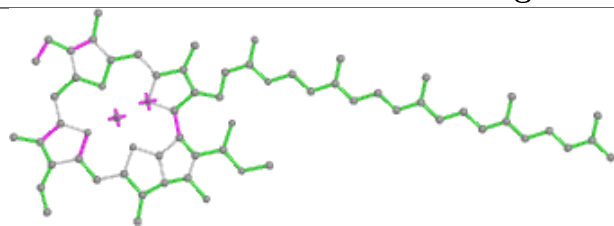
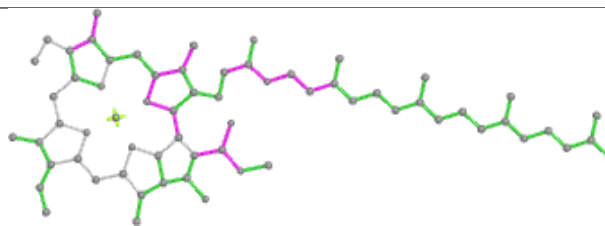
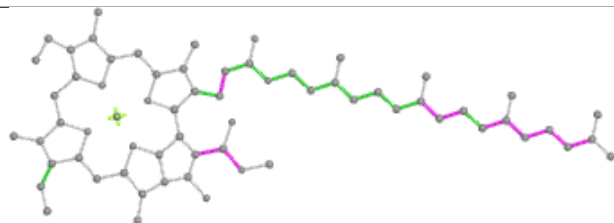
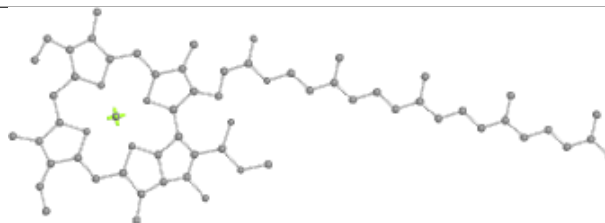
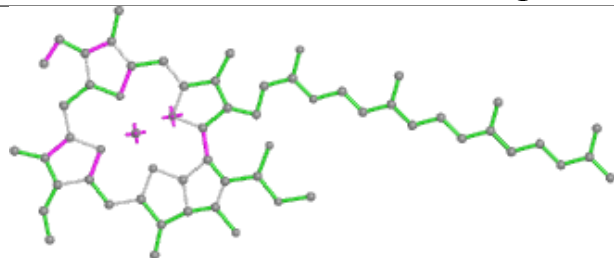
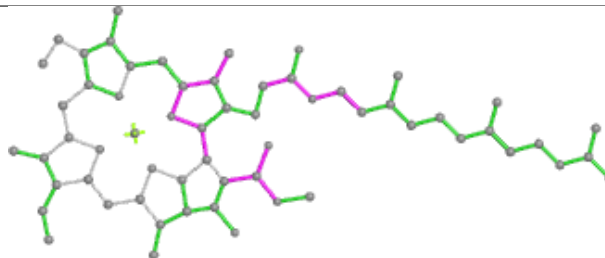
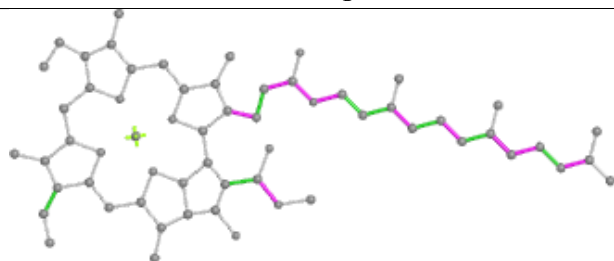
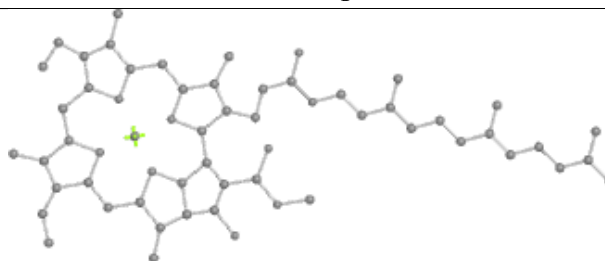
Bond angles

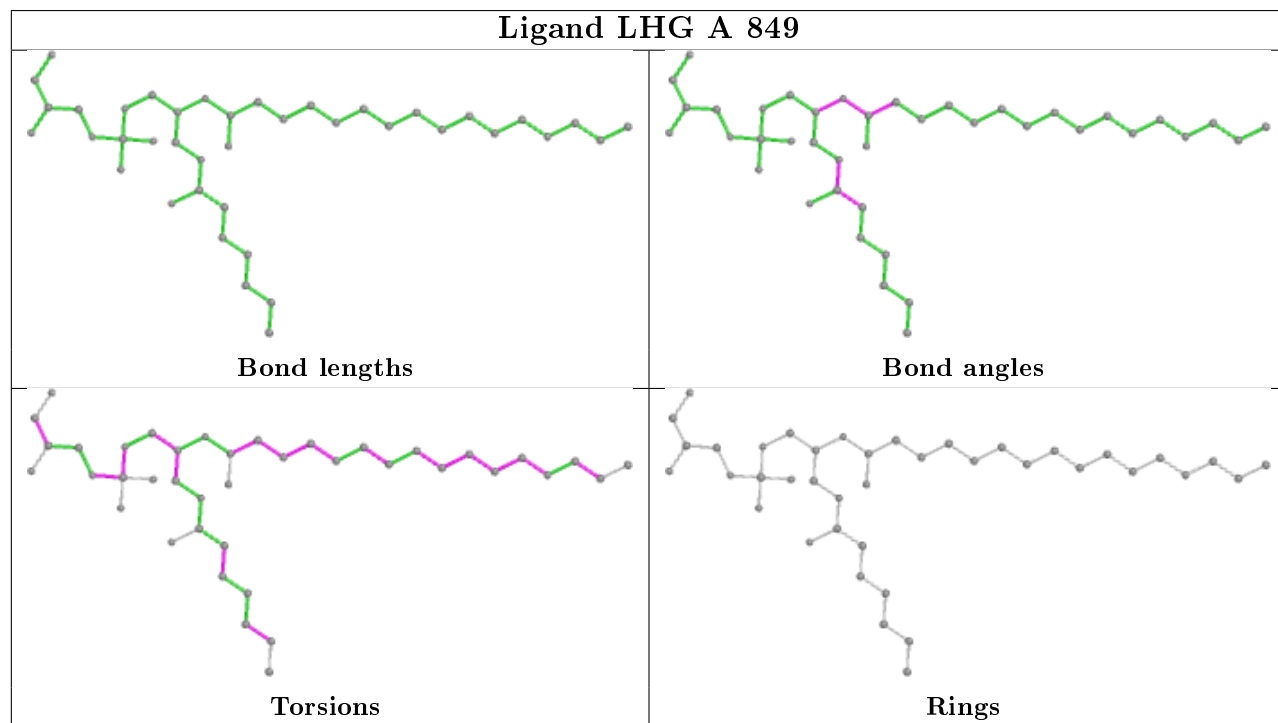
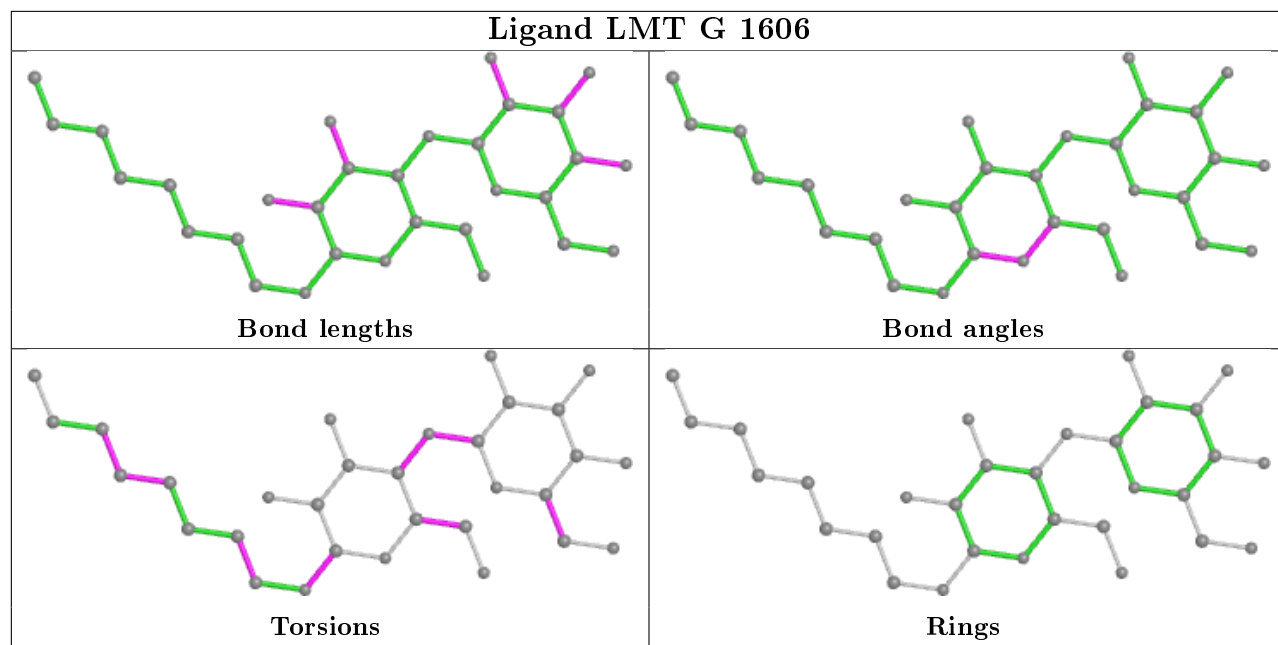


Torsions

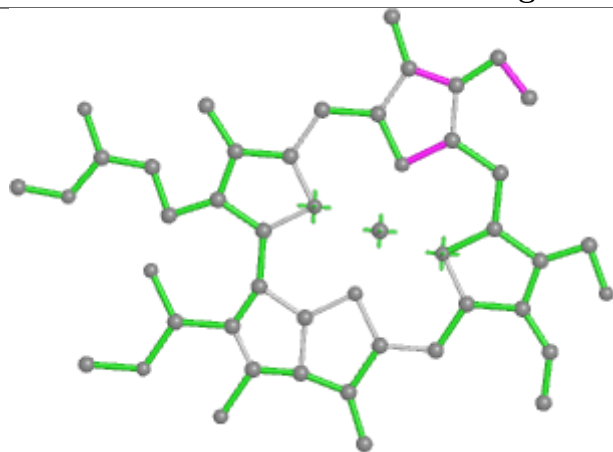


Rings

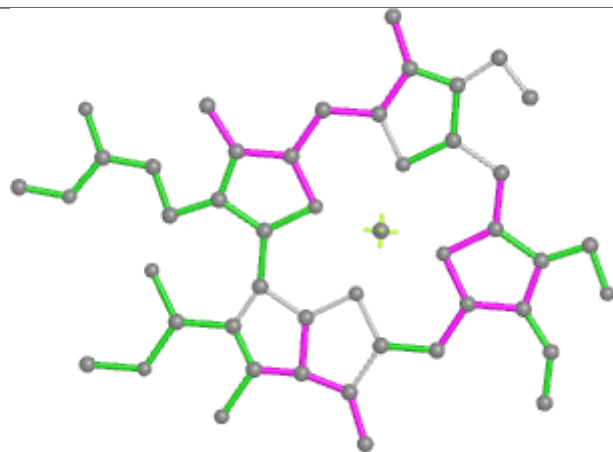
Ligand CLA B 804**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 820****Bond lengths****Bond angles****Torsions****Rings**



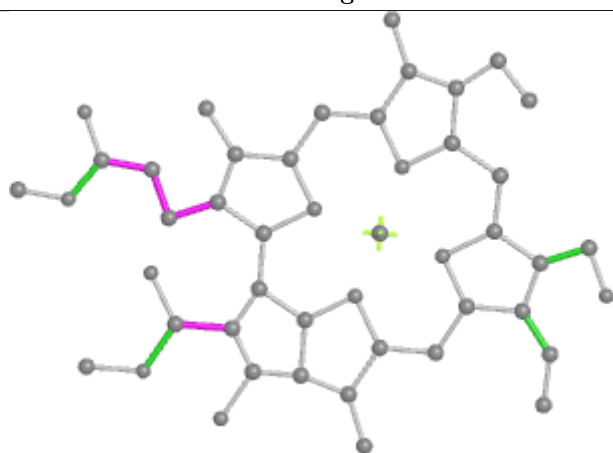
Ligand CHL 3 316



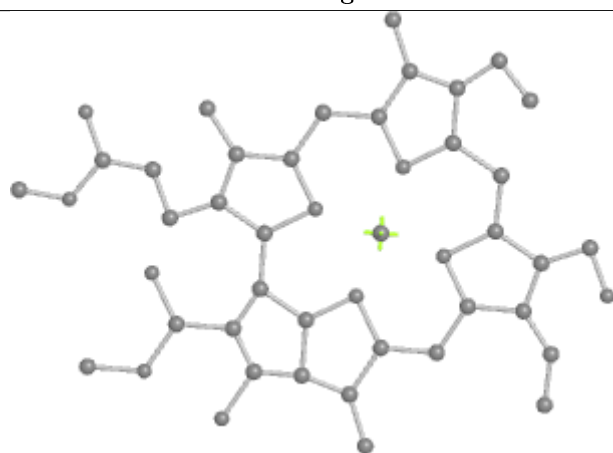
Bond lengths



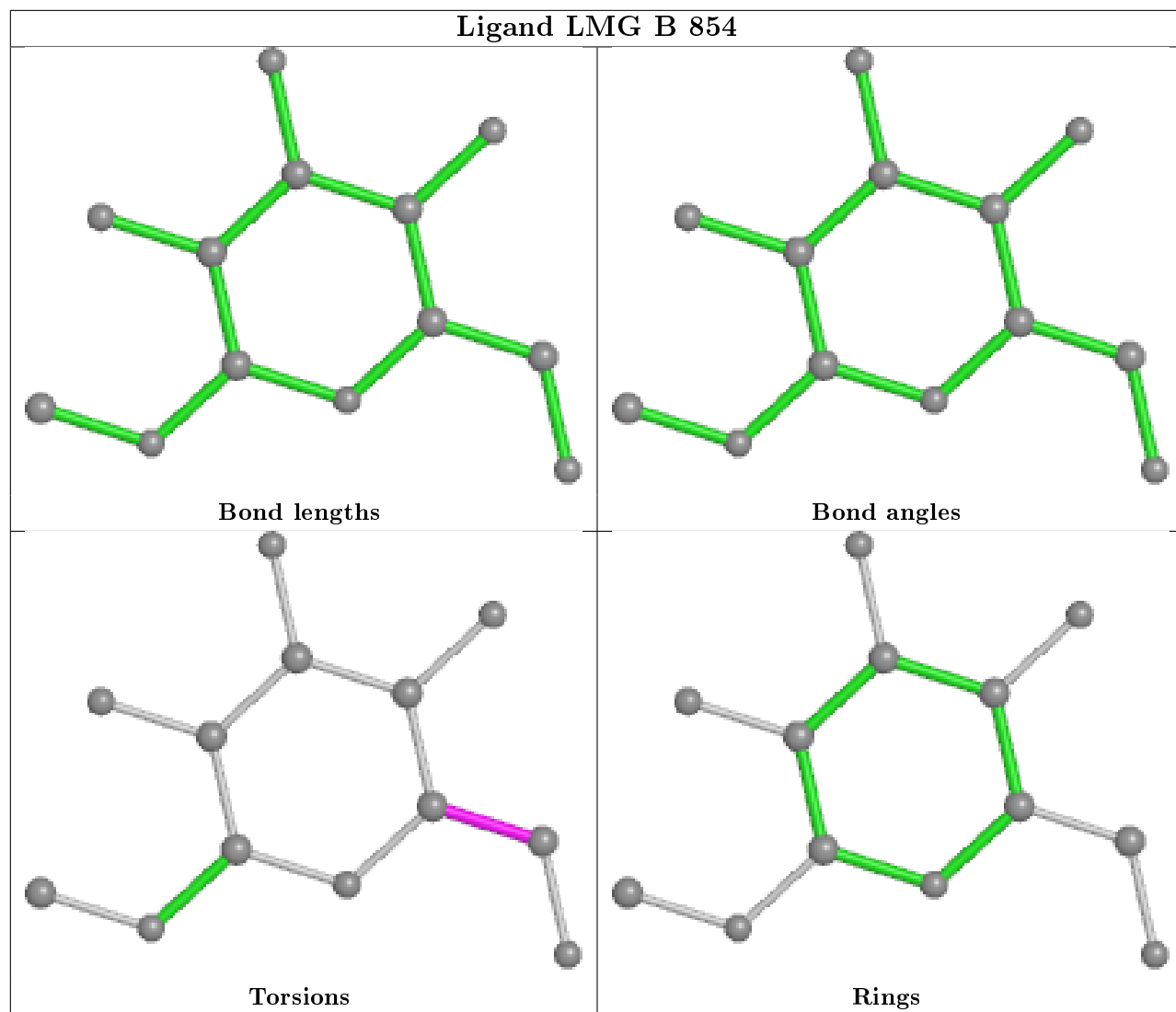
Bond angles



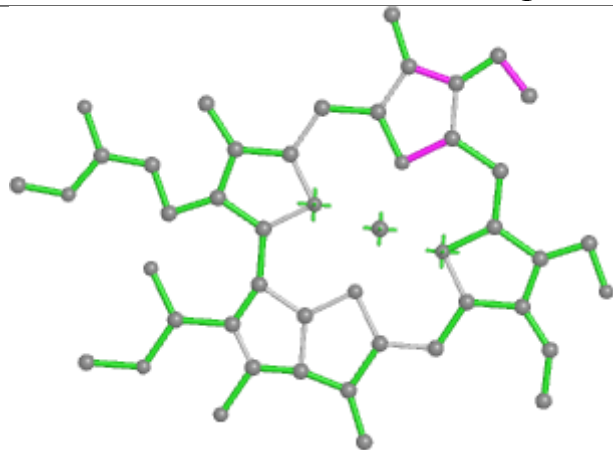
Torsions



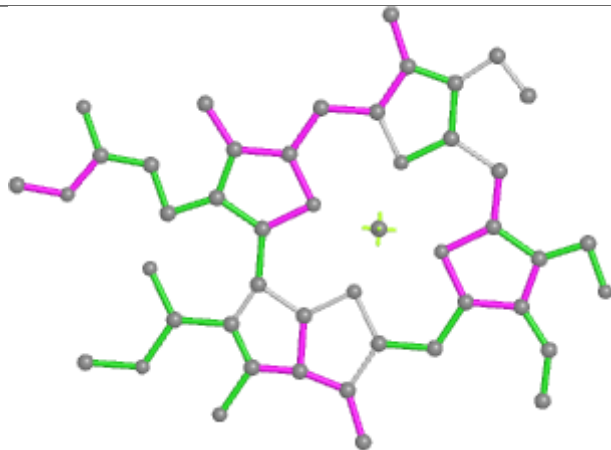
Rings



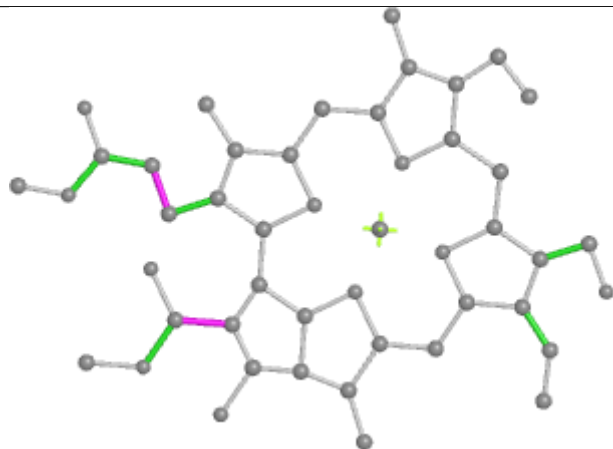
Ligand CHL 4 313



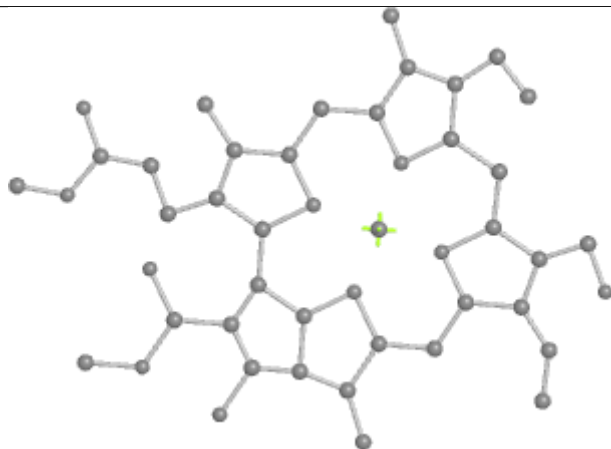
Bond lengths



Bond angles

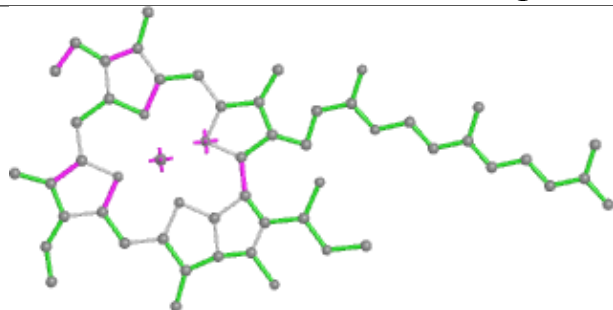


Torsions

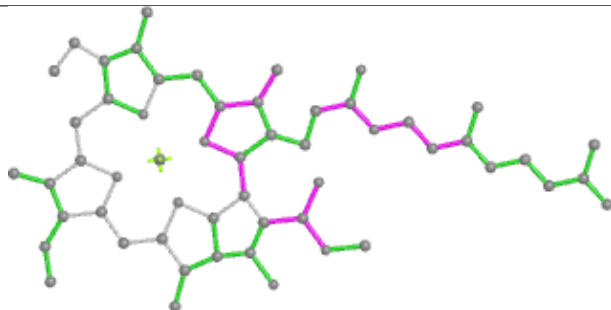


Rings

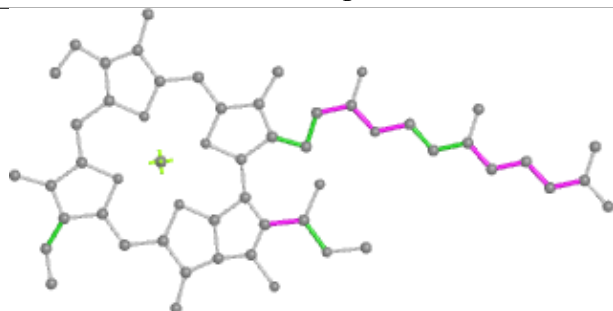
Ligand CLA B 824



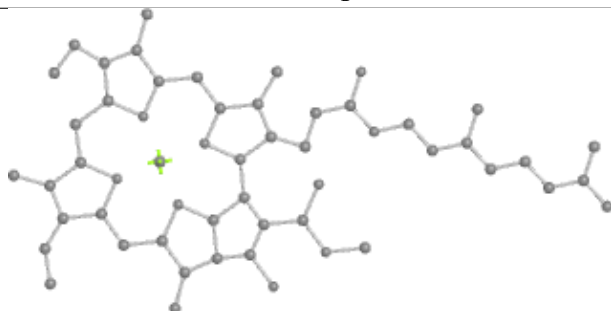
Bond lengths



Bond angles

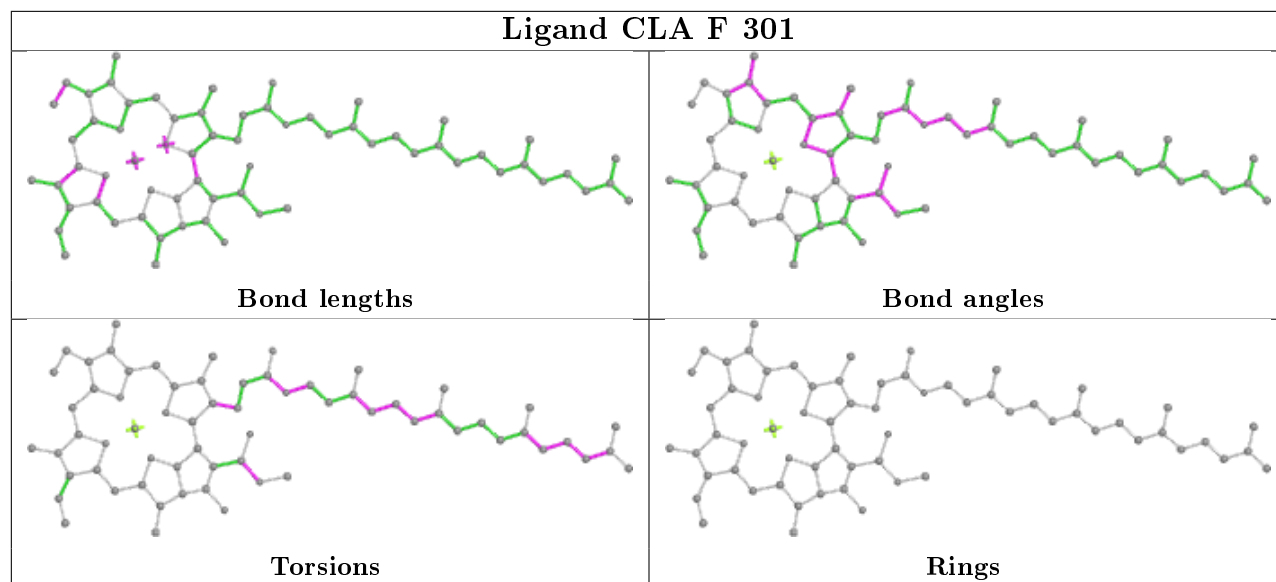


Torsions

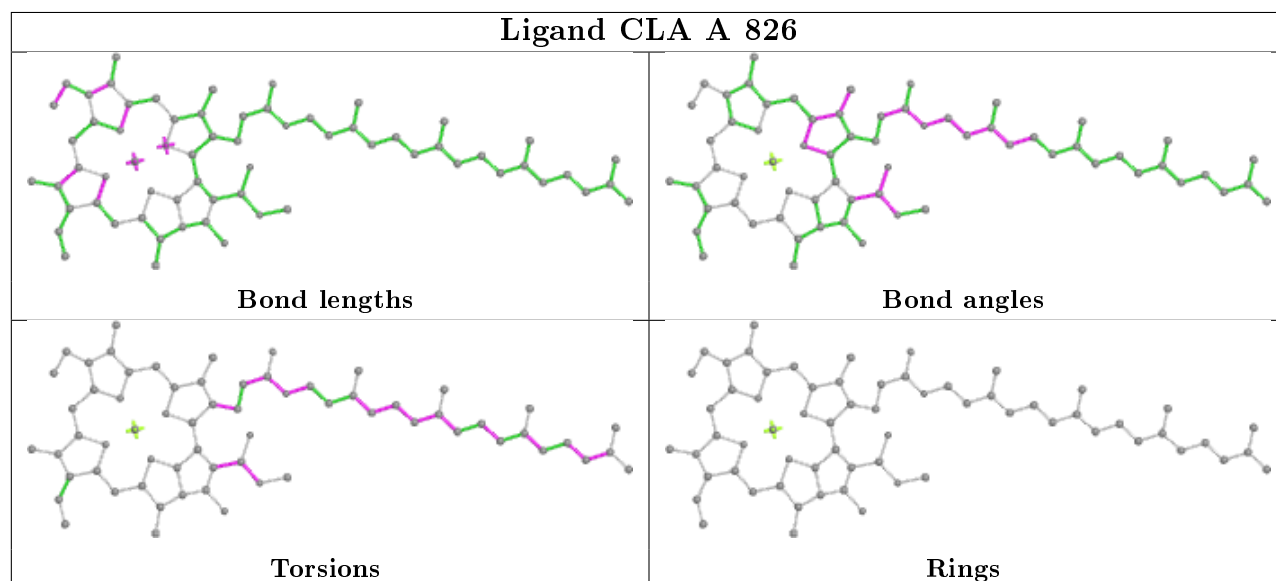


Rings

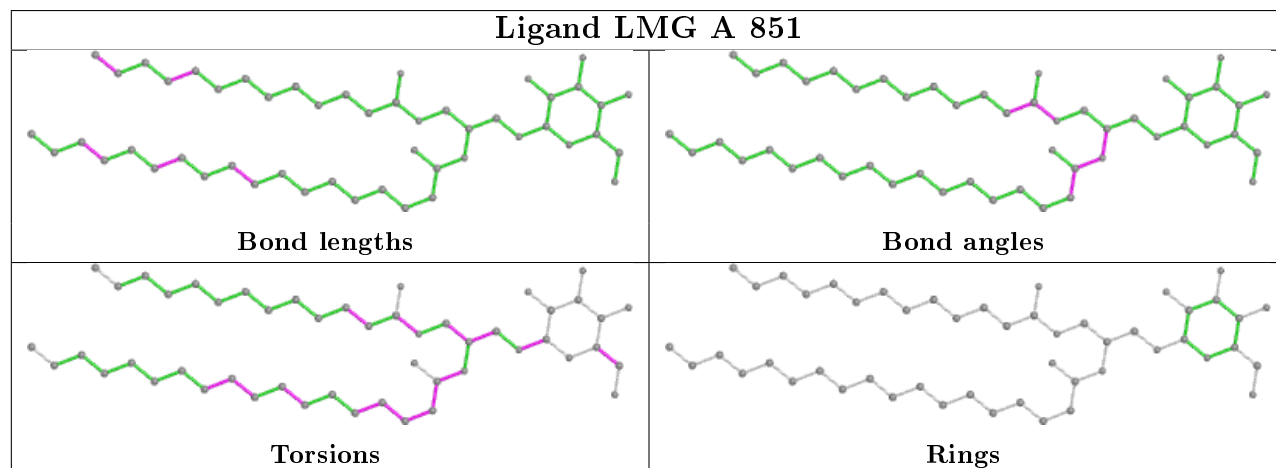
Ligand CLA F 301

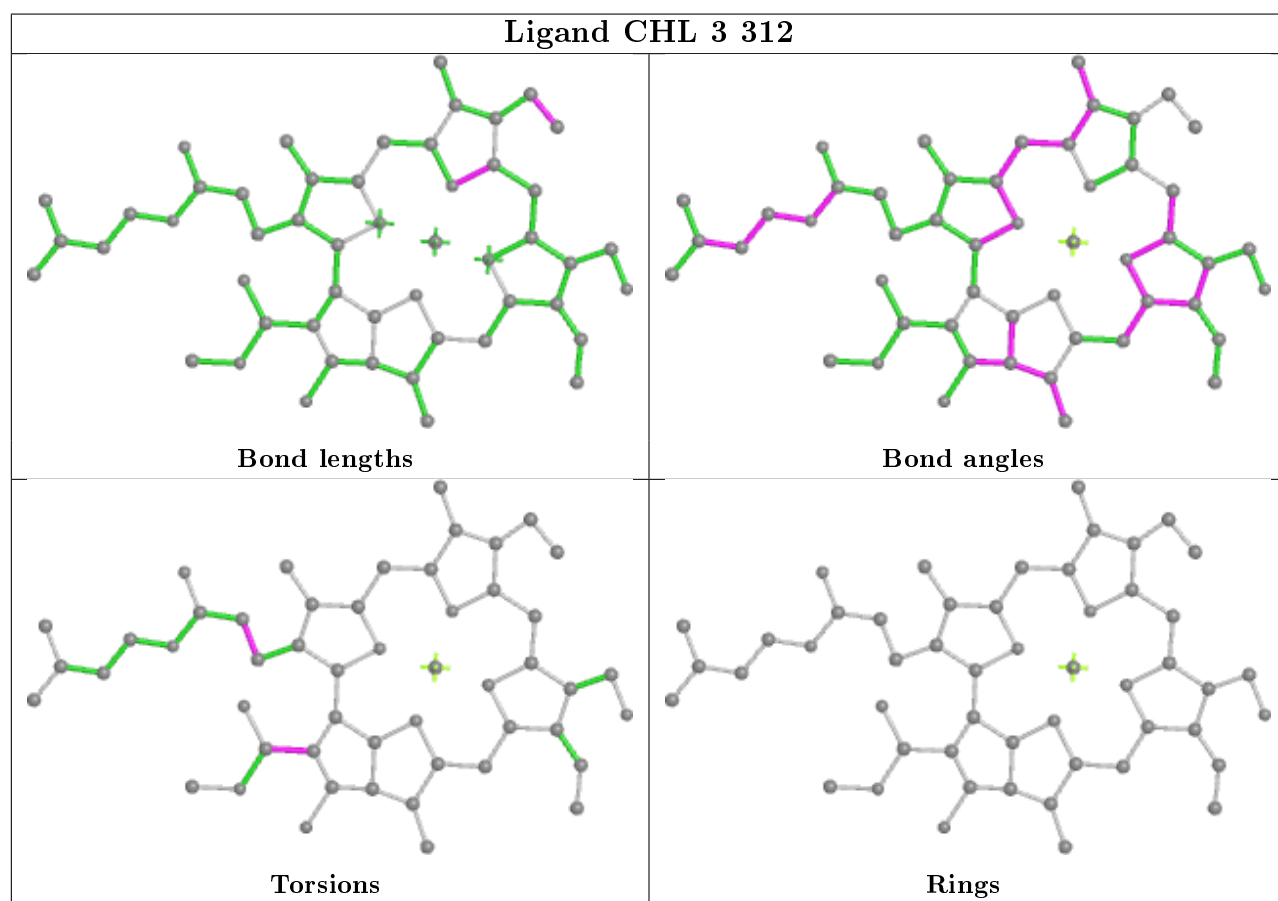
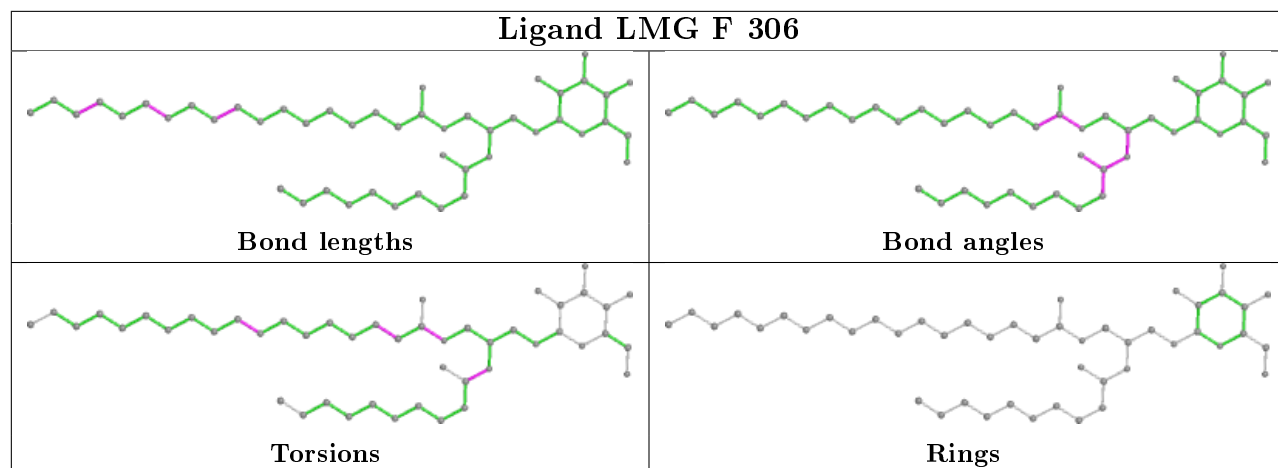


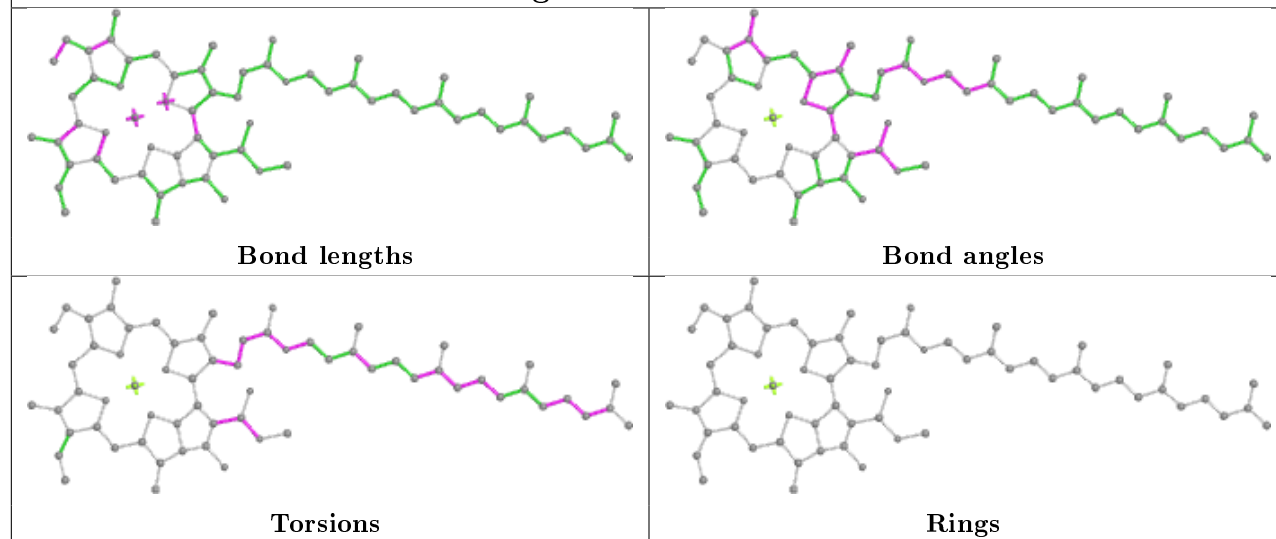
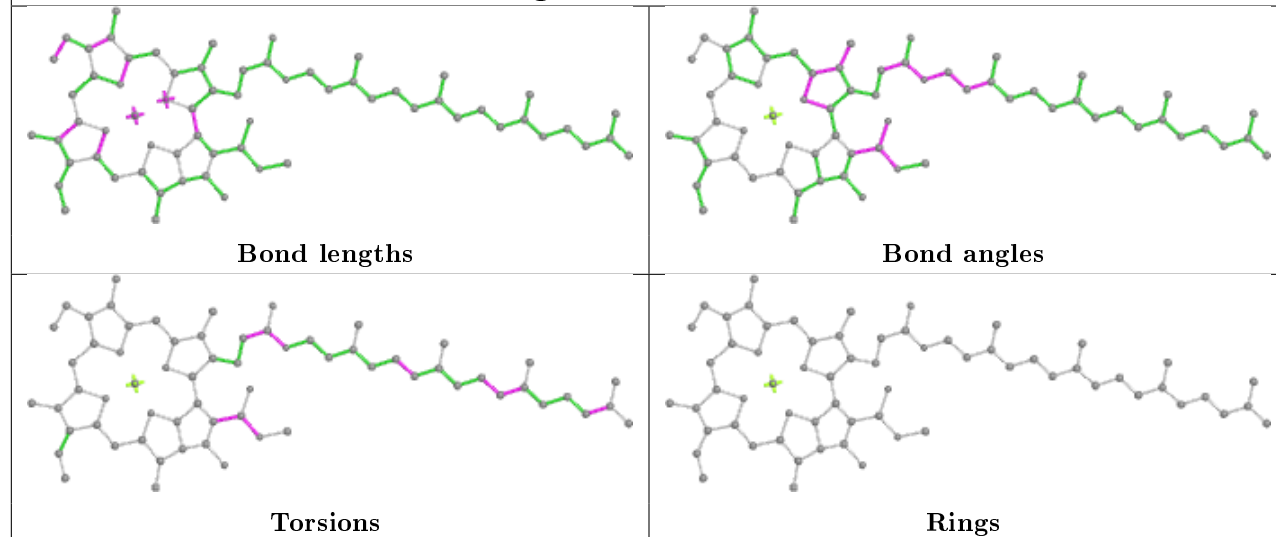
Ligand CLA A 826



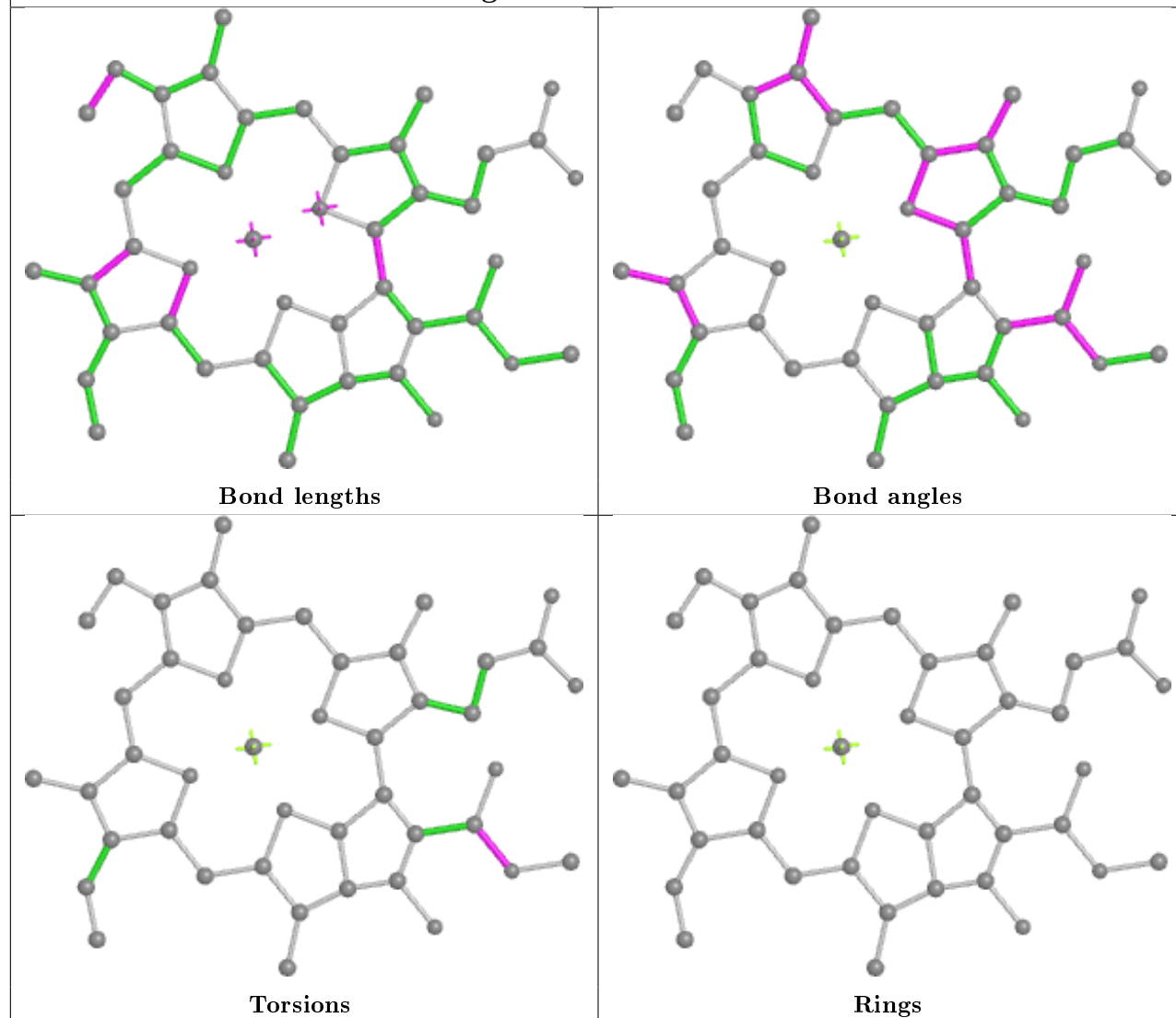
Ligand LMG A 851



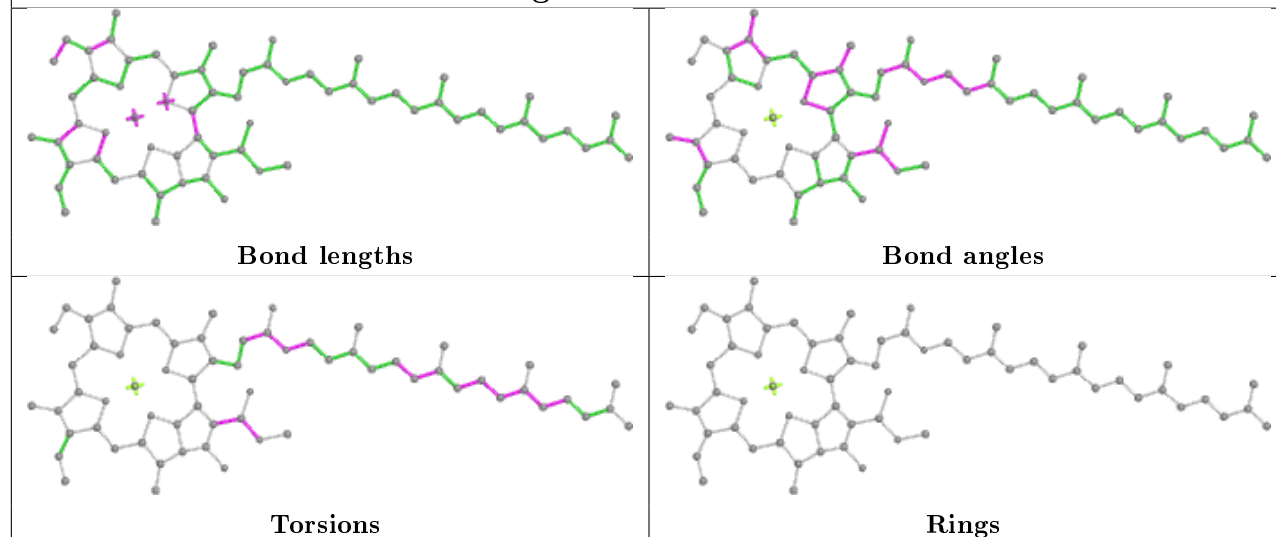


Ligand CLA B 828**Ligand CLA A 835**

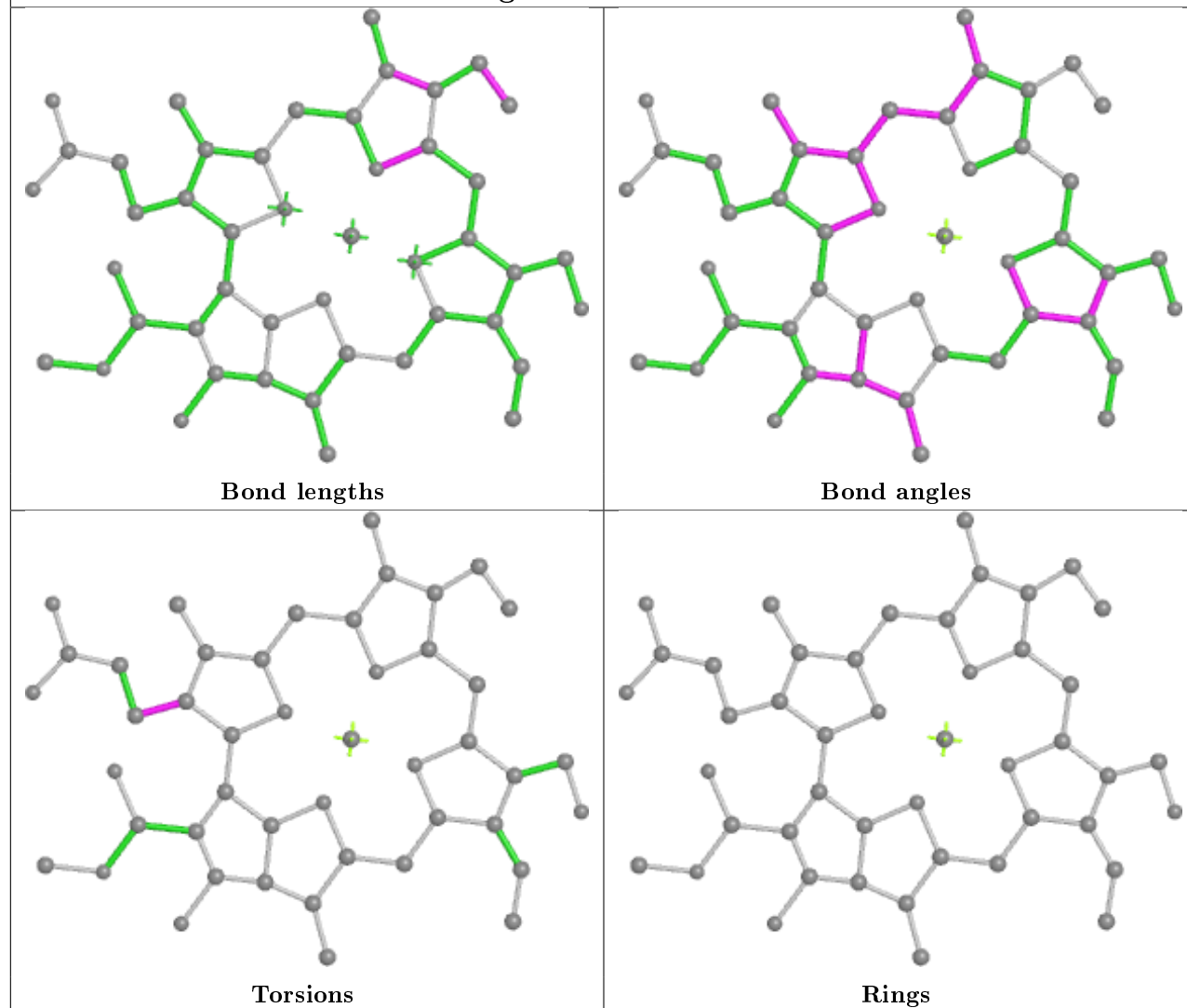
Ligand CLA K 1401



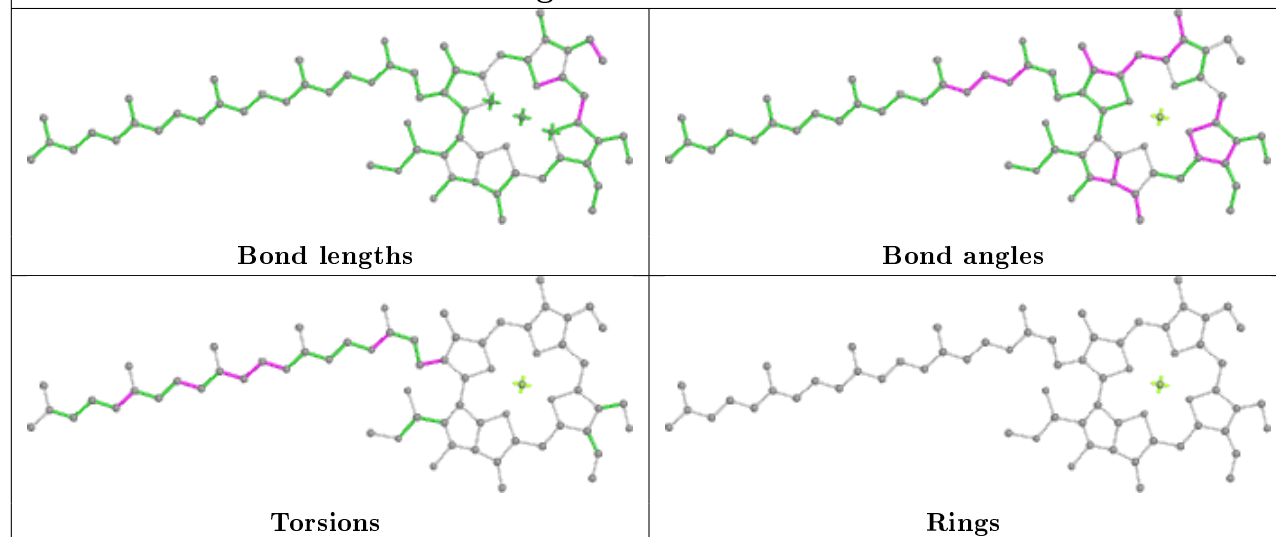
Ligand CLA A 828

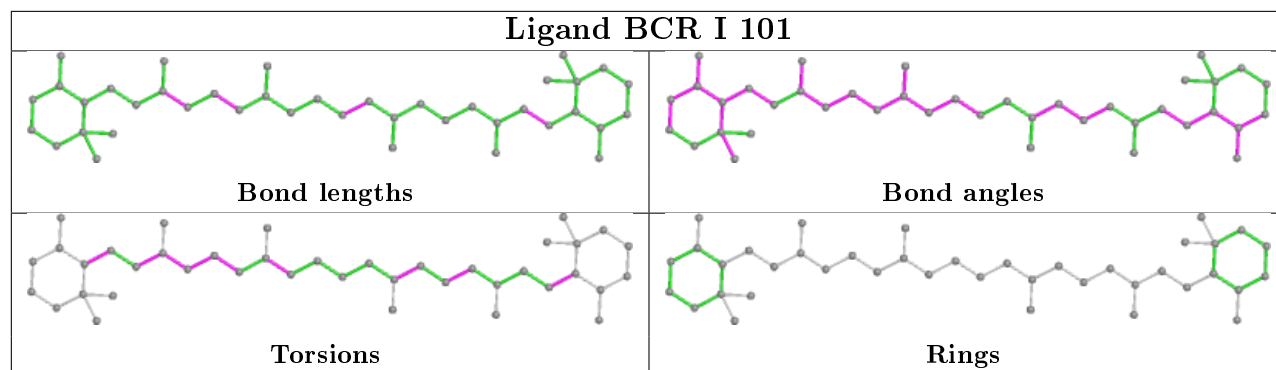
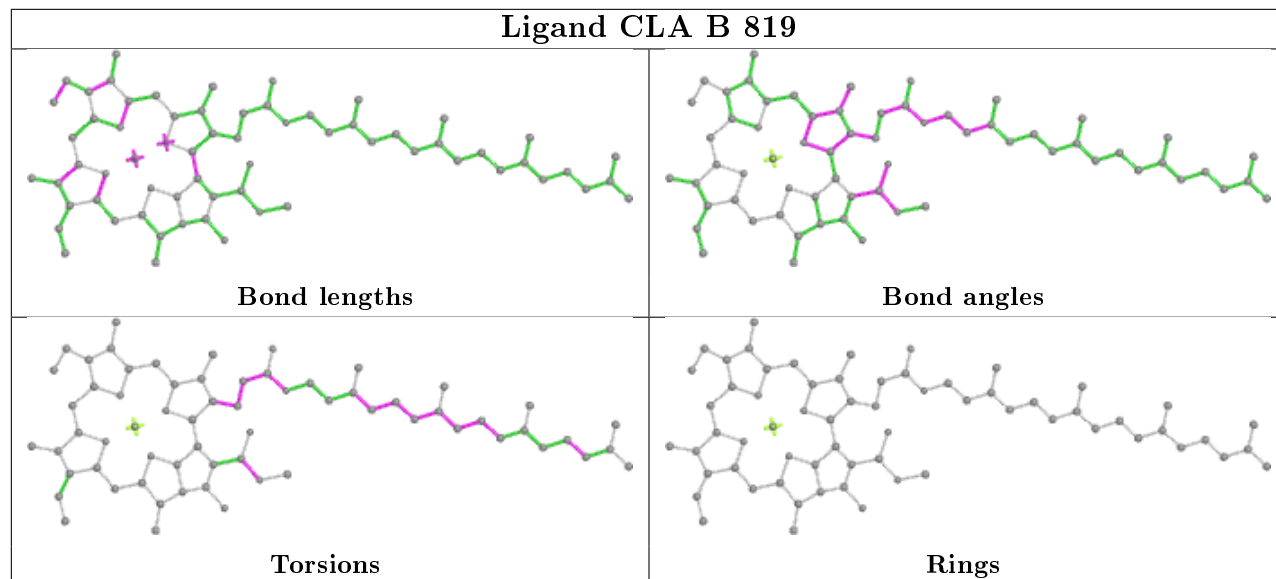
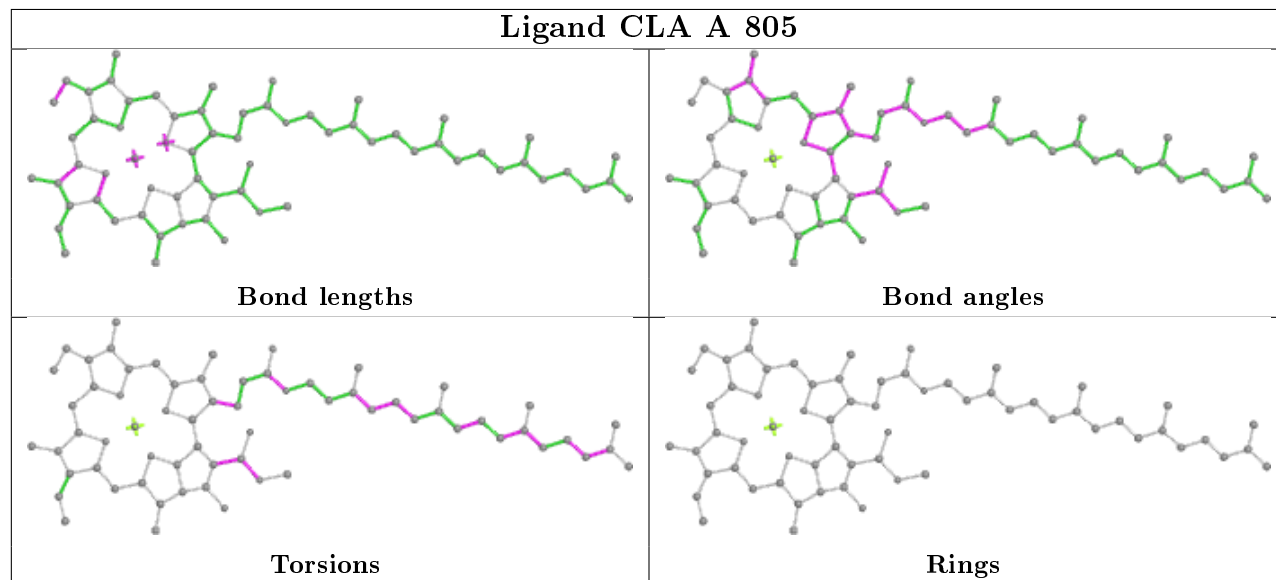


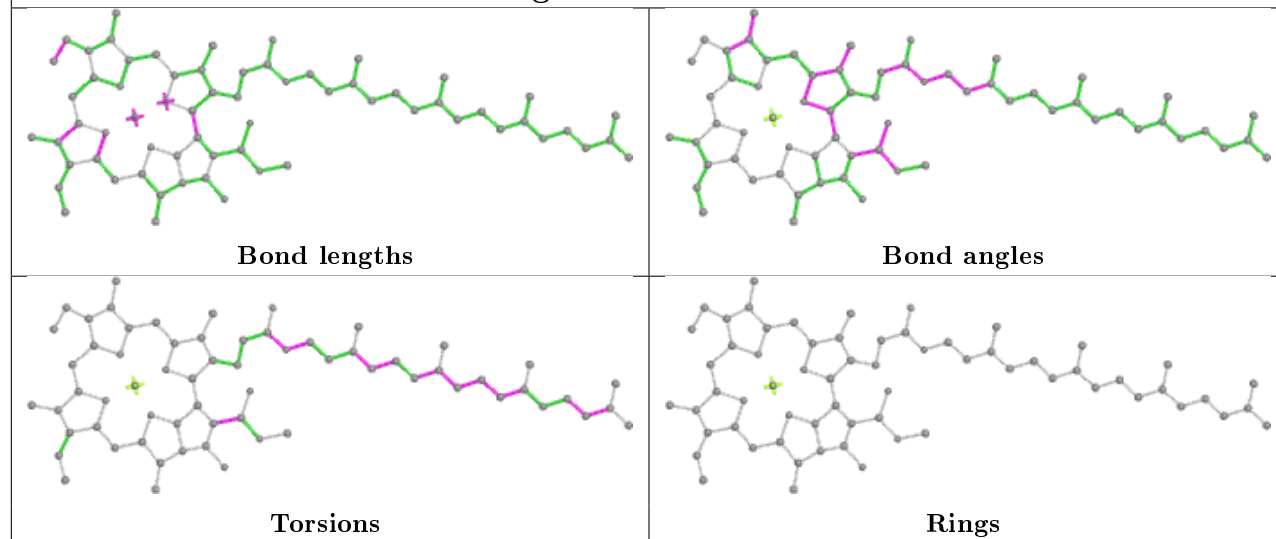
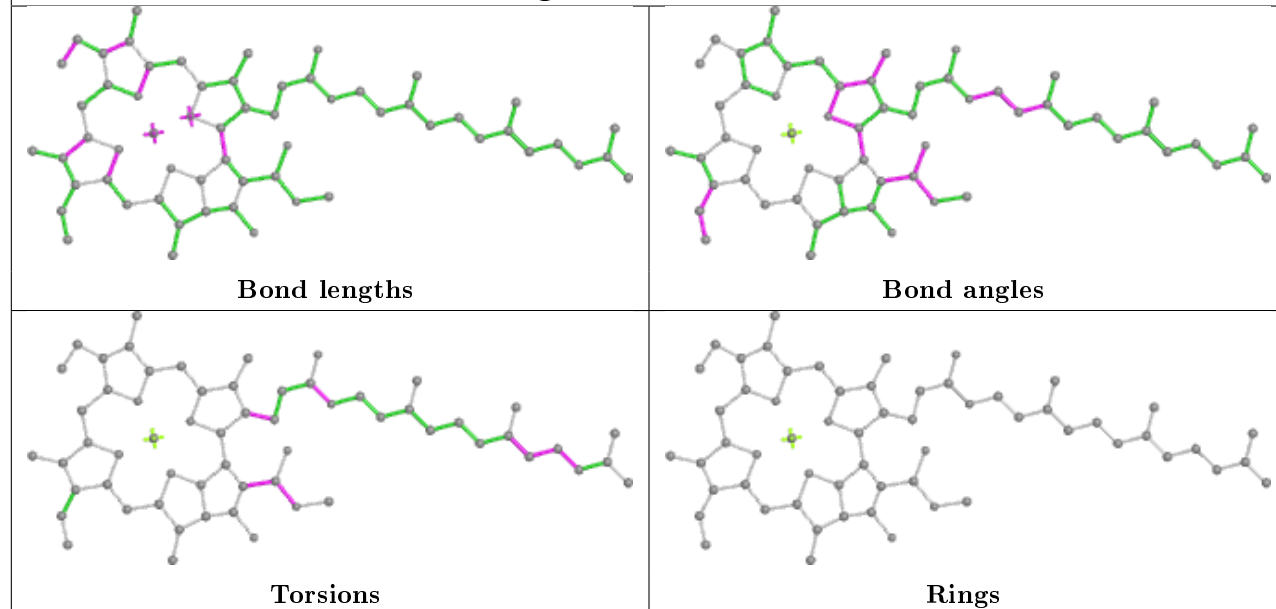
Ligand CHL 2 318

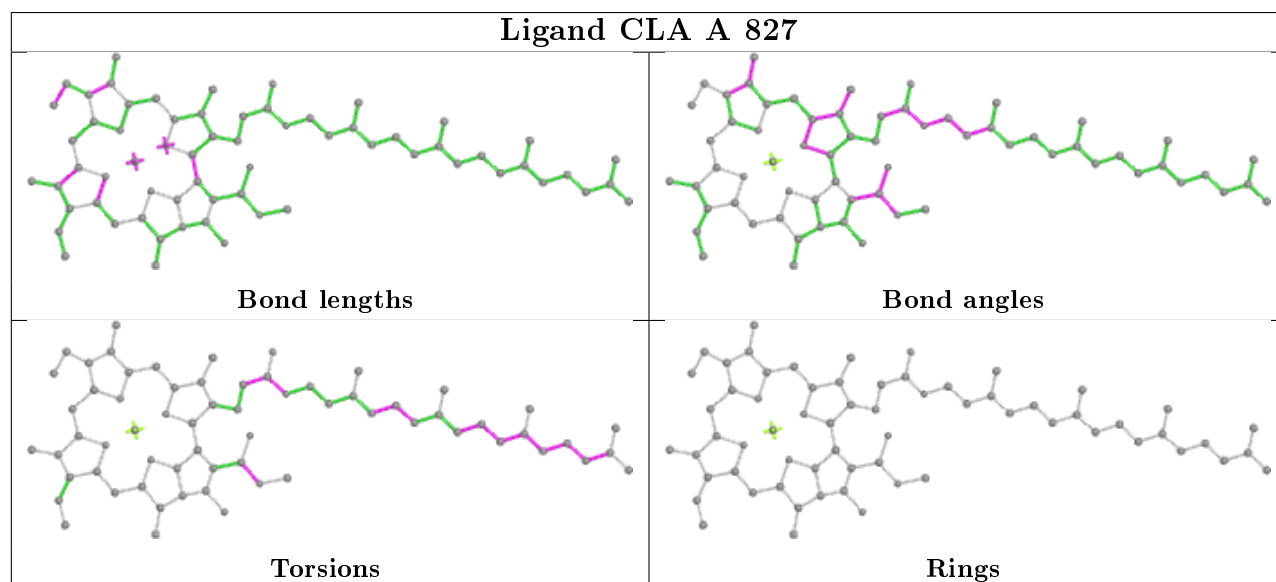
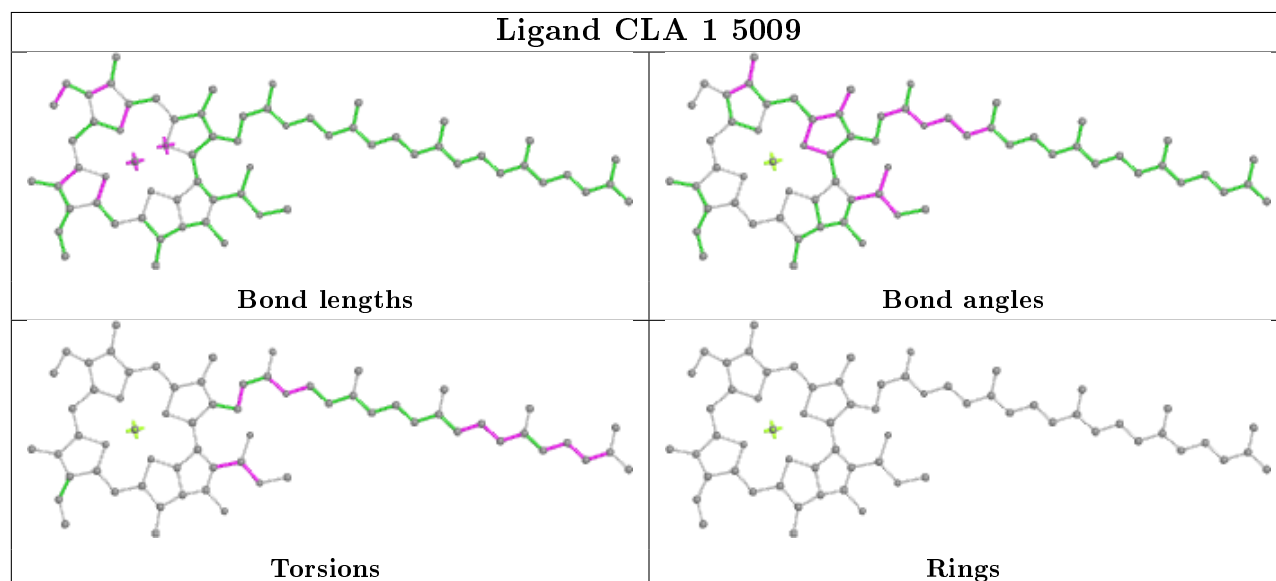
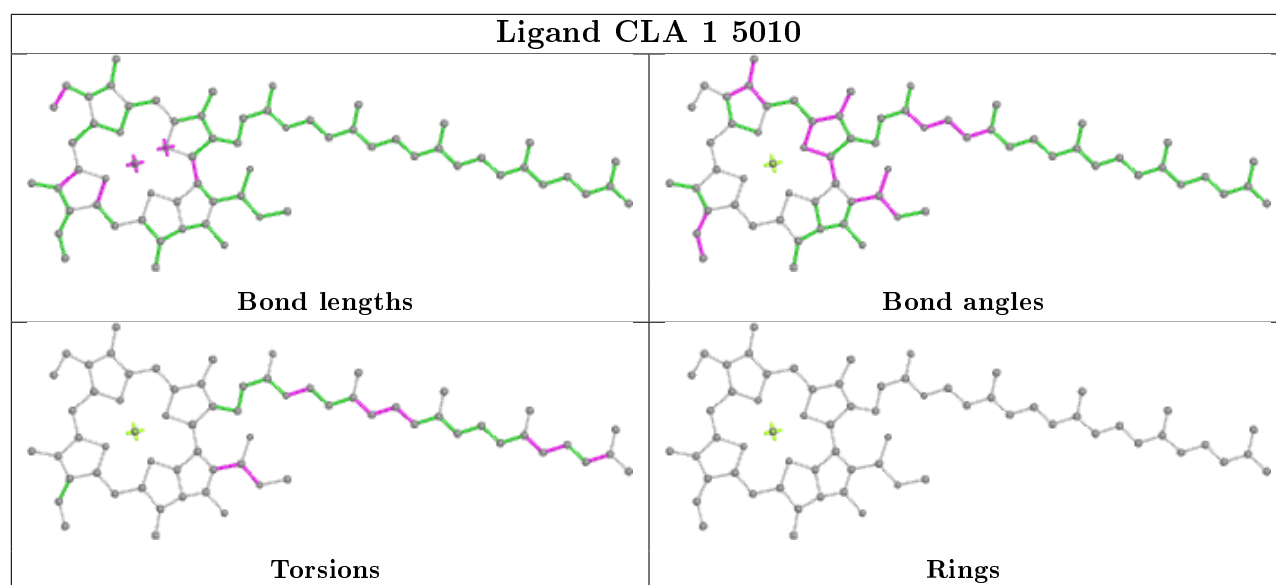


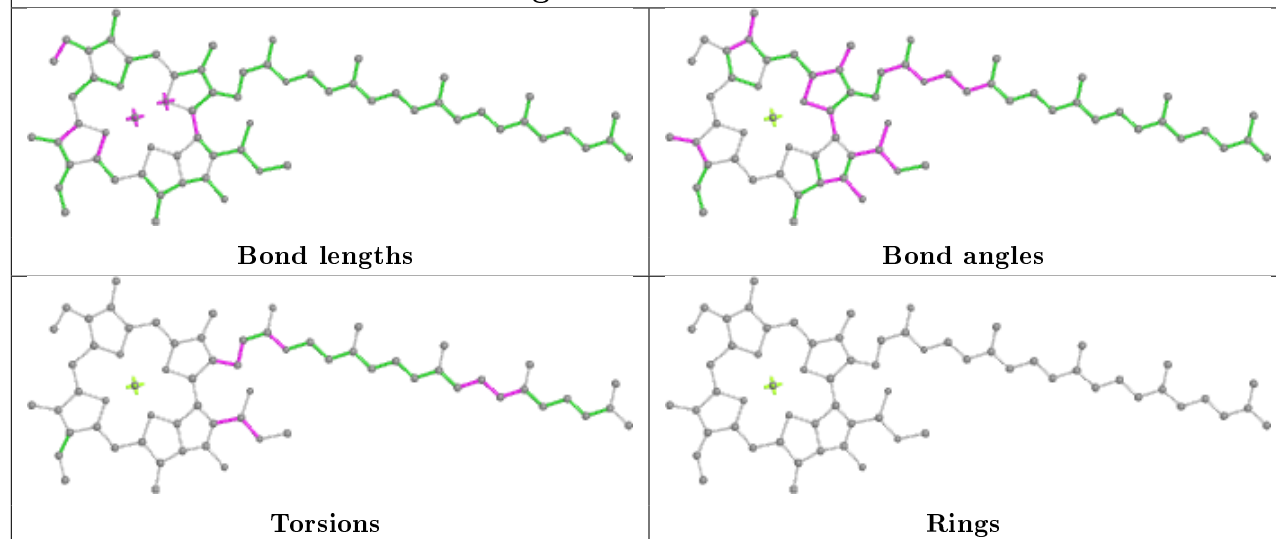
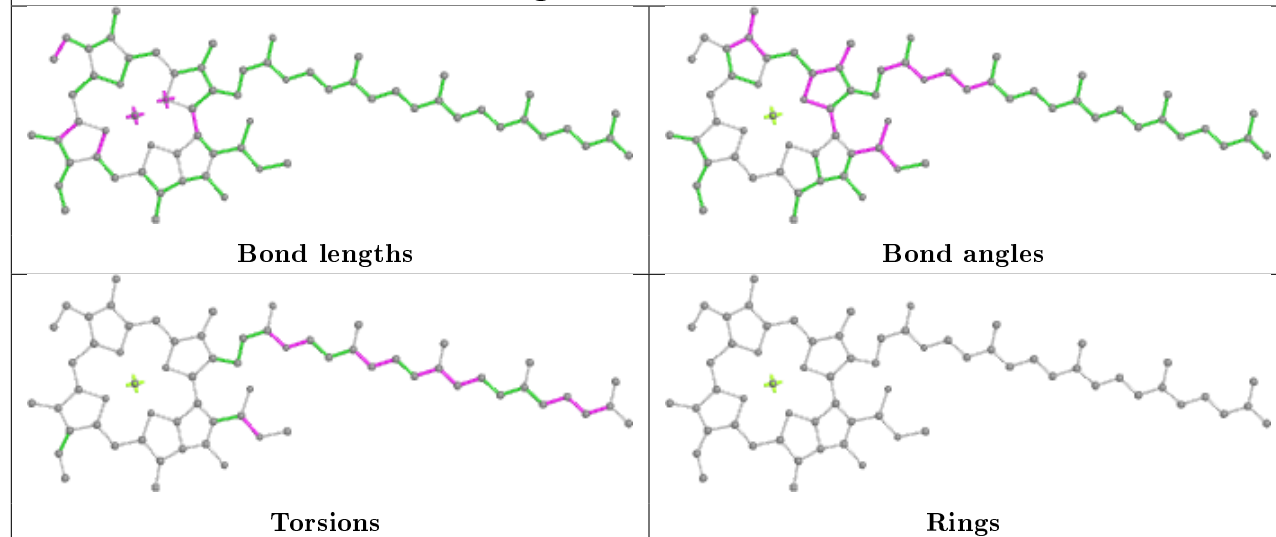
Ligand CHL 3 310



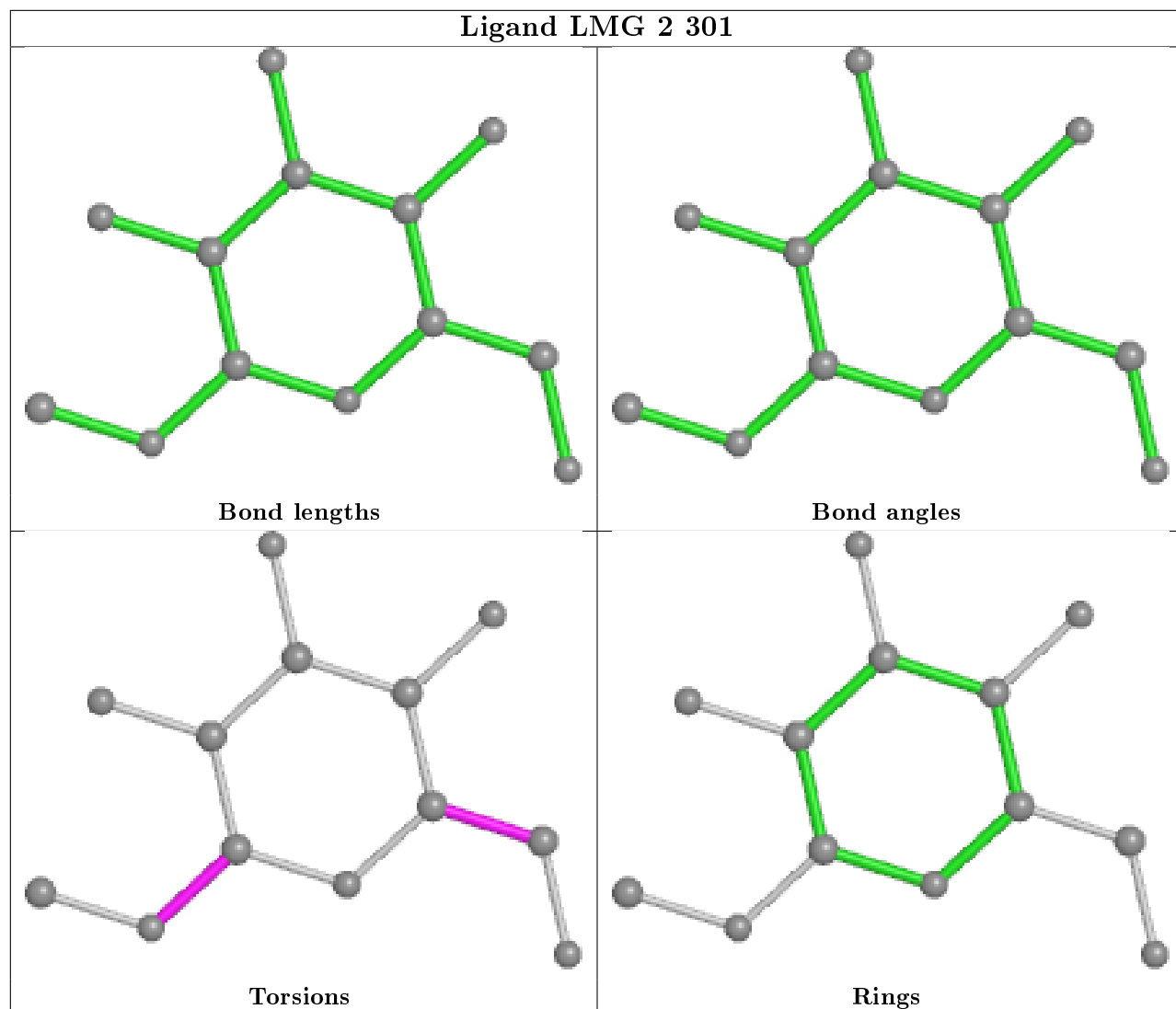
Ligand BCR I 101**Ligand CLA B 819****Ligand CLA A 805**

Ligand CLA A 823**Ligand CLA 4 309**

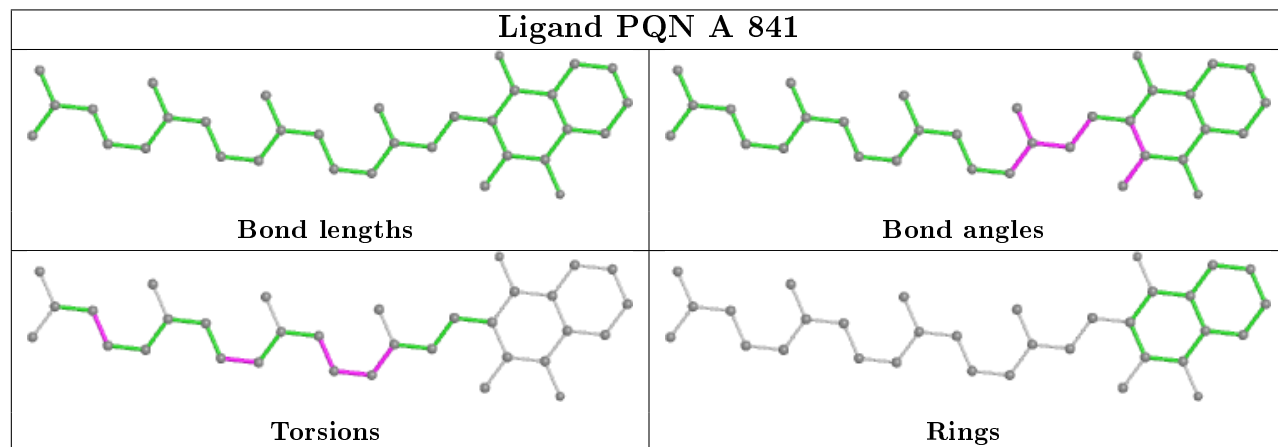


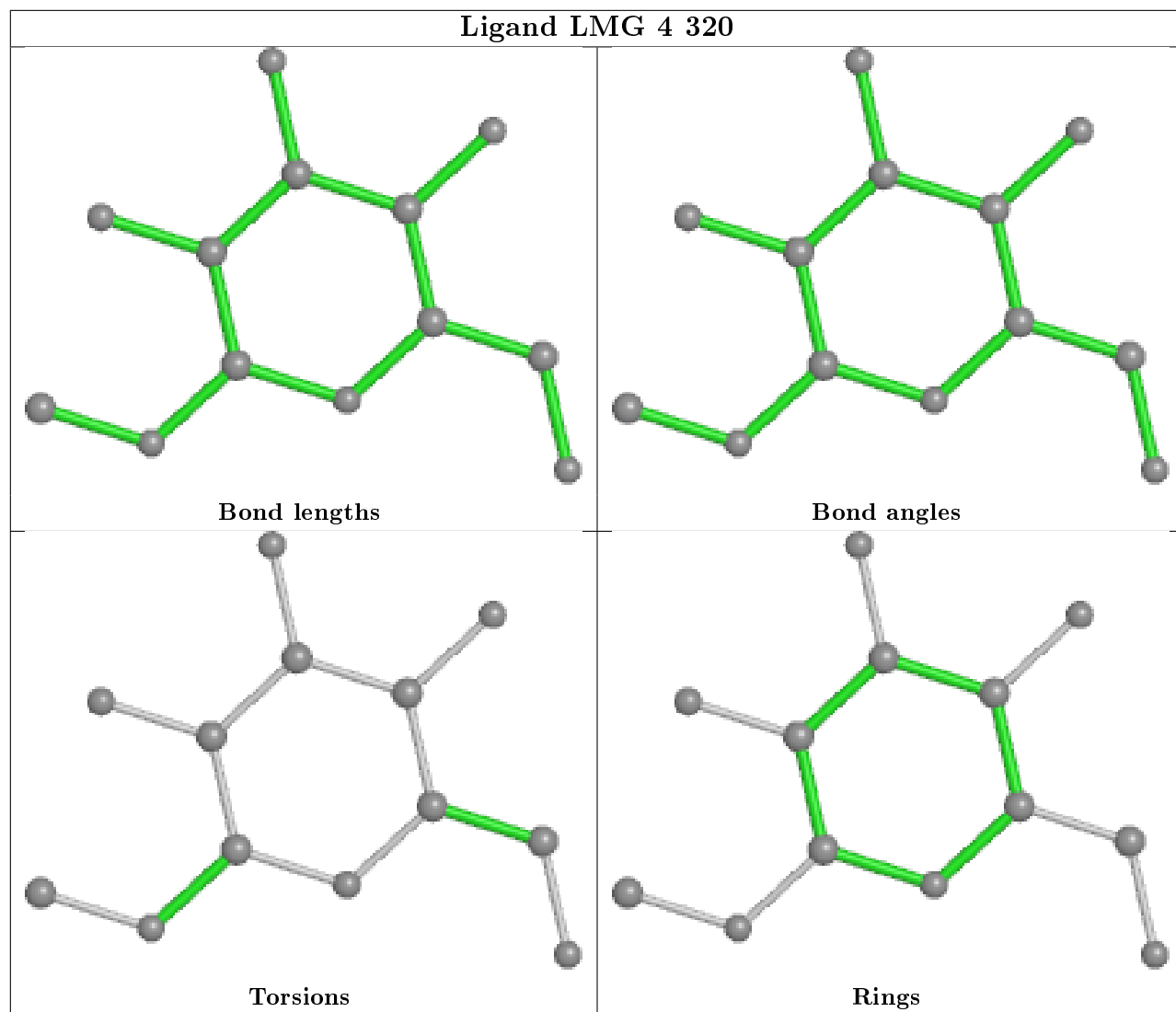
Ligand CLA B 827**Ligand CLA A 838**

Ligand LMG 2 301

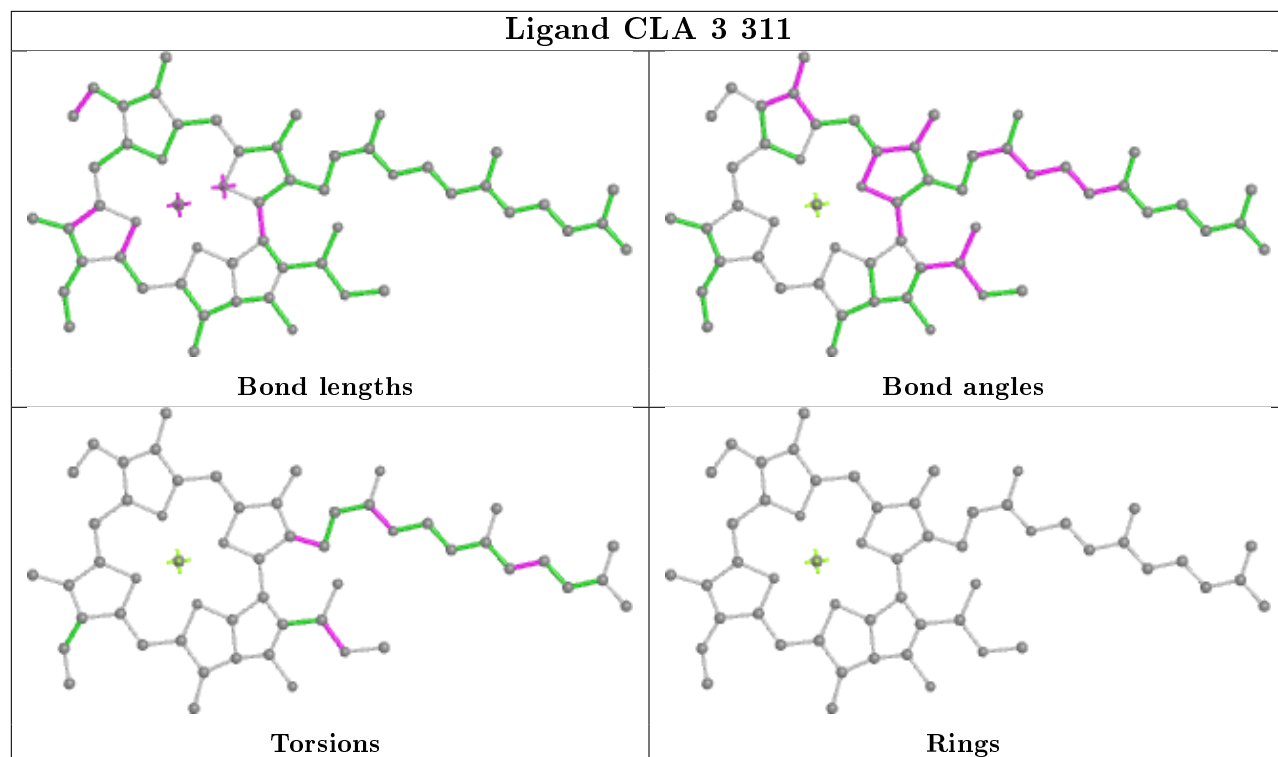


Ligand PQN A 841

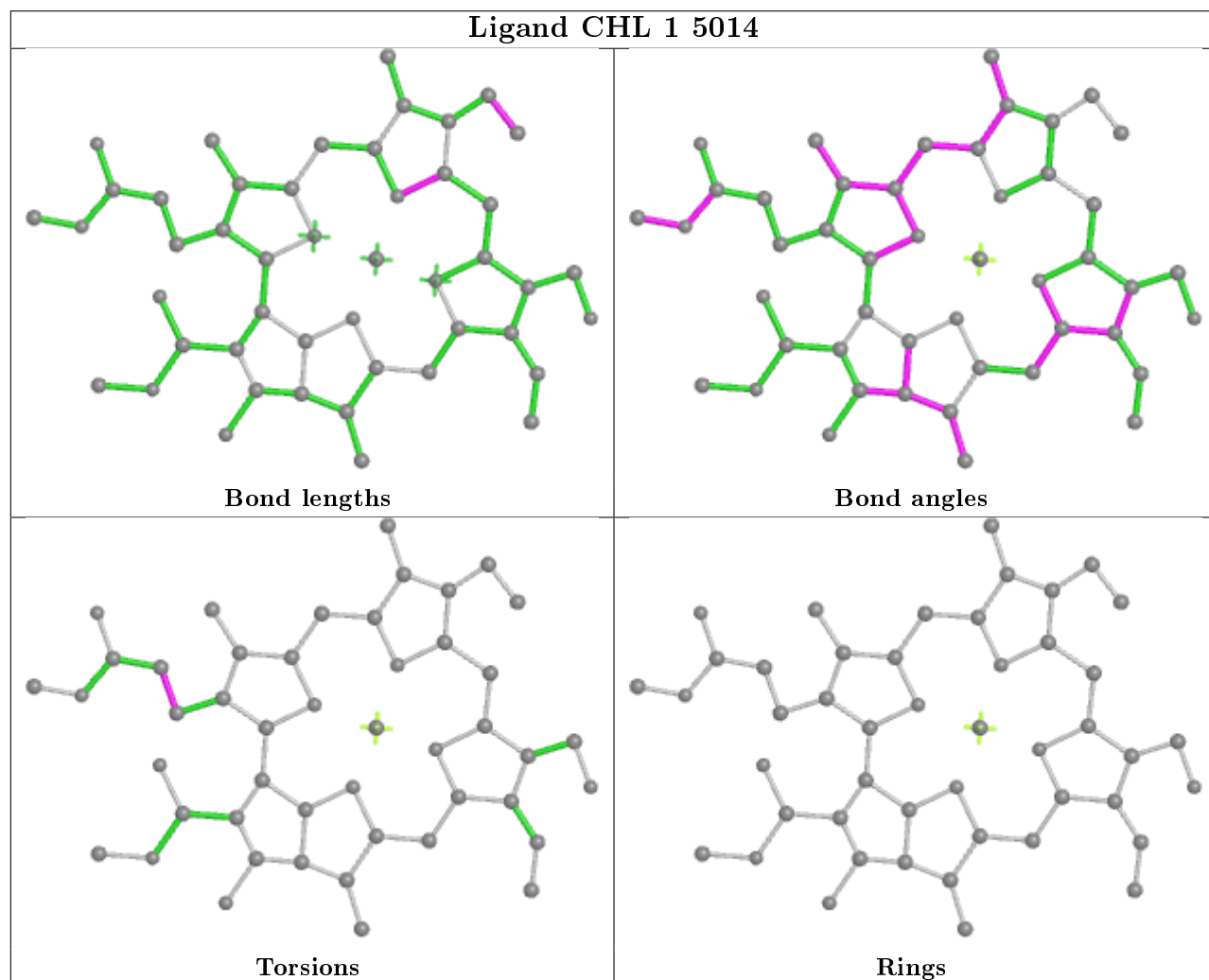


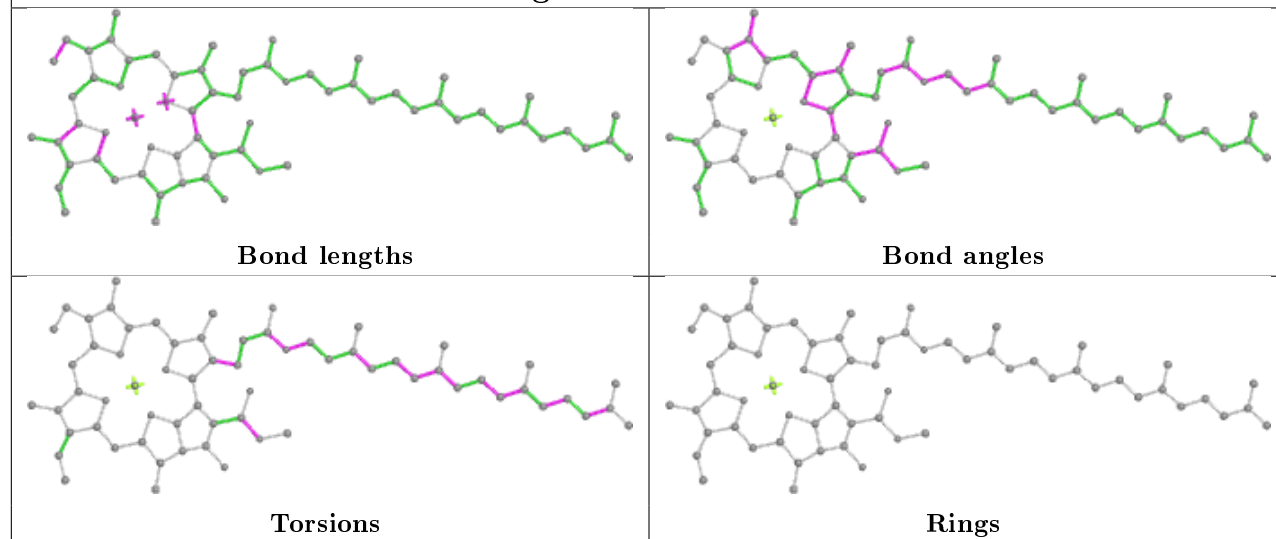
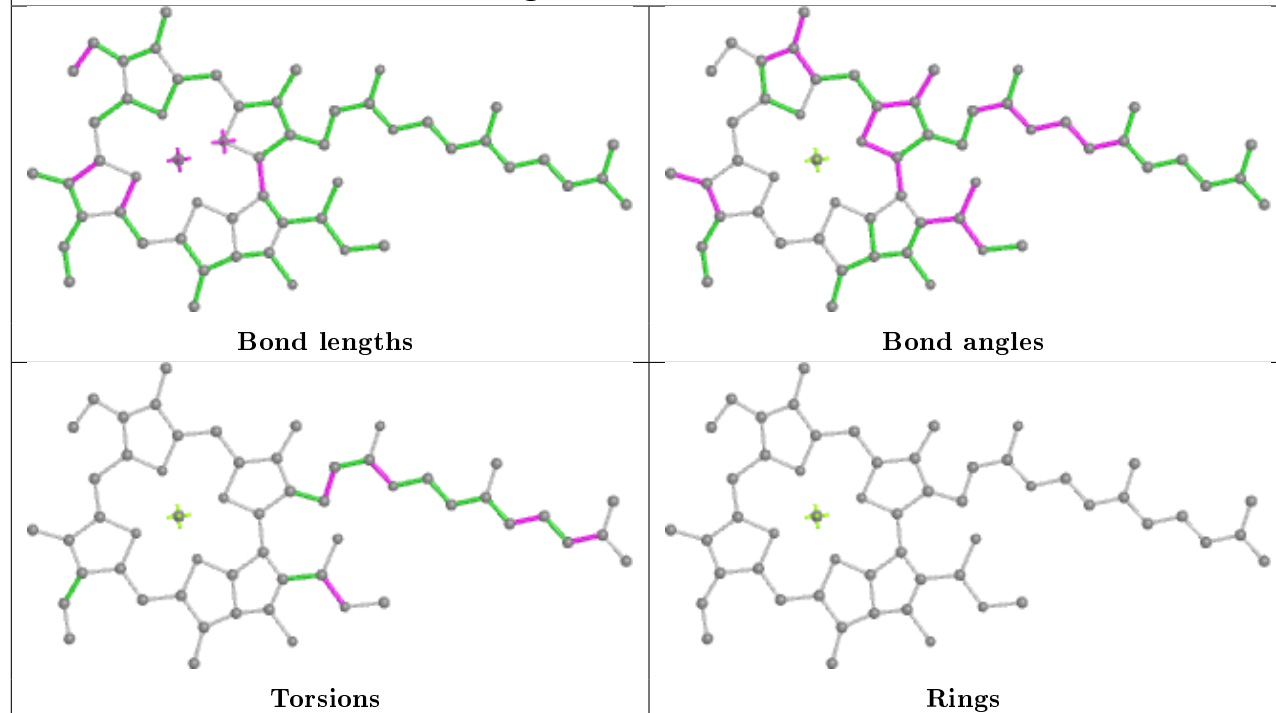


Ligand CLA 3 311

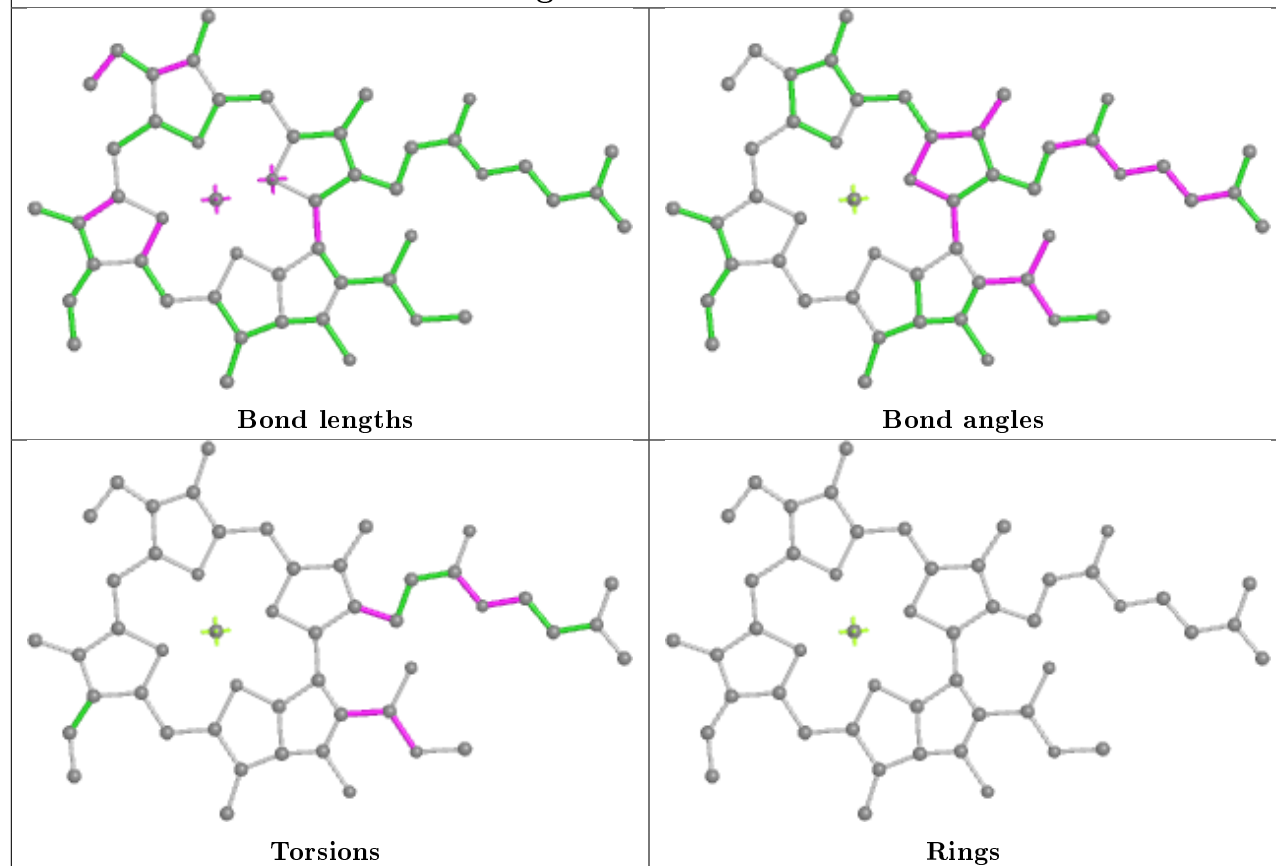


Ligand CHL 1 5014

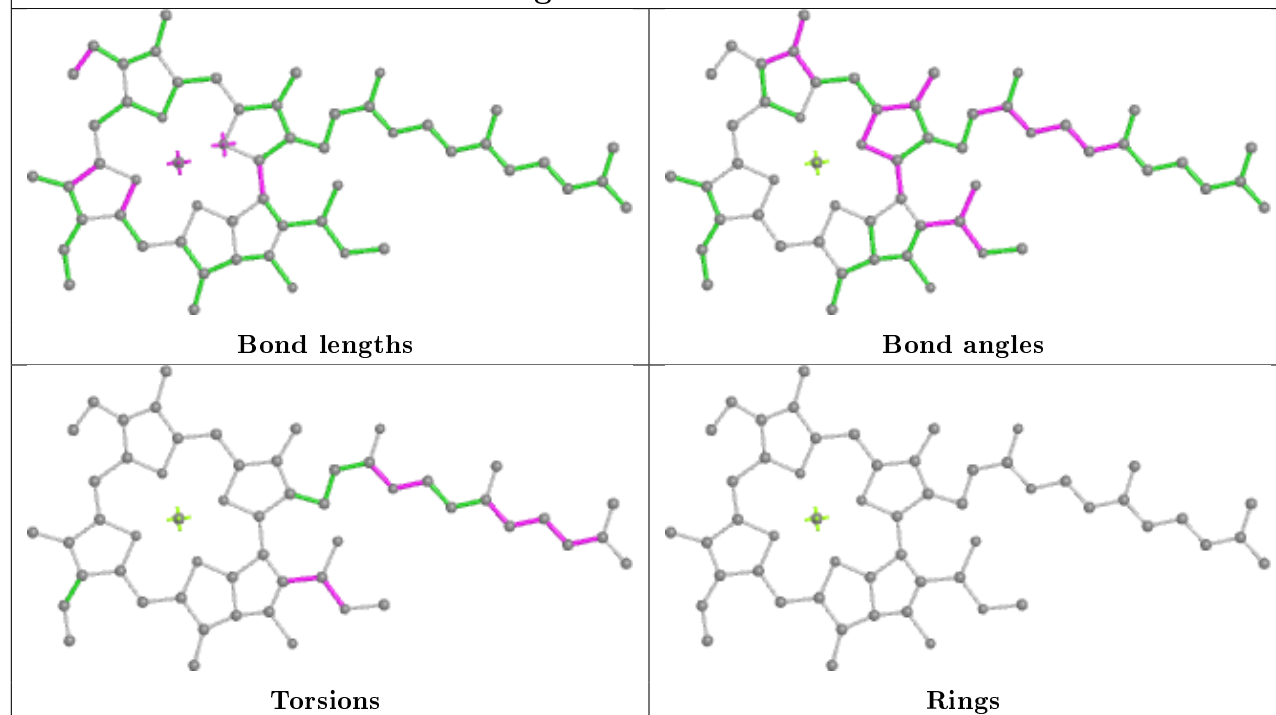


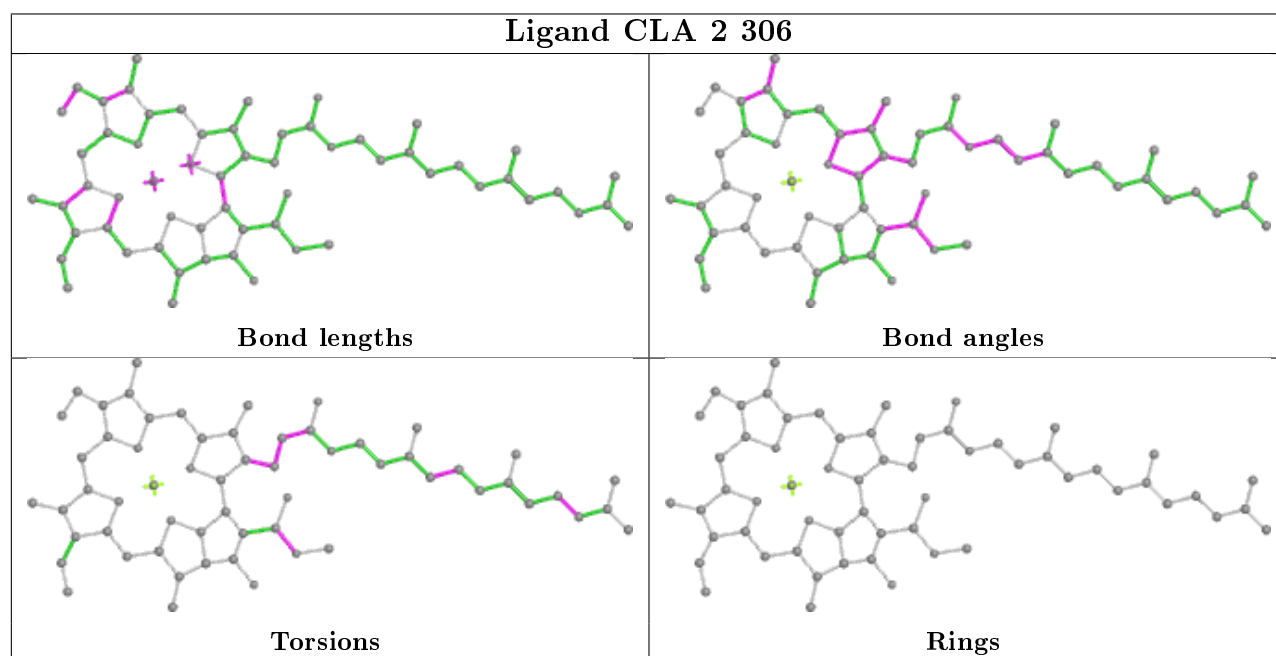
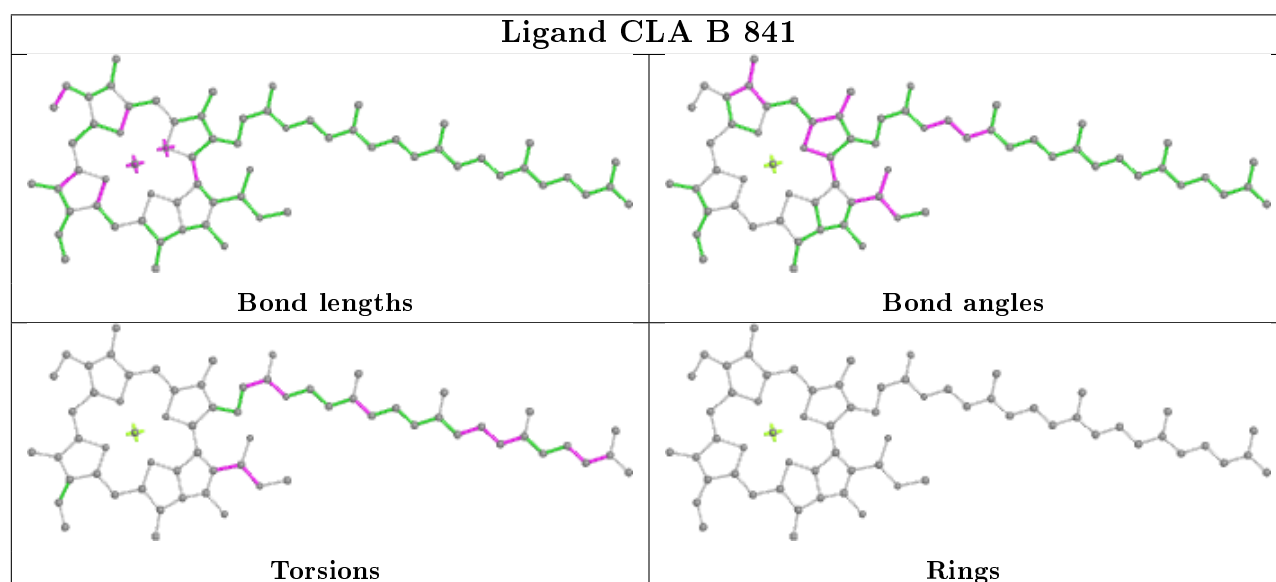
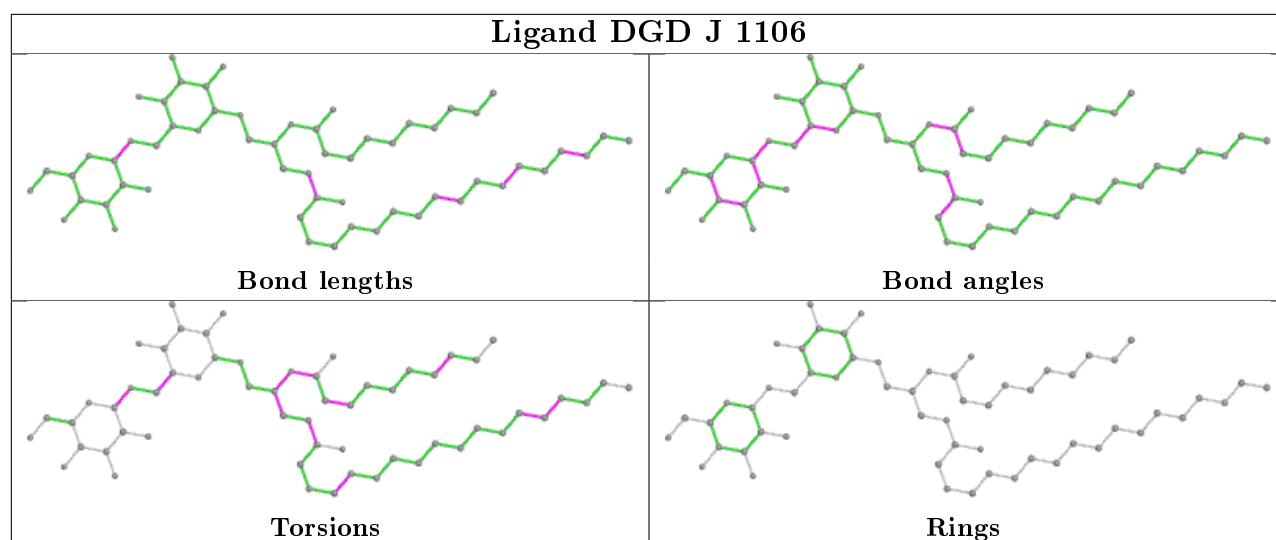
Ligand CLA A 808**Ligand CLA G 1601**

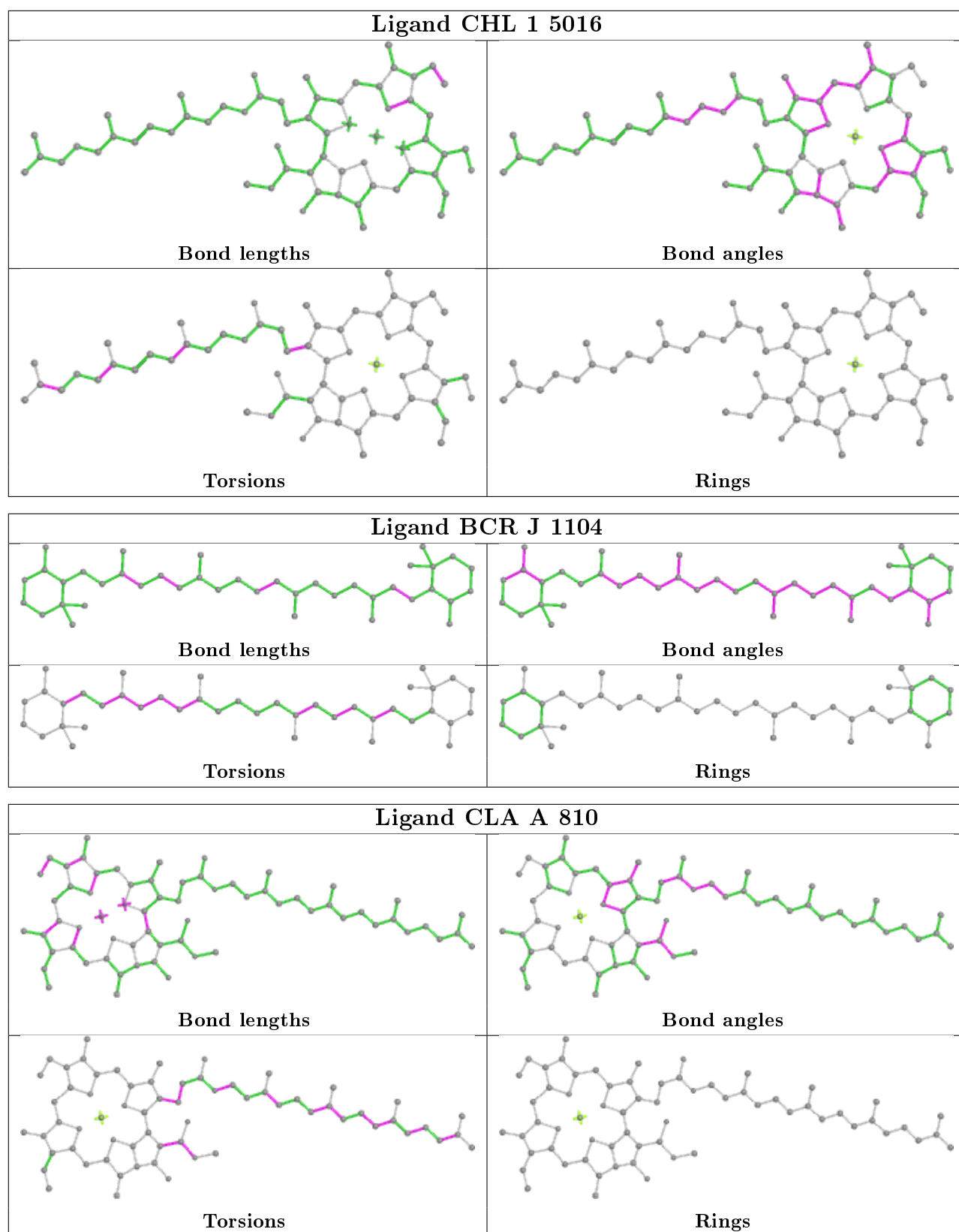
Ligand CLA 2 326



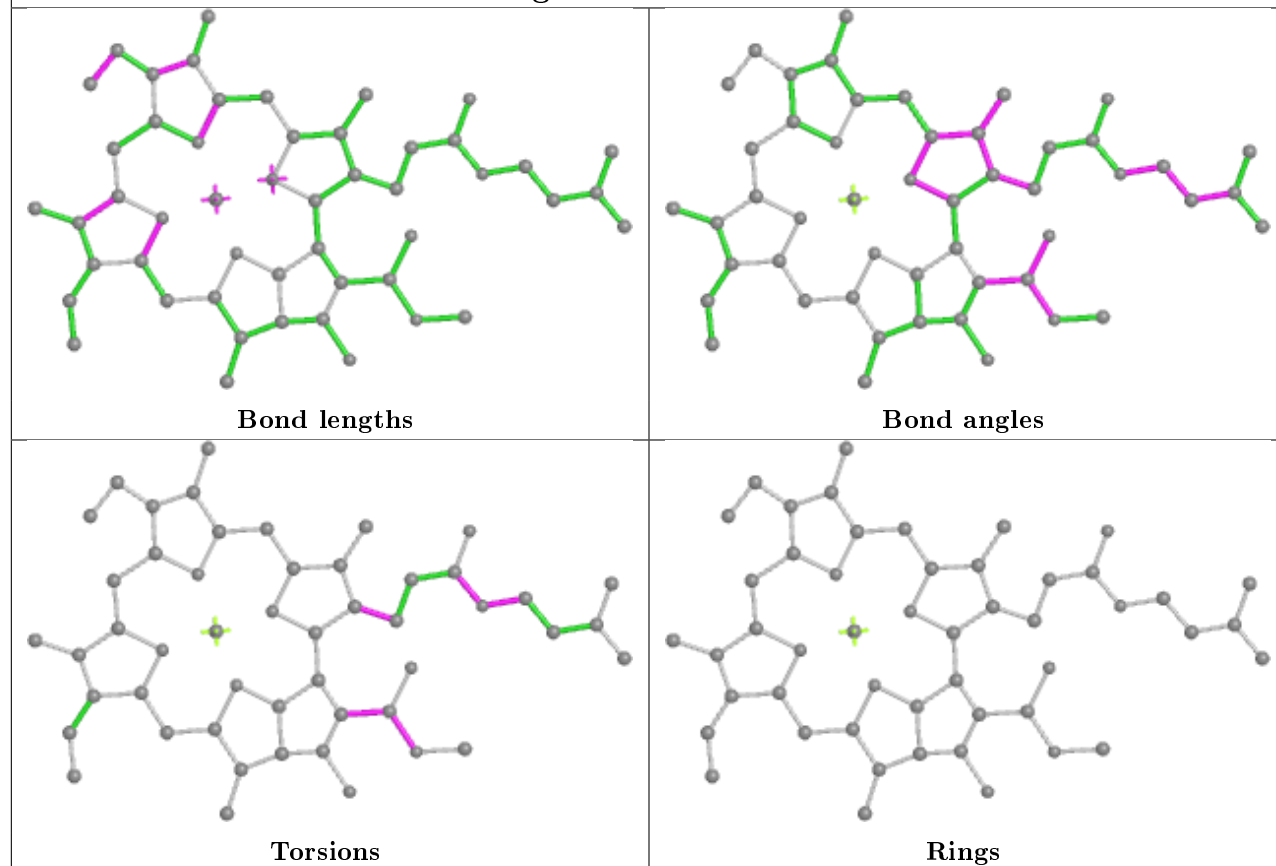
Ligand CLA L 301



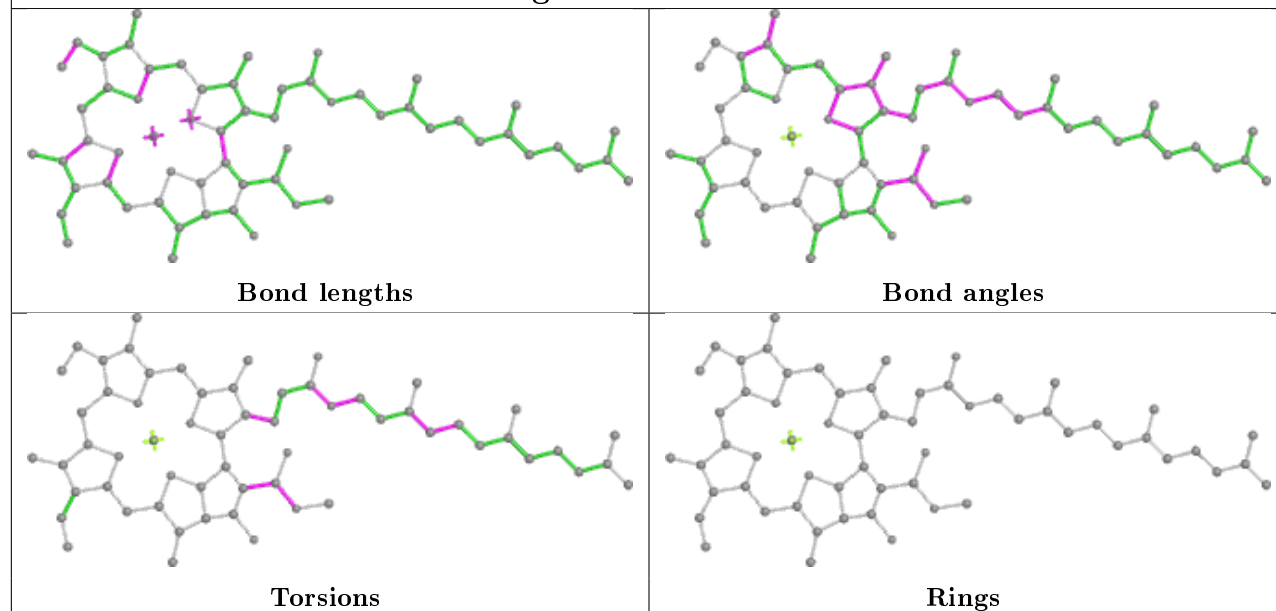




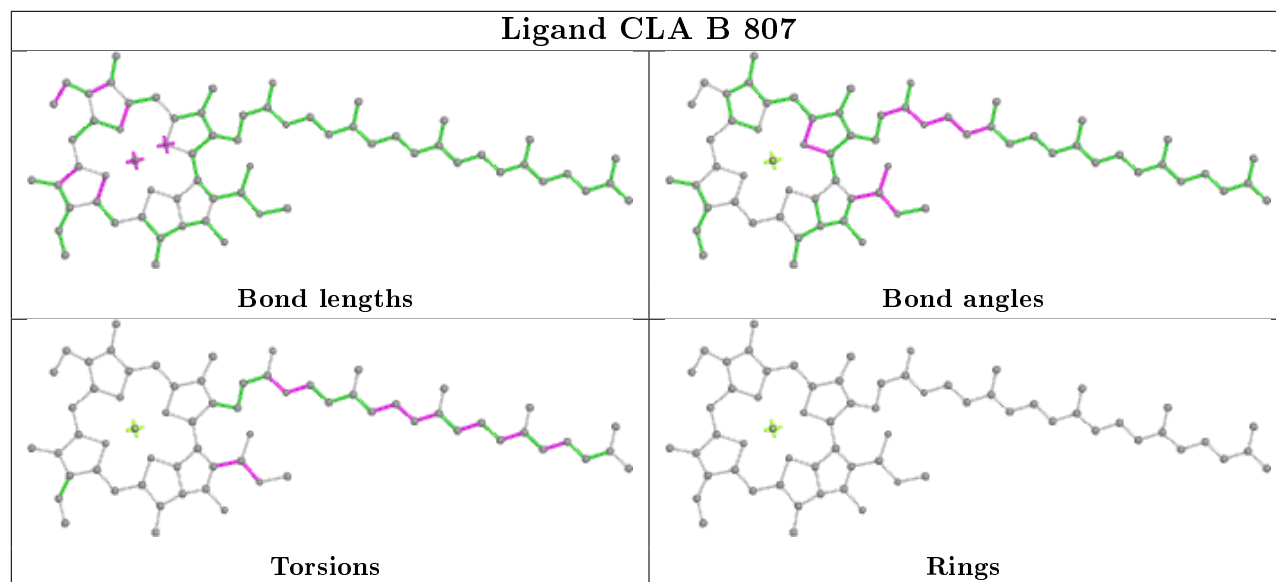
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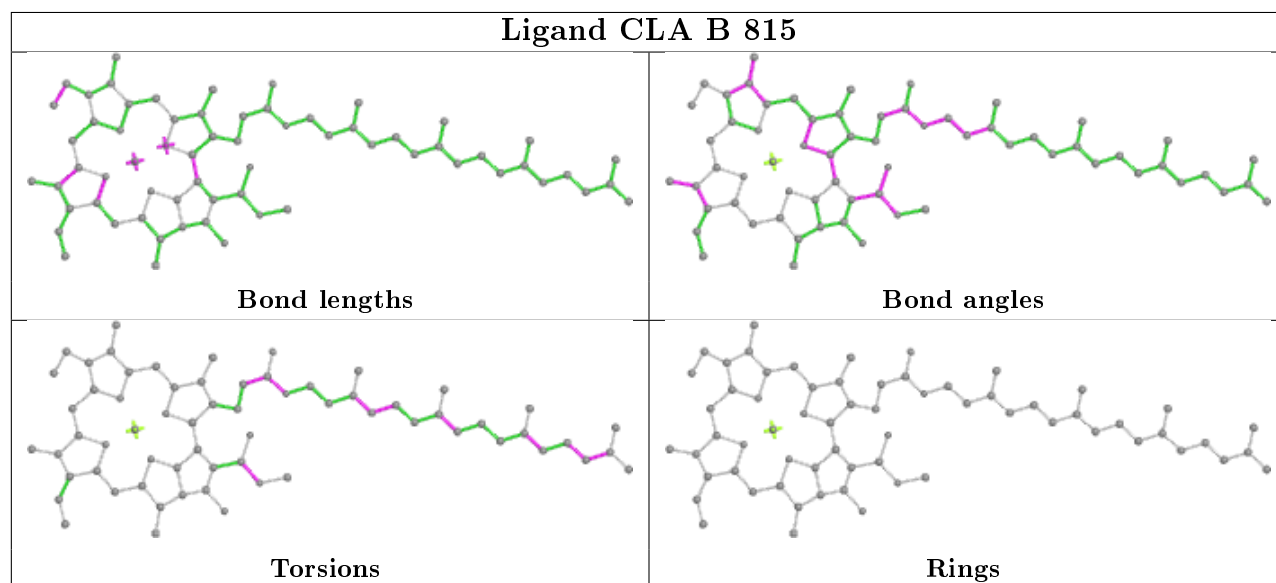
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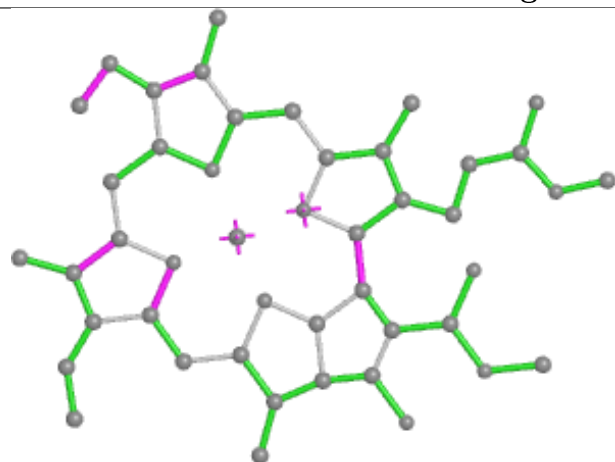
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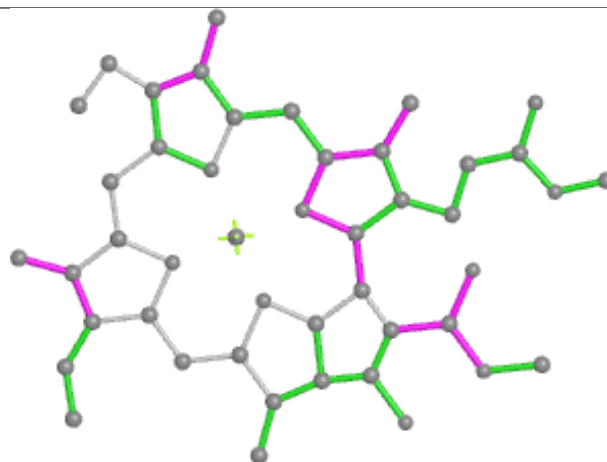
Ligand CLA B 815



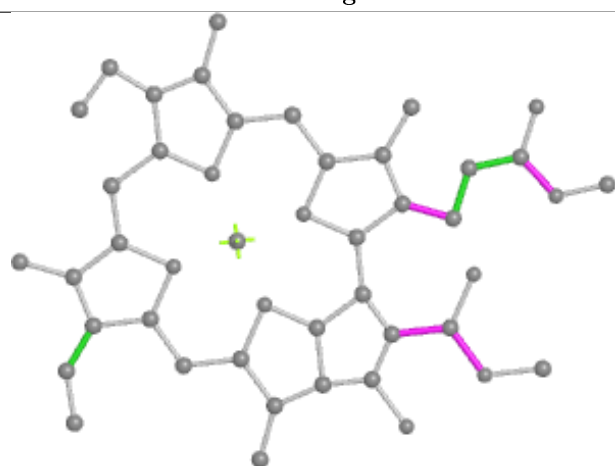
Ligand CLA 3 318



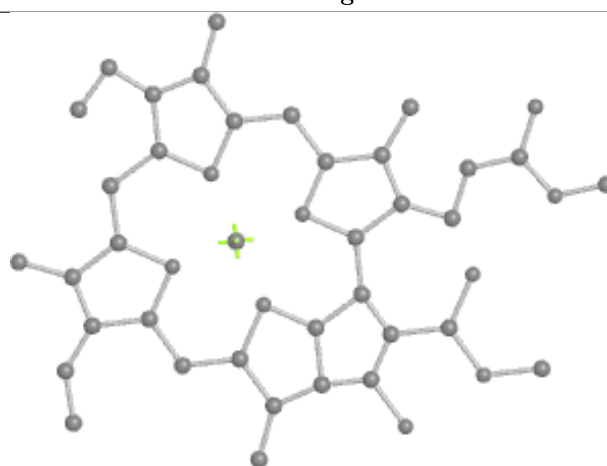
Bond lengths



Bond angles

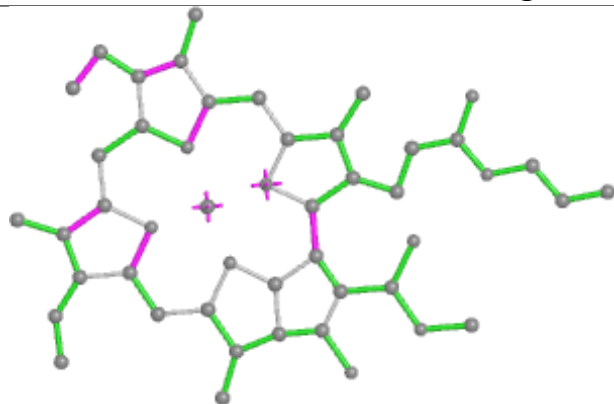


Torsions

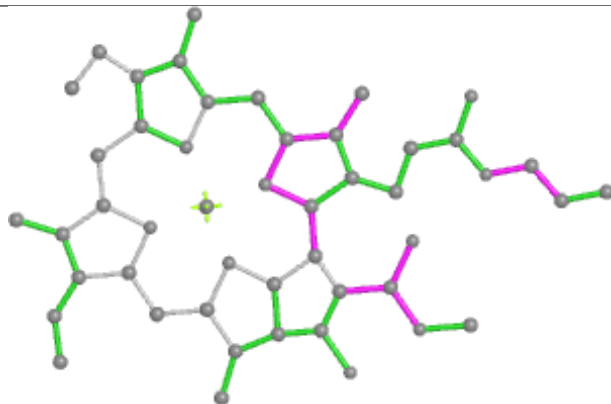


Rings

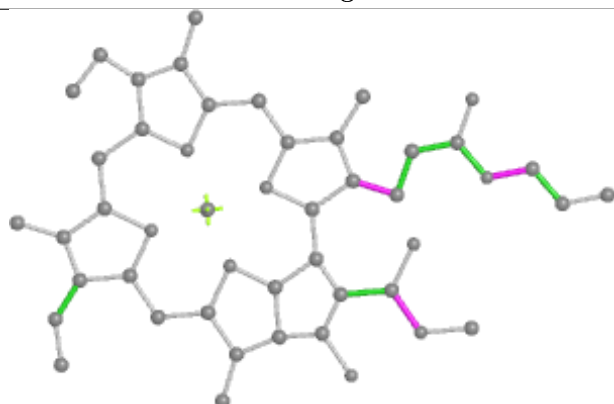
Ligand CLA 3 314



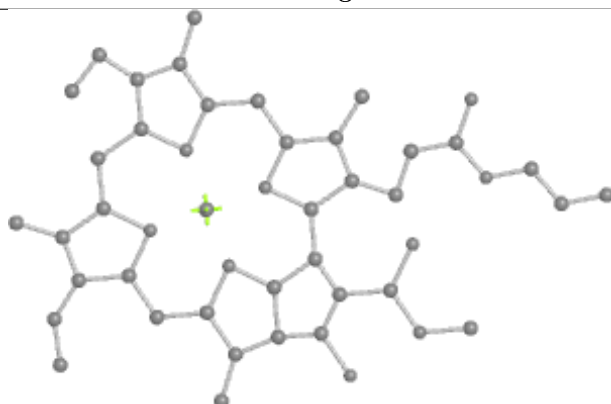
Bond lengths



Bond angles

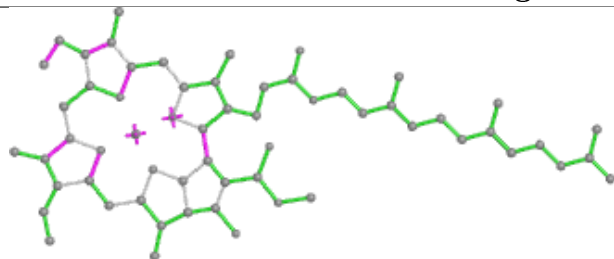


Torsions

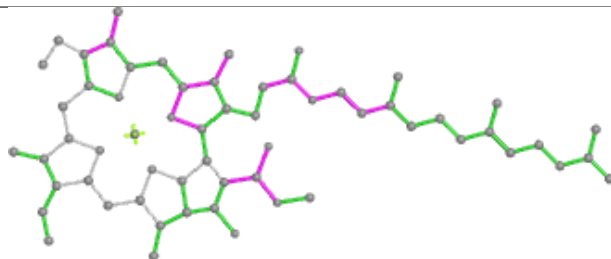


Rings

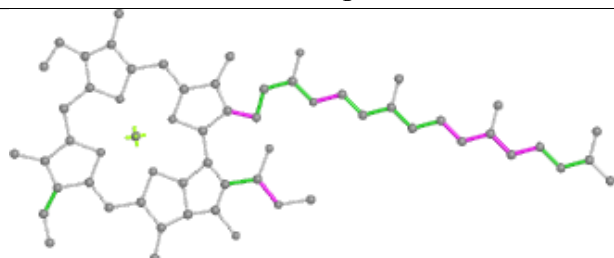
Ligand CLA B 817



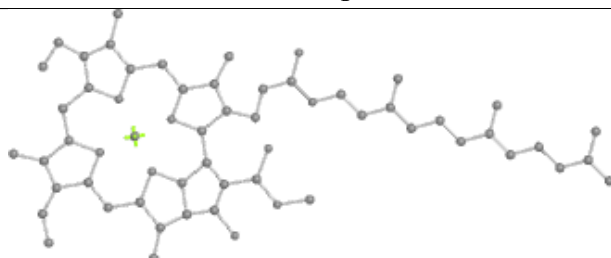
Bond lengths



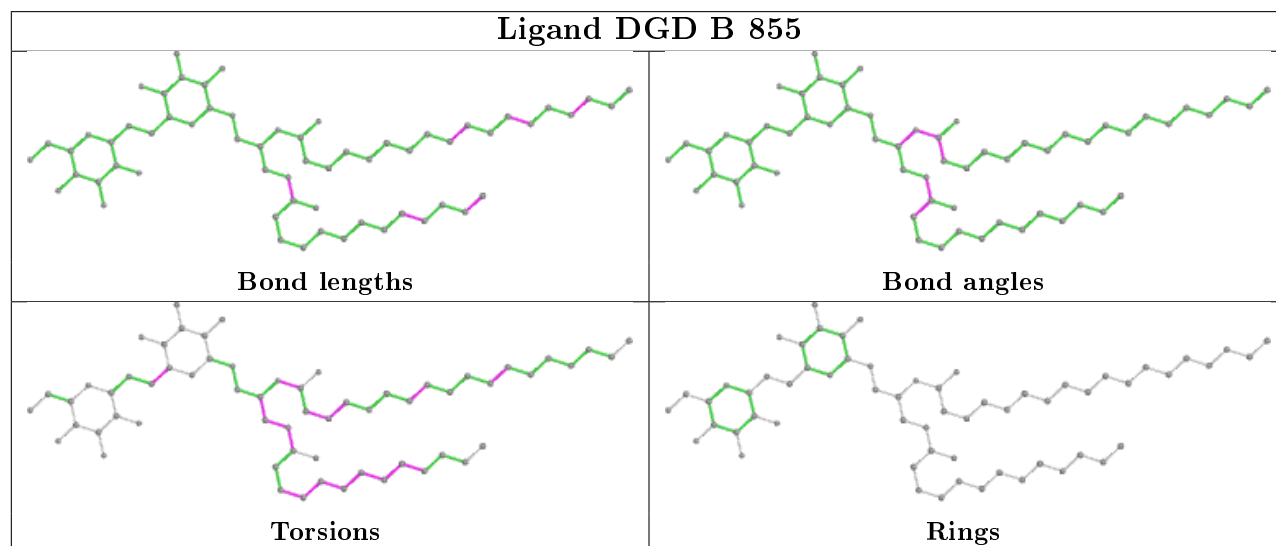
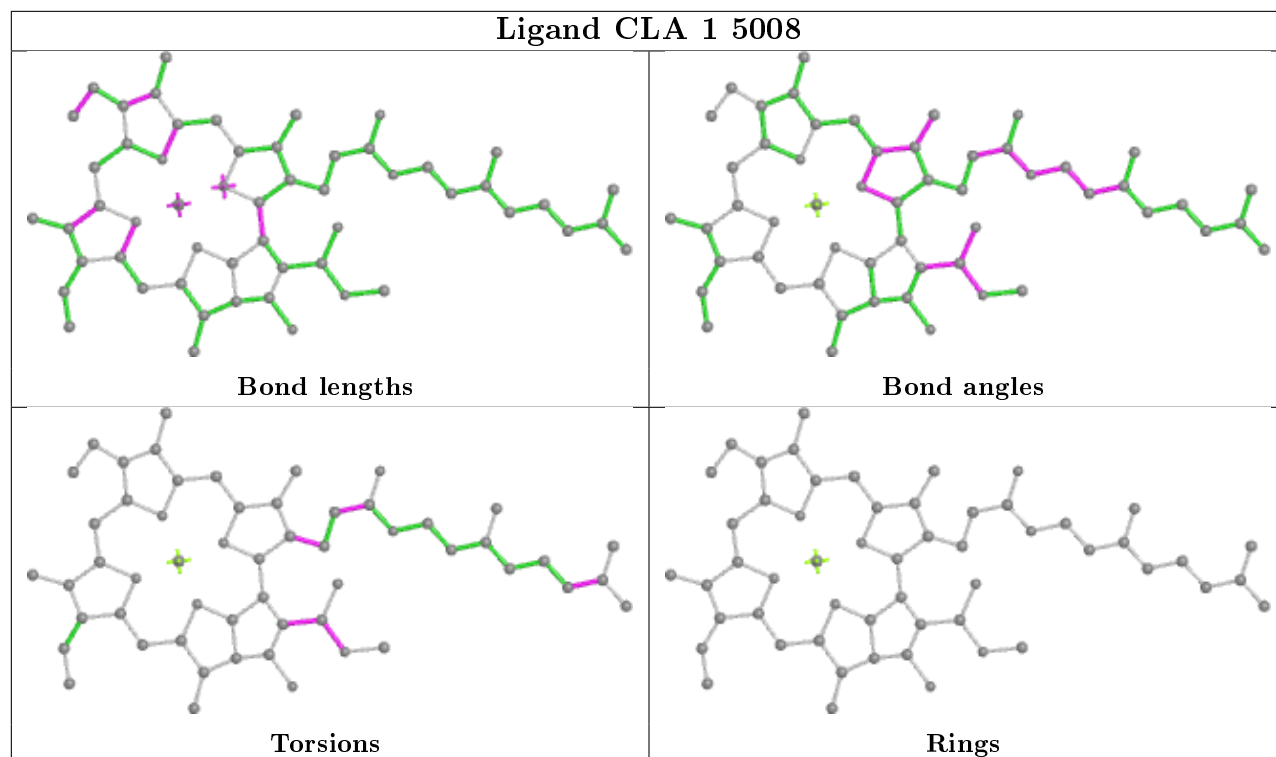
Bond angles

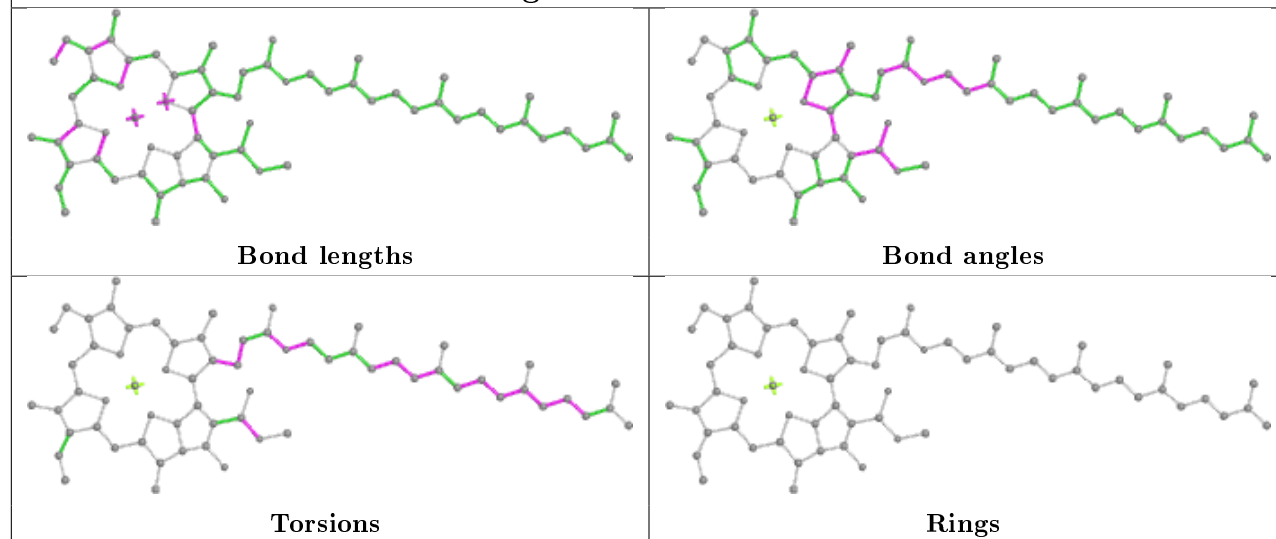
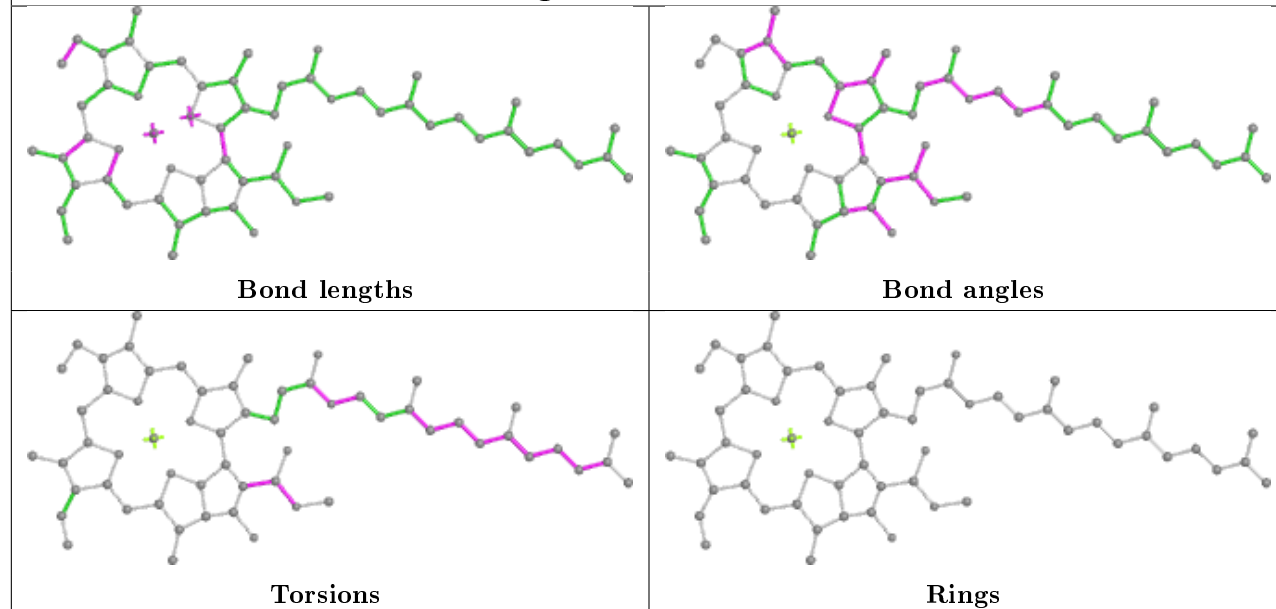


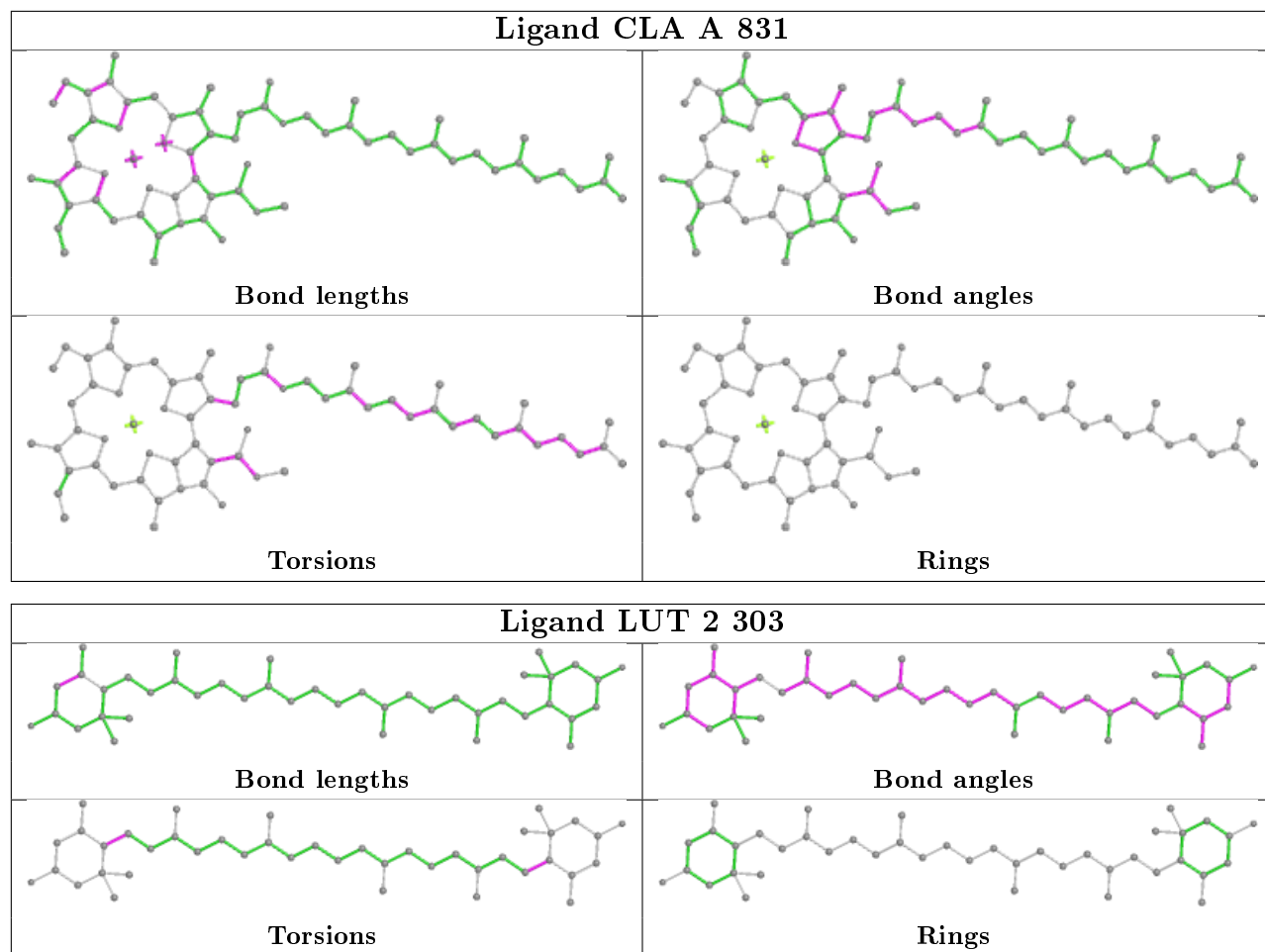
Torsions

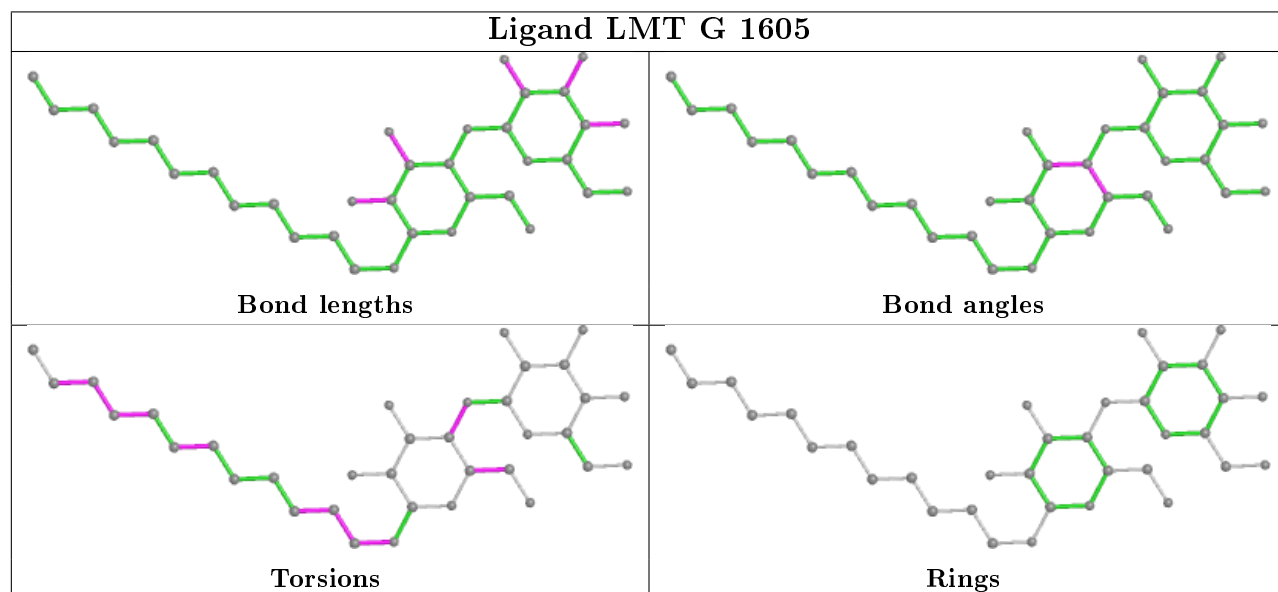
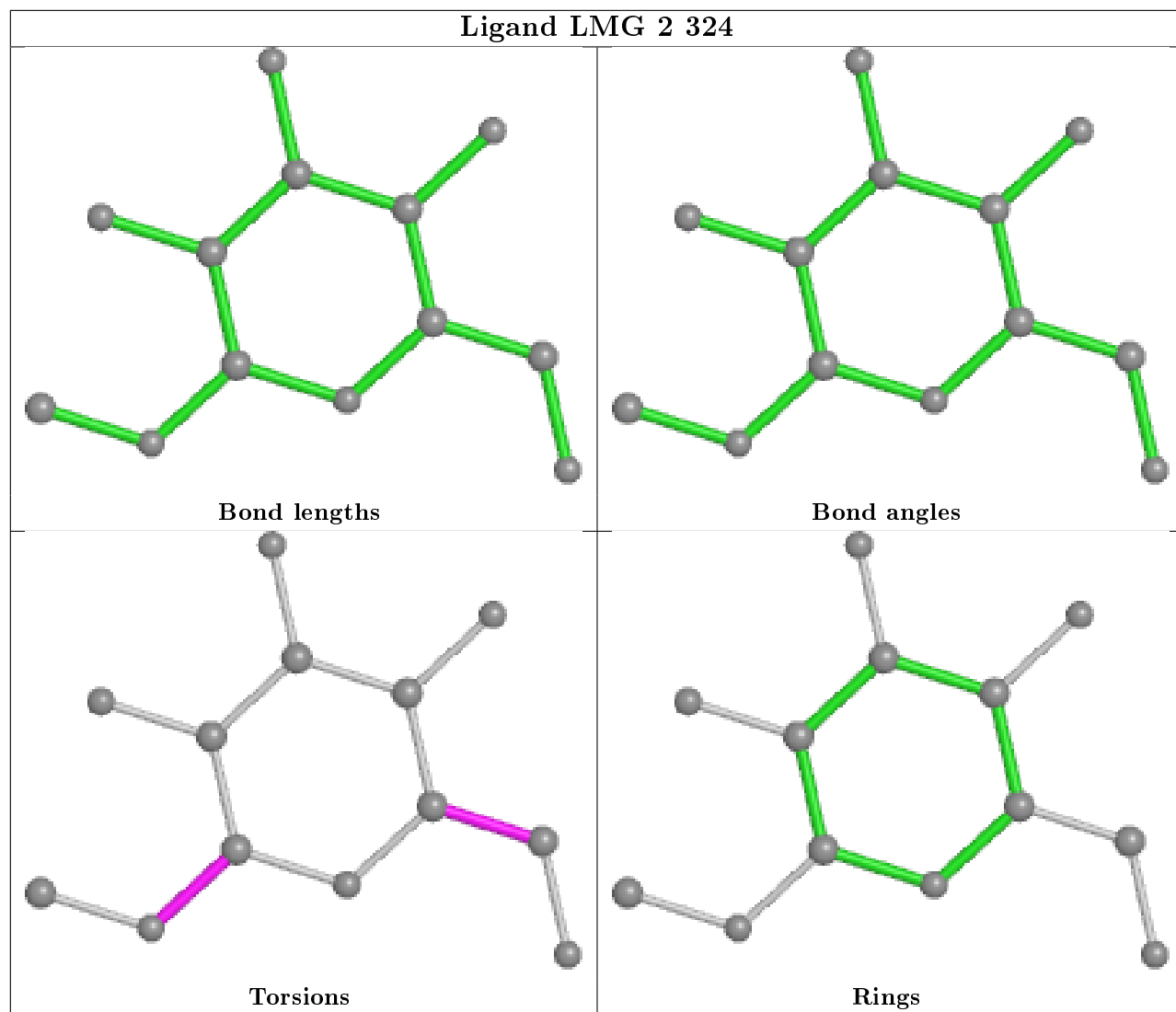


Rings

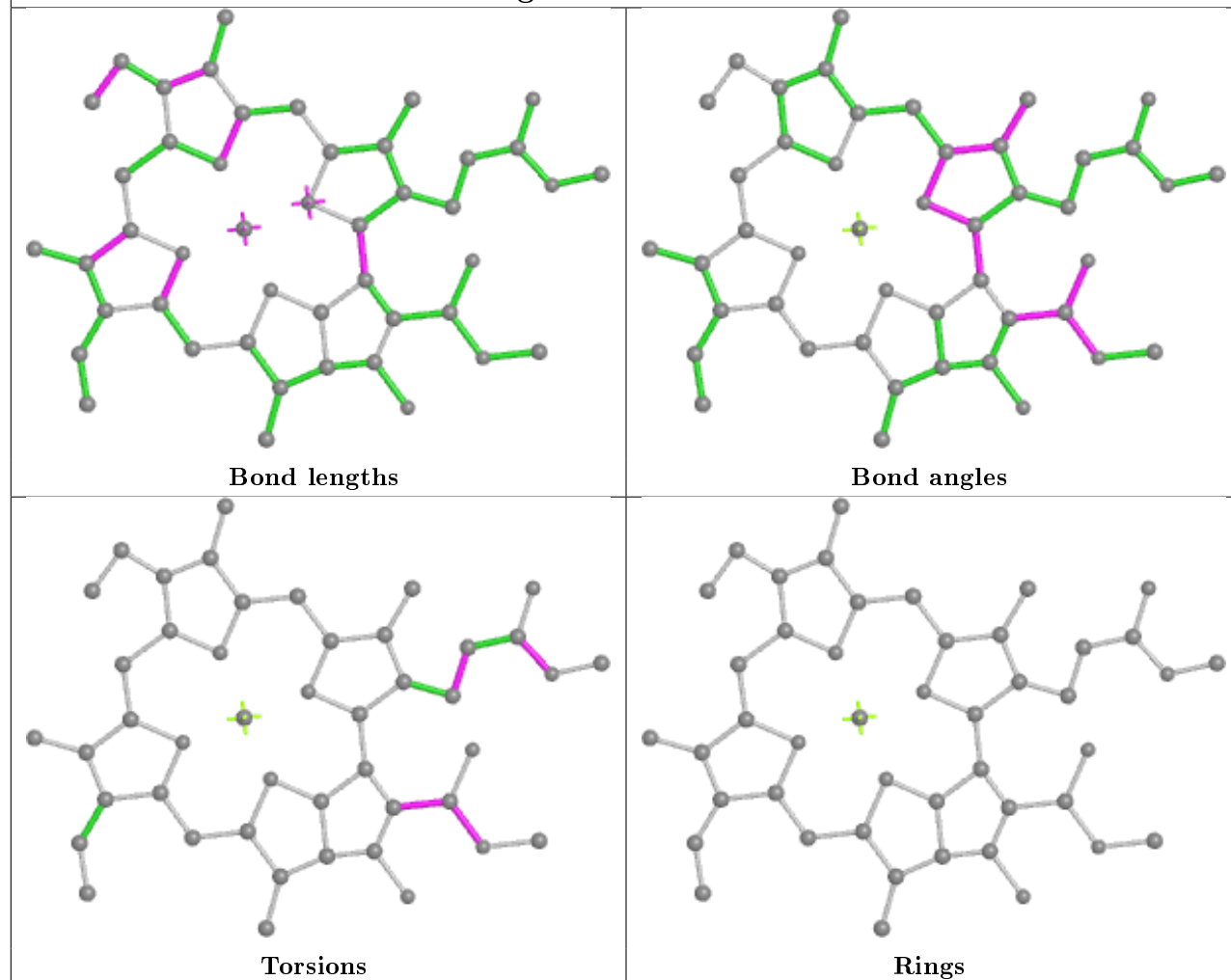


Ligand CLA G 1603**Ligand CLA 2 312**

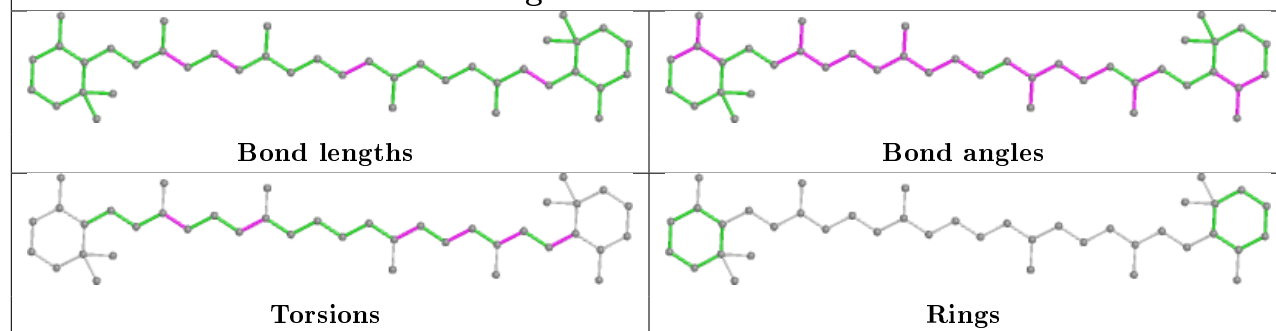


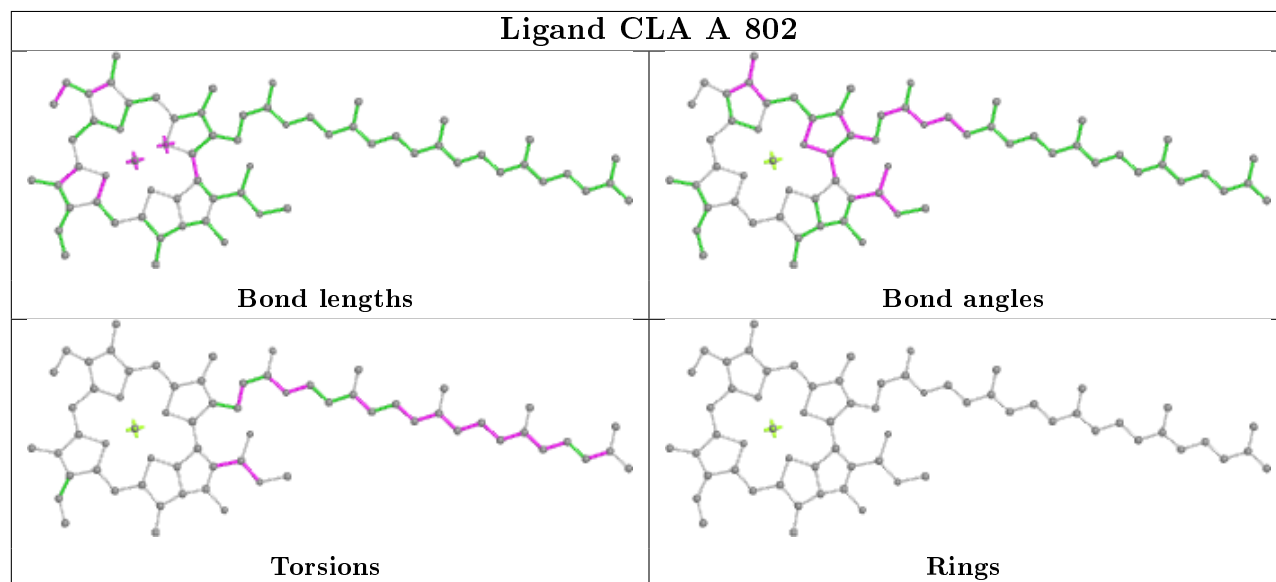
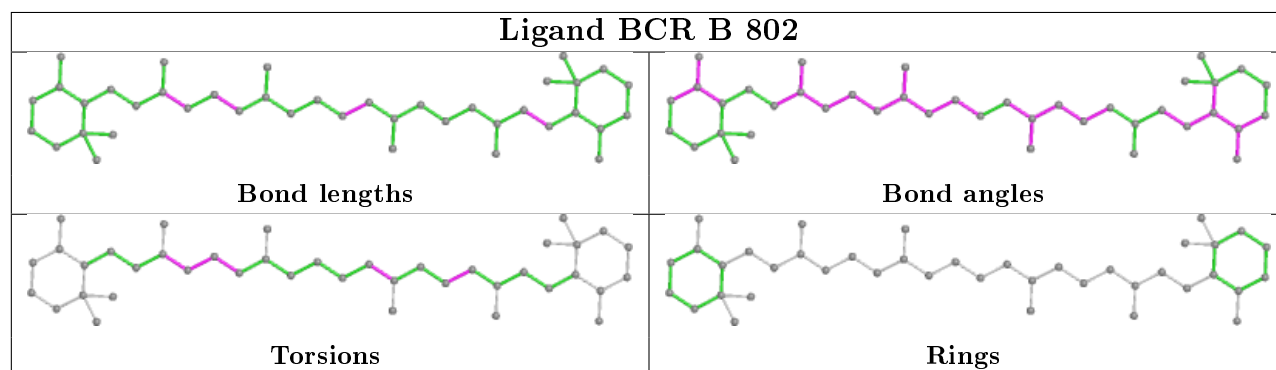
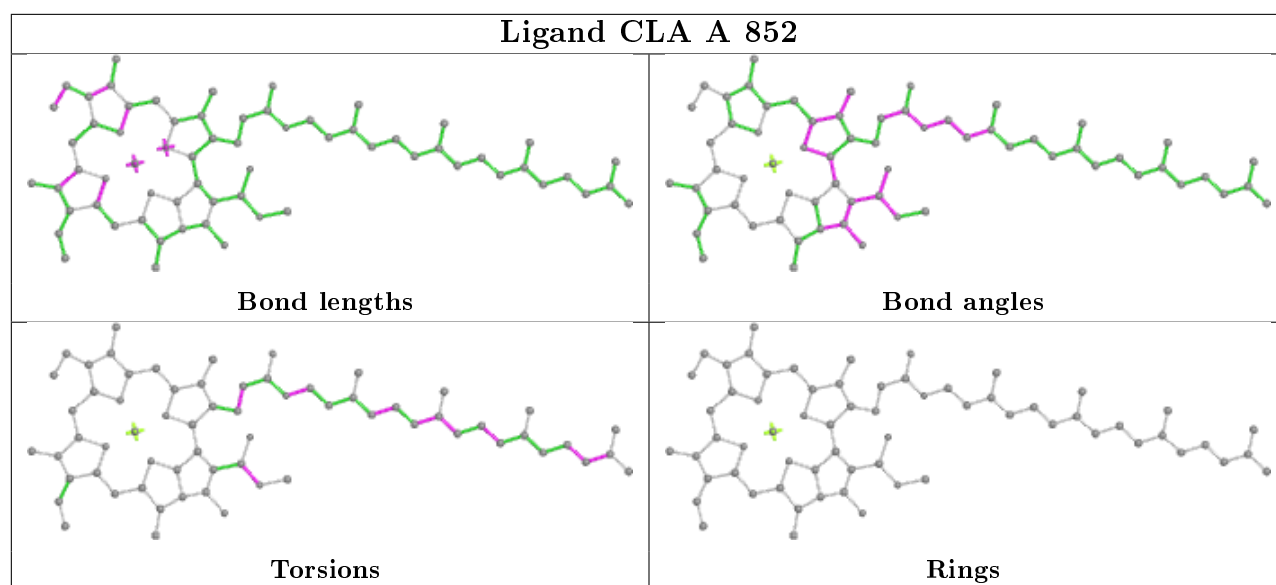


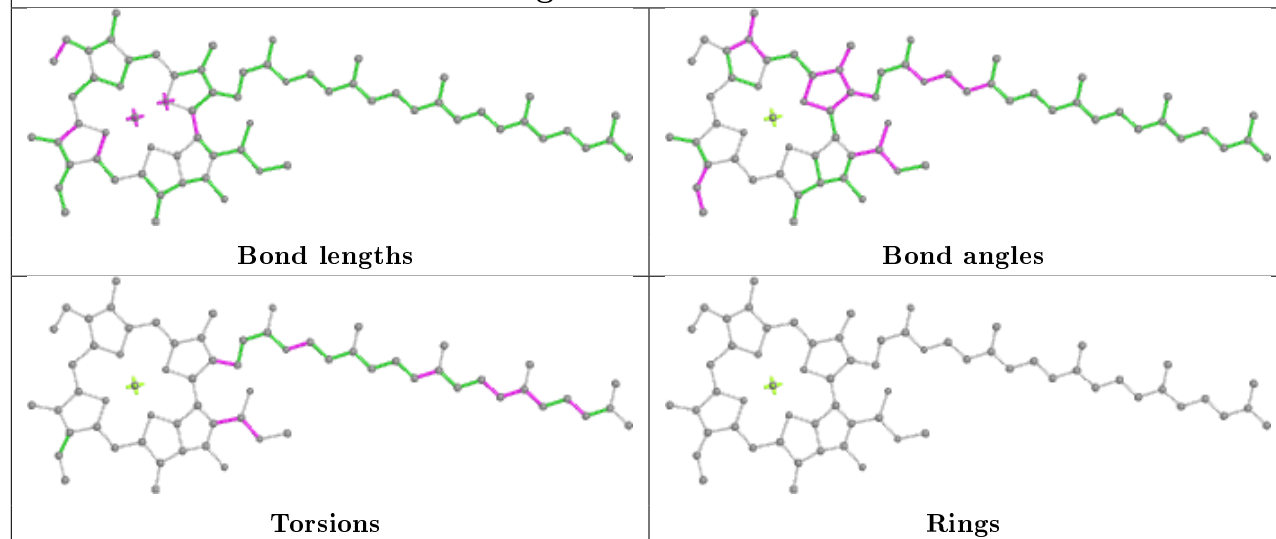
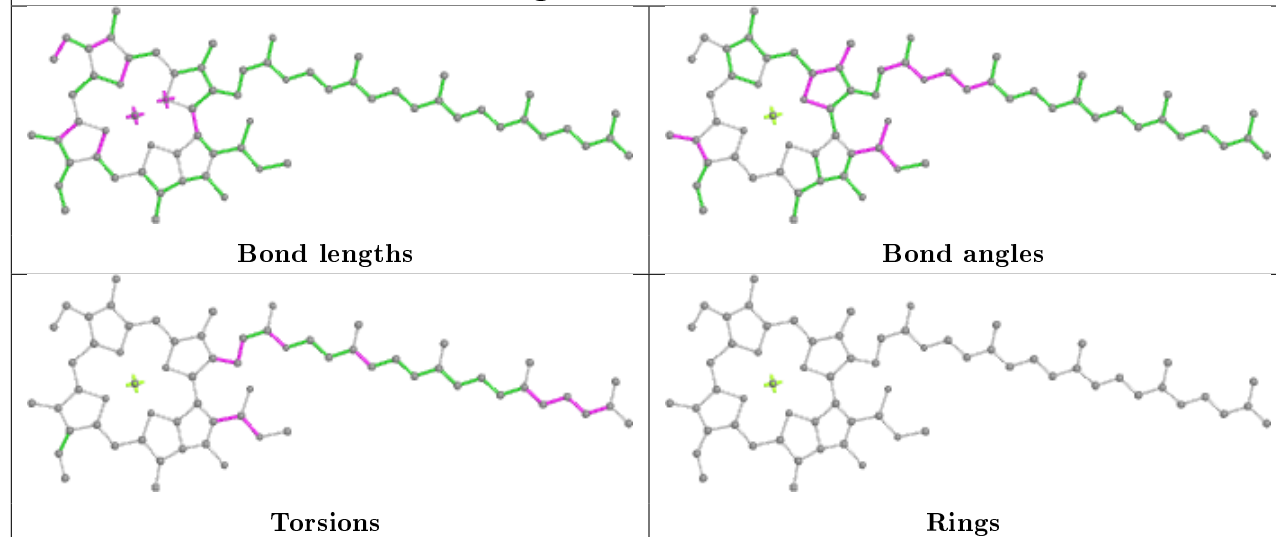
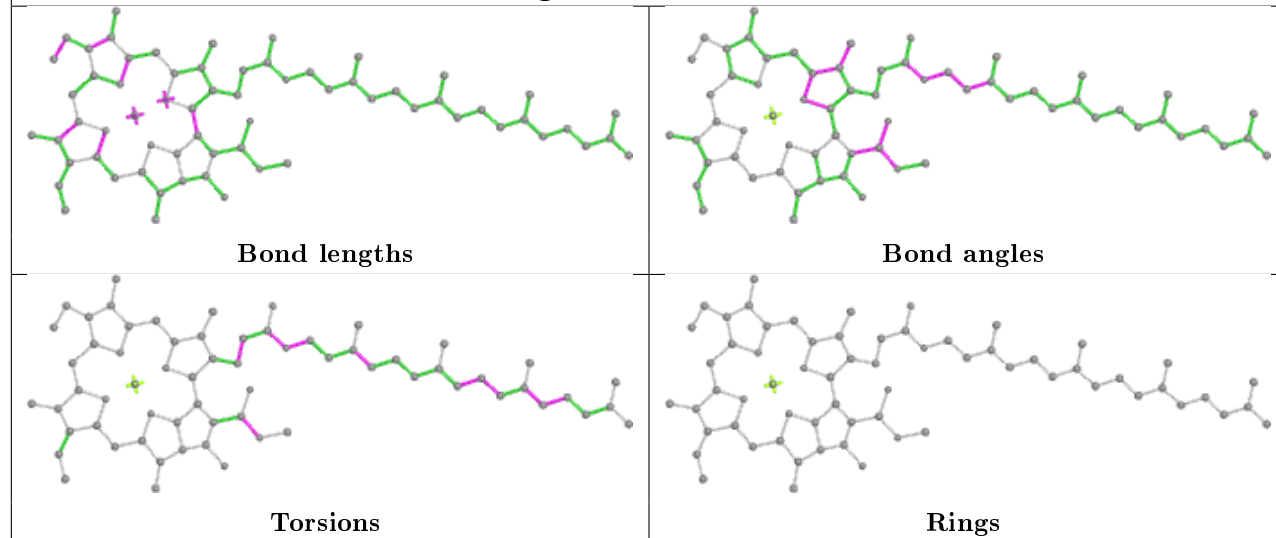
Ligand CLA 4 312

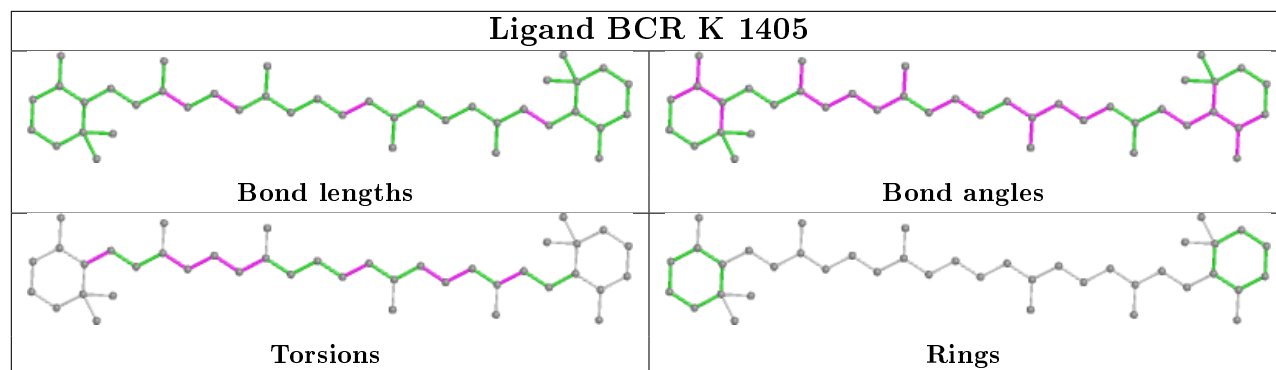
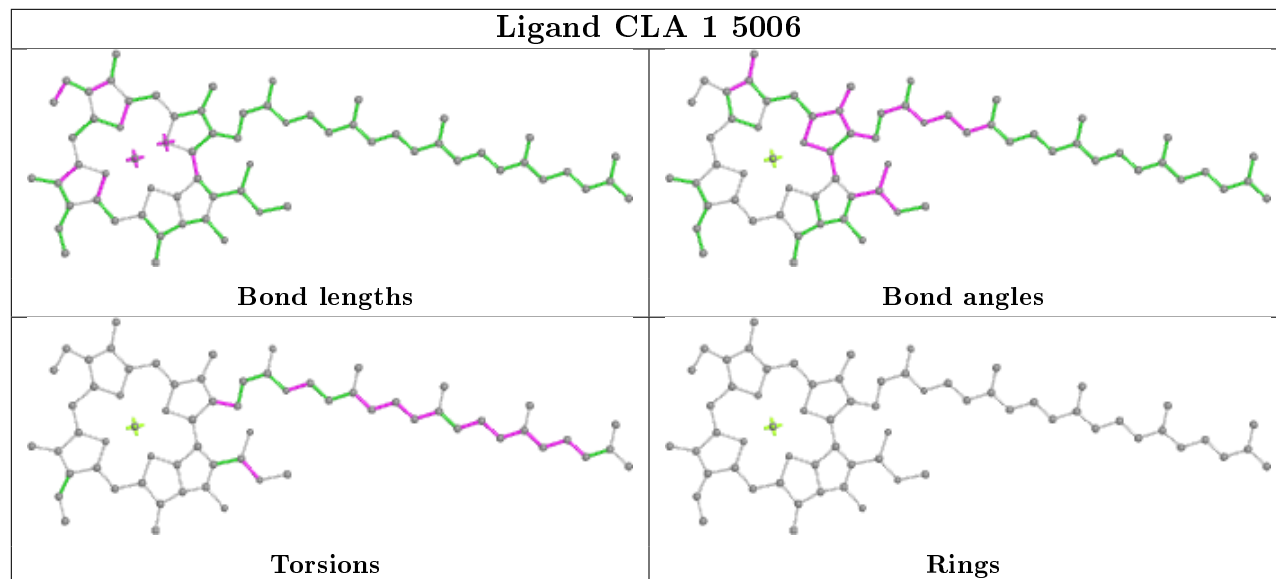
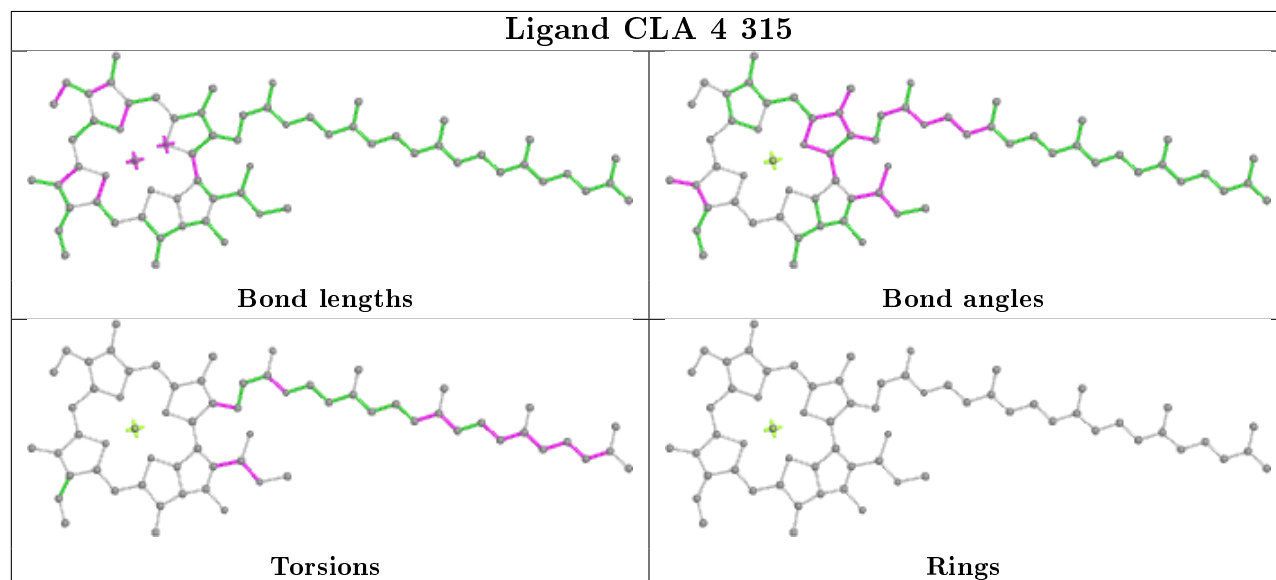


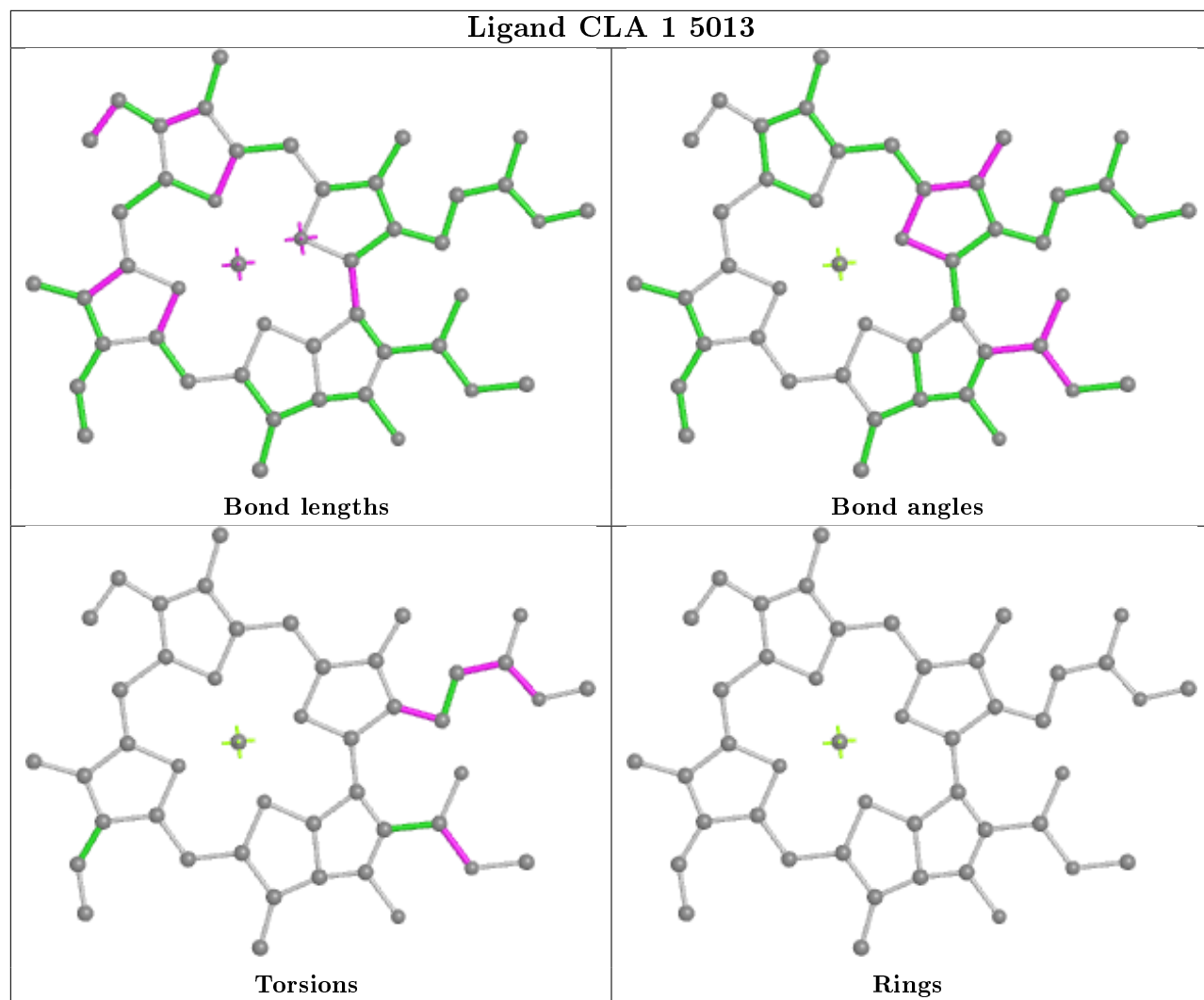
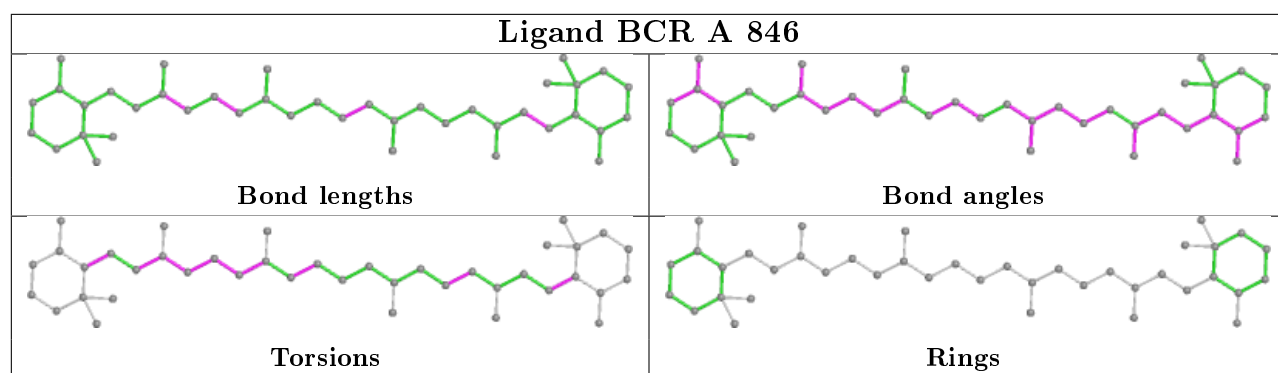
Ligand BCR 1 5005



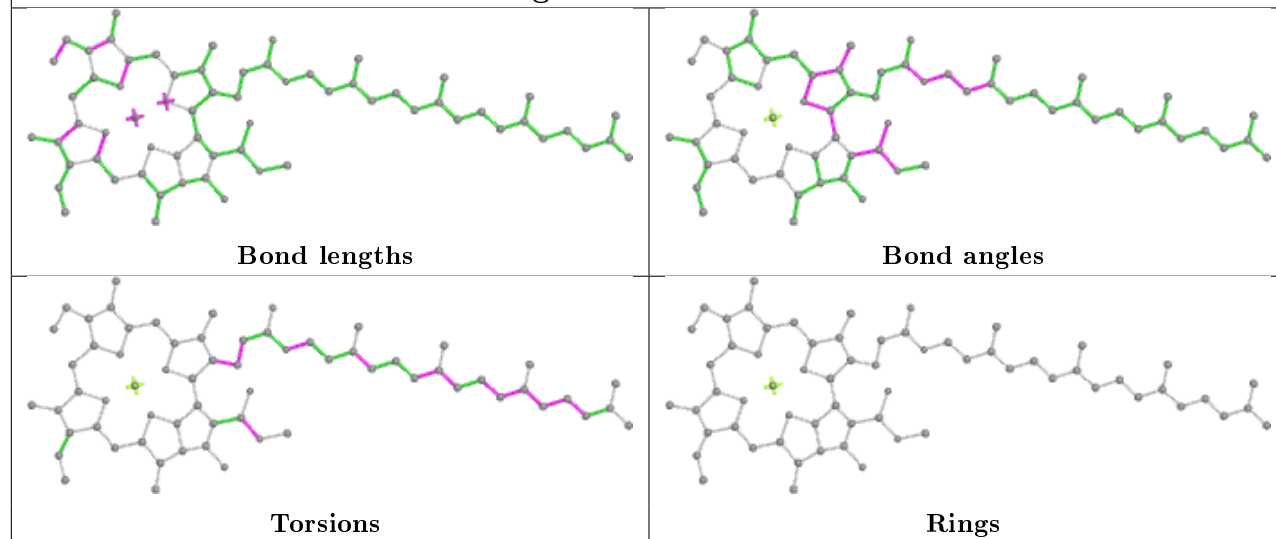


Ligand CLA 2 310**Ligand CLA B 806****Ligand CLA 4 307**

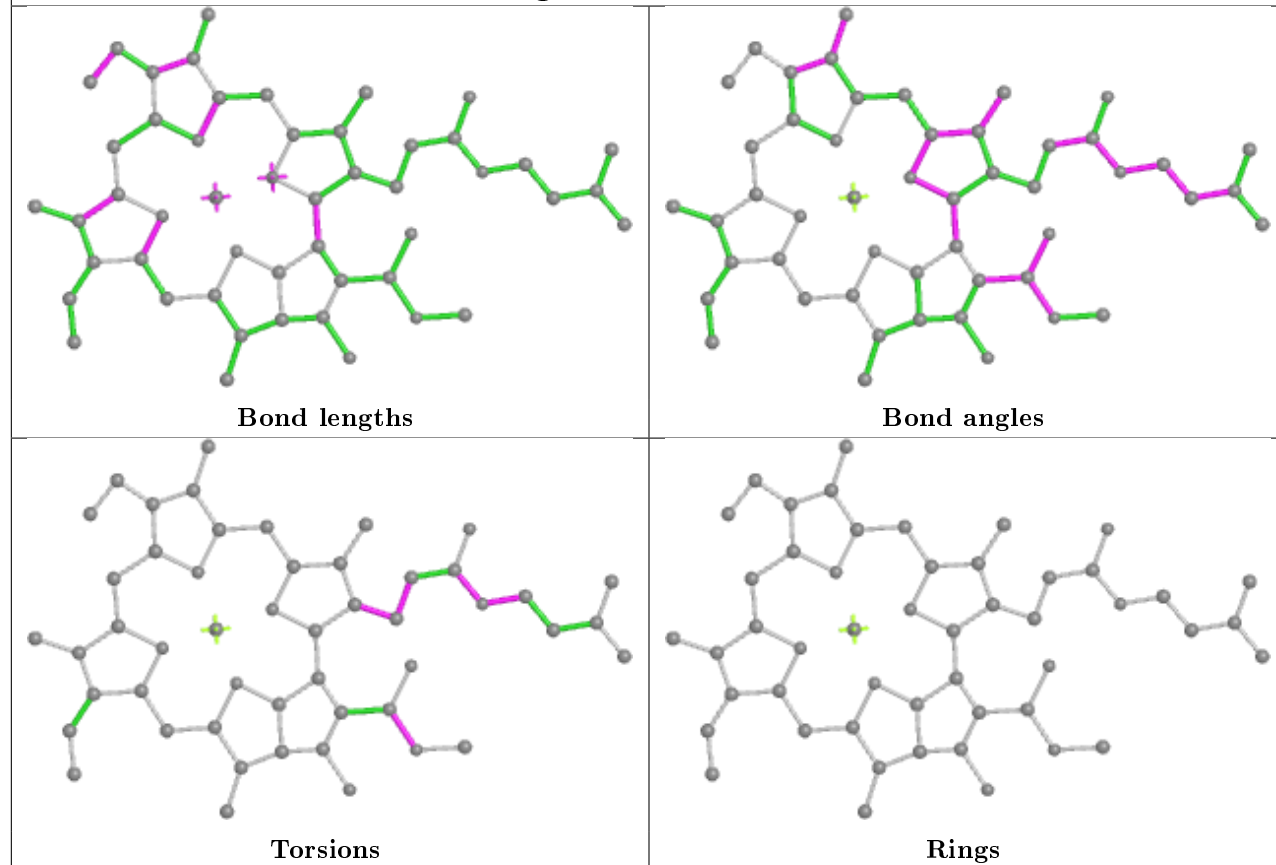
Ligand BCR K 1405**Ligand CLA 1 5006****Ligand CLA 4 315**



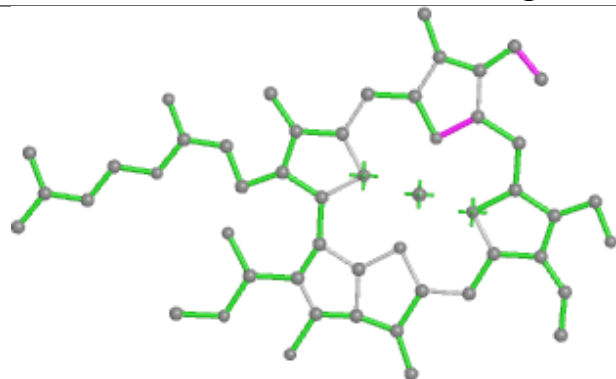
Ligand CLA A 832



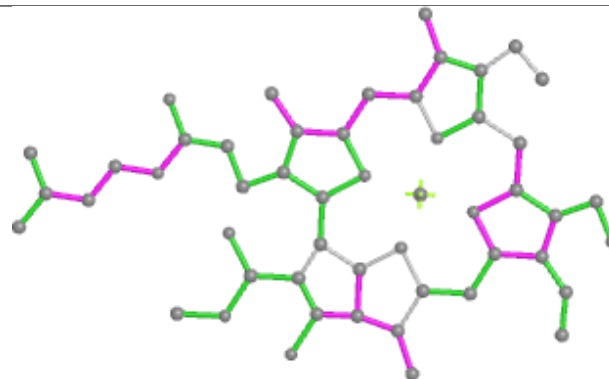
Ligand CLA L 306



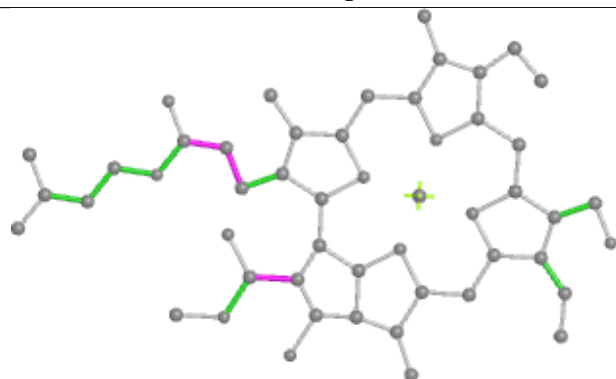
Ligand CHL 3 313



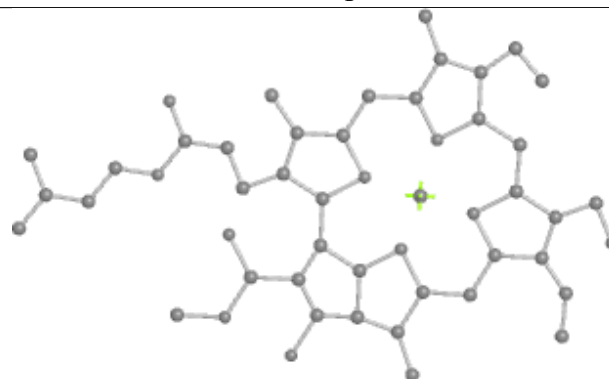
Bond lengths



Bond angles

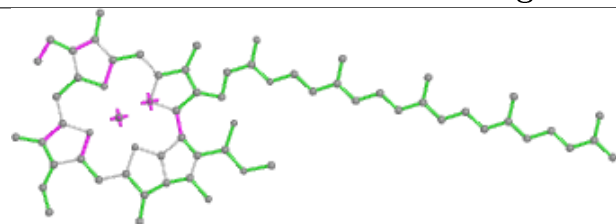


Torsions

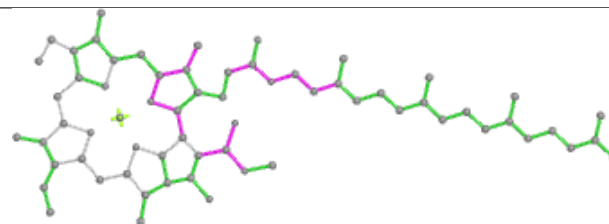


Rings

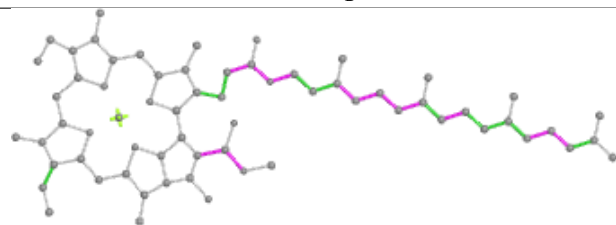
Ligand CLA B 822



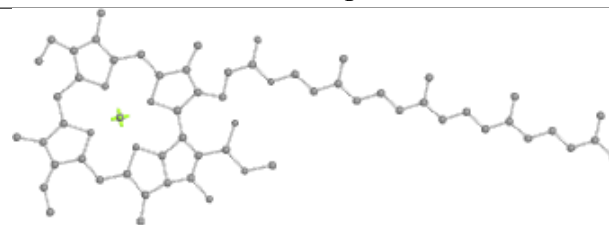
Bond lengths



Bond angles

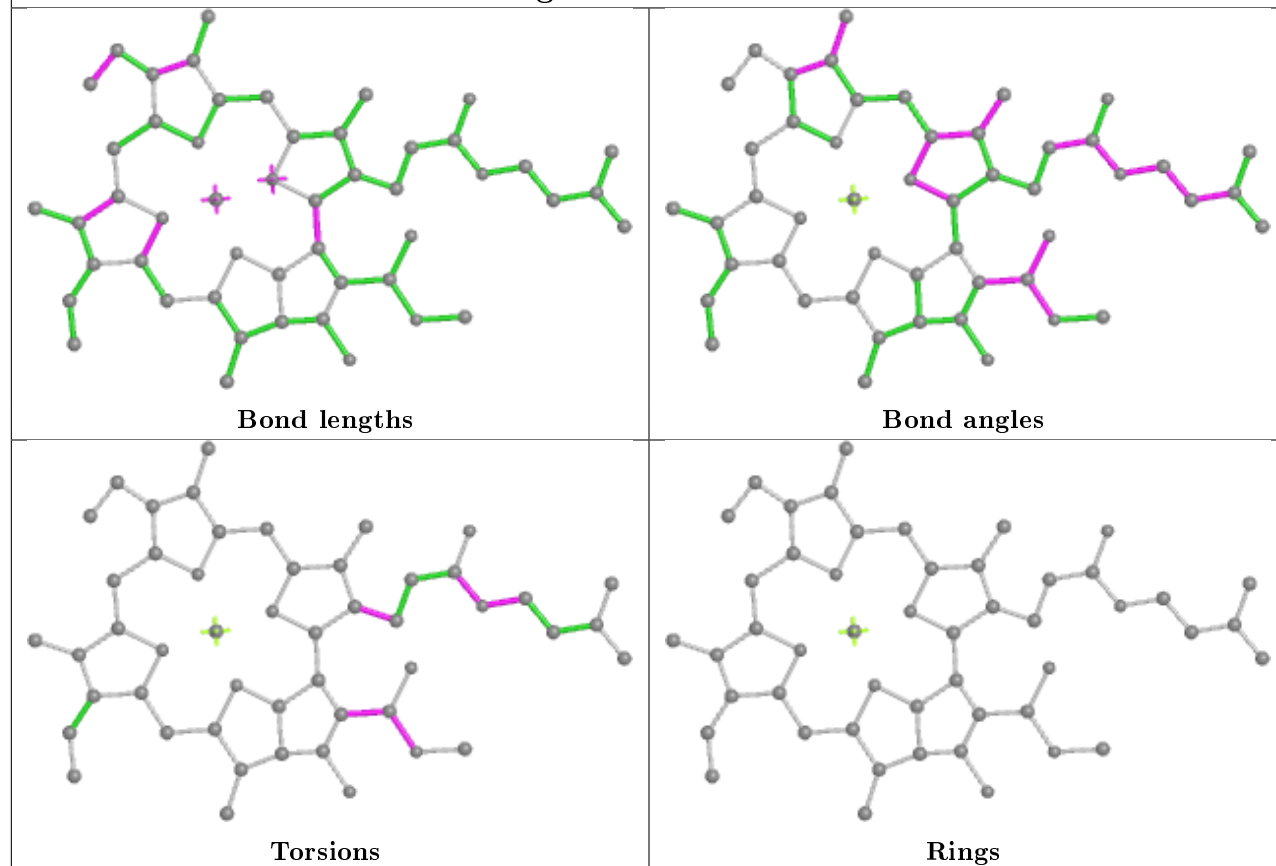


Torsions

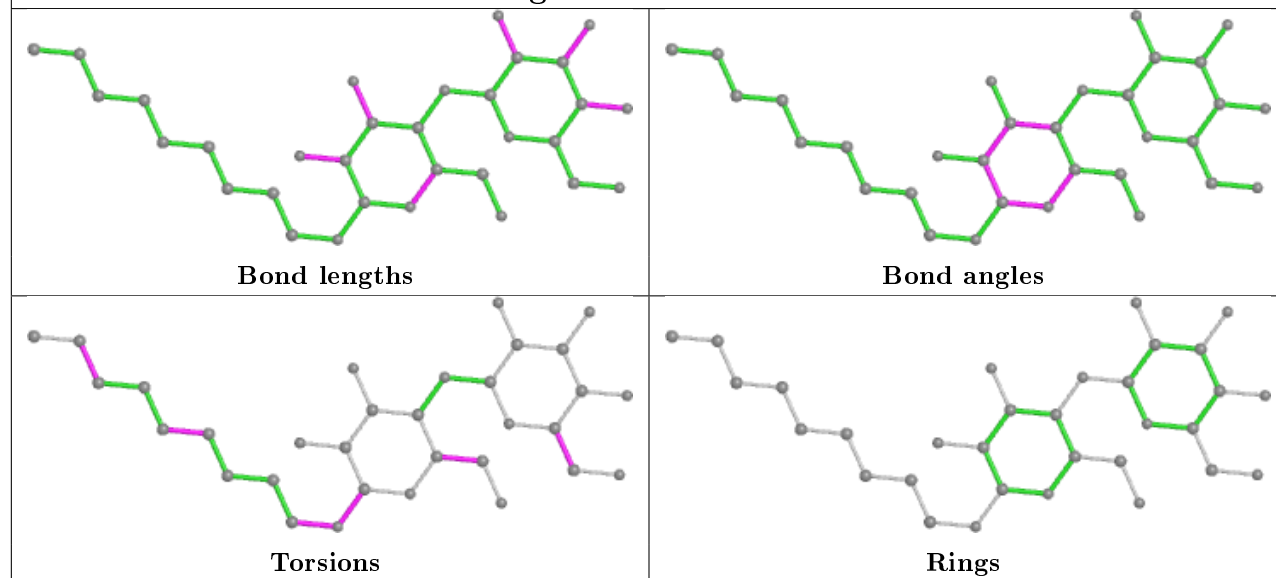


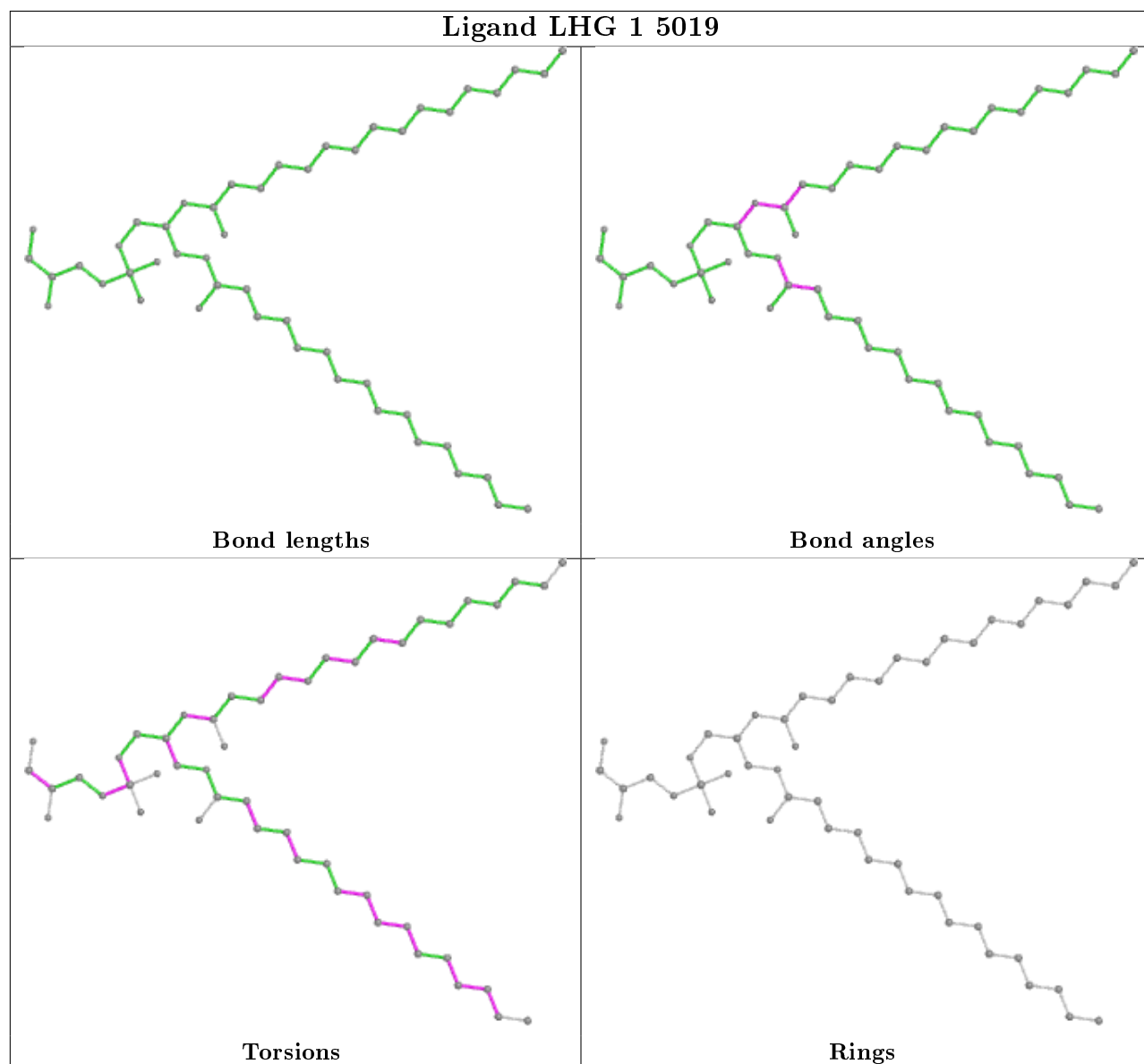
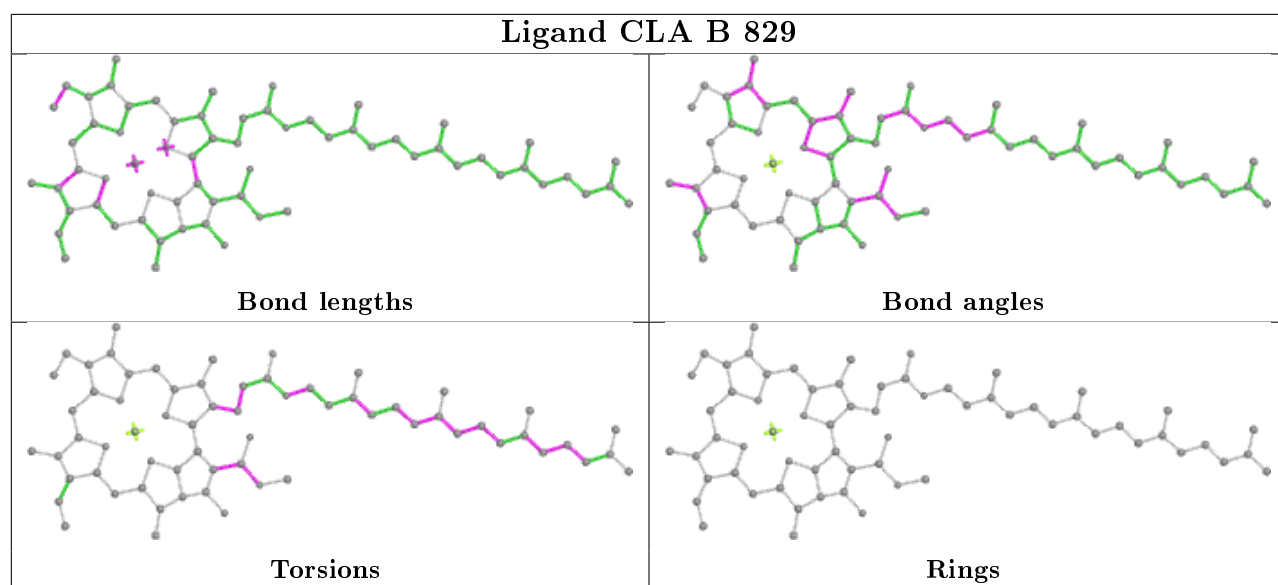
Rings

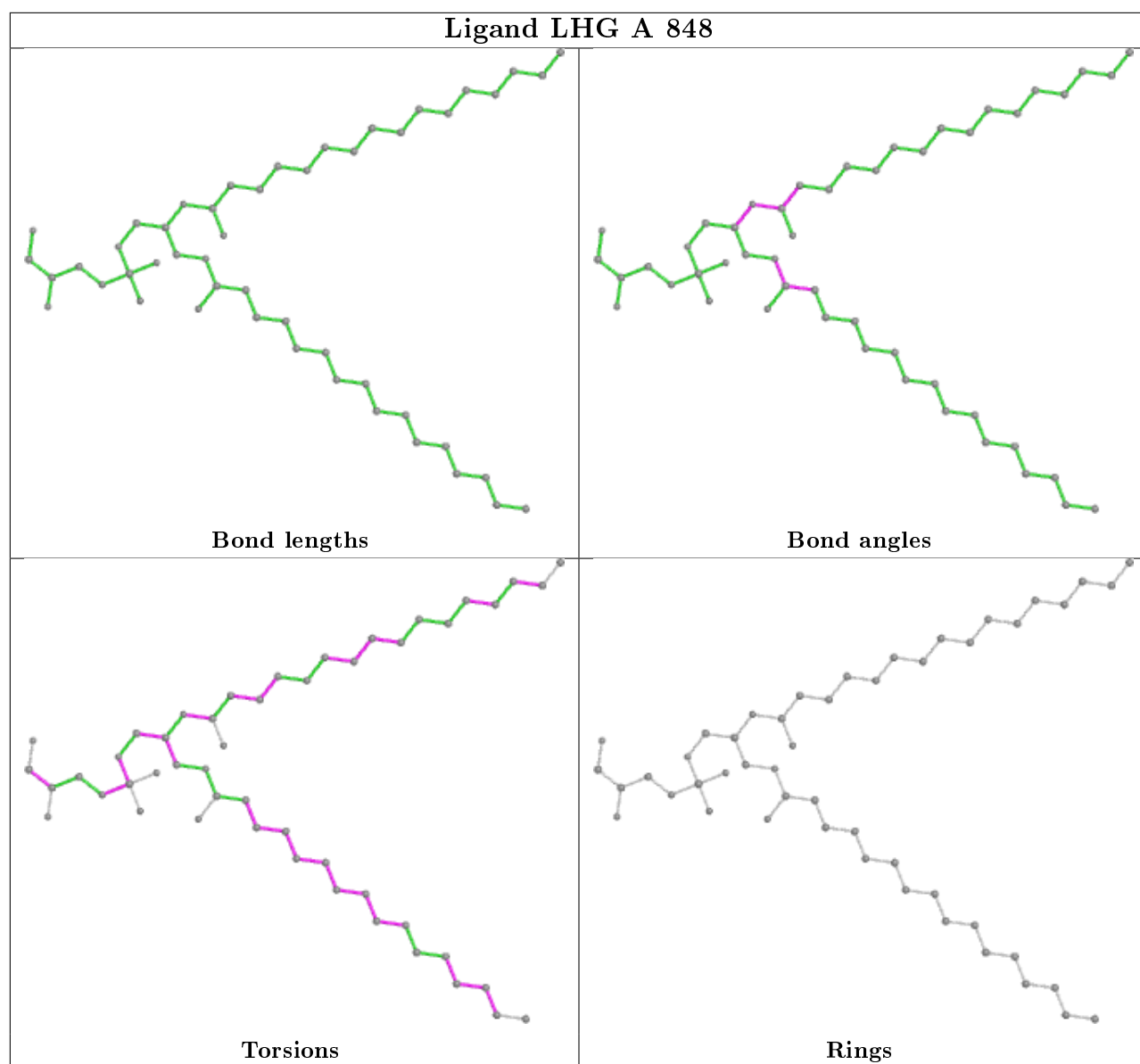
Ligand CLA 3 317

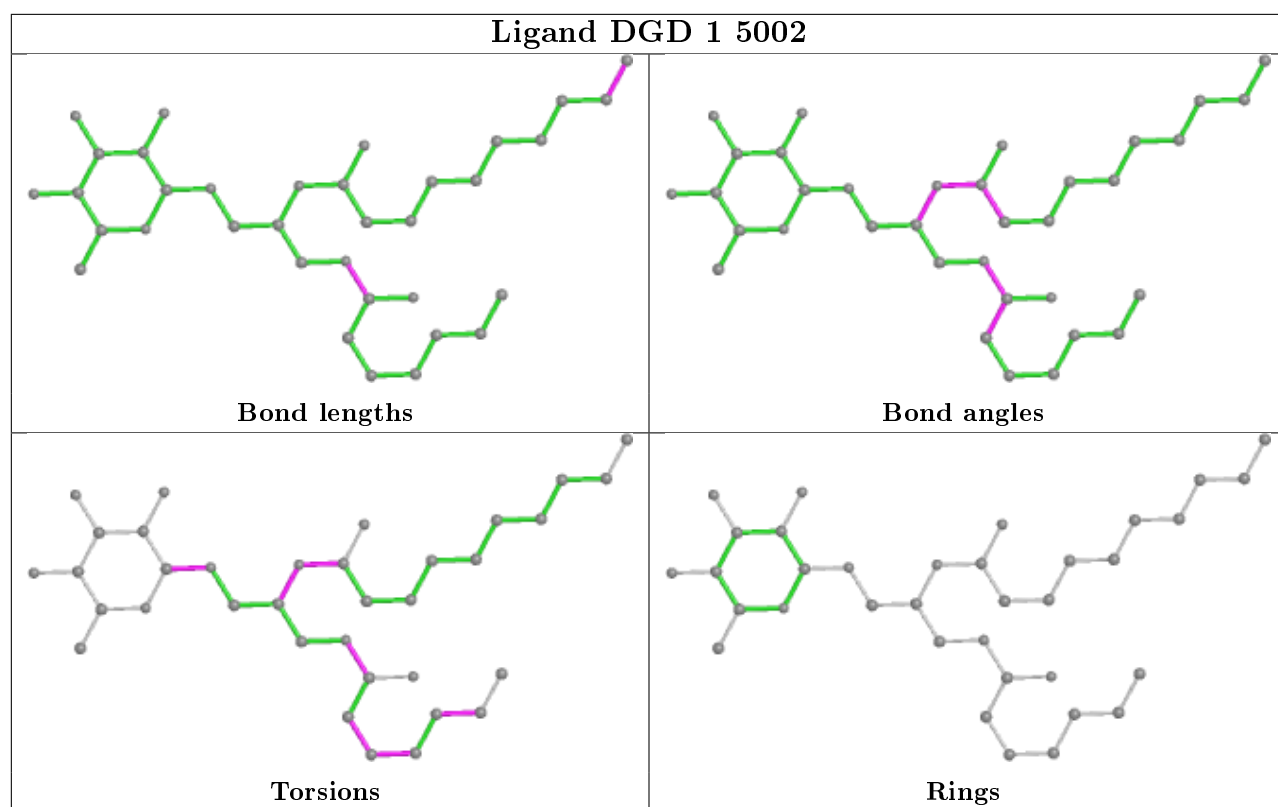


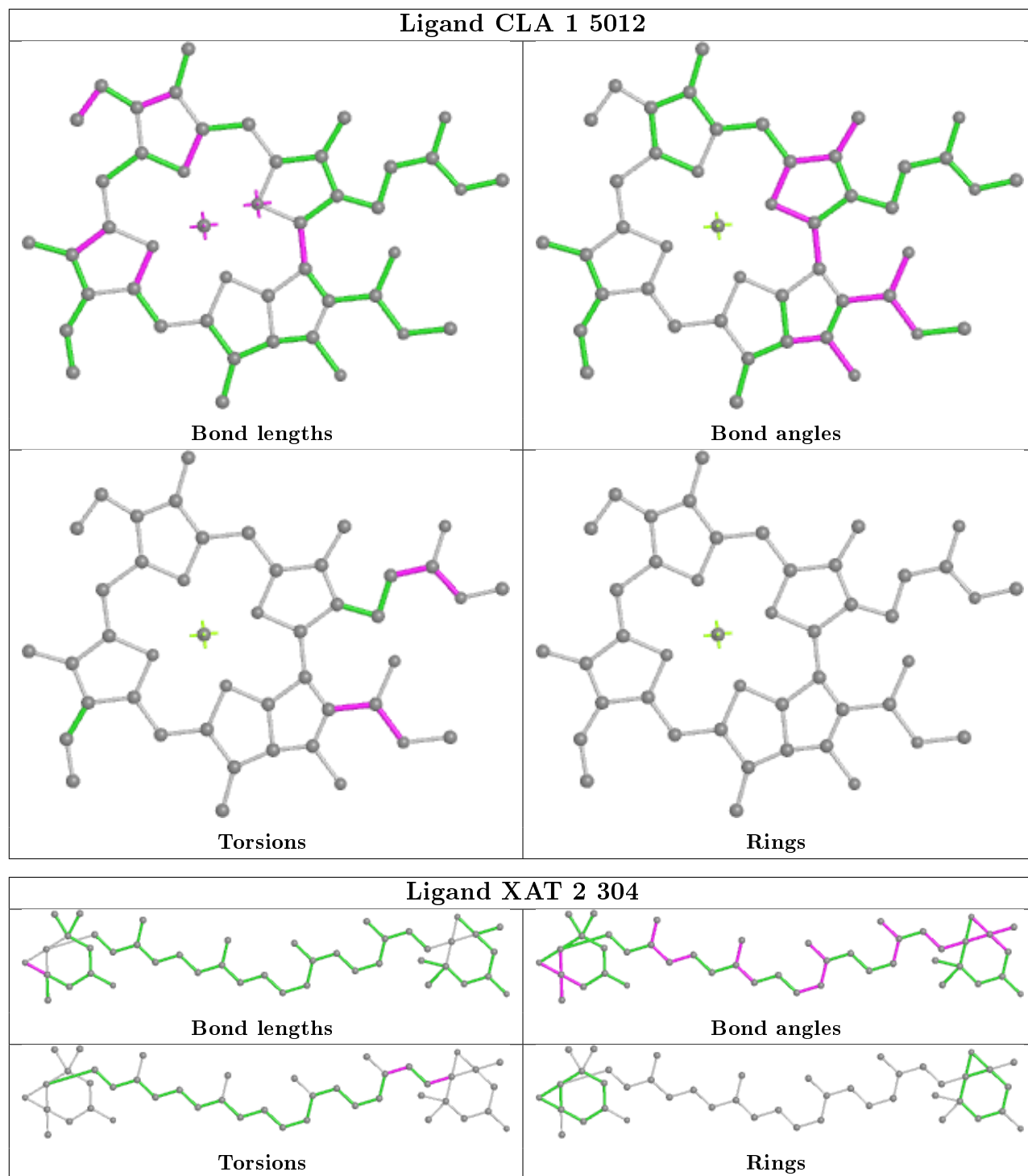
Ligand LMT B 853

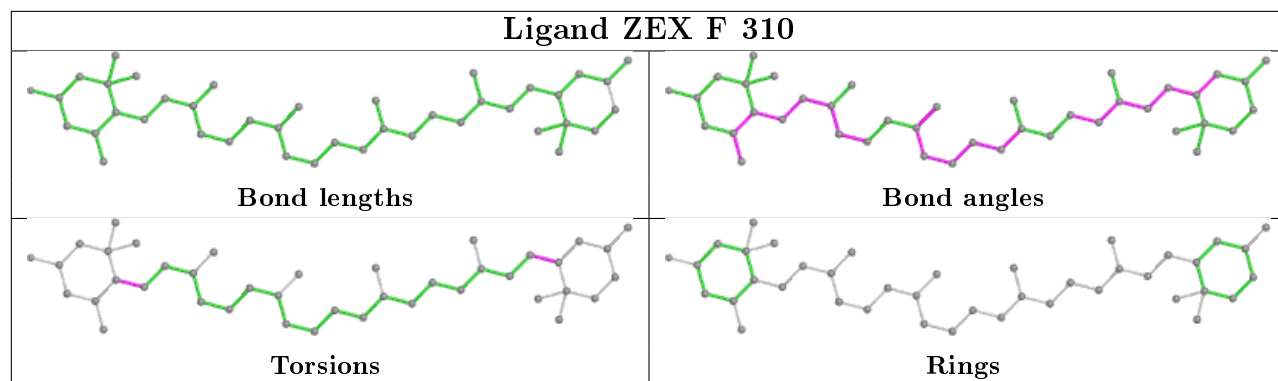
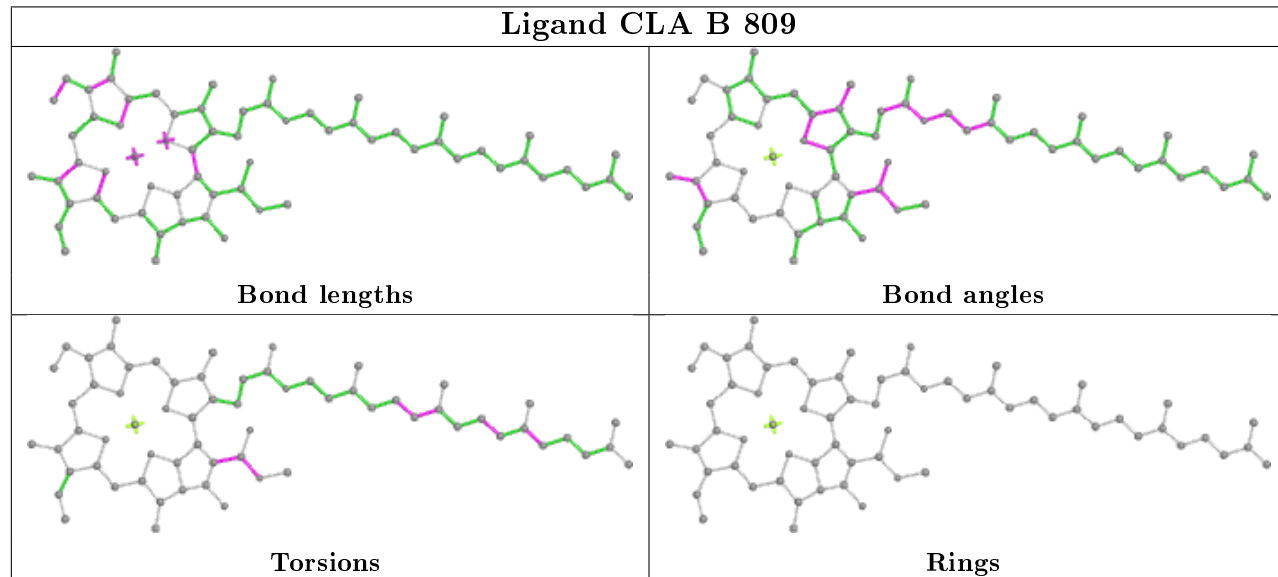
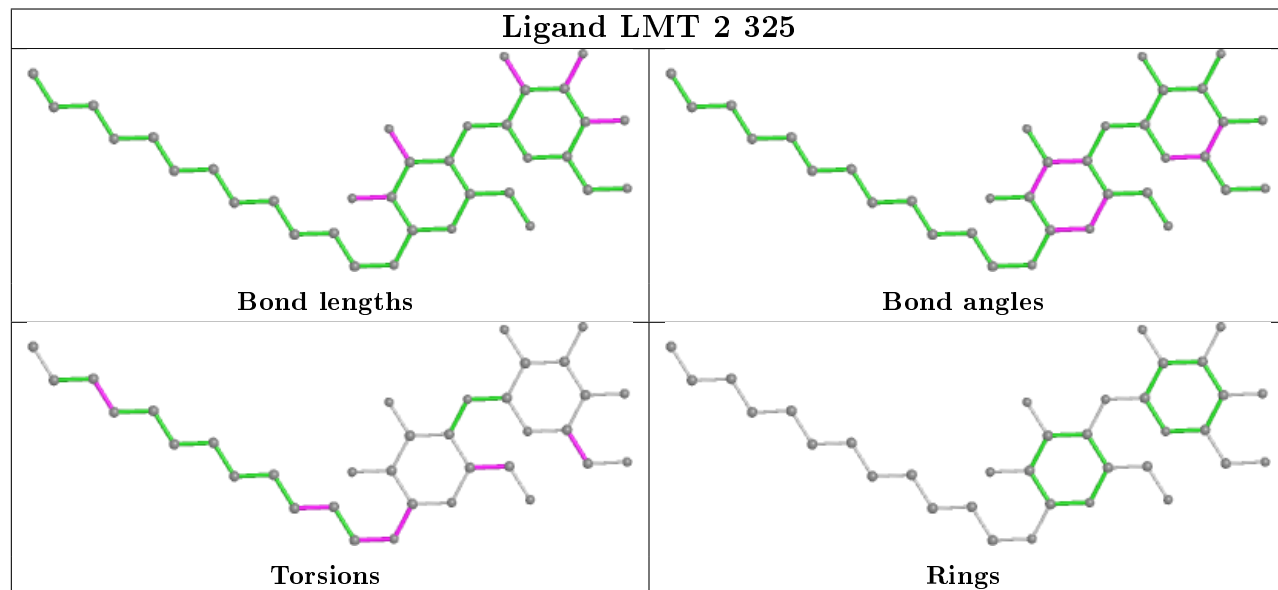


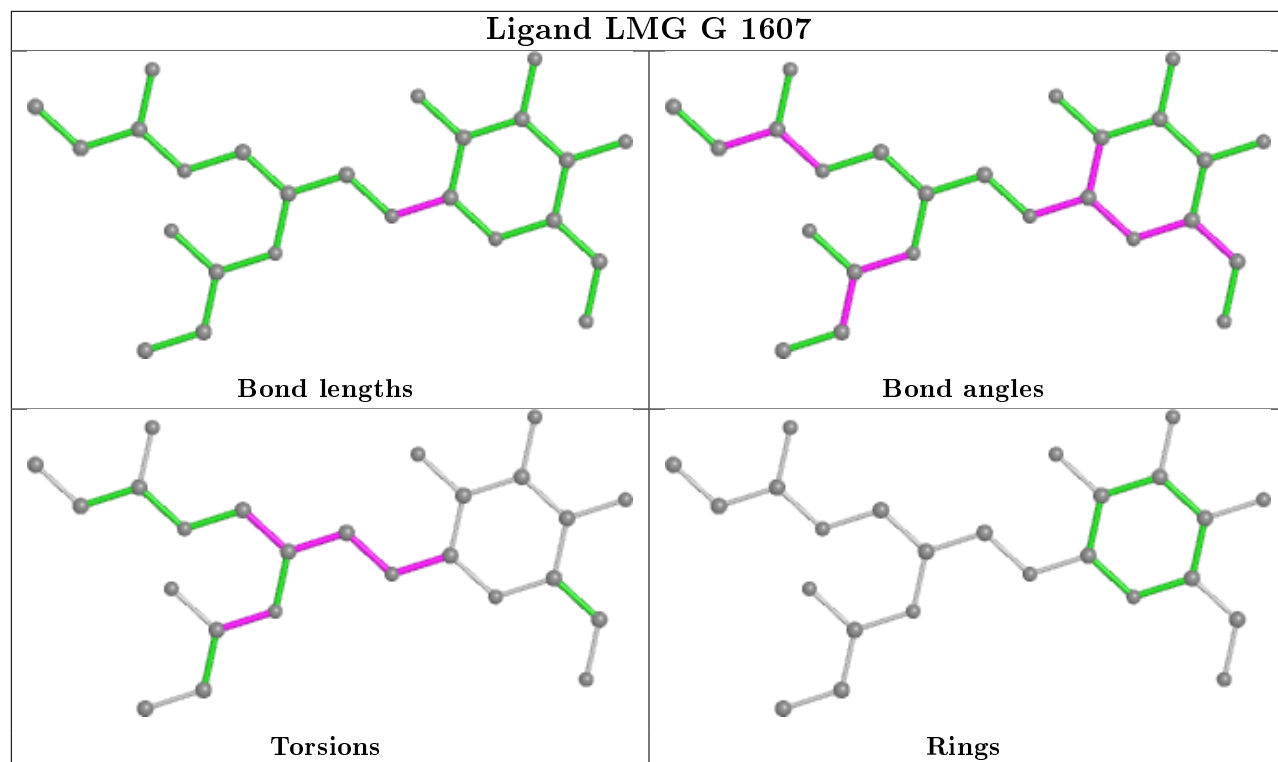




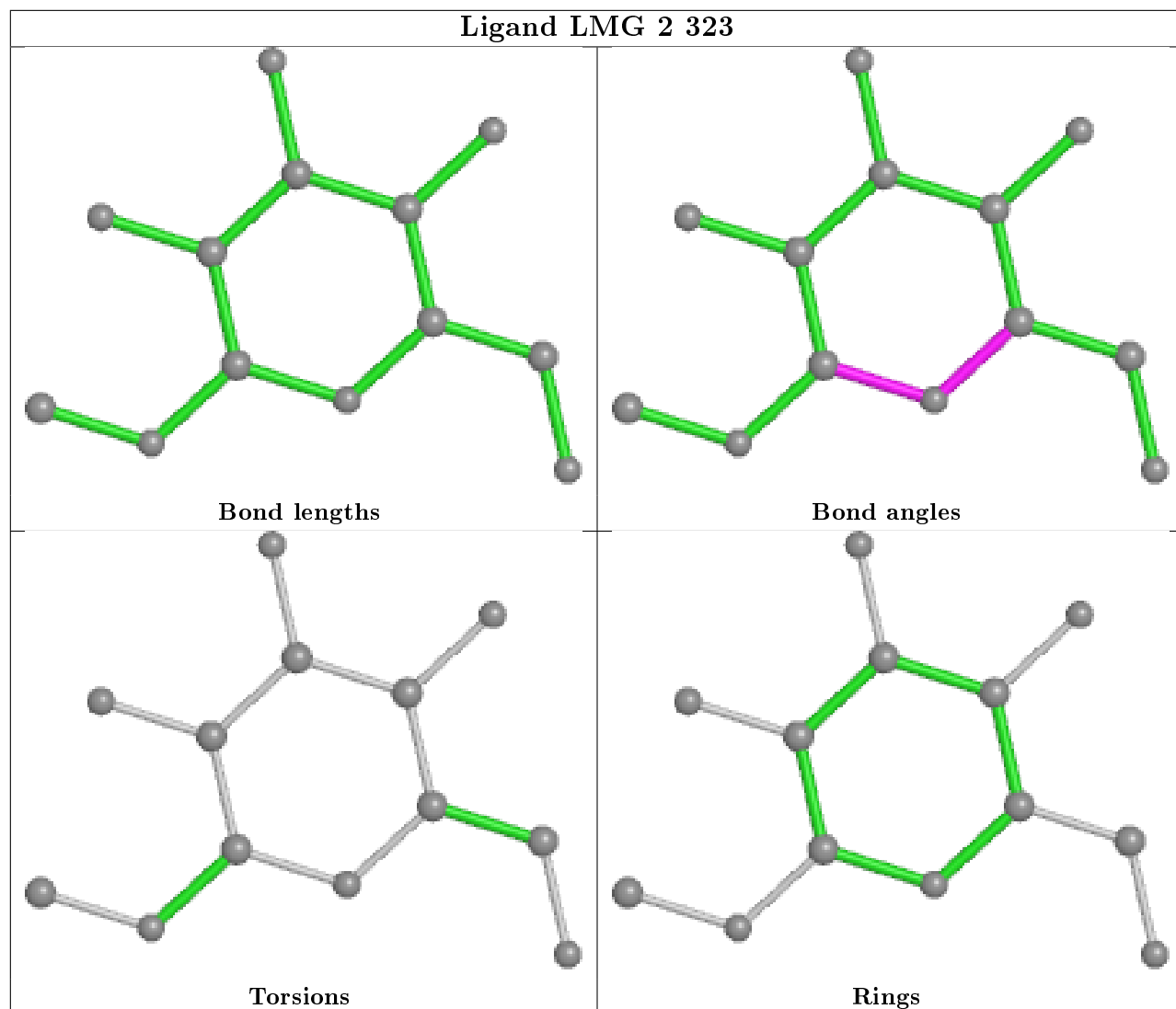




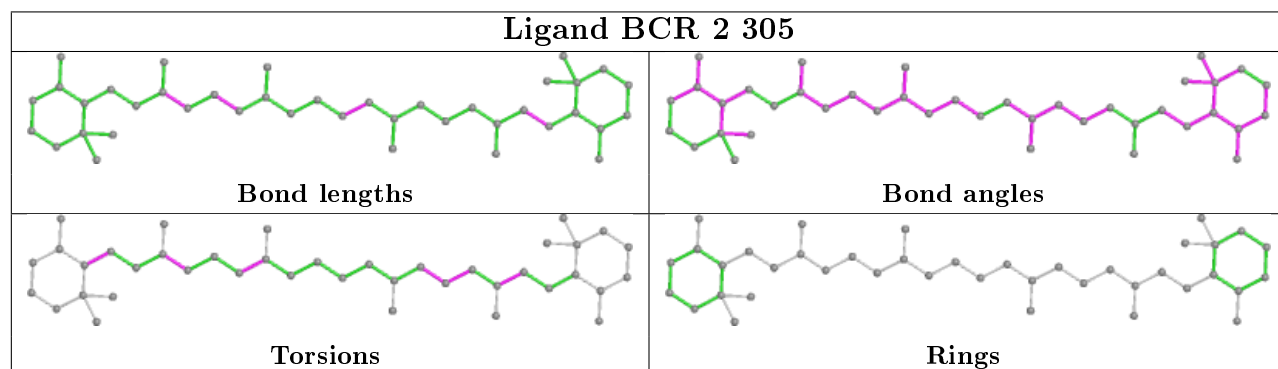
Ligand ZEX F 310**Ligand CLA B 809****Ligand LMT 2 325**

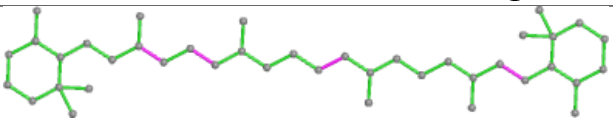
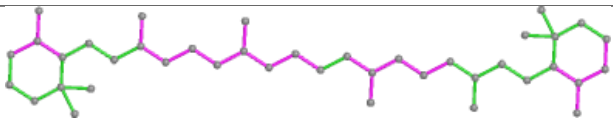
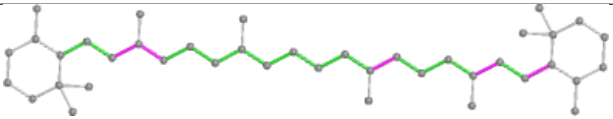
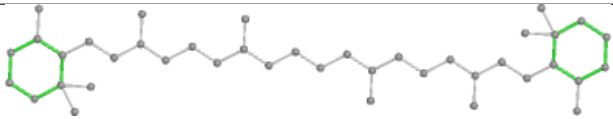


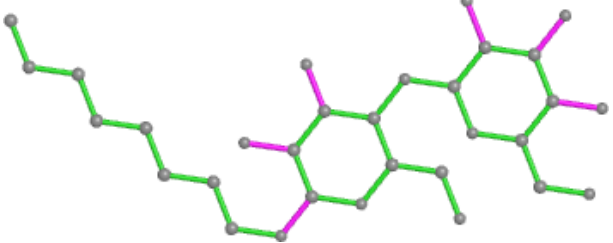
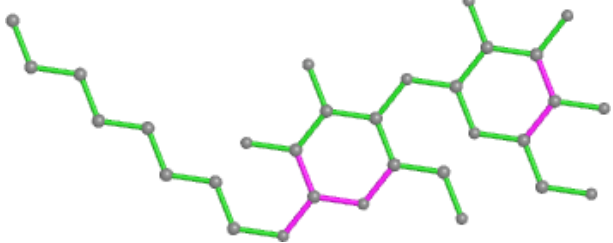
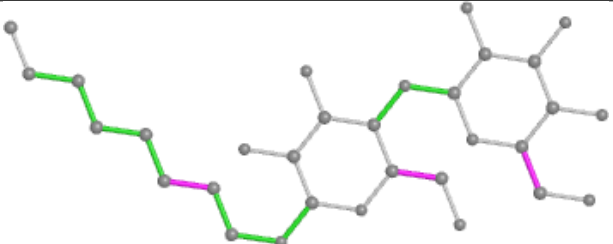
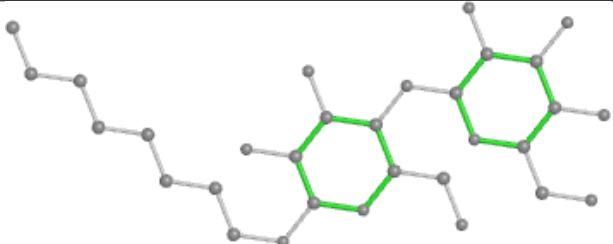
Ligand LMG 2 323

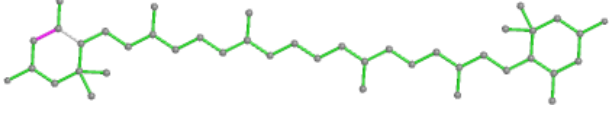
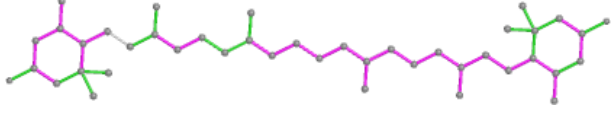
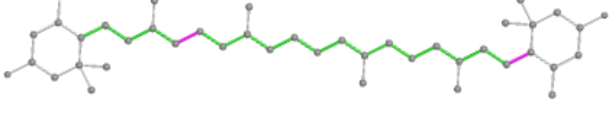
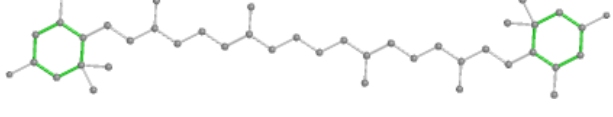


Ligand BCR 2 305

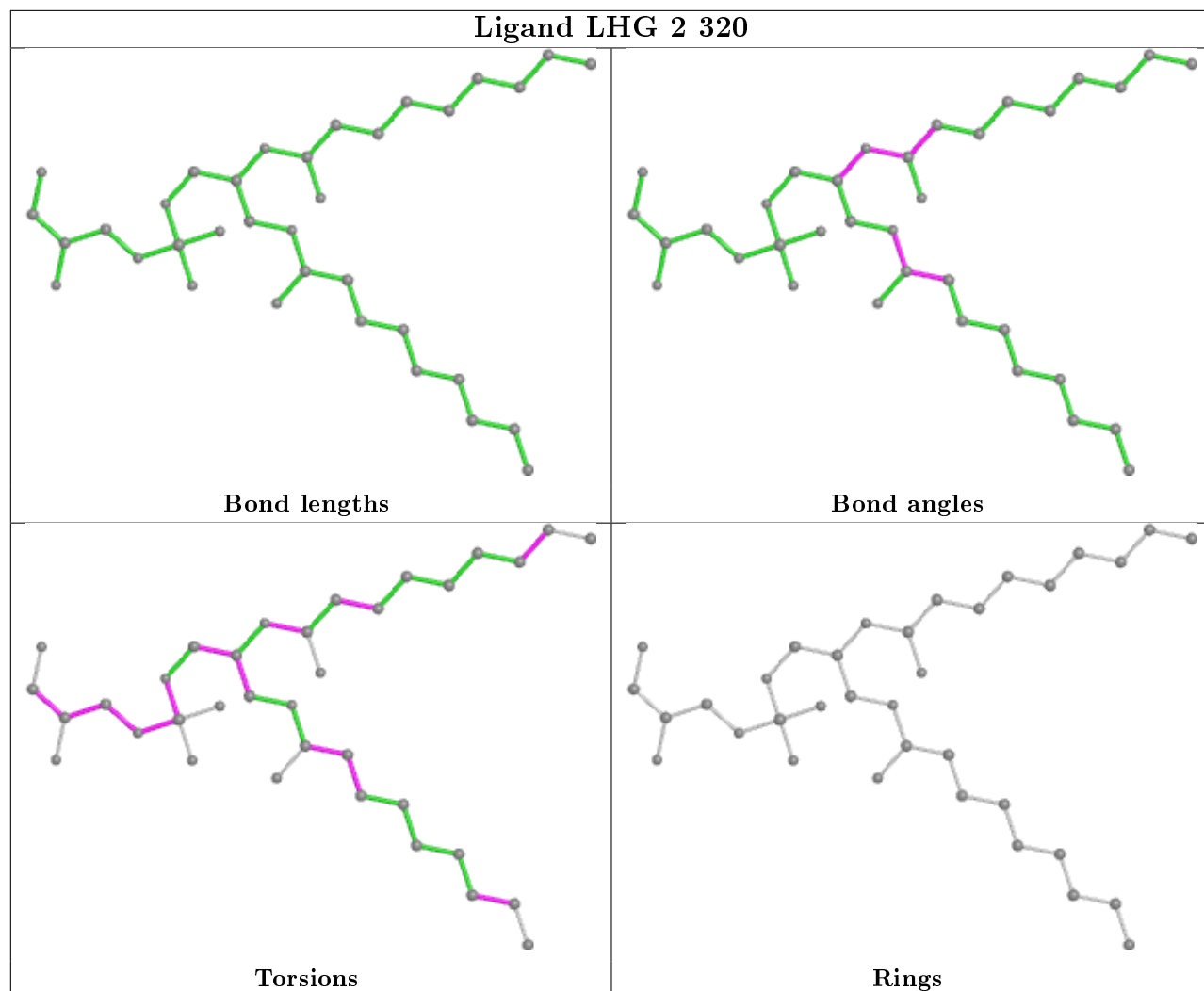


Ligand BCR A 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

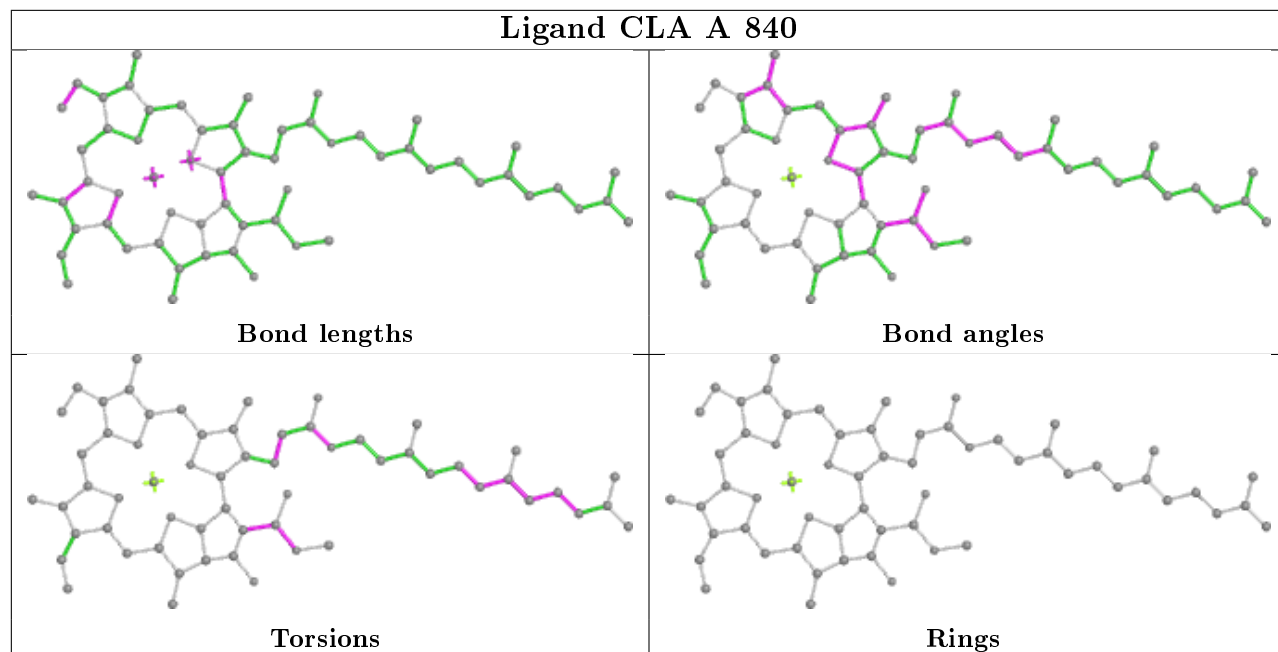
Ligand LMT B 856	
	
Bond lengths	Bond angles
	
Torsions	Rings

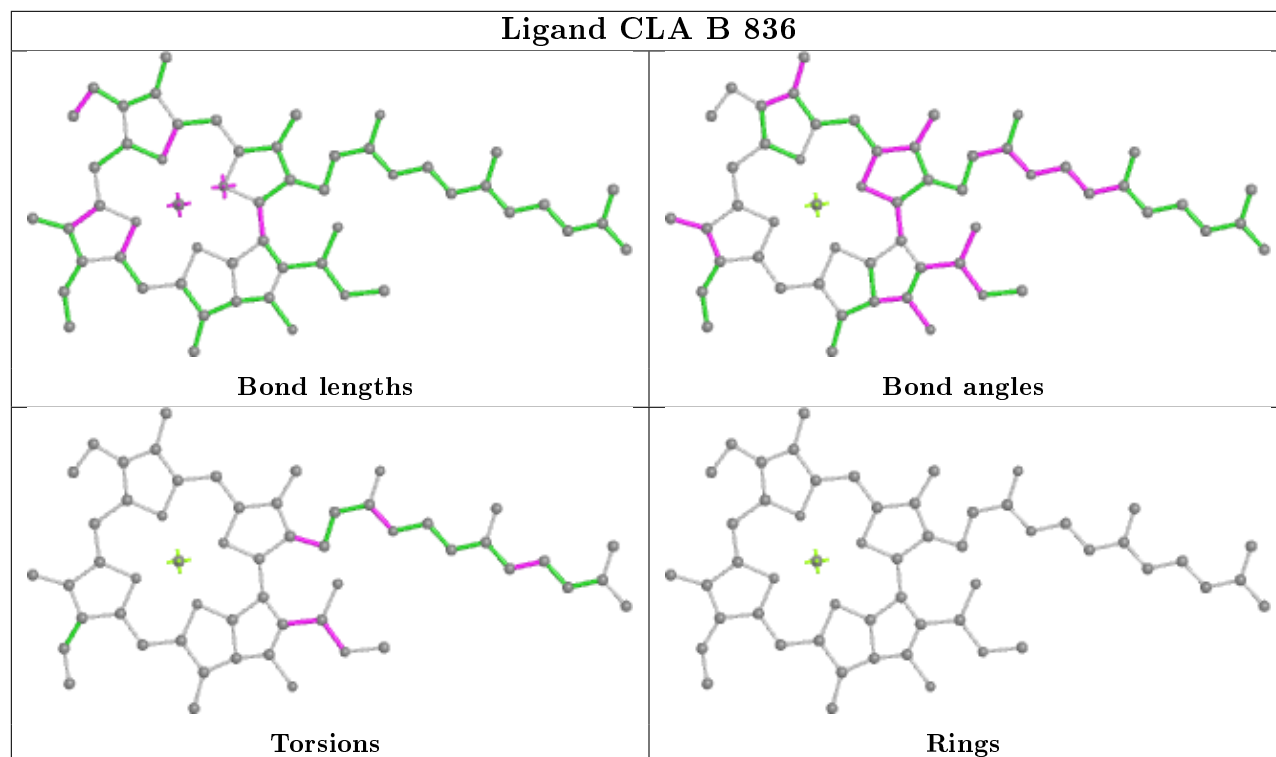
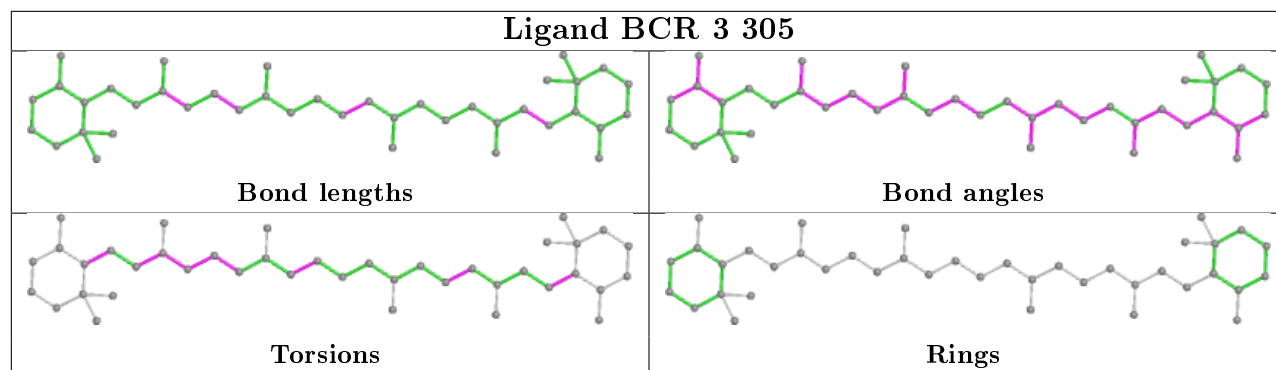
Ligand LUT 3 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG 2 320

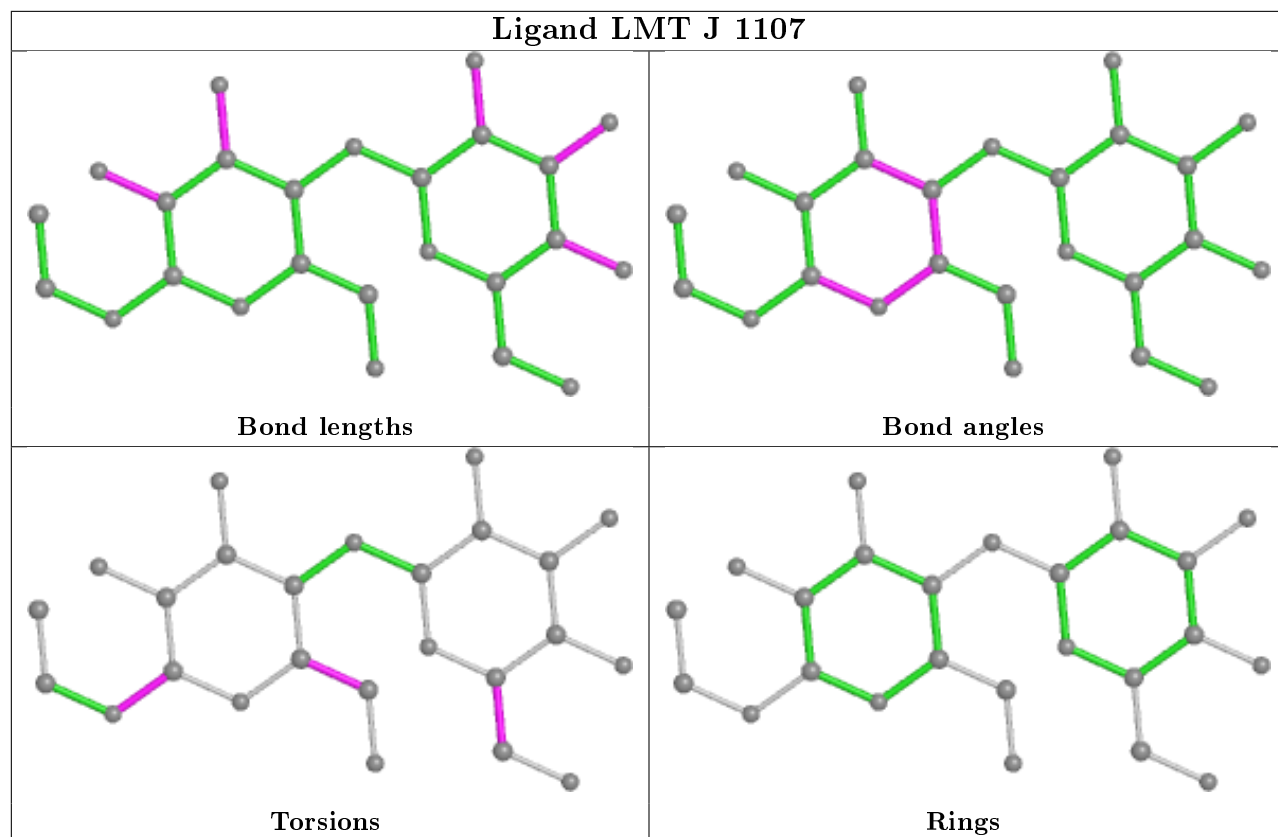


Ligand CLA A 840

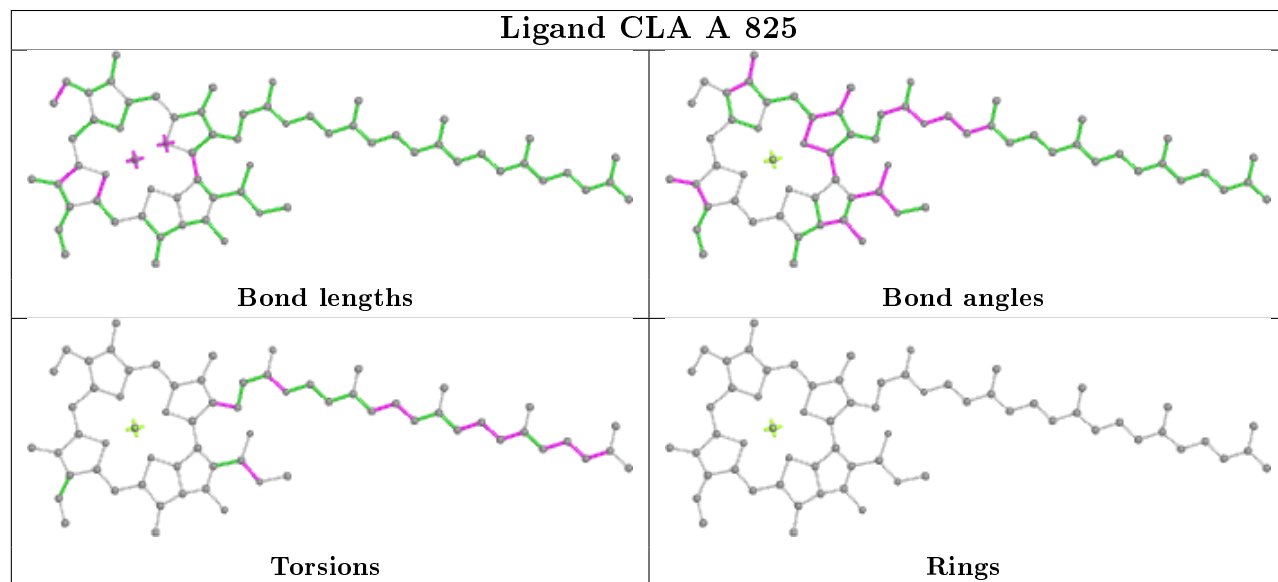


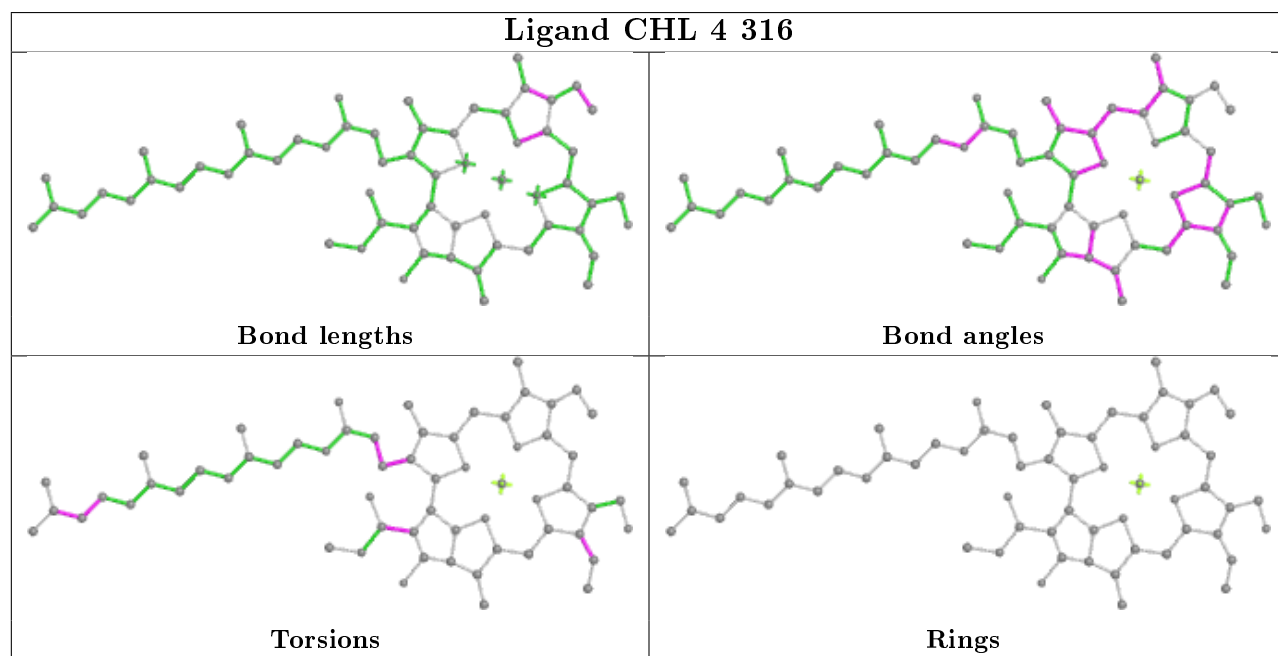
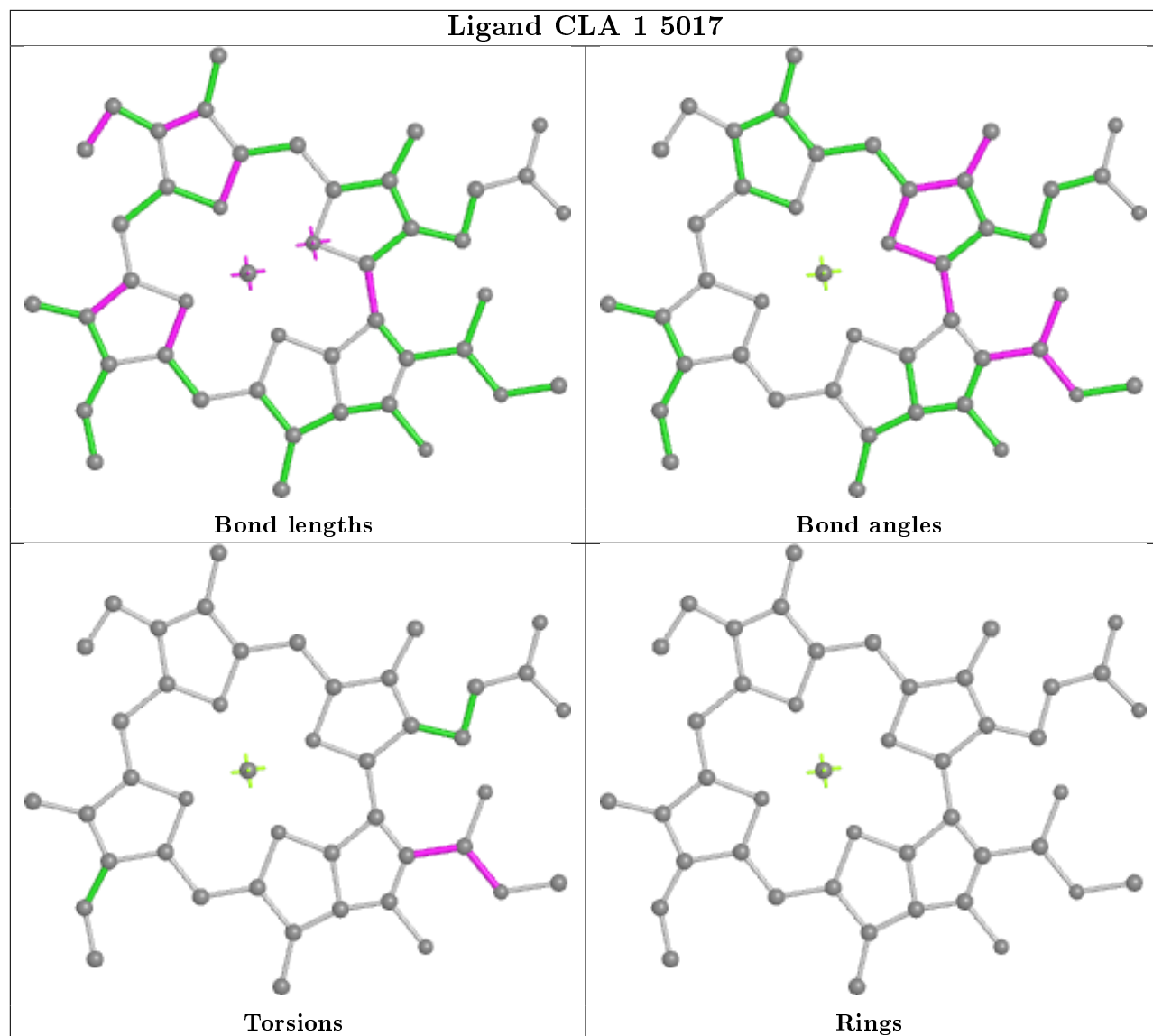


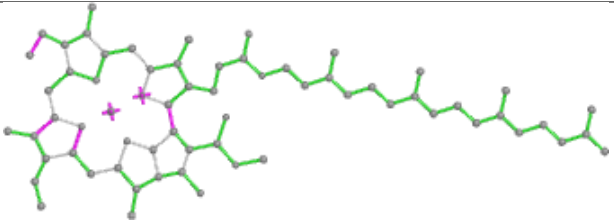
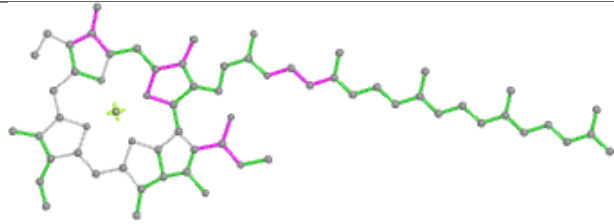
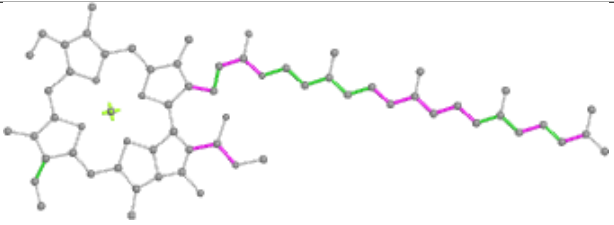
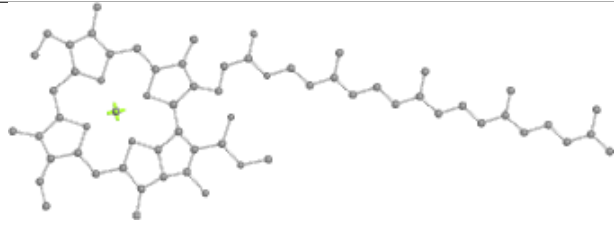
Ligand LMT J 1107

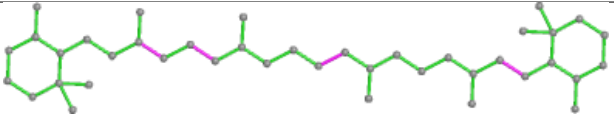
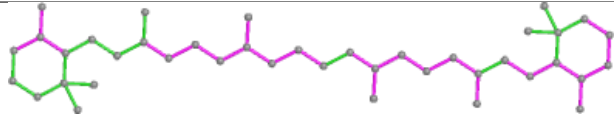
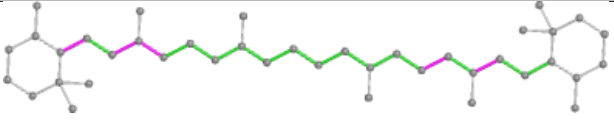
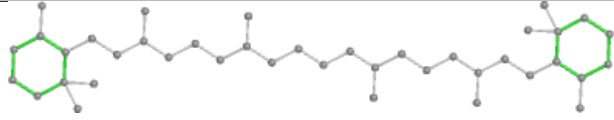


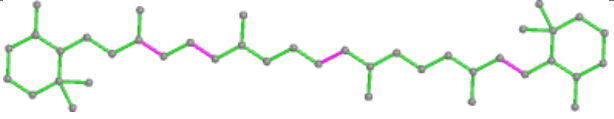
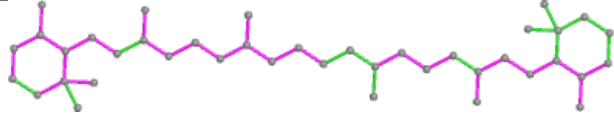
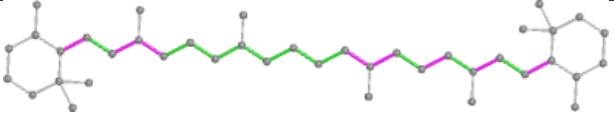
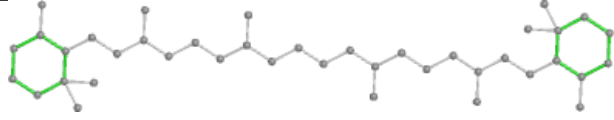
Ligand CLA A 825



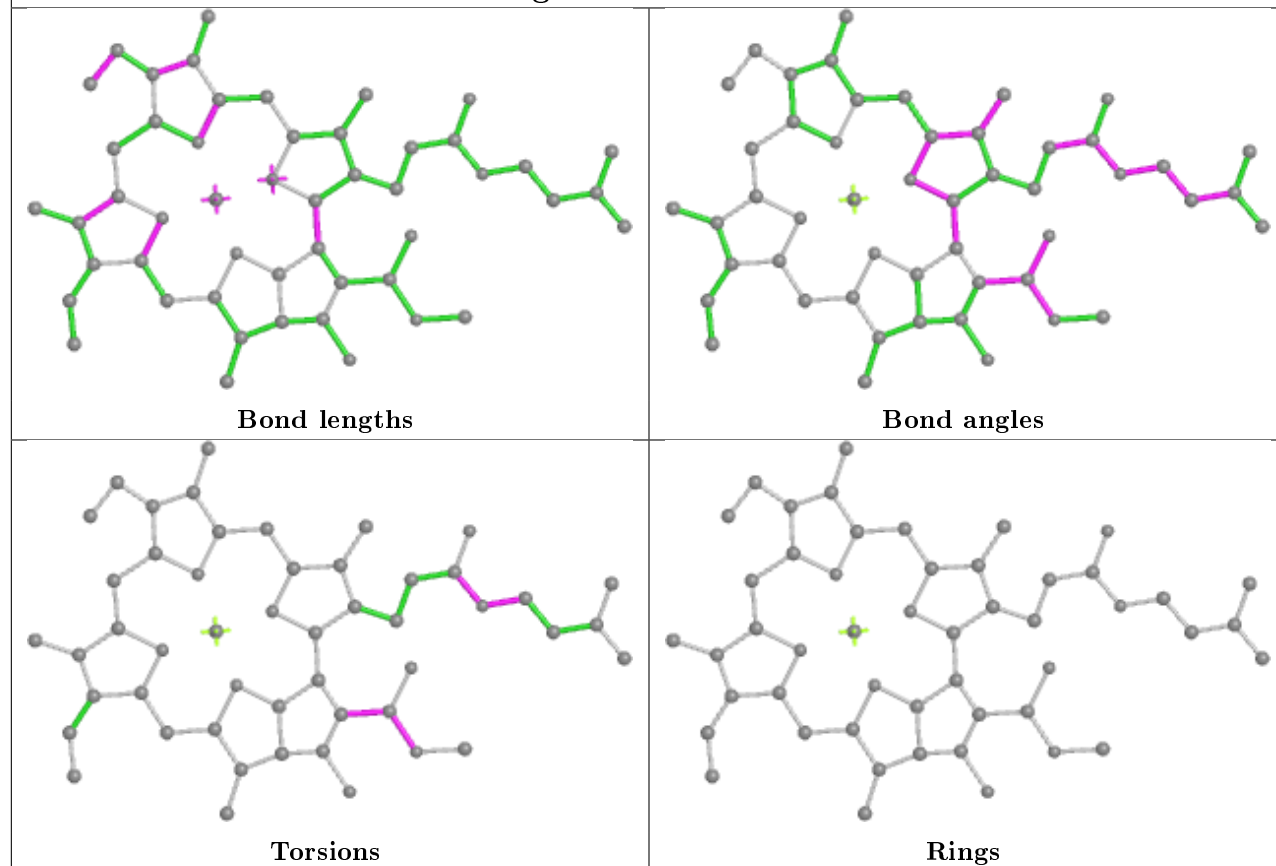


Ligand CLA B 826	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

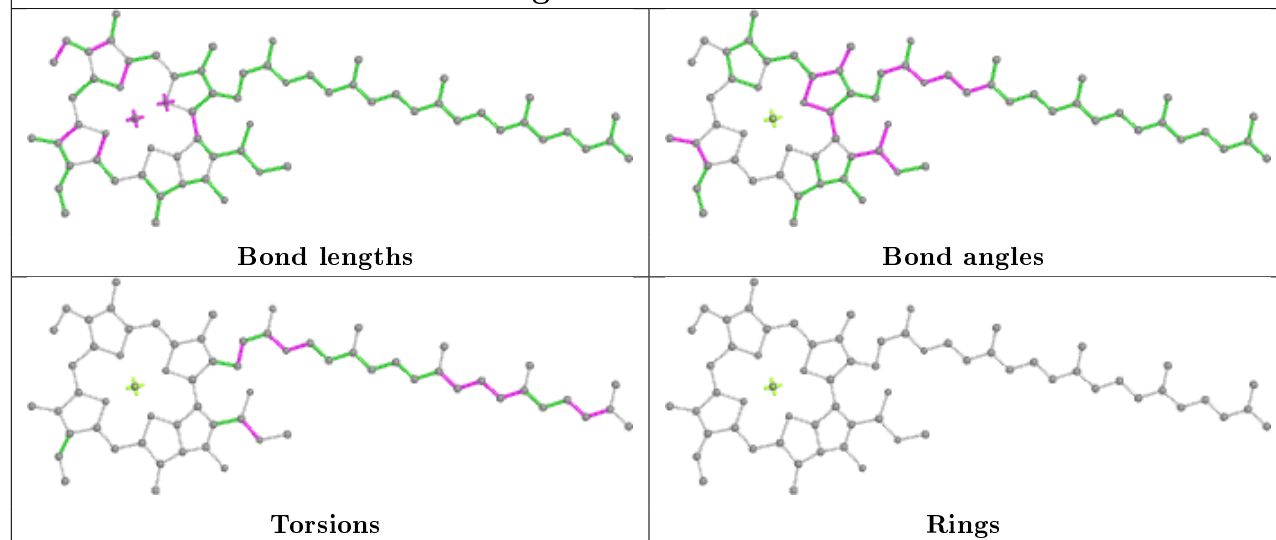
Ligand BCR A 855	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

Ligand BCR A 847	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

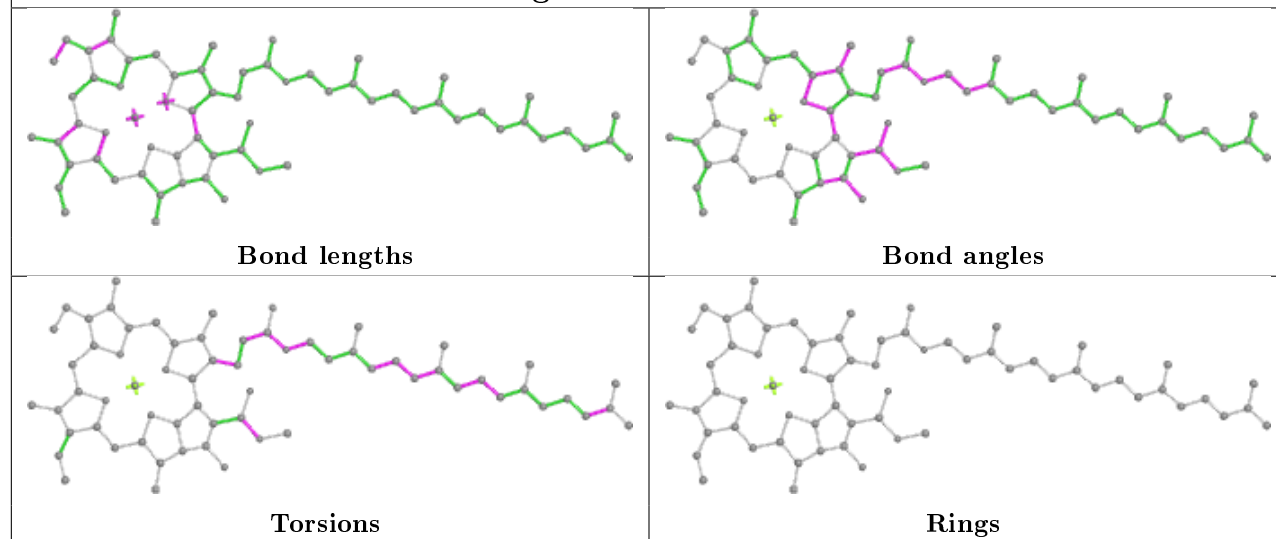
Ligand CLA A 818



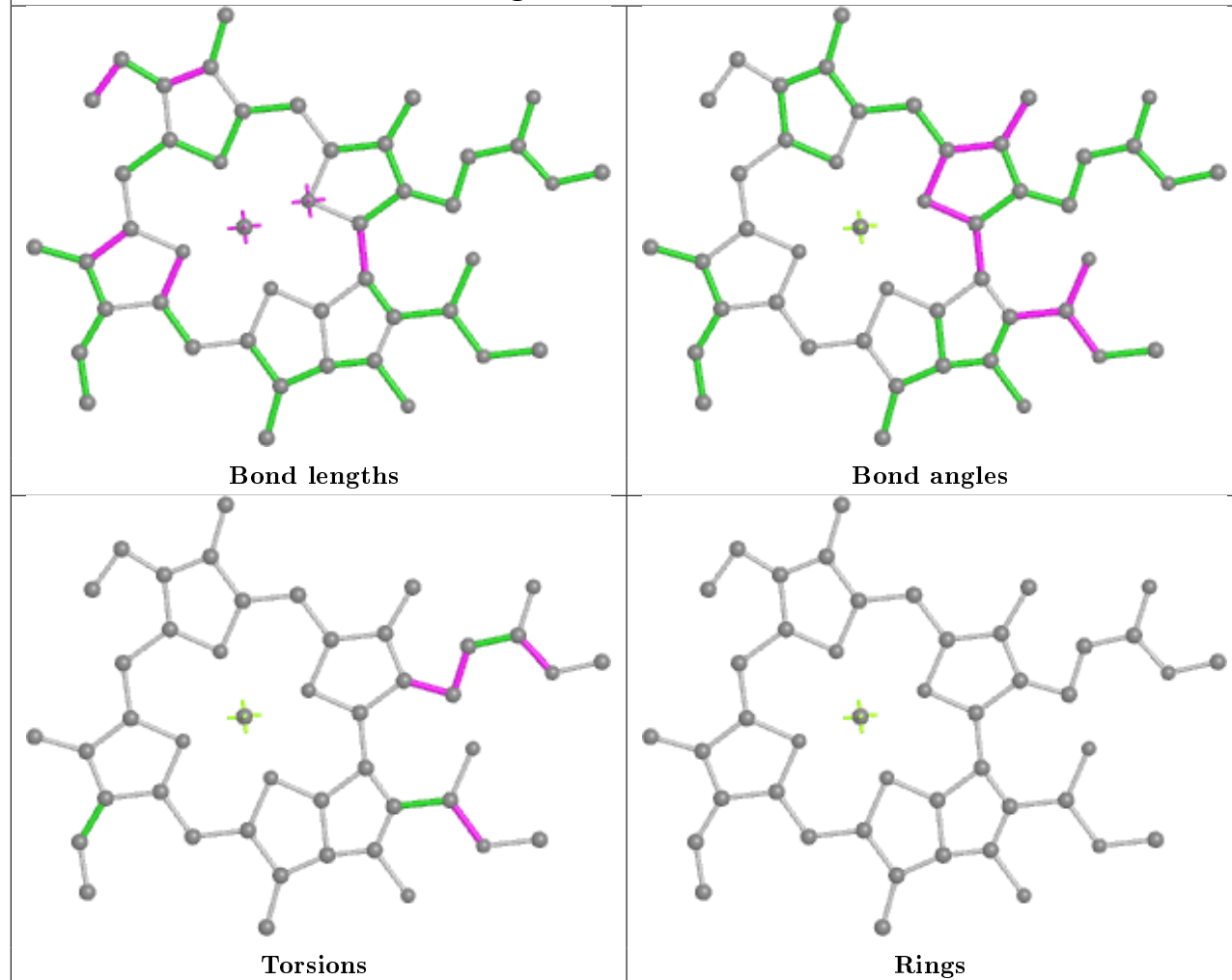
Ligand CLA B 818

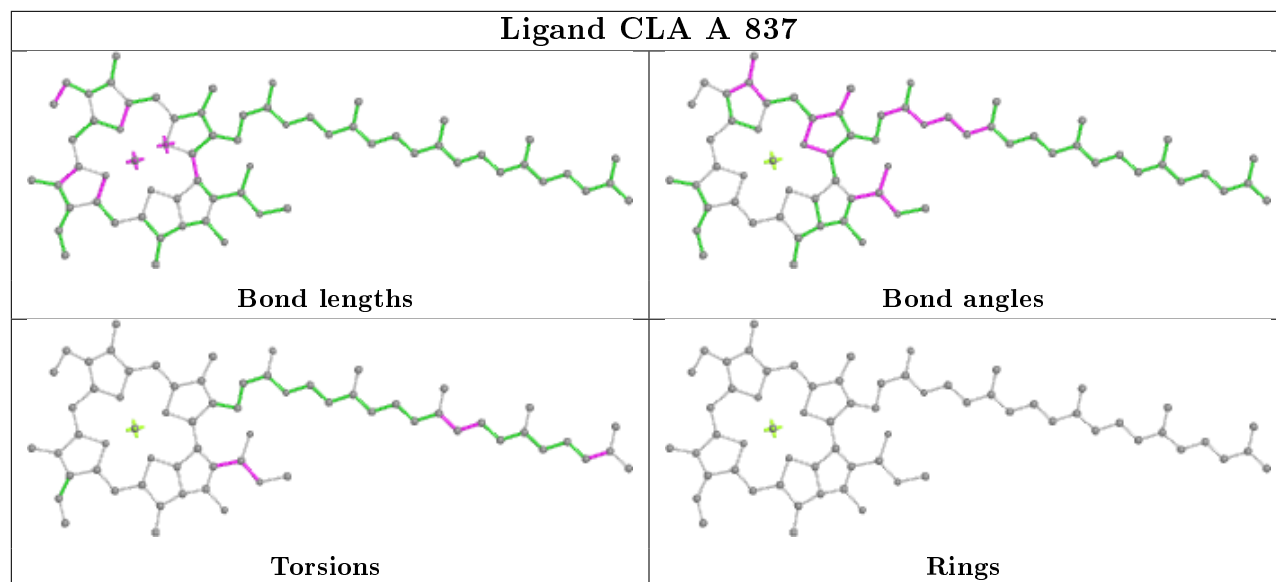
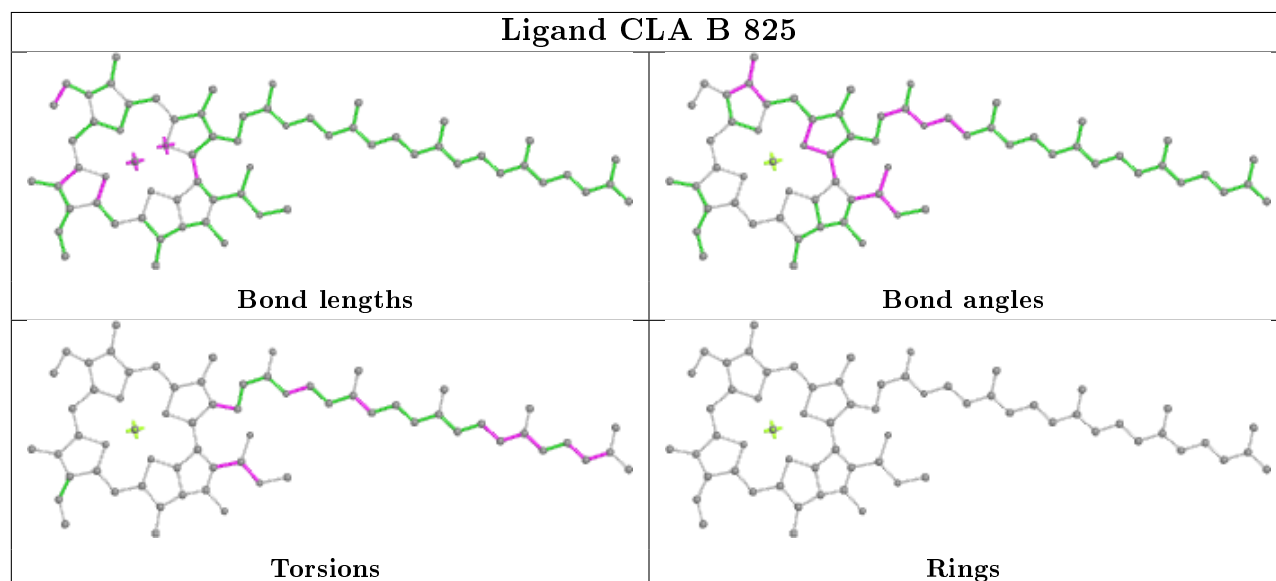
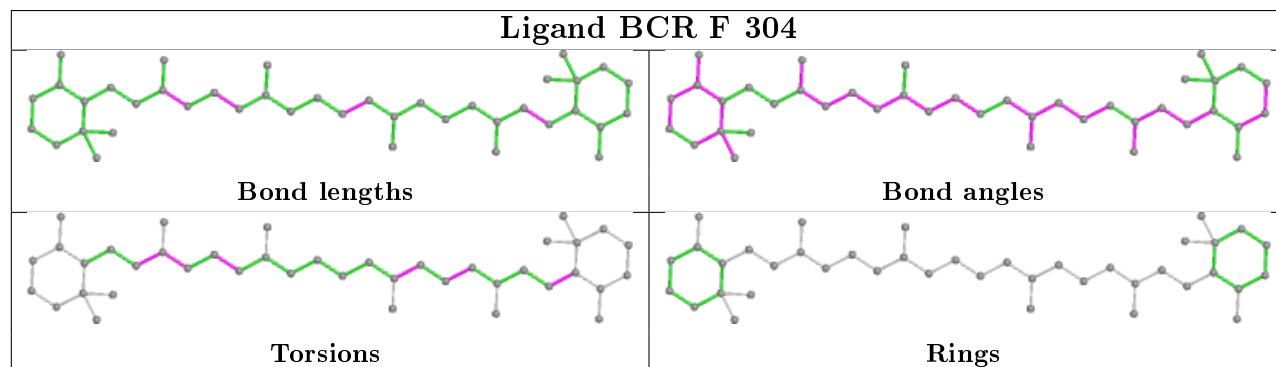


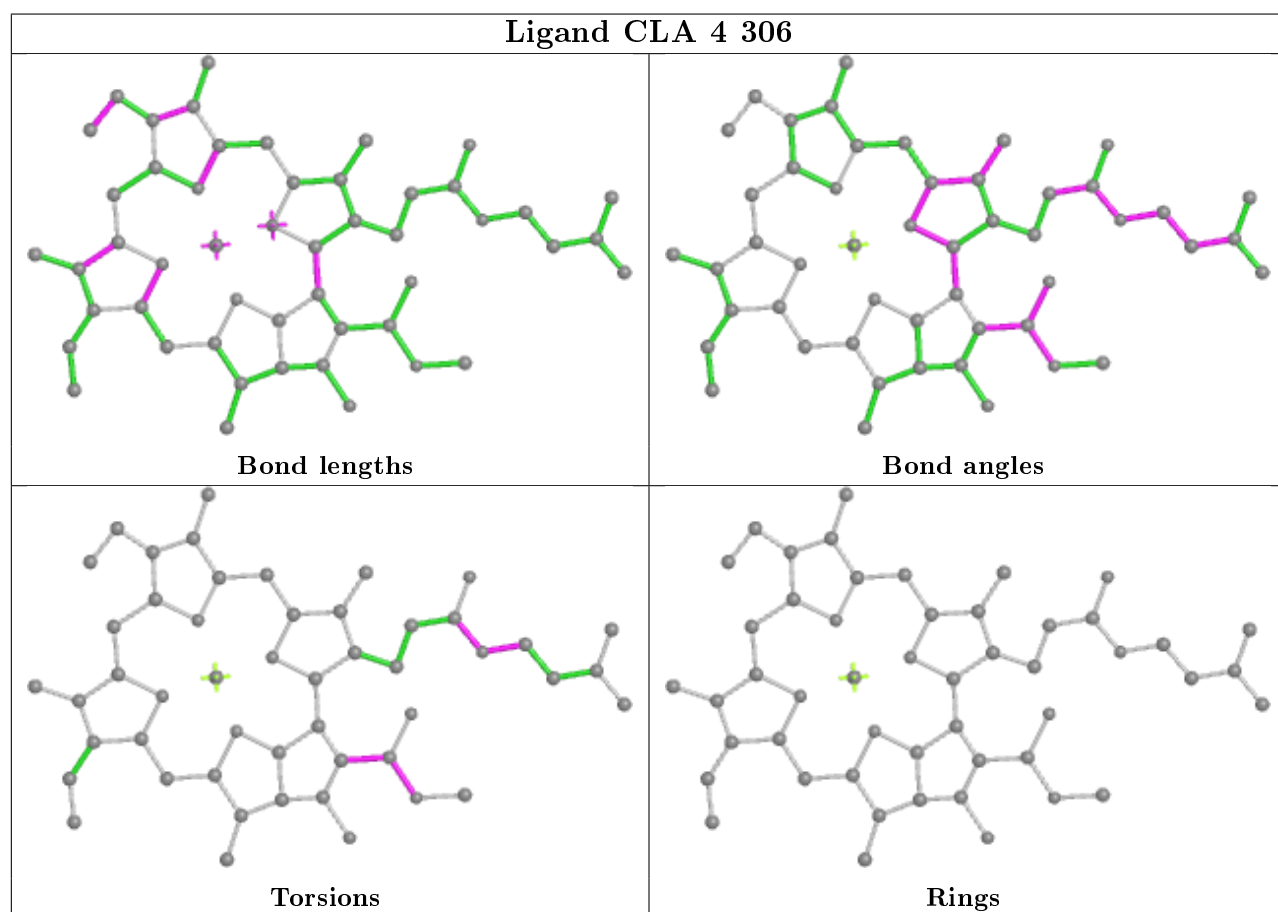
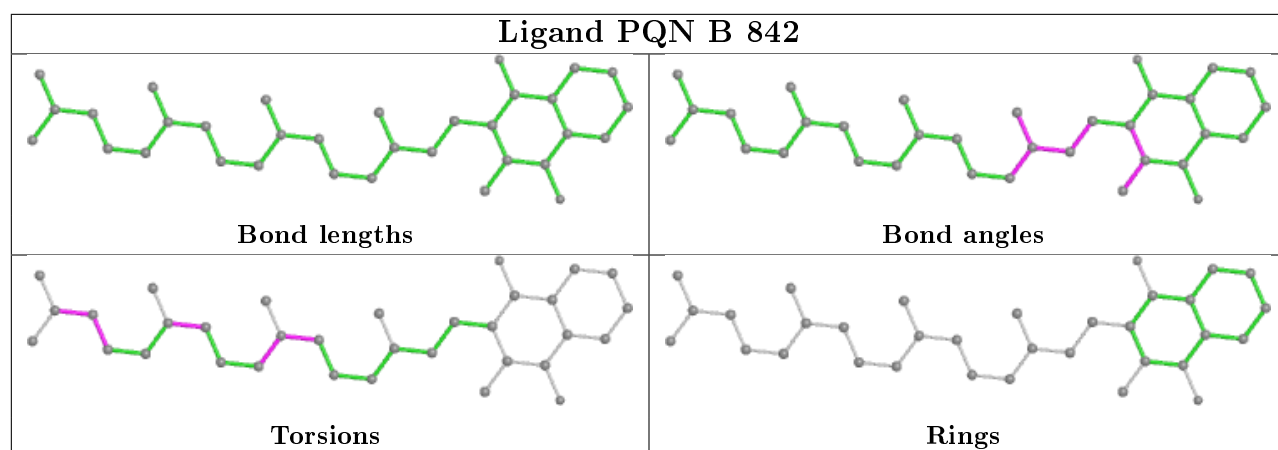
Ligand CLA B 811

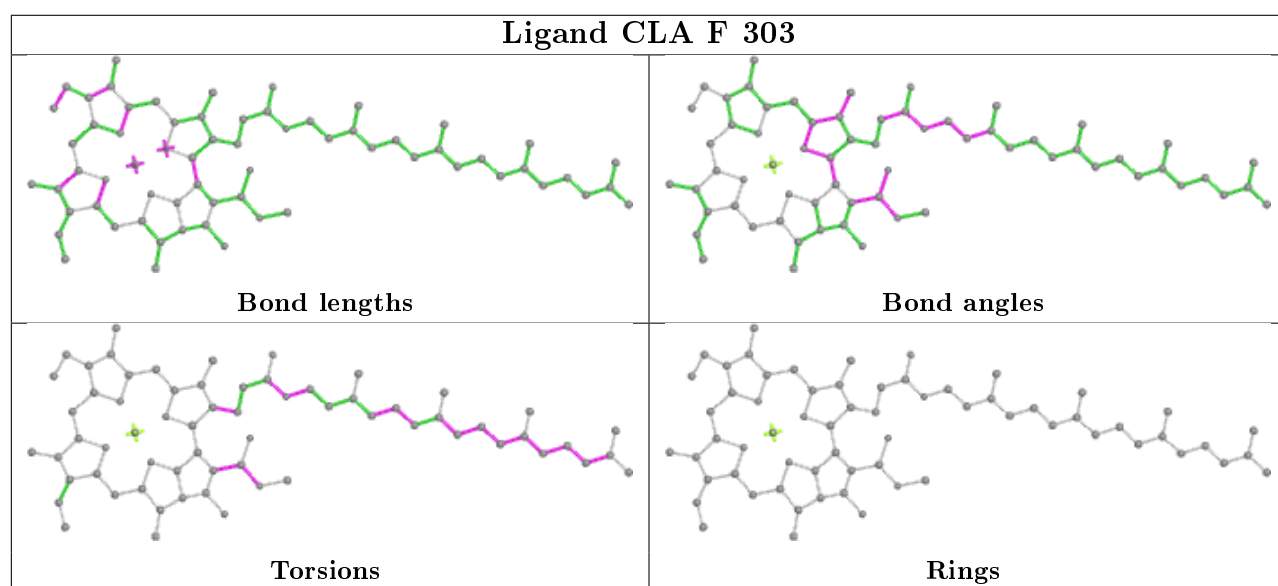
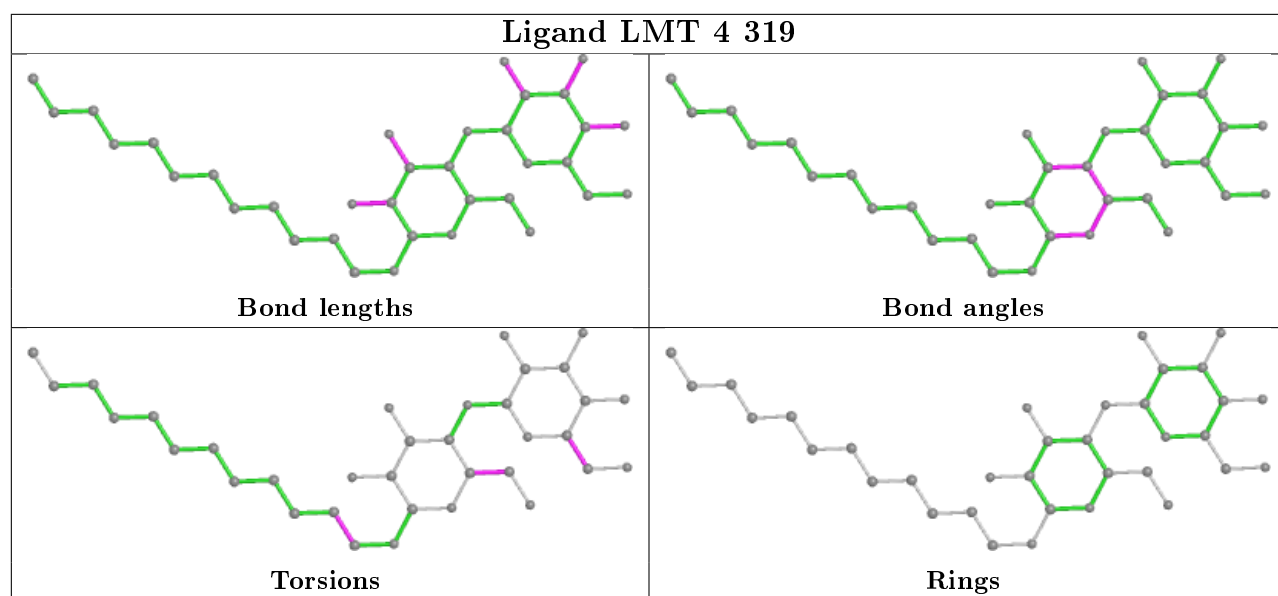


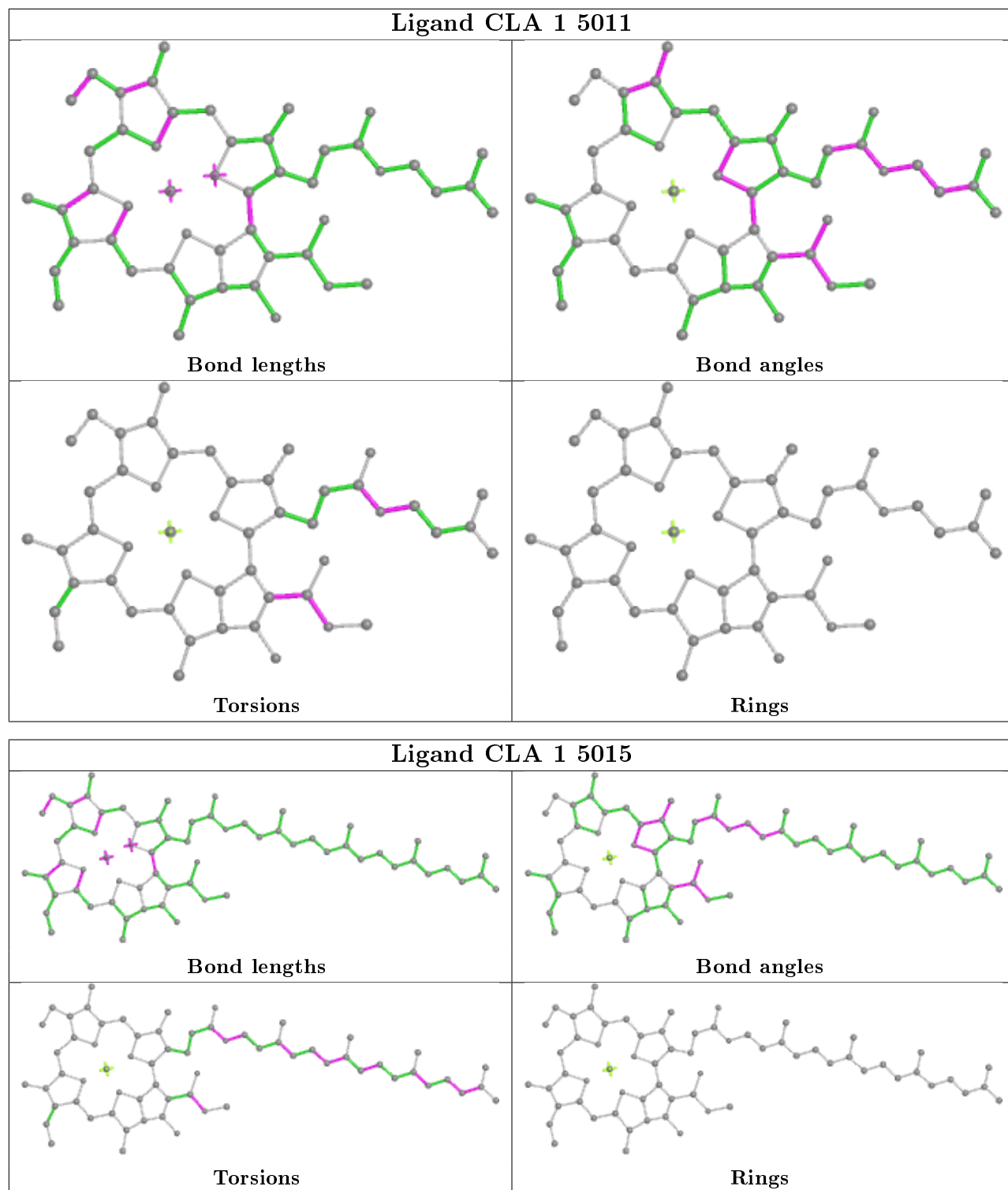
Ligand CLA 1 5007

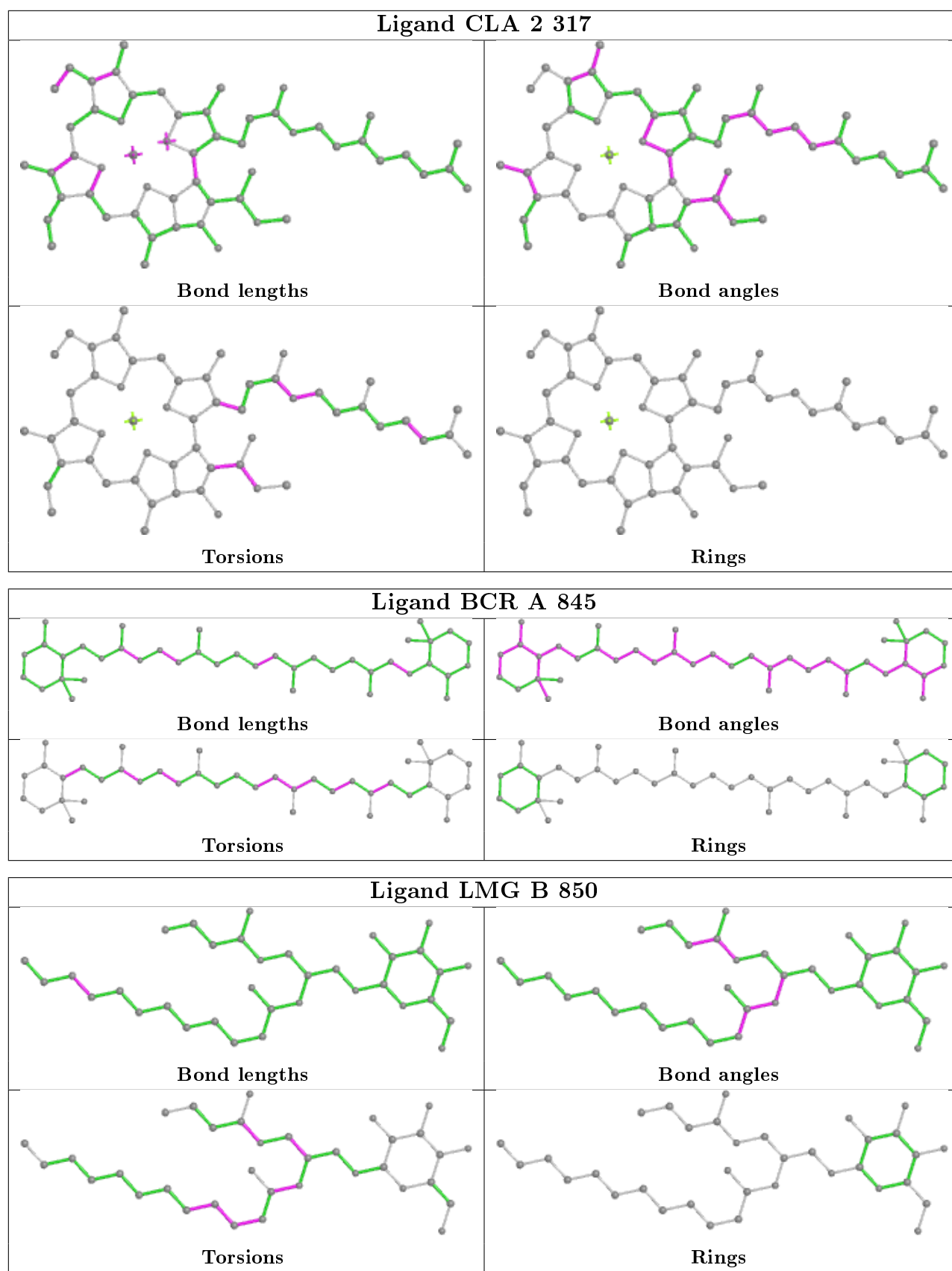


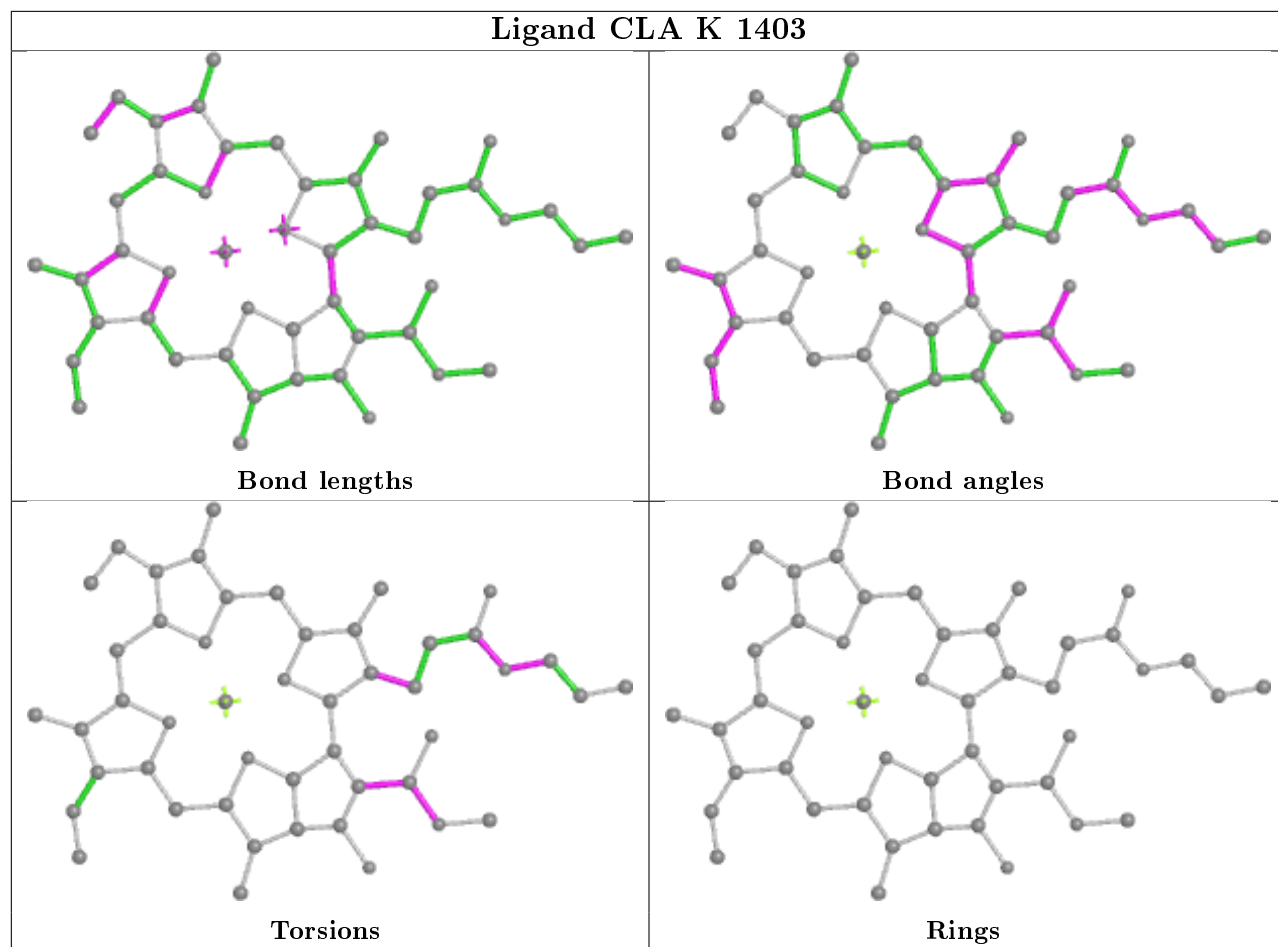
Ligand CLA A 837**Ligand CLA B 825****Ligand BCR F 304**



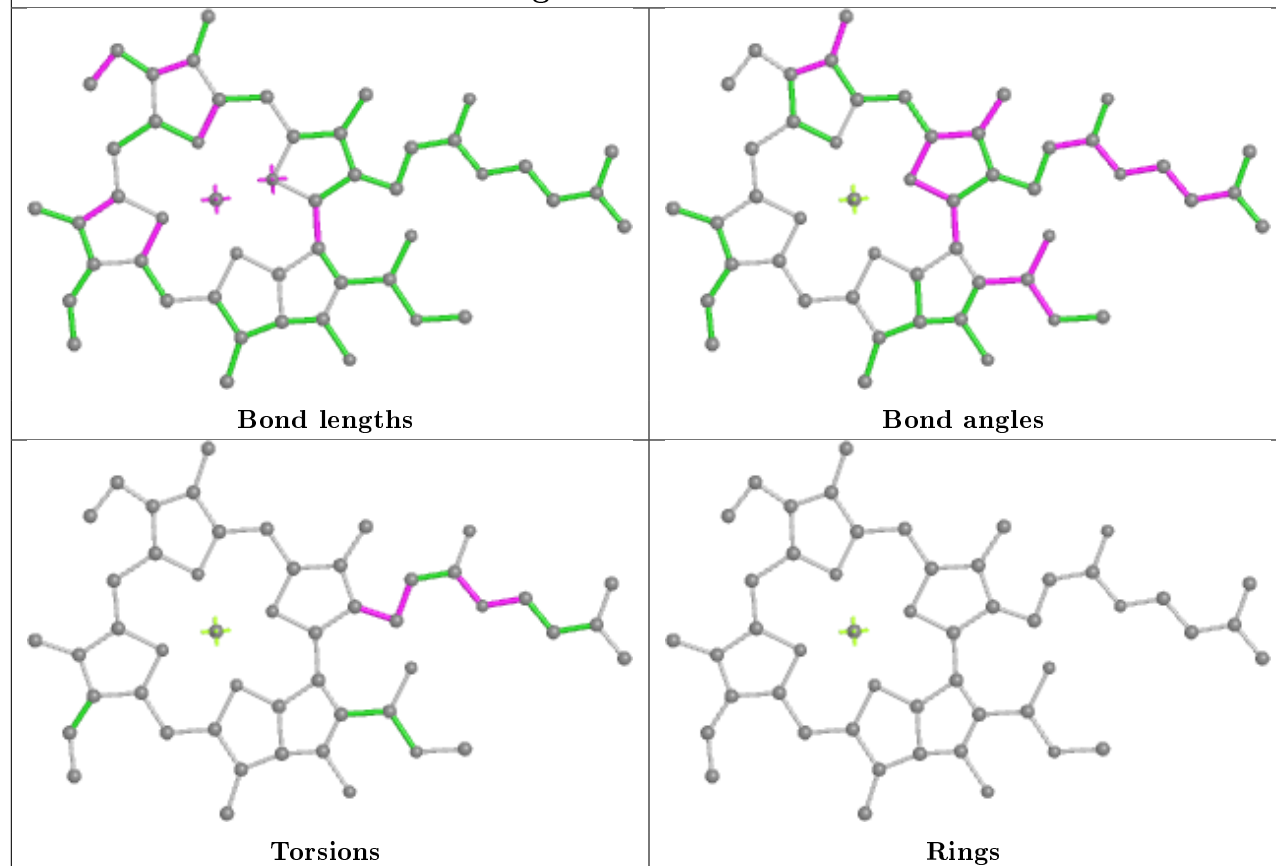




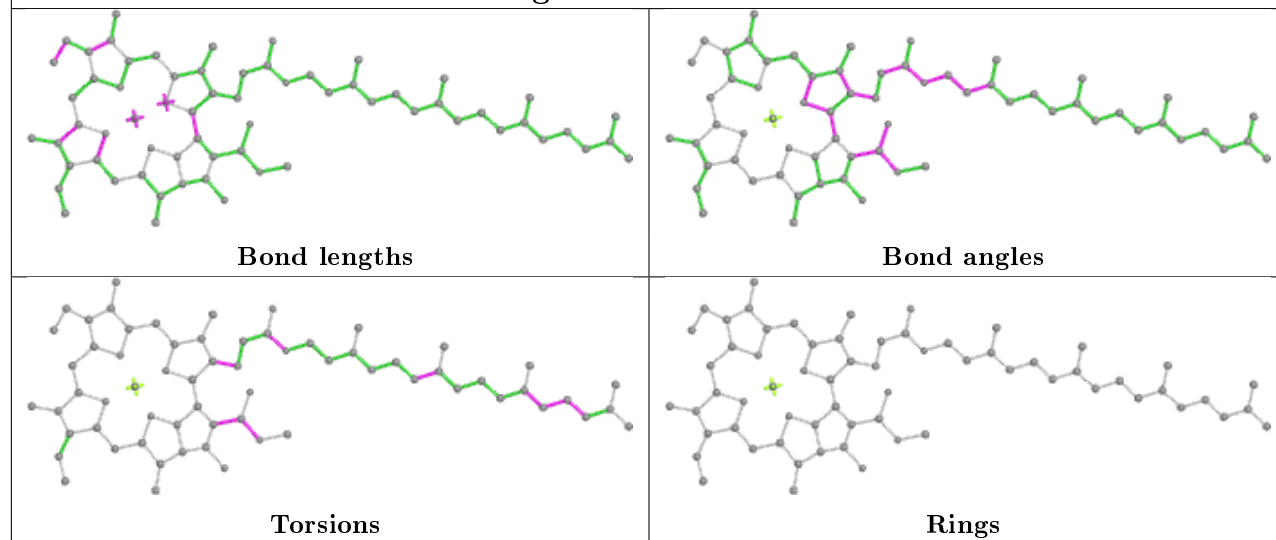


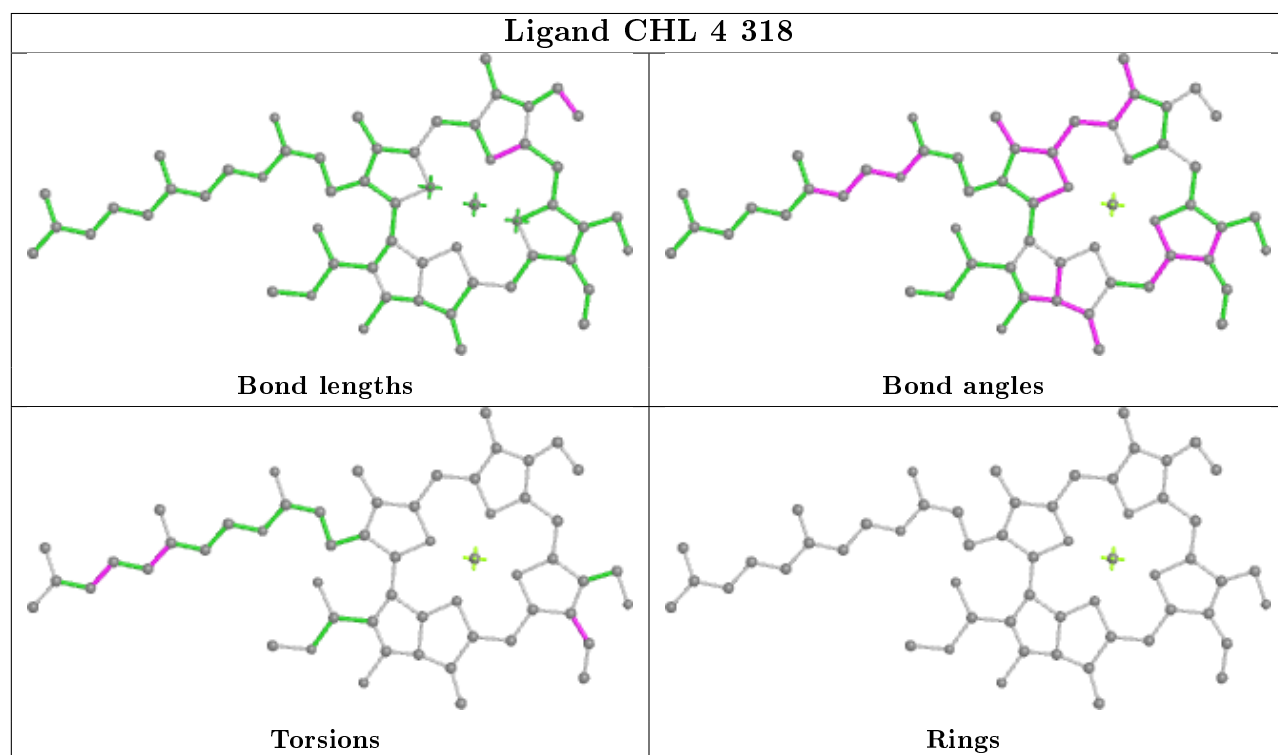
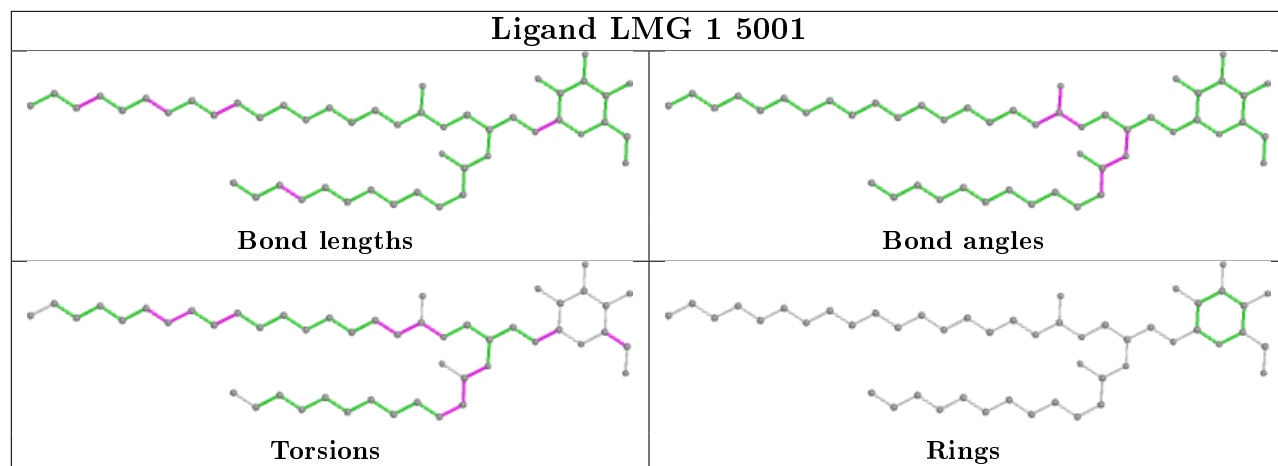


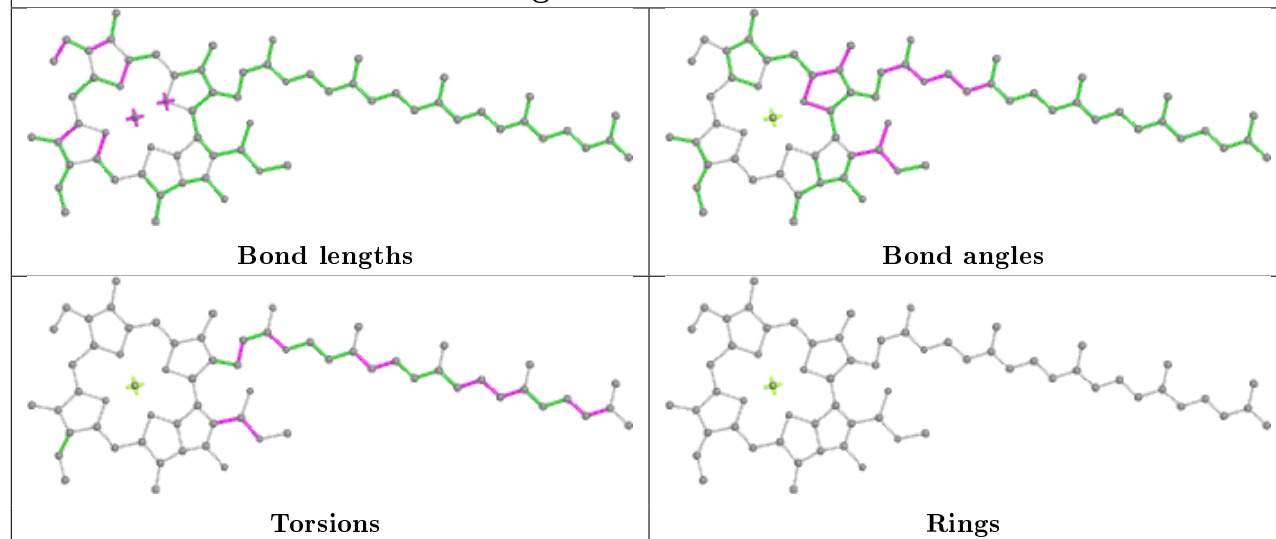
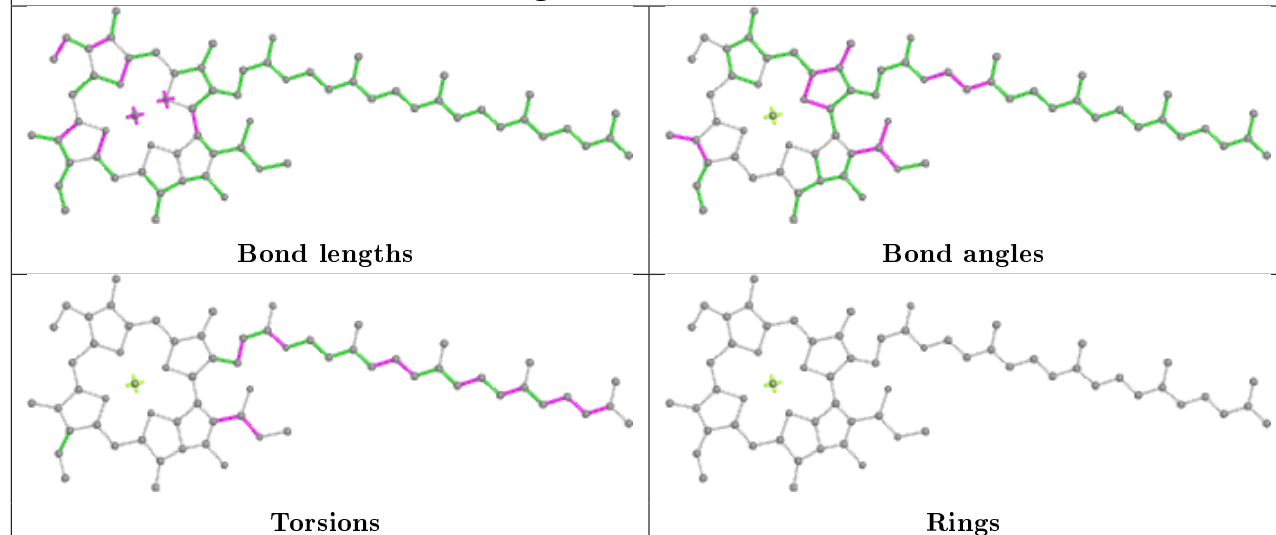
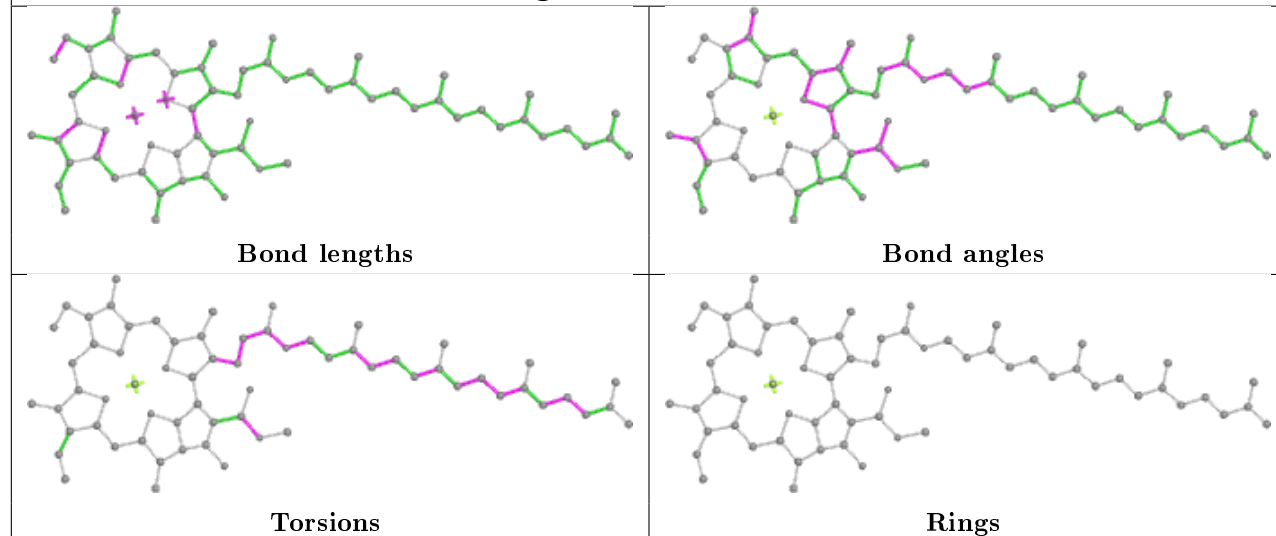
Ligand CLA B 838

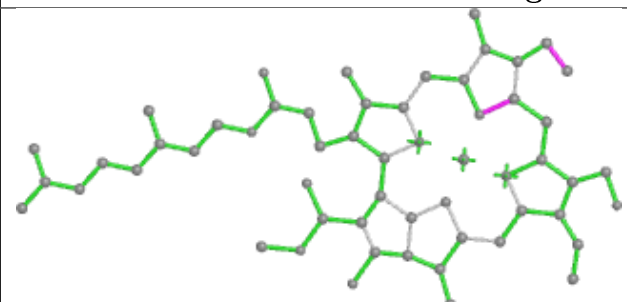
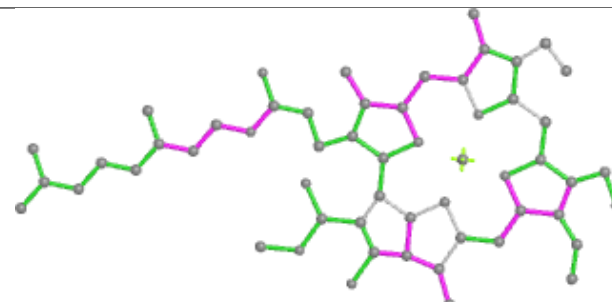
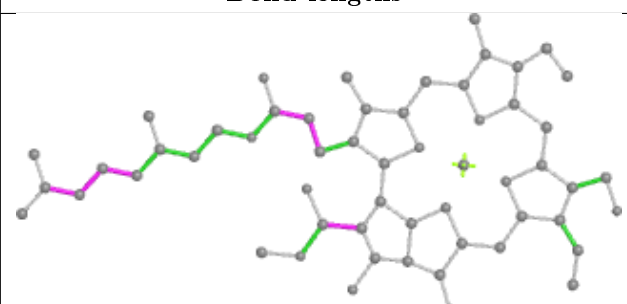
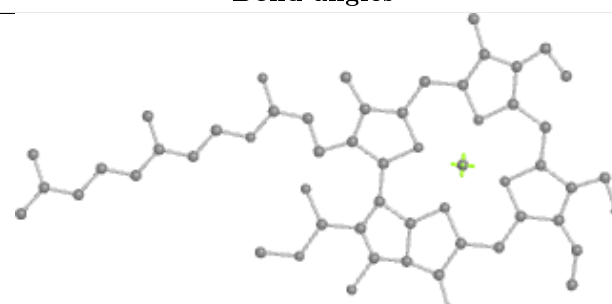


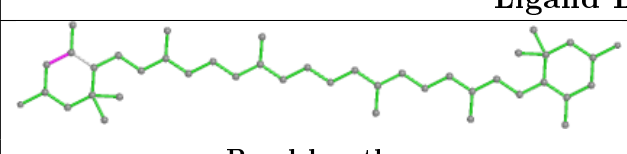
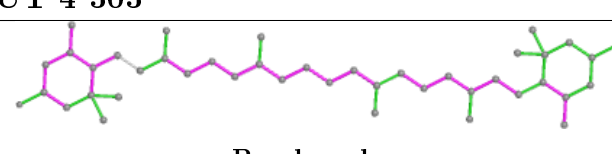
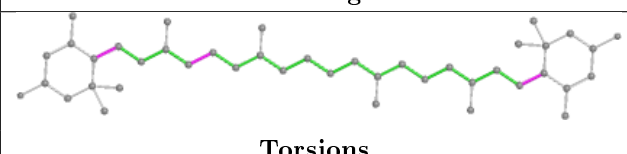
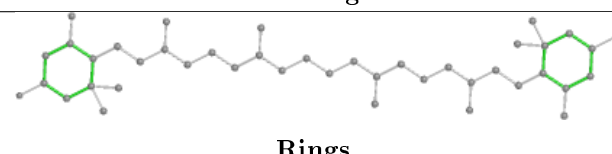
Ligand CLA B 820

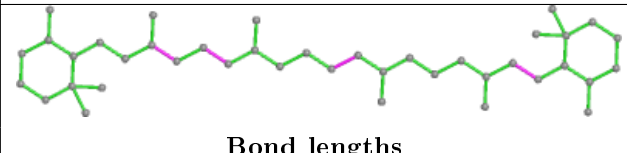
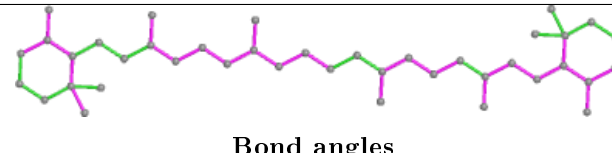
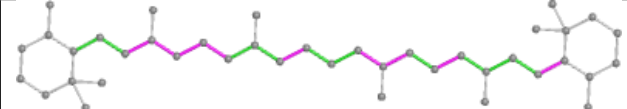
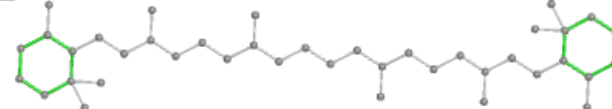


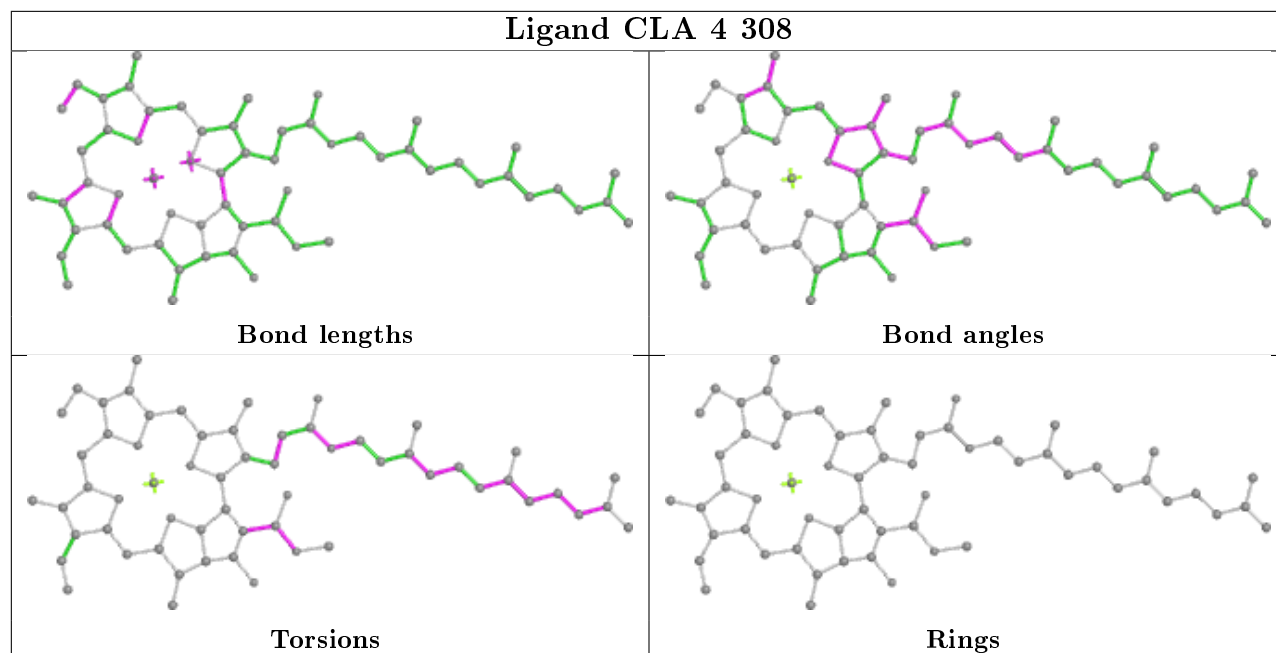
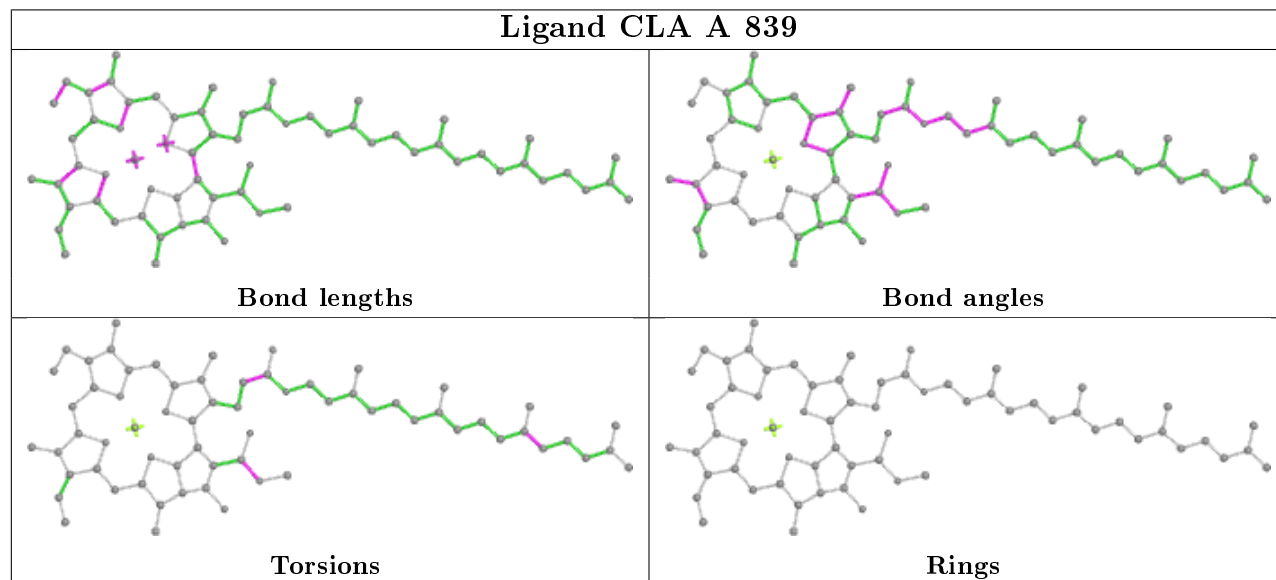
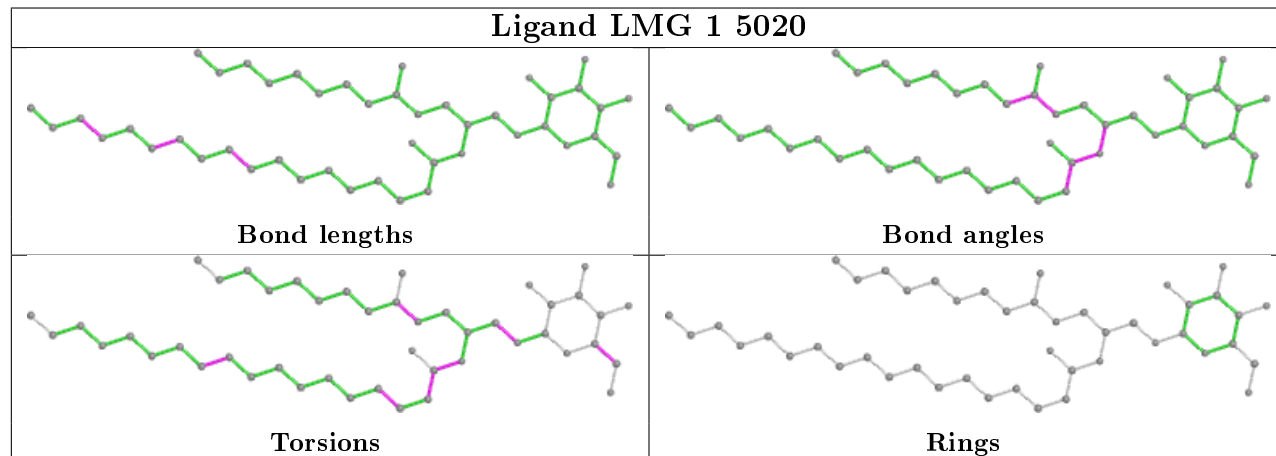


Ligand CLA A 853**Ligand CLA B 808****Ligand CLA F 302**

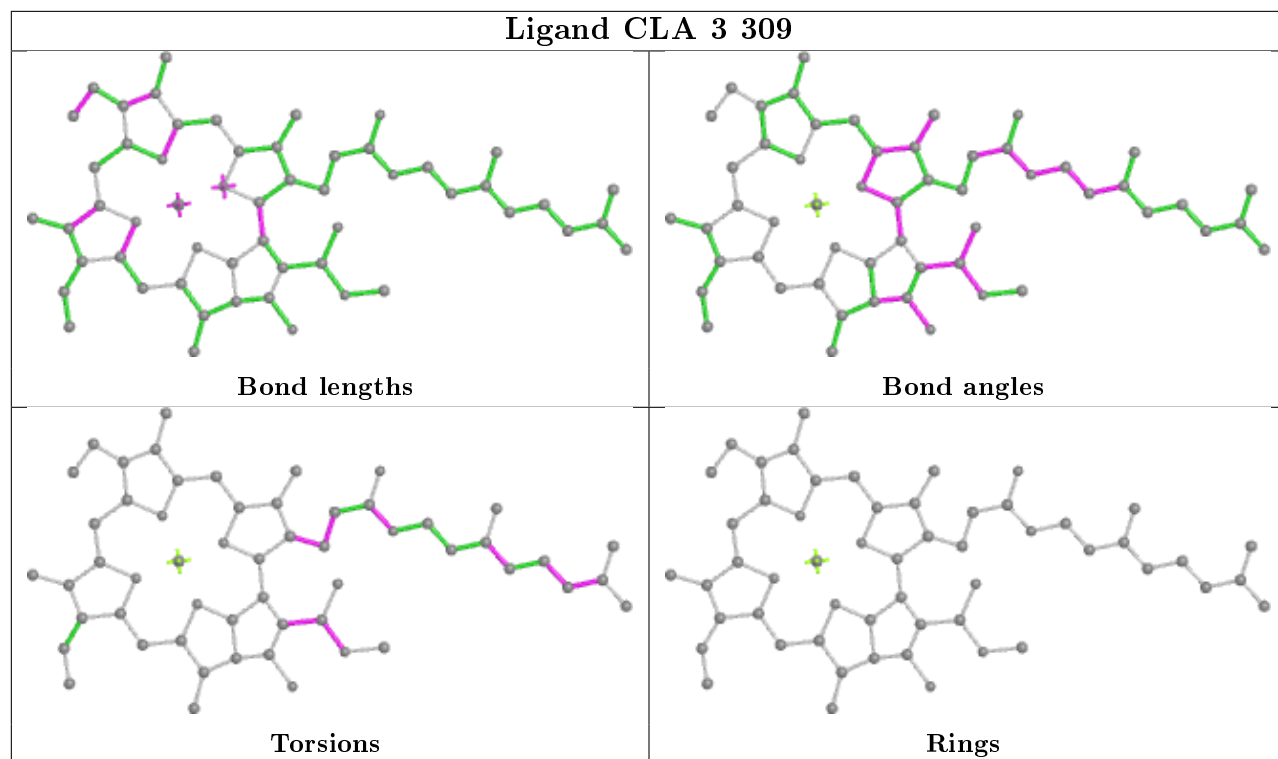
Ligand CHL 2 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 4 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

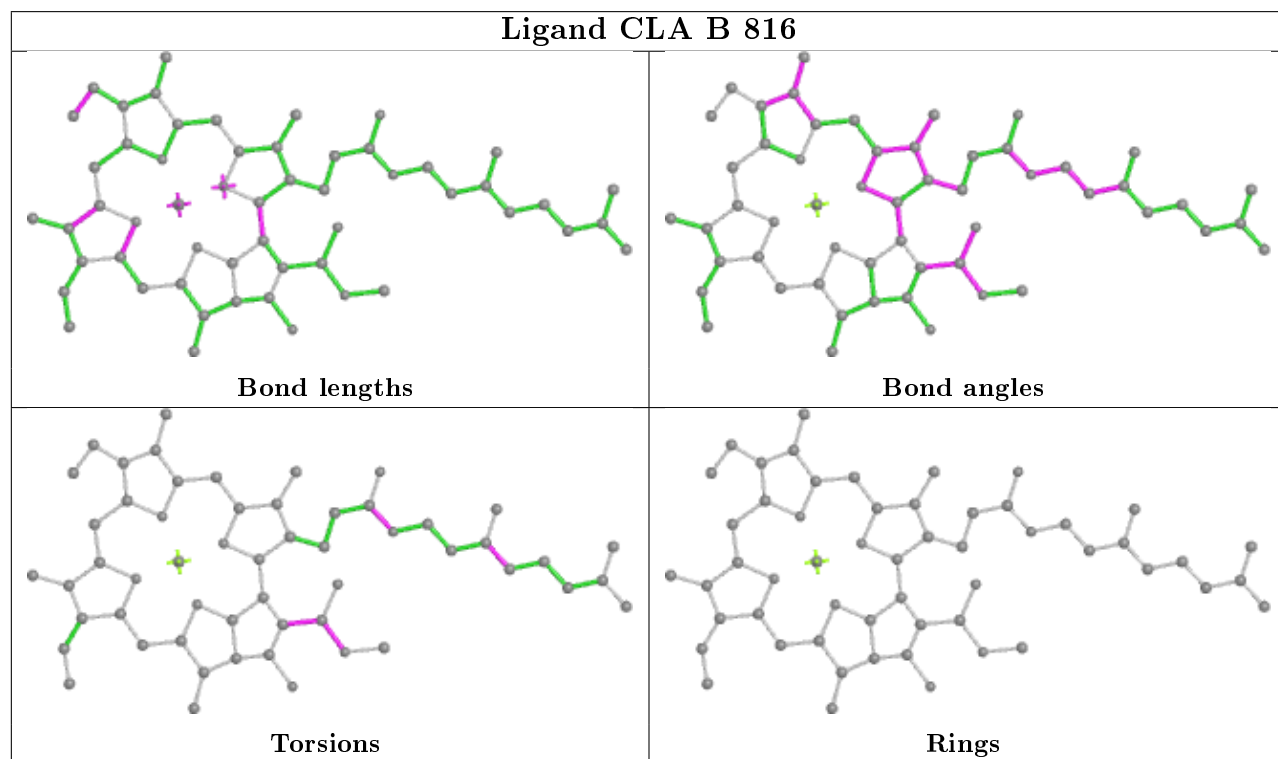
Ligand BCR F 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

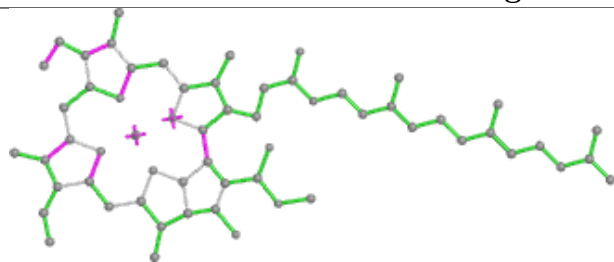
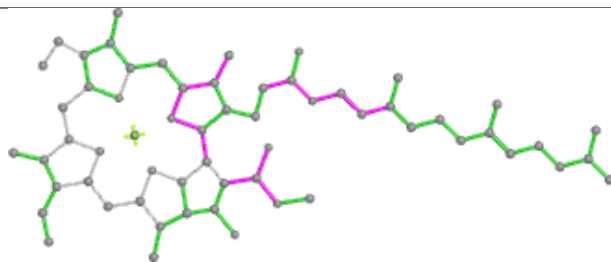
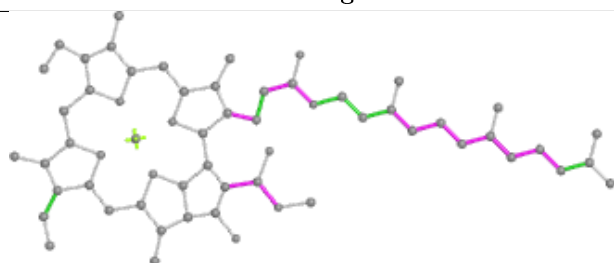
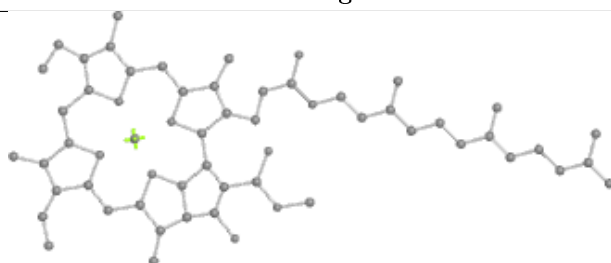
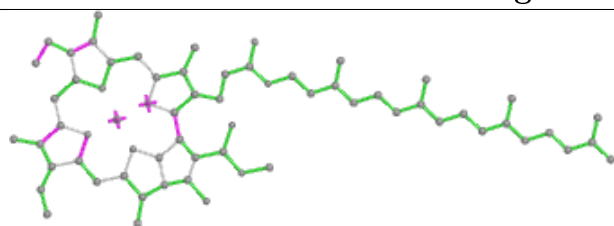
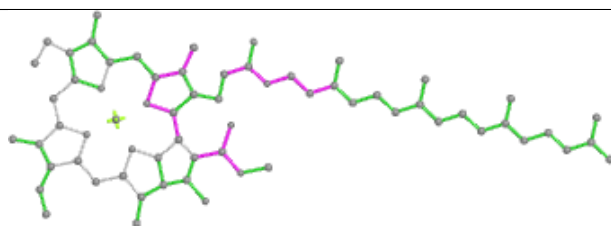
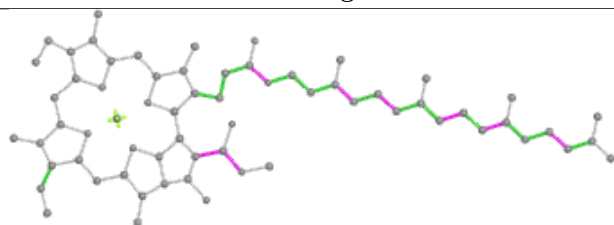
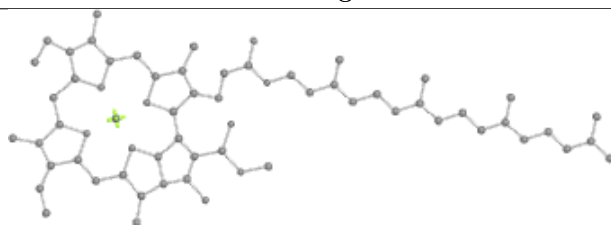
Ligand CLA 4 308**Ligand CLA A 839****Ligand LMG 1 5020**

Ligand CLA 3 309

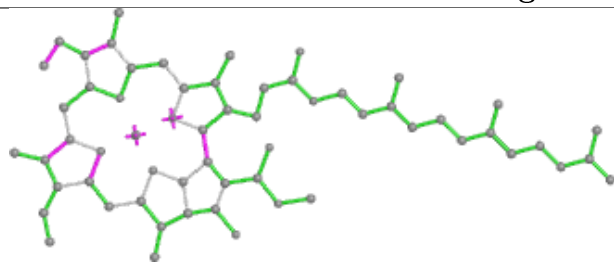


Ligand CLA B 816

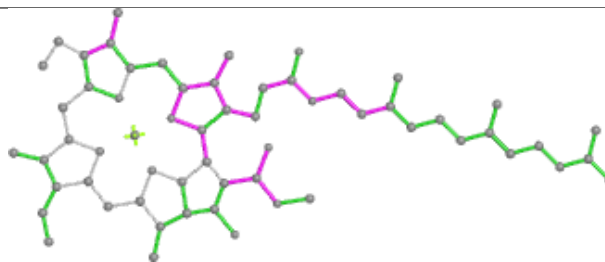


Ligand CLA K 1402**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 831****Bond lengths****Bond angles****Torsions****Rings**

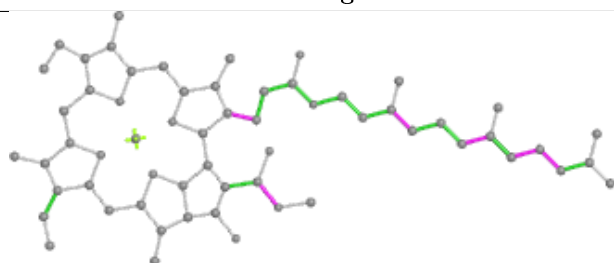
Ligand CLA 4 305



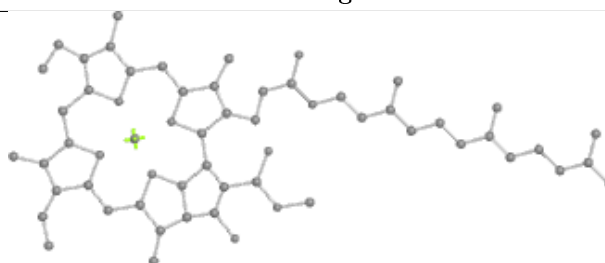
Bond lengths



Bond angles

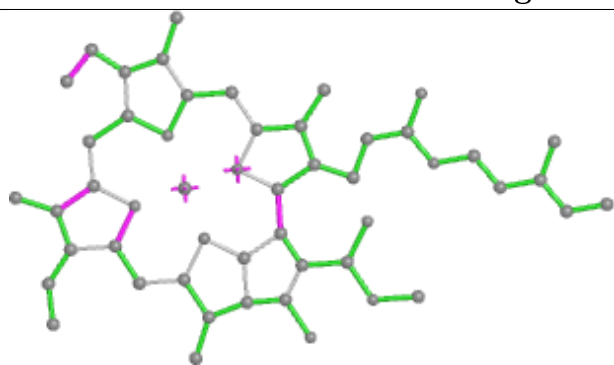


Torsions

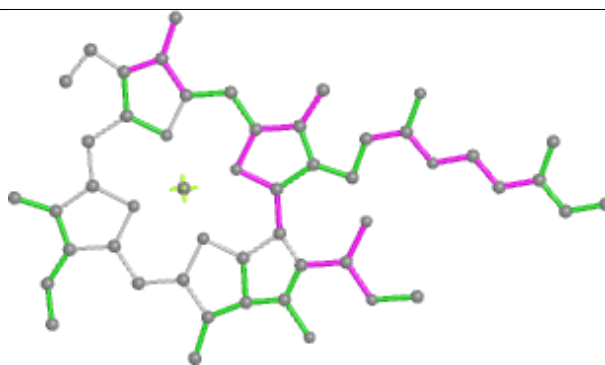


Rings

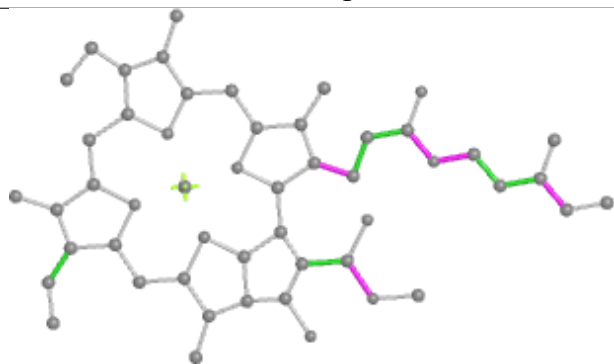
Ligand CLA A 834



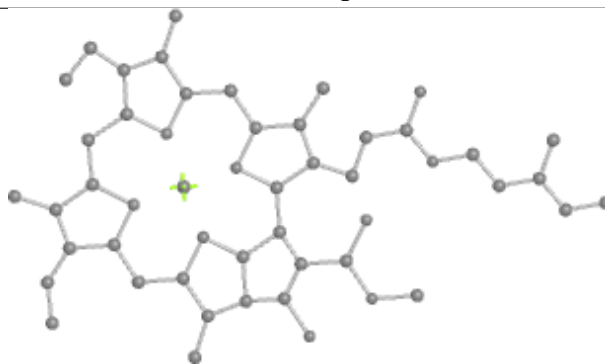
Bond lengths



Bond angles

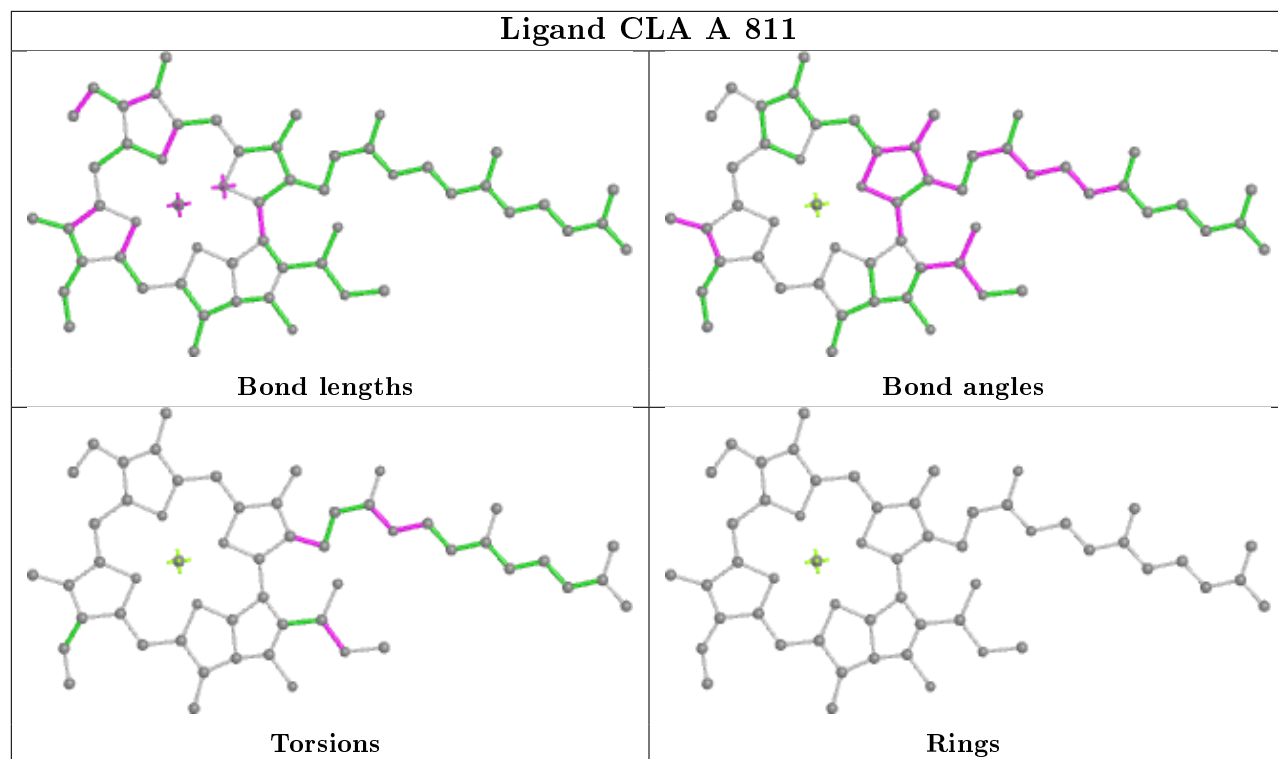


Torsions

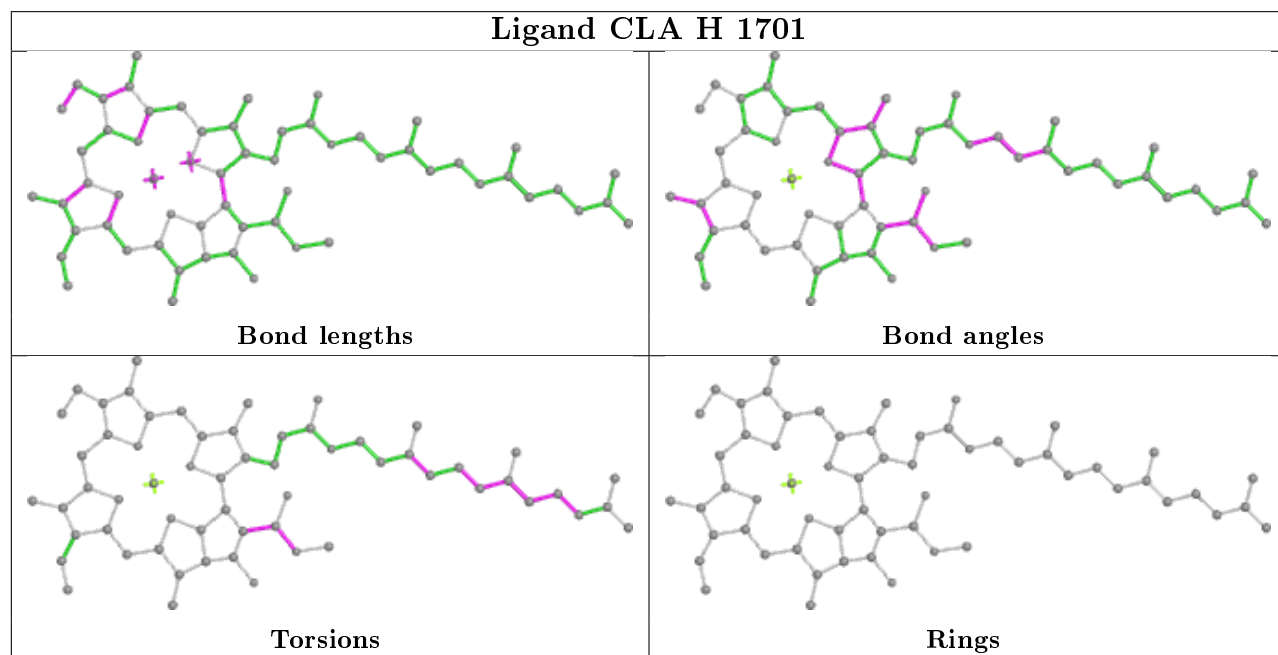


Rings

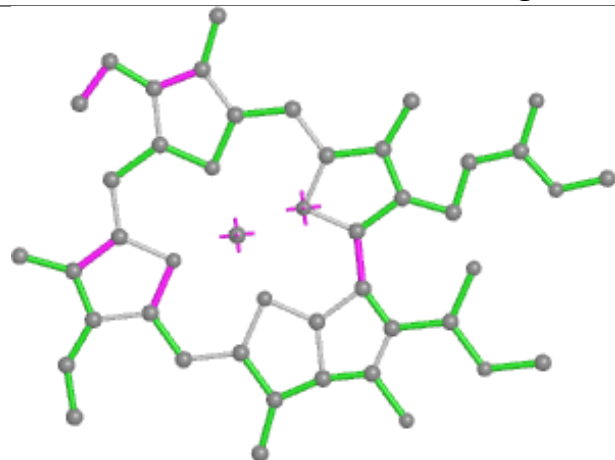
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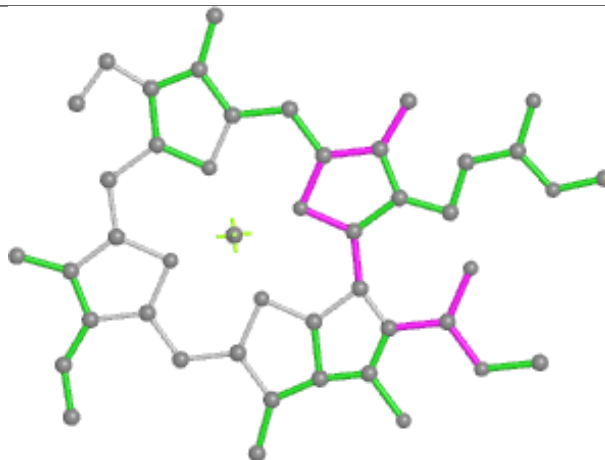
Ligand CLA H 1701



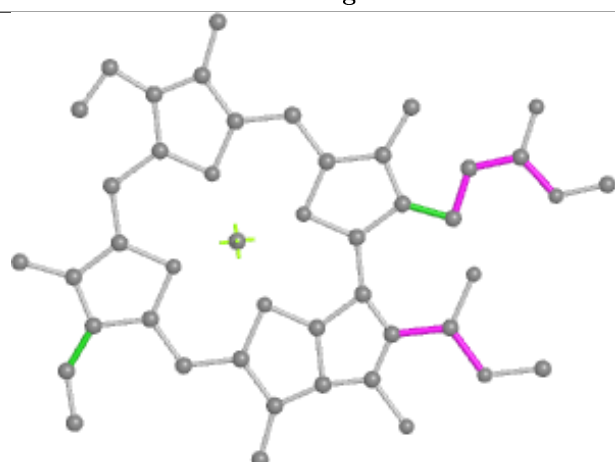
Ligand CLA A 814



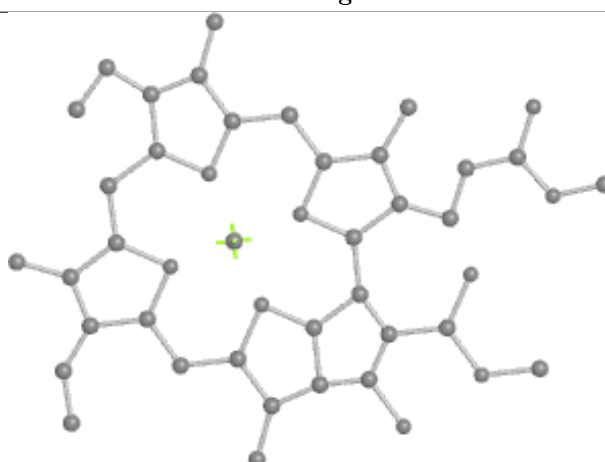
Bond lengths



Bond angles

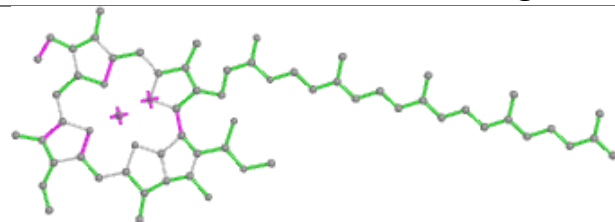


Torsions

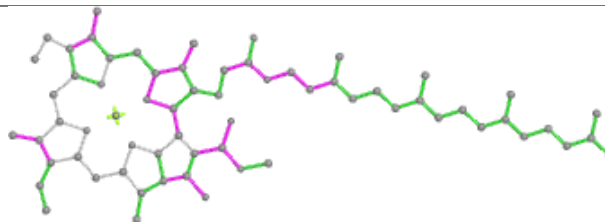


Rings

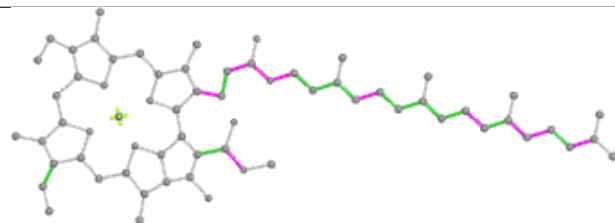
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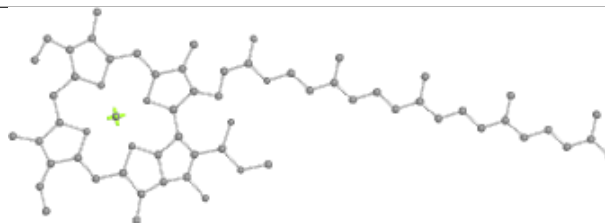
Bond lengths



Bond angles

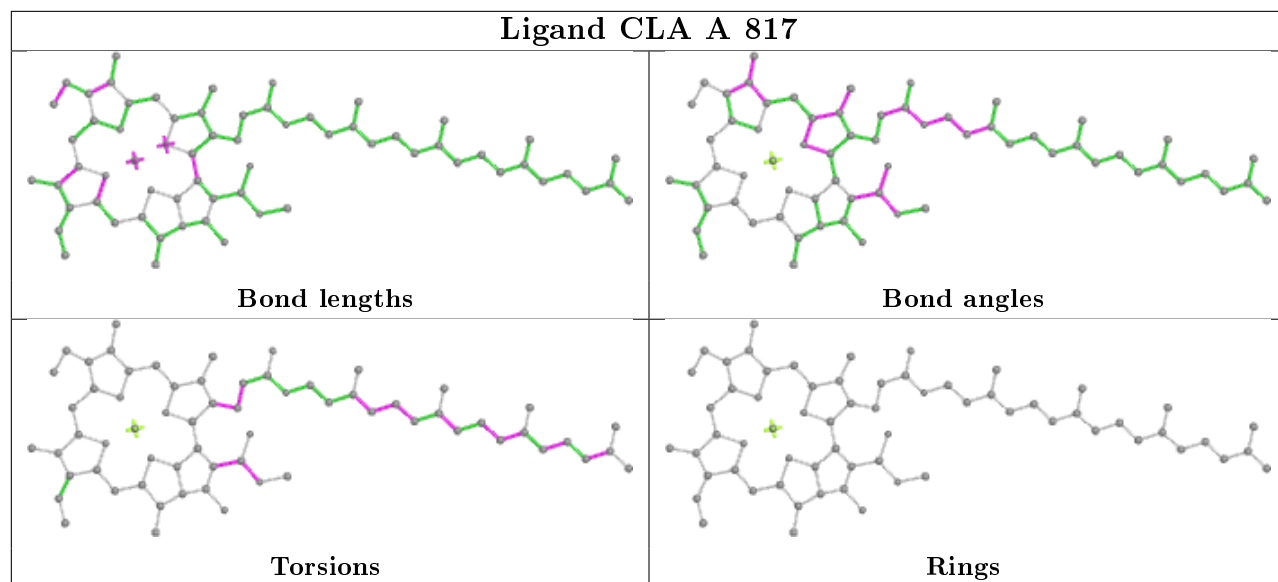


Torsions

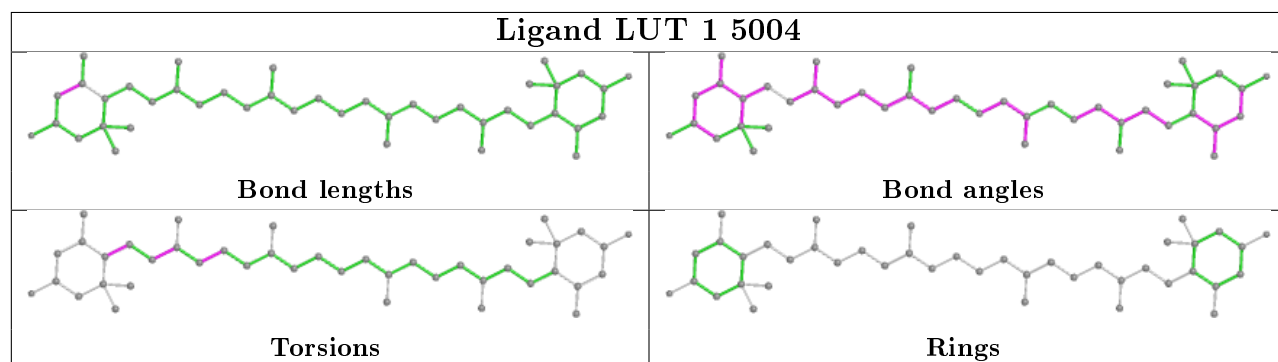


Rings

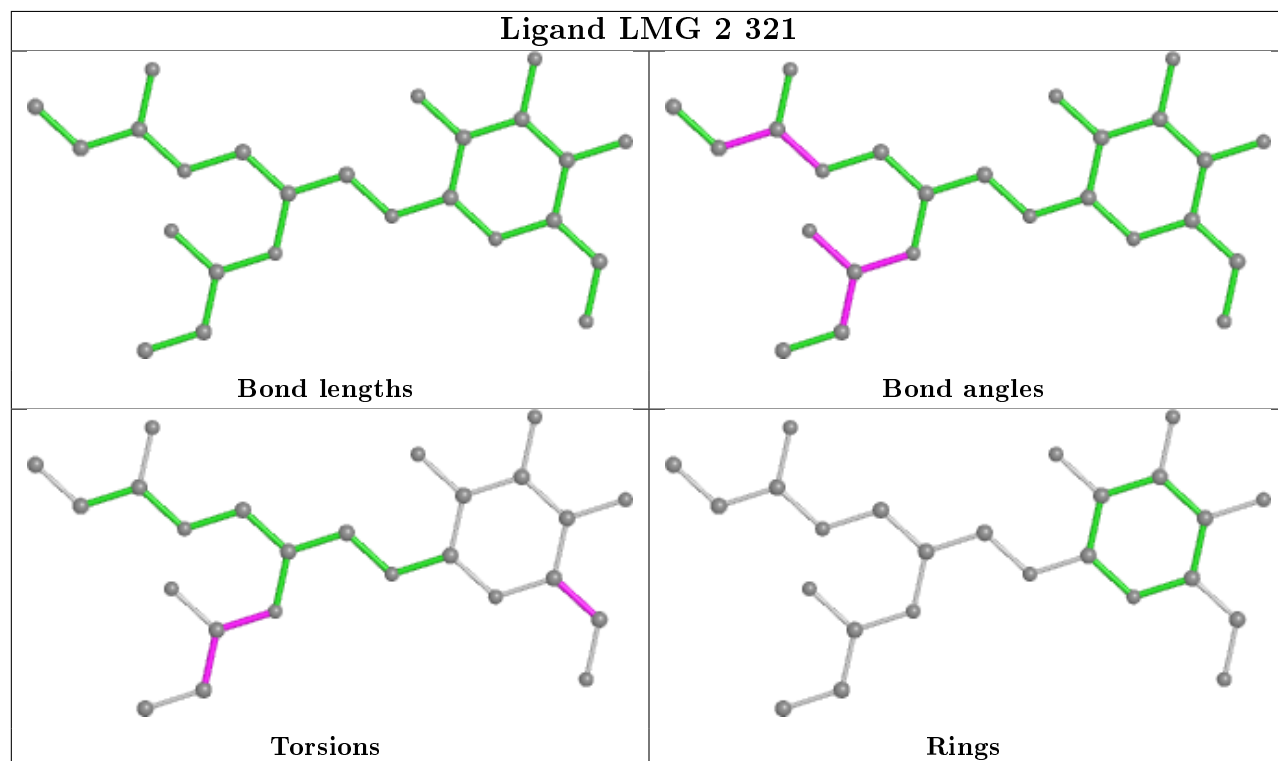
Ligand CLA A 817

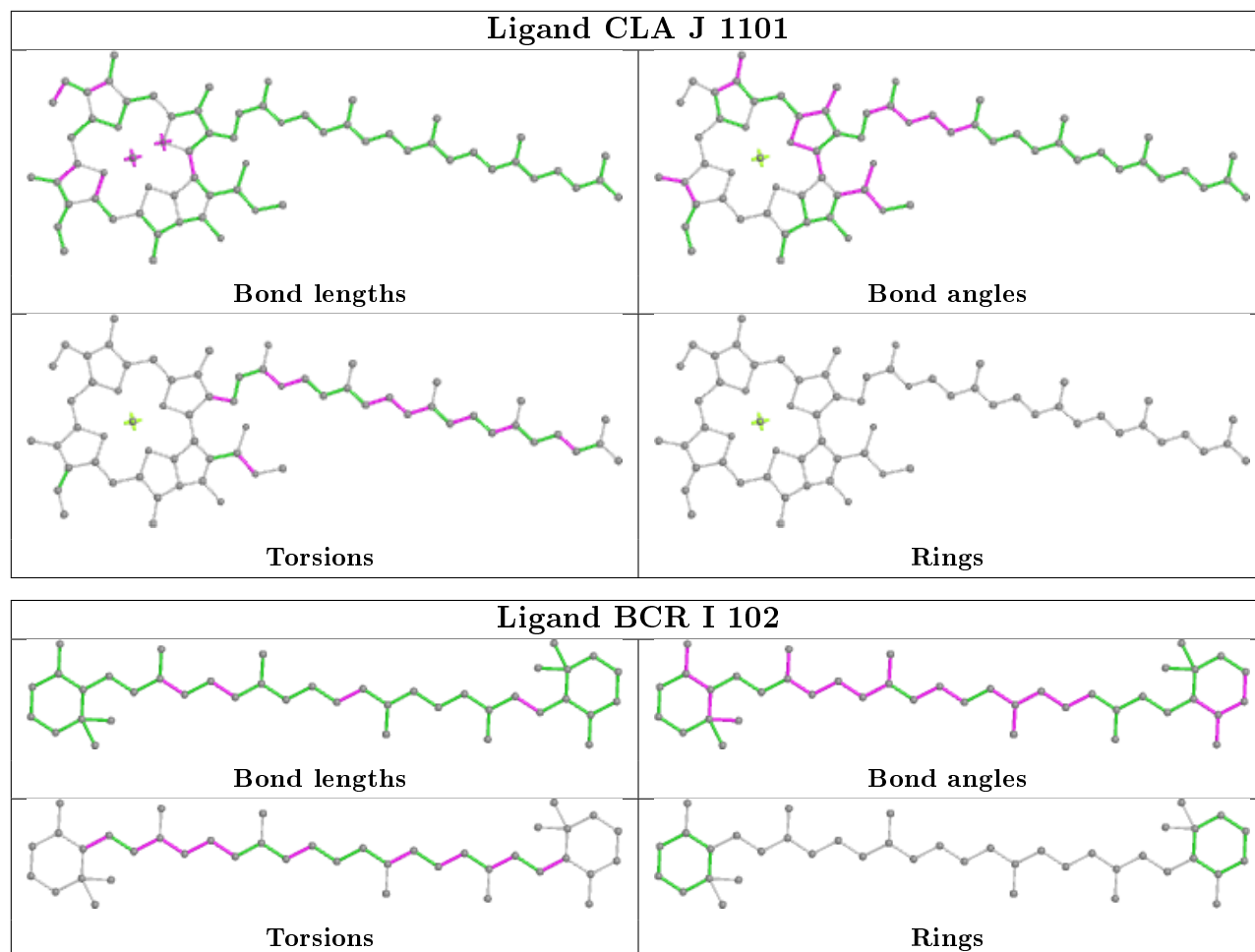


Ligand LUT 1 5004

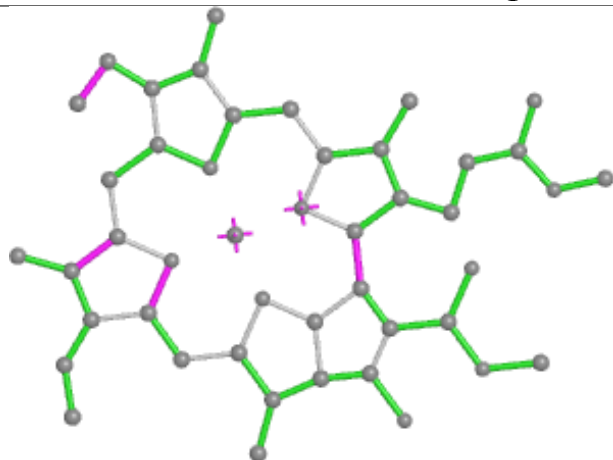


Ligand LMG 2 321

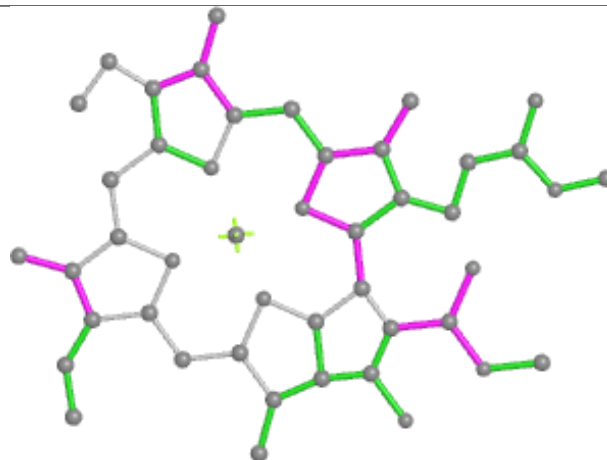




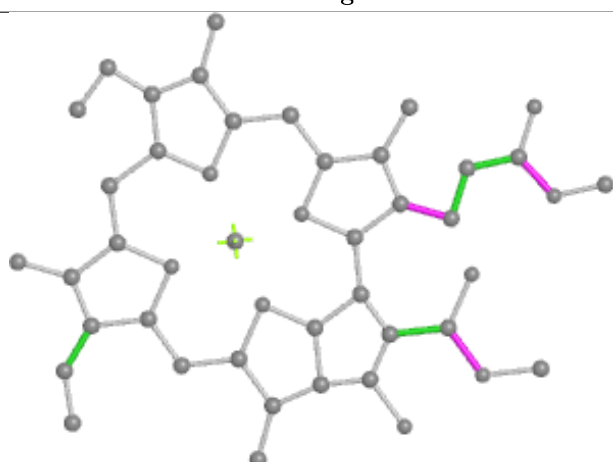
Ligand CLA G 1602



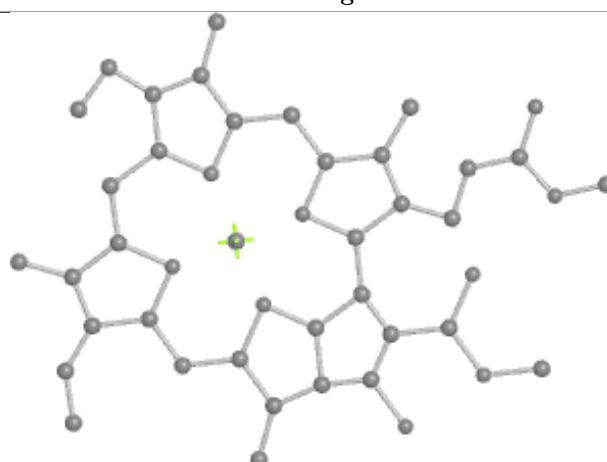
Bond lengths



Bond angles

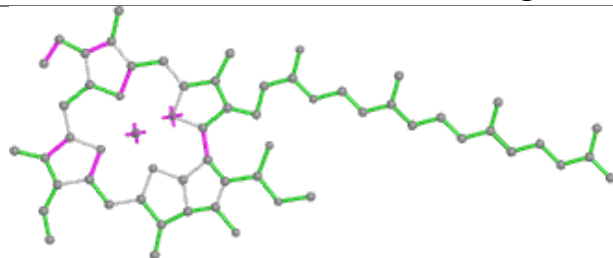


Torsions

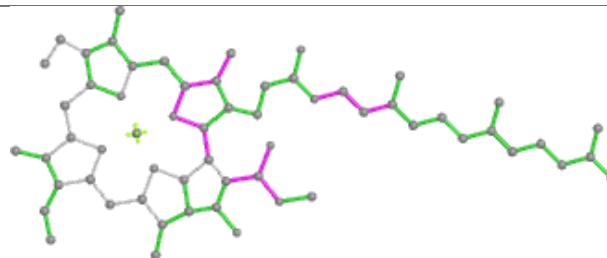


Rings

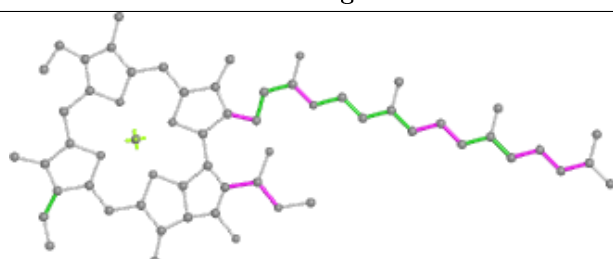
Ligand CLA 4 311



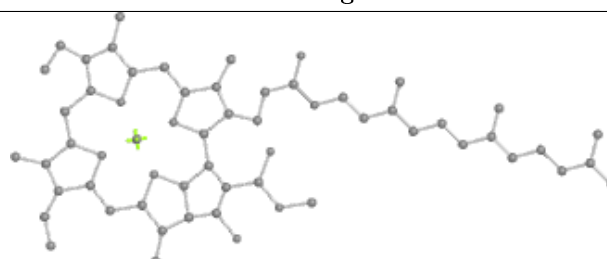
Bond lengths



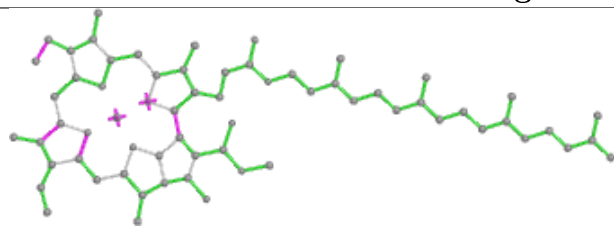
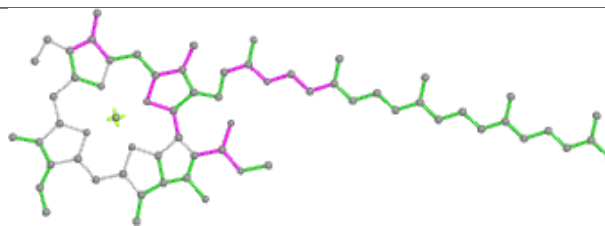
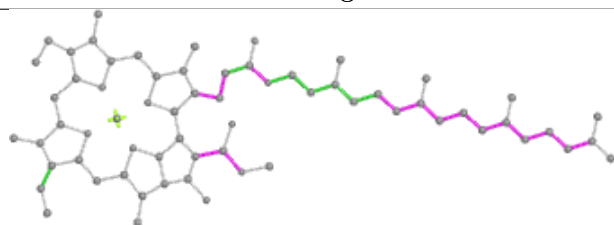
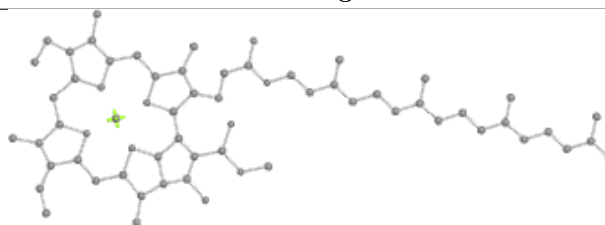
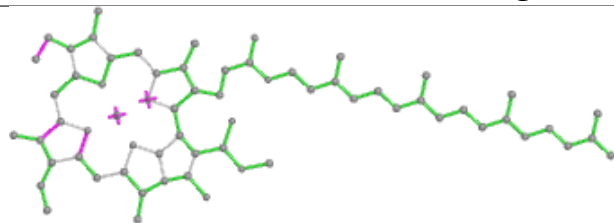
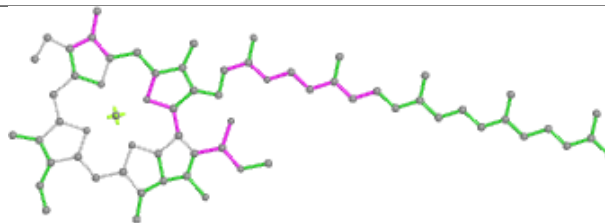
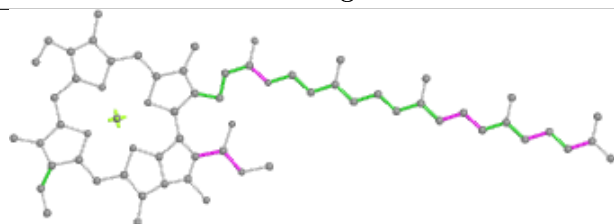
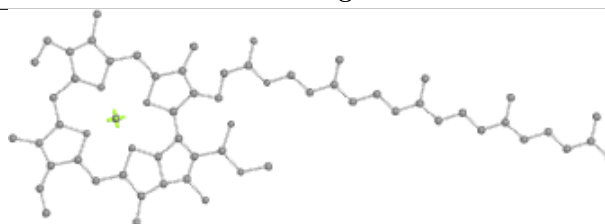
Bond angles

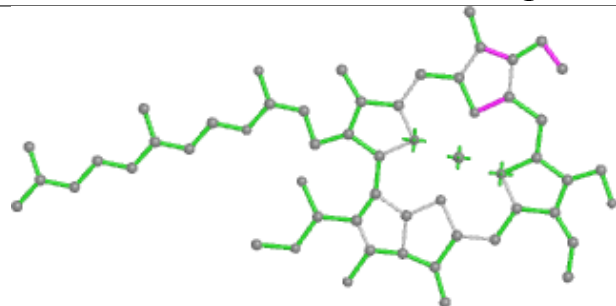
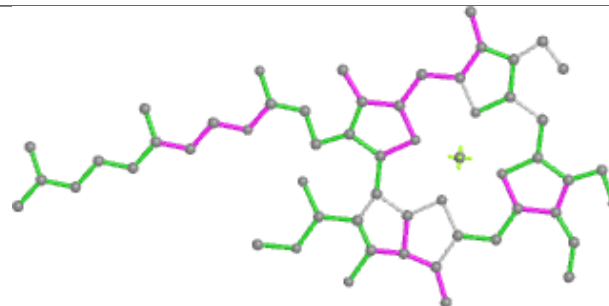
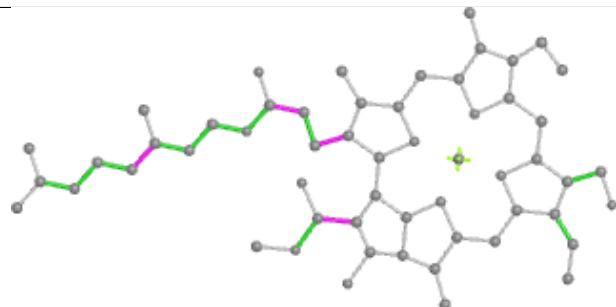
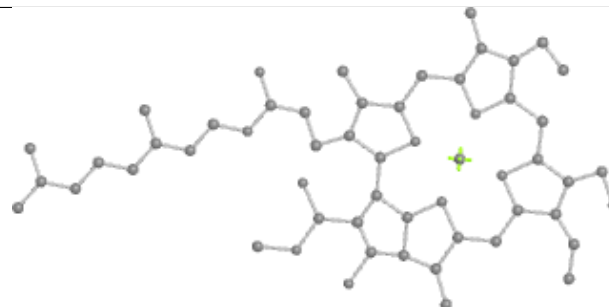
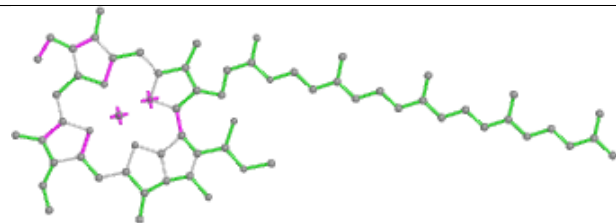
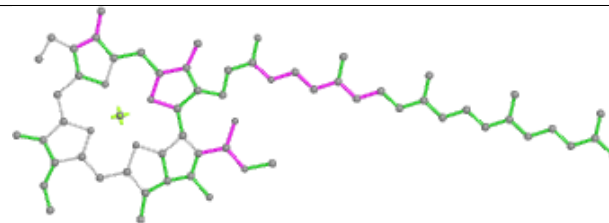
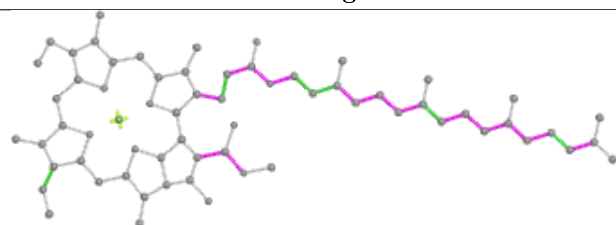
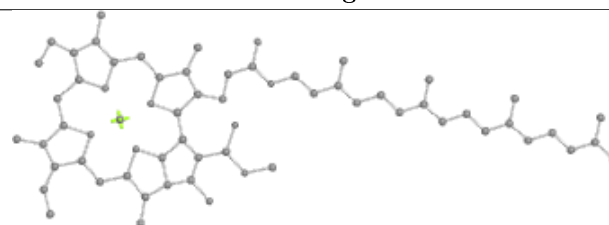


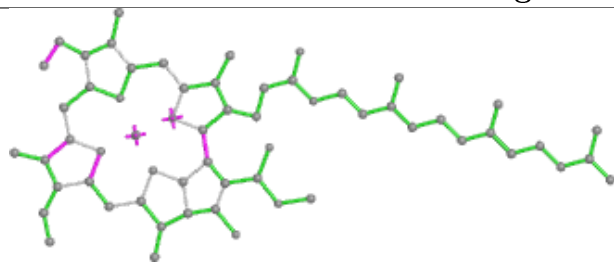
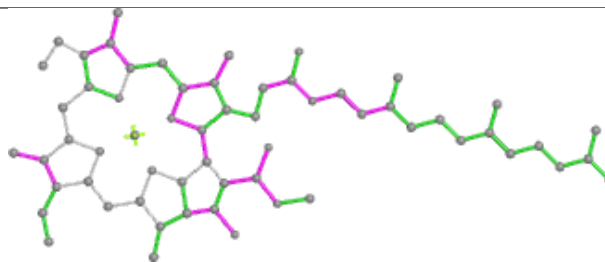
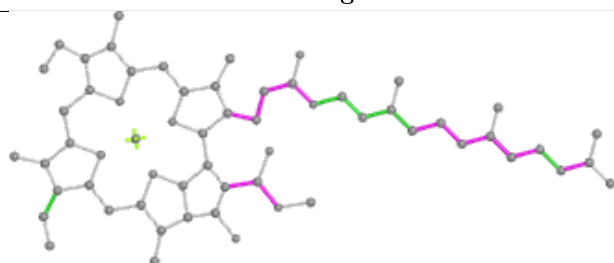
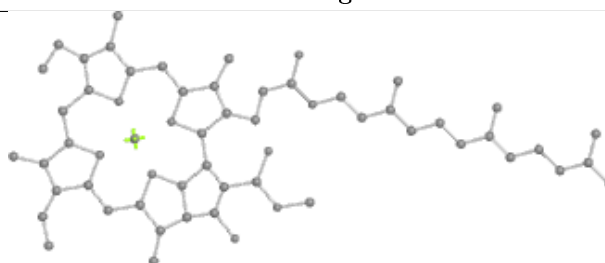
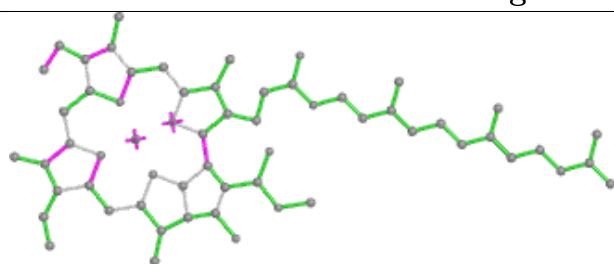
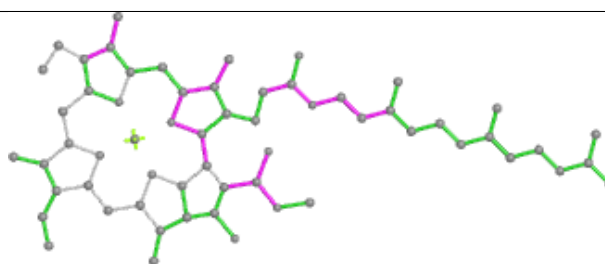
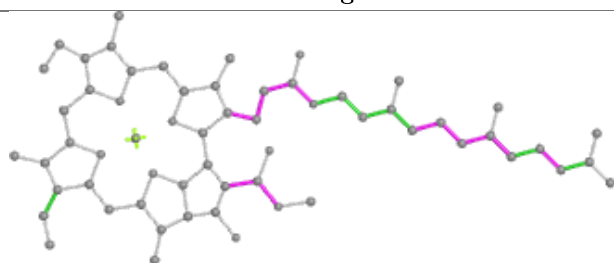
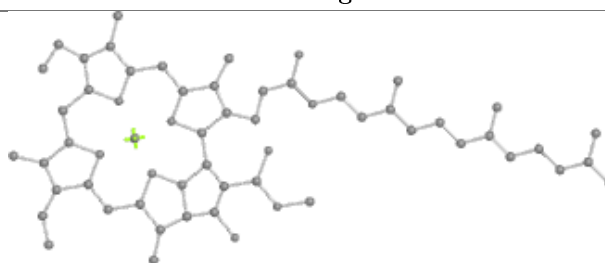
Torsions

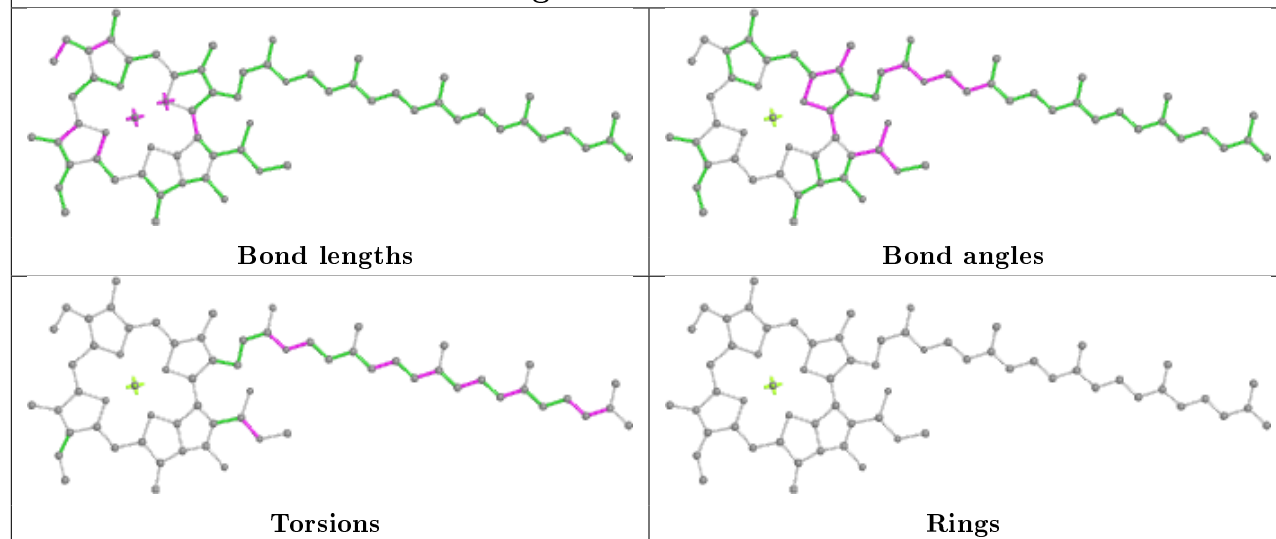
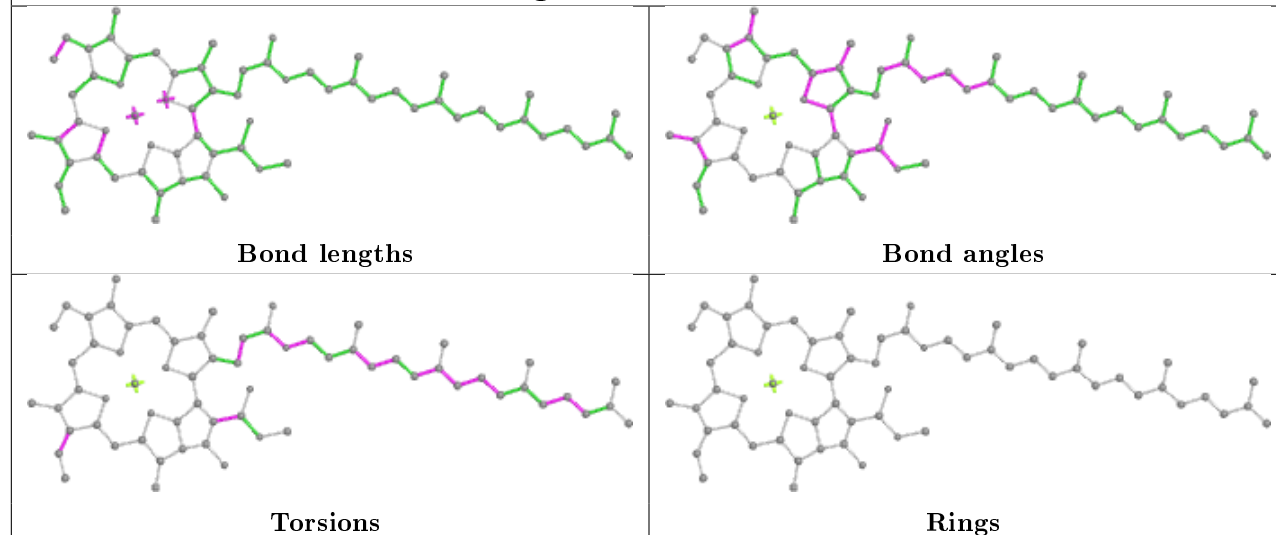
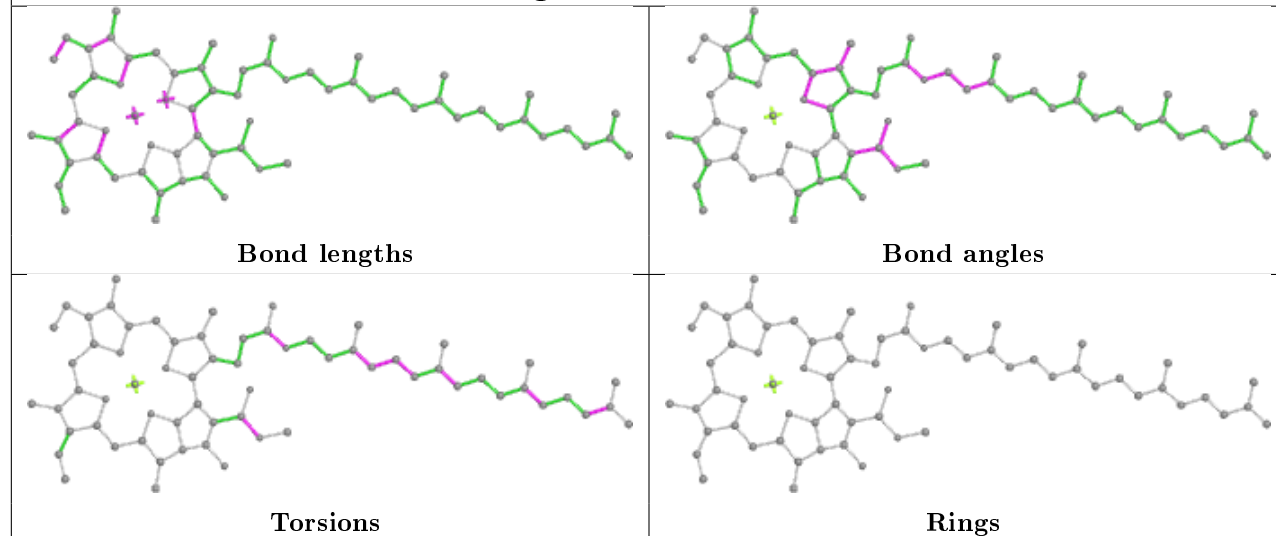


Rings

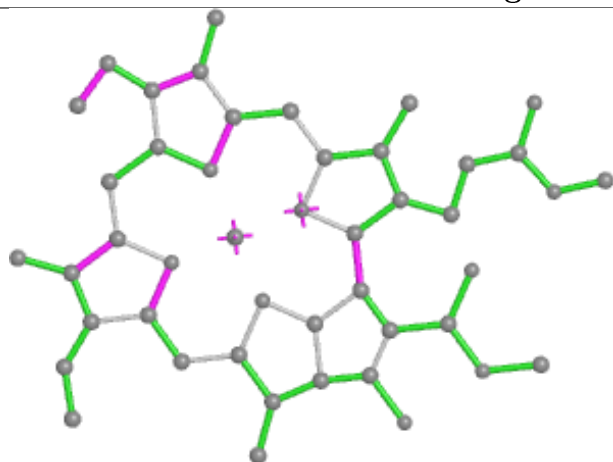
Ligand CLA B 805**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 803****Bond lengths****Bond angles****Torsions****Rings**

Ligand CHL 4 302**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 804****Bond lengths****Bond angles****Torsions****Rings**

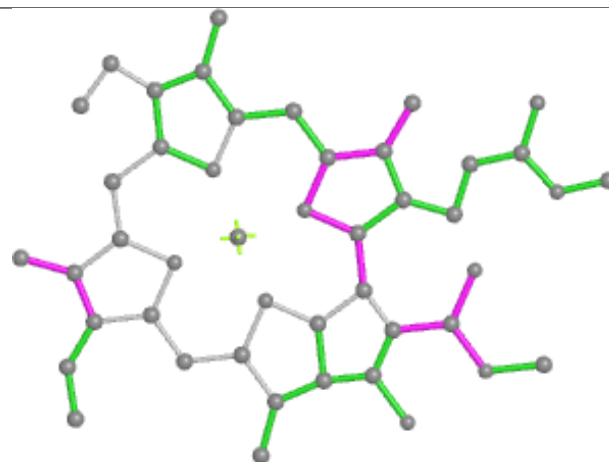
Ligand CLA B 832**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 1 5018****Bond lengths****Bond angles****Torsions****Rings**

Ligand CLA B 810**Ligand CLA A 812****Ligand CLA A 815**

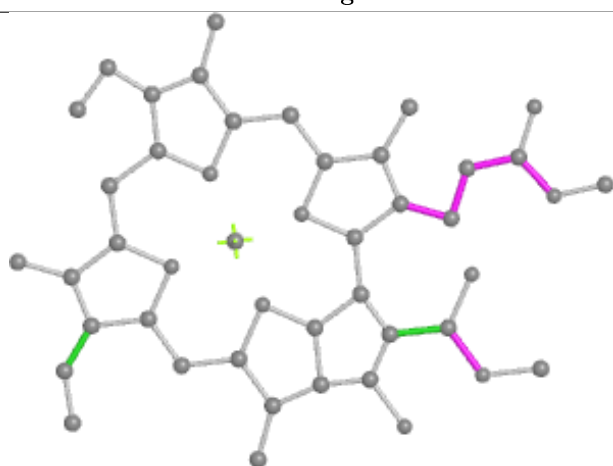
Ligand CLA K 1404



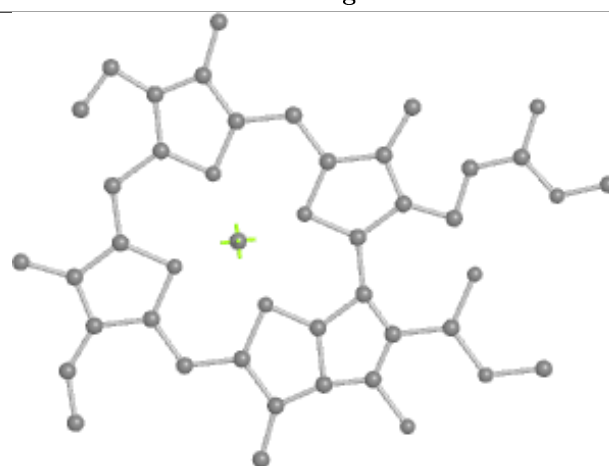
Bond lengths



Bond angles

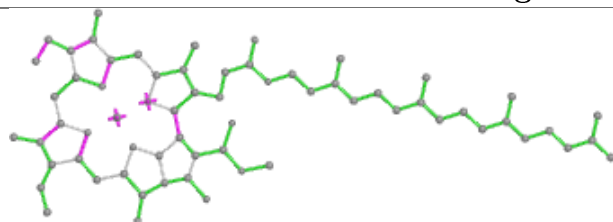


Torsions

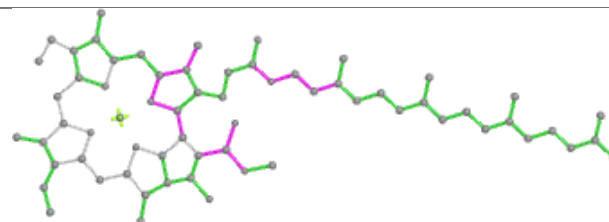


Rings

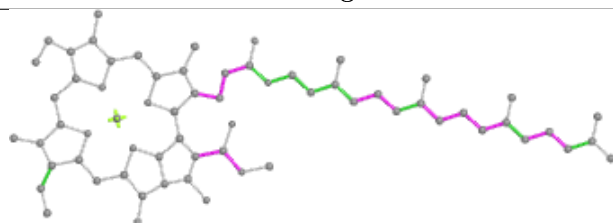
Ligand CLA A 803



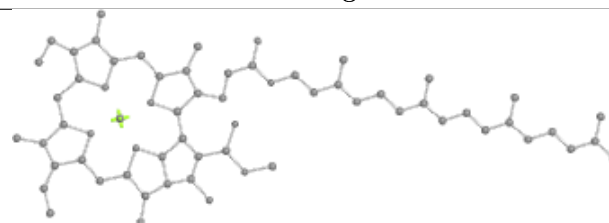
Bond lengths



Bond angles

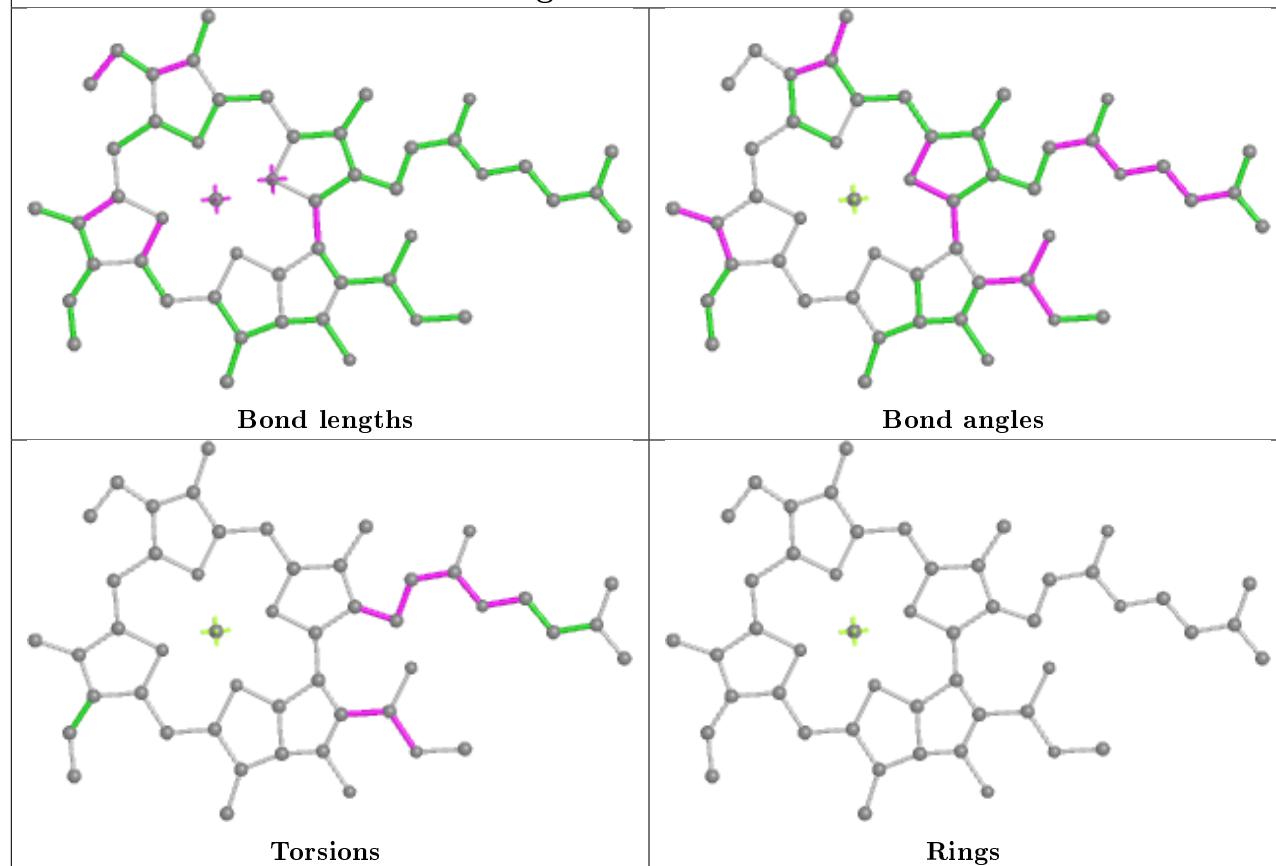


Torsions

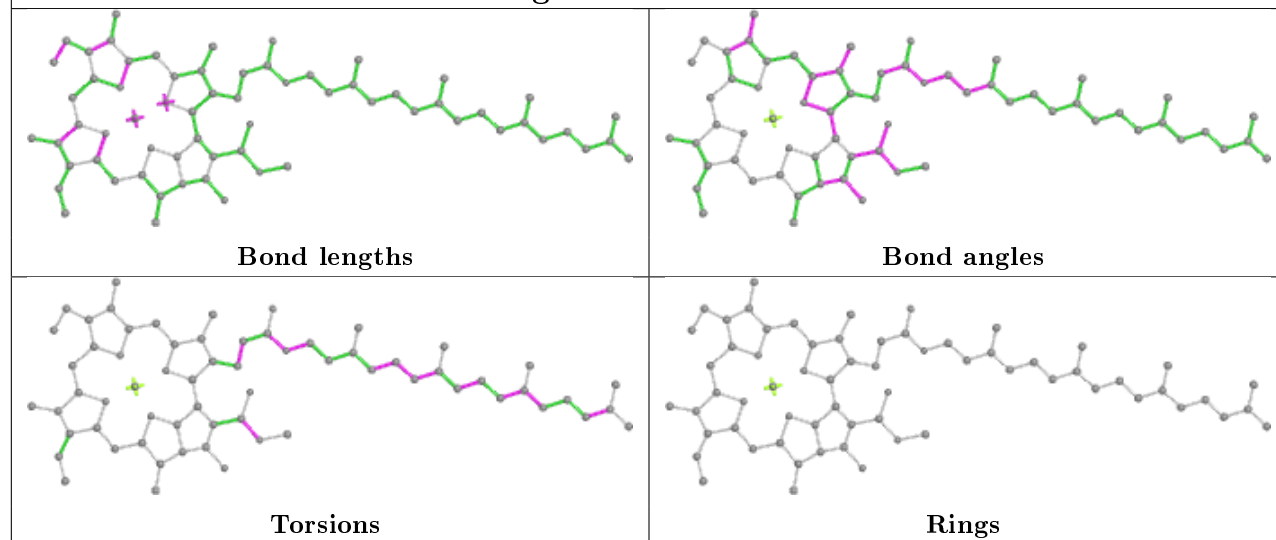


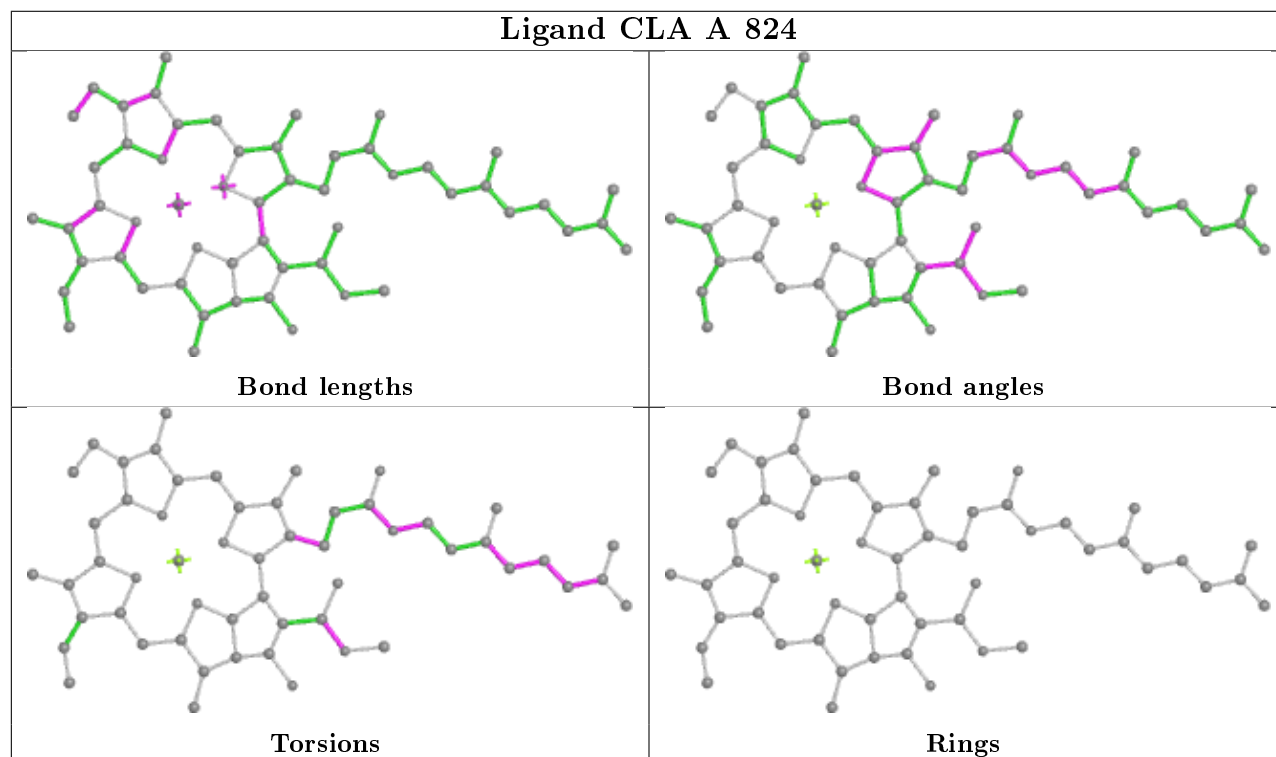
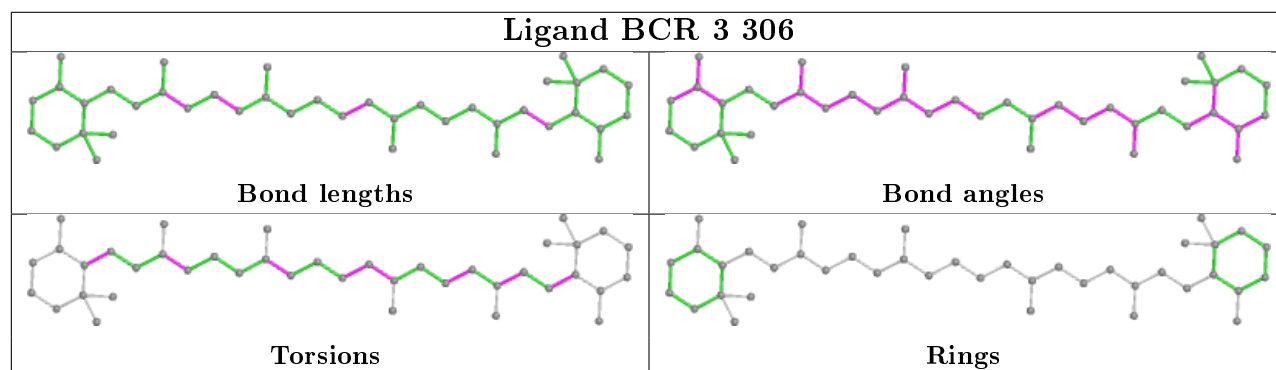
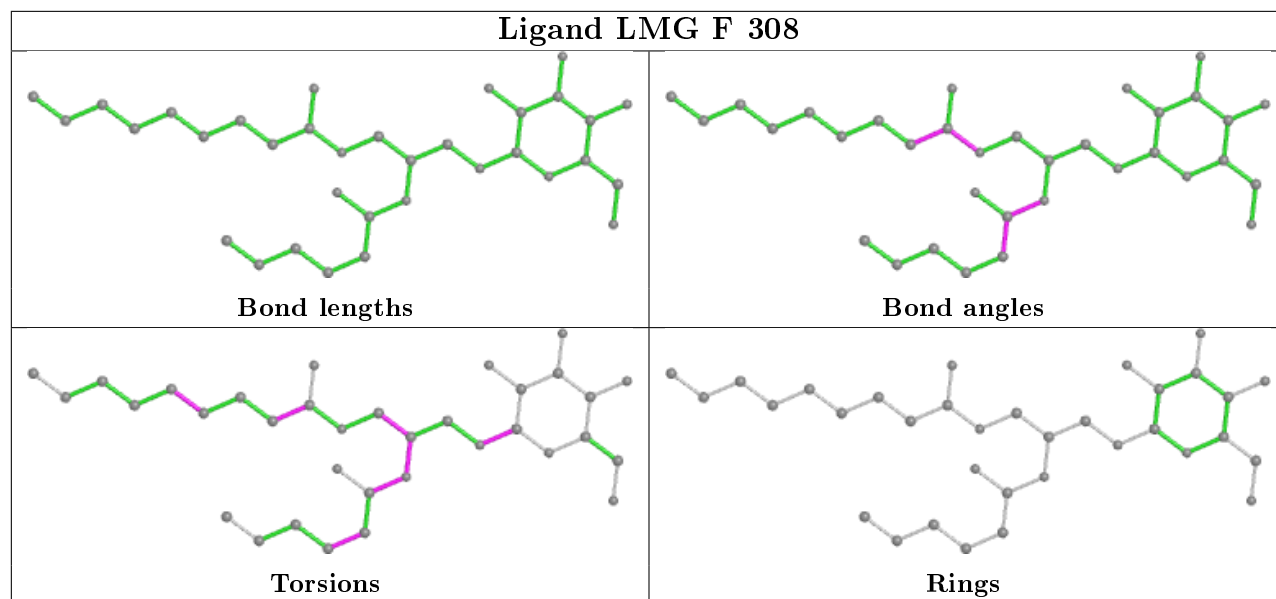
Rings

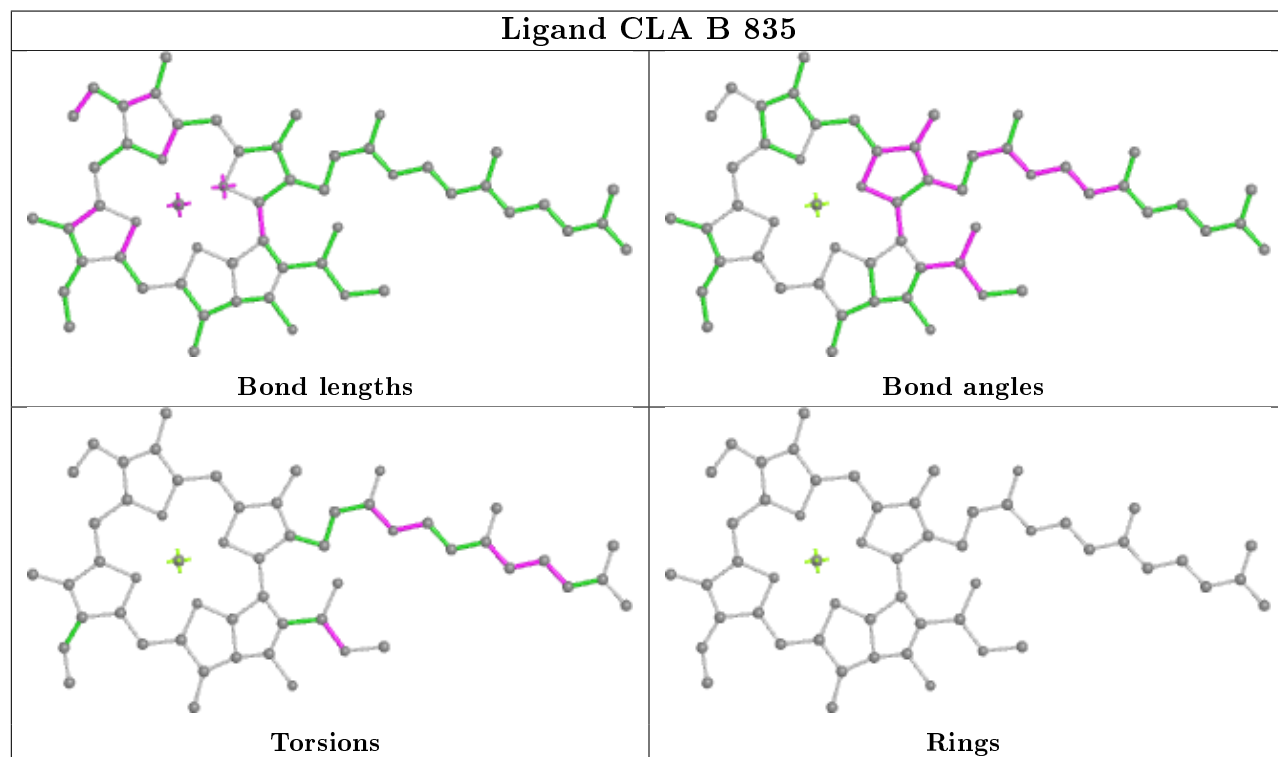
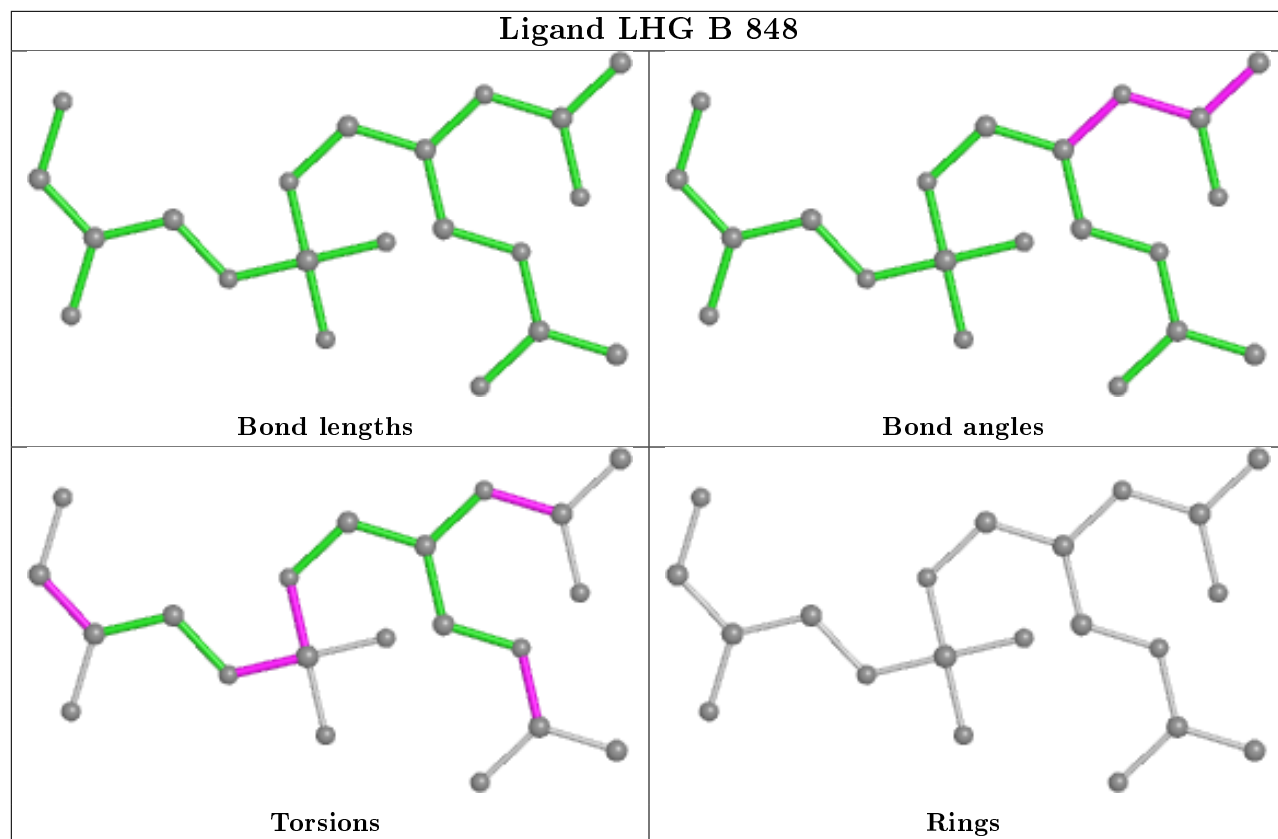
Ligand CLA 4 310

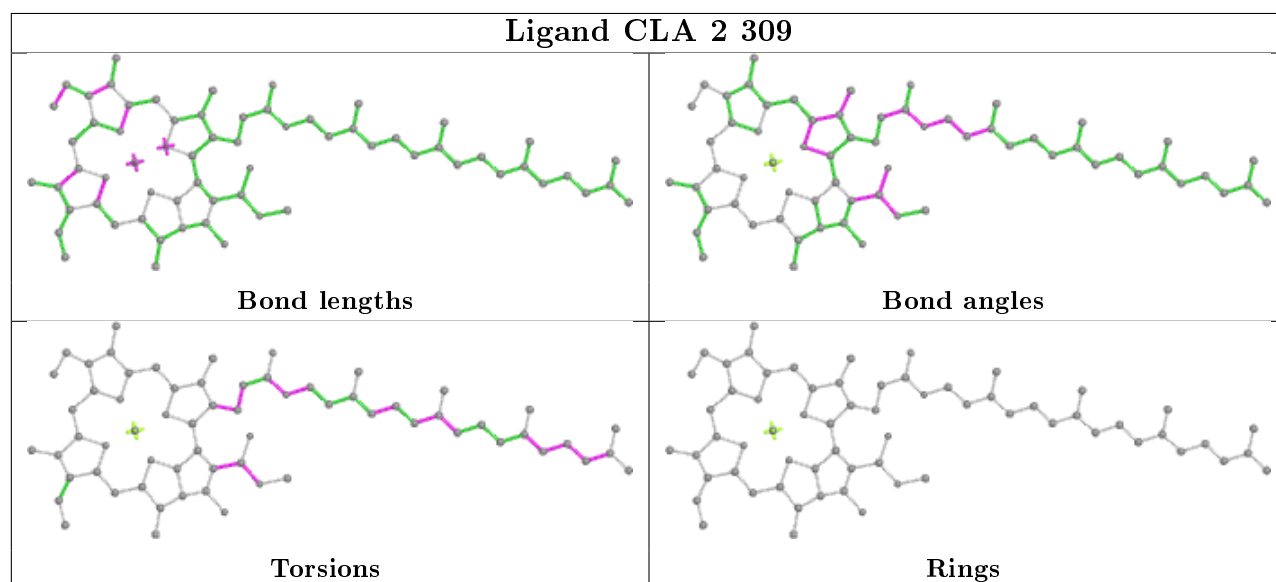
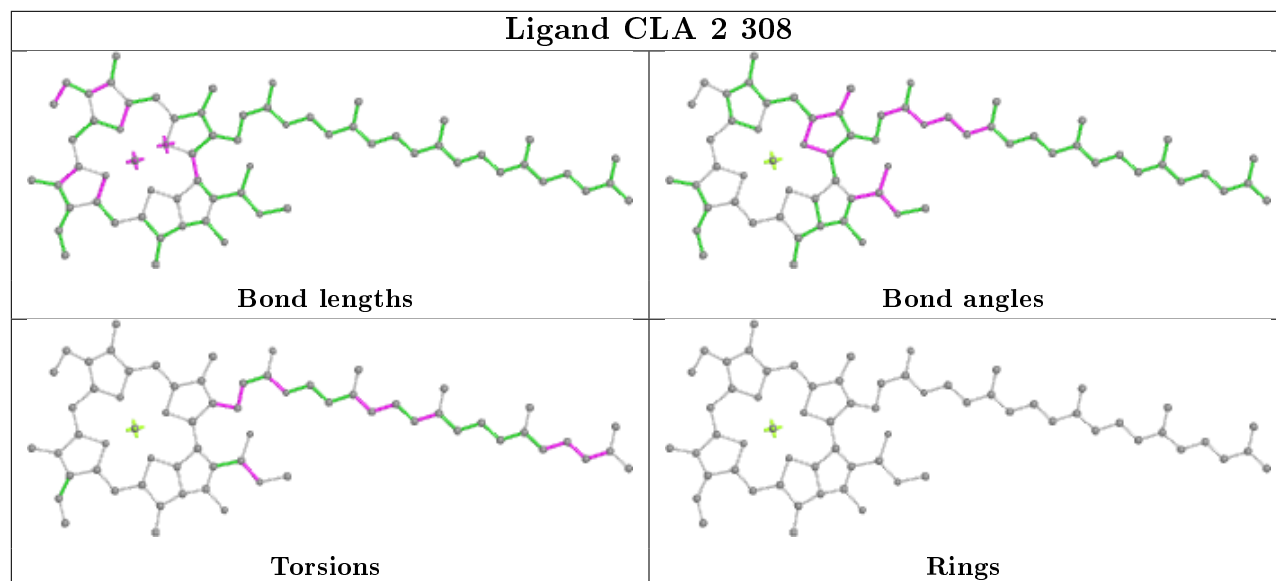
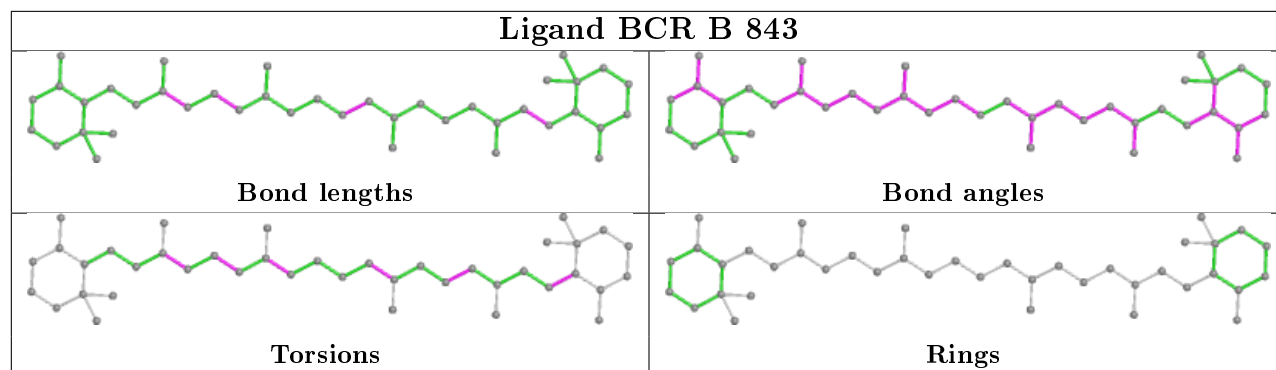


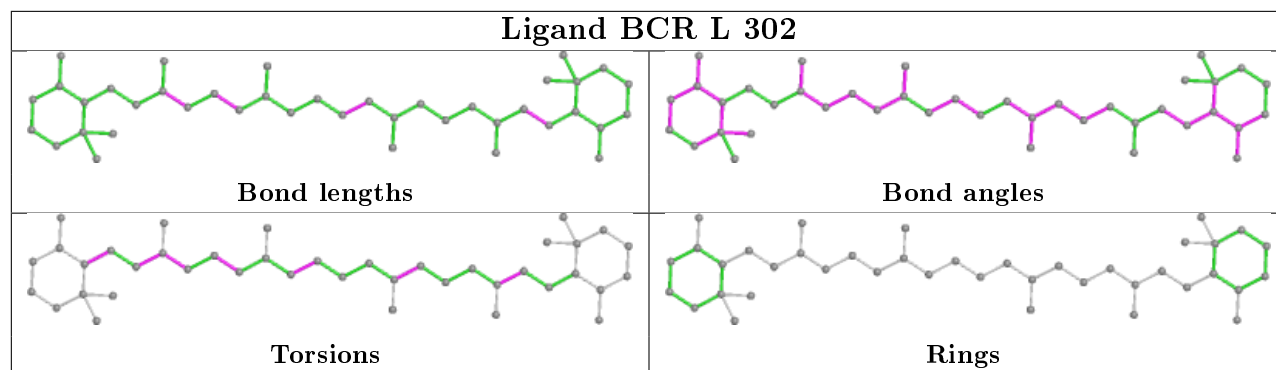
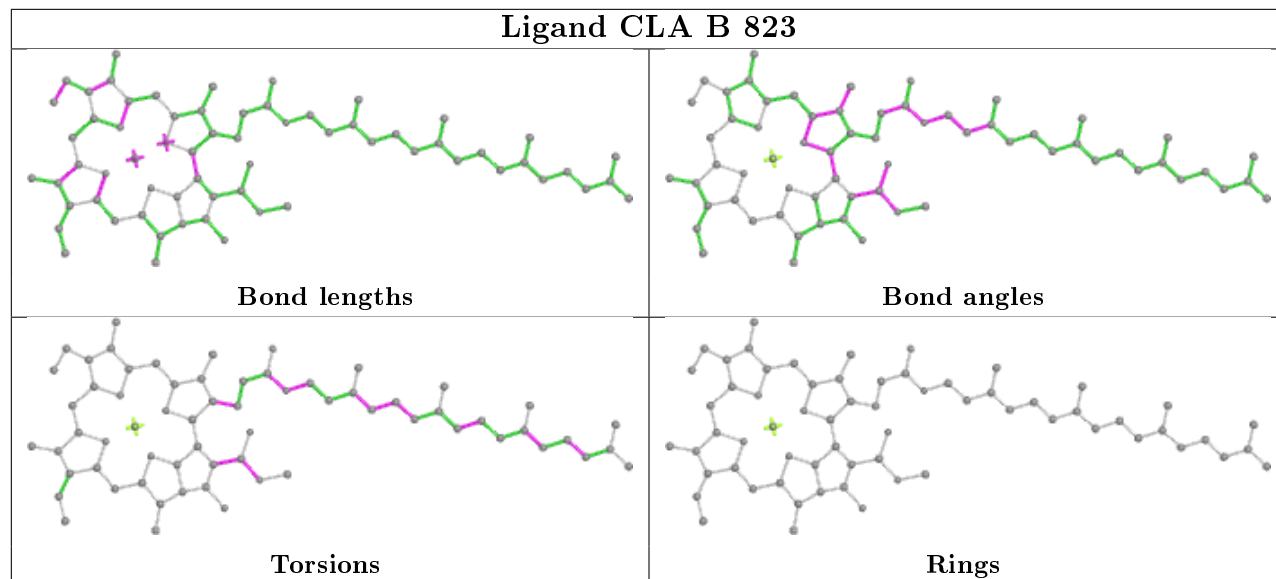
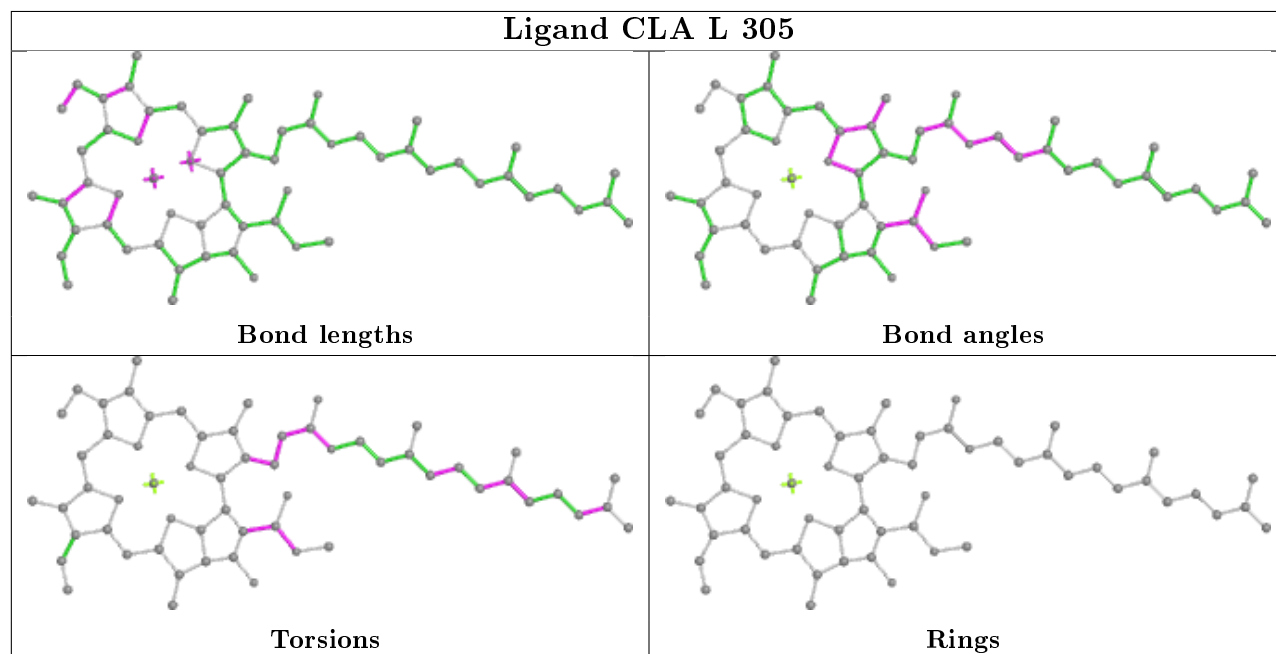
Ligand CLA A 829

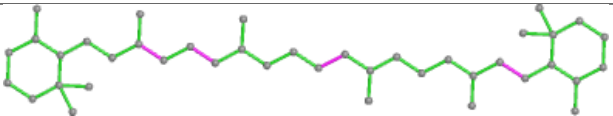
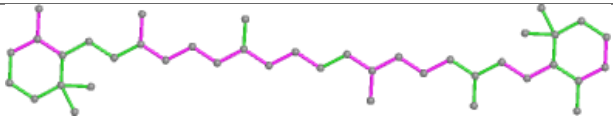
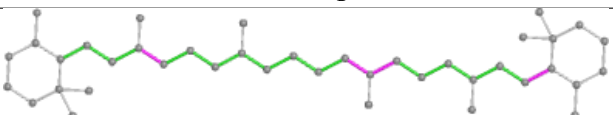
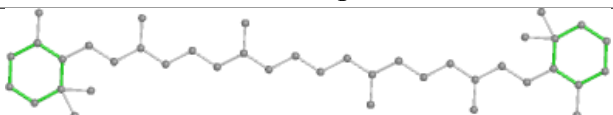
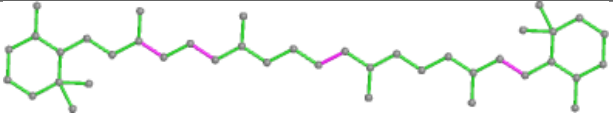
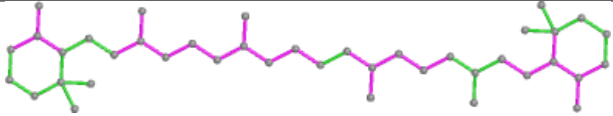
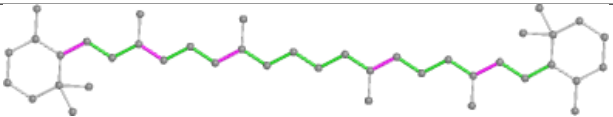
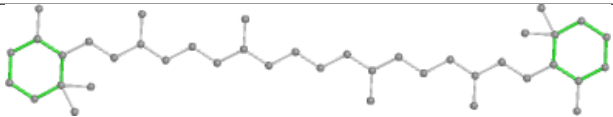
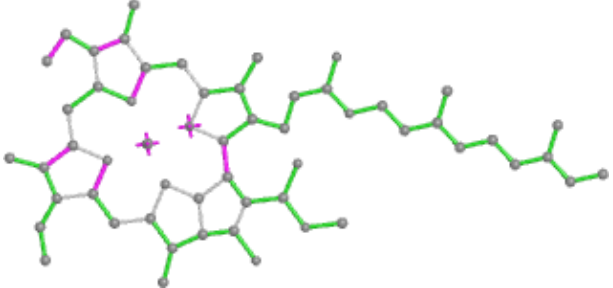
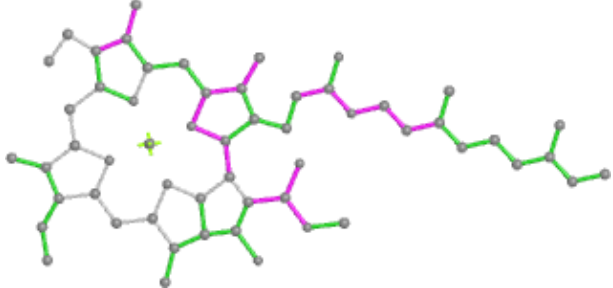
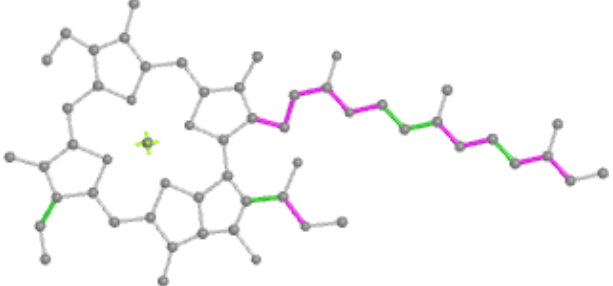
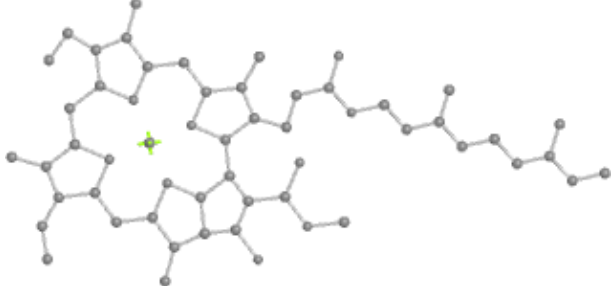


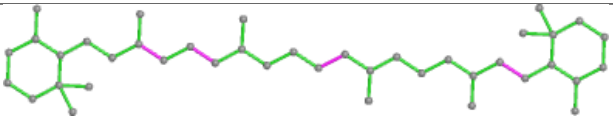
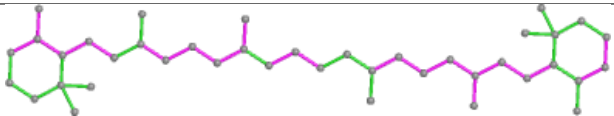
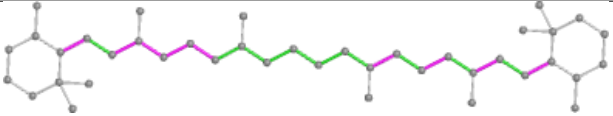
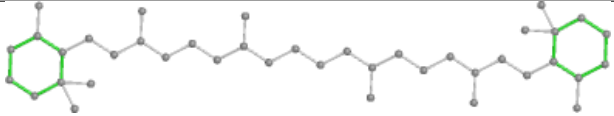


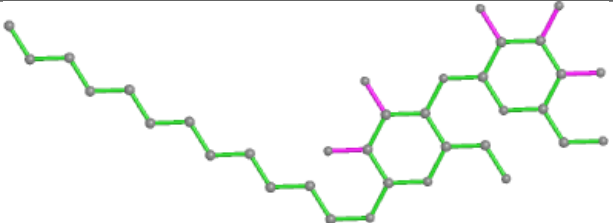
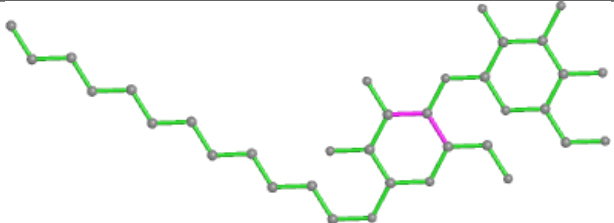
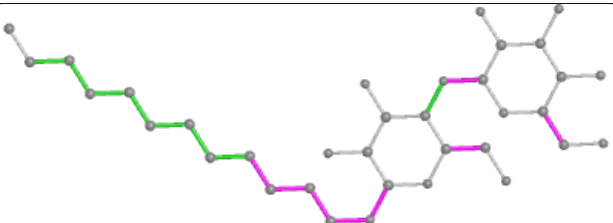
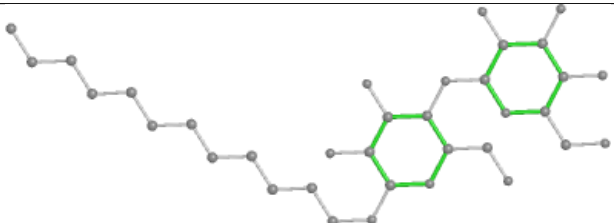


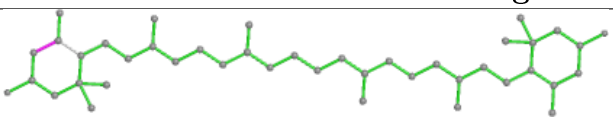
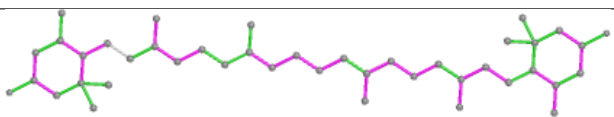
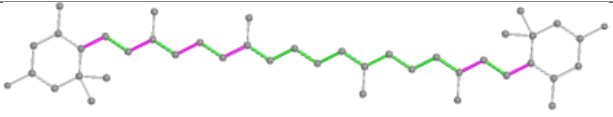
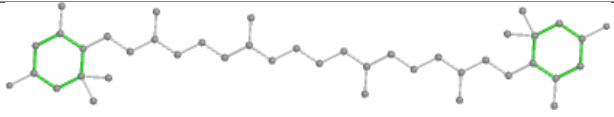


Ligand BCR L 302**Ligand CLA B 823****Ligand CLA L 305**

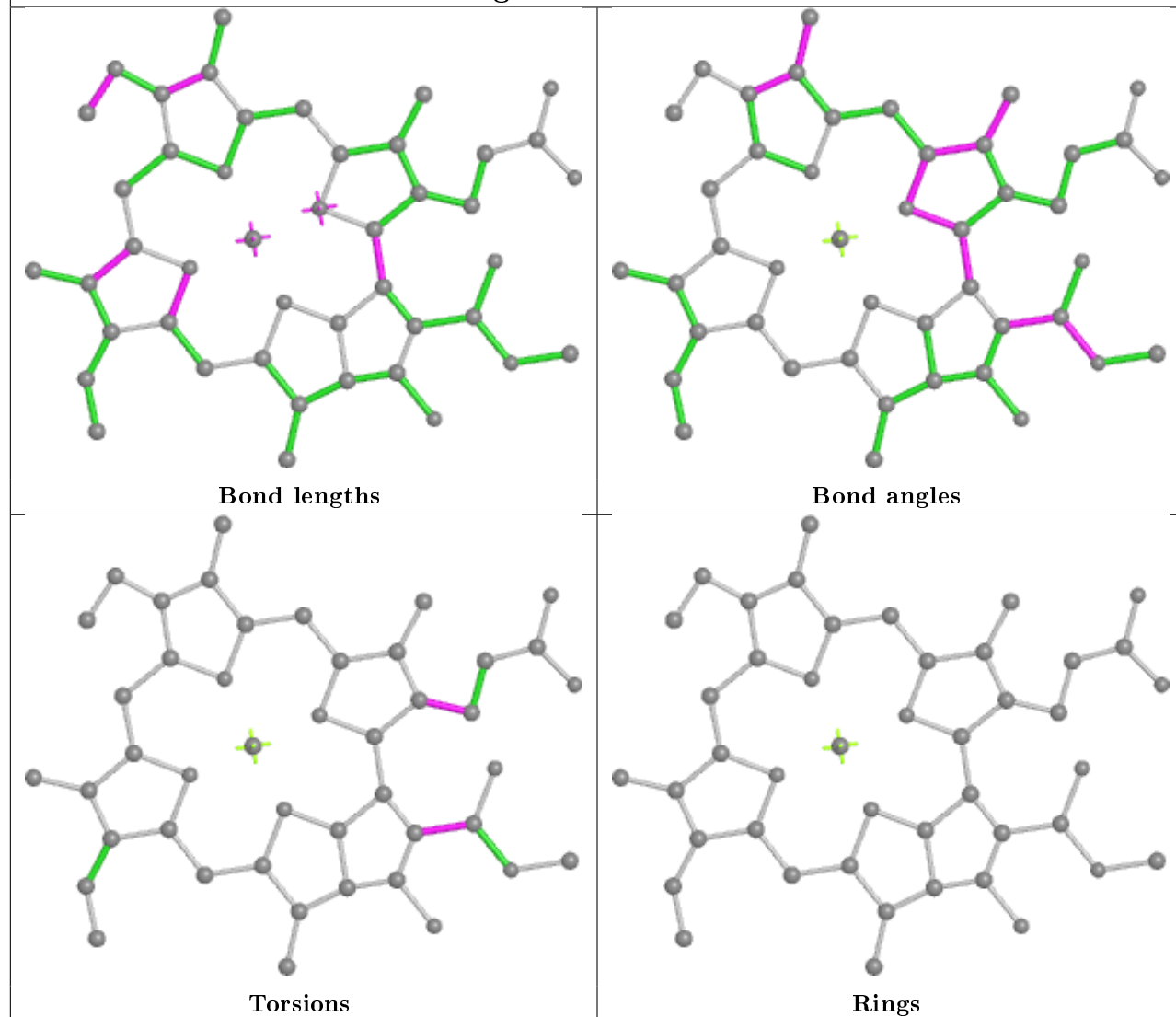
Ligand BCR G 1604	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA A 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

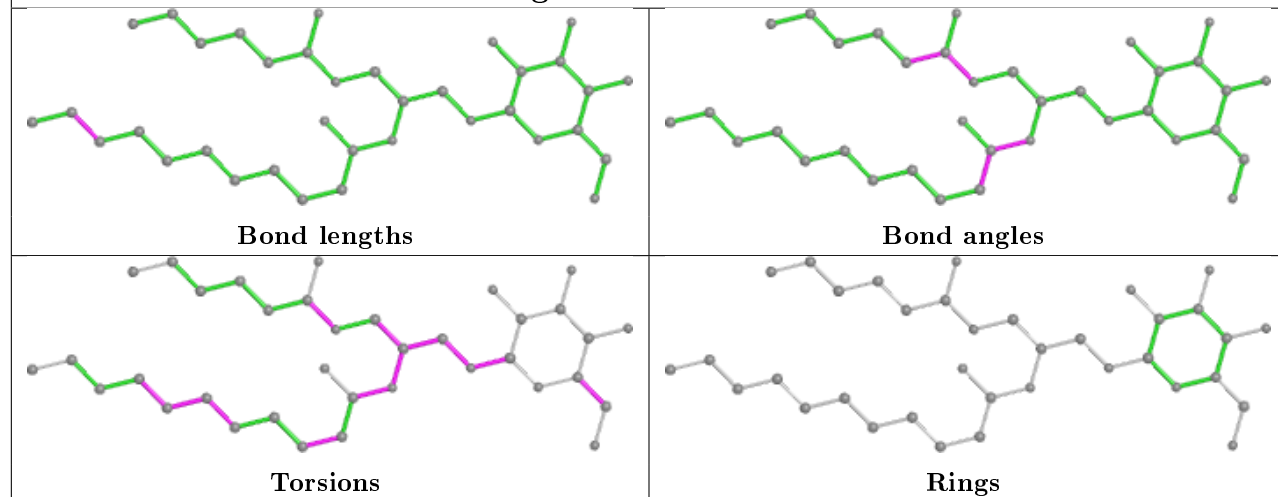
Ligand LMT A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 301



Ligand LMG 2 322



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	743/743 (100%)	-0.12	25 (3%)	45	19	68, 103, 151, 196	0
2	B	733/733 (100%)	-0.18	20 (2%)	54	26	67, 101, 138, 182	0
3	C	80/80 (100%)	-0.03	4 (5%)	28	10	77, 95, 158, 180	0
4	D	143/143 (100%)	0.00	12 (8%)	11	3	77, 105, 128, 151	0
5	E	66/66 (100%)	0.58	11 (16%)	1	0	85, 113, 168, 180	0
6	F	154/154 (100%)	-0.19	7 (4%)	33	12	82, 105, 141, 156	0
7	G	97/97 (100%)	-0.03	8 (8%)	11	3	109, 139, 165, 198	0
8	H	88/88 (100%)	-0.27	3 (3%)	45	19	100, 132, 160, 169	0
9	I	30/30 (100%)	-0.03	2 (6%)	17	5	97, 115, 132, 154	0
10	J	42/42 (100%)	-0.53	0	100	100	82, 96, 138, 171	0
11	K	80/80 (100%)	0.16	5 (6%)	20	6	142, 177, 208, 219	0
12	L	157/157 (100%)	-0.01	11 (7%)	16	5	96, 125, 173, 204	0
13	1	193/193 (100%)	0.59	32 (16%)	1	0	124, 156, 201, 228	0
14	2	208/208 (100%)	0.02	23 (11%)	5	1	106, 134, 168, 200	0
15	3	221/221 (100%)	0.29	25 (11%)	5	1	124, 161, 218, 248	0
16	4	198/198 (100%)	0.07	18 (9%)	9	3	110, 136, 174, 204	0
All	All	3233/3233 (100%)	-0.02	206 (6%)	19	6	67, 118, 178, 248	0

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	34	CYS	12.1
13	1	103	GLY	10.7
3	C	35	LYS	8.8
13	1	101	GLY	8.1
13	1	102	LEU	7.6

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 monosaccharides 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(\AA^2)	Q<0.9
23	LMT	J	1107	25/35	0.45	0.46	151,182,201,206	0
26	DGD	1	5002	35/66	0.52	0.67	125,209,233,236	0
24	LMG	2	302	13/55	0.55	0.39	130,165,187,190	0
22	LHG	B	849	49/49	0.59	0.53	101,139,196,220	0
24	LMG	B	850	35/55	0.59	0.30	74,146,176,185	0
24	LMG	A	851	50/55	0.64	0.58	136,173,197,203	0
23	LMT	2	325	35/35	0.65	0.38	157,224,241,245	0
25	GOL	4	321	6/6	0.66	0.65	135,146,153,158	0
24	LMG	2	301	13/55	0.68	0.46	148,168,192,202	0
24	LMG	B	851	33/55	0.68	0.38	133,208,223,227	0
21	BCR	2	305	40/40	0.71	0.57	131,154,181,186	0
24	LMG	1	5020	46/55	0.71	0.60	88,157,201,209	0
23	LMT	A	850	35/35	0.71	0.46	79,146,165,174	0
21	BCR	1	5005	40/40	0.72	0.57	135,175,224,229	0
24	LMG	G	1607	25/55	0.72	0.37	130,194,215,220	0
24	LMG	1	5001	49/55	0.72	0.38	91,156,219,221	0
18	CLA	K	1404	46/65	0.72	0.41	170,208,235,242	0
21	BCR	K	1405	40/40	0.74	0.54	138,166,194,201	0
21	BCR	L	302	40/40	0.74	0.44	118,167,216,221	0
21	BCR	3	306	40/40	0.75	0.79	134,160,182,188	0
24	LMG	4	320	13/55	0.75	0.41	166,194,213,219	0
24	LMG	2	323	13/55	0.76	0.19	126,164,190,192	0
21	BCR	G	1604	40/40	0.77	0.30	106,133,171,173	0
18	CLA	K	1401	45/65	0.77	0.36	133,166,181,194	0
21	BCR	B	845	40/40	0.78	0.44	92,121,179,183	0
23	LMT	B	852	35/35	0.79	0.54	114,212,231,232	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	LMT	G	1606	31/35	0.79	0.44	144,198,232,237	0
18	CLA	A	823	65/65	0.81	0.37	82,110,130,137	0
21	BCR	A	855	40/40	0.81	0.43	128,148,176,177	0
18	CLA	K	1402	60/65	0.81	0.48	100,164,183,192	0
27	CA	3	302	1/1	0.81	0.23	129,129,129,129	0
29	LUT	J	1105	42/42	0.81	0.33	89,122,148,163	0
29	LUT	3	303	42/42	0.81	0.49	145,166,176,181	0
29	LUT	3	304	42/42	0.81	0.34	116,146,169,173	0
24	LMG	2	322	36/55	0.82	0.35	111,177,212,217	0
24	LMG	F	307	36/55	0.82	0.46	125,159,194,197	0
23	LMT	4	319	35/35	0.82	0.36	95,179,207,207	0
25	GOL	A	854	6/6	0.82	0.80	124,136,142,142	0
24	LMG	2	321	25/55	0.82	0.18	114,144,164,168	0
18	CLA	3	314	48/65	0.83	0.36	159,194,205,208	0
18	CLA	J	1103	50/65	0.83	0.22	92,155,195,209	0
18	CLA	H	1701	60/65	0.83	0.29	148,175,199,206	0
18	CLA	1	5013	46/65	0.83	0.25	118,159,175,202	0
29	LUT	4	303	42/42	0.83	0.37	106,128,148,160	0
26	DGD	B	855	61/66	0.84	0.29	70,100,132,155	0
26	DGD	F	309	57/66	0.84	0.39	105,158,186,192	0
21	BCR	A	845	40/40	0.84	0.39	79,99,155,162	0
24	LMG	J	1102	30/55	0.84	0.29	103,123,146,159	0
21	BCR	B	844	40/40	0.84	0.35	81,109,151,165	0
21	BCR	L	307	40/40	0.84	0.47	102,130,153,164	0
24	LMG	B	854	13/55	0.84	0.20	131,170,201,202	0
23	LMT	G	1605	35/35	0.84	0.31	116,177,214,218	0
18	CLA	G	1603	65/65	0.85	0.27	127,161,197,202	0
21	BCR	A	846	40/40	0.85	0.32	72,100,129,147	0
29	LUT	2	303	42/42	0.85	0.38	114,132,145,159	0
18	CLA	1	5017	45/65	0.85	0.23	159,182,206,210	0
18	CLA	B	816	55/65	0.85	0.27	107,133,154,171	0
26	DGD	2	327	51/66	0.85	0.20	99,129,165,174	0
21	BCR	B	846	40/40	0.86	0.33	73,106,123,130	0
21	BCR	B	847	40/40	0.86	0.31	73,99,115,120	0
24	LMG	F	308	34/55	0.86	0.39	102,163,181,202	0
18	CLA	A	803	65/65	0.86	0.28	67,91,146,172	0
24	LMG	2	324	13/55	0.86	0.13	159,183,205,212	0
18	CLA	B	818	65/65	0.86	0.31	82,102,119,128	0
18	CLA	4	311	60/65	0.86	0.30	117,134,155,167	0
21	BCR	L	303	40/40	0.86	0.30	90,108,127,135	0
18	CLA	B	810	65/65	0.86	0.28	87,116,141,161	0
31	XAT	2	304	44/44	0.86	0.30	106,124,144,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	1	5015	65/65	0.87	0.26	140,176,193,202	0
28	ZEX	F	310	42/42	0.87	0.24	104,141,157,167	0
22	LHG	1	5019	49/49	0.87	0.26	112,135,168,176	0
29	LUT	1	5003	42/42	0.87	0.43	117,157,181,193	0
30	CHL	3	310	66/66	0.87	0.23	107,148,166,194	0
30	CHL	3	313	51/66	0.87	0.21	185,220,249,260	0
29	LUT	1	5004	42/42	0.87	0.34	105,145,165,174	0
21	BCR	B	843	40/40	0.88	0.35	104,121,144,166	0
18	CLA	L	304	50/65	0.88	0.23	123,151,170,179	0
18	CLA	3	307	55/65	0.88	0.26	148,169,183,191	0
30	CHL	3	312	51/66	0.88	0.19	141,157,177,183	0
18	CLA	4	312	46/65	0.88	0.17	115,145,160,175	0
21	BCR	3	305	40/40	0.88	0.24	120,134,155,161	0
18	CLA	A	840	60/65	0.89	0.27	101,147,196,206	0
18	CLA	2	311	50/65	0.89	0.30	116,139,154,158	0
23	LMT	B	853	32/35	0.89	0.37	121,153,174,179	0
30	CHL	1	5014	47/66	0.89	0.23	139,168,192,198	0
30	CHL	2	318	46/66	0.89	0.18	117,142,157,175	0
18	CLA	L	306	50/65	0.89	0.42	101,134,155,170	0
18	CLA	K	1403	48/65	0.89	0.31	166,197,226,242	0
26	DGD	J	1106	58/66	0.89	0.32	67,115,186,193	0
30	CHL	4	316	61/66	0.89	0.33	121,144,165,172	0
18	CLA	A	833	55/65	0.89	0.34	113,137,165,171	0
18	CLA	A	824	55/65	0.90	0.31	82,99,124,135	0
18	CLA	B	834	60/65	0.90	0.22	82,106,129,140	0
18	CLA	B	841	65/65	0.90	0.22	72,107,126,133	0
18	CLA	3	309	55/65	0.90	0.22	132,175,204,219	0
18	CLA	B	805	65/65	0.90	0.23	89,123,175,194	0
18	CLA	4	310	50/65	0.90	0.23	125,146,176,189	0
18	CLA	B	808	65/65	0.90	0.26	87,100,144,165	0
21	BCR	I	102	40/40	0.90	0.28	83,115,133,139	0
18	CLA	1	5008	55/65	0.90	0.20	114,142,159,162	0
18	CLA	A	825	65/65	0.90	0.27	85,116,136,143	0
18	CLA	A	814	46/65	0.90	0.26	127,143,167,179	0
31	XAT	4	304	44/44	0.90	0.26	92,127,146,156	0
18	CLA	1	5006	65/65	0.91	0.20	137,169,186,193	0
21	BCR	4	301	40/40	0.91	0.24	120,140,157,165	0
18	CLA	3	319	60/65	0.91	0.28	118,140,186,194	0
18	CLA	4	306	50/65	0.91	0.23	118,145,159,169	0
18	CLA	A	810	65/65	0.91	0.30	70,97,115,128	0
18	CLA	1	5009	65/65	0.91	0.29	91,137,151,157	0
18	CLA	B	801	65/65	0.91	0.26	63,84,96,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	CHL	2	315	56/66	0.91	0.25	109,151,170,175	0
21	BCR	A	844	40/40	0.91	0.31	87,115,169,186	0
30	CHL	2	319	56/66	0.91	0.15	117,147,181,192	0
18	CLA	A	829	65/65	0.91	0.26	78,118,173,180	0
18	CLA	B	835	55/65	0.91	0.21	99,115,163,178	0
27	CA	B	857	1/1	0.91	0.06	123,123,123,123	0
30	CHL	4	302	56/66	0.91	0.20	109,129,143,148	0
18	CLA	A	816	56/65	0.91	0.26	93,129,143,150	0
18	CLA	A	836	65/65	0.91	0.29	80,107,169,181	0
18	CLA	B	811	65/65	0.91	0.28	82,109,139,151	0
18	CLA	A	813	65/65	0.92	0.23	104,133,165,180	0
18	CLA	A	809	50/65	0.92	0.23	97,128,146,159	0
18	CLA	A	831	65/65	0.92	0.24	81,104,128,146	0
21	BCR	A	843	40/40	0.92	0.24	86,116,155,162	0
18	CLA	B	812	60/65	0.92	0.21	94,128,153,169	0
18	CLA	B	814	65/65	0.92	0.23	84,107,122,131	0
18	CLA	A	832	65/65	0.92	0.30	92,120,139,165	0
18	CLA	L	305	60/65	0.92	0.24	93,121,133,146	0
18	CLA	B	817	60/65	0.92	0.19	110,133,148,156	0
18	CLA	A	815	65/65	0.92	0.24	135,149,171,179	0
18	CLA	B	822	65/65	0.92	0.23	95,114,160,165	0
18	CLA	B	826	65/65	0.92	0.25	67,88,122,124	0
24	LMG	F	306	47/55	0.92	0.23	96,131,158,169	0
18	CLA	1	5011	50/65	0.92	0.26	146,167,182,191	0
18	CLA	B	827	65/65	0.92	0.24	74,94,112,120	0
18	CLA	A	806	60/65	0.92	0.22	79,112,152,161	0
18	CLA	A	818	50/65	0.92	0.28	101,128,151,163	0
30	CHL	1	5016	61/66	0.92	0.25	114,154,166,171	0
18	CLA	B	839	65/65	0.92	0.27	82,101,124,130	0
18	CLA	2	317	55/65	0.92	0.26	91,126,157,174	0
18	CLA	A	852	65/65	0.92	0.24	70,91,105,112	0
18	CLA	3	308	52/65	0.92	0.20	165,202,217,224	0
18	CLA	F	303	65/65	0.92	0.21	83,116,145,166	0
18	CLA	A	811	55/65	0.92	0.31	102,127,140,151	0
18	CLA	3	317	50/65	0.92	0.27	111,145,156,171	0
30	CHL	4	313	47/66	0.92	0.19	104,133,160,176	0
18	CLA	A	812	65/65	0.92	0.28	92,113,130,139	0
18	CLA	4	305	60/65	0.92	0.32	119,141,161,167	0
18	CLA	J	1101	65/65	0.92	0.18	65,87,114,129	0
18	CLA	B	830	65/65	0.93	0.21	77,98,128,139	0
18	CLA	B	815	65/65	0.93	0.24	96,116,136,155	0
18	CLA	A	835	65/65	0.93	0.25	89,114,148,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	L	301	55/65	0.93	0.25	89,120,136,145	0
18	CLA	B	837	65/65	0.93	0.19	68,88,105,114	0
21	BCR	F	304	40/40	0.93	0.22	67,85,100,105	0
18	CLA	3	311	55/65	0.93	0.25	113,139,155,160	0
18	CLA	A	804	65/65	0.93	0.21	78,91,114,138	0
21	BCR	J	1104	40/40	0.93	0.22	67,92,114,125	0
18	CLA	A	819	65/65	0.93	0.23	78,111,133,145	0
18	CLA	F	302	65/65	0.93	0.31	73,107,198,210	0
18	CLA	B	821	46/65	0.93	0.28	110,126,143,155	0
17	CL0	A	801	65/65	0.93	0.27	65,86,99,118	0
18	CLA	1	5010	65/65	0.93	0.25	89,146,162,180	0
18	CLA	B	823	65/65	0.93	0.24	87,114,150,162	0
18	CLA	A	834	51/65	0.93	0.40	81,106,134,147	0
18	CLA	4	315	65/65	0.93	0.29	107,134,164,176	0
19	PQN	B	842	33/33	0.93	0.24	67,84,105,120	0
18	CLA	B	804	65/65	0.93	0.30	69,90,105,117	0
18	CLA	B	828	65/65	0.93	0.31	72,100,128,141	0
22	LHG	2	320	35/49	0.93	0.21	101,131,149,160	0
18	CLA	1	5018	60/65	0.93	0.16	88,137,192,196	0
18	CLA	2	307	52/65	0.93	0.14	120,144,157,159	0
30	CHL	4	314	51/66	0.93	0.24	120,144,159,172	0
18	CLA	2	310	65/65	0.93	0.25	107,128,155,166	0
30	CHL	4	317	43/66	0.93	0.13	125,162,177,190	0
23	LMT	B	856	31/35	0.93	0.20	138,156,173,179	0
21	BCR	B	802	40/40	0.93	0.26	72,100,119,128	0
18	CLA	B	831	65/65	0.94	0.21	69,88,115,121	0
18	CLA	B	832	60/65	0.94	0.24	70,99,137,153	0
18	CLA	A	828	65/65	0.94	0.22	64,79,99,118	0
18	CLA	A	817	65/65	0.94	0.41	84,115,134,143	0
18	CLA	B	836	55/65	0.94	0.21	74,92,108,115	0
18	CLA	3	318	46/65	0.94	0.17	140,158,170,172	0
18	CLA	B	806	65/65	0.94	0.22	76,92,112,121	0
18	CLA	B	838	50/65	0.94	0.30	69,91,103,126	0
18	CLA	1	5007	46/65	0.94	0.15	122,149,167,180	0
22	LHG	A	848	49/49	0.94	0.23	63,90,107,112	0
18	CLA	4	307	65/65	0.94	0.17	109,135,157,165	0
18	CLA	4	309	60/65	0.94	0.24	83,123,138,143	0
18	CLA	B	819	65/65	0.94	0.28	82,104,123,132	0
18	CLA	B	840	65/65	0.94	0.30	74,97,120,127	0
18	CLA	A	830	65/65	0.94	0.27	77,95,108,122	0
18	CLA	B	809	65/65	0.94	0.22	79,108,122,129	0
19	PQN	A	841	33/33	0.94	0.23	63,82,97,104	0

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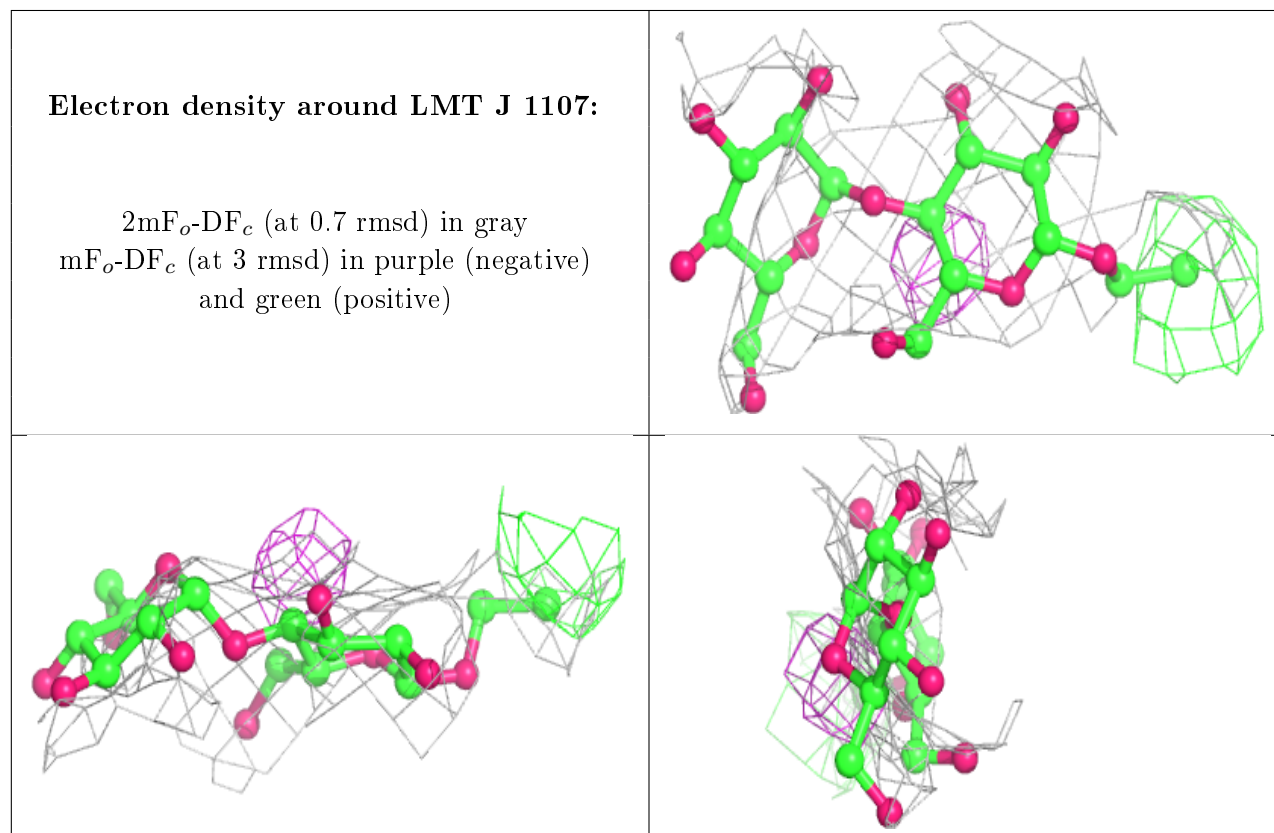
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	807	65/65	0.94	0.27	66,84,106,119	0
18	CLA	G	1601	55/65	0.94	0.19	120,147,172,177	0
18	CLA	G	1602	46/65	0.94	0.24	132,158,180,206	0
18	CLA	B	825	65/65	0.94	0.25	77,94,120,134	0
18	CLA	2	306	60/65	0.94	0.33	115,134,164,175	0
21	BCR	A	847	40/40	0.94	0.24	63,75,103,105	0
30	CHL	2	314	66/66	0.94	0.20	99,128,151,165	0
18	CLA	A	826	65/65	0.94	0.28	66,88,109,121	0
30	CHL	2	316	48/66	0.94	0.23	107,124,145,160	0
18	CLA	2	308	65/65	0.94	0.21	113,132,152,167	0
18	CLA	2	309	65/65	0.94	0.18	99,121,132,145	0
18	CLA	A	853	65/65	0.94	0.27	84,105,130,138	0
18	CLA	A	827	65/65	0.94	0.38	81,99,115,120	0
18	CLA	2	312	60/65	0.94	0.15	122,139,161,183	0
30	CHL	3	316	47/66	0.94	0.21	135,159,171,181	0
18	CLA	2	313	50/65	0.94	0.23	121,134,153,157	0
18	CLA	B	829	65/65	0.94	0.21	78,93,111,127	0
21	BCR	F	305	40/40	0.94	0.20	76,98,116,120	0
18	CLA	2	326	50/65	0.94	0.19	94,114,150,160	0
21	BCR	I	101	40/40	0.94	0.29	85,108,125,129	0
18	CLA	3	301	45/65	0.94	0.24	120,138,174,192	0
18	CLA	B	803	65/65	0.94	0.23	64,81,98,107	0
18	CLA	B	820	65/65	0.95	0.29	84,106,123,152	0
18	CLA	A	822	65/65	0.95	0.23	78,93,121,129	0
18	CLA	A	820	60/65	0.95	0.20	121,148,178,189	0
18	CLA	4	308	60/65	0.95	0.23	92,118,142,153	0
18	CLA	1	5012	46/65	0.95	0.12	117,149,168,183	0
18	CLA	A	821	60/65	0.95	0.22	122,149,190,193	0
22	LHG	A	849	40/49	0.95	0.23	88,125,152,155	0
18	CLA	B	824	55/65	0.95	0.21	82,105,123,133	0
18	CLA	3	315	65/65	0.95	0.22	115,153,164,191	0
18	CLA	A	838	65/65	0.95	0.18	64,84,119,134	0
30	CHL	4	318	56/66	0.95	0.26	109,134,178,182	0
18	CLA	B	807	65/65	0.95	0.23	73,93,108,115	0
18	CLA	B	813	46/65	0.95	0.23	107,126,142,166	0
18	CLA	A	802	65/65	0.96	0.27	62,77,96,111	0
18	CLA	B	833	58/65	0.96	0.20	65,87,107,117	0
18	CLA	A	837	65/65	0.96	0.19	63,77,94,114	0
22	LHG	B	848	21/49	0.96	0.15	88,113,140,155	0
18	CLA	A	805	65/65	0.96	0.23	65,86,103,115	0
18	CLA	A	808	65/65	0.96	0.20	67,85,132,144	0
18	CLA	F	301	65/65	0.96	0.22	65,87,105,109	0

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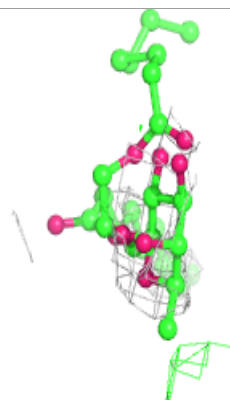
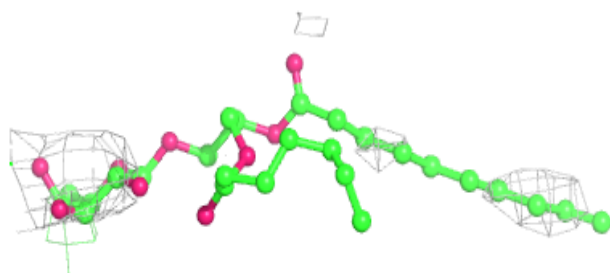
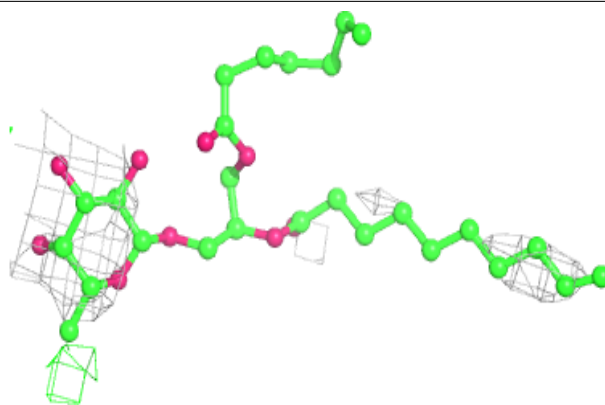
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	CLA	A	839	65/65	0.97	0.23	61,82,97,106	0
20	SF4	A	842	8/8	0.98	0.21	70,71,119,144	0
20	SF4	C	102	8/8	0.98	0.16	79,89,122,145	0
20	SF4	C	101	8/8	0.99	0.19	69,86,120,124	0

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.

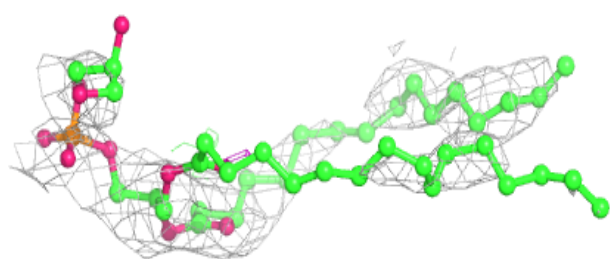
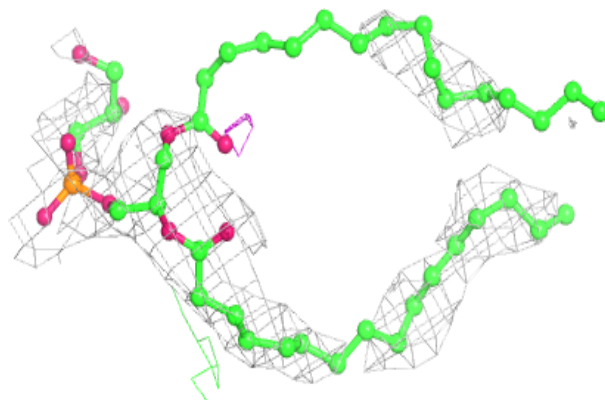


Electron density around DGD 1 5002:

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

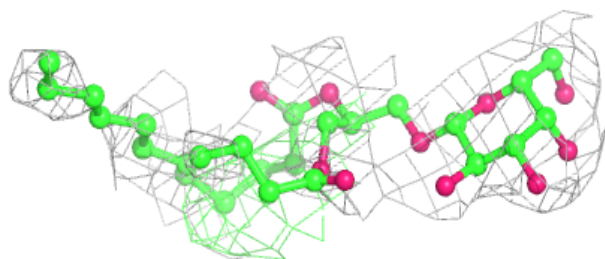
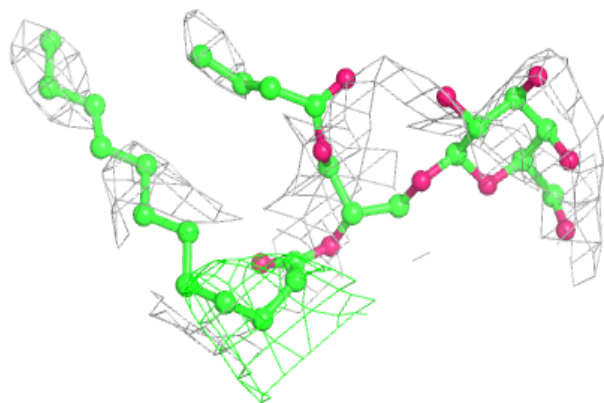
**Electron density around LHG B 849:**

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



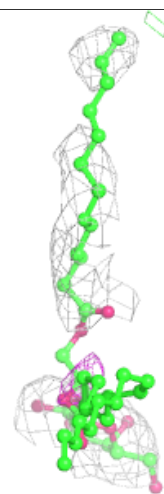
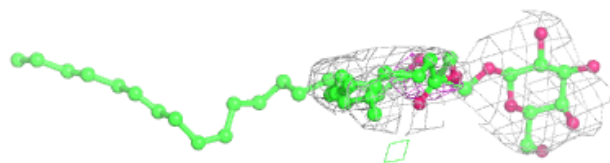
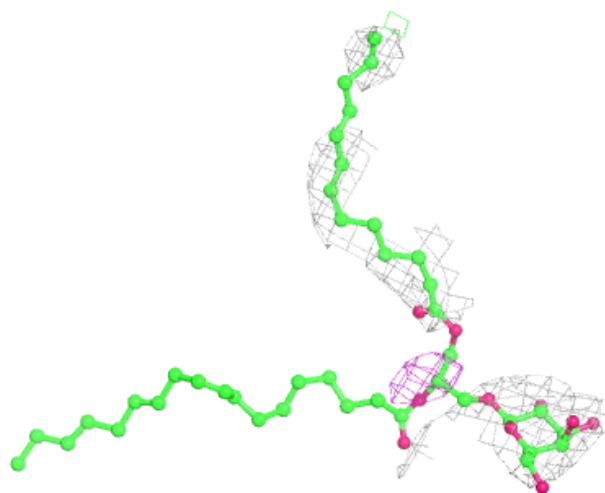
Electron density around LMG B 850:

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



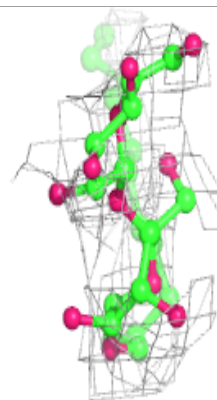
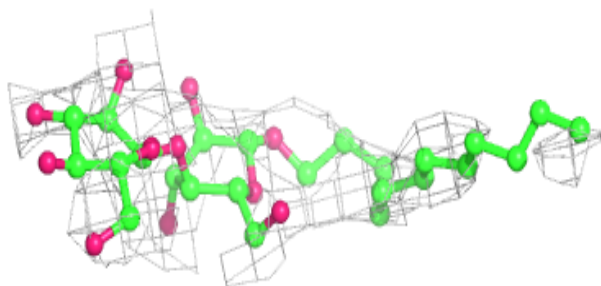
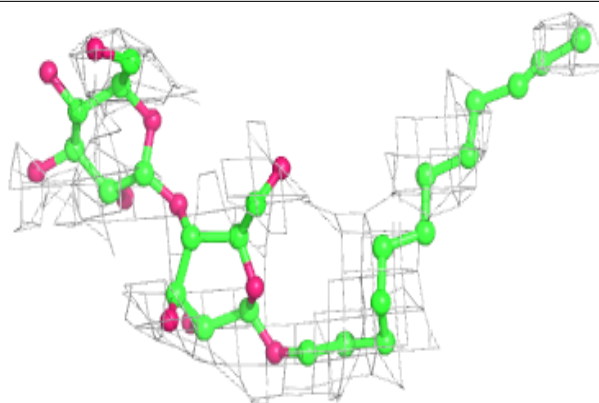
Electron density around LMG A 851:

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



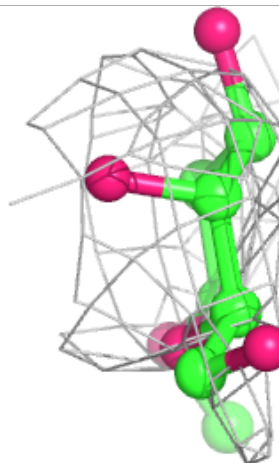
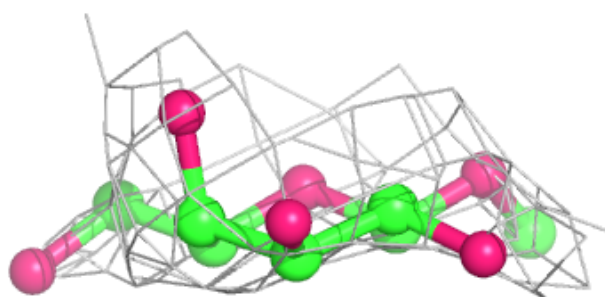
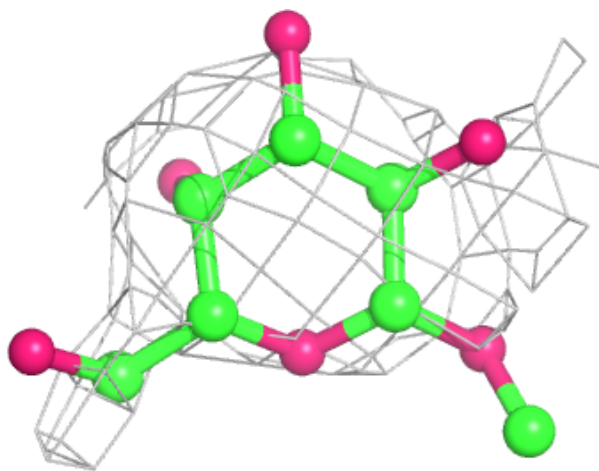
Electron density around LMT 2 325:

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



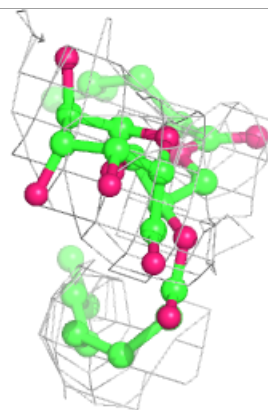
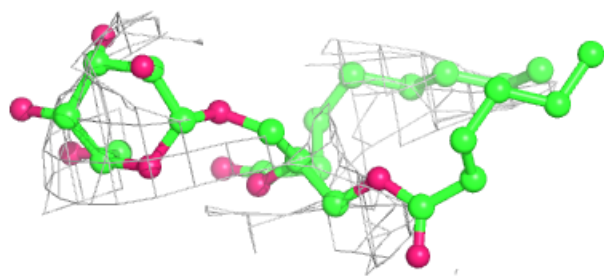
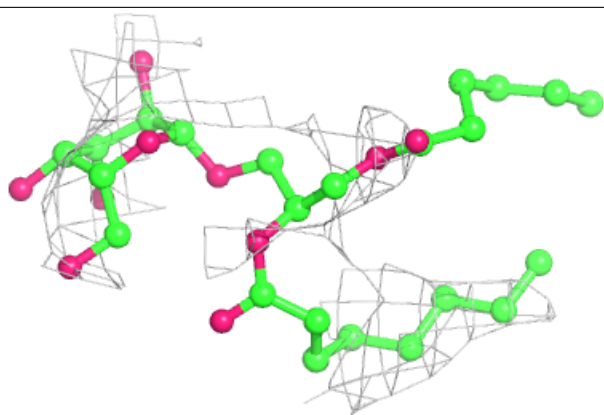
Electron density around LMG 2 301:

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

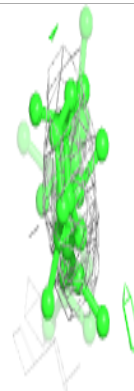
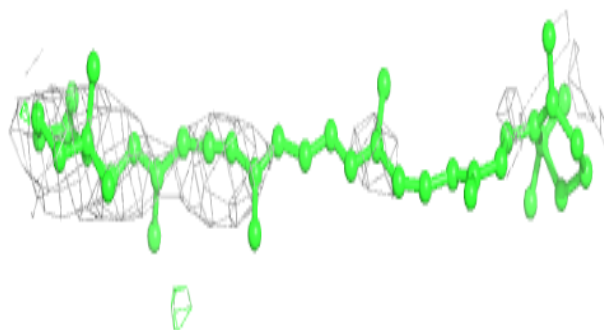
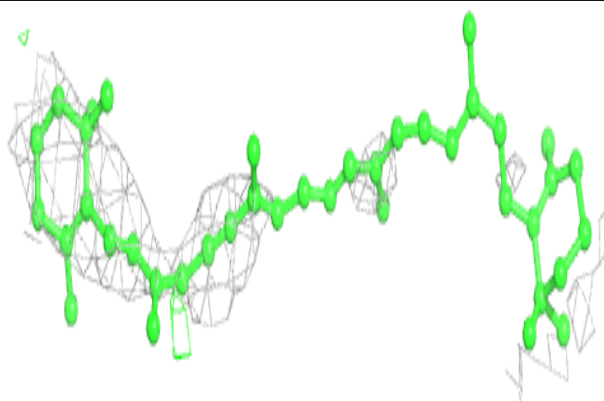


Electron density around LMG B 851:

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

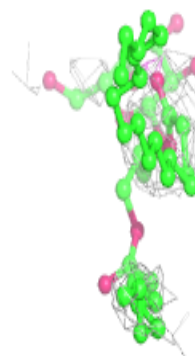
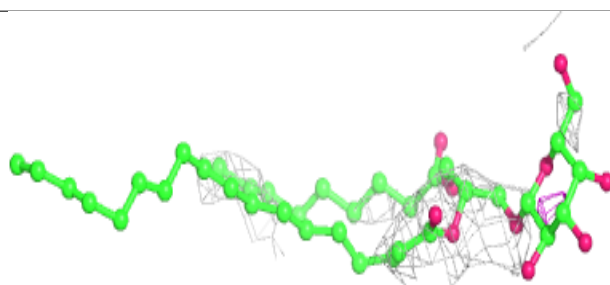
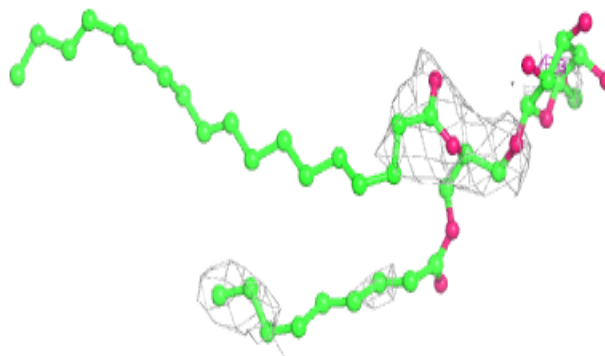
**Electron density around BCR 2 305:**

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

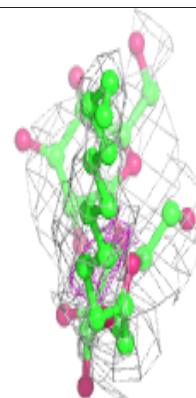
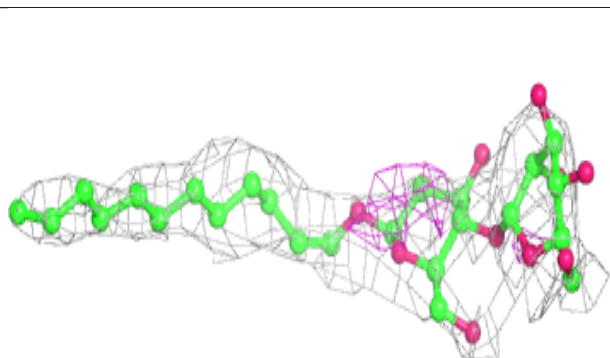
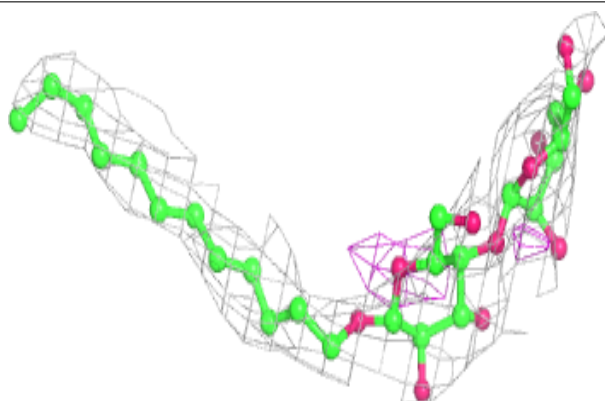


Electron density around LMG 1 5020:

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

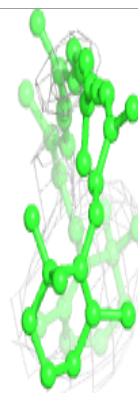
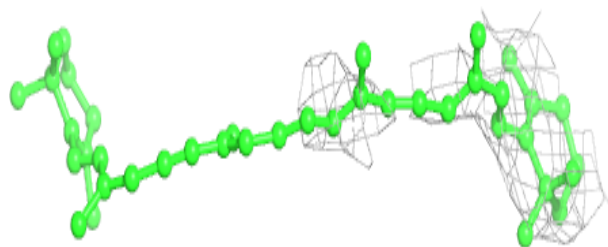
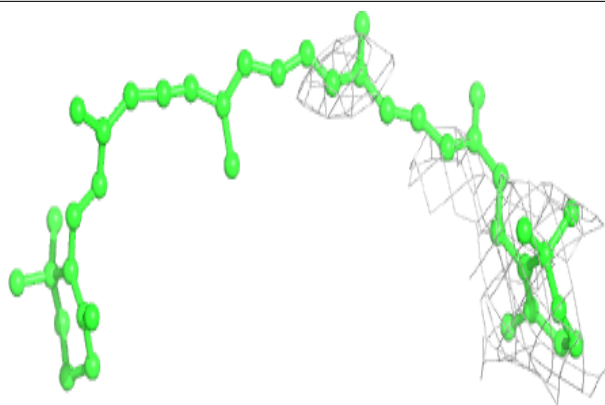
**Electron density around LMT A 850:**

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



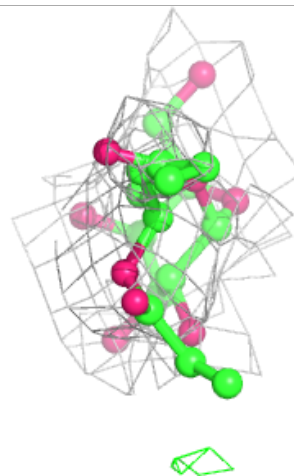
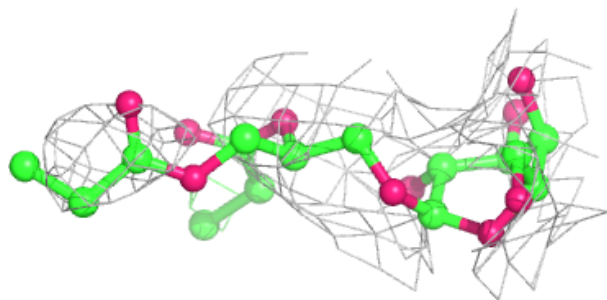
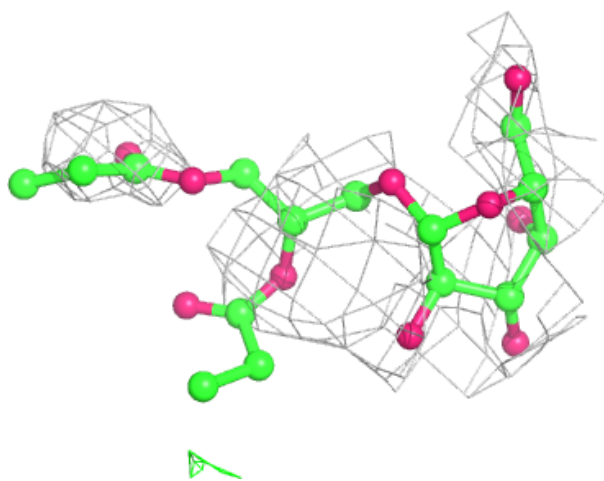
Electron density around BCR 1 5005:

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



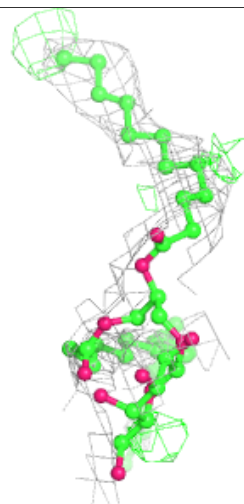
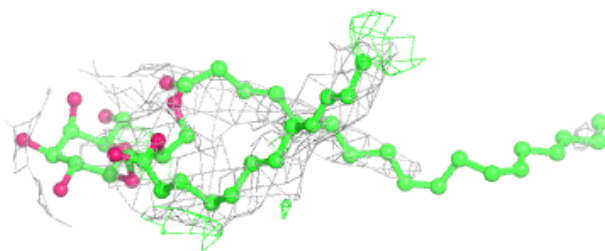
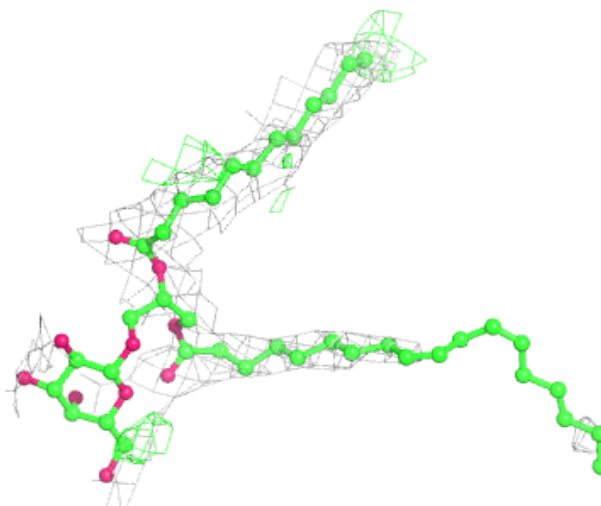
Electron density around LMG G 1607:

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



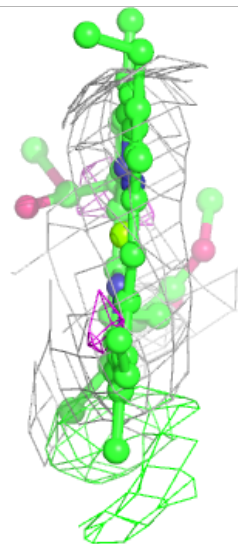
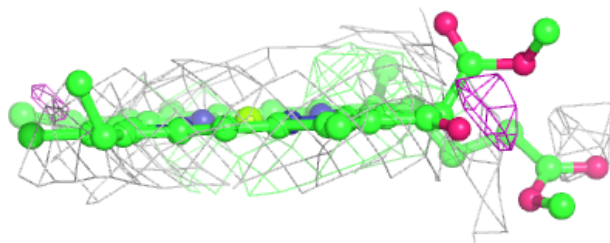
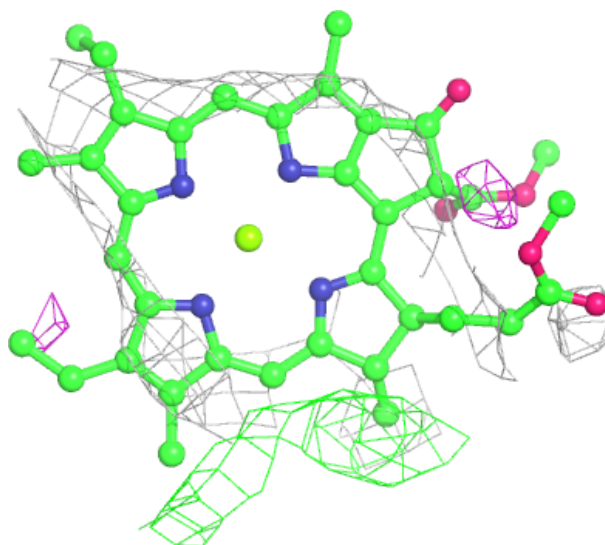
Electron density around LMG 1 5001:

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



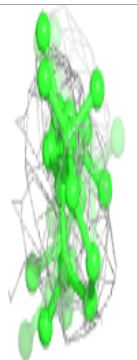
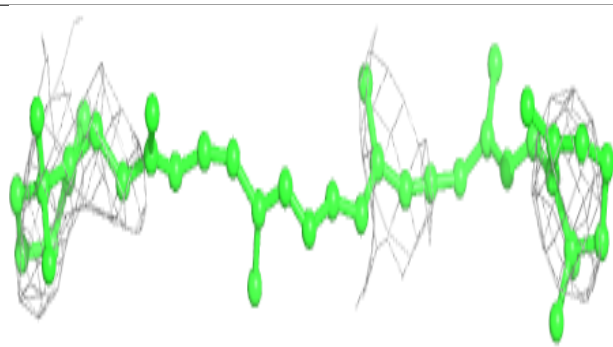
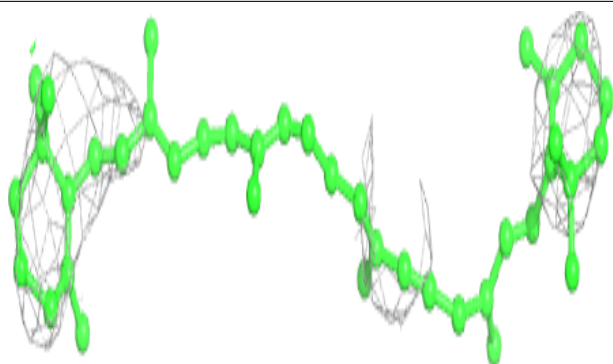
Electron density around CLA K 1404:

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

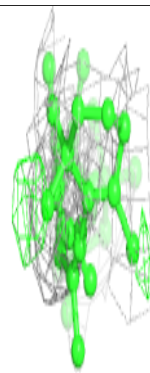
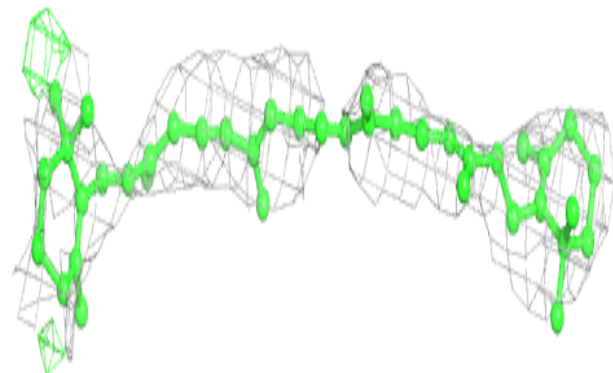
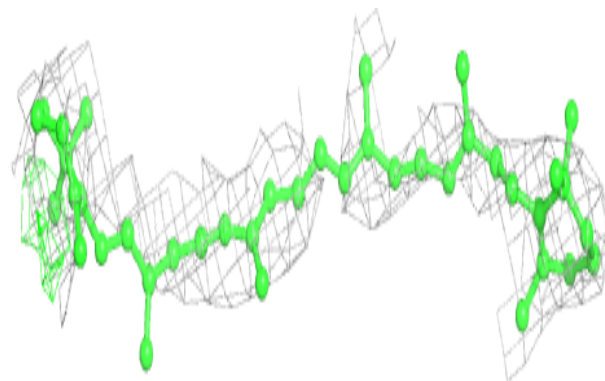


Electron density around BCR K 1405:

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

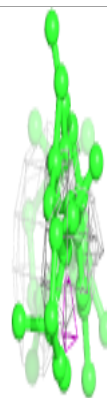
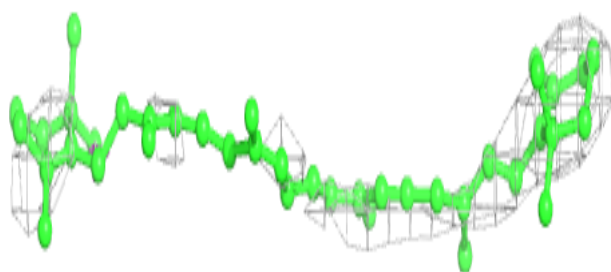
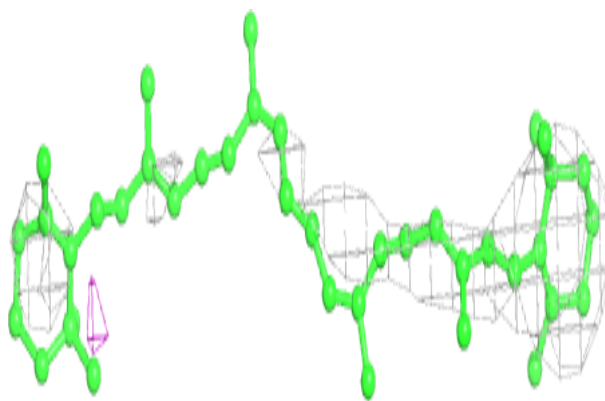
**Electron density around BCR L 302:**

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



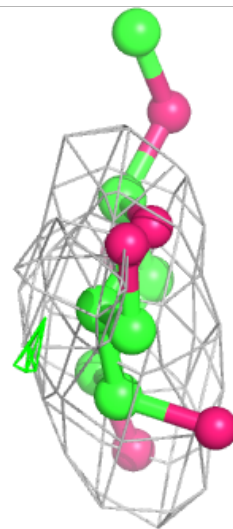
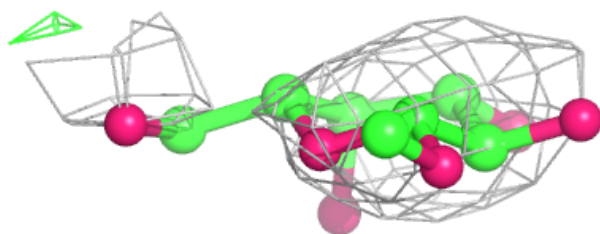
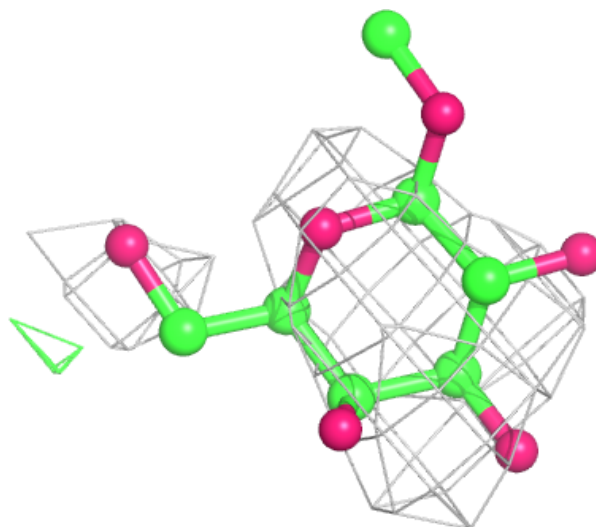
Electron density around BCR 3 306:

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



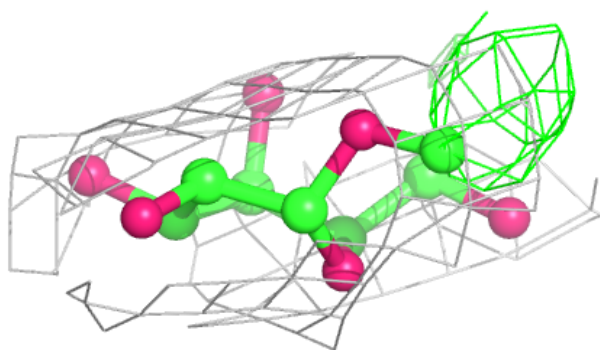
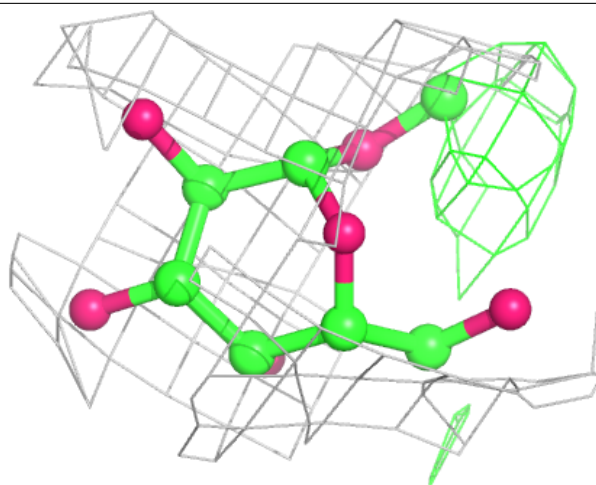
Electron density around LMG 4 320:

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



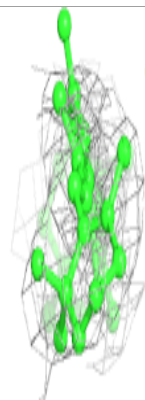
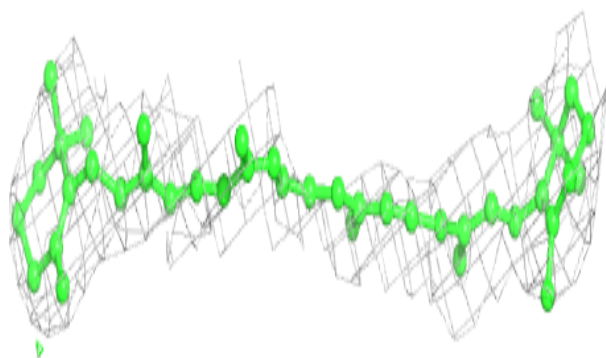
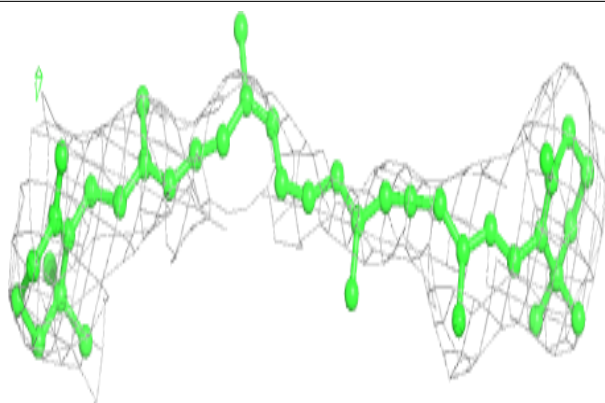
Electron density around LMG 2 323:

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

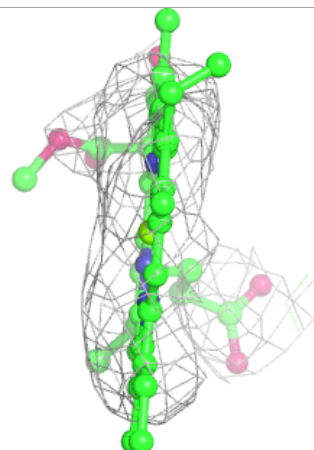
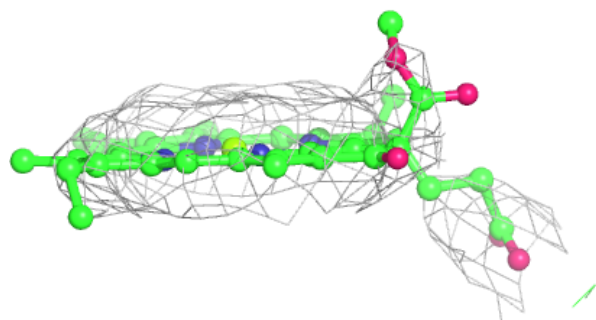
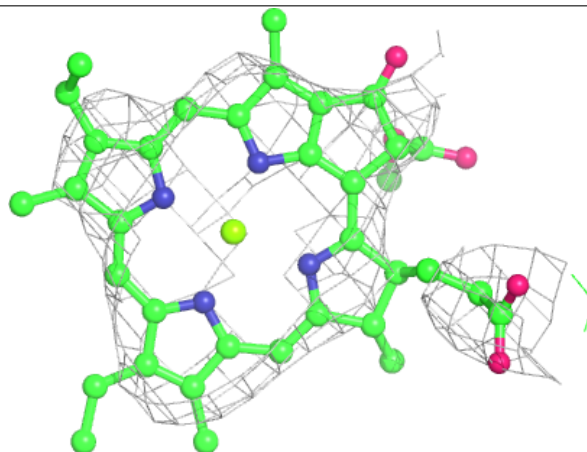


Electron density around BCR G 1604:

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

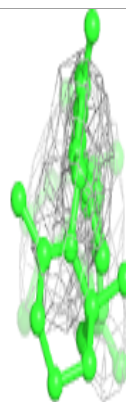
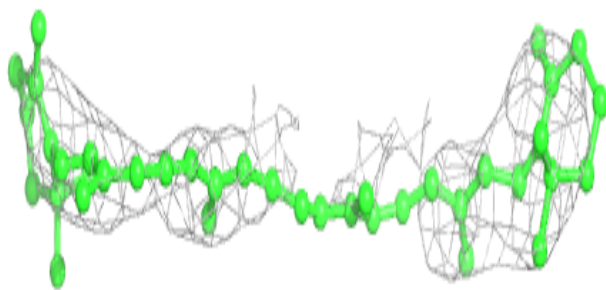
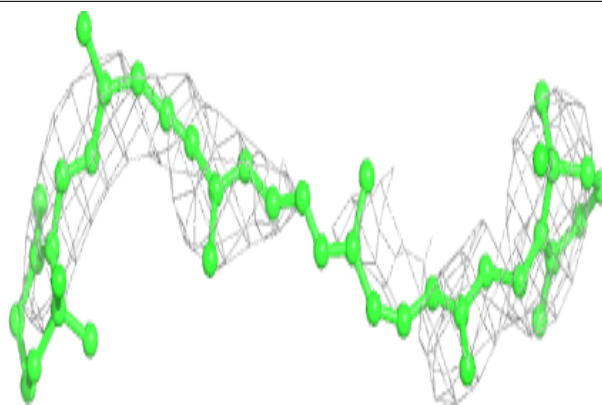
**Electron density around CLA K 1401:**

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

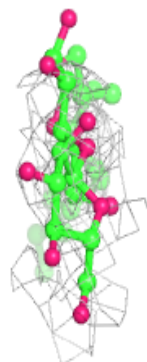
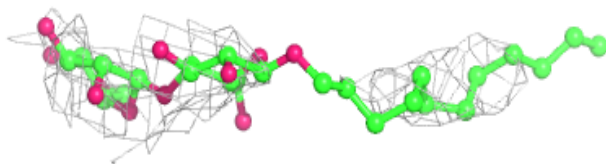
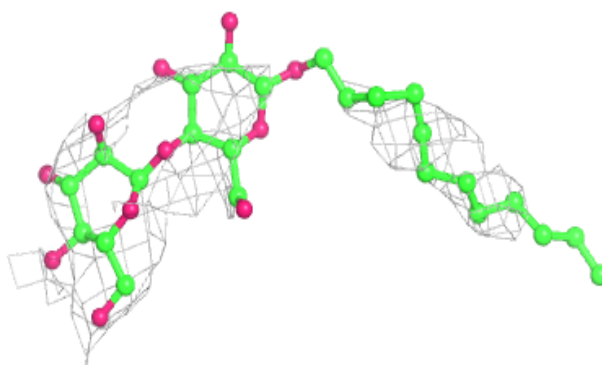


Electron density around BCR B 845:

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

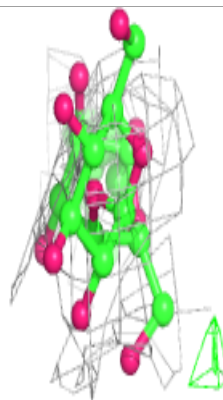
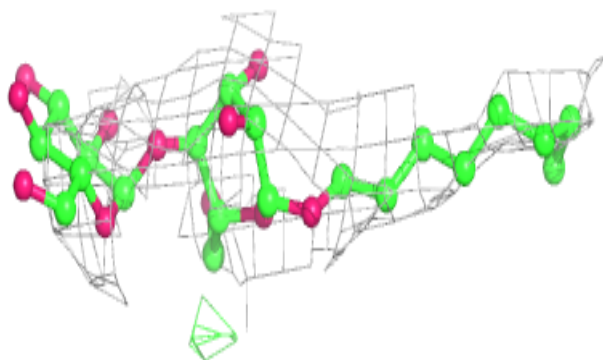
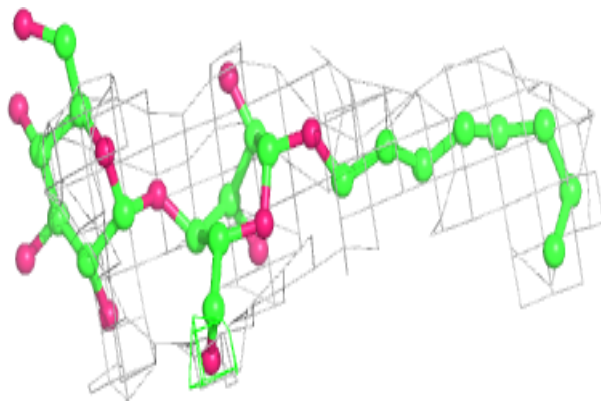
**Electron density around LMT B 852:**

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



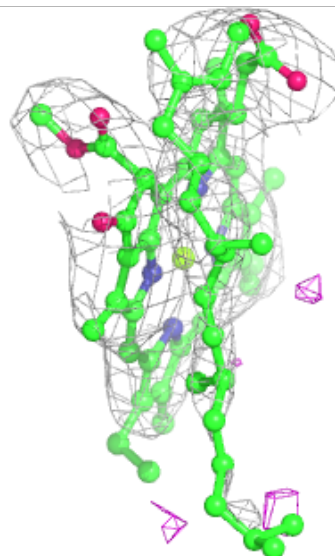
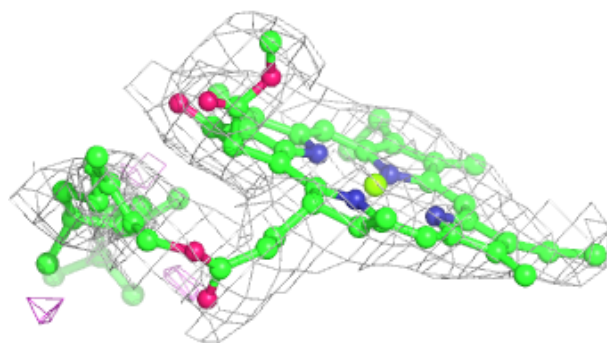
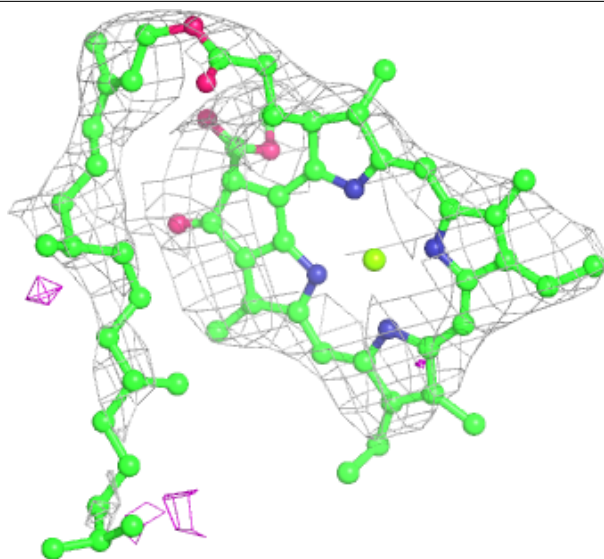
Electron density around LMT G 1606:

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



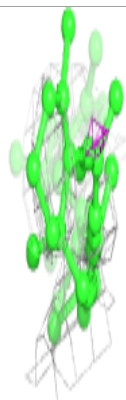
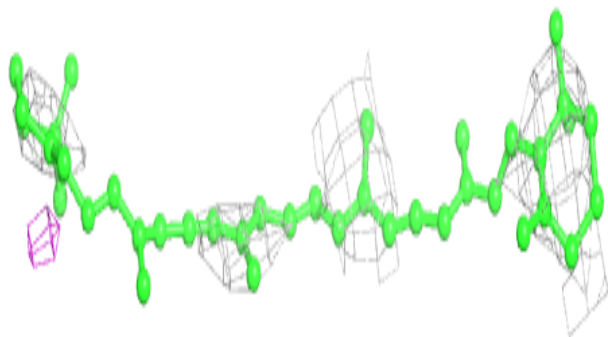
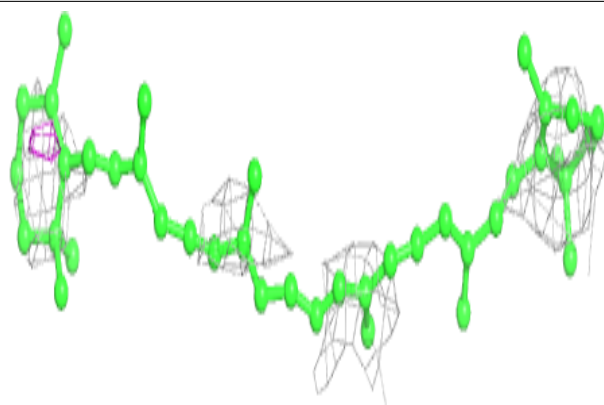
Electron density around CLA A 823:

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

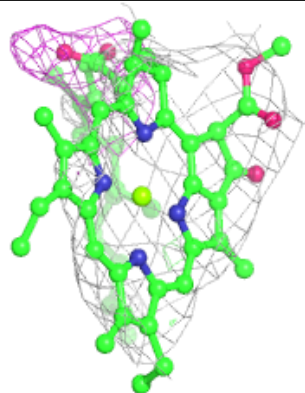
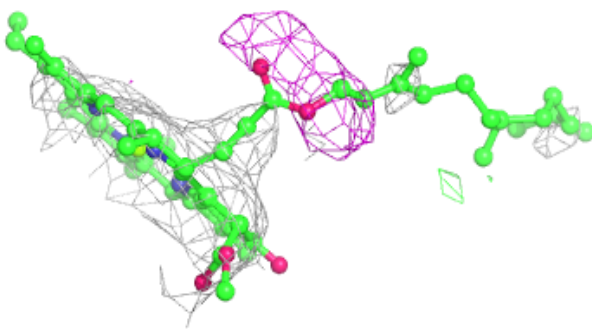
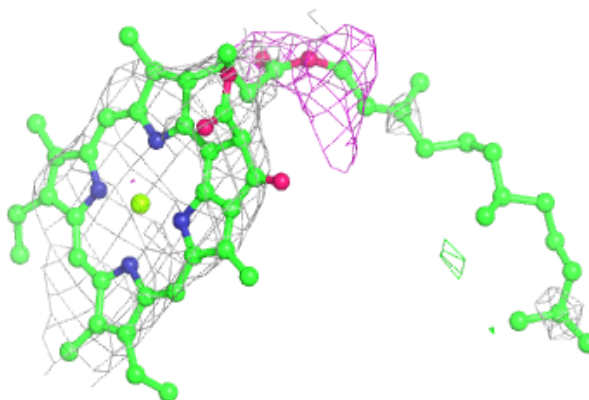


Electron density around BCR A 855:

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

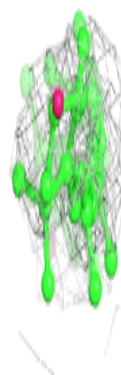
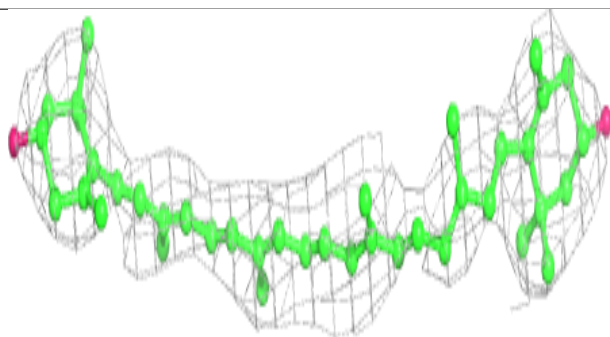
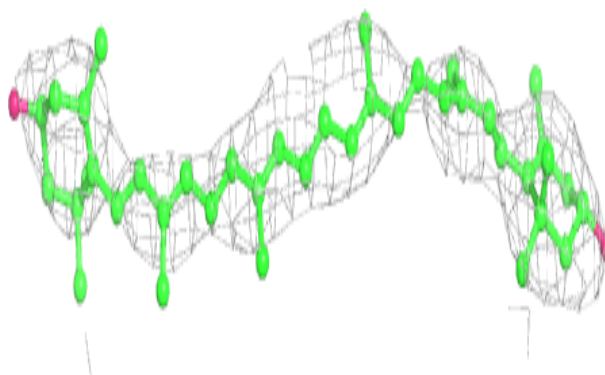
**Electron density around CLA K 1402:**

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

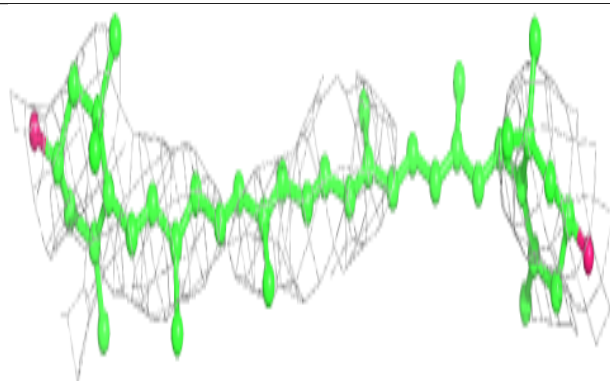
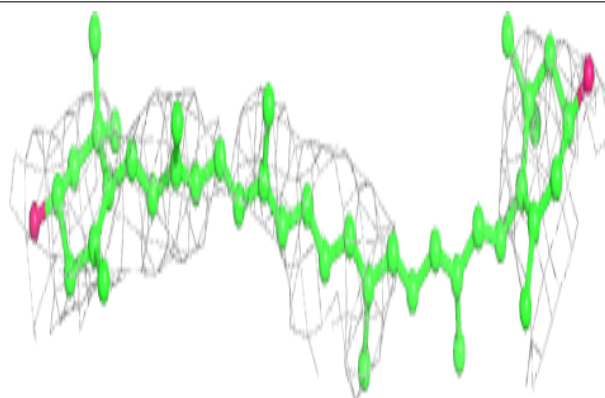


Electron density around LUT J 1105:

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

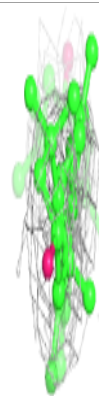
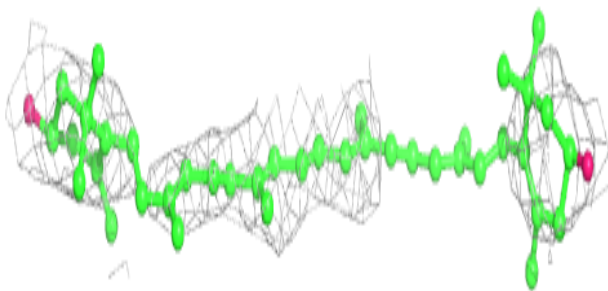
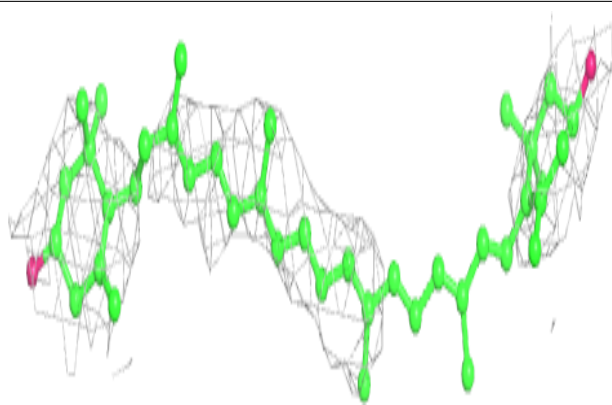
**Electron density around LUT 3 303:**

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

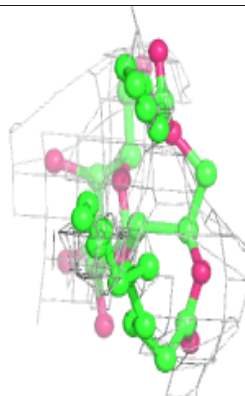
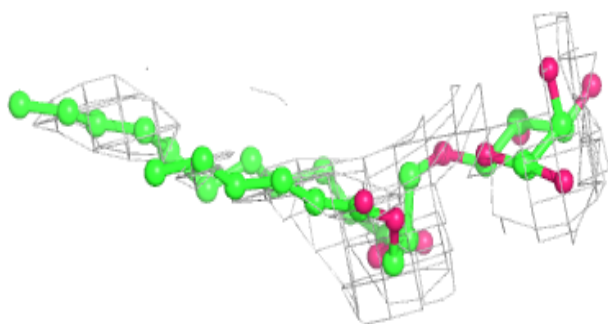
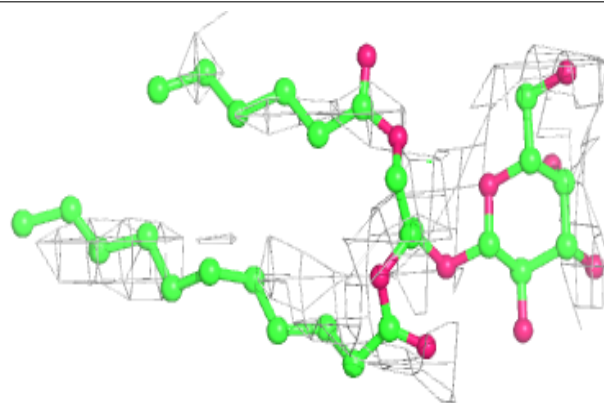


Electron density around LUT 3 304:

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

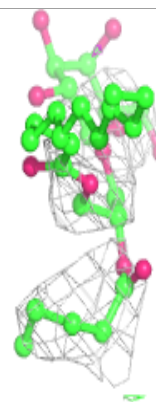
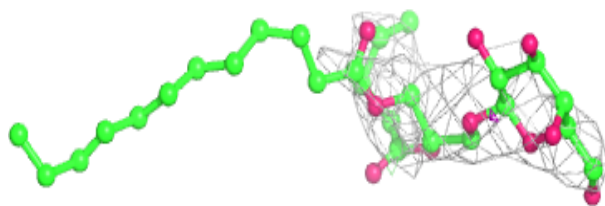
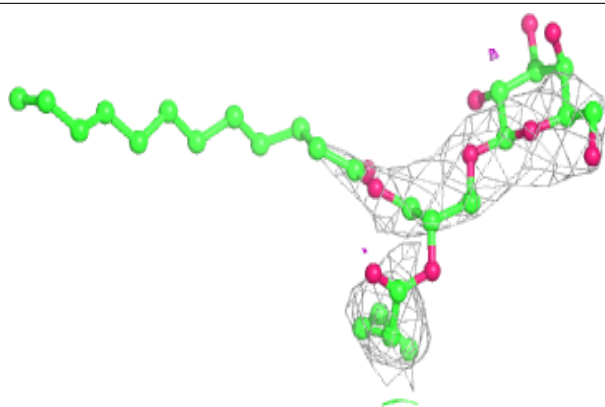
**Electron density around LMG 2 322:**

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

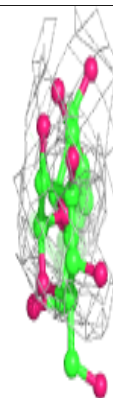
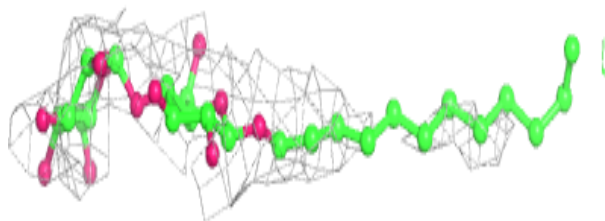
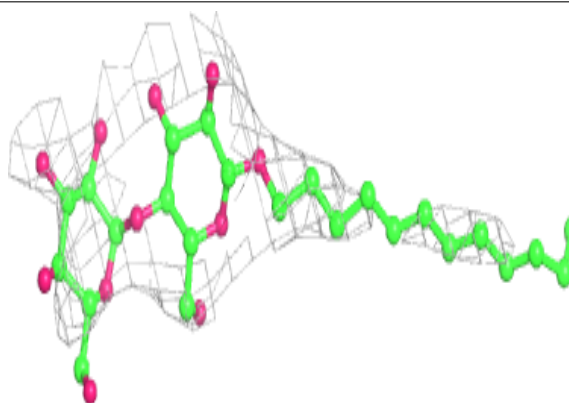


Electron density around LMG F 307:

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

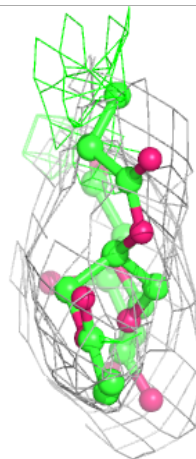
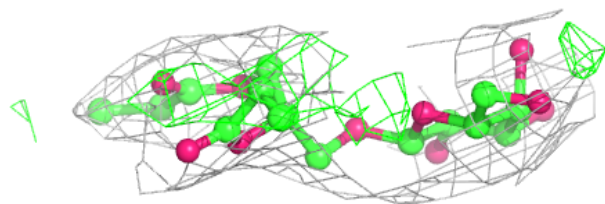
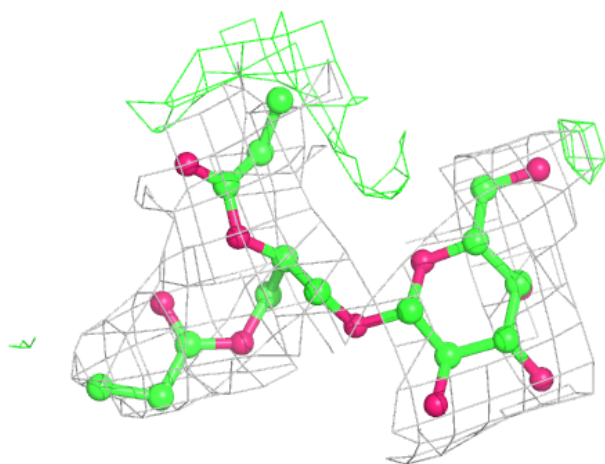
**Electron density around LMT 4 319:**

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



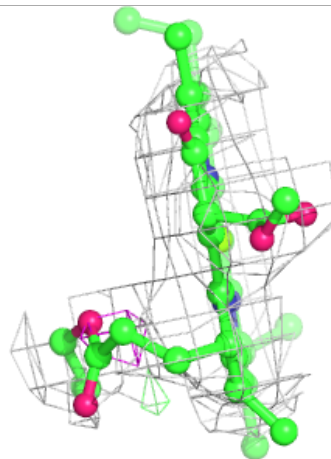
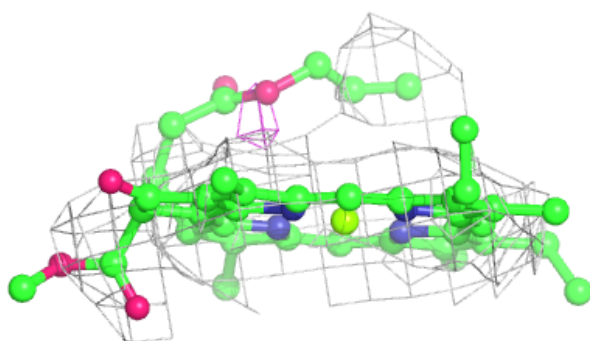
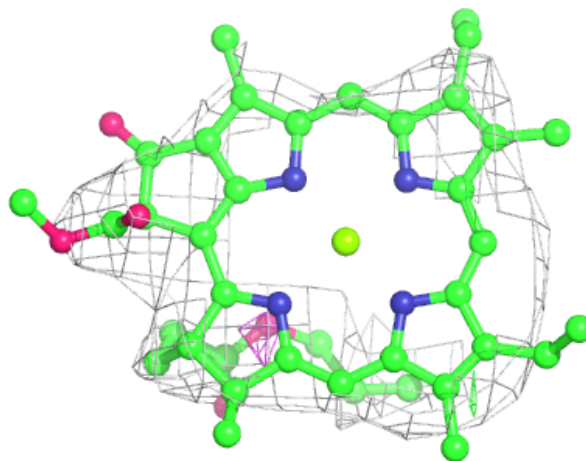
Electron density around LMG 2 321:

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



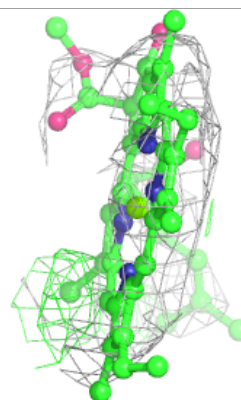
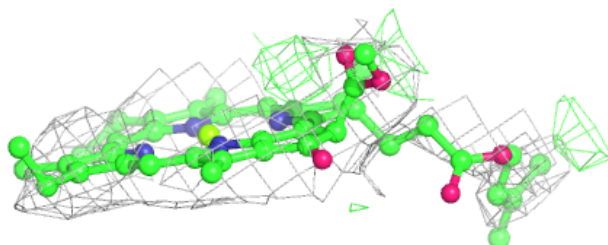
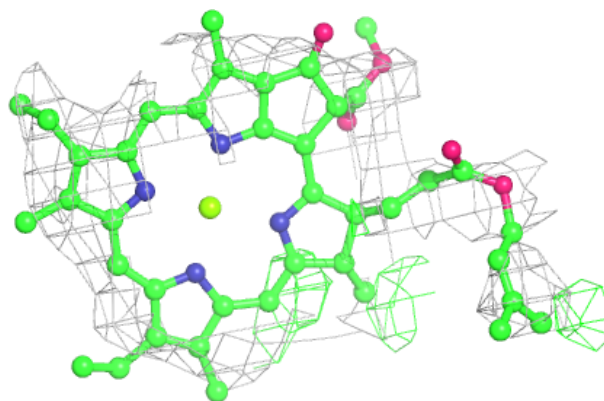
Electron density around CLA 3 314:

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

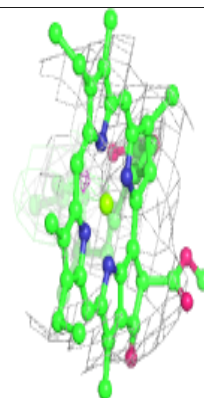
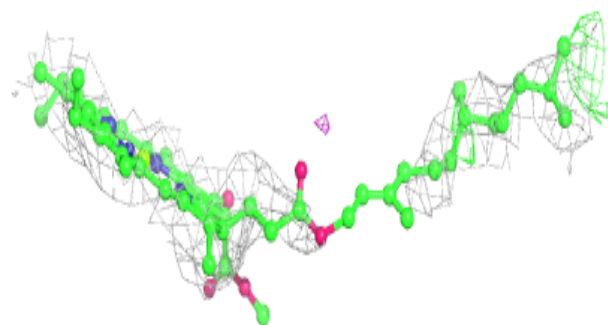
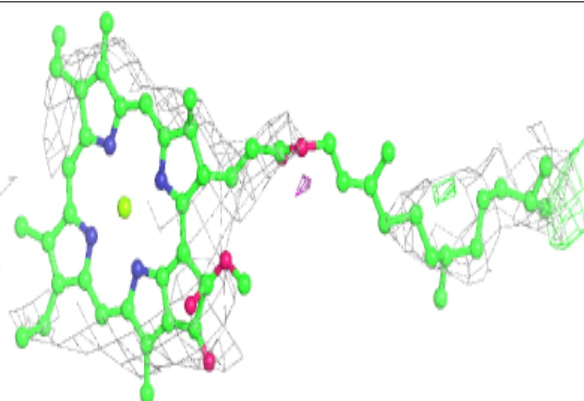


Electron density around CLA J 1103:

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

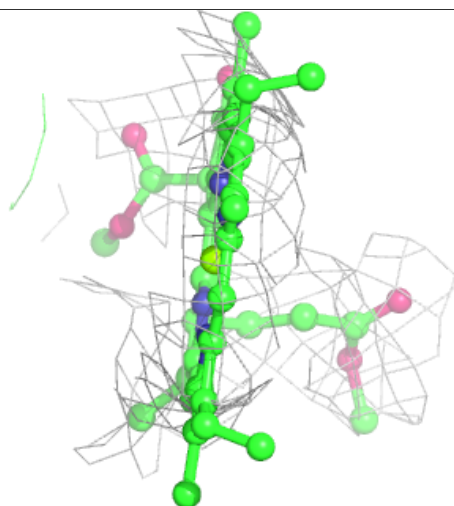
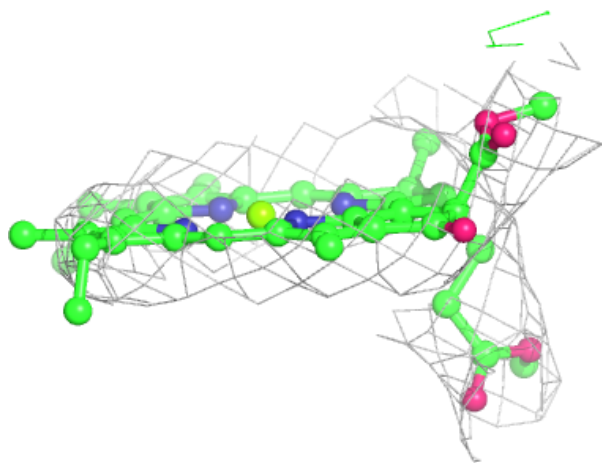
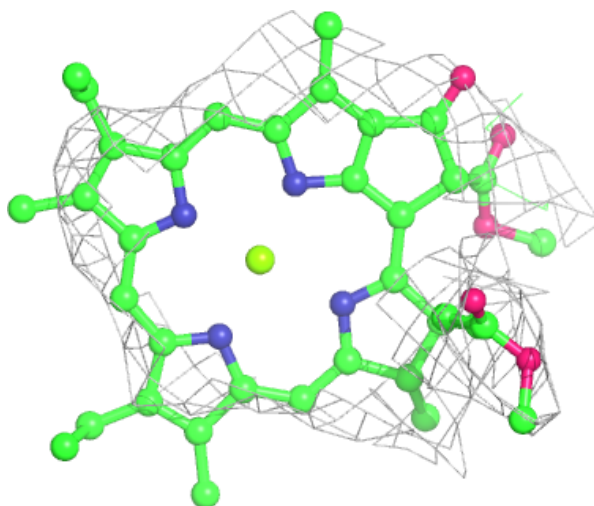
**Electron density around CLA H 1701:**

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



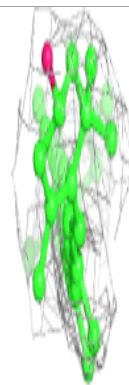
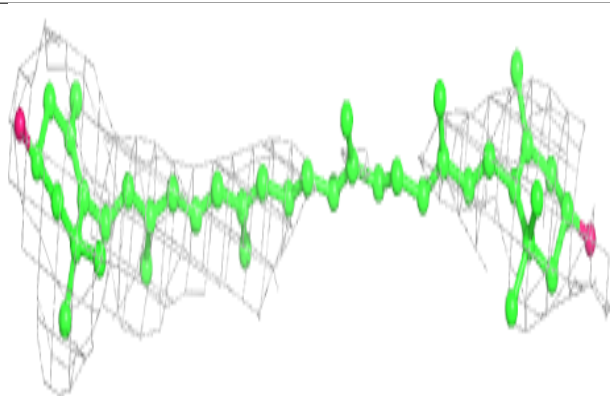
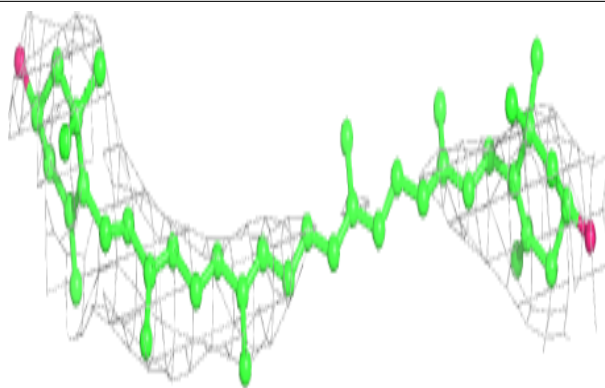
Electron density around CLA 1 5013:

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

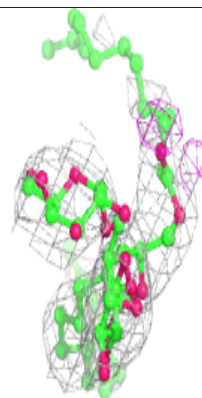
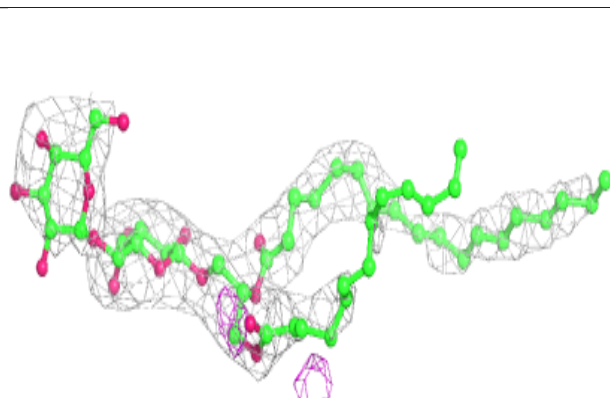
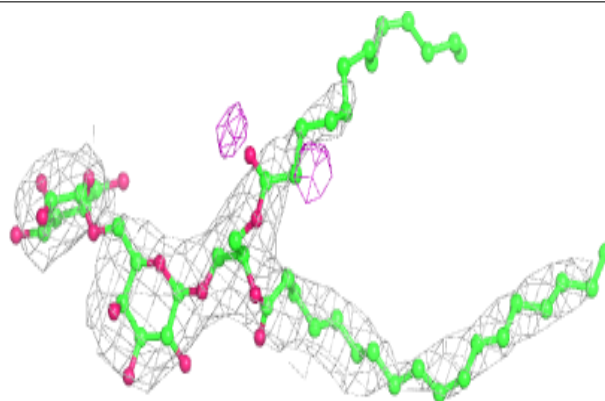


Electron density around LUT 4 303:

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

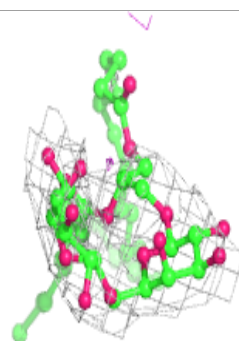
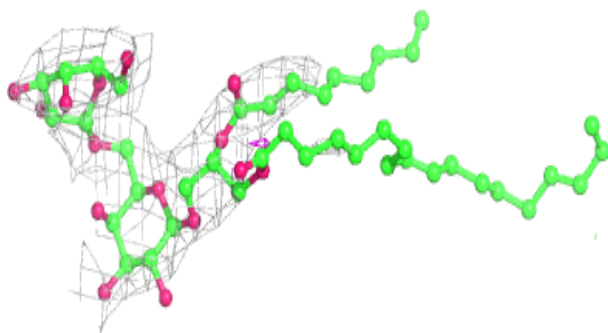
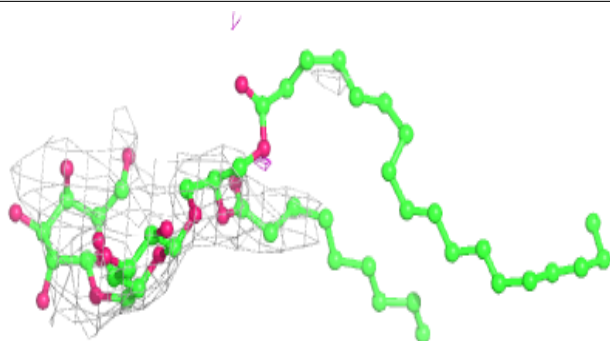
**Electron density around DGD B 855:**

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

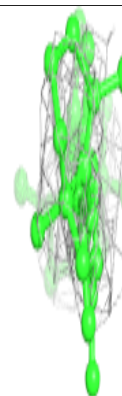
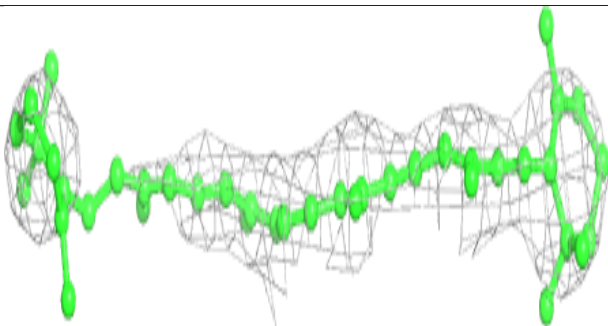
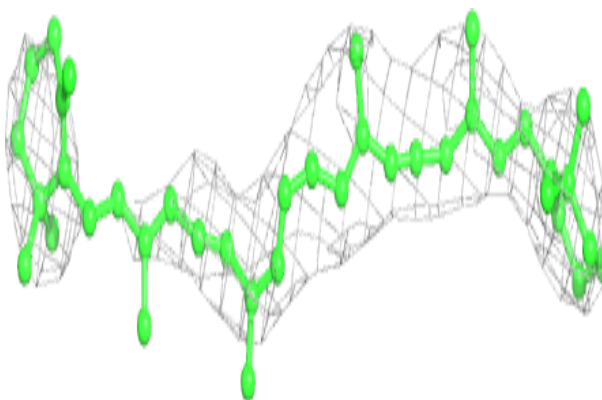


Electron density around DGD F 309:

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

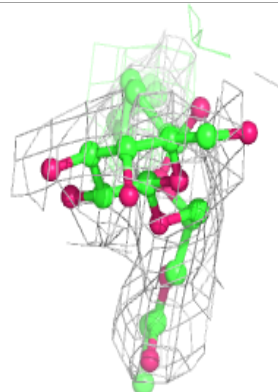
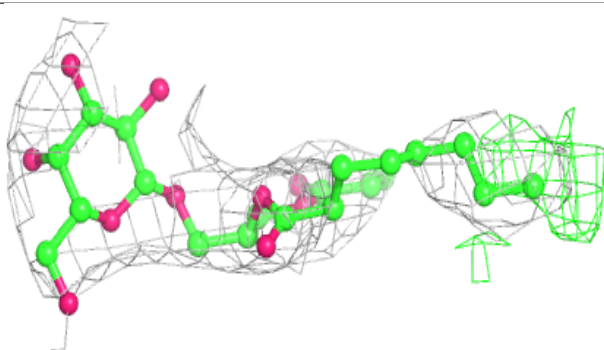
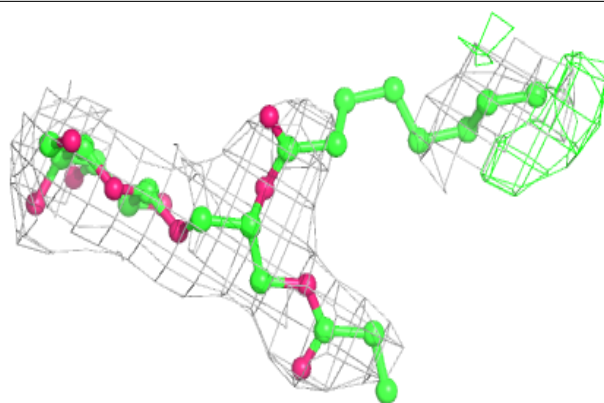
**Electron density around BCR A 845:**

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

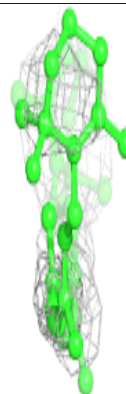
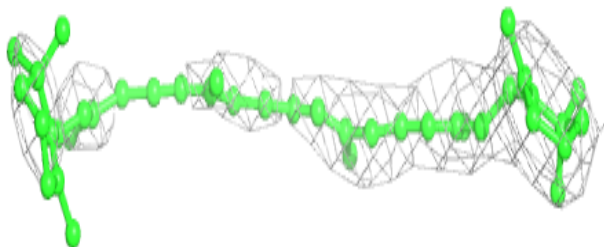
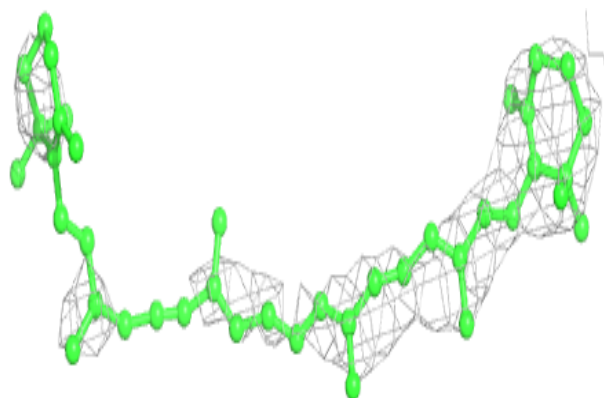


Electron density around LMG J 1102:

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

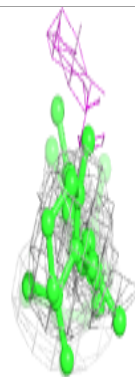
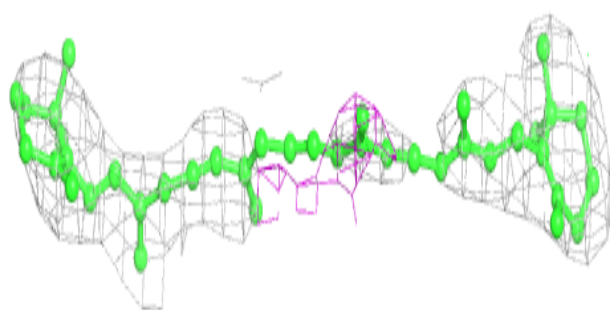
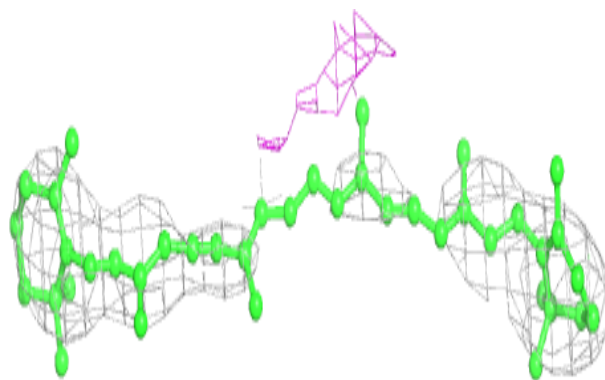
**Electron density around BCR B 844:**

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



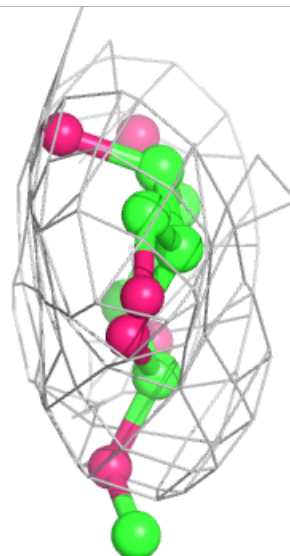
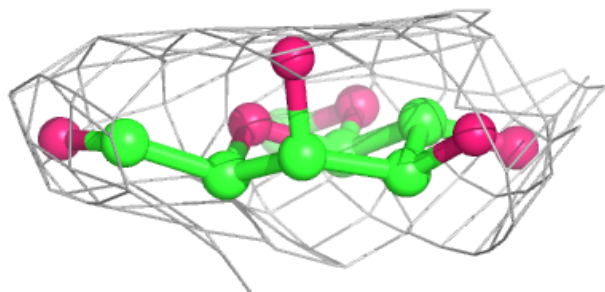
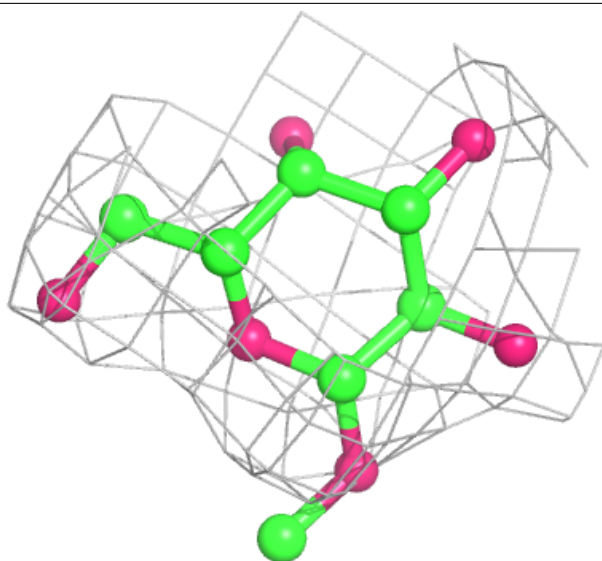
Electron density around BCR L 307:

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



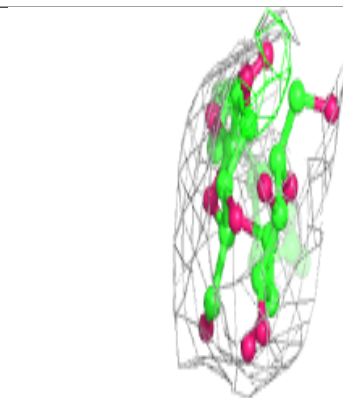
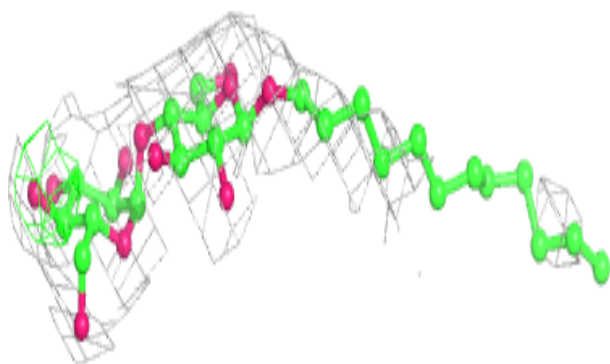
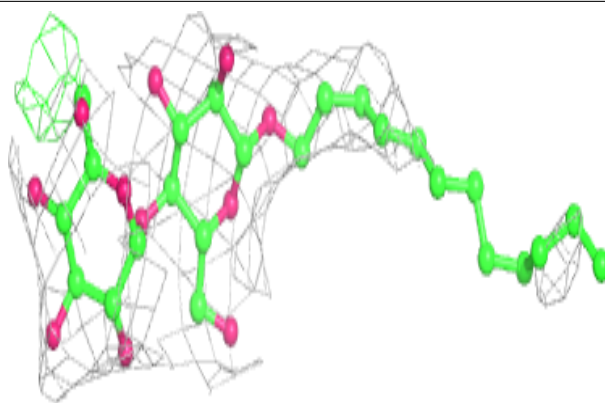
Electron density around LMG B 854:

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

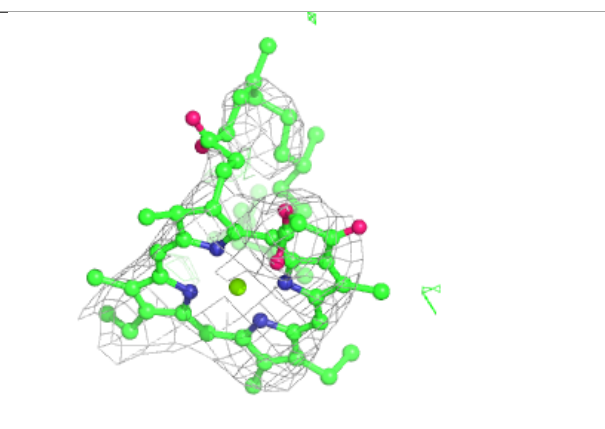
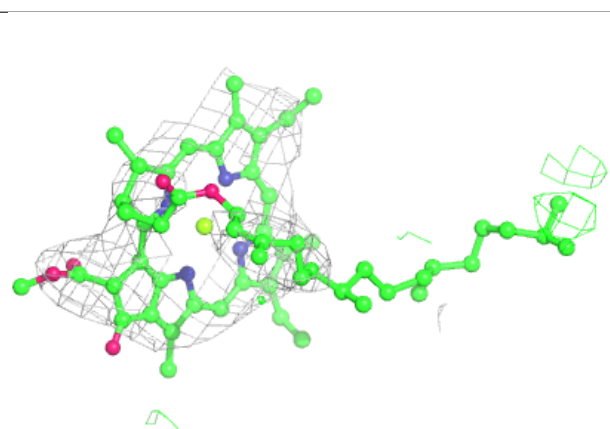
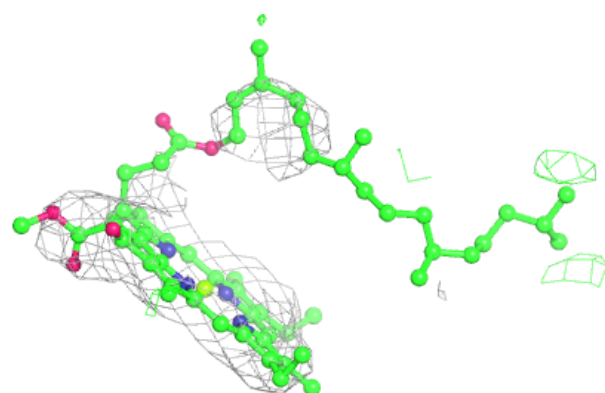


Electron density around LMT G 1605:

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

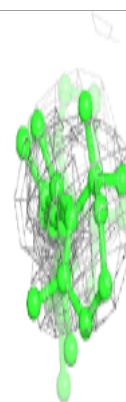
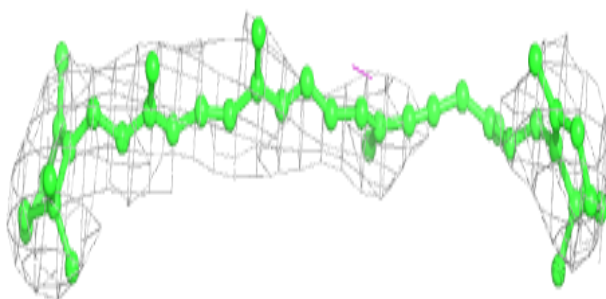
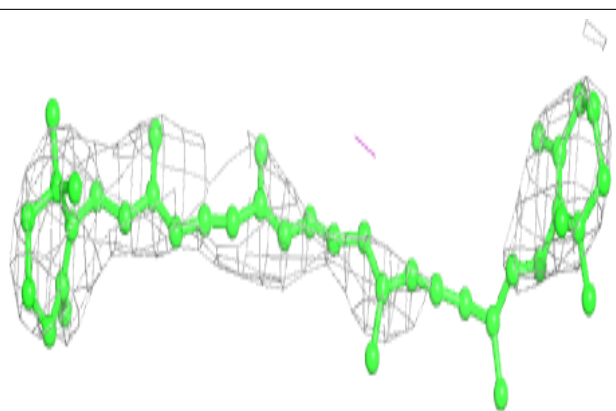
**Electron density around CLA G 1603:**

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

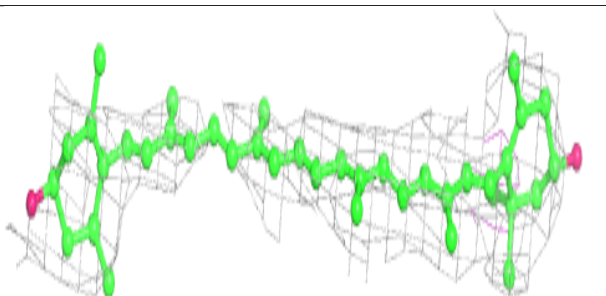
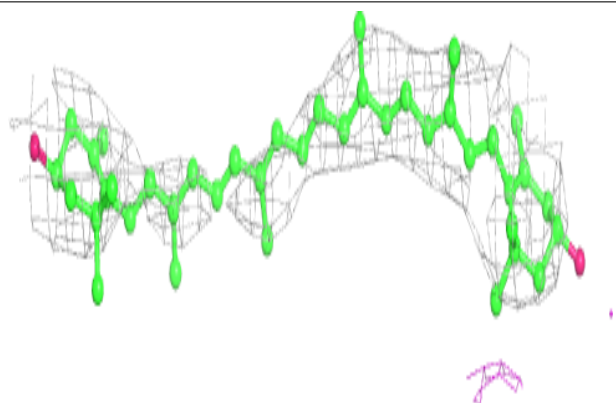


Electron density around BCR A 846:

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

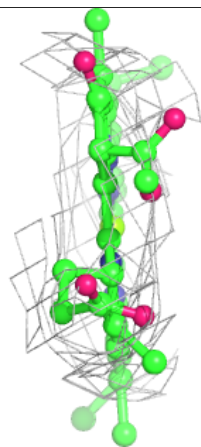
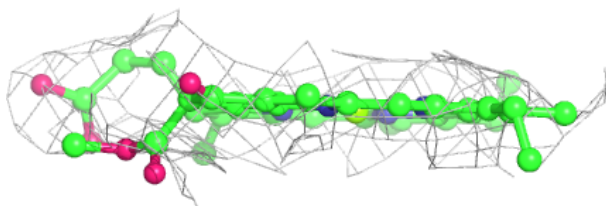
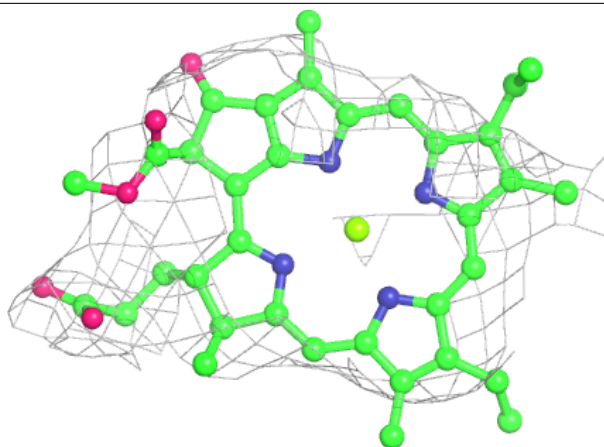
**Electron density around LUT 2 303:**

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



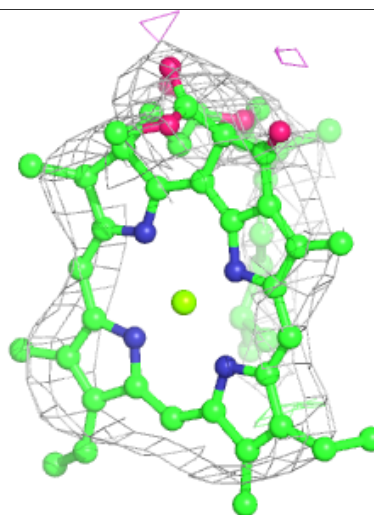
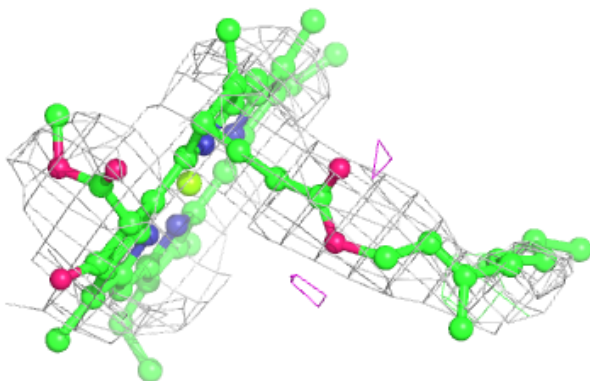
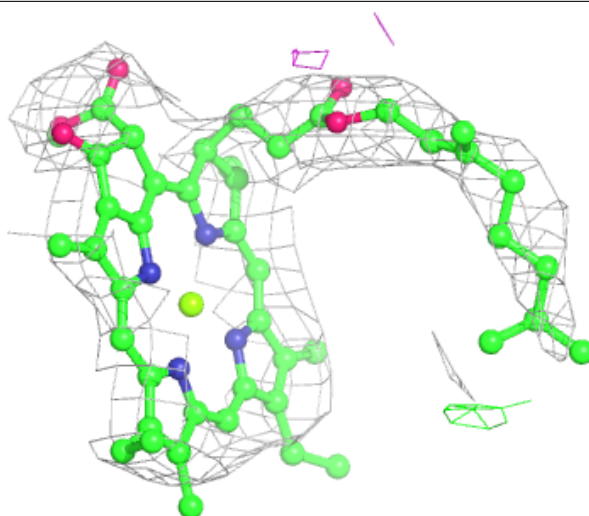
Electron density around CLA 1 5017:

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



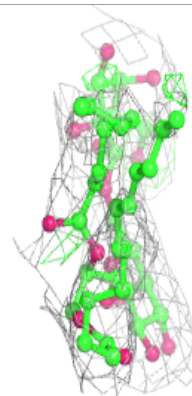
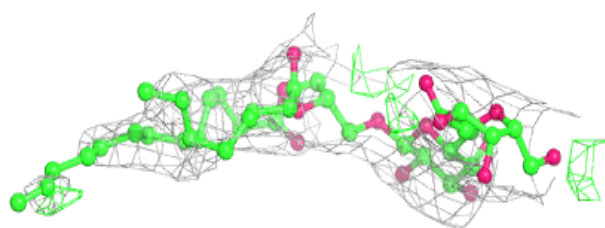
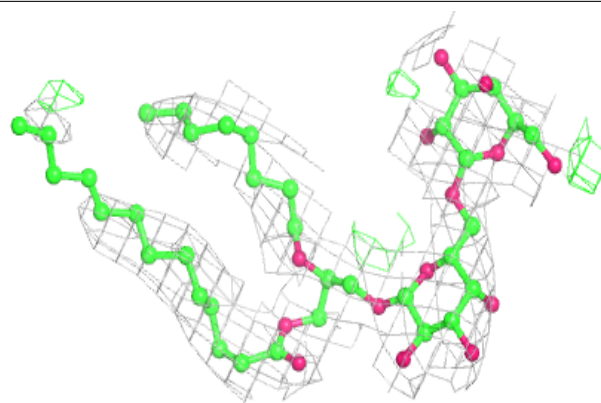
Electron density around CLA B 816:

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

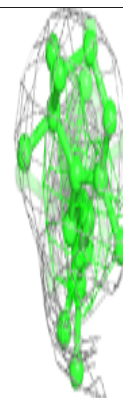
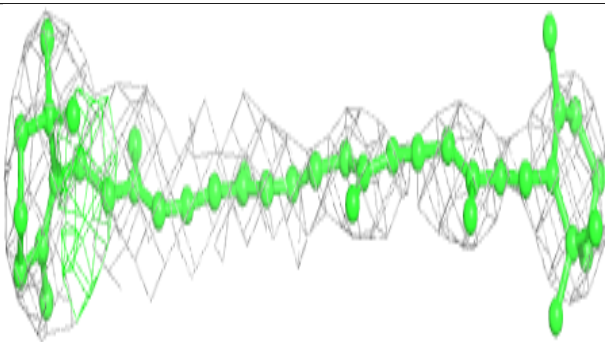
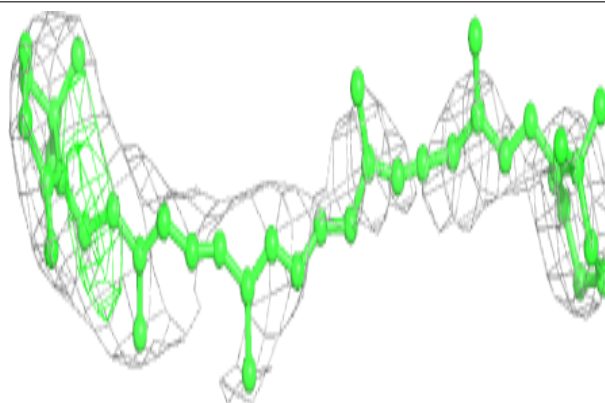


Electron density around DGD 2 327:

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

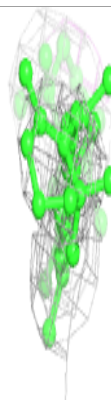
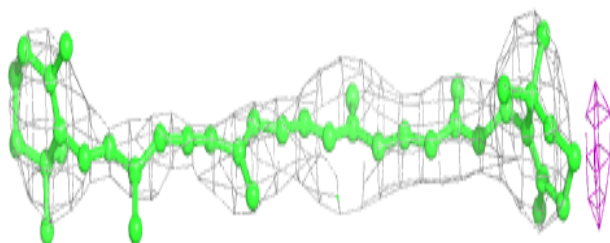
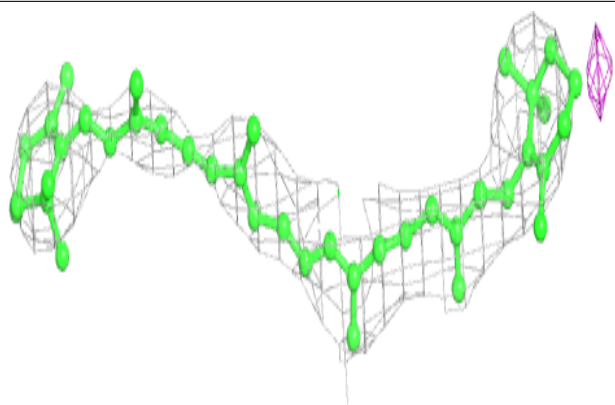
**Electron density around BCR B 846:**

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

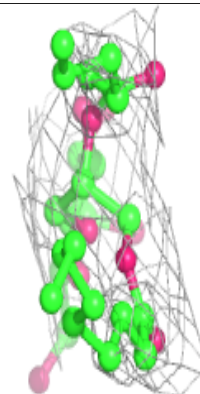
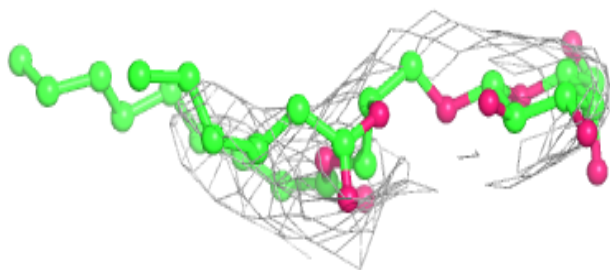
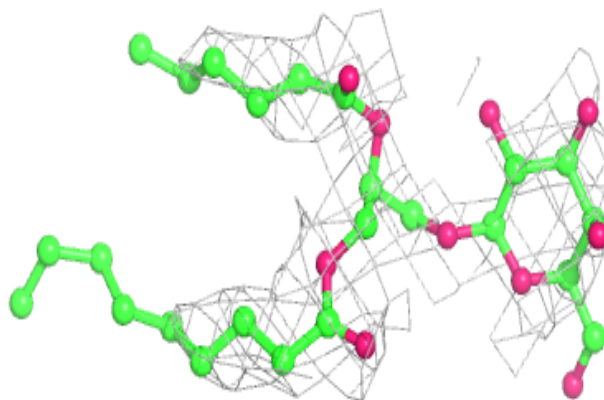


Electron density around BCR B 847:

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

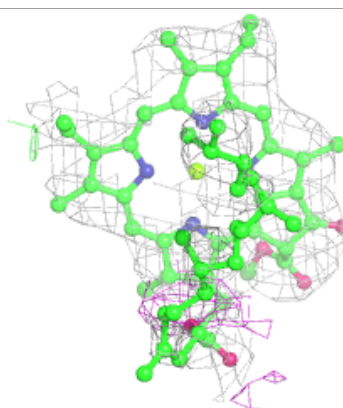
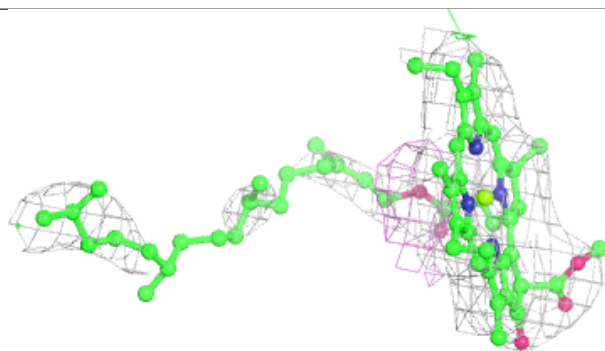
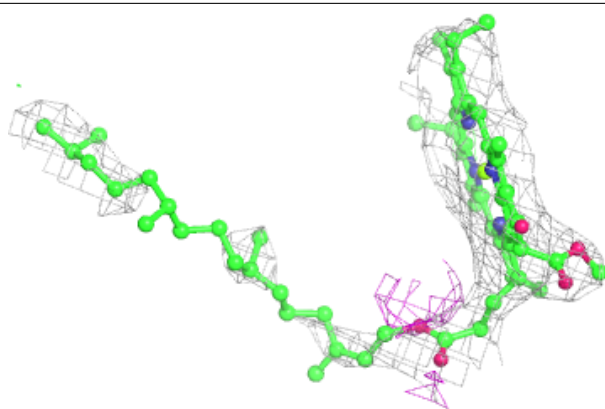
**Electron density around LMG F 308:**

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

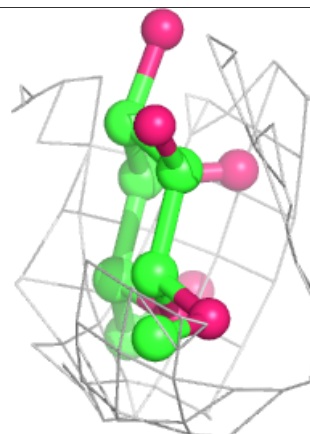
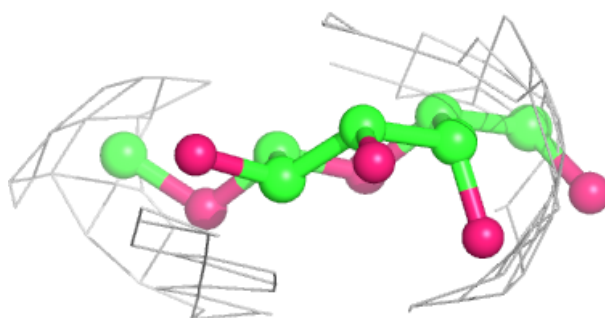
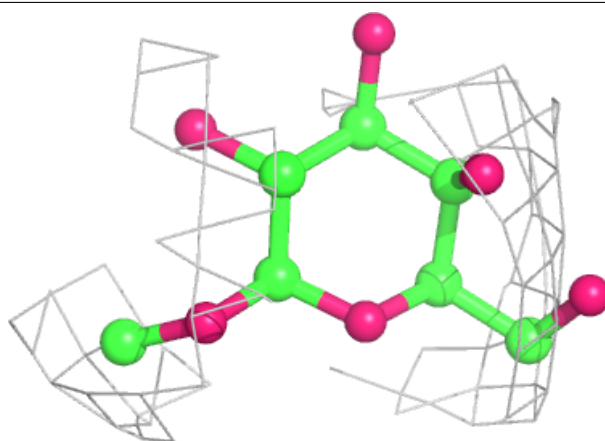


Electron density around CLA A 803:

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

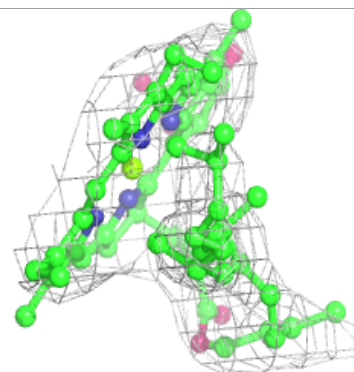
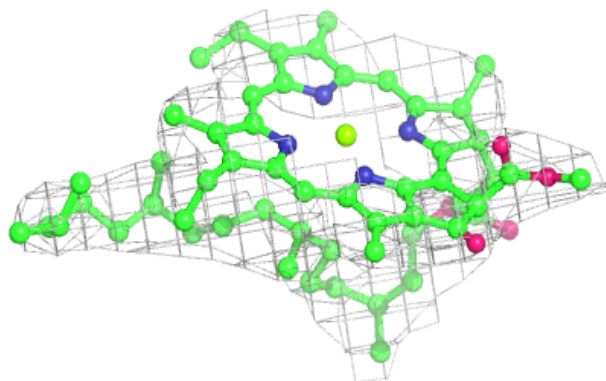
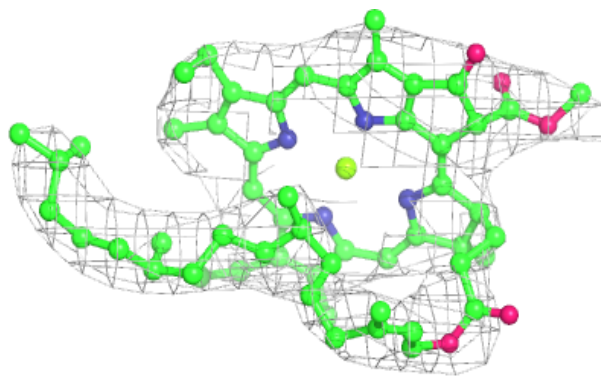
**Electron density around LMG 2 324:**

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

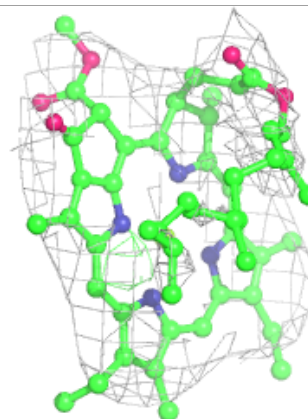
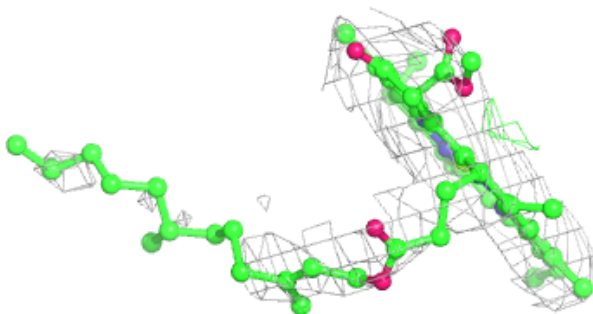
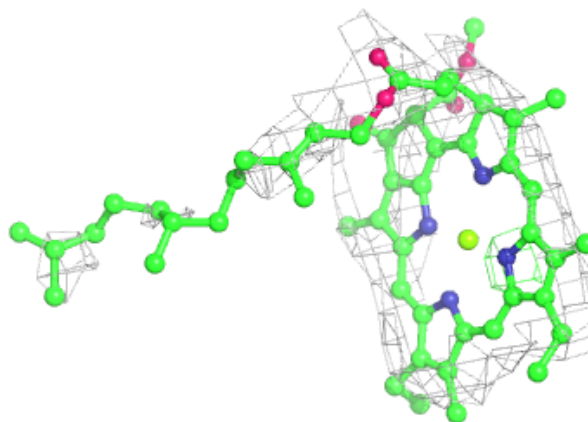


Electron density around CLA B 818:

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

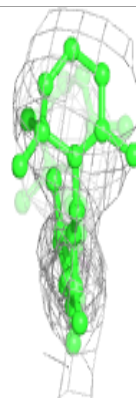
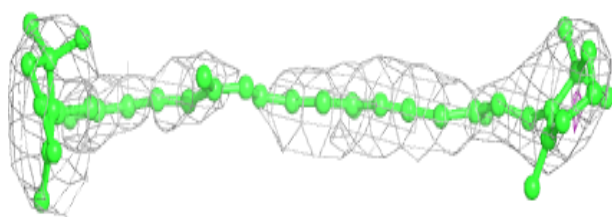
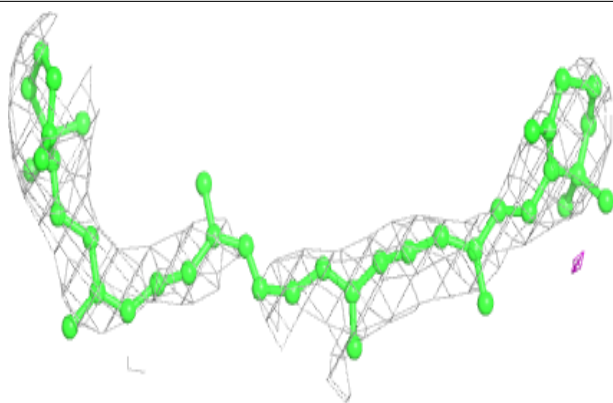
**Electron density around CLA 4 311:**

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

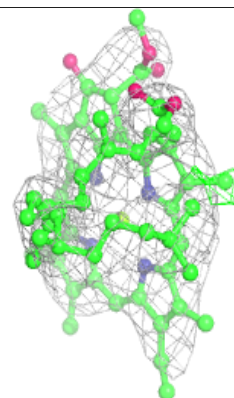
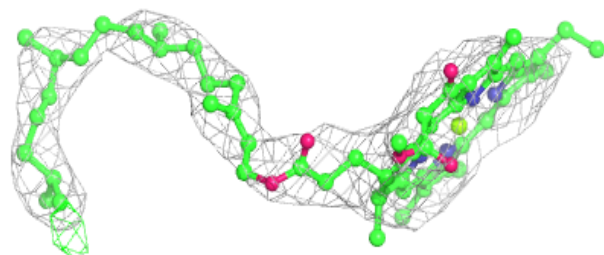
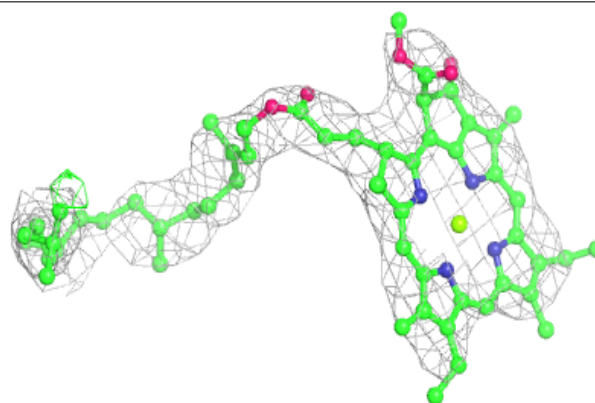


Electron density around BCR L 303:

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

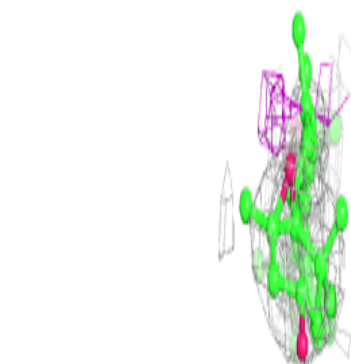
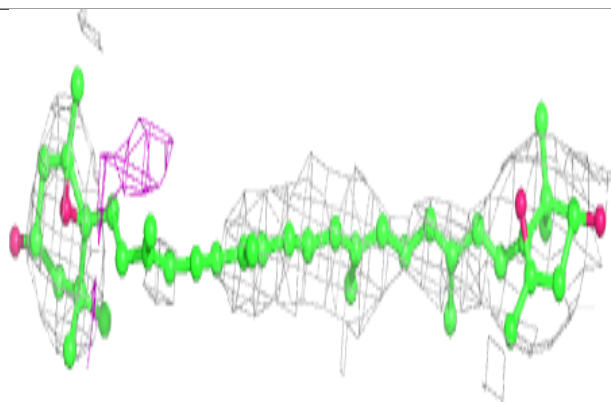
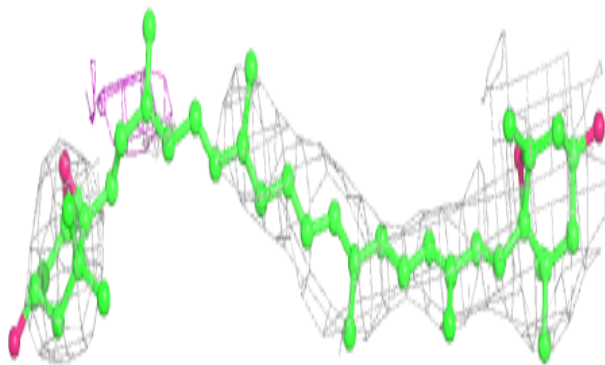
**Electron density around CLA B 810:**

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

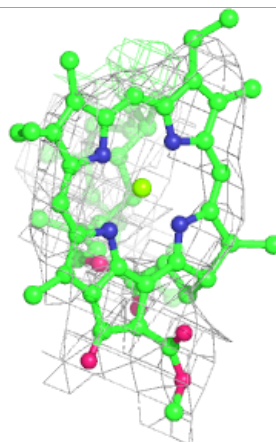
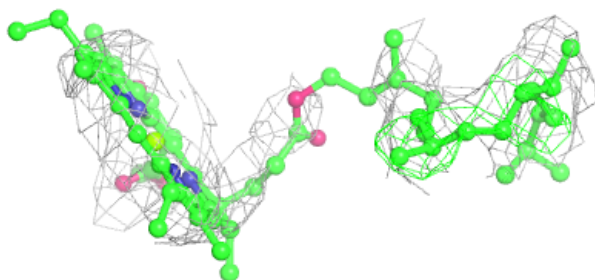
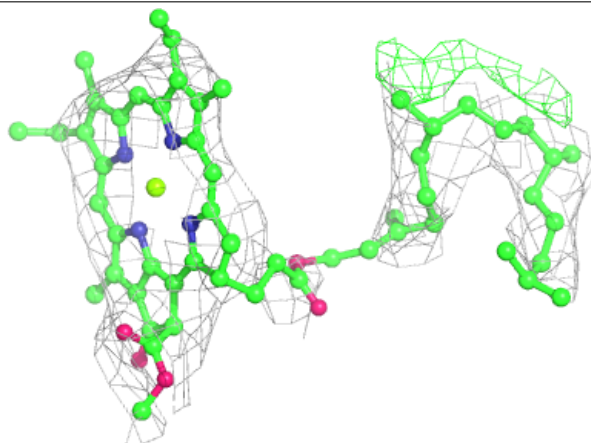


Electron density around XAT 2 304:

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

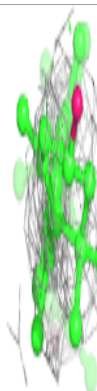
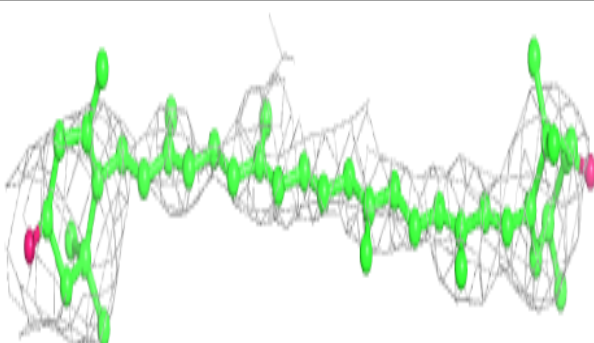
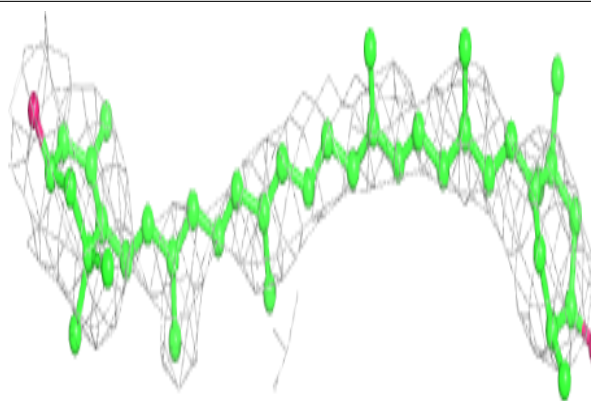
**Electron density around CLA 1 5015:**

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

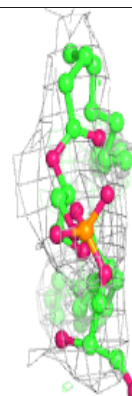
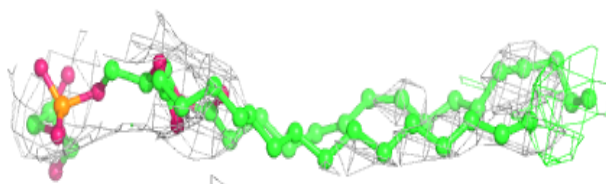


Electron density around ZEX F 310:

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

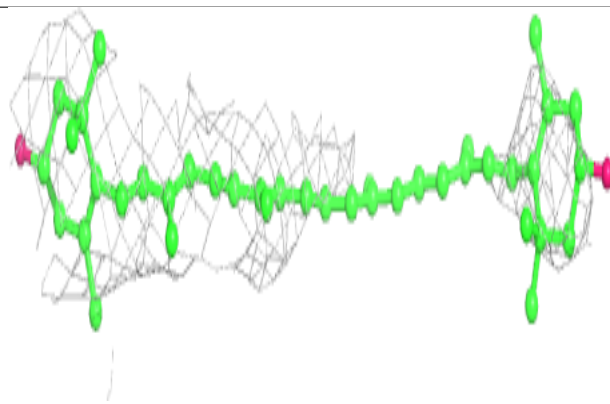
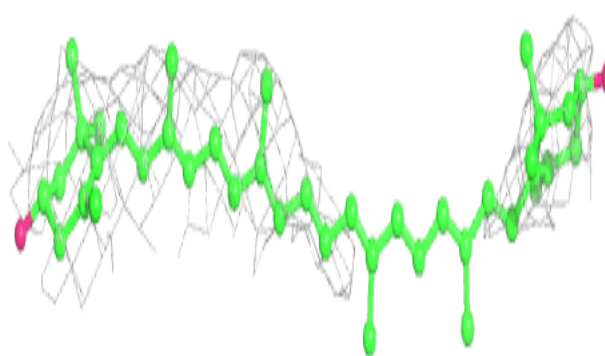
**Electron density around LHG 1 5019:**

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

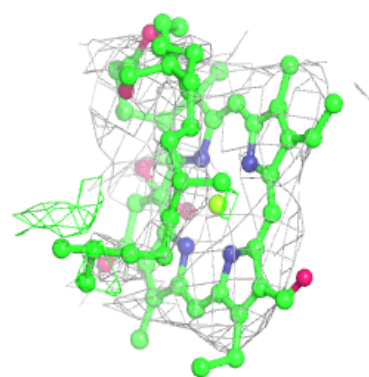
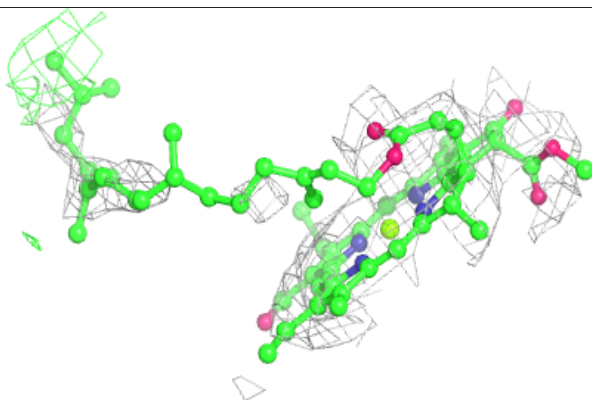
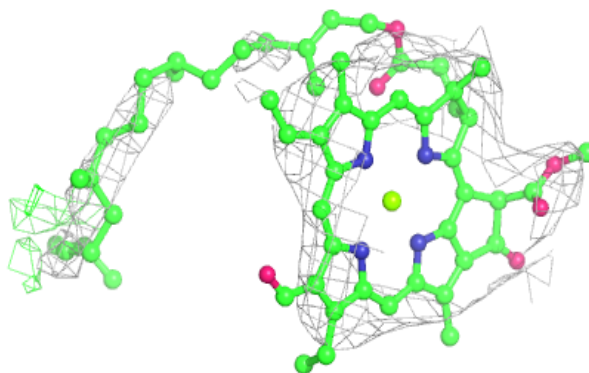


Electron density around LUT 1 5003:

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

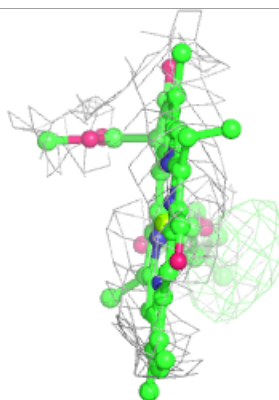
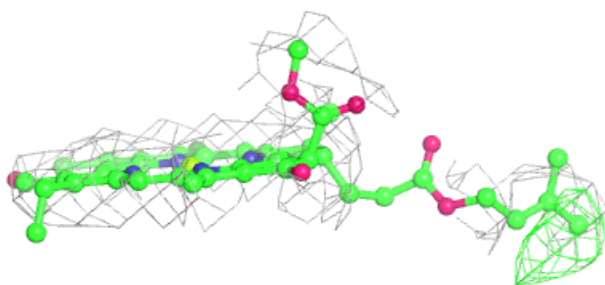
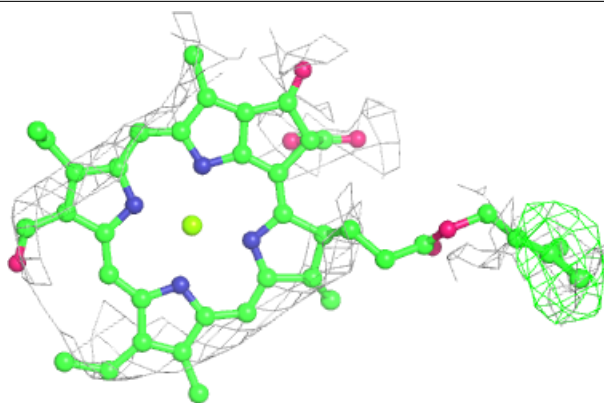
**Electron density around CHL 3 310:**

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

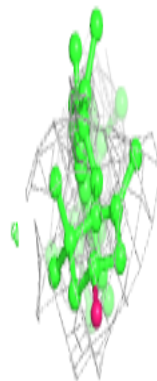
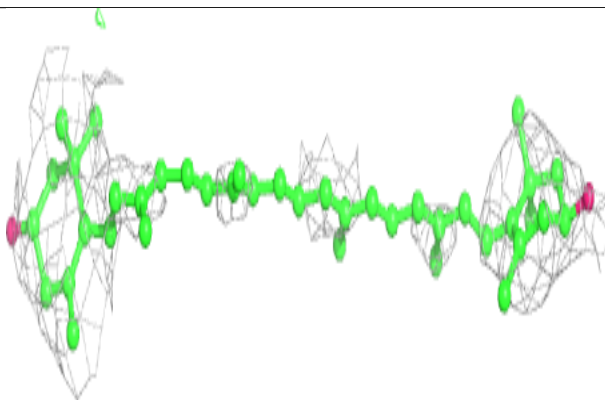
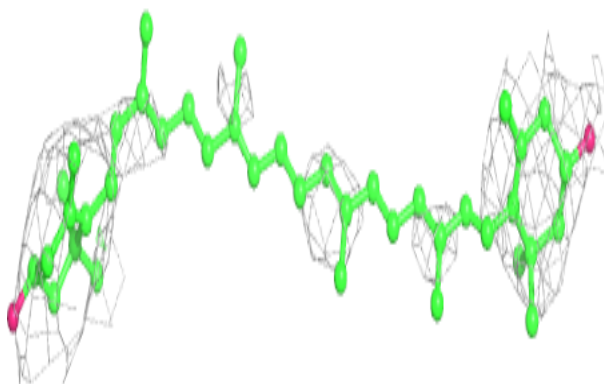


Electron density around CHL 3 313:

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

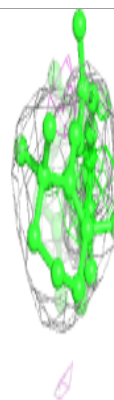
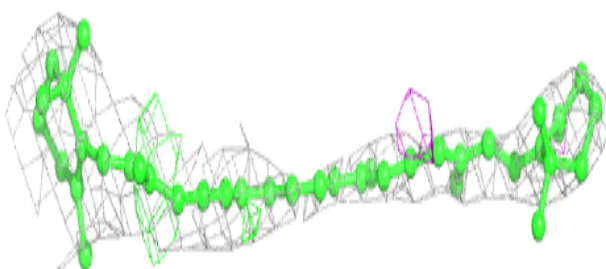
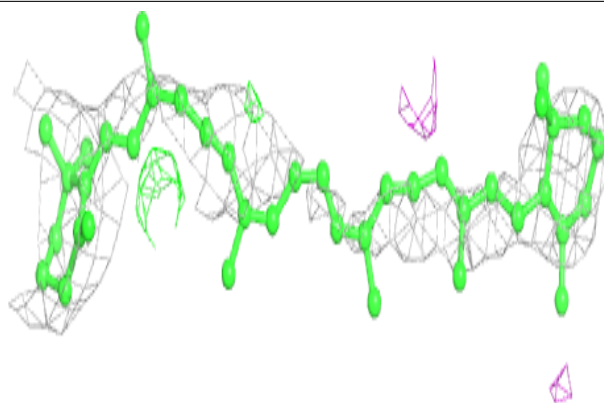
**Electron density around LUT 1 5004:**

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



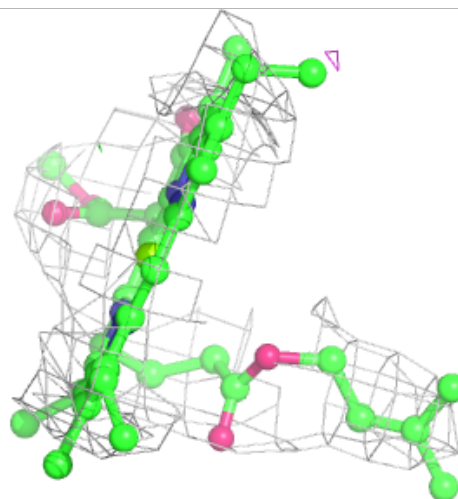
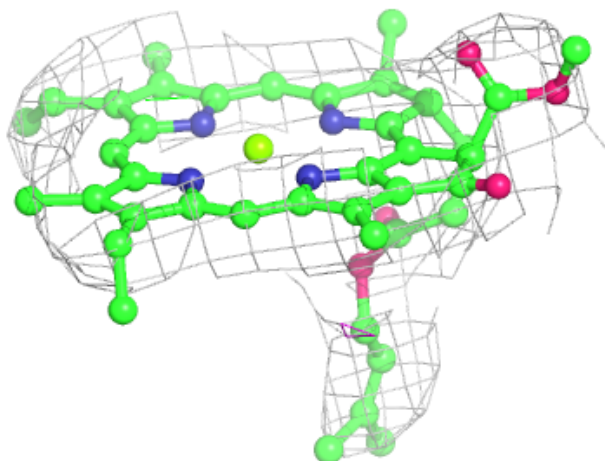
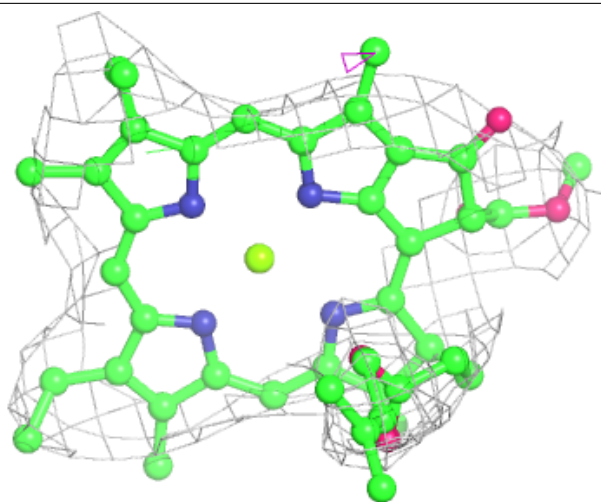
Electron density around BCR B 843:

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



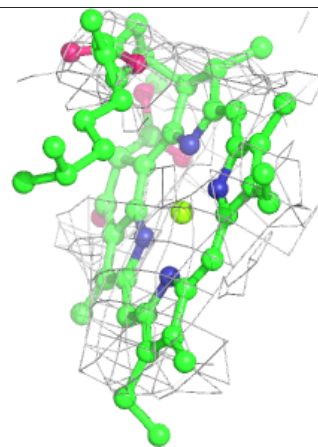
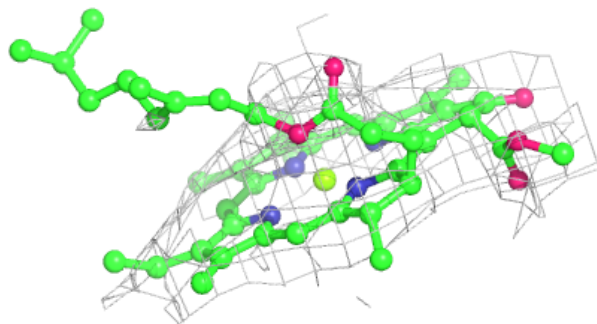
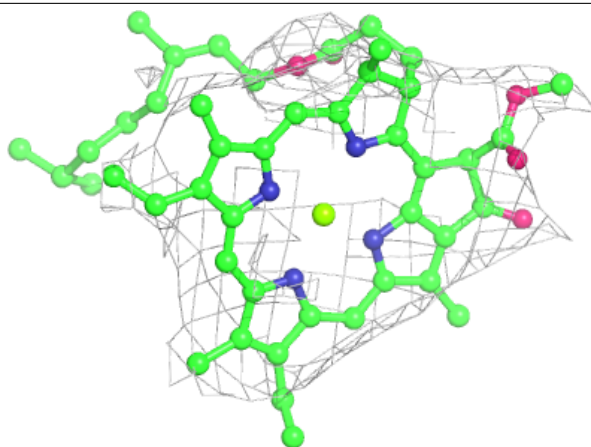
Electron density around CLA L 304:

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



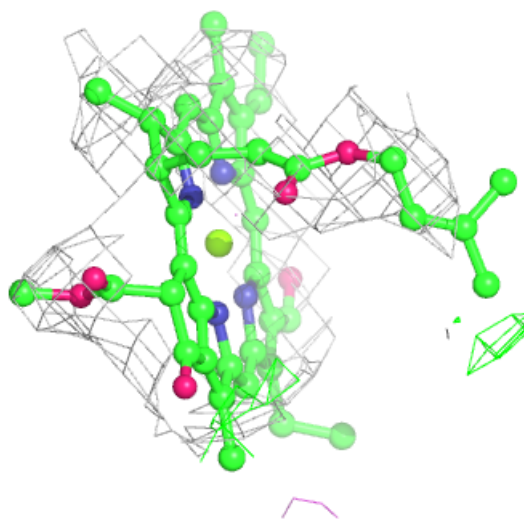
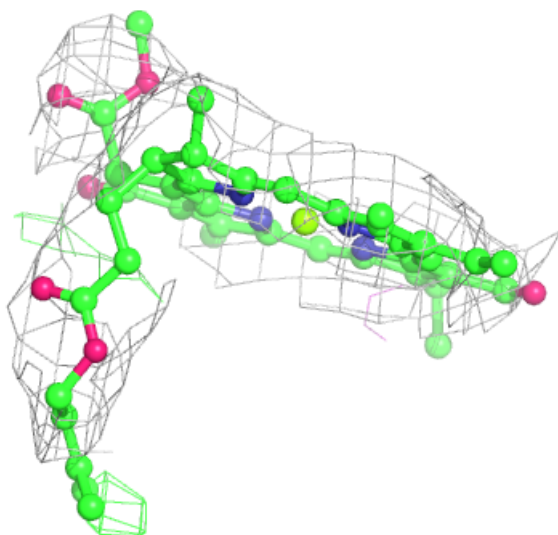
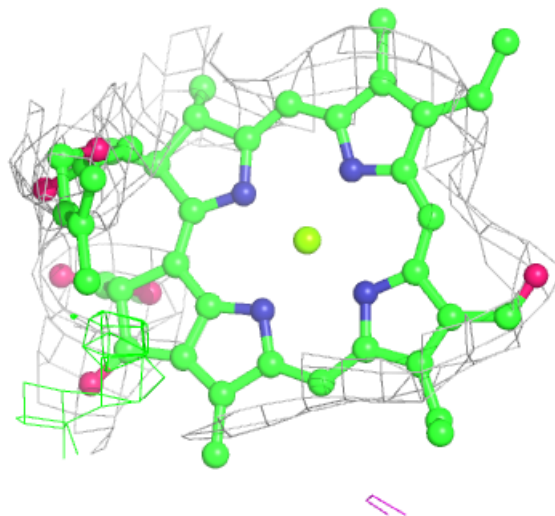
Electron density around CLA 3 307:

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



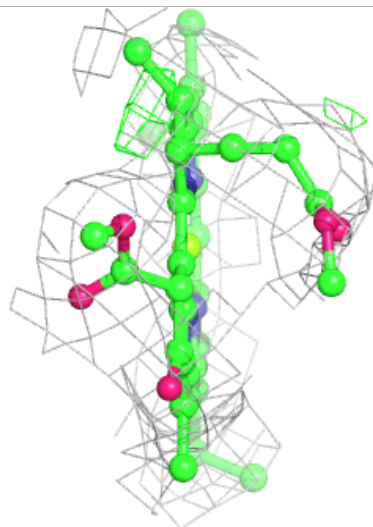
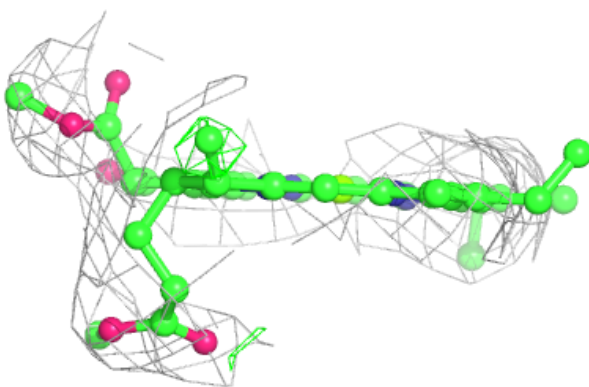
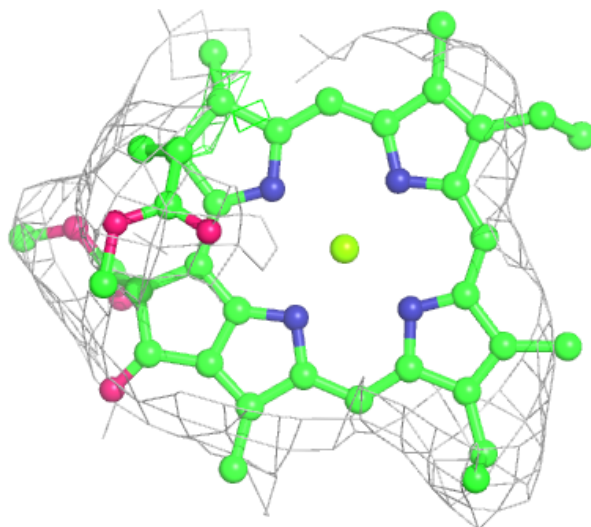
Electron density around CHL 3 312:

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



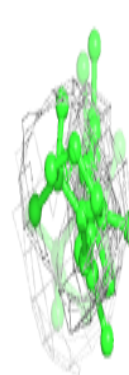
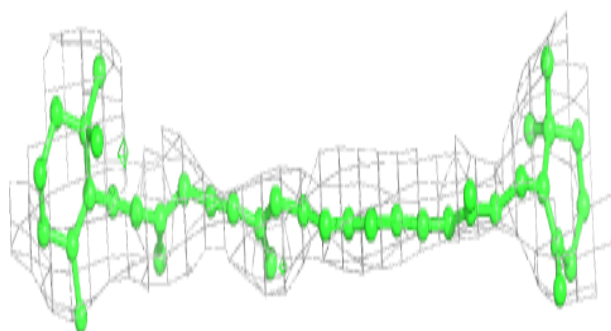
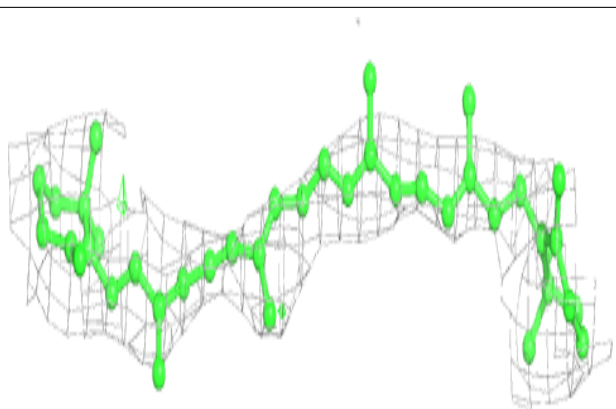
Electron density around CLA 4 312:

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

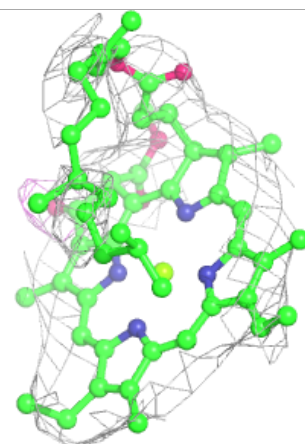
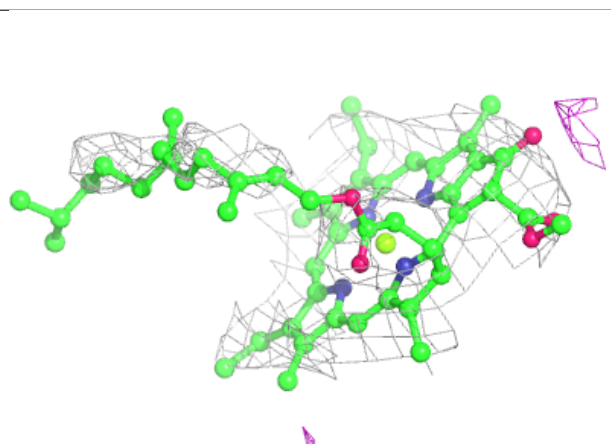
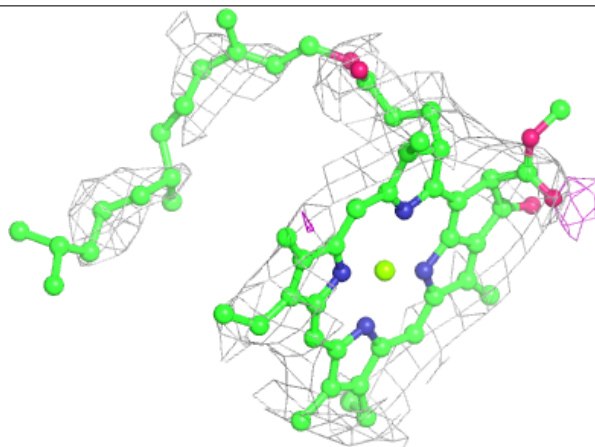


Electron density around BCR 3 305:

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

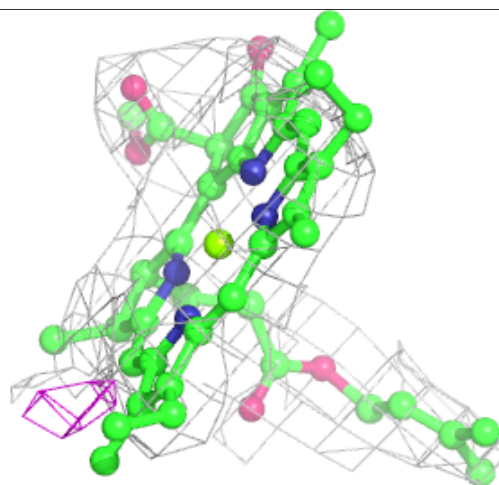
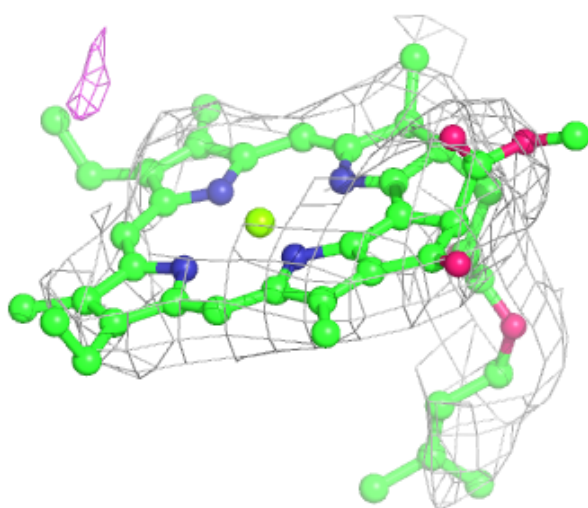
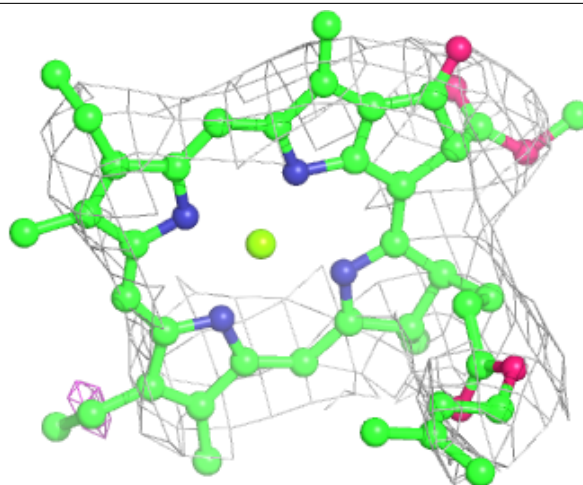
**Electron density around CLA A 840:**

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



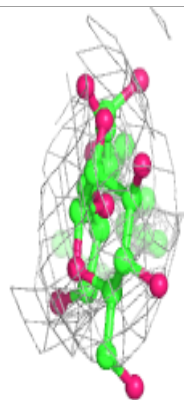
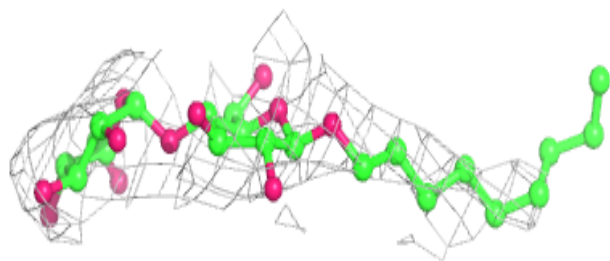
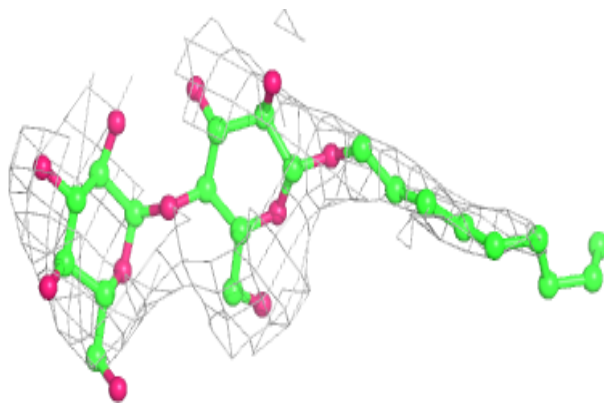
Electron density around CLA 2 311:

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



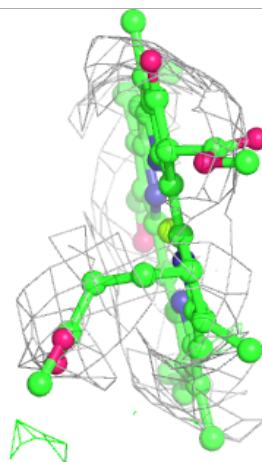
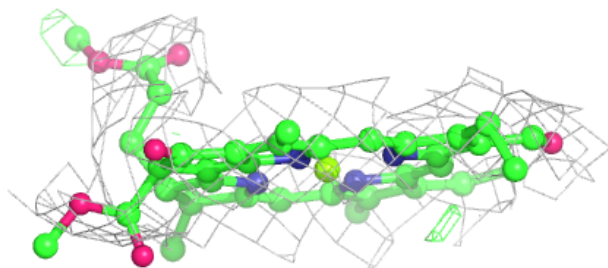
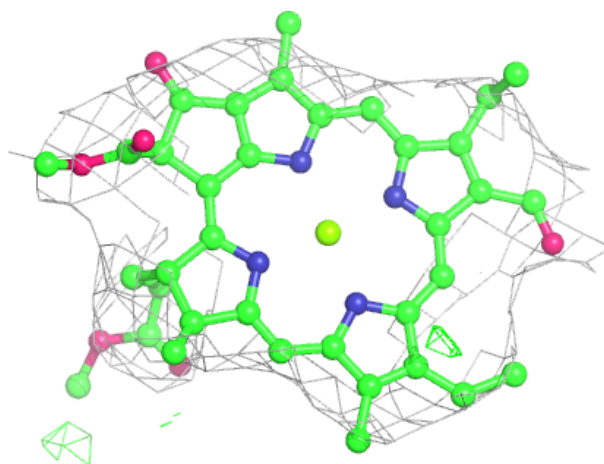
Electron density around LMT B 853:

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



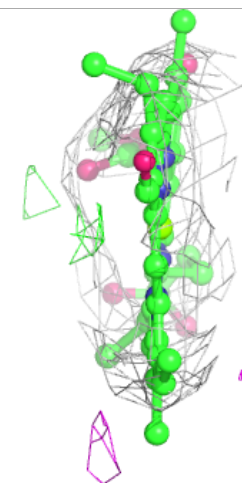
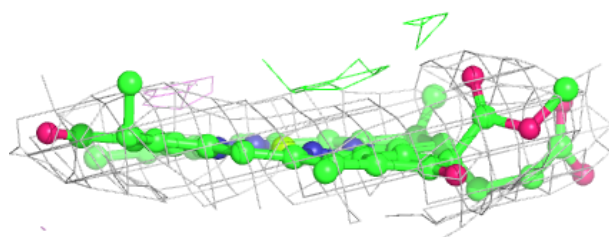
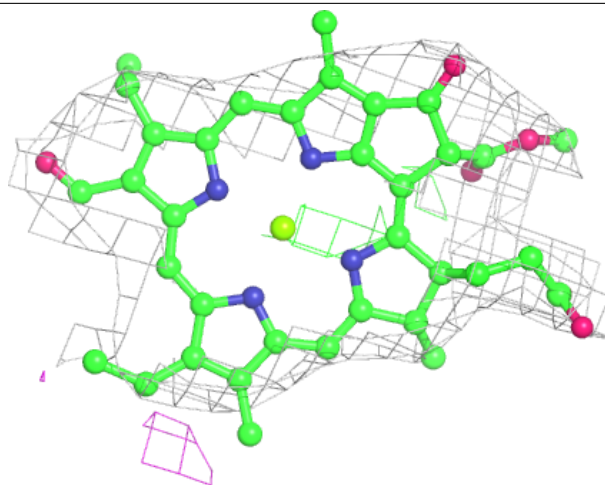
Electron density around CHL 1 5014:

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



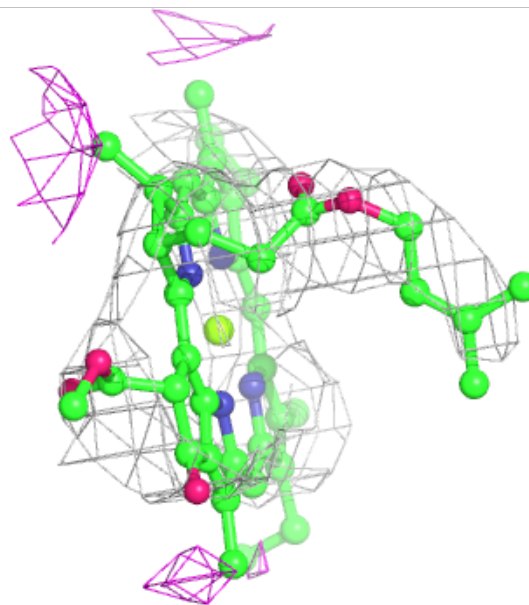
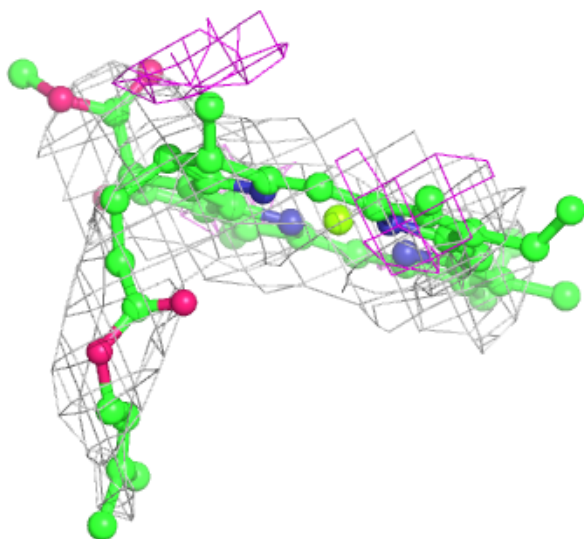
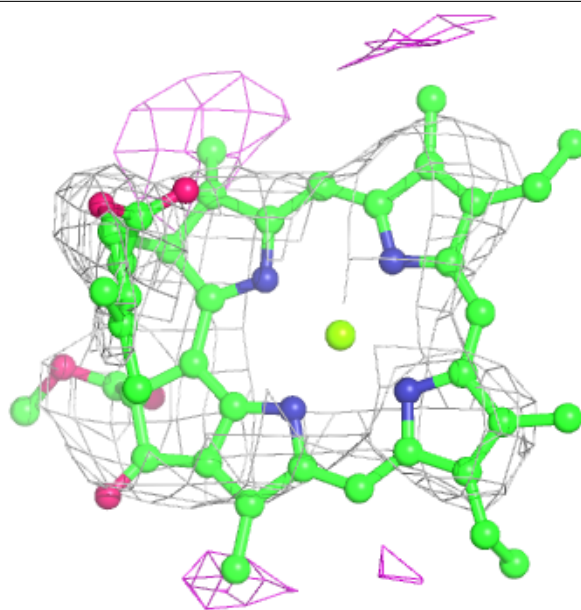
Electron density around CHL 2 318:

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



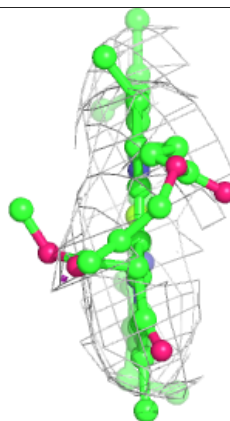
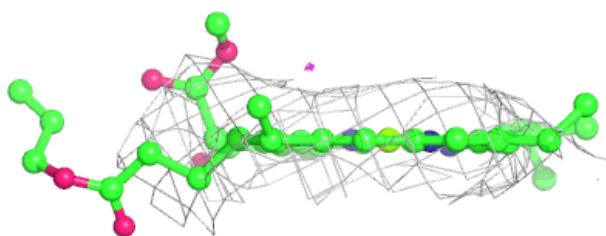
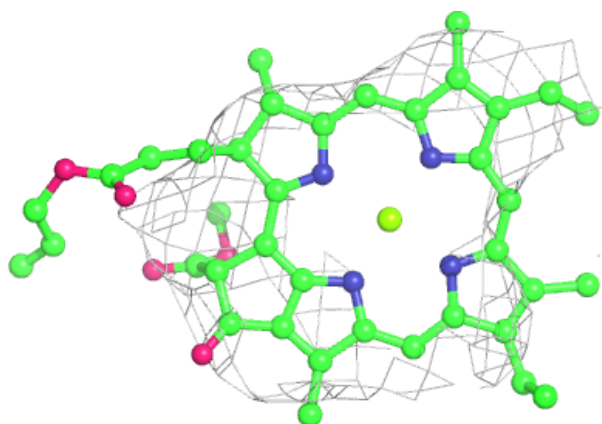
Electron density around CLA L 306:

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

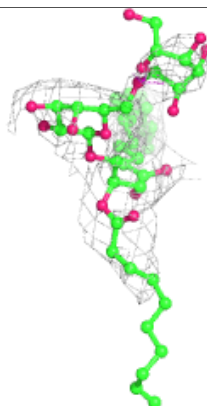
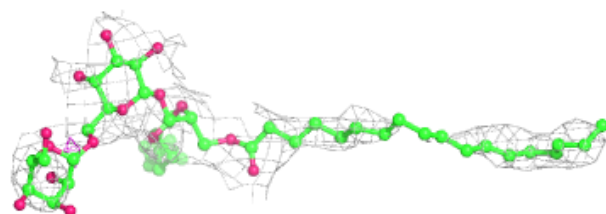
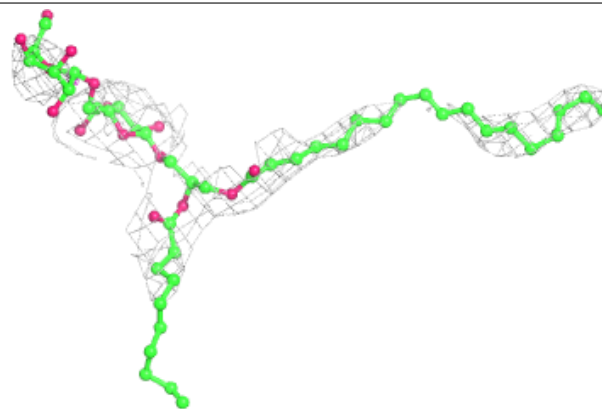


Electron density around CLA K 1403:

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

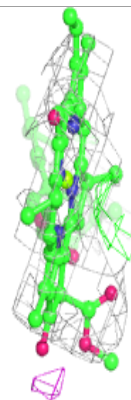
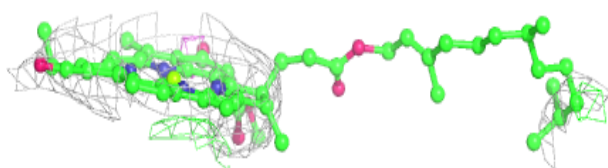
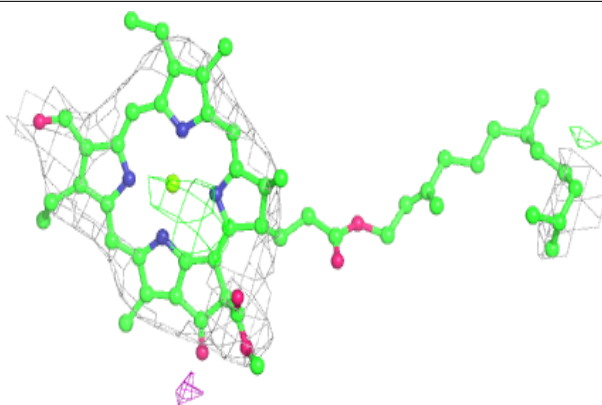
**Electron density around DGD J 1106:**

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



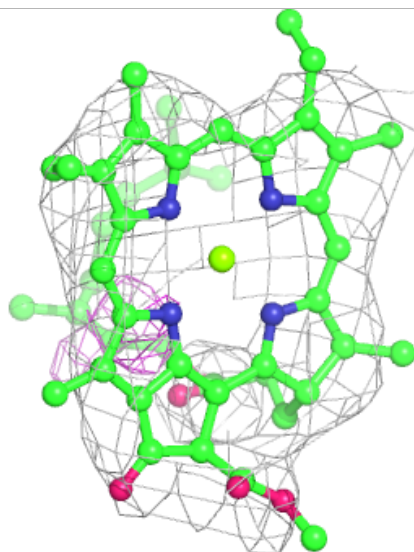
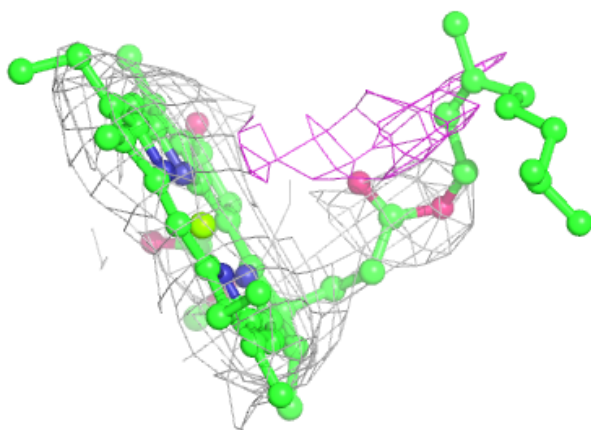
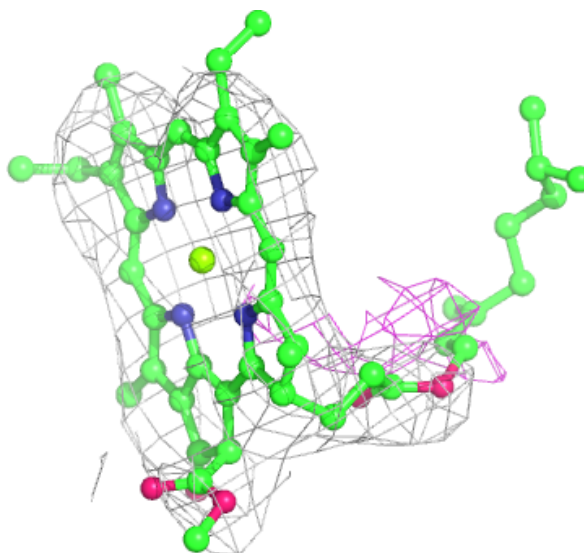
Electron density around CHL 4 316:

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



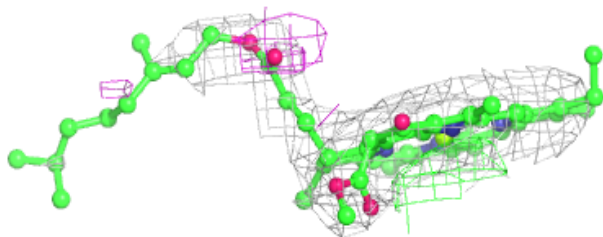
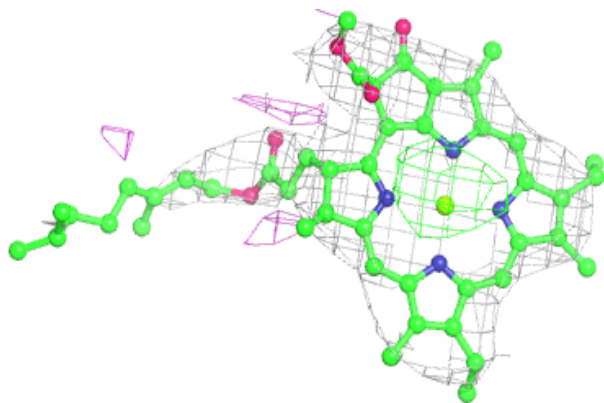
Electron density around CLA A 833:

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



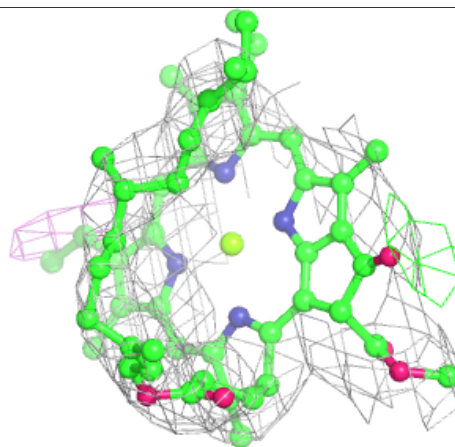
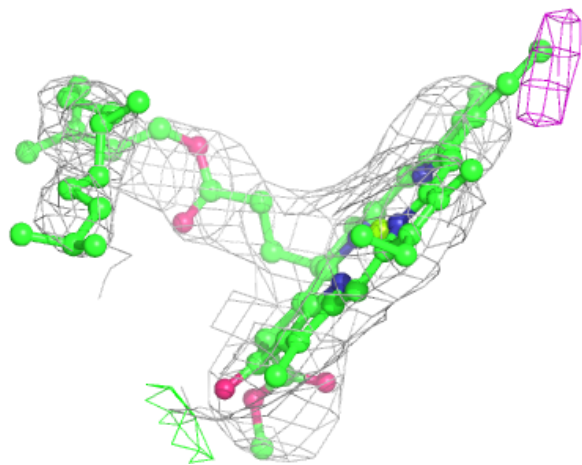
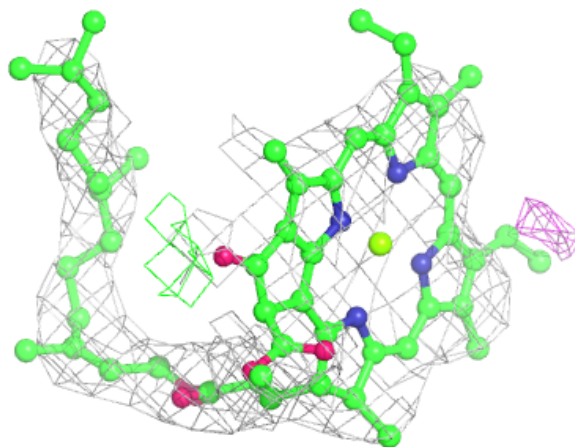
Electron density around CLA A 824:

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



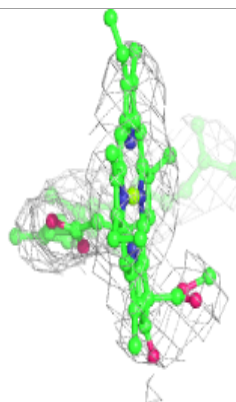
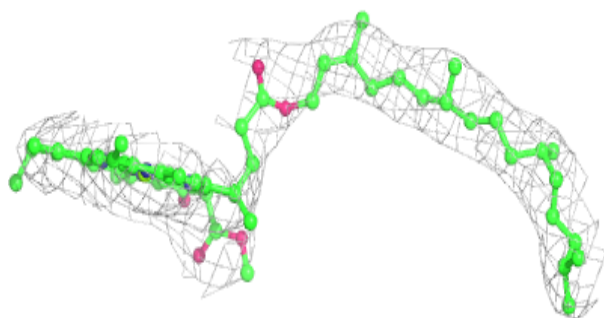
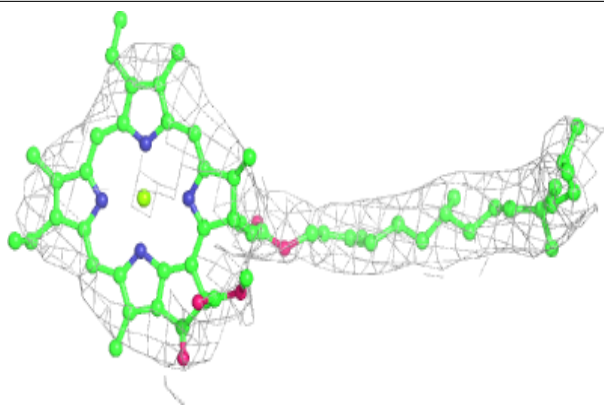
Electron density around CLA B 834:

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



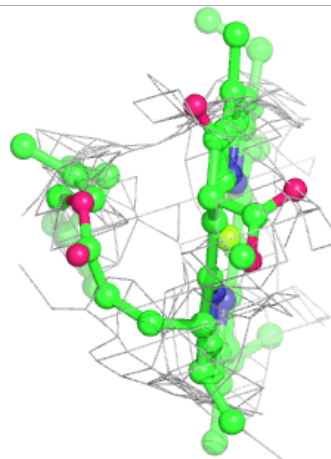
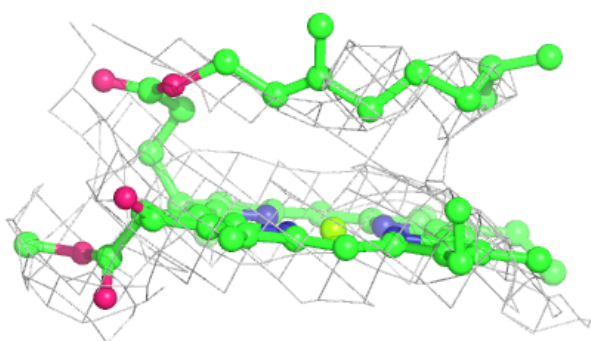
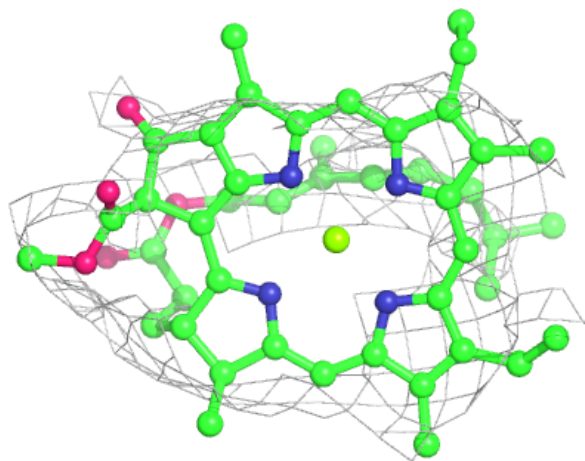
Electron density around CLA B 841:

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



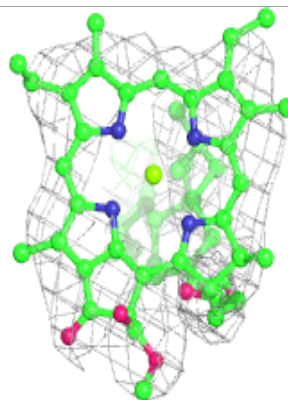
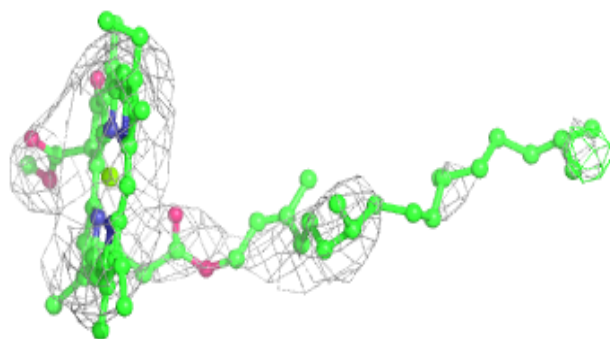
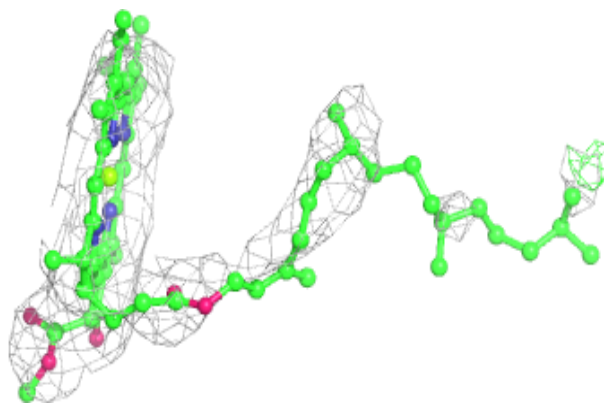
Electron density around CLA 3 309:

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



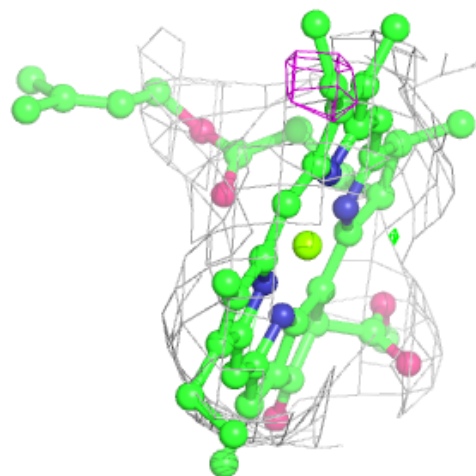
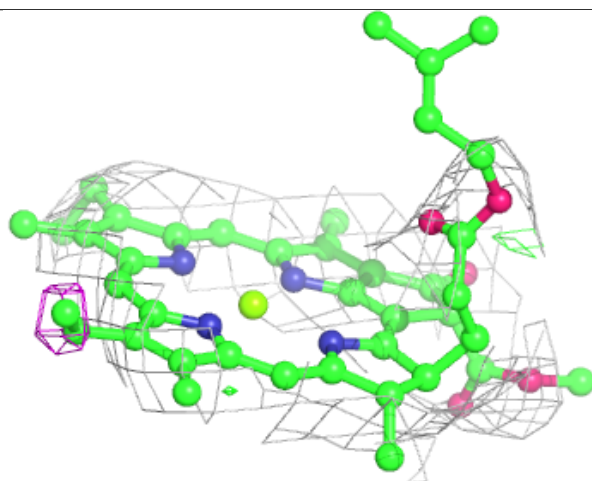
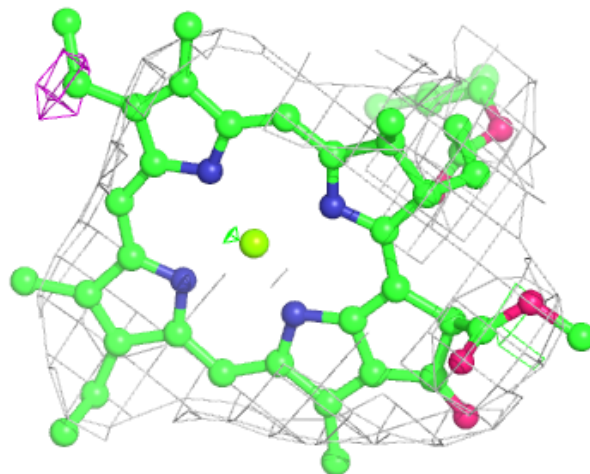
Electron density around CLA B 805:

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



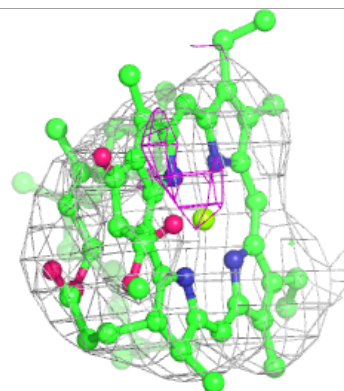
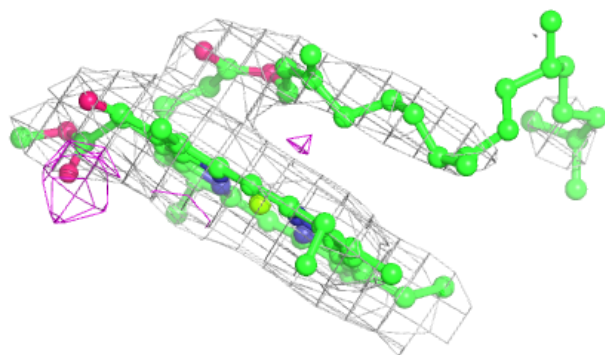
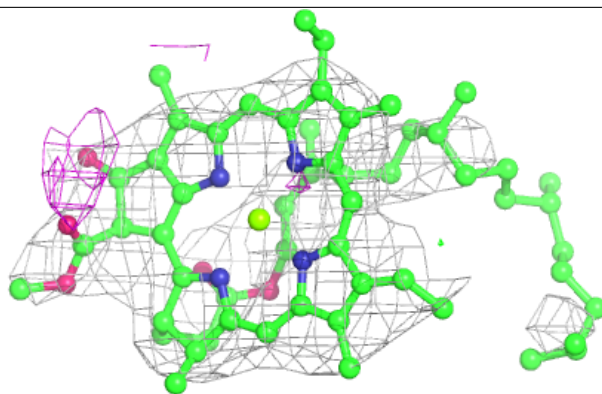
Electron density around CLA 4 310:

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

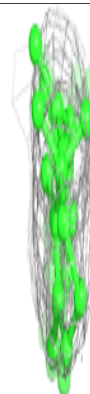
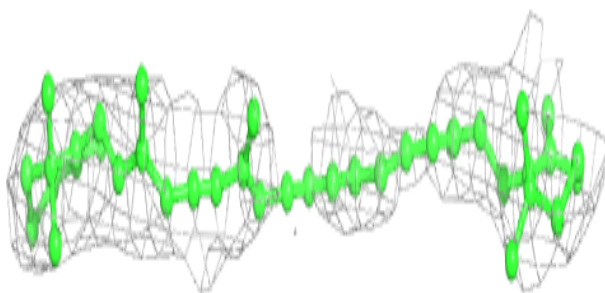
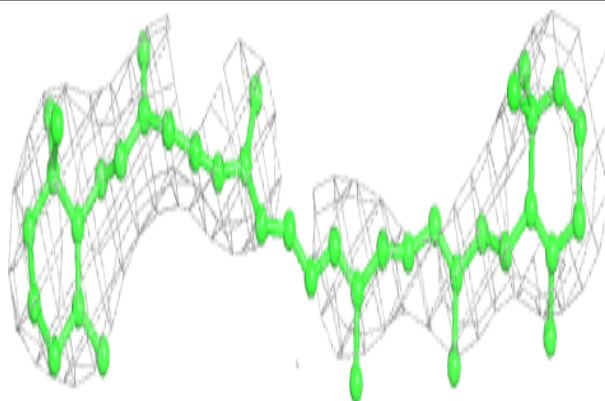


Electron density around CLA B 808:

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

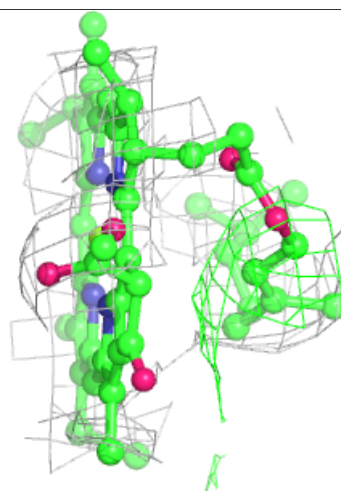
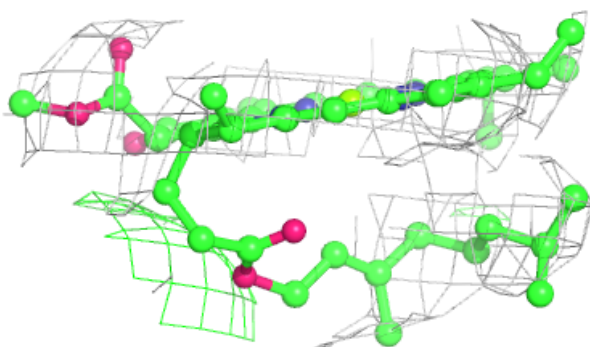
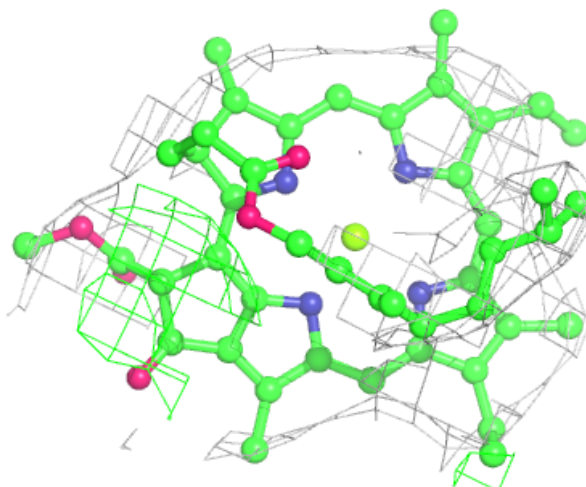
**Electron density around BCR I 102:**

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



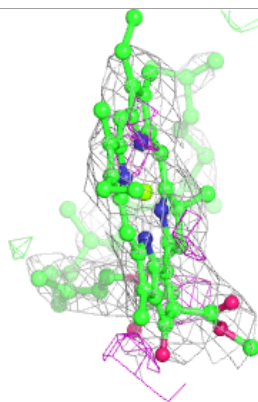
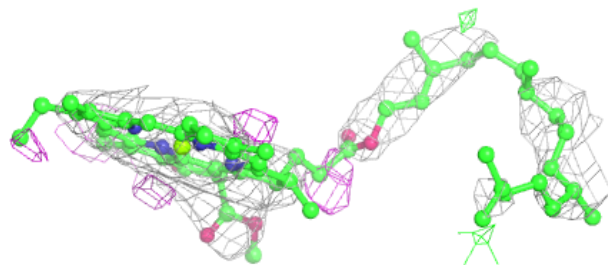
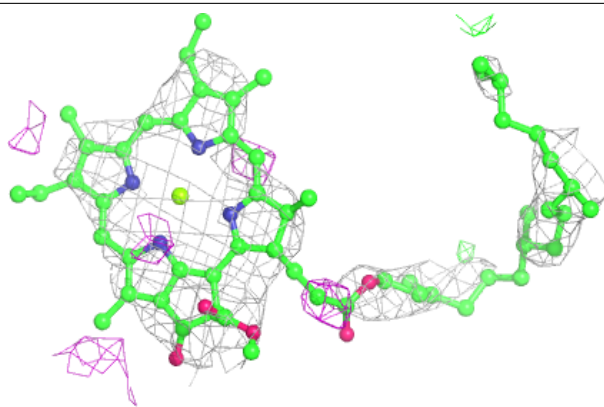
Electron density around CLA 1 5008:

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



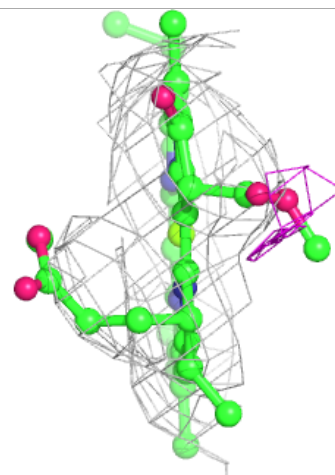
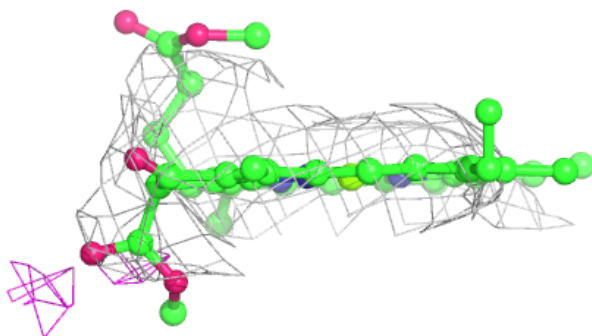
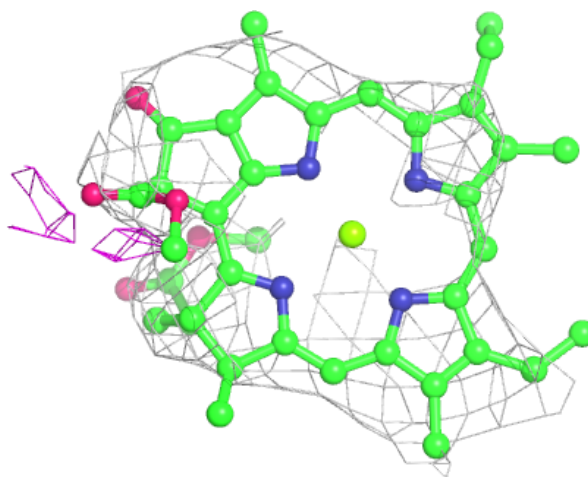
Electron density around CLA A 825:

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



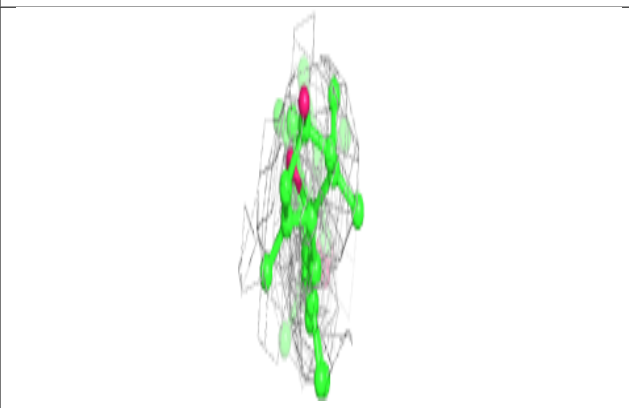
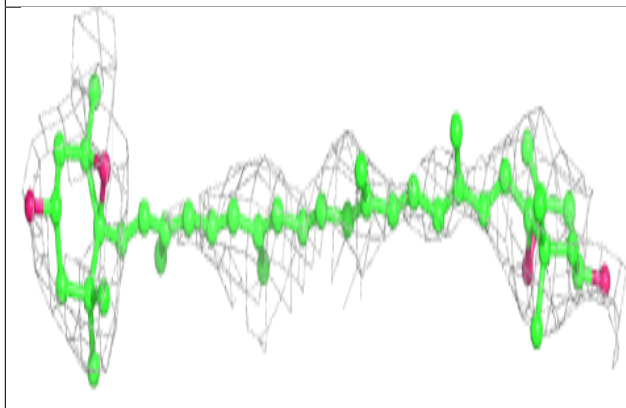
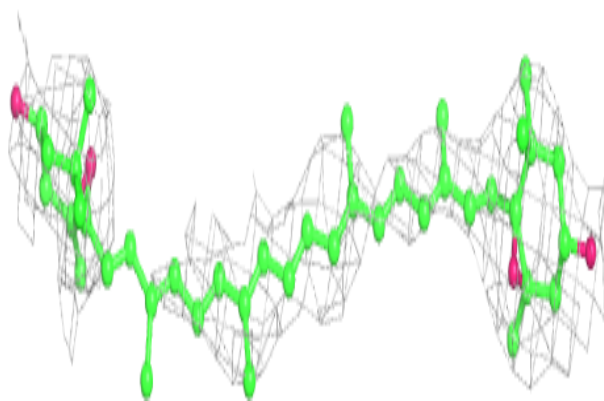
Electron density around CLA A 814:

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

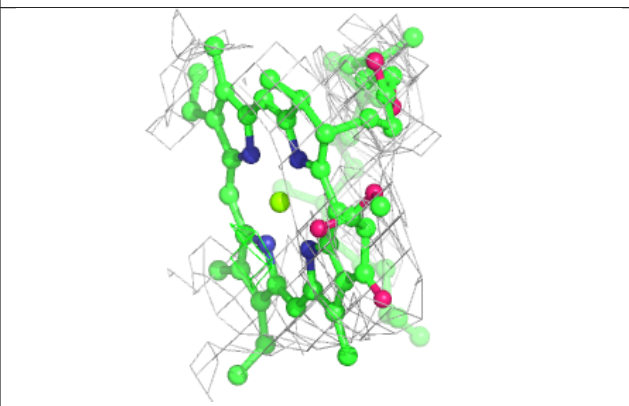
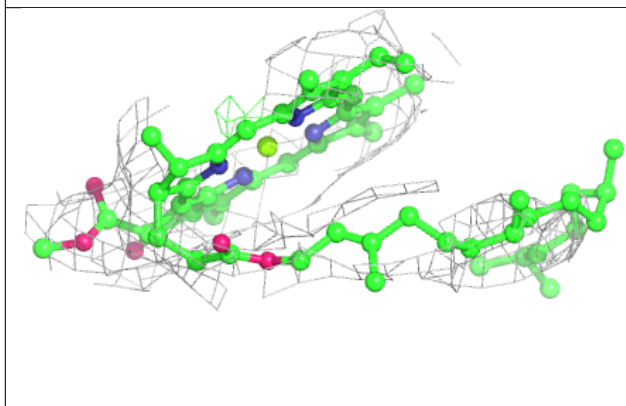
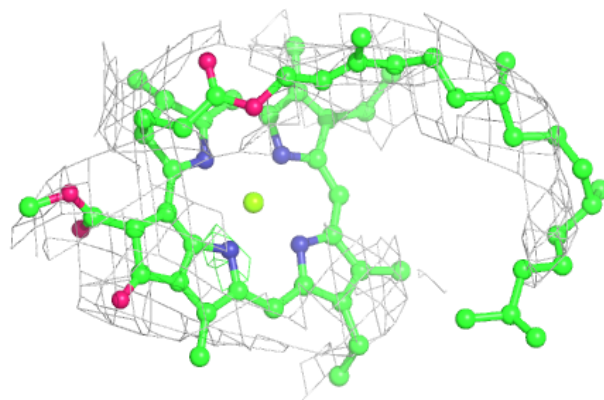


Electron density around XAT 4 304:

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

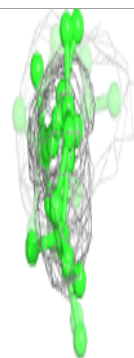
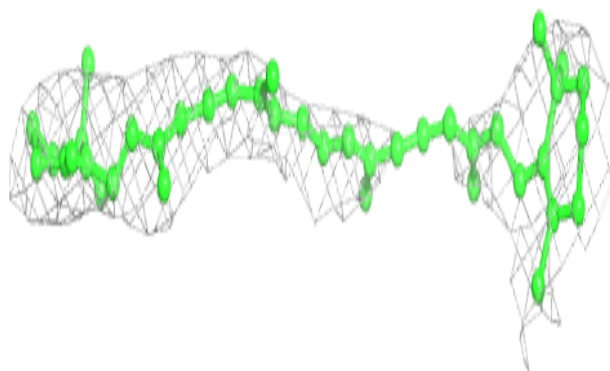
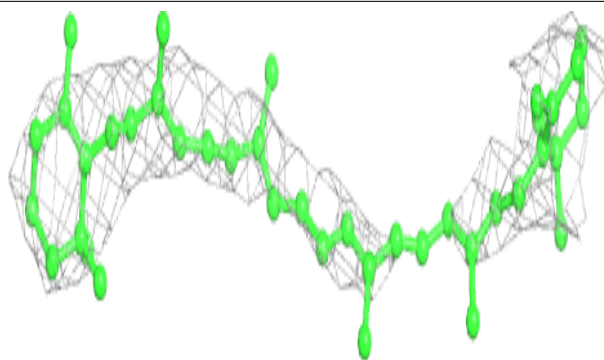
**Electron density around CLA 1 5006:**

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

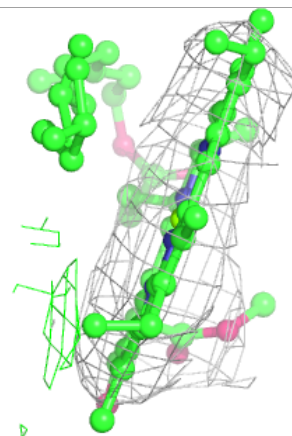
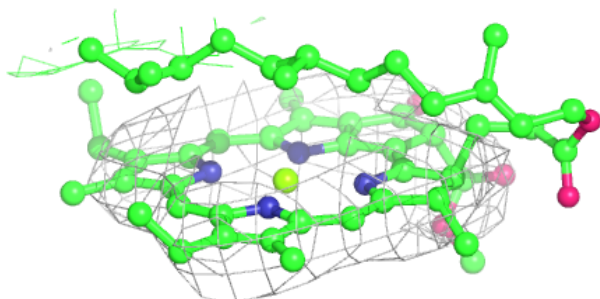
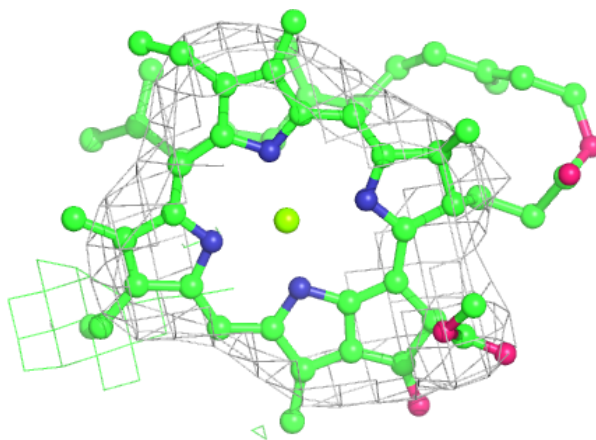


Electron density around BCR 4 301:

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

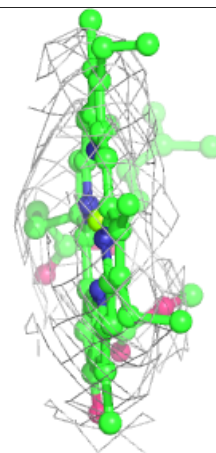
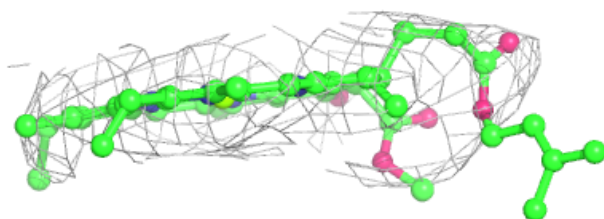
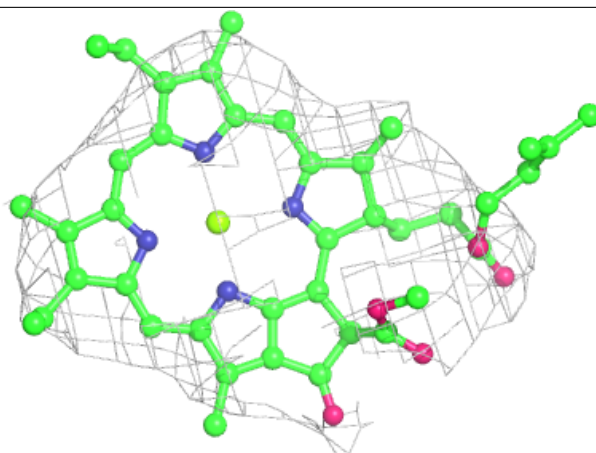
**Electron density around CLA 3 319:**

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

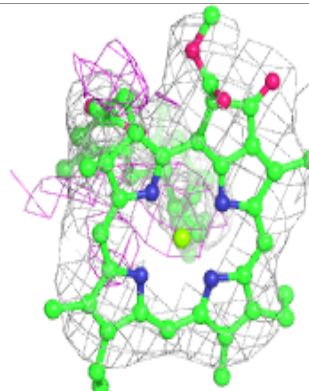
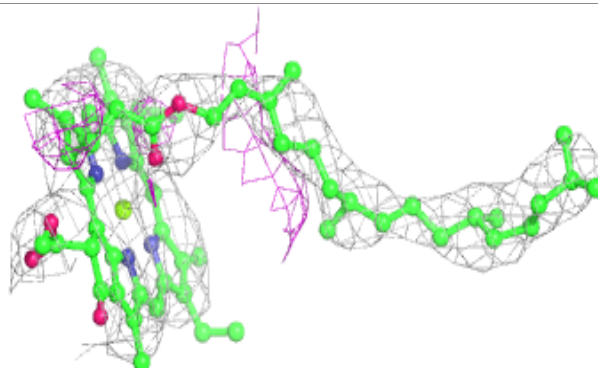
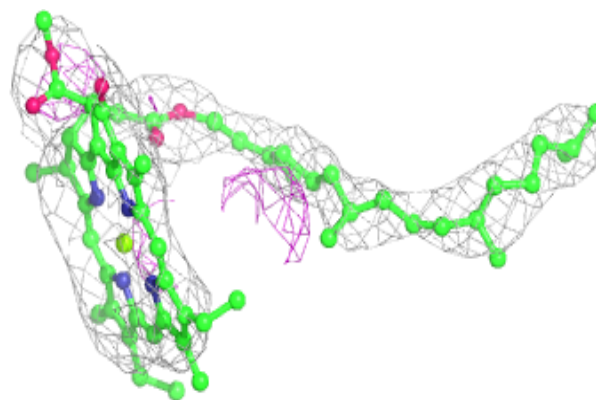


Electron density around CLA 4 306:

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

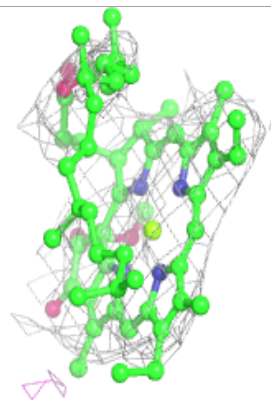
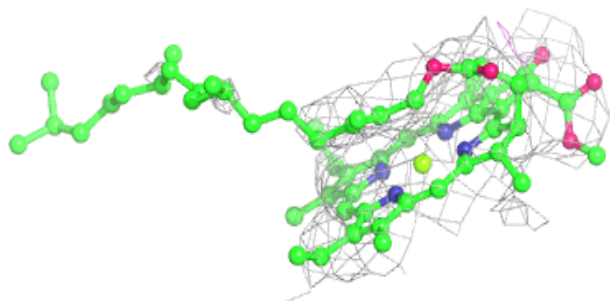
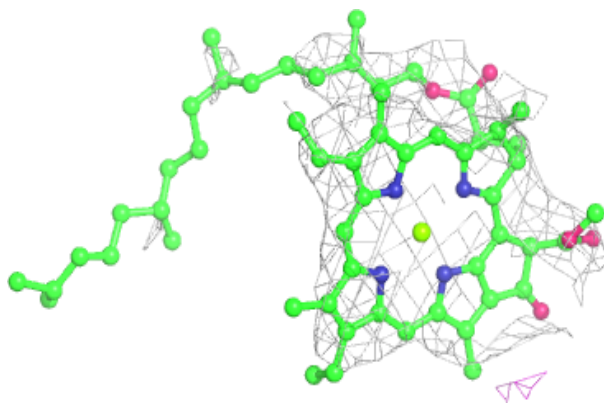
**Electron density around CLA A 810:**

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

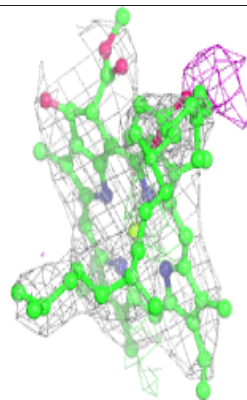
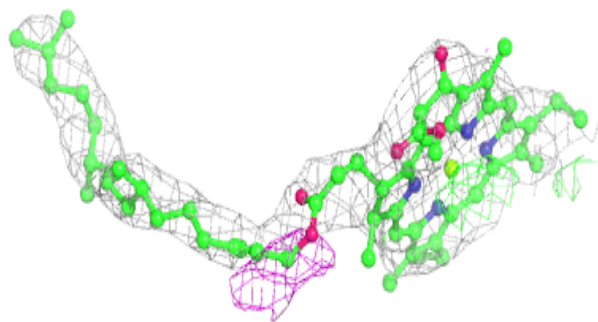
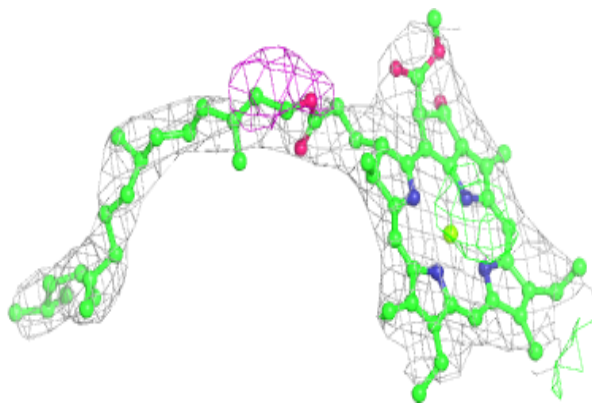


Electron density around CLA 1 5009:

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

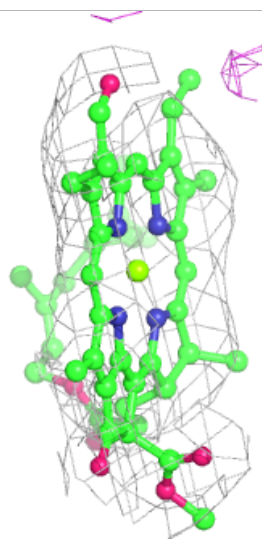
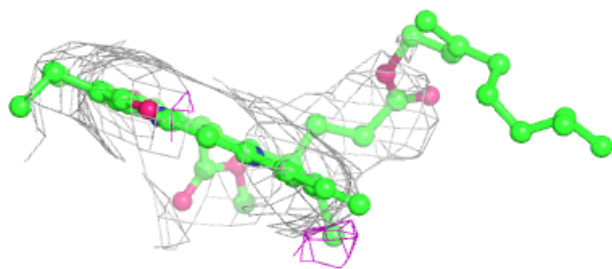
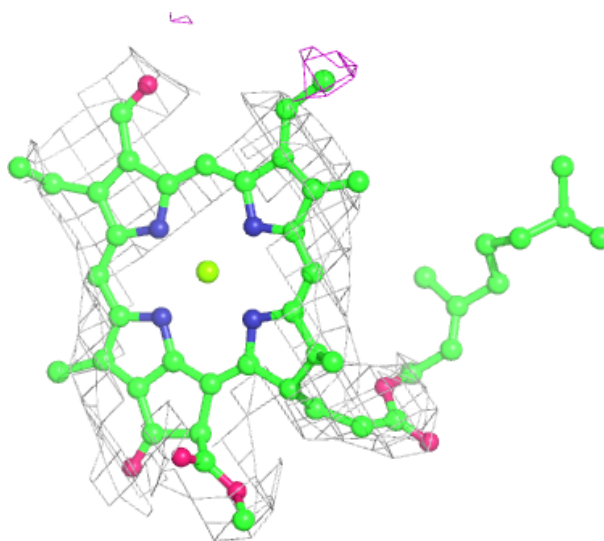
**Electron density around CLA B 801:**

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



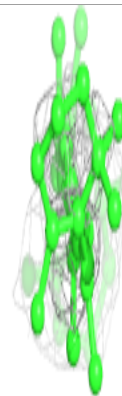
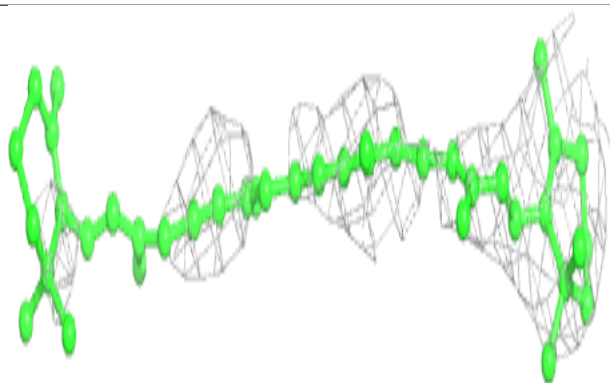
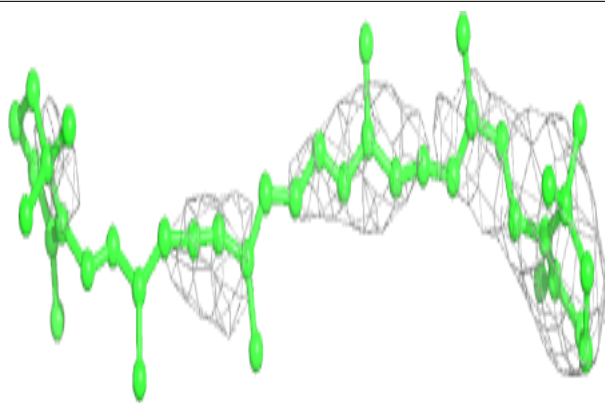
Electron density around CHL 2 315:

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

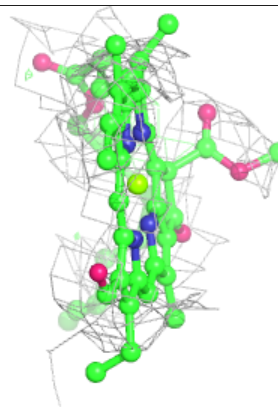
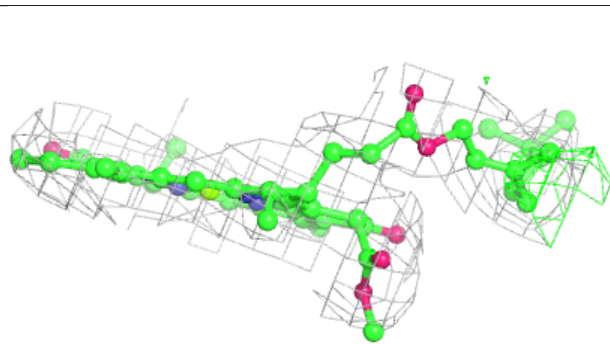
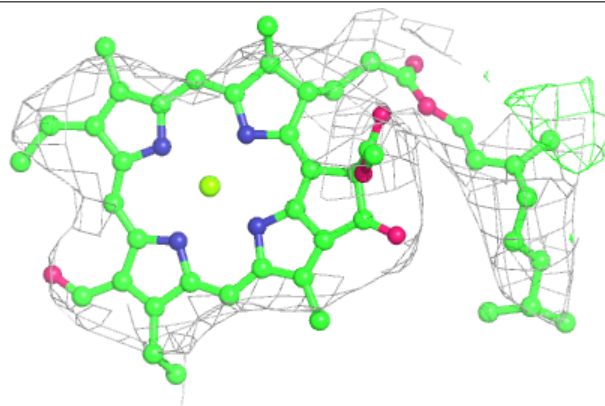


Electron density around BCR A 844:

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

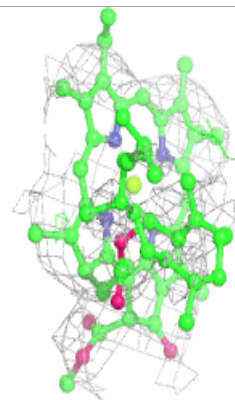
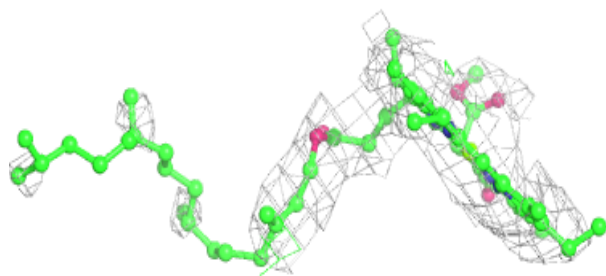
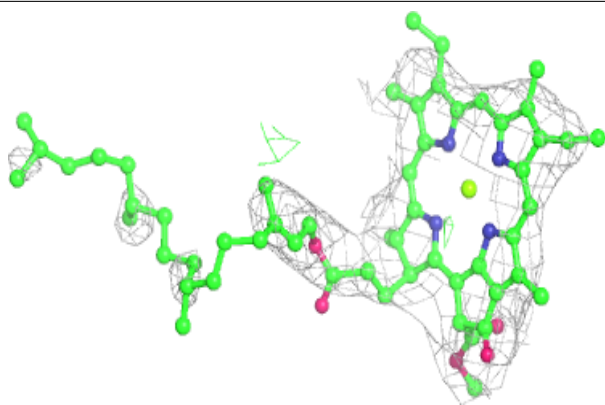
**Electron density around CHL 2 319:**

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



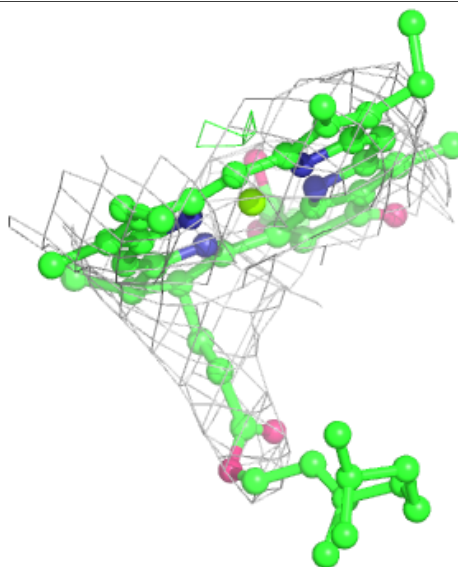
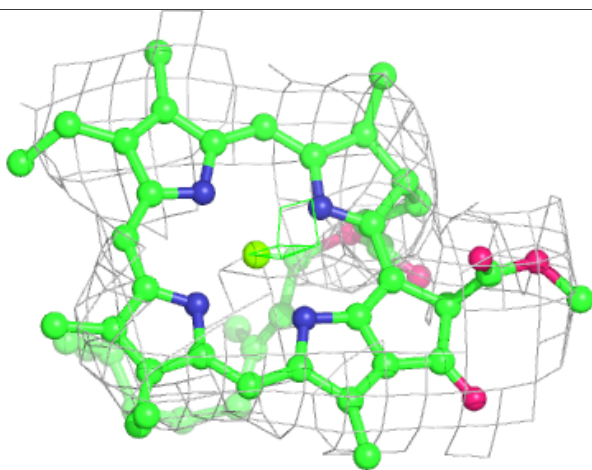
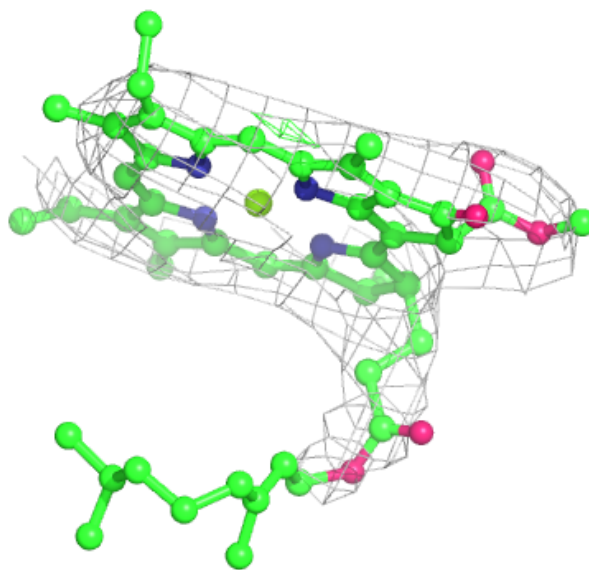
Electron density around CLA A 829:

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



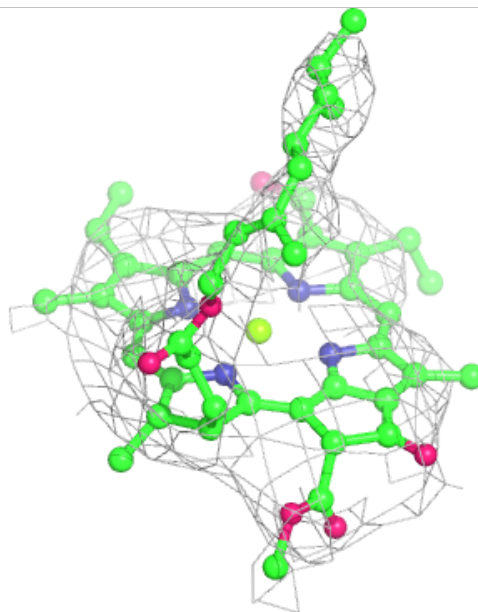
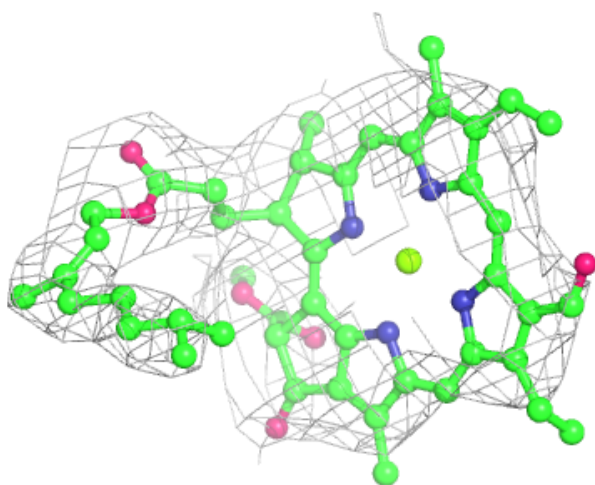
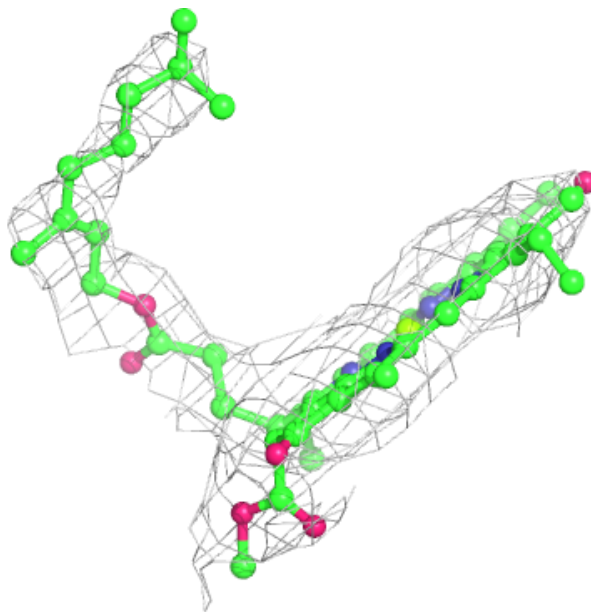
Electron density around CLA B 835:

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



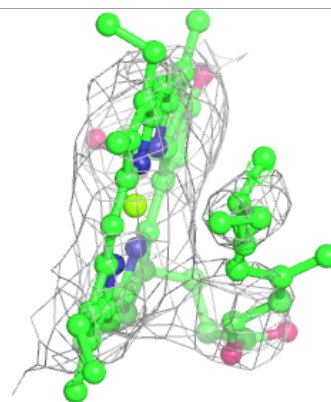
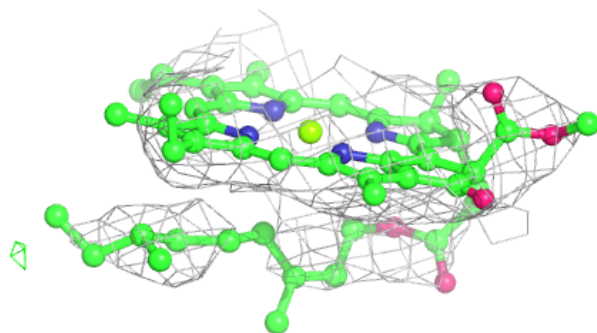
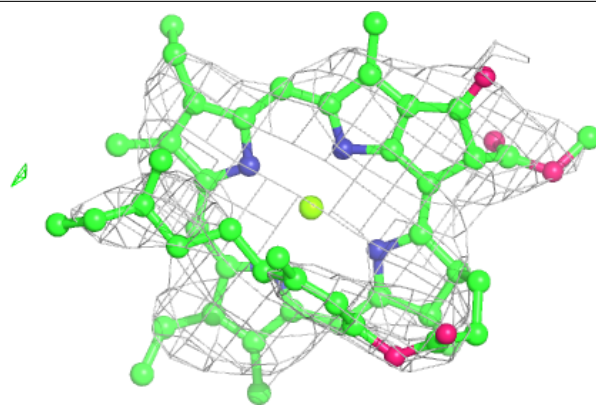
Electron density around CHL 4 302:

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



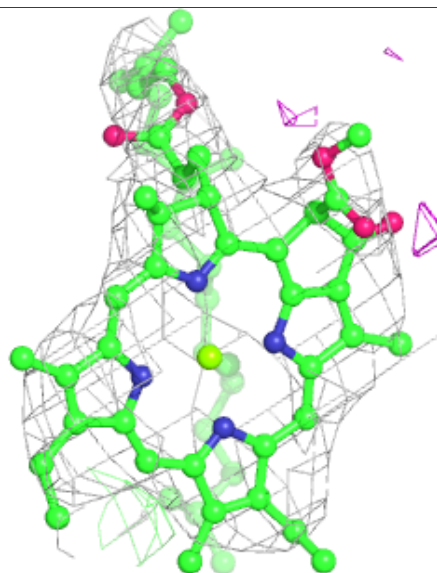
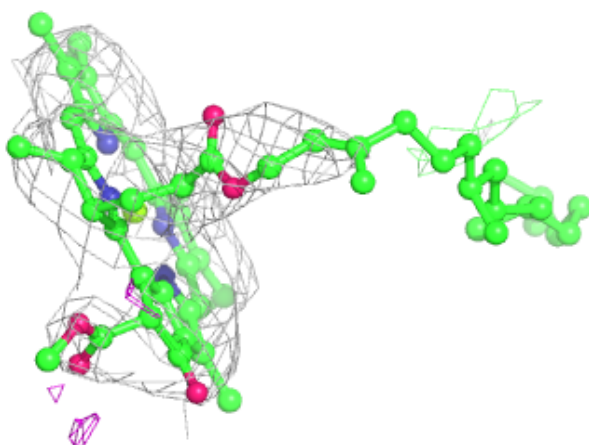
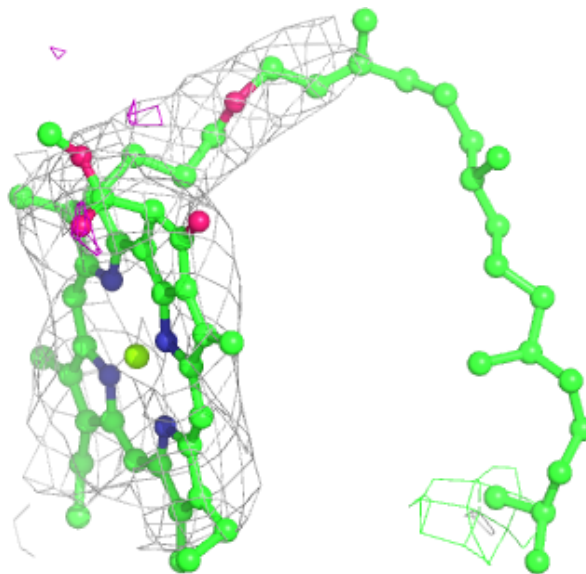
Electron density around CLA A 816:

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



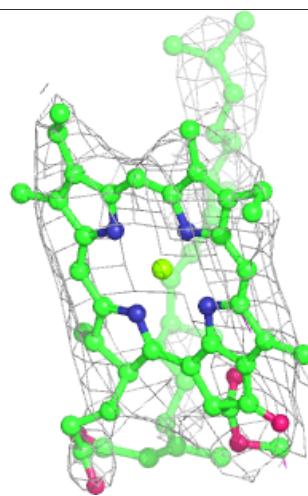
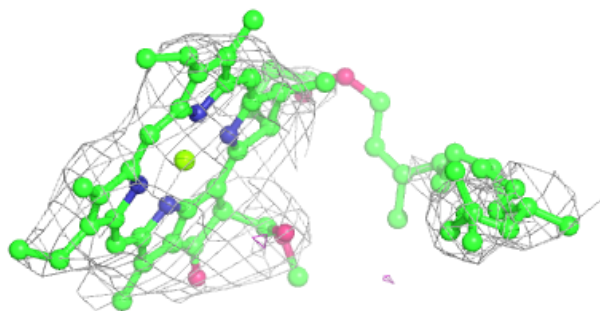
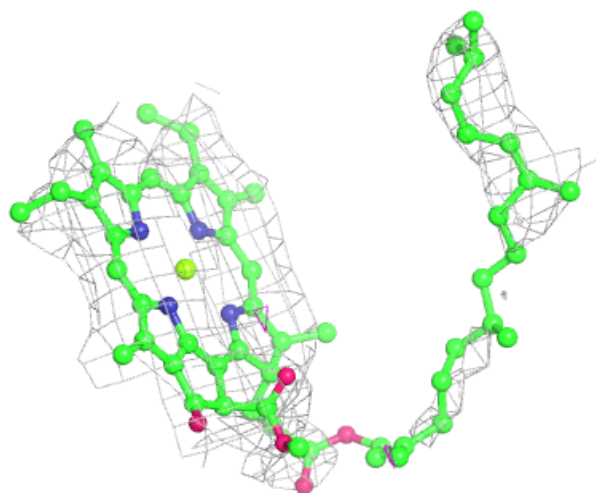
Electron density around CLA A 836:

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



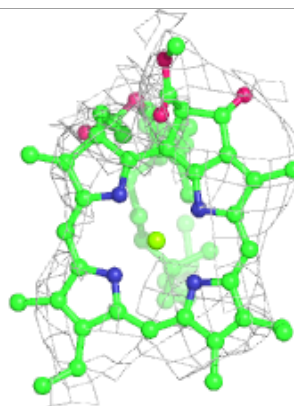
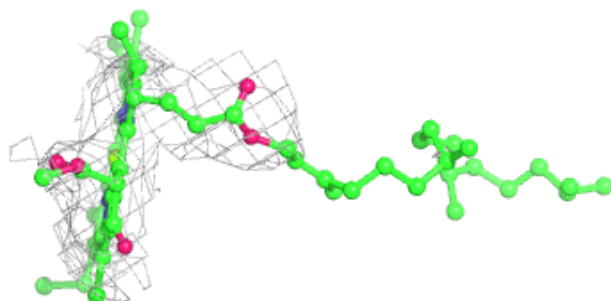
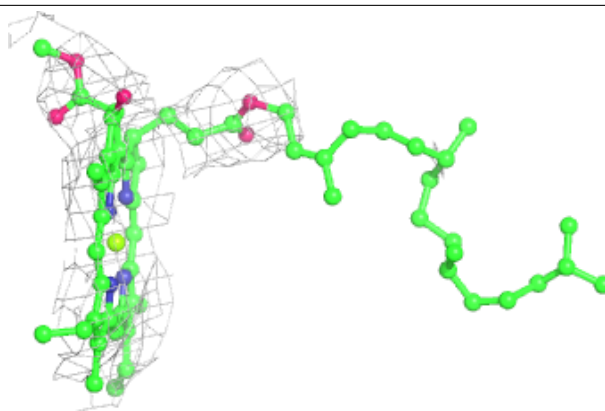
Electron density around CLA B 811:

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



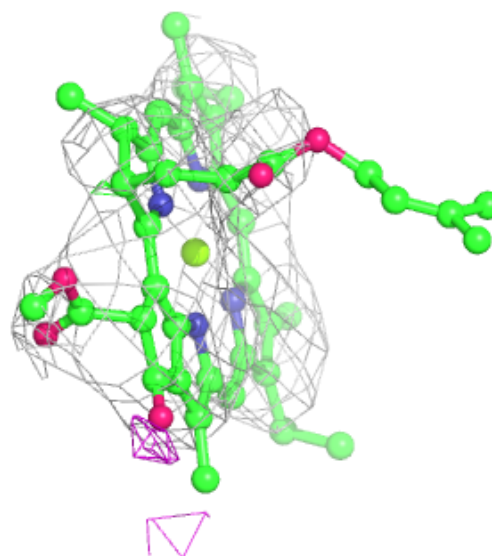
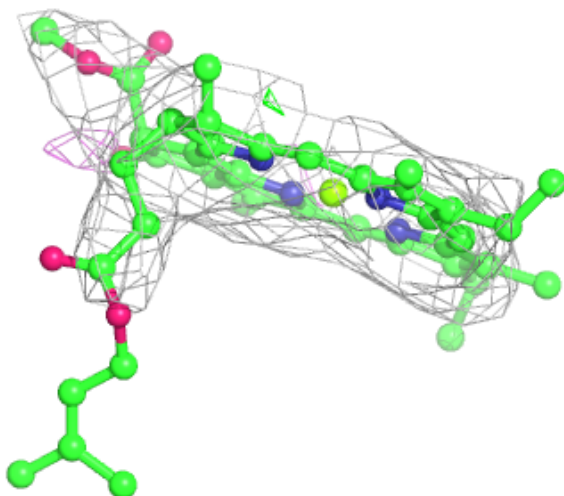
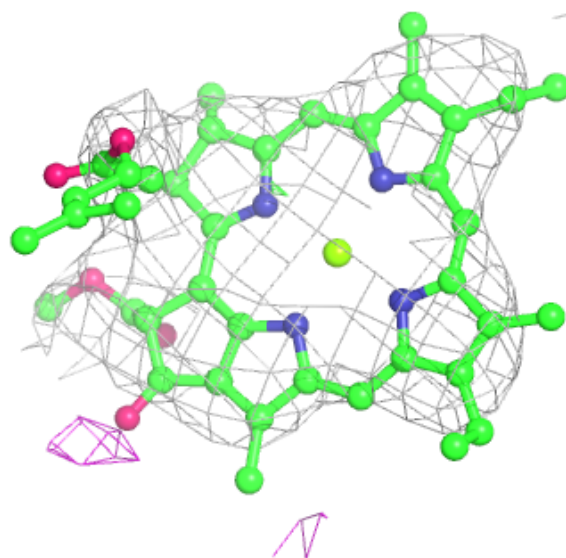
Electron density around CLA A 813:

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



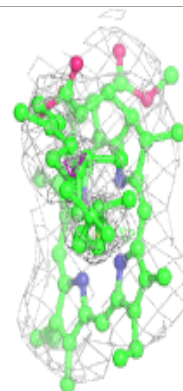
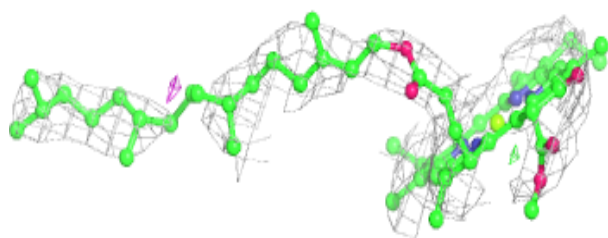
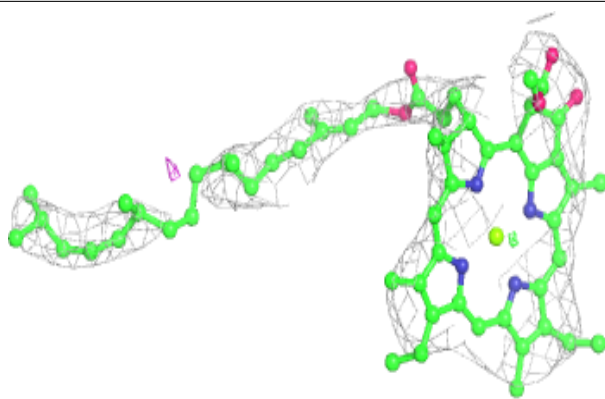
Electron density around CLA A 809:

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

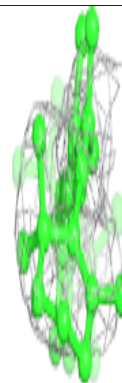
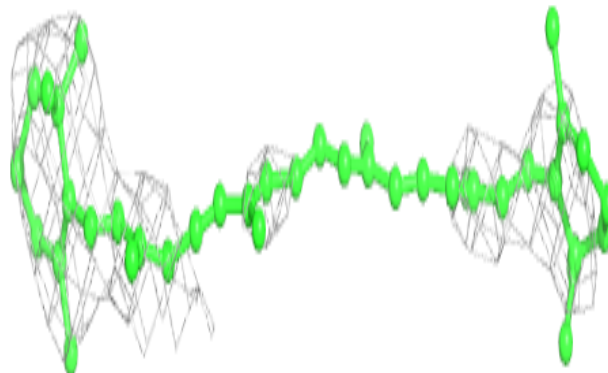
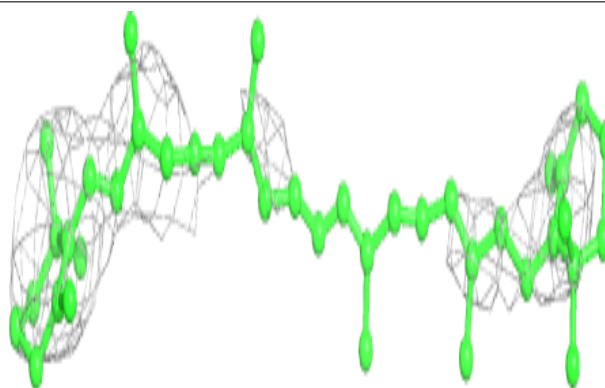


Electron density around CLA A 831:

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

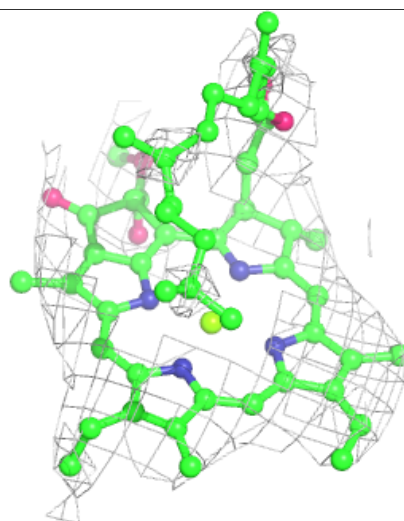
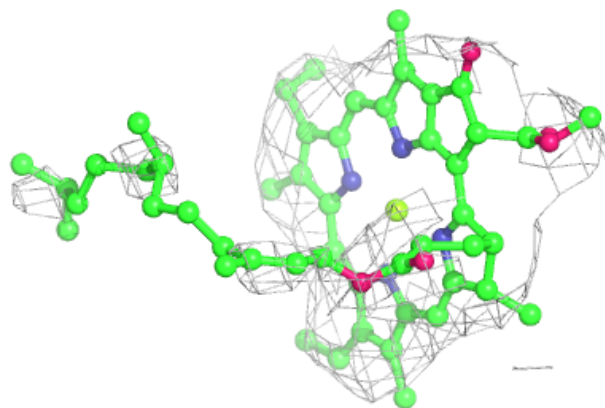
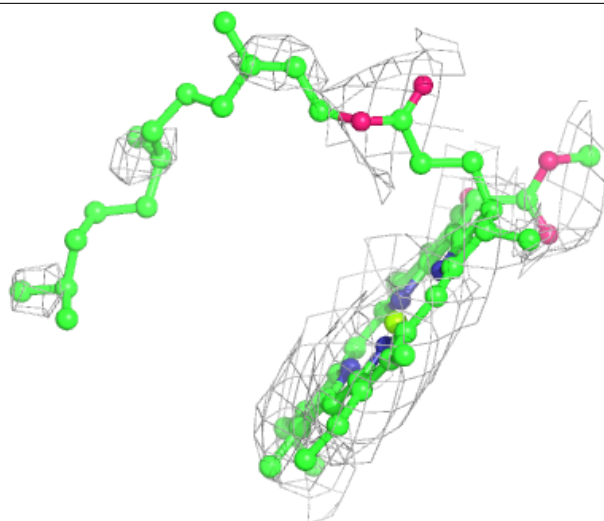
**Electron density around BCR A 843:**

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



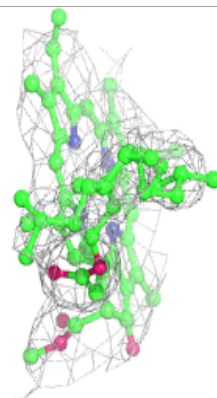
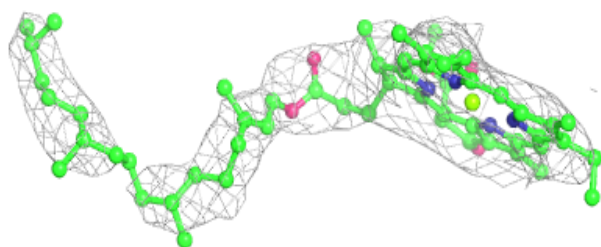
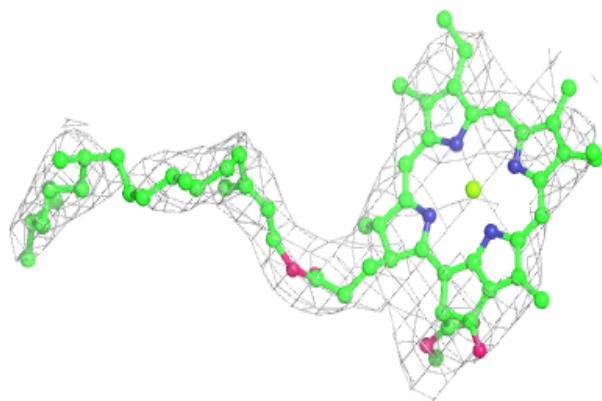
Electron density around CLA B 812:

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

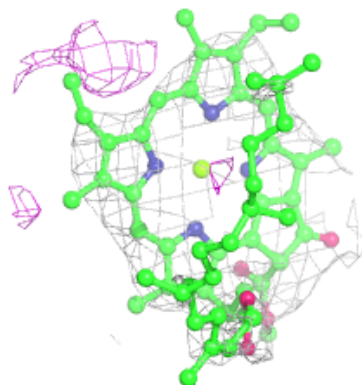
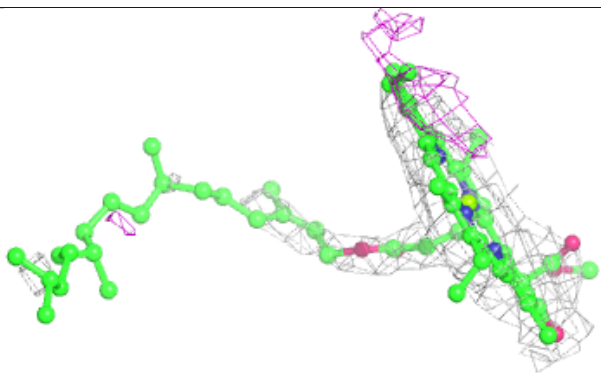
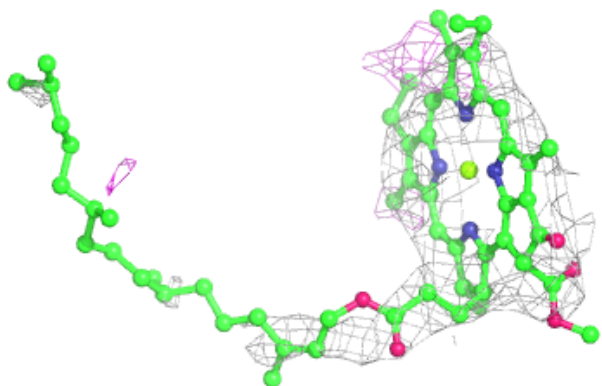


Electron density around CLA B 814:

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

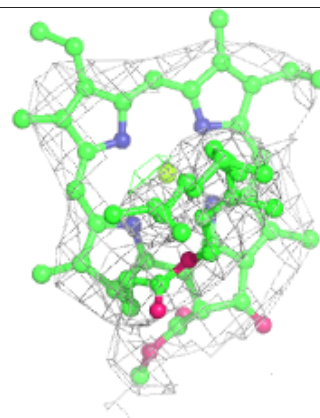
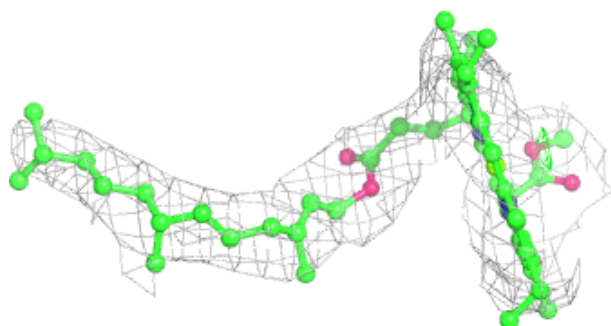
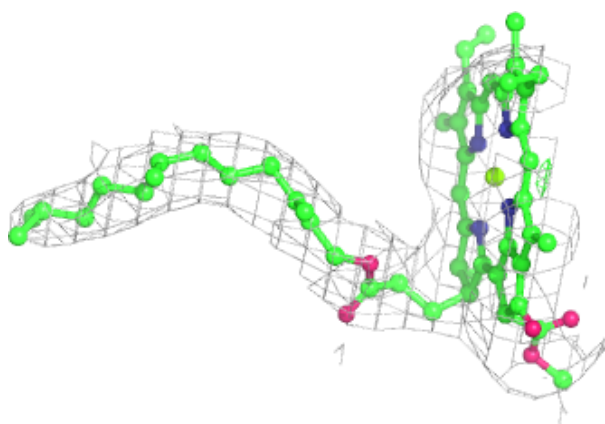
**Electron density around CLA A 832:**

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

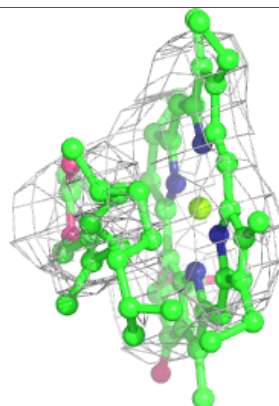
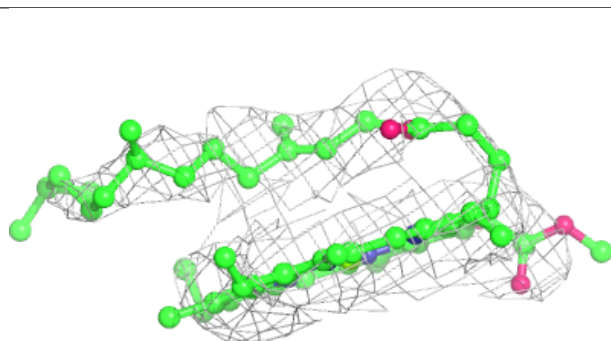
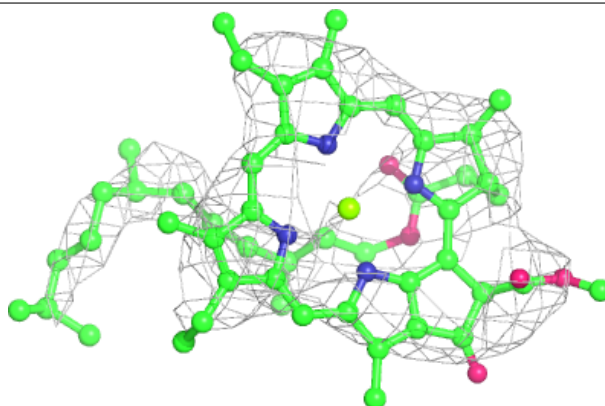


Electron density around CLA L 305:

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

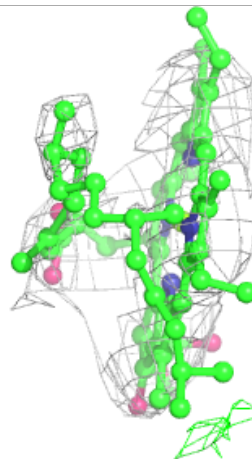
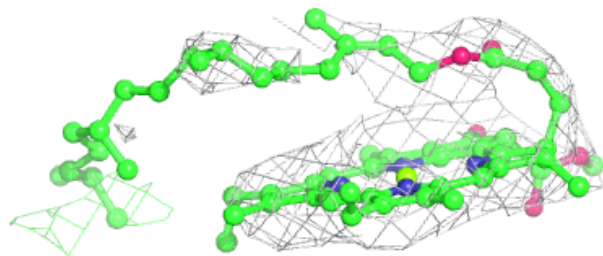
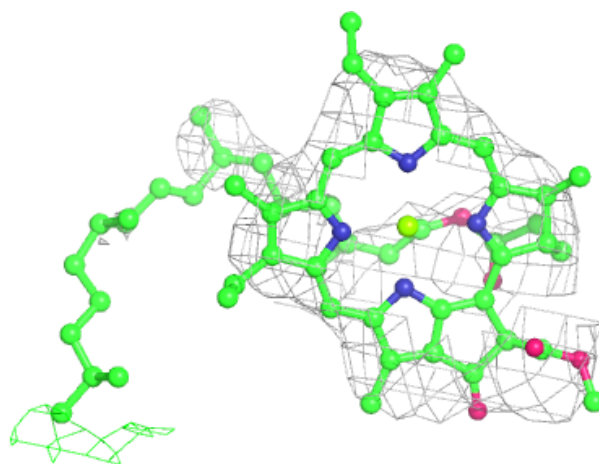
**Electron density around CLA B 817:**

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



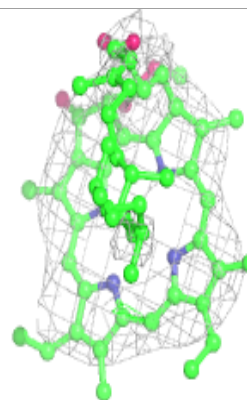
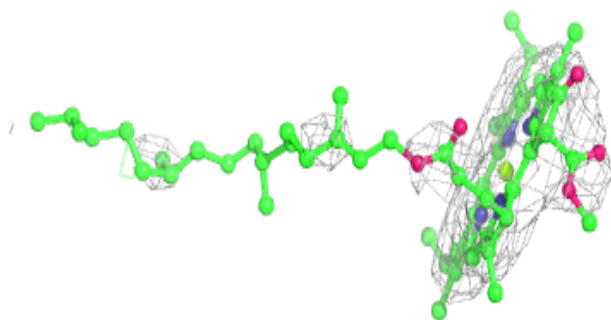
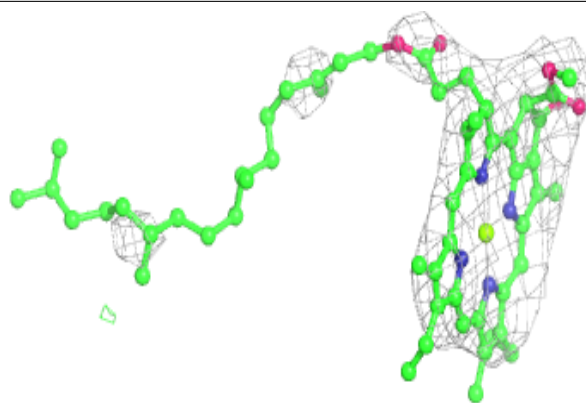
Electron density around CLA A 815:

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

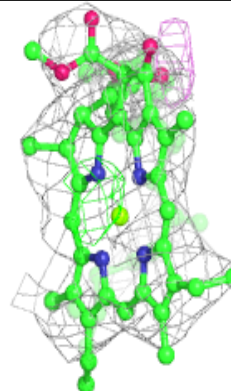
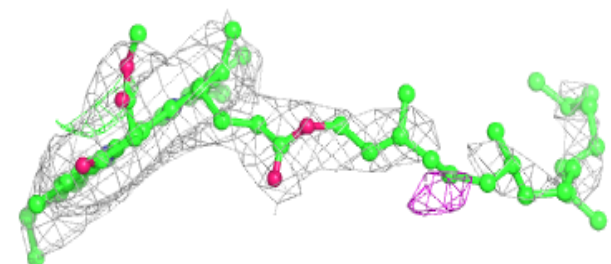
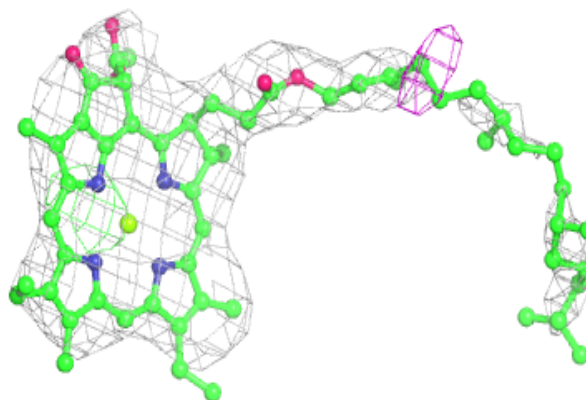


Electron density around CLA B 822:

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

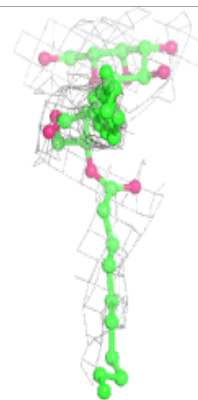
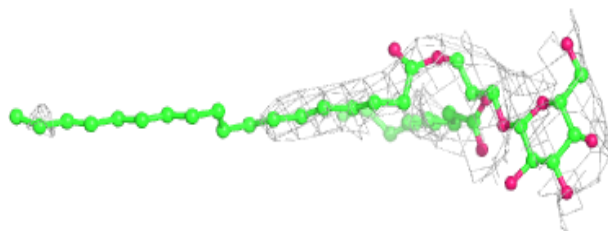
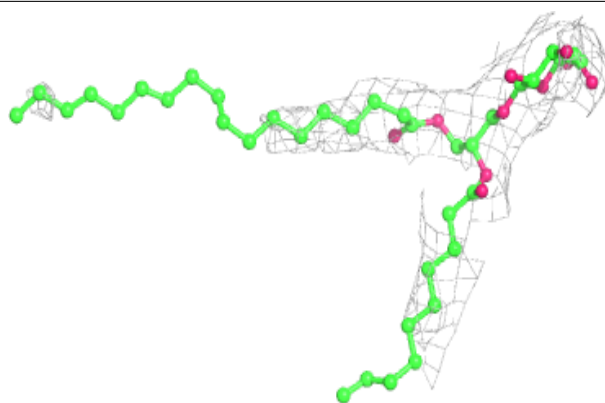
**Electron density around CLA B 826:**

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



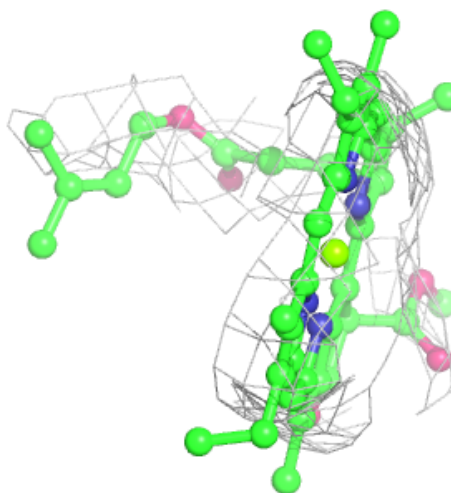
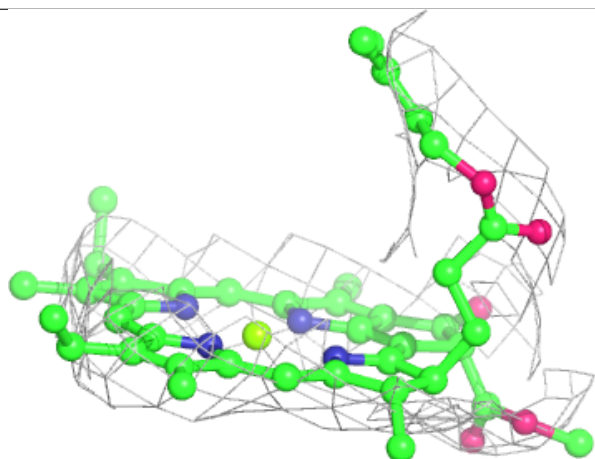
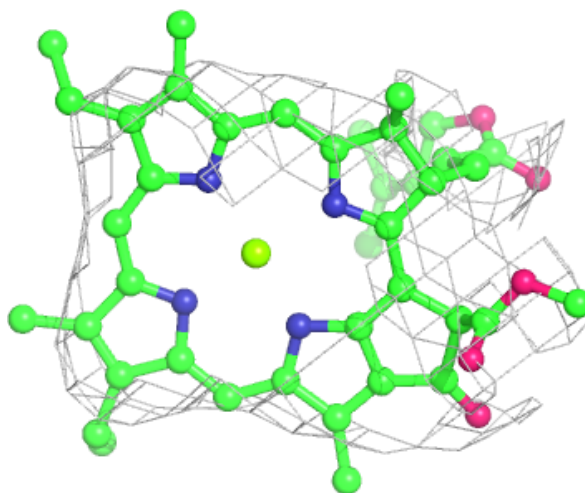
Electron density around LMG F 306:

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



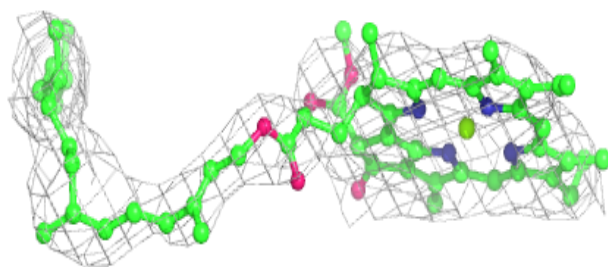
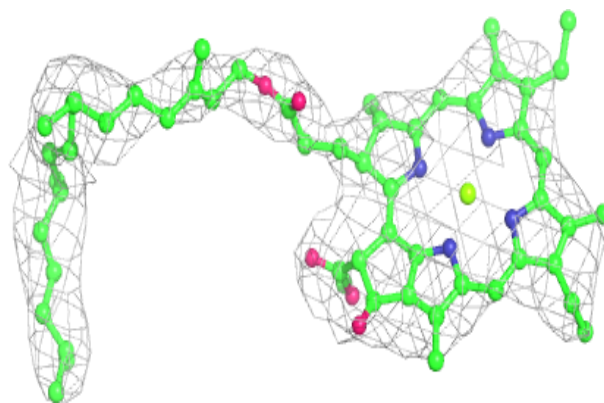
Electron density around CLA 1 5011:

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

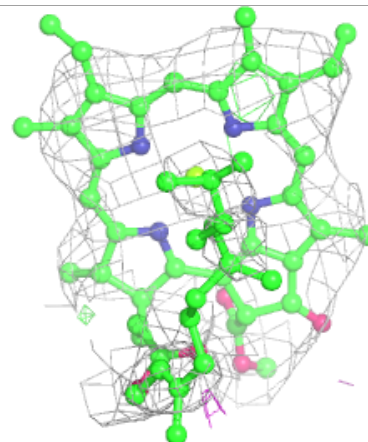
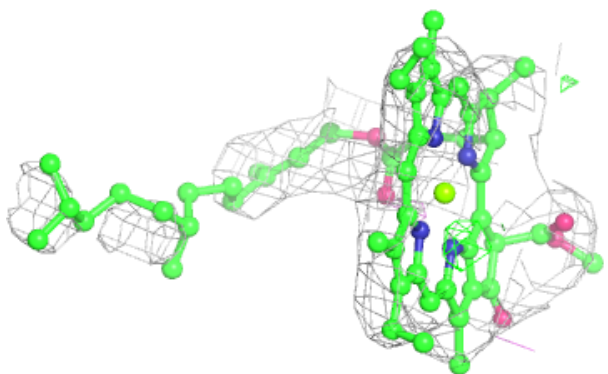
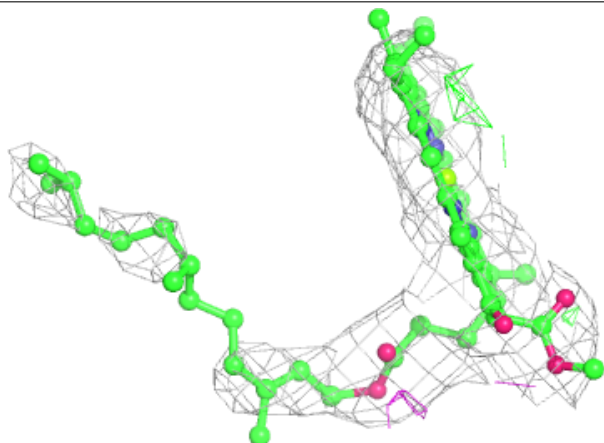


Electron density around CLA B 827:

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

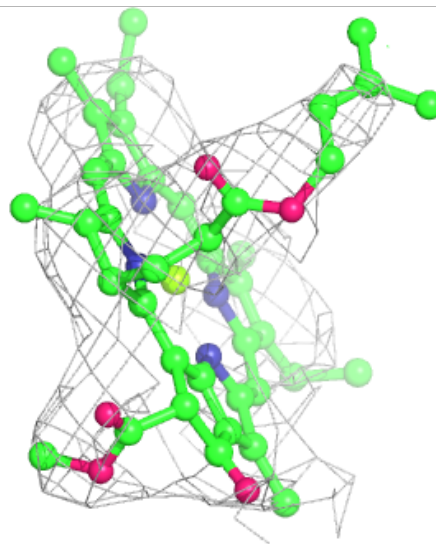
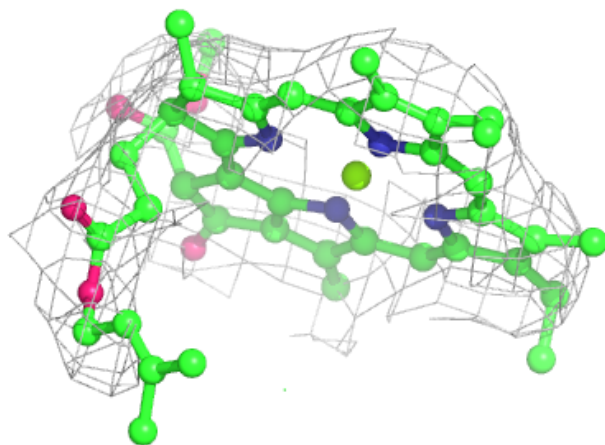
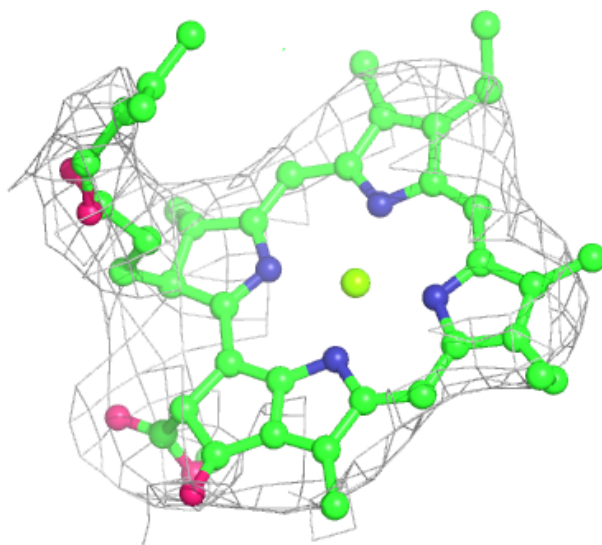
**Electron density around CLA A 806:**

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



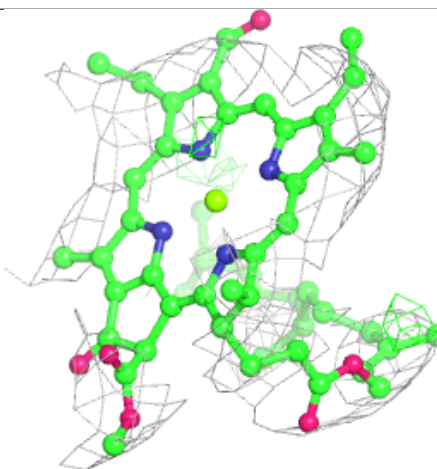
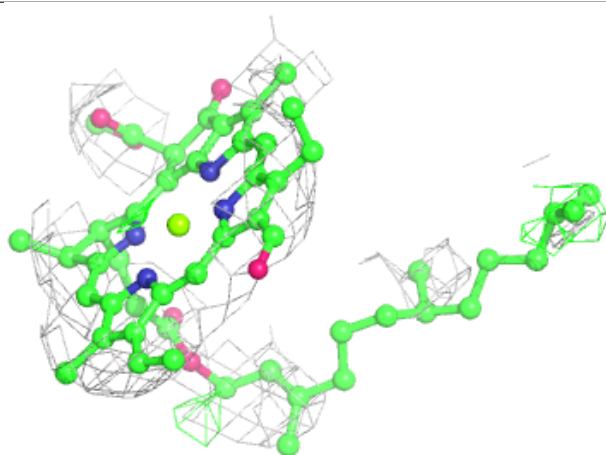
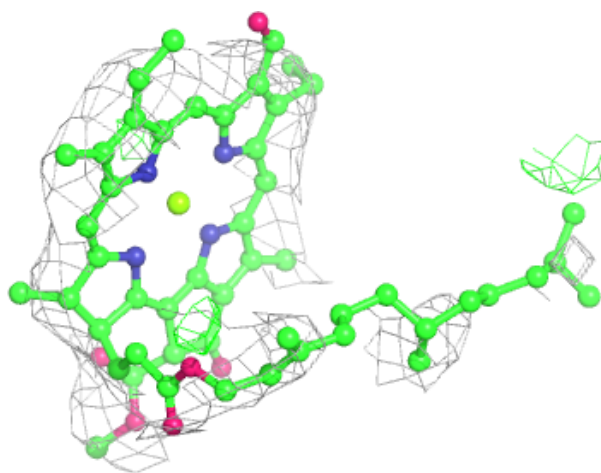
Electron density around CLA A 818:

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



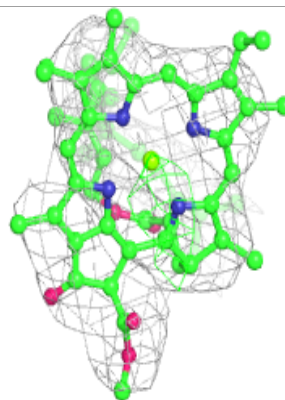
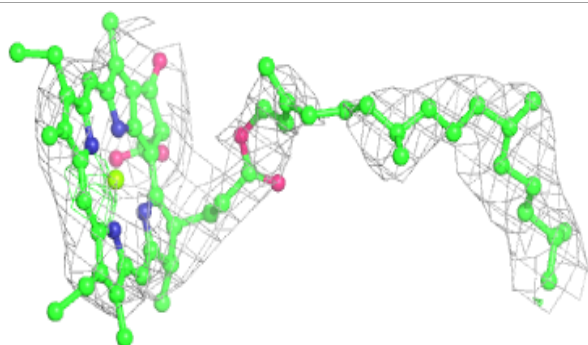
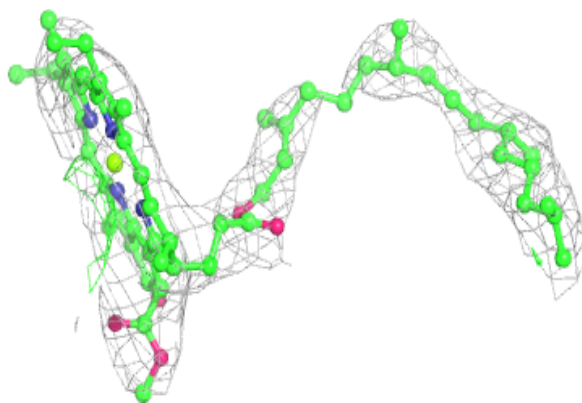
Electron density around CHL 1 5016:

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



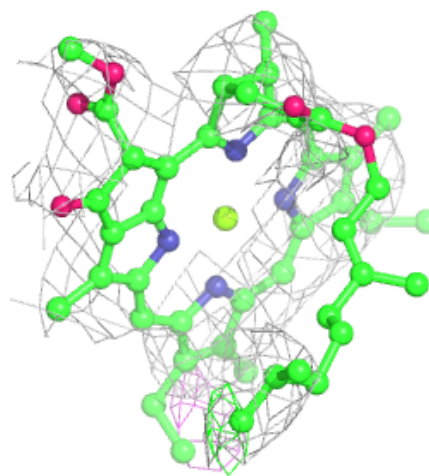
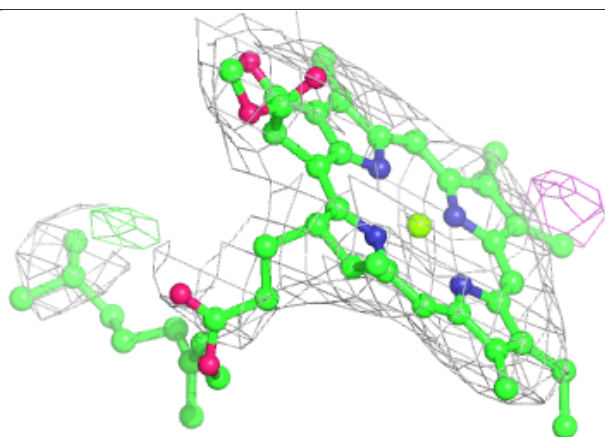
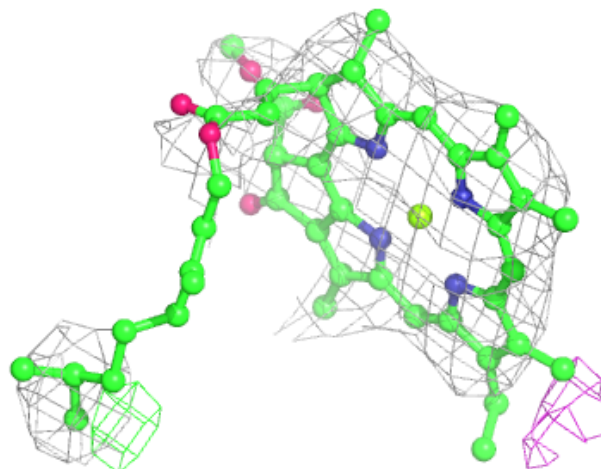
Electron density around CLA B 839:

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



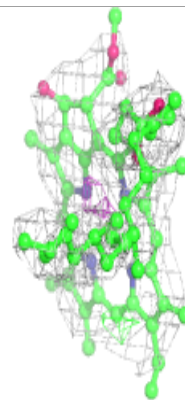
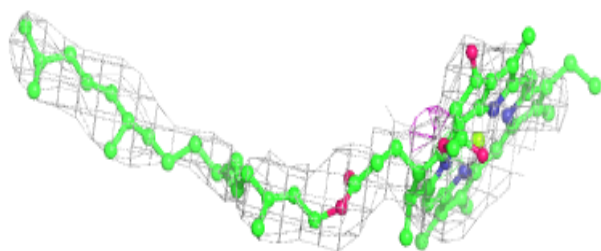
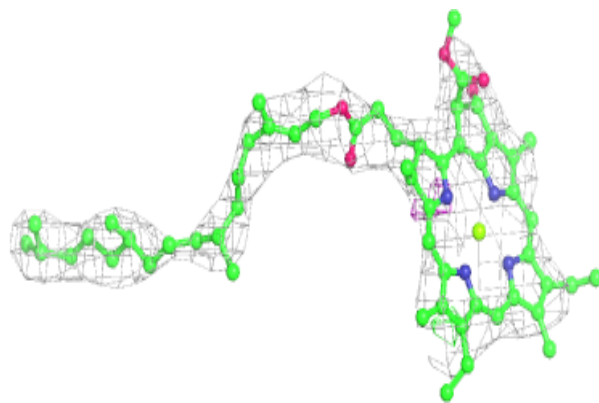
Electron density around CLA 2 317:

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

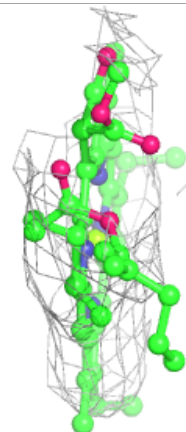
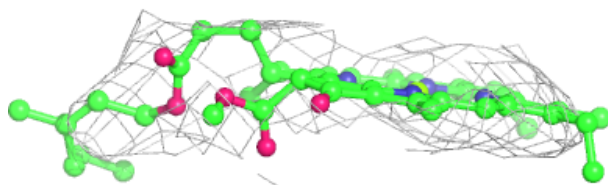
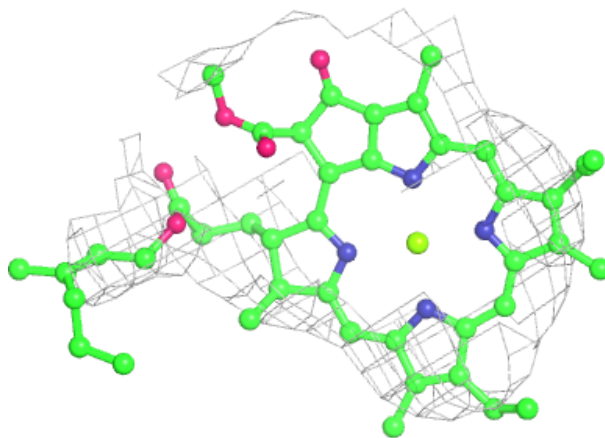


Electron density around CLA A 852:

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

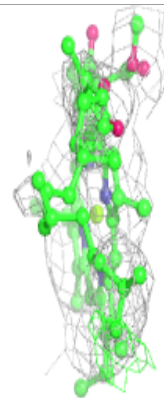
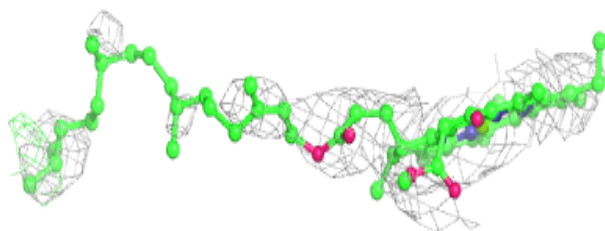
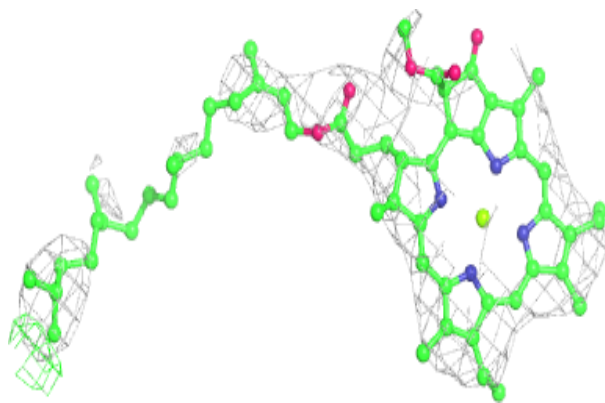
**Electron density around CLA 3 308:**

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

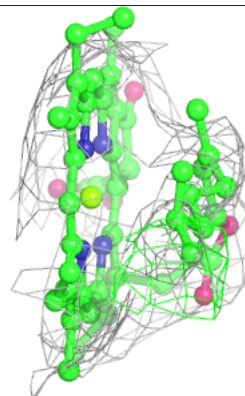
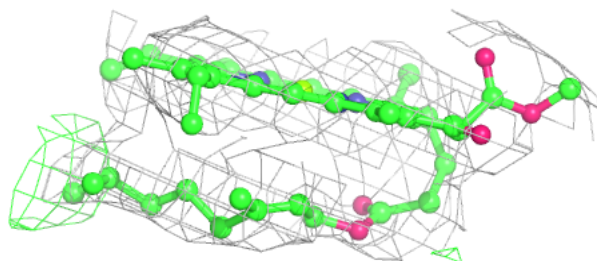
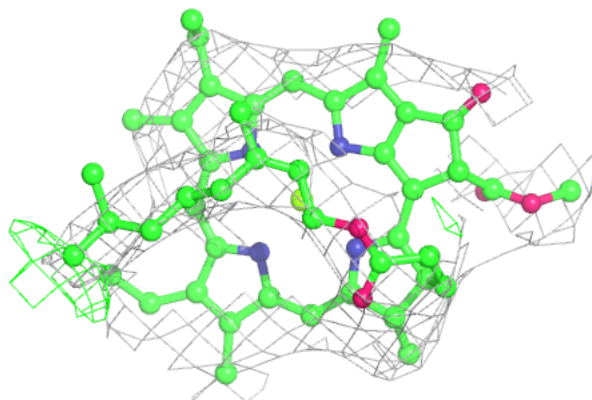


Electron density around CLA F 303:

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

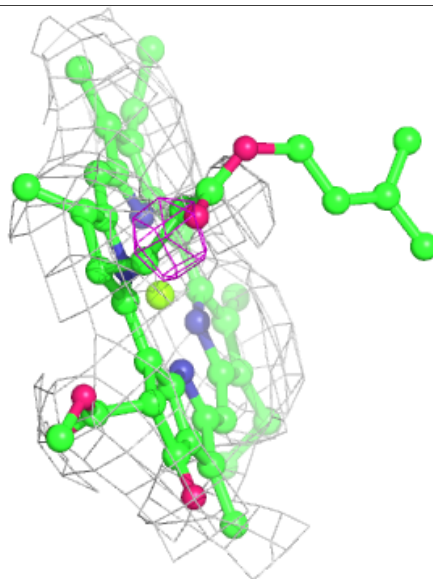
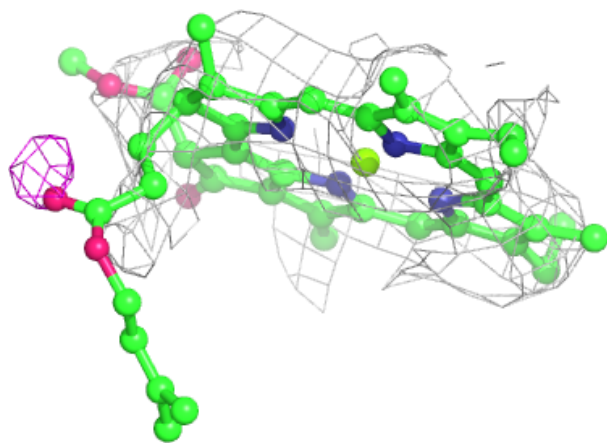
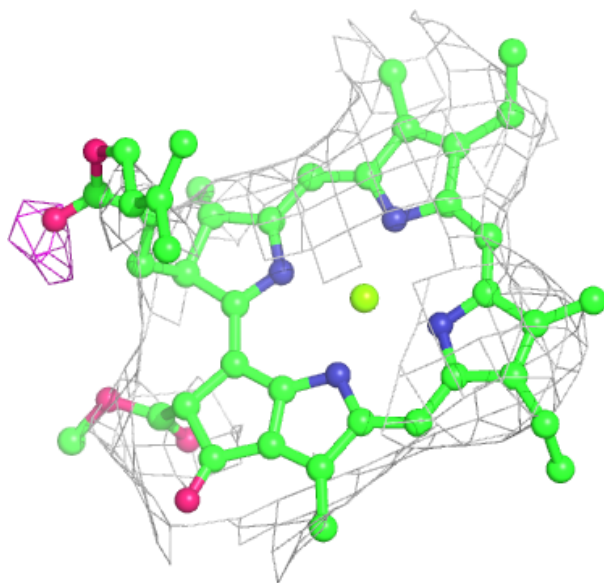
**Electron density around CLA A 811:**

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



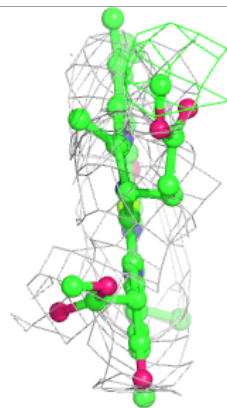
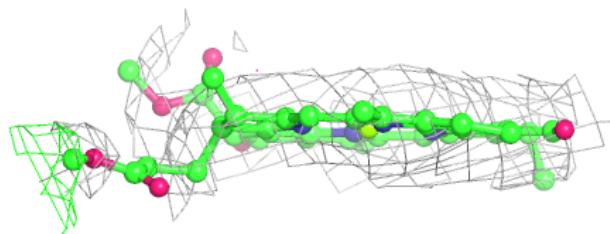
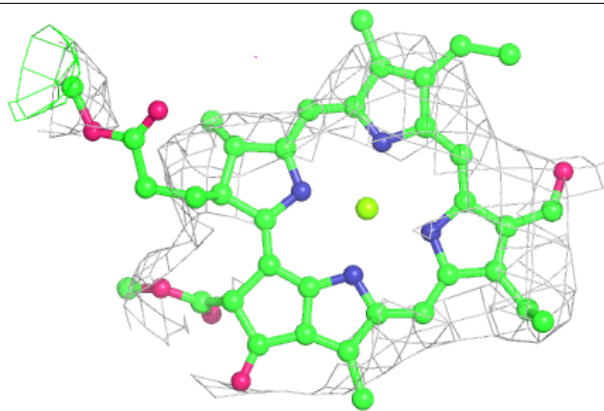
Electron density around CLA 3 317:

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



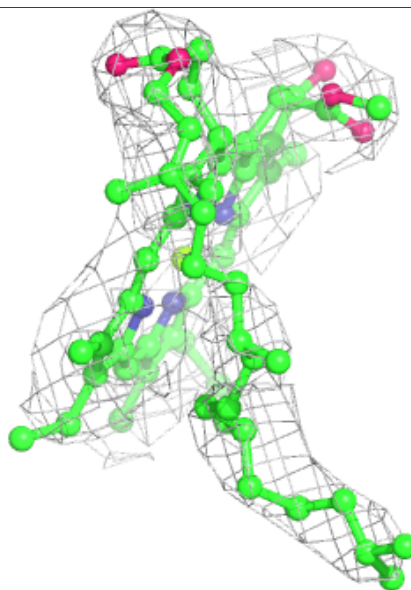
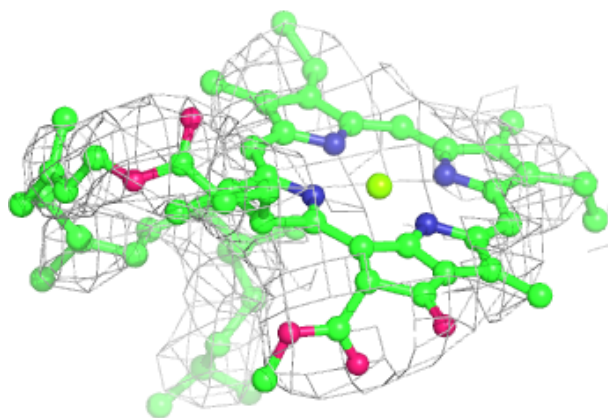
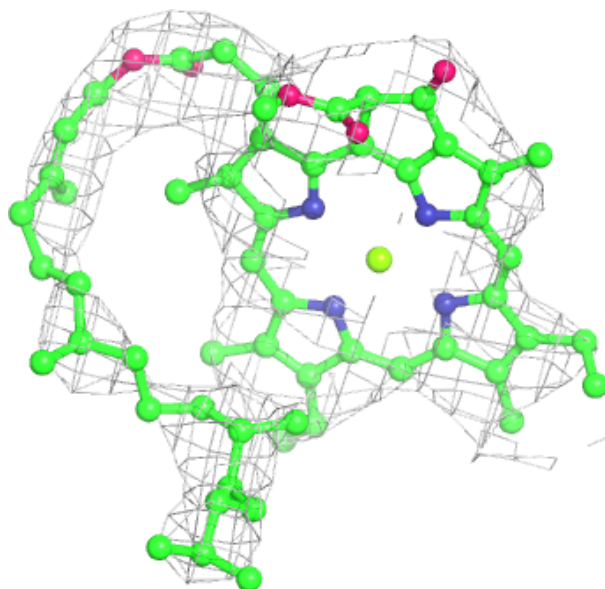
Electron density around CHL 4 313:

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



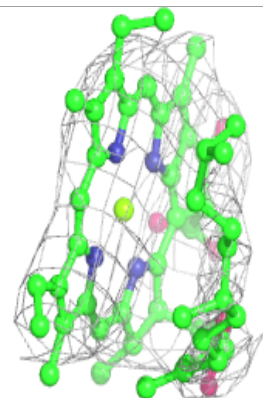
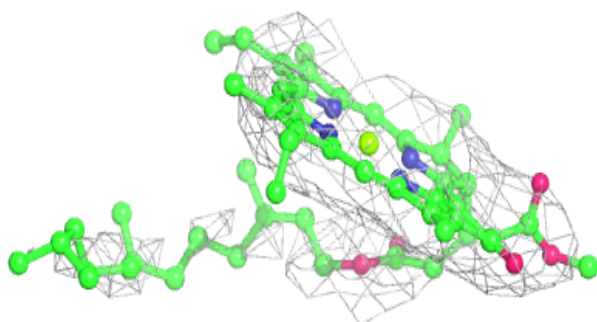
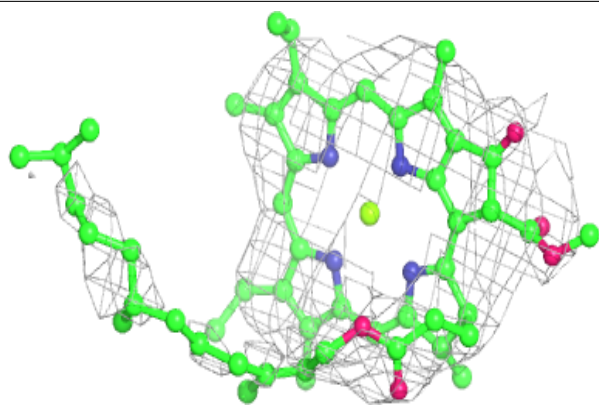
Electron density around CLA A 812:

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

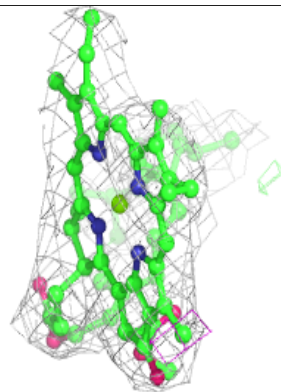
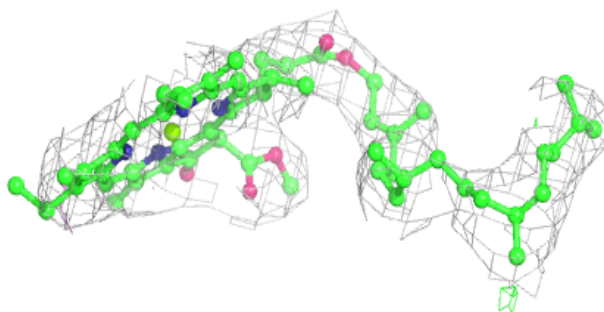
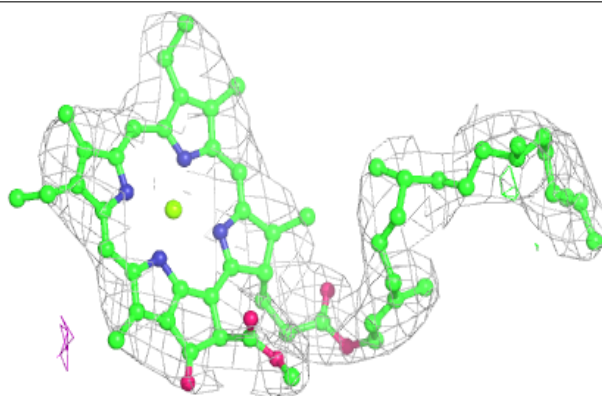


Electron density around CLA 4 305:

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

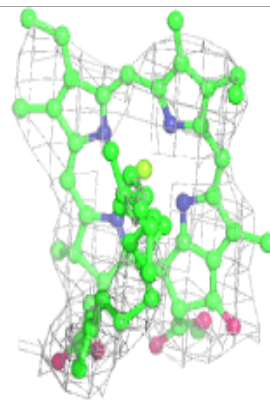
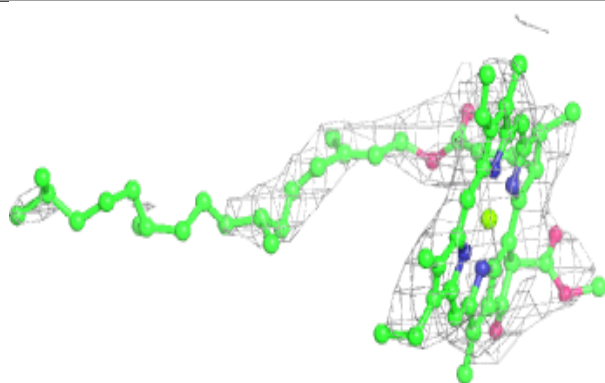
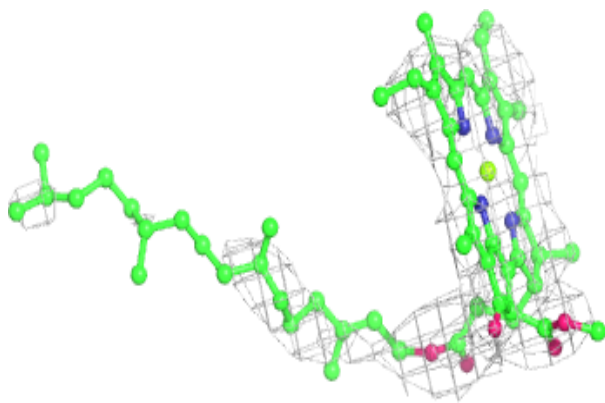
**Electron density around CLA J 1101:**

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

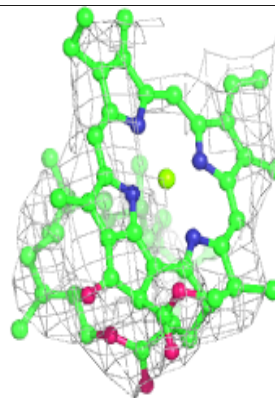
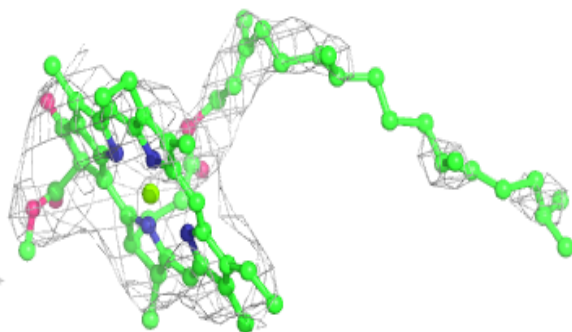
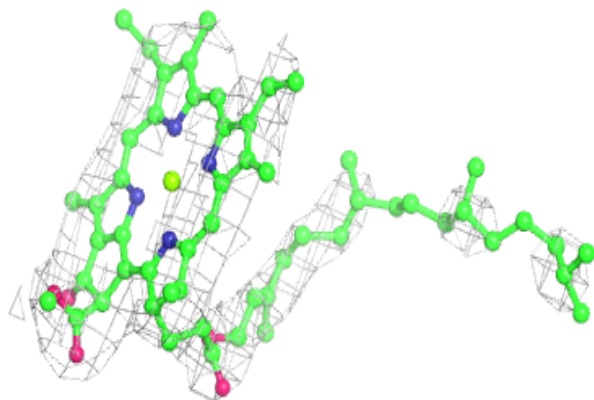


Electron density around CLA B 830:

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

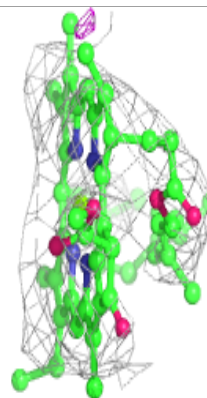
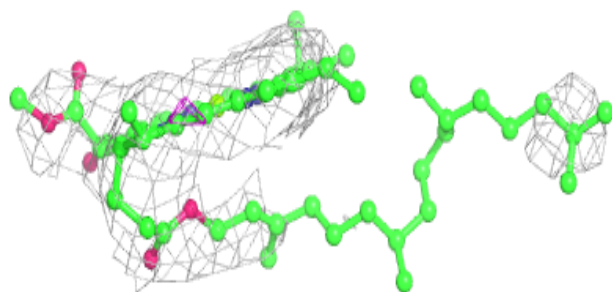
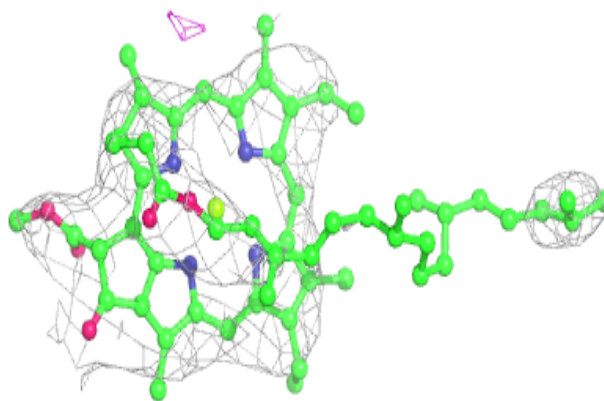
**Electron density around CLA B 815:**

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



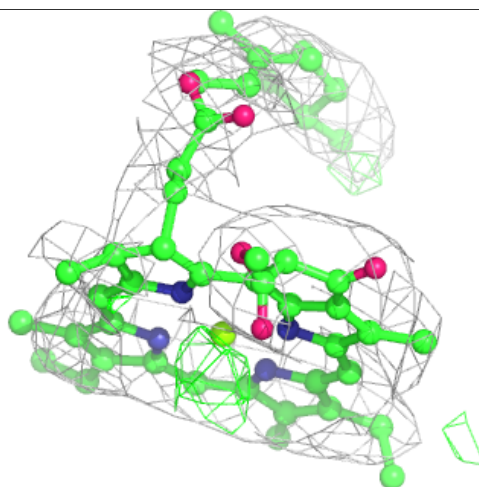
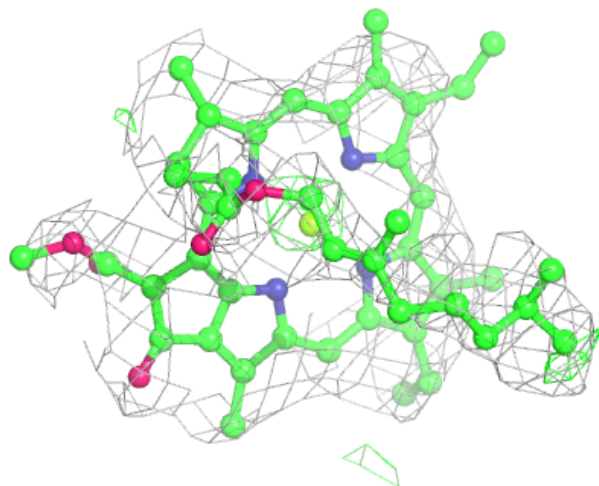
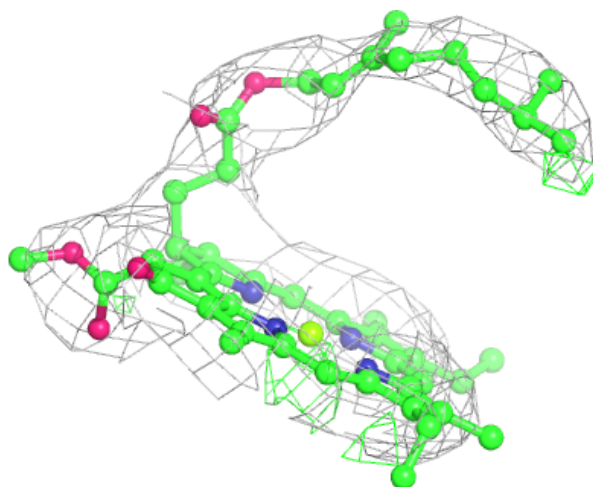
Electron density around CLA A 835:

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



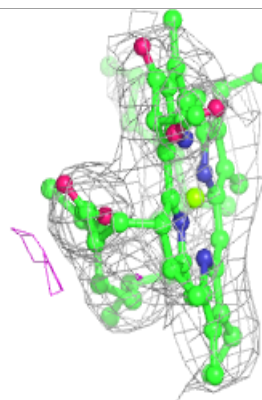
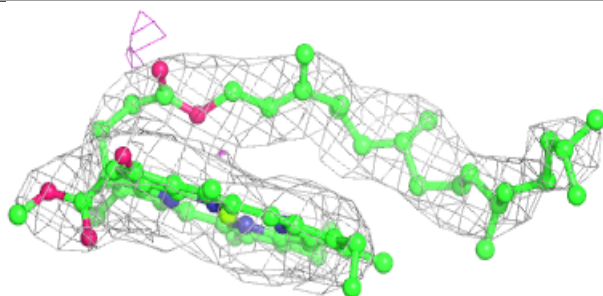
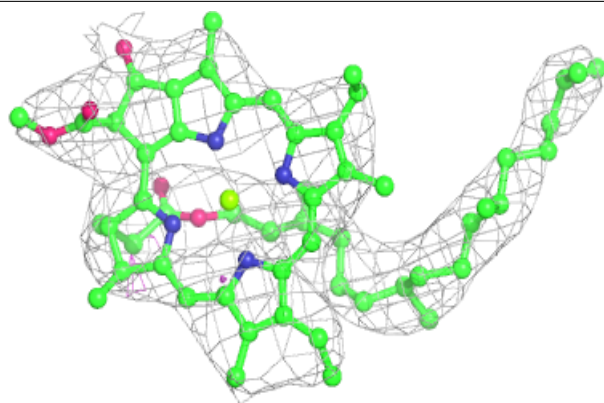
Electron density around CLA L 301:

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

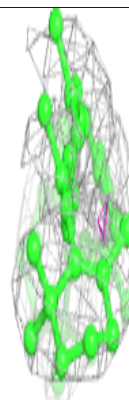
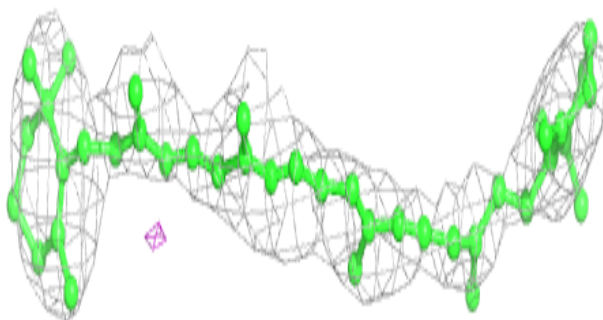
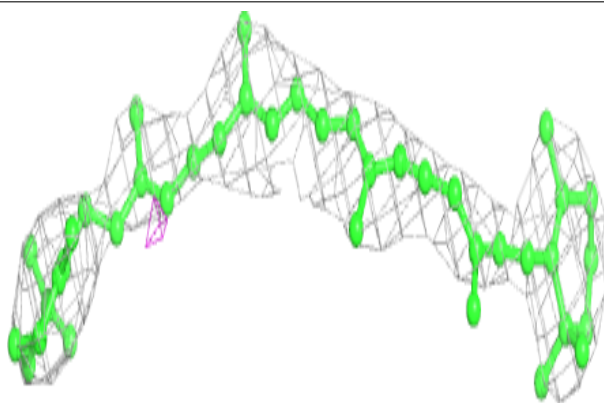


Electron density around CLA B 837:

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

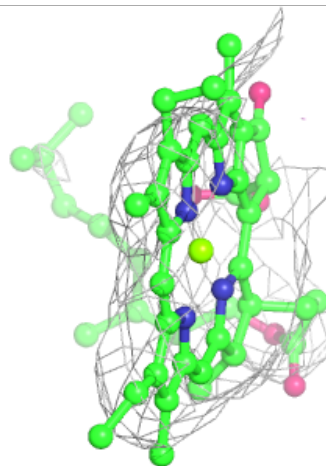
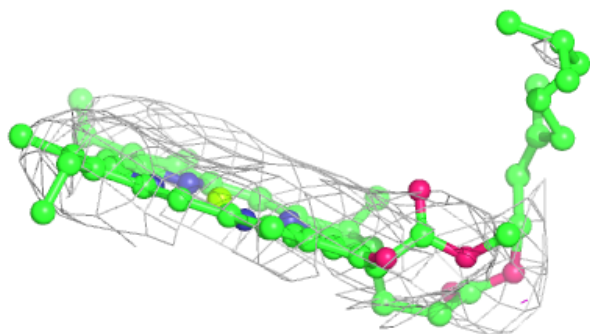
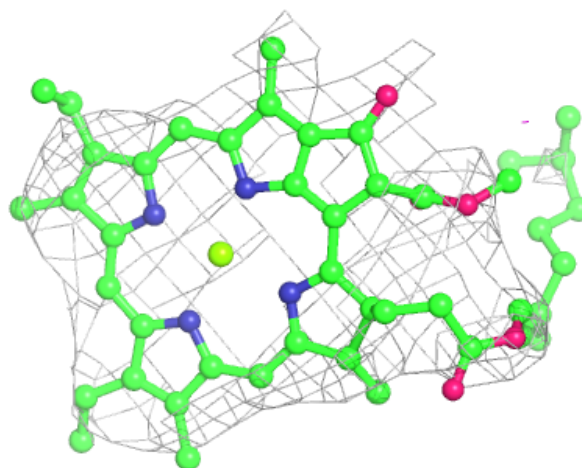
**Electron density around BCR F 304:**

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



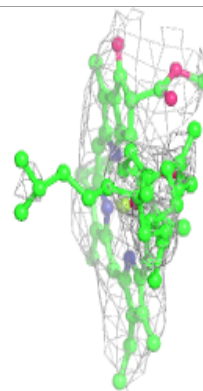
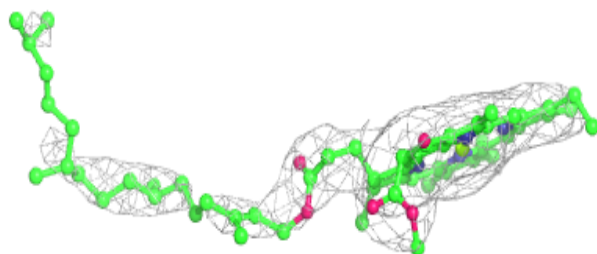
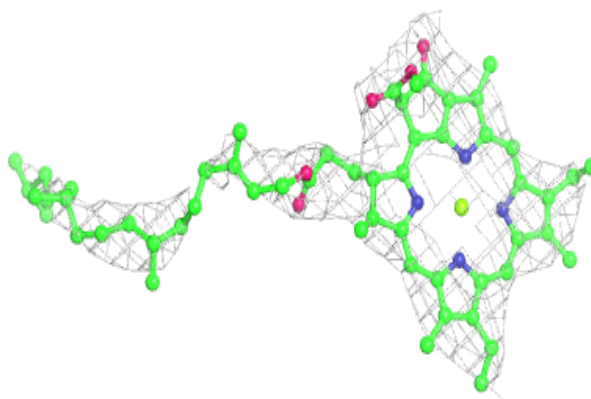
Electron density around CLA 3 311:

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

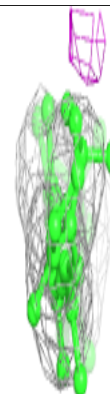
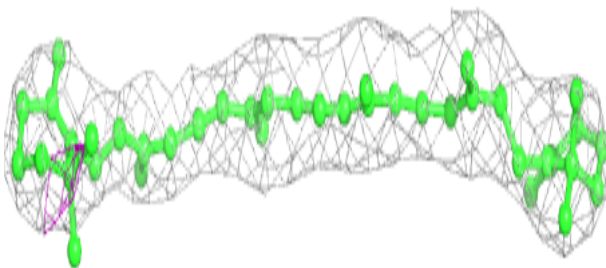
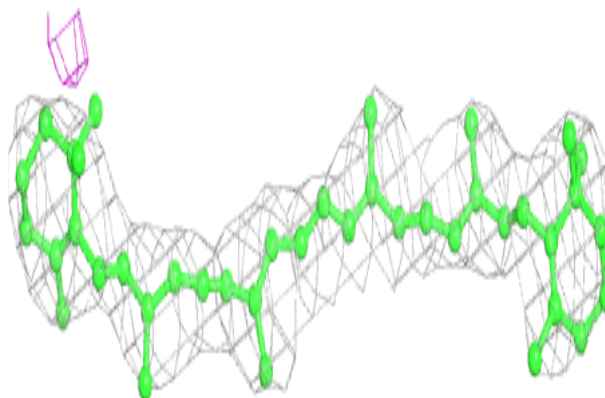


Electron density around CLA A 804:

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

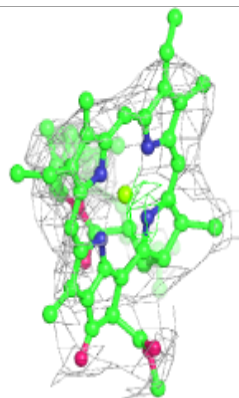
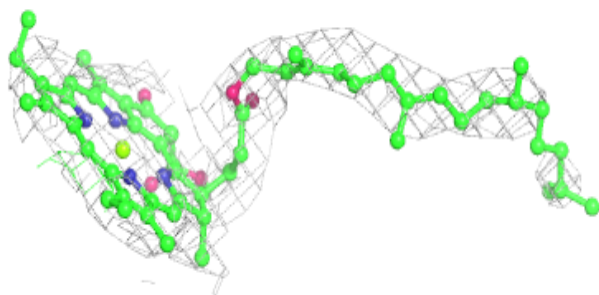
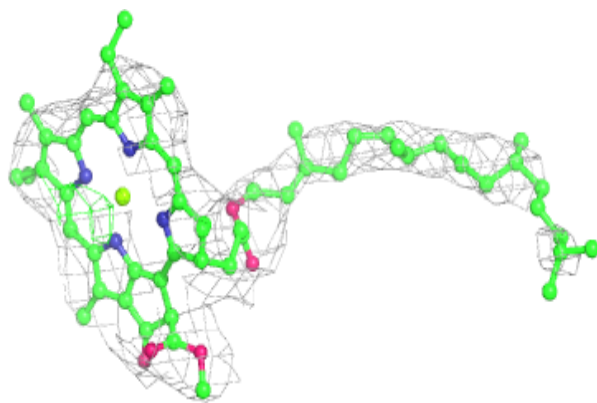
**Electron density around BCR J 1104:**

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

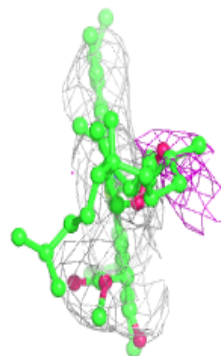
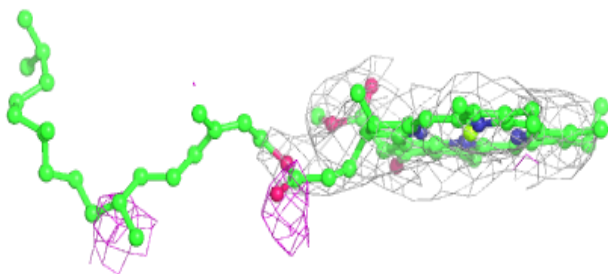
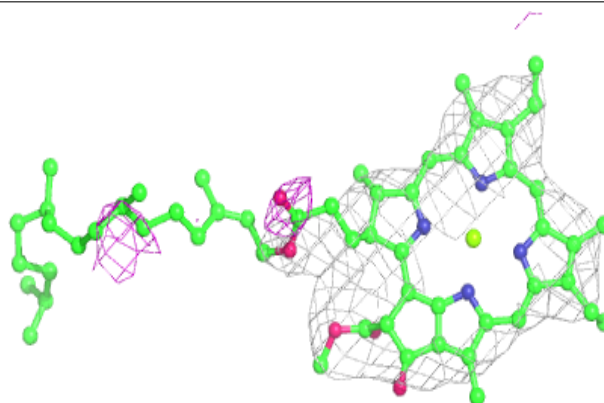


Electron density around CLA A 819:

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

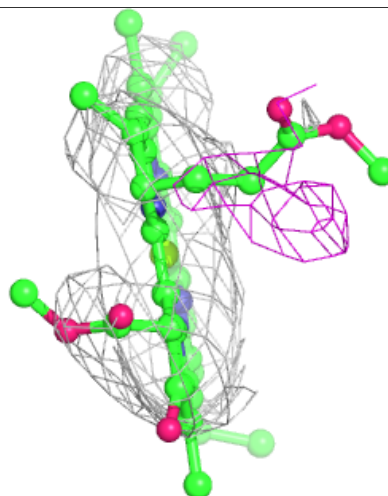
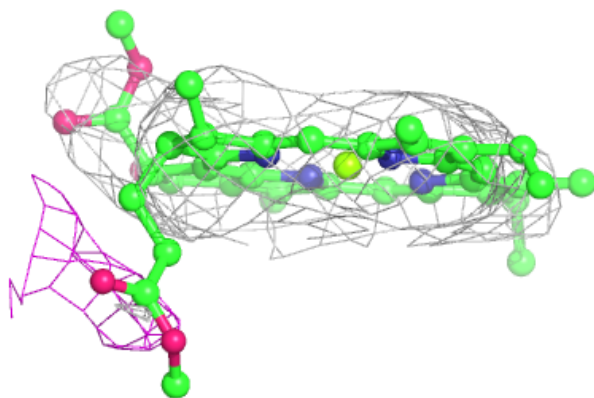
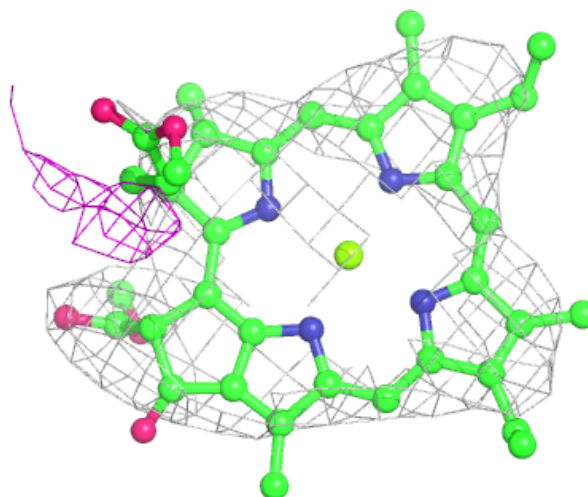
**Electron density around CLA F 302:**

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



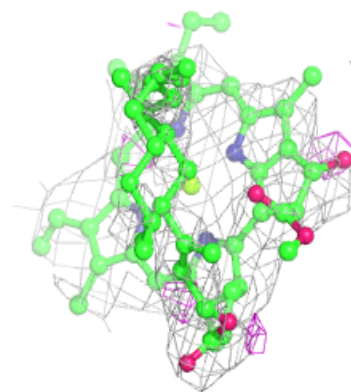
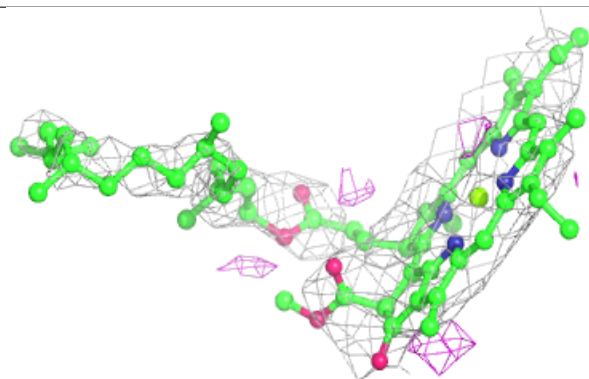
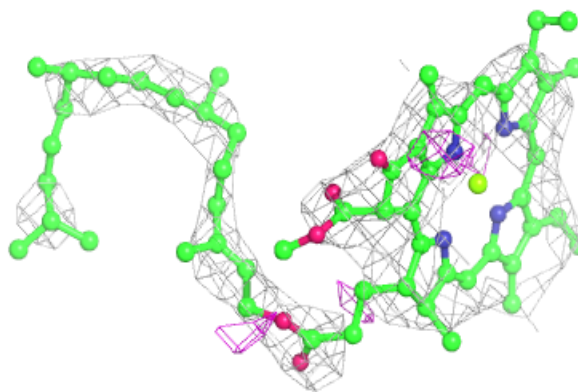
Electron density around CLA B 821:

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



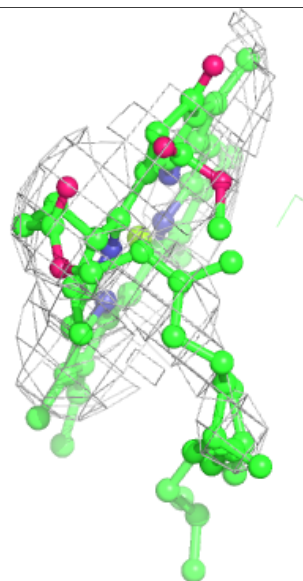
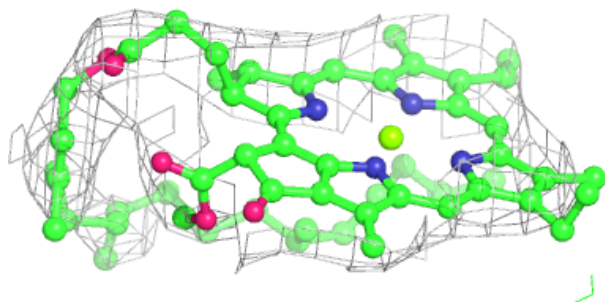
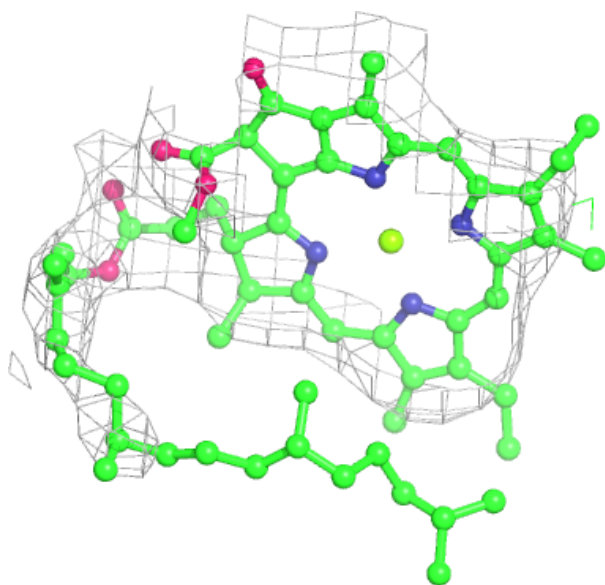
Electron density around CL0 A 801:

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



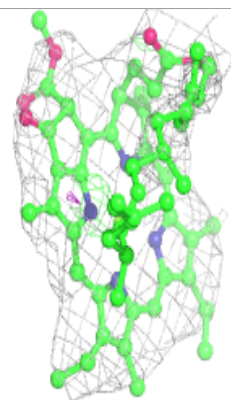
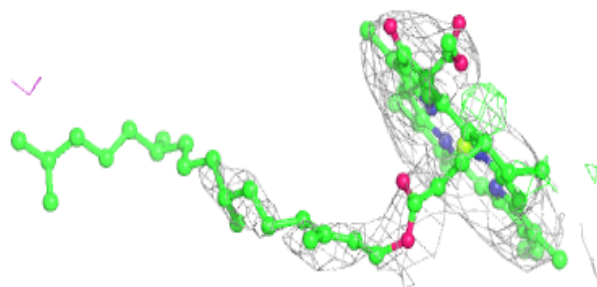
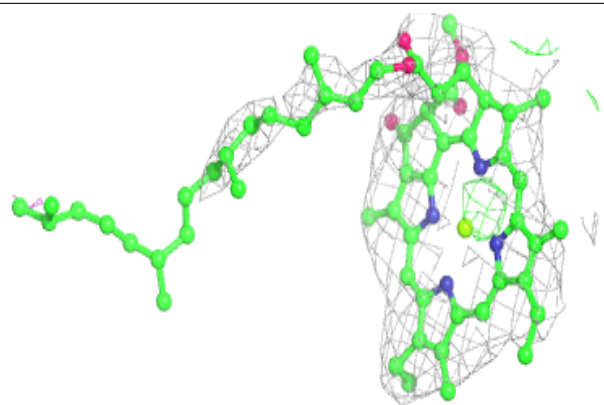
Electron density around CLA 1 5010:

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

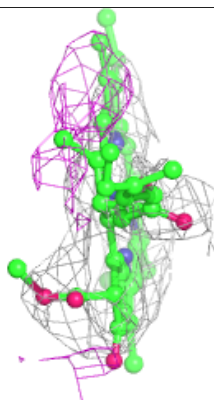
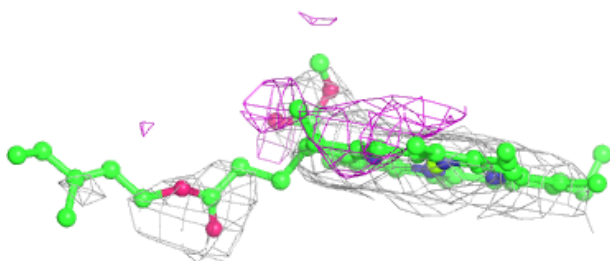
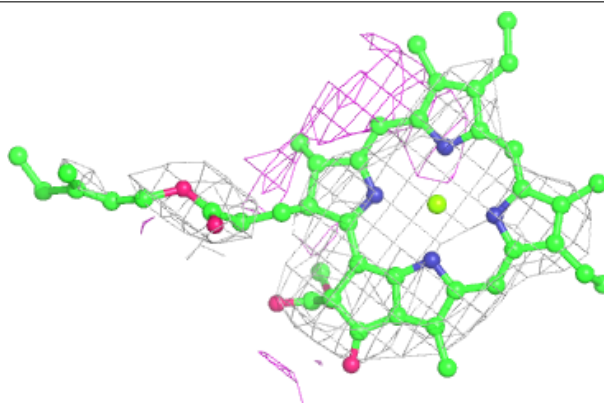


Electron density around CLA B 823:

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

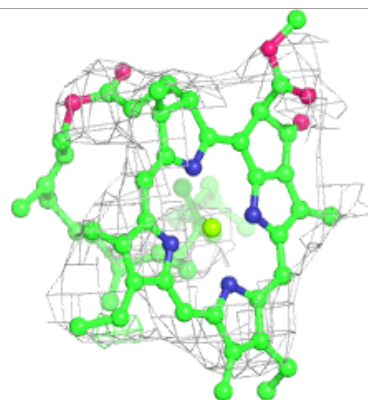
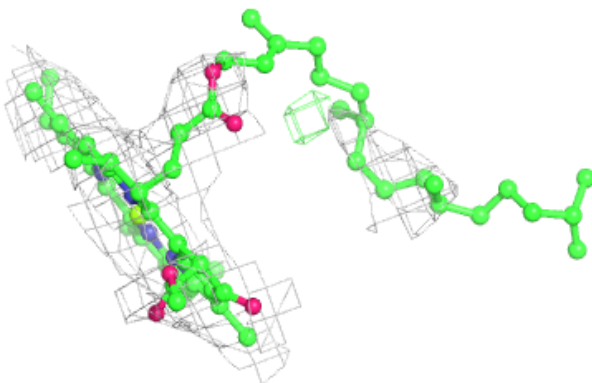
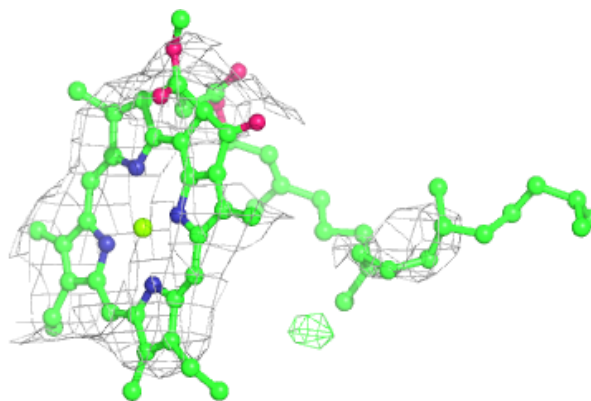
**Electron density around CLA A 834:**

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

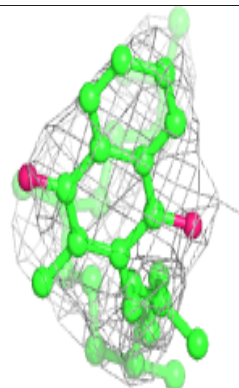
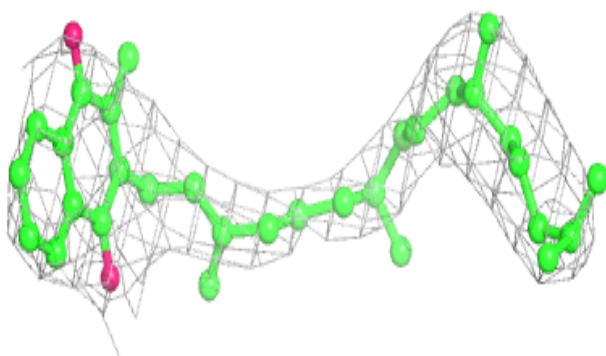
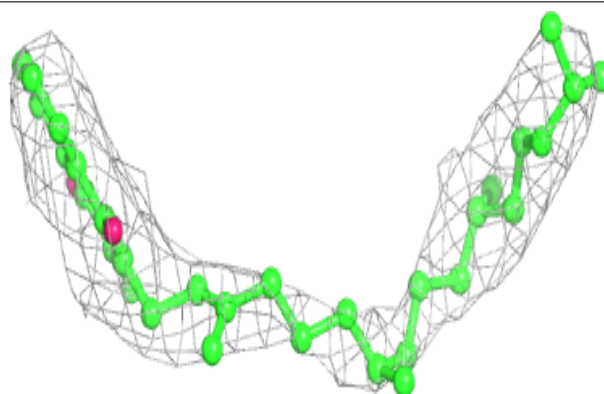


Electron density around CLA 4 315:

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

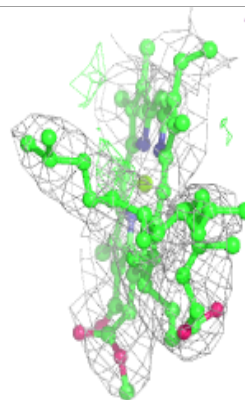
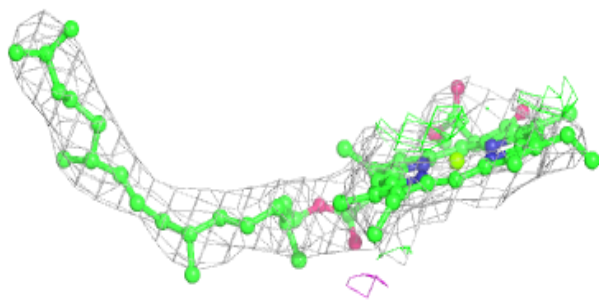
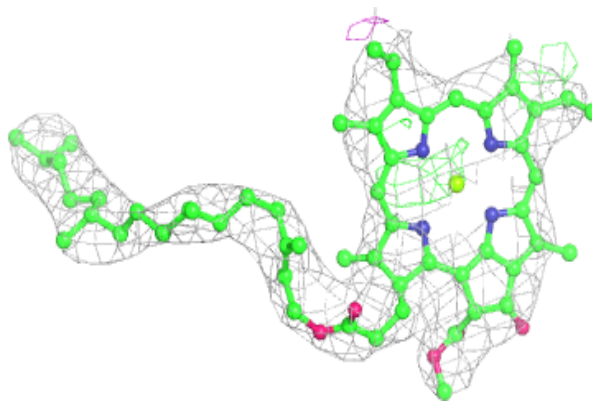
**Electron density around PQN B 842:**

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



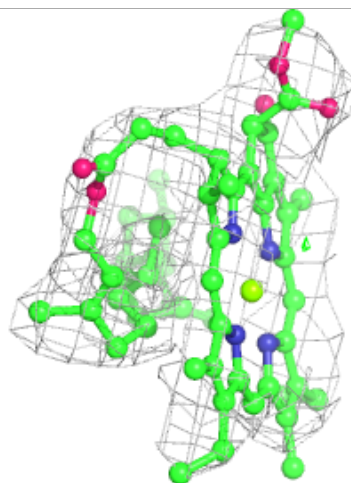
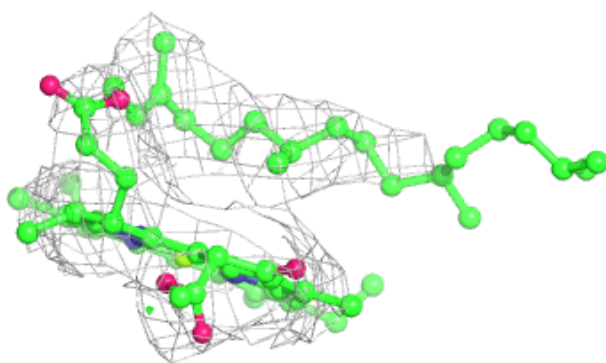
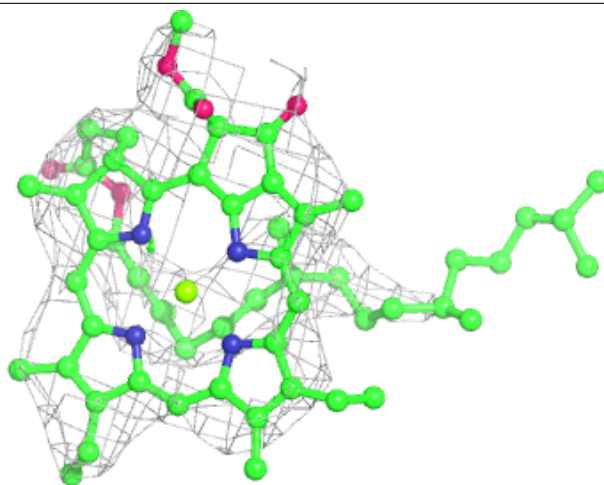
Electron density around CLA B 804:

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



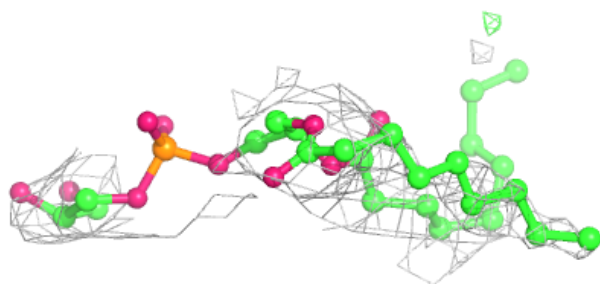
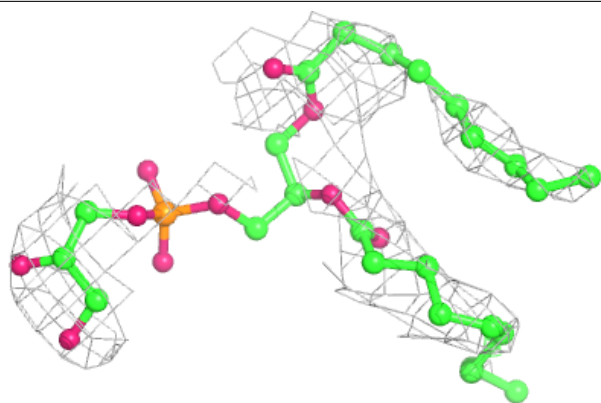
Electron density around CLA B 828:

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

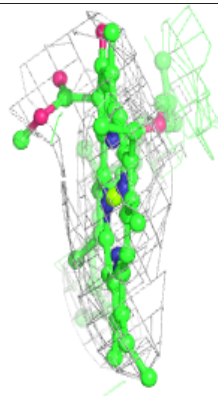
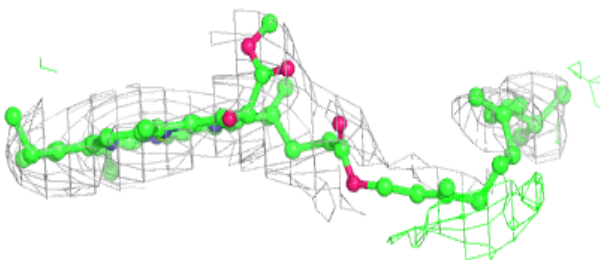
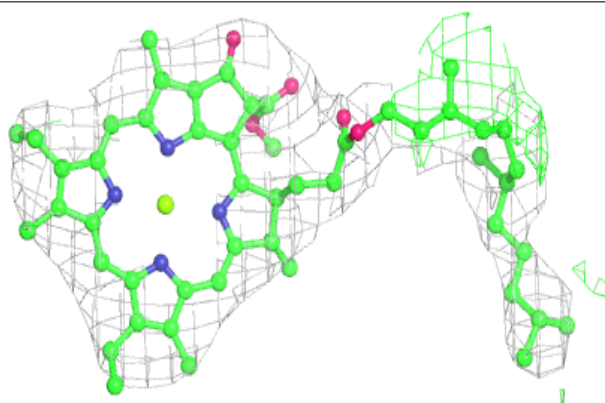


Electron density around LHG 2 320:

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

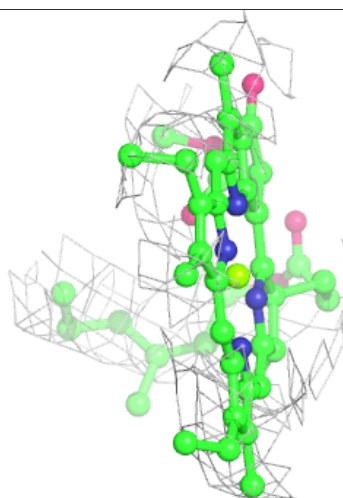
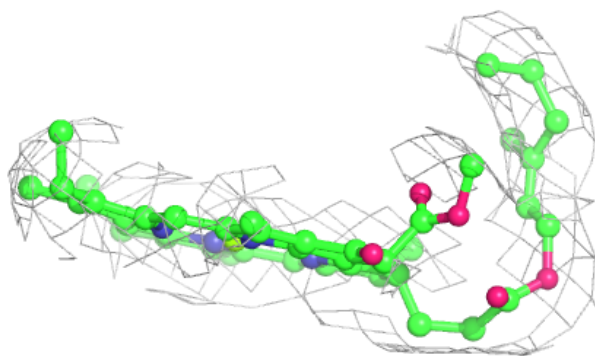
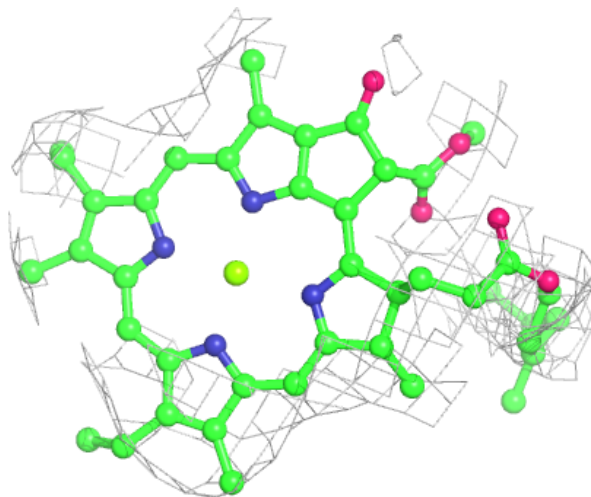
**Electron density around CLA 1 5018:**

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



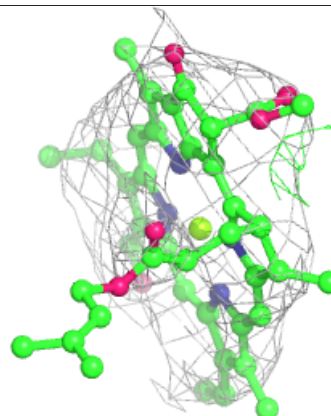
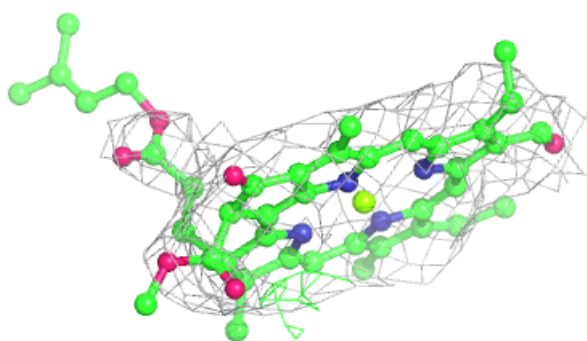
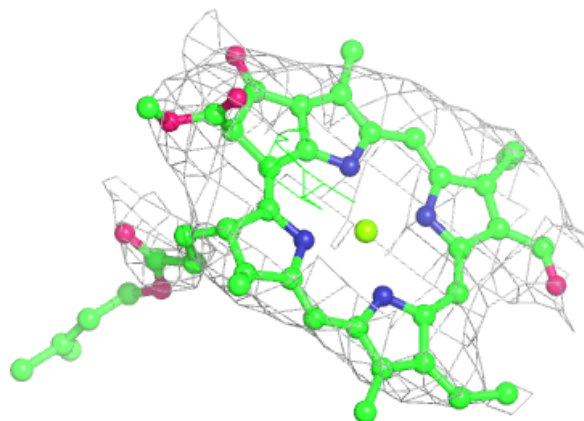
Electron density around CLA 2 307:

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



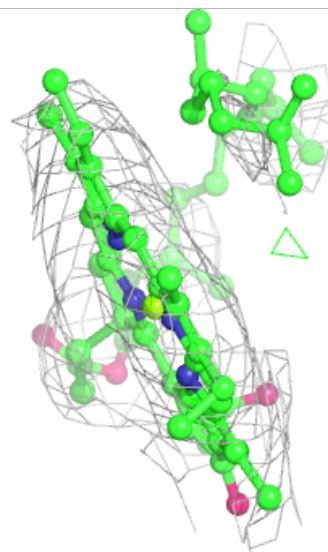
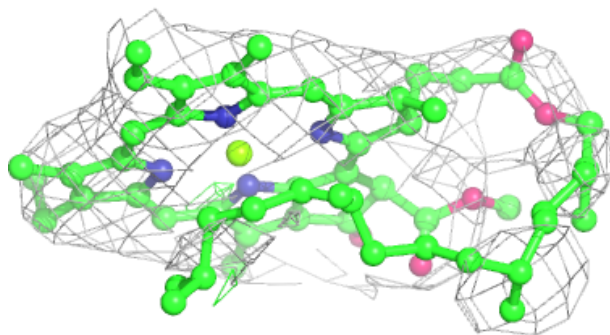
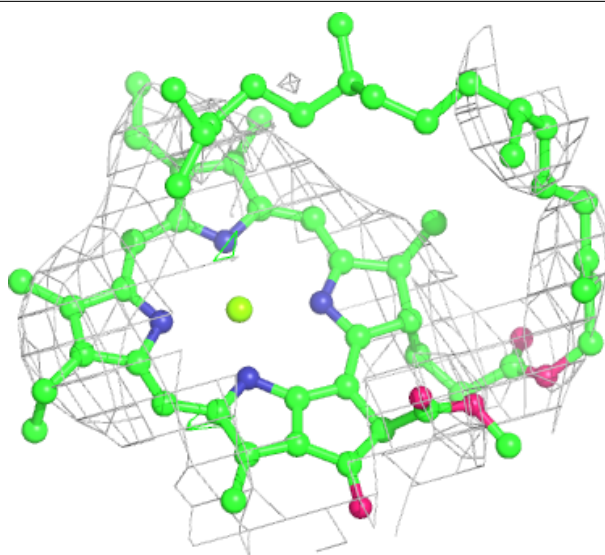
Electron density around CHL 4 314:

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



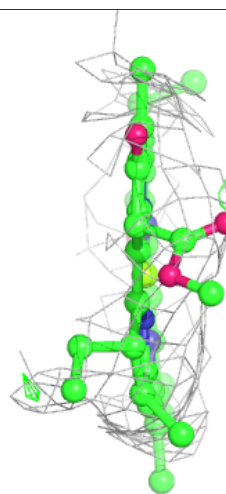
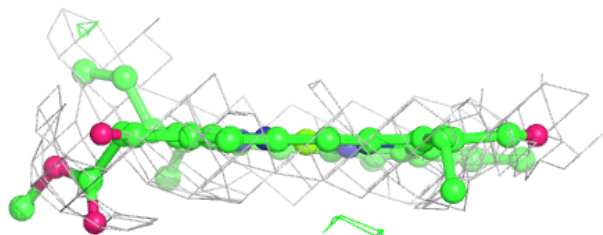
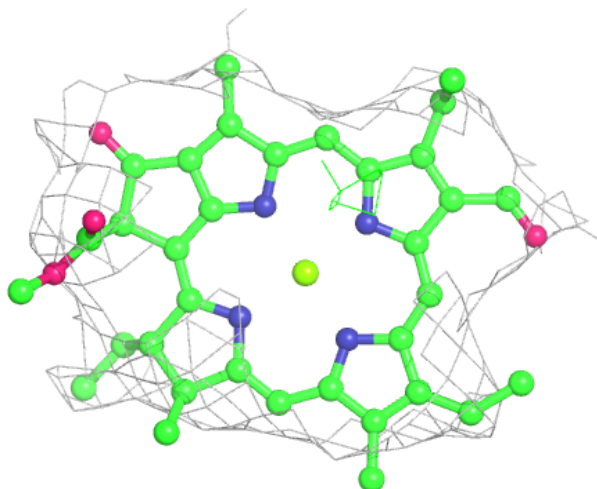
Electron density around CLA 2 310:

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



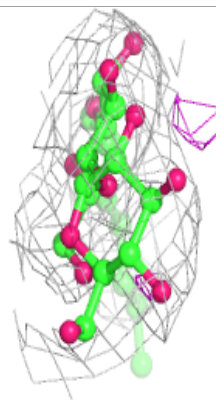
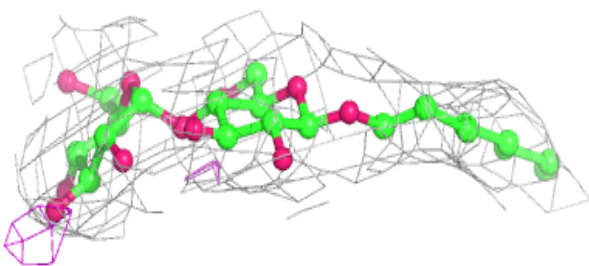
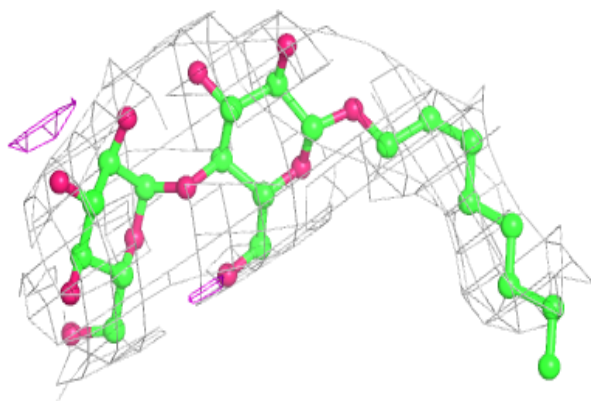
Electron density around CHL 4 317:

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

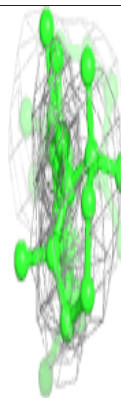
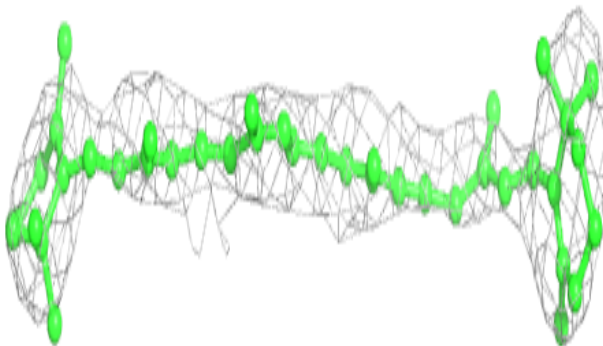
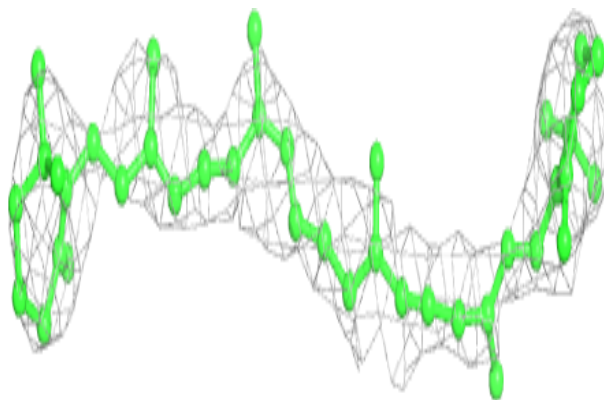


Electron density around LMT B 856:

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

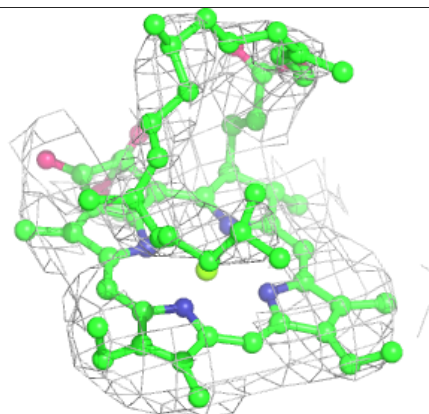
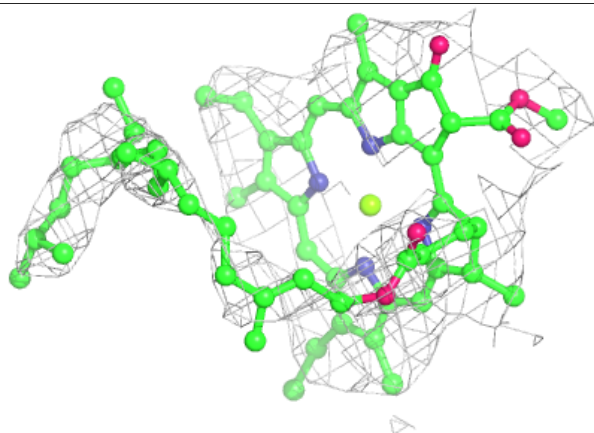
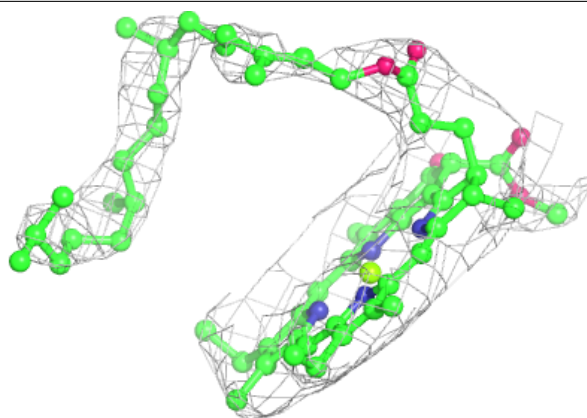
**Electron density around BCR B 802:**

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

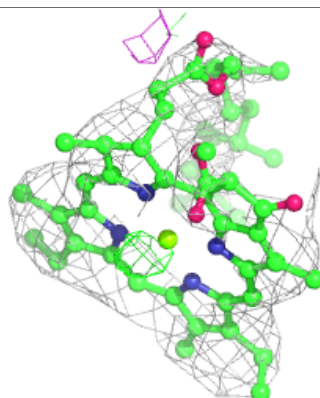
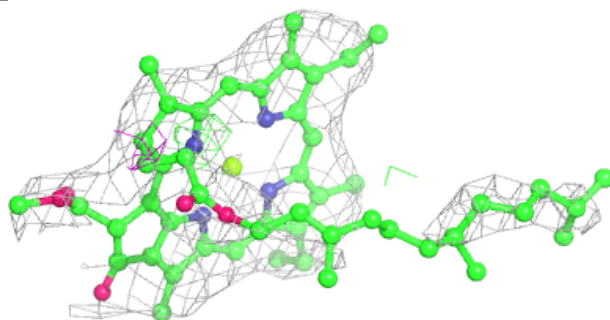
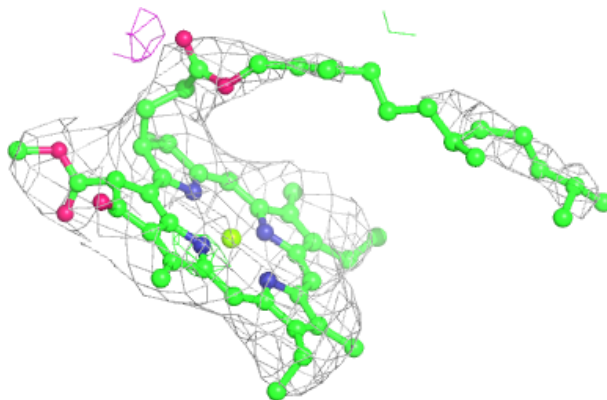


Electron density around CLA B 831:

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

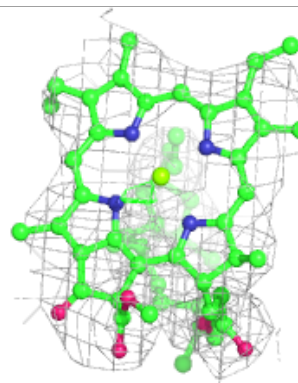
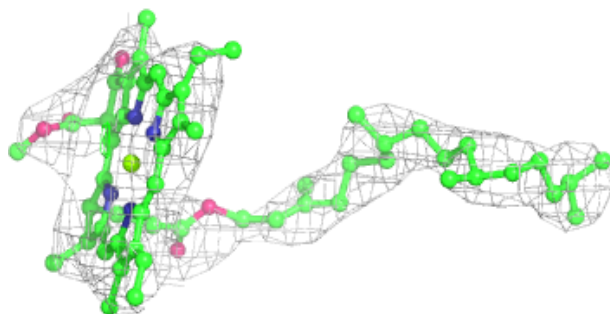
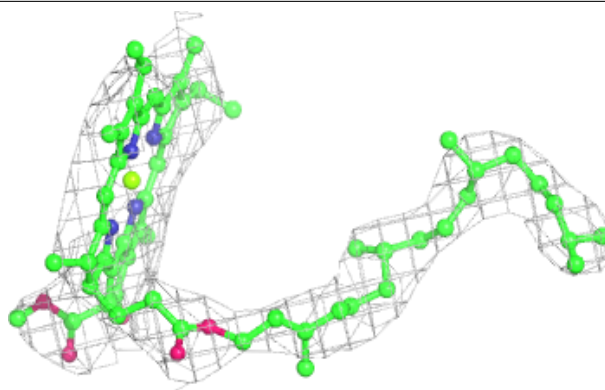
**Electron density around CLA B 832:**

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

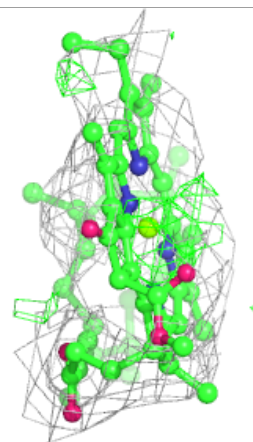
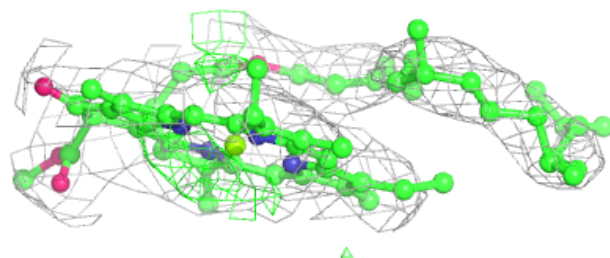
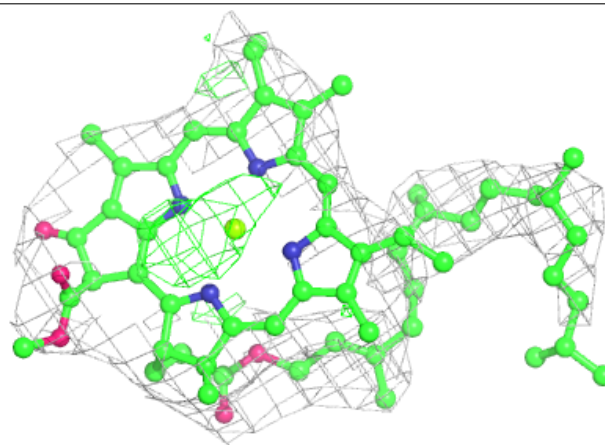


Electron density around CLA A 828:

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

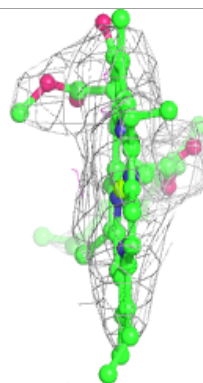
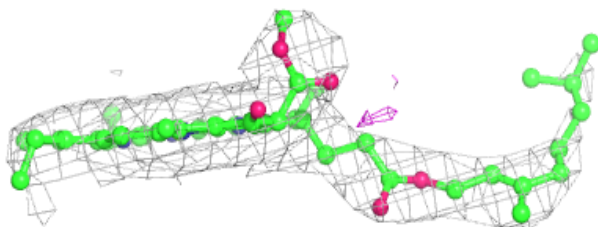
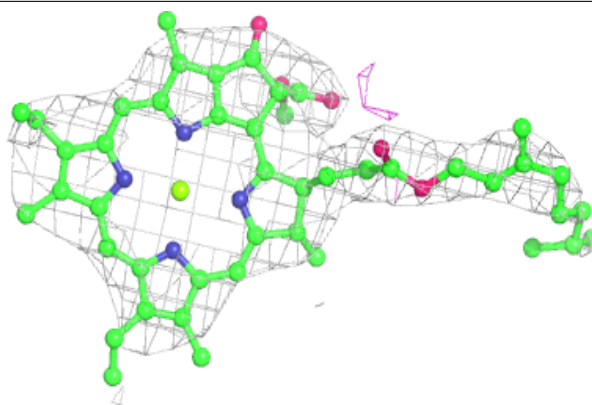
**Electron density around CLA A 817:**

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

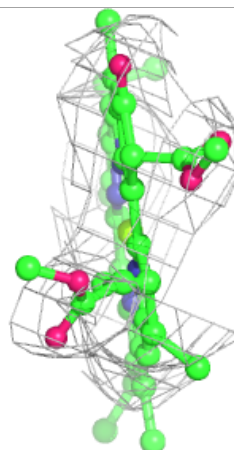
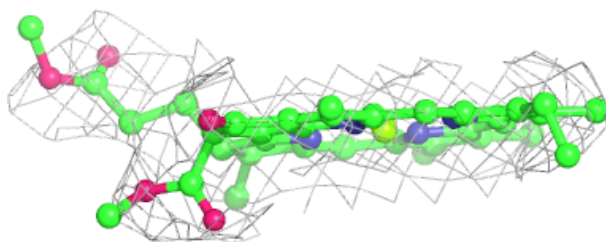
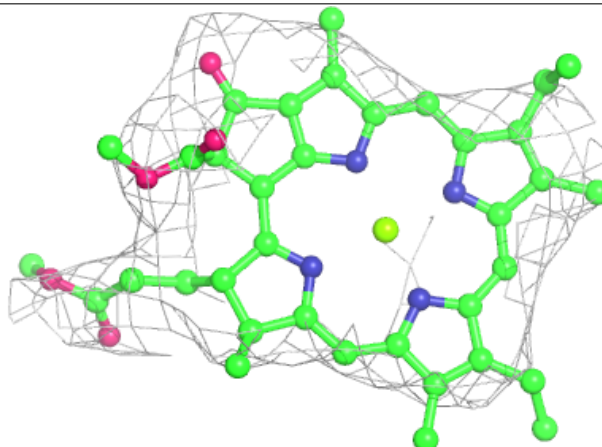


Electron density around CLA B 836:

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

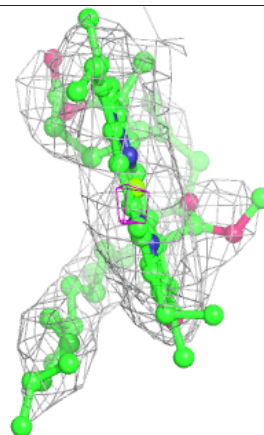
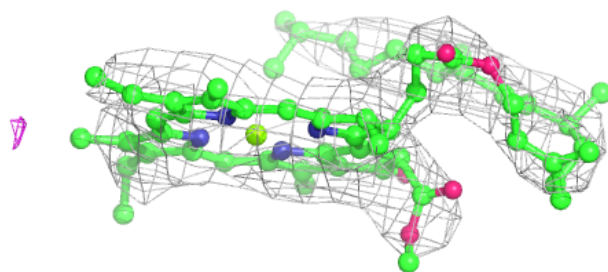
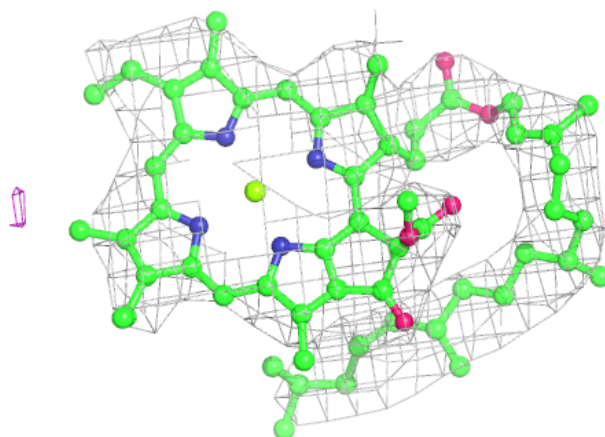
**Electron density around CLA 3 318:**

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



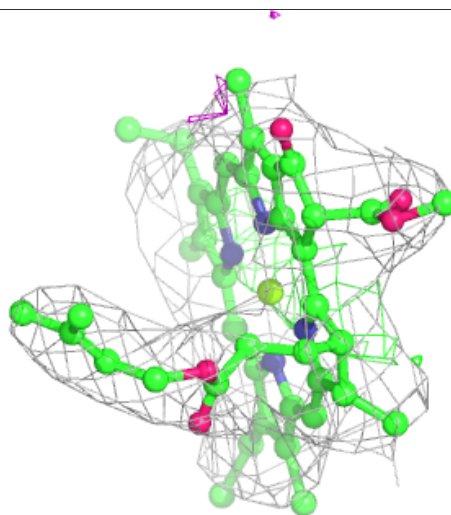
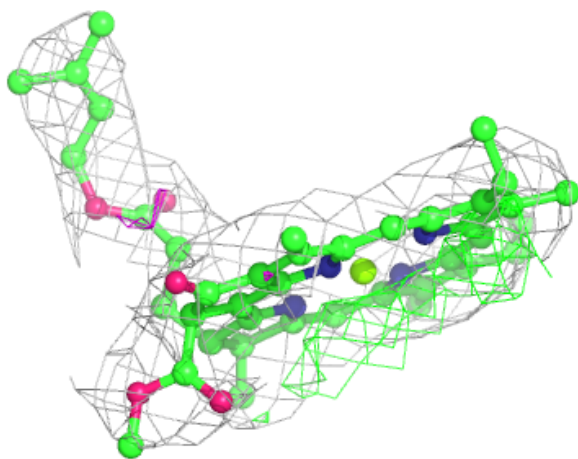
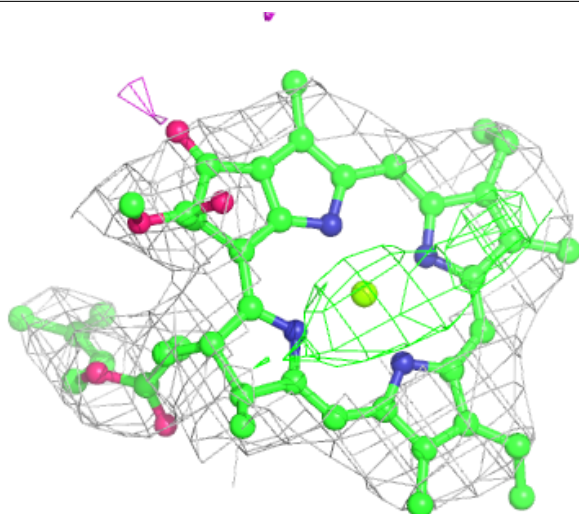
Electron density around CLA B 806:

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



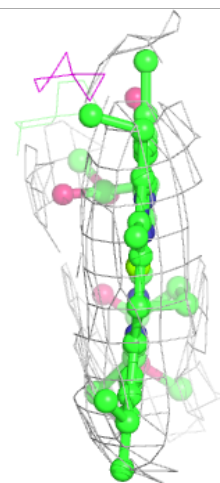
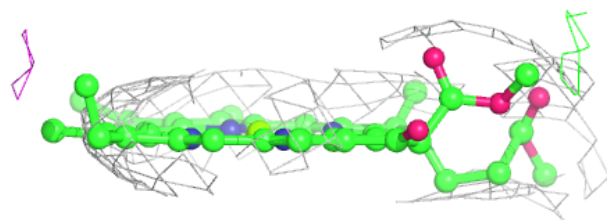
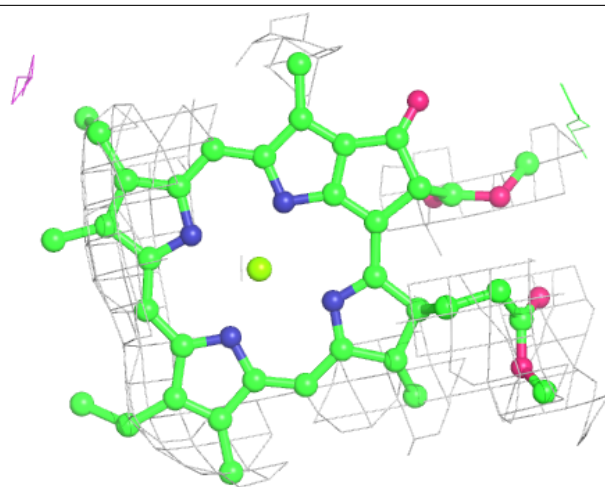
Electron density around CLA B 838:

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



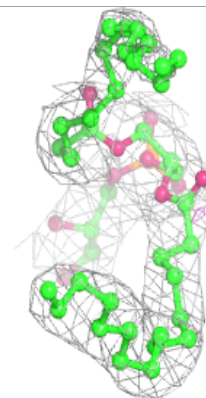
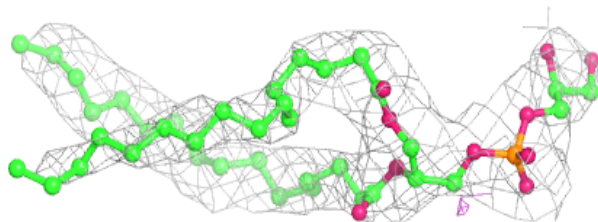
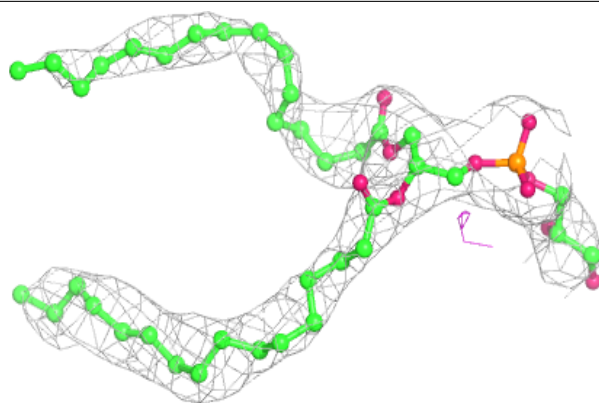
Electron density around CLA 1 5007:

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

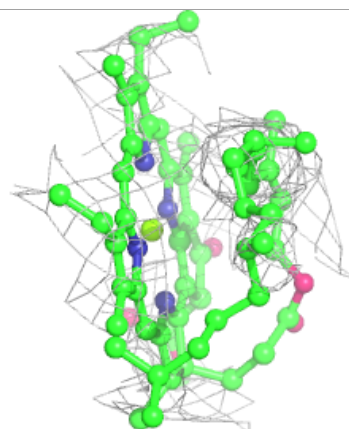
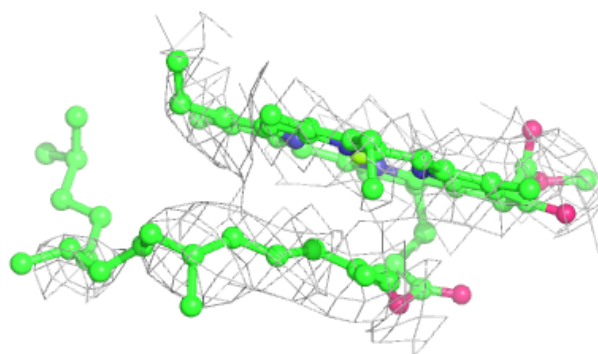
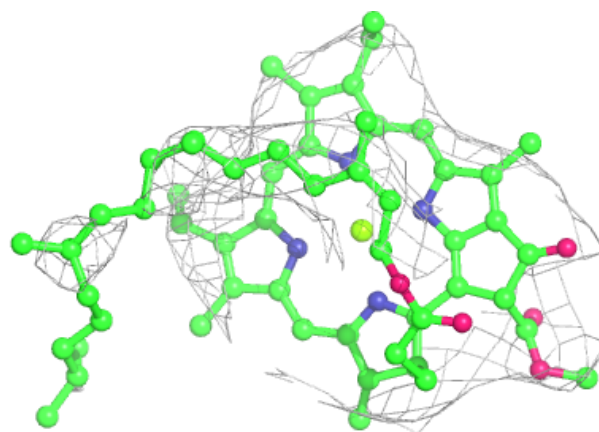


Electron density around LHG A 848:

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

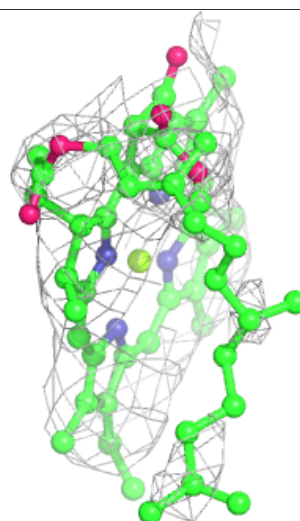
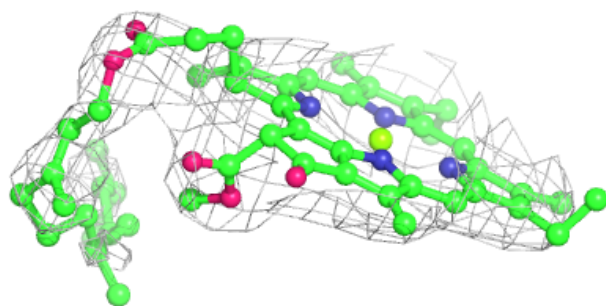
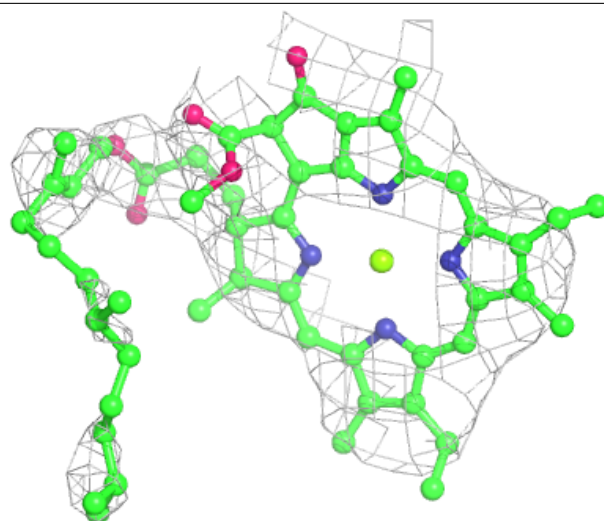
**Electron density around CLA 4 307:**

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



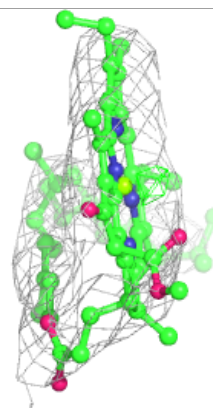
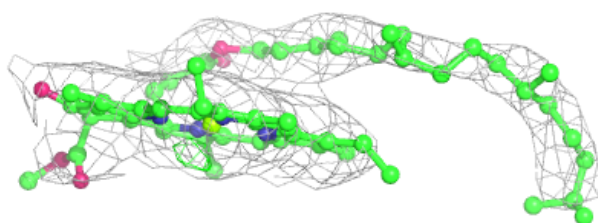
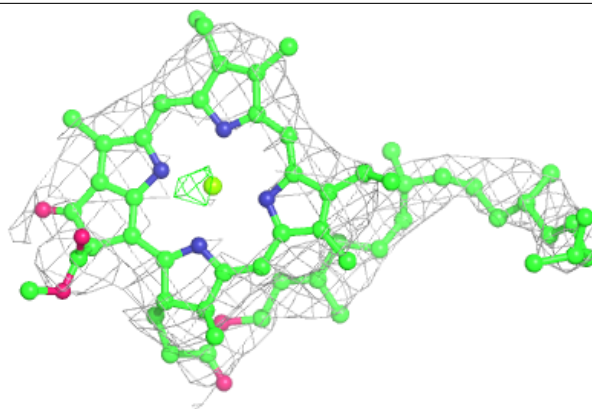
Electron density around CLA 4 309:

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

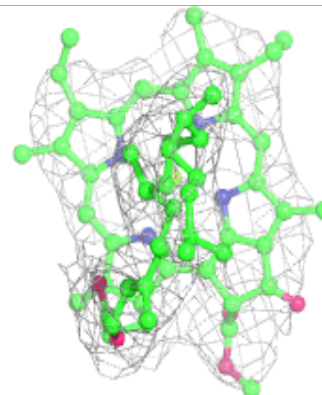
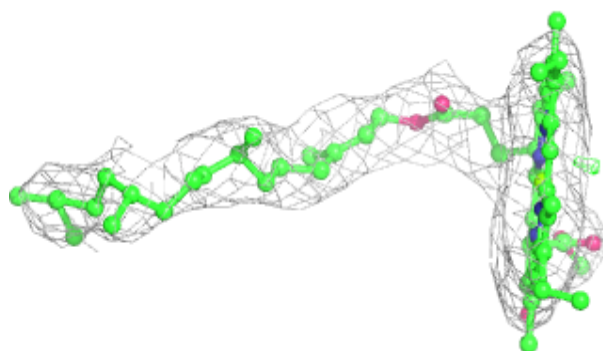
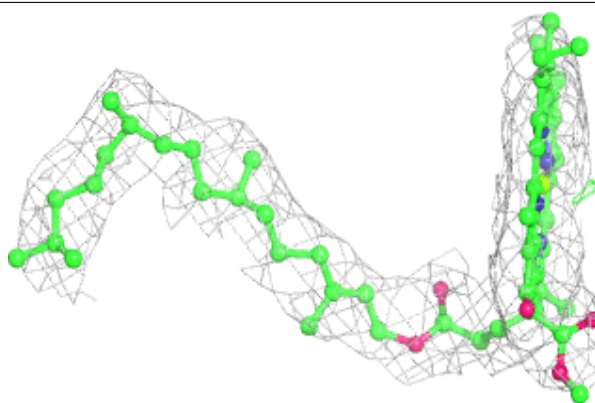


Electron density around CLA B 819:

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

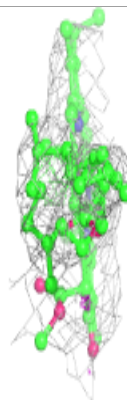
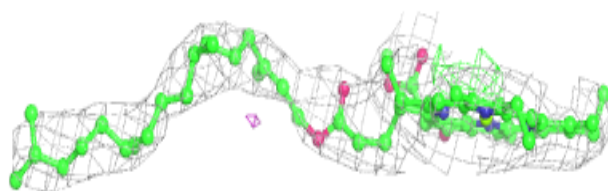
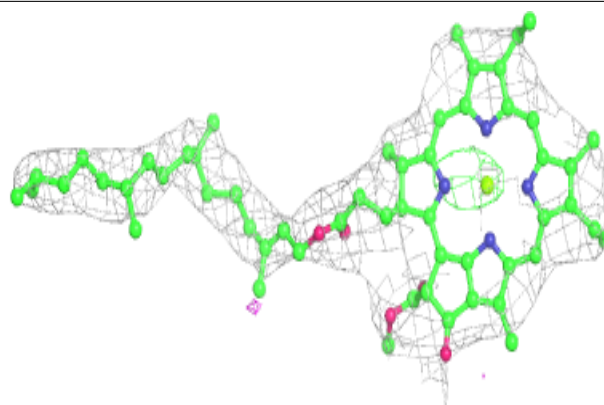
**Electron density around CLA B 840:**

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



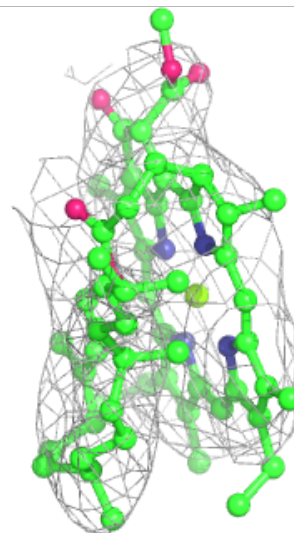
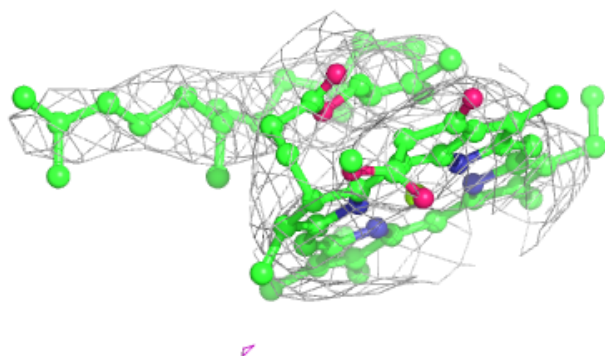
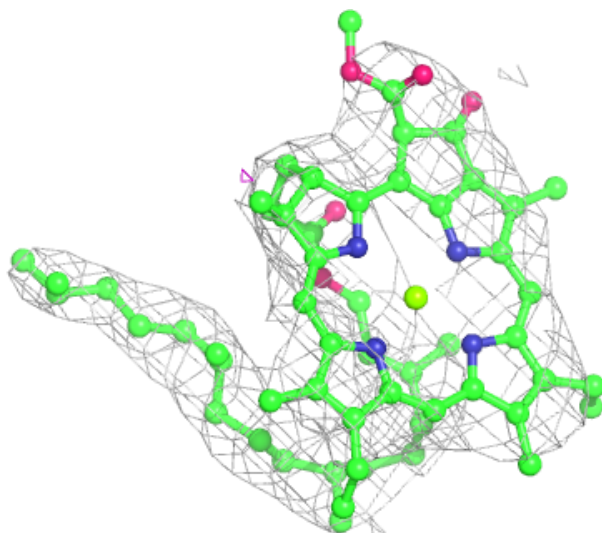
Electron density around CLA A 830:

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



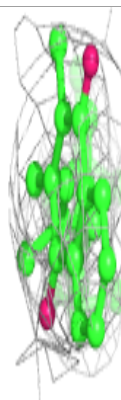
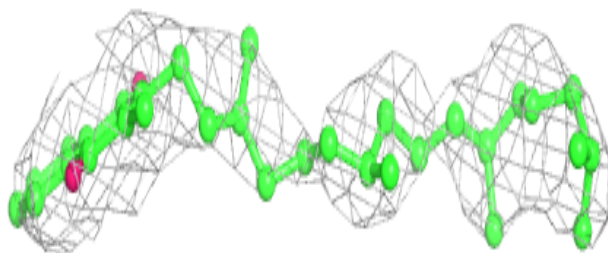
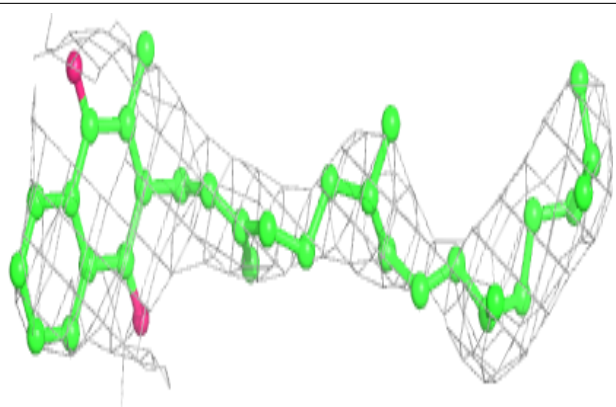
Electron density around CLA B 809:

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

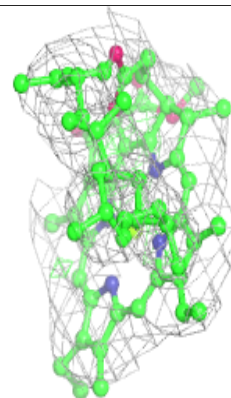
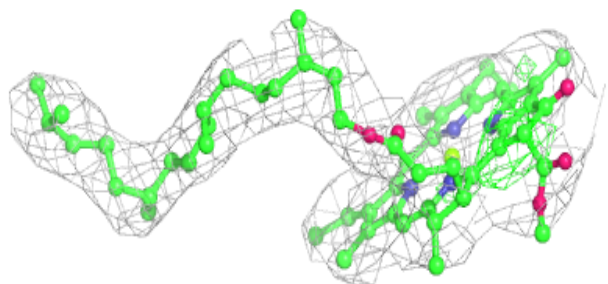
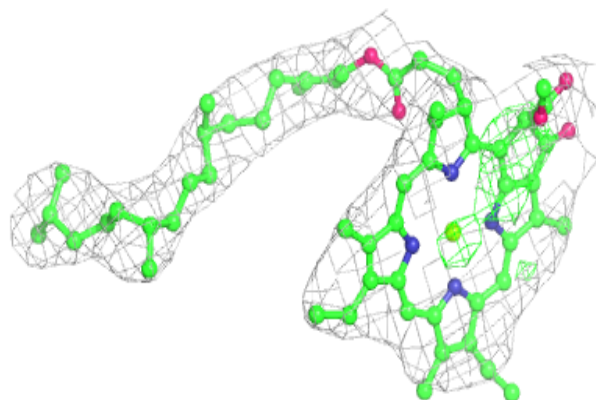


Electron density around PQN A 841:

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

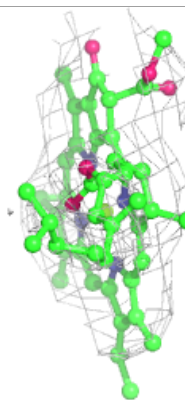
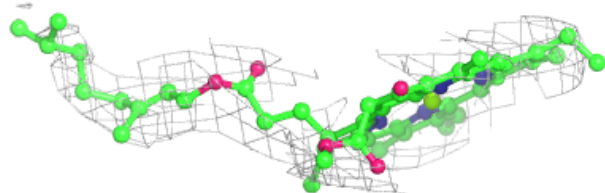
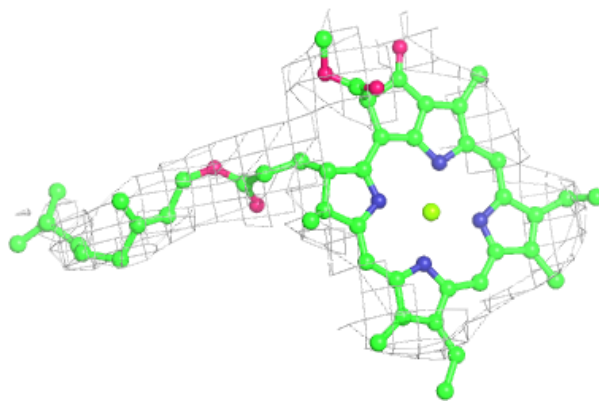
**Electron density around CLA A 807:**

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

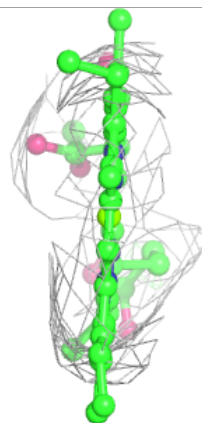
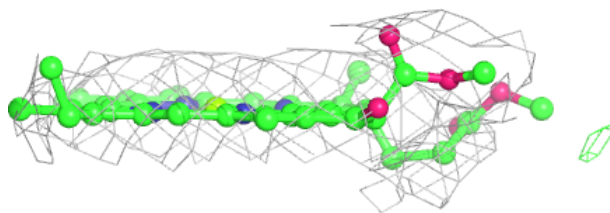
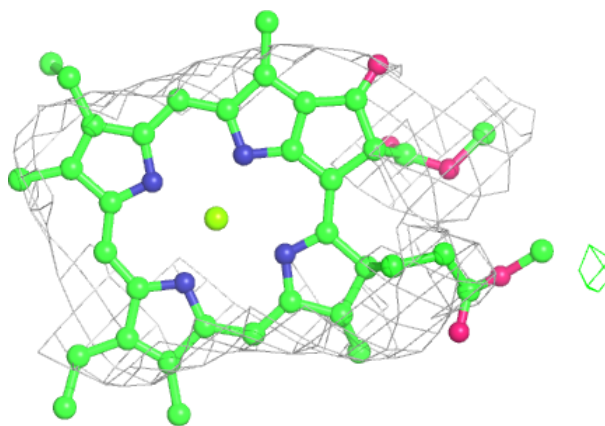


Electron density around CLA G 1601:

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

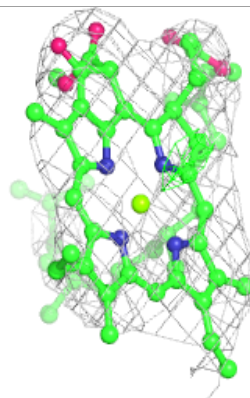
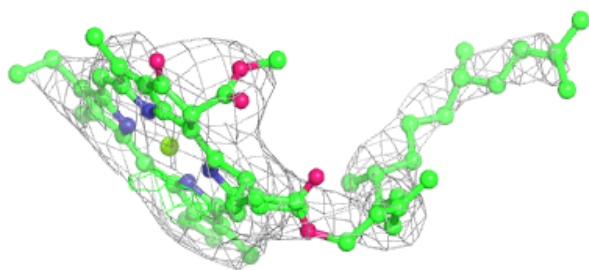
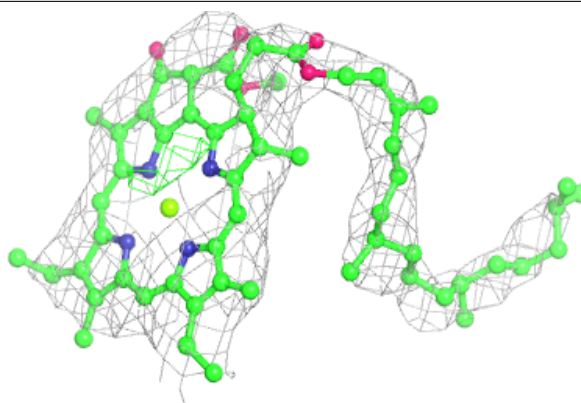
**Electron density around CLA G 1602:**

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

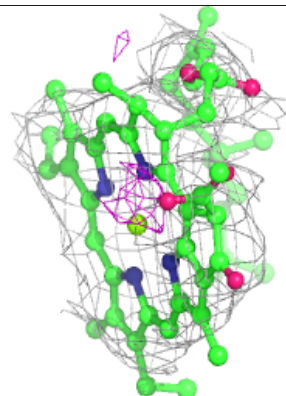
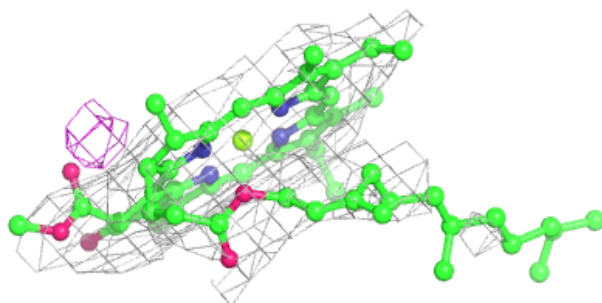
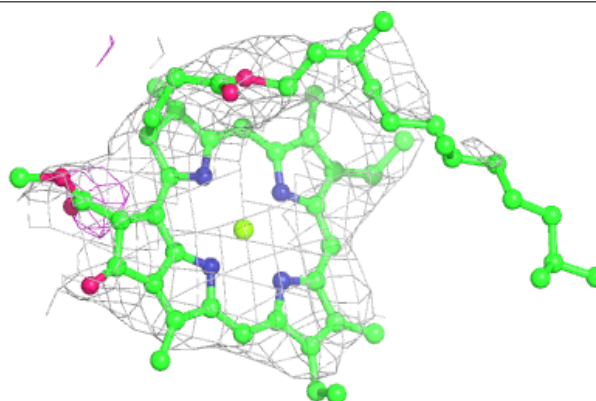


Electron density around CLA B 825:

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

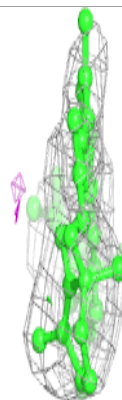
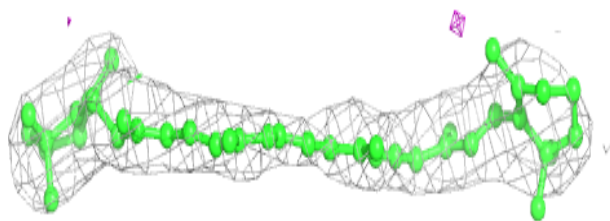
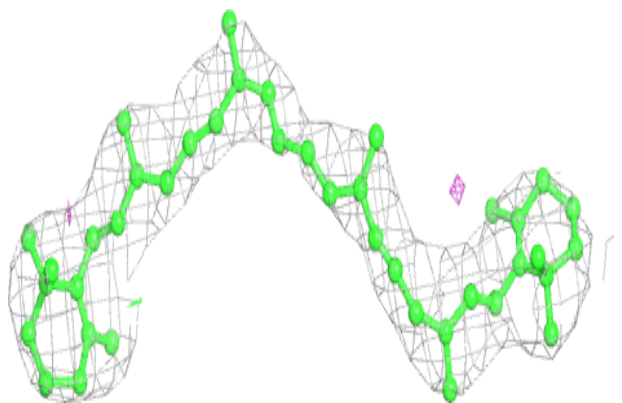
**Electron density around CLA 2 306:**

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



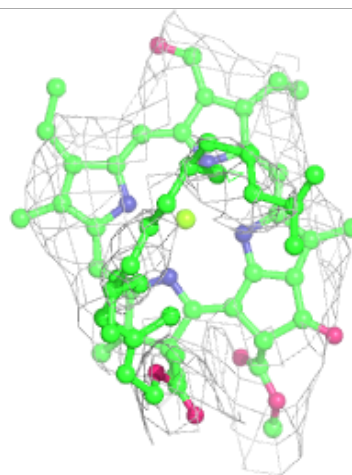
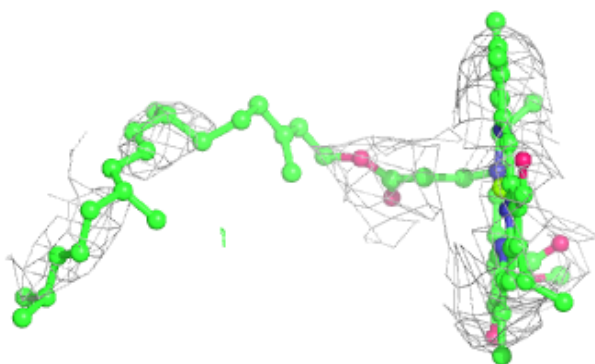
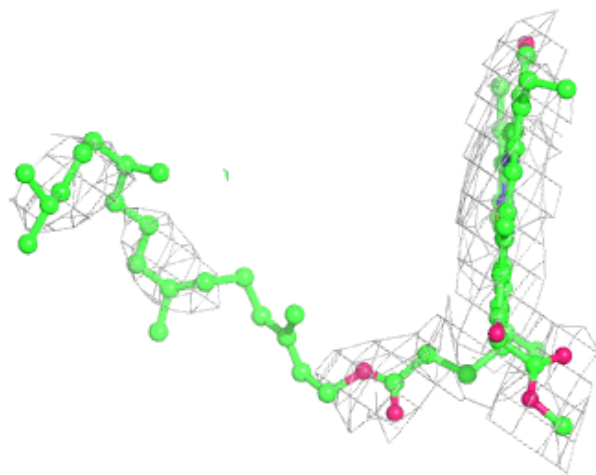
Electron density around BCR A 847:

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



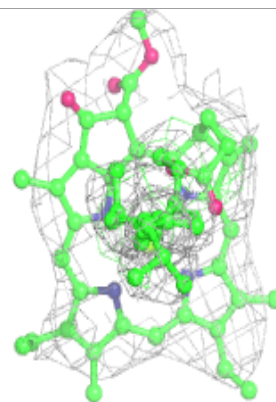
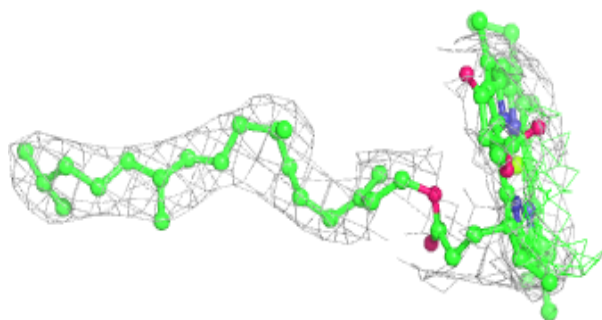
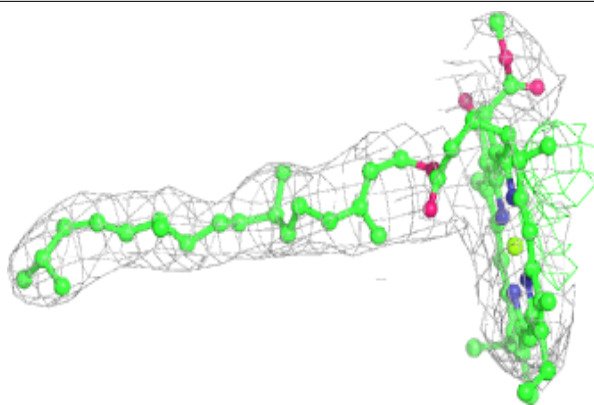
Electron density around CHL 2 314:

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

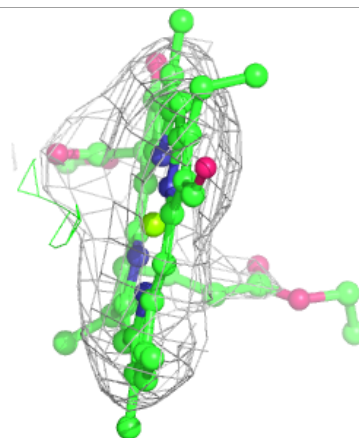
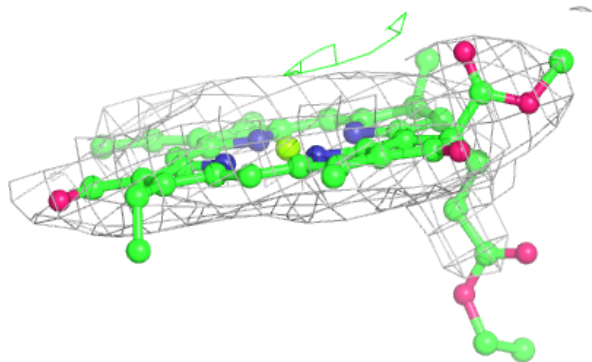
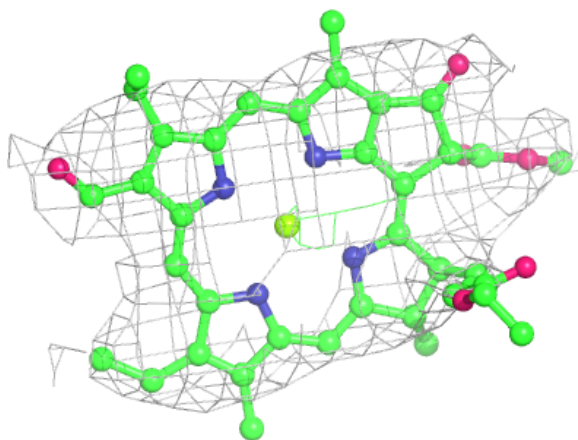


Electron density around CLA A 826:

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

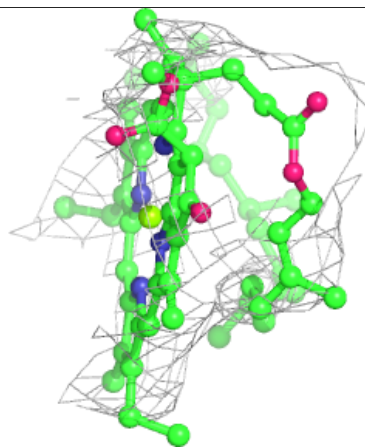
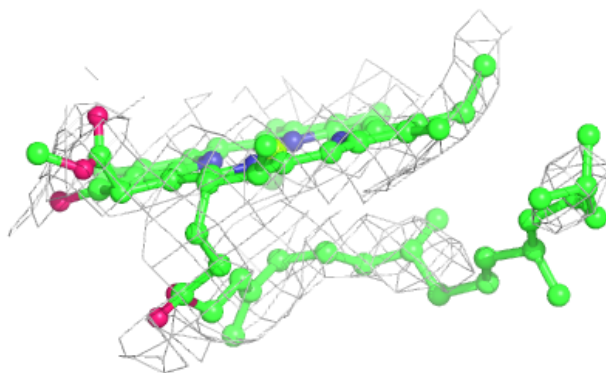
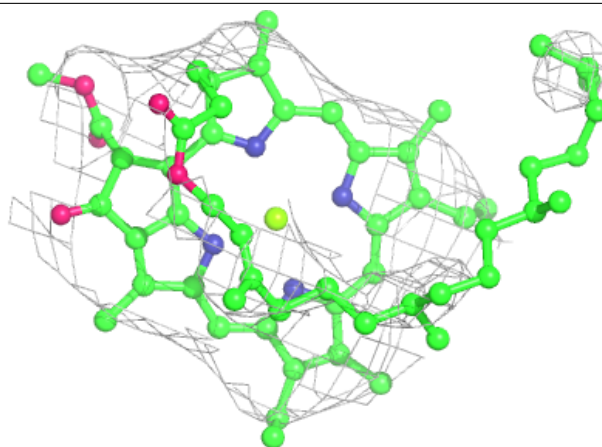
**Electron density around CHL 2 316:**

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

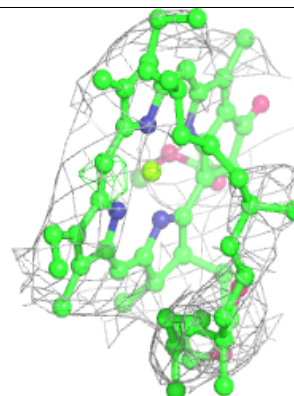
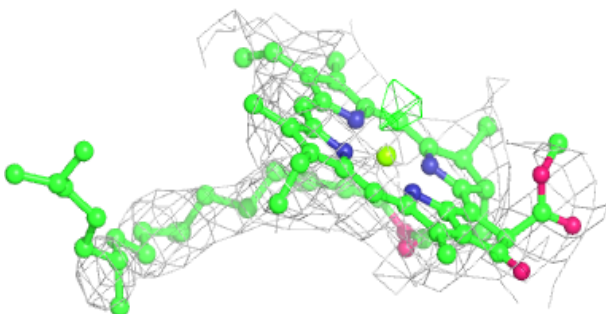
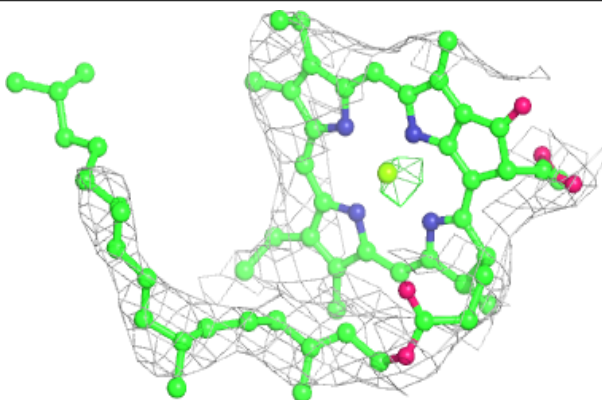


Electron density around CLA 2 308:

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

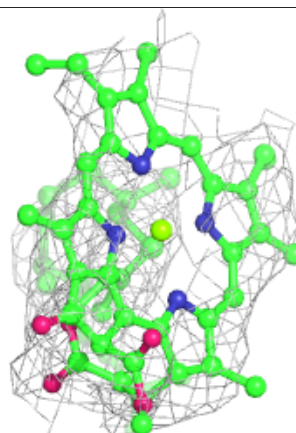
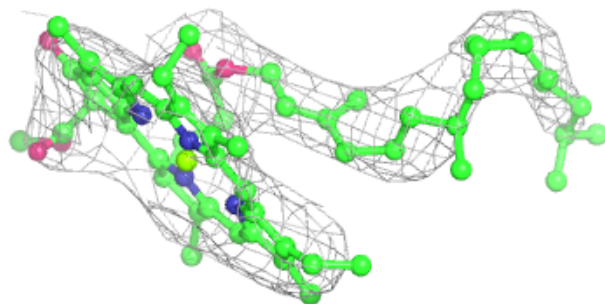
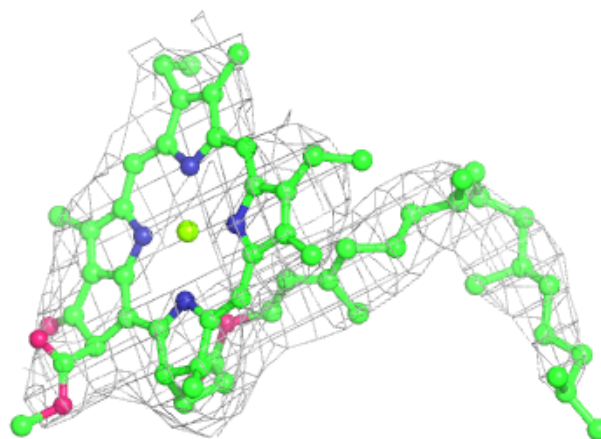
**Electron density around CLA 2 309:**

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



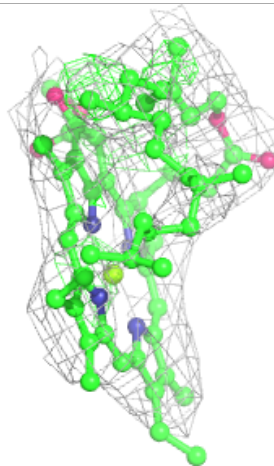
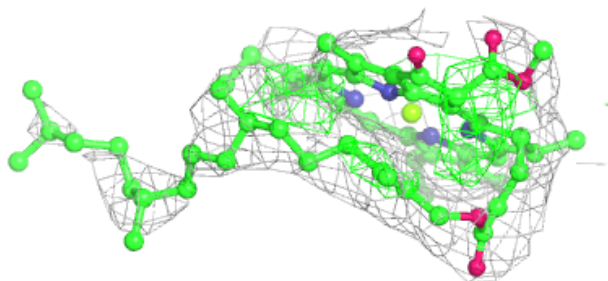
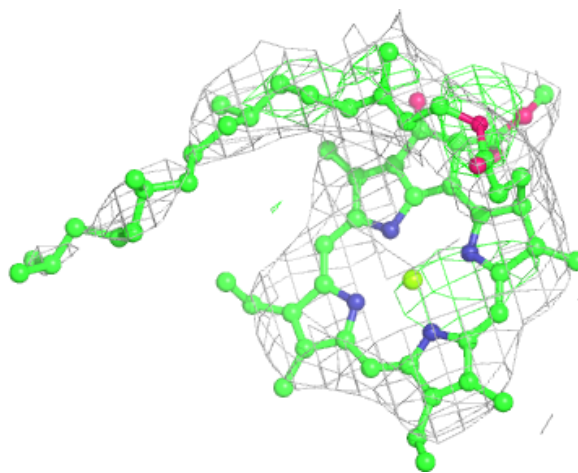
Electron density around CLA A 853:

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



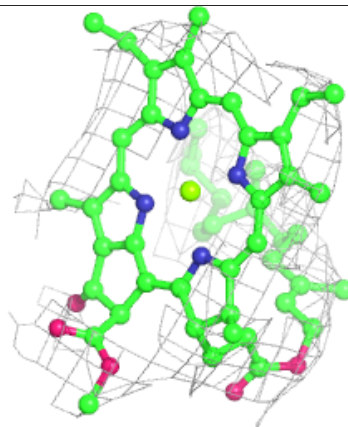
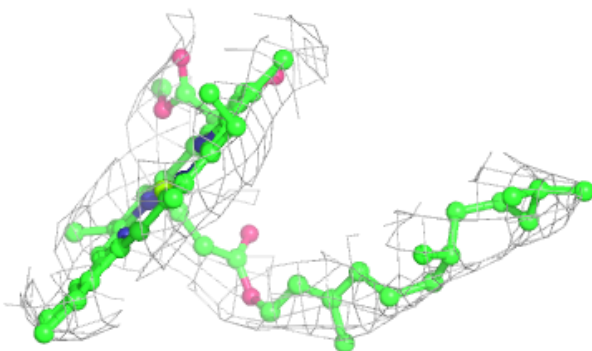
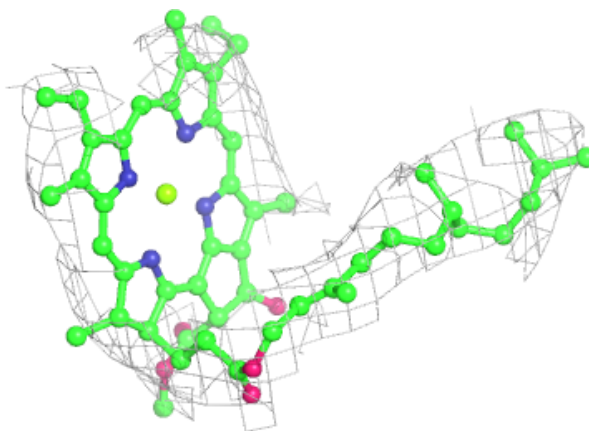
Electron density around CLA A 827:

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



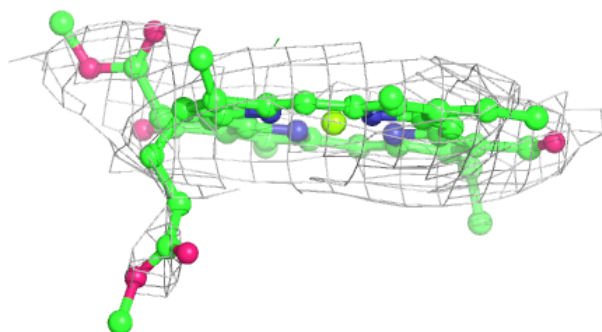
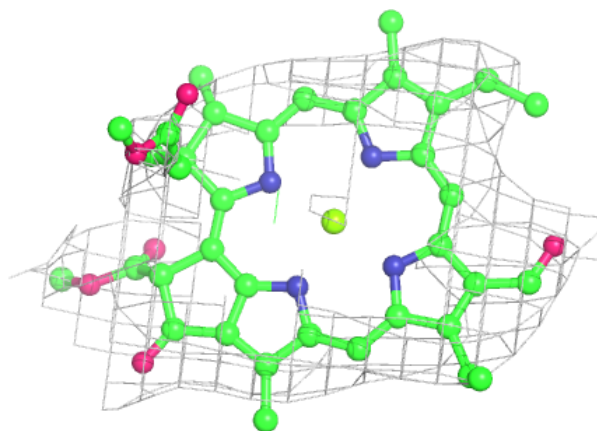
Electron density around CLA 2 312:

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



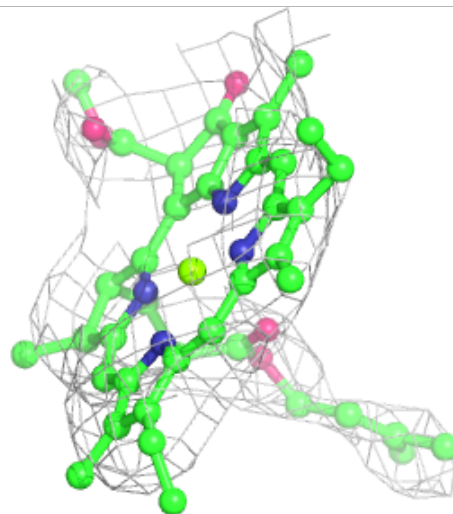
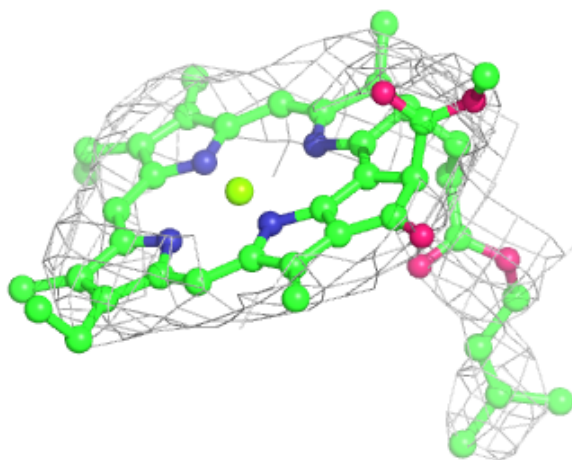
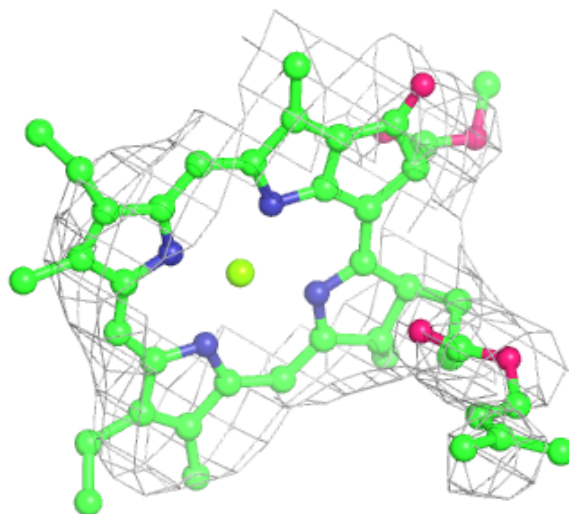
Electron density around CHL 3 316:

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



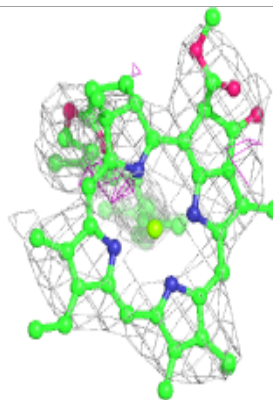
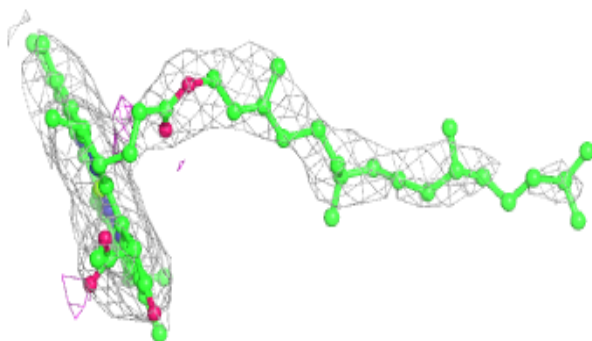
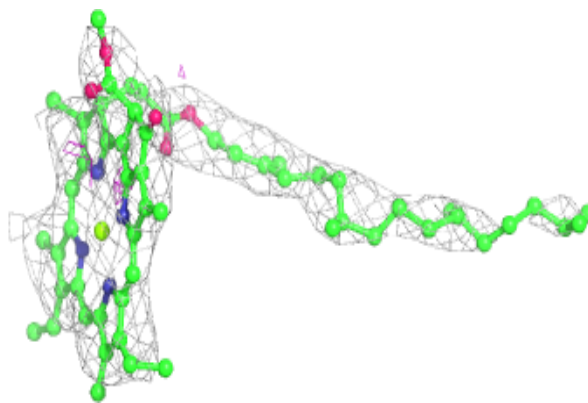
Electron density around CLA 2 313:

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

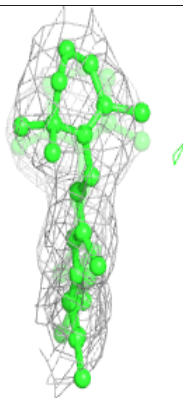
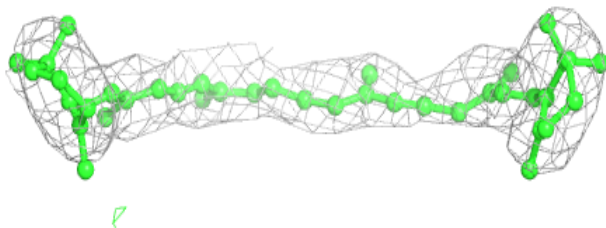
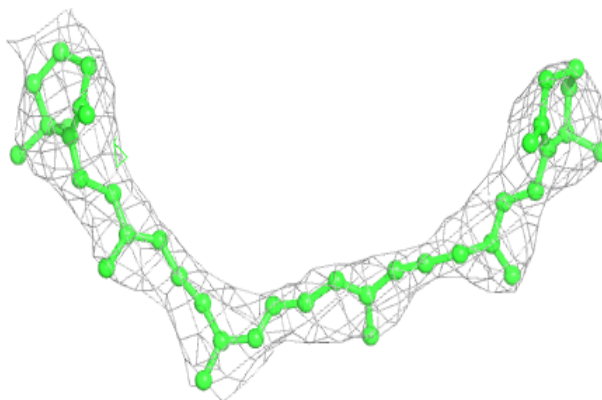


Electron density around CLA B 829:

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

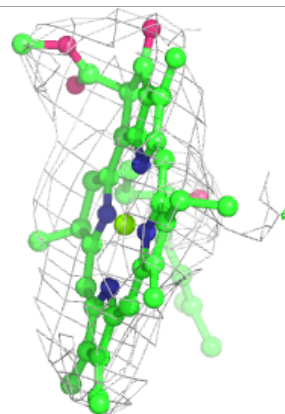
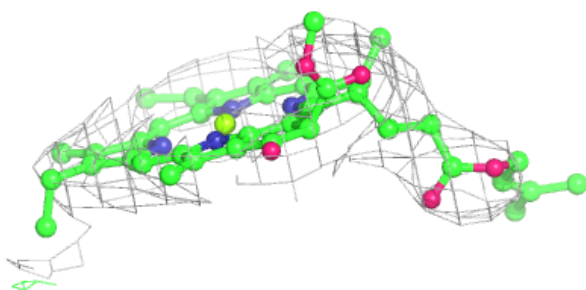
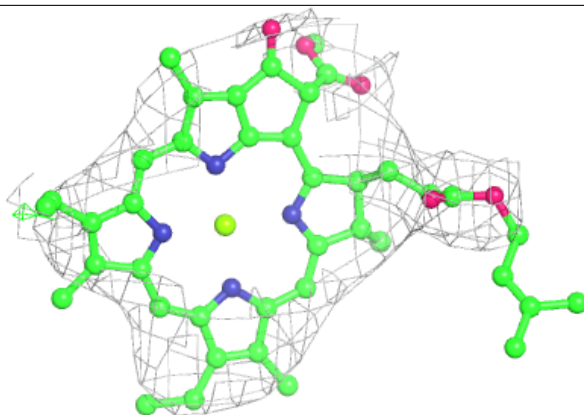
**Electron density around BCR F 305:**

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

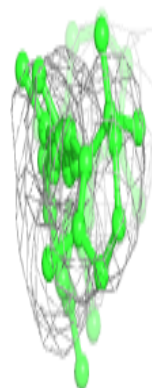
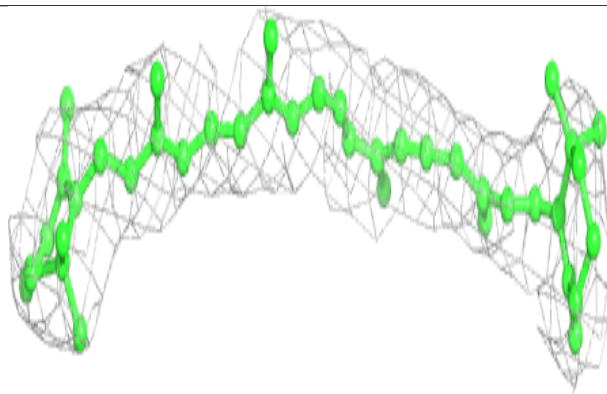
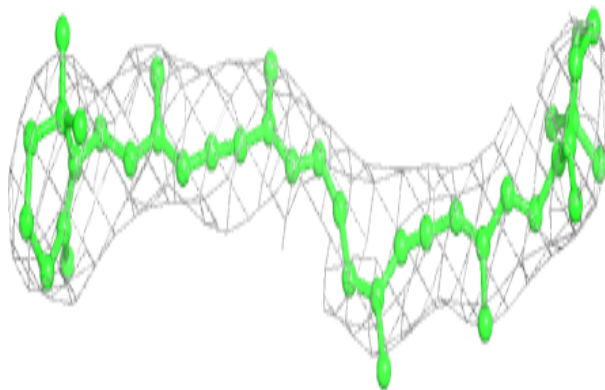


Electron density around CLA 2 326:

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

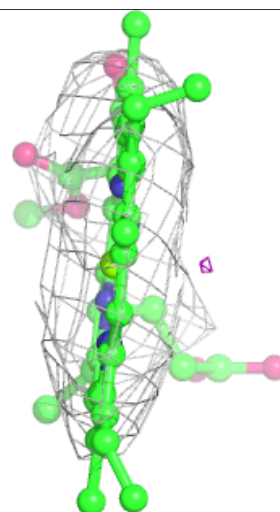
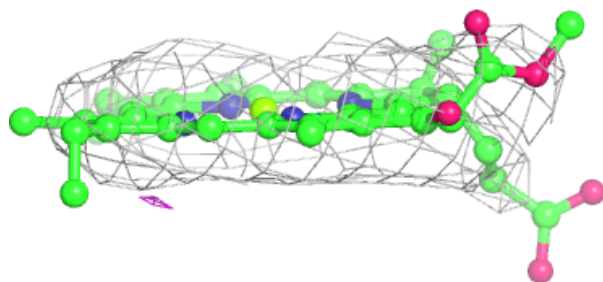
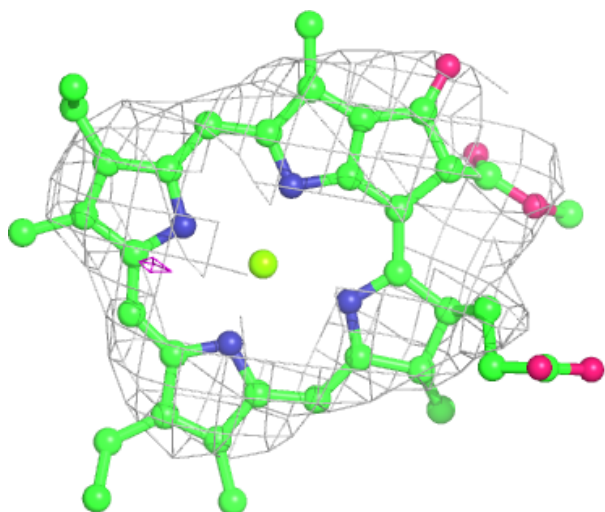
**Electron density around BCR I 101:**

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



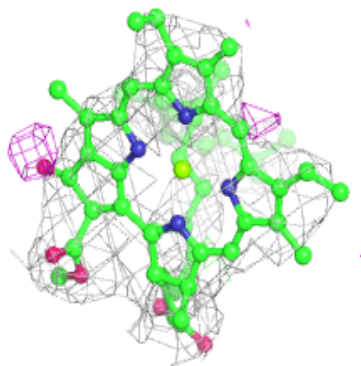
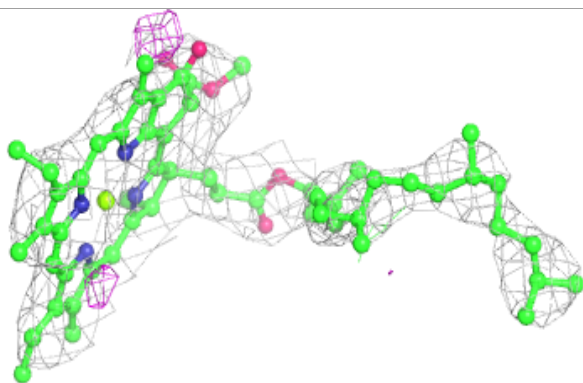
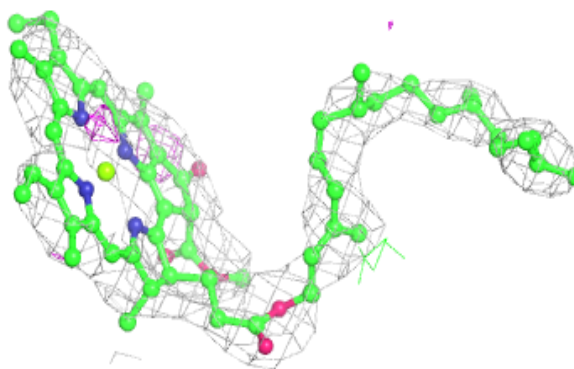
Electron density around CLA 3 301:

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



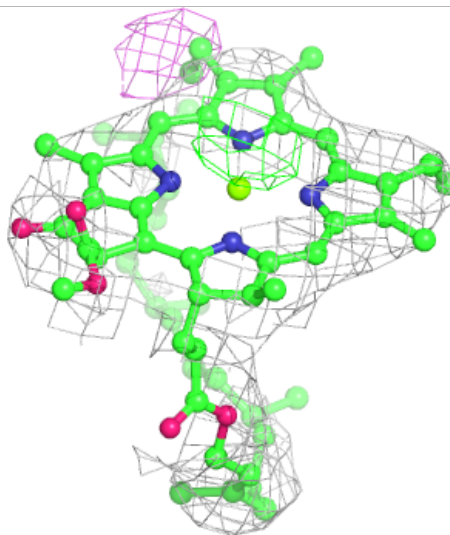
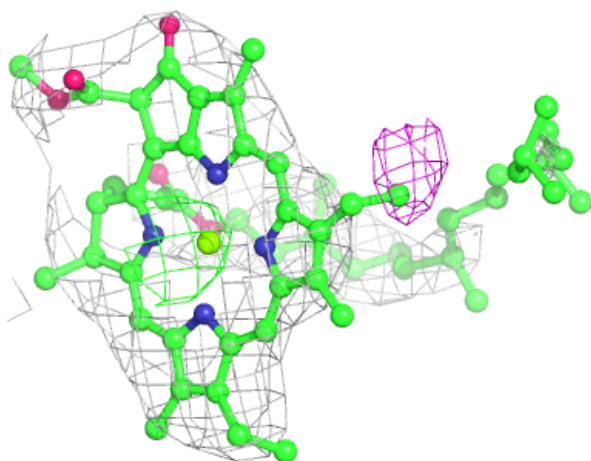
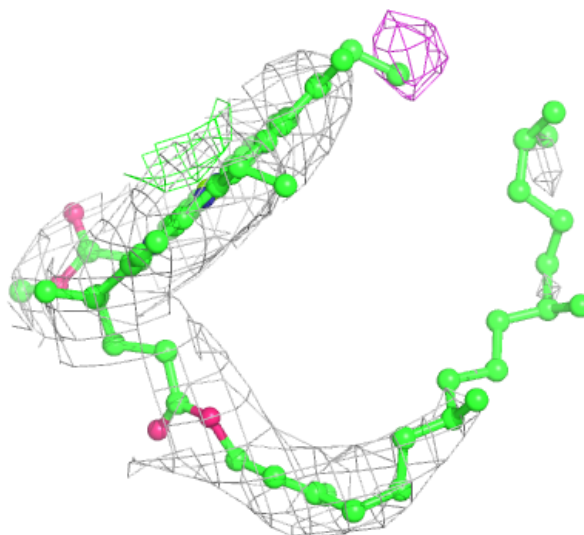
Electron density around CLA B 803:

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



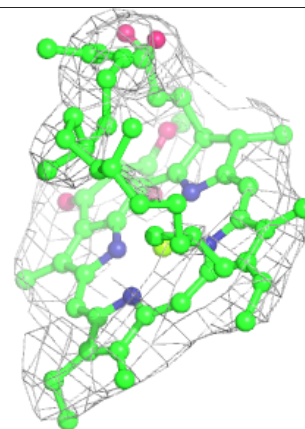
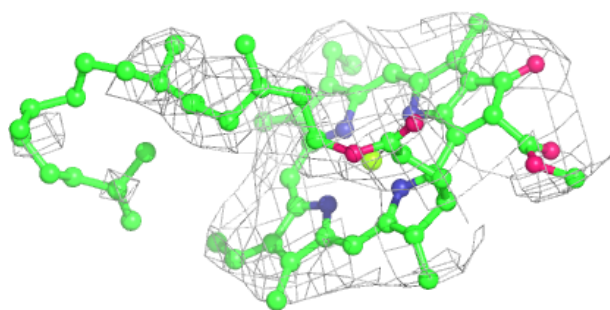
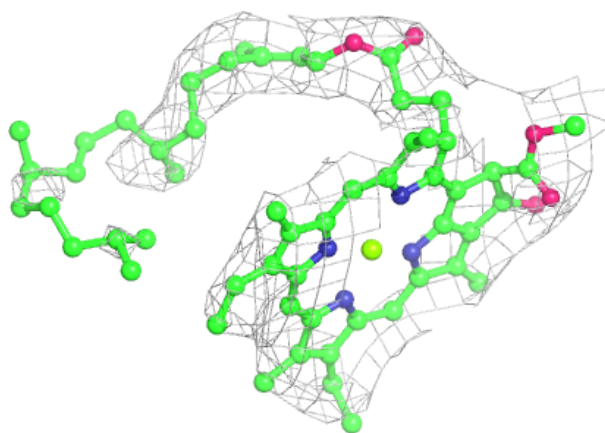
Electron density around CLA B 820:

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

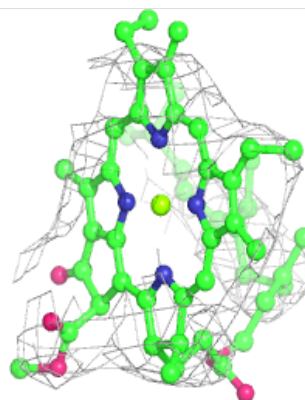
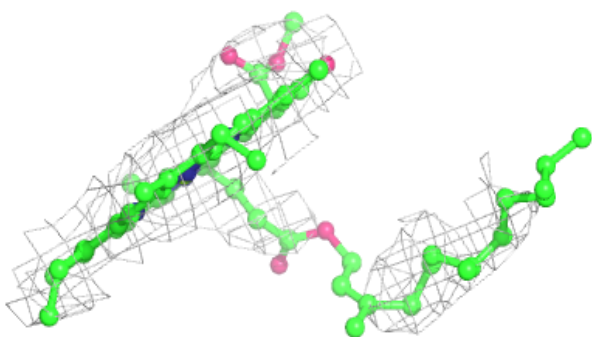
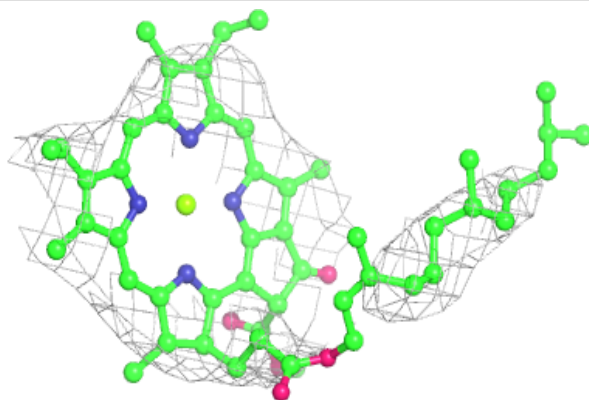


Electron density around CLA A 822:

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

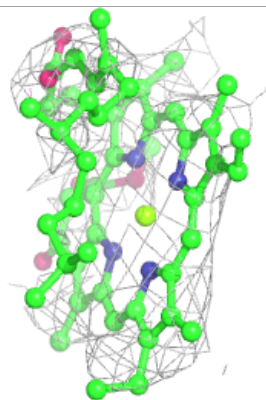
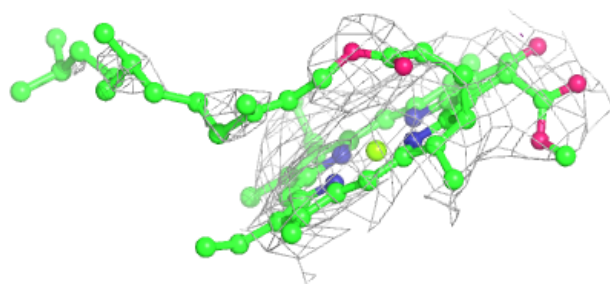
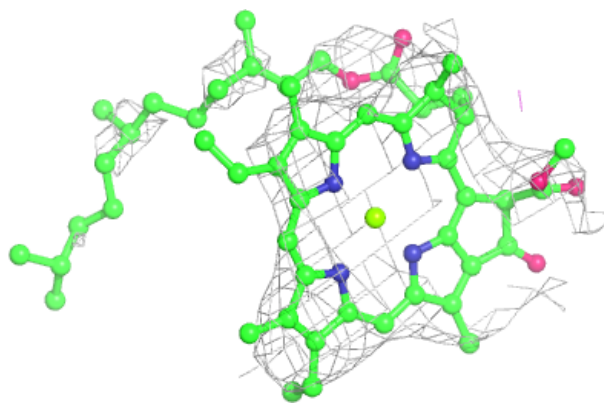
**Electron density around CLA A 820:**

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



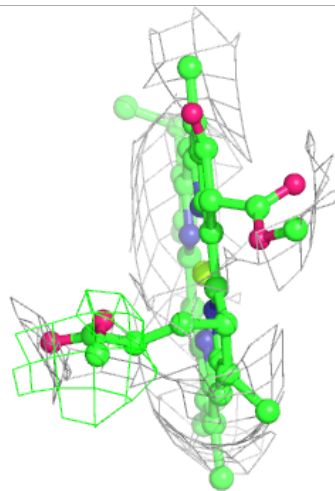
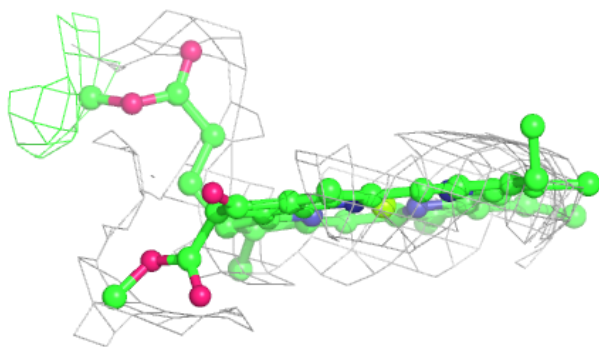
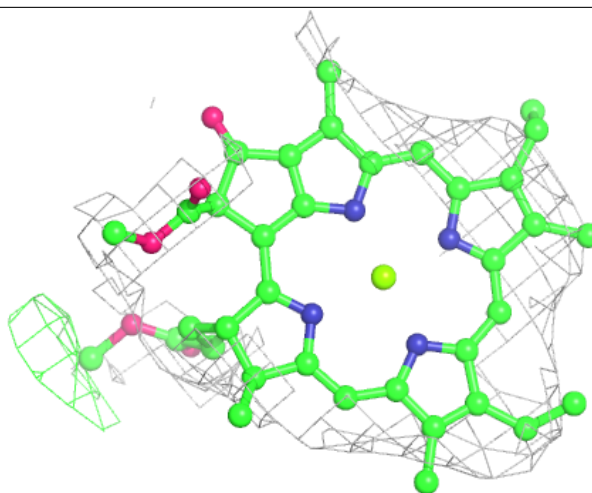
Electron density around CLA 4 308:

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



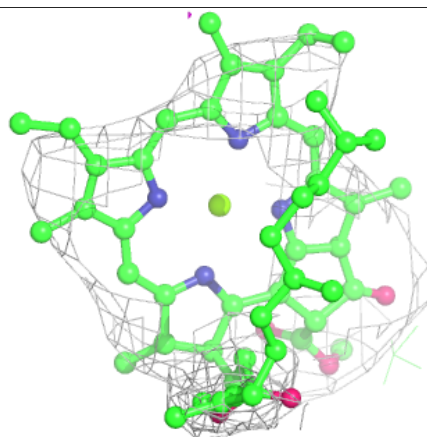
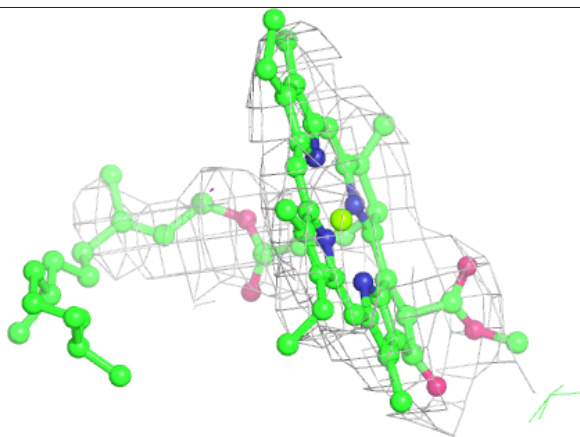
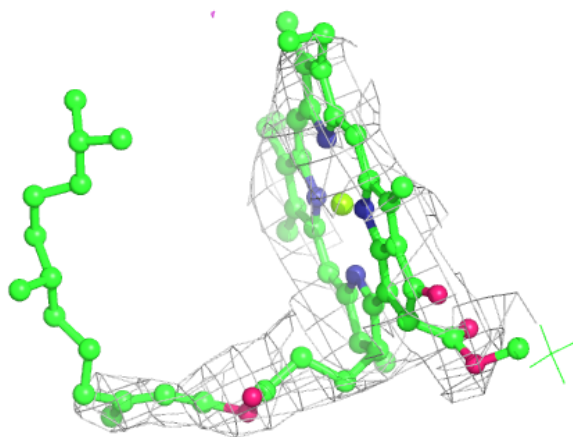
Electron density around CLA 1 5012:

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

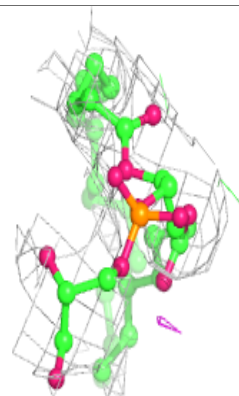
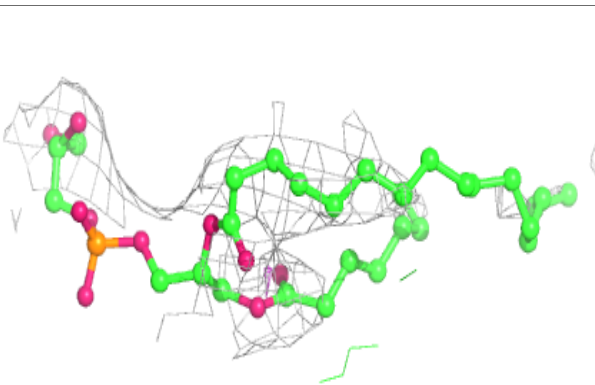
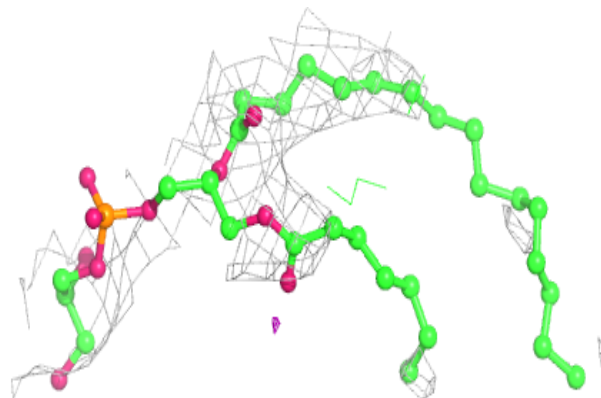


Electron density around CLA A 821:

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

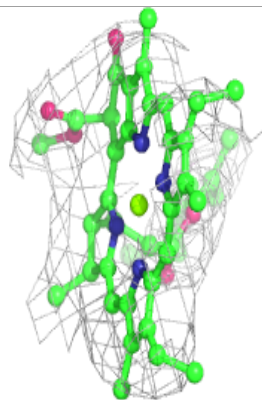
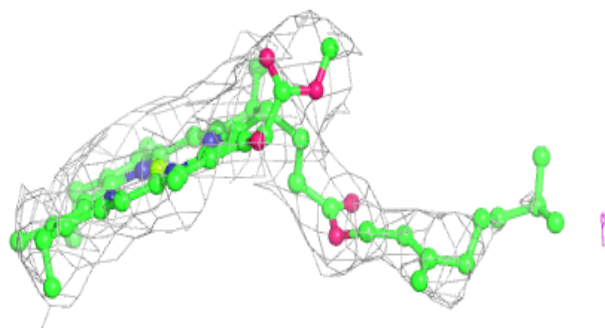
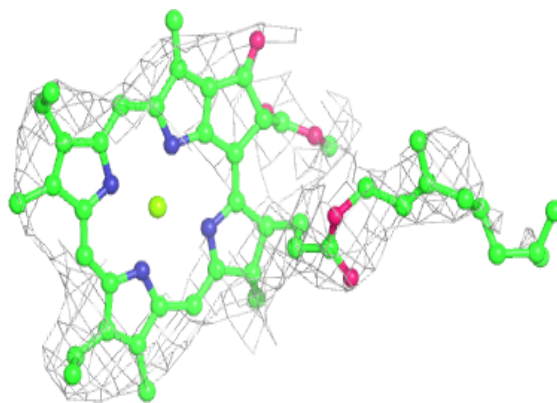
**Electron density around LHG A 849:**

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



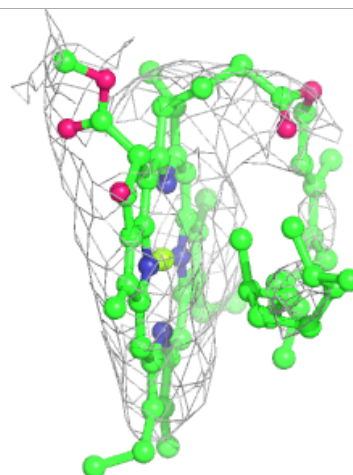
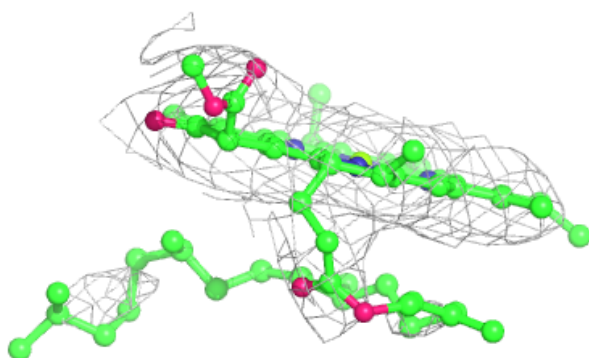
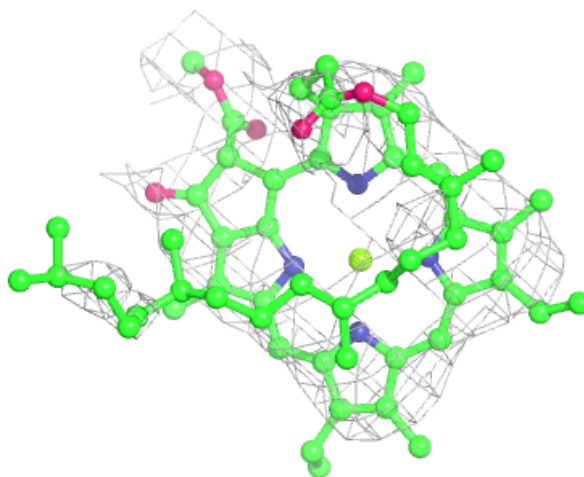
Electron density around CLA B 824:

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



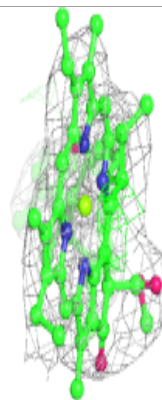
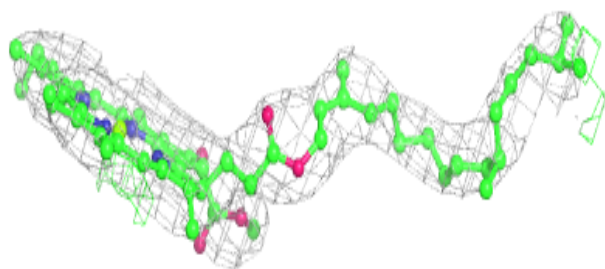
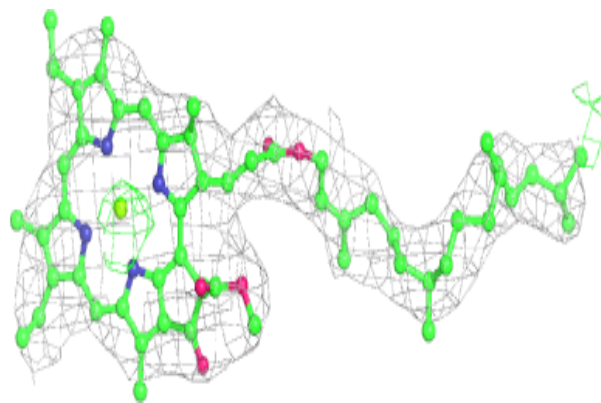
Electron density around CLA 3 315:

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

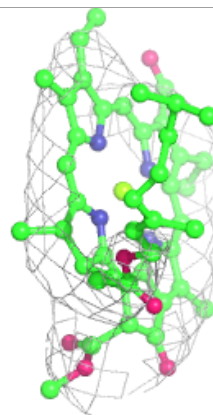
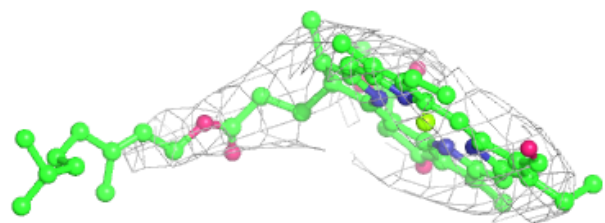
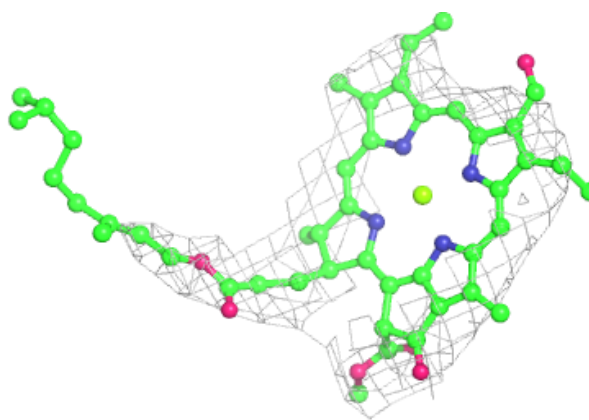


Electron density around CLA A 838:

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

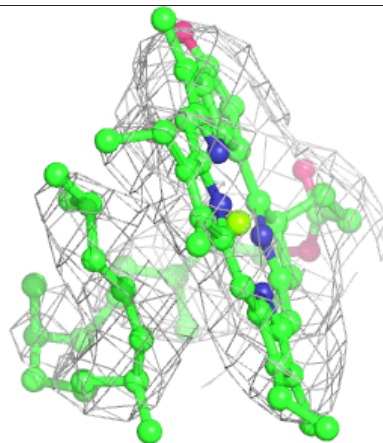
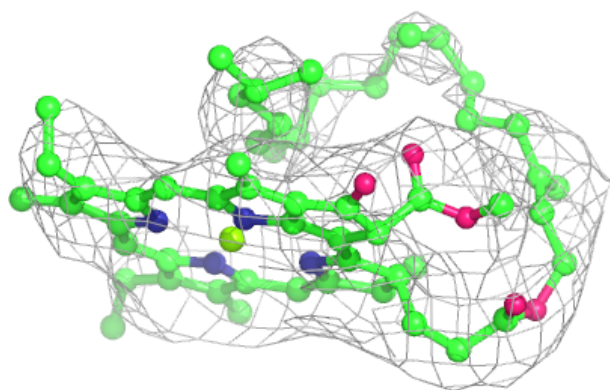
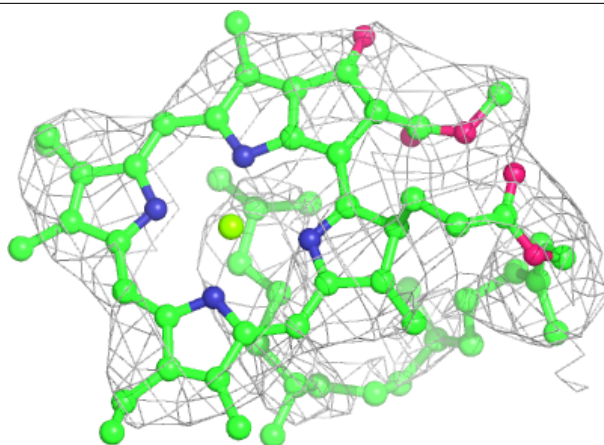
**Electron density around CHL 4 318:**

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



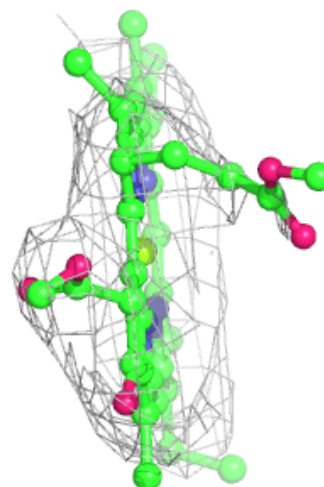
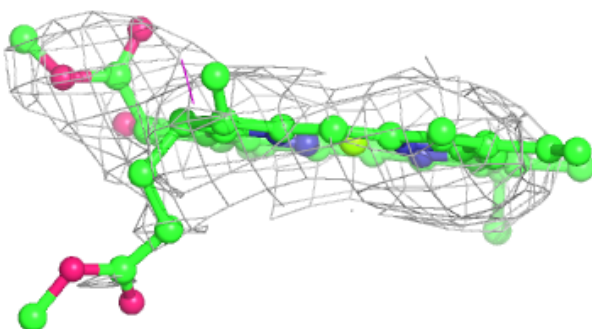
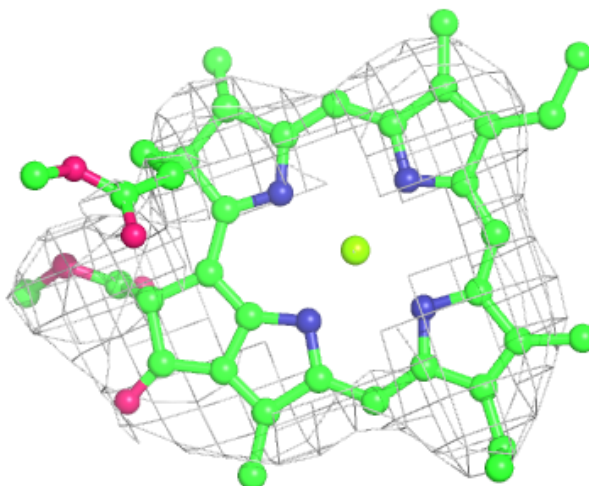
Electron density around CLA B 807:

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



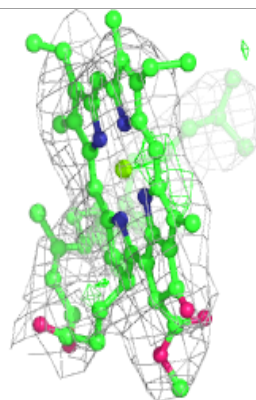
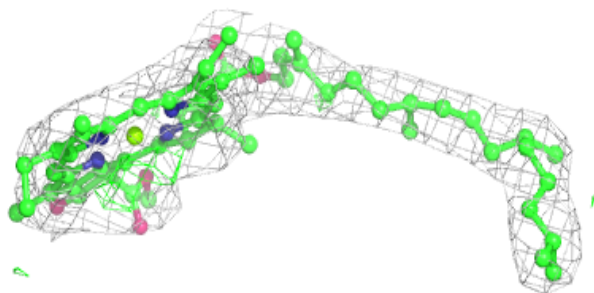
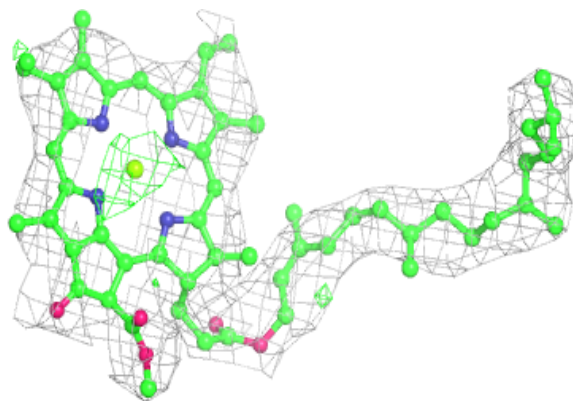
Electron density around CLA B 813:

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

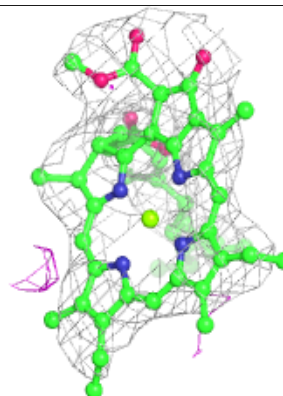
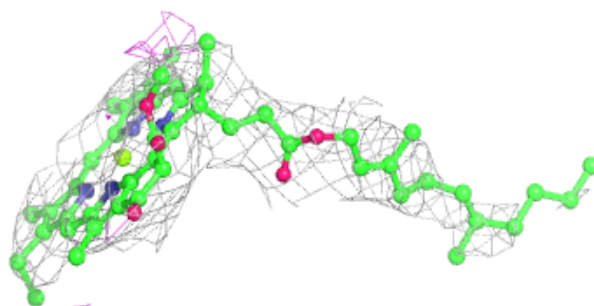
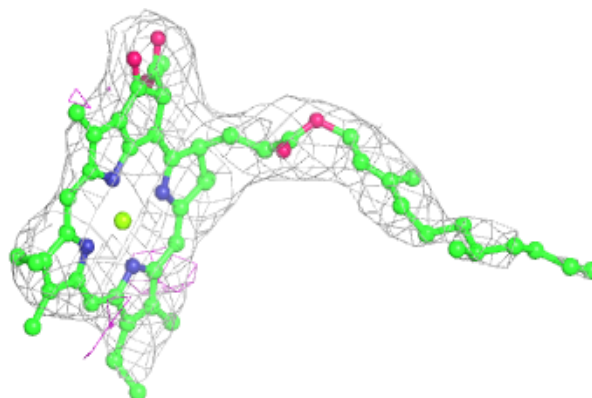


Electron density around CLA A 802:

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

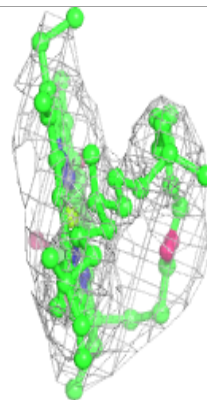
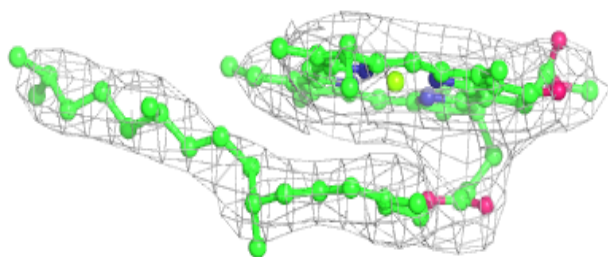
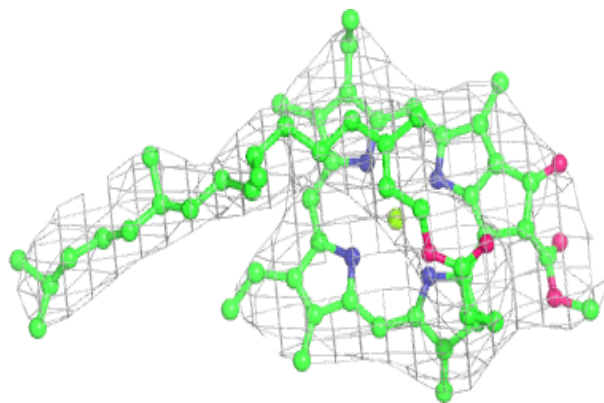
**Electron density around CLA B 833:**

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

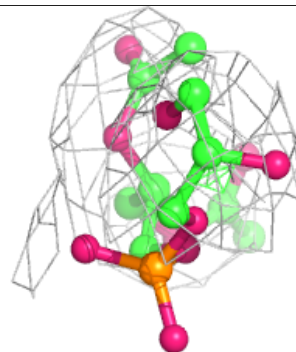
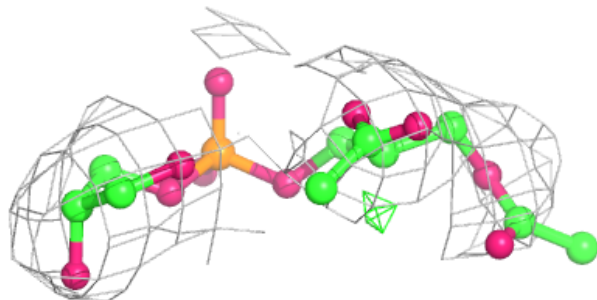


Electron density around CLA A 837:

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

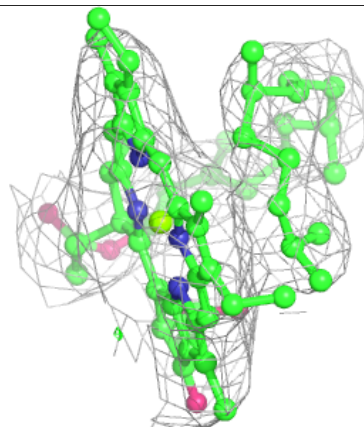
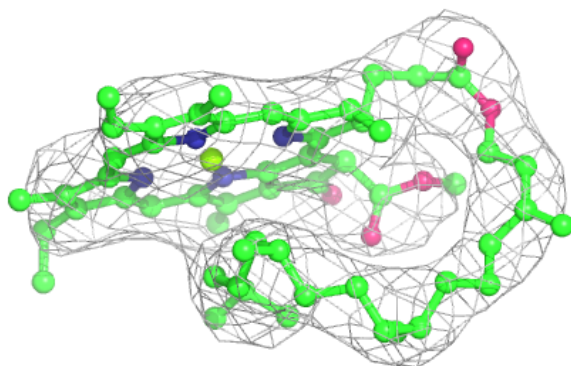
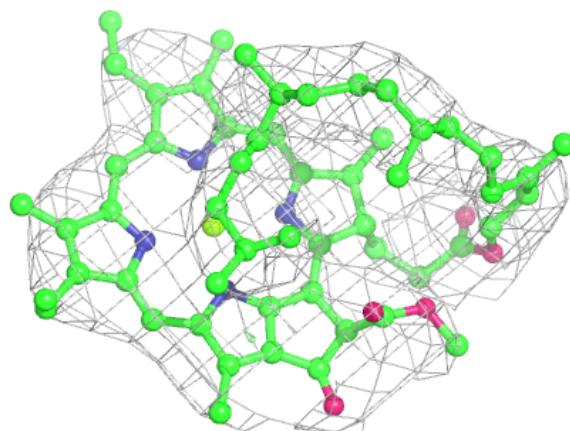
**Electron density around LHG B 848:**

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

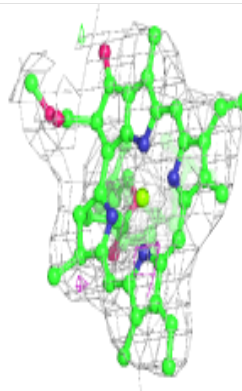
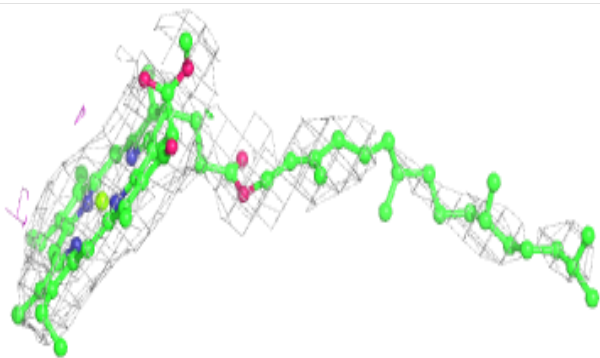
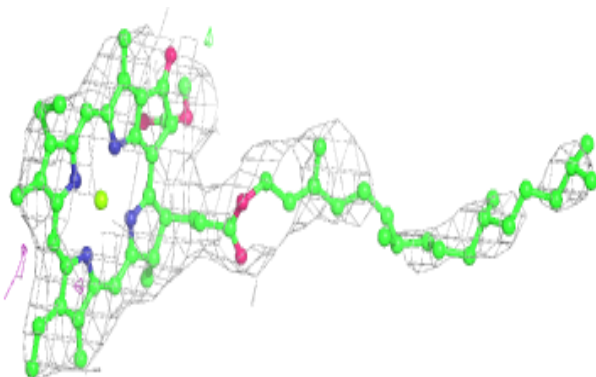


Electron density around CLA A 805:

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

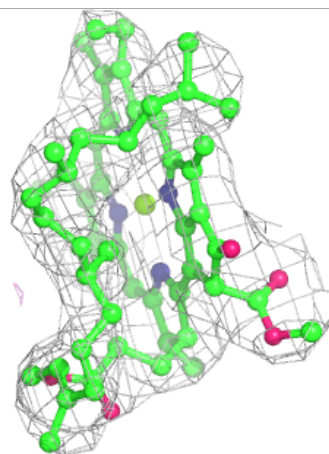
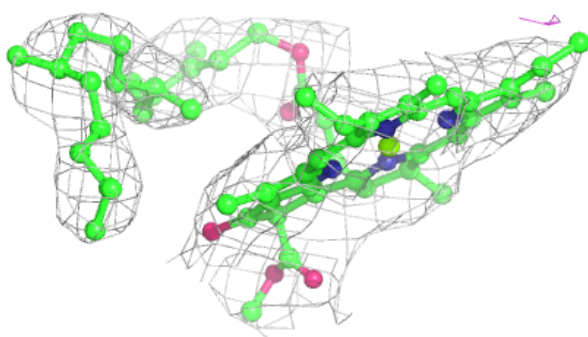
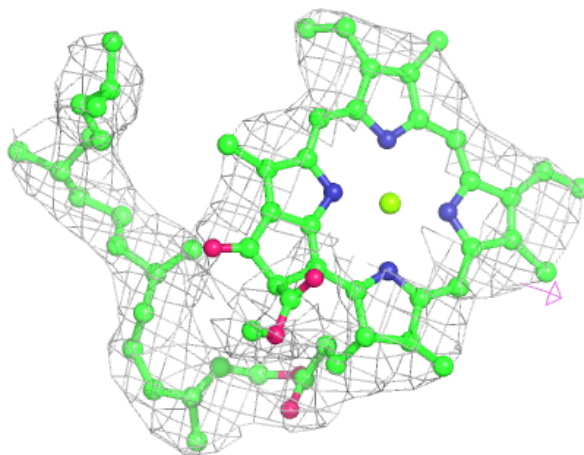
**Electron density around CLA A 808:**

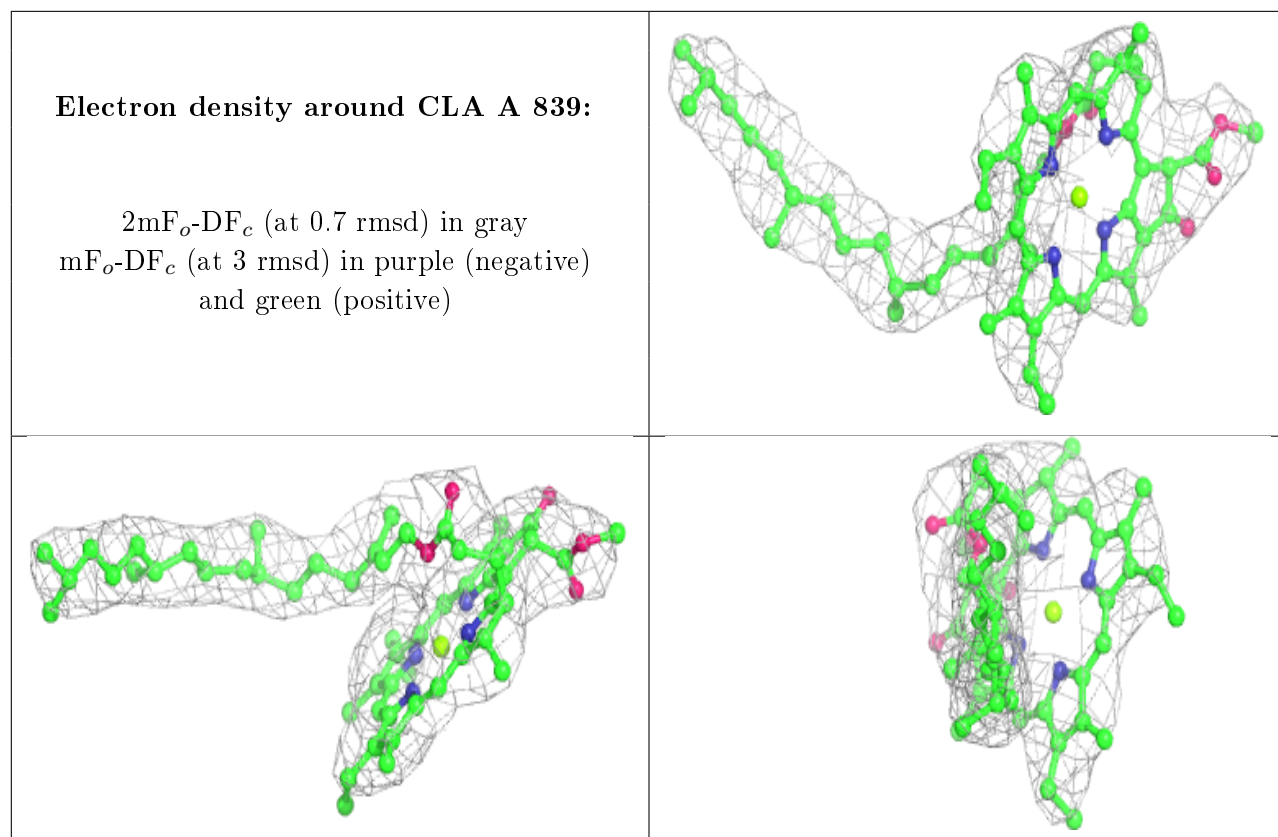
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA F 301:

$2mF_o-DF_c$ (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.