



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 5, 2026 – 02:41 PM EDT

PDB ID : 3KZI / pdb_00003kzi
Title : Crystal Structure of Monomeric Form of Cyanobacterial Photosystem II
Authors : Gabdulkhakov, A.; Guskov, A.; Broser, M.; Kern, J.; Zouni, A.; Saenger, W.
Deposited on : 2009-12-08
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

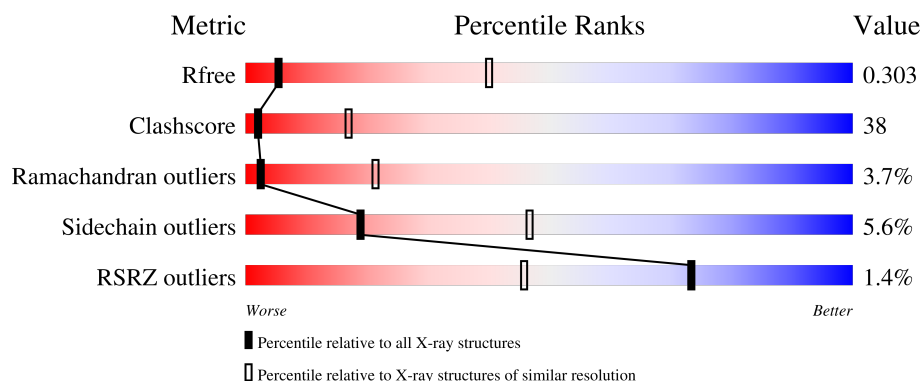
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



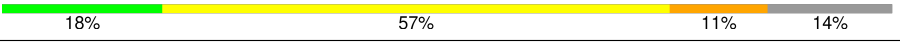
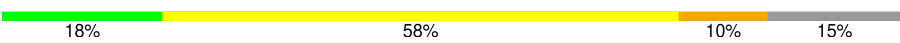
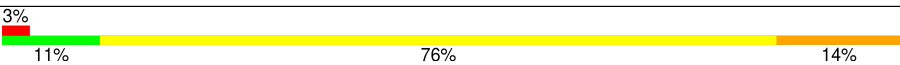
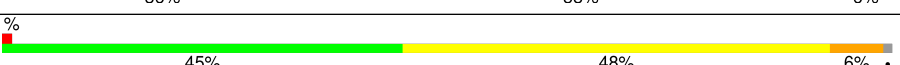
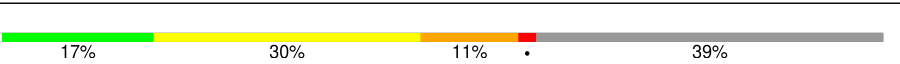
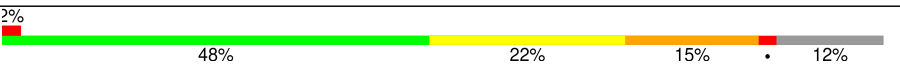
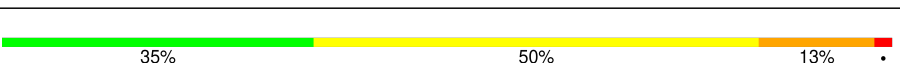
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	2% 41% 50% 6% • •
2	B	510	2% 49% 40% 6% • 5%
3	C	461	0% 37% 53% 7% •
4	D	352	3% 48% 41% 8% •
5	E	83	24% 54% 12% • 7%

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Mol	Chain	Length	Quality of chain
6	F	44	
7	H	65	
8	I	38	
9	J	40	
10	K	37	
11	L	37	
12	M	36	
13	O	246	
14	T	32	
15	U	104	
16	V	137	
17	y	46	
18	X	40	
19	Z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	362	X	-	-	-
21	CLA	A	363	X	-	-	-
21	CLA	A	364	X	-	-	-
21	CLA	A	366	X	-	-	-
21	CLA	B	511	X	-	-	-
21	CLA	B	512	X	-	-	-
21	CLA	B	513	X	-	X	-
21	CLA	B	514	X	-	-	-
21	CLA	B	515	X	-	-	-
21	CLA	B	516	X	-	-	-
21	CLA	B	517	X	-	-	-
21	CLA	B	518	X	-	-	-
21	CLA	B	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	520	X	-	-	-
21	CLA	B	521	X	-	-	-
21	CLA	B	522	X	-	-	-
21	CLA	B	523	X	-	-	-
21	CLA	B	524	X	-	-	-
21	CLA	B	525	X	-	-	-
21	CLA	B	526	X	-	-	-
21	CLA	C	477	X	-	-	-
21	CLA	C	478	X	-	-	-
21	CLA	C	479	X	-	-	-
21	CLA	C	480	X	-	-	-
21	CLA	C	481	X	-	-	-
21	CLA	C	482	X	-	-	-
21	CLA	C	483	X	-	-	-
21	CLA	C	484	X	-	-	-
21	CLA	C	485	X	-	-	-
21	CLA	C	486	X	-	X	-
21	CLA	C	487	X	-	-	-
21	CLA	C	488	X	-	-	-
21	CLA	D	354	X	-	-	-
21	CLA	D	356	X	-	-	-
21	CLA	K	483	X	-	-	-
22	PHO	A	365	X	-	-	-
22	PHO	D	355	X	-	-	-
23	MES	A	367	-	-	X	-
27	LMG	A	373	-	-	X	-
27	LMG	D	360	-	-	X	-
28	DGD	B	528	-	-	X	-
28	DGD	C	492	X	-	-	-
28	DGD	C	493	X	-	X	-
32	PL9	D	357	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 24678 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	485	Total	C	N	O	S	0	0	0
			3812	2505	635	659	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3455	2262	580	600	13			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	0	0	0
			635	417	103	115			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	38	Total	C	N	O	S	0	0	0
			307	207	50	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	35	Total	C	N	O	S	0	0	0
			254	172	38	44				

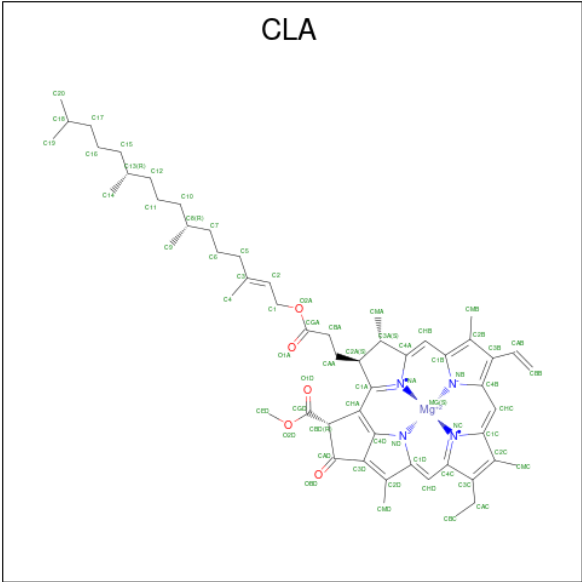
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



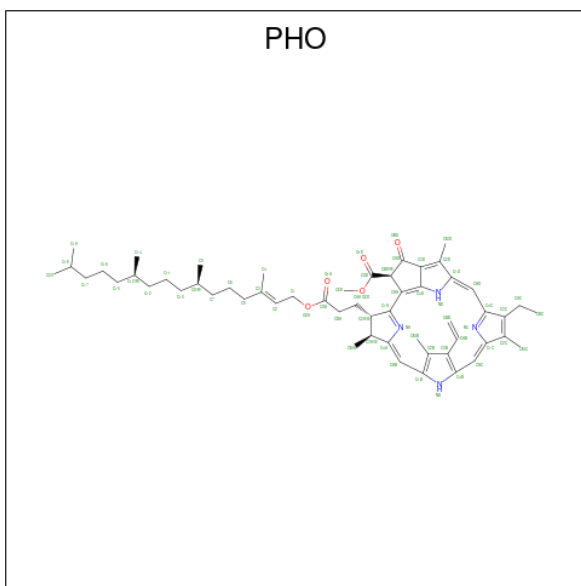
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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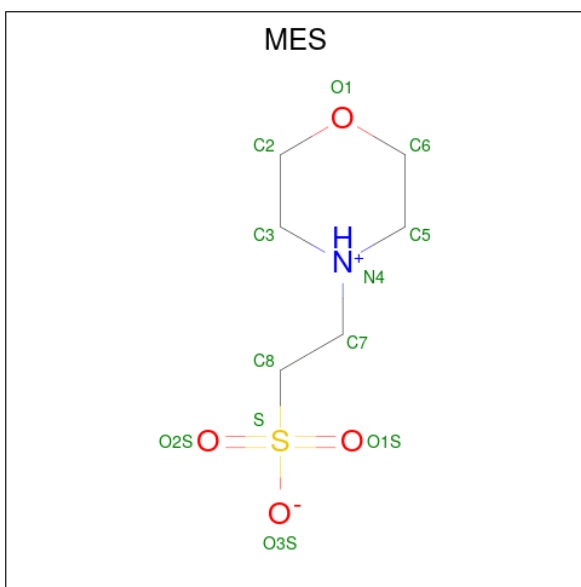
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N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

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



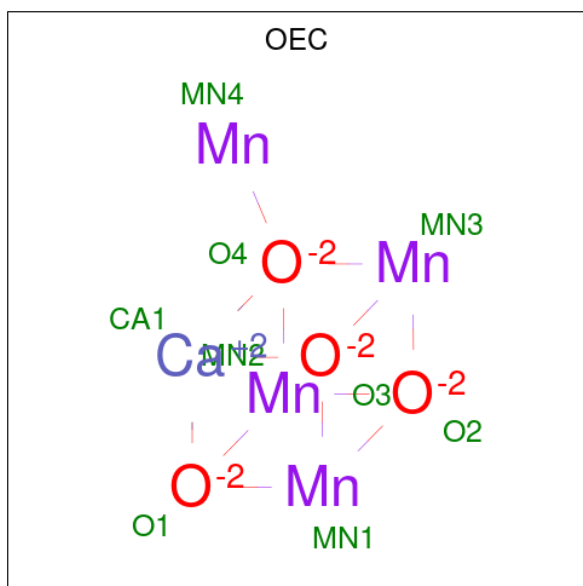
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 23 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



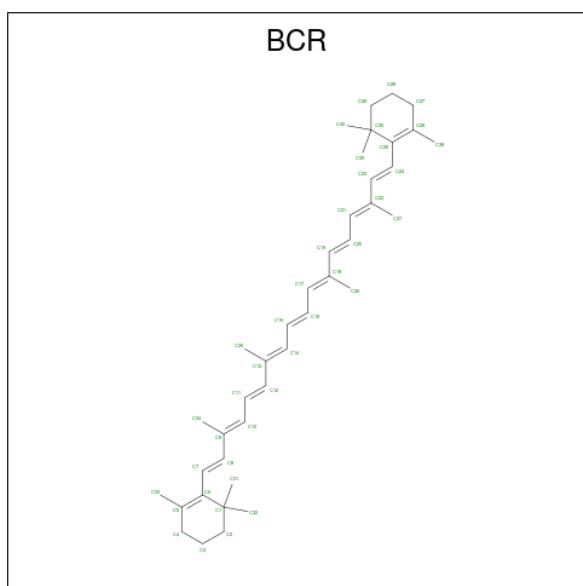
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 24 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).



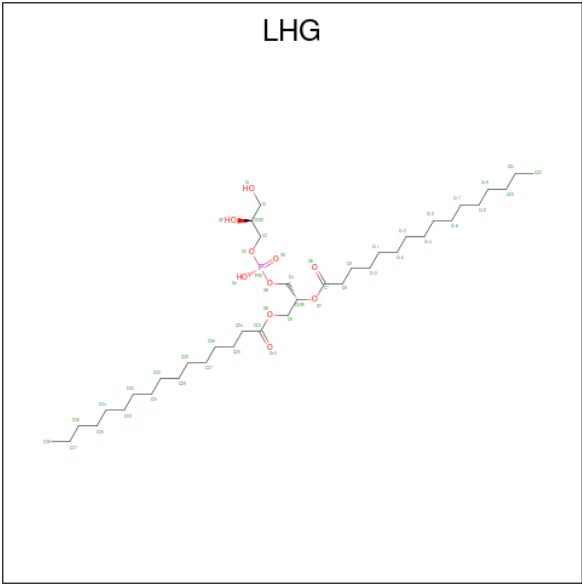
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total	Ca Mn	0	0
			5	1 4		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



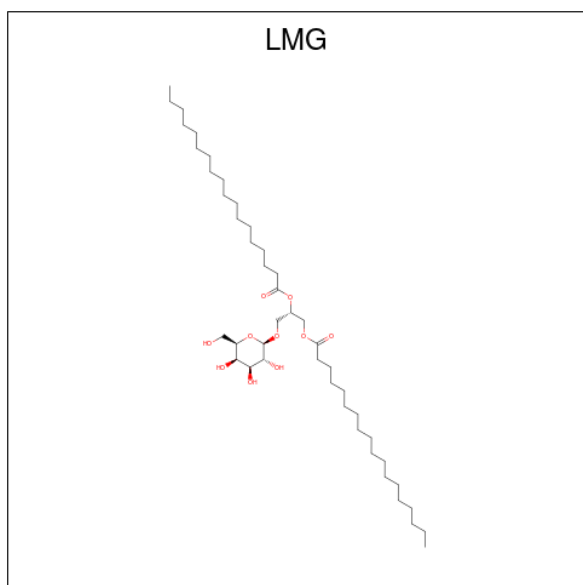
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	X	1	Total C 40 40	0	0
25	Z	1	Total C 40 40	0	0

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



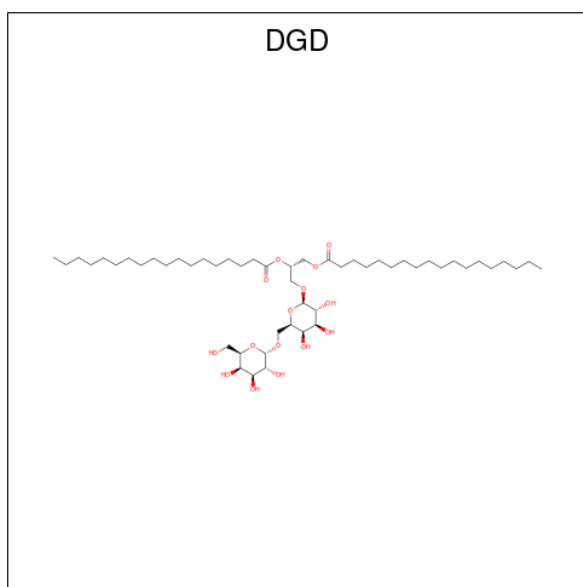
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



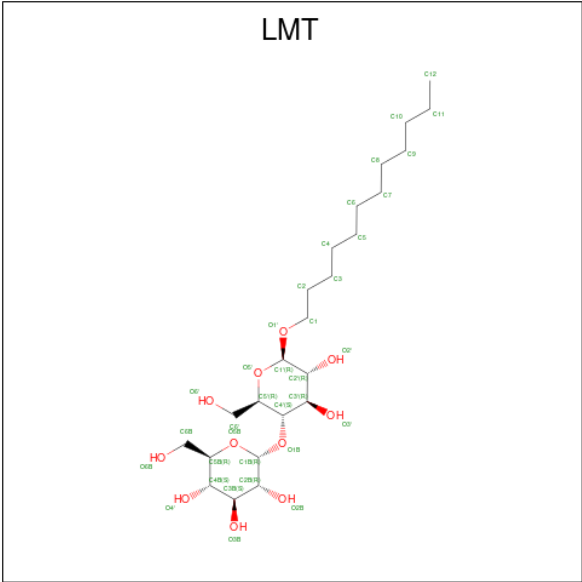
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O		0	0
			51	41	10			
27	B	1	Total	C	O		0	0
			49	39	10			
27	C	1	Total	C	O		0	0
			45	35	10			
27	D	1	Total	C	O		0	0
			46	36	10			
27	D	1	Total	C	O		0	0
			48	38	10			
27	I	1	Total	C	O		0	0
			43	33	10			
27	J	1	Total	C	O		0	0
			48	38	10			
27	M	1	Total	C	O		0	0
			42	32	10			

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



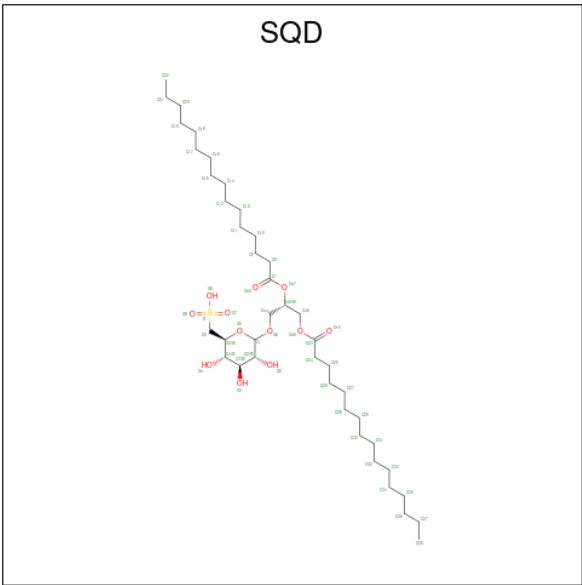
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			52	37	15		
28	B	1	Total	C	O	0	0
			66	51	15		
28	B	1	Total	C	O	0	0
			58	43	15		
28	C	1	Total	C	O	0	0
			56	41	15		
28	C	1	Total	C	O	0	0
			53	38	15		
28	C	1	Total	C	O	0	0
			62	47	15		
28	C	1	Total	C	O	0	0
			66	51	15		
28	D	1	Total	C	O	0	0
			63	48	15		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



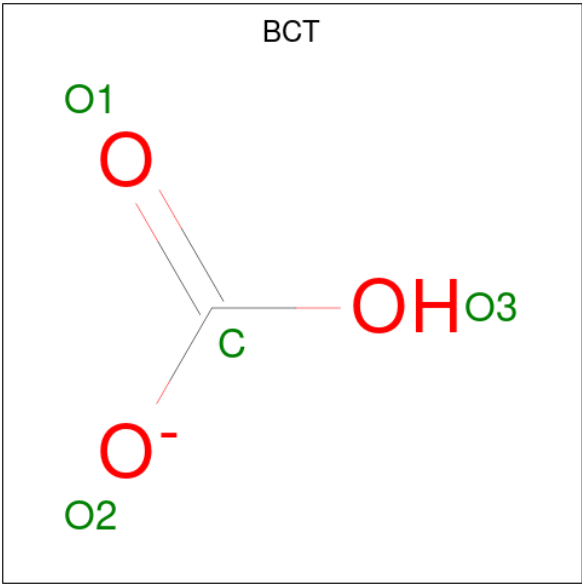
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			31	20	11		
29	I	1	Total	C	O	0	0
			35	24	11		
29	O	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



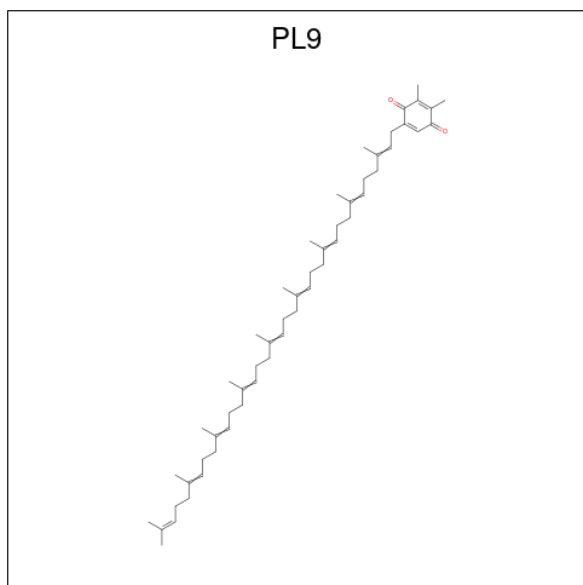
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	C	1	Total	C	O	S	0	0
			51	38	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



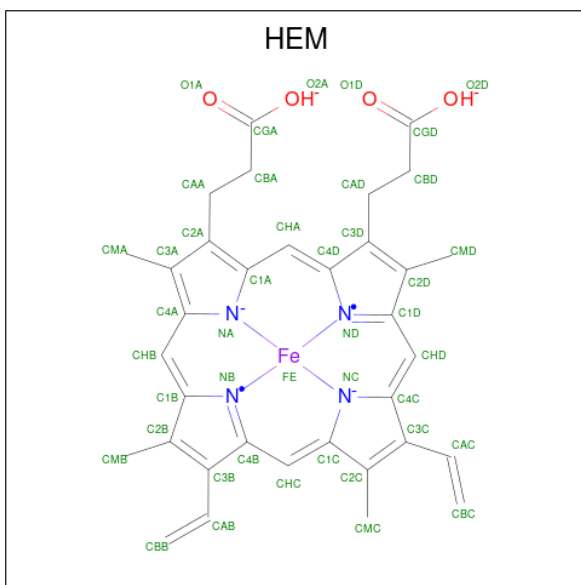
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			55	53	2		

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

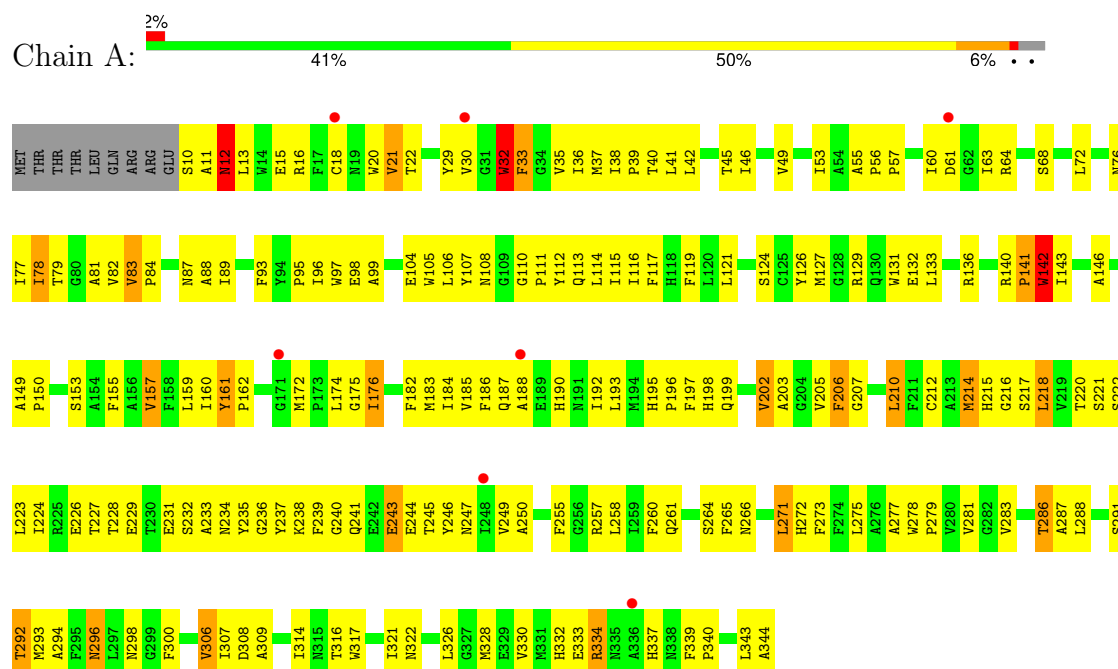
- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	F	1	Total Ca 1 1	0	0
34	K	1	Total Ca 1 1	0	0
34	O	1	Total Ca 1 1	0	0

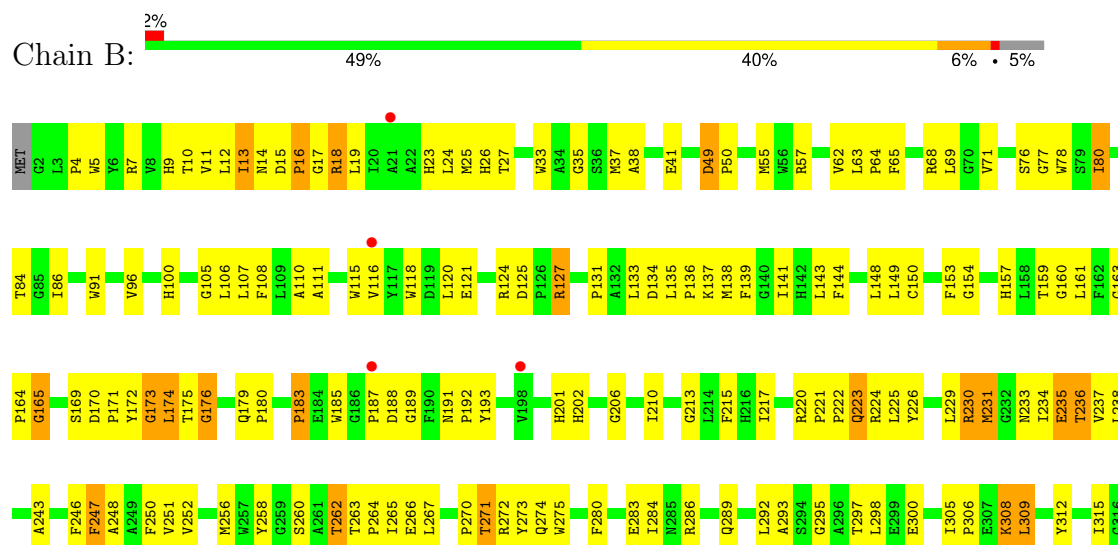
3 Residue-property plots [i](#)

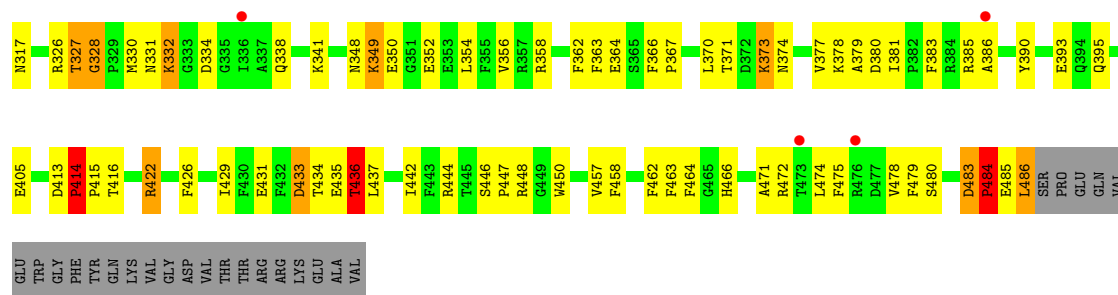
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Photosystem Q(B) protein 1

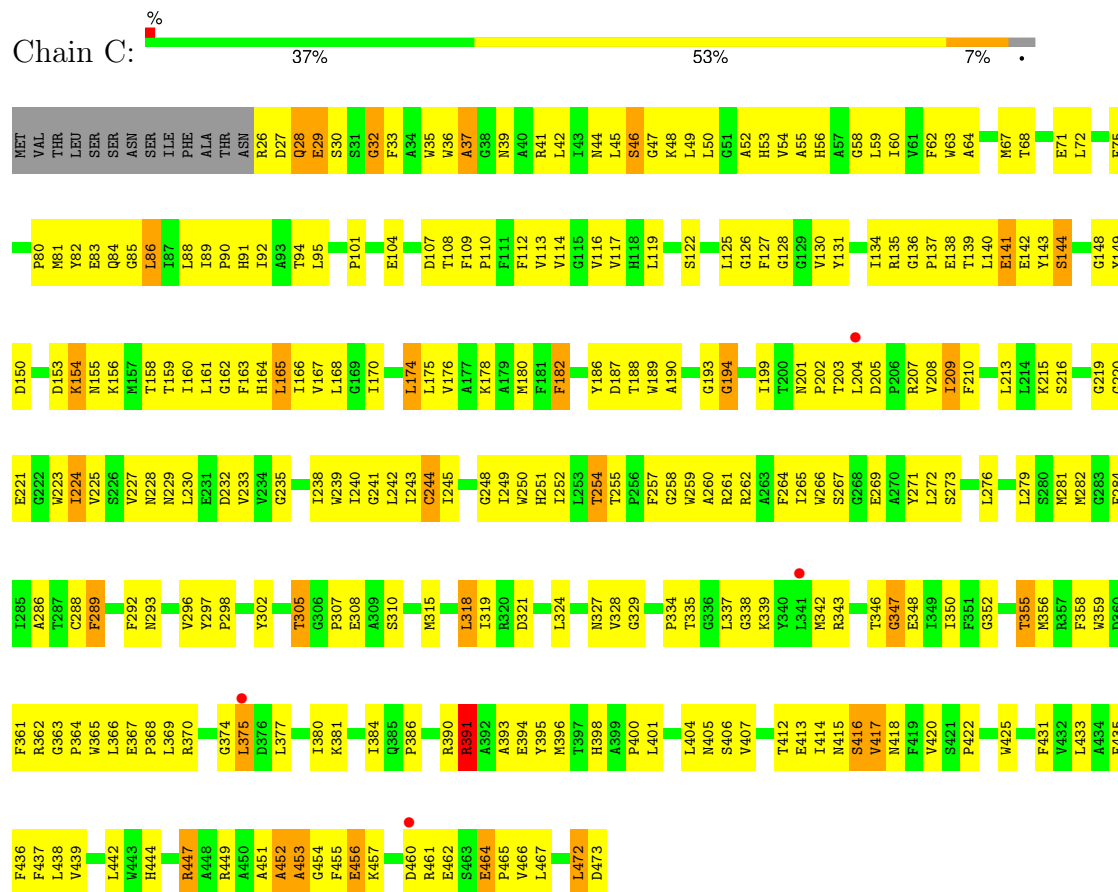


• Molecule 2: Photosystem II core light harvesting protein

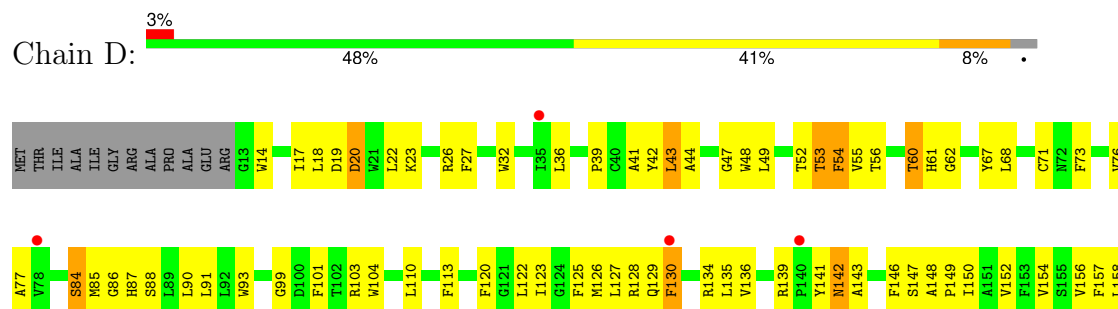


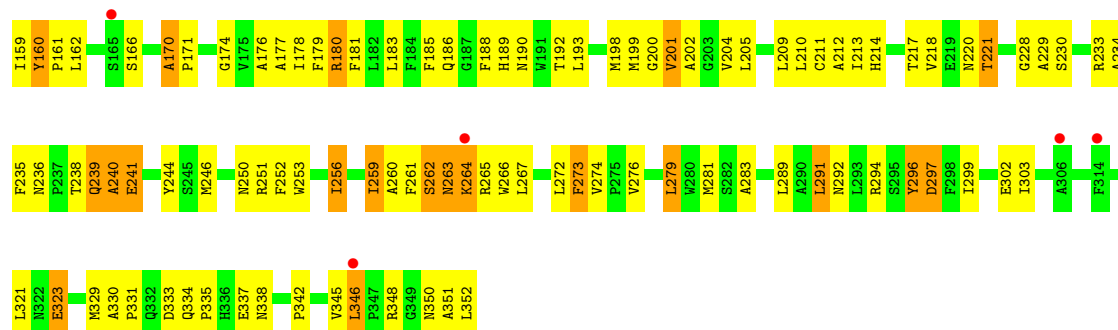


• Molecule 3: Photosystem II CP43 protein

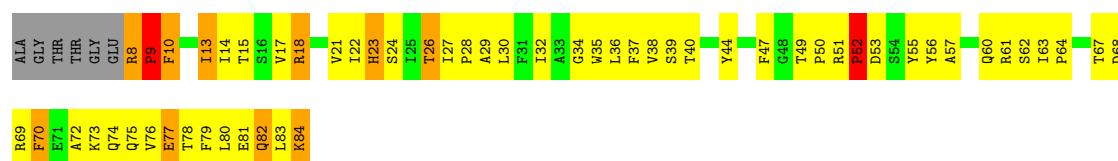


• Molecule 4: Photosystem II D2 protein

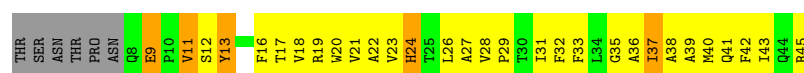




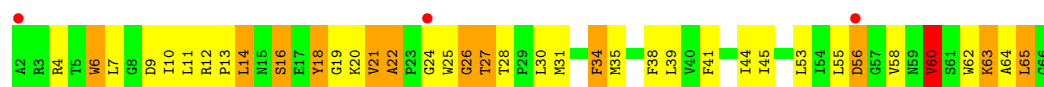
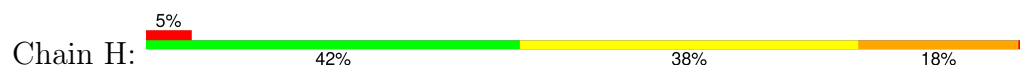
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H



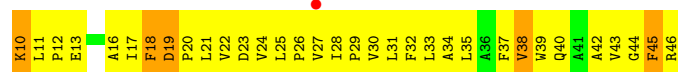
• Molecule 8: Photosystem II reaction center protein I



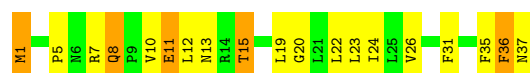
• Molecule 9: Photosystem II reaction center protein J



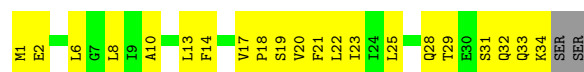
• Molecule 10: Photosystem II reaction center protein K



• Molecule 11: Photosystem II reaction center protein L



• Molecule 12: Photosystem II reaction center protein M



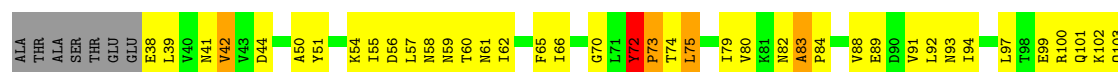
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



• Molecule 14: Photosystem II reaction center protein T



• Molecule 15: Photosystem II 12 kDa extrinsic protein





- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.89Å 224.69Å 337.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 29.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.87-3.60) 99.1 (29.87-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.297 , 0.308 0.296 , 0.303	Depositor DCC
R_{free} test set	1054 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	153.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24678	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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, FE2, LMG, LMT, BCR, BCT, MES, PL9, CA, OEC, CLA, HEM, DGD, SQD, PHO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	0/2713	1.06	19/3700 (0.5%)
2	B	0.54	0/3947	1.03	26/5379 (0.5%)
3	C	0.50	0/3567	1.00	13/4856 (0.3%)
4	D	0.58	0/2801	1.01	12/3818 (0.3%)
5	E	0.50	0/654	1.17	9/891 (1.0%)
6	F	0.80	0/317	0.99	0/433
7	H	0.48	0/520	0.93	2/709 (0.3%)
8	I	0.54	0/293	1.08	2/395 (0.5%)
9	J	0.48	0/255	1.17	2/346 (0.6%)
10	K	0.50	0/303	0.96	1/416 (0.2%)
11	L	0.50	0/311	1.02	1/422 (0.2%)
12	M	0.54	0/270	0.91	0/367
13	O	0.53	0/1876	1.03	13/2548 (0.5%)
14	T	0.56	0/265	0.97	0/359
15	U	0.55	0/785	1.10	6/1064 (0.6%)
16	V	0.51	0/1081	0.95	4/1468 (0.3%)
17	y	0.66	0/202	1.23	1/272 (0.4%)
18	X	0.48	0/257	0.90	0/348
19	Z	0.48	0/490	1.12	4/669 (0.6%)
All	All	0.54	0/20907	1.03	115/28460 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	34	ASP	N-CA-C	-9.30	101.71	113.43
17	y	22	LEU	N-CA-C	-9.06	101.48	112.54
3	C	182	PHE	N-CA-C	8.82	123.87	113.20
13	O	102	THR	N-CA-C	8.79	120.94	111.36
5	E	57	ALA	N-CA-C	-8.68	99.34	110.53

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain

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	2628	0	2524	258	0
2	B	3812	0	3683	274	0
3	C	3455	0	3378	387	0
4	D	2706	0	2608	244	0
5	E	635	0	625	82	0
6	F	307	0	312	52	0
7	H	507	0	521	69	0
8	I	286	0	308	25	0
9	J	249	0	262	52	0
10	K	293	0	305	63	0
11	L	304	0	316	29	0
12	M	267	0	289	34	0
13	O	1845	0	1801	127	0
14	T	256	0	262	26	0
15	U	774	0	773	51	0
16	V	1060	0	1068	51	0
17	y	201	0	226	32	0
18	X	254	0	282	30	0
19	Z	479	0	516	69	0
20	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A	260	0	288	48	0
21	B	1040	0	1152	131	0
21	C	780	0	864	134	0
21	D	130	0	144	18	0
21	K	65	0	72	12	0
22	A	64	0	74	6	0
22	D	64	0	74	15	0
23	A	12	0	13	13	0
24	A	5	0	0	0	0
25	A	40	0	56	9	0
25	B	120	0	168	8	0
25	C	80	0	112	24	0
25	D	40	0	56	8	0
25	J	80	0	112	19	0
25	X	40	0	56	5	0
25	Z	40	0	56	5	0
26	A	39	0	51	7	0
26	C	37	0	44	5	0
27	A	51	0	72	40	0
27	B	49	0	68	6	0
27	C	45	0	60	6	0
27	D	94	0	127	36	0
27	I	43	0	56	0	0
27	J	48	0	66	4	0
27	M	42	0	54	3	0
28	A	52	0	62	1	0
28	B	124	0	170	41	0
28	C	237	0	311	77	0
28	D	63	0	87	0	0
29	A	35	0	46	0	0
29	B	35	0	46	2	0
29	D	66	0	81	3	0
29	I	35	0	46	2	0
29	O	35	0	46	1	0
29	T	35	0	46	1	0
30	C	51	0	68	5	0
30	D	43	0	49	9	0
30	F	45	0	53	0	0
30	L	47	0	60	2	0
31	D	4	0	0	0	0
32	D	55	0	80	30	0
33	F	43	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	V	43	0	30	5	0
34	F	1	0	0	0	0
34	K	1	0	0	0	0
34	O	1	0	0	0	0
All	All	24678	0	25265	1891	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 38.

The worst 5 of 1891 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)
30:C:475:SQD:C3	30:C:475:SQD:C4	1.74	1.58
16:V:63:CYS:SG	33:V:164:HEM:HAB	1.65	1.35
27:A:373:LMG:H112	4:D:266:TRP:CH2	1.77	1.19
1:A:271:LEU:HD11	23:A:367:MES:C8	1.73	1.17
28:B:533:DGD:HAH1	12:M:17:VAL:HG21	1.21	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	5	31
2	B	483/510 (95%)	416 (86%)	54 (11%)	13 (3%)	4	27
3	C	446/461 (97%)	370 (83%)	60 (14%)	16 (4%)	2	22
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	4	27
5	E	75/83 (90%)	66 (88%)	5 (7%)	4 (5%)	1	14
6	F	36/44 (82%)	22 (61%)	9 (25%)	5 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	63/65 (97%)	45 (71%)	9 (14%)	9 (14%)	0	3
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1	13
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1	12
10	K	35/37 (95%)	26 (74%)	7 (20%)	2 (6%)	1	13
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	201 (83%)	29 (12%)	11 (5%)	2	17
14	T	28/32 (88%)	25 (89%)	3 (11%)	0	100	100
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	2	19
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	18	51
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	2
18	X	33/40 (82%)	25 (76%)	5 (15%)	3 (9%)	0	6
19	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1	16
All	All	2559/2714 (94%)	2121 (83%)	343 (13%)	95 (4%)	2	21

5 of 95 Ramachandran outliers are listed below:

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

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	271/280 (97%)	255 (94%)	16 (6%)	18	45
2	B	385/407 (95%)	368 (96%)	17 (4%)	25	52
3	C	348/362 (96%)	332 (95%)	16 (5%)	24	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	275/283 (97%)	257 (94%)	18 (6%)	15	43
5	E	69/72 (96%)	63 (91%)	6 (9%)	9	34
6	F	32/38 (84%)	31 (97%)	1 (3%)	35	59
7	H	53/54 (98%)	49 (92%)	4 (8%)	12	39
8	I	32/35 (91%)	30 (94%)	2 (6%)	16	44
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	53
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	30
11	L	35/35 (100%)	31 (89%)	4 (11%)	5	26
12	M	31/33 (94%)	30 (97%)	1 (3%)	34	58
13	O	202/208 (97%)	194 (96%)	8 (4%)	28	54
14	T	27/29 (93%)	26 (96%)	1 (4%)	30	56
15	U	84/89 (94%)	80 (95%)	4 (5%)	23	50
16	V	116/117 (99%)	112 (97%)	4 (3%)	32	57
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	17
18	X	28/33 (85%)	23 (82%)	5 (18%)	2	11
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	32
All	All	2114/2222 (95%)	1995 (94%)	119 (6%)	19	47

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	201	VAL
18	X	12	ILE
5	E	82	GLN
18	X	11	THR
19	Z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
11	L	8	GLN
13	O	222	GLN
12	M	33	GLN
13	O	135	GLN
15	U	82	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 4 are monoatomic - leaving 83 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	$\# Z > 2$
26	LHG	A	371	-	38,38,48	2.27	6 (15%)	41,44,54	1.41	4 (9%)
21	CLA	B	522	2	69,73,73	2.23	17 (24%)	82,113,113	1.70	11 (13%)
21	CLA	K	483	3	69,73,73	2.24	17 (24%)	82,113,113	1.78	13 (15%)
28	DGD	C	491	-	54,54,67	1.67	9 (16%)	68,68,81	2.94	24 (35%)
21	CLA	C	479	3	69,73,73	2.47	19 (27%)	82,113,113	1.91	13 (15%)
29	LMT	I	274	-	36,36,36	1.88	12 (33%)	47,47,47	1.34	7 (14%)
21	CLA	C	488	3	69,73,73	2.55	21 (30%)	82,113,113	1.85	15 (18%)
29	LMT	D	536	-	36,36,36	1.71	10 (27%)	47,47,47	1.61	8 (17%)
27	LMG	A	373	-	51,51,55	0.56	1 (1%)	59,59,63	1.10	5 (8%)
25	BCR	A	369	-	41,41,41	1.97	6 (14%)	56,56,56	2.13	23 (41%)
27	LMG	D	359	-	46,46,55	1.80	6 (13%)	54,54,63	2.54	17 (31%)
28	DGD	B	533	-	67,67,67	1.55	15 (22%)	81,81,81	1.83	19 (23%)
25	BCR	J	115	-	41,41,41	2.22	8 (19%)	56,56,56	3.32	17 (30%)
21	CLA	C	480	-	69,73,73	2.42	19 (27%)	82,113,113	1.97	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	B	527	-	41,41,41	1.83	7 (17%)	56,56,56	2.40	21 (37%)
21	CLA	B	518	2	69,73,73	2.55	19 (27%)	82,113,113	2.11	16 (19%)
21	CLA	B	520	-	69,73,73	2.29	19 (27%)	82,113,113	1.71	11 (13%)
21	CLA	C	483	-	69,73,73	2.59	23 (33%)	82,113,113	1.79	13 (15%)
27	LMG	B	531	-	49,49,55	1.74	6 (12%)	57,57,63	2.81	18 (31%)
21	CLA	B	519	2	69,73,73	2.34	17 (24%)	82,113,113	1.83	15 (18%)
21	CLA	B	524	2	69,73,73	2.56	22 (31%)	82,113,113	1.85	15 (18%)
28	DGD	C	474	-	57,57,67	2.11	15 (26%)	71,71,81	3.51	25 (35%)
21	CLA	A	362	1	69,73,73	2.15	19 (27%)	82,113,113	1.76	11 (13%)
21	CLA	B	514	2	69,73,73	2.33	16 (23%)	82,113,113	1.60	12 (14%)
25	BCR	B	530	-	41,41,41	2.56	9 (21%)	56,56,56	2.27	23 (41%)
25	BCR	Z	116	-	41,41,41	2.02	8 (19%)	56,56,56	2.14	21 (37%)
21	CLA	B	523	2	69,73,73	2.28	19 (27%)	82,113,113	1.67	13 (15%)
30	SQD	D	361	-	41,43,54	2.64	19 (46%)	51,54,65	2.81	16 (31%)
21	CLA	C	487	3	69,73,73	2.79	25 (36%)	82,113,113	1.85	11 (13%)
21	CLA	B	525	2	69,73,73	2.46	19 (27%)	82,113,113	1.83	12 (14%)
27	LMG	J	492	-	48,48,55	2.03	10 (20%)	56,56,63	1.88	17 (30%)
27	LMG	C	494	-	45,45,55	1.98	8 (17%)	53,53,63	2.20	16 (30%)
21	CLA	C	478	3	69,73,73	2.28	17 (24%)	82,113,113	1.75	15 (18%)
25	BCR	X	107	-	41,41,41	1.55	5 (12%)	56,56,56	2.46	21 (37%)
25	BCR	C	489	-	41,41,41	1.92	7 (17%)	56,56,56	2.13	19 (33%)
29	LMT	A	376	-	36,36,36	2.00	10 (27%)	47,47,47	1.47	8 (17%)
21	CLA	C	486	3	69,73,73	2.95	25 (36%)	82,113,113	1.79	15 (18%)
33	HEM	F	85	5	50,50,50	2.91	21 (42%)	67,82,82	2.49	20 (29%)
23	MES	A	367	-	12,12,12	1.51	1 (8%)	15,16,16	1.06	0
28	DGD	D	362	-	64,64,67	2.15	22 (34%)	78,78,81	2.47	21 (26%)
21	CLA	B	515	2	69,73,73	2.40	19 (27%)	82,113,113	1.78	14 (17%)
32	PL9	D	357	-	55,55,55	3.24	22 (40%)	68,69,69	2.85	27 (39%)
21	CLA	C	484	3	69,73,73	2.43	19 (27%)	82,113,113	1.82	14 (17%)
21	CLA	C	485	3	69,73,73	2.47	20 (28%)	82,113,113	1.76	13 (15%)
21	CLA	D	354	4	69,73,73	2.56	18 (26%)	82,113,113	1.68	14 (17%)
28	DGD	B	528	-	59,59,67	0.61	2 (3%)	73,73,81	1.07	8 (10%)
21	CLA	B	513	2	69,73,73	2.24	18 (26%)	82,113,113	1.88	14 (17%)
29	LMT	B	535	-	36,36,36	1.88	9 (25%)	47,47,47	1.15	2 (4%)
21	CLA	B	516	2	69,73,73	2.55	19 (27%)	82,113,113	1.96	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	517	-	69,73,73	2.69	22 (31%)	82,113,113	2.04	20 (24%)
25	BCR	B	529	-	41,41,41	2.18	7 (17%)	56,56,56	2.21	19 (33%)
27	LMG	I	220	-	43,43,55	2.09	12 (27%)	51,51,63	2.18	13 (25%)
28	DGD	C	492	-	63,63,67	1.43	11 (17%)	77,77,81	2.73	20 (25%)
28	DGD	A	375	-	53,53,67	2.09	13 (24%)	67,67,81	2.47	22 (32%)
25	BCR	J	112	-	41,41,41	1.93	7 (17%)	56,56,56	2.47	24 (42%)
30	SQD	C	475	-	49,51,54	2.71	27 (55%)	59,62,65	2.65	17 (28%)
21	CLA	A	363	-	69,73,73	2.22	19 (27%)	82,113,113	1.90	14 (17%)
28	DGD	C	493	-	67,67,67	1.51	16 (23%)	81,81,81	2.95	28 (34%)
21	CLA	B	526	2	69,73,73	2.65	22 (31%)	82,113,113	1.78	12 (14%)
21	CLA	B	512	2	69,73,73	2.15	17 (24%)	82,113,113	1.62	11 (13%)
21	CLA	C	481	3	69,73,73	2.73	22 (31%)	82,113,113	2.02	16 (19%)
30	SQD	L	213	-	45,47,54	2.70	25 (55%)	55,58,65	2.76	19 (34%)
26	LHG	C	476	-	36,36,48	2.44	6 (16%)	39,42,54	1.50	4 (10%)
27	LMG	M	217	-	42,42,55	2.02	8 (19%)	50,50,63	1.47	7 (14%)
21	CLA	D	356	4	69,73,73	2.38	20 (28%)	82,113,113	1.87	14 (17%)
33	HEM	V	164	16	50,50,50	2.72	25 (50%)	67,82,82	2.41	19 (28%)
21	CLA	B	511	-	69,73,73	2.82	28 (40%)	82,113,113	1.79	14 (17%)
21	CLA	C	482	3	69,73,73	2.86	23 (33%)	82,113,113	1.85	15 (18%)
21	CLA	C	477	3	69,73,73	2.35	16 (23%)	82,113,113	1.91	16 (19%)
29	LMT	T	226	-	36,36,36	1.80	9 (25%)	47,47,47	0.98	2 (4%)
31	BCT	D	353	20	3,3,3	0.53	0	2,3,3	0.36	0
22	PHO	D	355	-	58,69,69	3.74	16 (27%)	55,99,99	1.96	11 (20%)
21	CLA	B	521	2	69,73,73	2.45	17 (24%)	82,113,113	1.92	20 (24%)
29	LMT	D	363	-	32,32,36	1.83	7 (21%)	43,43,47	1.50	6 (13%)
21	CLA	A	364	-	69,73,73	2.33	20 (28%)	82,113,113	1.90	16 (19%)
25	BCR	D	358	-	41,41,41	1.76	7 (17%)	56,56,56	2.34	21 (37%)
21	CLA	A	366	1	69,73,73	2.34	20 (28%)	82,113,113	1.77	11 (13%)
25	BCR	C	490	-	41,41,41	1.99	6 (14%)	56,56,56	2.26	24 (42%)
29	LMT	O	274	-	36,36,36	2.01	12 (33%)	47,47,47	1.41	8 (17%)
30	SQD	F	224	-	43,45,54	2.74	22 (51%)	53,56,65	2.73	20 (37%)
22	PHO	A	365	-	58,69,69	4.00	16 (27%)	55,99,99	2.06	11 (20%)
27	LMG	D	360	-	48,48,55	0.57	1 (2%)	56,56,63	1.12	6 (10%)

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
26	LHG	A	371	-	-	16/43/43/53	-
21	CLA	B	522	2	1/1/15/20	14/39/115/115	-
21	CLA	K	483	3	1/1/15/20	6/39/115/115	-
28	DGD	C	491	-	-	5/42/82/95	0/2/2/2
21	CLA	C	479	3	1/1/15/20	12/39/115/115	-
29	LMT	I	274	-	-	2/21/61/61	0/2/2/2
21	CLA	C	488	3	1/1/15/20	7/39/115/115	-
29	LMT	D	536	-	-	1/21/61/61	0/2/2/2
27	LMG	A	373	-	-	20/46/66/70	0/1/1/1
25	BCR	A	369	-	-	5/29/63/63	0/2/2/2
27	LMG	D	359	-	-	5/41/61/70	0/1/1/1
28	DGD	B	533	-	-	9/55/95/95	0/2/2/2
25	BCR	J	115	-	-	3/29/63/63	0/2/2/2
21	CLA	C	480	-	1/1/15/20	14/39/115/115	-
25	BCR	B	527	-	-	4/29/63/63	0/2/2/2
21	CLA	B	518	2	1/1/15/20	8/39/115/115	-
21	CLA	B	520	-	1/1/15/20	14/39/115/115	-
21	CLA	C	483	-	1/1/15/20	10/39/115/115	-
27	LMG	B	531	-	-	4/44/64/70	0/1/1/1
21	CLA	B	519	2	1/1/15/20	7/39/115/115	-
21	CLA	B	524	2	1/1/15/20	12/39/115/115	-
28	DGD	C	474	-	-	7/45/85/95	0/2/2/2
21	CLA	A	362	1	1/1/15/20	9/39/115/115	-
21	CLA	B	514	2	1/1/15/20	10/39/115/115	-
25	BCR	B	530	-	-	4/29/63/63	0/2/2/2
25	BCR	Z	116	-	-	2/29/63/63	0/2/2/2
21	CLA	B	523	2	1/1/15/20	11/39/115/115	-
30	SQD	D	361	-	-	16/38/58/69	0/1/1/1
21	CLA	C	487	3	1/1/15/20	8/39/115/115	-
21	CLA	B	525	2	1/1/15/20	9/39/115/115	-
27	LMG	J	492	-	-	5/43/63/70	0/1/1/1
27	LMG	C	494	-	-	3/40/60/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	C	478	3	1/1/15/20	7/39/115/115	-
25	BCR	X	107	-	-	3/29/63/63	0/2/2/2
25	BCR	C	489	-	-	5/29/63/63	0/2/2/2
29	LMT	A	376	-	-	3/21/61/61	0/2/2/2
21	CLA	C	486	3	1/1/15/20	6/39/115/115	-
33	HEM	F	85	5	-	8/14/54/54	-
23	MES	A	367	-	-	3/6/14/14	0/1/1/1
28	DGD	D	362	-	-	10/52/92/95	0/2/2/2
21	CLA	B	515	2	1/1/15/20	8/39/115/115	-
32	PL9	D	357	-	-	17/53/73/73	0/1/1/1
21	CLA	C	484	3	1/1/15/20	12/39/115/115	-
21	CLA	C	485	3	1/1/15/20	10/39/115/115	-
21	CLA	D	354	4	1/1/15/20	10/39/115/115	-
28	DGD	B	528	-	-	18/47/87/95	0/2/2/2
21	CLA	B	513	2	1/1/15/20	10/39/115/115	-
29	LMT	B	535	-	-	3/21/61/61	0/2/2/2
21	CLA	B	516	2	1/1/15/20	10/39/115/115	-
21	CLA	B	517	-	1/1/15/20	8/39/115/115	-
25	BCR	B	529	-	-	0/29/63/63	0/2/2/2
27	LMG	I	220	-	-	4/38/58/70	0/1/1/1
28	DGD	C	492	-	1/1/13/13	8/51/91/95	0/2/2/2
28	DGD	A	375	-	-	6/41/81/95	0/2/2/2
25	BCR	J	112	-	-	1/29/63/63	0/2/2/2
30	SQD	C	475	-	-	22/46/66/69	0/1/1/1
21	CLA	A	363	-	1/1/15/20	9/39/115/115	-
28	DGD	C	493	-	1/1/13/13	9/55/95/95	0/2/2/2
21	CLA	B	526	2	1/1/15/20	9/39/115/115	-
21	CLA	B	512	2	1/1/15/20	7/39/115/115	-
21	CLA	C	481	3	1/1/15/20	11/39/115/115	-
30	SQD	L	213	-	-	16/42/62/69	0/1/1/1
26	LHG	C	476	-	-	16/41/41/53	-
27	LMG	M	217	-	-	3/37/57/70	0/1/1/1
21	CLA	D	356	4	1/1/15/20	8/39/115/115	-
33	HEM	V	164	16	-	10/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	511	-	1/1/15/20	16/39/115/115	-
21	CLA	C	482	3	1/1/15/20	10/39/115/115	-
21	CLA	C	477	3	1/1/15/20	10/39/115/115	-
29	LMT	T	226	-	-	1/21/61/61	0/2/2/2
22	PHO	D	355	-	1/1/17/22	16/37/103/103	0/5/6/6
21	CLA	B	521	2	1/1/15/20	9/39/115/115	-
29	LMT	D	363	-	-	1/17/57/61	0/2/2/2
21	CLA	A	364	-	1/1/15/20	11/39/115/115	-
25	BCR	D	358	-	-	3/29/63/63	0/2/2/2
21	CLA	A	366	1	1/1/15/20	6/39/115/115	-
25	BCR	C	490	-	-	3/29/63/63	0/2/2/2
29	LMT	O	274	-	-	3/21/61/61	0/2/2/2
30	SQD	F	224	-	-	18/40/60/69	0/1/1/1
22	PHO	A	365	-	1/1/17/22	6/37/103/103	0/5/6/6
27	LMG	D	360	-	-	20/43/63/70	0/1/1/1

The worst 5 of 1199 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	365	PHO	C3A-C2A	-17.56	1.39	1.54
22	D	355	PHO	C3A-C2A	-17.49	1.39	1.54
32	D	357	PL9	C28-C29	11.74	1.60	1.33
22	A	365	PHO	C1D-C2D	11.48	1.52	1.39
21	C	486	CLA	MG-NA	11.31	2.33	2.06

The worst 5 of 1197 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	474	DGD	O1G-C1G-C2G	12.52	144.47	108.40
25	J	115	BCR	C32-C1-C6	-10.90	93.14	110.24
28	C	492	DGD	O5D-C1E-C2E	10.88	124.80	108.27
33	F	85	HEM	CMA-C3A-C4A	10.64	141.62	125.42
28	C	491	DGD	O5D-C1E-C2E	10.63	124.41	108.27

5 of 39 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	362	CLA	C8
21	A	363	CLA	C8

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Mol	Chain	Res	Type	Atom
21	A	366	CLA	C8
21	A	364	CLA	C8
21	B	511	CLA	C8

5 of 685 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	511	CLA	C11-C12-C13-C14
21	B	516	CLA	C4-C3-C5-C6
21	B	524	CLA	CAD-CBD-CGD-O2D
21	C	477	CLA	CAD-CBD-CGD-O1D
21	C	477	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

77 monomers are involved in 672 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	371	LHG	7	0
21	B	522	CLA	10	0
21	K	483	CLA	12	0
28	C	491	DGD	17	0
21	C	479	CLA	19	0
29	I	274	LMT	2	0
21	C	488	CLA	6	0
29	D	536	LMT	1	0
27	A	373	LMG	40	0
25	A	369	BCR	9	0
27	D	359	LMG	6	0
28	B	533	DGD	18	0
25	J	115	BCR	7	0
21	C	480	CLA	14	0
25	B	527	BCR	1	0
21	B	518	CLA	12	0
21	B	520	CLA	7	0
21	C	483	CLA	11	0
27	B	531	LMG	6	0
21	B	519	CLA	6	0
21	B	524	CLA	5	0
28	C	474	DGD	8	0
21	A	362	CLA	19	0
21	B	514	CLA	9	0
25	B	530	BCR	2	0

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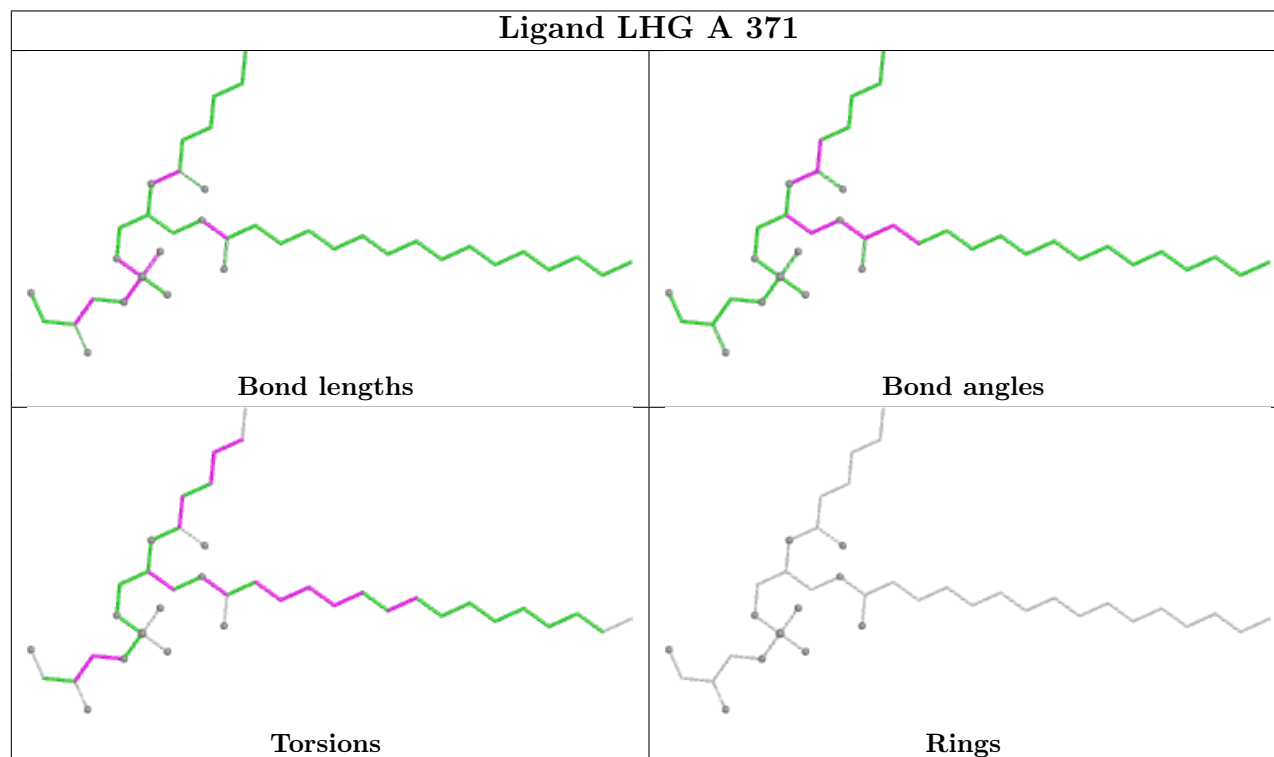
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	116	BCR	5	0
21	B	523	CLA	5	0
30	D	361	SQD	9	0
21	C	487	CLA	15	0
21	B	525	CLA	6	0
27	J	492	LMG	4	0
27	C	494	LMG	6	0
21	C	478	CLA	13	0
25	X	107	BCR	5	0
25	C	489	BCR	17	0
21	C	486	CLA	21	0
33	F	85	HEM	6	0
23	A	367	MES	13	0
21	B	515	CLA	9	0
32	D	357	PL9	30	0
21	C	484	CLA	13	0
21	C	485	CLA	2	0
21	D	354	CLA	15	0
28	B	528	DGD	23	0
21	B	513	CLA	23	0
29	B	535	LMT	2	0
21	B	516	CLA	7	0
21	B	517	CLA	19	0
25	B	529	BCR	5	0
28	C	492	DGD	14	0
28	A	375	DGD	1	0
25	J	112	BCR	12	0
30	C	475	SQD	5	0
21	A	363	CLA	14	0
28	C	493	DGD	40	0
21	B	526	CLA	4	0
21	B	512	CLA	9	0
21	C	481	CLA	16	0
30	L	213	SQD	2	0
26	C	476	LHG	5	0
27	M	217	LMG	3	0
21	D	356	CLA	3	0
33	V	164	HEM	5	0
21	B	511	CLA	3	0
21	C	482	CLA	7	0
21	C	477	CLA	9	0
29	T	226	LMT	1	0

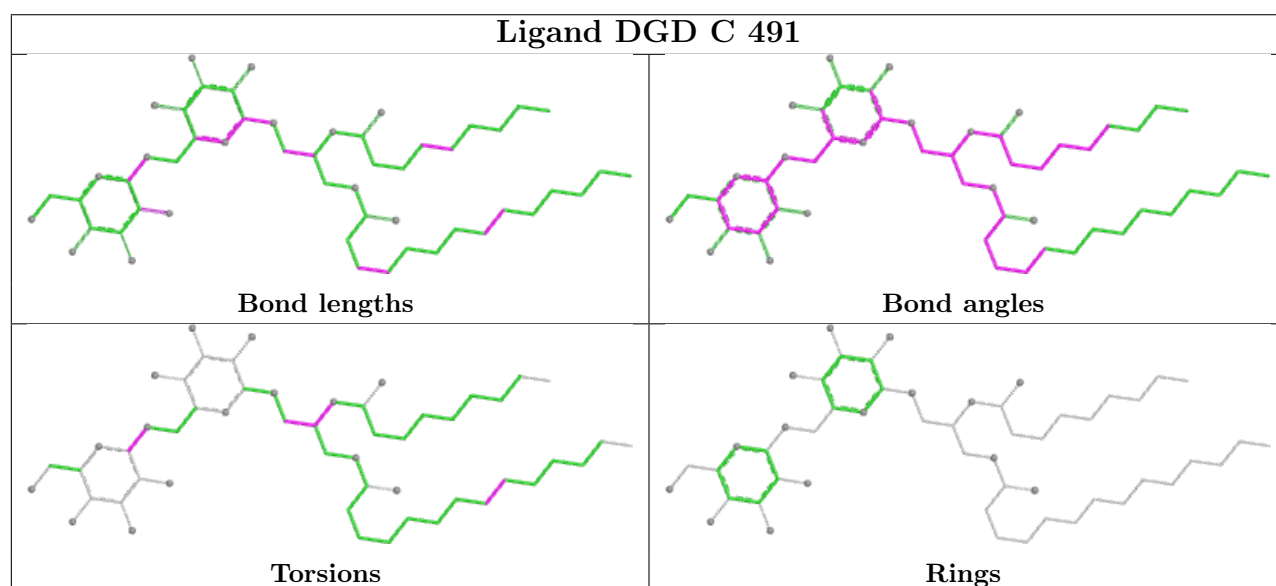
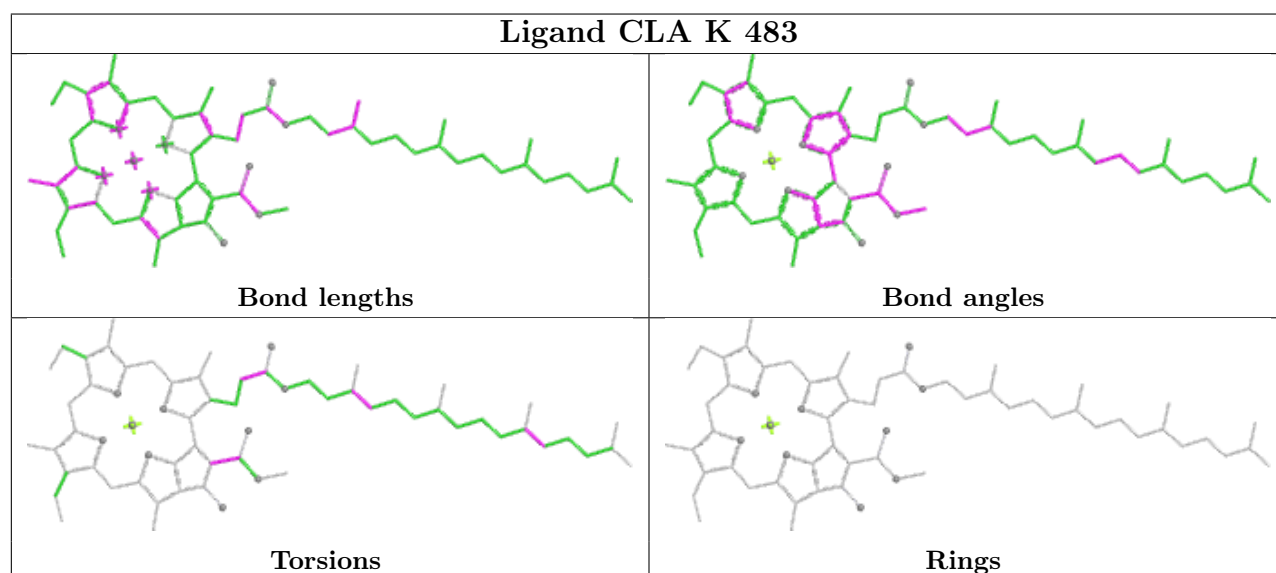
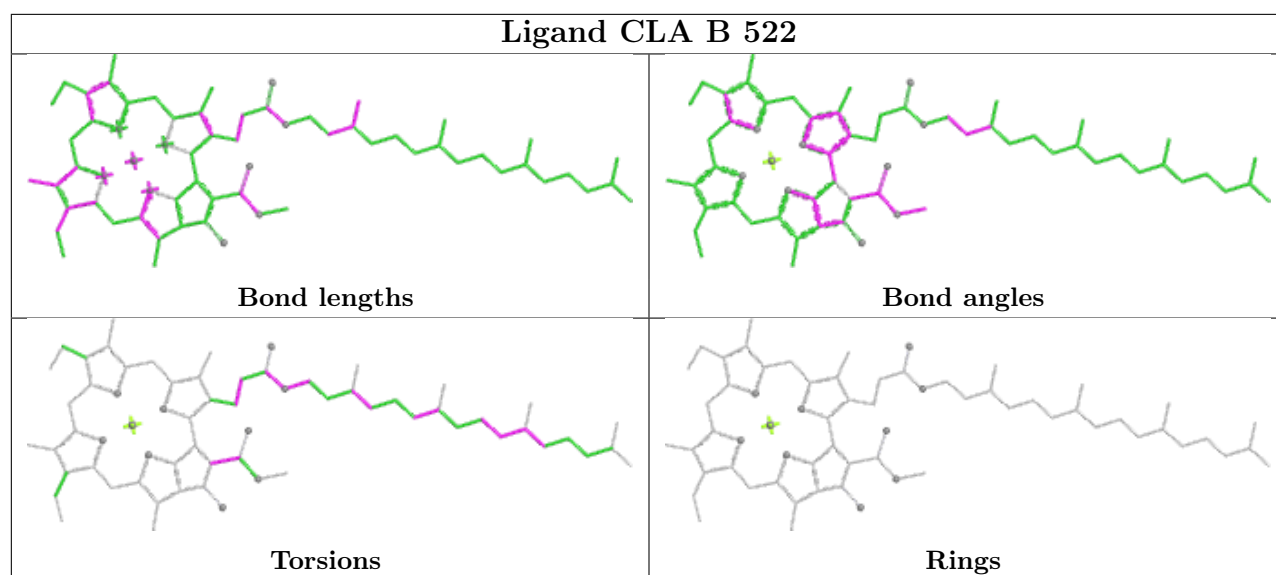
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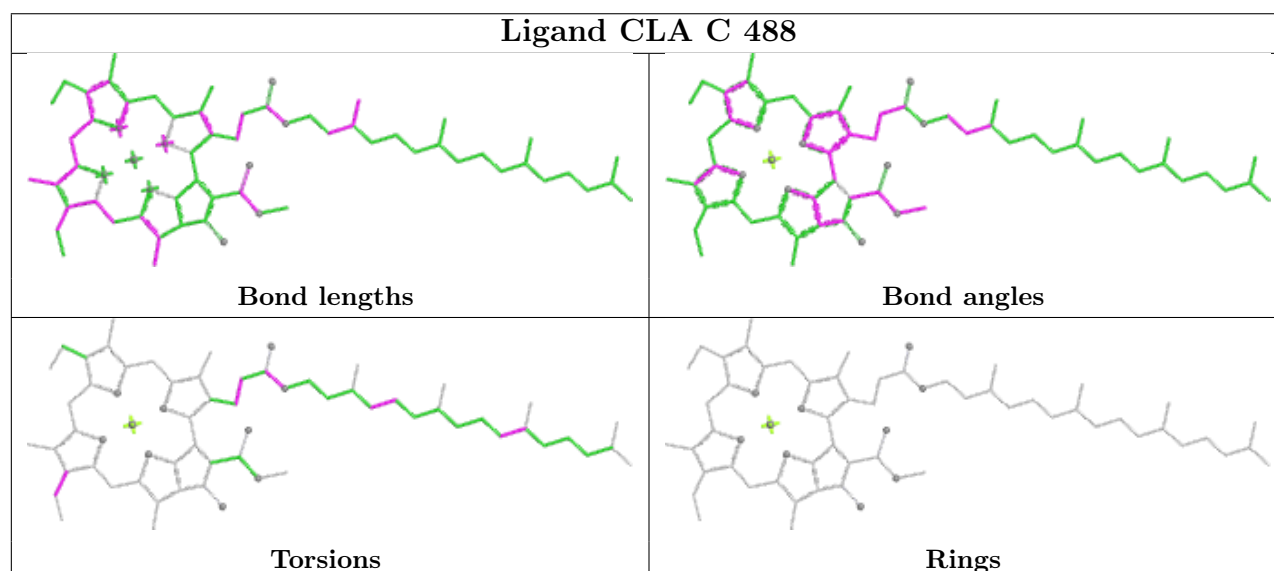
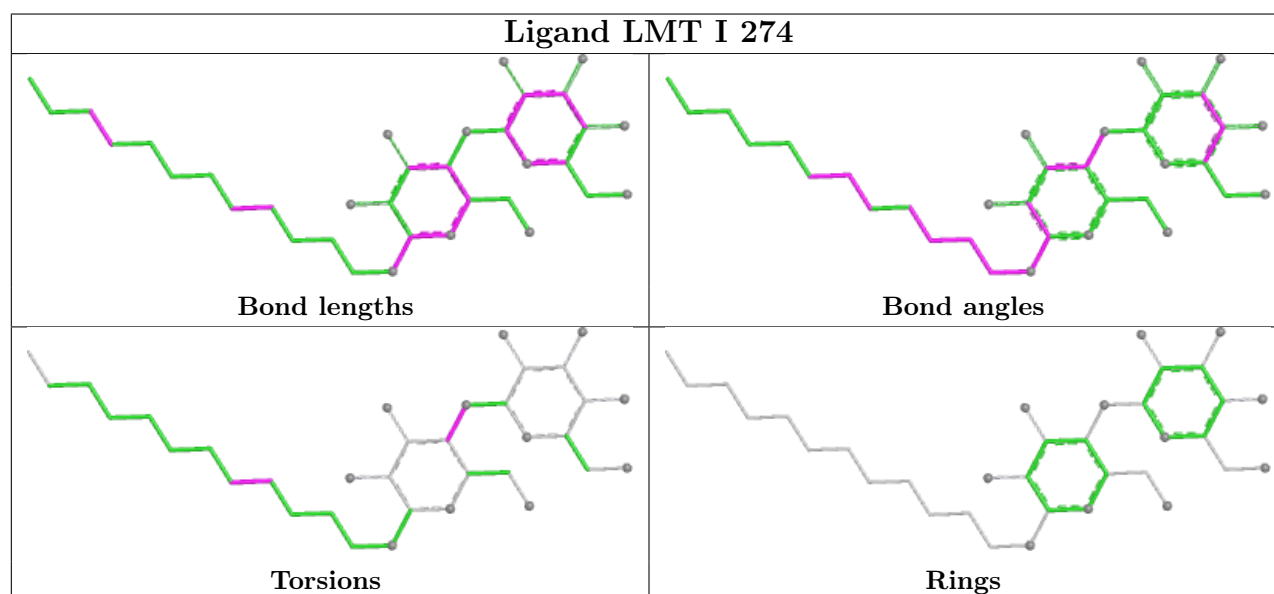
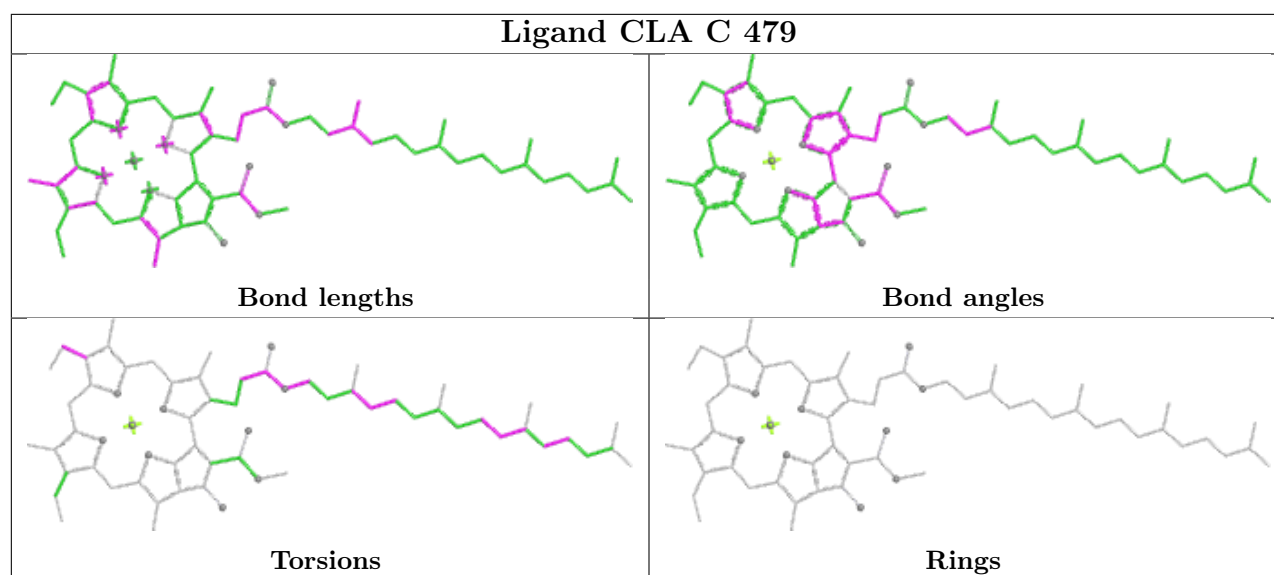
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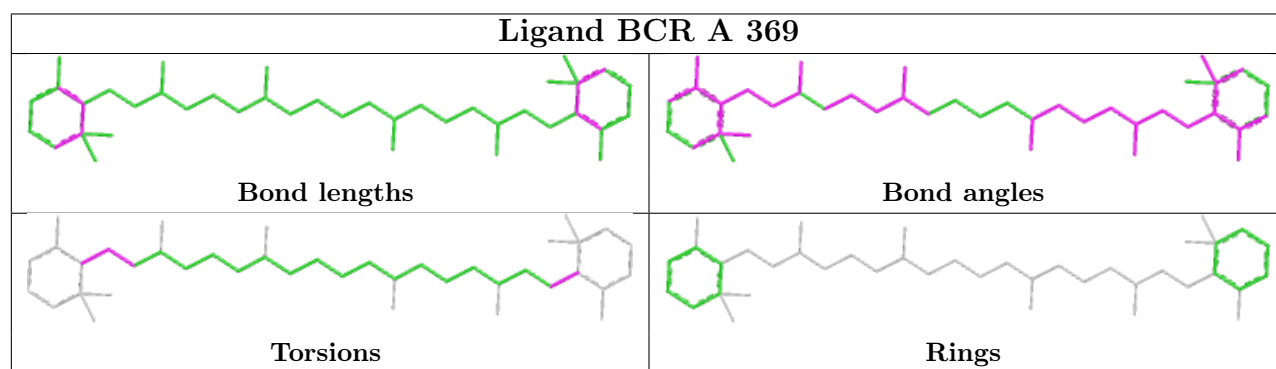
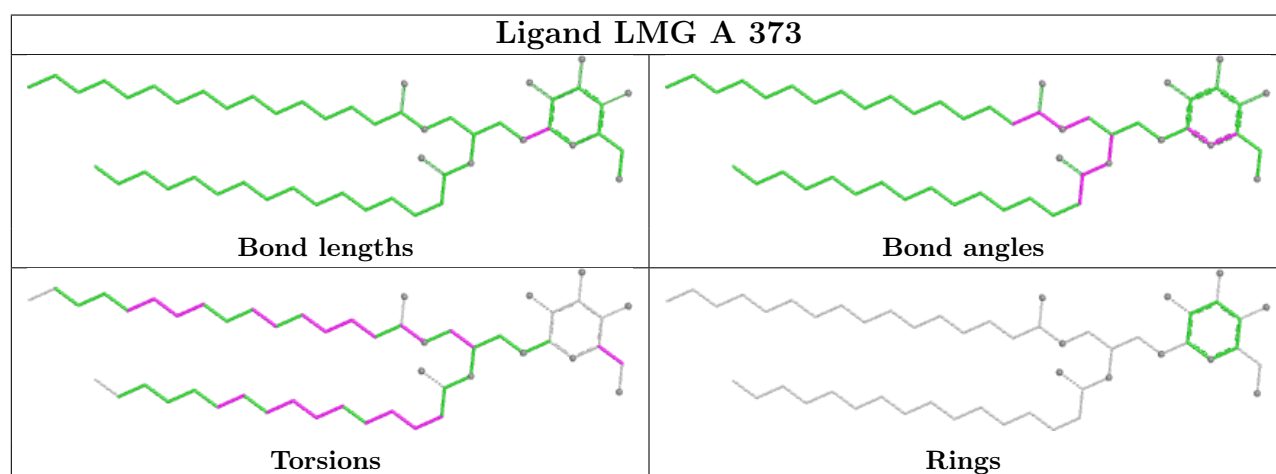
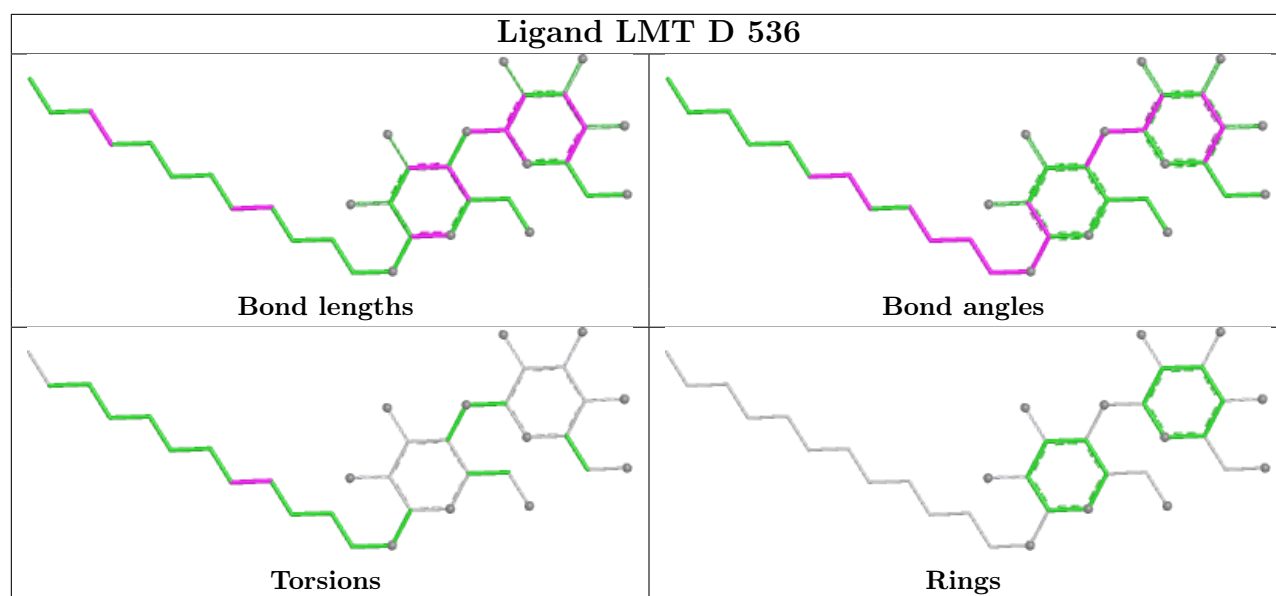
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	D	355	PHO	15	0
21	B	521	CLA	13	0
29	D	363	LMT	2	0
21	A	364	CLA	7	0
25	D	358	BCR	8	0
21	A	366	CLA	9	0
25	C	490	BCR	7	0
29	O	274	LMT	1	0
22	A	365	PHO	6	0
27	D	360	LMG	30	0

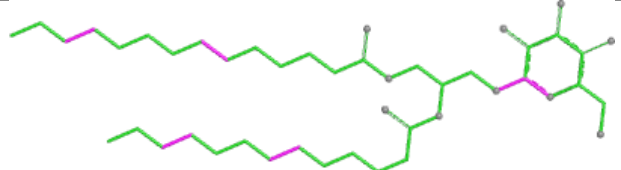
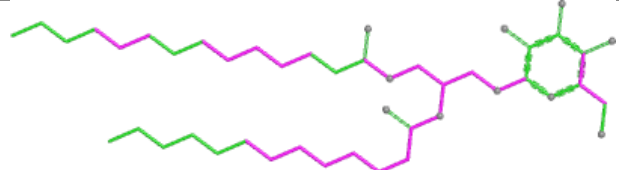
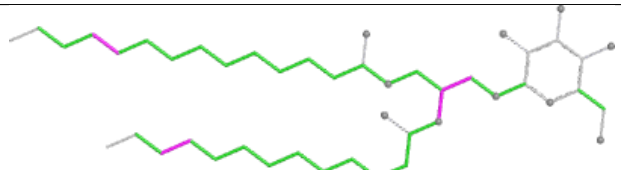
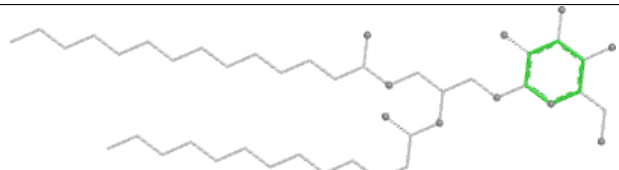
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

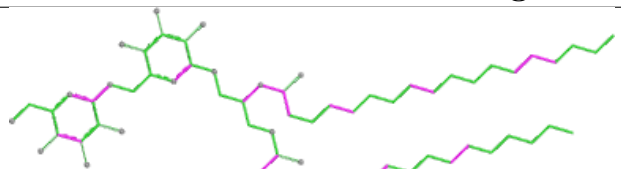
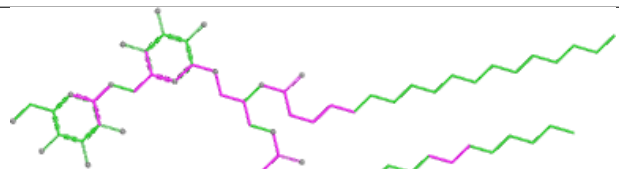
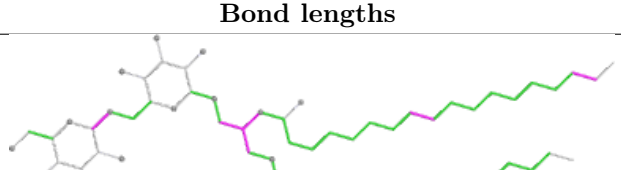
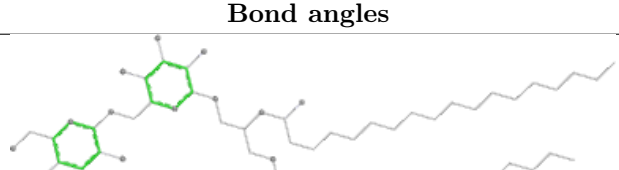


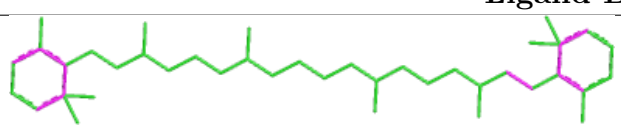
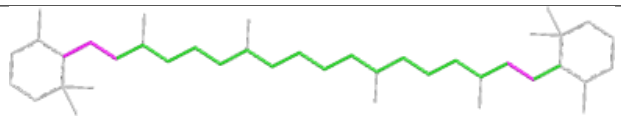
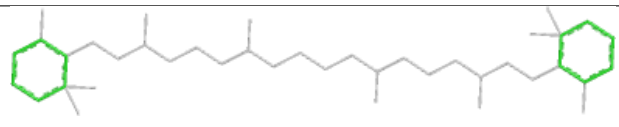


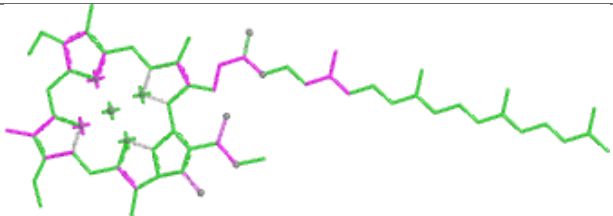
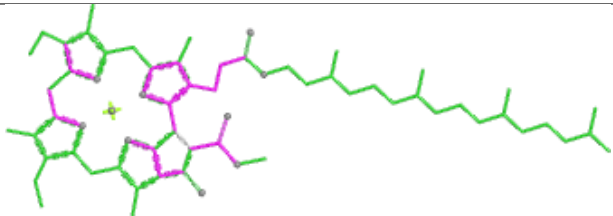
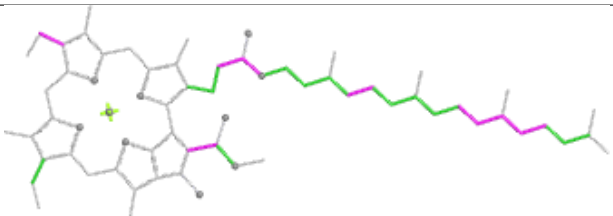
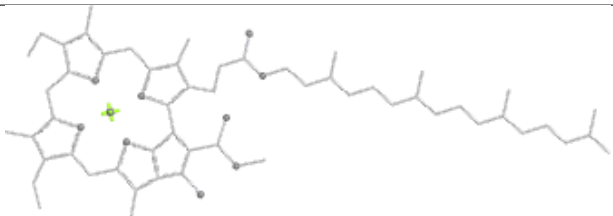


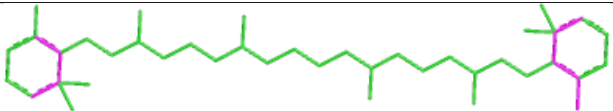
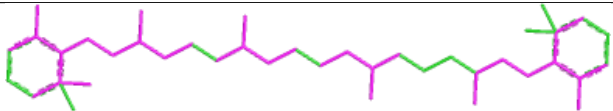
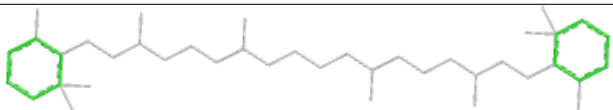


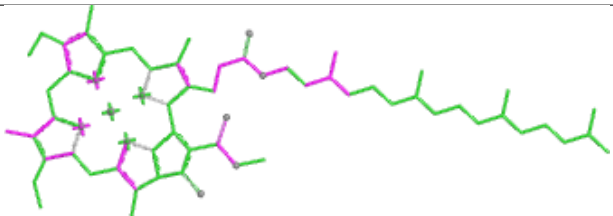
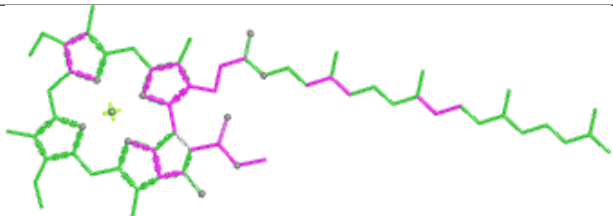
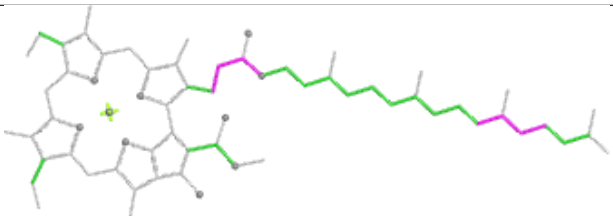
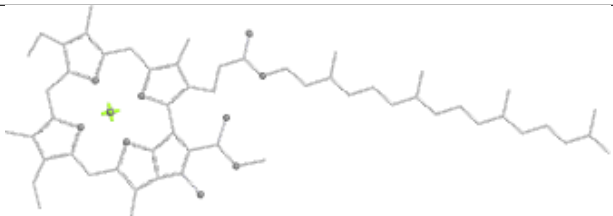
Ligand LMG D 359	
	
Bond lengths	Bond angles
	
Torsions	Rings

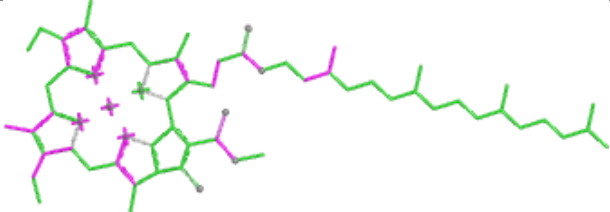
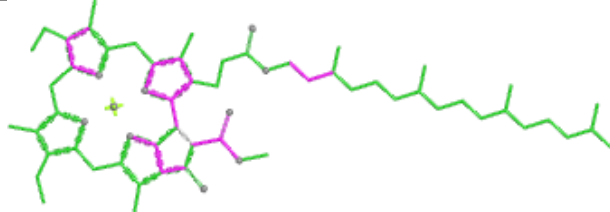
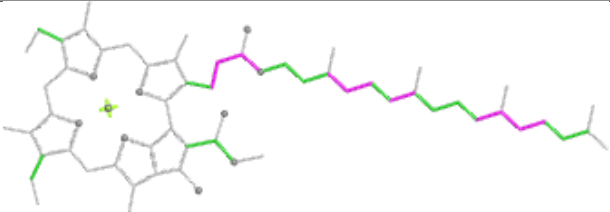
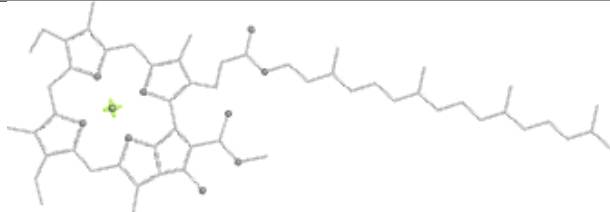
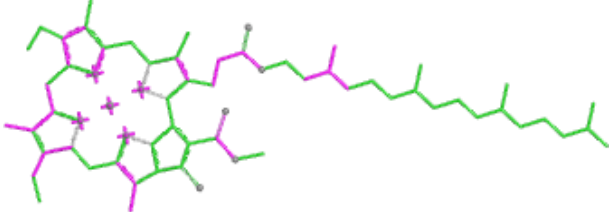
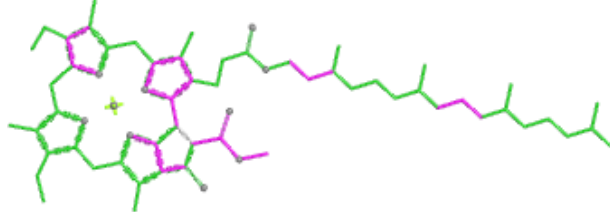
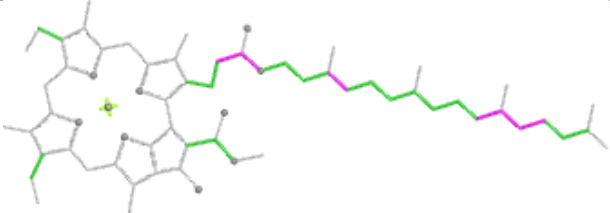
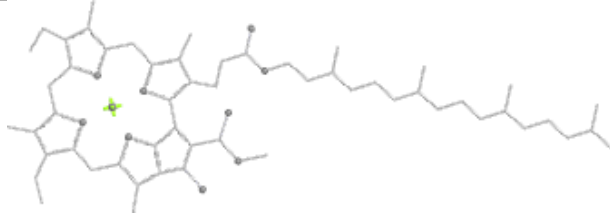
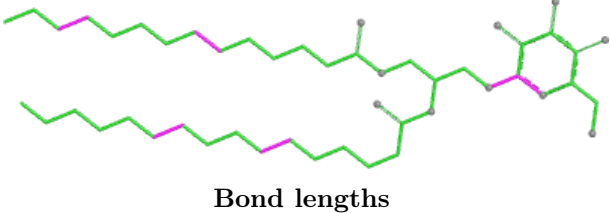
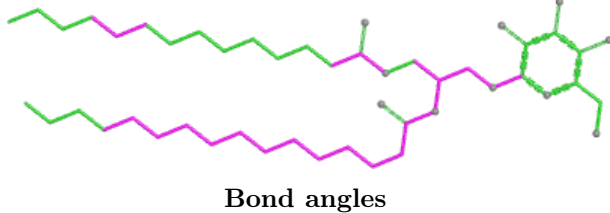
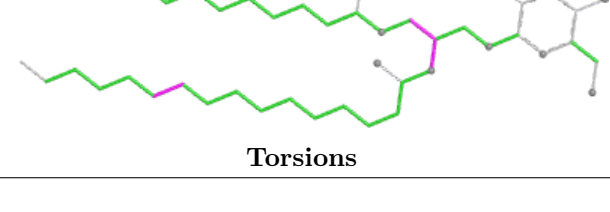
Ligand DGD B 533	
	
Bond lengths	Bond angles
	
Torsions	Rings

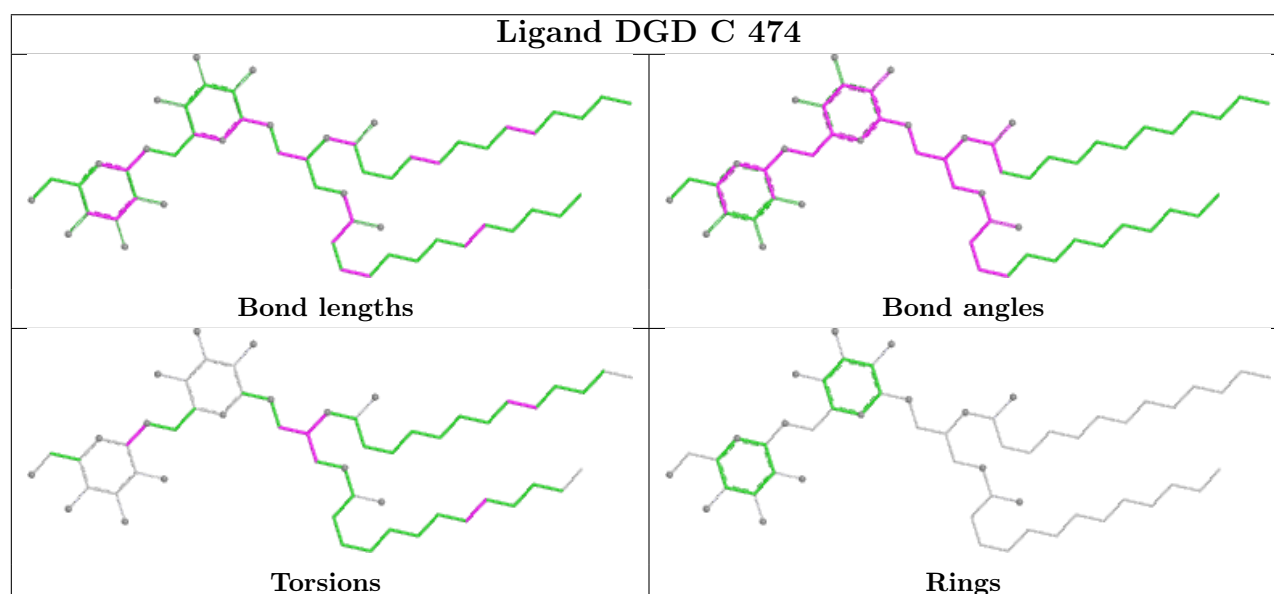
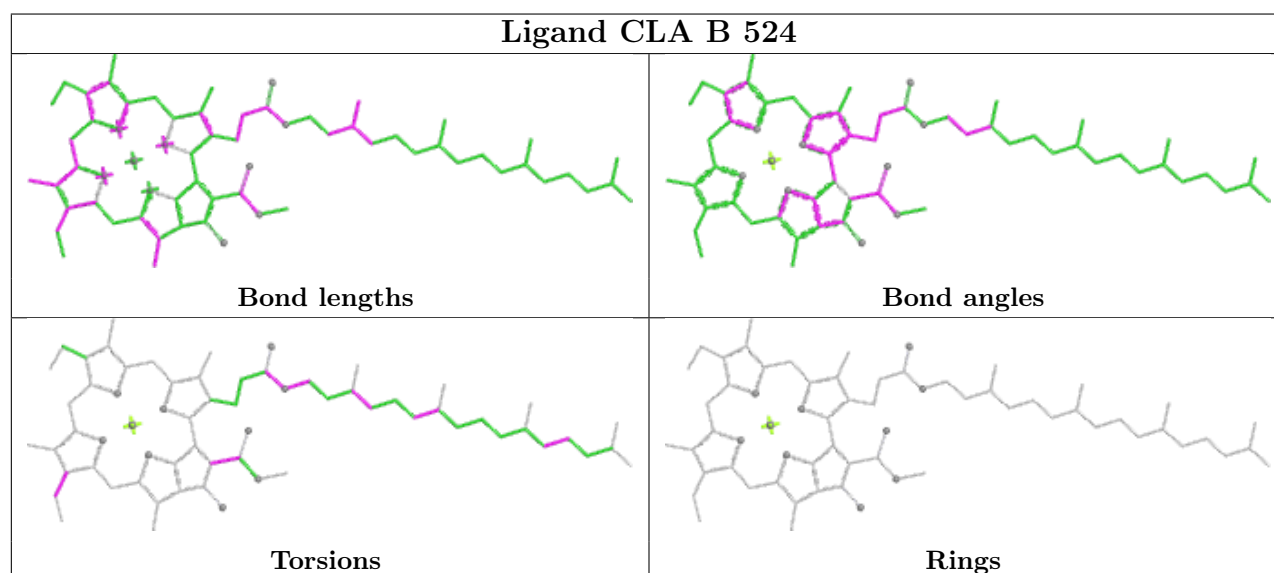
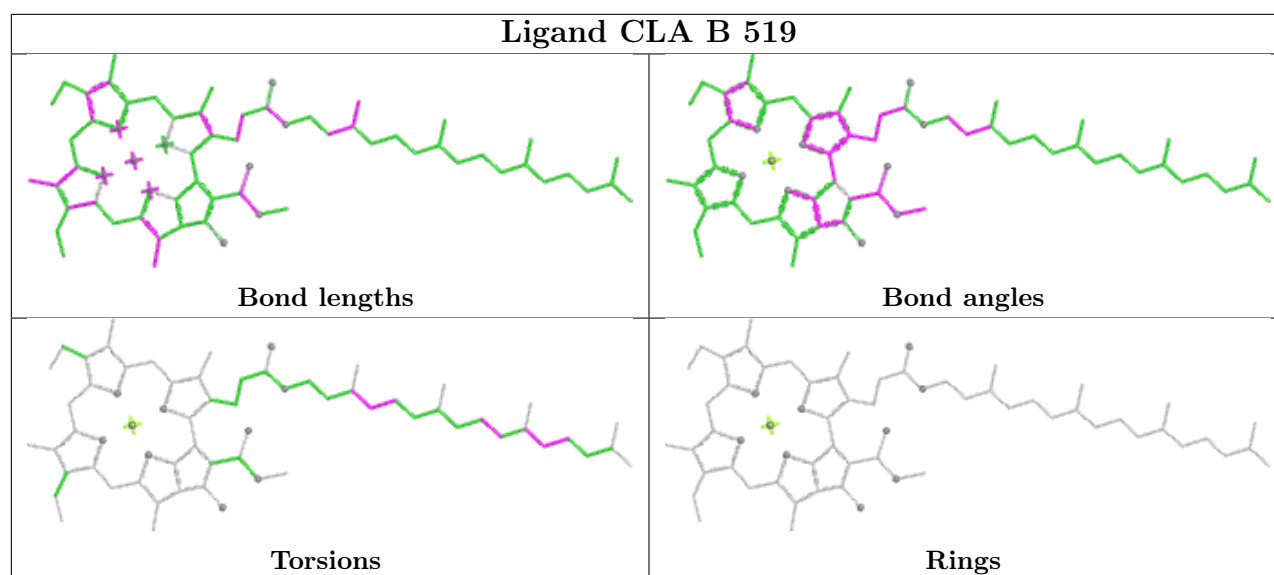
Ligand BCR J 115	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 480	
	
Bond lengths	Bond angles
	
Torsions	Rings

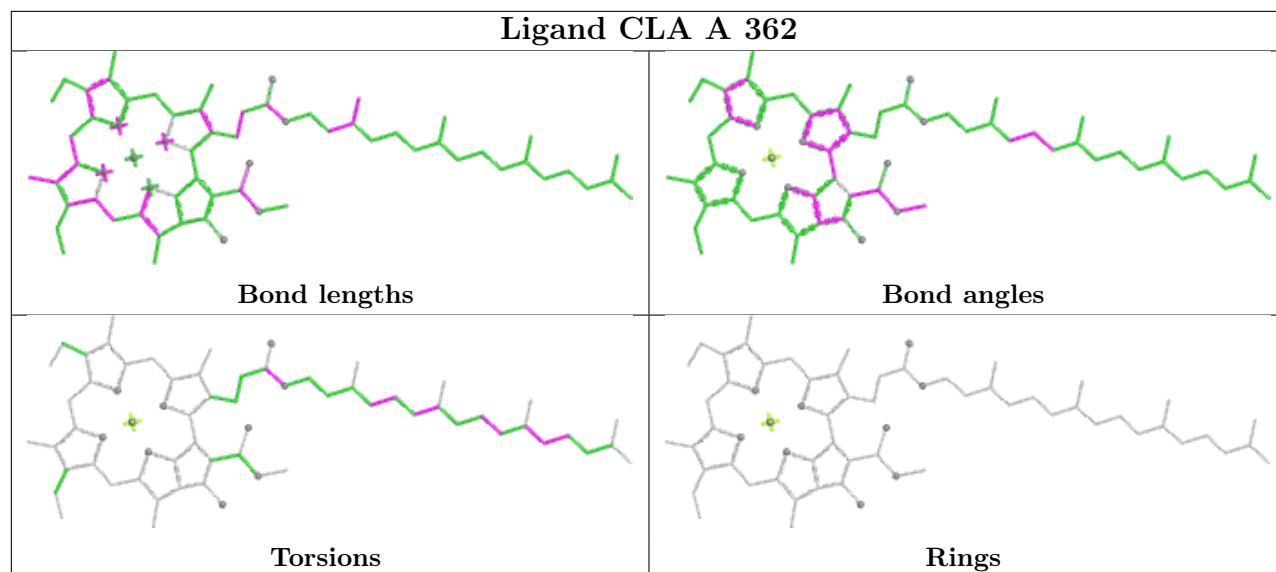
Ligand BCR B 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

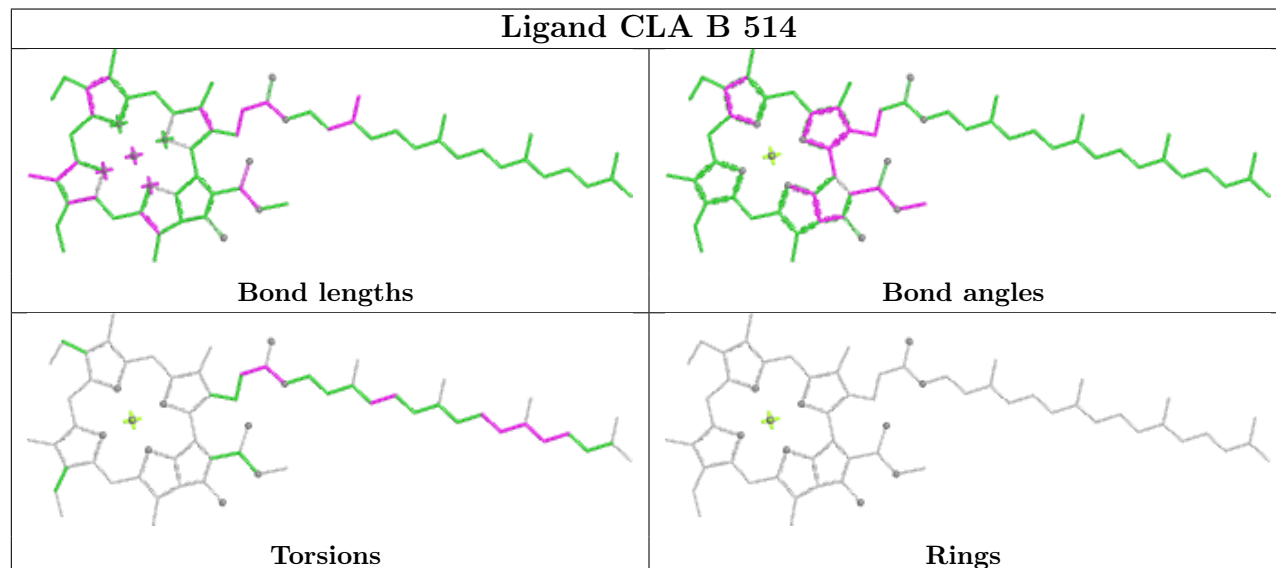
Ligand CLA B 520	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 483	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG B 531	
 Bond lengths	 Bond angles
 Torsions	 Rings



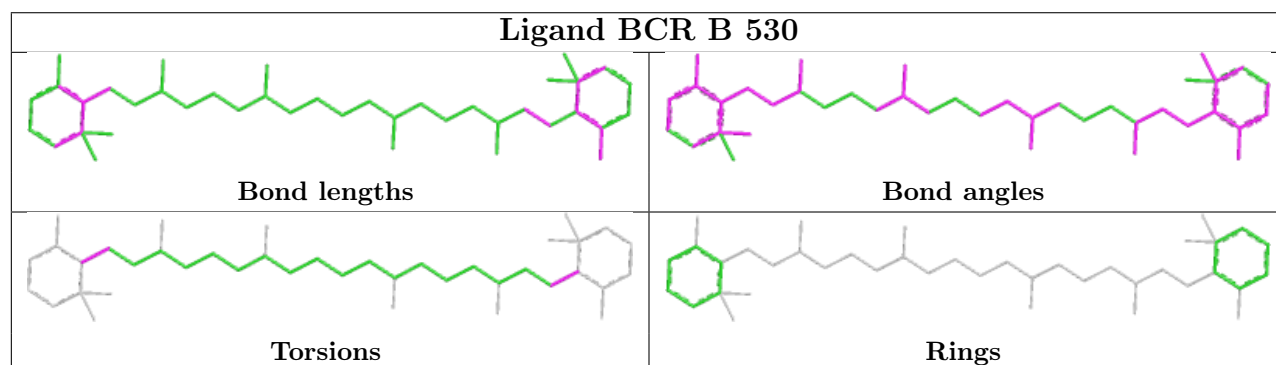
Ligand CLA A 362

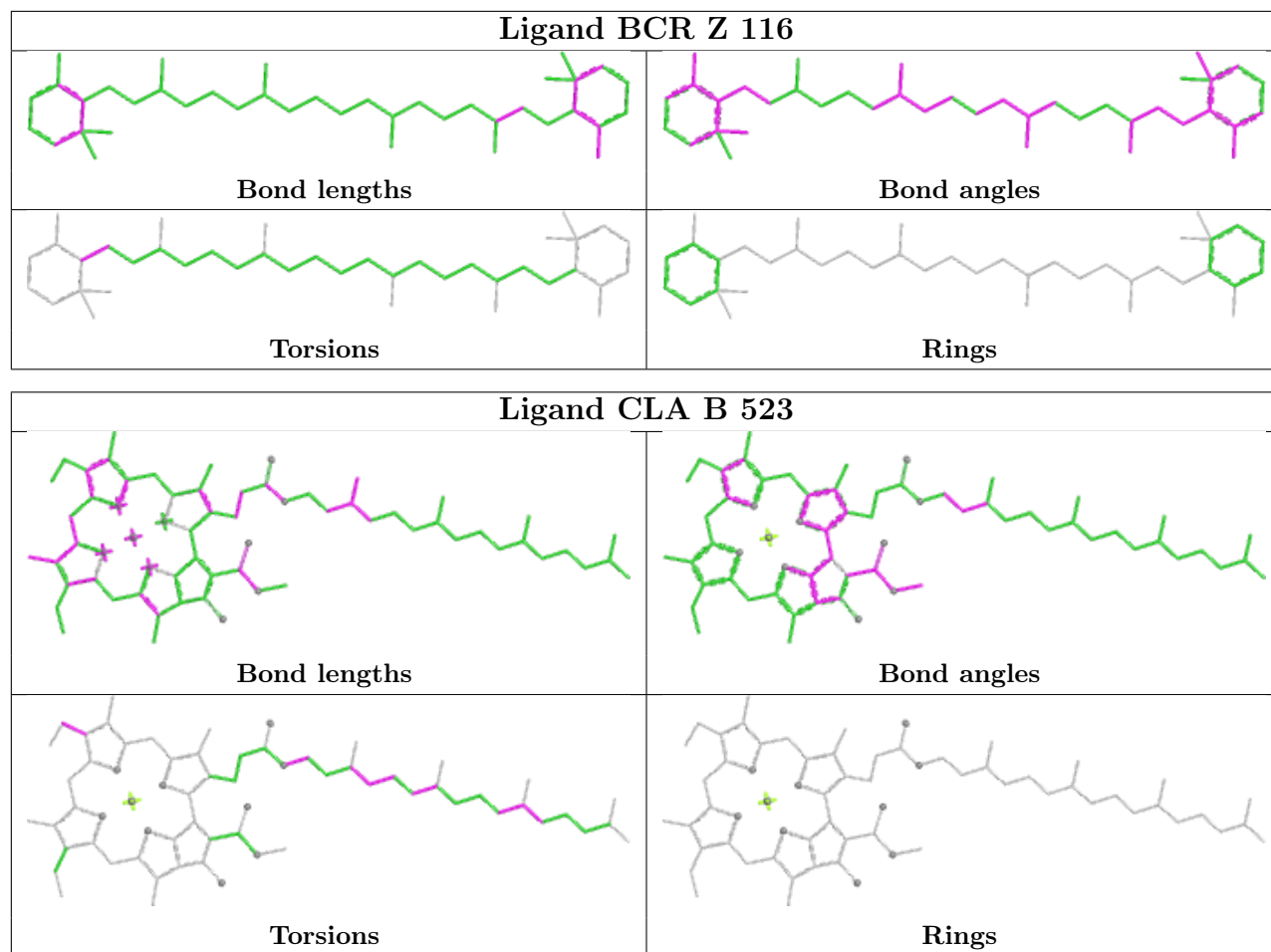


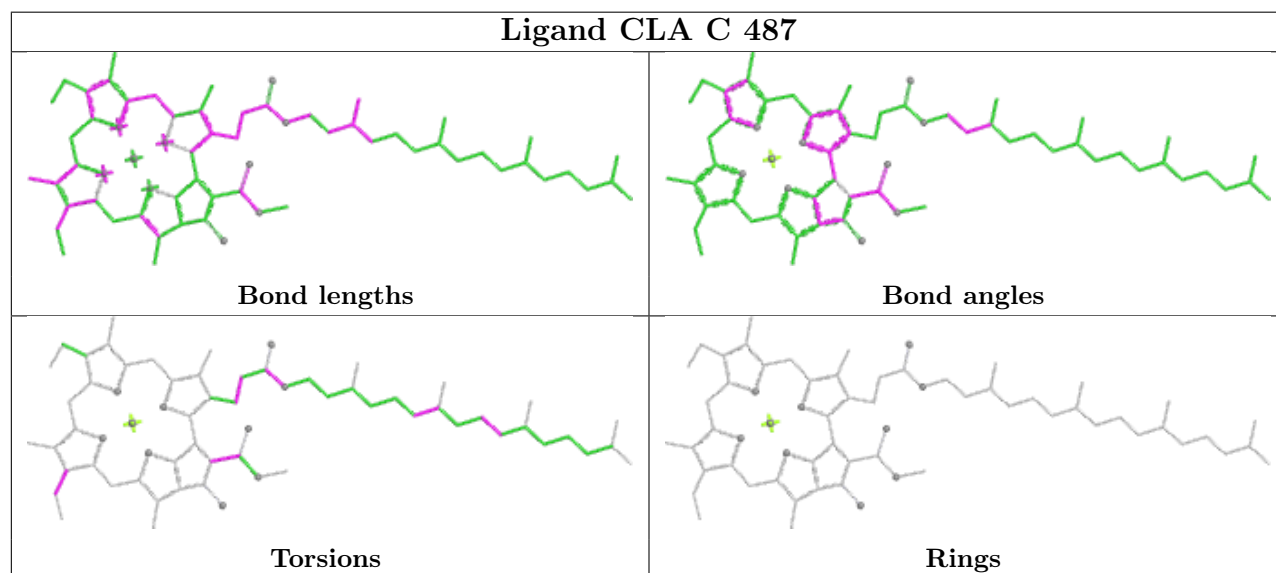
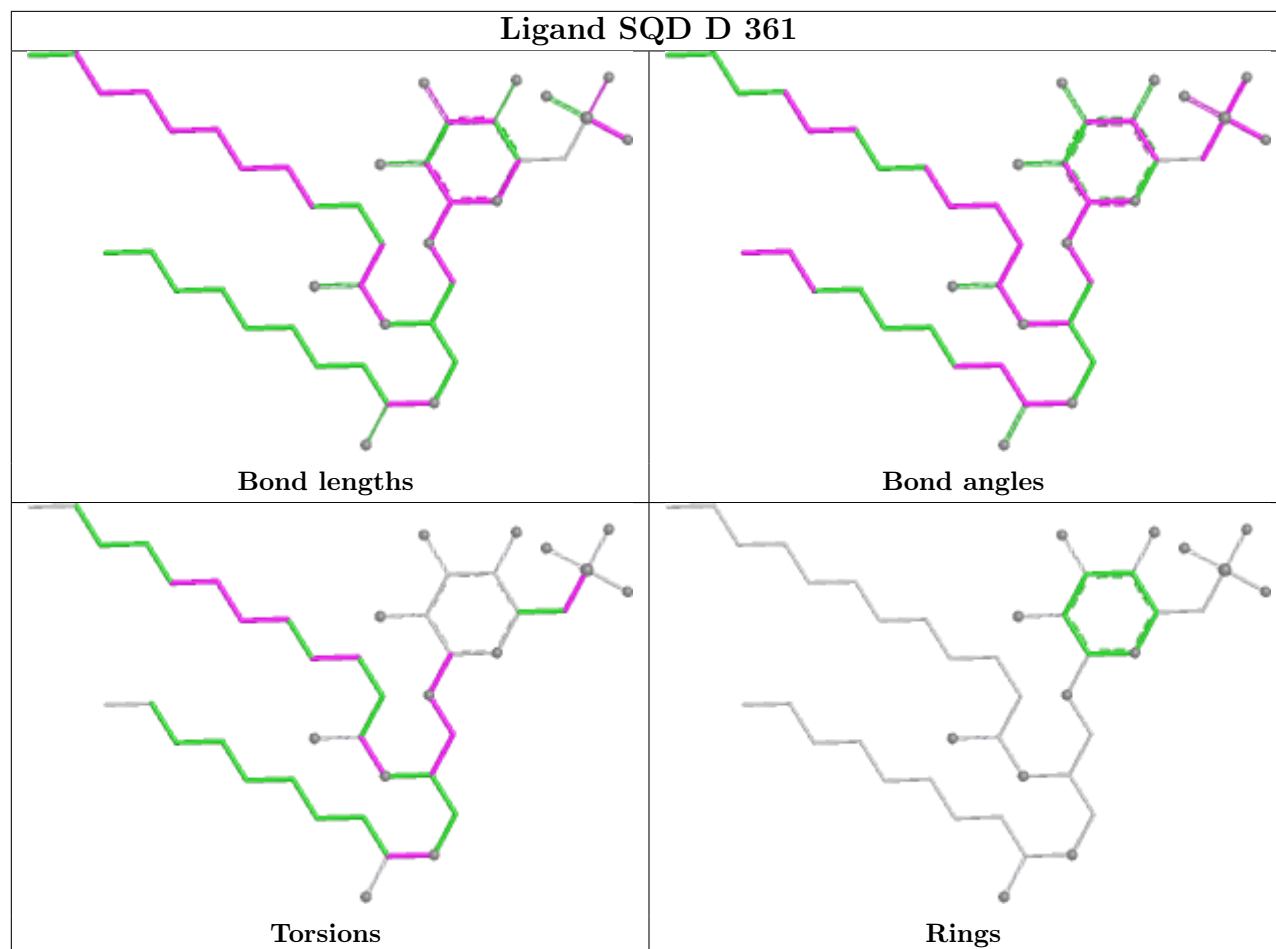
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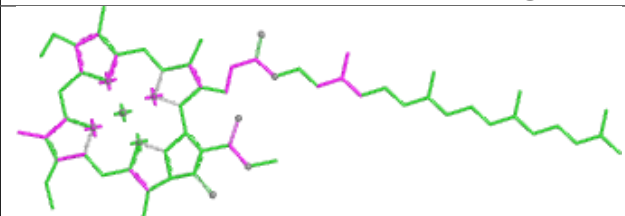
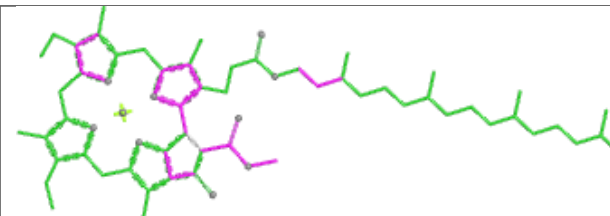
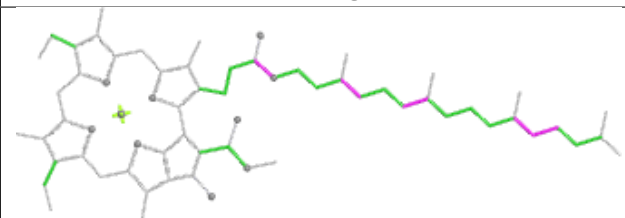
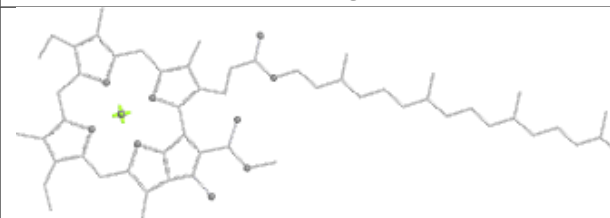


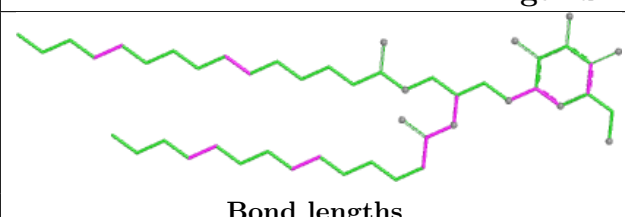
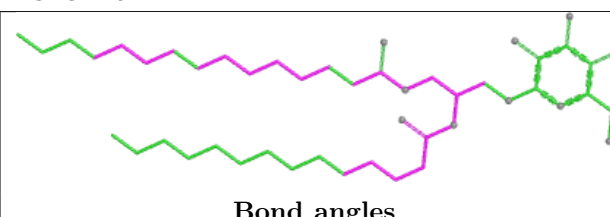
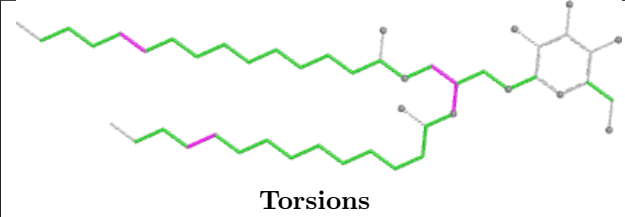
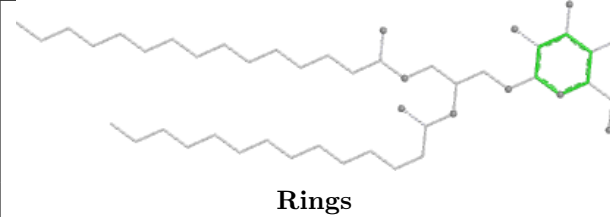
Ligand BCR B 530

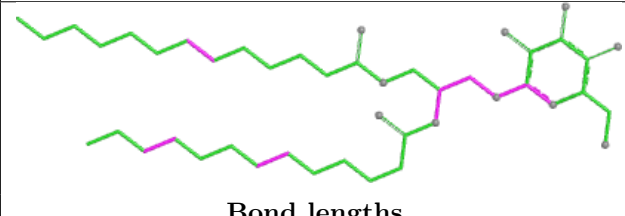
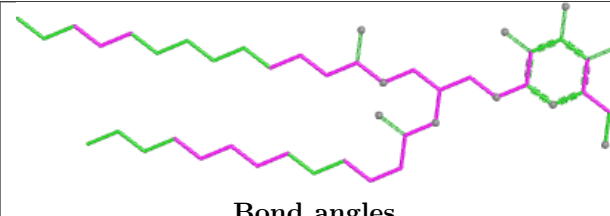
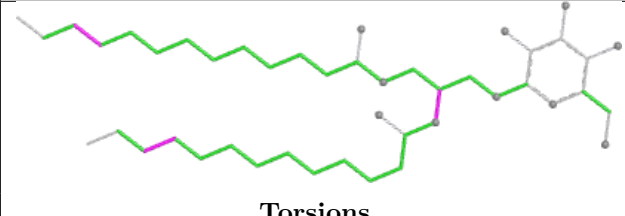
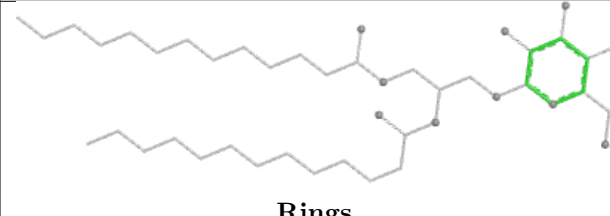


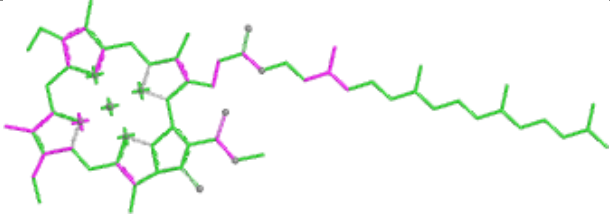
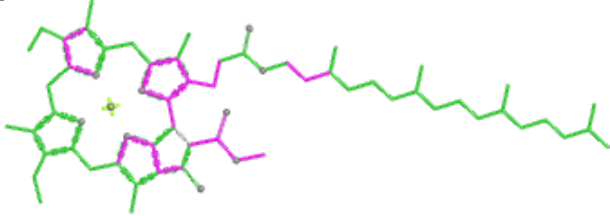
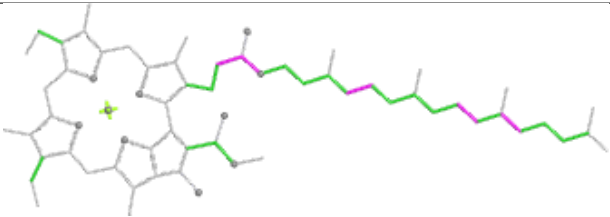
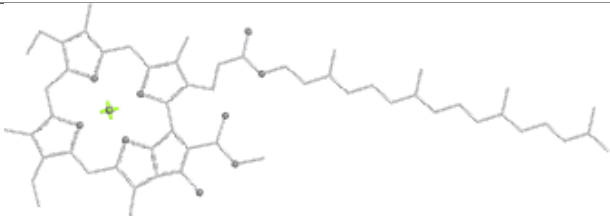
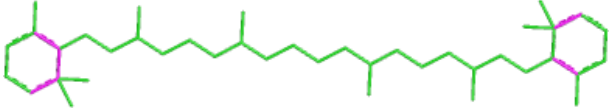
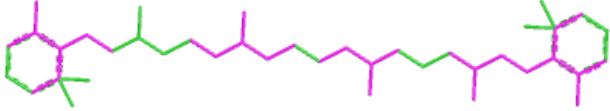
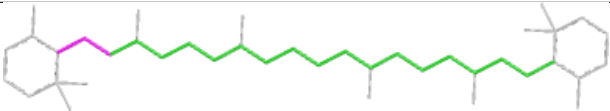
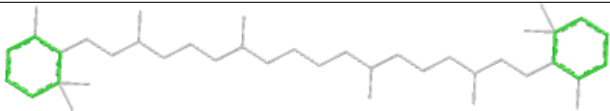
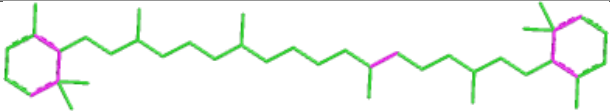
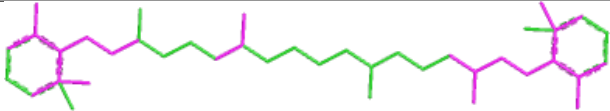
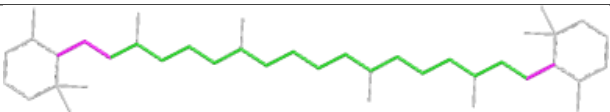
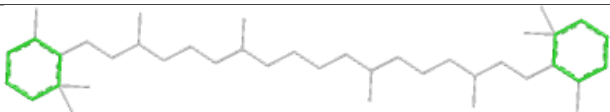


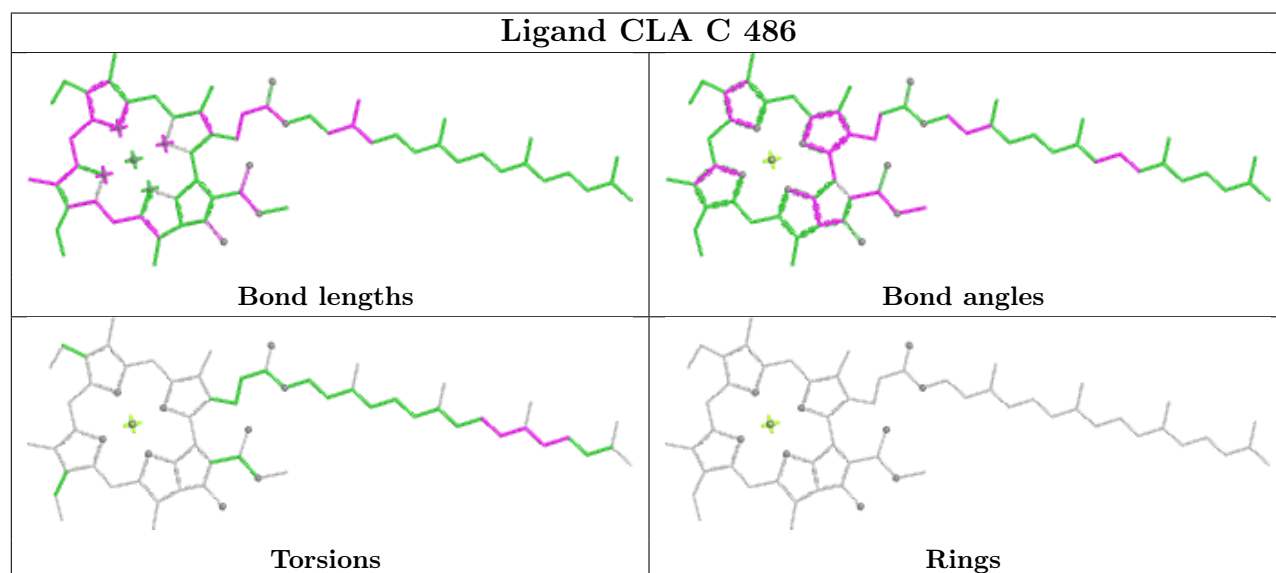
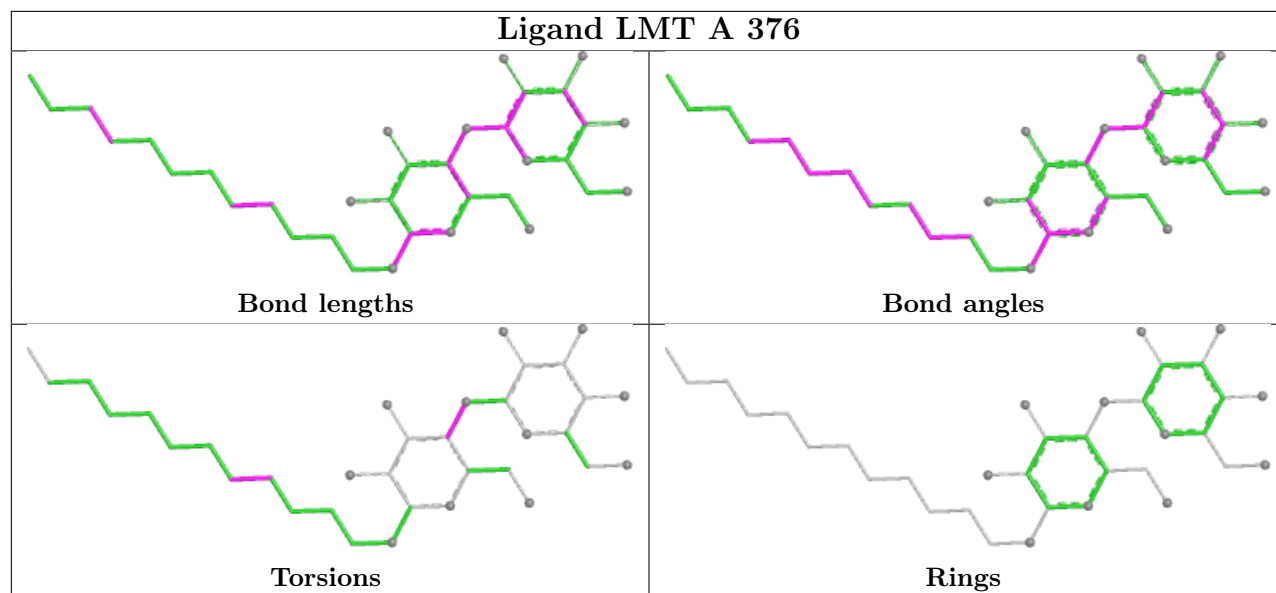


Ligand CLA B 525	
	
Bond lengths	Bond angles
	
Torsions	Rings

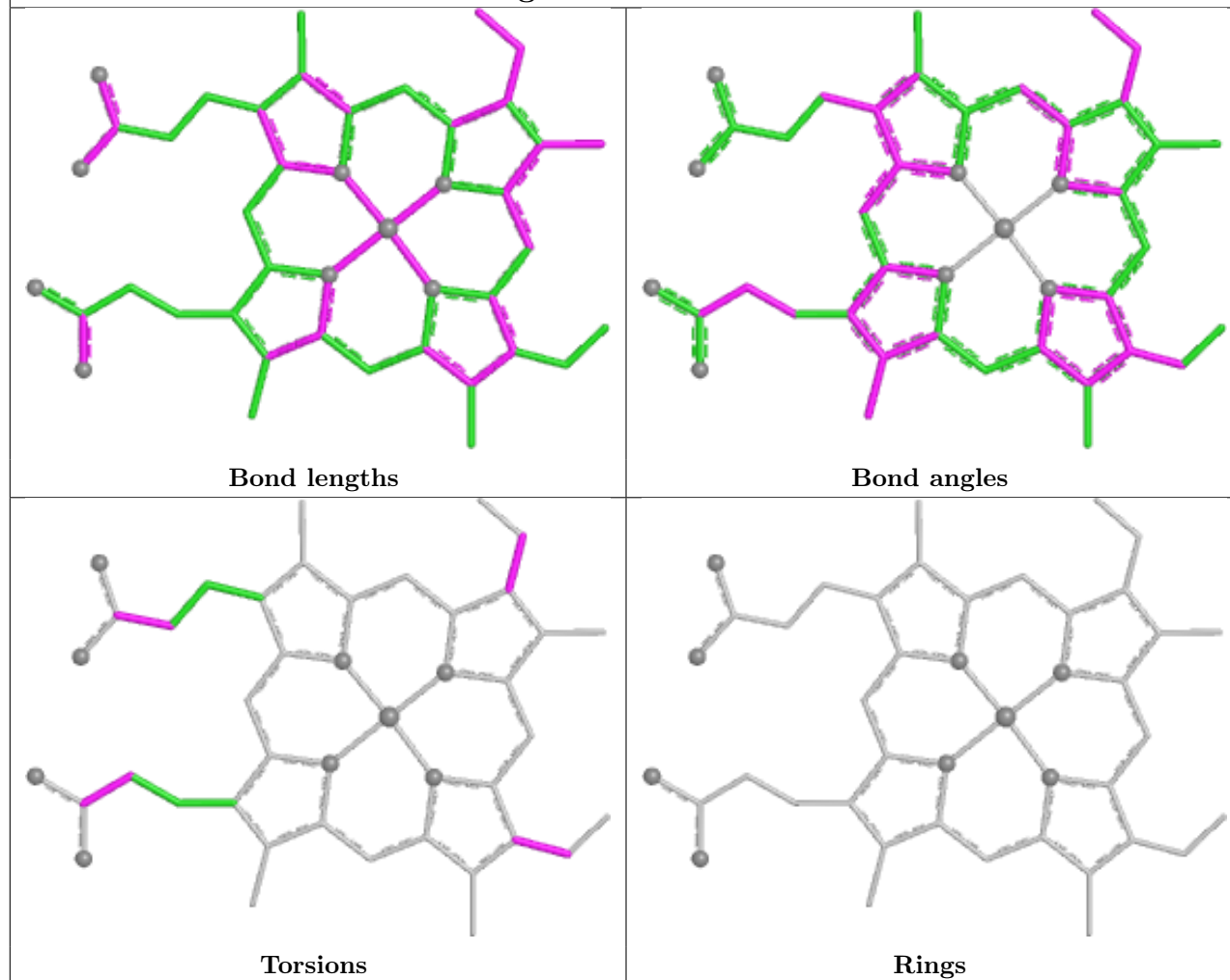
Ligand LMG J 492	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG C 494	
	
Bond lengths	Bond angles
	
Torsions	Rings

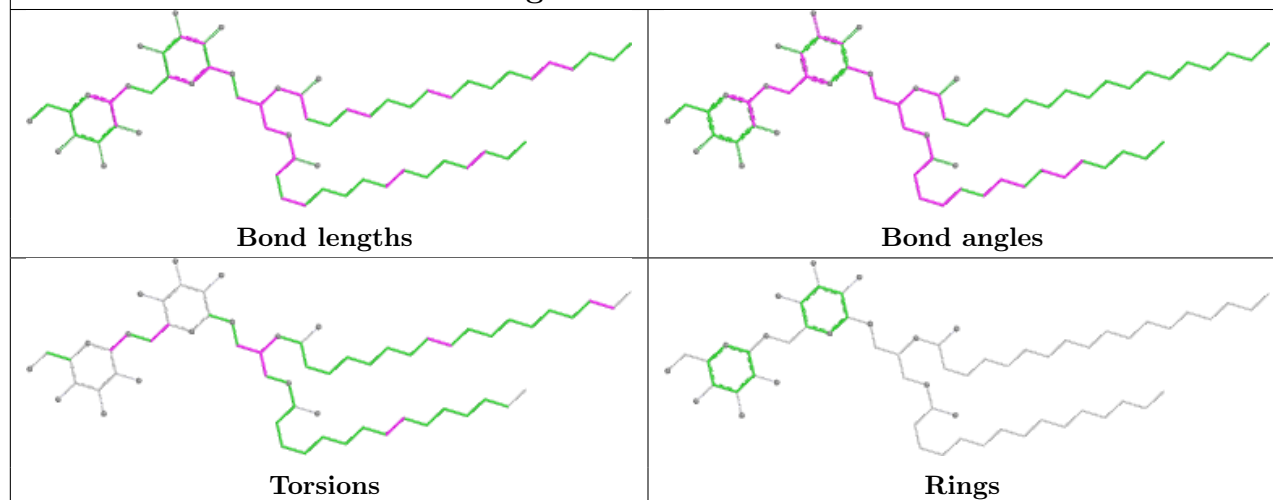
Ligand CLA C 478	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR X 107	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 489	
 Bond lengths	 Bond angles
 Torsions	 Rings

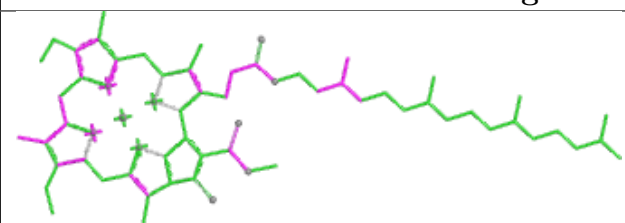
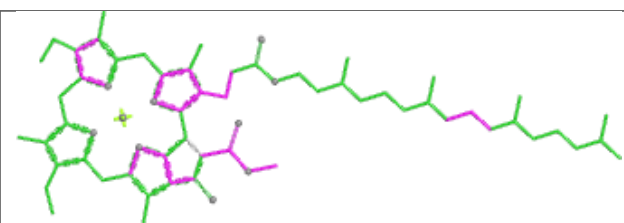
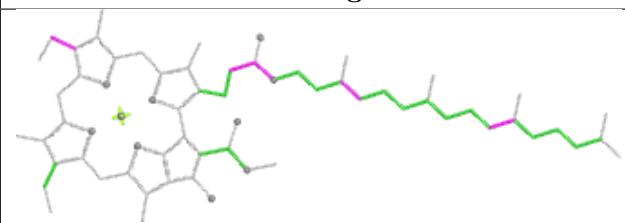
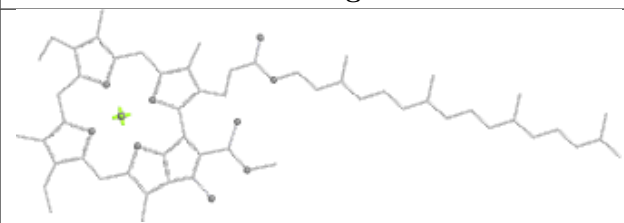


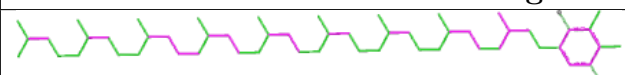
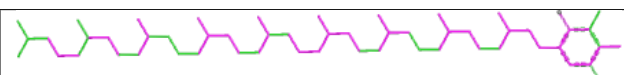
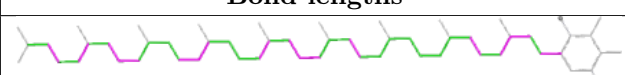
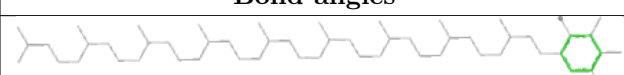
Ligand HEM F 85

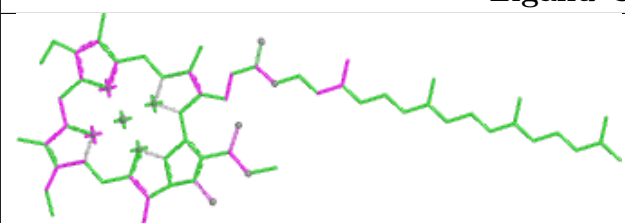
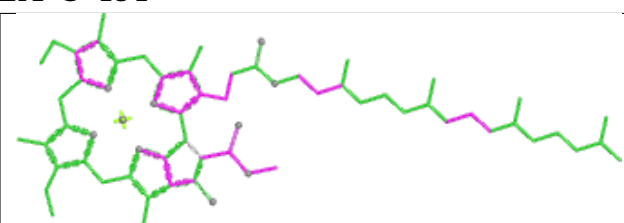
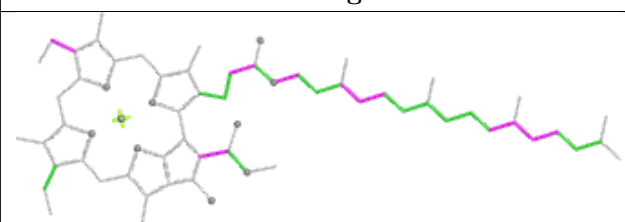
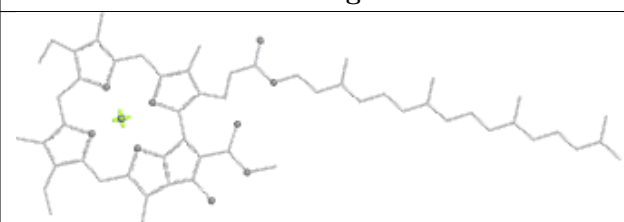


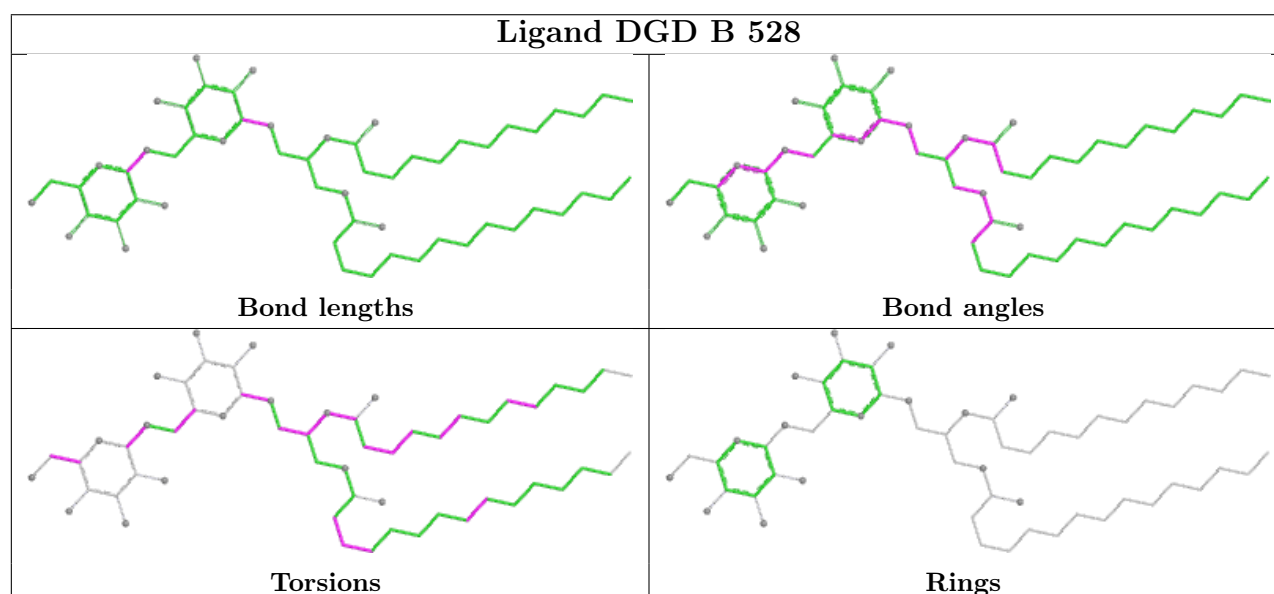
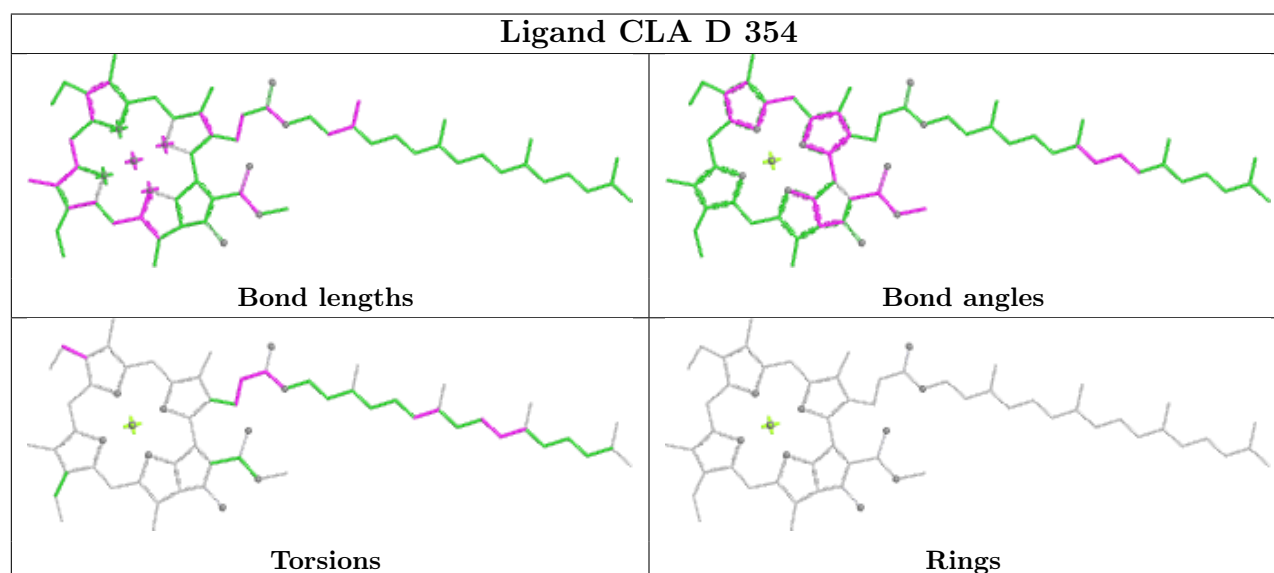
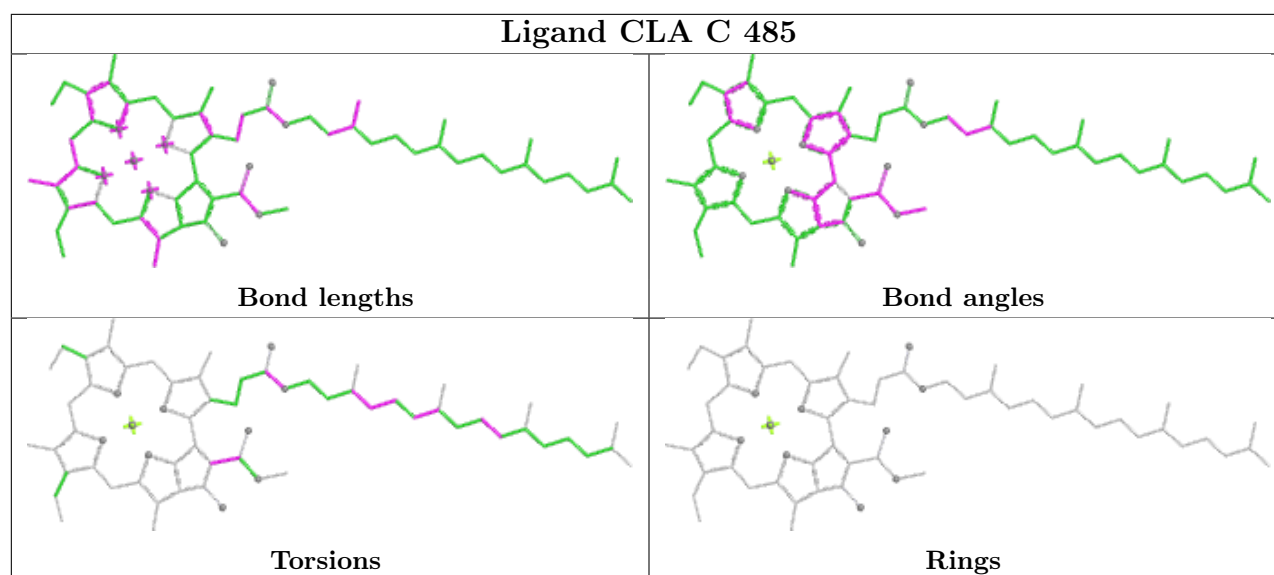
Ligand DGD D 362

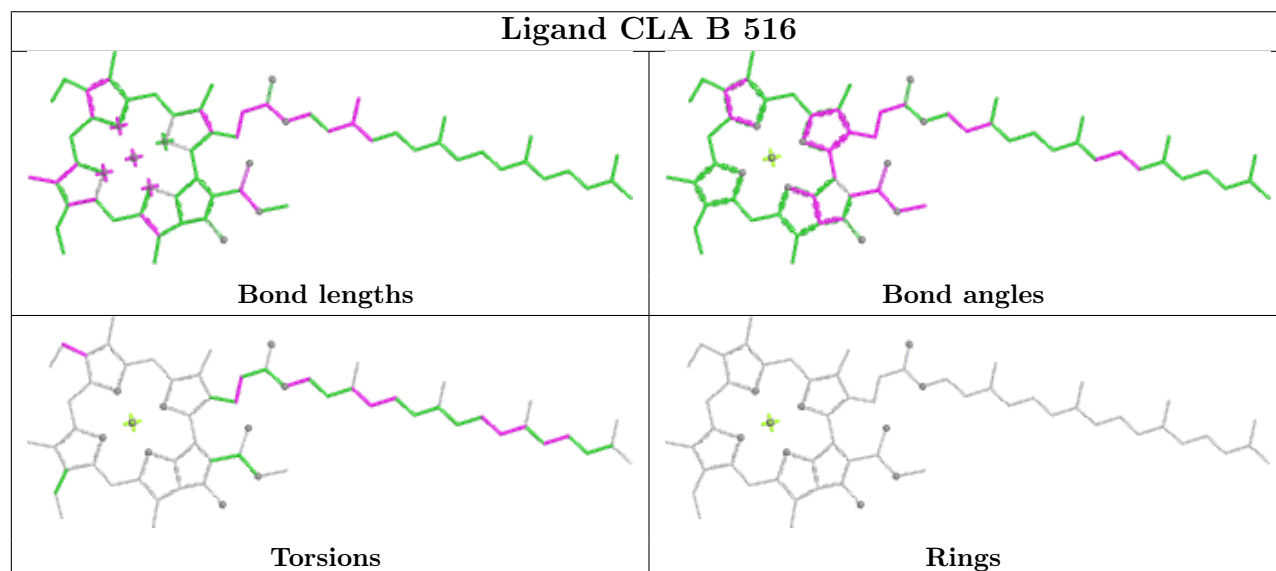
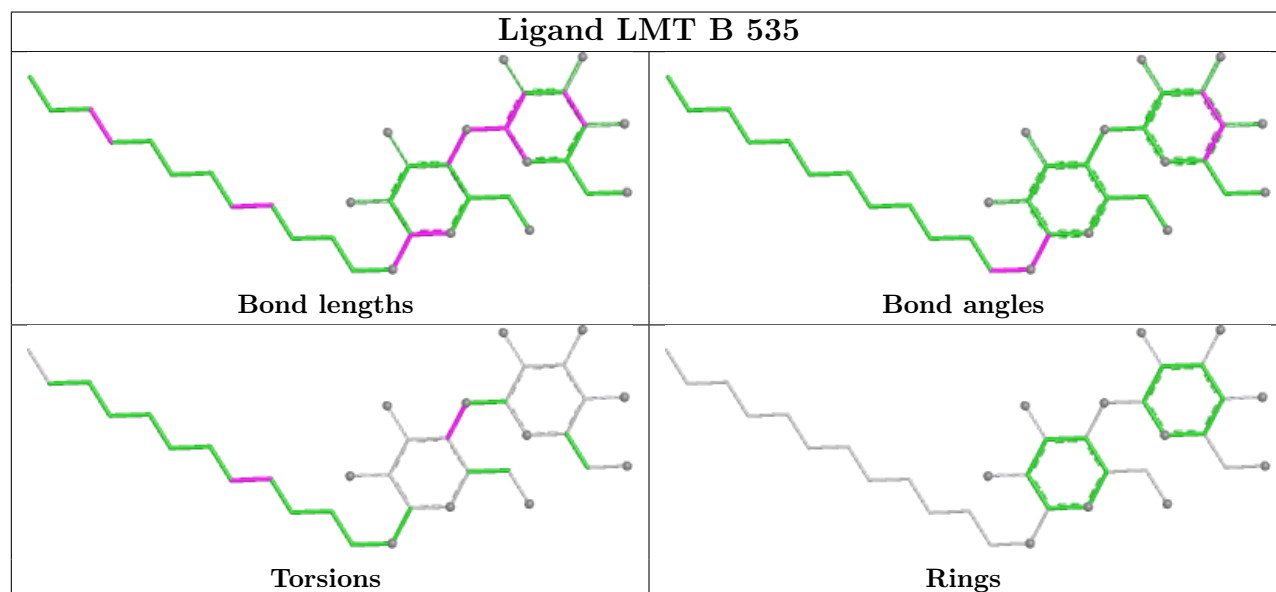
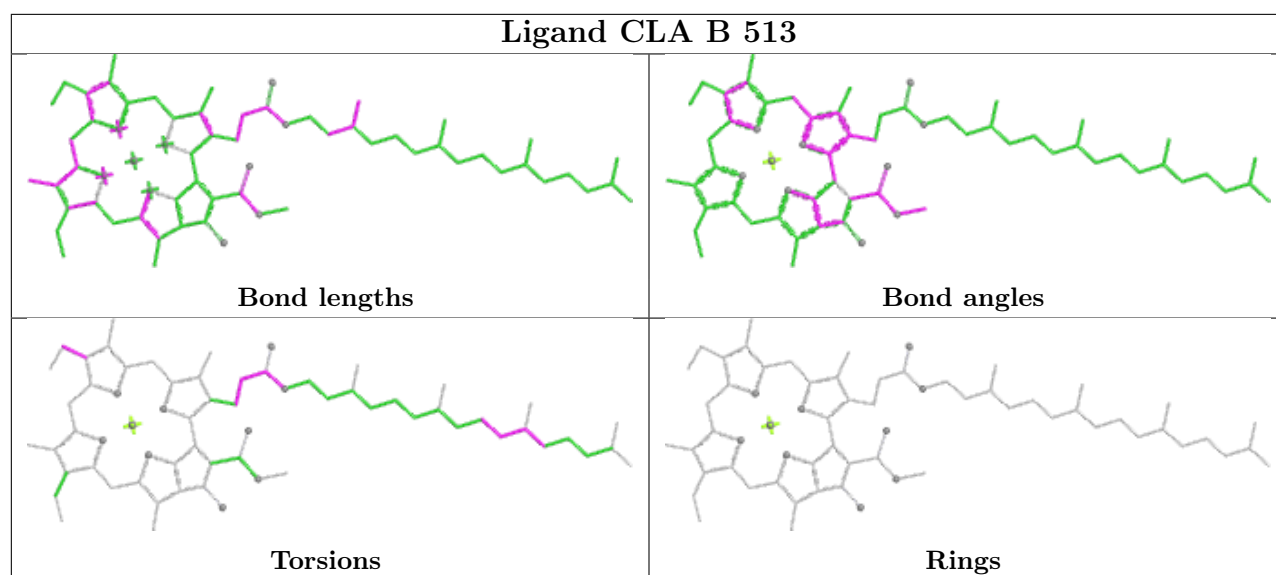


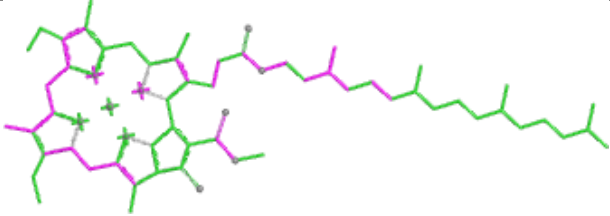
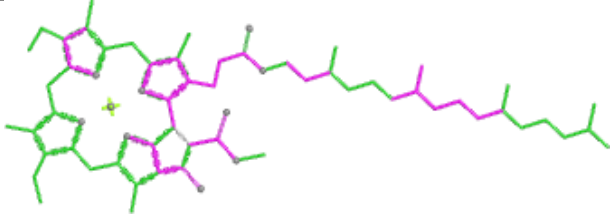
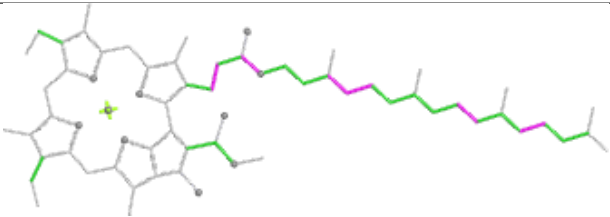
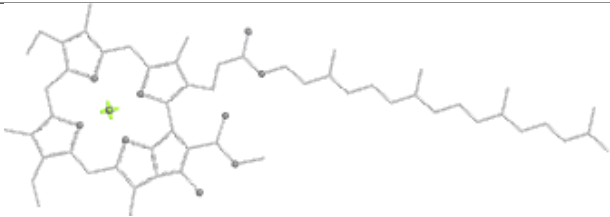
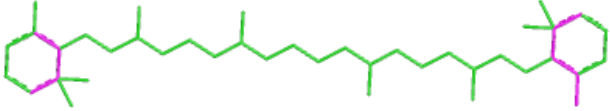
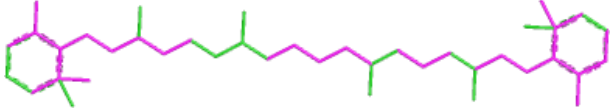
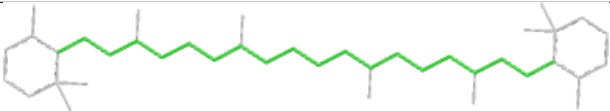
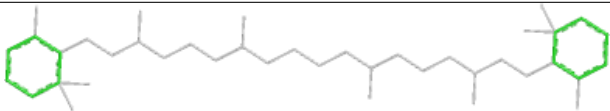
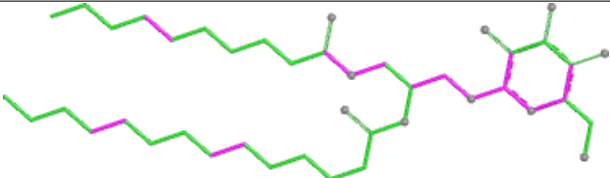
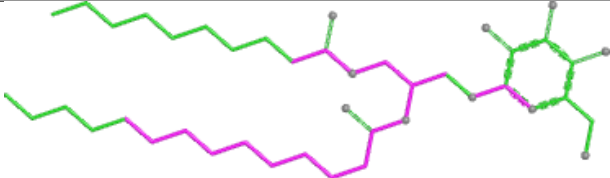
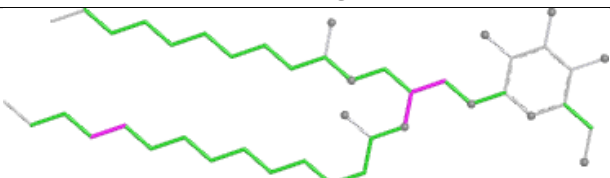
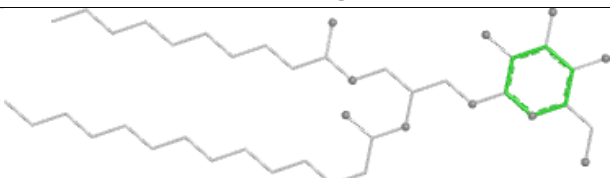
Ligand CLA B 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

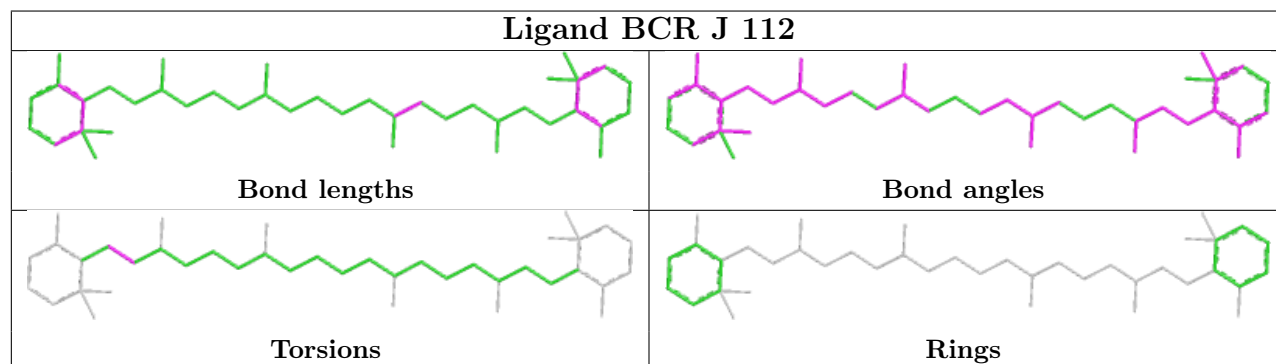
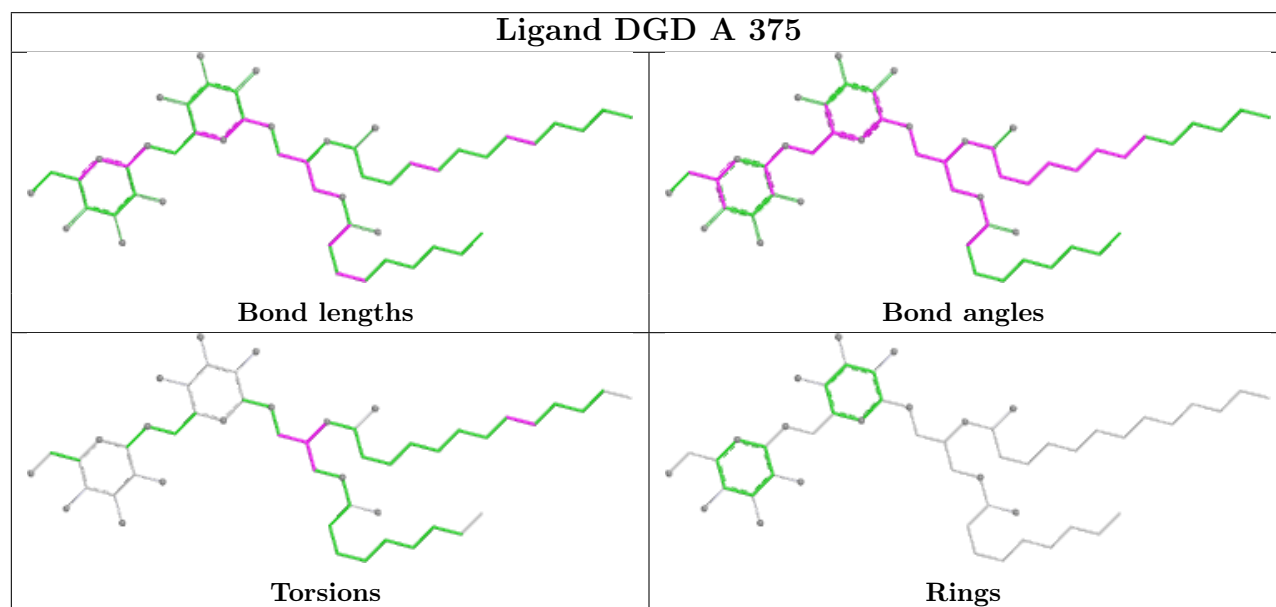
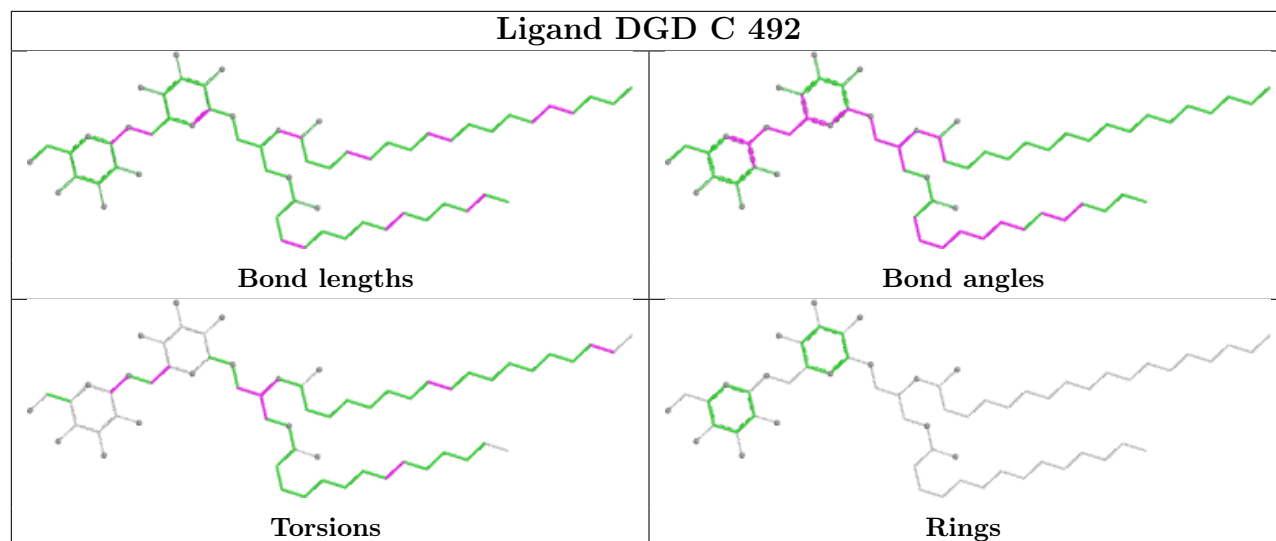
Ligand PL9 D 357	
	
Bond lengths	Bond angles
	
Torsions	Rings

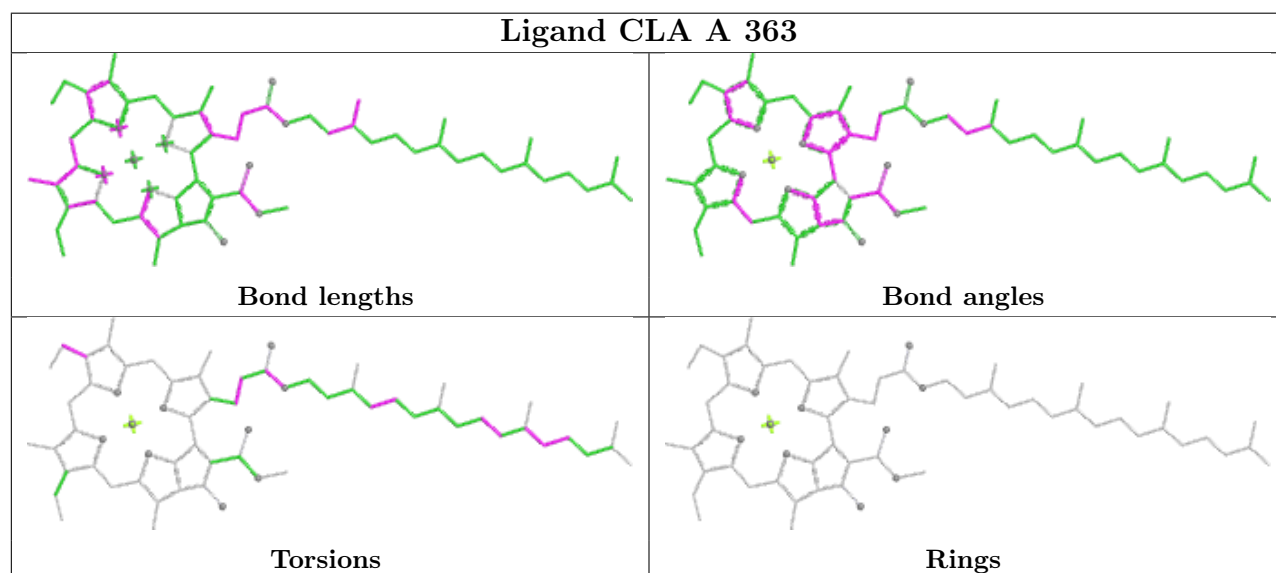
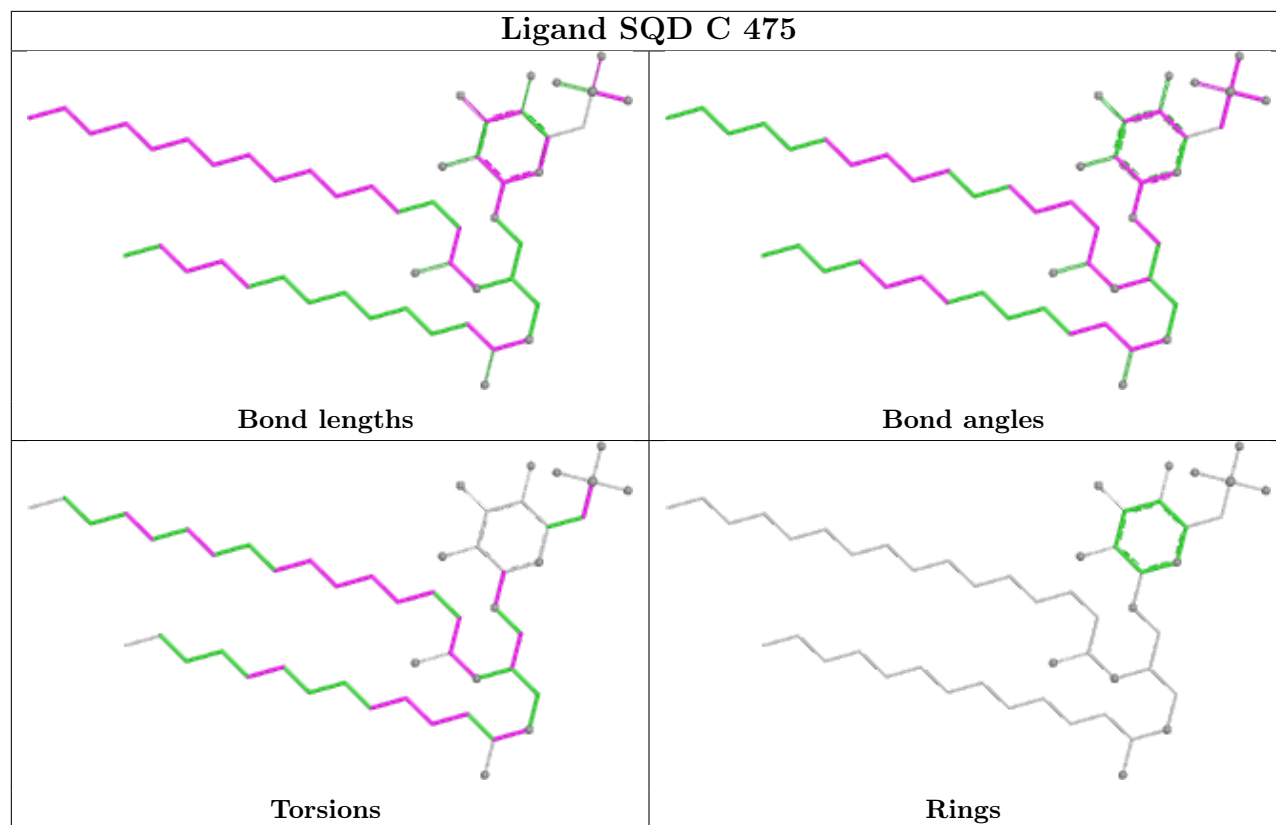
Ligand CLA C 484	
	
Bond lengths	Bond angles
	
Torsions	Rings

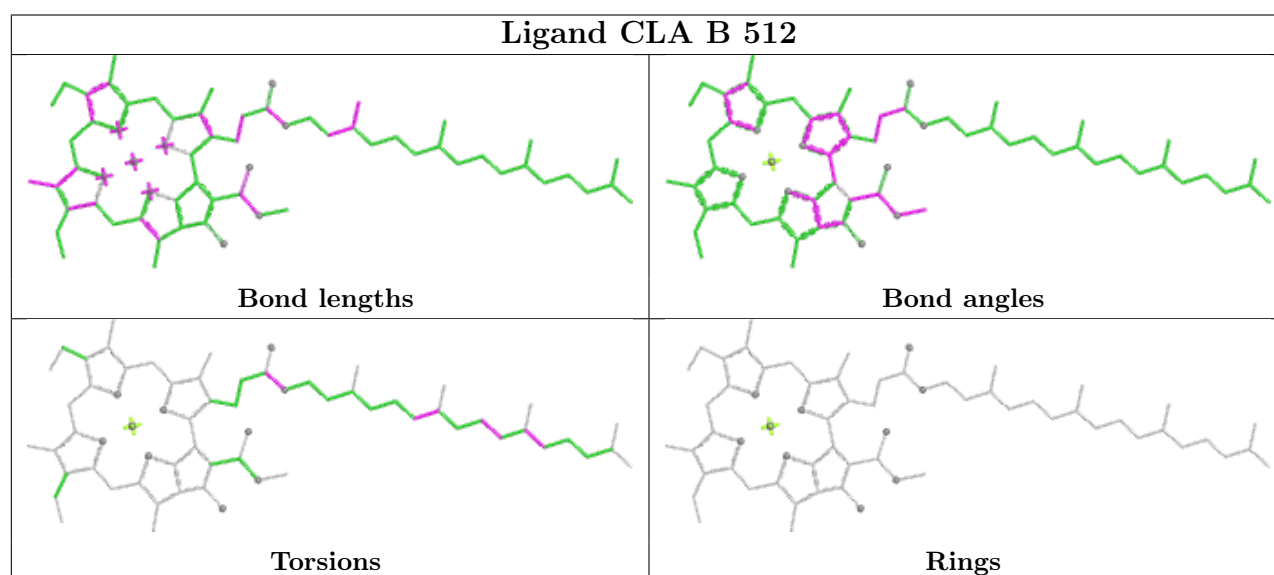
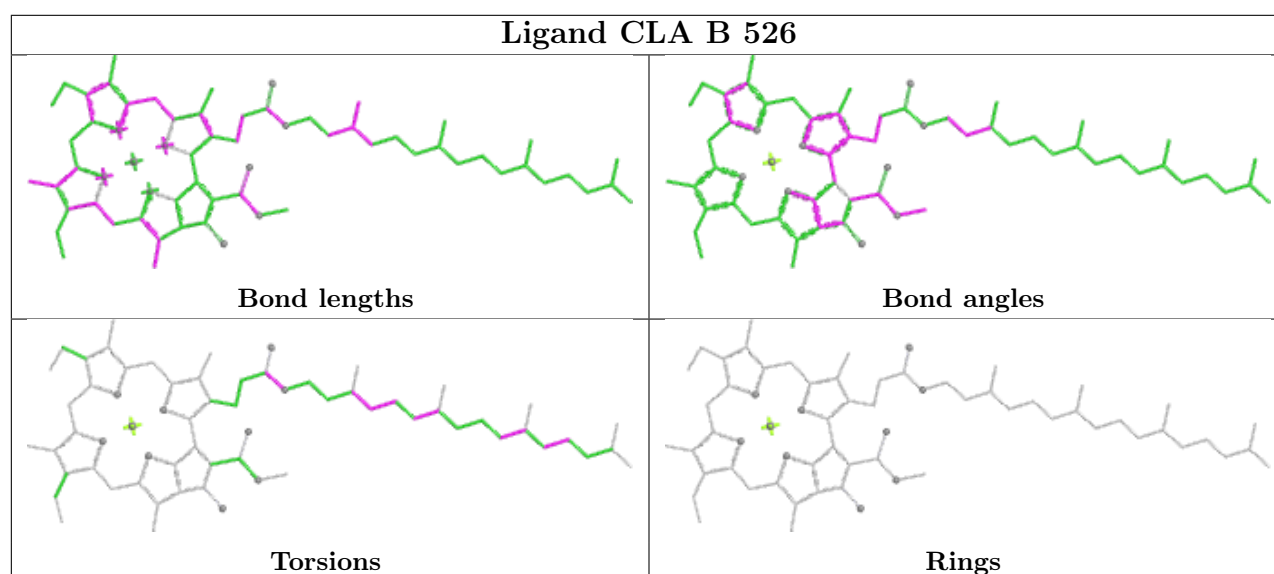
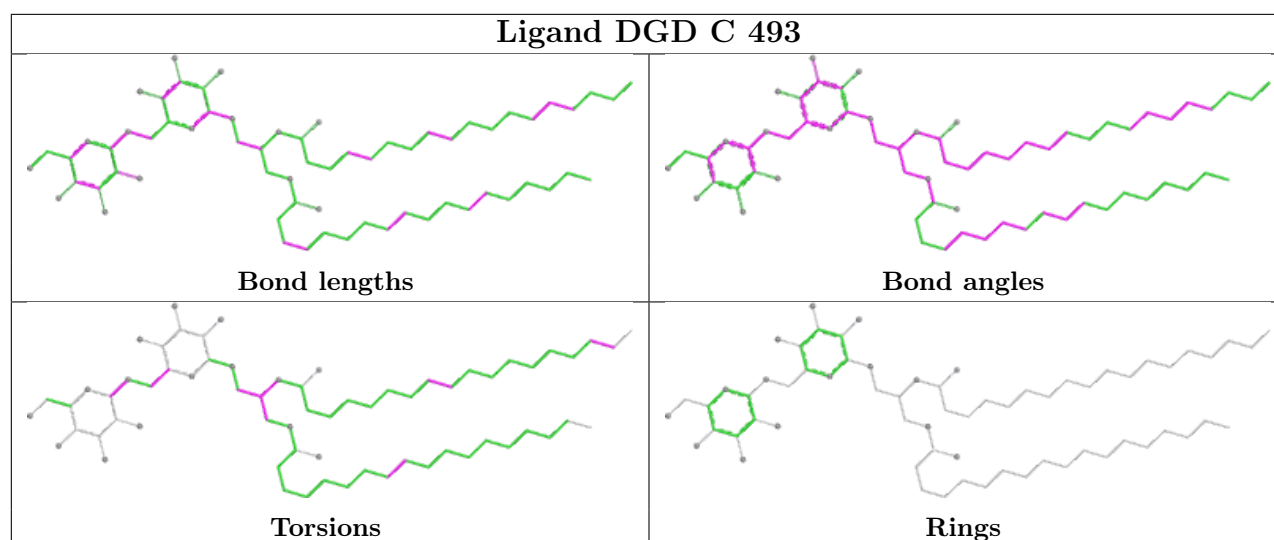


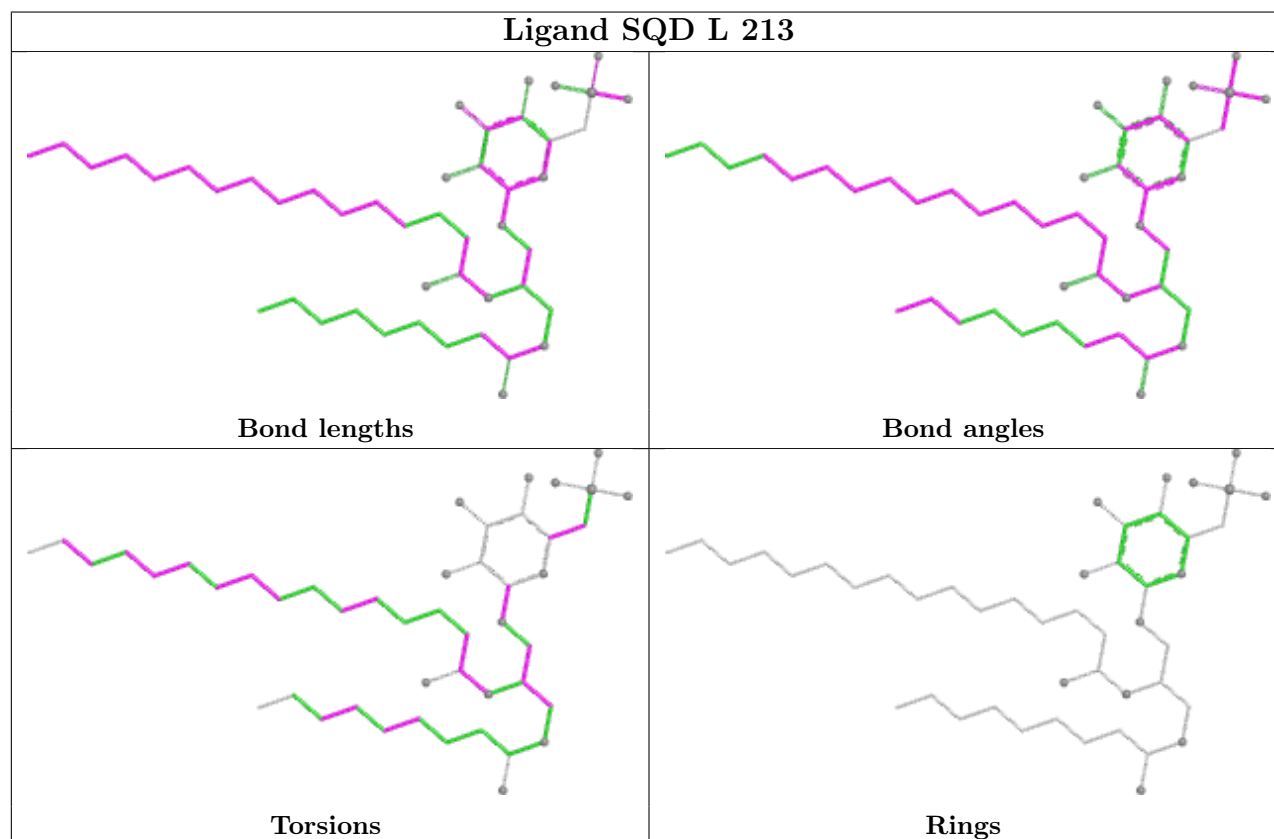
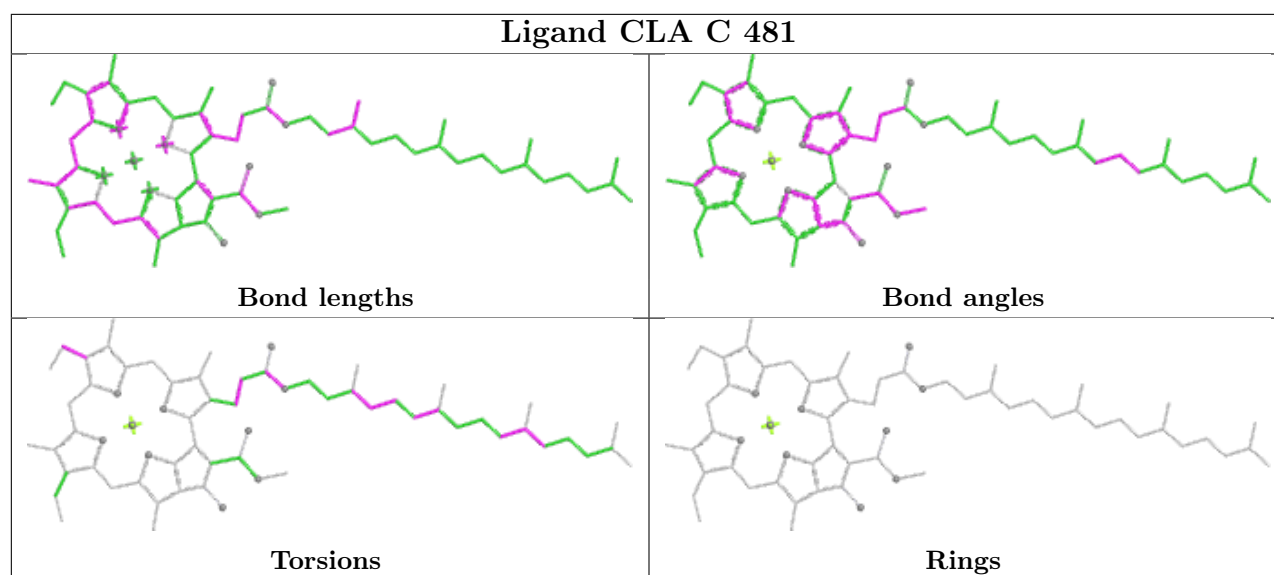


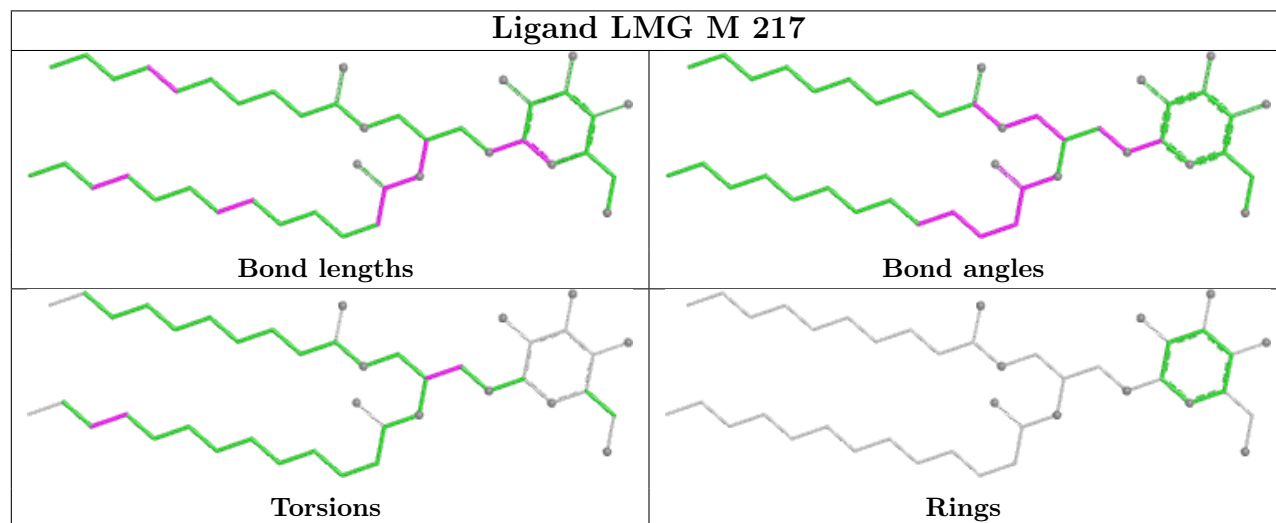
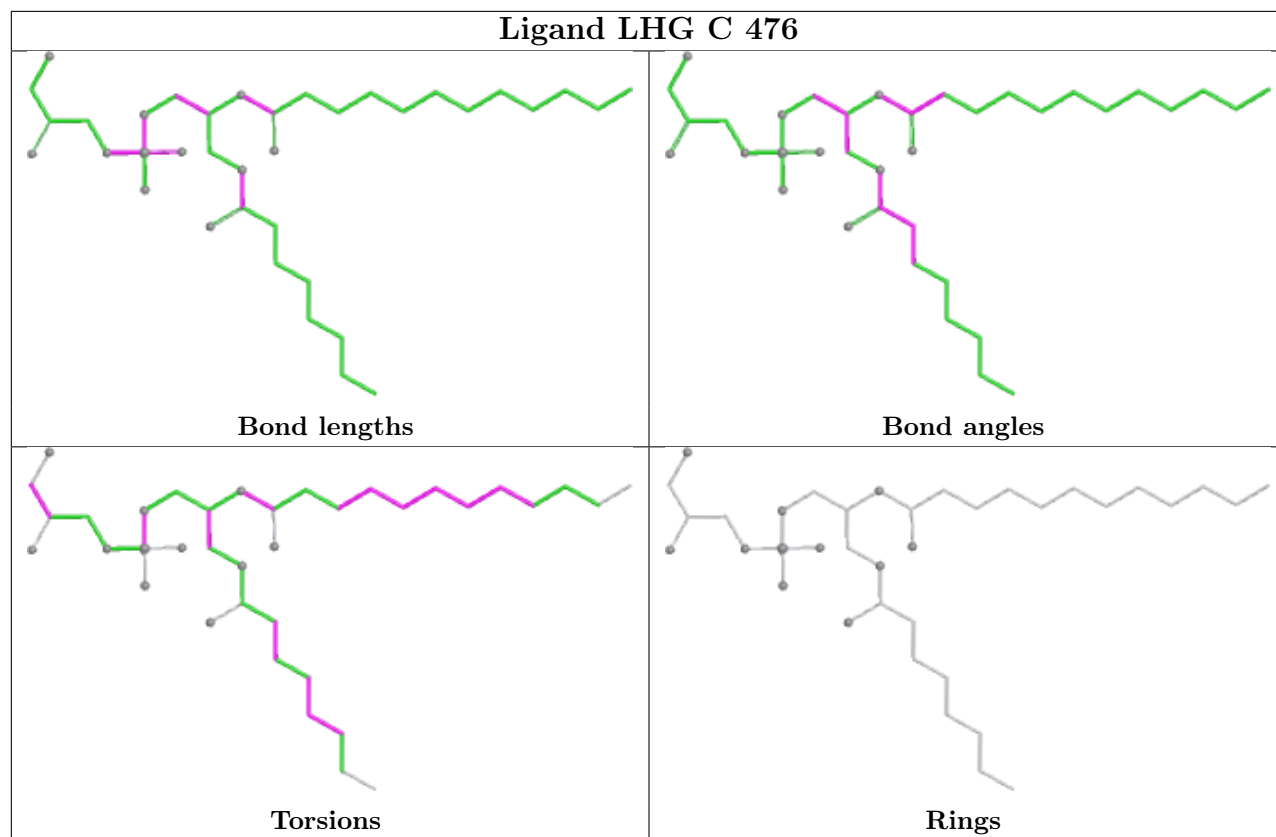
Ligand CLA B 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 529	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG I 220	
 Bond lengths	 Bond angles
 Torsions	 Rings



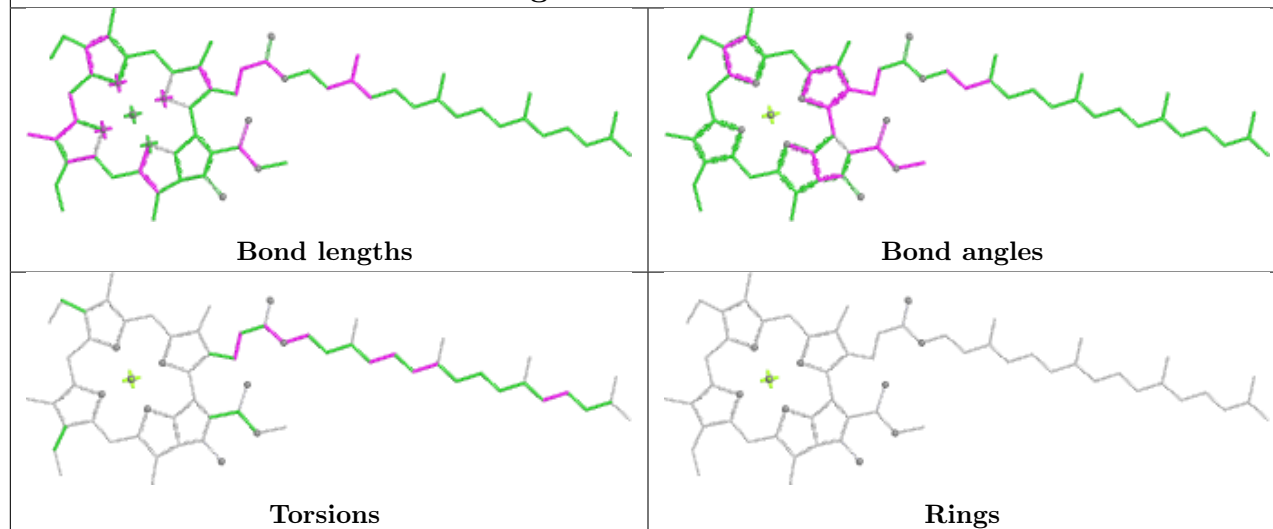




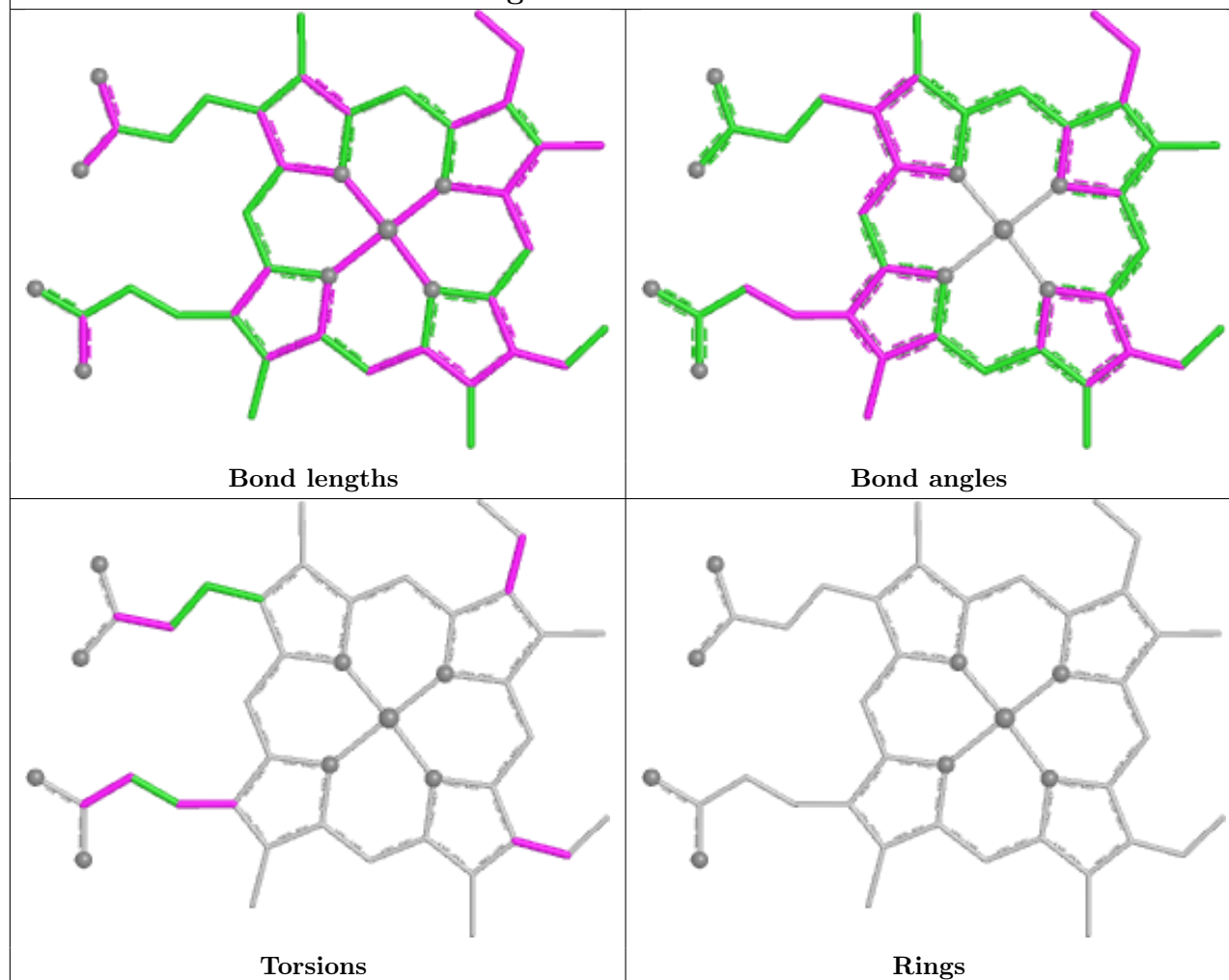


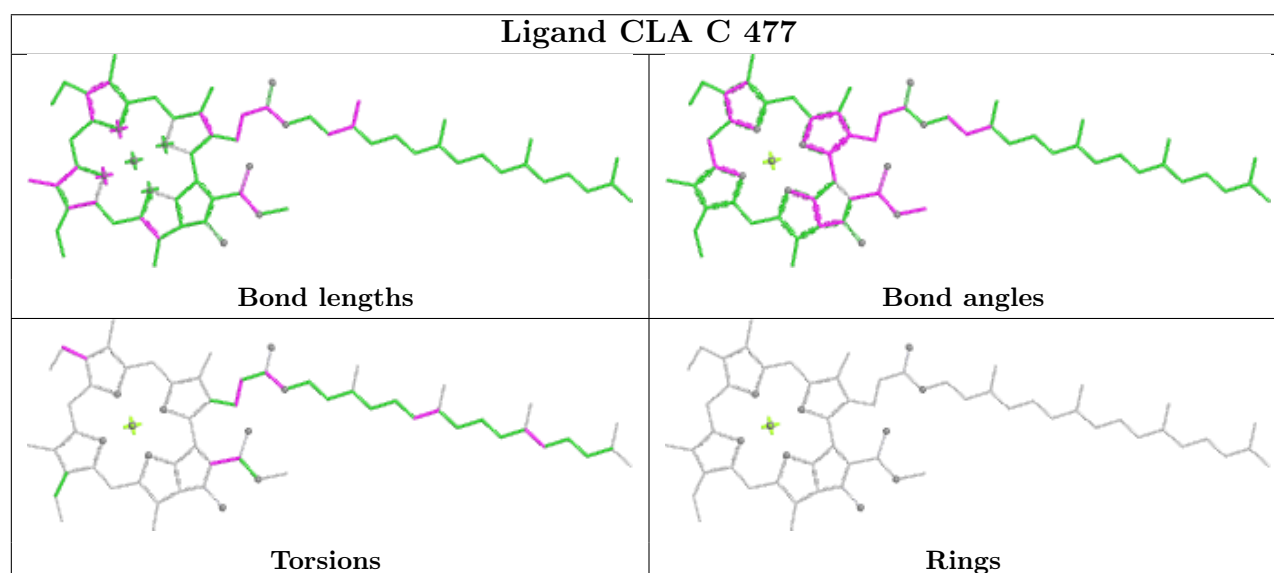
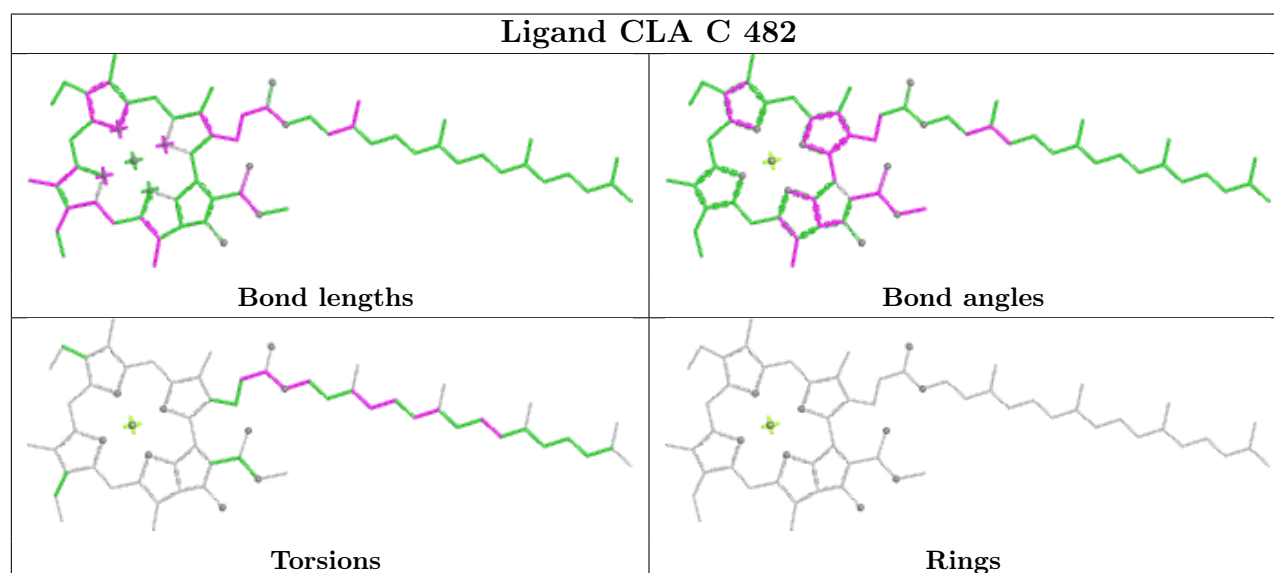
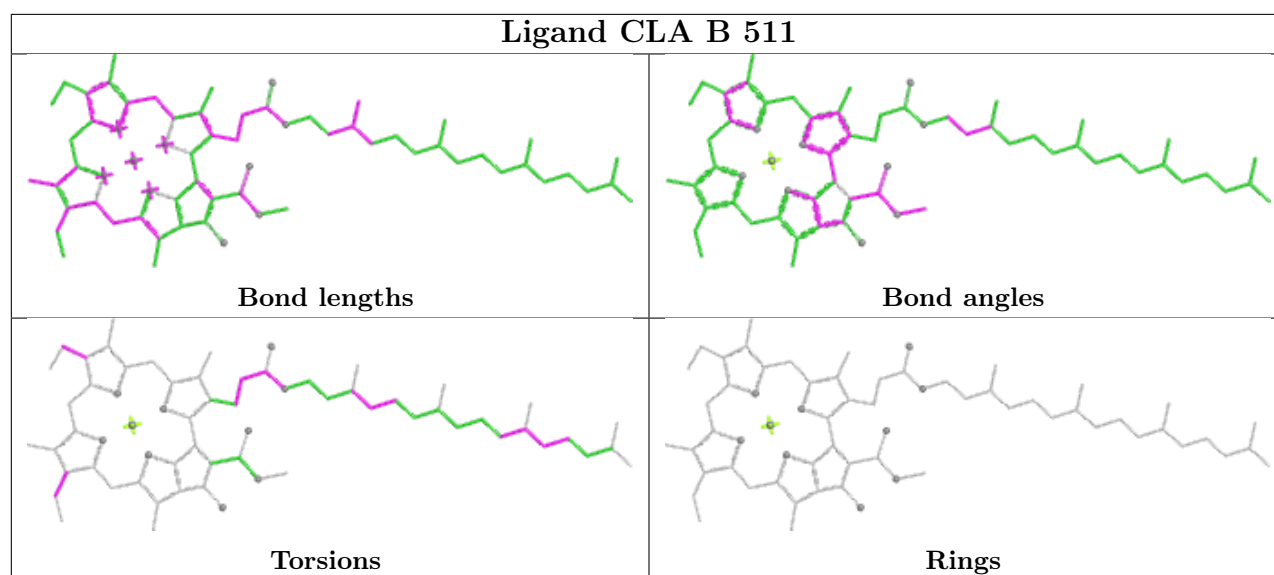


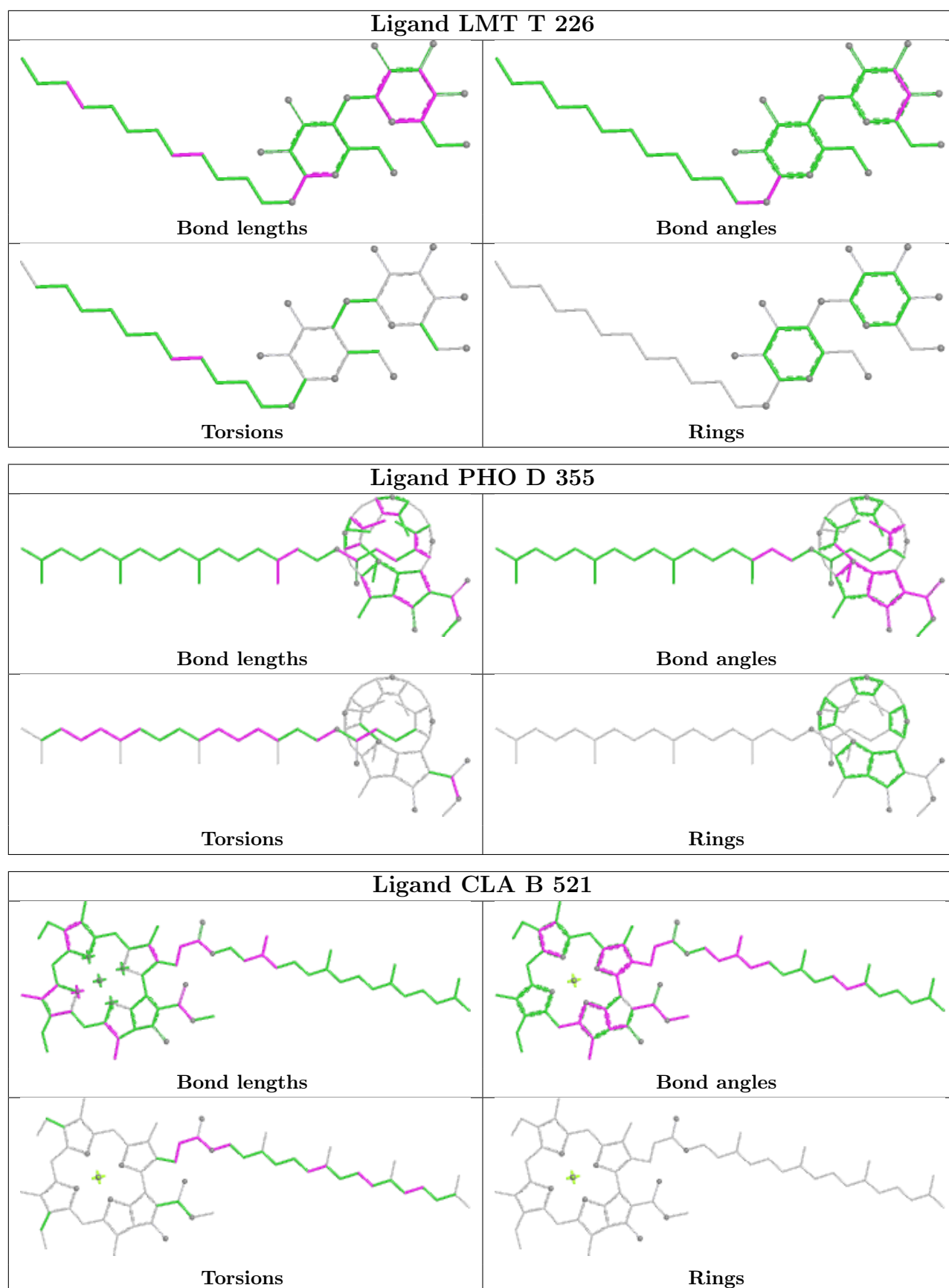
Ligand CLA D 356

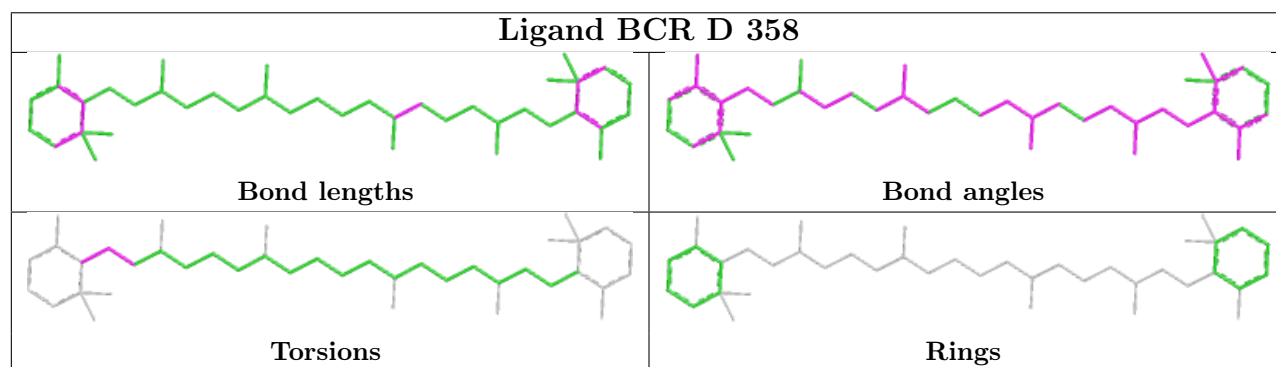
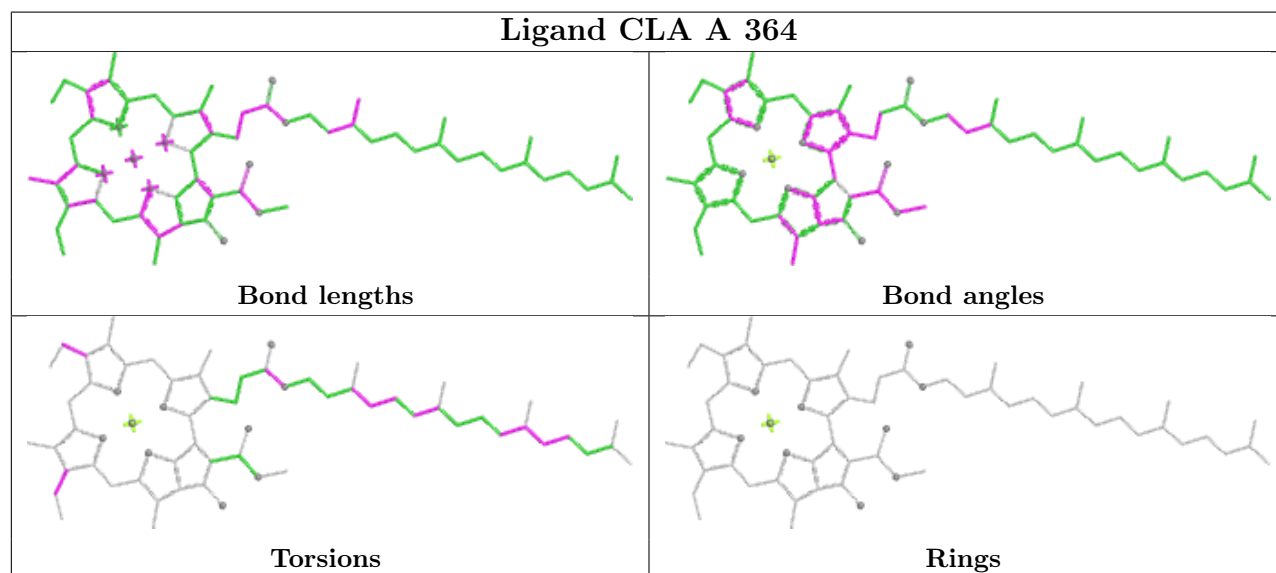
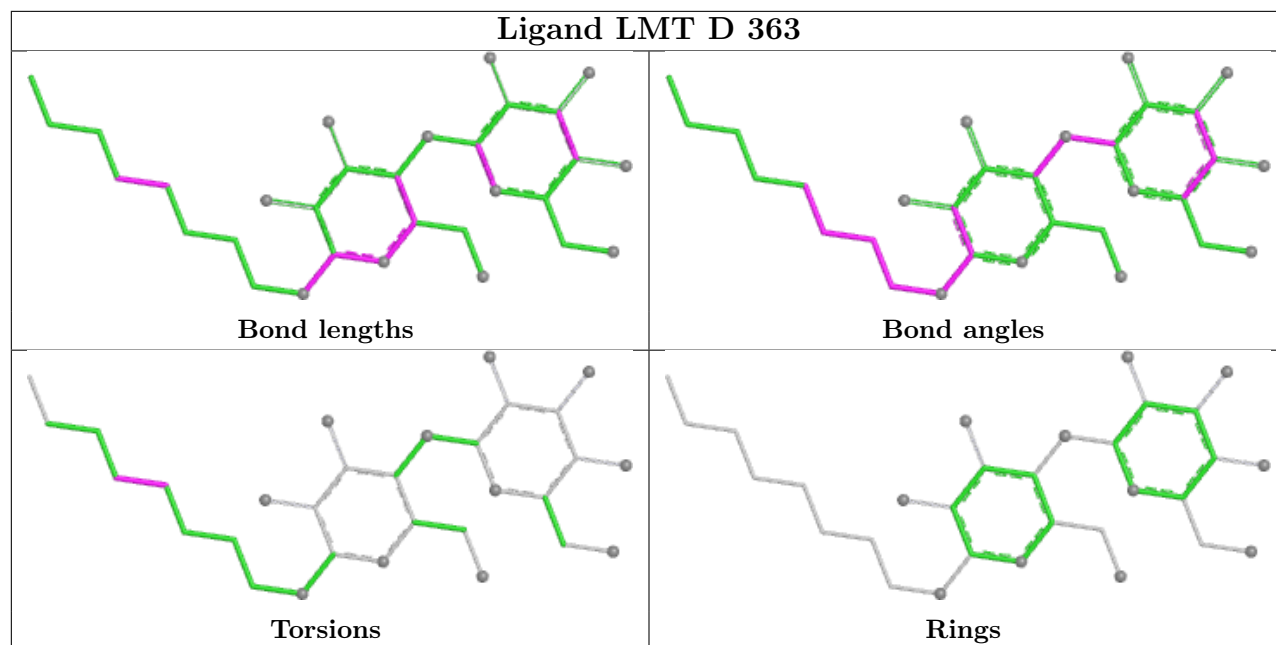


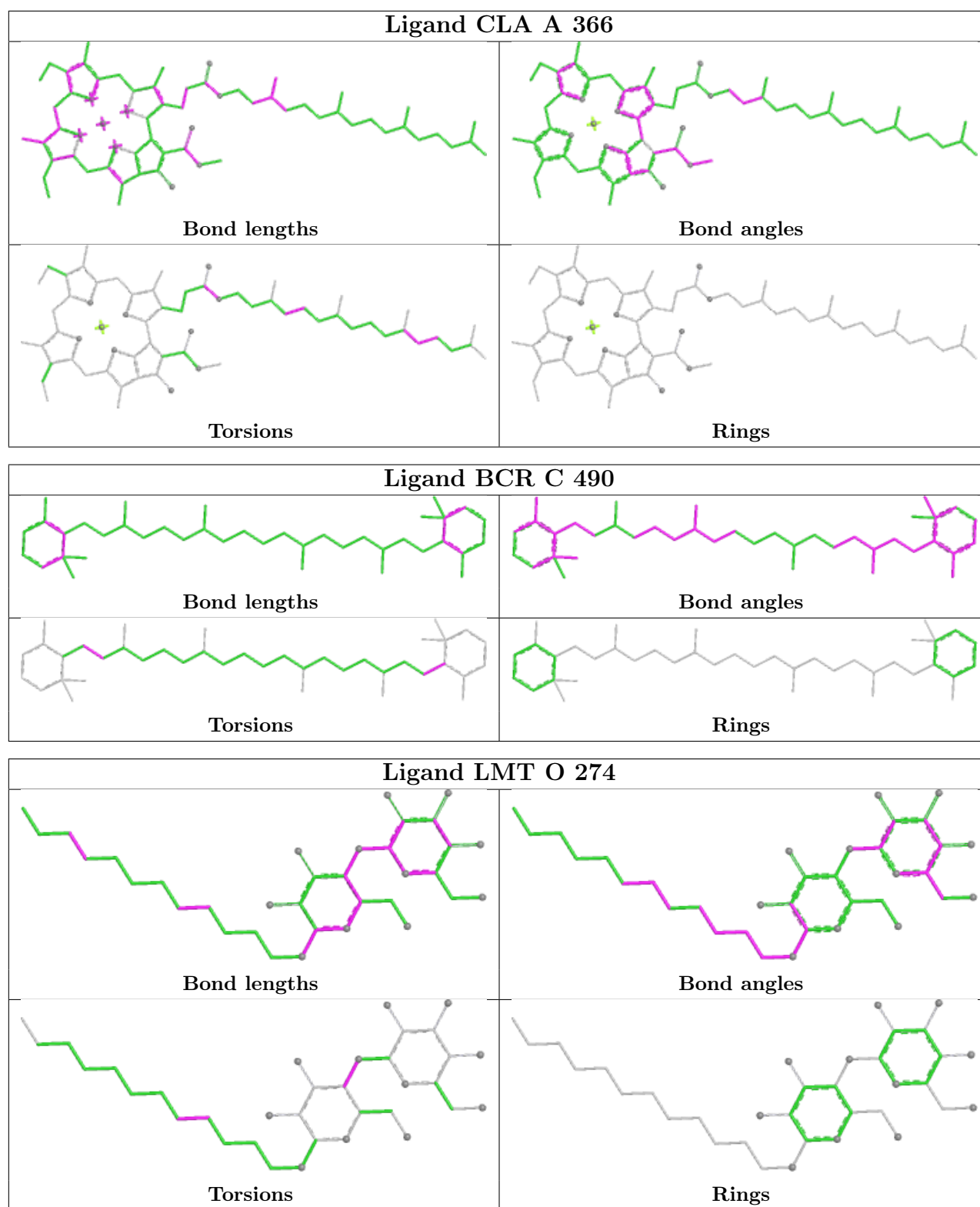
Ligand HEM V 164



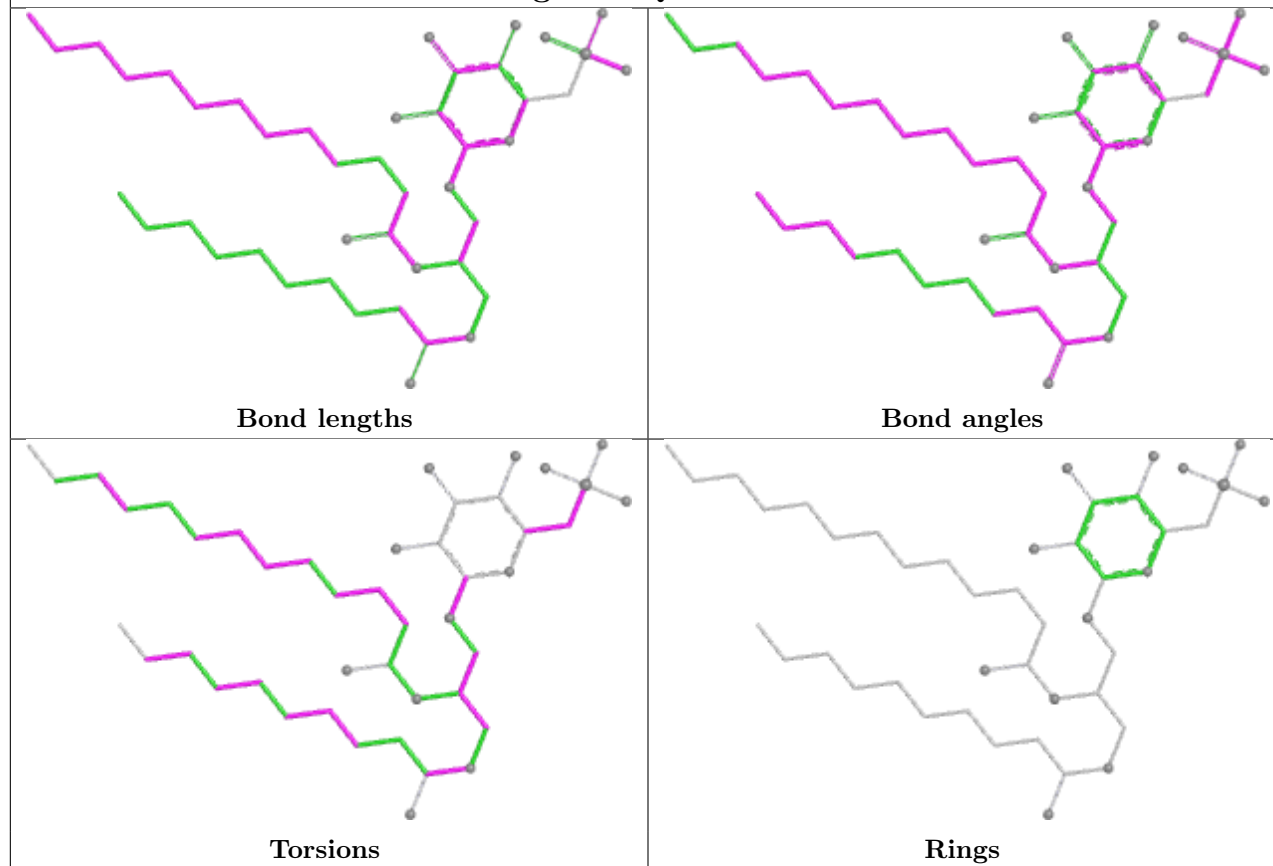




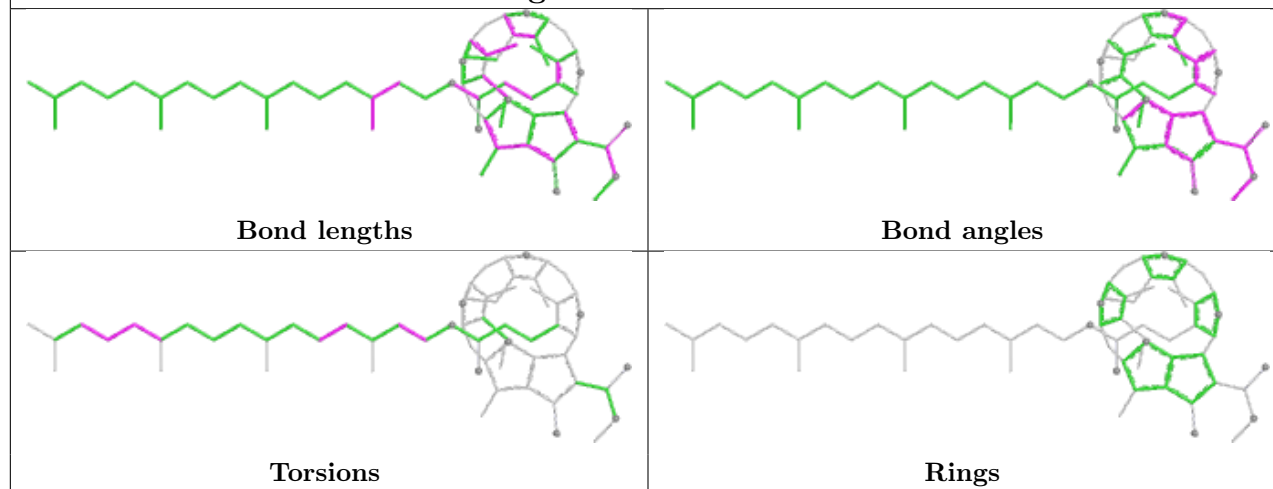


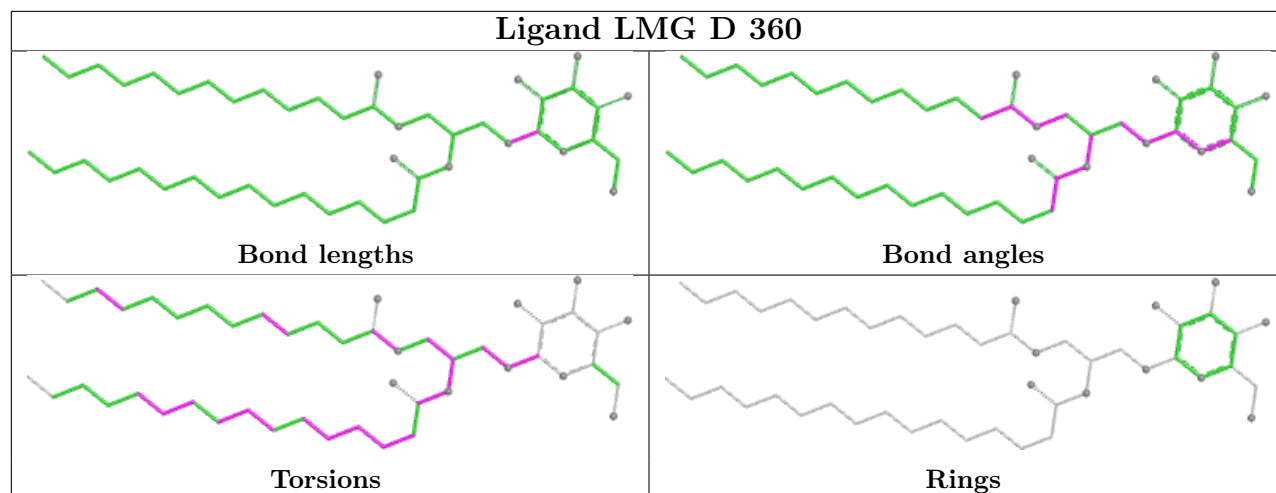


Ligand SQD F 224



Ligand PHO A 365





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.00	7 (2%) 63 37	134, 163, 180, 180	0
2	B	485/510 (95%)	-0.03	8 (1%) 70 43	129, 158, 178, 180	0
3	C	448/461 (97%)	-0.03	4 (0%) 81 56	136, 168, 180, 180	0
4	D	340/352 (96%)	0.09	9 (2%) 57 33	126, 154, 179, 180	0
5	E	77/83 (92%)	-0.16	0 100 100	138, 157, 179, 180	0
6	F	38/44 (86%)	-0.29	0 100 100	138, 157, 169, 177	0
7	H	65/65 (100%)	0.06	3 (4%) 37 21	139, 164, 177, 180	0
8	I	35/38 (92%)	-0.34	0 100 100	163, 172, 180, 180	0
9	J	34/40 (85%)	-0.28	0 100 100	141, 155, 169, 171	0
10	K	37/37 (100%)	0.07	1 (2%) 56 32	156, 166, 179, 180	0
11	L	37/37 (100%)	-0.34	0 100 100	152, 168, 180, 180	0
12	M	34/36 (94%)	0.03	0 100 100	153, 165, 180, 180	0
13	O	243/246 (98%)	-0.06	2 (0%) 82 58	143, 174, 180, 180	0
14	T	30/32 (93%)	-0.27	0 100 100	152, 169, 180, 180	0
15	U	97/104 (93%)	-0.08	0 100 100	141, 160, 171, 179	0
16	V	137/137 (100%)	0.02	2 (1%) 72 44	136, 160, 171, 174	0
17	y	28/46 (60%)	-0.22	0 100 100	158, 175, 180, 180	0
18	X	35/40 (87%)	-0.15	1 (2%) 53 30	144, 156, 174, 178	0
19	Z	62/62 (100%)	-0.05	0 100 100	166, 178, 180, 180	0
All	All	2597/2714 (95%)	-0.03	37 (1%) 73 46	126, 164, 180, 180	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	341	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
7	H	56	ASP	3.8
4	D	130	PHE	3.7
1	A	30	VAL	3.5
4	D	35	ILE	3.4

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	LHG	C	476	37/49	0.39	0.12	143,176,180,180	0
27	LMG	M	217	42/55	0.43	0.13	166,180,180,180	0
30	SQD	F	224	45/54	0.65	0.15	152,179,180,180	0
25	BCR	J	115	40/40	0.67	0.14	171,180,180,180	0
29	LMT	T	226	35/35	0.68	0.11	156,180,180,180	0
29	LMT	O	274	35/35	0.68	0.08	180,180,180,180	0
27	LMG	I	220	43/55	0.69	0.10	158,180,180,180	0
30	SQD	L	213	47/54	0.69	0.10	155,178,180,180	0
28	DGD	D	362	63/66	0.71	0.12	177,180,180,180	0
28	DGD	A	375	52/66	0.72	0.09	164,180,180,180	0
29	LMT	A	376	35/35	0.72	0.12	162,180,180,180	0
27	LMG	C	494	45/55	0.73	0.10	168,180,180,180	0
34	CA	K	56	1/1	0.73	0.08	180,180,180,180	0
29	LMT	B	535	35/35	0.74	0.11	163,180,180,180	0
29	LMT	D	536	35/35	0.75	0.17	168,173,180,180	0
27	LMG	D	360	48/55	0.76	0.17	140,169,176,177	0
30	SQD	C	475	51/54	0.77	0.10	156,172,180,180	0
29	LMT	D	363	31/35	0.77	0.13	170,180,180,180	0
34	CA	O	273	1/1	0.77	0.17	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	CLA	B	526	65/65	0.78	0.12	167,177,180,180	0
21	CLA	B	511	65/65	0.78	0.15	148,179,180,180	0
28	DGD	C	492	62/66	0.78	0.12	153,171,180,180	0
28	DGD	C	474	56/66	0.79	0.13	158,180,180,180	0
28	DGD	C	493	66/66	0.80	0.13	159,174,180,180	0
29	LMT	I	274	35/35	0.82	0.11	170,180,180,180	0
28	DGD	B	533	66/66	0.82	0.12	166,179,180,180	0
25	BCR	B	530	40/40	0.83	0.13	173,180,180,180	0
21	CLA	C	482	65/65	0.83	0.15	148,179,180,180	0
27	LMG	D	359	46/55	0.83	0.13	142,163,180,180	0
25	BCR	C	490	40/40	0.84	0.16	164,169,180,180	0
25	BCR	B	527	40/40	0.85	0.13	161,169,176,178	0
27	LMG	A	373	51/55	0.85	0.18	169,174,180,180	0
27	LMG	J	492	48/55	0.85	0.15	155,175,180,180	0
28	DGD	B	528	58/66	0.85	0.16	126,136,172,173	0
25	BCR	B	529	40/40	0.86	0.15	166,169,173,174	0
21	CLA	C	488	65/65	0.87	0.10	169,176,179,180	0
21	CLA	A	363	65/65	0.87	0.13	154,161,175,177	0
27	LMG	B	531	49/55	0.87	0.16	160,167,175,176	0
21	CLA	B	524	65/65	0.87	0.11	157,180,180,180	0
25	BCR	Z	116	40/40	0.88	0.16	163,165,170,171	0
30	SQD	D	361	43/54	0.88	0.11	160,173,180,180	0
21	CLA	C	486	65/65	0.88	0.15	143,180,180,180	0
25	BCR	J	112	40/40	0.89	0.18	157,160,172,173	0
21	CLA	A	364	65/65	0.90	0.12	126,141,175,177	0
21	CLA	C	477	65/65	0.90	0.14	163,169,179,180	0
21	CLA	C	481	65/65	0.90	0.12	152,180,180,180	0
21	CLA	B	525	65/65	0.91	0.12	148,167,180,180	0
21	CLA	C	487	65/65	0.91	0.13	176,180,180,180	0
21	CLA	C	479	65/65	0.91	0.13	162,180,180,180	0
24	OEC	A	368	5/9	0.91	0.11	118,138,151,154	0
21	CLA	C	484	65/65	0.91	0.12	168,177,180,180	0
25	BCR	X	107	40/40	0.91	0.14	154,158,161,163	0
21	CLA	D	356	65/65	0.92	0.13	149,154,162,164	0
28	DGD	C	491	53/66	0.92	0.14	155,160,166,168	0
23	MES	A	367	12/12	0.92	0.11	136,144,152,153	0
21	CLA	C	480	65/65	0.92	0.10	151,159,180,180	0
25	BCR	A	369	40/40	0.92	0.14	164,171,178,178	0
21	CLA	C	485	65/65	0.92	0.14	170,176,178,180	0
21	CLA	B	516	65/65	0.92	0.10	152,155,180,180	0
31	BCT	D	353	4/4	0.92	0.07	169,170,170,171	0
21	CLA	A	366	65/65	0.92	0.09	152,162,164,166	0

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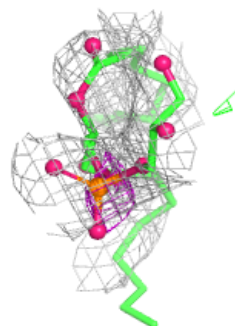
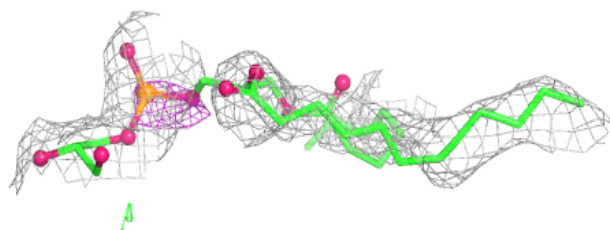
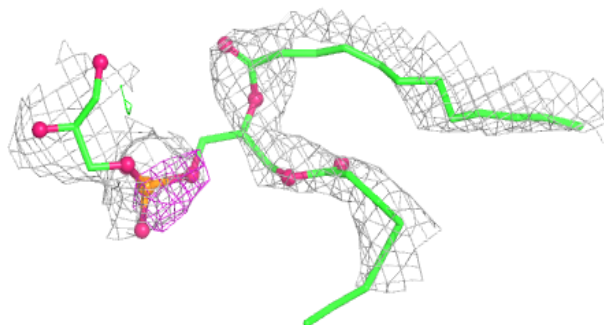
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	CLA	C	483	65/65	0.92	0.12	164,180,180,180	0
21	CLA	K	483	65/65	0.93	0.10	155,160,174,176	0
25	BCR	C	489	40/40	0.93	0.16	152,169,171,171	0
21	CLA	C	478	65/65	0.93	0.11	153,155,166,170	0
32	PL9	D	357	55/55	0.93	0.13	146,153,161,162	0
26	LHG	A	371	39/49	0.93	0.11	156,175,179,180	0
21	CLA	B	518	65/65	0.93	0.12	150,164,167,169	0
22	PHO	A	365	64/64	0.94	0.10	143,154,162,164	0
22	PHO	D	355	64/64	0.94	0.11	140,162,169,171	0
21	CLA	B	521	65/65	0.94	0.11	149,169,175,179	0
21	CLA	D	354	65/65	0.94	0.14	135,154,164,168	0
25	BCR	D	358	40/40	0.94	0.11	135,151,162,162	0
33	HEM	F	85	43/43	0.94	0.11	154,159,162,163	0
21	CLA	B	517	65/65	0.94	0.11	144,160,164,167	0
21	CLA	B	512	65/65	0.94	0.14	142,165,172,173	0
21	CLA	B	514	65/65	0.95	0.13	139,146,168,169	0
21	CLA	B	519	65/65	0.95	0.11	152,157,158,159	0
21	CLA	A	362	65/65	0.95	0.12	149,154,159,163	0
21	CLA	B	522	65/65	0.95	0.12	134,144,163,165	0
21	CLA	B	523	65/65	0.95	0.10	134,142,169,170	0
21	CLA	B	513	65/65	0.95	0.12	133,170,171,172	0
21	CLA	B	515	65/65	0.96	0.12	142,162,168,170	0
34	CA	F	225	1/1	0.97	0.07	142,142,142,142	0
21	CLA	B	520	65/65	0.97	0.14	150,162,165,167	0
33	HEM	V	164	43/43	0.97	0.11	89,102,122,129	0
20	FE2	A	361	1/1	0.99	0.03	160,160,160,160	0

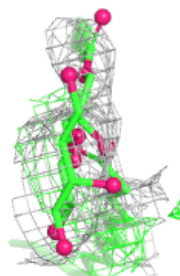
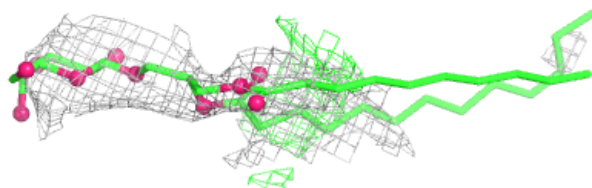
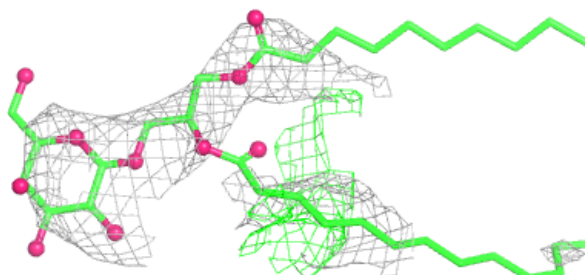
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LHG C 476:

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

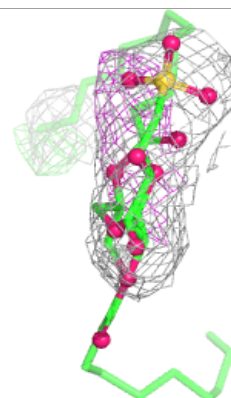
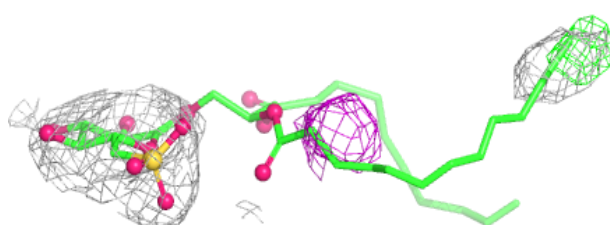
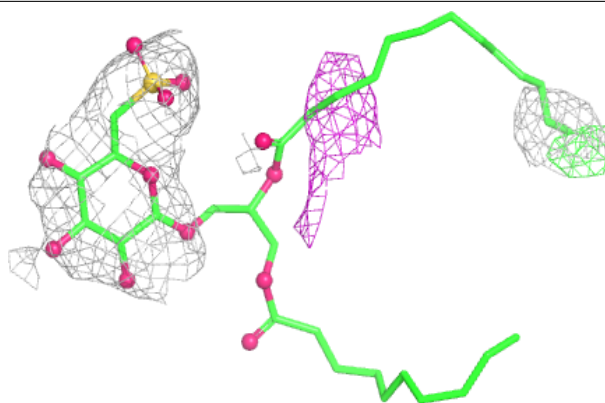
**Electron density around LMG M 217:**

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

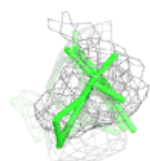
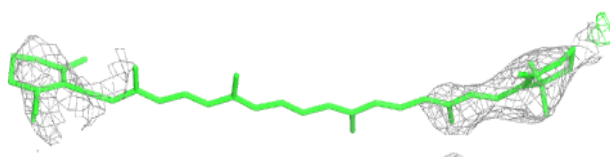
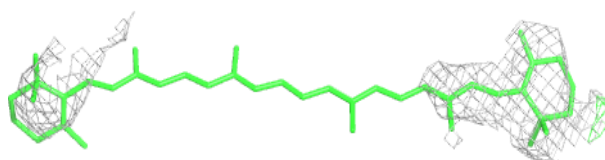


Electron density around SQD F 224:

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

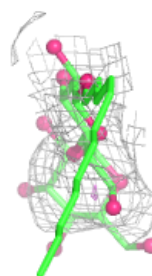
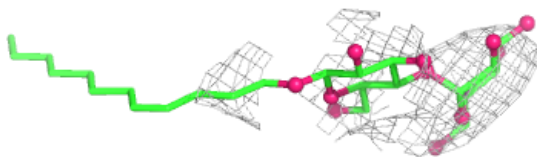
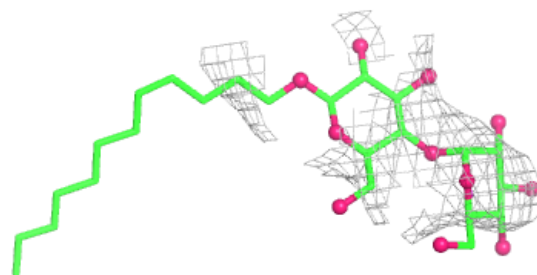
**Electron density around BCR J 115:**

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

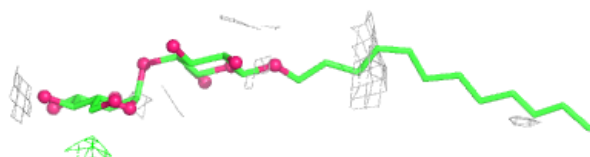
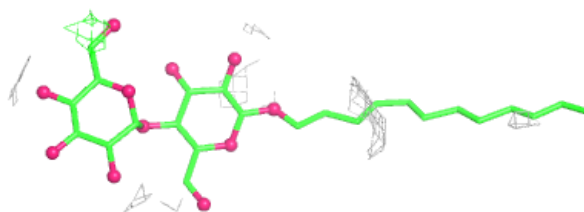


Electron density around LMT T 226:

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

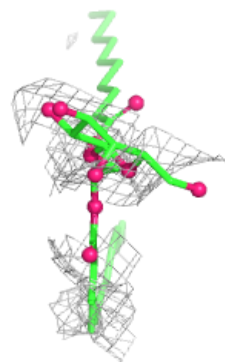
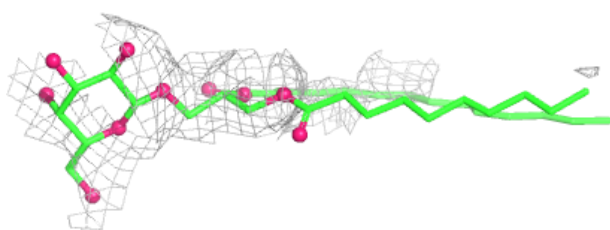
**Electron density around LMT O 274:**

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

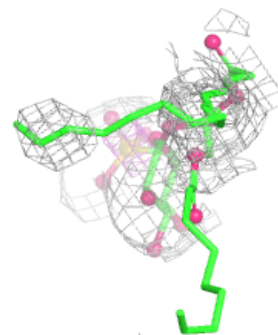
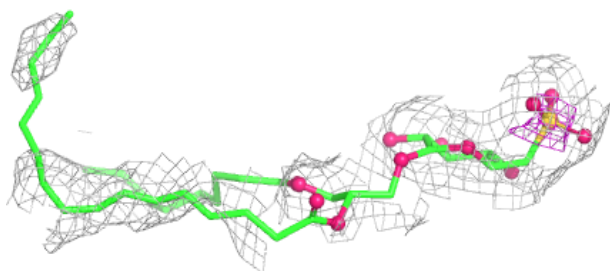
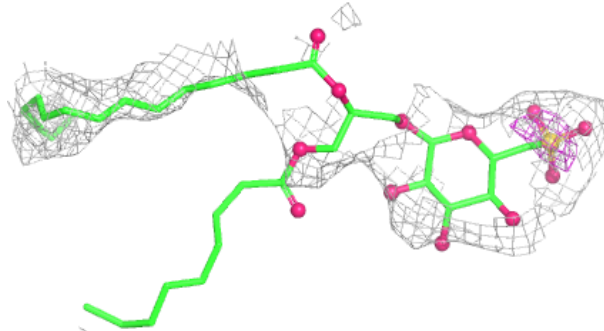


Electron density around LMG I 220:

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

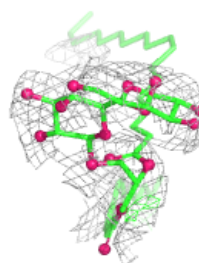
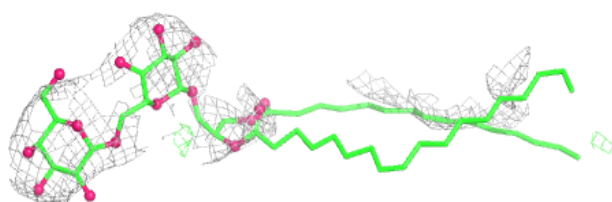
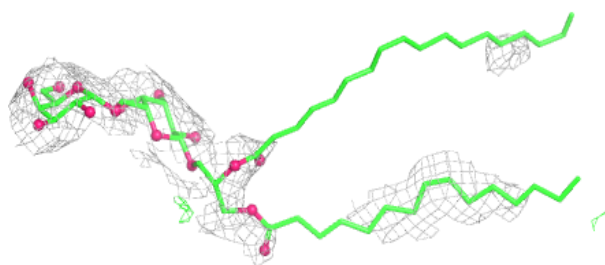
**Electron density around SQD L 213:**

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

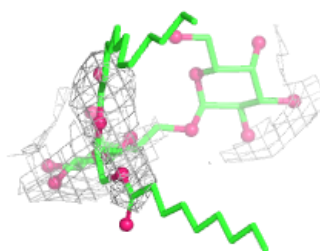
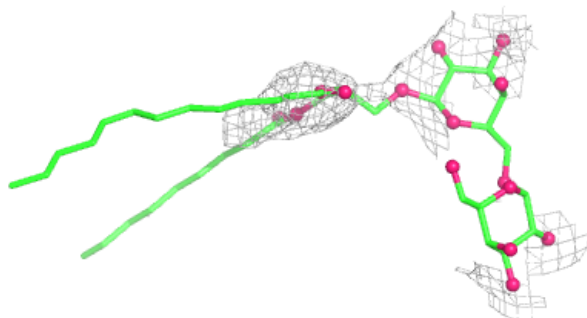


Electron density around DGD D 362:

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

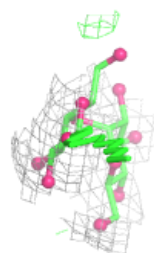
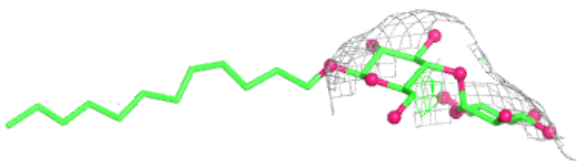
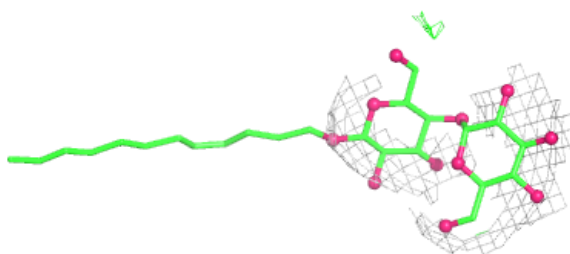
**Electron density around DGD A 375:**

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

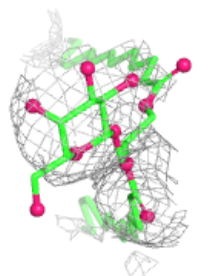
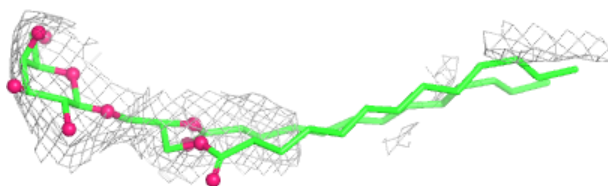
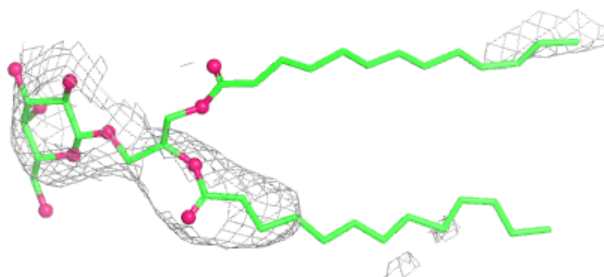


Electron density around LMT A 376:

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

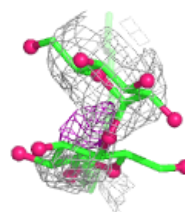
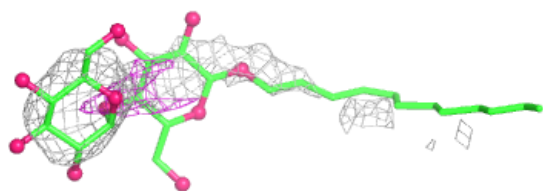
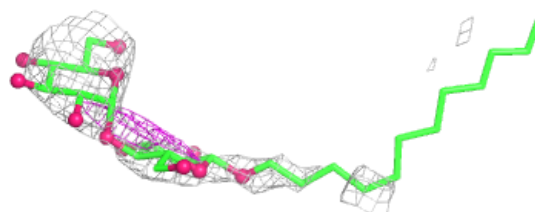
**Electron density around LMG C 494:**

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

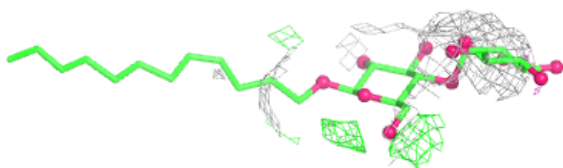
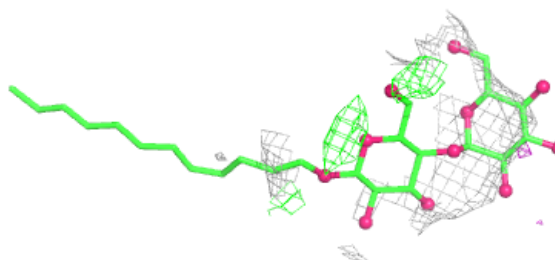


Electron density around LMT B 535:

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

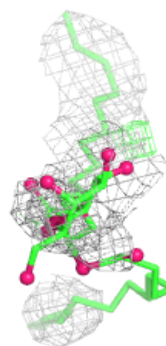
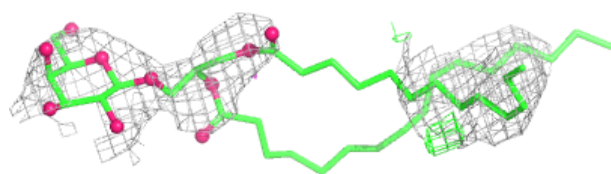
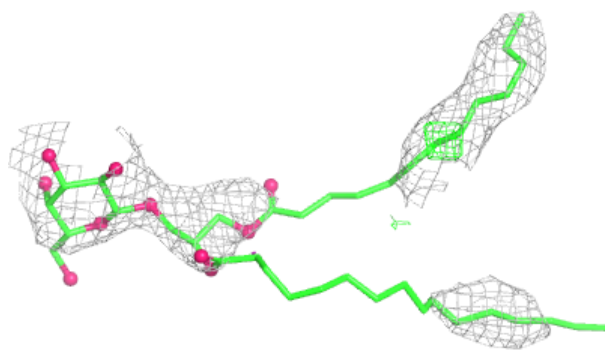
**Electron density around LMT D 536:**

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



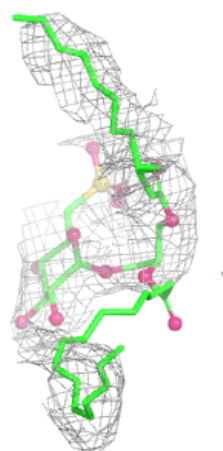
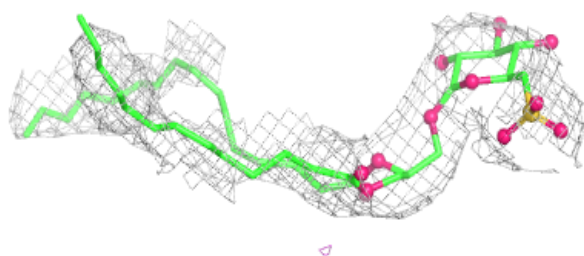
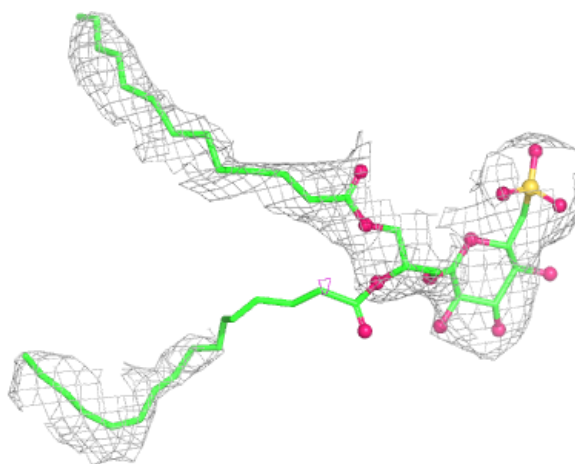
Electron density around LMG D 360:

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



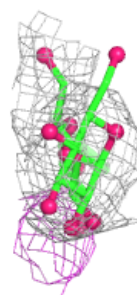
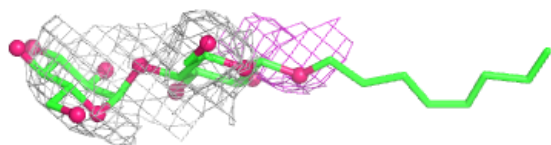
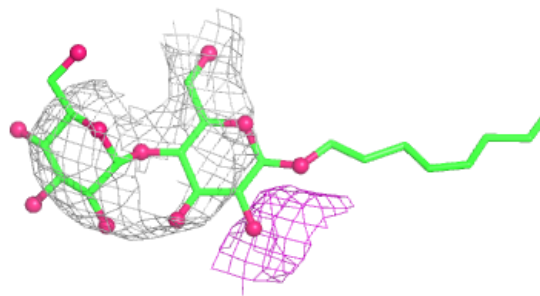
Electron density around SQD C 475:

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



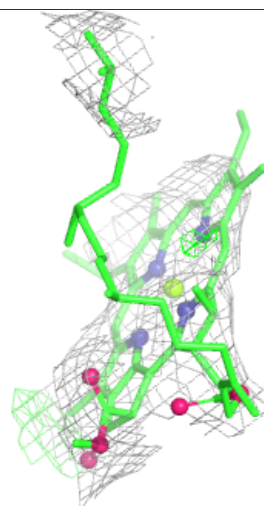
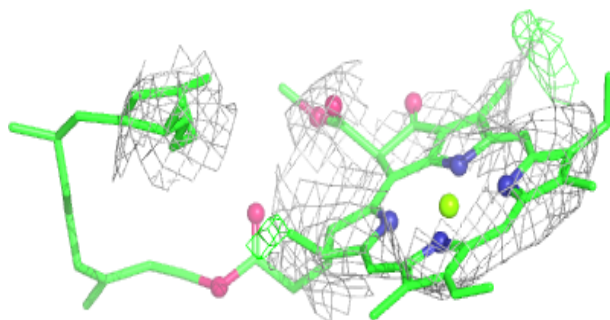
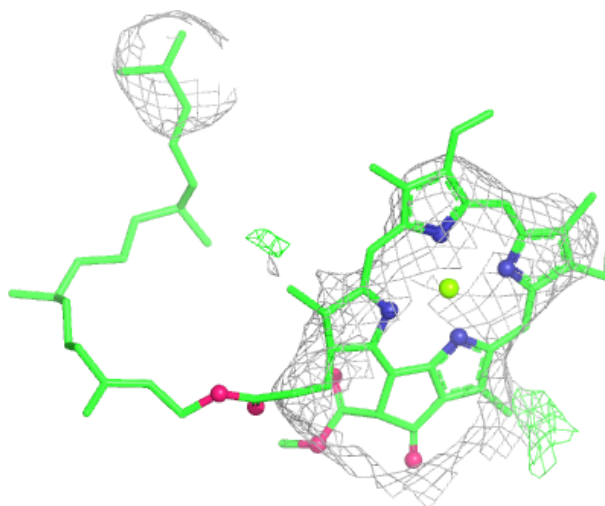
Electron density around LMT D 363:

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



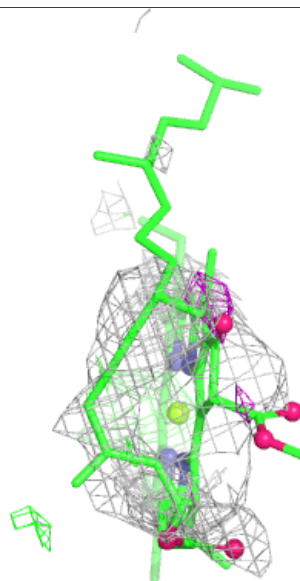
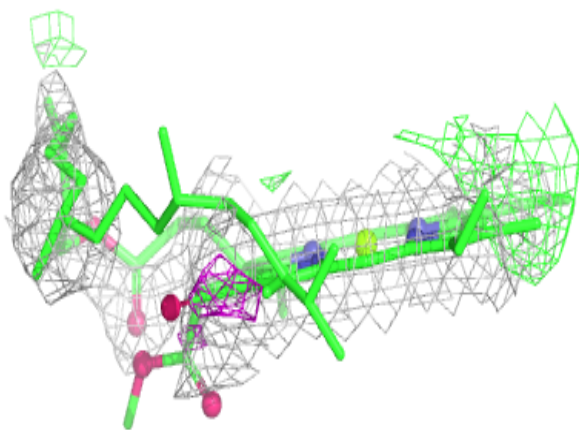
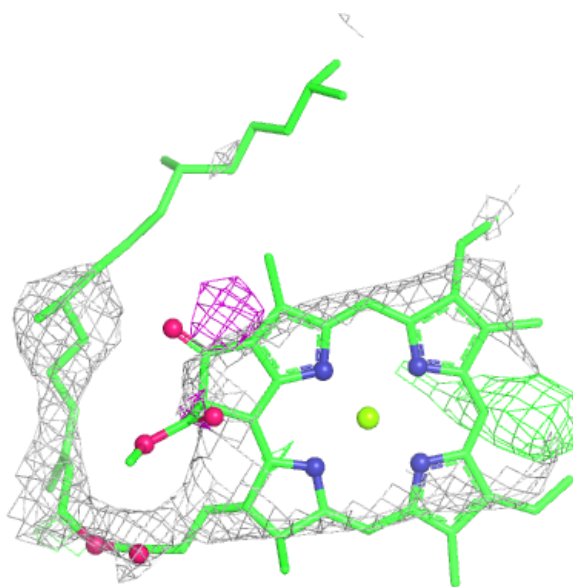
Electron density around CLA B 526:

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



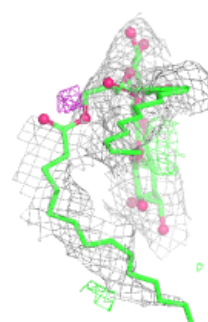
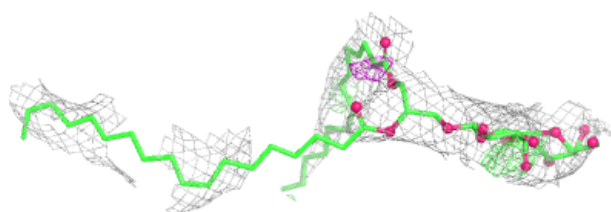
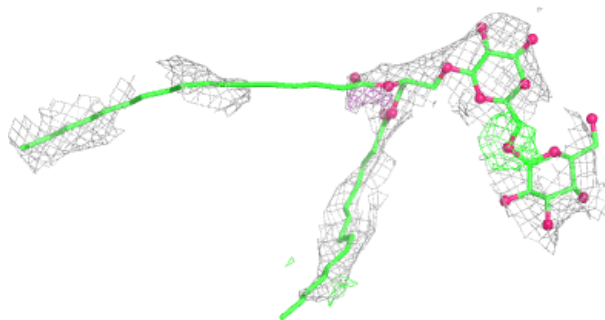
Electron density around CLA B 511:

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

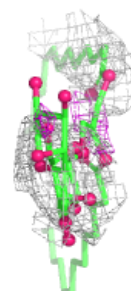
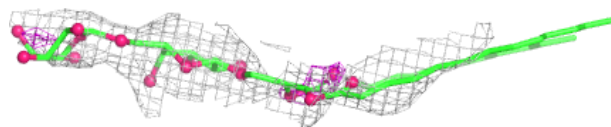
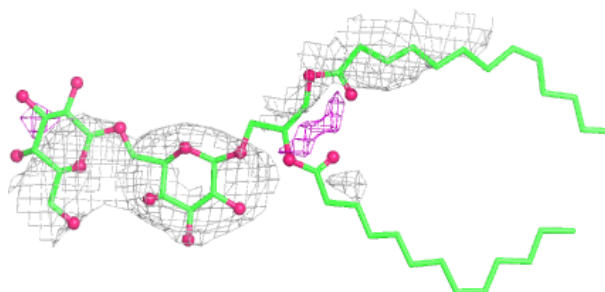


Electron density around DGD C 492:

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

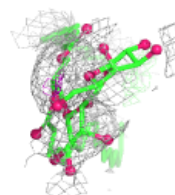
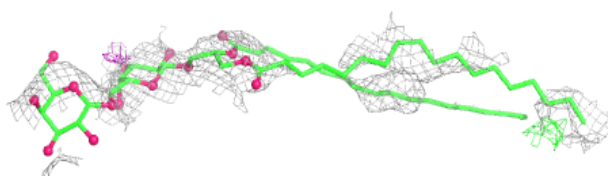
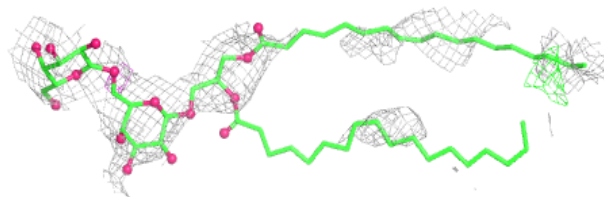
**Electron density around DGD C 474:**

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

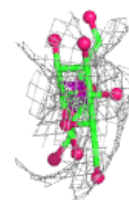
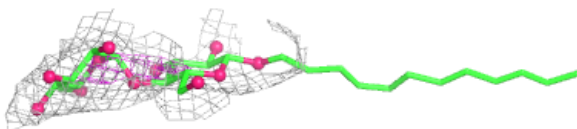
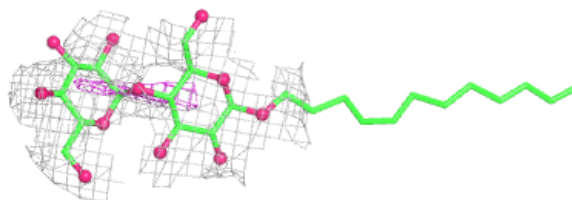


Electron density around DGD C 493:

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

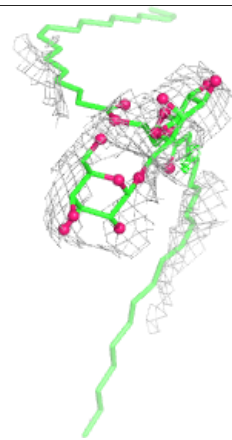
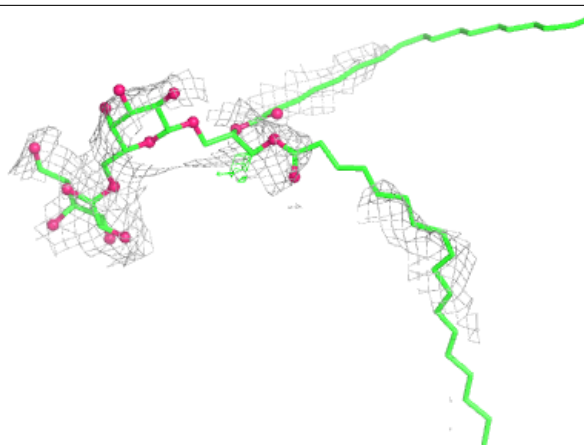
**Electron density around LMT I 274:**

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

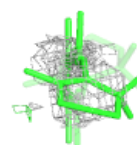
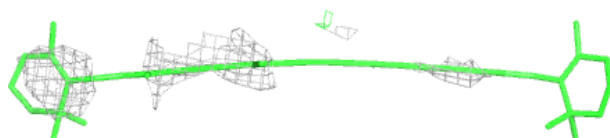
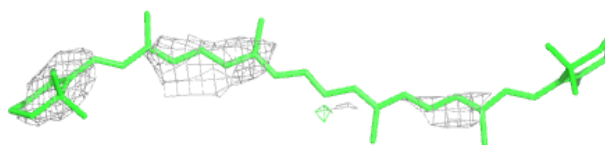


Electron density around DGD B 533:

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

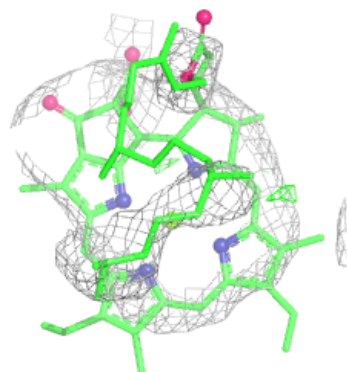
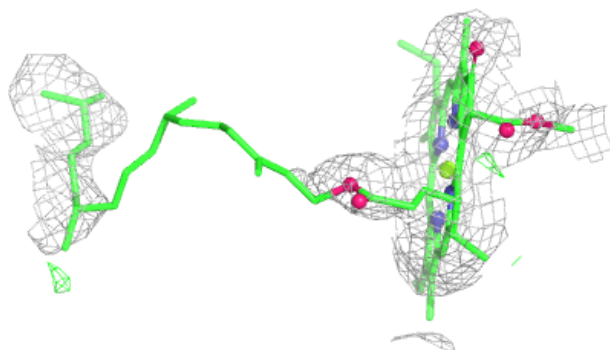
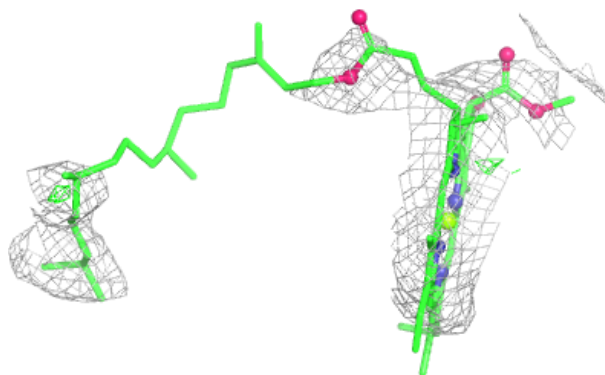
**Electron density around BCR B 530:**

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

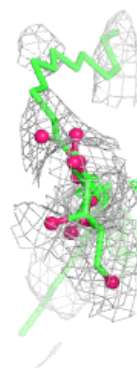
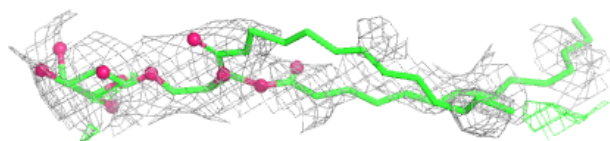
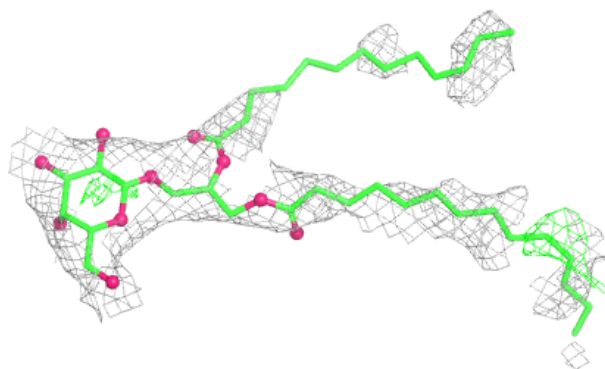


Electron density around CLA C 482:

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

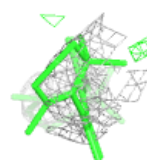
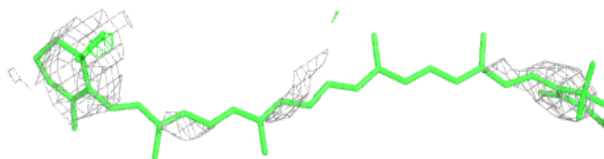
**Electron density around LMG D 359:**

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

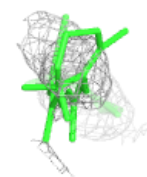
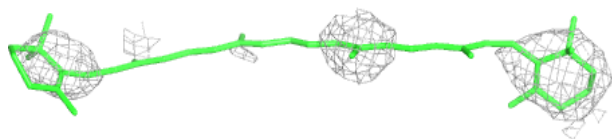
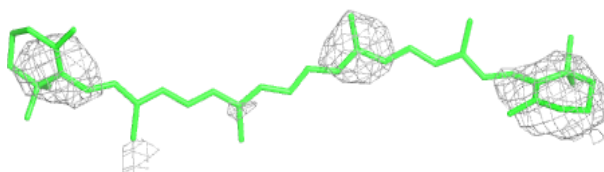


Electron density around BCR C 490:

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

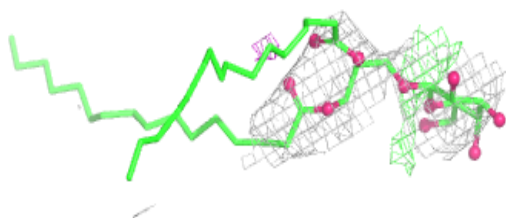
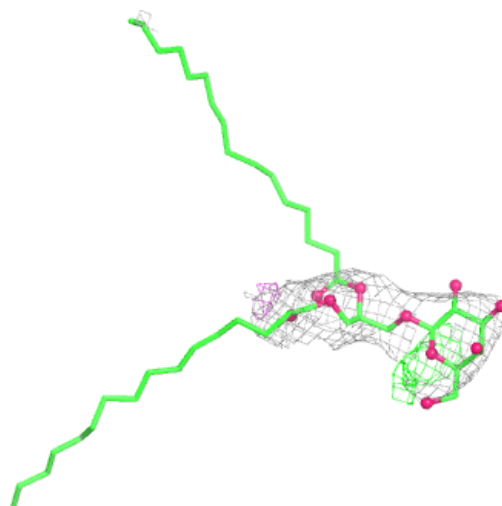
**Electron density around BCR B 527:**

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



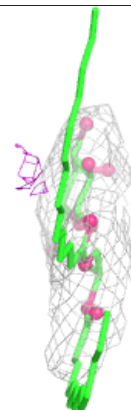
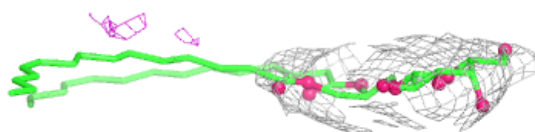
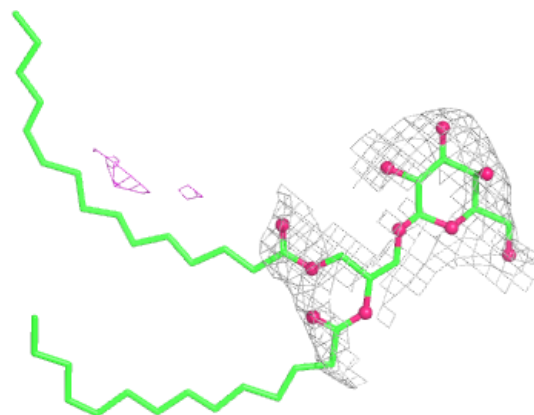
Electron density around LMG A 373:

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

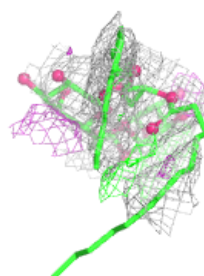
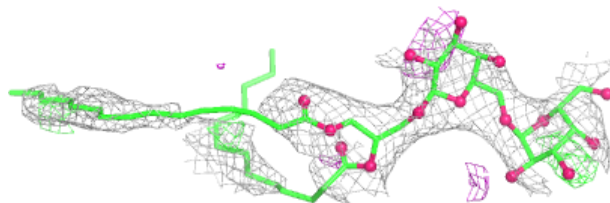
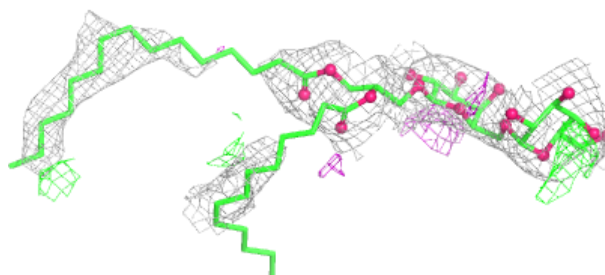


Electron density around LMG J 492:

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

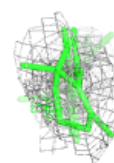
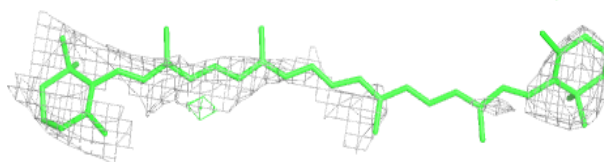
**Electron density around DGD B 528:**

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

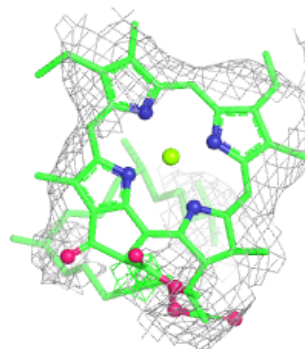
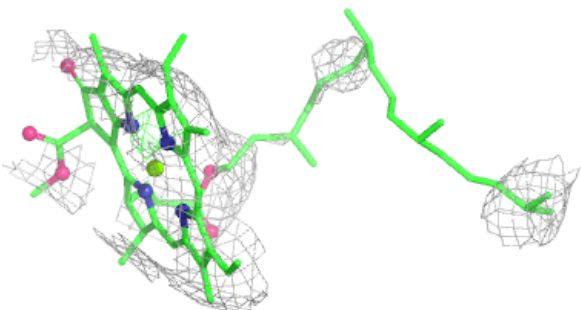
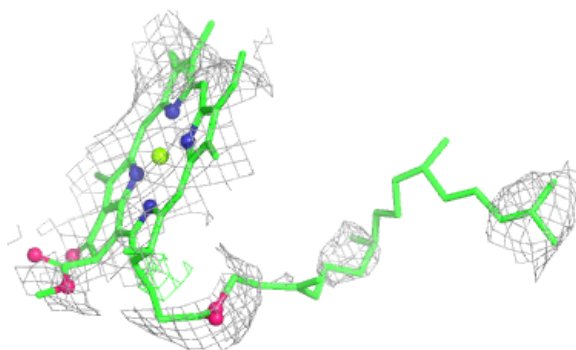


Electron density around BCR B 529:

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

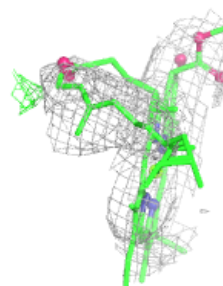
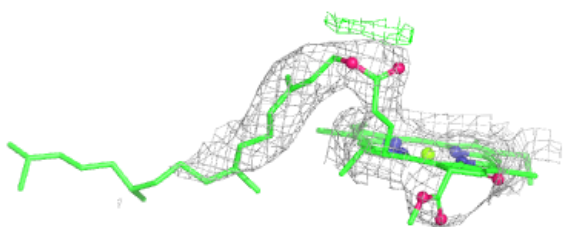
**Electron density around CLA C 488:**

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

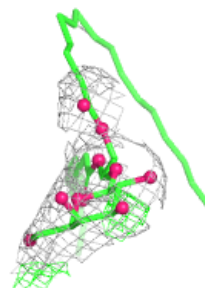
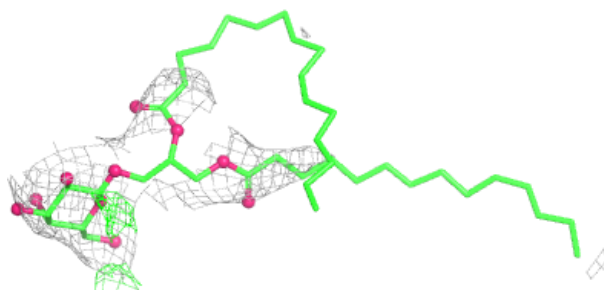


Electron density around CLA A 363:

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

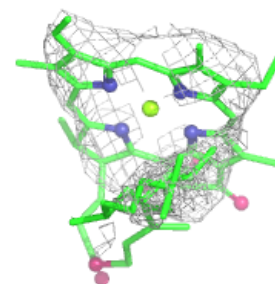
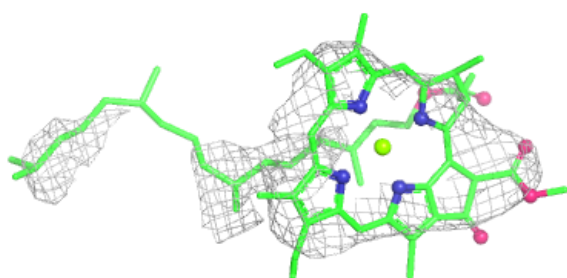
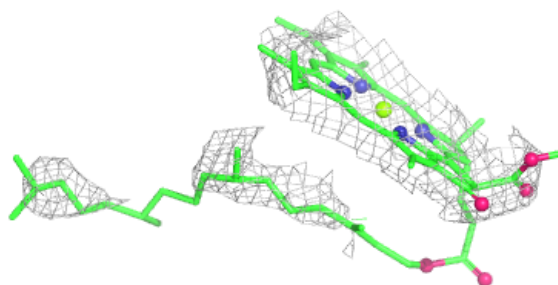
**Electron density around LMG B 531:**

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

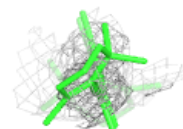
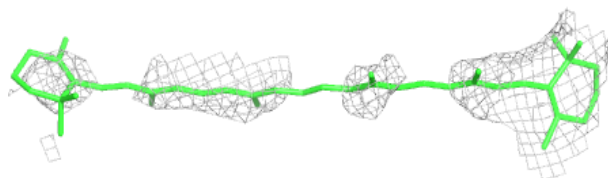
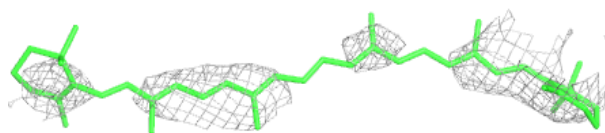


Electron density around CLA B 524:

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

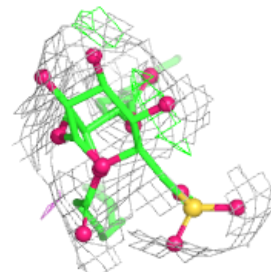
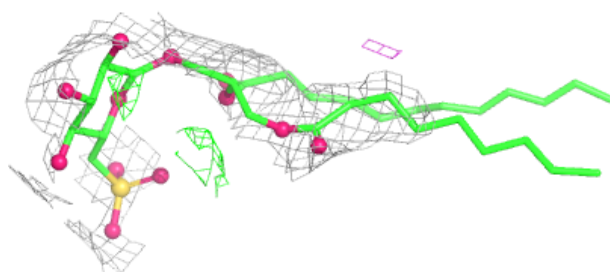
**Electron density around BCR Z 116:**

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

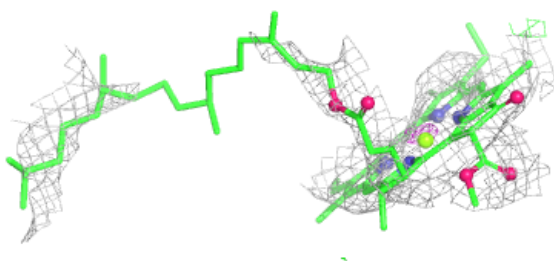
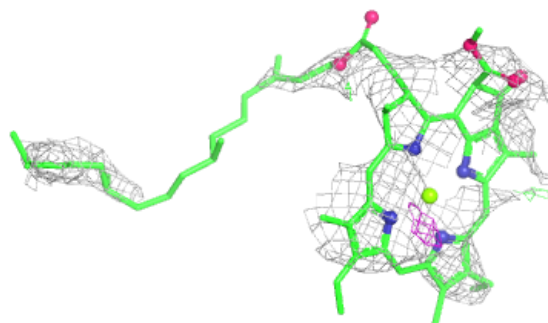


Electron density around SQD D 361:

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

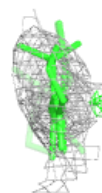
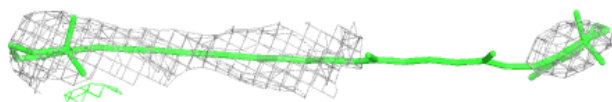
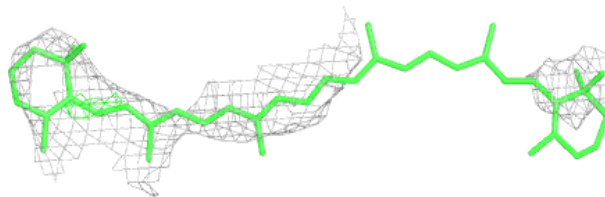
**Electron density around CLA C 486:**

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

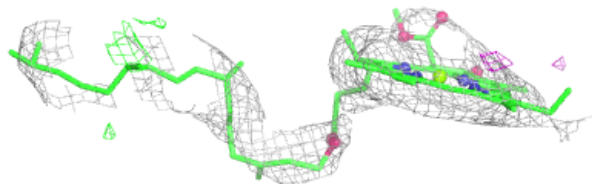
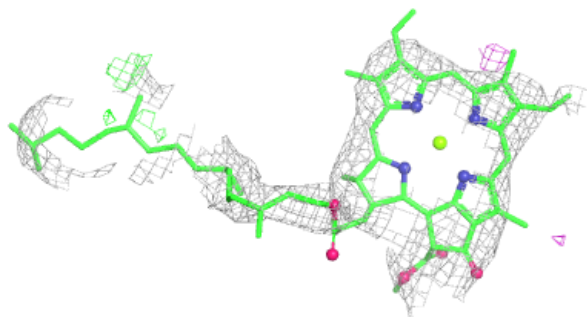


Electron density around BCR J 112:

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

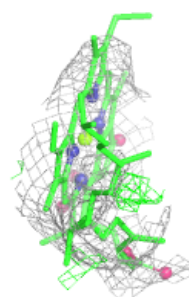
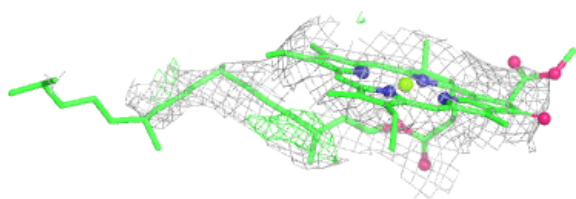
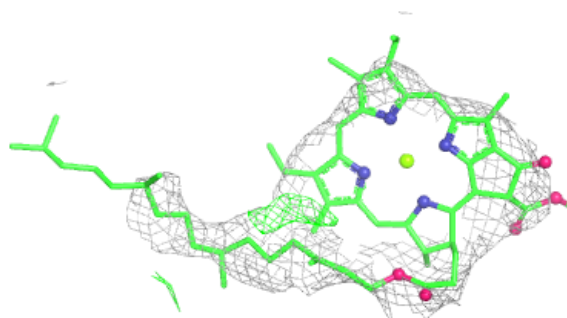
**Electron density around CLA A 364:**

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

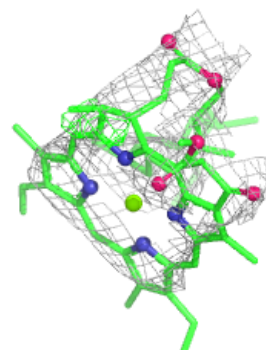
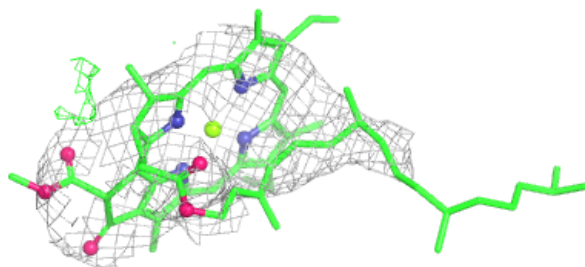


Electron density around CLA C 477:

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

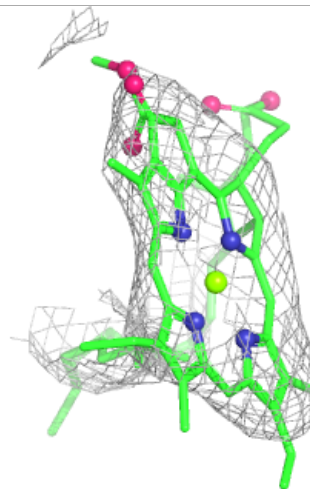
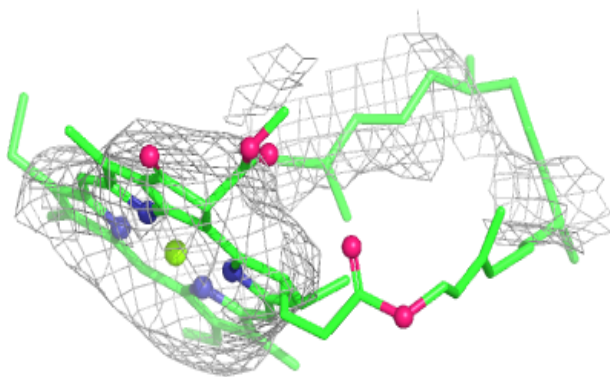
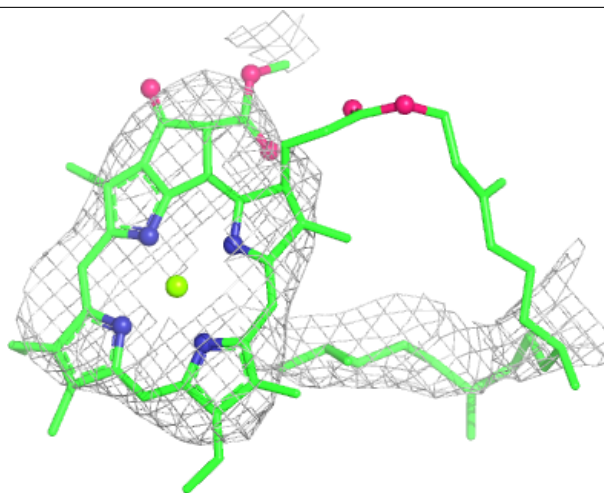
**Electron density around CLA C 481:**

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



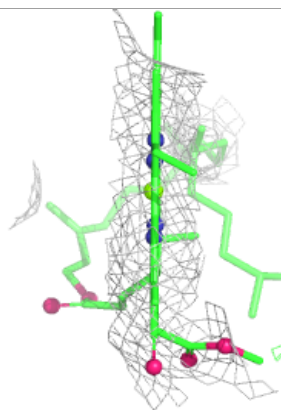
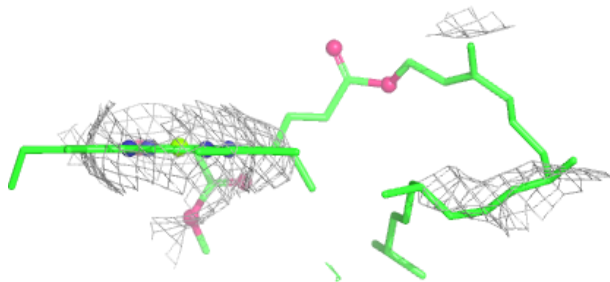
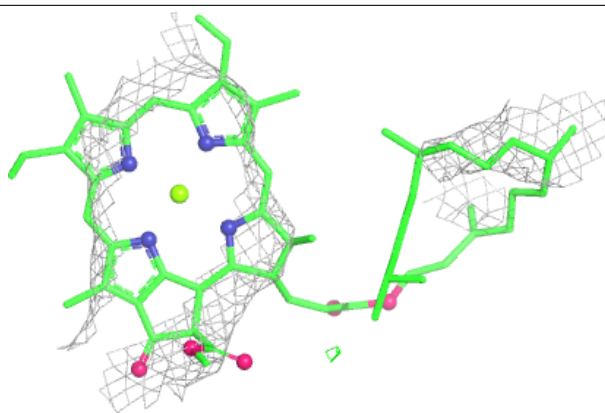
Electron density around CLA B 525:

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



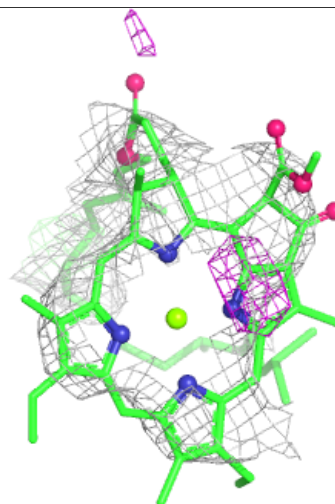
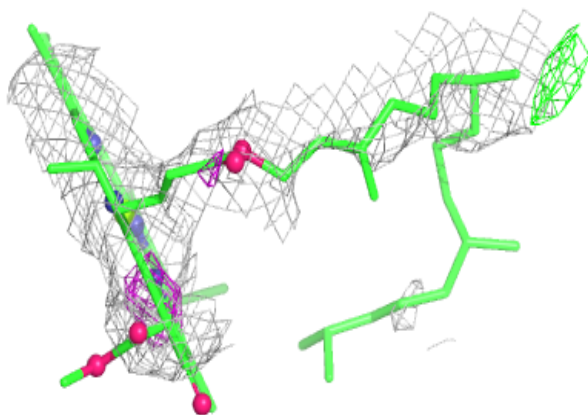
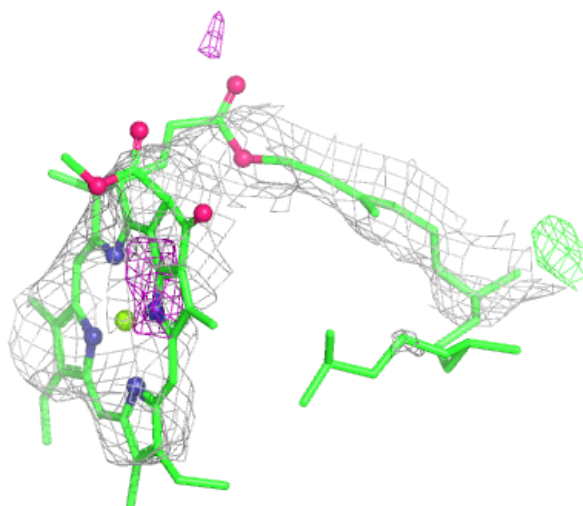
Electron density around CLA C 487:

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



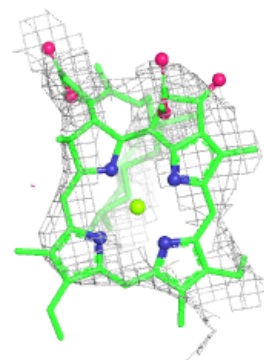
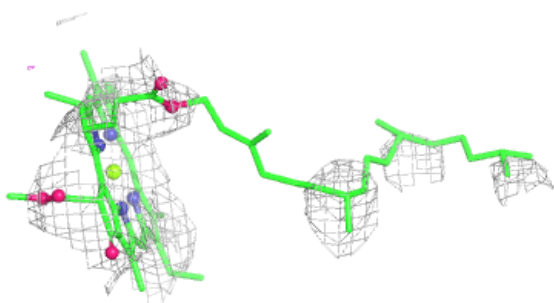
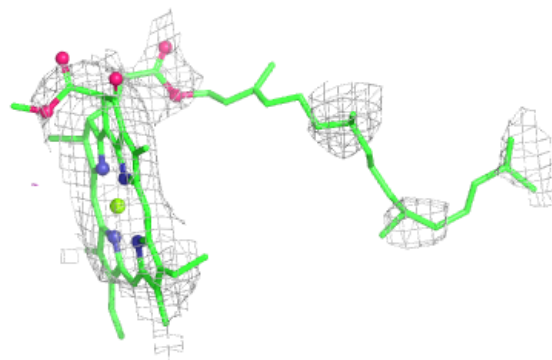
Electron density around CLA C 479:

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

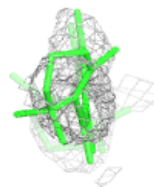
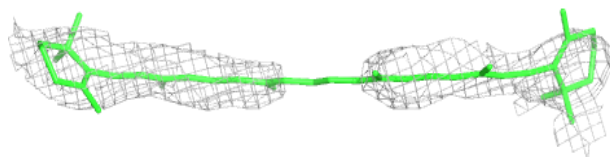
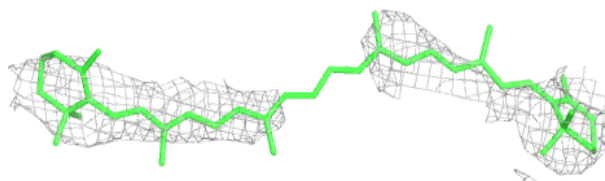


Electron density around CLA C 484:

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

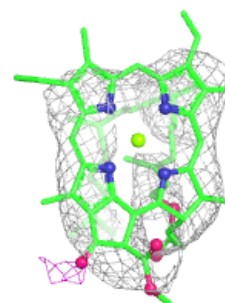
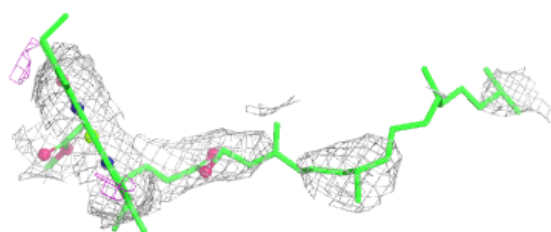
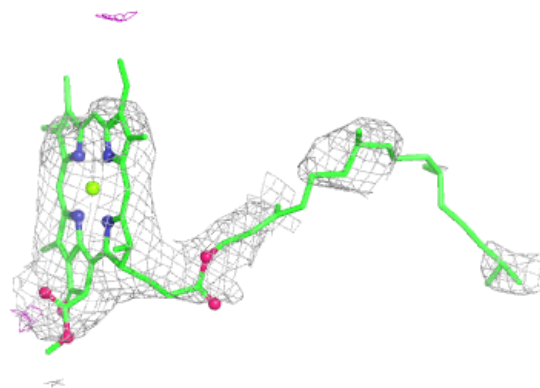
**Electron density around BCR X 107:**

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

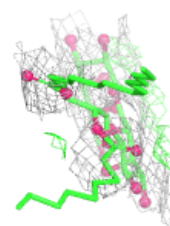
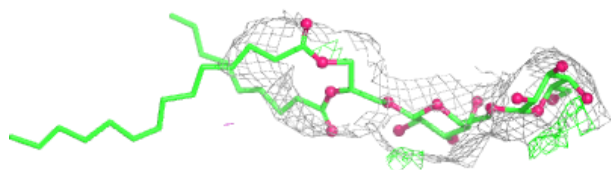
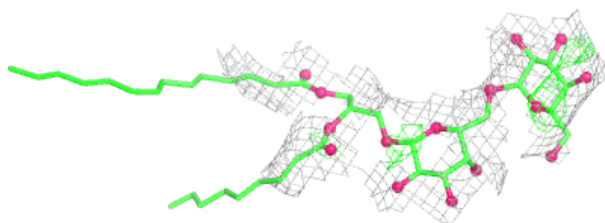


Electron density around CLA D 356:

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

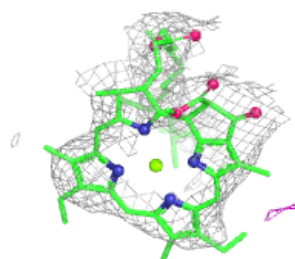
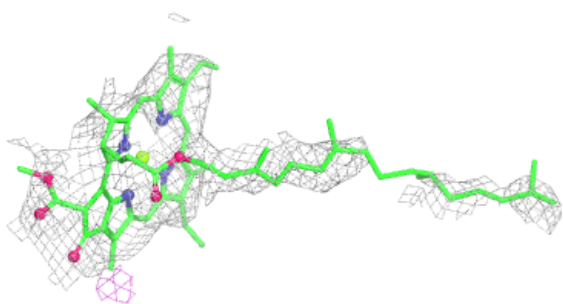
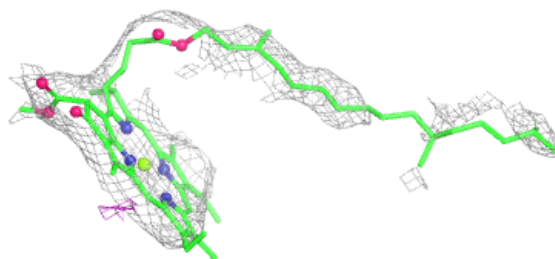
**Electron density around DGD C 491:**

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

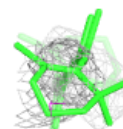
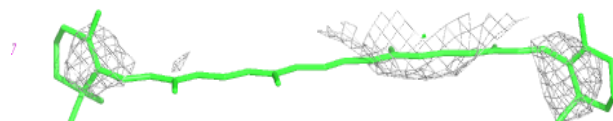
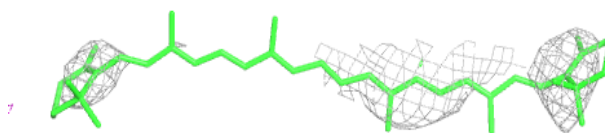


Electron density around CLA C 480:

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

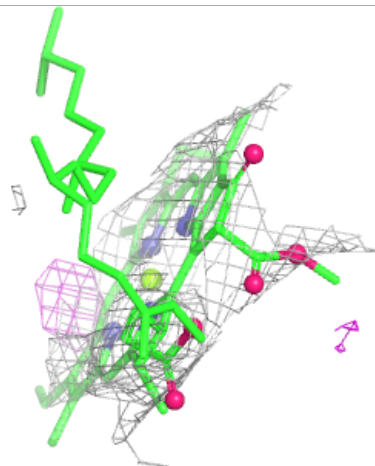
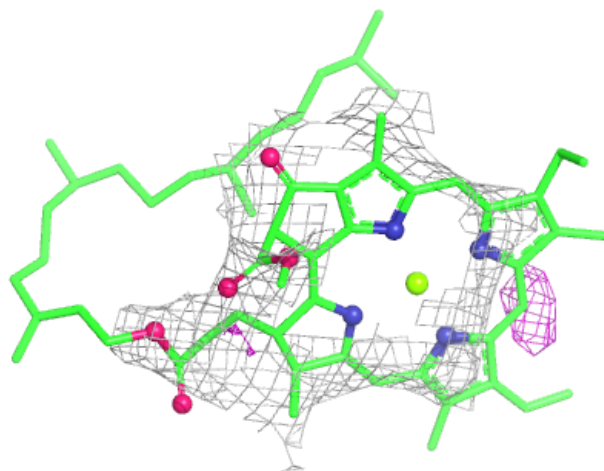
**Electron density around BCR A 369:**

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



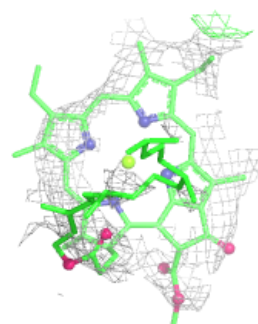
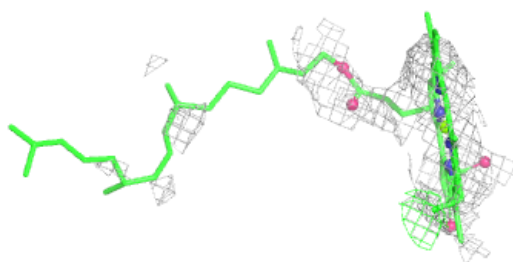
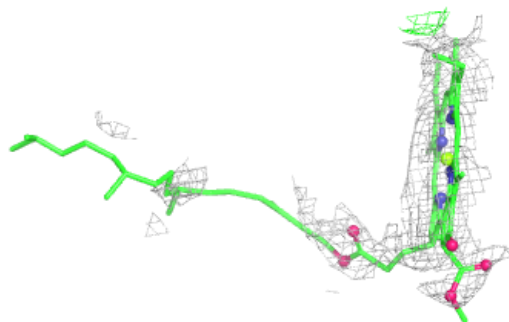
Electron density around CLA C 485:

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

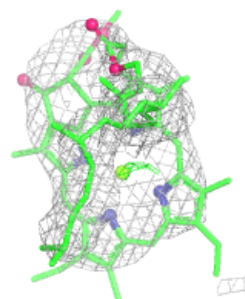
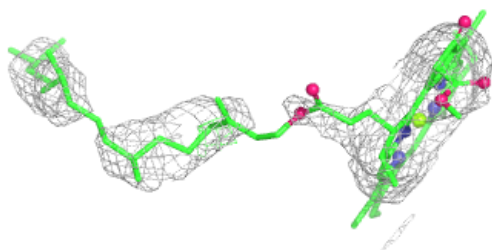
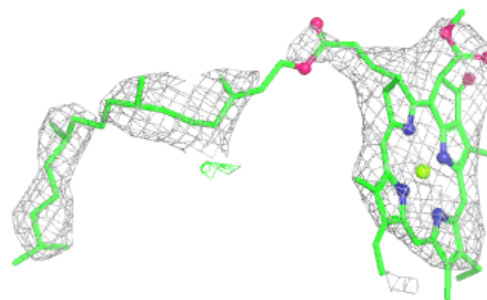


Electron density around CLA B 516:

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

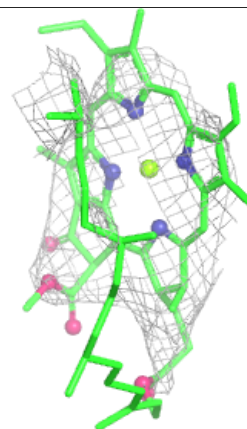
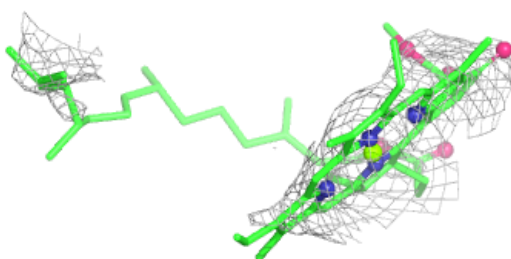
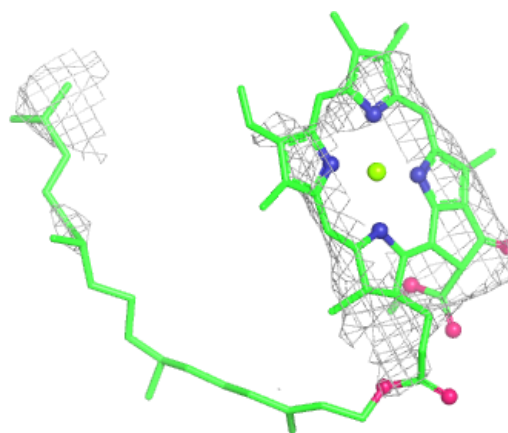
**Electron density around CLA A 366:**

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



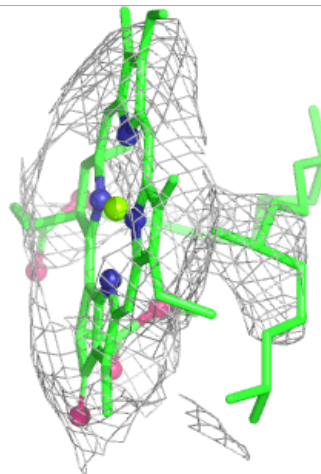
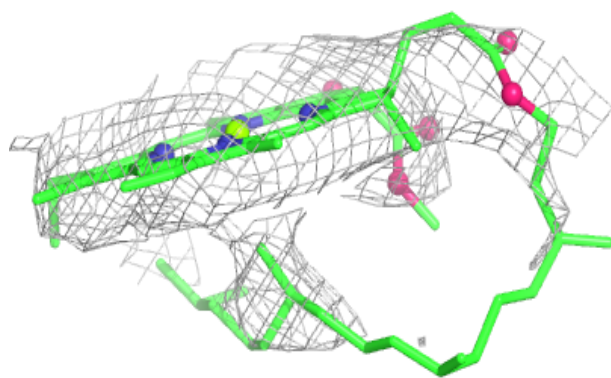
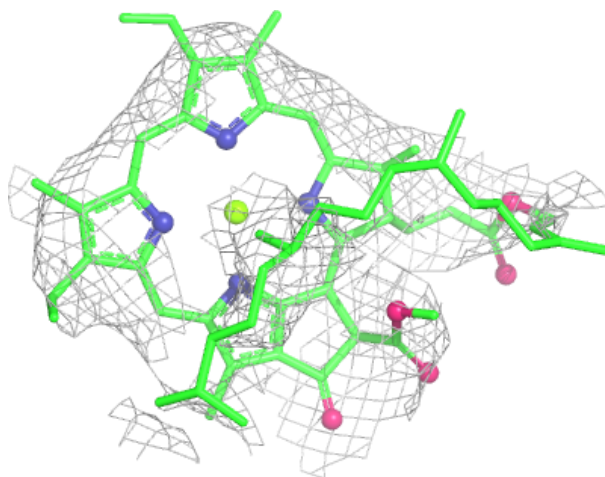
Electron density around CLA C 483:

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



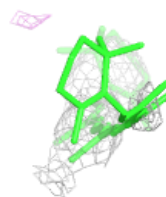
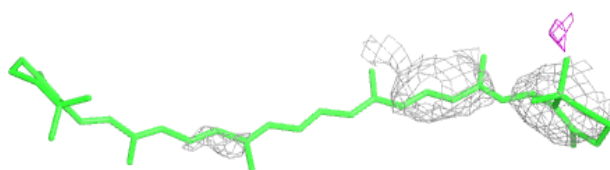
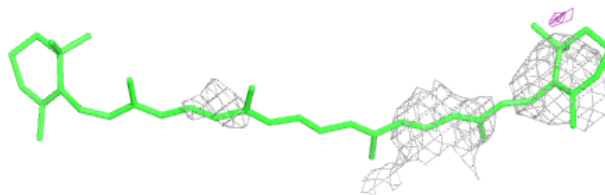
Electron density around CLA K 483:

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

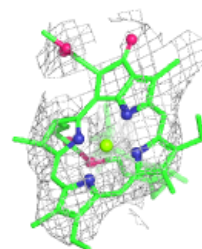
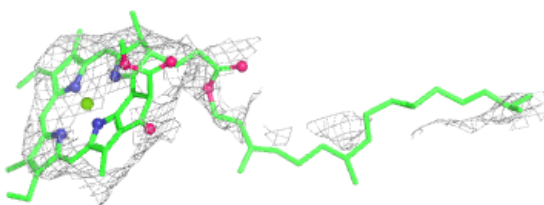


Electron density around BCR C 489:

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

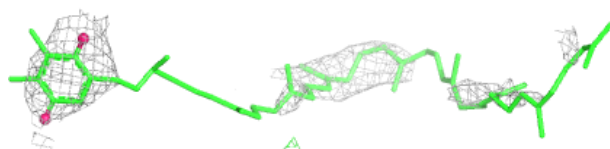
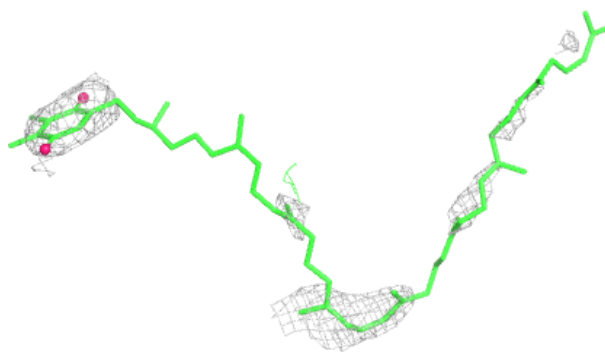
**Electron density around CLA C 478:**

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

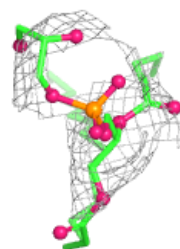
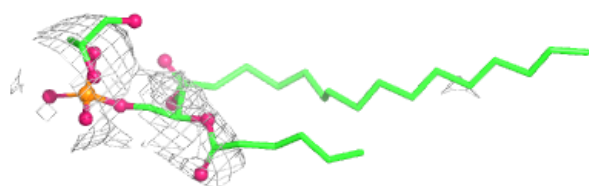
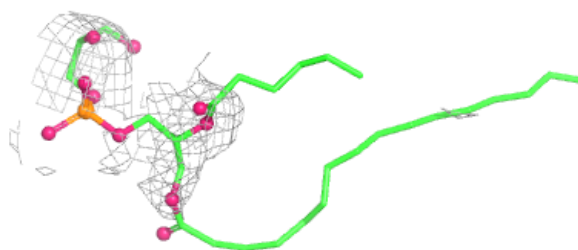


Electron density around PL9 D 357:

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

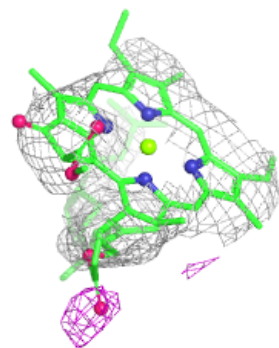
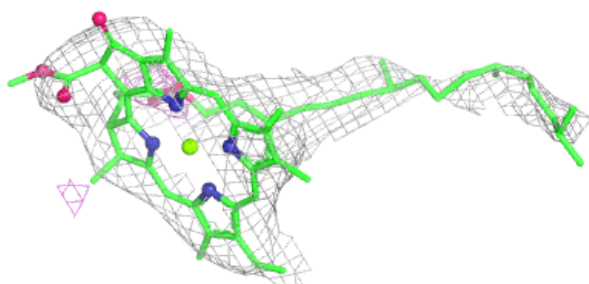
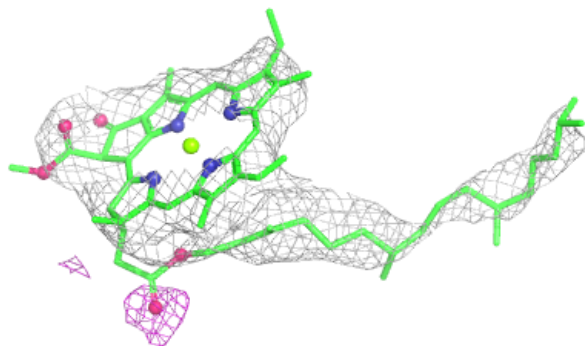
**Electron density around LHG A 371:**

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

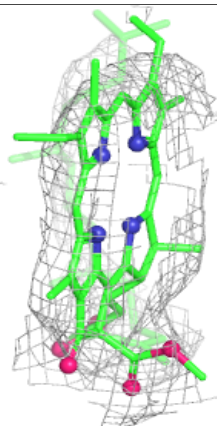
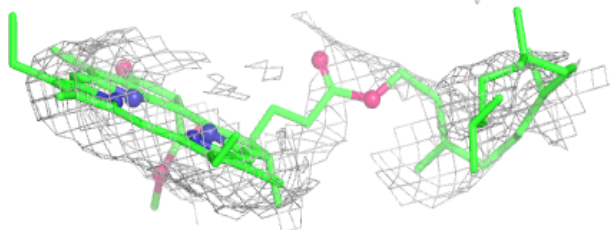
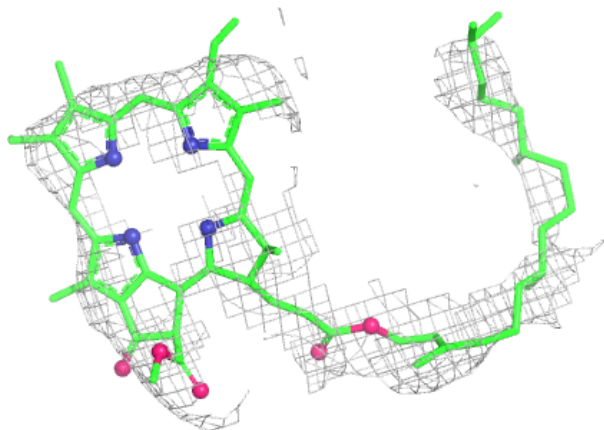


Electron density around CLA B 518:

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

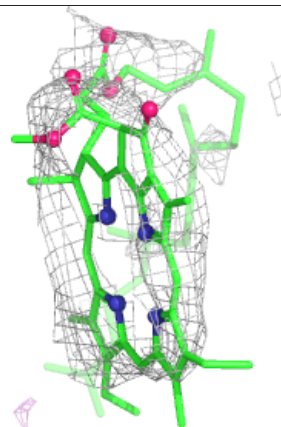
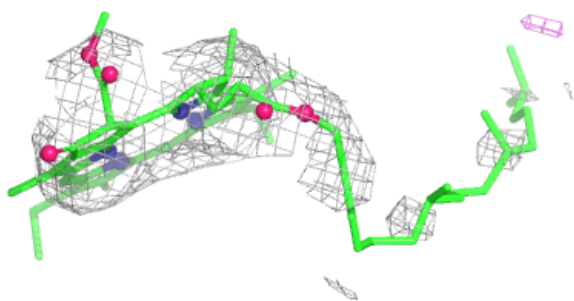
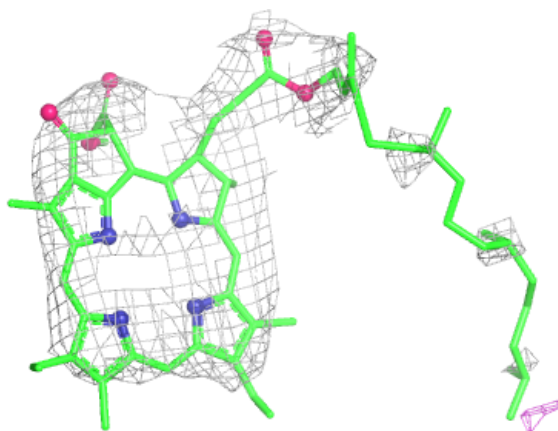
**Electron density around PHO A 365:**

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



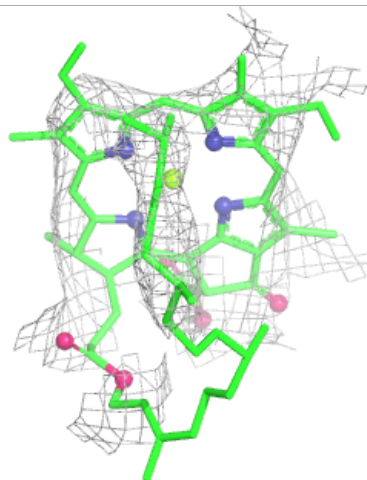
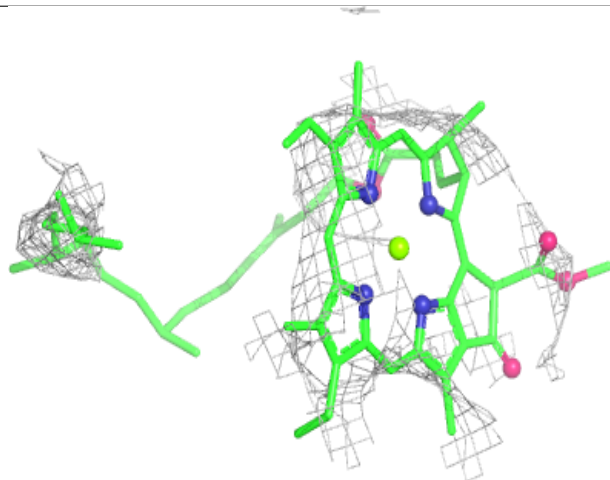
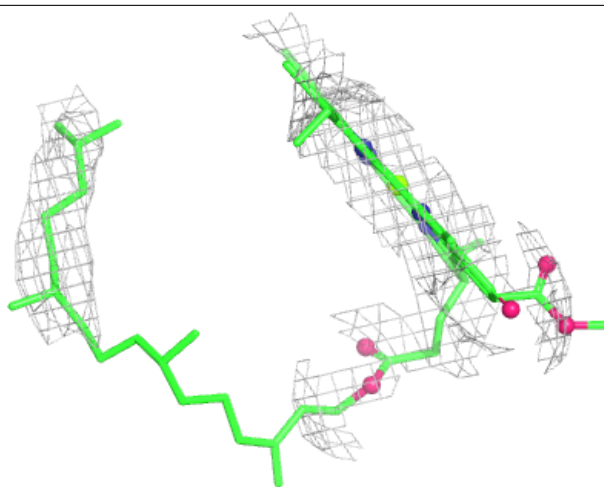
Electron density around PHO D 355:

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



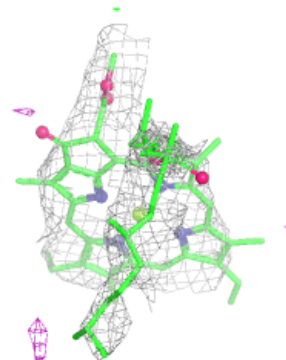
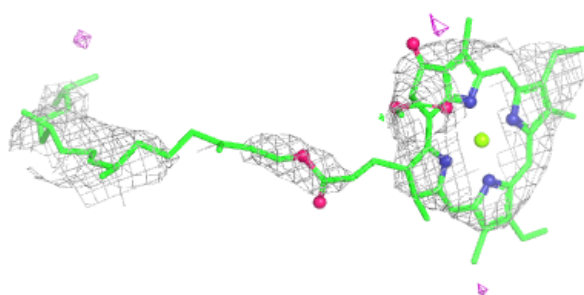
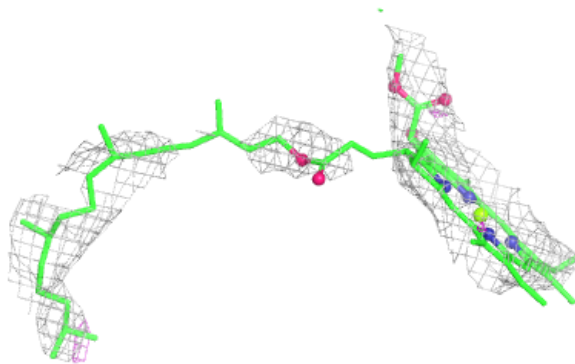
Electron density around CLA B 521:

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

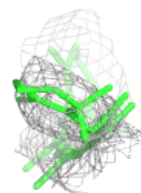
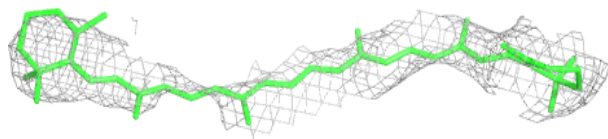
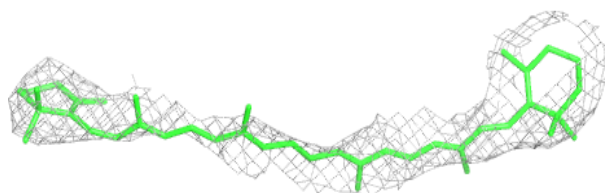


Electron density around CLA D 354:

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

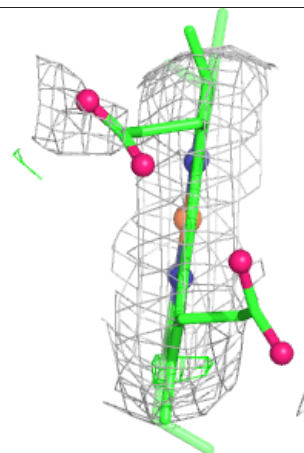
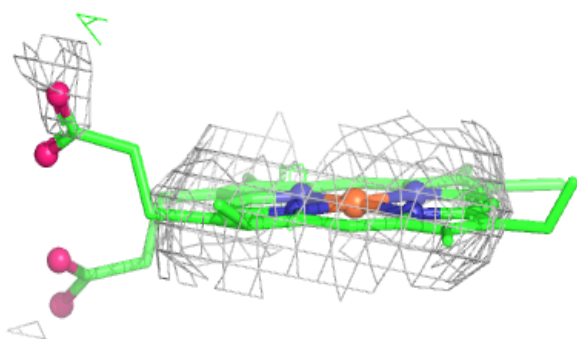
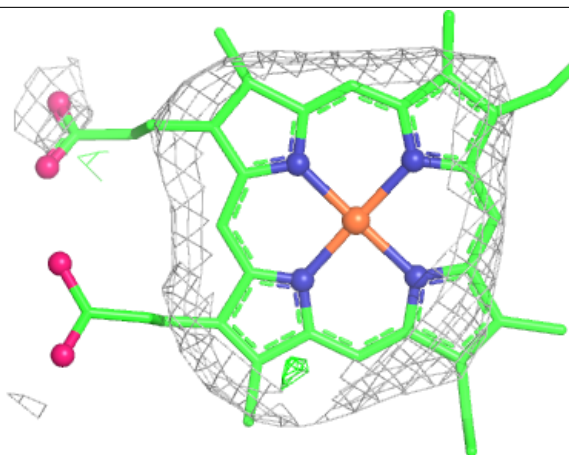
**Electron density around BCR D 358:**

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



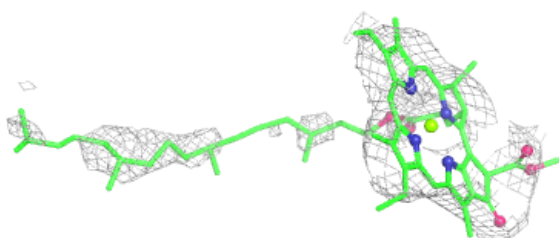
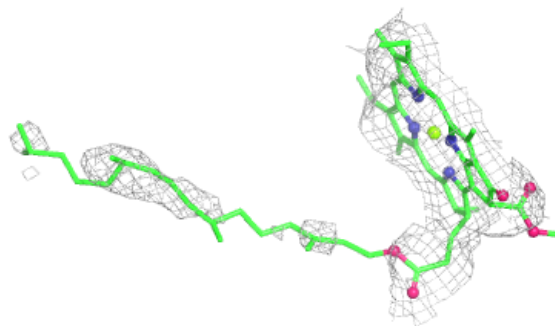
Electron density around HEM F 85:

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

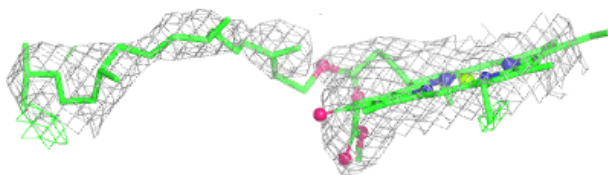
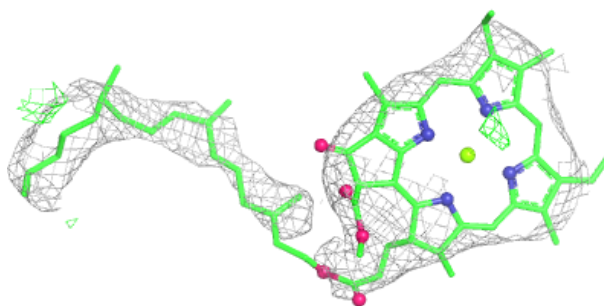


Electron density around CLA B 517:

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

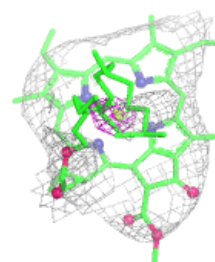
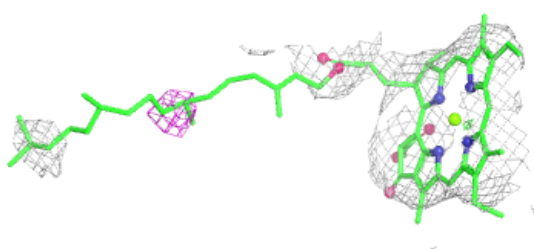
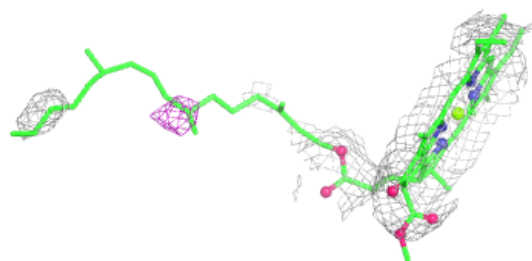
**Electron density around CLA B 512:**

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

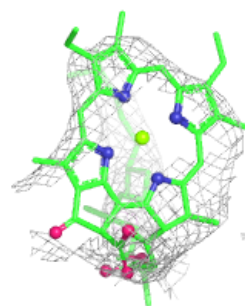
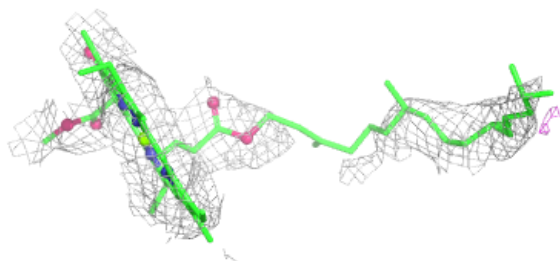
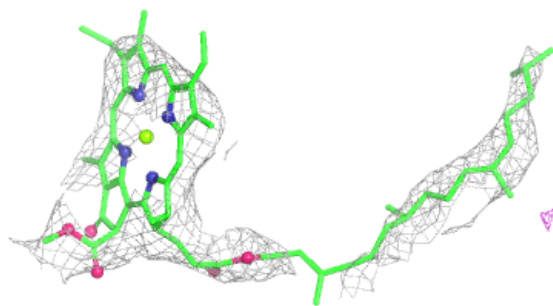


Electron density around CLA B 514:

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

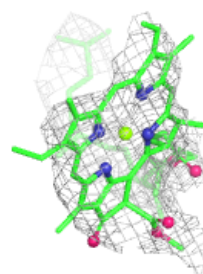
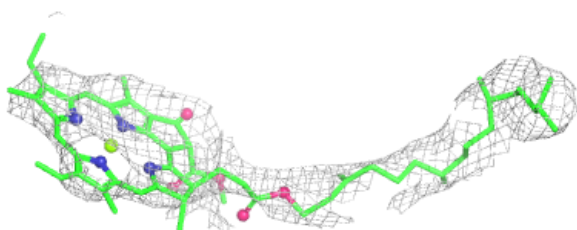
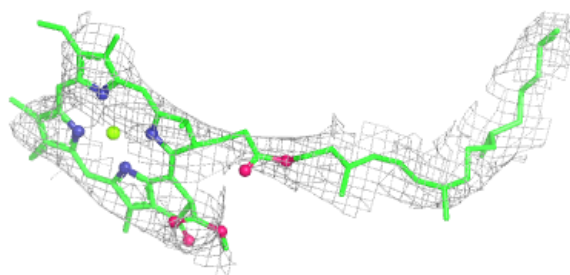
**Electron density around CLA B 519:**

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

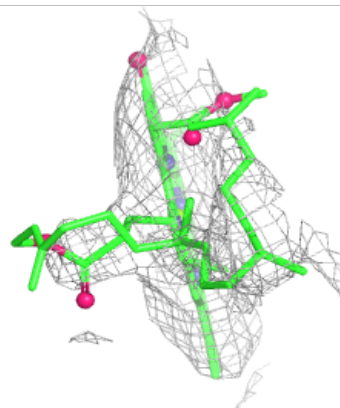
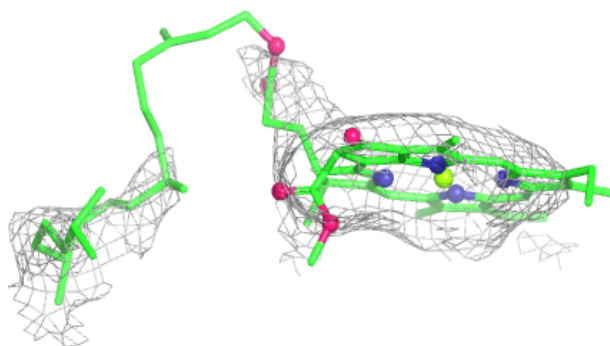
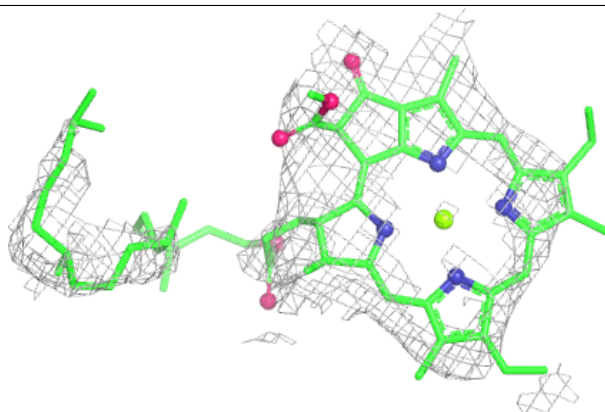


Electron density around CLA A 362:

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

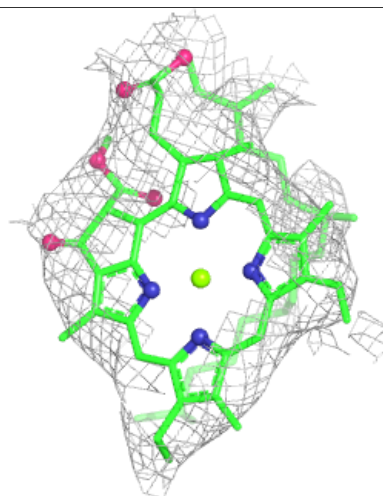
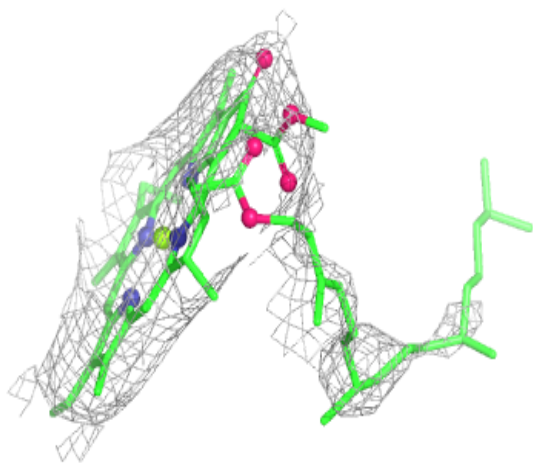
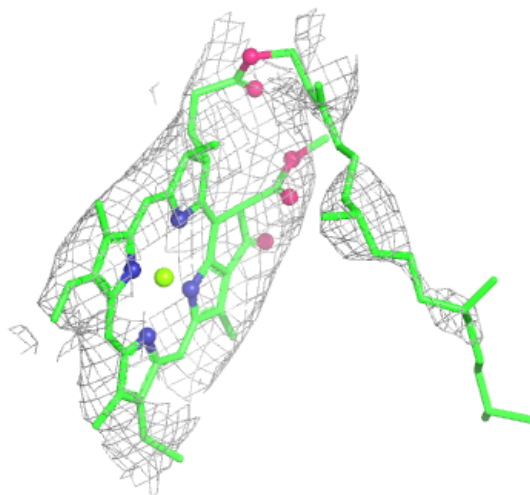
**Electron density around CLA B 522:**

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



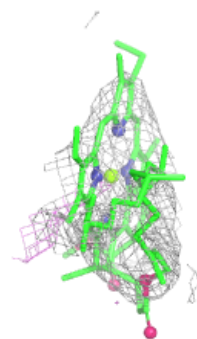
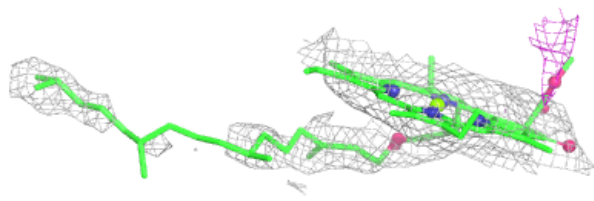
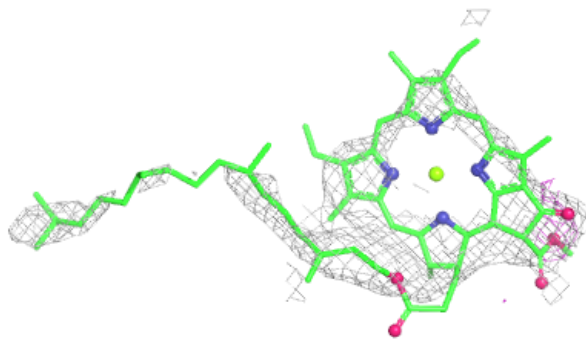
Electron density around CLA B 523:

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

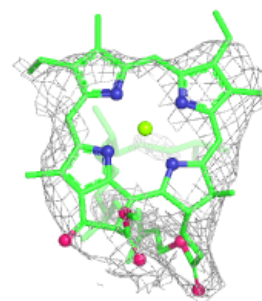
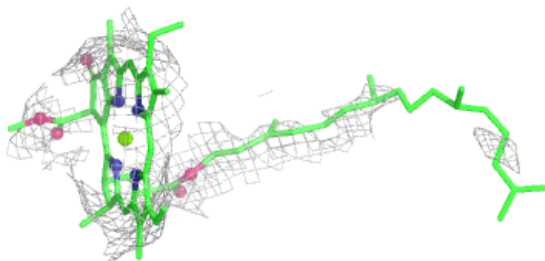
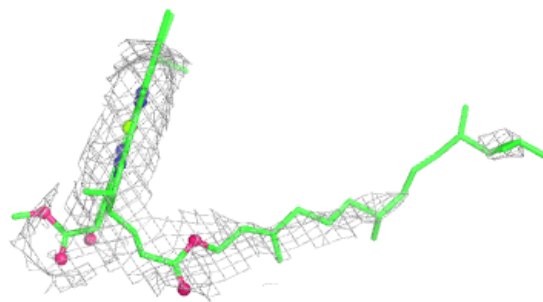


Electron density around CLA B 513:

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

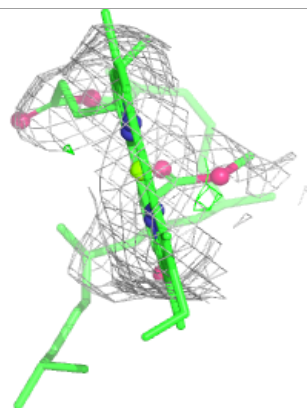
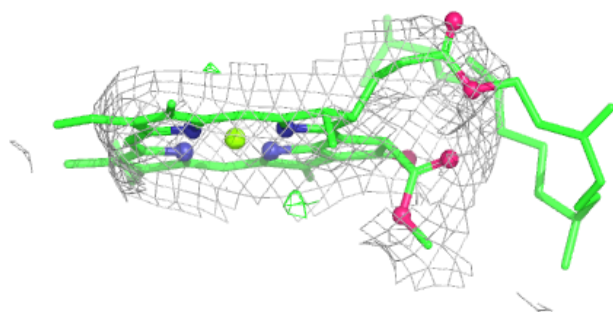
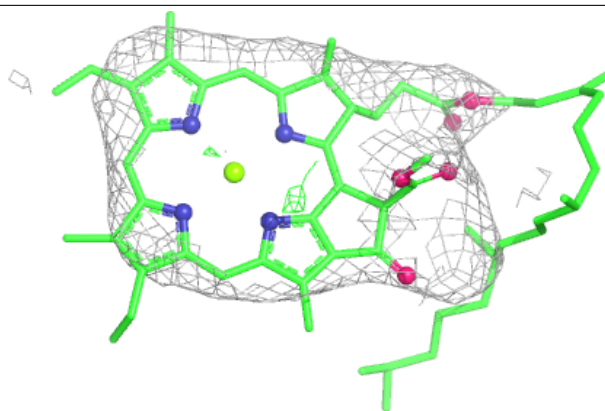
**Electron density around CLA B 515:**

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

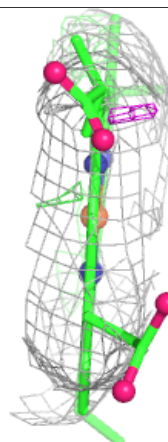
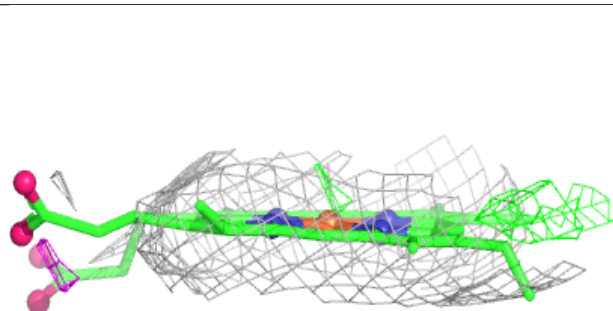
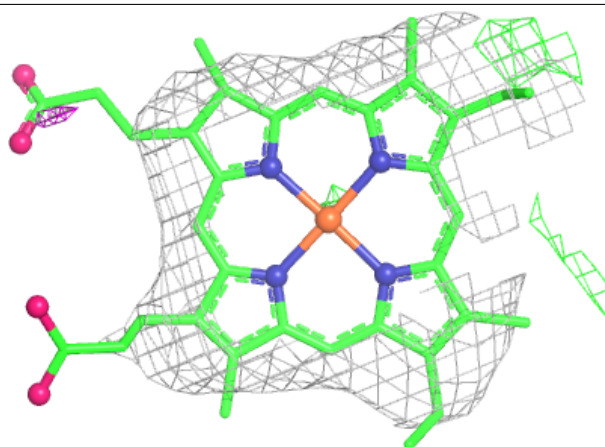


Electron density around CLA B 520:

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

**Electron density around HEM V 164:**

$2mF_o-DF_c$ (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.