wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 11:28 am BST

PDB ID	:	5E79 / pdb_00005e79
Title	:	Macromolecular diffractive imaging using imperfect crystals
Authors	:	Ayyer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on	:	2015-10-12
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

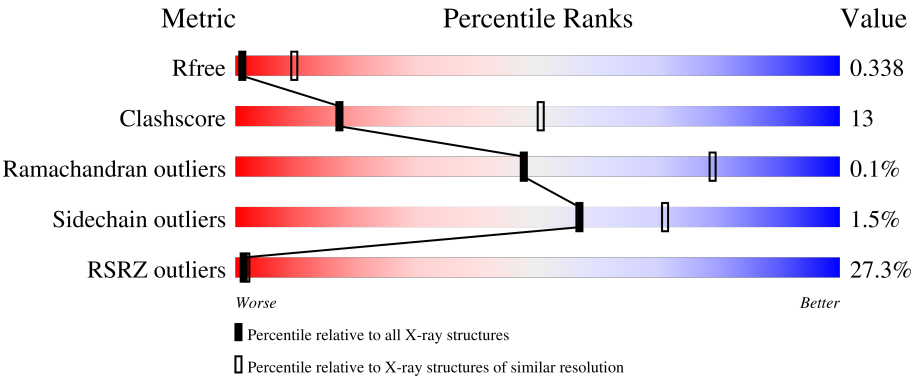
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	334	21% 77% 23%
1	a	334	33% 80% 20%
2	B	504	19% 77% 22%

Continued on next page...

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	b	504	32% 78% 21%
3	C	451	20% 80% 19%
3	c	451	34% 84% 16%
4	D	342	21% 75% 25%
4	d	342	32% 77% 23%
5	E	81	25% 77% 23%
5	e	81	46% 89% 11%
6	F	34	18% 50% 47%
6	f	34	32% 65% 35%
7	H	65	25% 74% 23%
7	h	65	38% 68% 31%
8	I	38	34% 74% 26%
8	i	38	42% 87% 13%
9	J	38	24% 95% 5%
9	j	38	37% 84% 16%
10	K	37	8% 70% 24% 5%
10	k	37	30% 57% 32% 8%
11	L	37	22% 68% 32%
11	l	37	32% 70% 27%
12	M	34	29% 74% 26%
12	m	34	35% 74% 21% 6%
13	O	243	23% 84% 16%
13	o	243	39% 84% 15%
14	T	30	13% 60% 40%
14	t	30	23% 70% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	U	97	15% 88% 12%
15	u	97	31% 88% 12%
16	V	137	20% 88% 12%
16	v	137	26% 91% 9%
17	Y	29	24% 86% 14%
17	y	29	38% 86% 14%
18	X	39	15% 82% 18%
18	x	39	28% 77% 23%
19	Z	62	29% 94% 6%
19	z	62	47% 90% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	U	201	-	-	-	X
22	CL	a	604	-	-	-	X
22	CL	u	201	-	-	-	X
26	BCR	A	610	-	X	-	-
26	BCR	B	618	-	X	X	-
26	BCR	B	619	-	X	-	-
26	BCR	B	620	-	X	-	-
26	BCR	C	514	-	X	-	-
26	BCR	F	101	-	X	-	-
26	BCR	H	101	-	X	-	-
26	BCR	I	101	-	X	-	-
26	BCR	K	101	-	X	-	-
26	BCR	K	102	-	X	-	-
26	BCR	T	101	-	X	X	-
26	BCR	a	610	-	X	-	-
26	BCR	b	619	-	X	X	-
26	BCR	b	620	-	X	-	-
26	BCR	b	621	-	X	-	-
26	BCR	c	514	-	X	-	-
26	BCR	c	515	-	X	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	BCR	c	521	-	X	-	-
26	BCR	f	101	-	X	X	-
26	BCR	h	101	-	X	-	-
26	BCR	k	101	-	X	-	-
26	BCR	t	101	-	X	X	-
27	PL9	D	405	-	X	-	-
27	PL9	a	611	-	-	-	X
27	PL9	d	404	-	X	-	-
29	LMG	Z	101	-	-	-	X
29	LMG	c	520	-	-	-	X
30	LHG	E	102	-	-	-	X
31	CA	b	602	-	-	-	X

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 50074 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	3	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			668	436	107	125			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	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	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	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	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	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	5	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	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	1	0
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	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	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

- 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	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total 1072	C 680	N 180	O 208	S 4	0	1	0
16	v	137	Total 1072	C 680	N 180	O 208	S 4	0	1	0

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total 215	C 142	N 37	O 33	S 3	0	0	0
17	y	29	Total 215	C 142	N 37	O 33	S 3	0	0	0

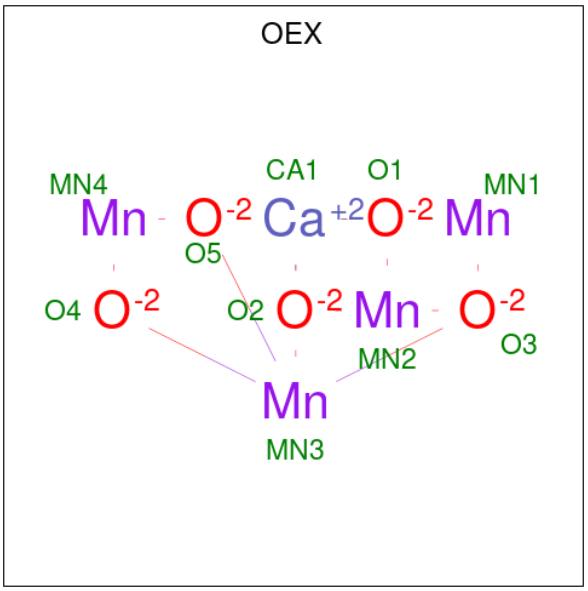
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total 292	C 196	N 46	O 50	0	1	0
18	x	39	Total 292	C 196	N 46	O 50	0	1	0

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

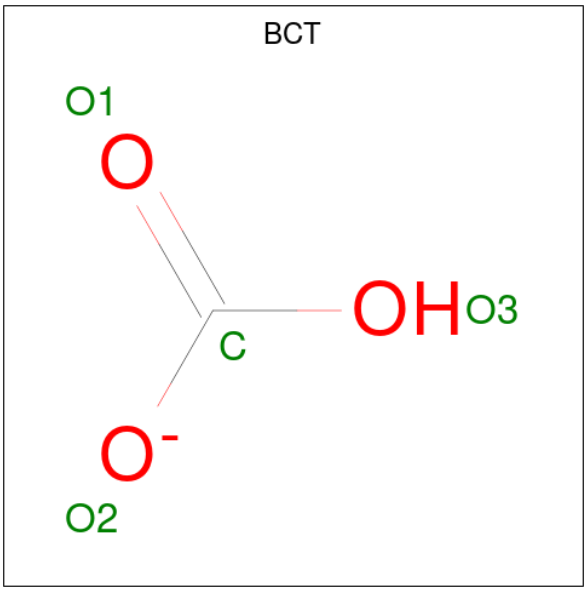
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

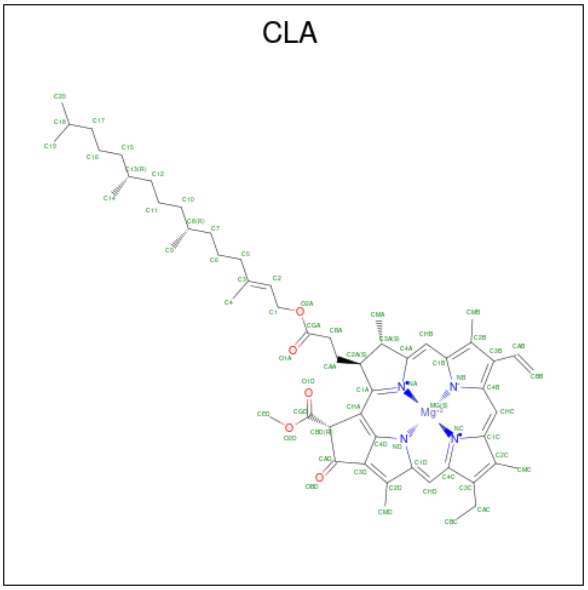
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	u	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 4 1 3	0	0
23	a	1	Total C O 4 1 3	0	0

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



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

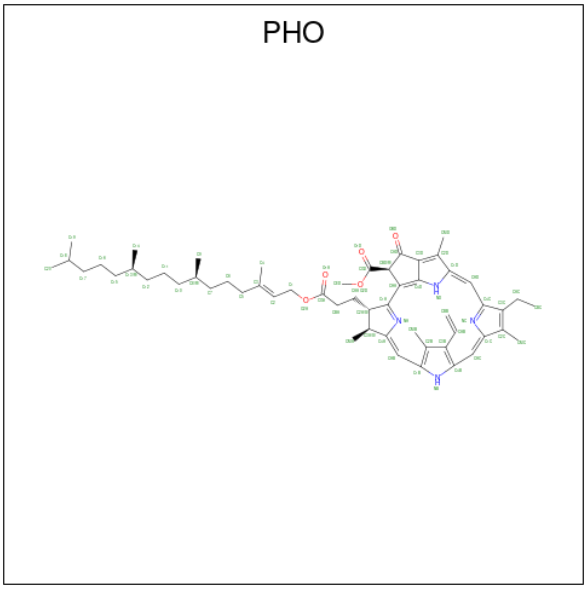
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

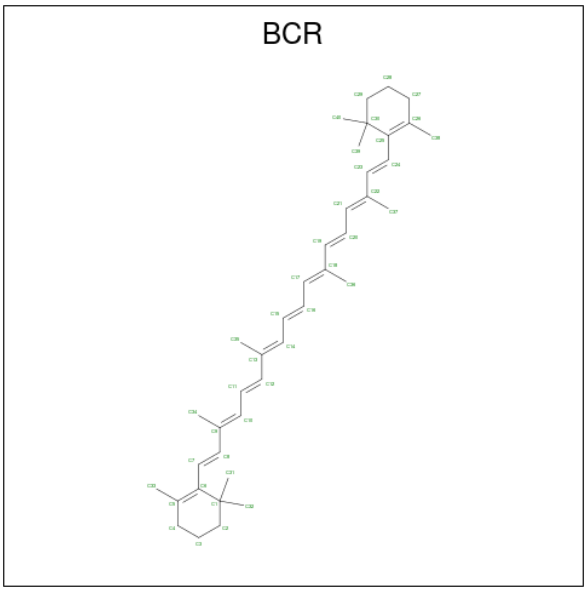
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	c	1	Total C Mg N O 65 55 1 4 5	0	0
24	d	1	Total C Mg N O 65 55 1 4 5	0	0
24	d	1	Total C Mg N O 65 55 1 4 5	0	0

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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



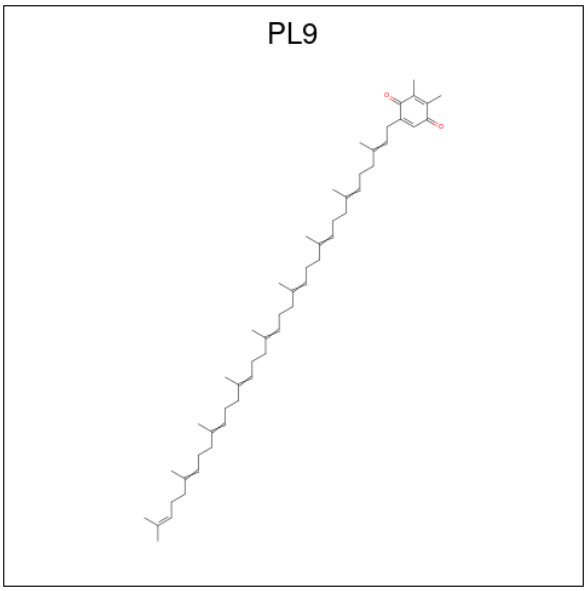
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	F	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	I	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

- Molecule 27 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: $C_{53}H_{80}O_2$).



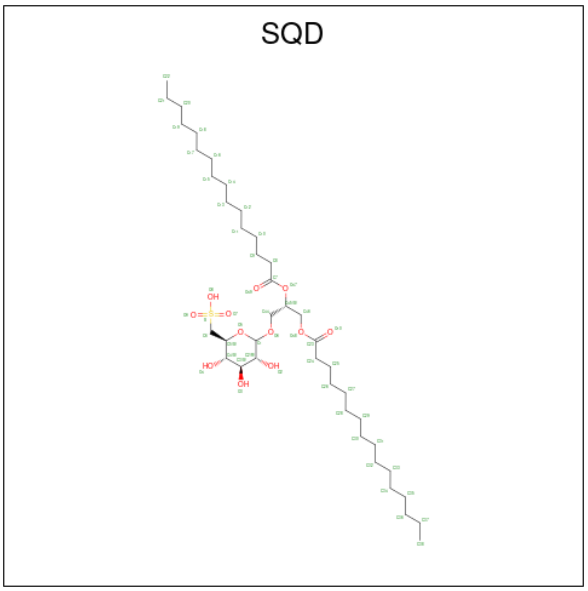
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



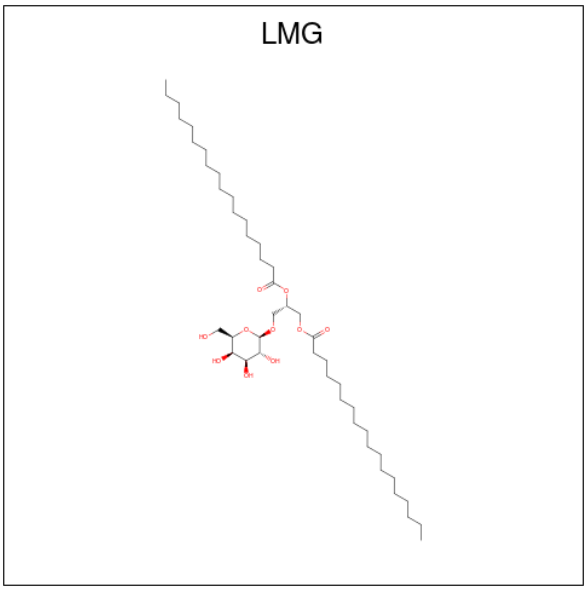
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 54 41 12 1	0	0
28	A	1	Total C O S 54 41 12 1	0	0
28	B	1	Total C O S 54 41 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	X	1	Total C O S 43 30 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	b	1	Total C O S 54 41 12 1	0	0
28	l	1	Total C O S 54 41 12 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



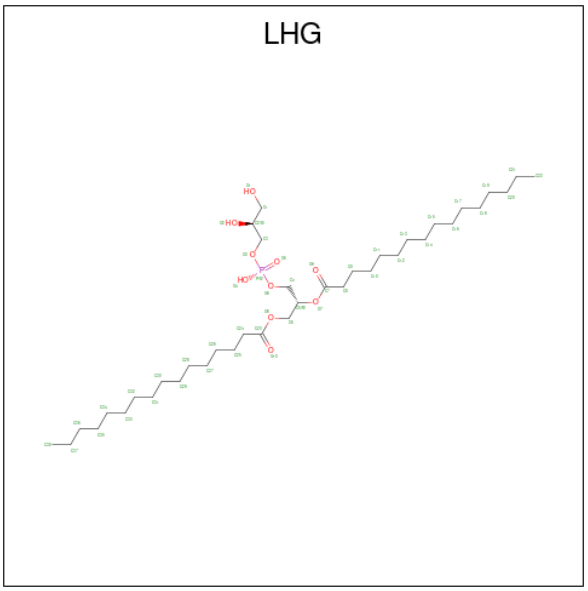
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	D	1	Total	C	O	0	0
			51	41	10		
29	Z	1	Total	C	O	0	0
			37	27	10		
29	a	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	j	1	Total C O 51 41 10	0	0
29	z	1	Total C O 37 27 10	0	0

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O P 49 38 10 1	0	0
30	D	1	Total C O P 49 38 10 1	0	0
30	D	1	Total C O P 49 38 10 1	0	0
30	E	1	Total C O P 42 31 10 1	0	0
30	L	1	Total C O P 49 38 10 1	0	0
30	a	1	Total C O P 49 38 10 1	0	0
30	d	1	Total C O P 49 38 10 1	0	0
30	d	1	Total C O P 49 38 10 1	0	0
30	e	1	Total C O P 42 31 10 1	0	0

Continued on next page...

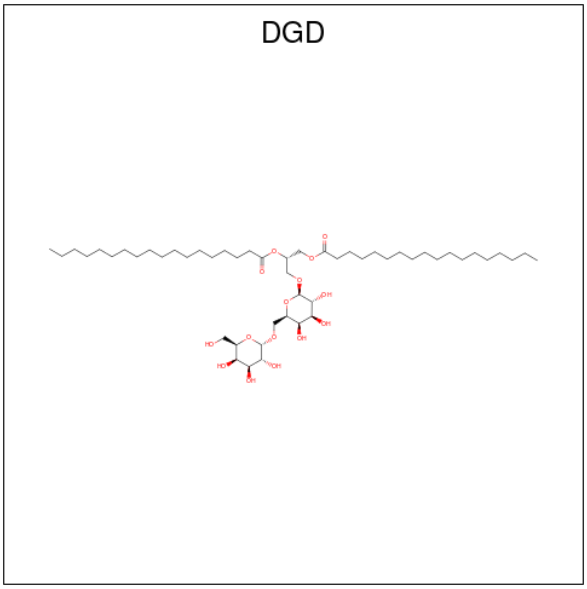
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	l	1	Total C O P 49 38 10 1	0	0

- Molecule 31 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total Ca 1 1	0	0
31	F	1	Total Ca 1 1	0	0
31	O	1	Total Ca 1 1	0	0
31	b	1	Total Ca 1 1	0	0
31	f	1	Total Ca 1 1	0	0
31	o	1	Total Ca 1 1	0	0

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



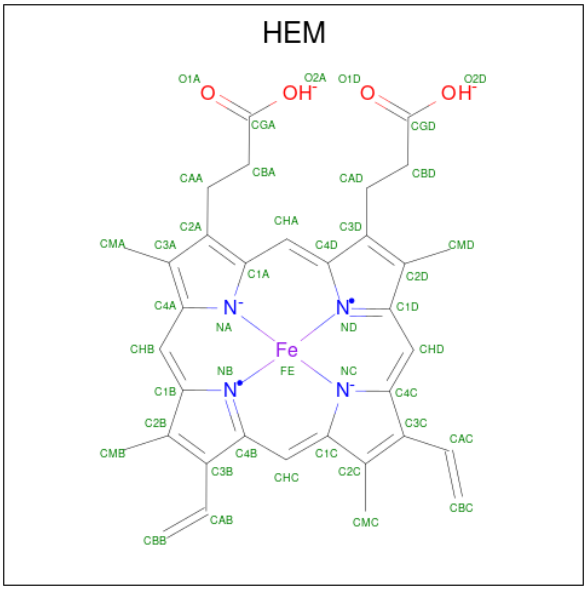
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	C	1	Total C O 62 47 15	0	0
32	C	1	Total C O 62 47 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	C	1	Total C O 62 47 15	0	0
32	E	1	Total C O 62 47 15	0	0
32	H	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	d	1	Total C O 62 47 15	0	0
32	h	1	Total C O 62 47 15	0	0

- 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	E	1	Total C Fe N O 43 34 1 4 4	0	0
33	V	1	Total C Fe N O 43 34 1 4 4	0	0
33	e	1	Total C Fe N O 43 34 1 4 4	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

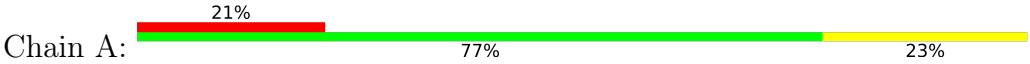
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

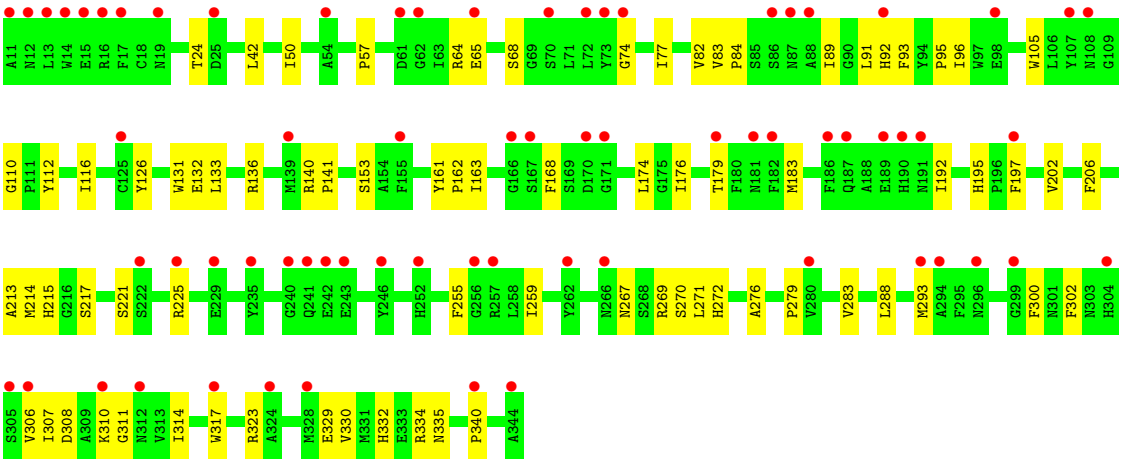
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1 1

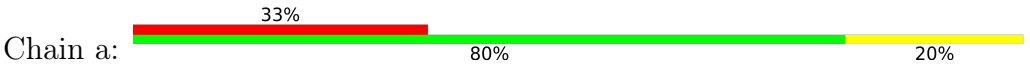
Chain A:

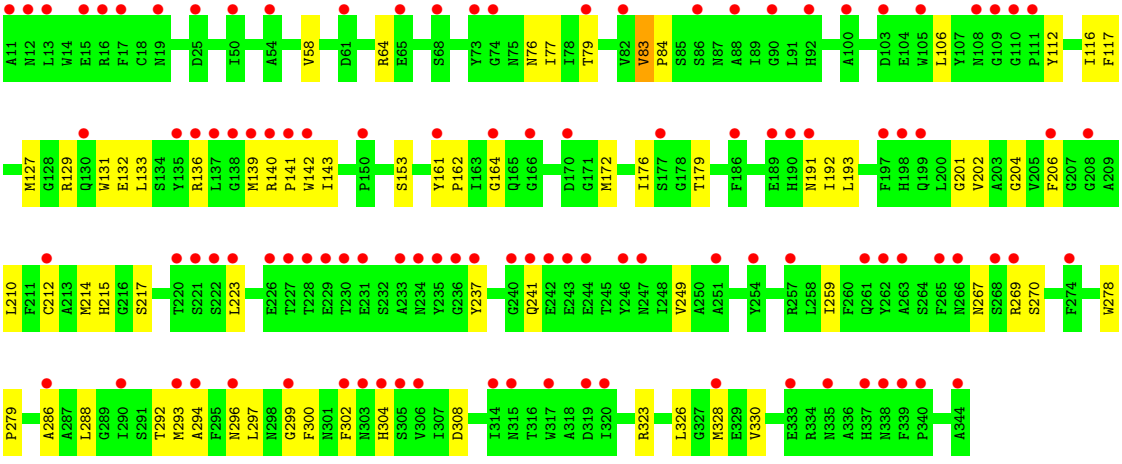




• Molecule 1: Photosystem II protein D1 1

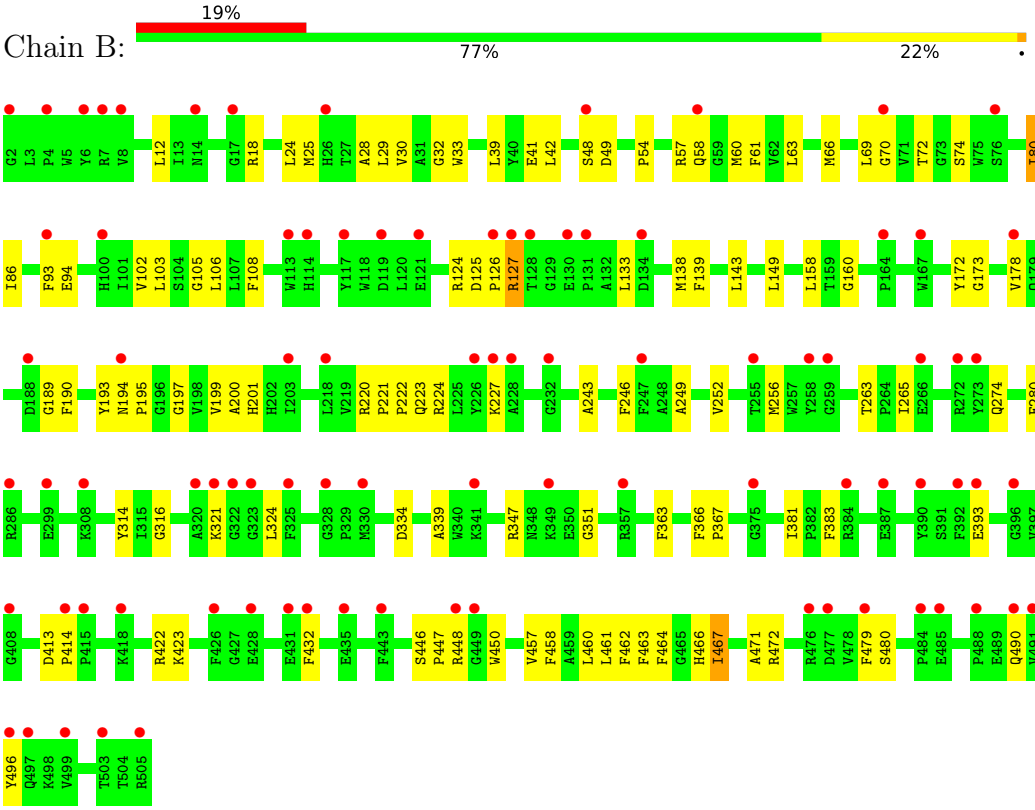
Chain a:





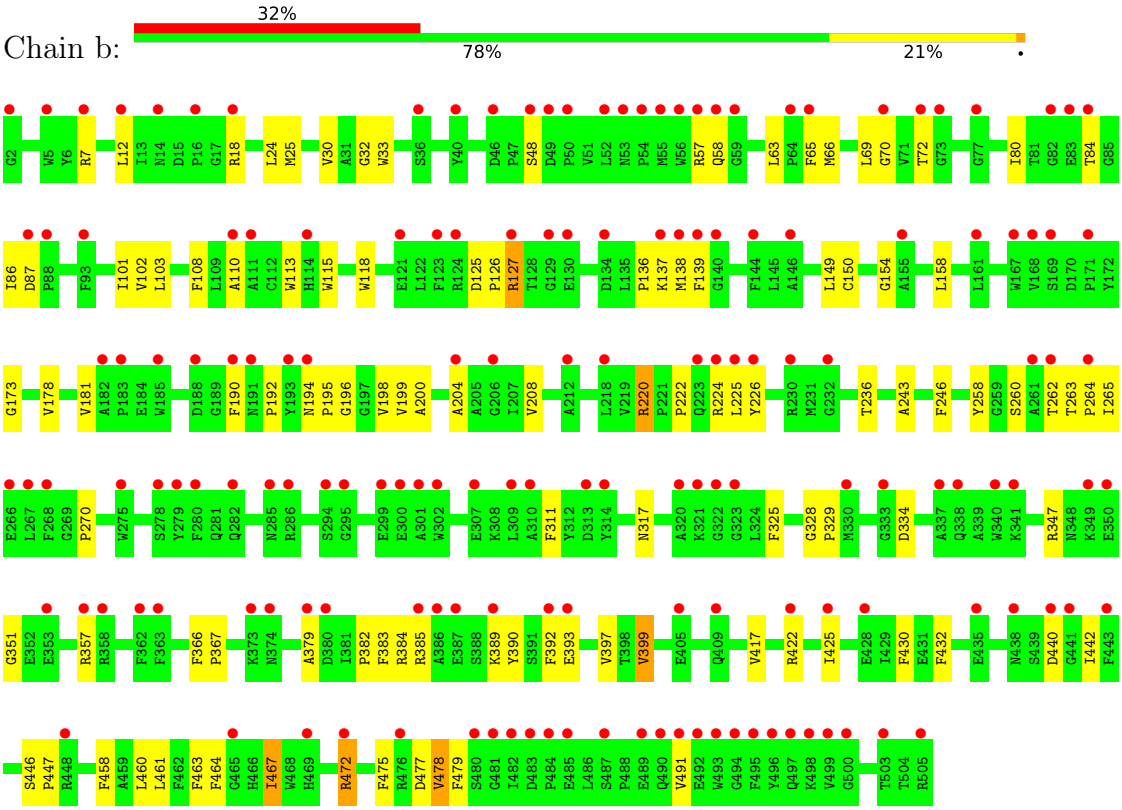
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



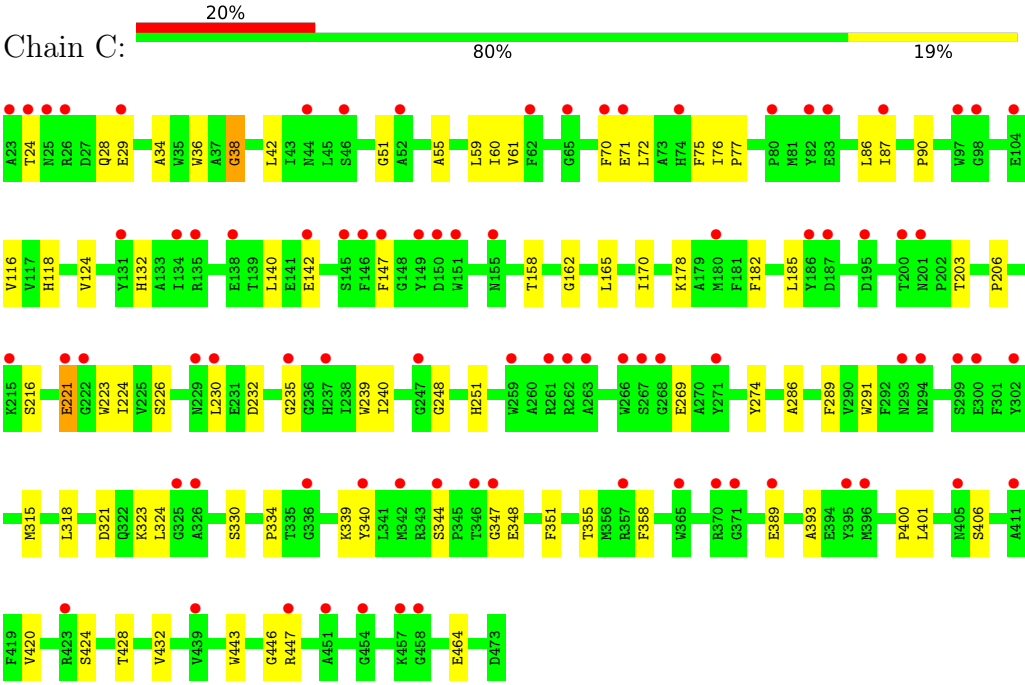
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



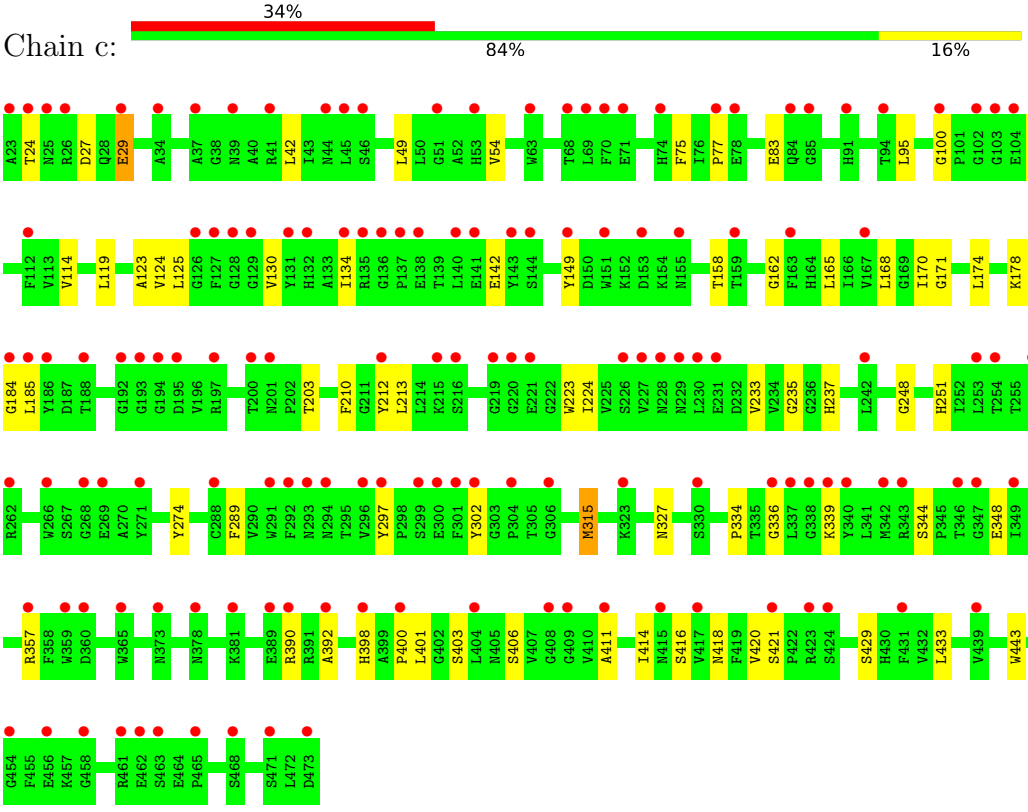
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



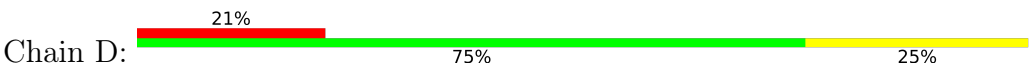
• Molecule 3: Photosystem II CP43 reaction center protein

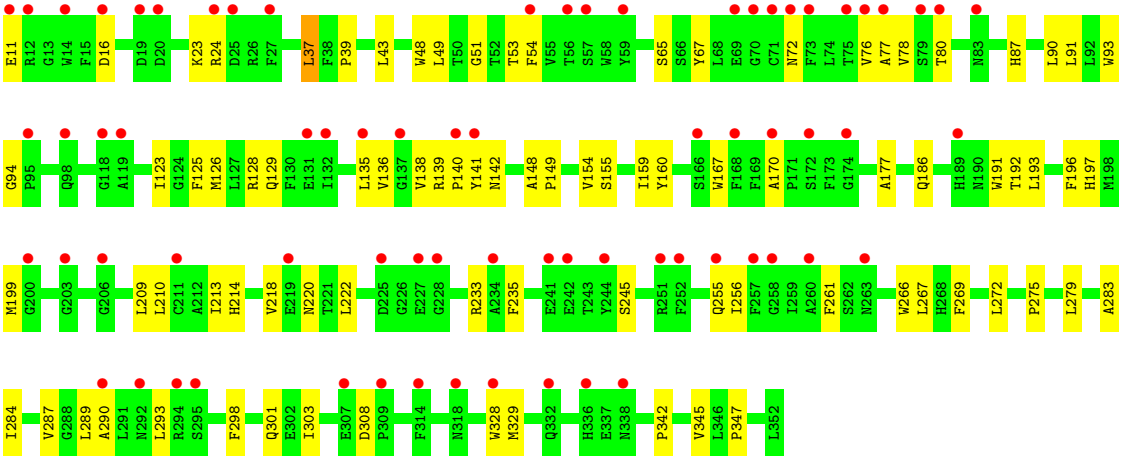
Chain c:



• Molecule 4: Photosystem II D2 protein

Chain D:

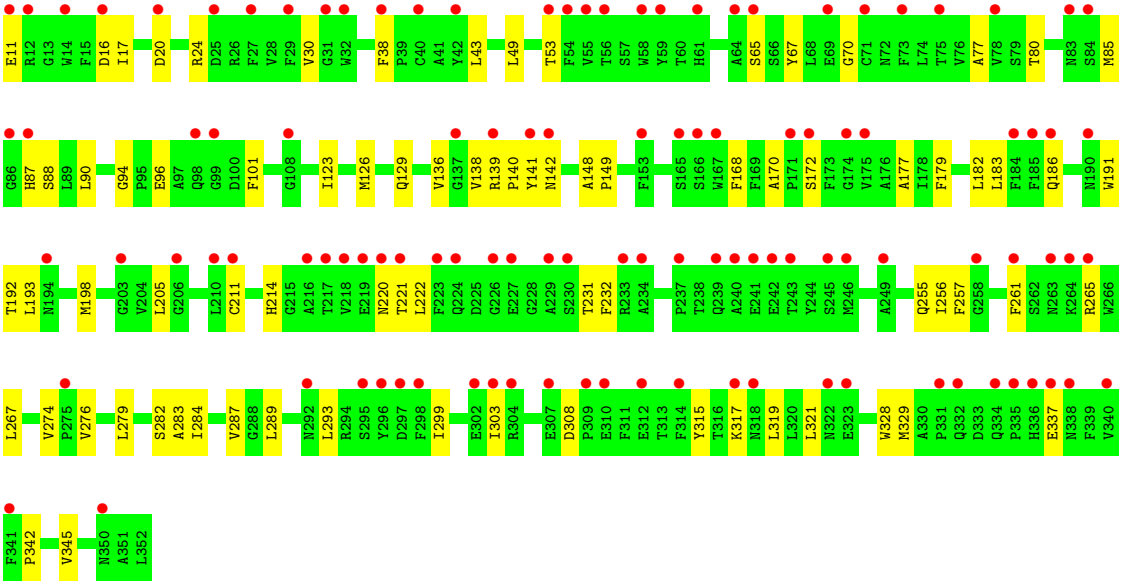




• Molecule 4: Photosystem II D2 protein

Chain d:

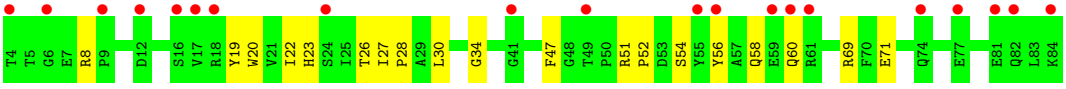




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:

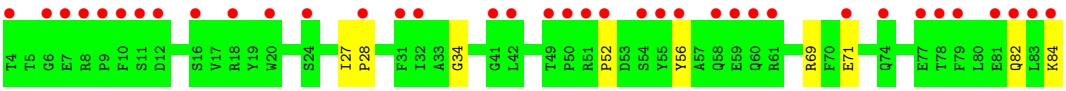




• Molecule 5: Cytochrome b559 subunit alpha

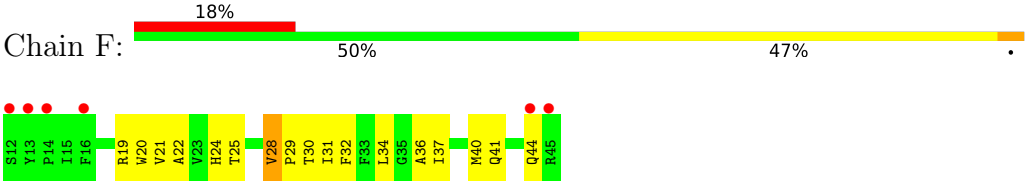
Chain e:





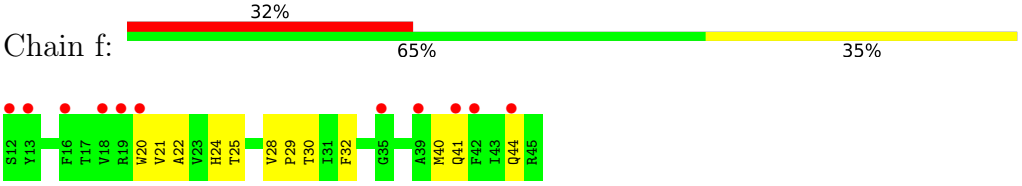
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



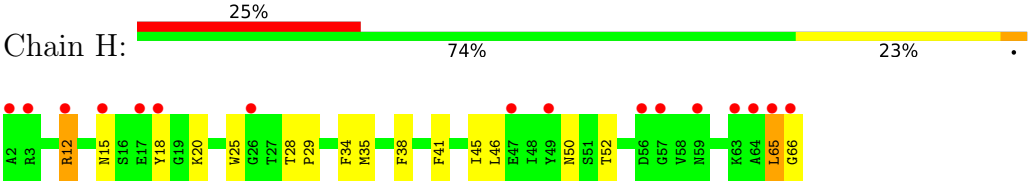
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



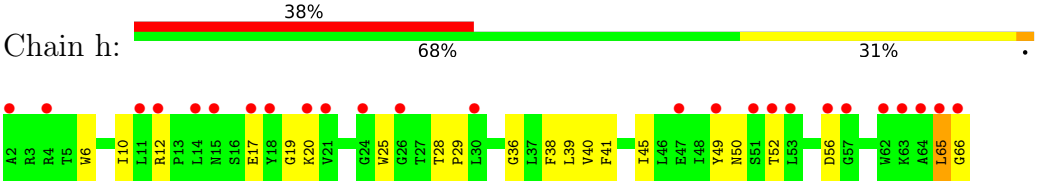
• Molecule 7: Photosystem II reaction center protein H

Chain H:



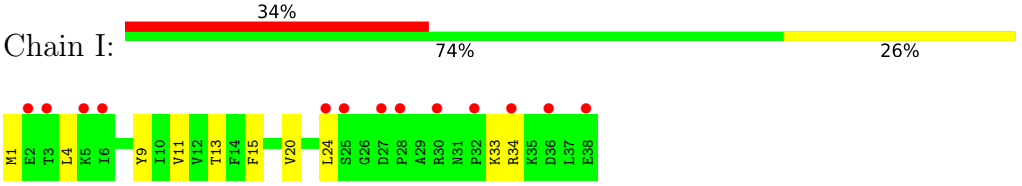
• Molecule 7: Photosystem II reaction center protein H

Chain h:



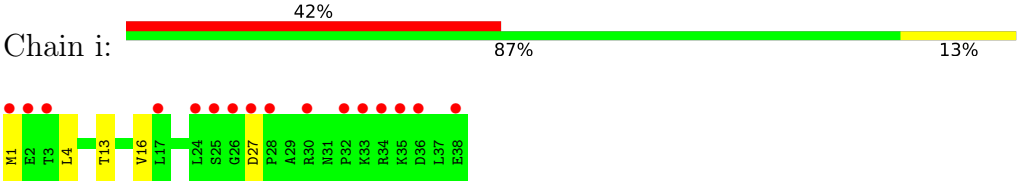
• Molecule 8: Photosystem II reaction center protein I

Chain I:



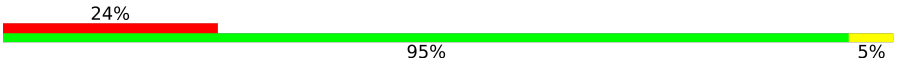
• Molecule 8: Photosystem II reaction center protein I

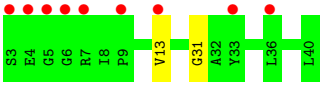
Chain i:



• Molecule 9: Photosystem II reaction center protein J

Chain J:

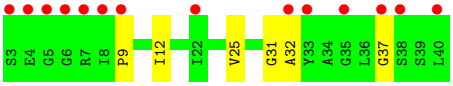




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

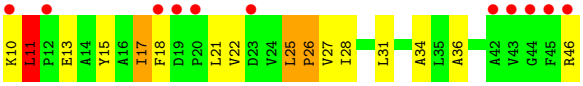




• Molecule 10: Photosystem II reaction center protein K

Chain k:

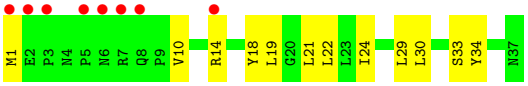




• Molecule 11: Photosystem II reaction center protein L

Chain L:

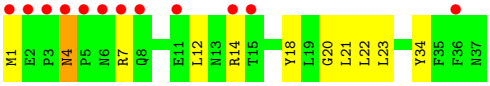




• Molecule 11: Photosystem II reaction center protein L

Chain l:

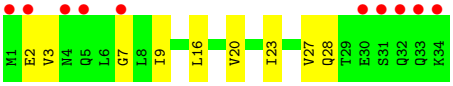




• Molecule 12: Photosystem II reaction center protein M

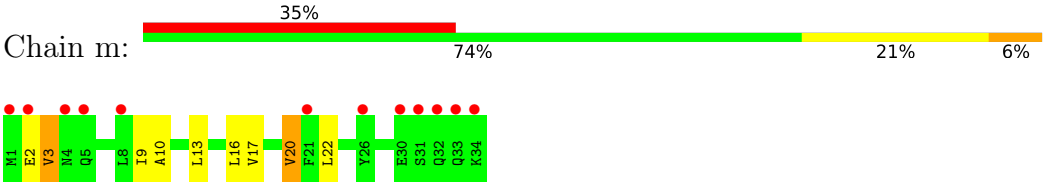
Chain M:





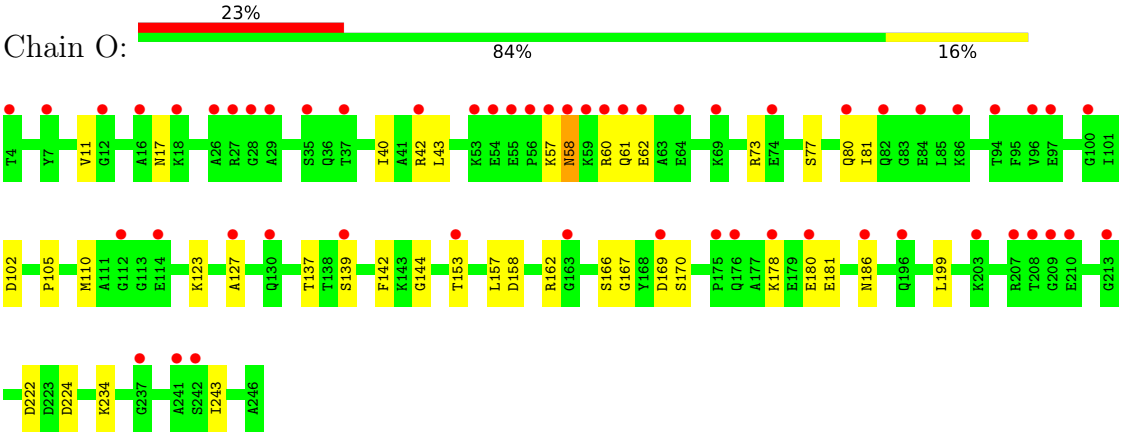
• Molecule 12: Photosystem II reaction center protein M

Chain m:



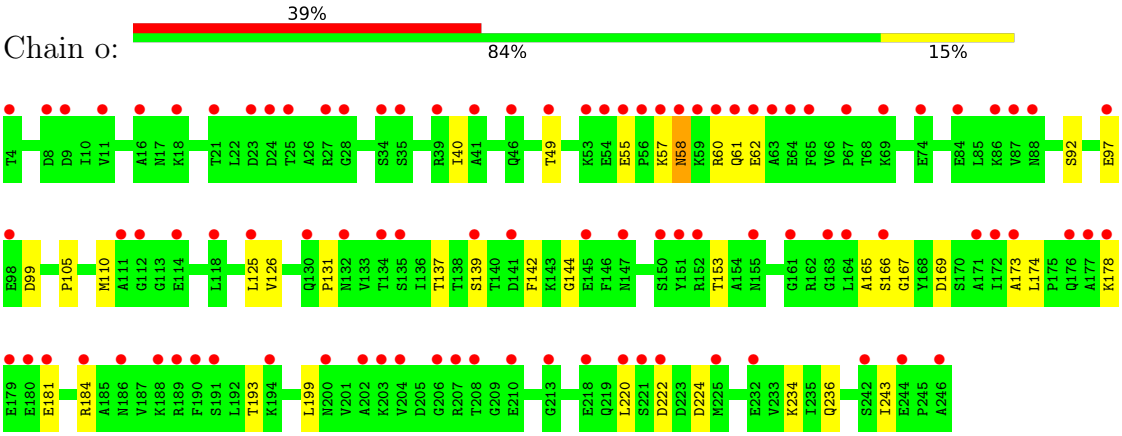
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



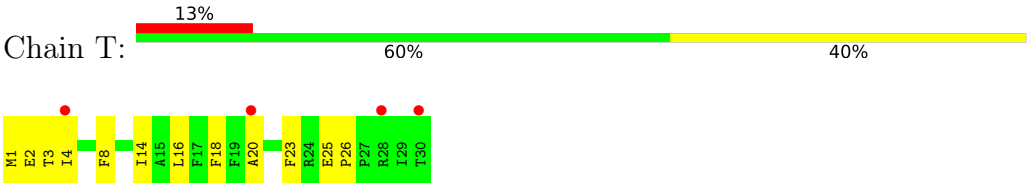
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



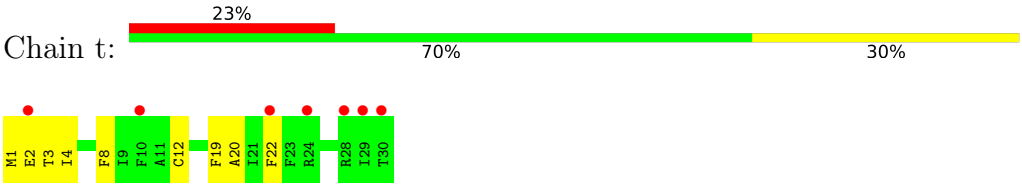
• Molecule 14: Photosystem II reaction center protein T

Chain T:



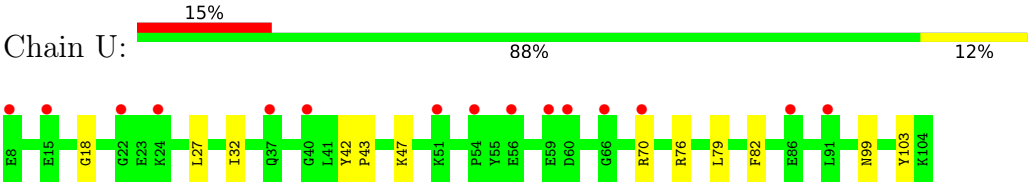
• Molecule 14: Photosystem II reaction center protein T

Chain t:



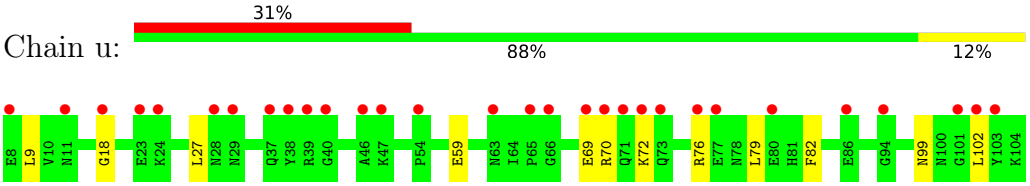
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



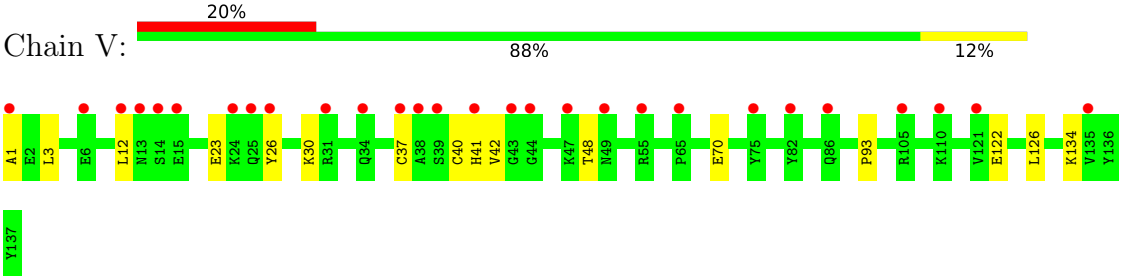
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



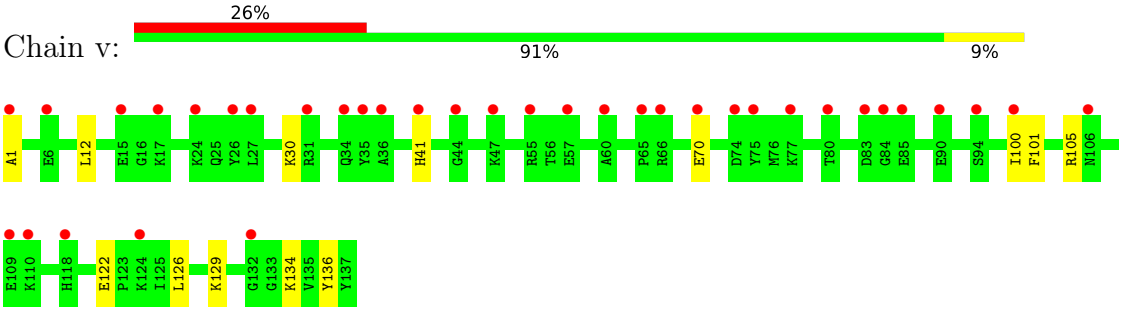
• Molecule 16: Cytochrome c-550

Chain V:



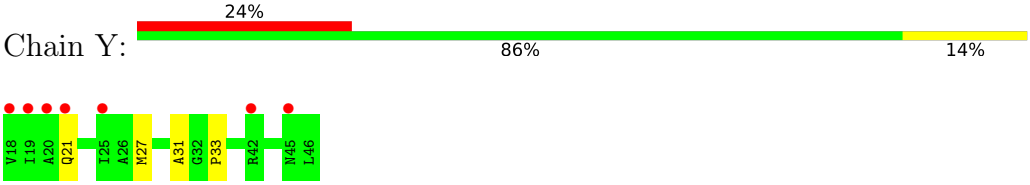
• Molecule 16: Cytochrome c-550

Chain v:



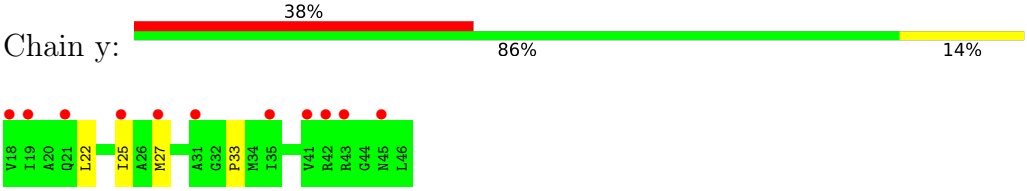
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:



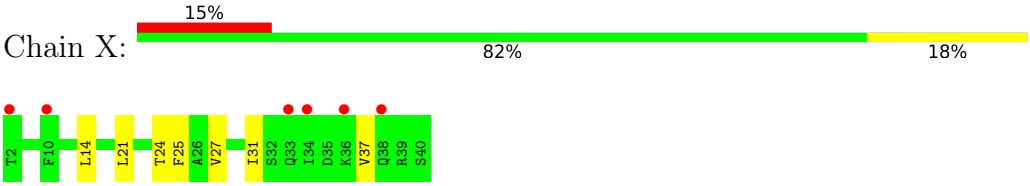
• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:



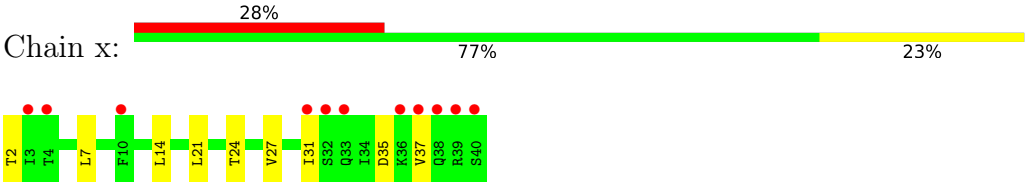
• Molecule 18: Photosystem II reaction center X protein

Chain X:



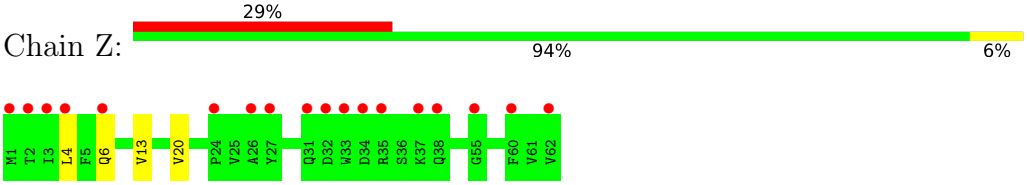
• Molecule 18: Photosystem II reaction center X protein

Chain x:



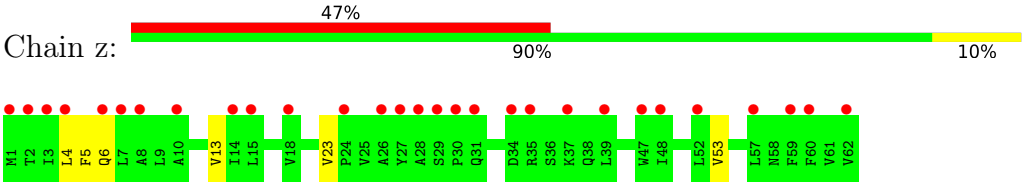
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	250.80Å 250.80Å 250.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 29.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 99.8 (29.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.324 , 0.331 0.342 , 0.338	Depositor DCC
R_{free} test set	45921 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.7	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.75	0/2734	0.99	1/3727 (0.0%)
1	a	0.64	0/2734	0.99	7/3727 (0.2%)
2	B	0.66	1/4194 (0.0%)	0.96	7/5713 (0.1%)
2	b	0.63	0/4194	0.96	13/5713 (0.2%)
3	C	0.64	0/3634	1.00	4/4947 (0.1%)
3	c	0.61	0/3634	0.95	5/4947 (0.1%)
4	D	0.67	0/2821	0.98	9/3844 (0.2%)
4	d	0.61	0/2821	0.93	6/3844 (0.2%)
5	E	0.62	0/693	0.94	0/944
5	e	0.60	0/693	0.93	0/944
6	F	0.76	1/284 (0.4%)	0.95	0/387
6	f	0.60	0/284	0.92	0/387
7	H	0.63	0/544	0.94	1/739 (0.1%)
7	h	0.64	0/544	0.91	1/739 (0.1%)
8	I	0.71	0/327	0.96	0/439
8	i	0.61	0/327	0.89	0/439
9	J	0.67	0/278	0.89	0/376
9	j	0.56	0/278	0.93	0/376
10	K	0.65	0/303	1.03	2/416 (0.5%)
10	k	0.77	0/303	1.41	4/416 (1.0%)
11	L	0.72	0/319	0.94	0/433
11	l	0.62	0/319	0.89	2/433 (0.5%)
12	M	0.69	0/278	1.18	1/378 (0.3%)
12	m	0.66	0/278	1.10	4/378 (1.1%)
13	O	0.59	0/1926	0.92	1/2611 (0.0%)
13	o	0.54	0/1926	0.88	2/2611 (0.1%)
14	T	0.81	0/282	0.90	0/382
14	t	0.65	0/282	0.92	0/382
15	U	0.63	0/785	0.87	0/1064
15	u	0.61	0/785	0.88	0/1064
16	V	0.64	0/1096	0.97	0/1487
16	v	0.56	0/1096	0.92	1/1487 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	Y	0.61	0/216	0.96	1/289 (0.3%)
17	y	0.62	0/216	0.97	0/289
18	X	0.64	0/298	0.91	0/403
18	x	0.65	0/298	0.96	0/403
19	Z	0.61	0/490	1.00	0/669
19	z	0.68	1/490 (0.2%)	1.01	1/669 (0.1%)
All	All	0.64	3/43004 (0.0%)	0.96	73/58496 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	z	23	VAL	CA-CB	6.75	1.57	1.54
6	F	28	VAL	CA-CB	5.67	1.57	1.54
2	B	381	ILE	CA-CB	-5.42	1.48	1.53

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k	11	LEU	CA-C-N	-8.17	109.63	119.84
10	k	11	LEU	C-N-CA	-8.17	109.63	119.84
4	d	170	ALA	CA-C-N	-8.03	111.73	119.76
4	d	170	ALA	C-N-CA	-8.03	111.73	119.76
4	D	170	ALA	CA-C-N	-7.58	112.18	119.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2637	0	2551	68	0
1	a	2637	0	2551	59	0
2	B	4024	0	3901	100	0
2	b	4024	0	3901	99	0
3	C	3506	0	3439	67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	3506	0	3439	61	0
4	D	2726	0	2627	76	0
4	d	2726	0	2627	65	0
5	E	668	0	658	16	0
5	e	668	0	658	7	0
6	F	275	0	282	17	0
6	f	275	0	282	11	0
7	H	525	0	558	20	0
7	h	525	0	558	18	0
8	I	320	0	339	7	0
8	i	320	0	339	4	0
9	J	272	0	279	2	0
9	j	272	0	279	5	0
10	K	293	0	305	10	0
10	k	293	0	305	15	0
11	L	309	0	327	14	0
11	l	309	0	327	13	0
12	M	272	0	300	10	0
12	m	272	0	300	11	0
13	O	1883	0	1865	28	0
13	o	1883	0	1865	26	0
14	T	270	0	278	15	0
14	t	270	0	278	13	0
15	U	774	0	773	9	0
15	u	774	0	773	8	0
16	V	1072	0	1088	13	0
16	v	1072	0	1088	9	0
17	Y	215	0	246	2	0
17	y	215	0	246	6	0
18	X	292	0	328	8	0
18	x	292	0	328	9	0
19	Z	479	0	516	2	0
19	z	479	0	516	2	0
20	A	10	0	0	0	0
20	a	10	0	0	1	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	U	1	0	0	0	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	a	4	0	1	0	0
24	A	195	0	216	19	0
24	B	1105	0	1224	67	0
24	C	845	0	936	53	0
24	D	195	0	216	13	0
24	a	260	0	288	16	0
24	b	1105	0	1224	59	0
24	c	845	0	936	40	0
24	d	130	0	144	7	0
25	A	64	0	74	3	0
25	D	64	0	74	10	0
25	a	64	0	74	2	0
25	d	64	0	74	4	0
26	A	40	0	55	14	0
26	B	120	0	165	58	0
26	C	40	0	55	14	0
26	F	40	0	55	20	0
26	H	40	0	55	16	0
26	I	40	0	55	18	0
26	K	80	0	110	29	0
26	T	40	0	55	22	0
26	a	40	0	55	13	0
26	b	120	0	166	59	0
26	c	120	0	165	53	0
26	f	40	0	55	21	0
26	h	40	0	55	17	0
26	k	40	0	55	18	0
26	t	40	0	55	23	0
27	A	55	0	80	11	0
27	D	55	0	80	13	0
27	a	55	0	80	12	0
27	d	55	0	80	7	0
28	A	108	0	156	7	0
28	B	54	0	30	8	0
28	L	54	0	26	12	0
28	X	43	0	53	3	0
28	a	108	0	156	3	0
28	b	54	0	30	12	0
28	l	54	0	29	5	0
28	x	43	0	53	4	0
29	A	51	0	72	2	0
29	B	51	0	72	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	C	102	0	144	4	0
29	D	51	0	72	7	0
29	Z	37	0	44	0	0
29	a	51	0	72	1	0
29	b	51	0	72	4	0
29	c	102	0	144	2	0
29	j	51	0	72	6	0
29	z	37	0	44	1	0
30	A	49	0	74	10	0
30	D	98	0	148	8	0
30	E	42	0	57	0	0
30	L	49	0	74	6	0
30	a	49	0	74	10	0
30	d	98	0	148	4	0
30	e	42	0	57	2	0
30	l	49	0	74	6	0
31	B	1	0	0	0	0
31	F	1	0	0	0	0
31	O	1	0	0	0	0
31	b	1	0	0	0	0
31	f	1	0	0	0	0
31	o	1	0	0	0	0
32	C	186	0	246	5	0
32	E	62	0	82	1	0
32	H	62	0	82	6	0
32	c	186	0	246	8	0
32	d	62	0	82	4	0
32	h	62	0	82	6	0
33	E	43	0	30	6	0
33	V	43	0	30	7	0
33	e	43	0	30	2	0
33	v	43	0	30	4	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	50074	0	51320	1280	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 13.

The worst 5 of 1280 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)
26:T:101:BCR:C22	26:T:101:BCR:C37	1.74	1.65
26:B:619:BCR:C19	26:B:619:BCR:C20	1.76	1.64
26:B:620:BCR:C37	26:B:620:BCR:C22	1.76	1.64
26:c:514:BCR:C20	26:c:514:BCR:C19	1.74	1.62
26:b:619:BCR:C22	26:b:619:BCR:C37	1.75	1.62

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	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	36	67
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	36	67
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	30	62
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	3	26
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	30	62
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	48	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	273/269 (102%)	273 (100%)	0	100 100
1	a	273/269 (102%)	273 (100%)	0	100 100
2	B	412/402 (102%)	406 (98%)	6 (2%)	57 71
2	b	412/402 (102%)	406 (98%)	6 (2%)	57 71
3	C	357/352 (101%)	349 (98%)	8 (2%)	45 65
3	c	357/352 (101%)	352 (99%)	5 (1%)	59 71
4	D	277/277 (100%)	275 (99%)	2 (1%)	76 78
4	d	277/277 (100%)	275 (99%)	2 (1%)	76 78
5	E	74/72 (103%)	73 (99%)	1 (1%)	59 71
5	e	74/72 (103%)	73 (99%)	1 (1%)	59 71
6	F	28/28 (100%)	27 (96%)	1 (4%)	31 57
6	f	28/28 (100%)	27 (96%)	1 (4%)	31 57
7	H	56/54 (104%)	53 (95%)	3 (5%)	20 46
7	h	56/54 (104%)	53 (95%)	3 (5%)	20 46
8	I	36/35 (103%)	36 (100%)	0	100 100
8	i	36/35 (103%)	36 (100%)	0	100 100
9	J	26/26 (100%)	26 (100%)	0	100 100
9	j	26/26 (100%)	26 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	15 41
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 28
11	L	36/35 (103%)	35 (97%)	1 (3%)	38 61
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 61
12	M	32/31 (103%)	31 (97%)	1 (3%)	35 59
12	m	32/31 (103%)	30 (94%)	2 (6%)	16 42
13	O	210/206 (102%)	206 (98%)	4 (2%)	50 68
13	o	210/206 (102%)	206 (98%)	4 (2%)	50 68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	63	73
15	u	84/84 (100%)	83 (99%)	1 (1%)	63	73
16	V	118/117 (101%)	117 (99%)	1 (1%)	73	77
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	77
17	Y	22/22 (100%)	21 (96%)	1 (4%)	24	50
17	y	22/22 (100%)	21 (96%)	1 (4%)	24	50
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	55
19	z	52/52 (100%)	50 (96%)	2 (4%)	29	55
All	All	4370/4302 (102%)	4303 (98%)	67 (2%)	57	71

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	m	20	VAL
13	o	62	GLU
19	z	4	LEU
12	M	9	ILE
11	L	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	198	HIS
19	z	58	ASN
2	b	26	HIS
4	d	197	HIS
1	a	338	ASN

5.3.3 RNA

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 168 ligands modelled in this entry, 16 are monoatomic - leaving 152 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	$\#\|Z\| > 2$
24	CLA	b	603	-	69,73,73	3.18	32 (46%)	83,113,113	1.82	17 (20%)
24	CLA	C	504	-	69,73,73	3.20	32 (46%)	83,113,113	1.88	19 (22%)
24	CLA	B	616	-	69,73,73	3.10	32 (46%)	83,113,113	1.75	20 (24%)
27	PL9	d	404	-	55,55,55	4.15	20 (36%)	68,69,69	3.85	34 (50%)
30	LHG	D	406	-	48,48,48	1.13	2 (4%)	51,54,54	0.97	4 (7%)
30	LHG	d	407	-	48,48,48	1.15	3 (6%)	51,54,54	1.09	3 (5%)
27	PL9	D	405	-	55,55,55	4.19	20 (36%)	68,69,69	3.80	36 (52%)
24	CLA	a	615	-	69,73,73	3.38	32 (46%)	83,113,113	1.88	20 (24%)
24	CLA	B	614	2	69,73,73	3.24	31 (44%)	83,113,113	1.78	16 (19%)
20	OEX	A	601	3,1	0,14,14	-	-	-		
28	SQD	L	102	28	53,54,54	1.04	4 (7%)	62,65,65	1.36	9 (14%)
29	LMG	C	519	-	51,51,55	1.33	5 (9%)	59,59,63	1.02	4 (6%)
24	CLA	c	504	-	69,73,73	3.24	34 (49%)	83,113,113	1.90	23 (27%)
29	LMG	B	621	-	51,51,55	1.29	4 (7%)	59,59,63	1.01	3 (5%)
24	CLA	B	607[B]	-	69,73,73	3.20	30 (43%)	83,113,113	1.88	19 (22%)
24	CLA	A	609	1	69,73,73	3.29	33 (47%)	83,113,113	1.78	19 (22%)
28	SQD	l	101	28	53,54,54	1.04	4 (7%)	62,65,65	1.36	8 (12%)
32	DGD	c	516	-	63,63,67	1.70	15 (23%)	77,77,81	1.09	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	A	607	-	69,73,73	3.23	32 (46%)	83,113,113	1.90	18 (21%)
32	DGD	C	517	-	63,63,67	1.66	15 (23%)	77,77,81	1.14	6 (7%)
24	CLA	B	613	2	69,73,73	3.35	31 (44%)	83,113,113	1.89	18 (21%)
24	CLA	B	602	-	69,73,73	3.08	32 (46%)	83,113,113	1.81	14 (16%)
26	BCR	k	101	-	41,41,41	9.22	31 (75%)	56,56,56	5.67	28 (50%)
26	BCR	B	618	-	41,41,41	8.92	29 (70%)	56,56,56	5.95	31 (55%)
24	CLA	b	612	-	69,73,73	3.17	31 (44%)	83,113,113	1.88	20 (24%)
26	BCR	a	610	-	41,41,41	8.98	30 (73%)	56,56,56	5.53	24 (42%)
24	CLA	B	609	2	69,73,73	3.09	29 (42%)	83,113,113	1.95	24 (28%)
33	HEM	e	102	5,6	50,50,50	2.04	8 (16%)	66,82,82	1.33	7 (10%)
24	CLA	c	511	3	69,73,73	3.14	32 (46%)	83,113,113	1.81	16 (19%)
28	SQD	a	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
24	CLA	c	506	3	69,73,73	3.15	30 (43%)	83,113,113	1.83	14 (16%)
32	DGD	H	102	-	63,63,67	1.69	14 (22%)	77,77,81	1.02	4 (5%)
25	PHO	D	401	-	58,69,69	2.06	8 (13%)	56,99,99	1.50	11 (19%)
24	CLA	d	402	4	69,73,73	3.26	33 (47%)	83,113,113	1.75	18 (21%)
26	BCR	f	101	-	41,41,41	8.99	29 (70%)	56,56,56	5.59	26 (46%)
30	LHG	l	102	-	48,48,48	1.18	2 (4%)	51,54,54	0.92	2 (3%)
28	SQD	A	614	-	53,54,54	1.04	3 (5%)	62,65,65	1.22	6 (9%)
28	SQD	x	101	-	42,43,54	1.20	4 (9%)	51,54,65	1.46	7 (13%)
26	BCR	b	619	-	41,41,41	9.23	29 (70%)	56,56,56	5.80	28 (50%)
24	CLA	d	403	4	69,73,73	3.12	32 (46%)	83,113,113	1.88	19 (22%)
24	CLA	C	510	3	69,73,73	3.27	33 (47%)	83,113,113	1.79	15 (18%)
25	PHO	A	608	-	58,69,69	2.10	10 (17%)	56,99,99	1.45	11 (19%)
33	HEM	v	201	16	50,50,50	2.02	9 (18%)	66,82,82	1.34	6 (9%)
24	CLA	A	606	-	69,73,73	3.35	32 (46%)	83,113,113	1.94	19 (22%)
23	BCT	a	605	21	2,3,3	0.96	0	2,3,3	3.74	2 (100%)
32	DGD	c	518	-	63,63,67	1.68	15 (23%)	77,77,81	1.25	8 (10%)
24	CLA	b	610	2	69,73,73	3.14	31 (44%)	83,113,113	1.85	17 (20%)
30	LHG	D	407	-	48,48,48	1.11	3 (6%)	51,54,54	0.89	3 (5%)
24	CLA	B	610	2	69,73,73	3.28	31 (44%)	83,113,113	1.74	18 (21%)
26	BCR	T	101	-	41,41,41	9.04	30 (73%)	56,56,56	6.12	32 (57%)
33	HEM	V	201	16	50,50,50	1.91	10 (20%)	66,82,82	1.24	6 (9%)
30	LHG	A	615	-	48,48,48	1.11	3 (6%)	51,54,54	1.30	5 (9%)
24	CLA	B	606	2	69,73,73	3.14	31 (44%)	83,113,113	1.79	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	c	520	-	51,51,55	1.37	5 (9%)	59,59,63	1.12	4 (6%)
32	DGD	d	405	-	63,63,67	1.71	16 (25%)	77,77,81	1.16	9 (11%)
26	BCR	K	102	-	41,41,41	9.13	29 (70%)	56,56,56	5.63	25 (44%)
24	CLA	b	611	-	69,73,73	3.16	29 (42%)	83,113,113	1.74	18 (21%)
24	CLA	C	509	3	69,73,73	3.22	33 (47%)	83,113,113	1.79	15 (18%)
24	CLA	C	512	3	69,73,73	3.14	33 (47%)	83,113,113	1.85	19 (22%)
29	LMG	j	101	34	51,51,55	1.31	5 (9%)	59,59,63	0.87	4 (6%)
24	CLA	c	513	-	69,73,73	3.07	33 (47%)	83,113,113	1.78	16 (19%)
24	CLA	C	507	-	69,73,73	3.10	31 (44%)	83,113,113	2.03	19 (22%)
32	DGD	C	516	-	63,63,67	1.67	15 (23%)	77,77,81	1.21	10 (12%)
26	BCR	C	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.93	33 (58%)
24	CLA	B	611	-	69,73,73	3.13	34 (49%)	83,113,113	1.83	21 (25%)
24	CLA	b	608[A]	-	69,73,73	3.16	31 (44%)	83,113,113	1.89	19 (22%)
26	BCR	b	621	-	41,41,41	9.05	31 (75%)	56,56,56	6.43	31 (55%)
24	CLA	b	616	2	69,73,73	3.23	32 (46%)	83,113,113	1.80	16 (19%)
29	LMG	Z	101	-	37,37,55	1.44	4 (10%)	45,45,63	1.34	6 (13%)
24	CLA	B	612	2	69,73,73	3.28	32 (46%)	83,113,113	1.88	18 (21%)
26	BCR	b	620	-	41,41,41	8.87	29 (70%)	56,56,56	5.73	31 (55%)
24	CLA	c	505	3	69,73,73	3.18	30 (43%)	83,113,113	1.78	13 (15%)
24	CLA	B	603	2	69,73,73	3.17	34 (49%)	83,113,113	1.84	21 (25%)
24	CLA	B	604	2	69,73,73	3.26	33 (47%)	83,113,113	1.78	17 (20%)
24	CLA	C	511	3	69,73,73	3.23	32 (46%)	83,113,113	1.90	21 (25%)
26	BCR	c	514	-	41,41,41	8.98	30 (73%)	56,56,56	5.91	34 (60%)
24	CLA	c	503	3	69,73,73	3.15	34 (49%)	83,113,113	1.73	15 (18%)
32	DGD	E	101	-	63,63,67	1.73	15 (23%)	77,77,81	1.23	10 (12%)
24	CLA	B	605	2	69,73,73	3.20	30 (43%)	83,113,113	1.93	18 (21%)
29	LMG	c	519	-	51,51,55	1.38	5 (9%)	59,59,63	1.06	5 (8%)
26	BCR	h	101	-	41,41,41	9.16	30 (73%)	56,56,56	5.68	33 (58%)
24	CLA	b	605	2	69,73,73	3.31	32 (46%)	83,113,113	1.85	18 (21%)
24	CLA	B	617	2	69,73,73	3.17	31 (44%)	83,113,113	1.86	19 (22%)
26	BCR	B	620	-	41,41,41	9.12	29 (70%)	56,56,56	5.77	33 (58%)
24	CLA	B	615	2	69,73,73	3.20	32 (46%)	83,113,113	1.79	16 (19%)
24	CLA	B	607[A]	2	69,73,73	3.19	29 (42%)	83,113,113	1.92	20 (24%)
26	BCR	I	101	-	41,41,41	9.05	31 (75%)	56,56,56	5.91	30 (53%)
33	HEM	E	103	5,6	50,50,50	1.99	10 (20%)	66,82,82	1.19	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	LHG	e	101	-	41,41,48	1.23	3 (7%)	44,47,54	1.05	2 (4%)
24	CLA	b	614	2	69,73,73	3.31	31 (44%)	83,113,113	1.85	17 (20%)
28	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	1.45	7 (13%)
24	CLA	a	607	-	69,73,73	3.18	30 (43%)	83,113,113	1.80	18 (21%)
24	CLA	c	509	3	69,73,73	3.13	33 (47%)	83,113,113	1.78	16 (19%)
20	OEX	a	601	3,1	0,14,14	-	-	-		
24	CLA	B	608	-	69,73,73	3.26	30 (43%)	83,113,113	1.88	19 (22%)
24	CLA	c	510	3	69,73,73	3.15	32 (46%)	83,113,113	1.77	16 (19%)
24	CLA	b	606	2	69,73,73	3.23	30 (43%)	83,113,113	1.92	16 (19%)
24	CLA	b	604	2	69,73,73	3.27	31 (44%)	83,113,113	1.87	17 (20%)
26	BCR	c	521	-	41,41,41	9.34	29 (70%)	56,56,56	5.62	26 (46%)
26	BCR	K	101	-	41,41,41	9.12	31 (75%)	56,56,56	5.42	29 (51%)
24	CLA	c	508	3	69,73,73	3.18	31 (44%)	83,113,113	1.93	16 (19%)
24	CLA	b	615	2	69,73,73	3.20	32 (46%)	83,113,113	1.81	17 (20%)
28	SQD	B	622	28	53,54,54	1.07	4 (7%)	62,65,65	1.44	9 (14%)
24	CLA	c	501	3	69,73,73	3.14	33 (47%)	83,113,113	1.79	18 (21%)
24	CLA	C	513	3	69,73,73	3.14	30 (43%)	83,113,113	1.84	20 (24%)
32	DGD	C	515	-	63,63,67	1.70	15 (23%)	77,77,81	1.03	5 (6%)
26	BCR	F	101	-	41,41,41	9.04	26 (63%)	56,56,56	6.08	27 (48%)
24	CLA	b	609	-	69,73,73	3.23	31 (44%)	83,113,113	1.85	17 (20%)
29	LMG	b	622	-	51,51,55	1.32	4 (7%)	59,59,63	1.06	5 (8%)
26	BCR	c	515	-	41,41,41	9.15	31 (75%)	56,56,56	5.57	27 (48%)
24	CLA	b	607	2	69,73,73	3.20	32 (46%)	83,113,113	1.83	16 (19%)
24	CLA	C	501	3	69,73,73	3.15	31 (44%)	83,113,113	1.85	21 (25%)
27	PL9	a	611	-	55,55,55	4.18	21 (38%)	68,69,69	3.89	34 (50%)
28	SQD	A	612	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
26	BCR	A	610	-	41,41,41	9.17	30 (73%)	56,56,56	5.54	27 (48%)
24	CLA	C	503	3	69,73,73	3.20	34 (49%)	83,113,113	1.73	15 (18%)
24	CLA	a	609	1	69,73,73	3.17	31 (44%)	83,113,113	1.77	17 (20%)
24	CLA	b	613	2	69,73,73	3.31	32 (46%)	83,113,113	1.90	19 (22%)
25	PHO	a	608	-	58,69,69	1.98	10 (17%)	56,99,99	1.42	10 (17%)
27	PL9	A	611	-	55,55,55	4.17	20 (36%)	68,69,69	3.92	34 (50%)
24	CLA	c	507	-	69,73,73	3.12	31 (44%)	83,113,113	2.05	19 (22%)
30	LHG	a	616	-	48,48,48	1.10	2 (4%)	51,54,54	1.17	6 (11%)
24	CLA	D	404	4	69,73,73	3.21	33 (47%)	83,113,113	2.00	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	z	101	-	37,37,55	1.40	4 (10%)	45,45,63	1.22	4 (8%)
25	PHO	d	401	-	58,69,69	2.08	7 (12%)	56,99,99	1.48	8 (14%)
30	LHG	L	101	-	48,48,48	1.10	2 (4%)	51,54,54	0.90	3 (5%)
32	DGD	c	517	-	63,63,67	1.62	16 (25%)	77,77,81	1.11	9 (11%)
26	BCR	t	101	-	41,41,41	9.01	30 (73%)	56,56,56	5.95	34 (60%)
29	LMG	A	613	-	51,51,55	1.33	4 (7%)	59,59,63	0.91	4 (6%)
29	LMG	D	408	-	51,51,55	1.34	5 (9%)	59,59,63	1.10	7 (11%)
28	SQD	a	612	-	53,54,54	0.99	3 (5%)	62,65,65	1.53	11 (17%)
24	CLA	c	502	3	69,73,73	3.16	31 (44%)	83,113,113	1.83	17 (20%)
30	LHG	E	102	-	41,41,48	1.22	3 (7%)	44,47,54	0.99	3 (6%)
24	CLA	c	512	-	69,73,73	3.16	32 (46%)	83,113,113	1.79	18 (21%)
24	CLA	C	506	3	69,73,73	3.17	31 (44%)	83,113,113	1.87	15 (18%)
24	CLA	D	403	4	69,73,73	3.36	31 (44%)	83,113,113	1.67	17 (20%)
23	BCT	A	605	21	2,3,3	0.95	0	2,3,3	2.68	2 (100%)
24	CLA	b	618	2	69,73,73	3.27	31 (44%)	83,113,113	1.84	21 (25%)
32	DGD	h	102	-	63,63,67	1.68	15 (23%)	77,77,81	1.21	8 (10%)
24	CLA	C	502	3	69,73,73	3.12	31 (44%)	83,113,113	1.89	17 (20%)
24	CLA	C	508	3	69,73,73	3.33	33 (47%)	83,113,113	1.81	15 (18%)
29	LMG	C	518	-	51,51,55	1.42	6 (11%)	59,59,63	1.29	10 (16%)
24	CLA	D	402	-	69,73,73	3.32	35 (50%)	83,113,113	1.81	21 (25%)
29	LMG	a	613	-	51,51,55	1.33	5 (9%)	59,59,63	0.99	3 (5%)
30	LHG	d	406	-	48,48,48	1.11	2 (4%)	51,54,54	1.02	3 (5%)
26	BCR	B	619	-	41,41,41	8.94	30 (73%)	56,56,56	5.62	29 (51%)
26	BCR	H	101	-	41,41,41	9.06	30 (73%)	56,56,56	5.72	30 (53%)
24	CLA	b	617	2	69,73,73	3.12	33 (47%)	83,113,113	1.78	17 (20%)
24	CLA	C	505	3	69,73,73	3.11	30 (43%)	83,113,113	1.83	16 (19%)
28	SQD	b	601	28	53,54,54	1.08	4 (7%)	62,65,65	1.44	9 (14%)
24	CLA	b	608[B]	-	69,73,73	3.17	30 (43%)	83,113,113	1.86	20 (24%)
24	CLA	a	606	1	69,73,73	3.30	30 (43%)	83,113,113	1.90	19 (22%)

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
24	CLA	b	603	-	-	20/39/115/115	-
24	CLA	C	504	-	-	14/39/115/115	-
24	CLA	B	616	-	-	15/39/115/115	-
27	PL9	d	404	-	-	26/53/73/73	0/1/1/1
30	LHG	D	406	-	-	19/53/53/53	-
30	LHG	d	407	-	-	18/53/53/53	-
27	PL9	D	405	-	-	26/53/73/73	0/1/1/1
24	CLA	a	615	-	-	7/39/115/115	-
24	CLA	B	614	2	-	3/39/115/115	-
28	SQD	L	102	28	-	28/49/69/69	0/1/1/1
29	LMG	C	519	-	-	20/46/66/70	0/1/1/1
24	CLA	c	504	-	-	11/39/115/115	-
29	LMG	B	621	-	-	21/46/66/70	0/1/1/1
24	CLA	B	607[B]	-	-	12/39/115/115	-
24	CLA	A	609	1	-	19/39/115/115	-
28	SQD	l	101	28	-	28/49/69/69	0/1/1/1
32	DGD	c	516	-	-	22/51/91/95	0/2/2/2
24	CLA	A	607	-	-	11/39/115/115	-
32	DGD	C	517	-	-	17/51/91/95	0/2/2/2
24	CLA	B	613	2	-	7/39/115/115	-
24	CLA	B	602	-	-	21/39/115/115	-
26	BCR	k	101	-	-	20/29/63/63	0/2/2/2
26	BCR	B	618	-	-	23/29/63/63	0/2/2/2
24	CLA	b	612	-	-	10/39/115/115	-
26	BCR	a	610	-	-	22/29/63/63	0/2/2/2
24	CLA	B	609	2	-	4/39/115/115	-
33	HEM	e	102	5,6	-	3/14/54/54	-
24	CLA	c	511	3	-	4/39/115/115	-
28	SQD	a	614	-	-	23/49/69/69	0/1/1/1
24	CLA	c	506	3	-	13/39/115/115	-
32	DGD	H	102	-	-	20/51/91/95	0/2/2/2
25	PHO	D	401	-	-	3/37/103/103	0/5/6/6
24	CLA	d	402	4	-	3/39/115/115	-
26	BCR	f	101	-	-	18/29/63/63	0/2/2/2
30	LHG	l	102	-	-	23/53/53/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	614	-	-	23/49/69/69	0/1/1/1
28	SQD	x	101	-	-	16/38/58/69	0/1/1/1
26	BCR	b	619	-	-	21/29/63/63	0/2/2/2
24	CLA	d	403	4	-	16/39/115/115	-
24	CLA	C	510	3	-	12/39/115/115	-
25	PHO	A	608	-	-	4/37/103/103	0/5/6/6
33	HEM	v	201	16	-	2/14/54/54	-
24	CLA	A	606	-	-	1/39/115/115	-
32	DGD	c	518	-	-	21/51/91/95	0/2/2/2
24	CLA	b	610	2	-	5/39/115/115	-
30	LHG	D	407	-	-	19/53/53/53	-
24	CLA	B	610	2	-	6/39/115/115	-
26	BCR	T	101	-	-	25/29/63/63	0/2/2/2
33	HEM	V	201	16	-	2/14/54/54	-
30	LHG	A	615	-	-	16/53/53/53	-
24	CLA	B	606	2	-	7/39/115/115	-
29	LMG	c	520	-	-	22/46/66/70	0/1/1/1
32	DGD	d	405	-	-	34/51/91/95	0/2/2/2
26	BCR	K	102	-	-	20/29/63/63	0/2/2/2
24	CLA	b	611	-	-	7/39/115/115	-
24	CLA	C	509	3	-	7/39/115/115	-
24	CLA	C	512	3	-	9/39/115/115	-
29	LMG	j	101	34	-	17/46/66/70	0/1/1/1
24	CLA	c	513	-	-	11/39/115/115	-
24	CLA	C	507	-	-	11/39/115/115	-
32	DGD	C	516	-	-	31/51/91/95	0/2/2/2
26	BCR	C	514	-	-	25/29/63/63	0/2/2/2
24	CLA	B	611	-	-	9/39/115/115	-
24	CLA	b	608[A]	-	-	10/39/115/115	-
26	BCR	b	621	-	-	20/29/63/63	0/2/2/2
24	CLA	b	616	2	-	13/39/115/115	-
29	LMG	Z	101	-	-	17/31/51/70	0/1/1/1
24	CLA	B	612	2	-	5/39/115/115	-
26	BCR	b	620	-	-	19/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	505	3	-	8/39/115/115	-
24	CLA	B	603	2	-	6/39/115/115	-
24	CLA	B	604	2	-	6/39/115/115	-
24	CLA	C	511	3	-	6/39/115/115	-
26	BCR	c	514	-	-	24/29/63/63	0/2/2/2
24	CLA	c	503	3	-	3/39/115/115	-
32	DGD	E	101	-	-	35/51/91/95	0/2/2/2
24	CLA	B	605	2	-	11/39/115/115	-
29	LMG	c	519	-	-	21/46/66/70	0/1/1/1
26	BCR	h	101	-	-	25/29/63/63	0/2/2/2
24	CLA	b	605	2	-	7/39/115/115	-
24	CLA	B	617	2	-	16/39/115/115	-
26	BCR	B	620	-	-	19/29/63/63	0/2/2/2
24	CLA	B	615	2	-	15/39/115/115	-
24	CLA	B	607[A]	2	-	11/39/115/115	-
26	BCR	I	101	-	-	21/29/63/63	0/2/2/2
33	HEM	E	103	5,6	-	3/14/54/54	-
30	LHG	e	101	-	-	24/46/46/53	-
24	CLA	b	614	2	-	7/39/115/115	-
28	SQD	X	101	-	-	16/38/58/69	0/1/1/1
24	CLA	a	607	-	-	11/39/115/115	-
24	CLA	c	509	3	-	11/39/115/115	-
24	CLA	B	608	-	-	9/39/115/115	-
24	CLA	c	510	3	-	11/39/115/115	-
24	CLA	b	606	2	-	10/39/115/115	-
24	CLA	b	604	2	-	7/39/115/115	-
26	BCR	c	521	-	-	22/29/63/63	0/2/2/2
26	BCR	K	101	-	-	19/29/63/63	0/2/2/2
24	CLA	c	508	3	-	4/39/115/115	-
24	CLA	b	615	2	-	7/39/115/115	-
28	SQD	B	622	28	-	29/49/69/69	0/1/1/1
24	CLA	c	501	3	-	12/39/115/115	-
24	CLA	C	513	3	-	12/39/115/115	-
32	DGD	C	515	-	-	23/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	F	101	-	-	21/29/63/63	0/2/2/2
24	CLA	b	609	-	-	4/39/115/115	-
29	LMG	b	622	-	-	19/46/66/70	0/1/1/1
26	BCR	c	515	-	-	20/29/63/63	0/2/2/2
24	CLA	b	607	2	-	6/39/115/115	-
24	CLA	C	501	3	-	12/39/115/115	-
27	PL9	a	611	-	-	24/53/73/73	0/1/1/1
28	SQD	A	612	-	-	16/49/69/69	0/1/1/1
26	BCR	A	610	-	-	23/29/63/63	0/2/2/2
24	CLA	C	503	3	-	8/39/115/115	-
24	CLA	a	609	1	-	14/39/115/115	-
24	CLA	b	613	2	-	4/39/115/115	-
25	PHO	a	608	-	-	3/37/103/103	0/5/6/6
27	PL9	A	611	-	-	25/53/73/73	0/1/1/1
24	CLA	c	507	-	-	11/39/115/115	-
30	LHG	a	616	-	-	17/53/53/53	-
24	CLA	D	404	4	-	15/39/115/115	-
29	LMG	z	101	-	-	18/31/51/70	0/1/1/1
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
30	LHG	L	101	-	-	19/53/53/53	-
32	DGD	c	517	-	-	26/51/91/95	0/2/2/2
26	BCR	t	101	-	-	26/29/63/63	0/2/2/2
29	LMG	A	613	-	-	32/46/66/70	0/1/1/1
29	LMG	D	408	-	-	20/46/66/70	0/1/1/1
28	SQD	a	612	-	-	16/49/69/69	0/1/1/1
24	CLA	c	502	3	-	12/39/115/115	-
30	LHG	E	102	-	-	26/46/46/53	-
24	CLA	c	512	-	-	7/39/115/115	-
24	CLA	C	506	3	-	17/39/115/115	-
24	CLA	D	403	4	-	6/39/115/115	-
24	CLA	b	618	2	-	16/39/115/115	-
32	DGD	h	102	-	-	17/51/91/95	0/2/2/2
24	CLA	C	502	3	-	11/39/115/115	-
24	CLA	C	508	3	-	6/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	C	518	-	-	22/46/66/70	0/1/1/1
24	CLA	D	402	-	-	6/39/115/115	-
29	LMG	a	613	-	-	30/46/66/70	0/1/1/1
30	LHG	d	406	-	-	15/53/53/53	-
26	BCR	B	619	-	-	23/29/63/63	0/2/2/2
26	BCR	H	101	-	-	21/29/63/63	0/2/2/2
24	CLA	b	617	2	-	13/39/115/115	-
24	CLA	C	505	3	-	9/39/115/115	-
28	SQD	b	601	28	-	29/49/69/69	0/1/1/1
24	CLA	b	608[B]	-	-	12/39/115/115	-
24	CLA	a	606	1	-	3/39/115/115	-

The worst 5 of 3352 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C14-C13	28.80	1.74	1.35
26	F	101	BCR	C14-C13	27.15	1.71	1.35
26	c	515	BCR	C14-C13	27.13	1.71	1.35
26	K	102	BCR	C14-C13	26.70	1.71	1.35
26	B	620	BCR	C14-C13	26.66	1.71	1.35

The worst 5 of 2390 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	621	BCR	C15-C16-C17	25.00	174.68	123.47
26	k	101	BCR	C15-C16-C17	24.97	174.62	123.47
26	T	101	BCR	C15-C16-C17	24.91	174.50	123.47
26	t	101	BCR	C15-C16-C17	24.76	174.19	123.47
26	A	610	BCR	C15-C16-C17	23.82	172.26	123.47

There are no chirality outliers.

5 of 2210 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	607	CLA	CHA-CBD-CGD-O2D
24	A	609	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	C1A-C2A-CAA-CBA
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

144 monomers are involved in 796 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	603	CLA	4	0
24	C	504	CLA	4	0
24	B	616	CLA	3	0
27	d	404	PL9	7	0
30	D	406	LHG	5	0
30	d	407	LHG	1	0
27	D	405	PL9	13	0
24	a	615	CLA	5	0
24	B	614	CLA	7	0
28	L	102	SQD	12	0
29	C	519	LMG	2	0
24	c	504	CLA	3	0
29	B	621	LMG	2	0
24	B	607[B]	CLA	5	0
24	A	609	CLA	7	0
28	l	101	SQD	5	0
32	c	516	DGD	1	0
24	A	607	CLA	5	0
32	C	517	DGD	3	0
24	B	613	CLA	4	0
24	B	602	CLA	3	0
26	k	101	BCR	18	0
26	B	618	BCR	24	0
24	b	612	CLA	3	0
26	a	610	BCR	13	0
24	B	609	CLA	2	0
33	e	102	HEM	2	0
24	c	511	CLA	1	0
28	a	614	SQD	2	0
24	c	506	CLA	3	0
32	H	102	DGD	6	0
25	D	401	PHO	10	0
24	d	402	CLA	4	0
26	f	101	BCR	21	0
30	l	102	LHG	6	0
28	A	614	SQD	5	0
28	x	101	SQD	4	0
26	b	619	BCR	26	0
24	d	403	CLA	3	0
24	C	510	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	608	PHO	3	0
33	v	201	HEM	4	0
24	A	606	CLA	7	0
32	c	518	DGD	3	0
24	b	610	CLA	1	0
30	D	407	LHG	3	0
24	B	610	CLA	2	0
26	T	101	BCR	22	0
33	V	201	HEM	7	0
30	A	615	LHG	10	0
24	B	606	CLA	11	0
32	d	405	DGD	4	0
26	K	102	BCR	15	0
24	C	509	CLA	3	0
24	C	512	CLA	4	0
29	j	101	LMG	6	0
24	c	513	CLA	2	0
24	C	507	CLA	6	0
32	C	516	DGD	2	0
26	C	514	BCR	14	0
24	B	611	CLA	4	0
24	b	608[A]	CLA	4	0
26	b	621	BCR	19	0
24	b	616	CLA	8	0
24	B	612	CLA	3	0
26	b	620	BCR	15	0
24	c	505	CLA	5	0
24	B	603	CLA	3	0
24	B	604	CLA	5	0
24	C	511	CLA	4	0
26	c	514	BCR	14	0
24	c	503	CLA	8	0
32	E	101	DGD	1	0
24	B	605	CLA	8	0
29	c	519	LMG	2	0
26	h	101	BCR	17	0
24	b	605	CLA	5	0
24	B	617	CLA	4	0
26	B	620	BCR	16	0
24	B	615	CLA	6	0
24	B	607[A]	CLA	1	0
26	I	101	BCR	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	E	103	HEM	6	0
30	e	101	LHG	2	0
24	b	614	CLA	2	0
28	X	101	SQD	3	0
24	a	607	CLA	4	0
24	c	509	CLA	3	0
20	a	601	OEX	1	0
24	B	608	CLA	6	0
24	c	510	CLA	3	0
24	b	606	CLA	8	0
24	b	604	CLA	4	0
26	c	521	BCR	19	0
26	K	101	BCR	14	0
24	c	508	CLA	3	0
24	b	615	CLA	2	0
28	B	622	SQD	8	0
24	c	501	CLA	10	0
24	C	513	CLA	2	0
26	F	101	BCR	20	0
24	b	609	CLA	5	0
29	b	622	LMG	4	0
26	c	515	BCR	20	0
24	b	607	CLA	12	0
24	C	501	CLA	10	0
27	a	611	PL9	12	0
28	A	612	SQD	2	0
26	A	610	BCR	14	0
24	C	503	CLA	7	0
24	a	609	CLA	5	0
24	b	613	CLA	3	0
25	a	608	PHO	2	0
27	A	611	PL9	11	0
24	c	507	CLA	3	0
30	a	616	LHG	10	0
24	D	404	CLA	6	0
29	z	101	LMG	1	0
25	d	401	PHO	4	0
30	L	101	LHG	6	0
32	c	517	DGD	5	0
26	t	101	BCR	23	0
29	A	613	LMG	2	0
29	D	408	LMG	7	0

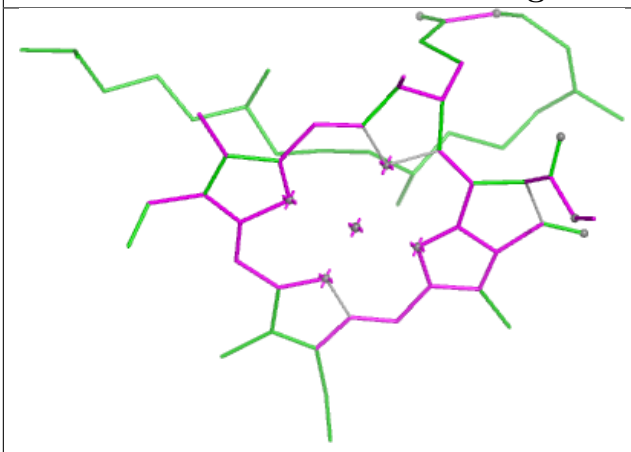
Continued on next page...

Continued from previous page...

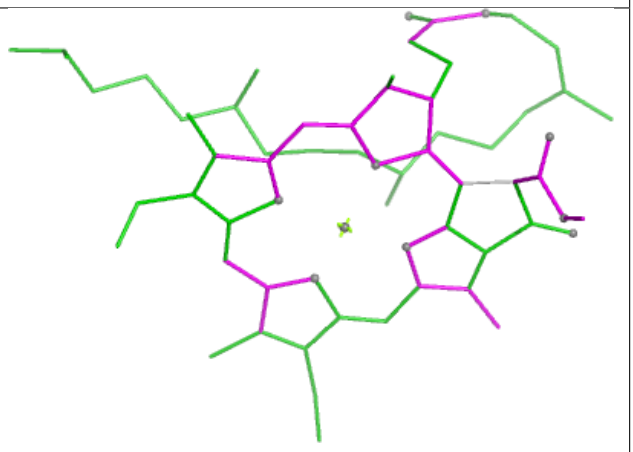
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	612	SQD	1	0
24	c	502	CLA	4	0
24	c	512	CLA	2	0
24	C	506	CLA	9	0
24	D	403	CLA	5	0
24	b	618	CLA	2	0
32	h	102	DGD	6	0
24	C	502	CLA	5	0
24	C	508	CLA	6	0
29	C	518	LMG	2	0
24	D	402	CLA	2	0
29	a	613	LMG	1	0
30	d	406	LHG	3	0
26	B	619	BCR	20	0
26	H	101	BCR	16	0
24	b	617	CLA	4	0
24	C	505	CLA	6	0
28	b	601	SQD	12	0
24	b	608[B]	CLA	2	0
24	a	606	CLA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

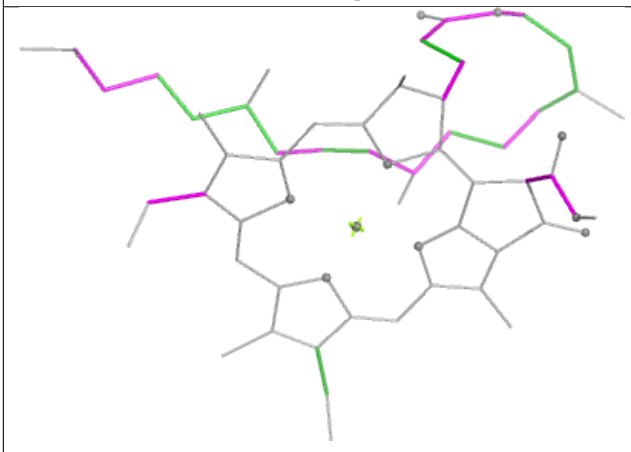
Ligand CLA b 603



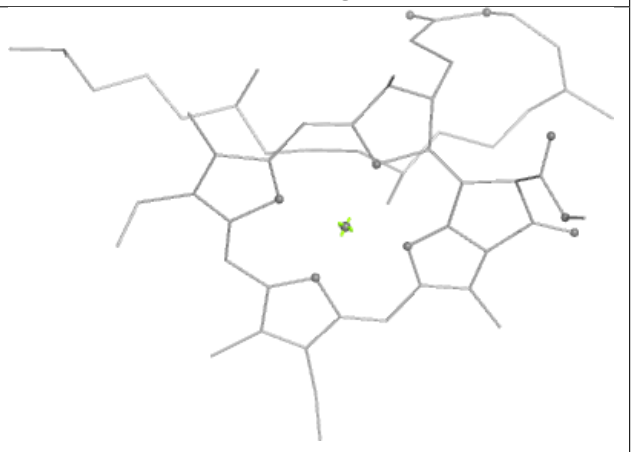
Bond lengths



Bond angles

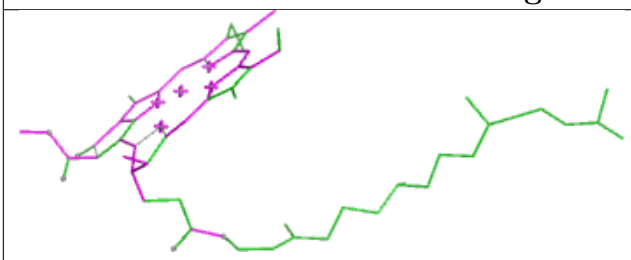


Torsions

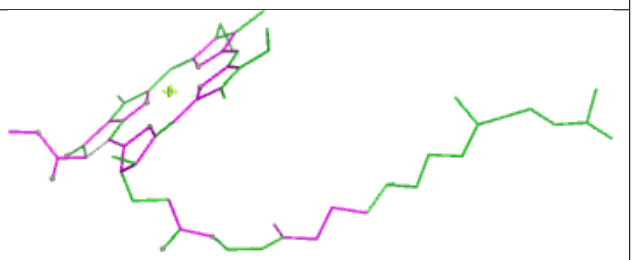


Rings

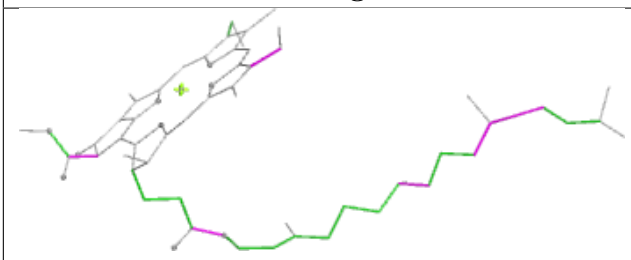
Ligand CLA C 504



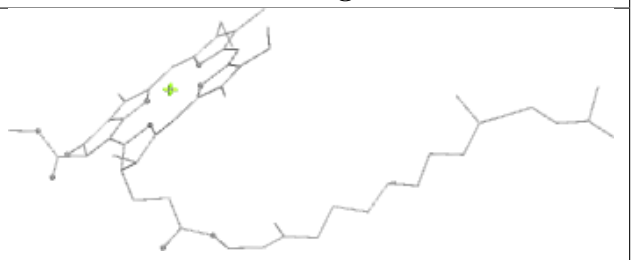
Bond lengths



Bond angles

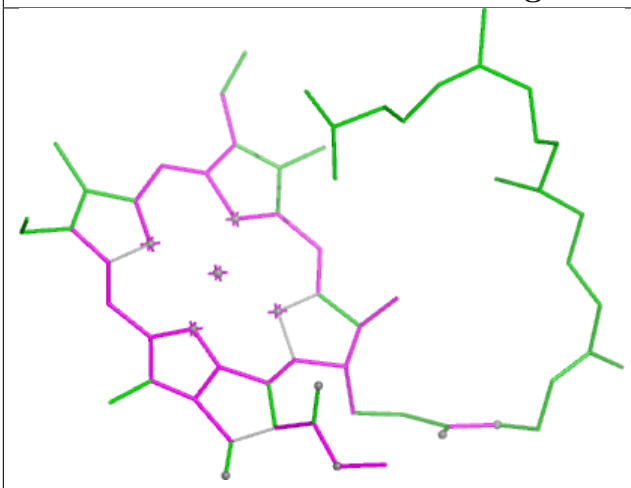


Torsions

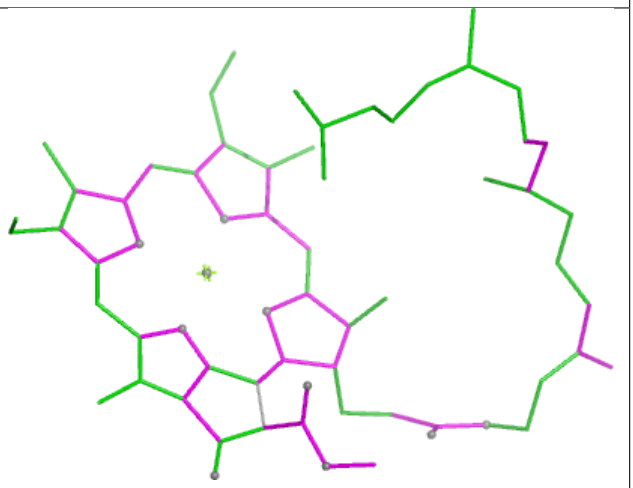


Rings

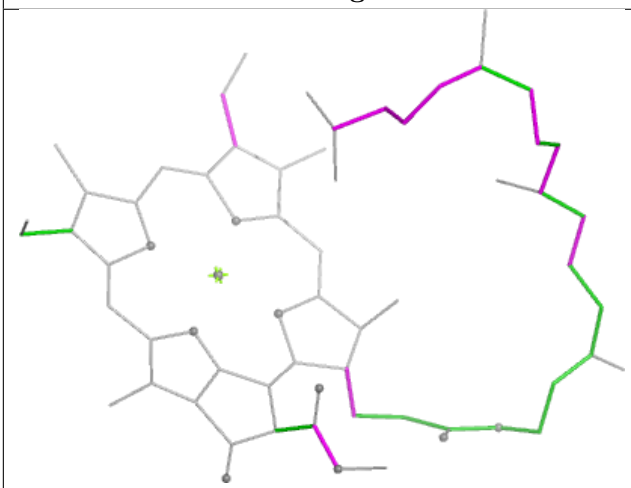
Ligand CLA B 616



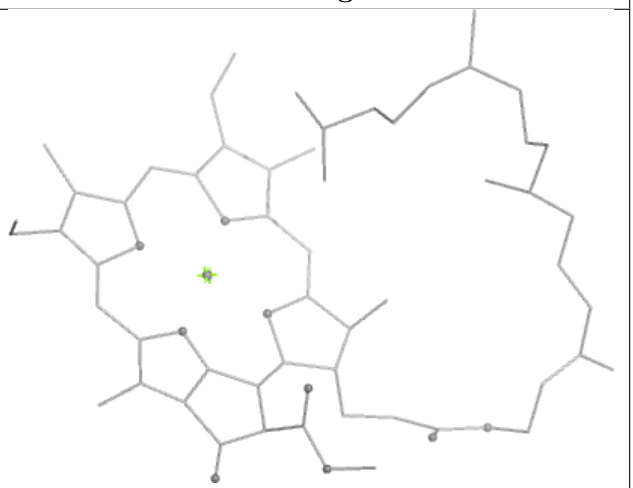
Bond lengths



Bond angles

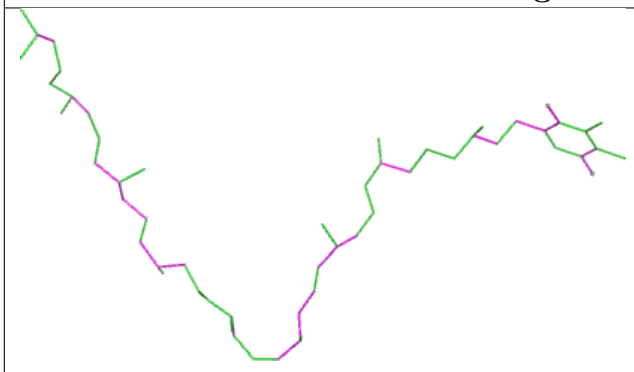


Torsions

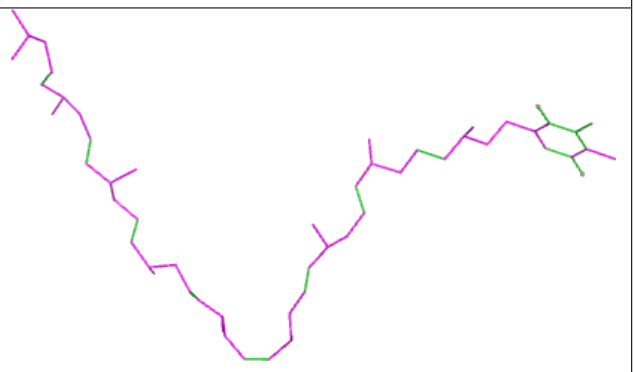


Rings

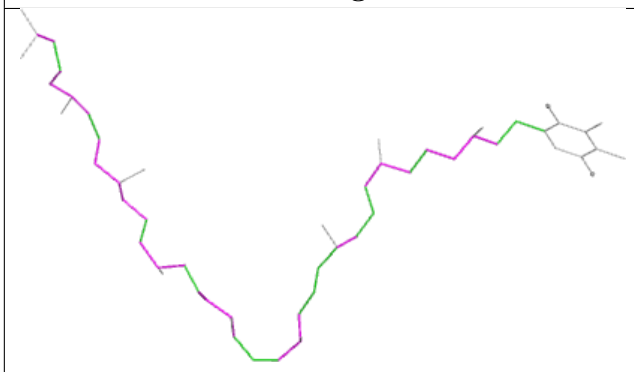
Ligand PL9 d 404



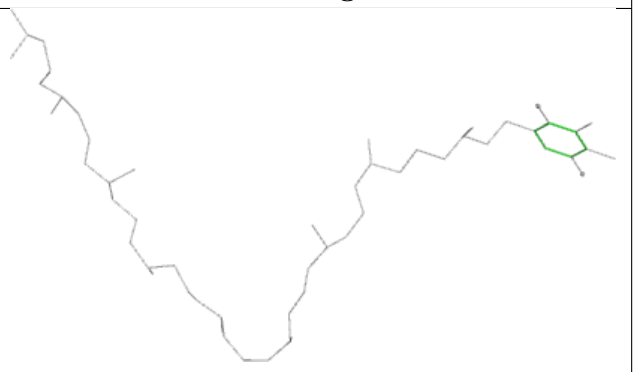
Bond lengths



Bond angles

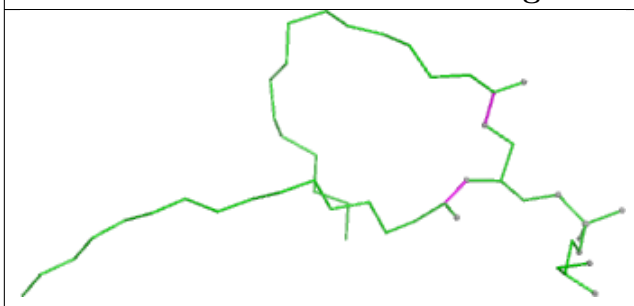


Torsions

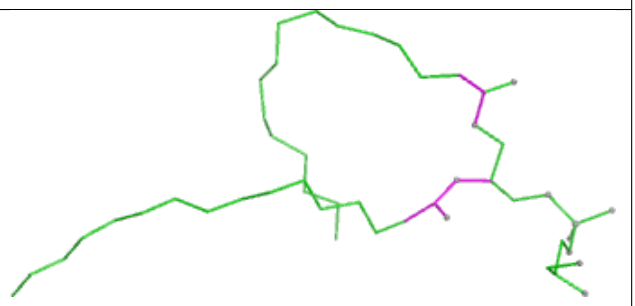


Rings

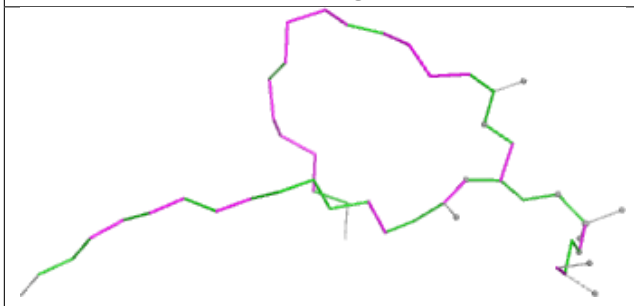
Ligand LHG D 406



Bond lengths



Bond angles

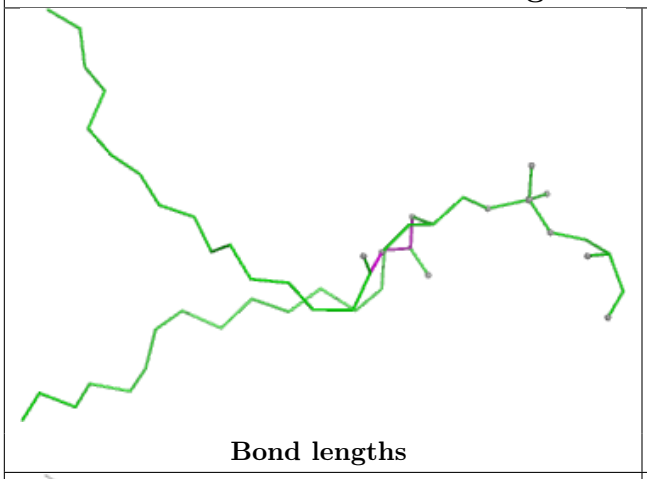


Torsions

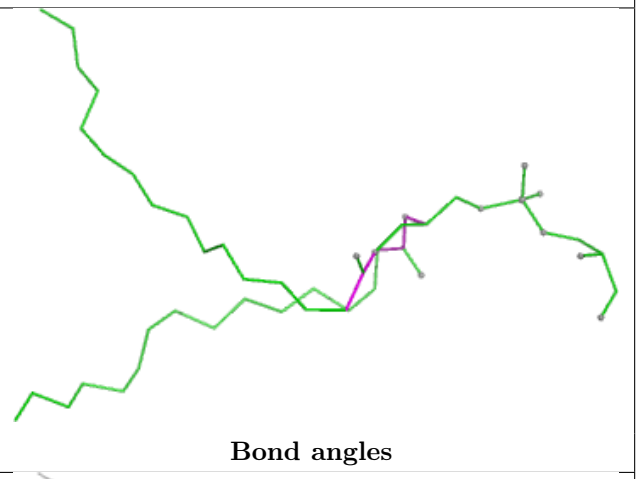


Rings

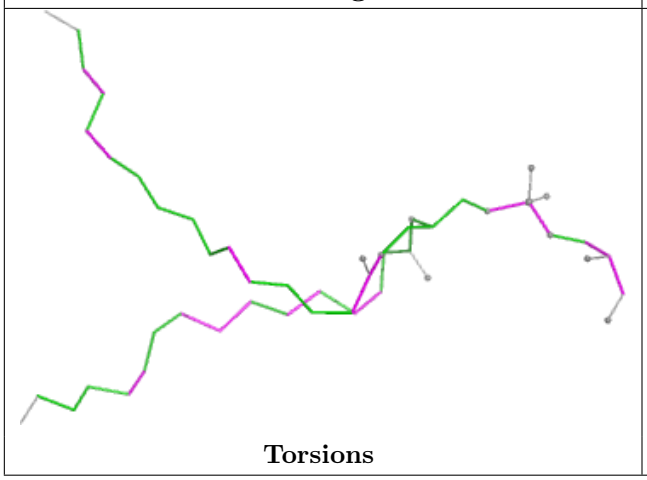
Ligand LHG d 407



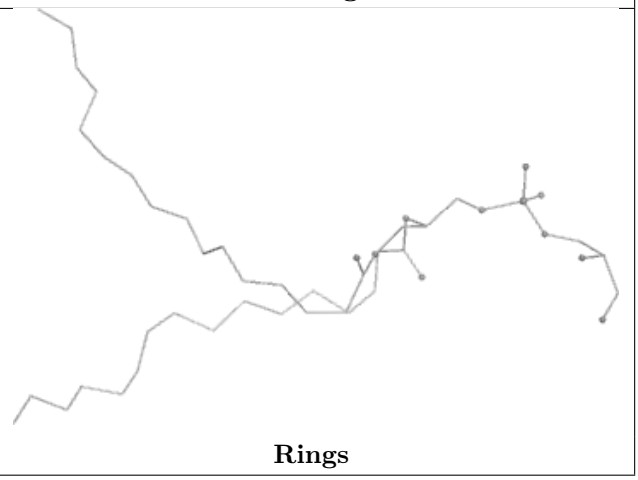
Bond lengths



Bond angles

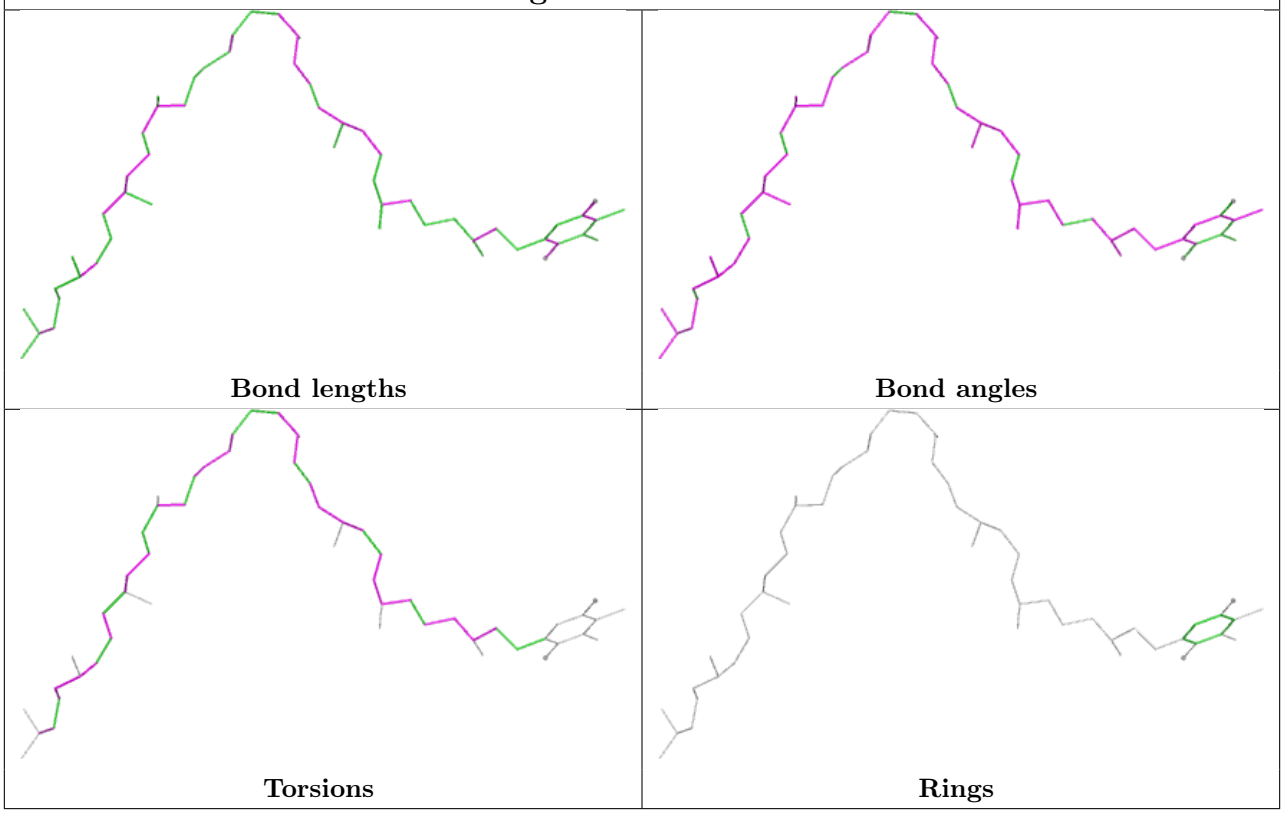


Torsions

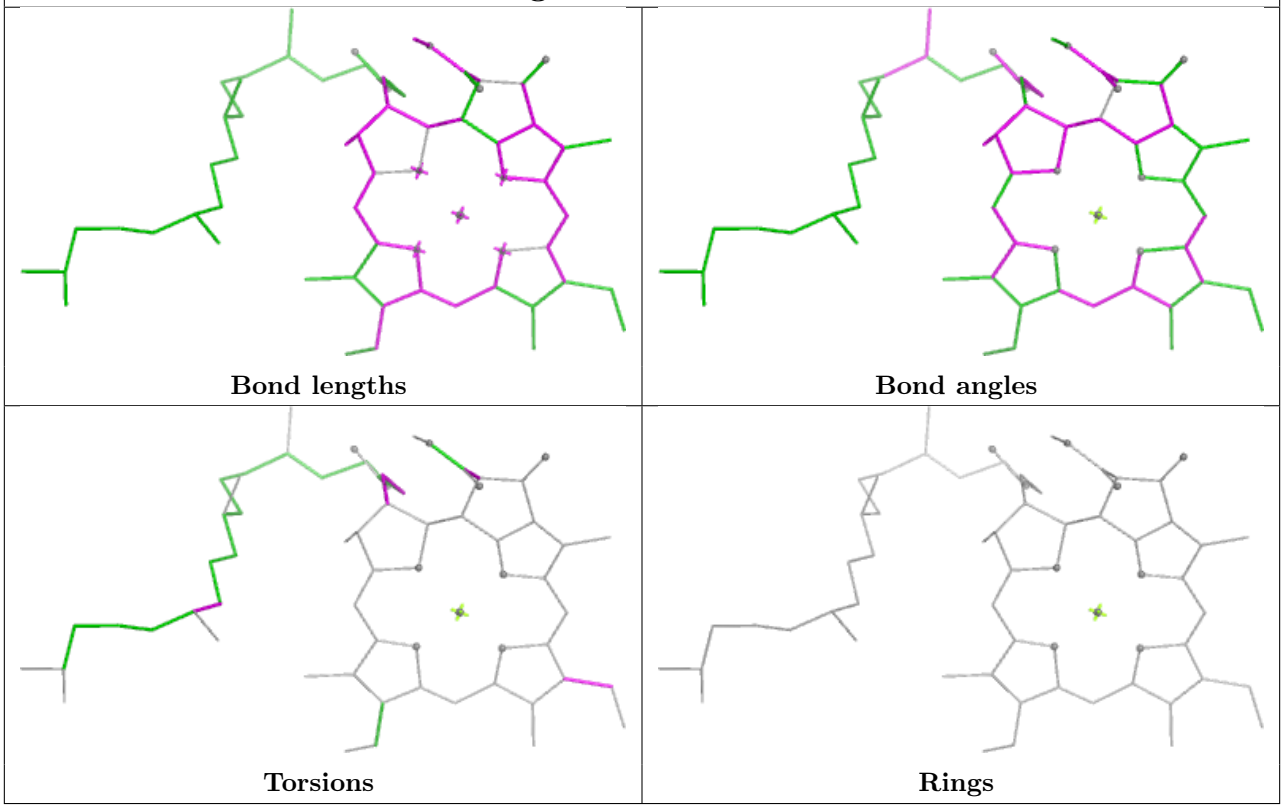


Rings

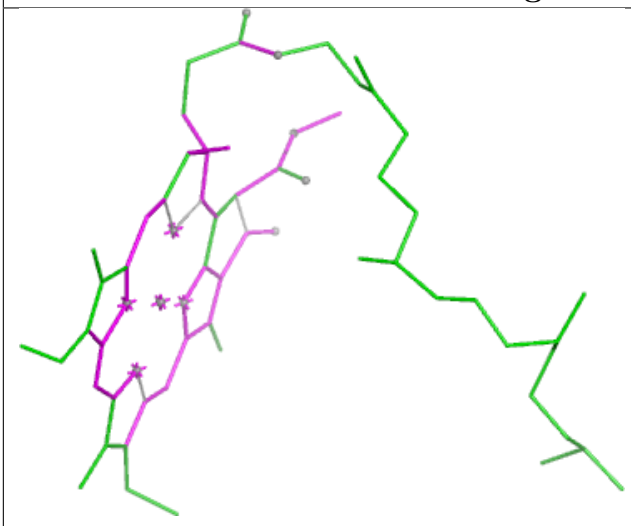
Ligand PL9 D 405



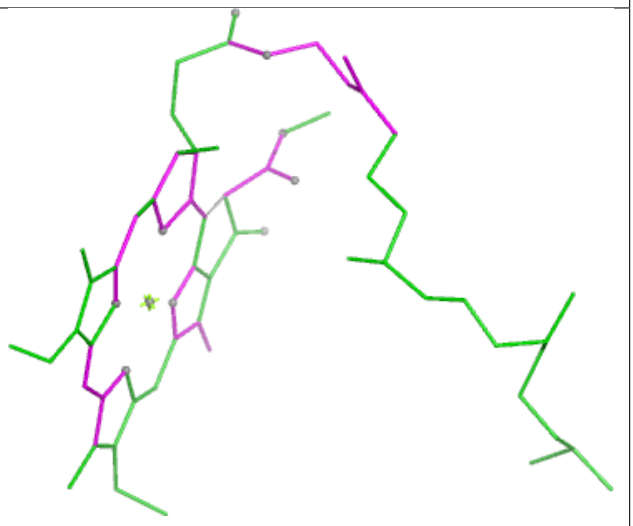
Ligand CLA a 615



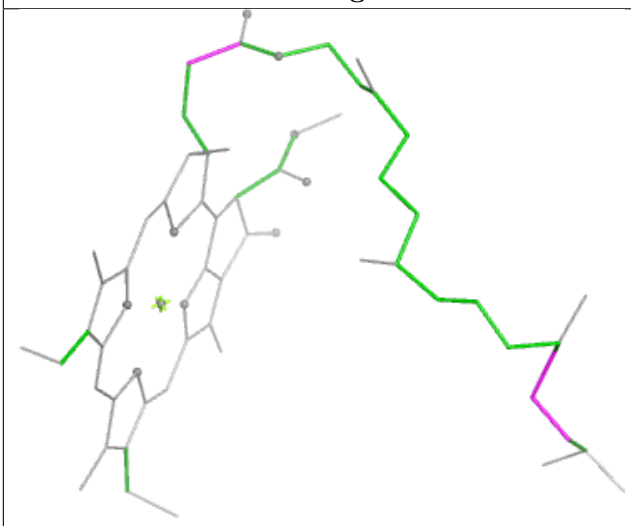
Ligand CLA B 614



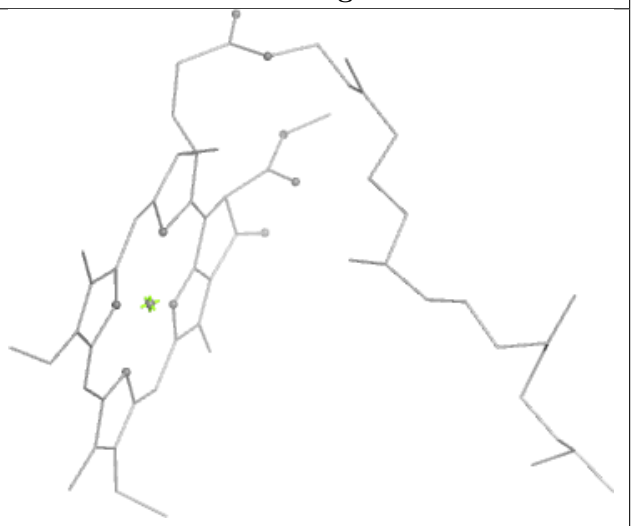
Bond lengths



Bond angles

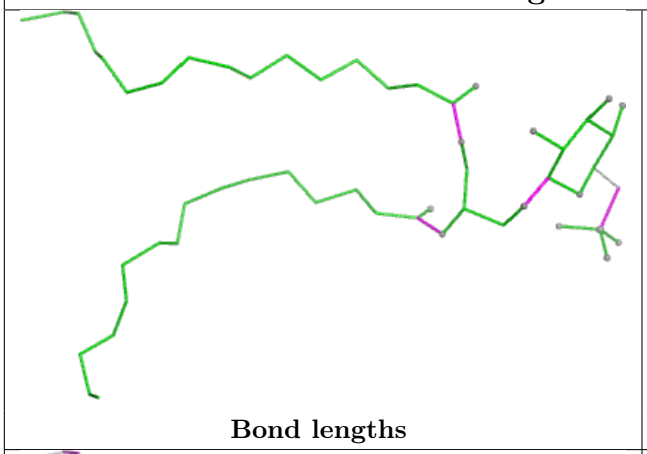


Torsions

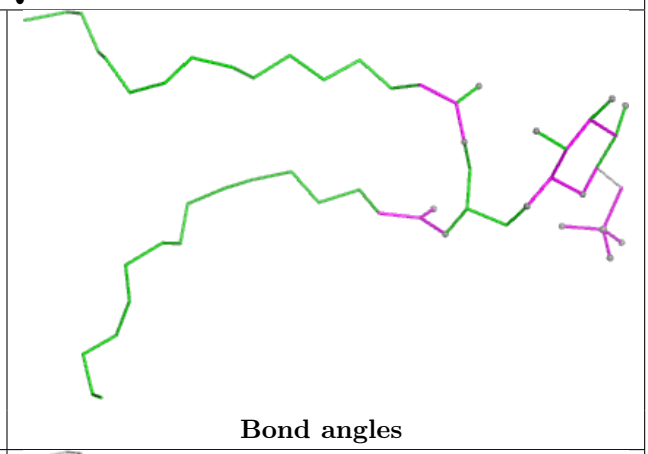


Rings

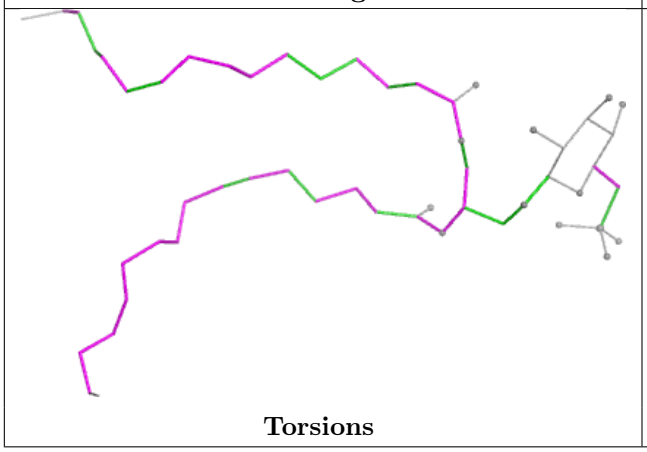
Ligand SQD L 102



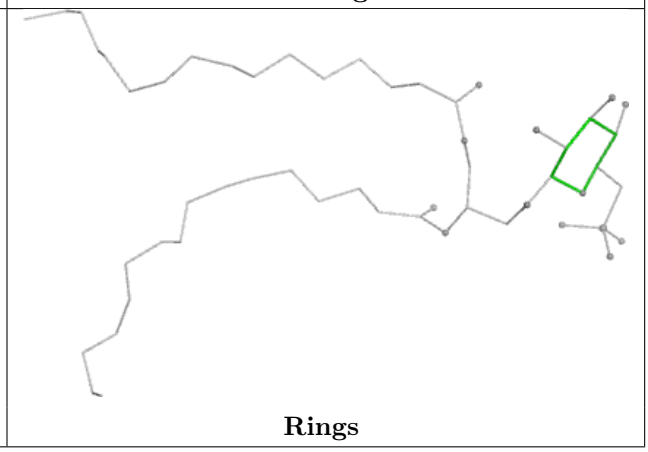
Bond lengths



Bond angles

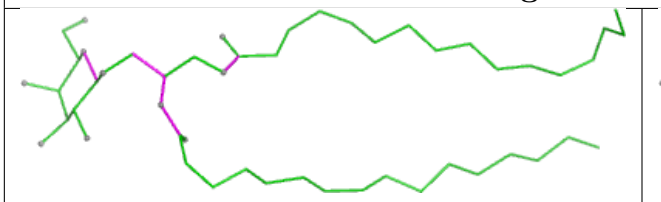


Torsions

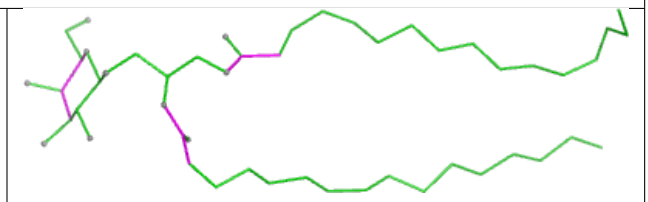


Rings

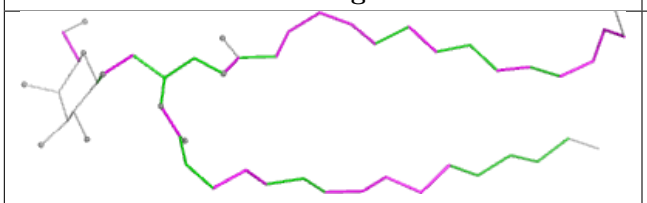
Ligand LMG C 519



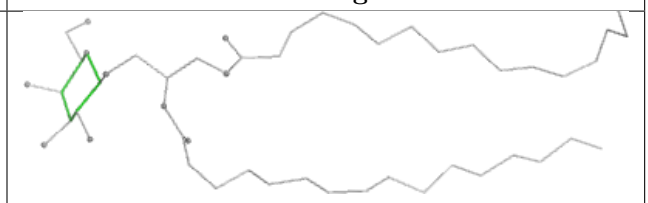
Bond lengths



Bond angles

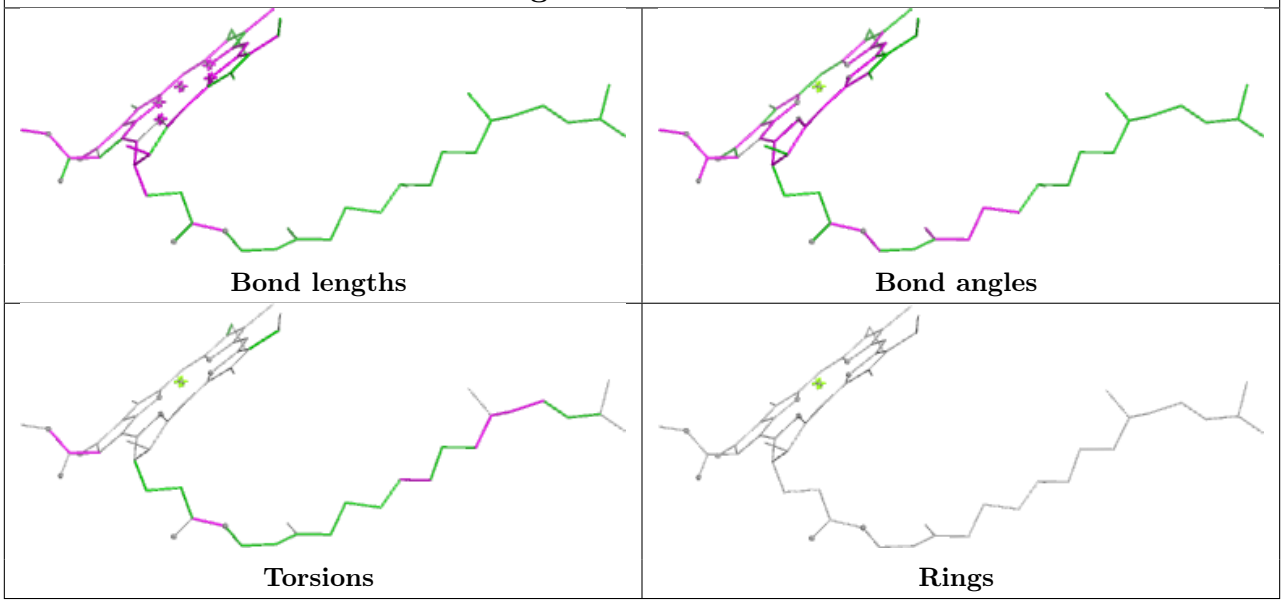


Torsions

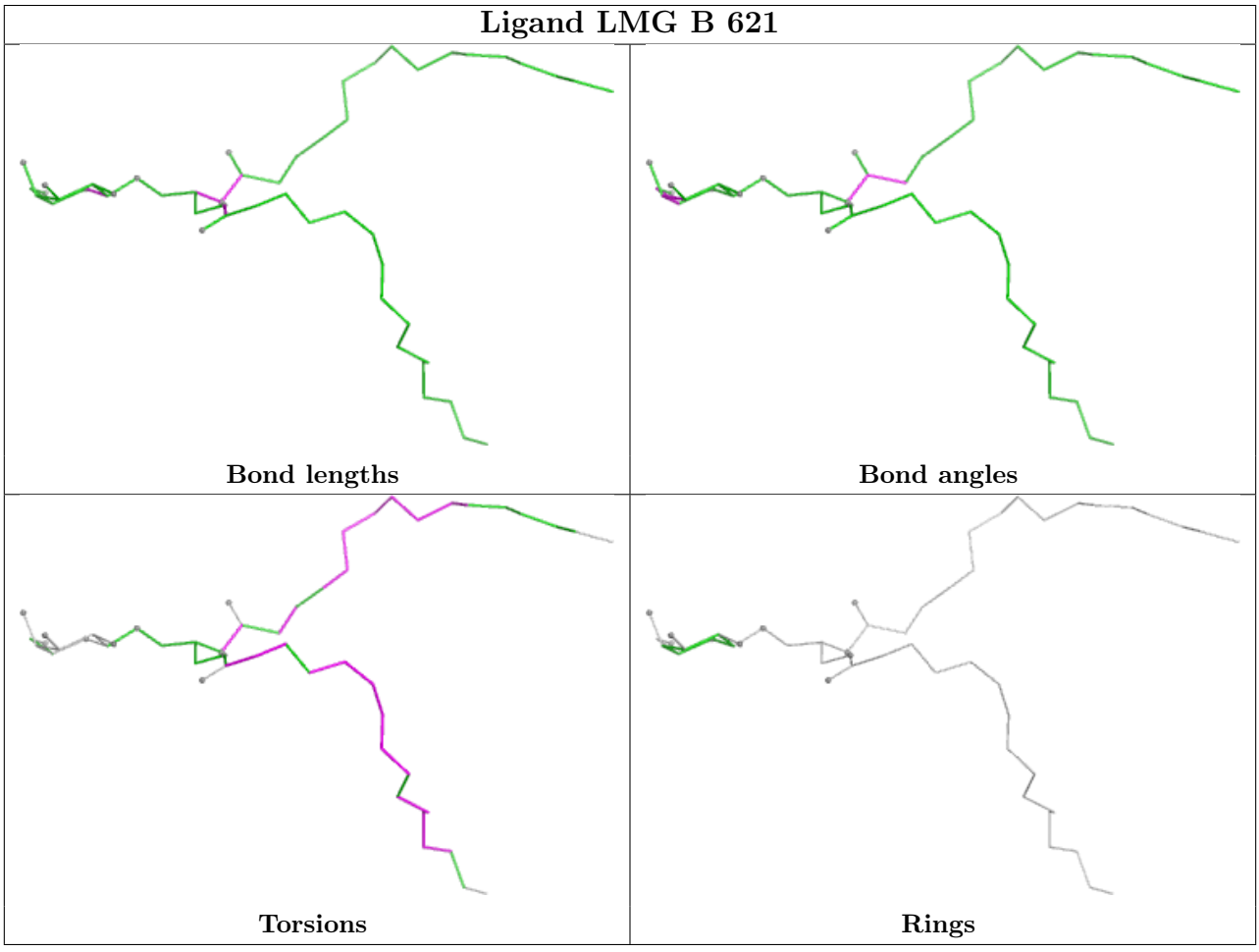


Rings

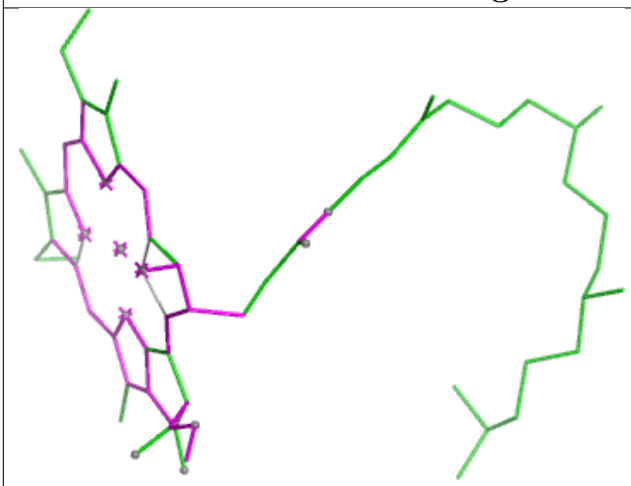
Ligand CLA c 504



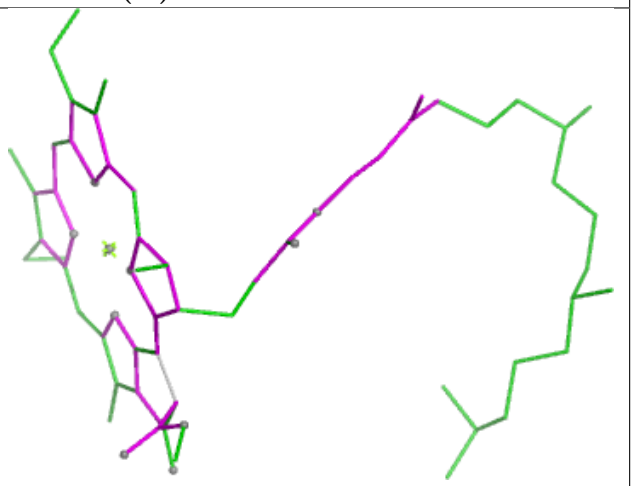
Ligand LMG B 621



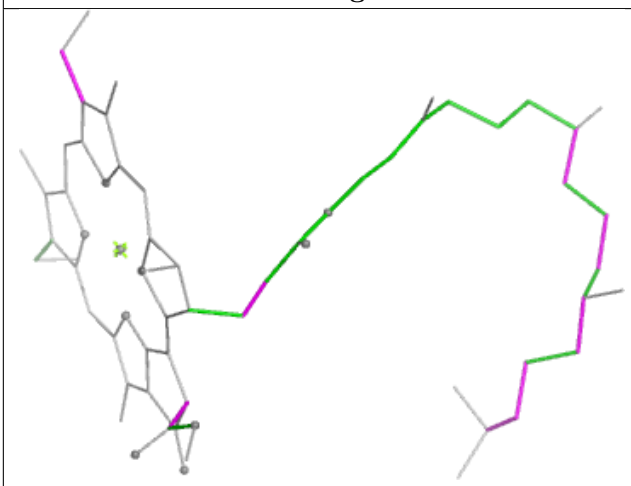
Ligand CLA B 607 (B)



Bond lengths



Bond angles

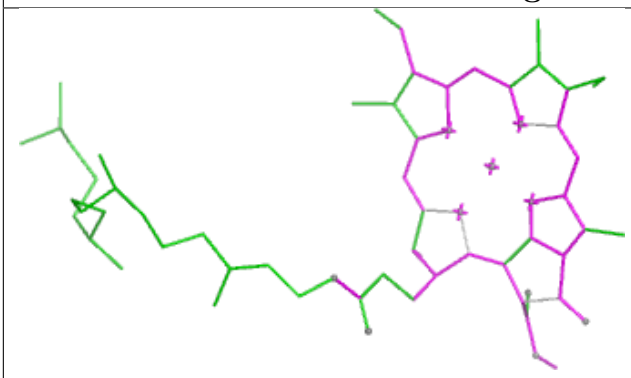


Torsions

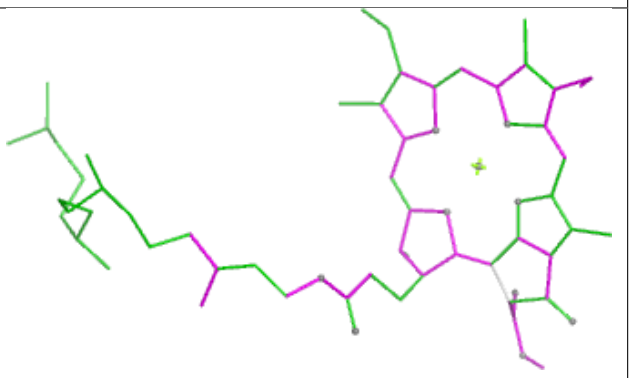


Rings

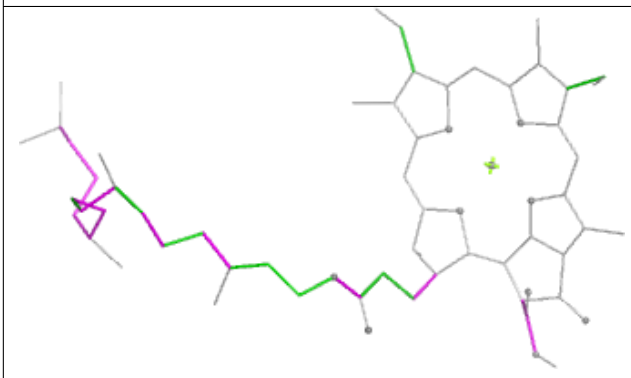
Ligand CLA A 609



Bond lengths



Bond angles

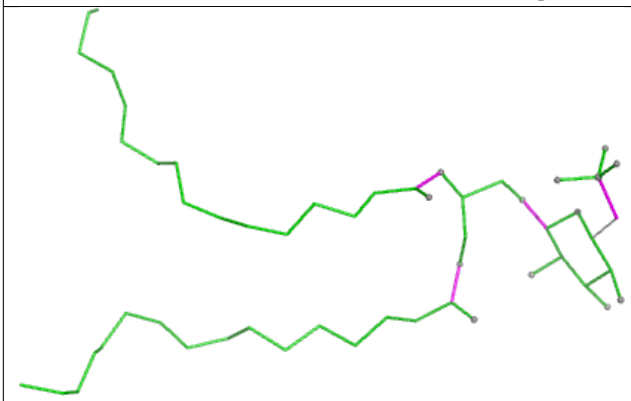


Torsions

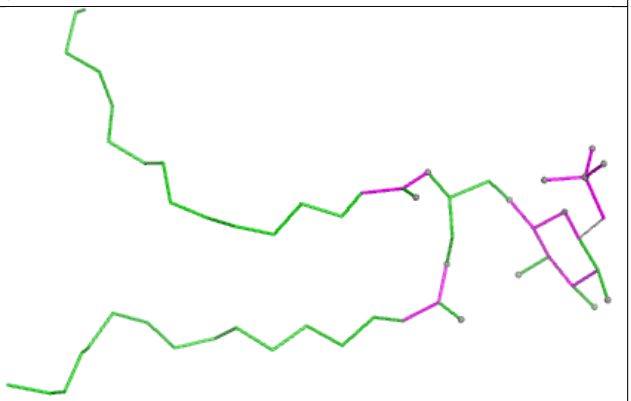


Rings

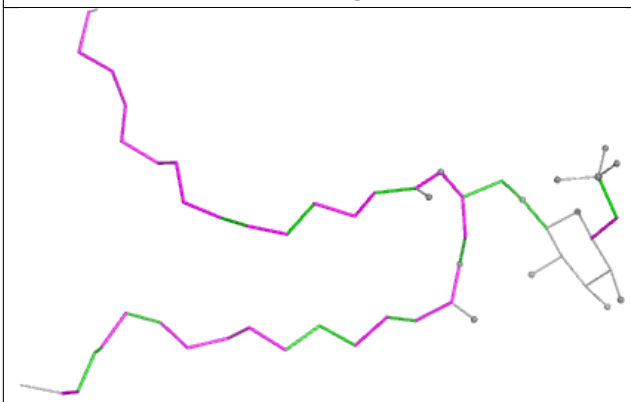
Ligand SQD l 101



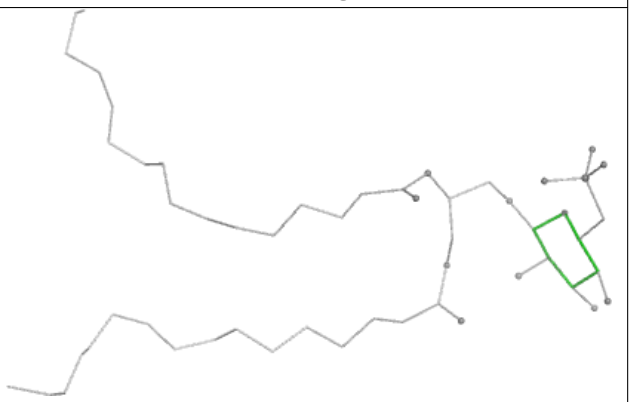
Bond lengths



Bond angles

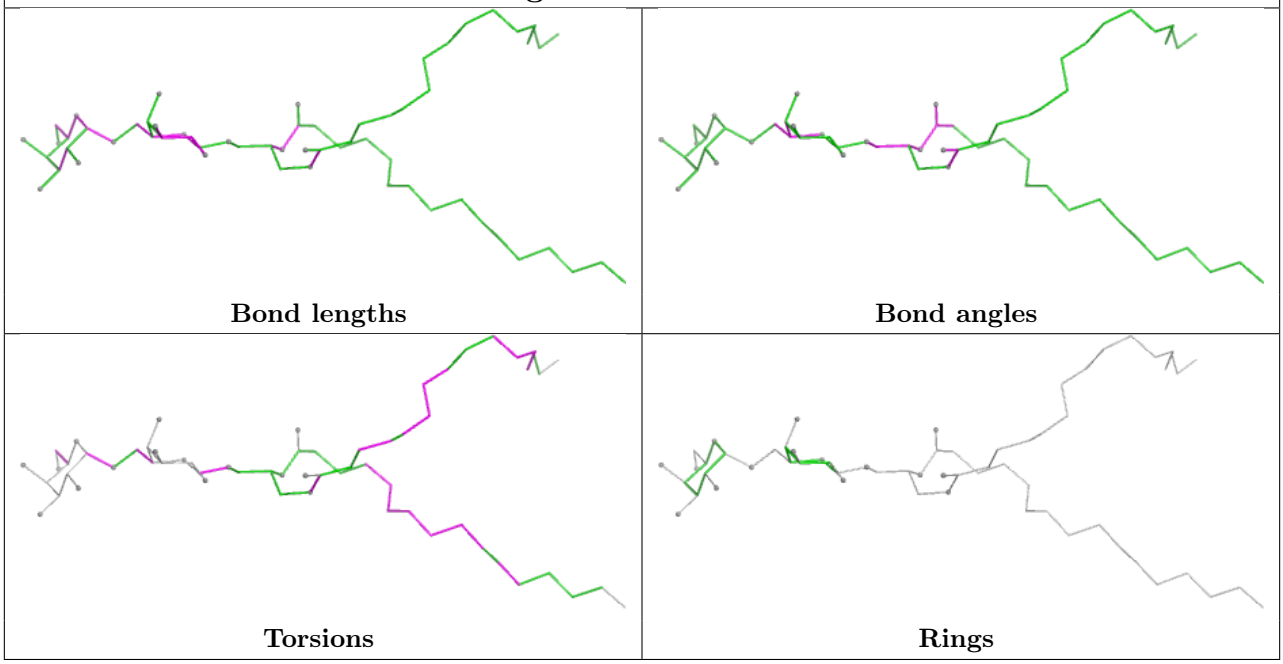


Torsions

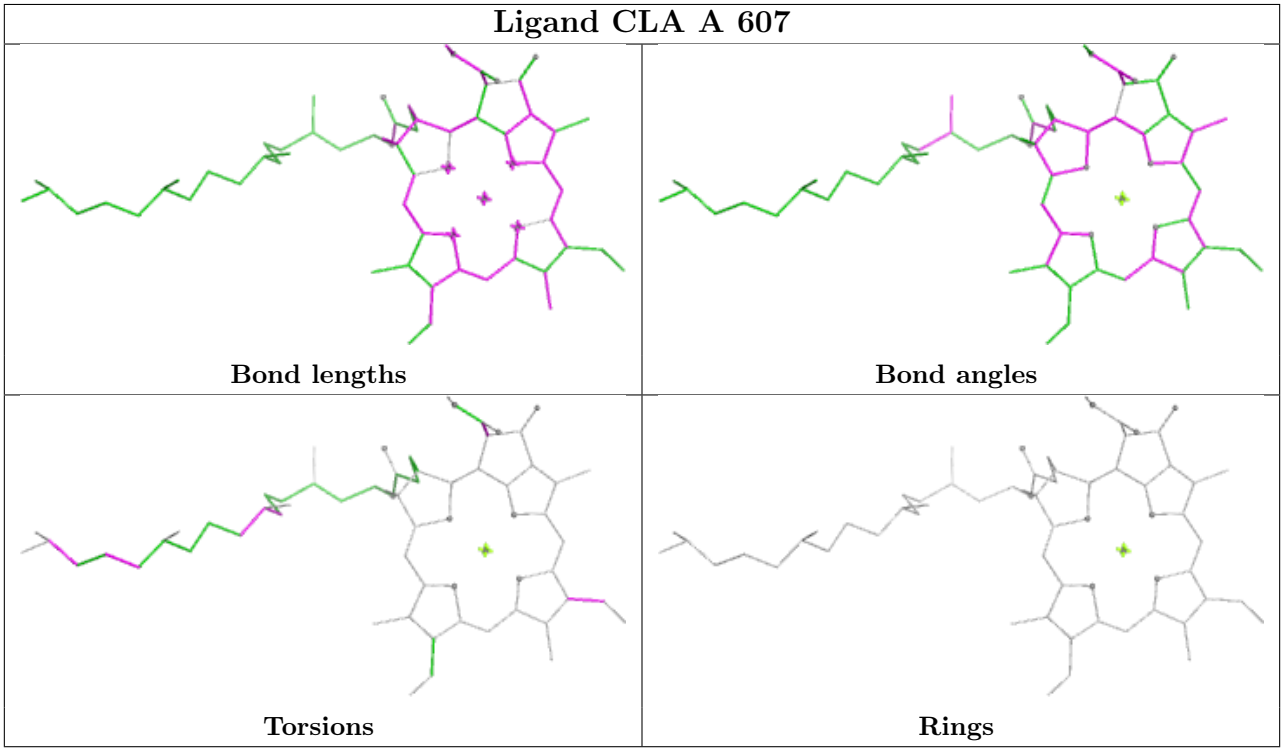


Rings

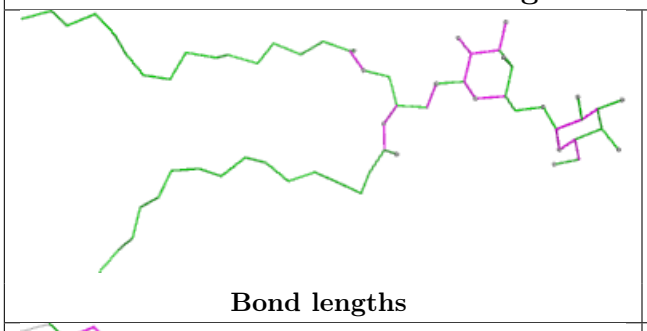
Ligand DGD c 516



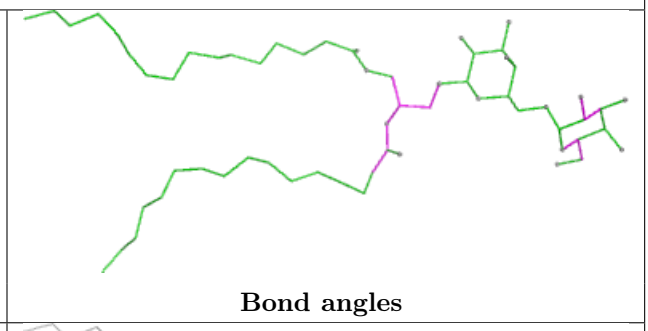
Ligand CLA A 607



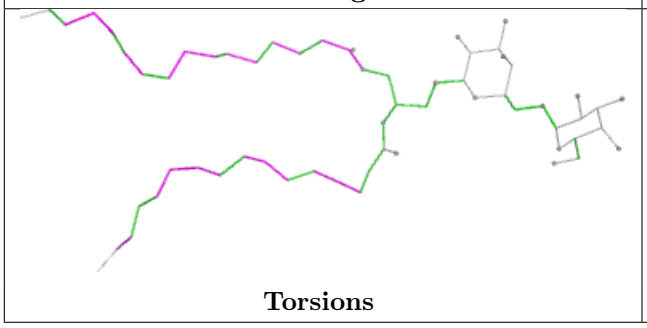
Ligand DGD C 517



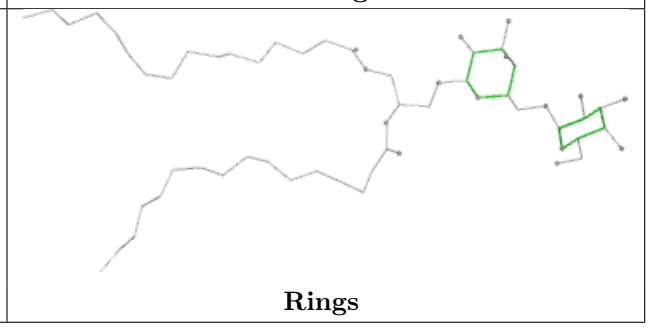
Bond lengths



Bond angles

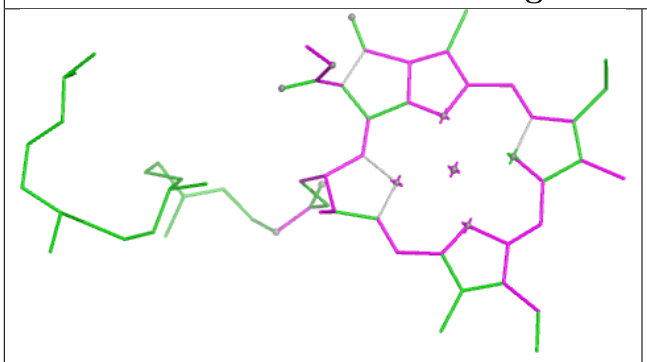


Torsions

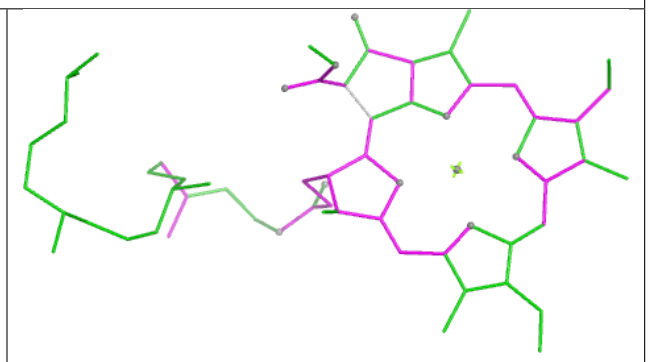


Rings

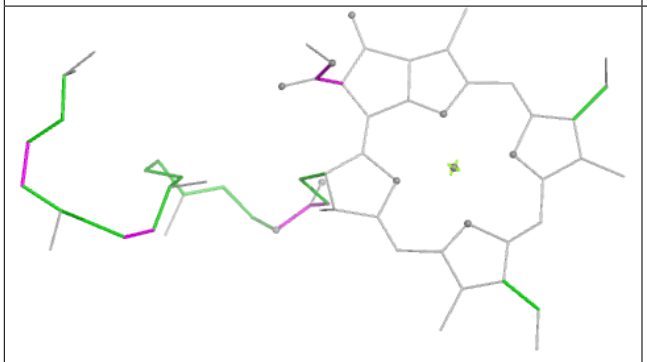
Ligand CLA B 613



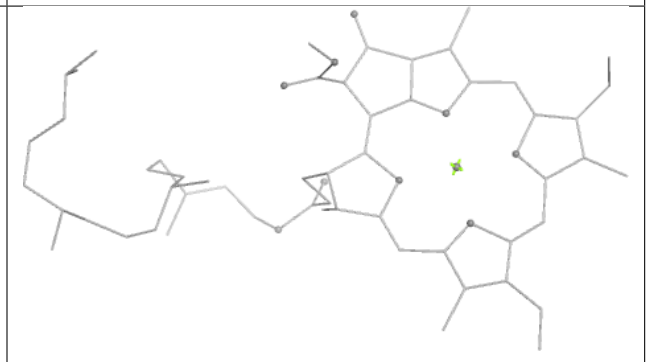
Bond lengths



Bond angles

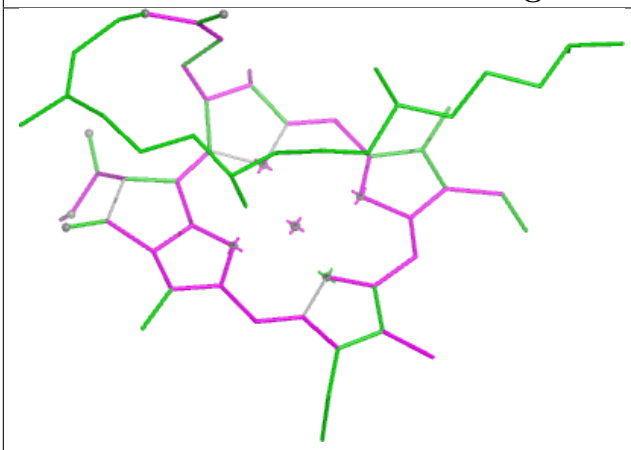


Torsions

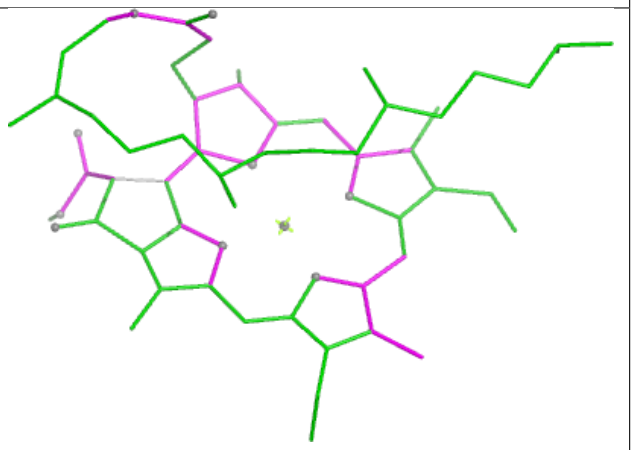


Rings

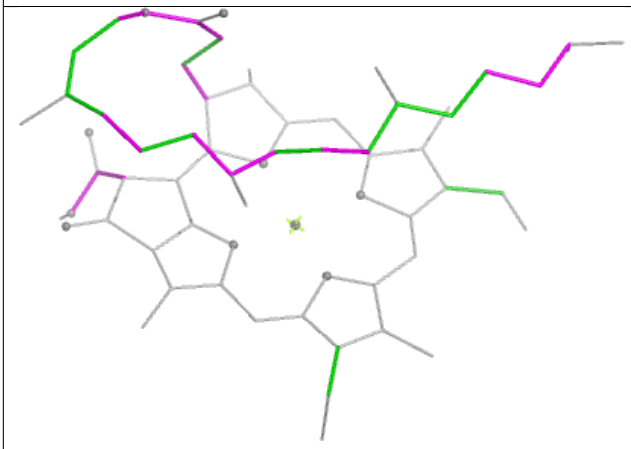
Ligand CLA B 602



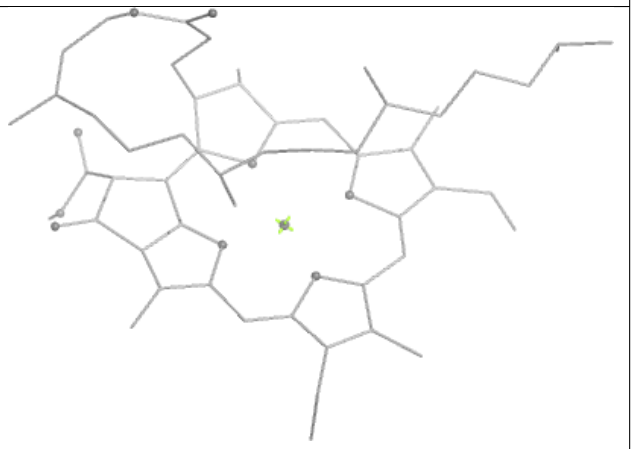
Bond lengths



Bond angles

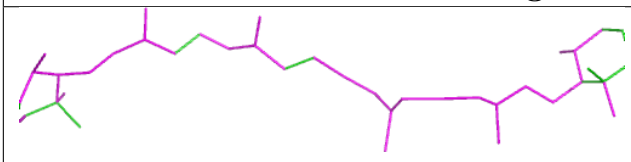


Torsions

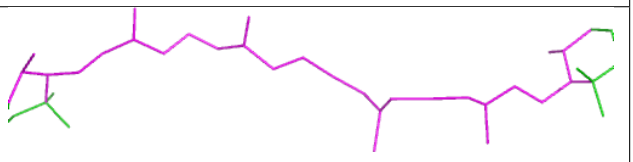


Rings

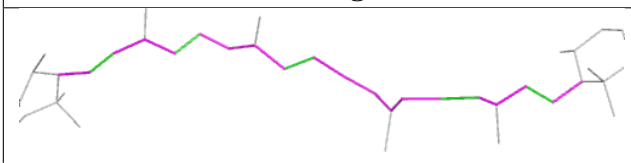
Ligand BCR k 101



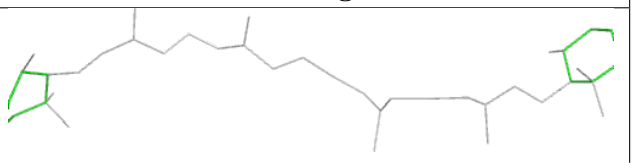
Bond lengths



Bond angles

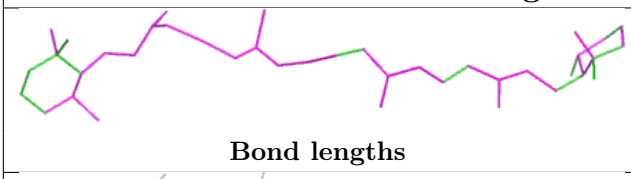


Torsions

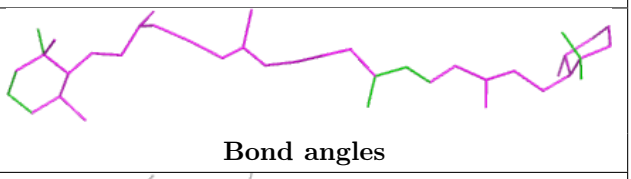


Rings

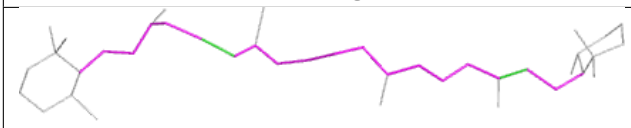
Ligand BCR B 618



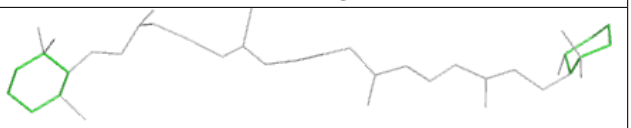
Bond lengths



Bond angles

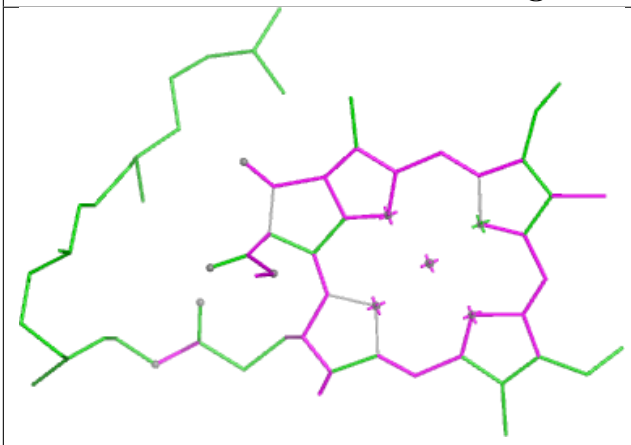


Torsions

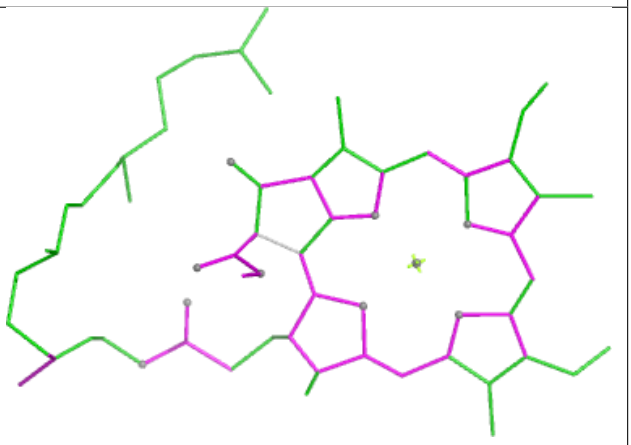


Rings

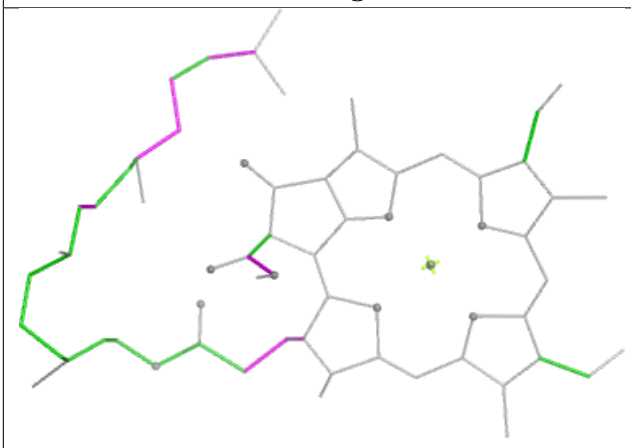
Ligand CLA b 612



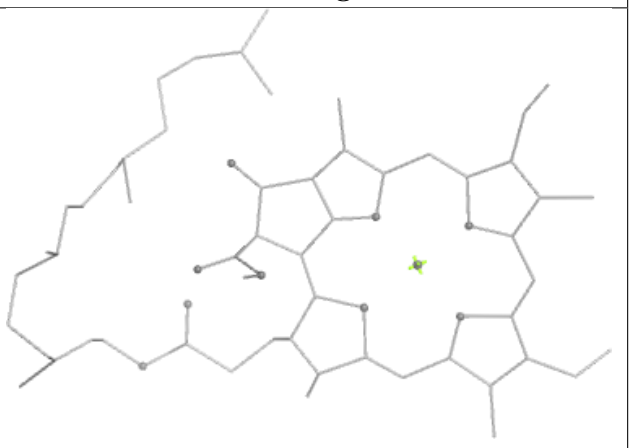
Bond lengths



Bond angles

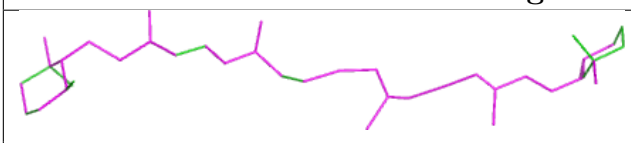


Torsions

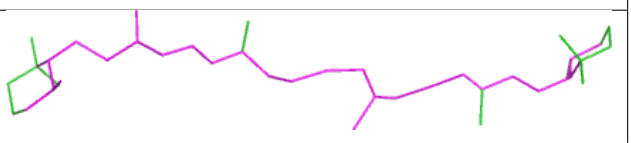


Rings

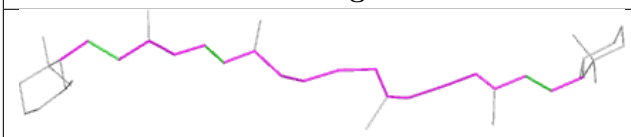
Ligand BCR a 610



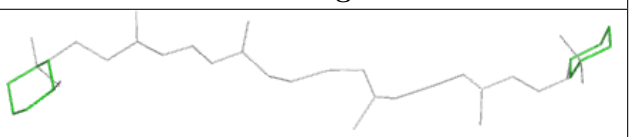
Bond lengths



Bond angles

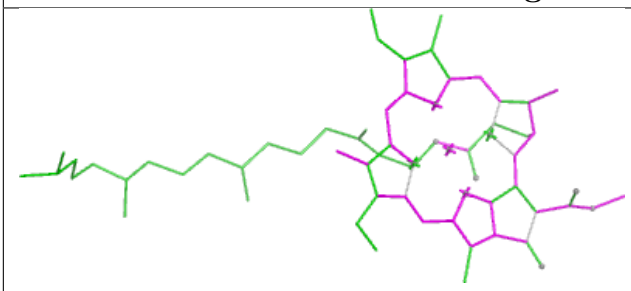


Torsions

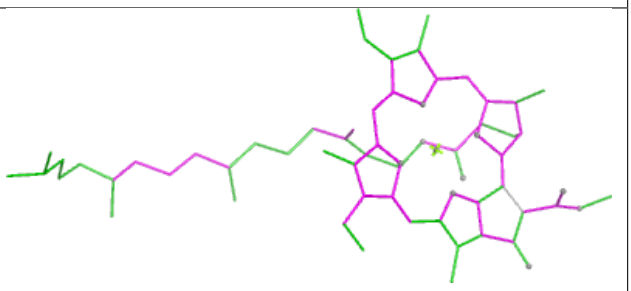


Rings

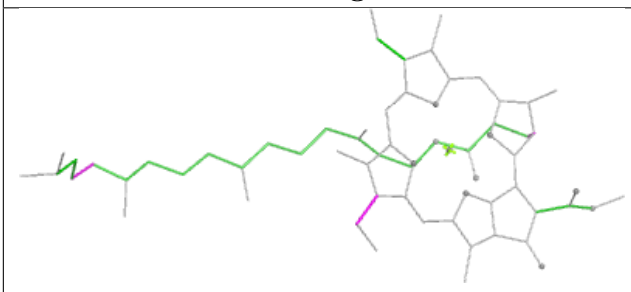
Ligand CLA B 609



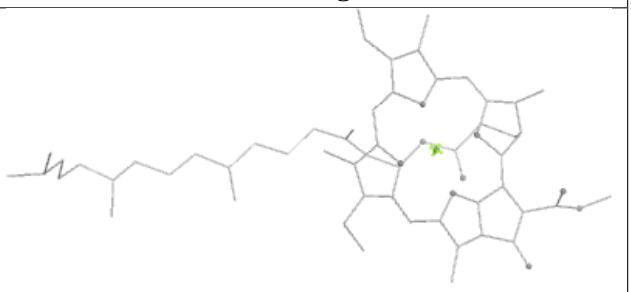
Bond lengths



Bond angles

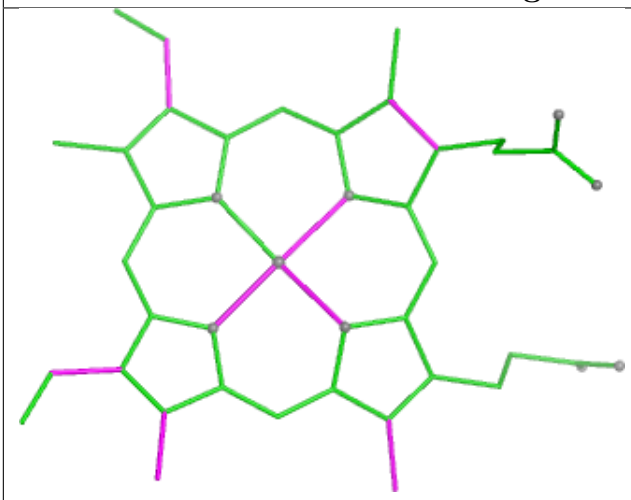


Torsions

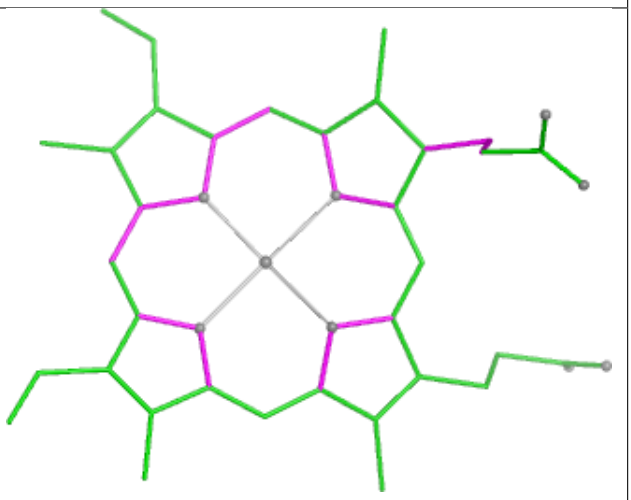


Rings

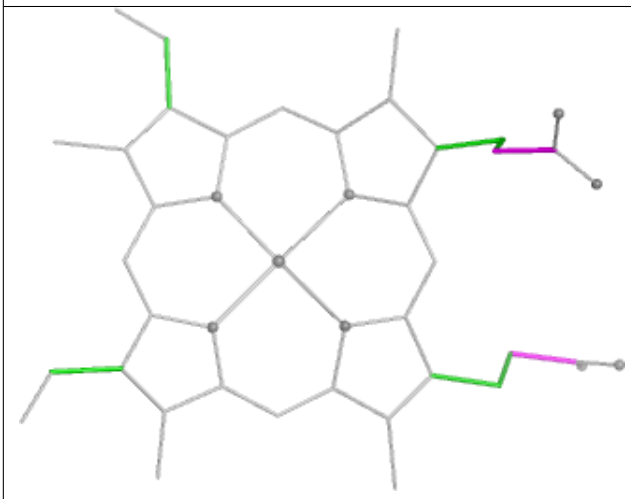
Ligand HEM e 102



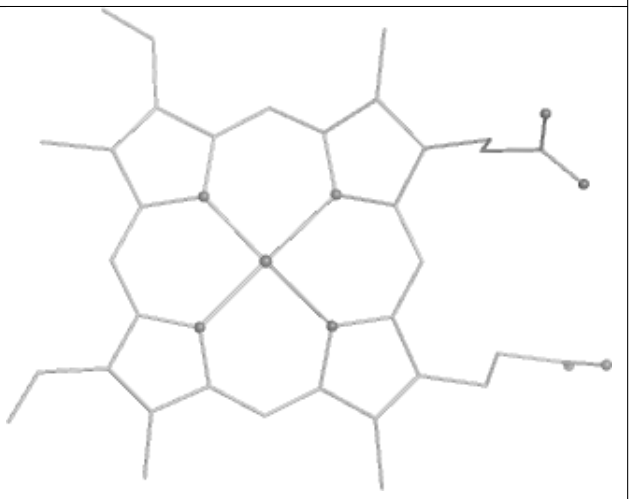
Bond lengths



Bond angles

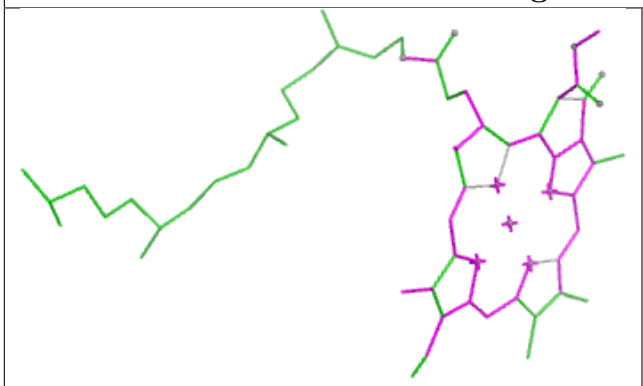


Torsions

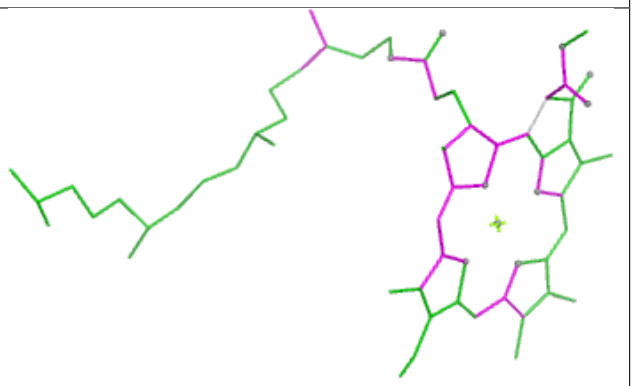


Rings

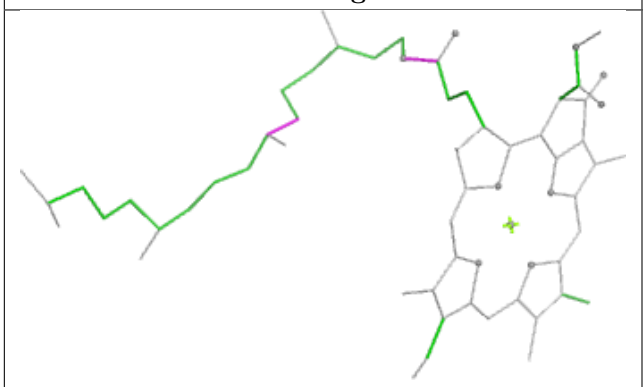
Ligand CLA c 511



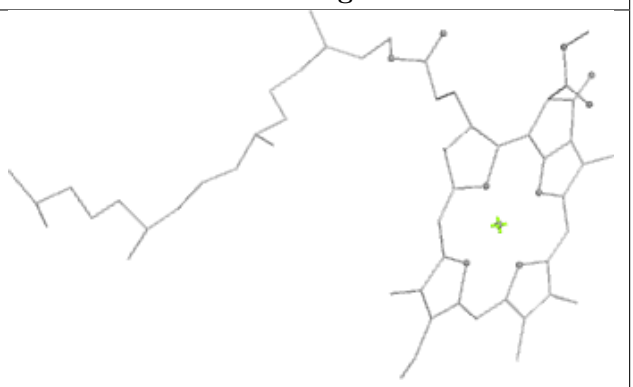
Bond lengths



Bond angles

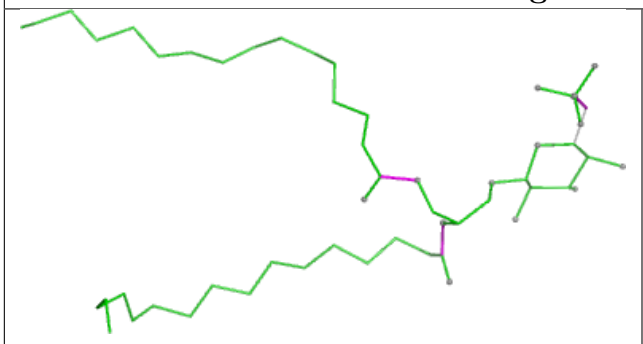


Torsions

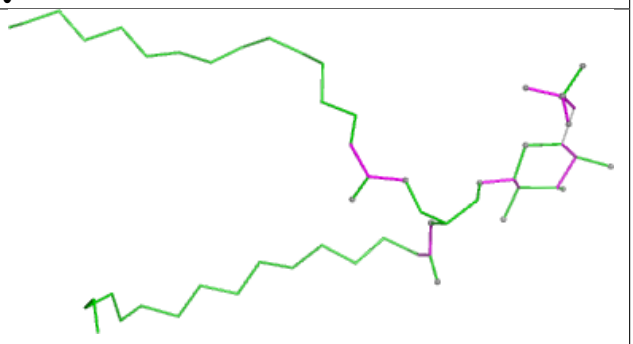


Rings

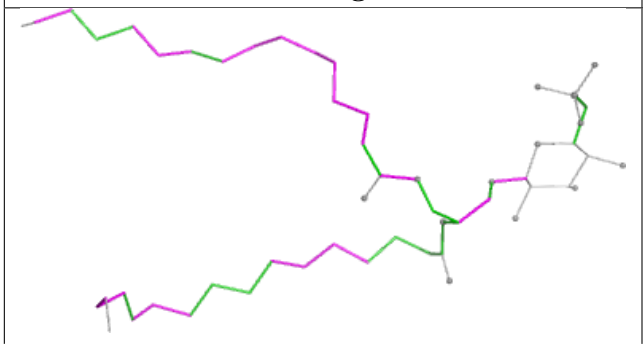
Ligand SQD a 614



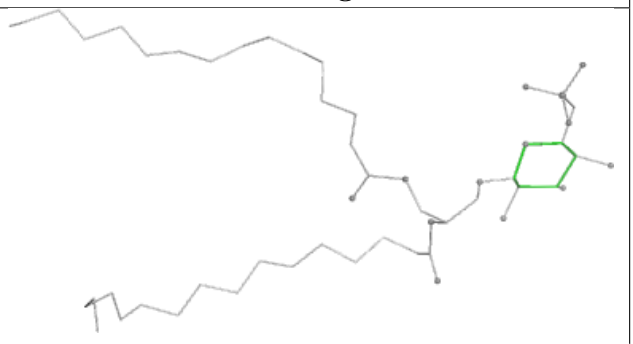
Bond lengths



Bond angles

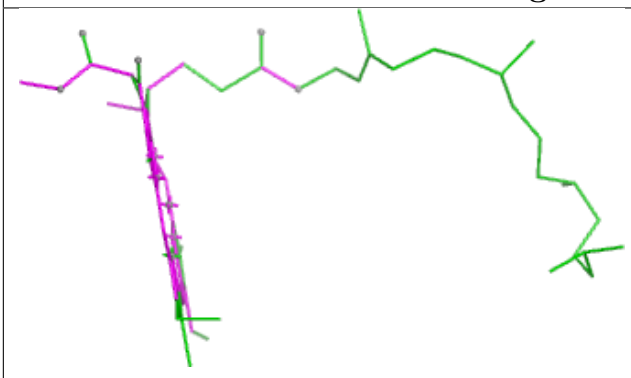


Torsions

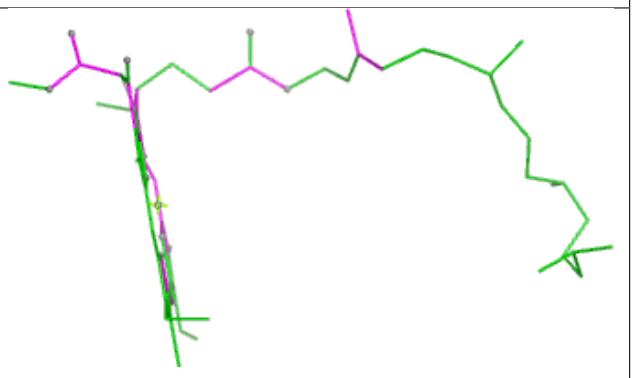


Rings

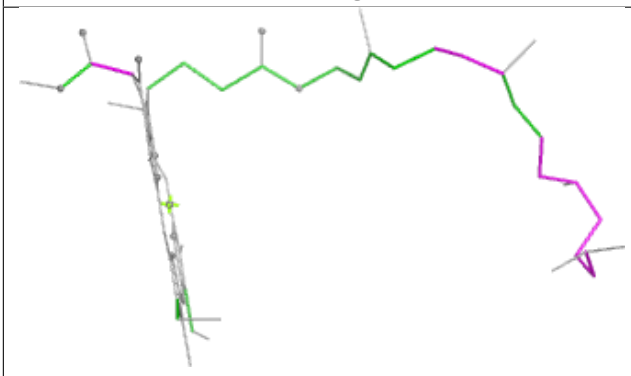
Ligand CLA c 506



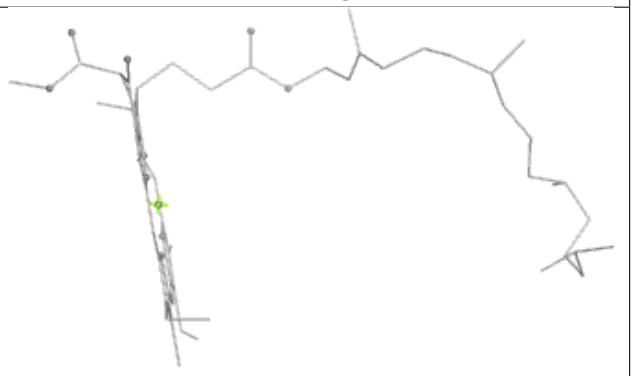
Bond lengths



Bond angles

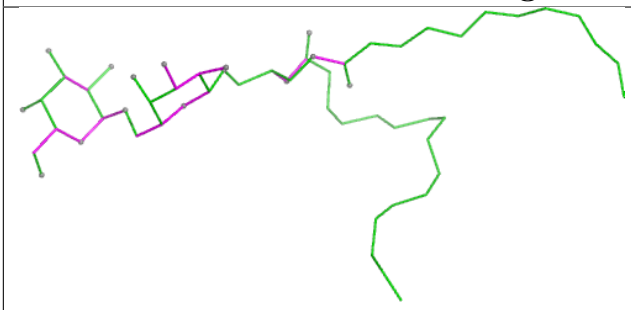


Torsions

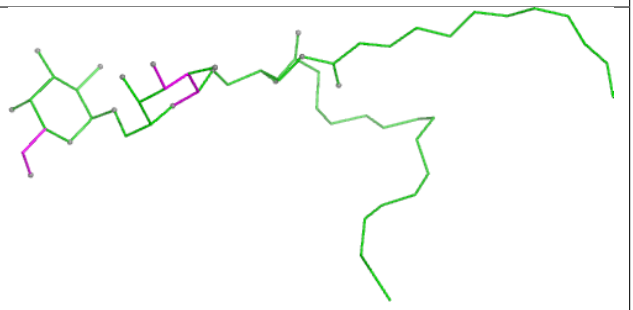


Rings

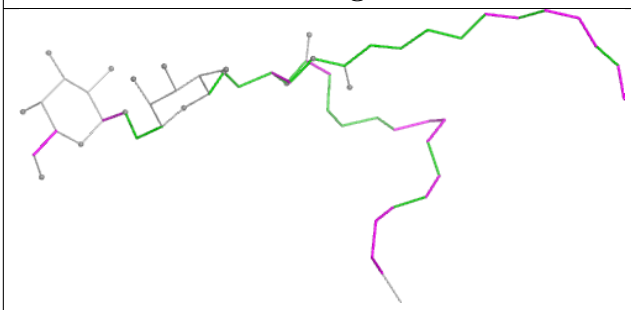
Ligand DGD H 102



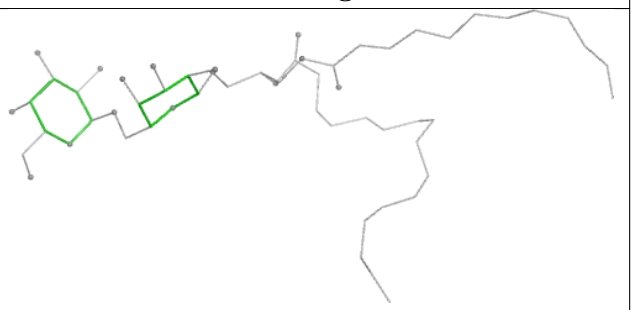
Bond lengths



Bond angles

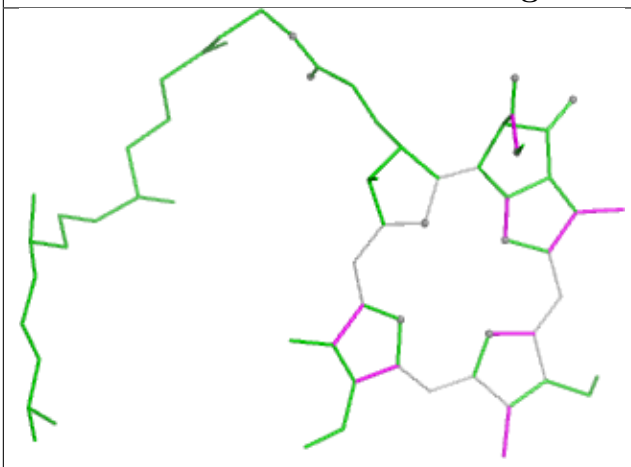


Torsions

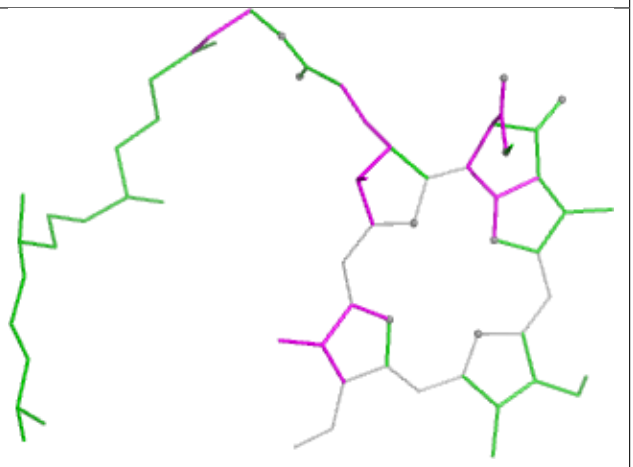


Rings

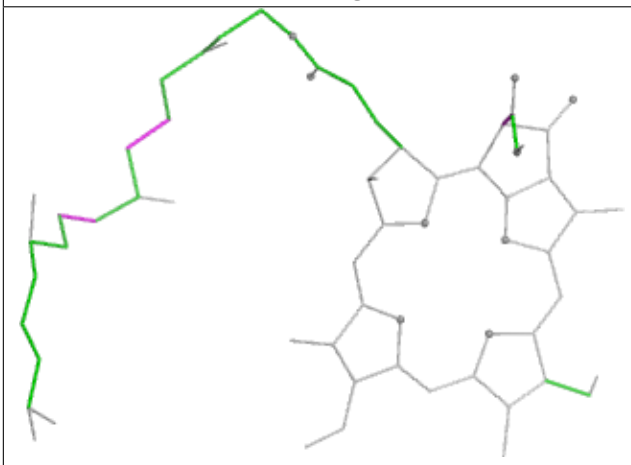
Ligand PHO D 401



Bond lengths



Bond angles

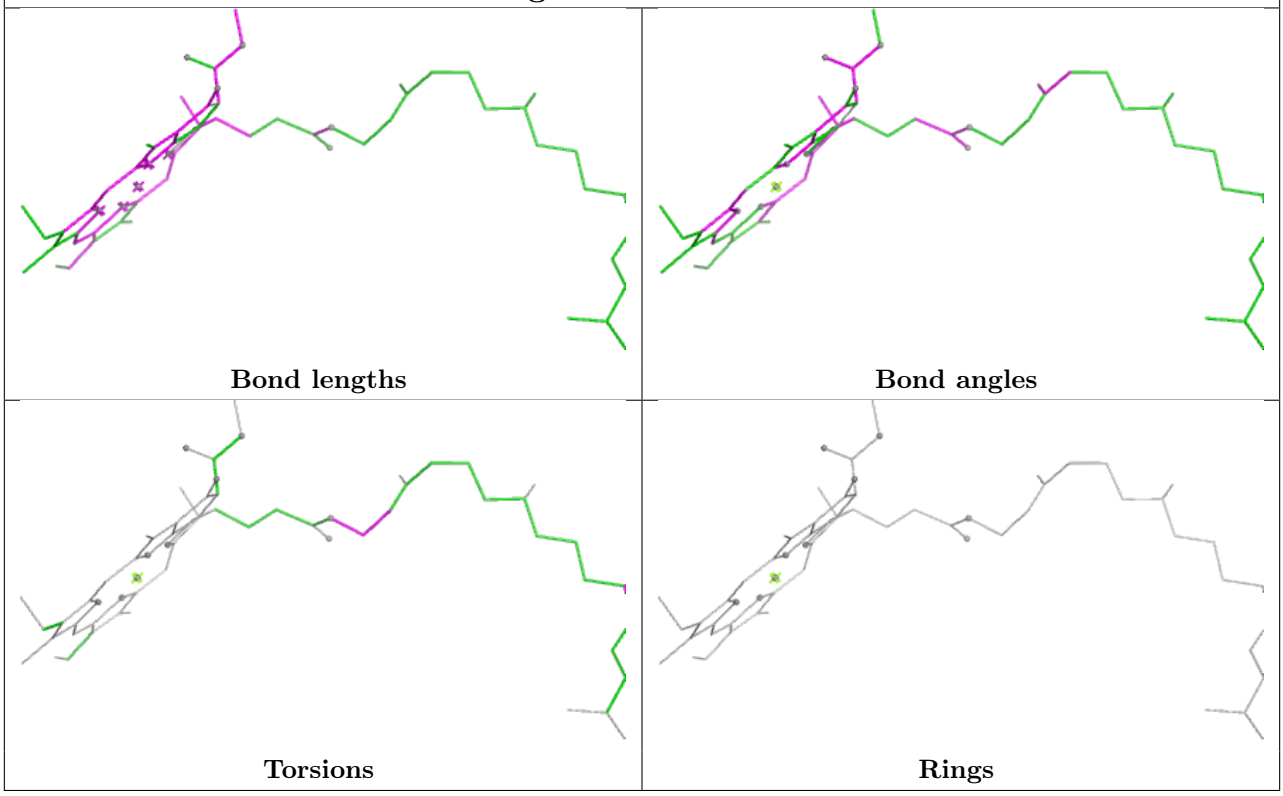


Torsions

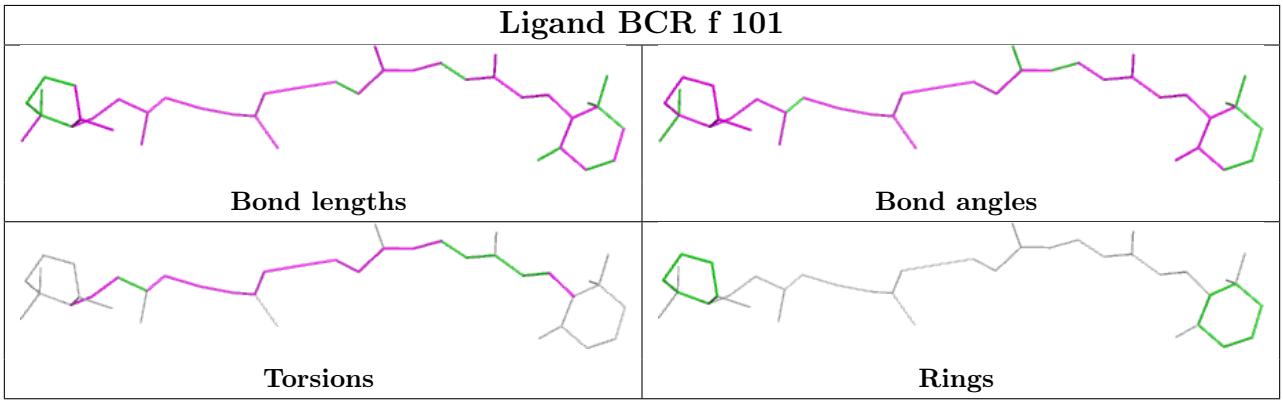


Rings

Ligand CLA d 402



Ligand BCR f 101



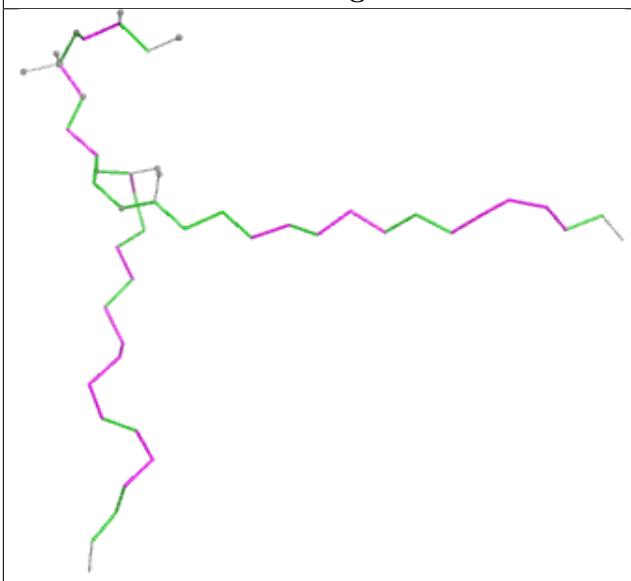
Ligand LHG l 102



Bond lengths



Bond angles

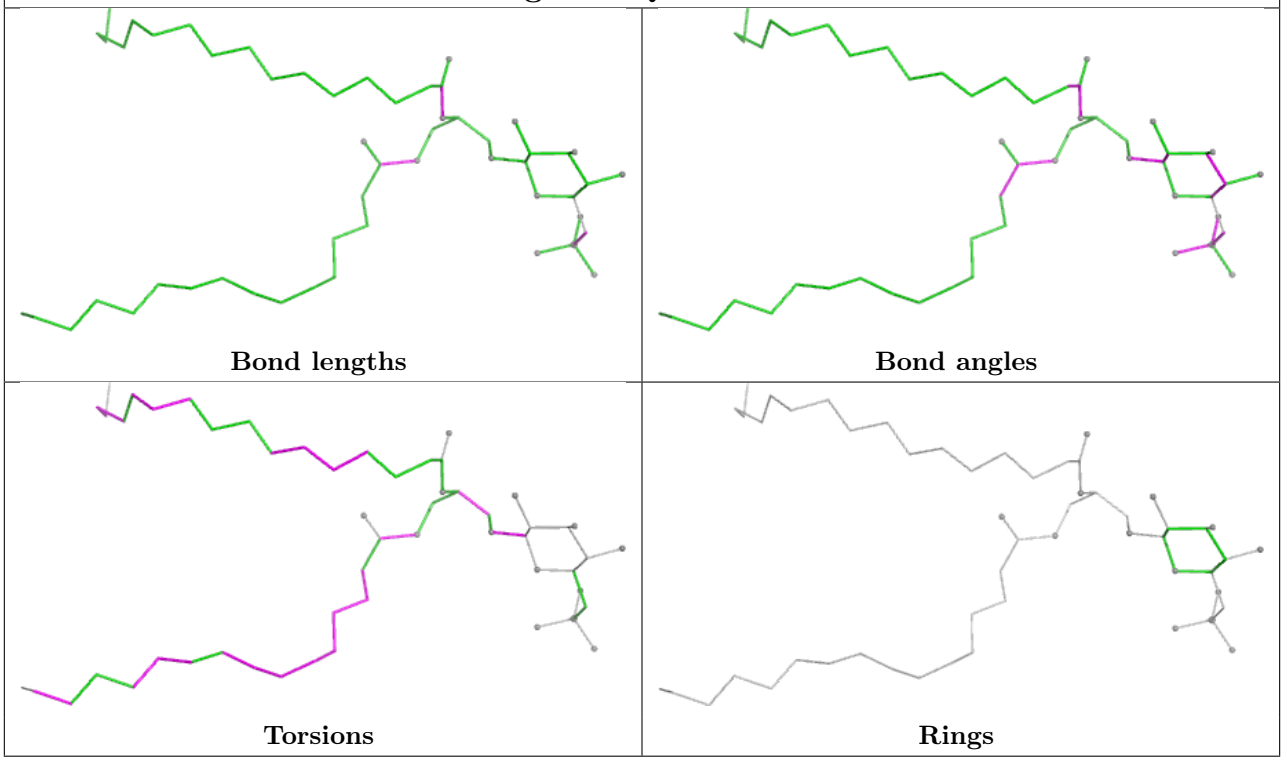


Torsions

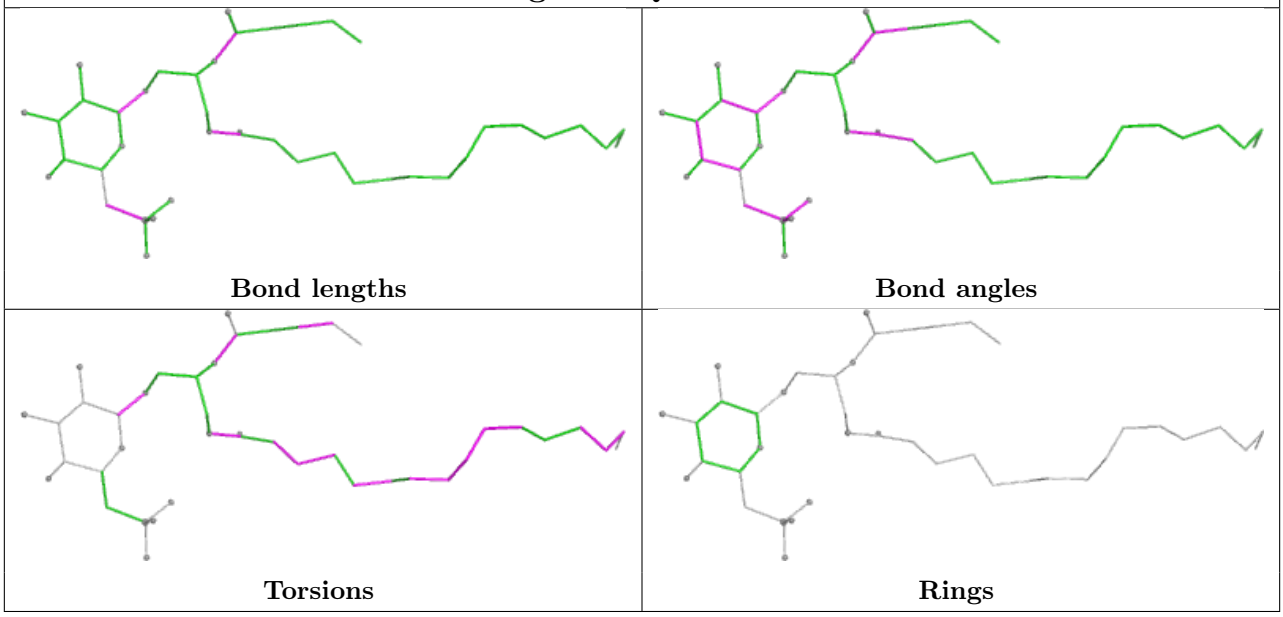


Rings

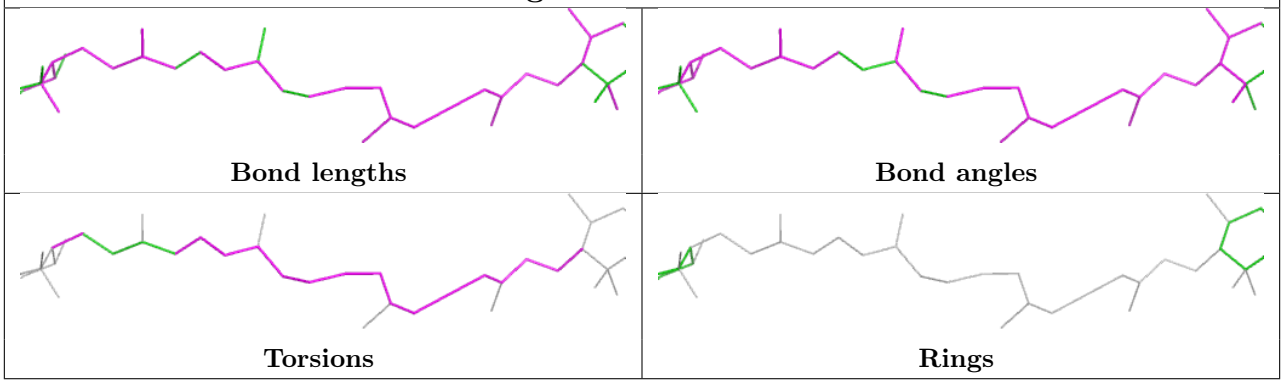
Ligand SQD A 614



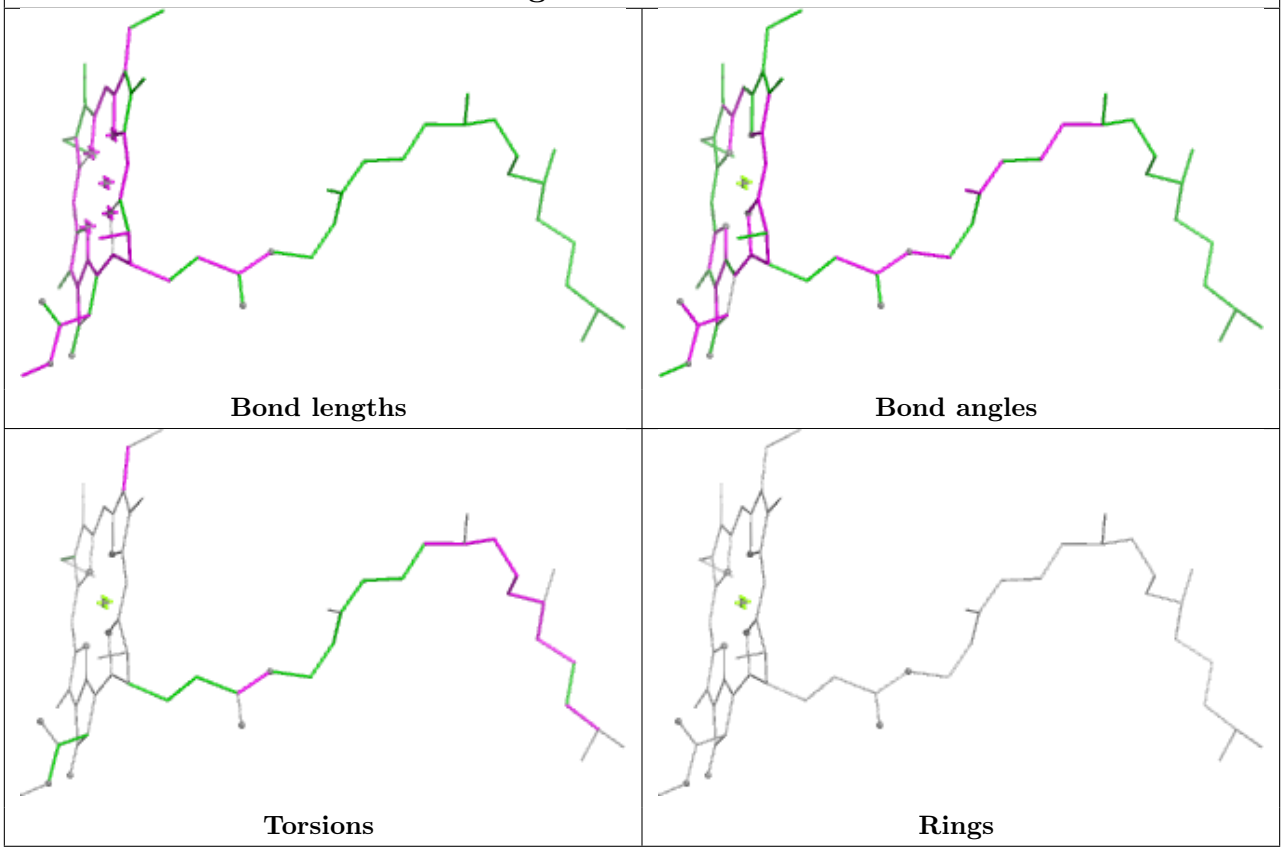
Ligand SQD x 101



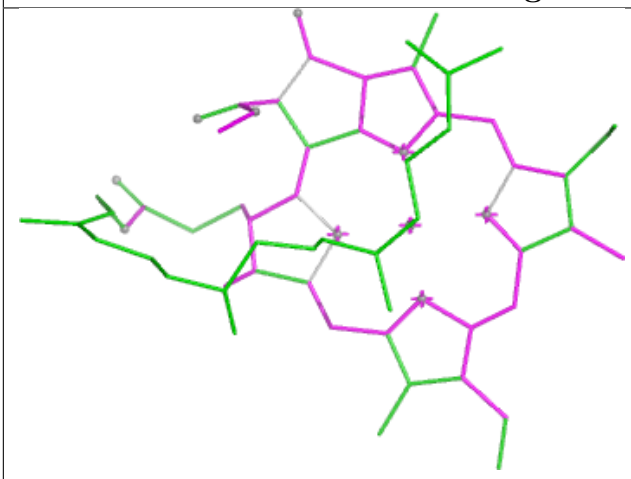
Ligand BCR b 619



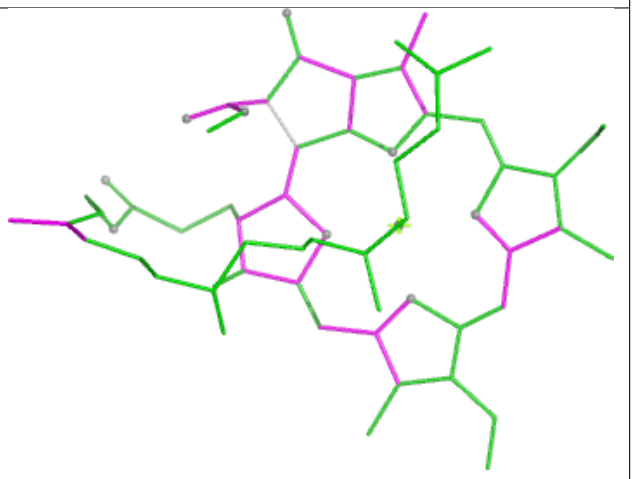
Ligand CLA d 403



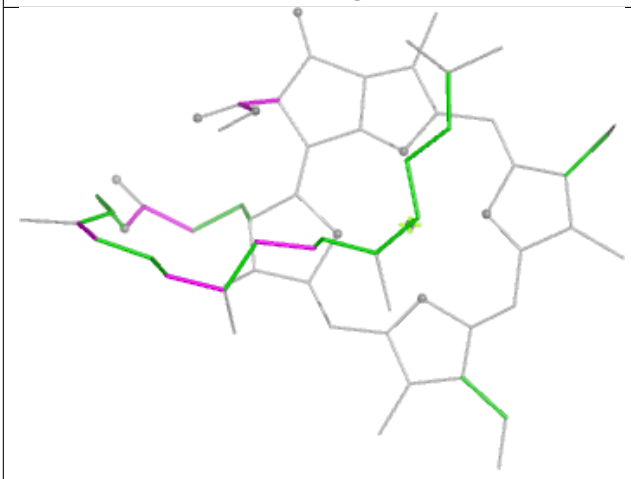
Ligand CLA C 510



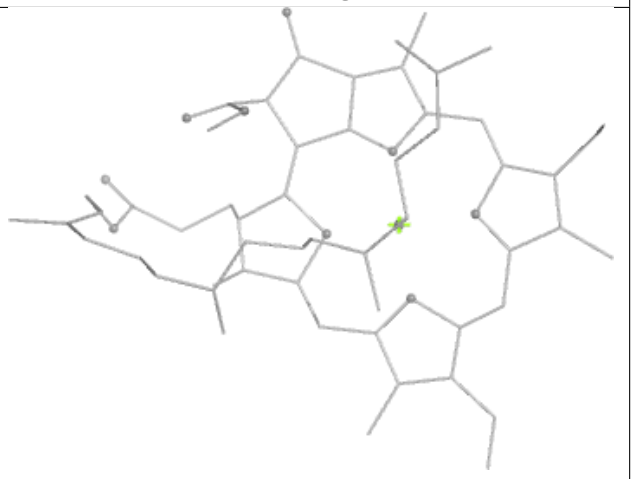
Bond lengths



Bond angles

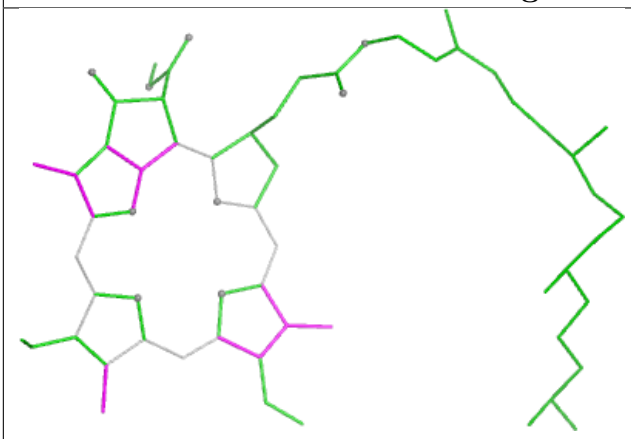


Torsions

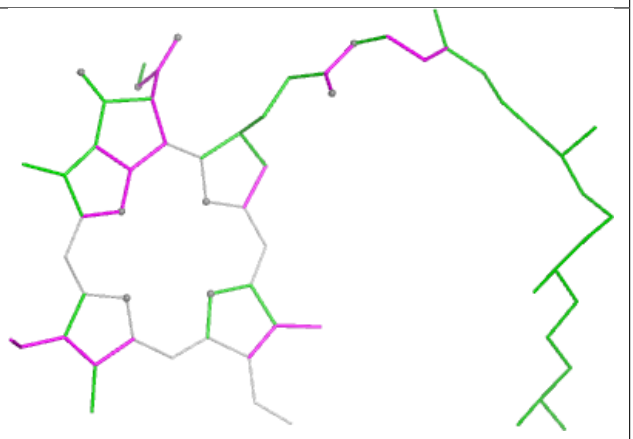


Rings

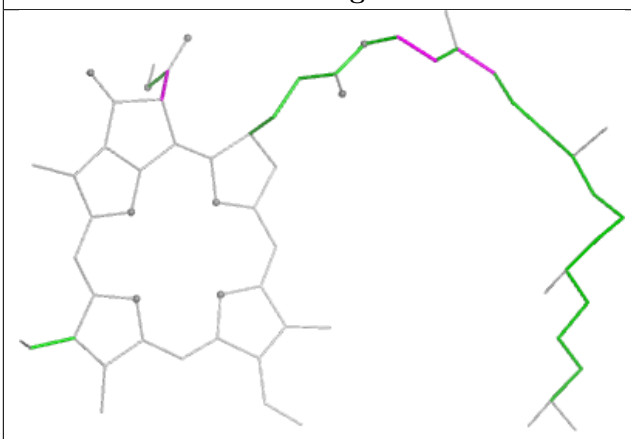
Ligand PHO A 608



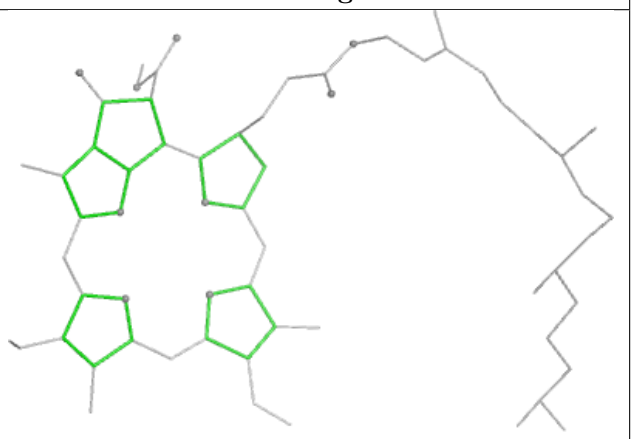
Bond lengths



Bond angles

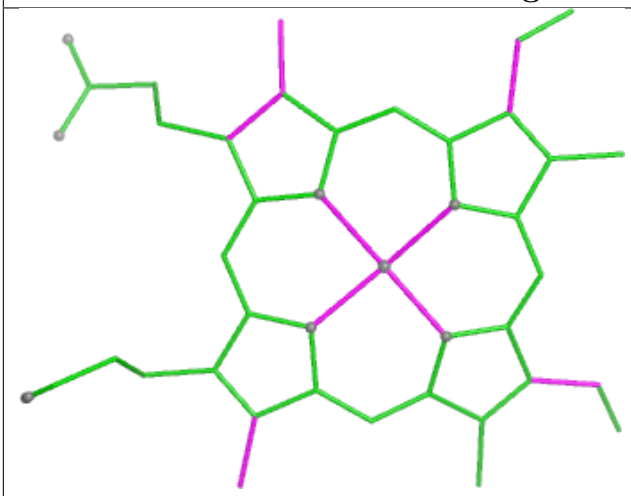


Torsions

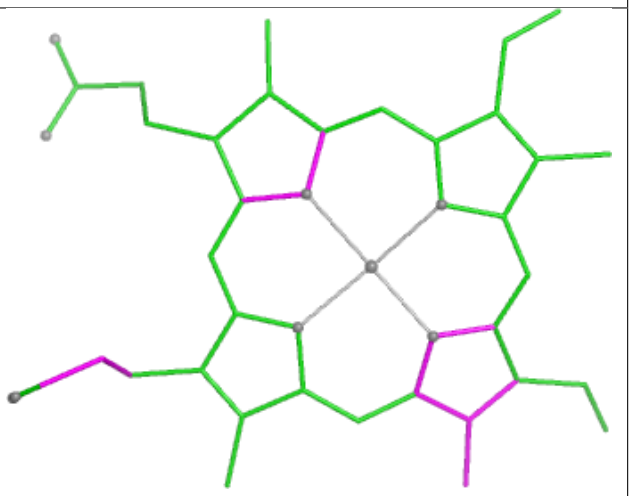


Rings

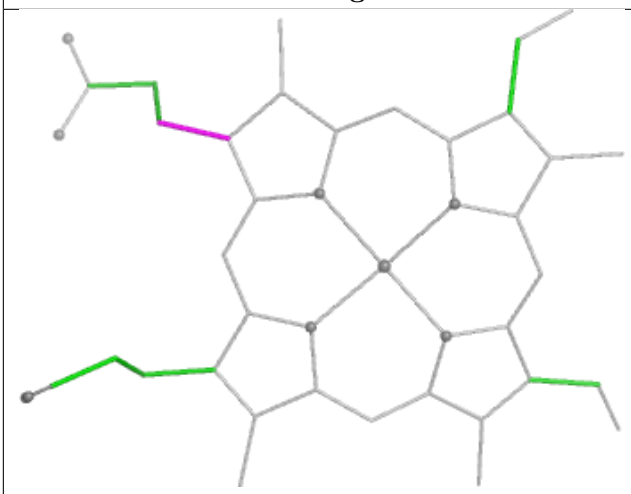
Ligand HEM v 201



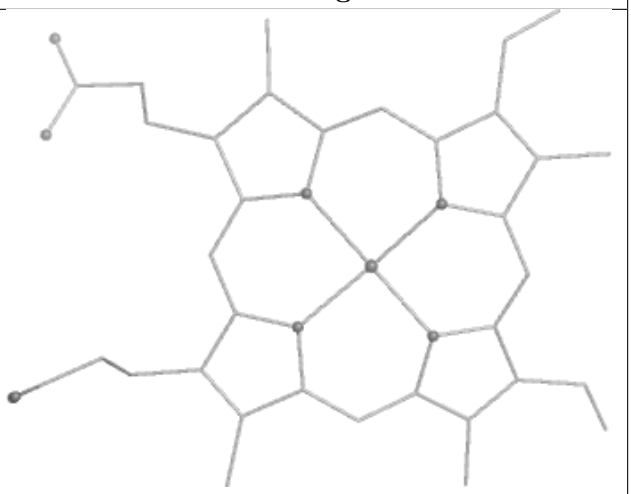
Bond lengths



Bond angles

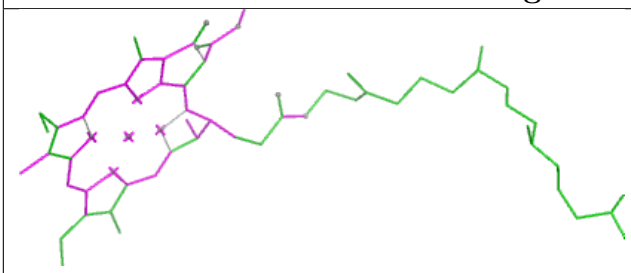


Torsions

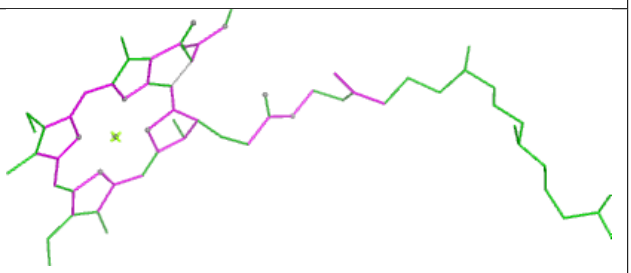


Rings

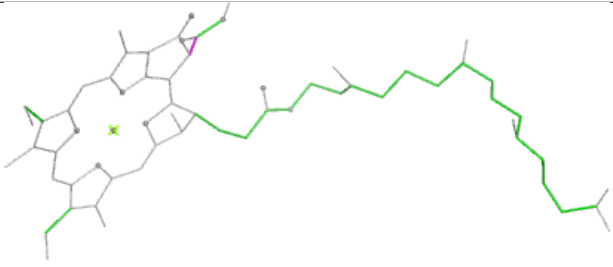
Ligand CLA A 606



Bond lengths



Bond angles

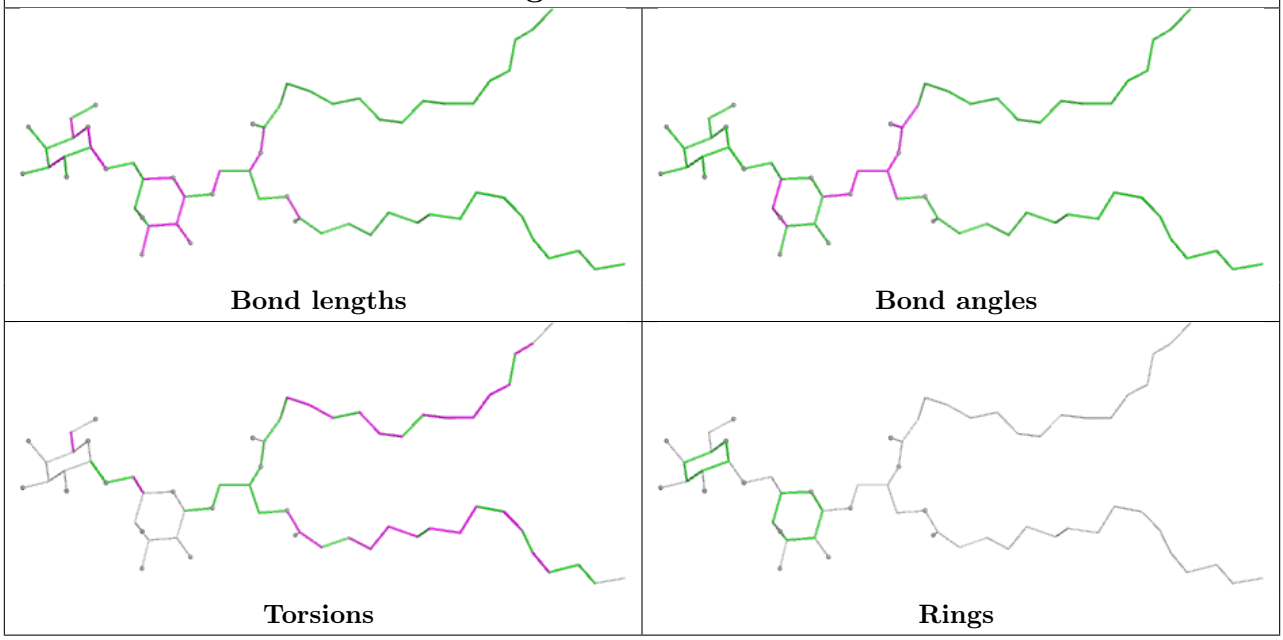


Torsions

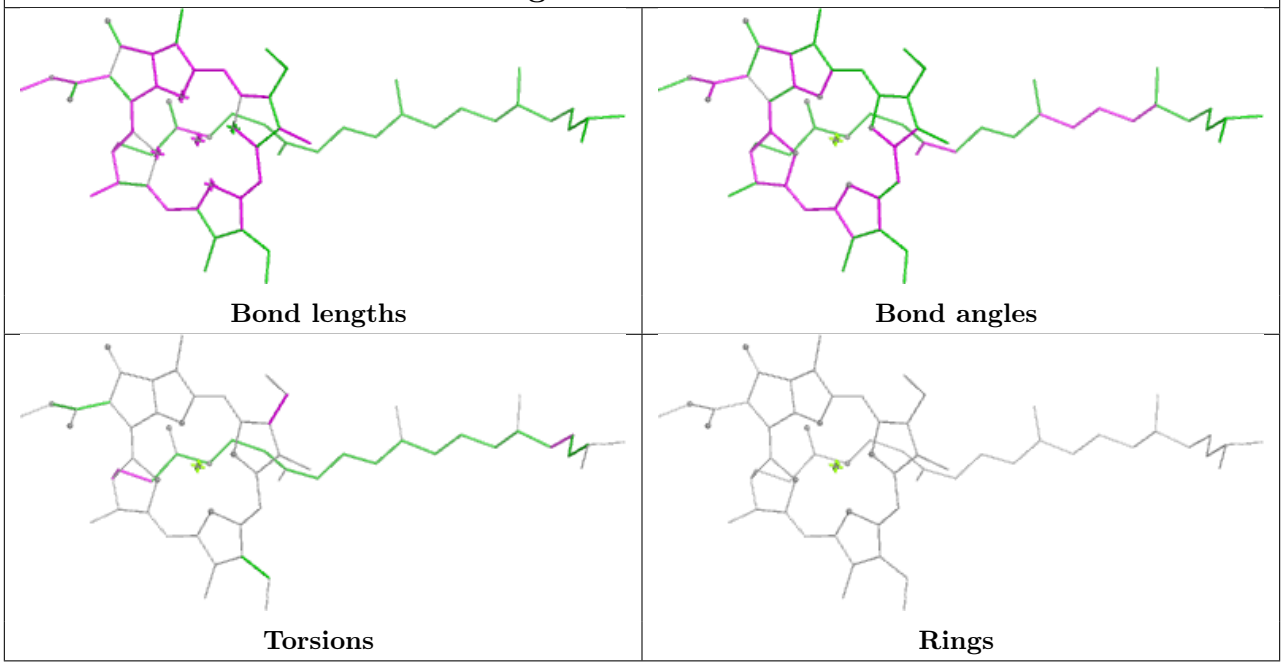


Rings

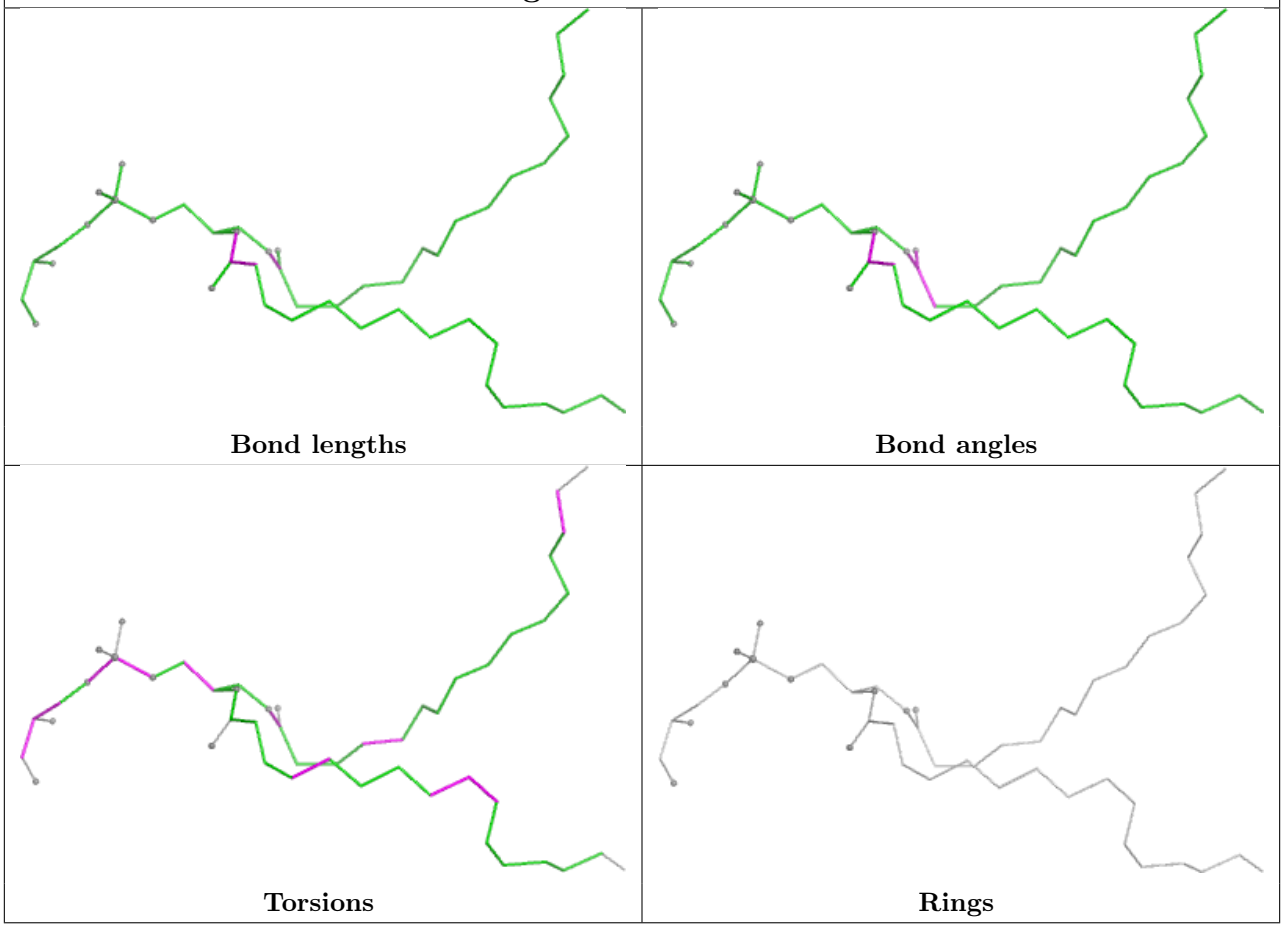
Ligand DGD c 518



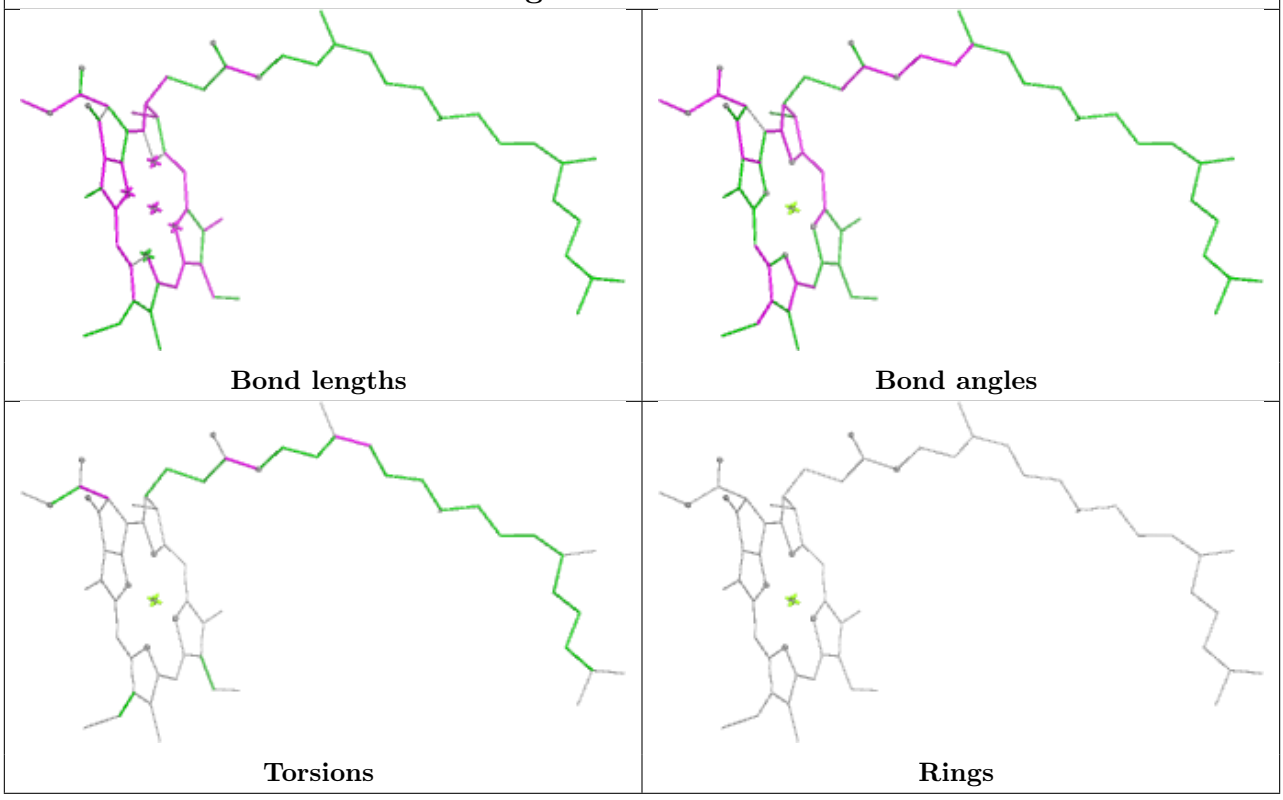
Ligand CLA b 610



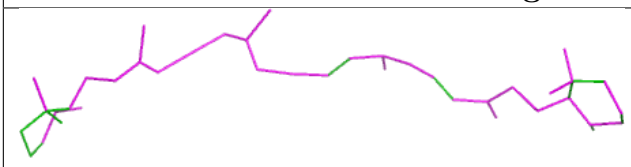
Ligand LHG D 407



Ligand CLA B 610



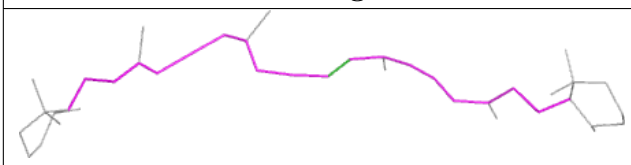
Ligand BCR T 101



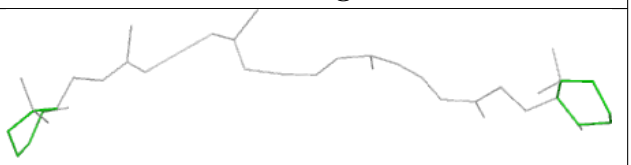
Bond lengths



Bond angles

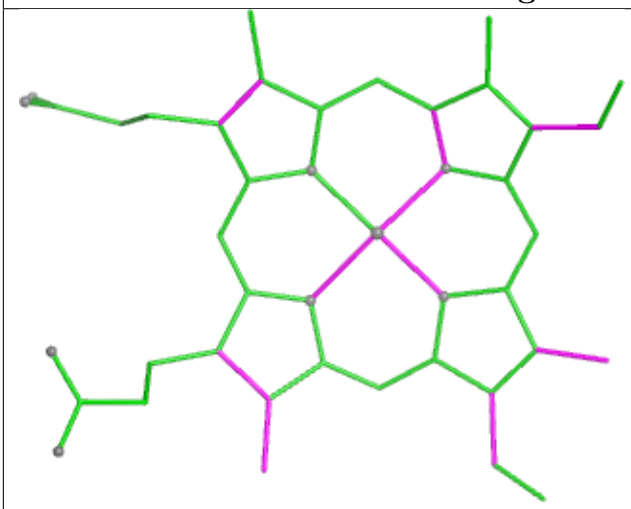


Torsions

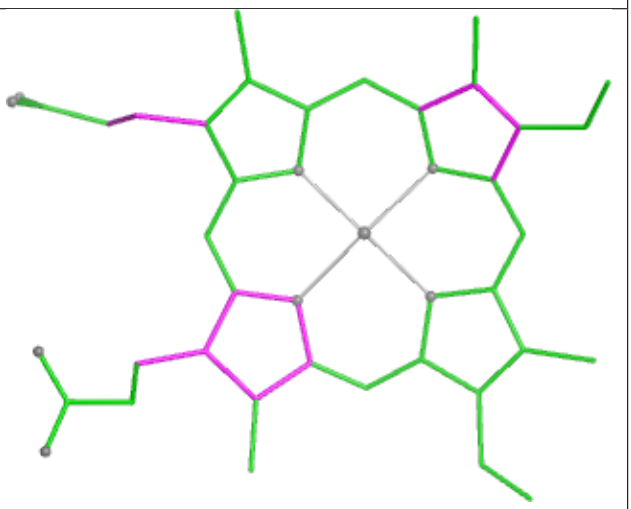


Rings

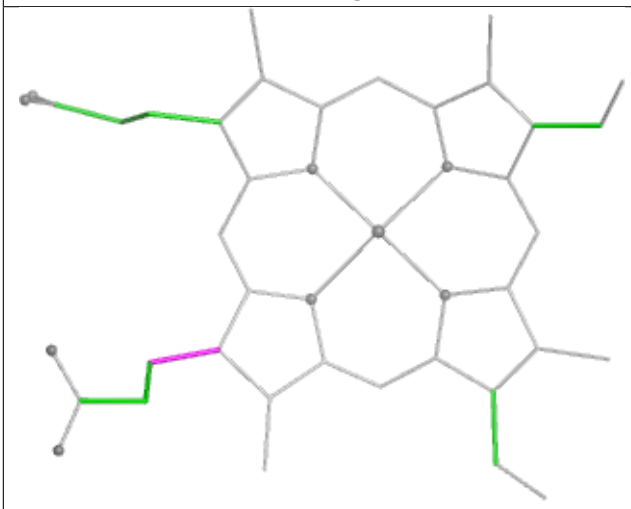
Ligand HEM V 201



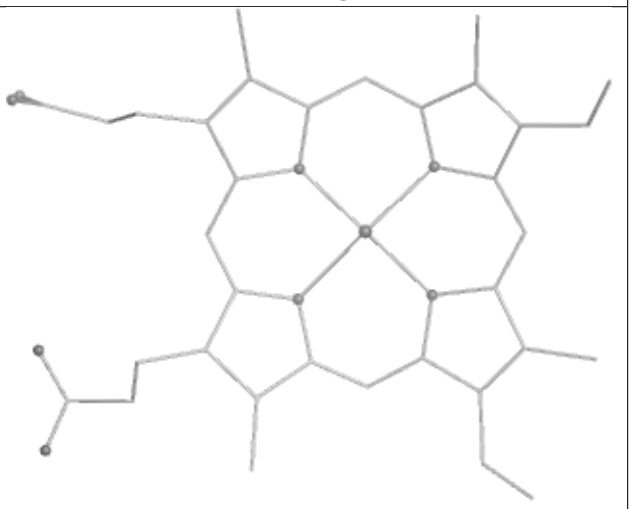
Bond lengths



Bond angles

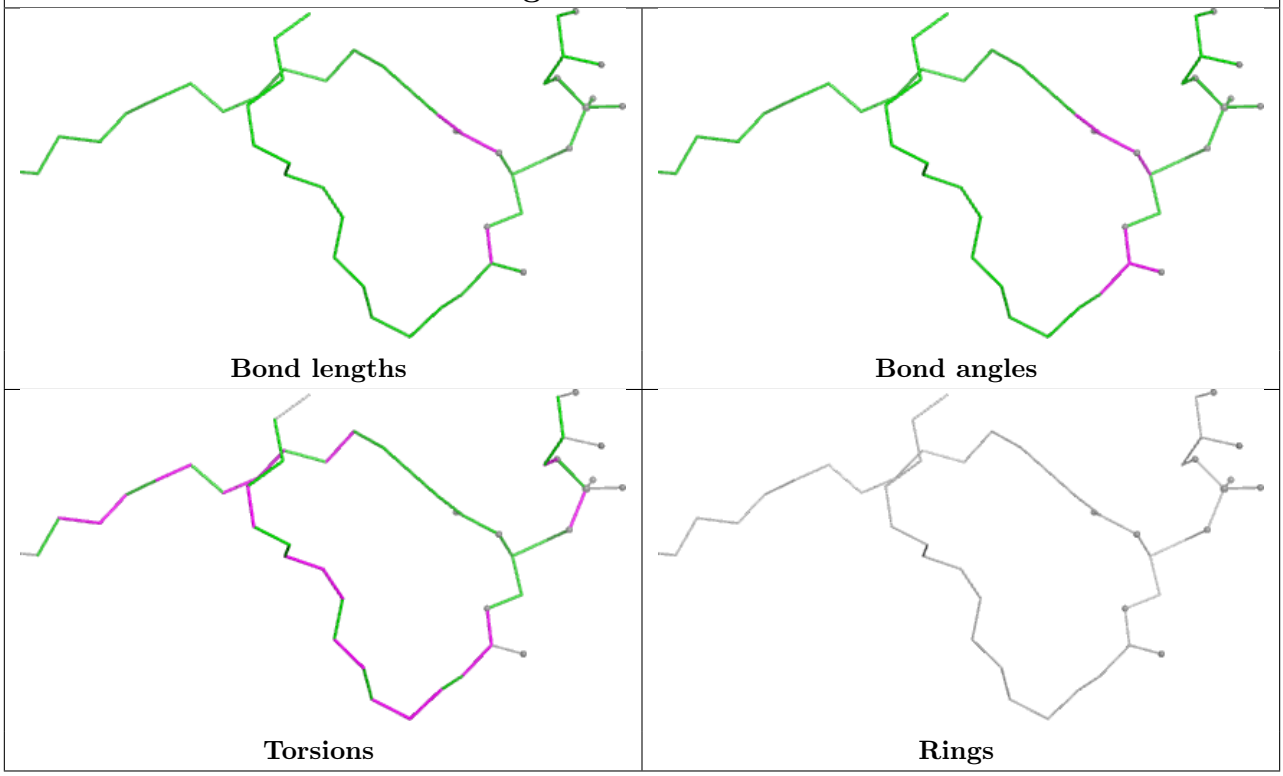


Torsions

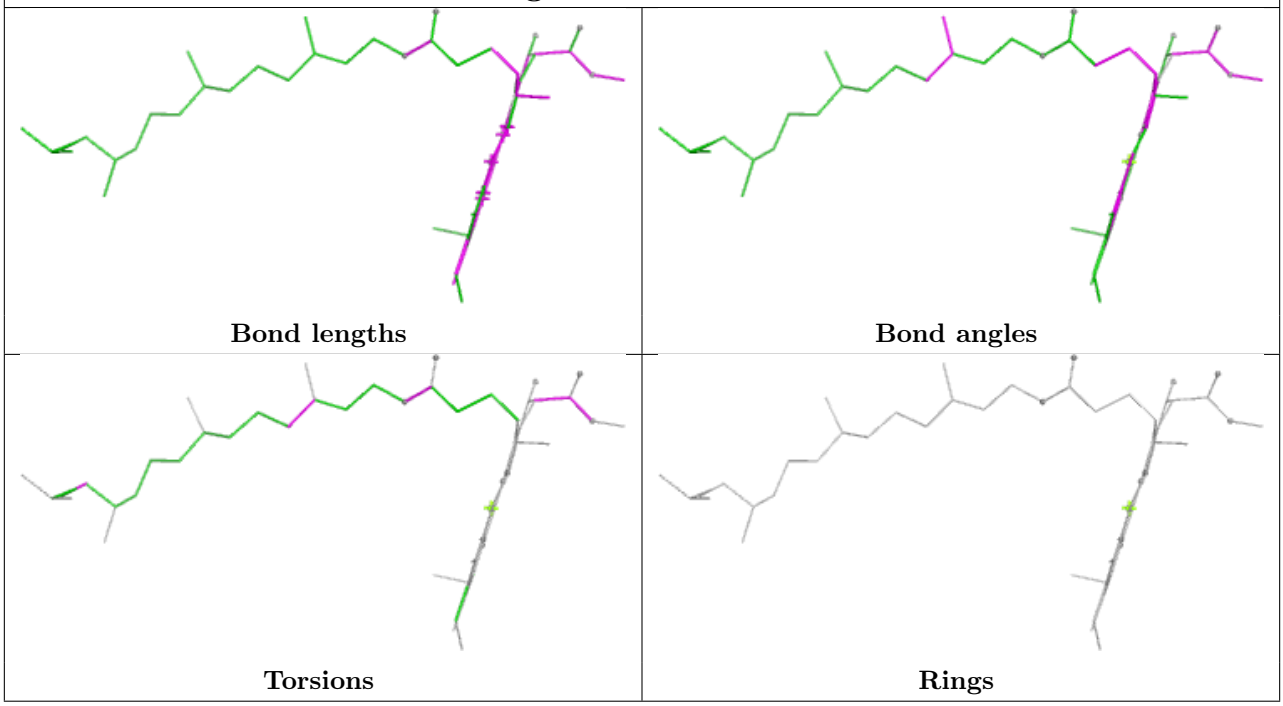


Rings

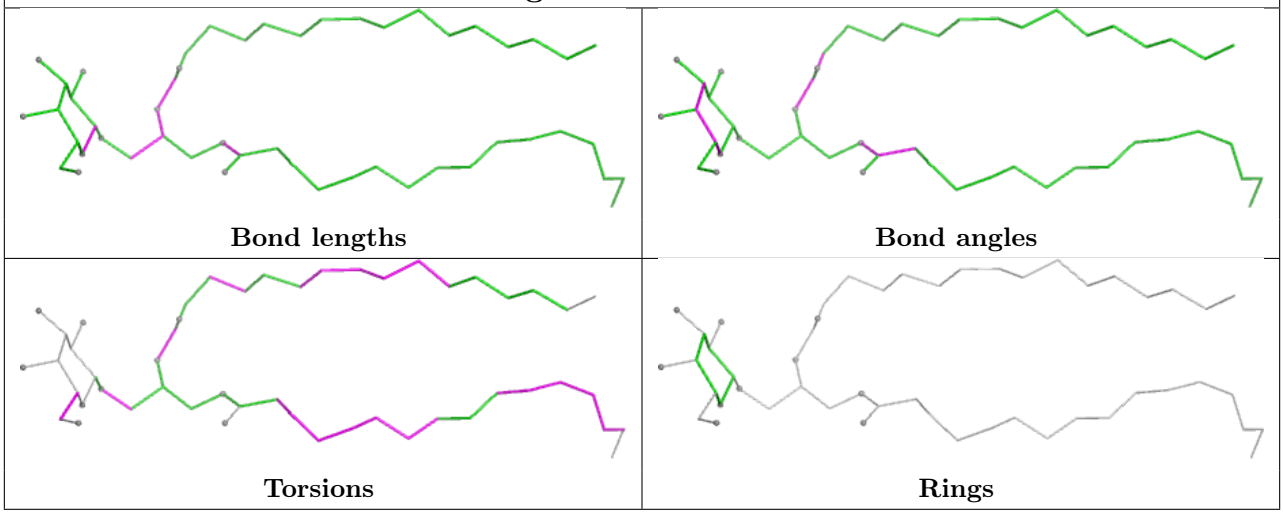
Ligand LHG A 615



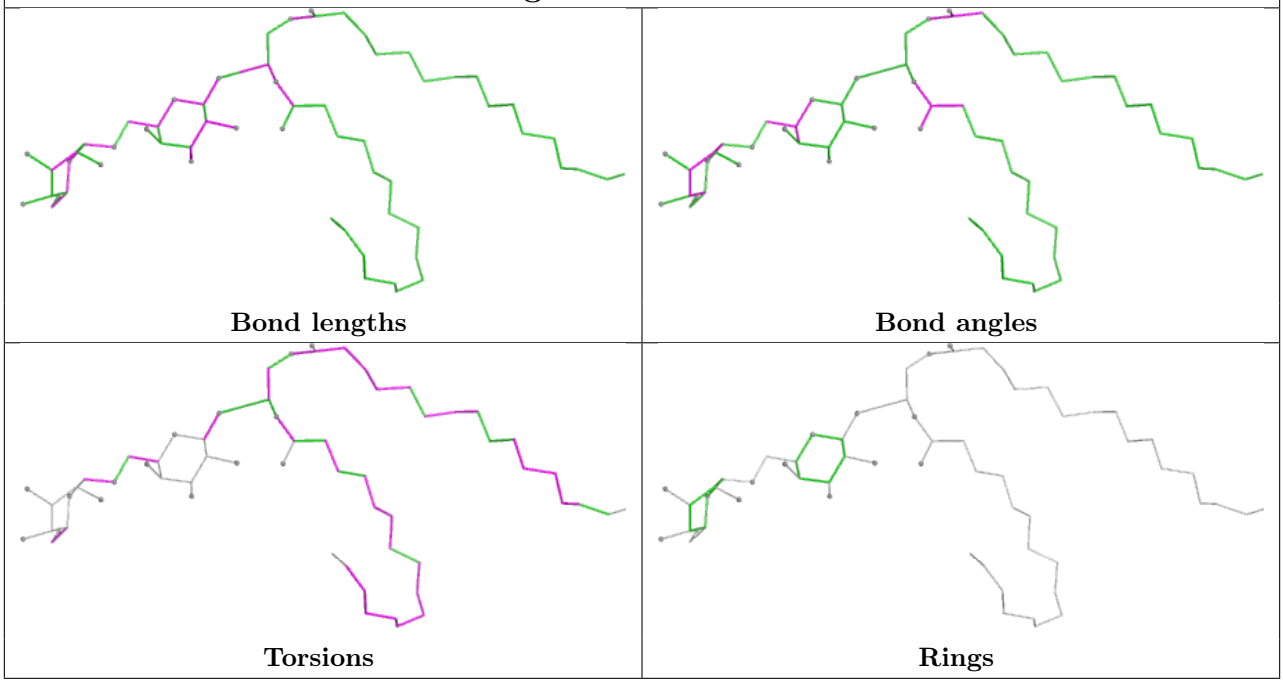
Ligand CLA B 606



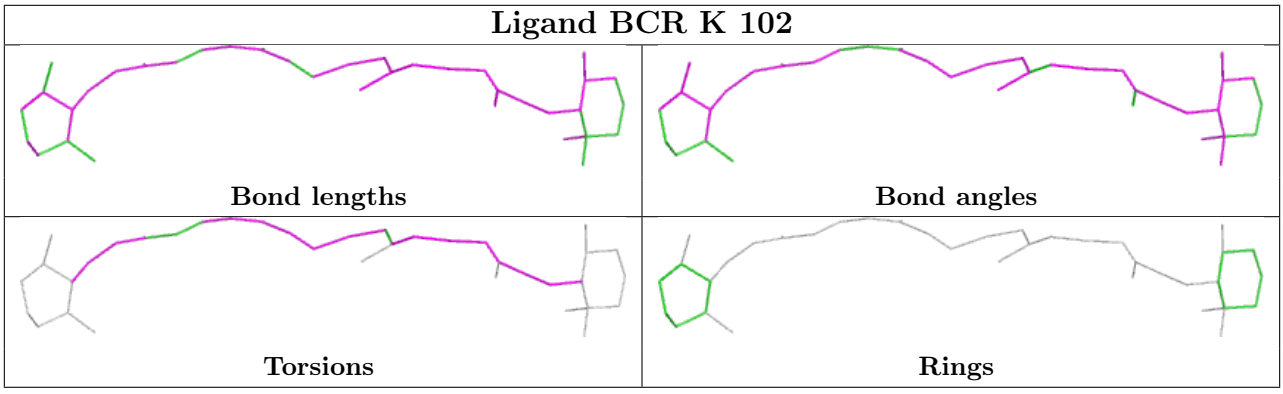
Ligand LMG c 520



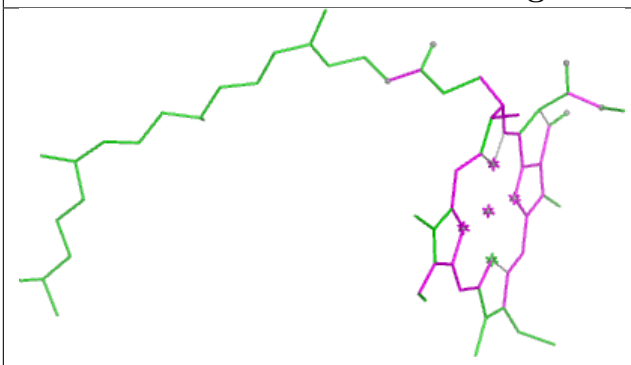
Ligand DGD d 405



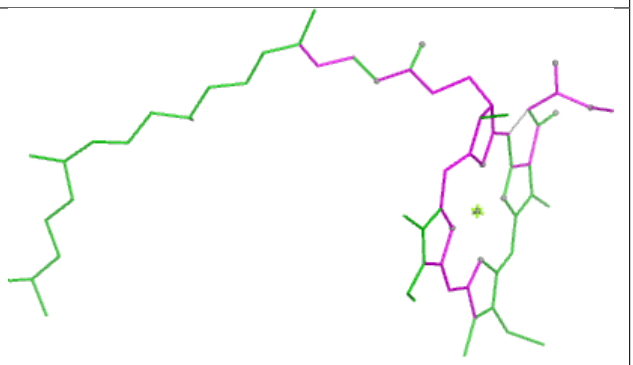
Ligand BCR K 102



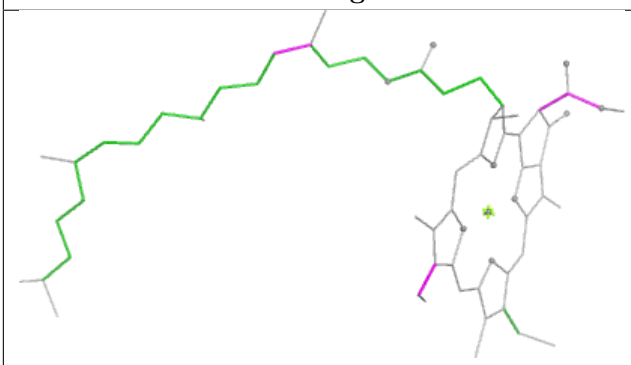
Ligand CLA b 611



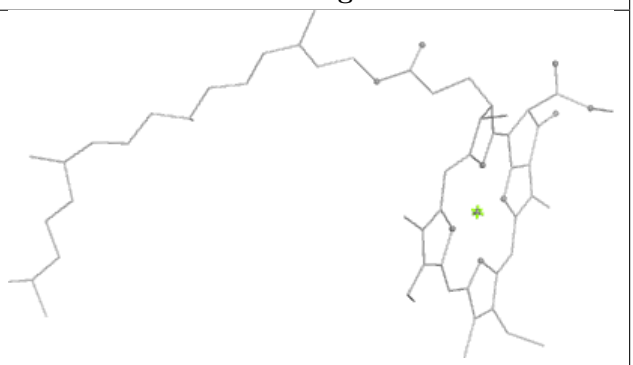
Bond lengths



Bond angles

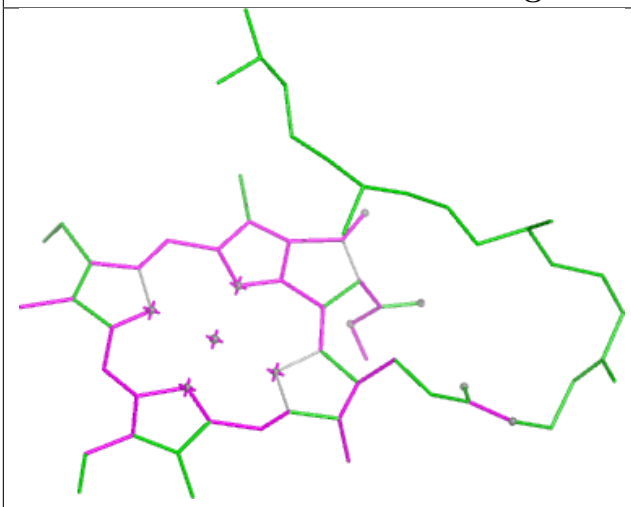


Torsions

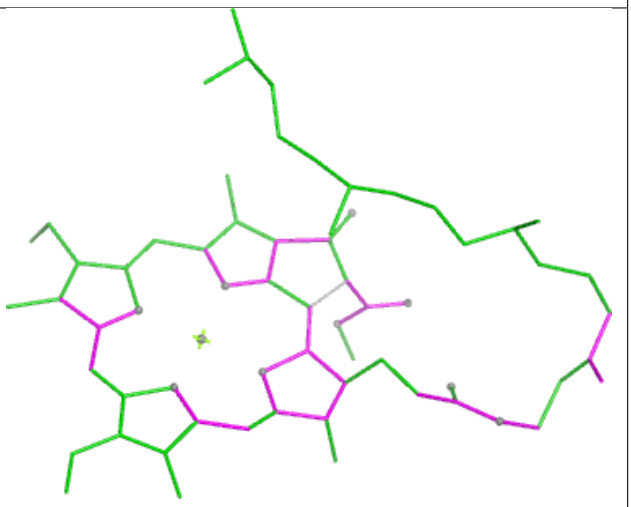


Rings

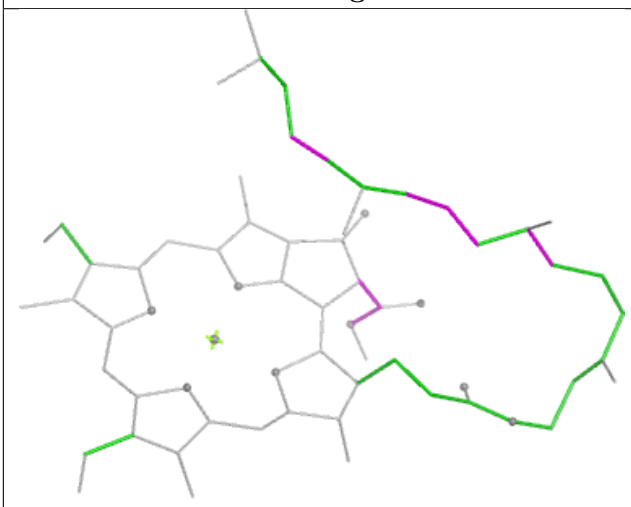
Ligand CLA C 509



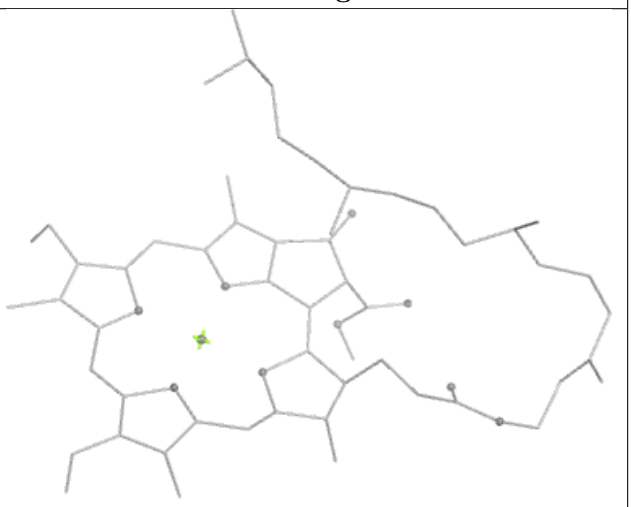
Bond lengths



Bond angles

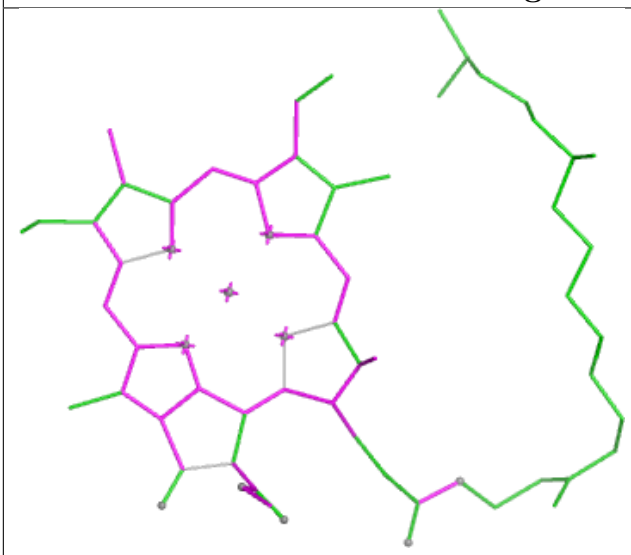


Torsions

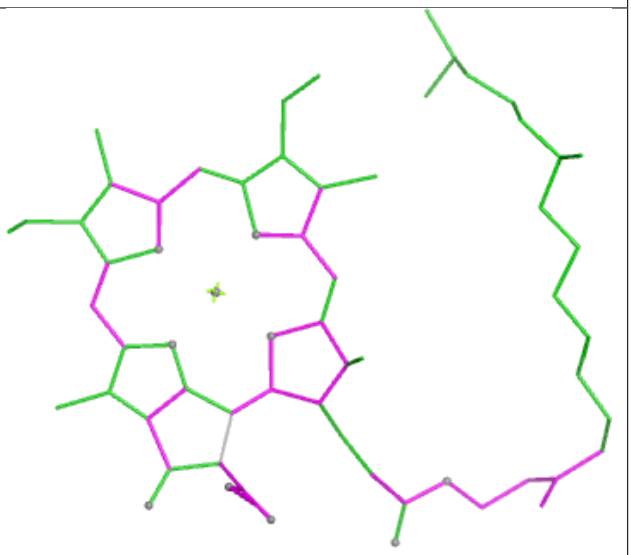


Rings

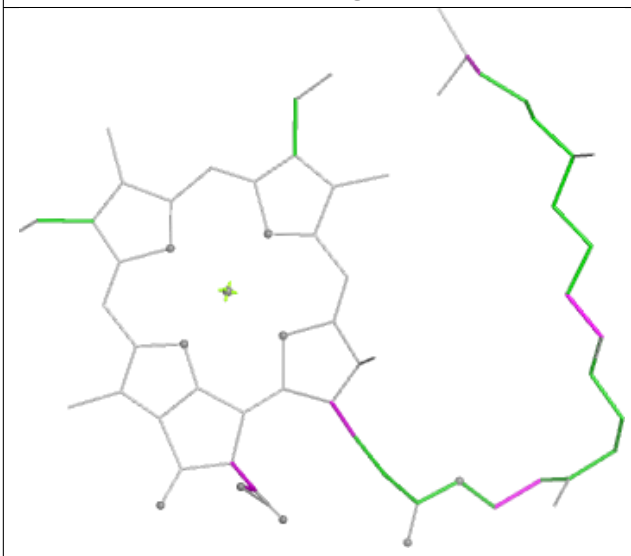
Ligand CLA C 512



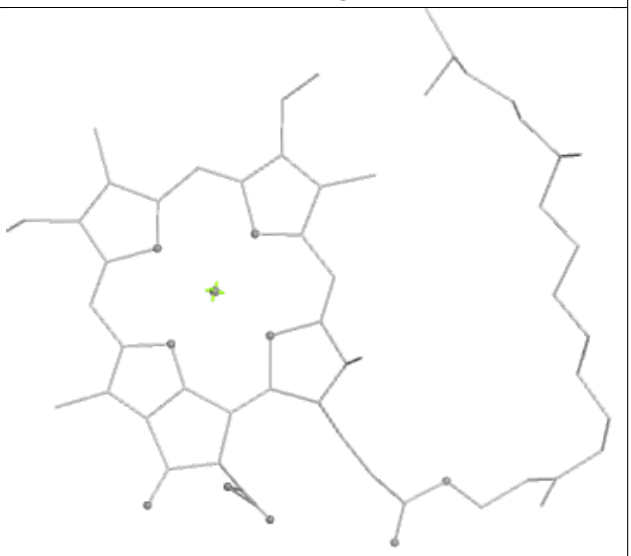
Bond lengths



Bond angles

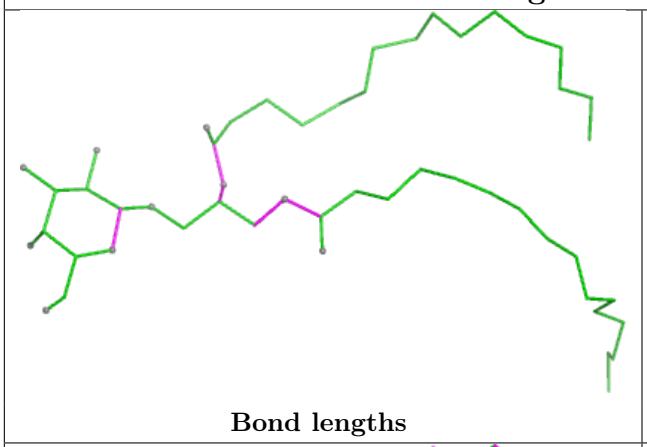


Torsions

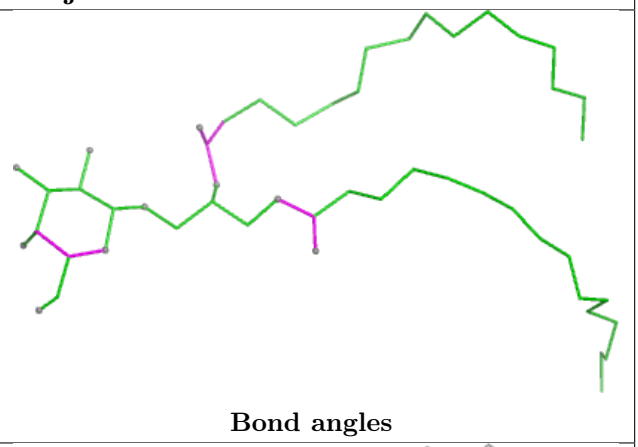


Rings

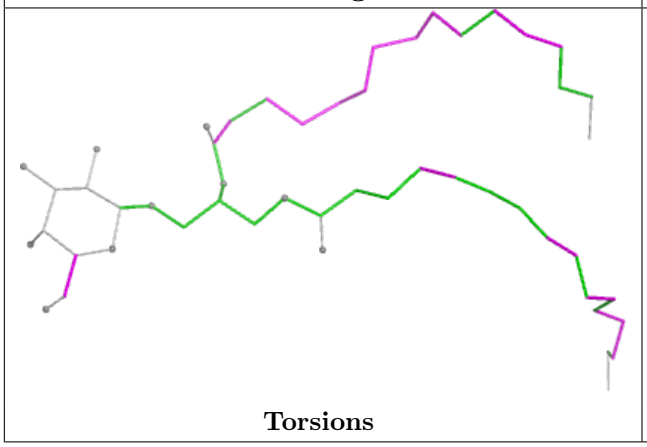
Ligand LMG j 101



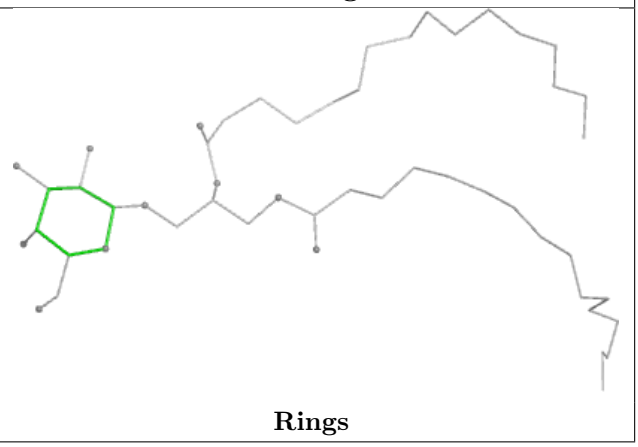
Bond lengths



Bond angles

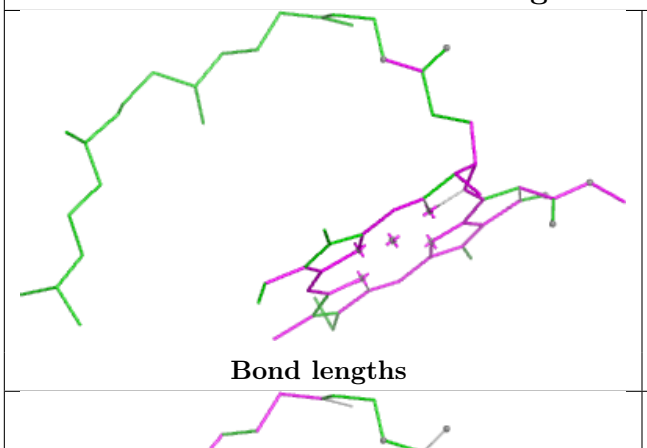


Torsions

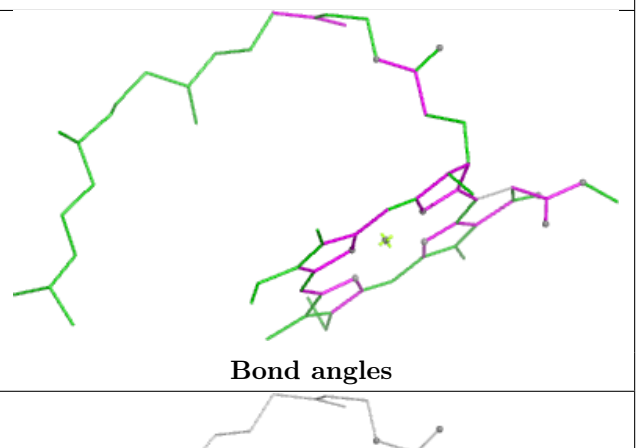


Rings

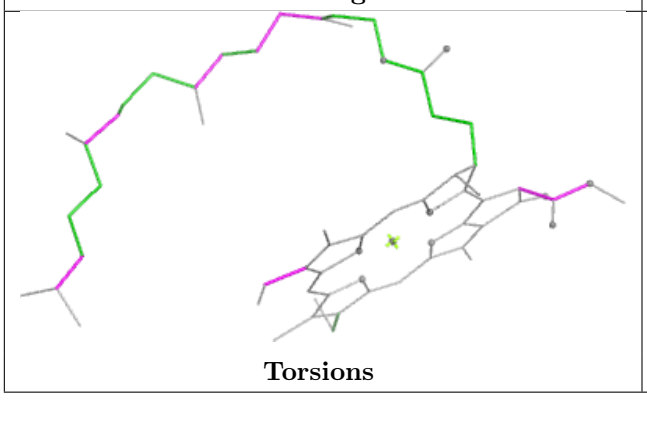
Ligand CLA c 513



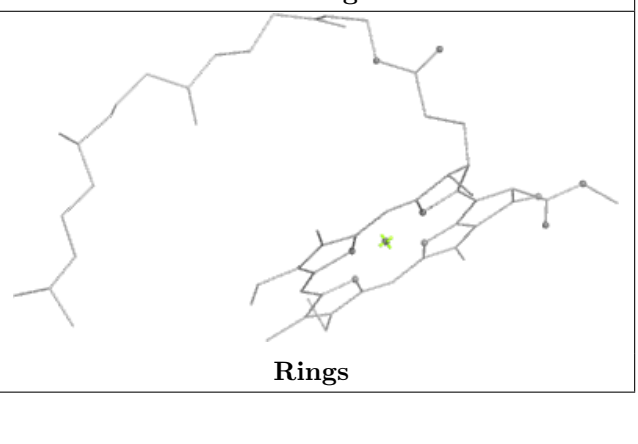
Bond lengths



Bond angles

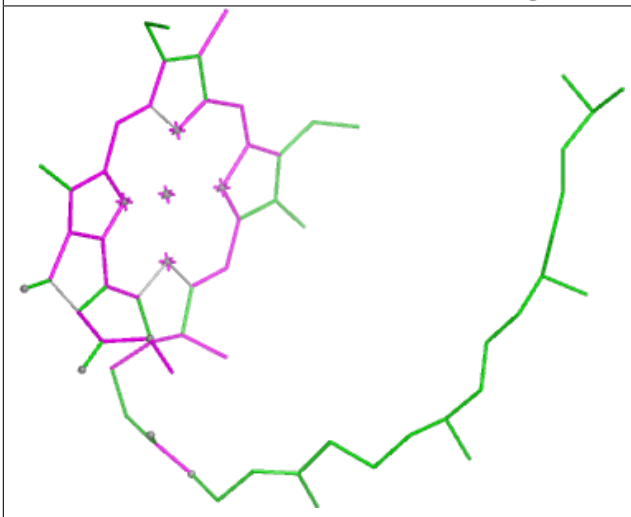


Torsions

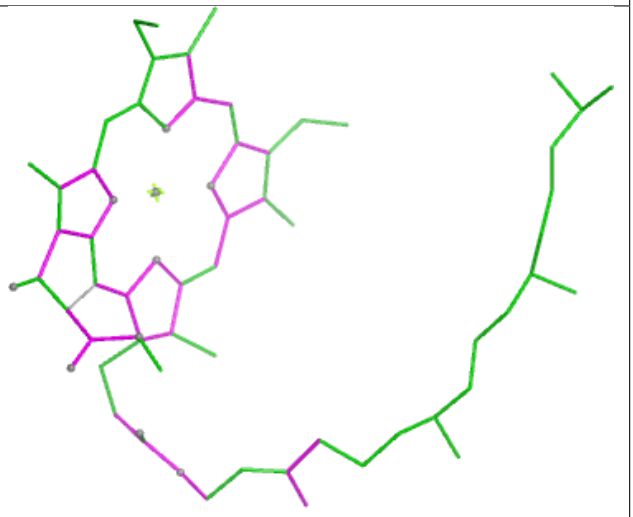


Rings

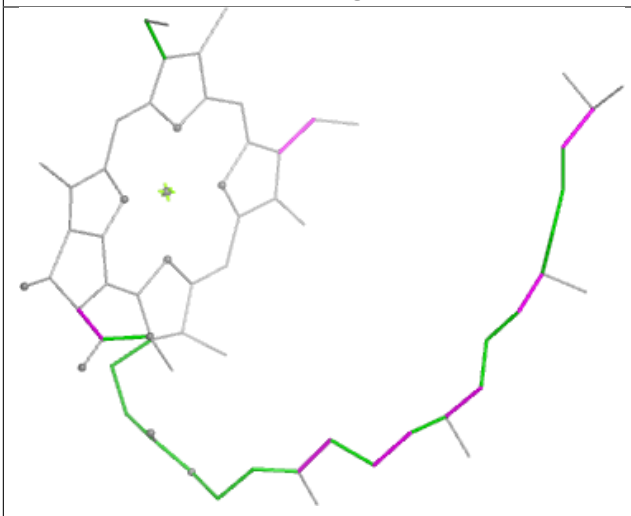
Ligand CLA C 507



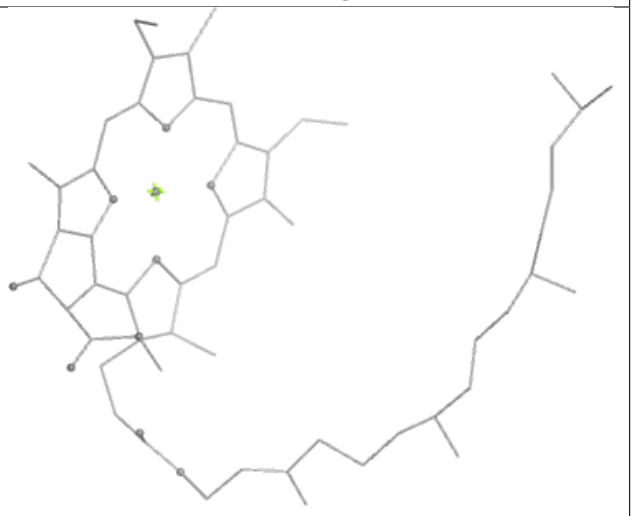
Bond lengths



Bond angles

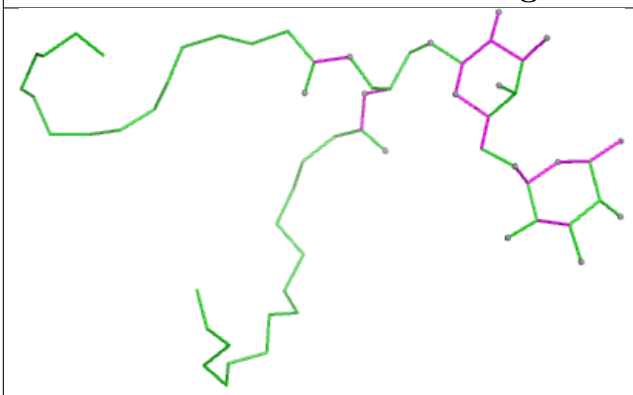


Torsions

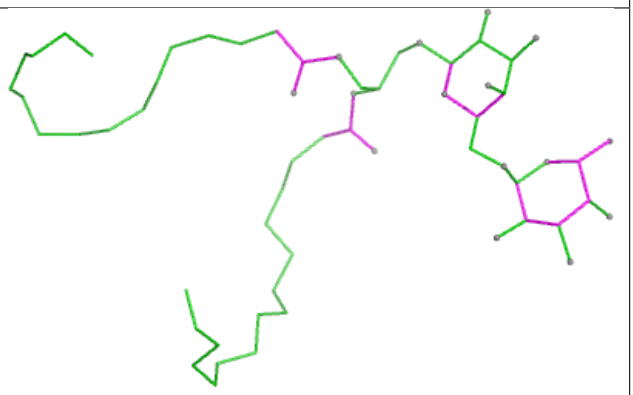


Rings

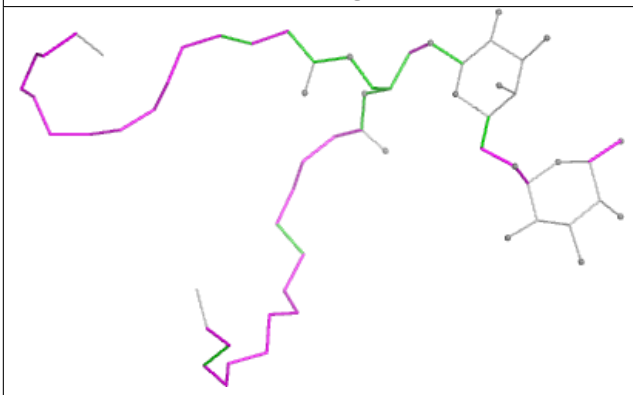
Ligand DGD C 516



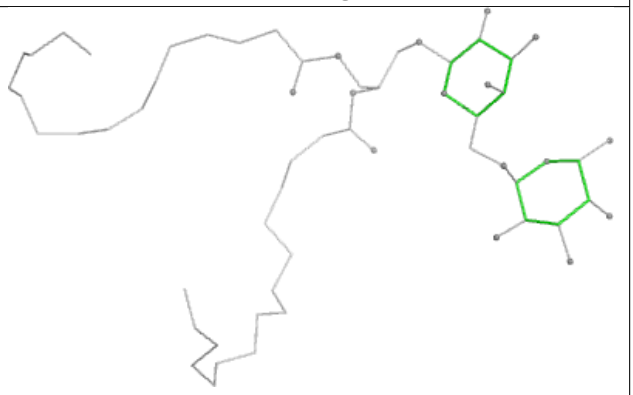
Bond lengths



Bond angles

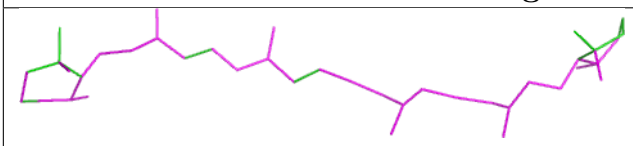


Torsions

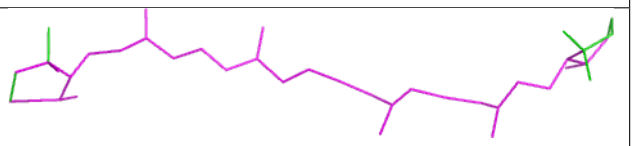


Rings

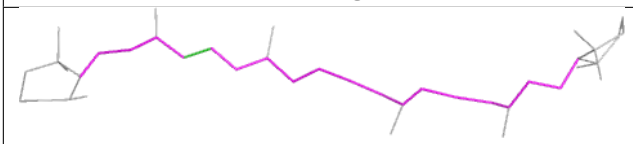
Ligand BCR C 514



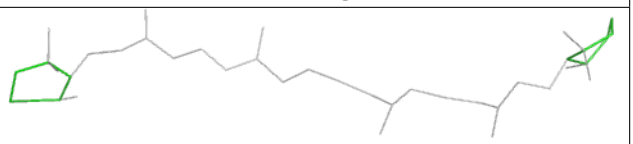
Bond lengths



Bond angles

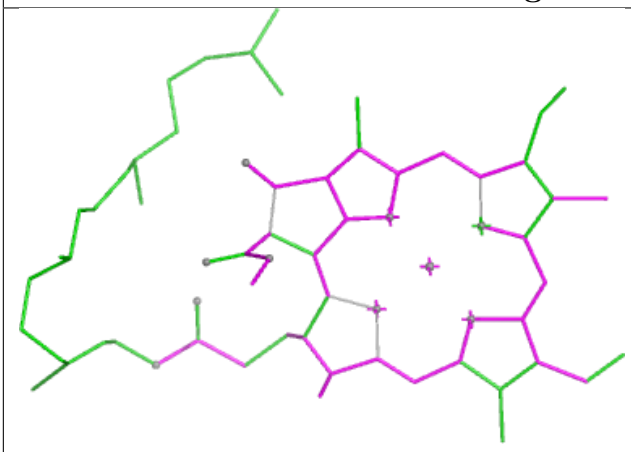


Torsions

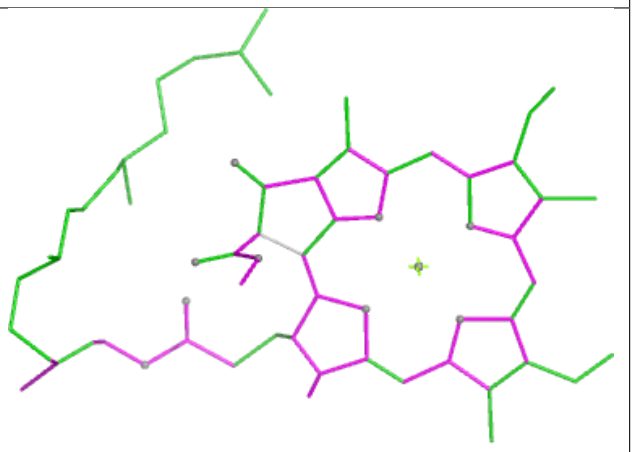


Rings

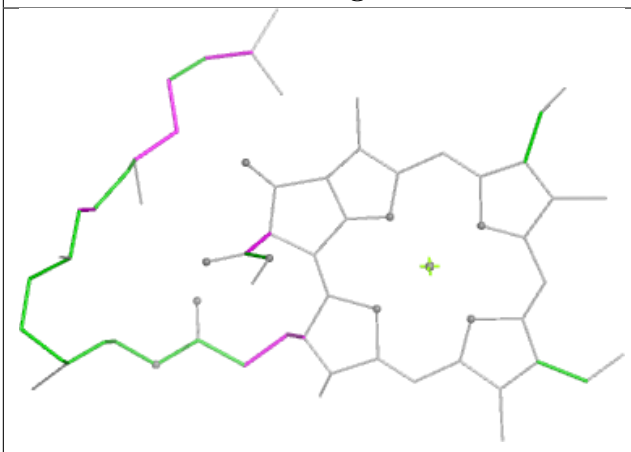
Ligand CLA B 611



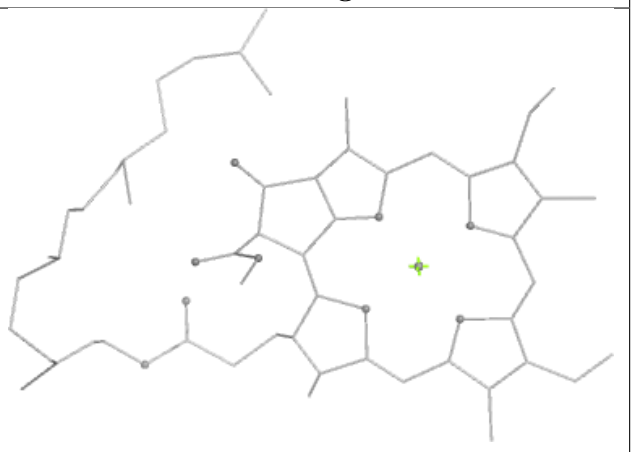
Bond lengths



Bond angles

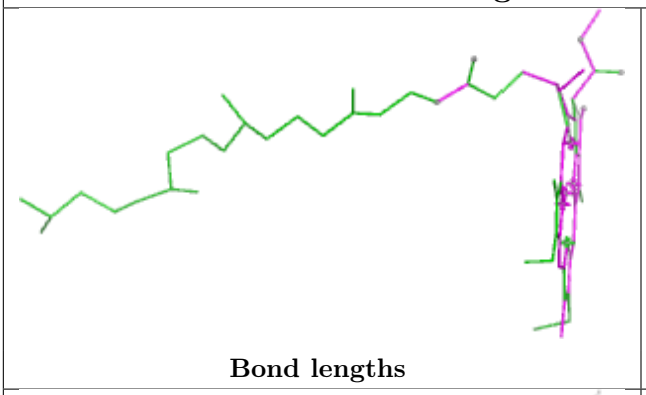


Torsions

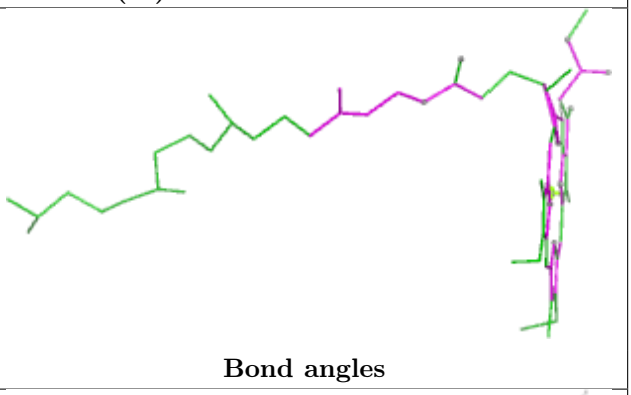


Rings

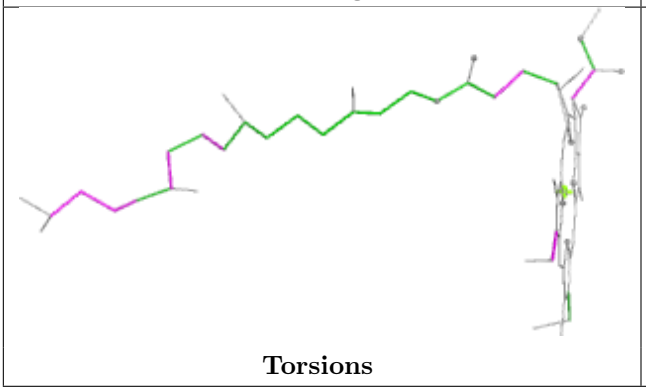
Ligand CLA b 608 (A)



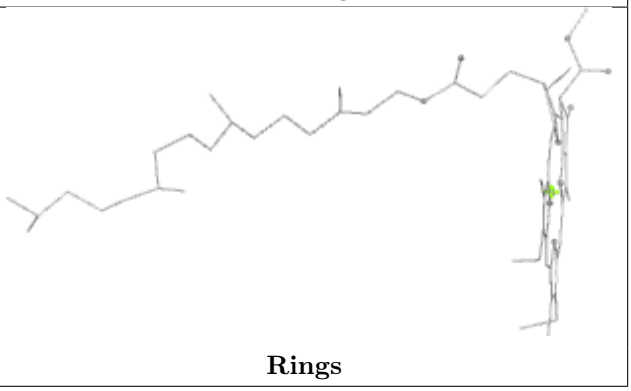
Bond lengths



Bond angles

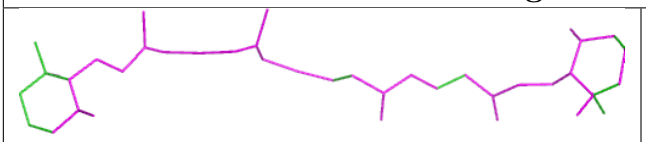


Torsions

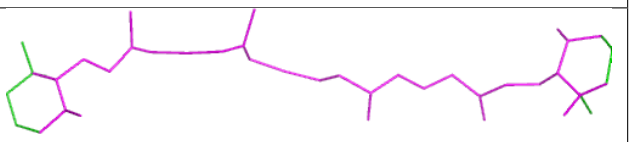


Rings

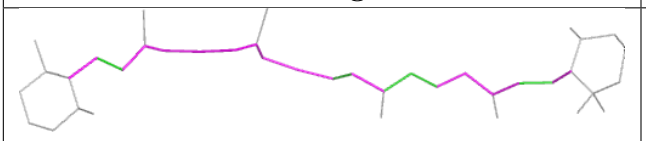
Ligand BCR b 621



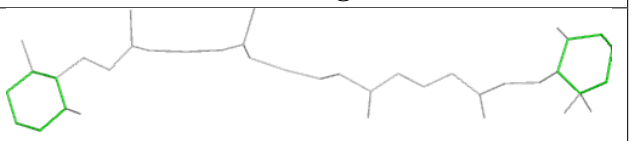
Bond lengths



Bond angles

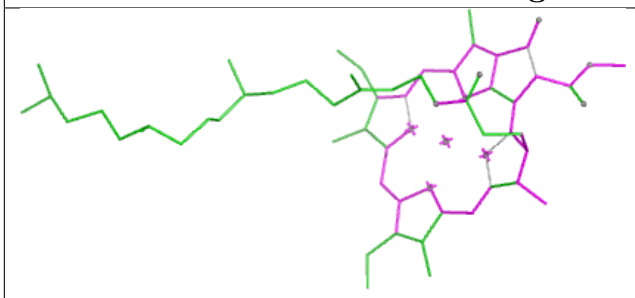


Torsions

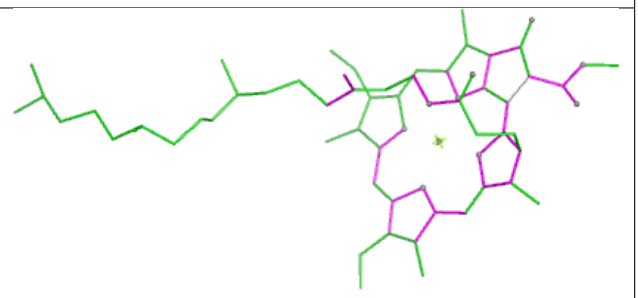


Rings

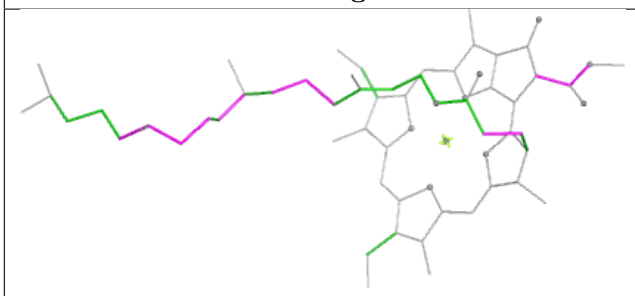
Ligand CLA b 616



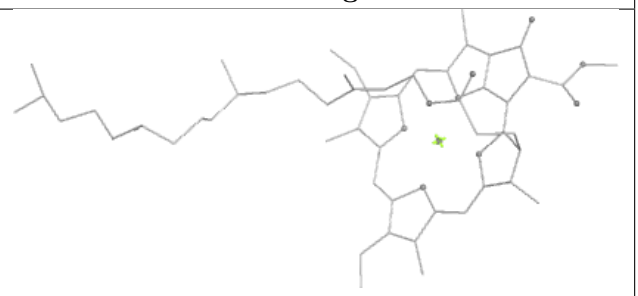
Bond lengths



Bond angles

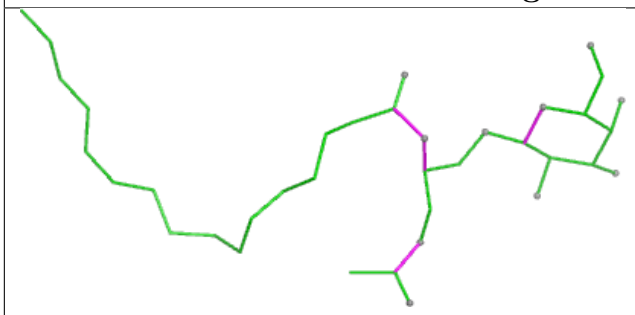


Torsions

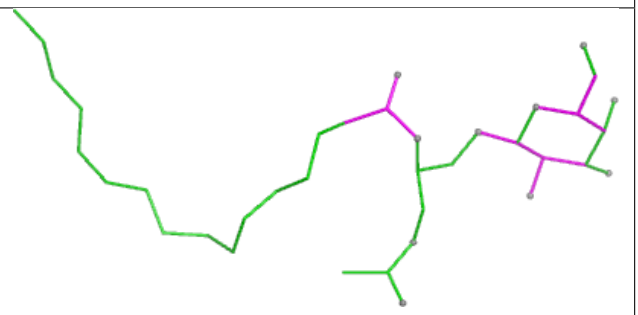


Rings

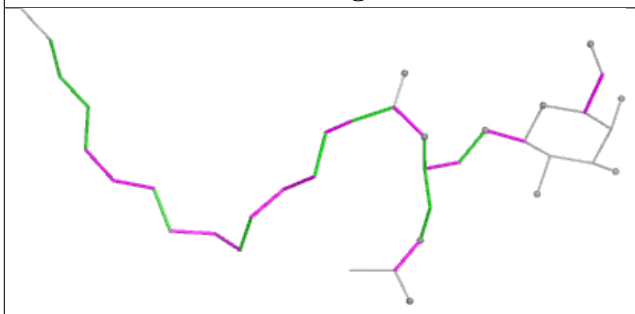
Ligand LMG Z 101



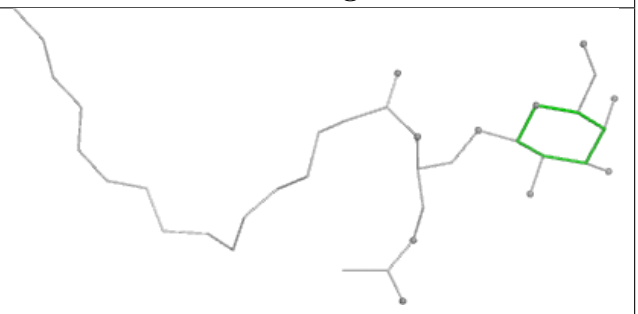
Bond lengths



Bond angles

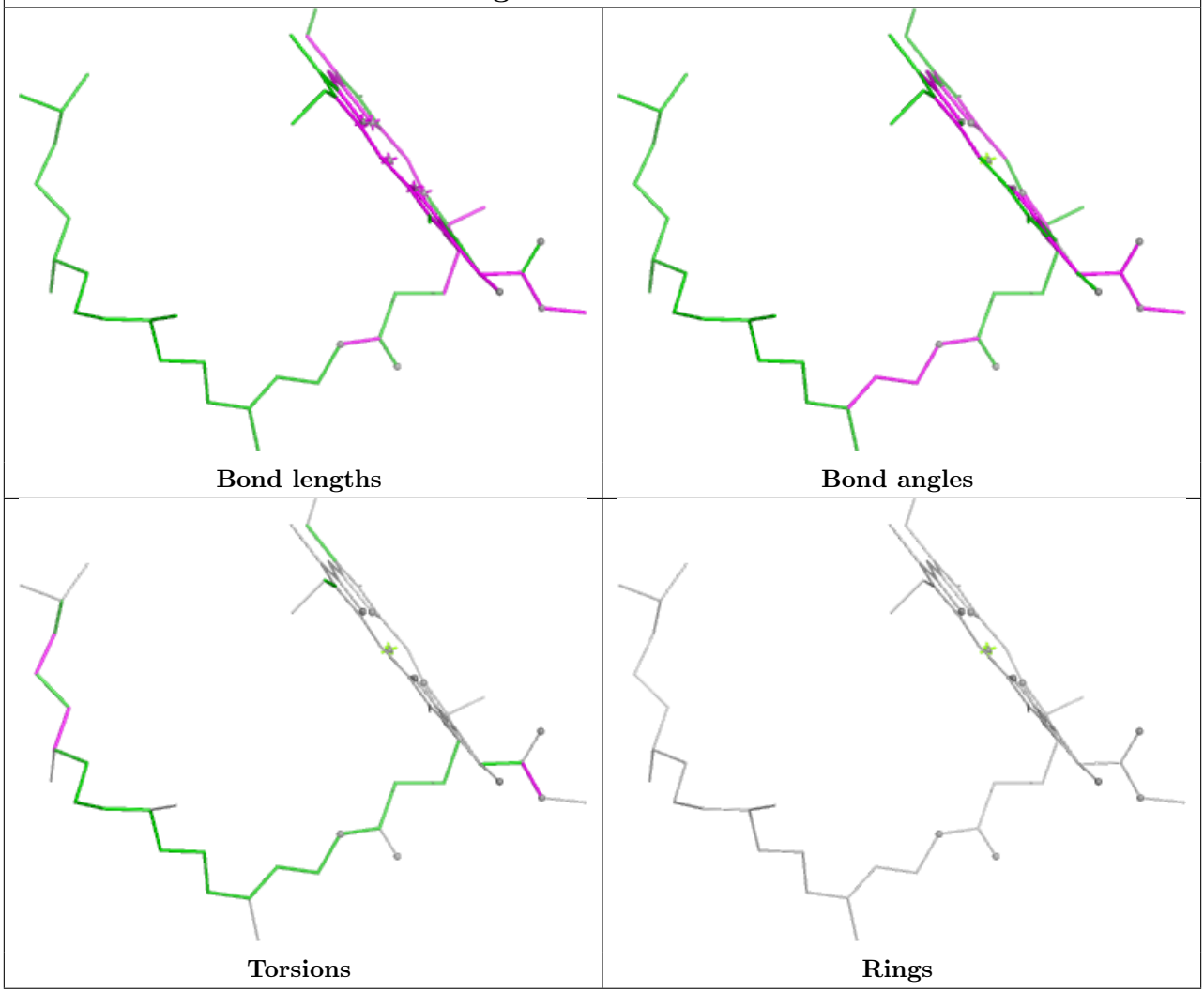


Torsions

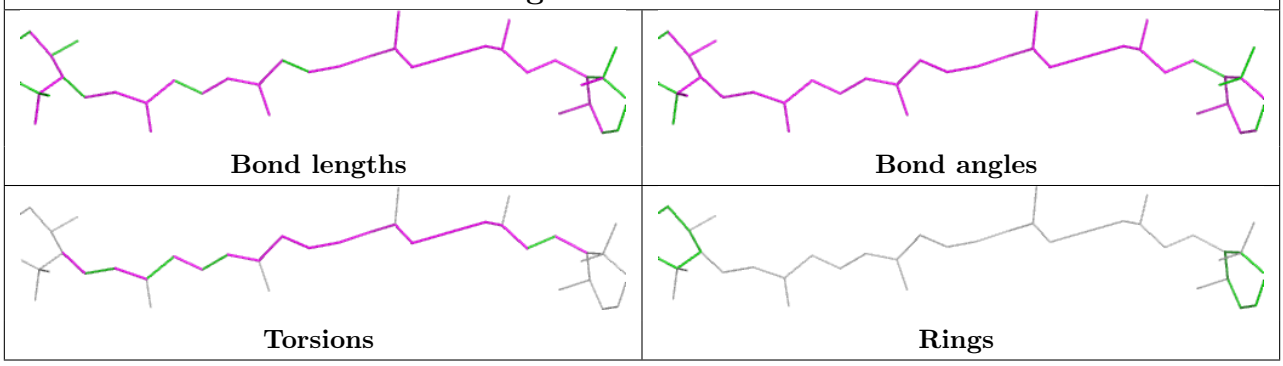


Rings

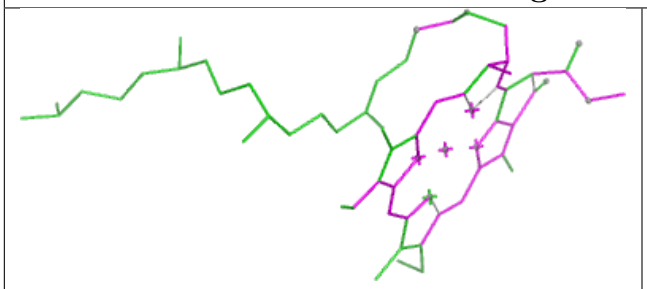
Ligand CLA B 612



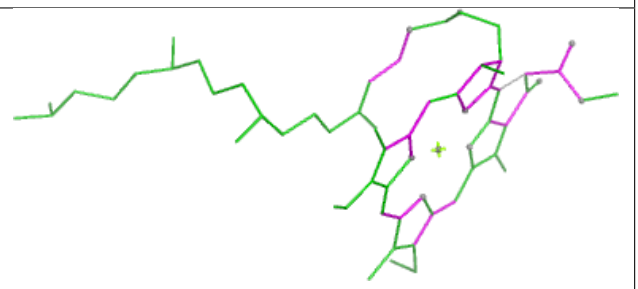
Ligand BCR b 620



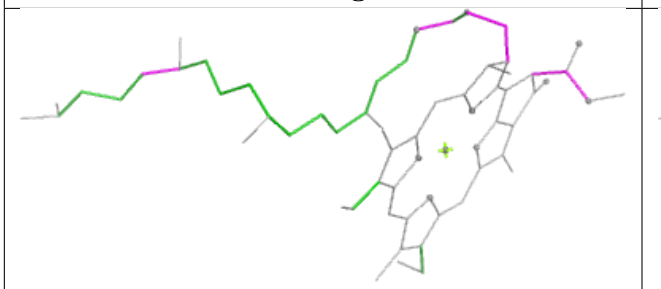
Ligand CLA c 505



Bond lengths



Bond angles

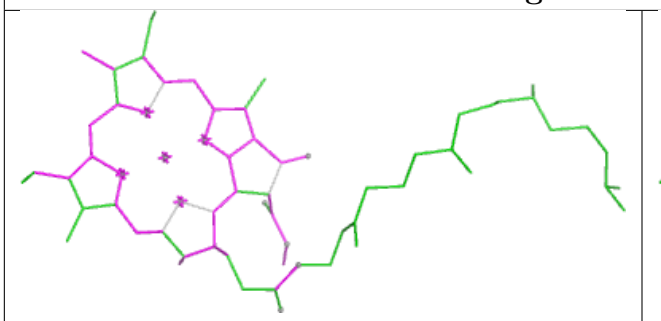


Torsions

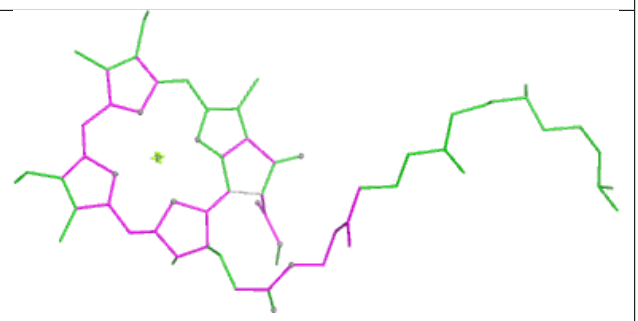


Rings

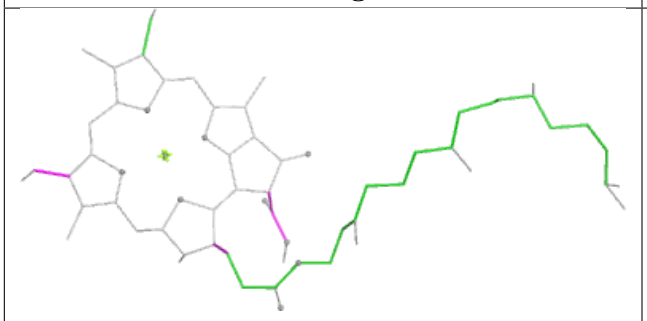
Ligand CLA B 603



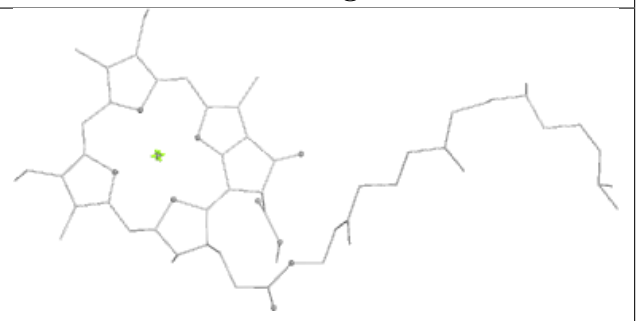
Bond lengths



Bond angles

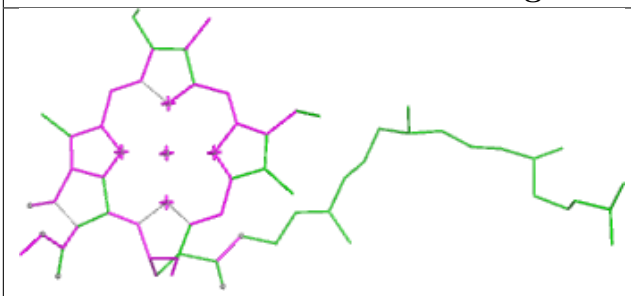


Torsions

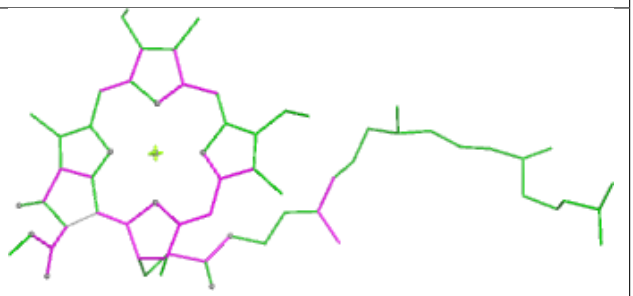


Rings

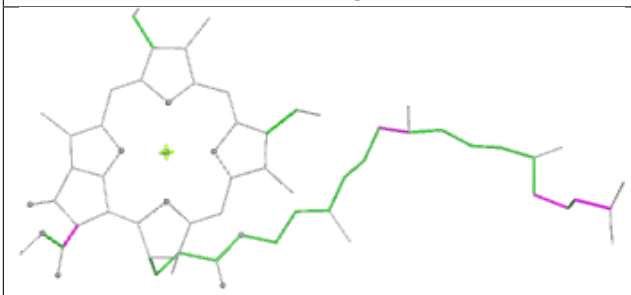
Ligand CLA B 604



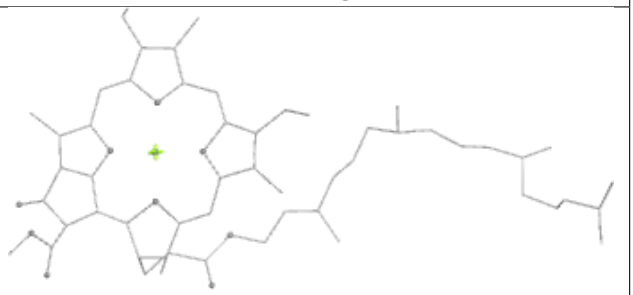
Bond lengths



Bond angles

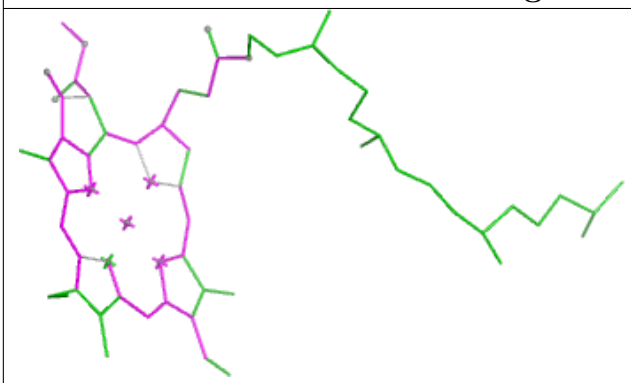


Torsions

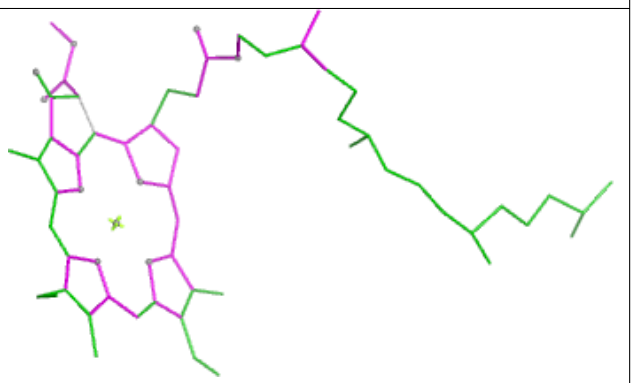


Rings

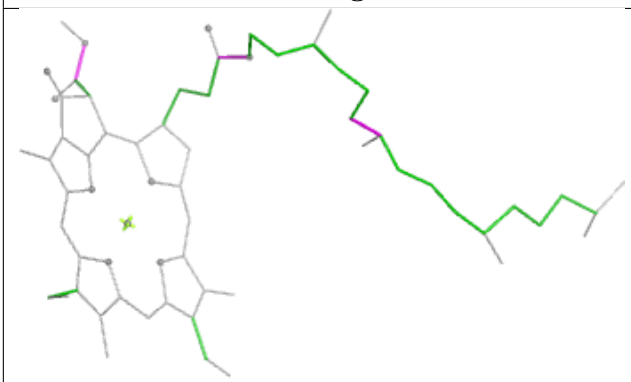
Ligand CLA C 511



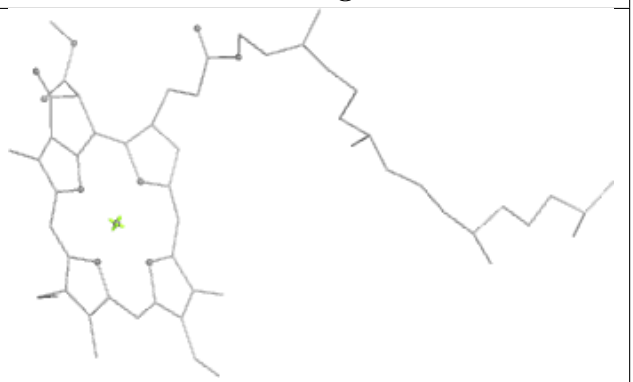
Bond lengths



Bond angles

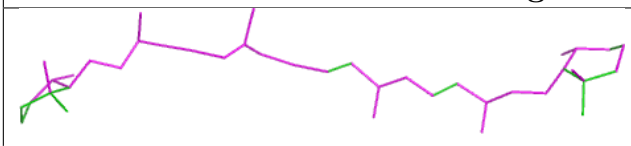


Torsions

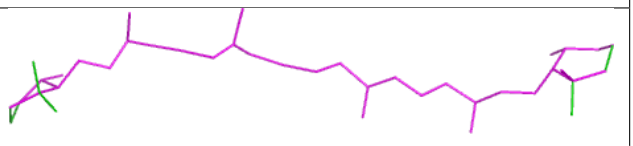


Rings

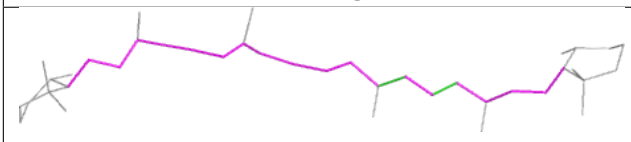
Ligand BCR c 514



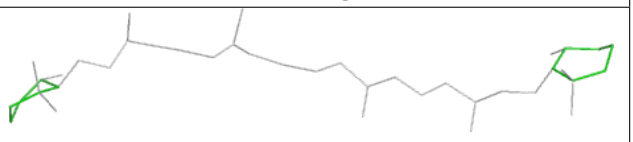
Bond lengths



Bond angles

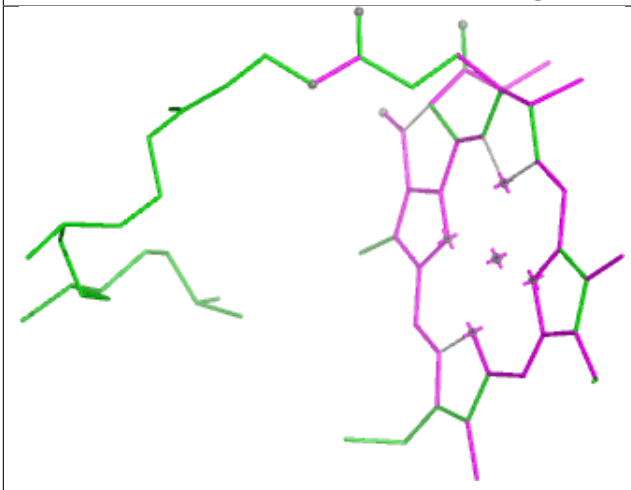


Torsions

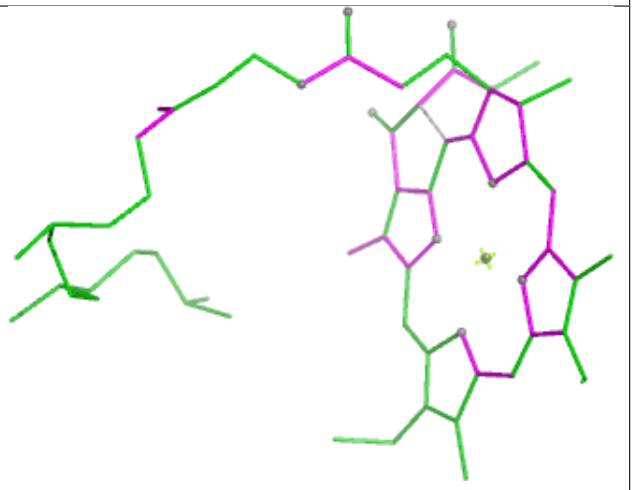


Rings

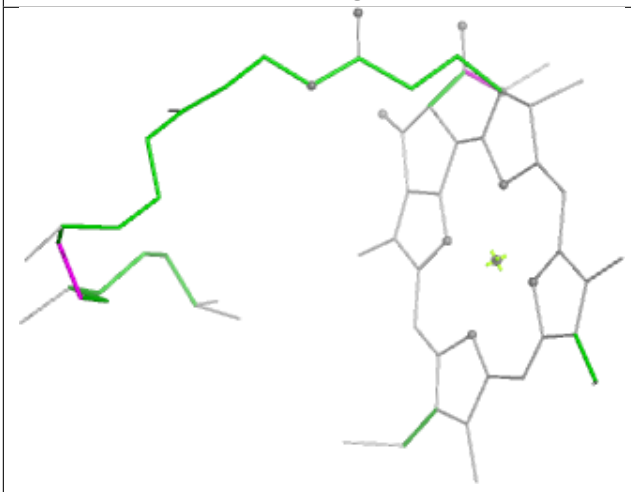
Ligand CLA c 503



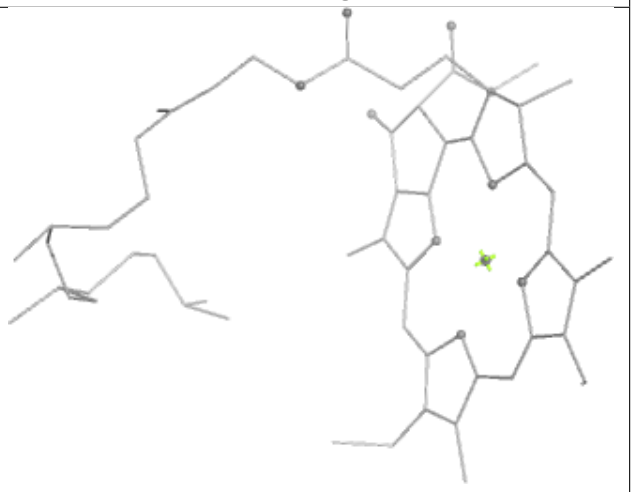
Bond lengths



Bond angles

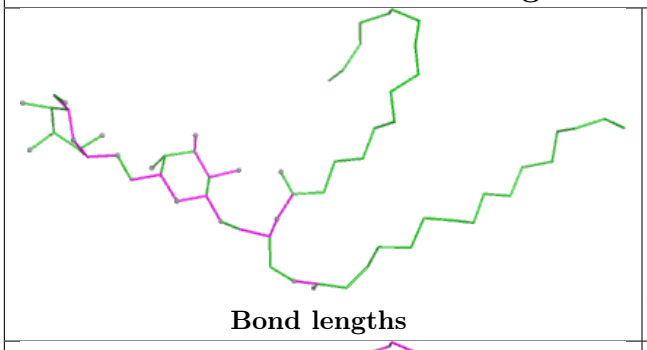


Torsions

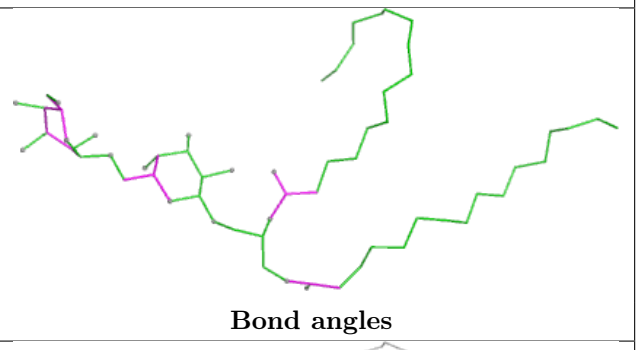


Rings

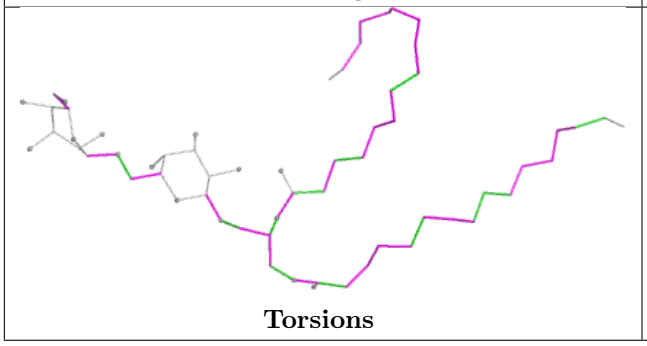
Ligand DGD E 101



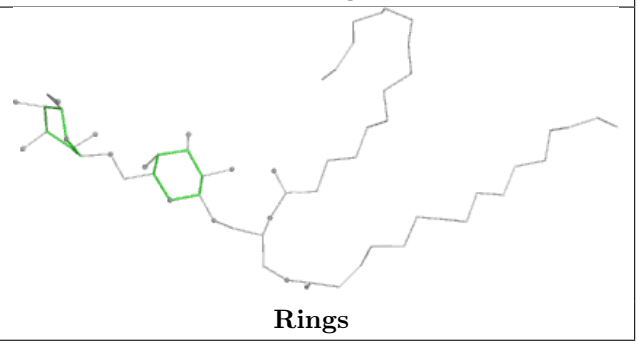
Bond lengths



Bond angles

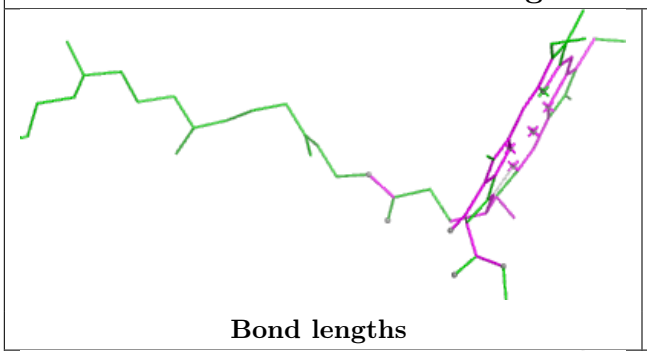


Torsions

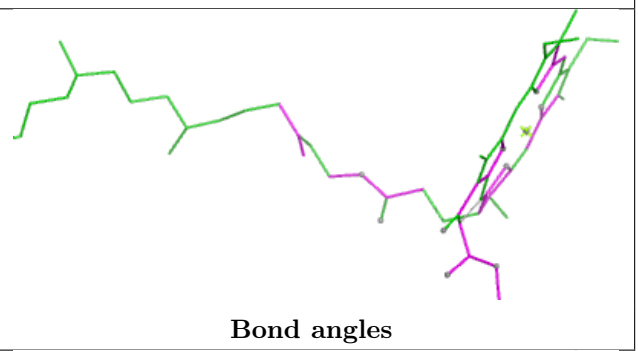


Rings

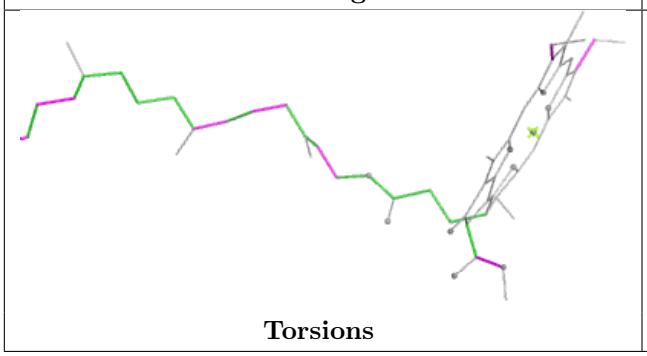
Ligand CLA B 605



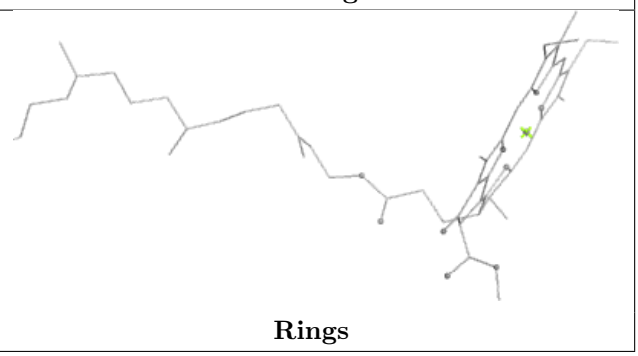
Bond lengths



Bond angles

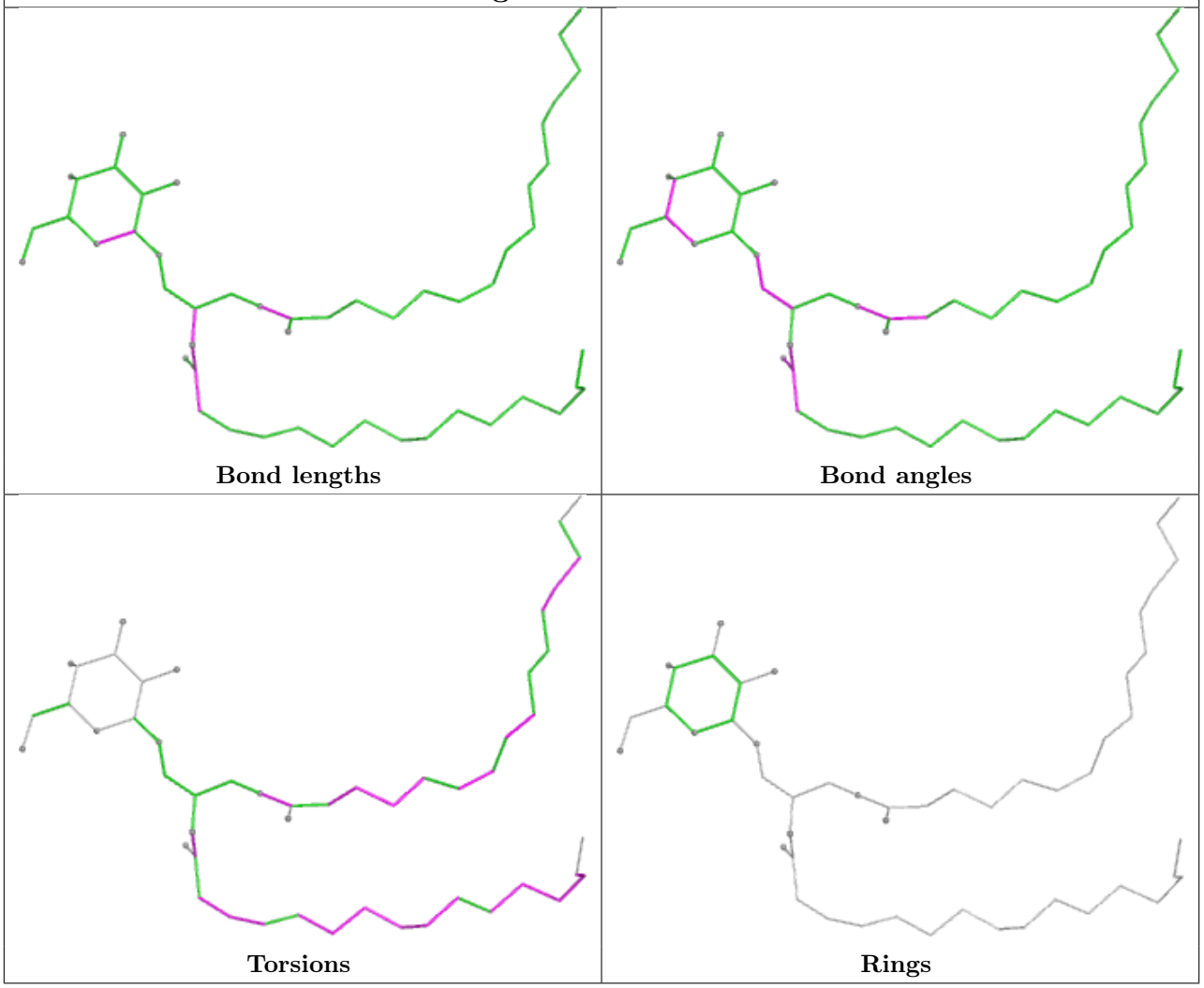


Torsions

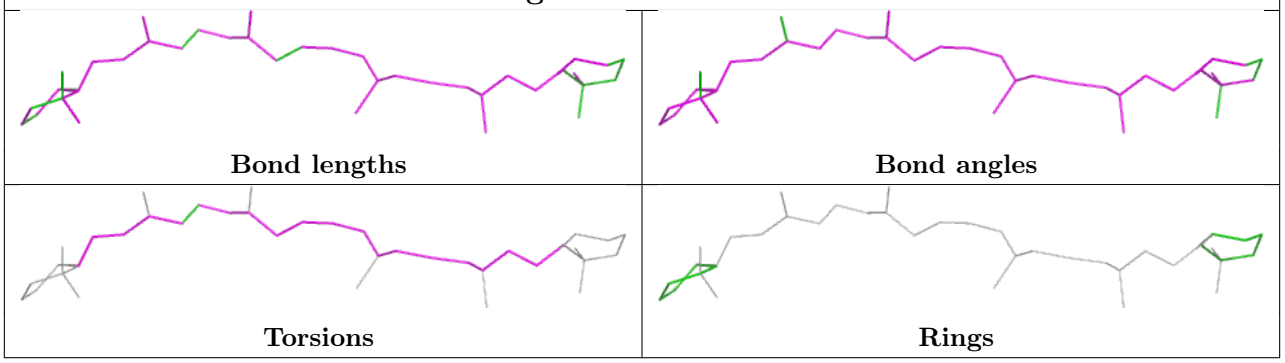


Rings

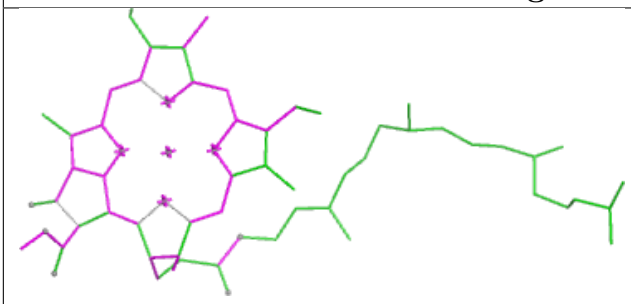
Ligand LMG c 519



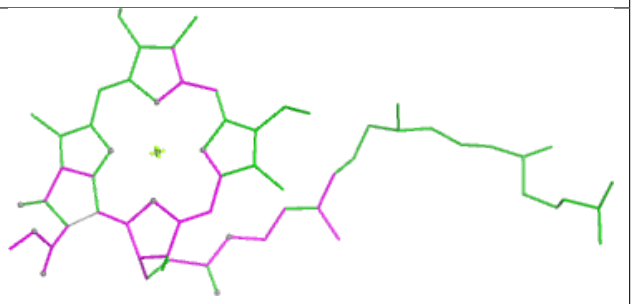
Ligand BCR h 101



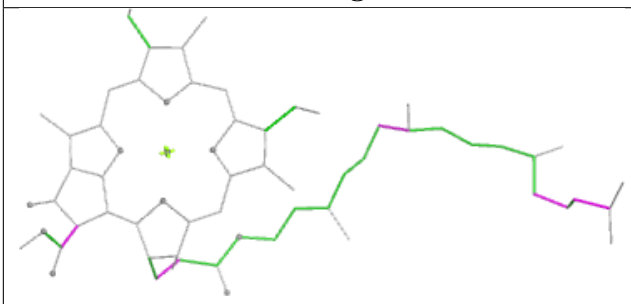
Ligand CLA b 605



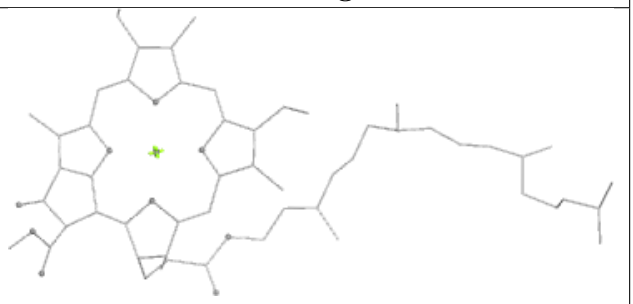
Bond lengths



Bond angles

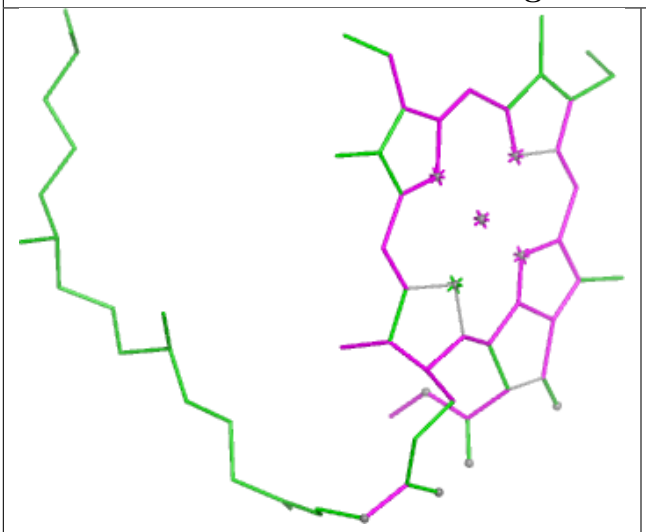


Torsions

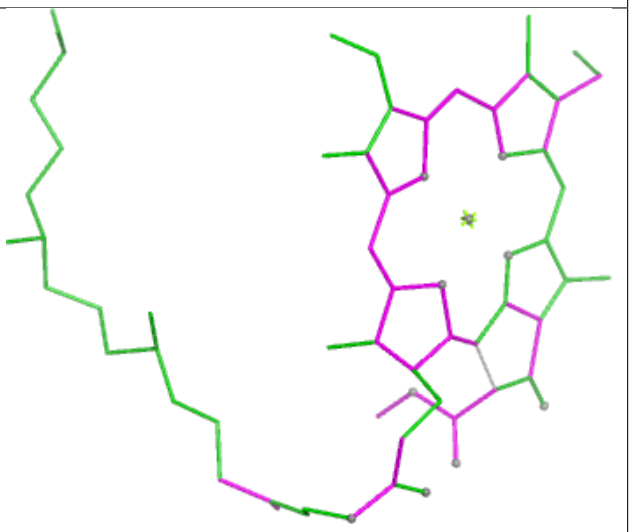


Rings

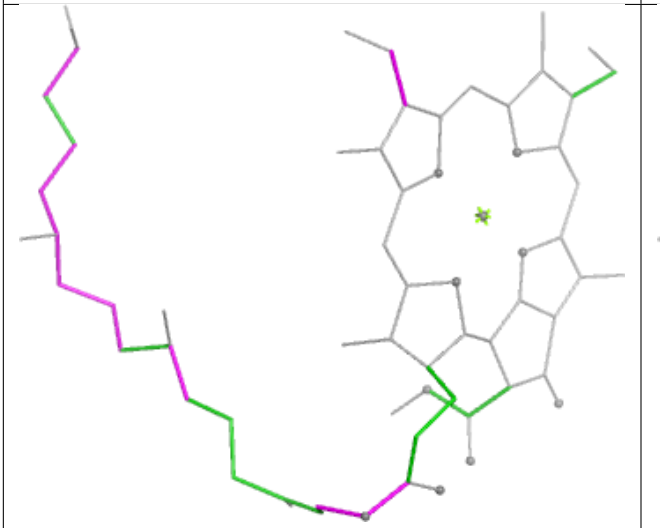
Ligand CLA B 617



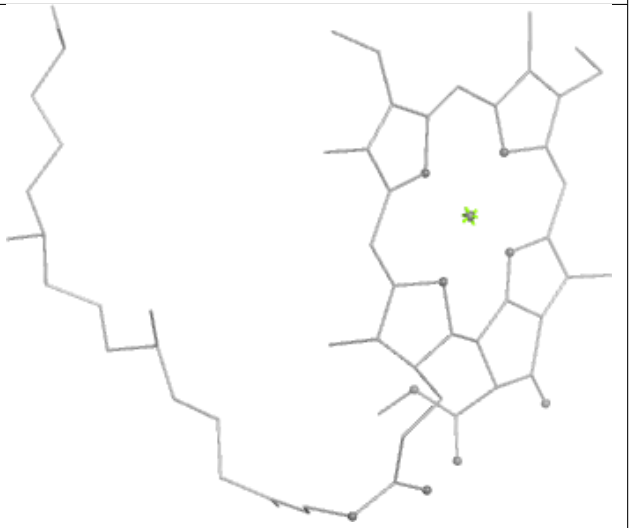
Bond lengths



Bond angles

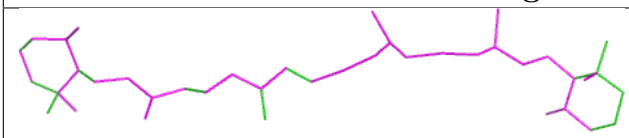


Torsions

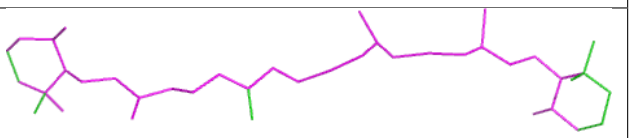


Rings

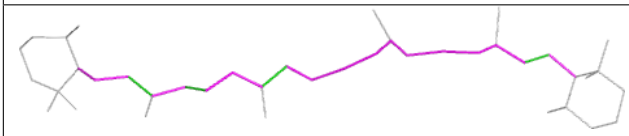
Ligand BCR B 620



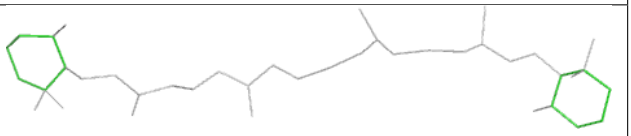
Bond lengths



Bond angles

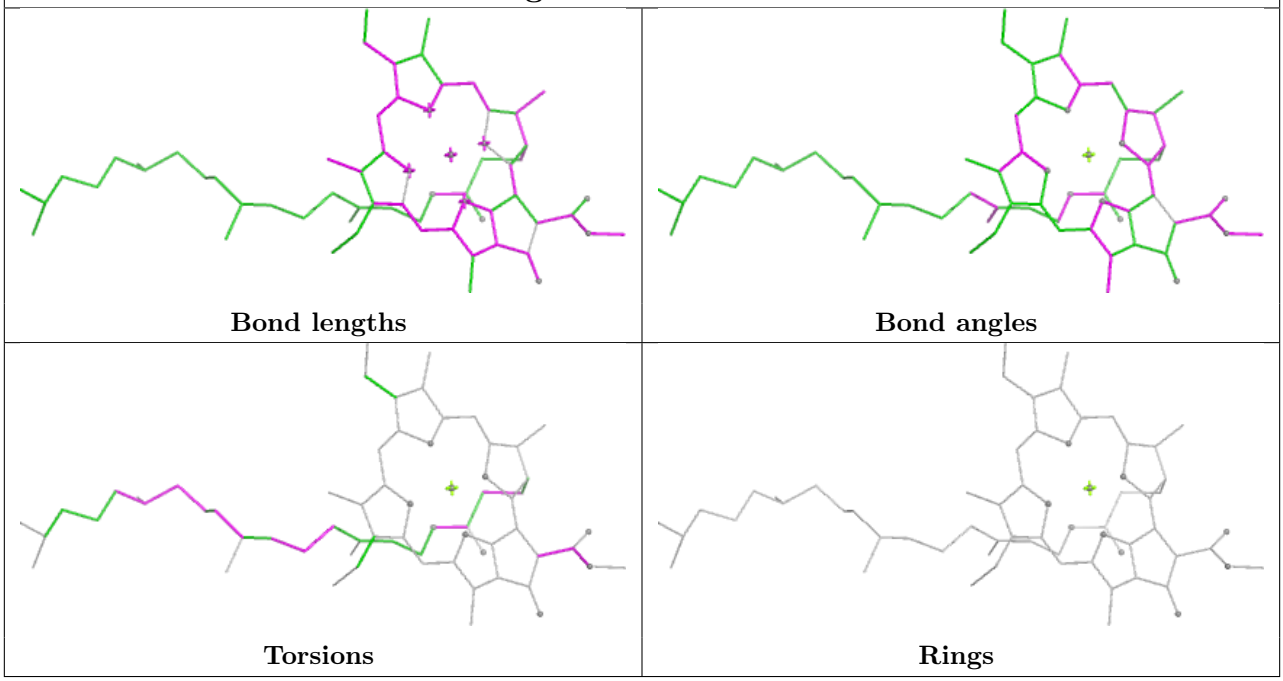


Torsions

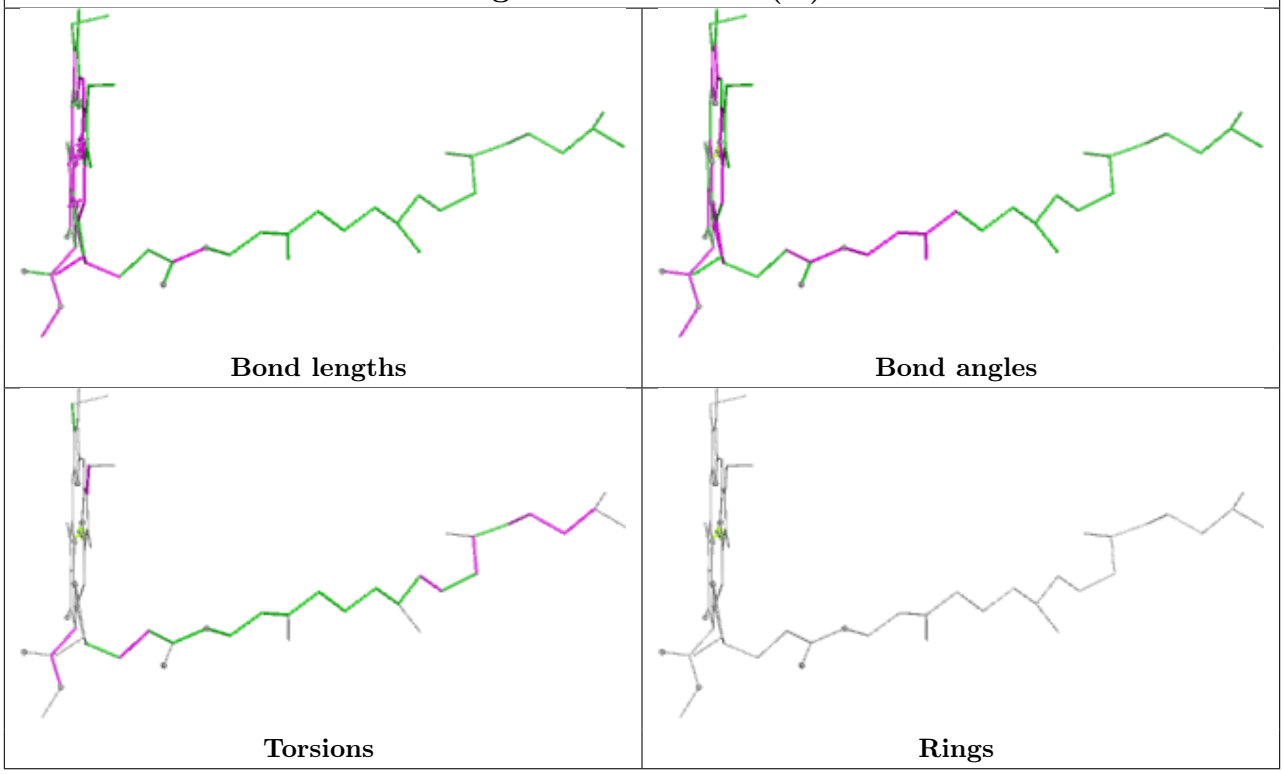


Rings

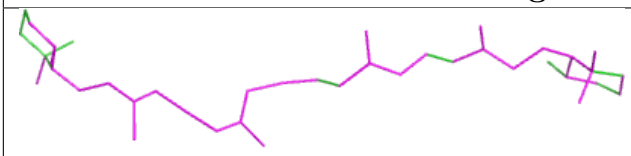
Ligand CLA B 615



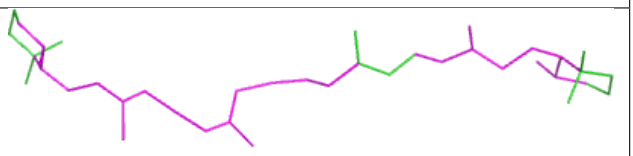
Ligand CLA B 607 (A)



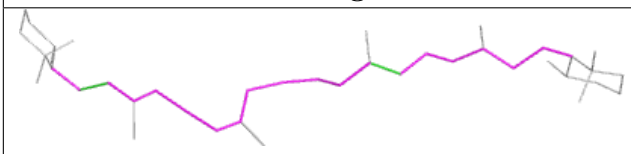
Ligand BCR I 101



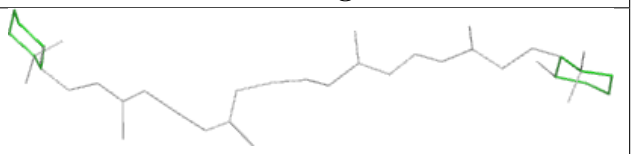
Bond lengths



Bond angles

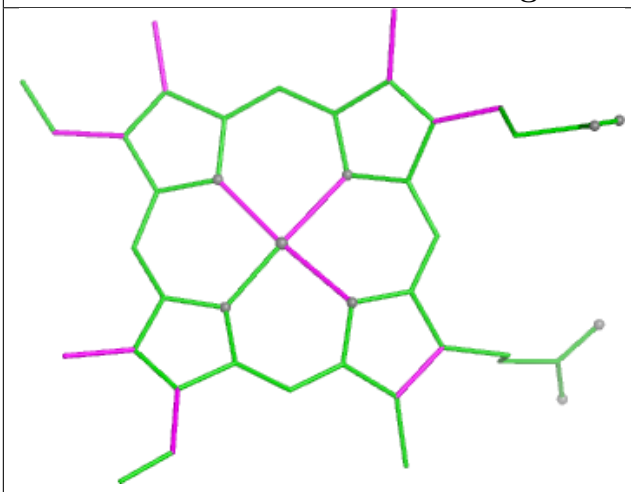


Torsions

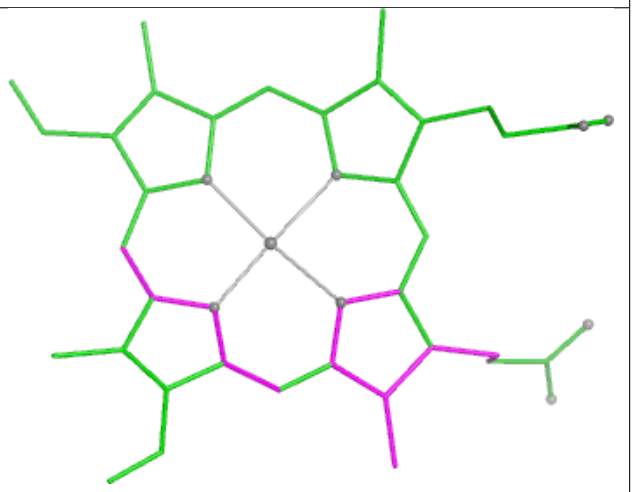


Rings

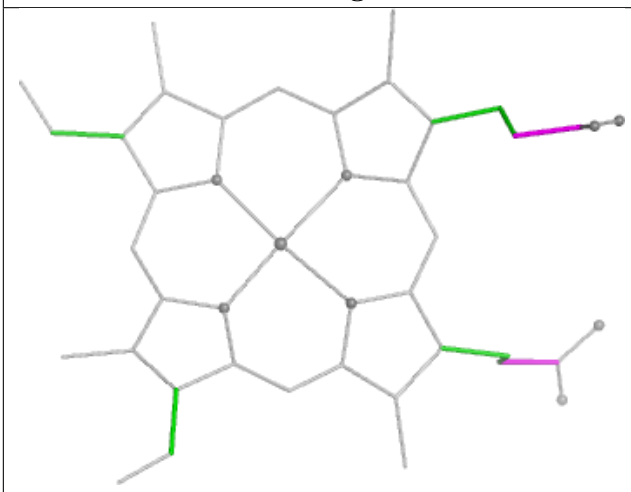
Ligand HEM E 103



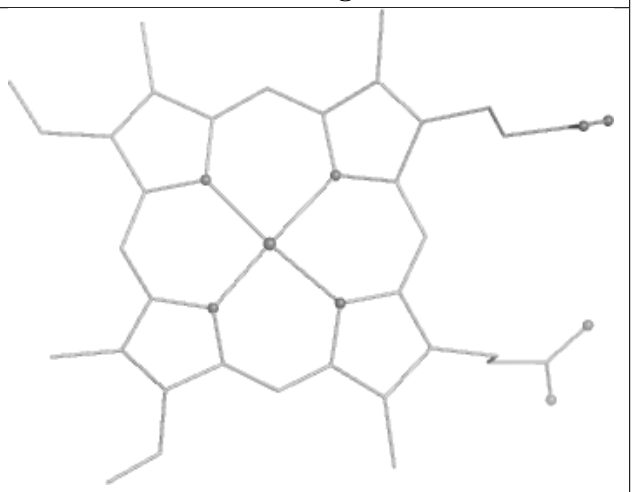
Bond lengths



Bond angles

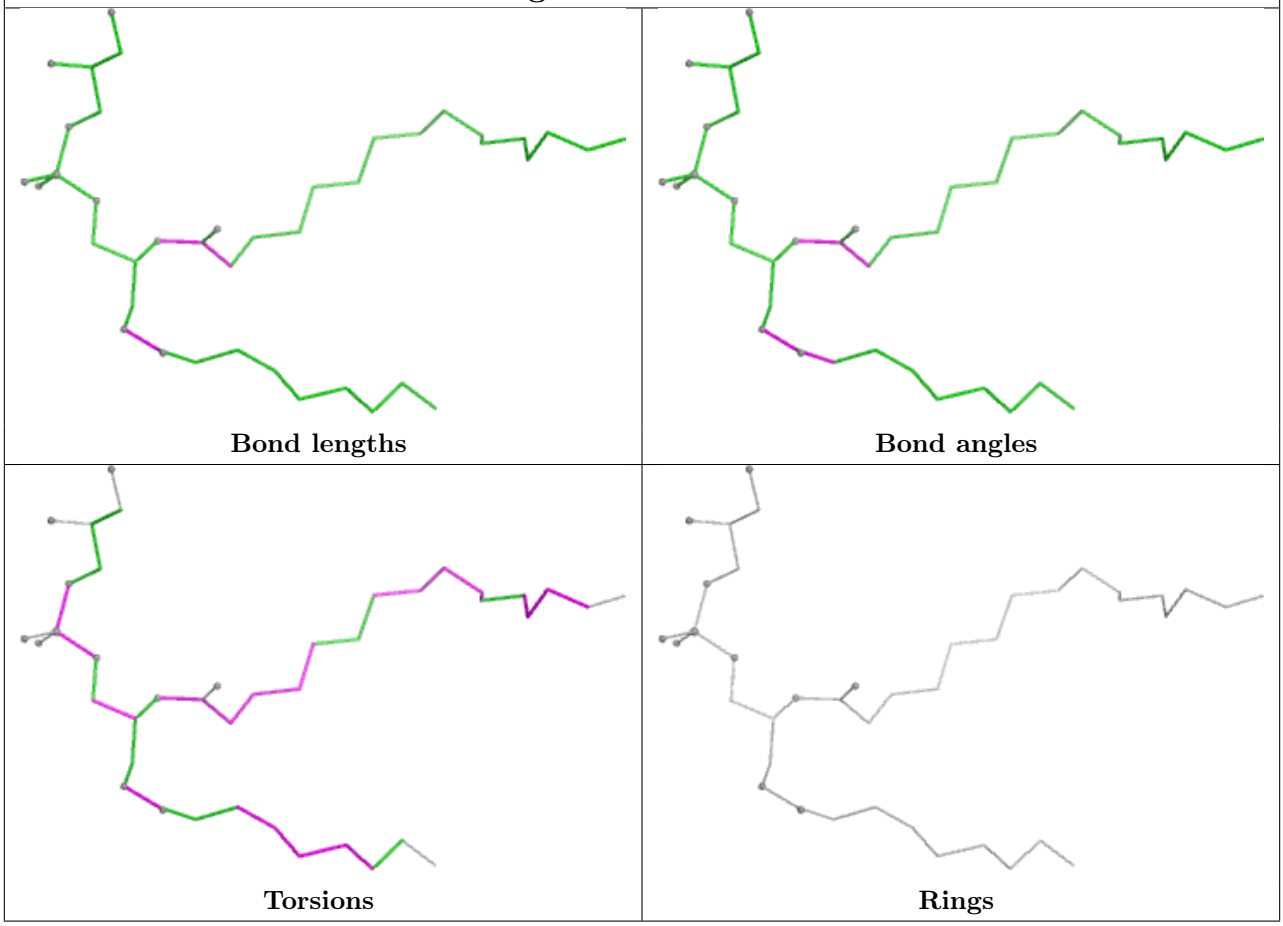


Torsions

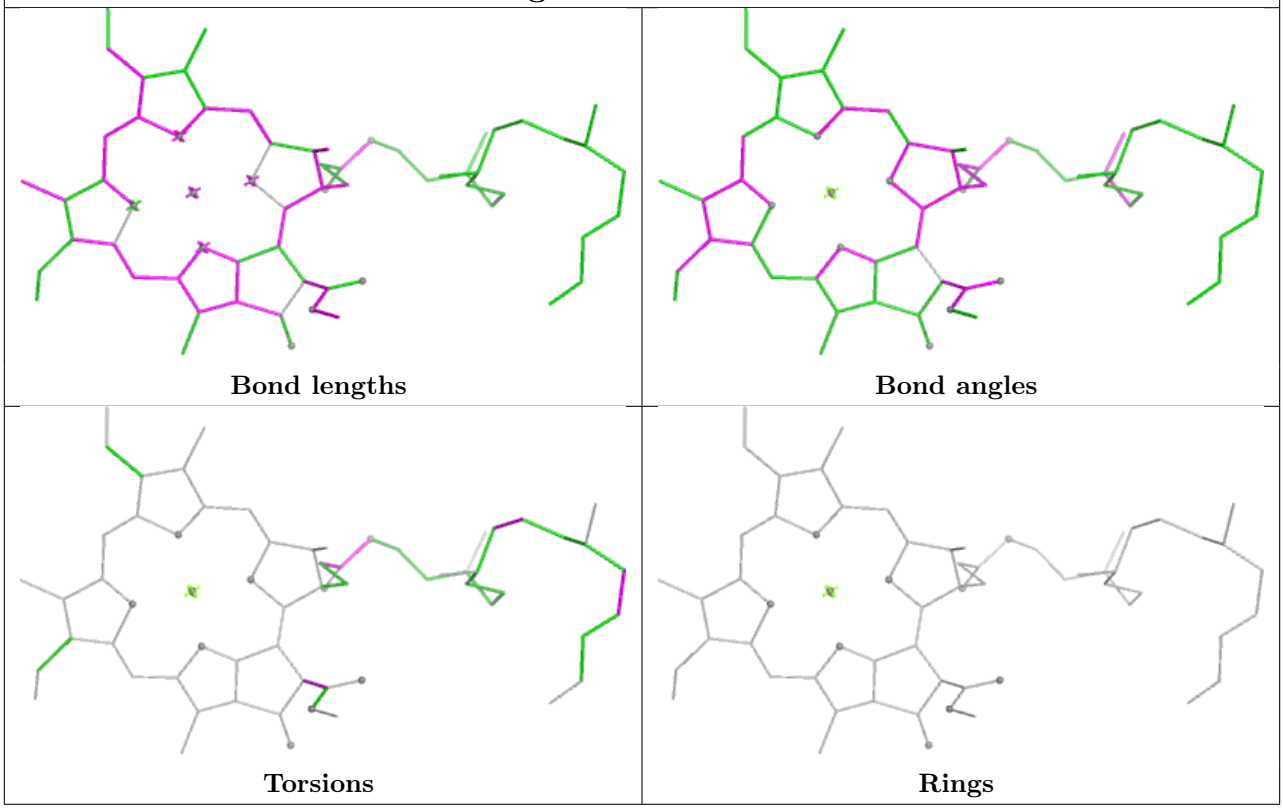


Rings

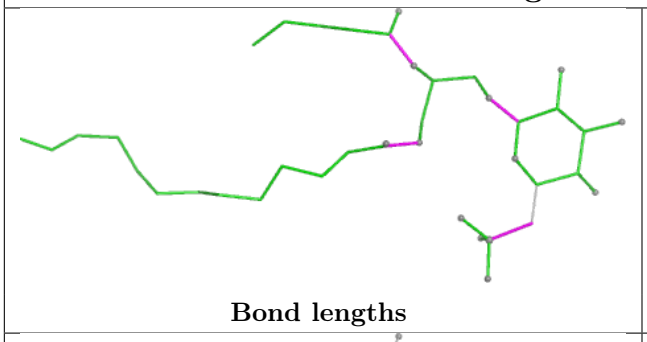
Ligand LHG e 101



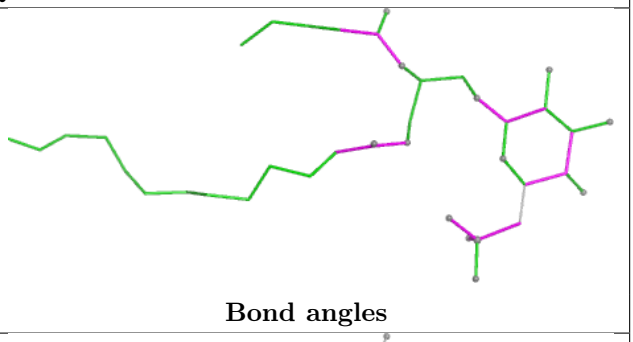
Ligand CLA b 614



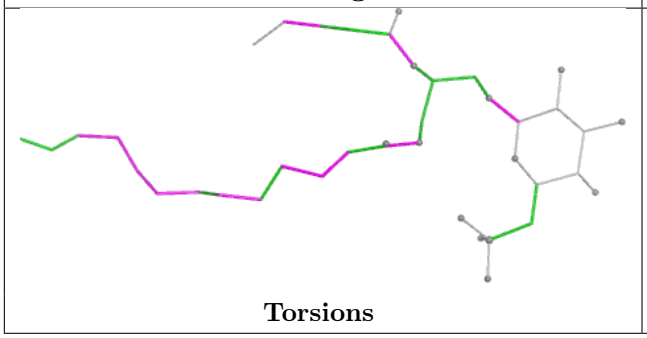
Ligand SQD X 101



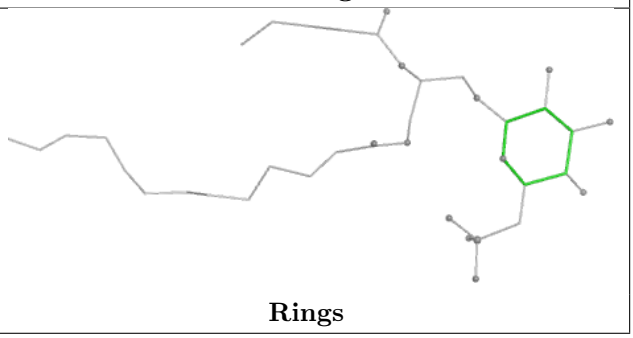
Bond lengths



Bond angles

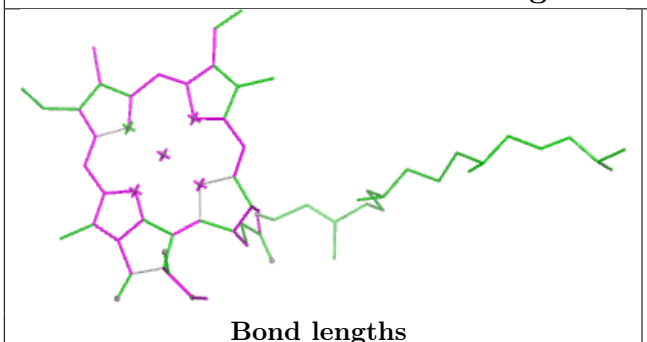


Torsions

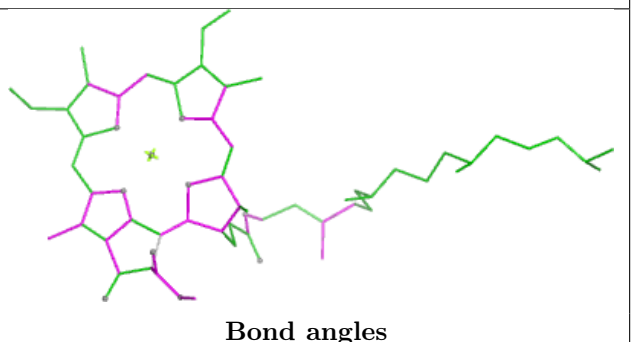


Rings

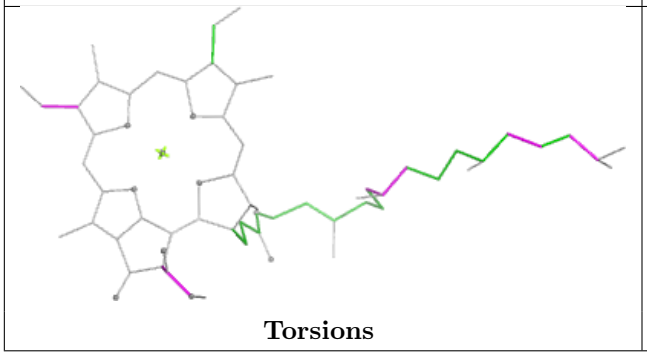
Ligand CLA a 607



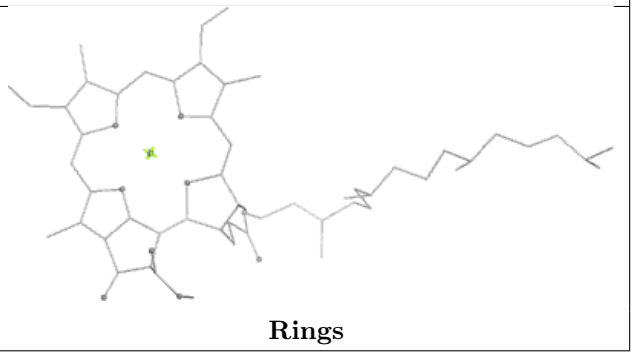
Bond lengths



Bond angles

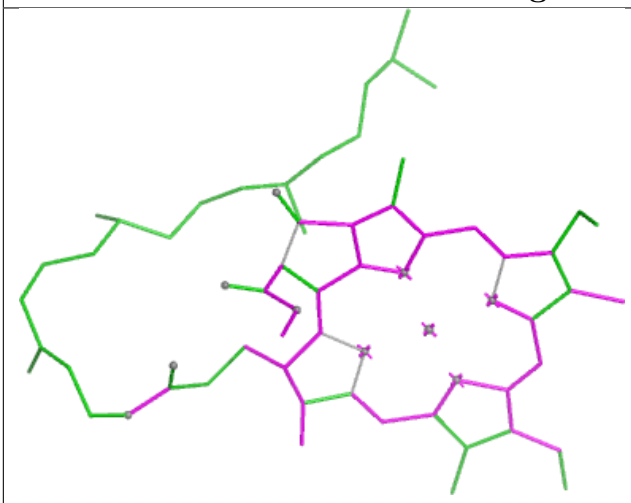


Torsions

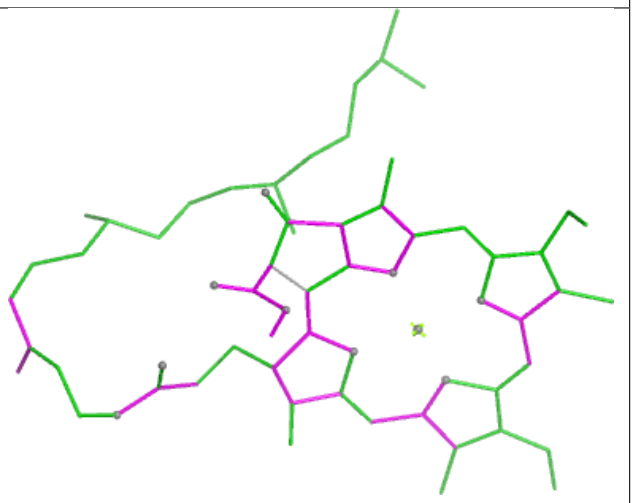


Rings

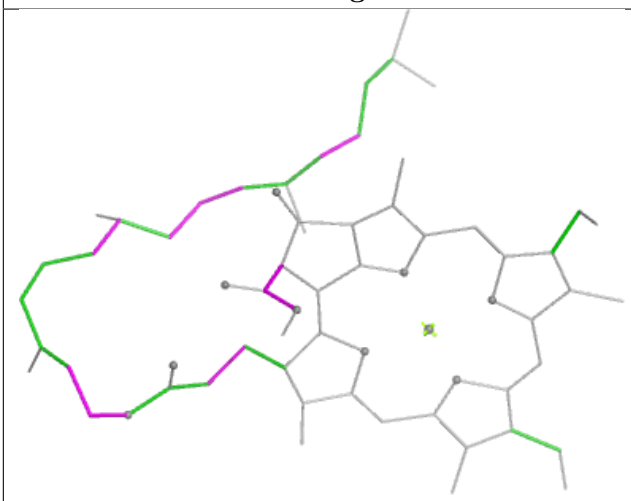
Ligand CLA c 509



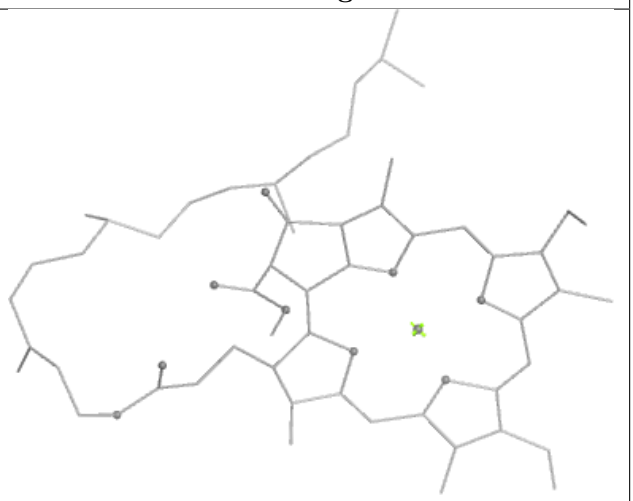
Bond lengths



Bond angles

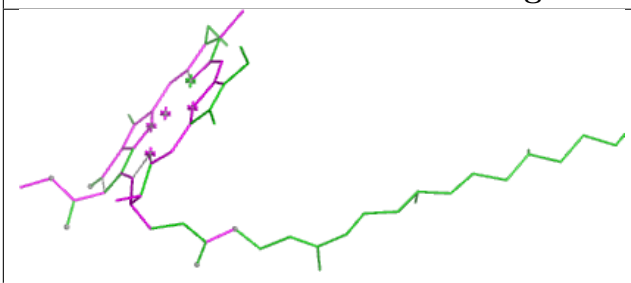


Torsions

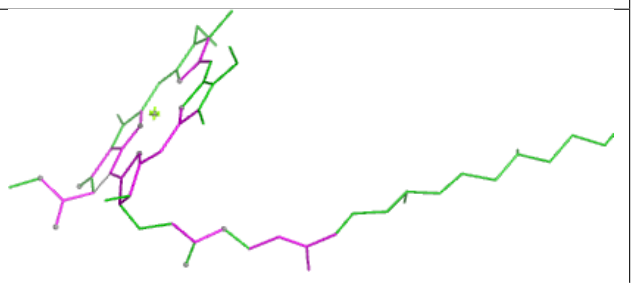


Rings

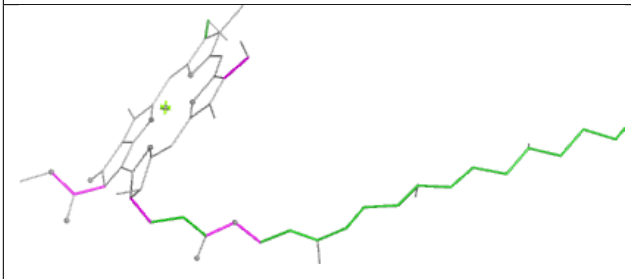
Ligand CLA B 608



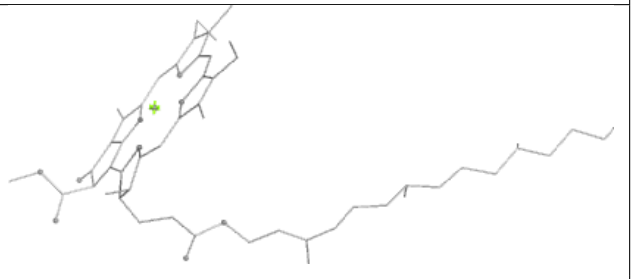
Bond lengths



Bond angles

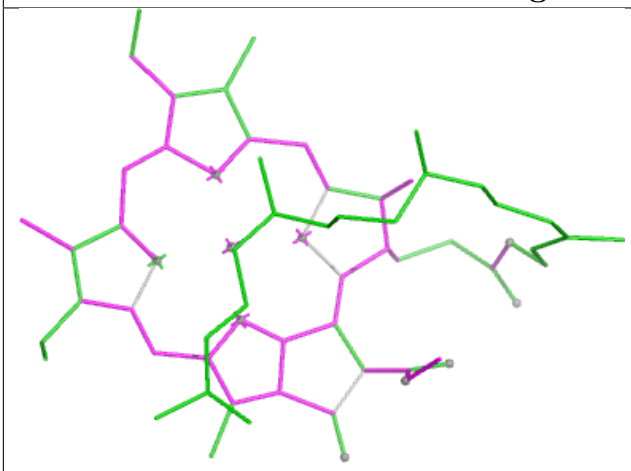


Torsions

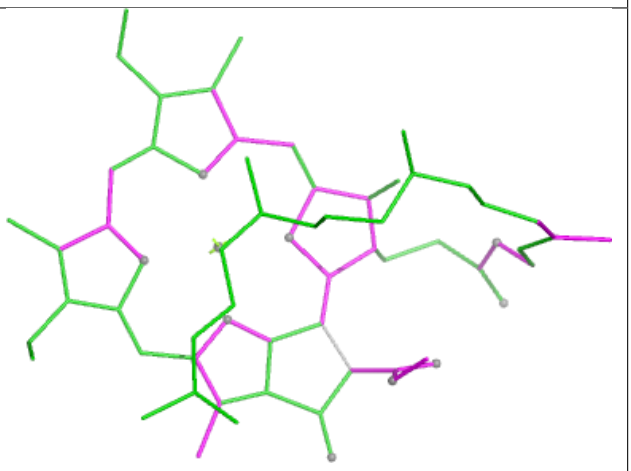


Rings

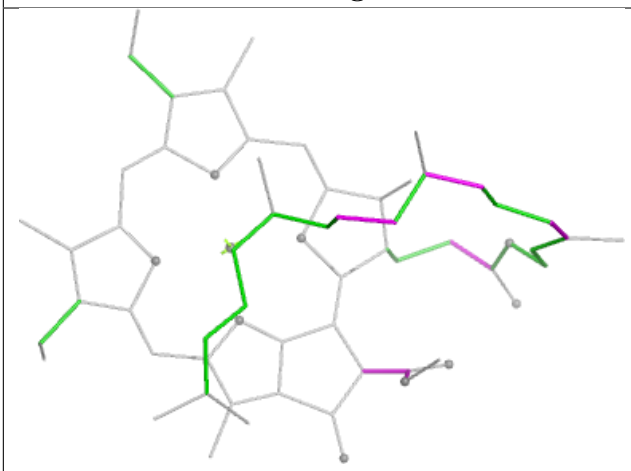
Ligand CLA c 510



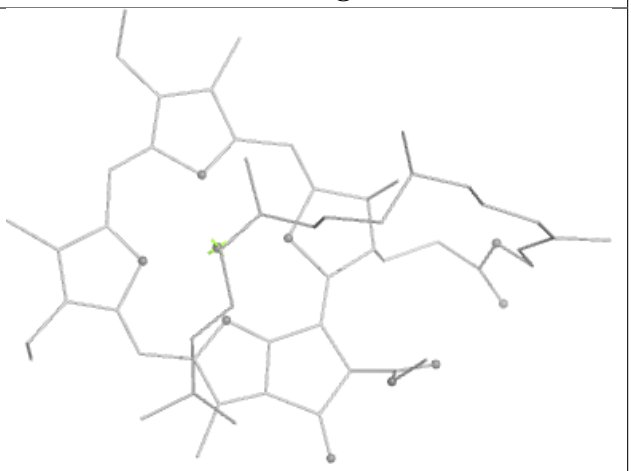
Bond lengths



Bond angles

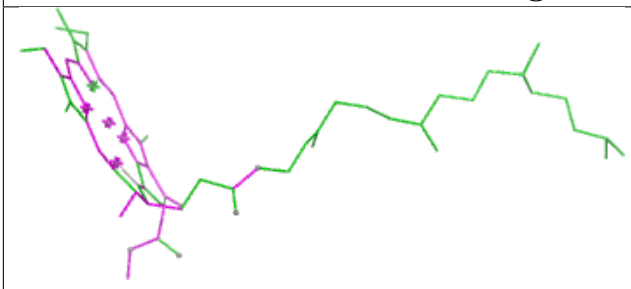


Torsions

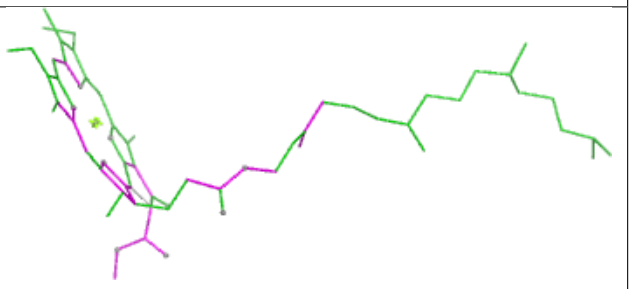


Rings

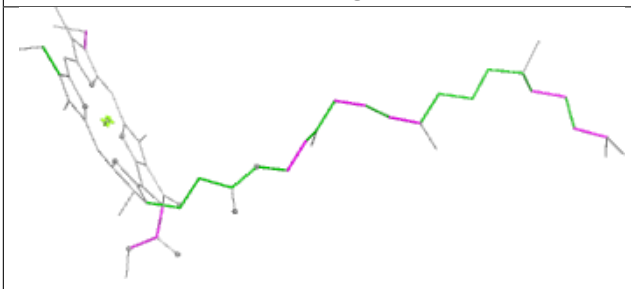
Ligand CLA b 606



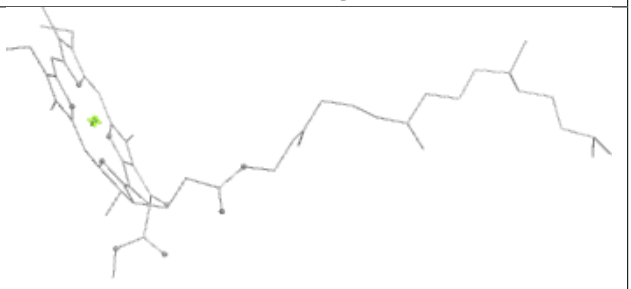
Bond lengths



Bond angles

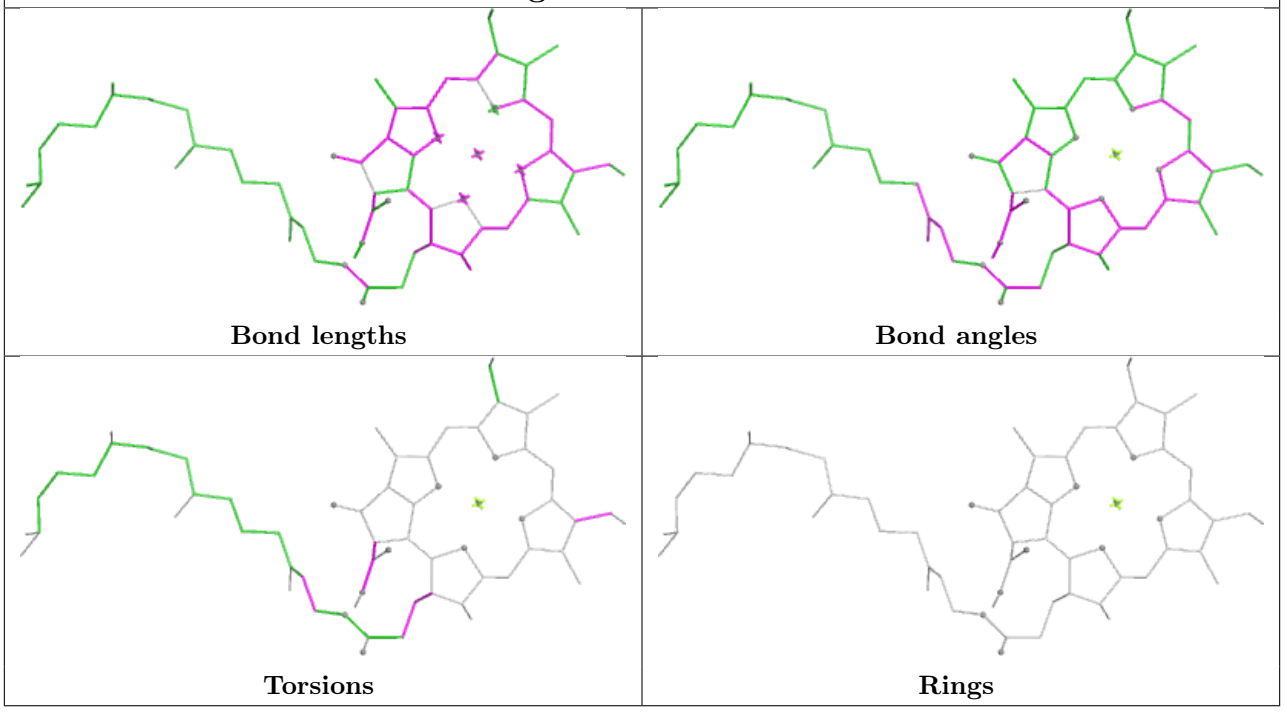


Torsions

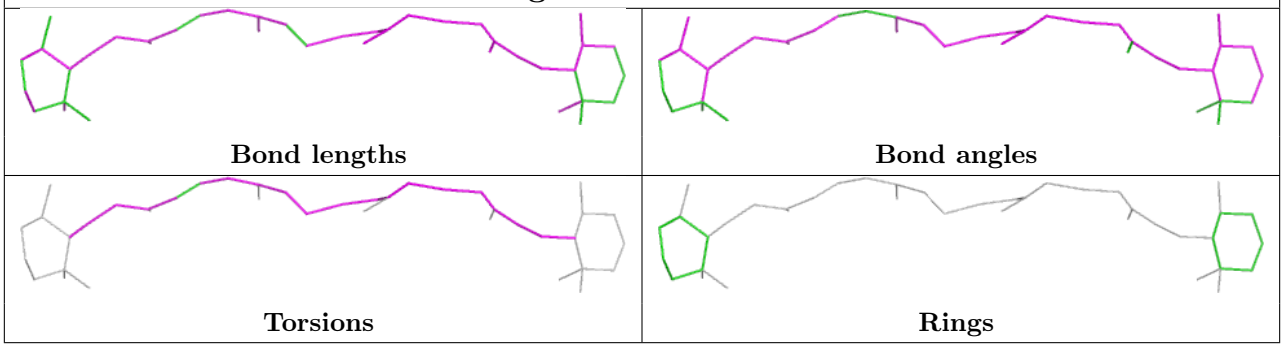


Rings

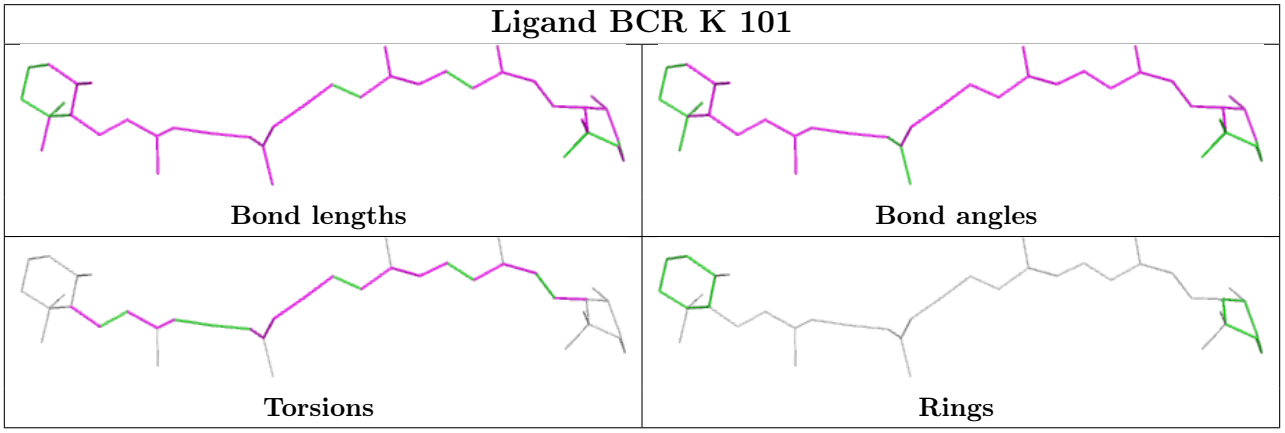
Ligand CLA b 604



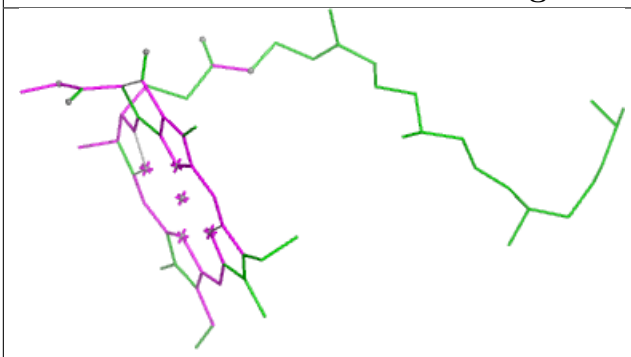
Ligand BCR c 521



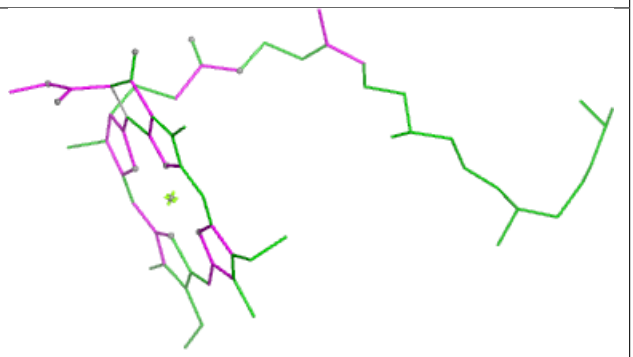
Ligand BCR K 101



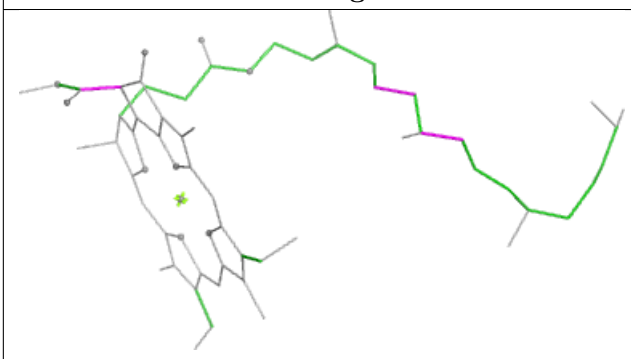
Ligand CLA c 508



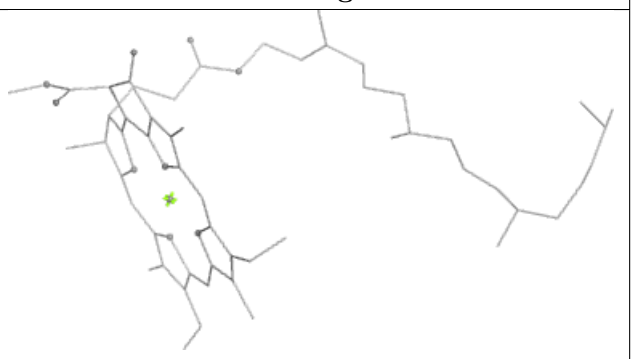
Bond lengths



Bond angles

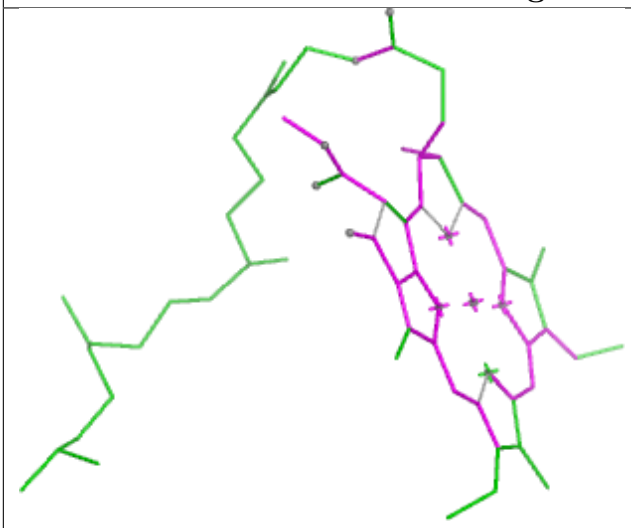


Torsions



Rings

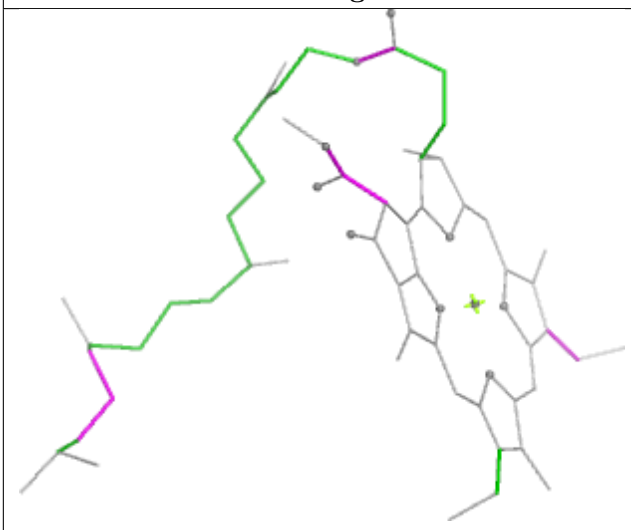
Ligand CLA b 615



Bond lengths



Bond angles

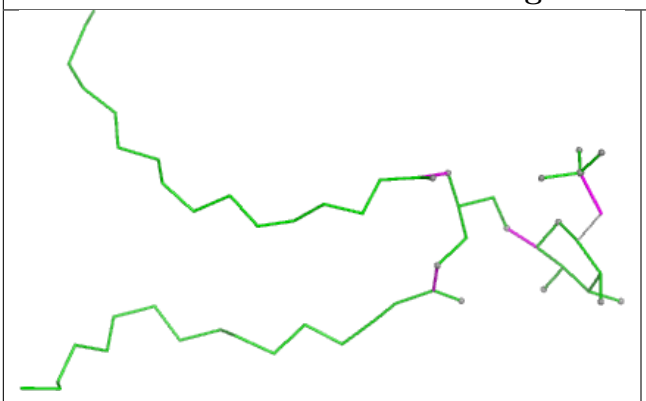


Torsions

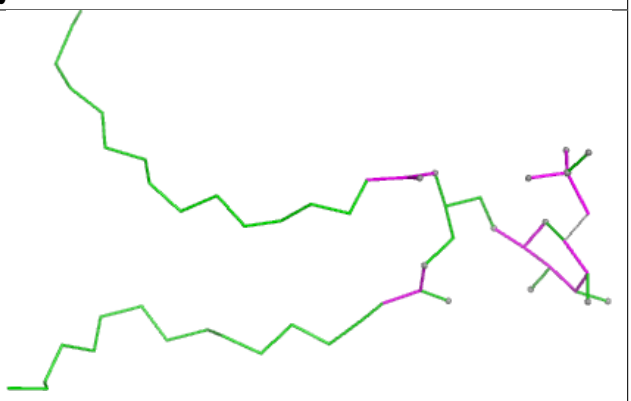


Rings

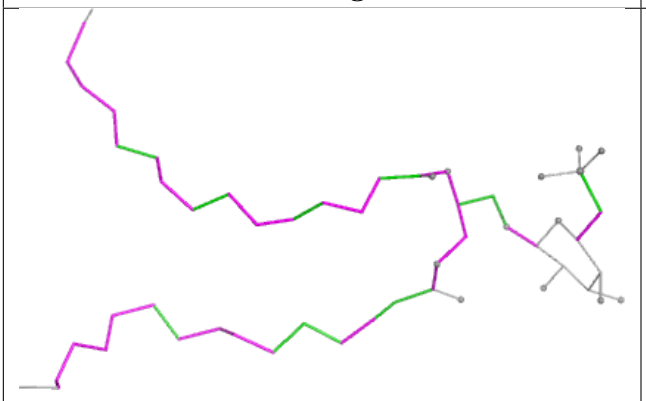
Ligand SQD B 622



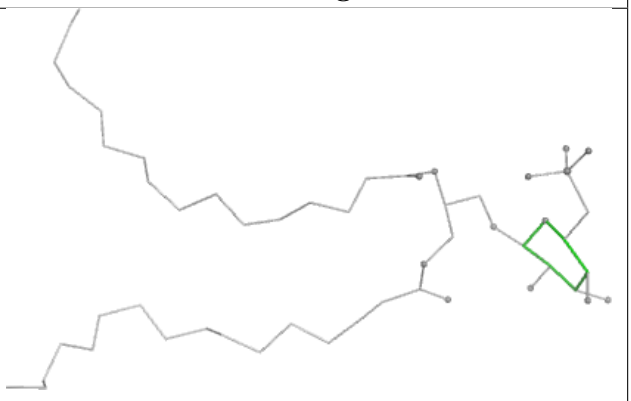
Bond lengths



Bond angles

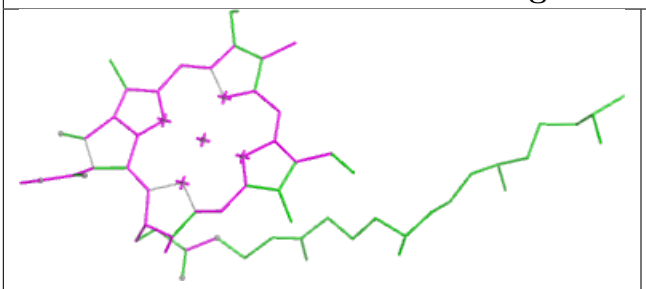


Torsions

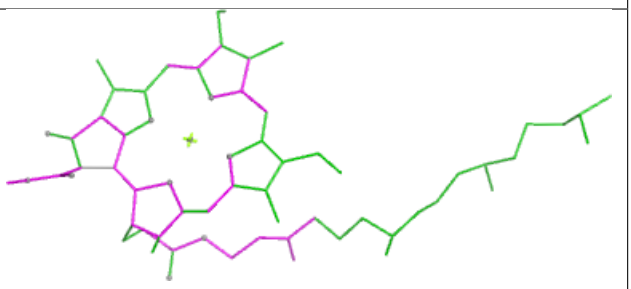


Rings

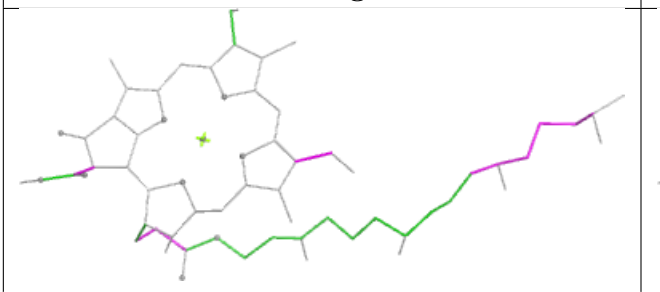
Ligand CLA c 501



Bond lengths



Bond angles

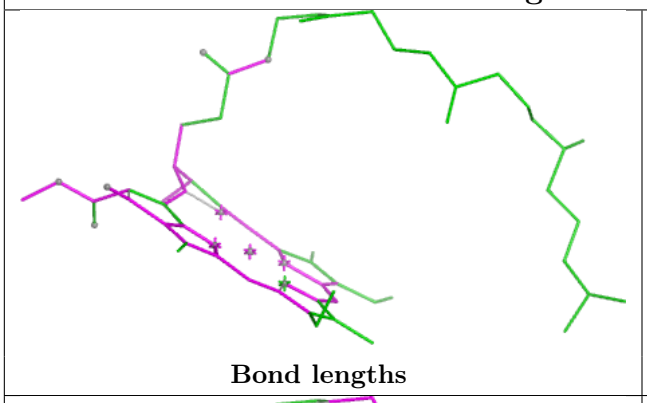


Torsions

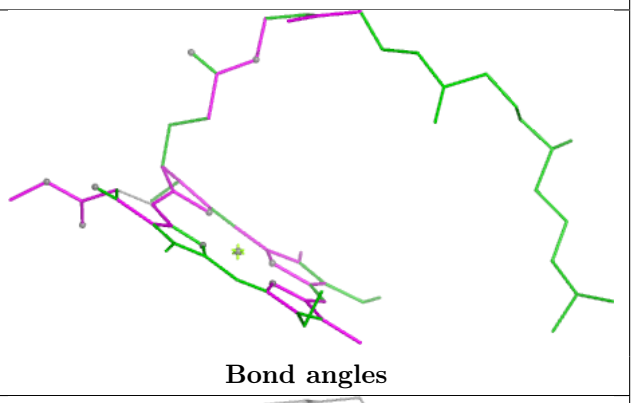


Rings

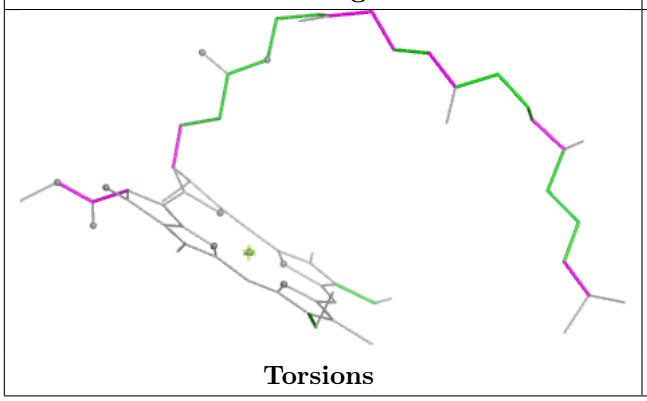
Ligand CLA C 513



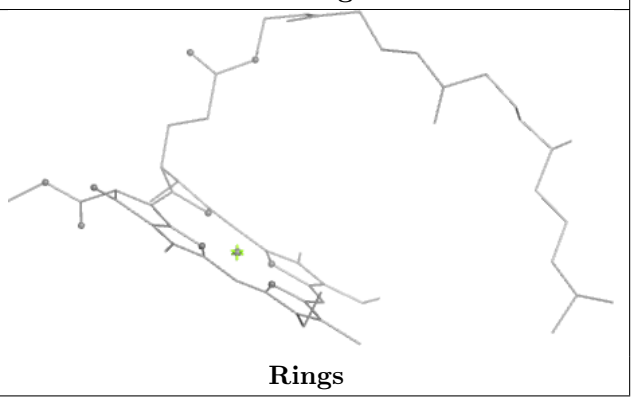
Bond lengths



Bond angles

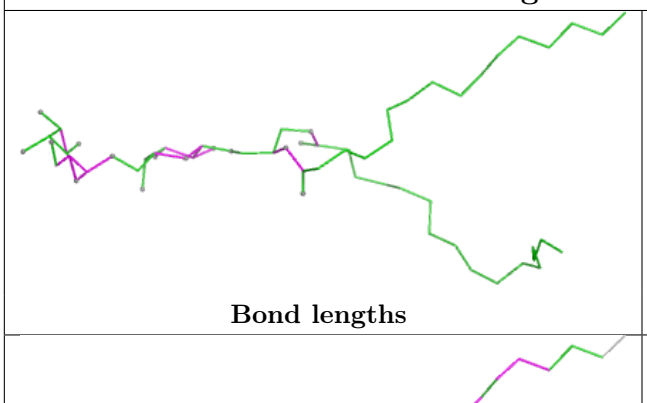


Torsions

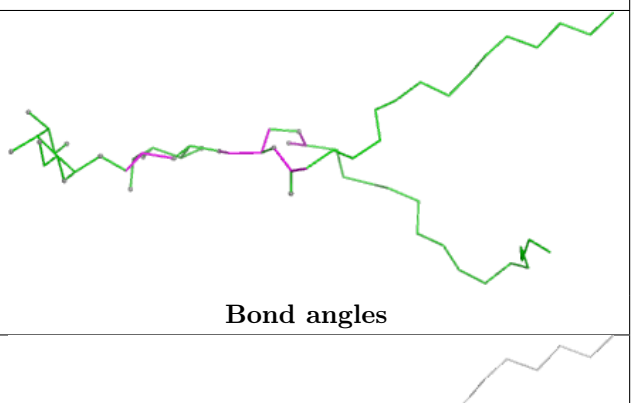


Rings

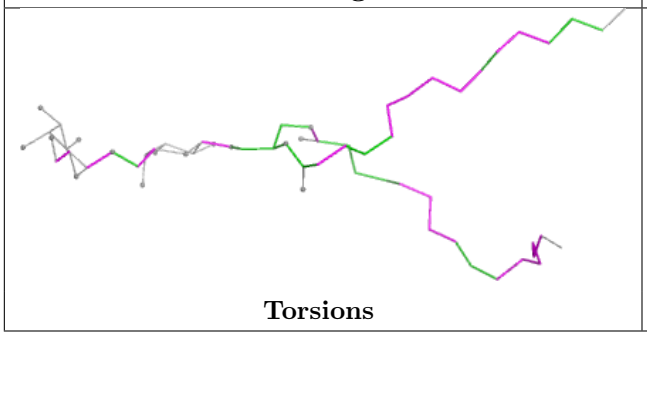
Ligand DGD C 515



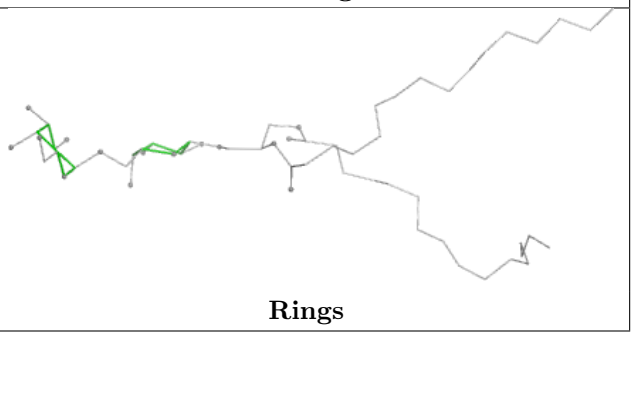
Bond lengths



Bond angles

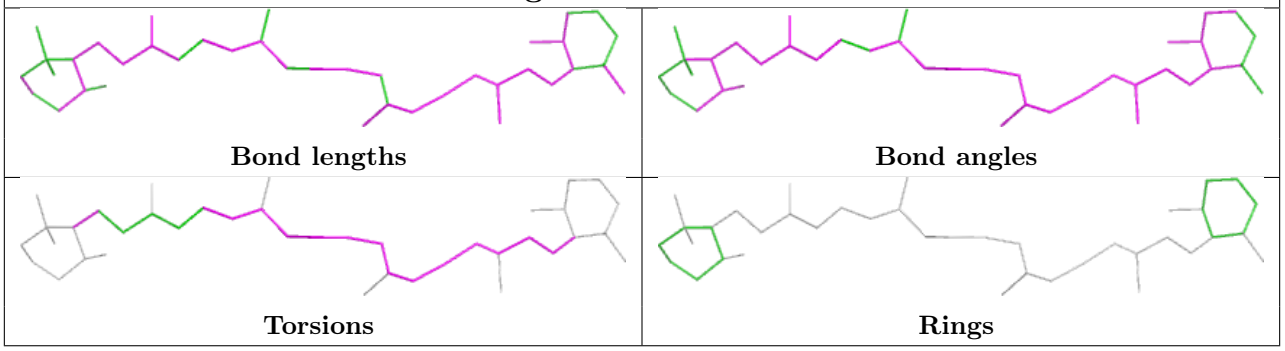


Torsions

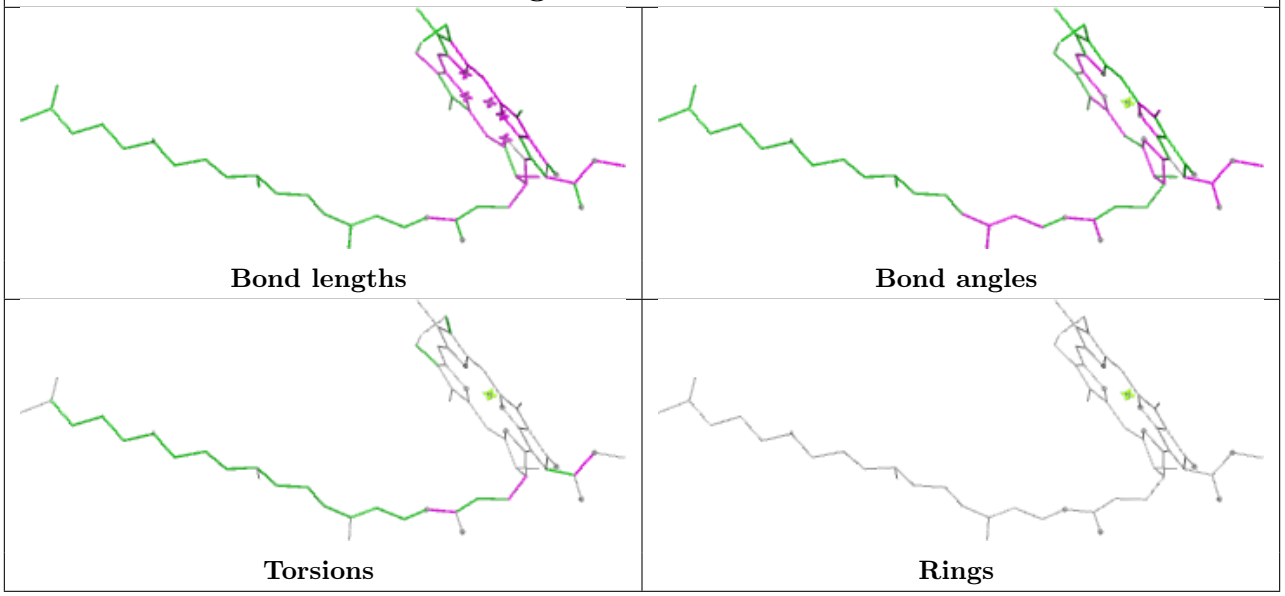


Rings

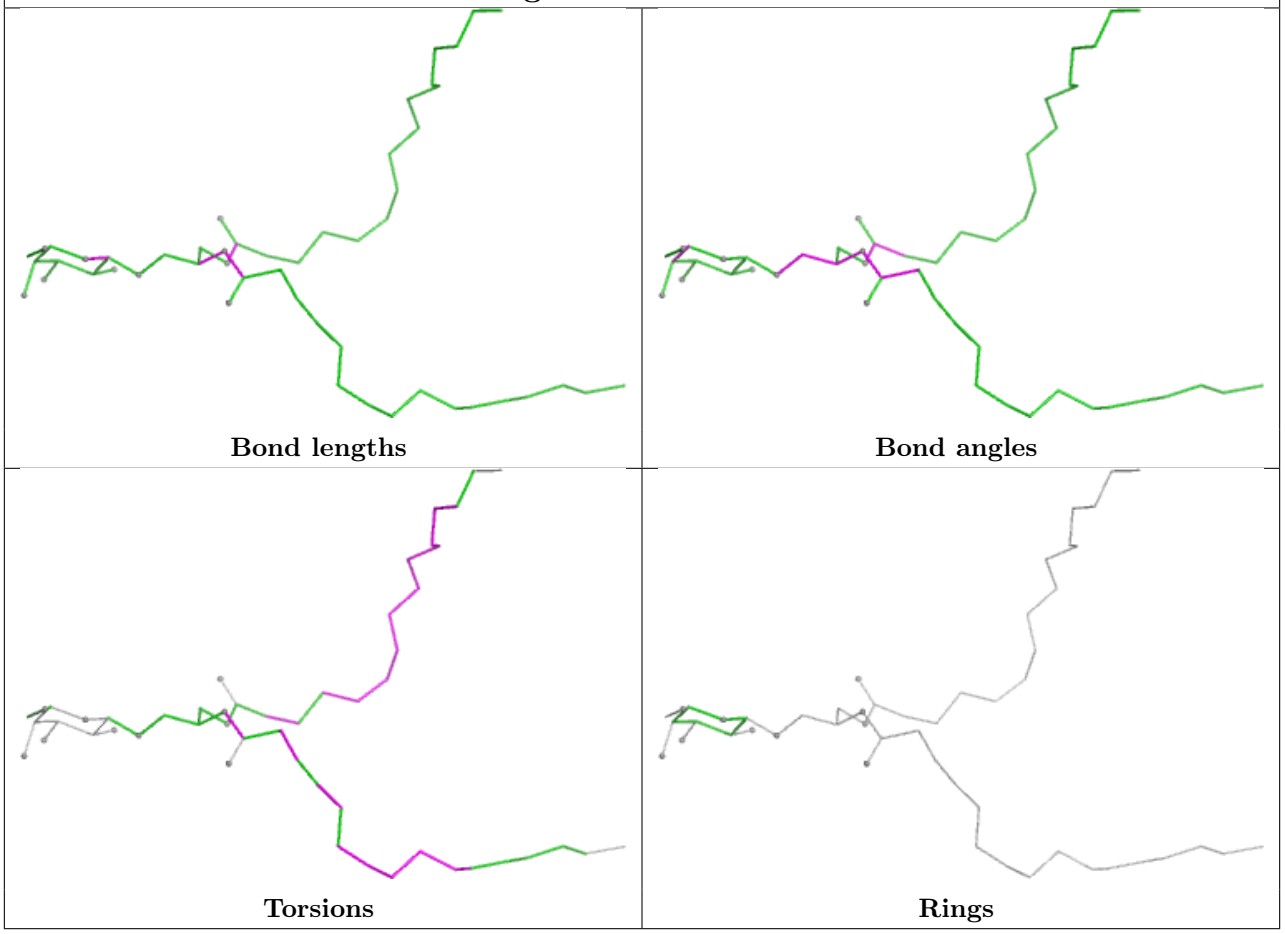
Ligand BCR F 101



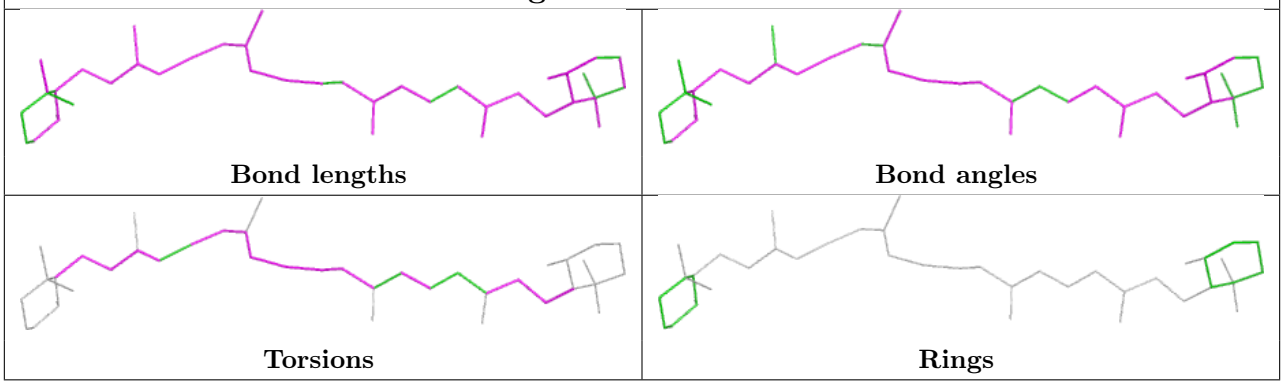
Ligand CLA b 609



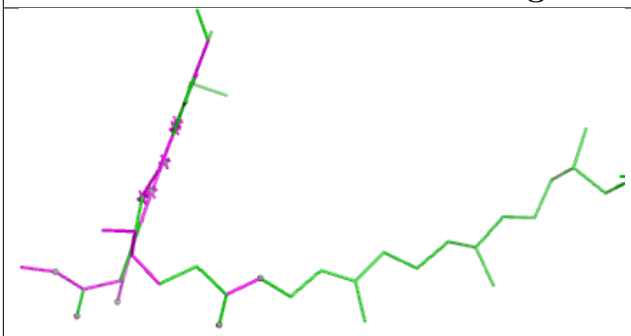
Ligand LMG b 622



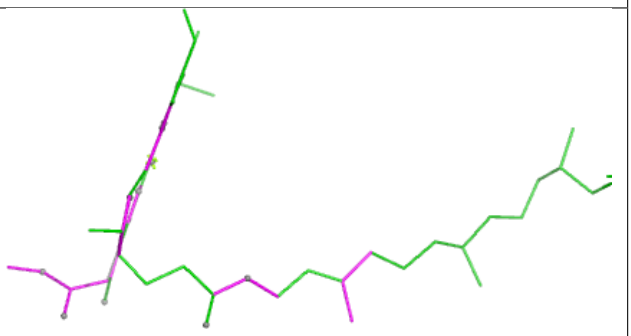
Ligand BCR c 515



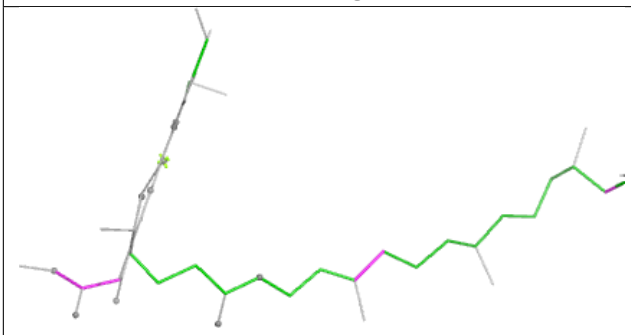
Ligand CLA b 607



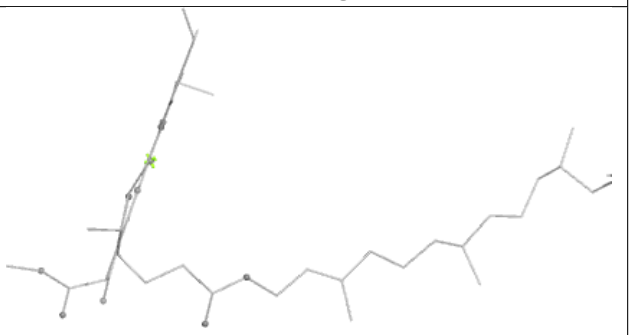
Bond lengths



Bond angles

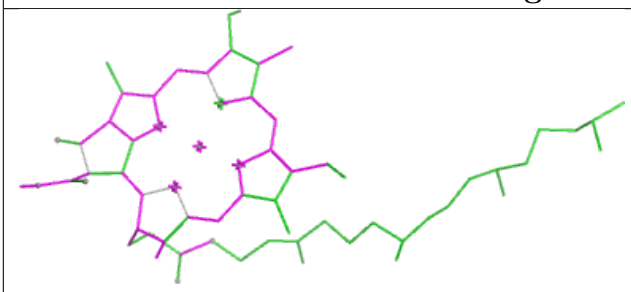


Torsions

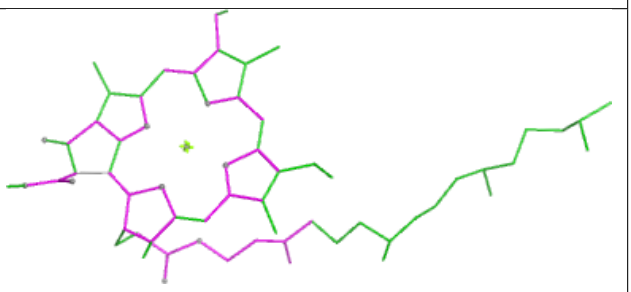


Rings

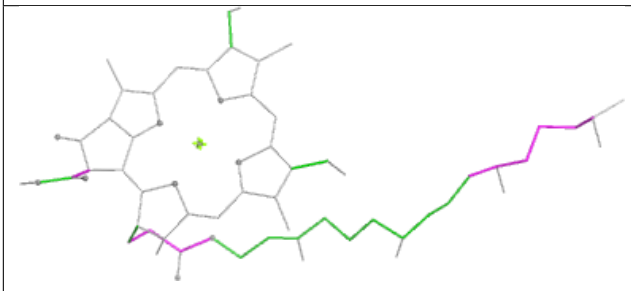
Ligand CLA C 501



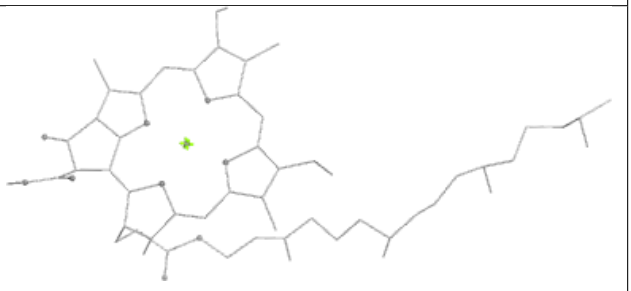
Bond lengths



Bond angles

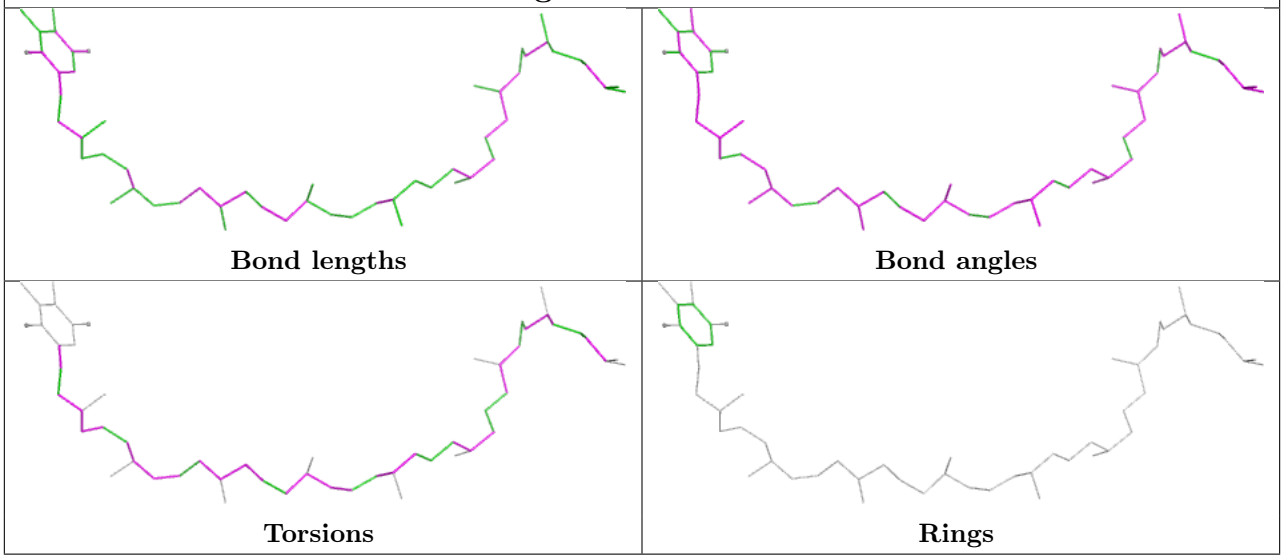


Torsions

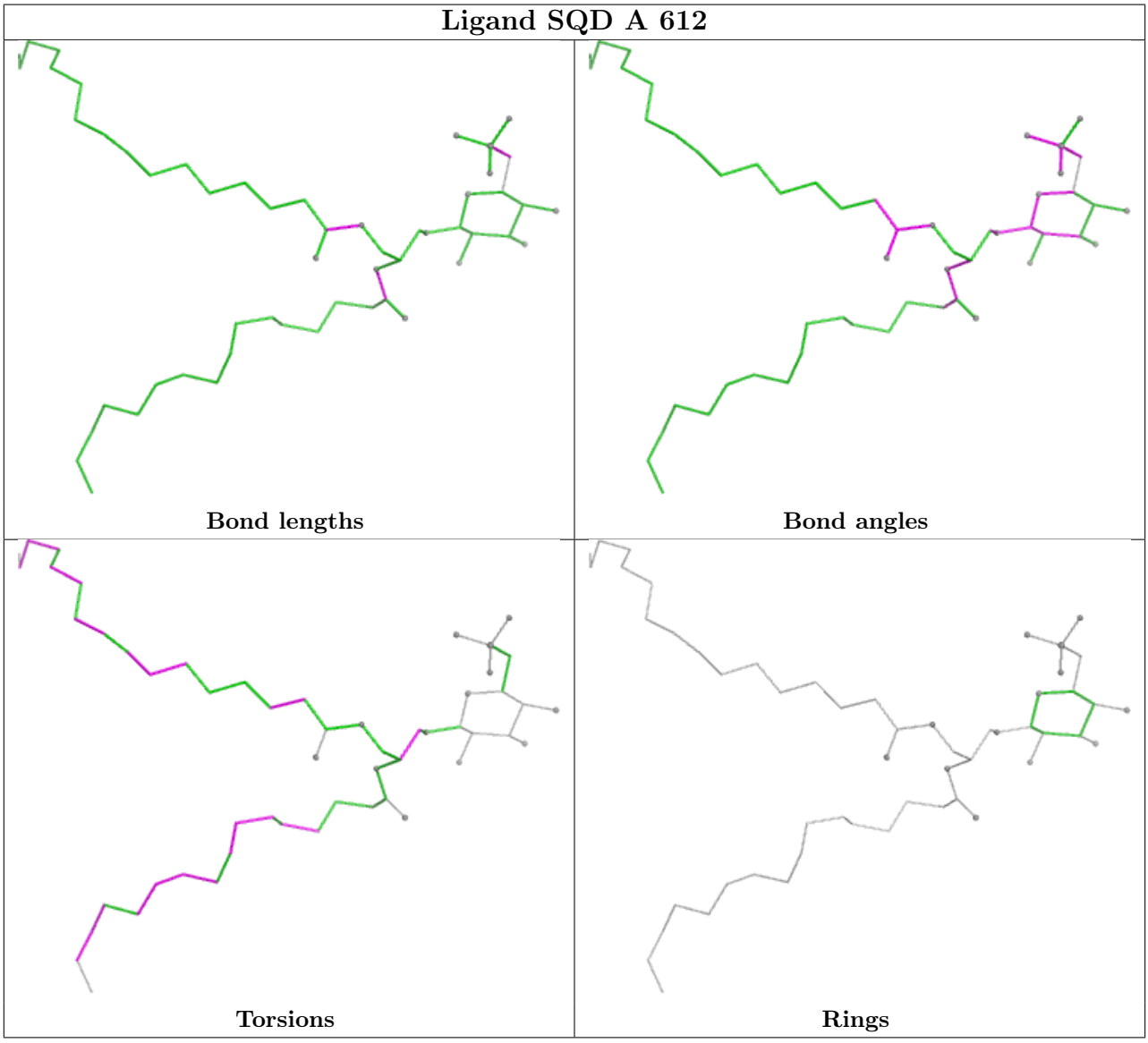


Rings

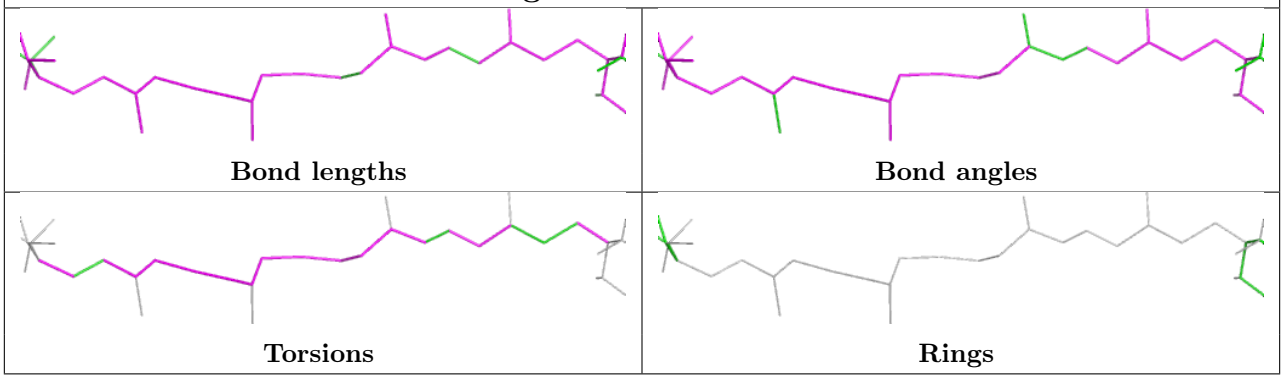
Ligand PL9 a 611



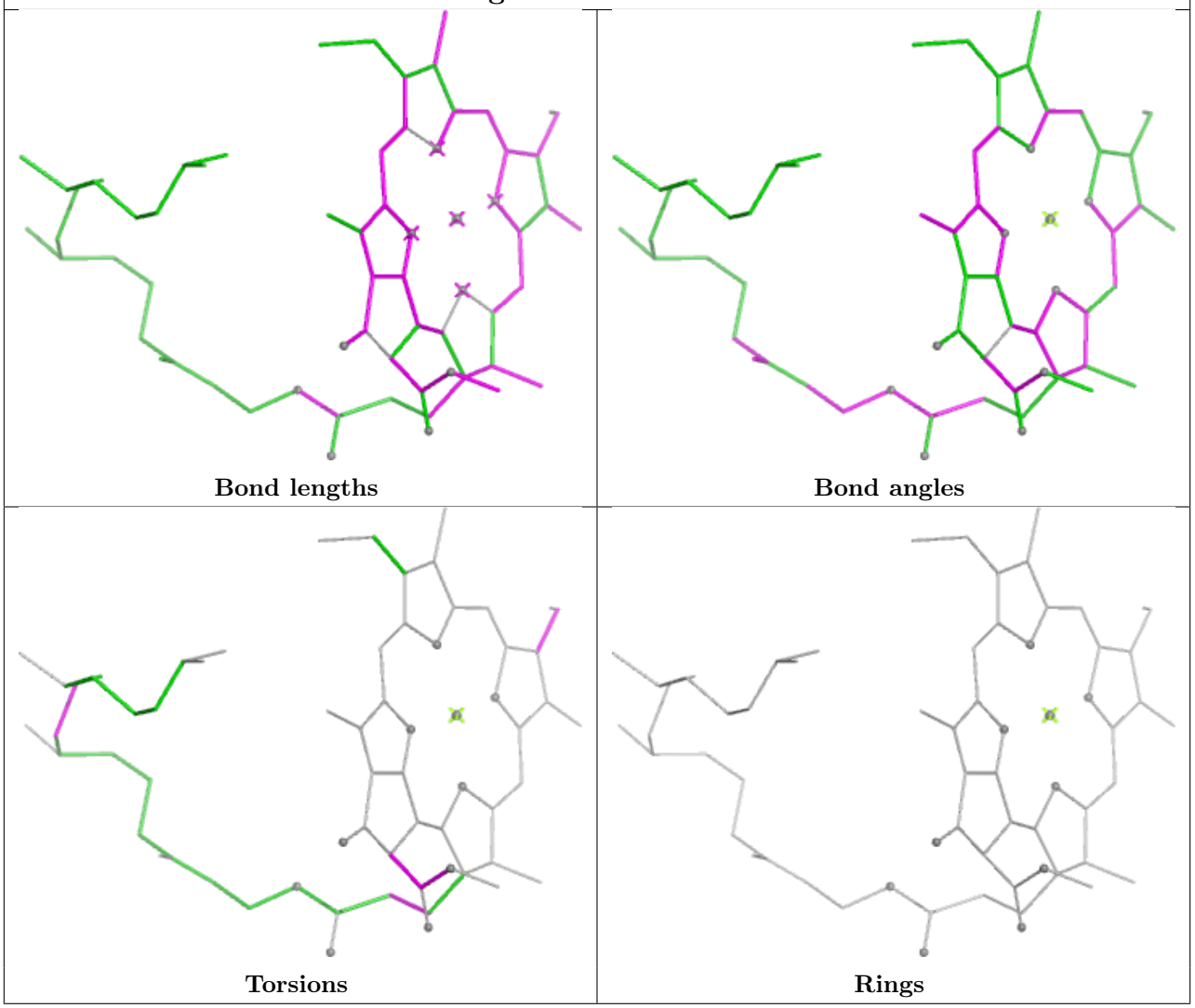
Ligand SQD A 612



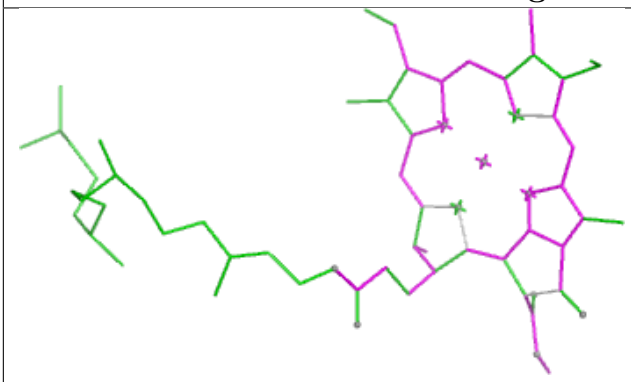
Ligand BCR A 610



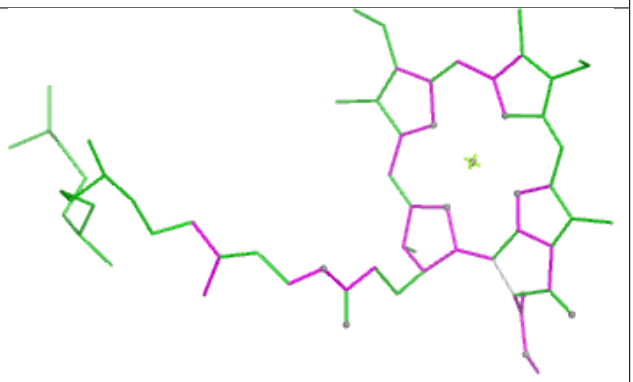
Ligand CLA C 503



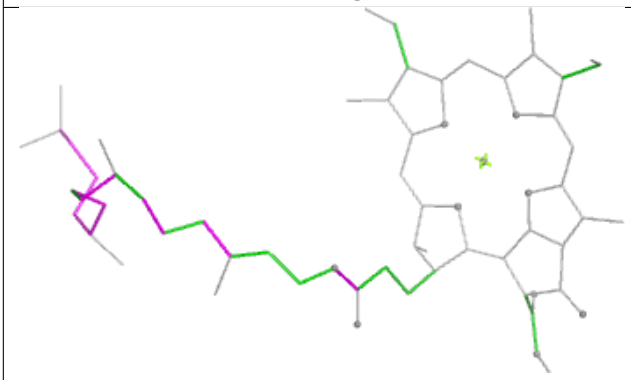
Ligand CLA a 609



Bond lengths



Bond angles

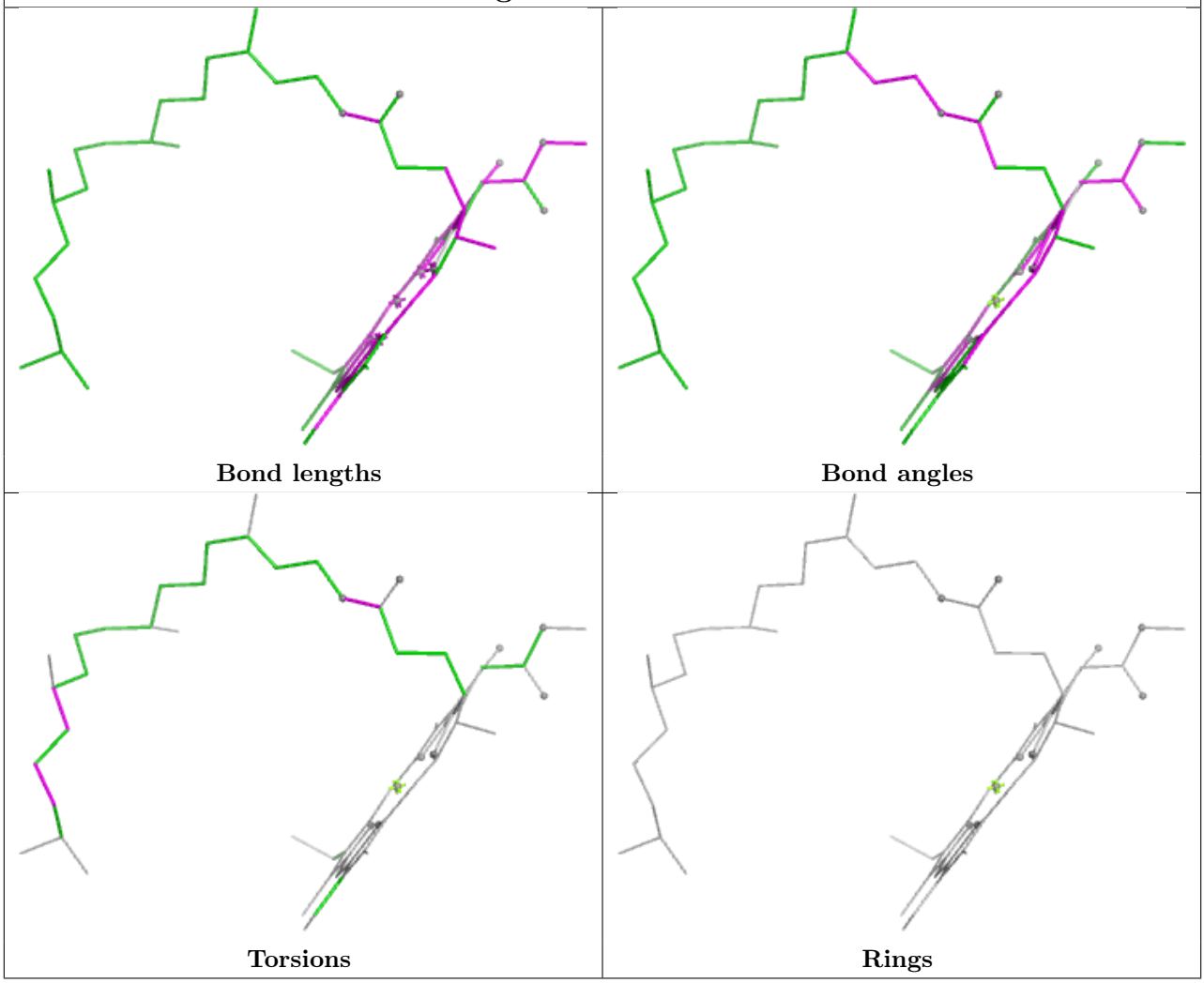


Torsions



Rings

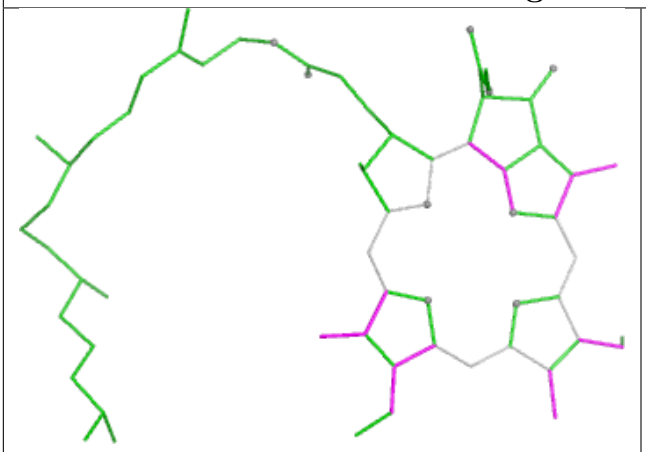
Ligand CLA b 613



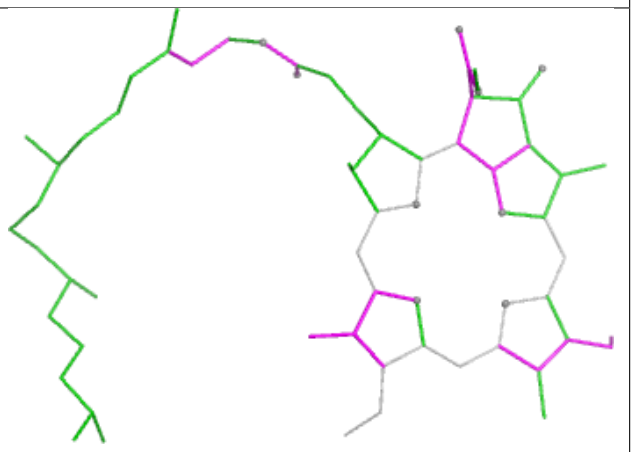
Bond lengths | Bond angles

Torsions | Rings

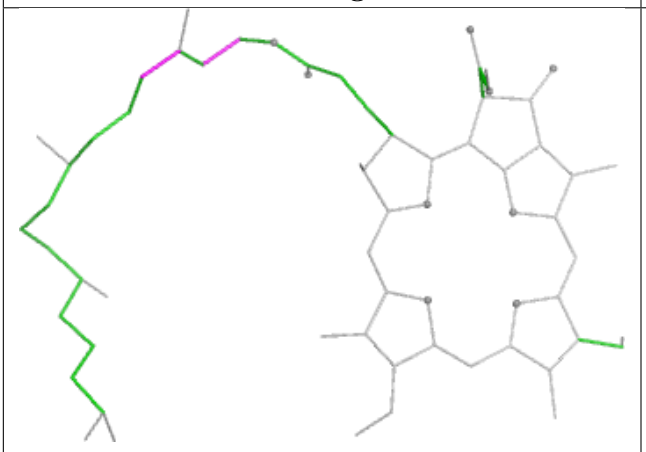
Ligand PHO a 608



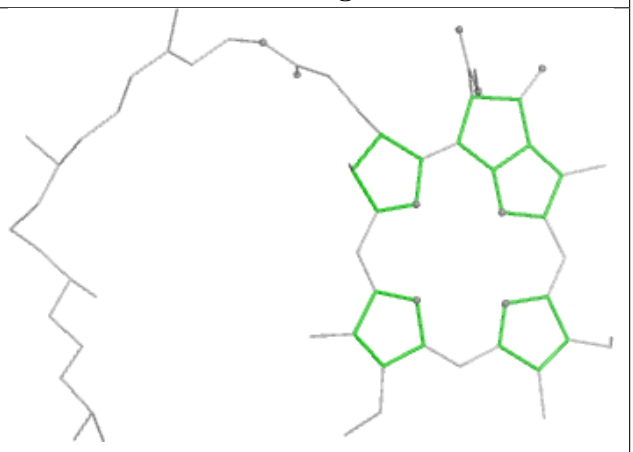
Bond lengths



Bond angles

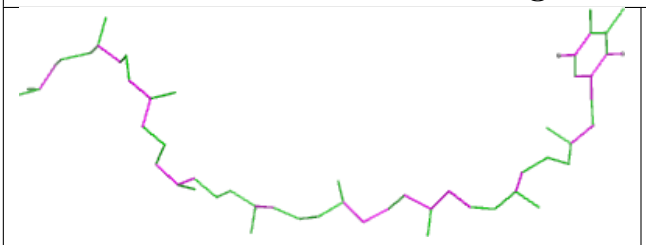


Torsions

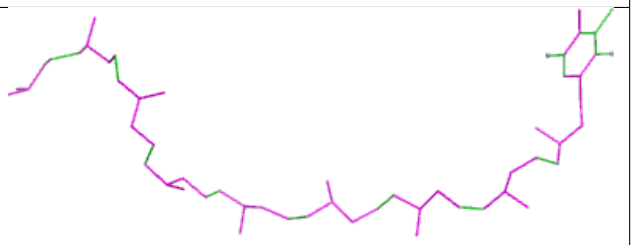


Rings

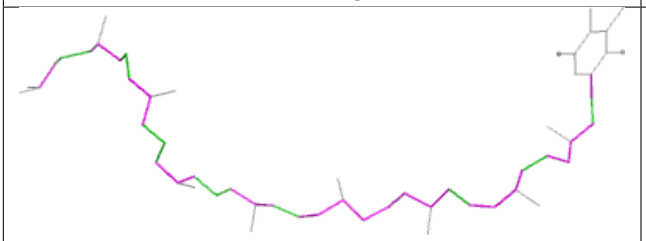
Ligand PL9 A 611



Bond lengths



Bond angles

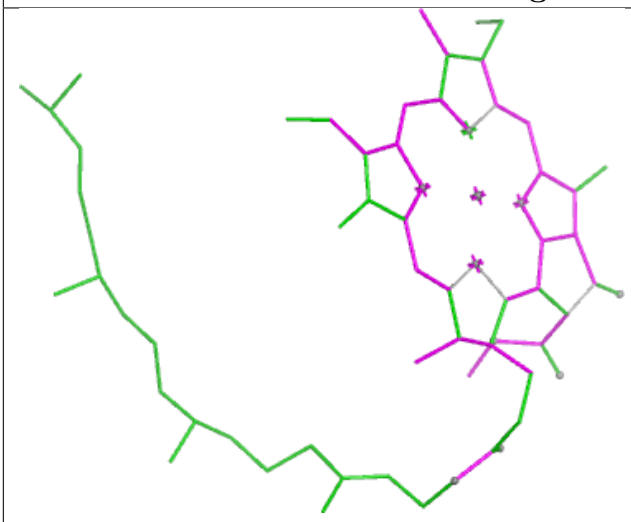


Torsions

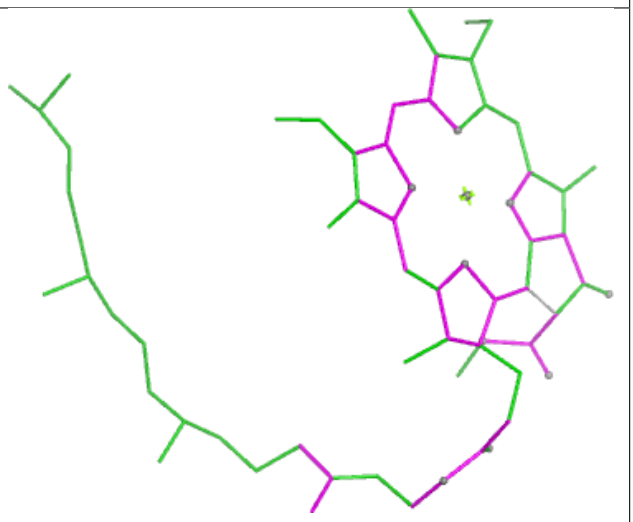


Rings

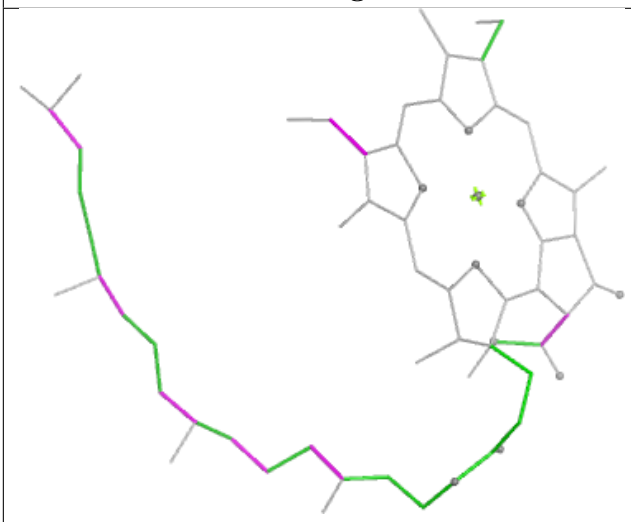
Ligand CLA c 507



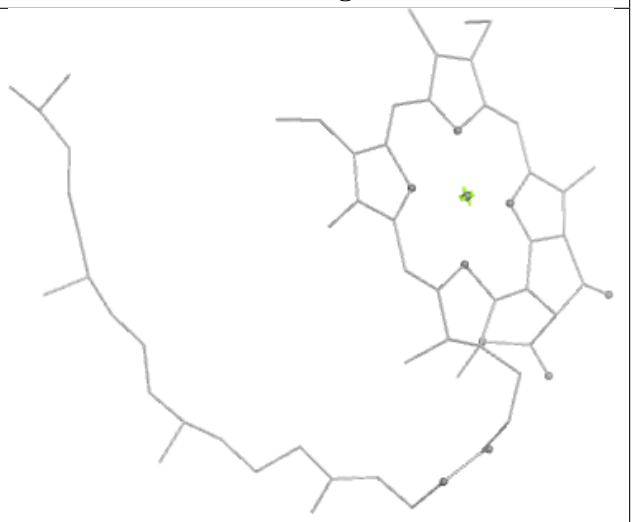
Bond lengths



Bond angles

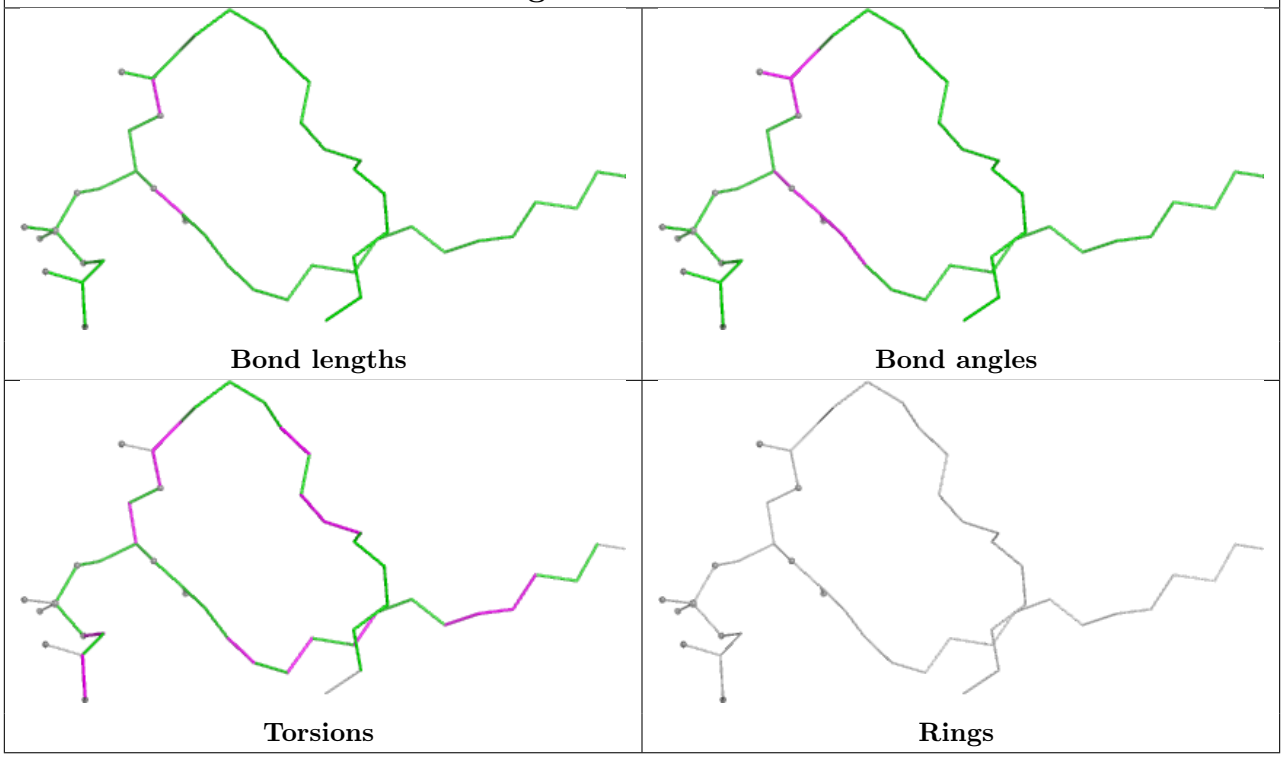


Torsions

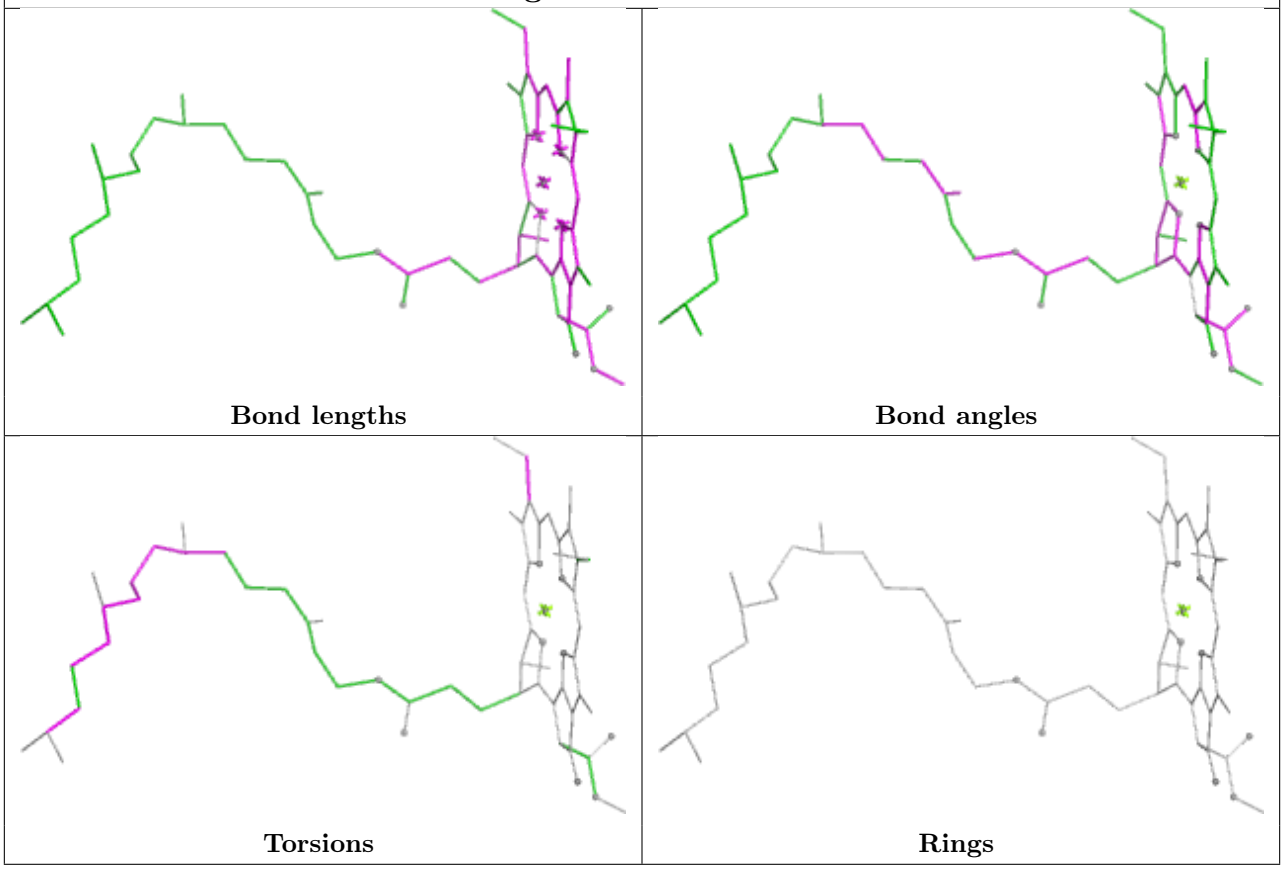


Rings

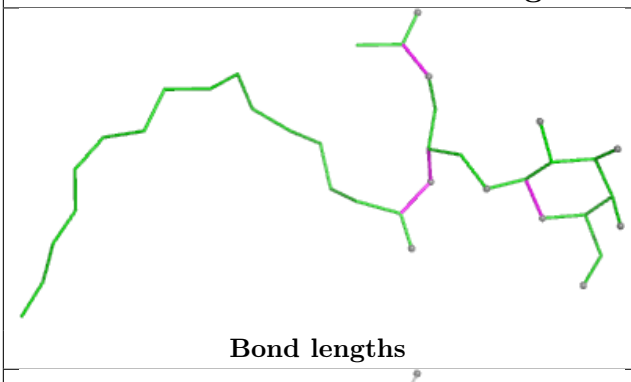
Ligand LHG a 616



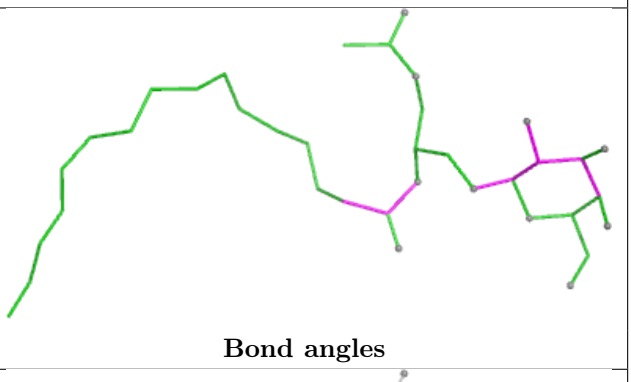
Ligand CLA D 404



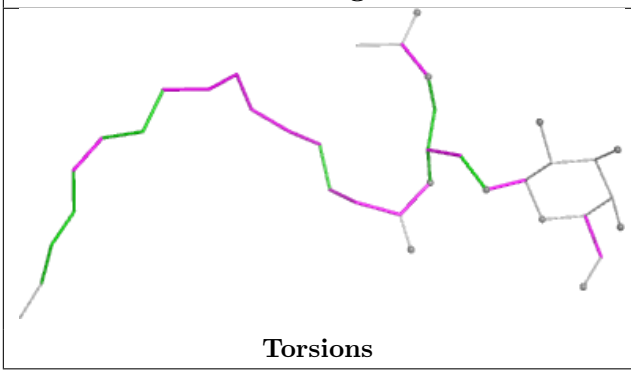
Ligand LMG z 101



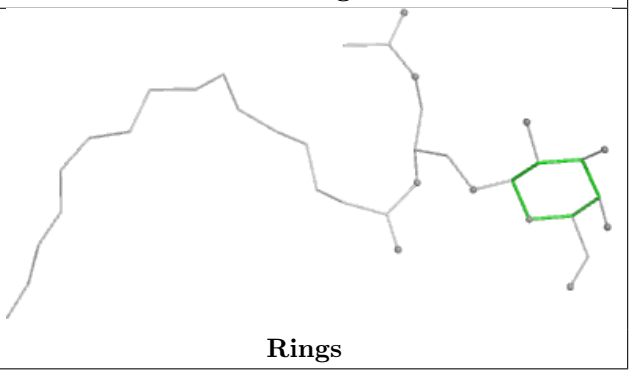
Bond lengths



Bond angles

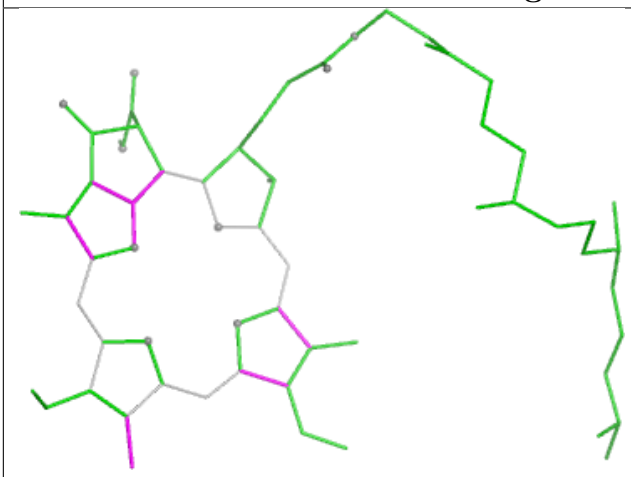


Torsions

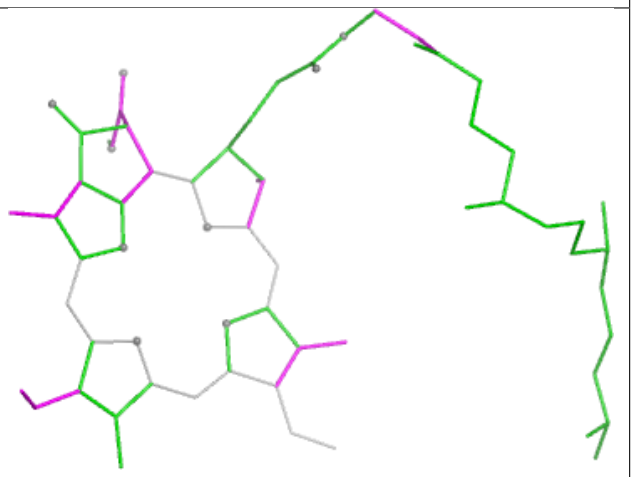


Rings

Ligand PHO d 401



Bond lengths



Bond angles

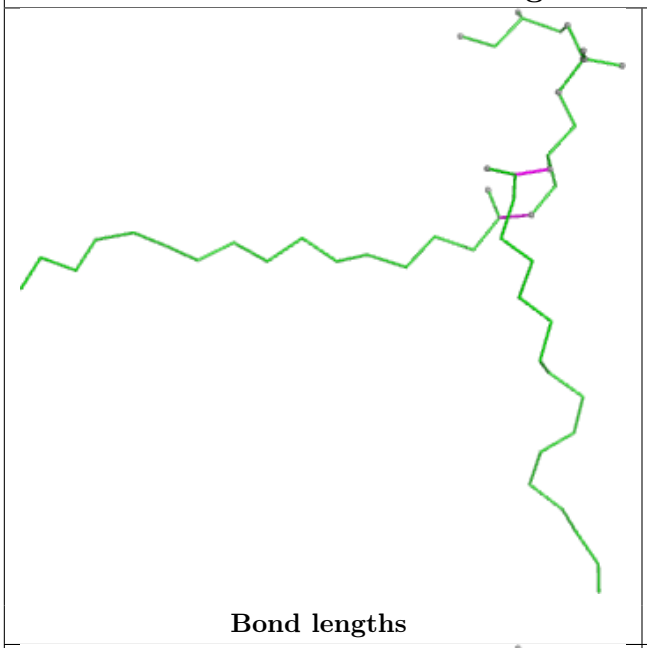


Torsions

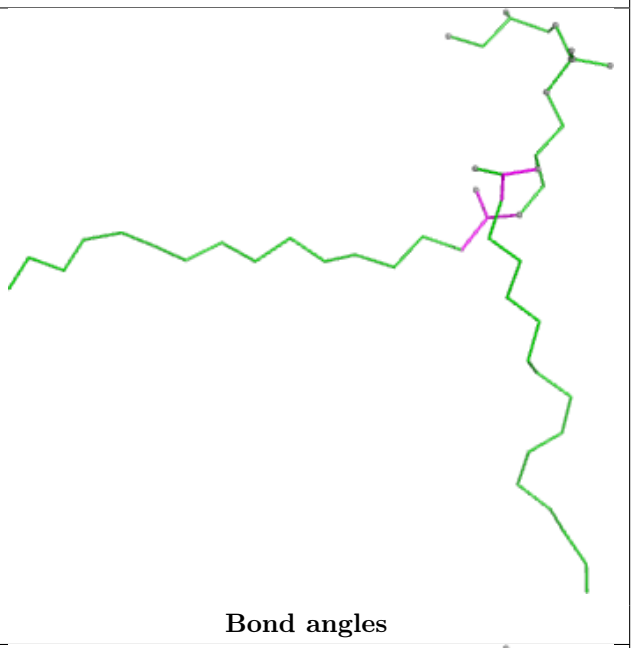


Rings

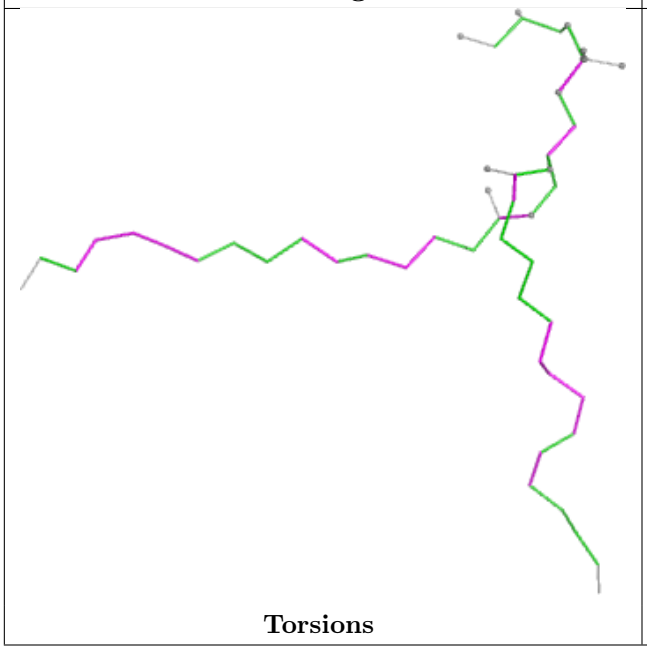
Ligand LHG L 101



Bond lengths



Bond angles

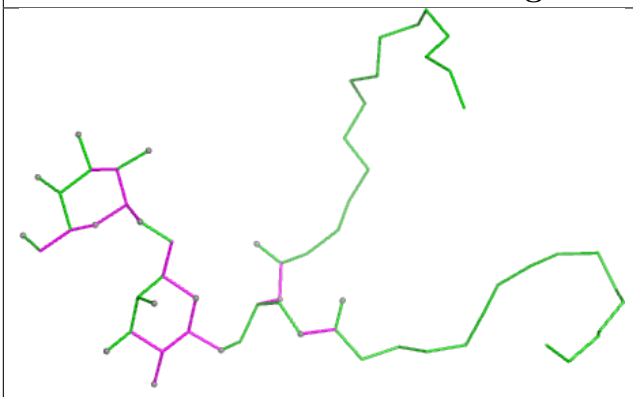


Torsions

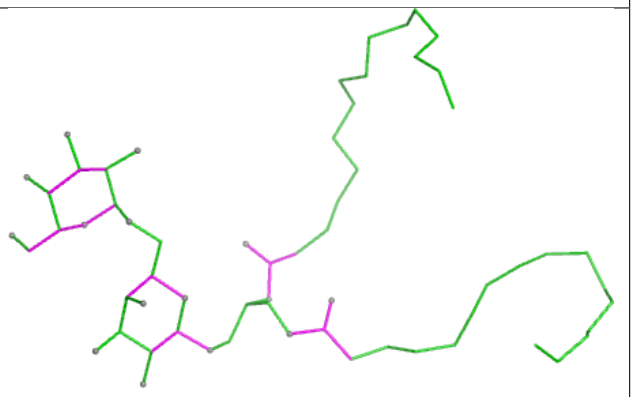


Rings

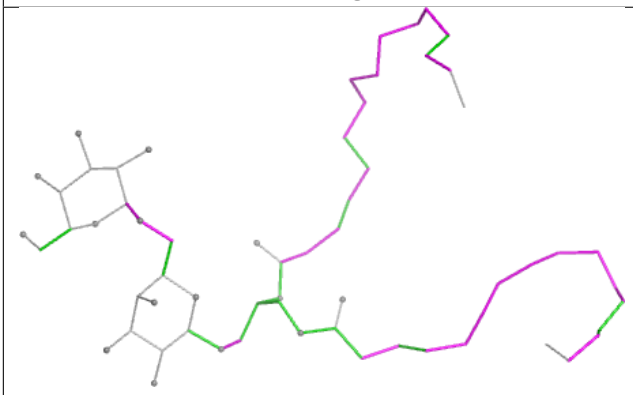
Ligand DGD c 517



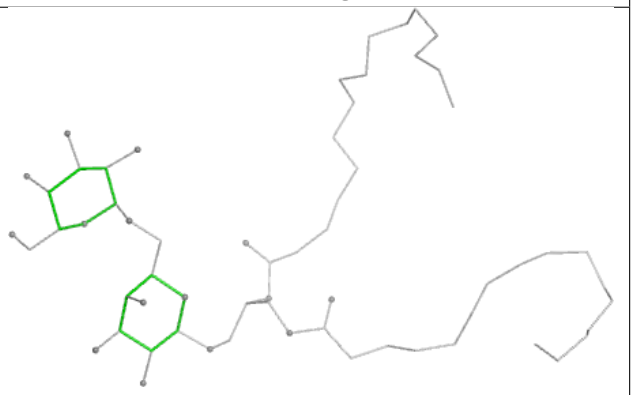
Bond lengths



Bond angles

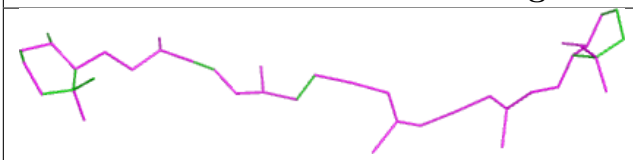


Torsions



Rings

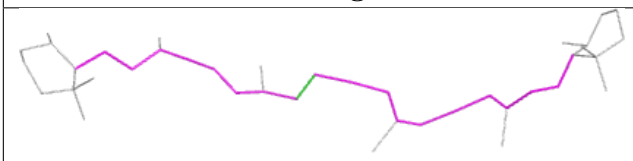
Ligand BCR t 101



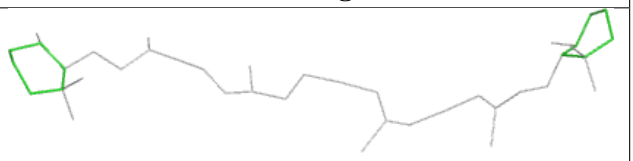
Bond lengths



Bond angles

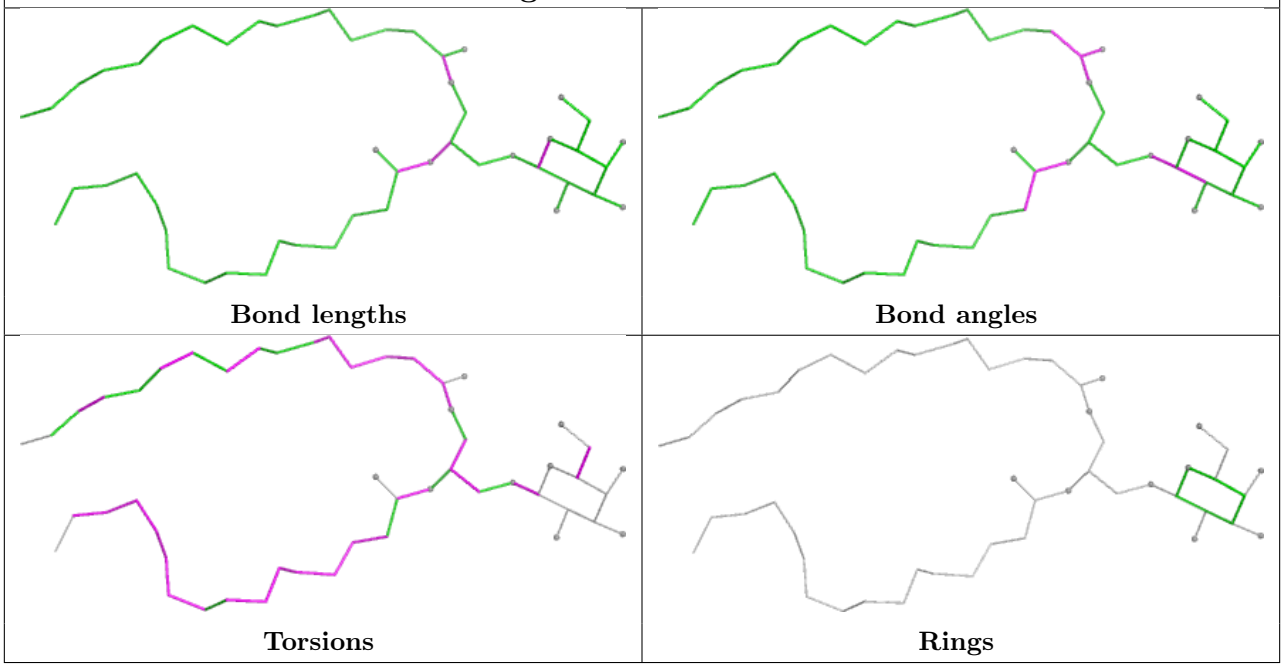


Torsions

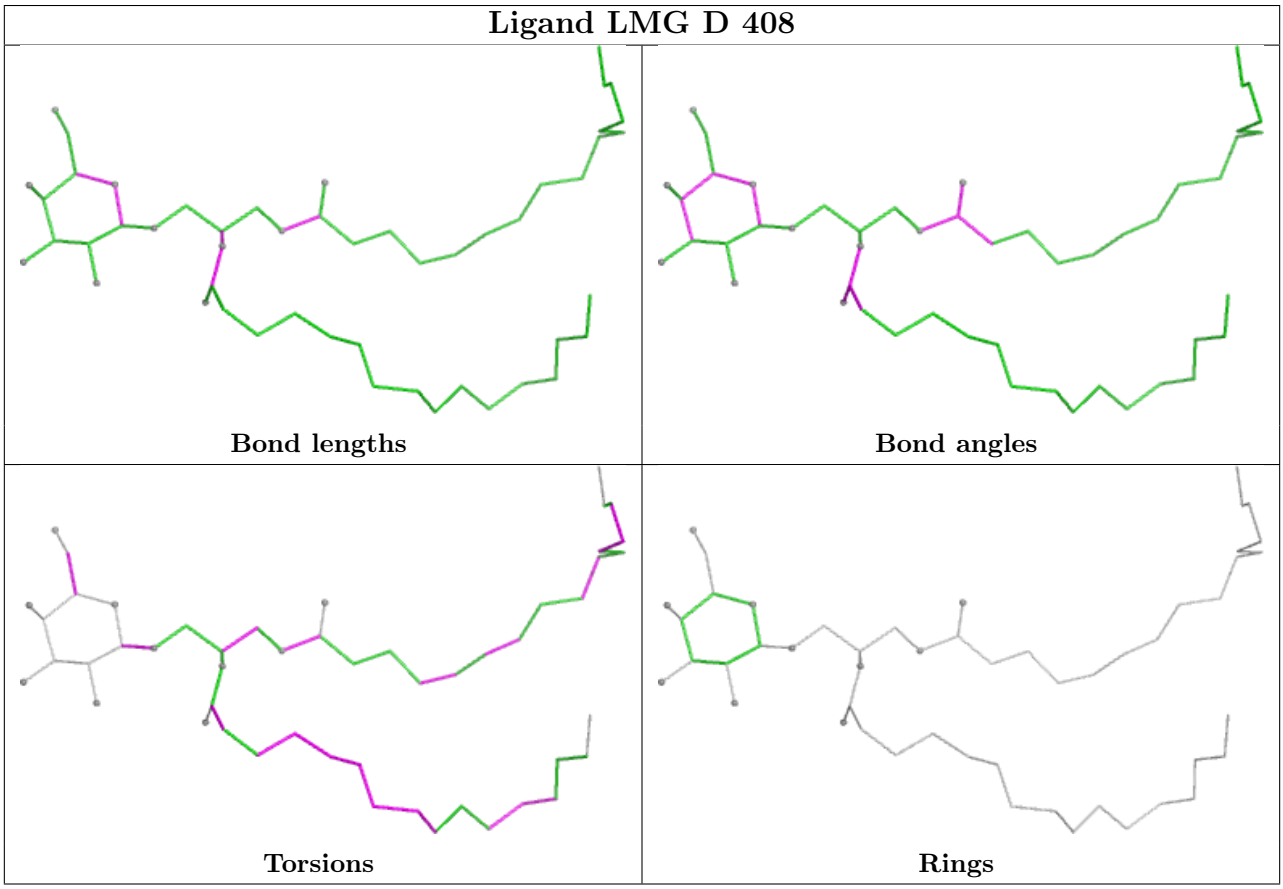


Rings

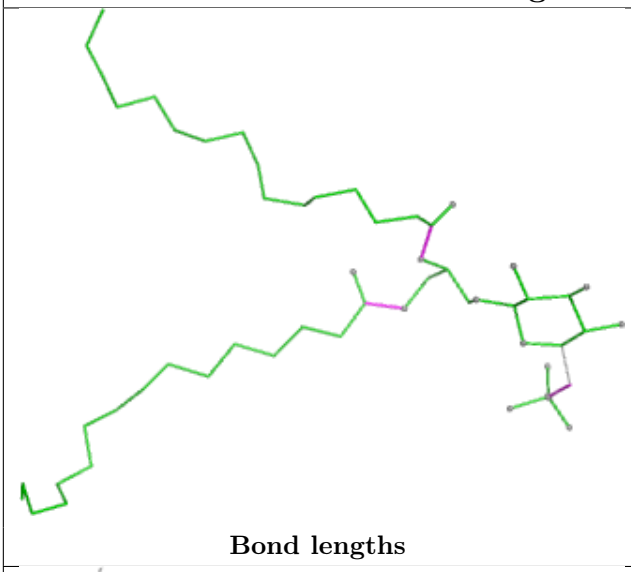
Ligand LMG A 613



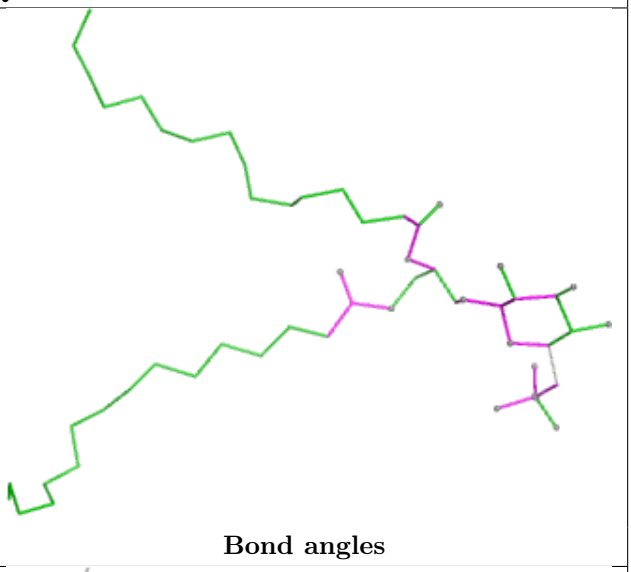
Ligand LMG D 408



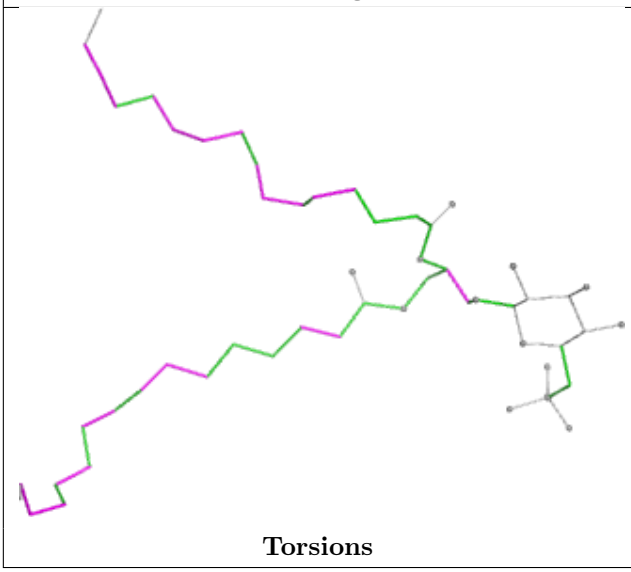
Ligand SQD a 612



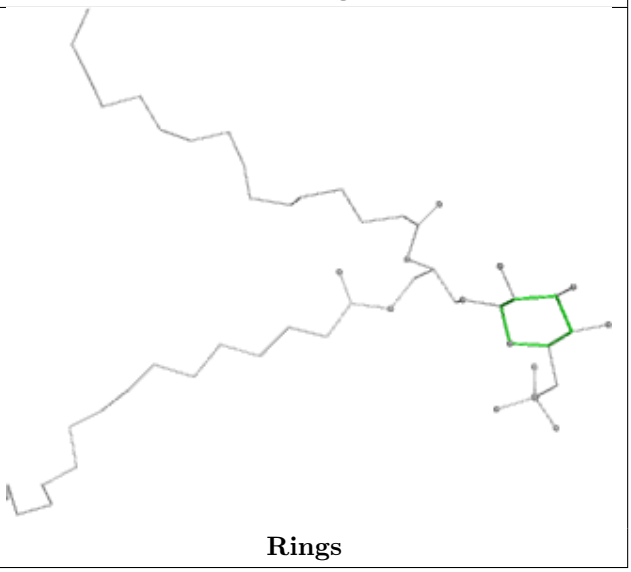
Bond lengths



Bond angles

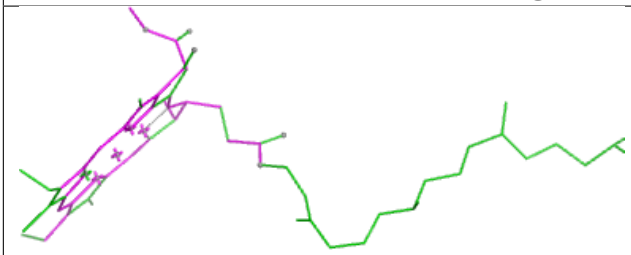


Torsions

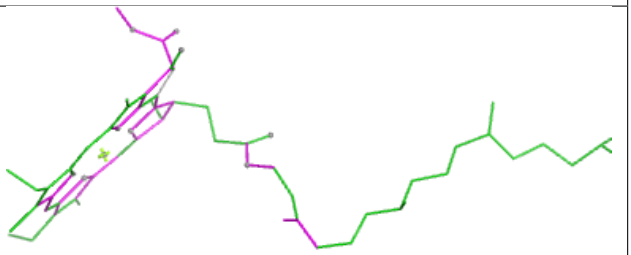


Rings

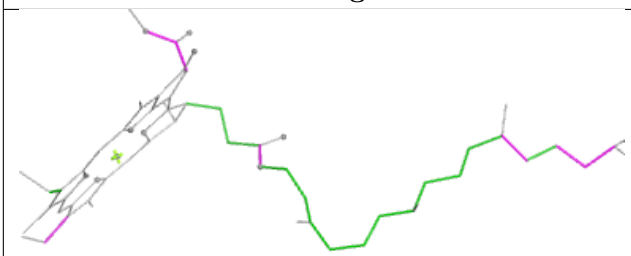
Ligand CLA c 502



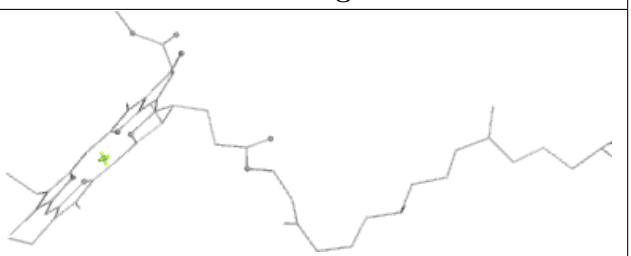
Bond lengths



Bond angles

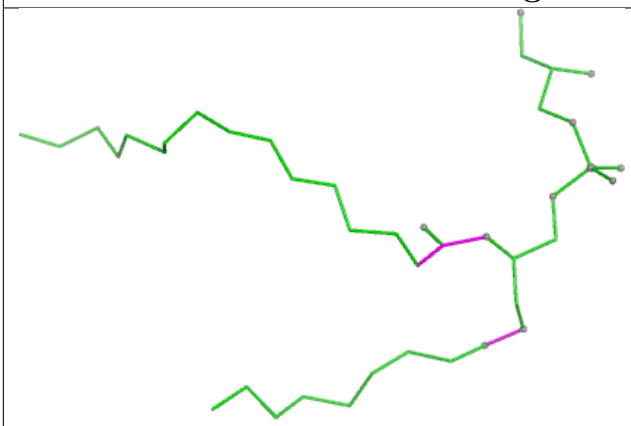


Torsions

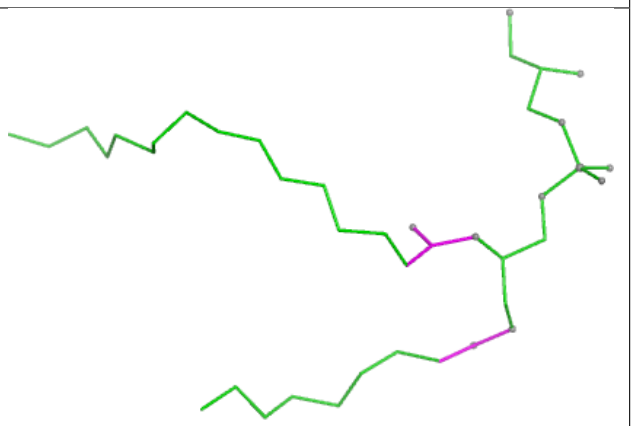


Rings

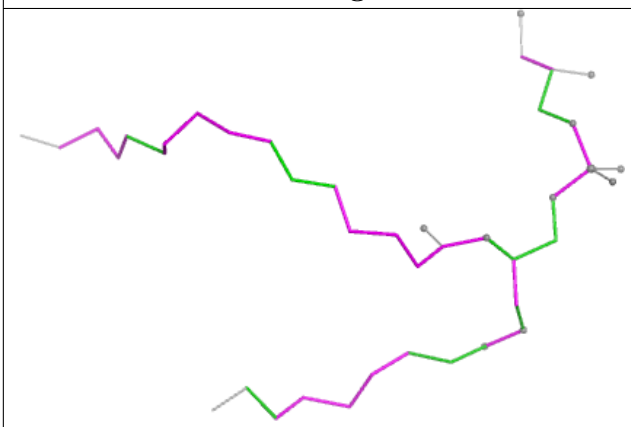
Ligand LHG E 102



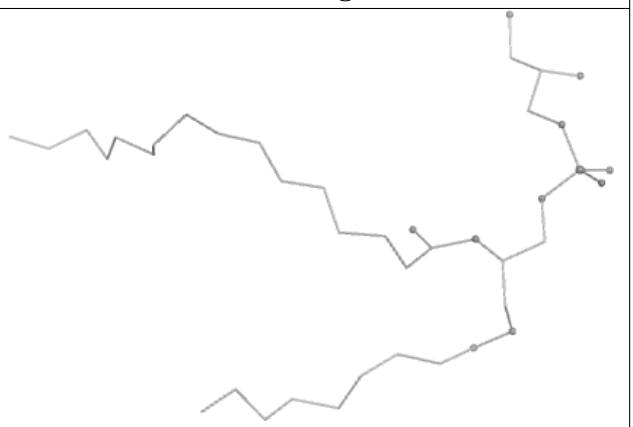
Bond lengths



Bond angles

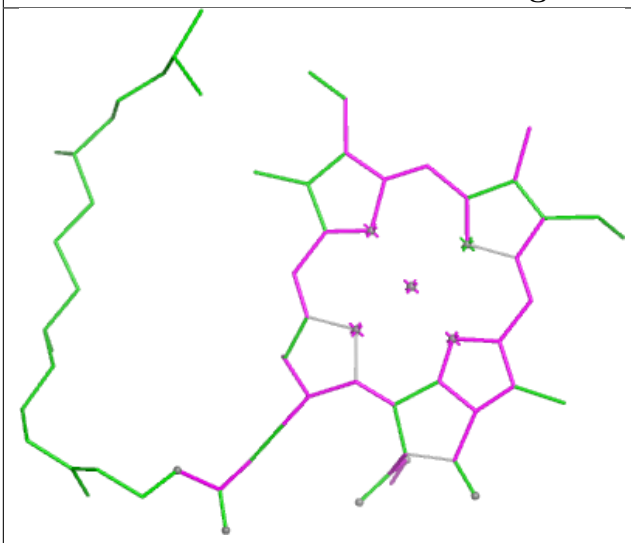


Torsions

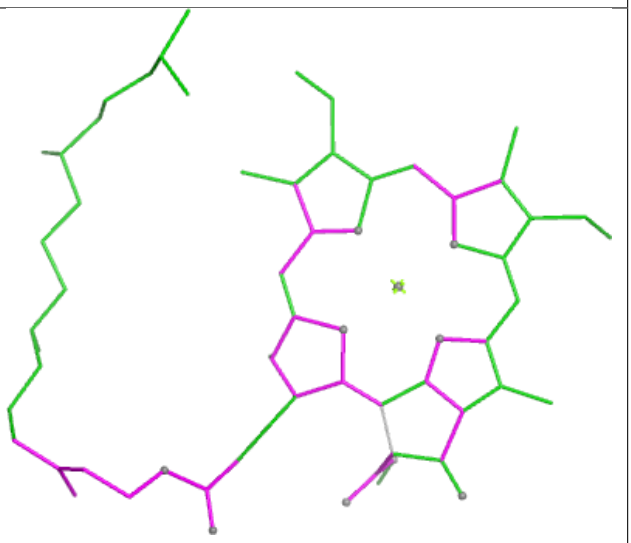


Rings

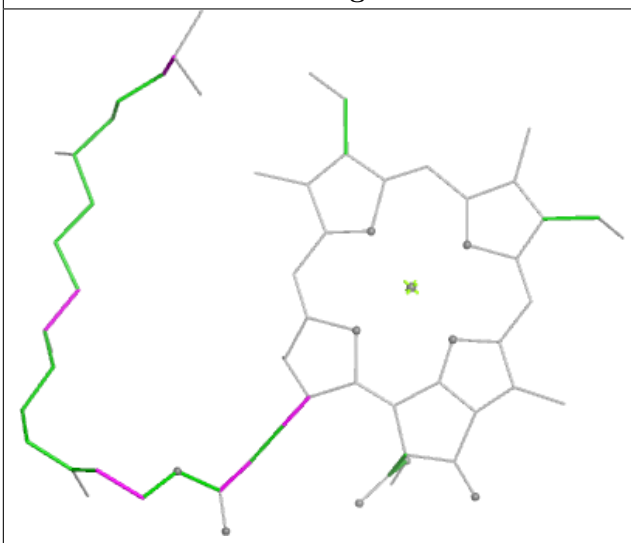
Ligand CLA c 512



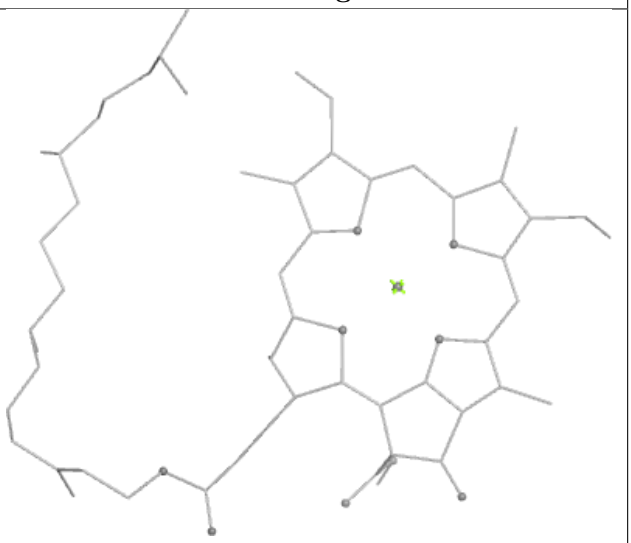
Bond lengths



Bond angles

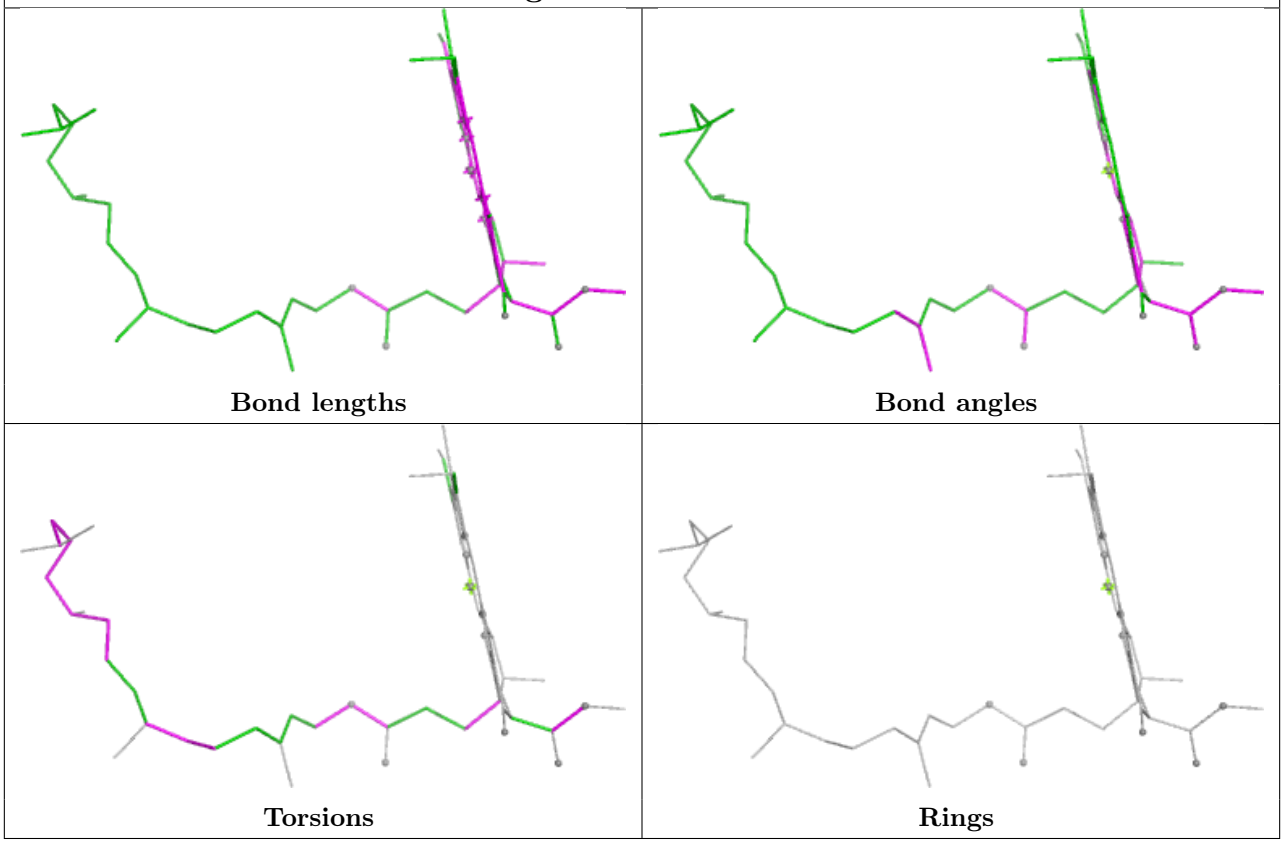


Torsions

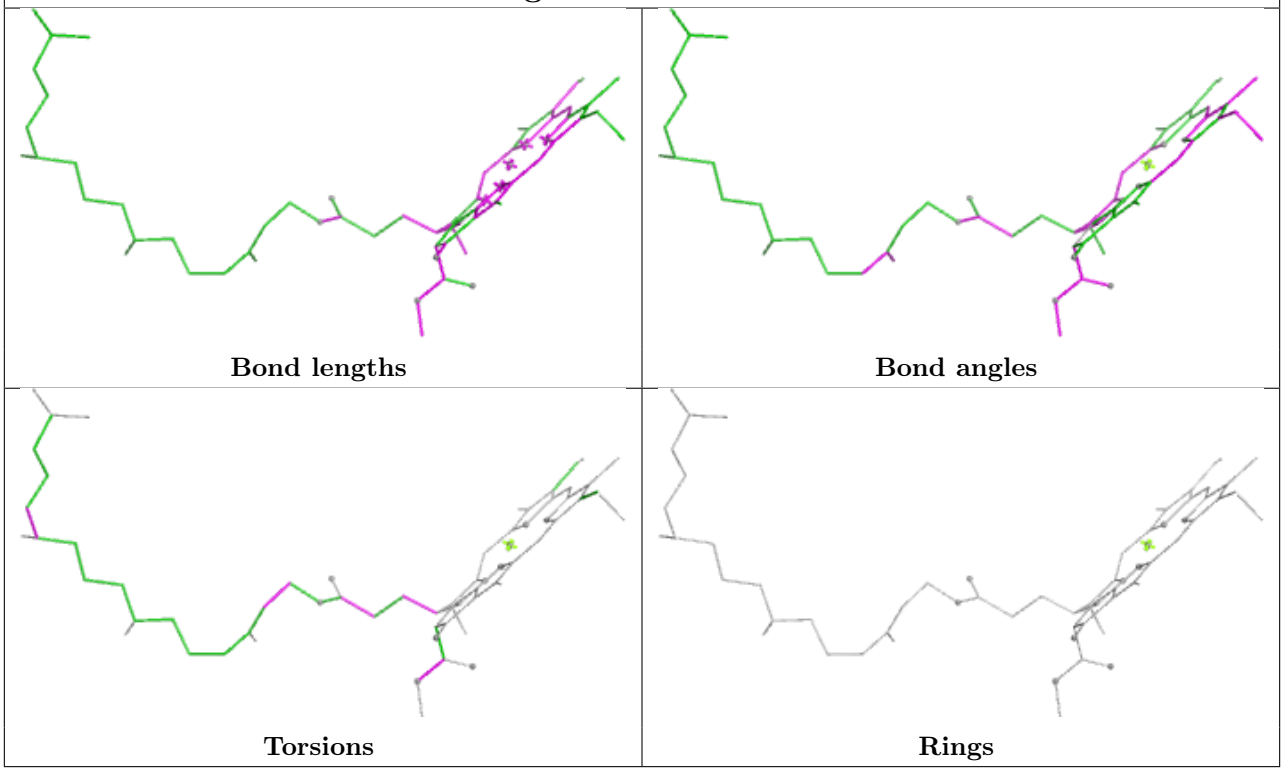


Rings

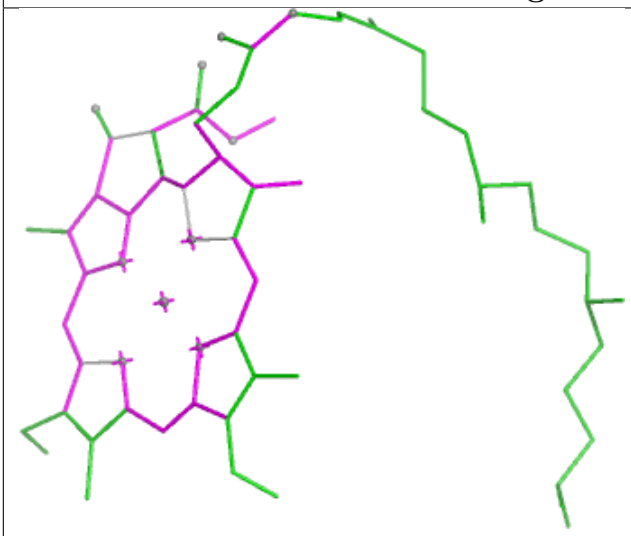
Ligand CLA C 506



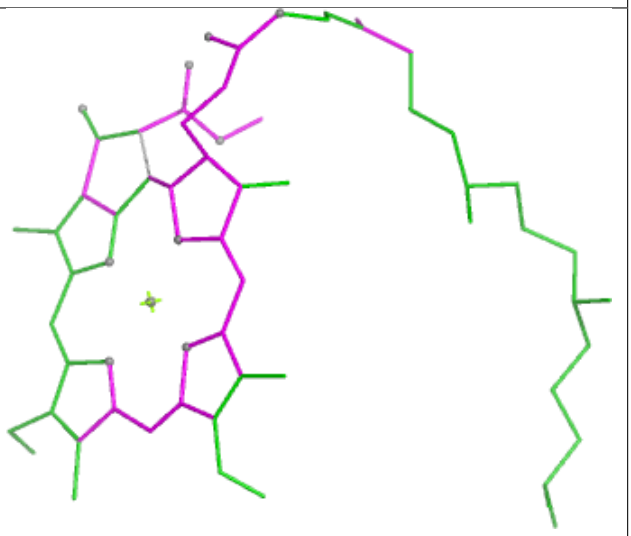
Ligand CLA D 403



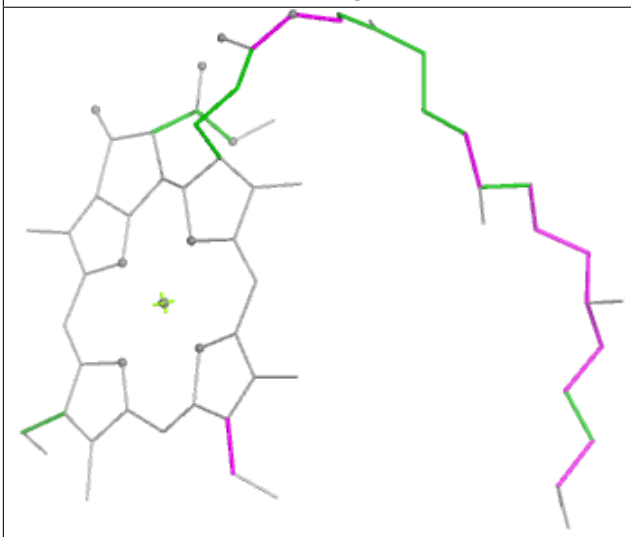
Ligand CLA b 618



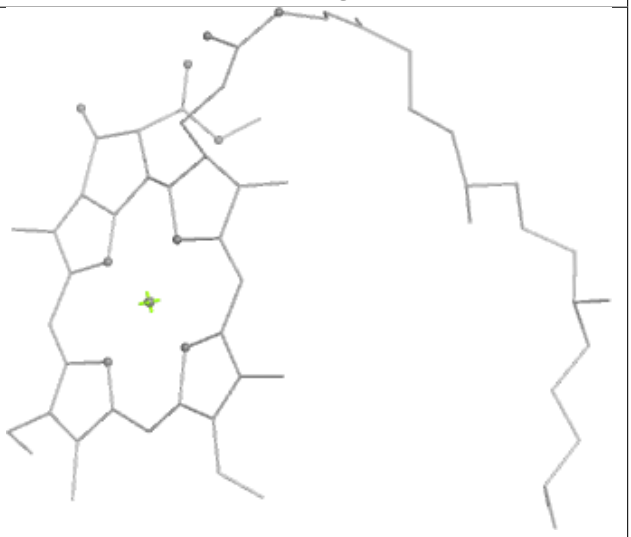
Bond lengths



Bond angles

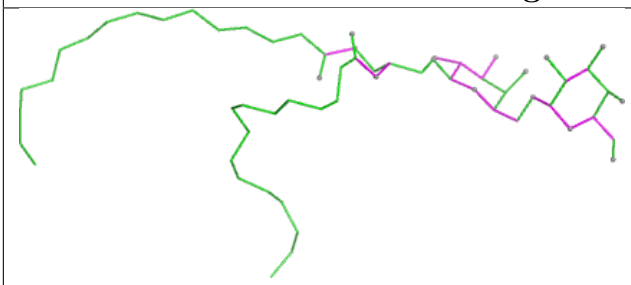


Torsions

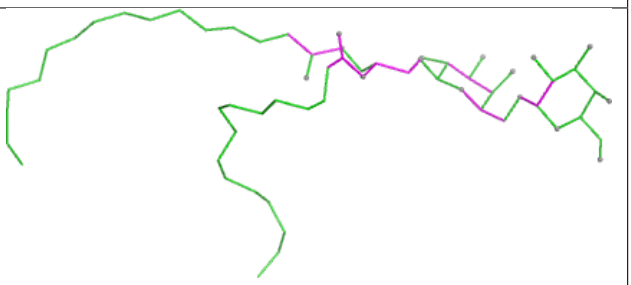


Rings

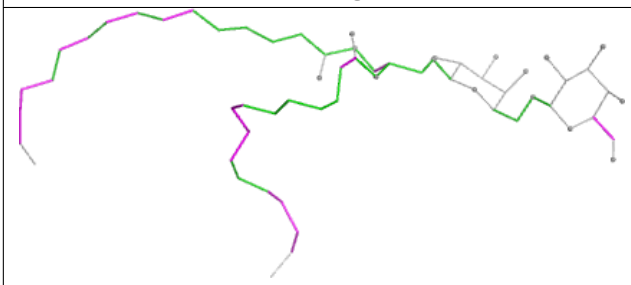
Ligand DGD h 102



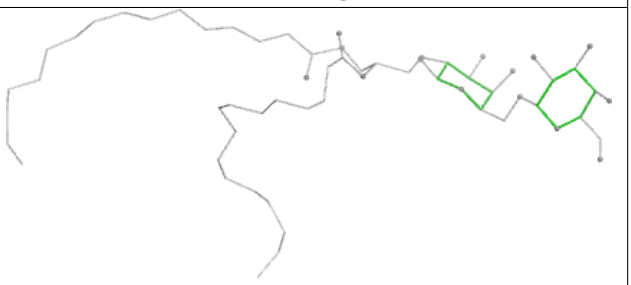
Bond lengths



Bond angles

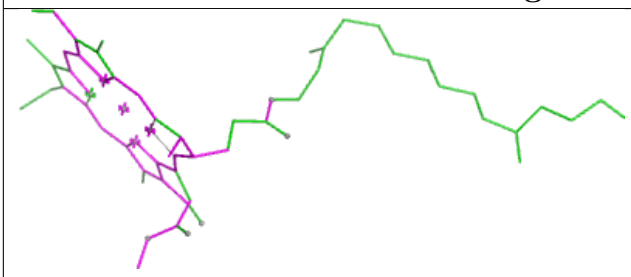


Torsions

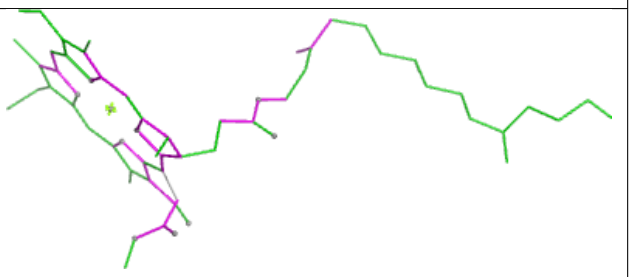


Rings

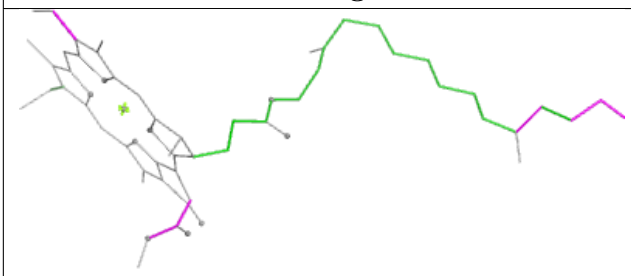
Ligand CLA C 502



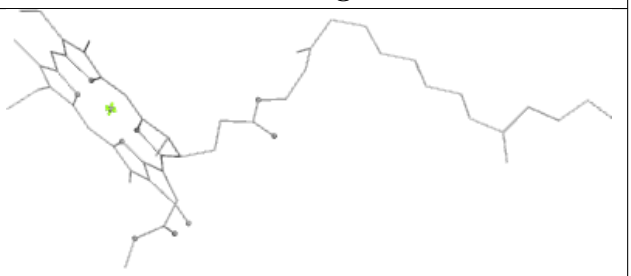
Bond lengths



Bond angles

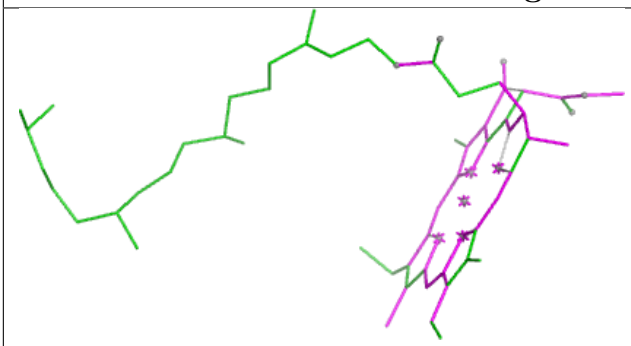


Torsions

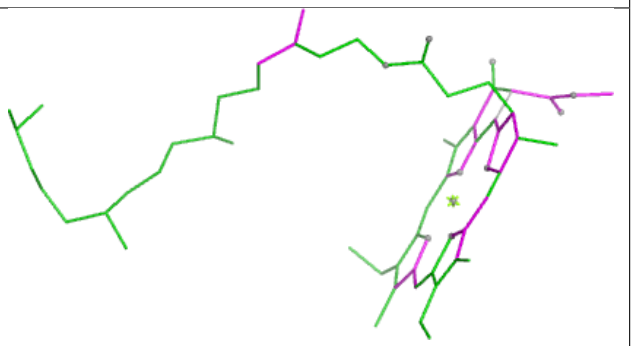


Rings

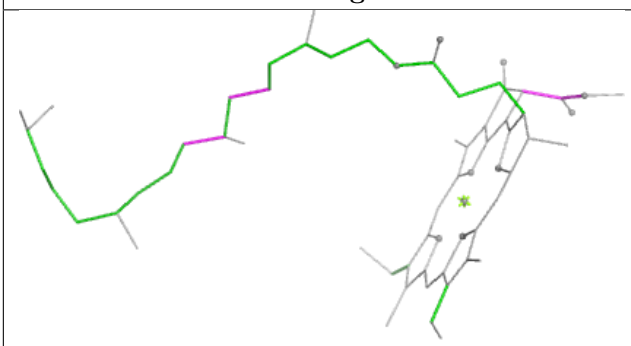
Ligand CLA C 508



Bond lengths



Bond angles

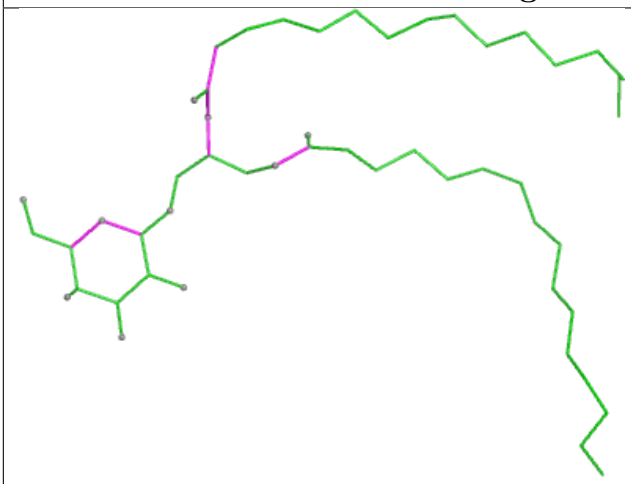


Torsions

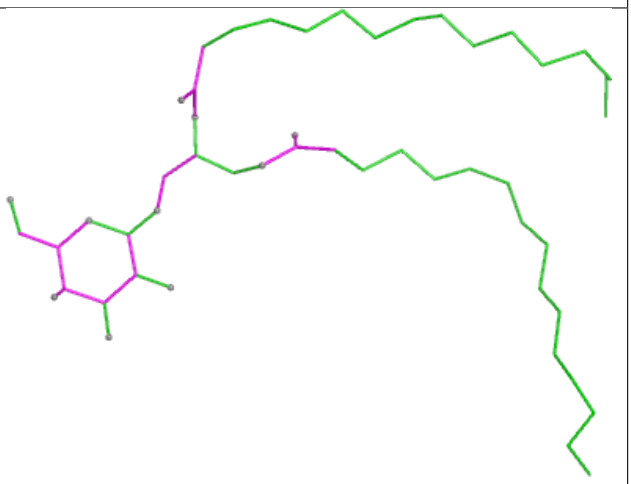


Rings

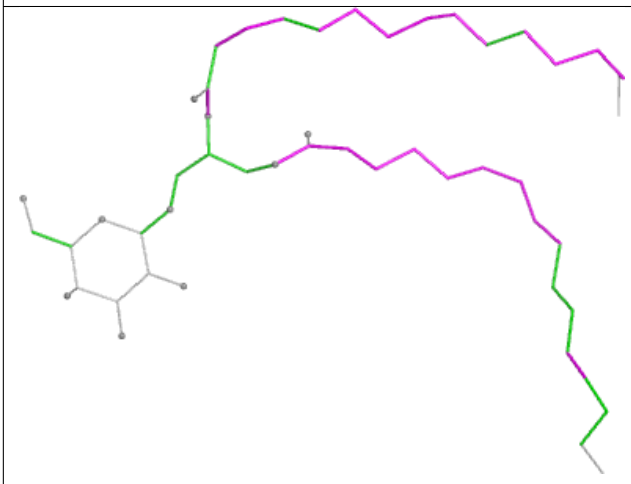
Ligand LMG C 518



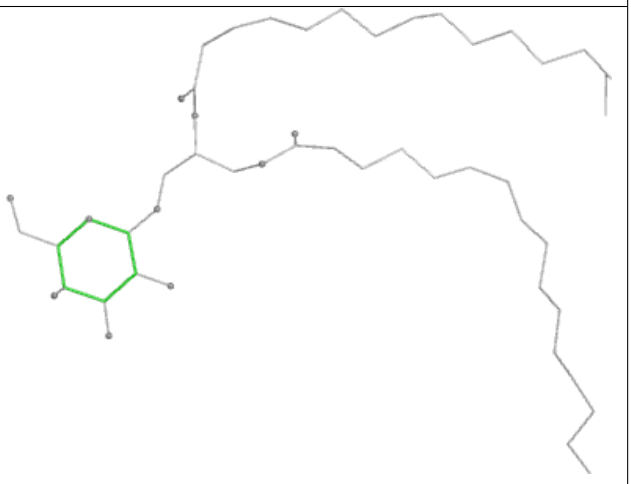
Bond lengths



Bond angles

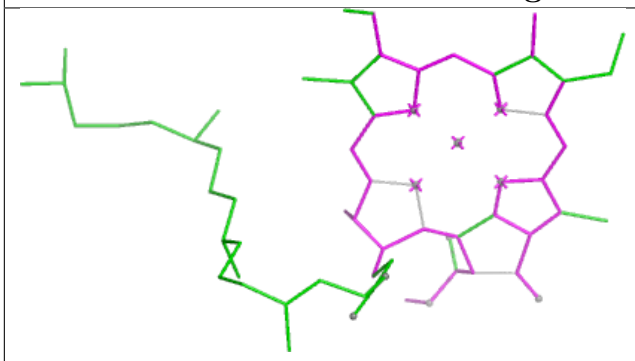


Torsions

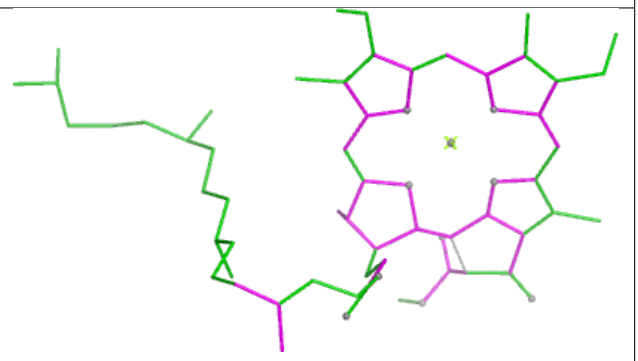


Rings

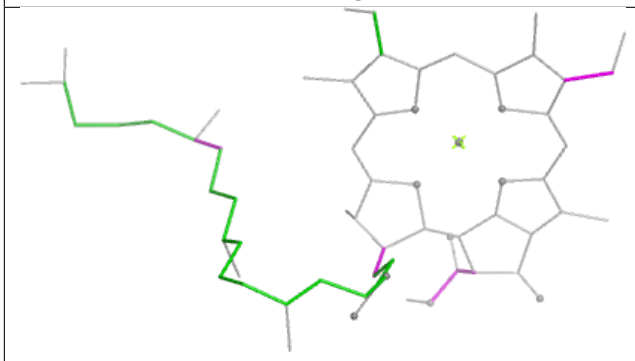
Ligand CLA D 402



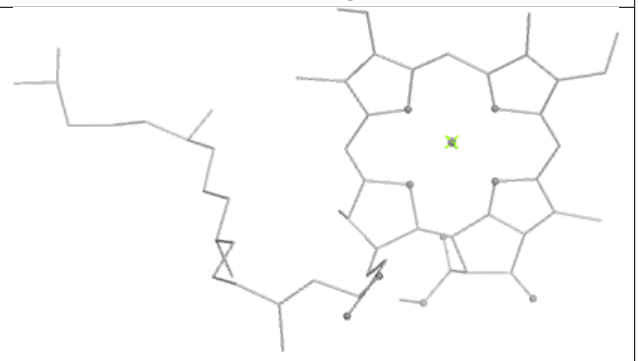
Bond lengths



Bond angles

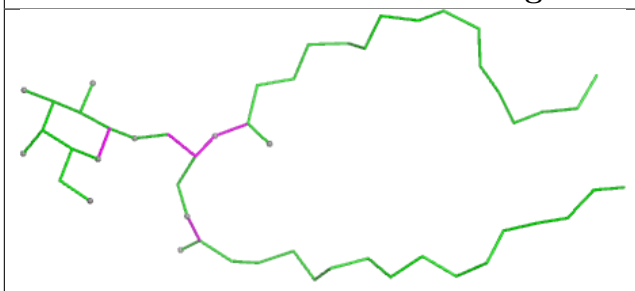


Torsions

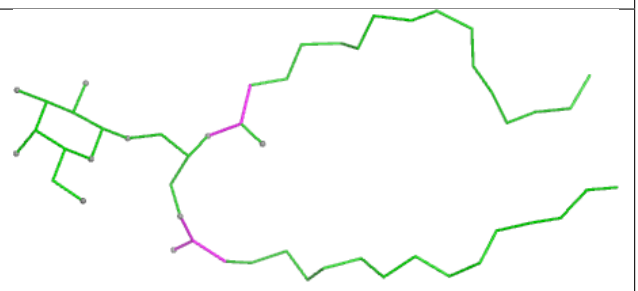


Rings

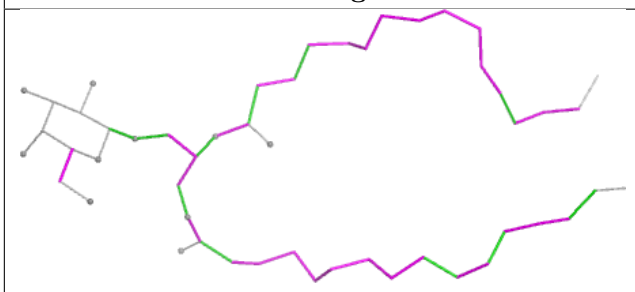
Ligand LMG a 613



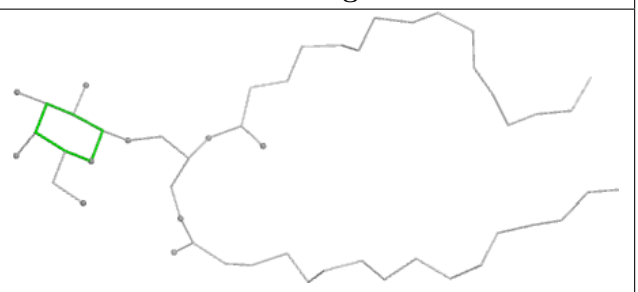
Bond lengths



Bond angles

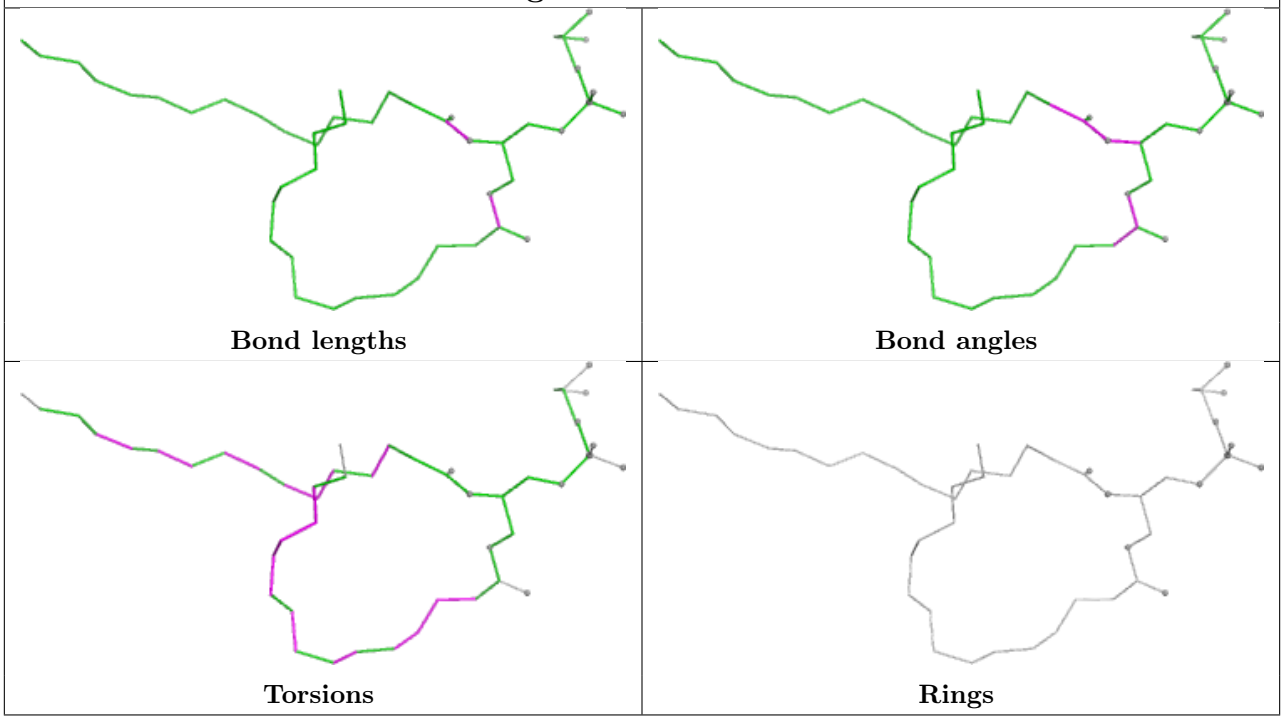


Torsions

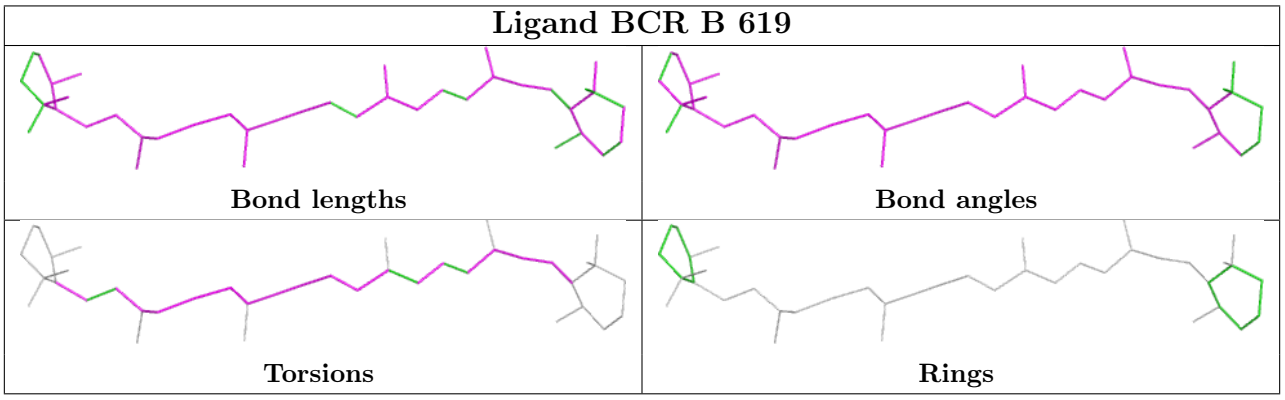


Rings

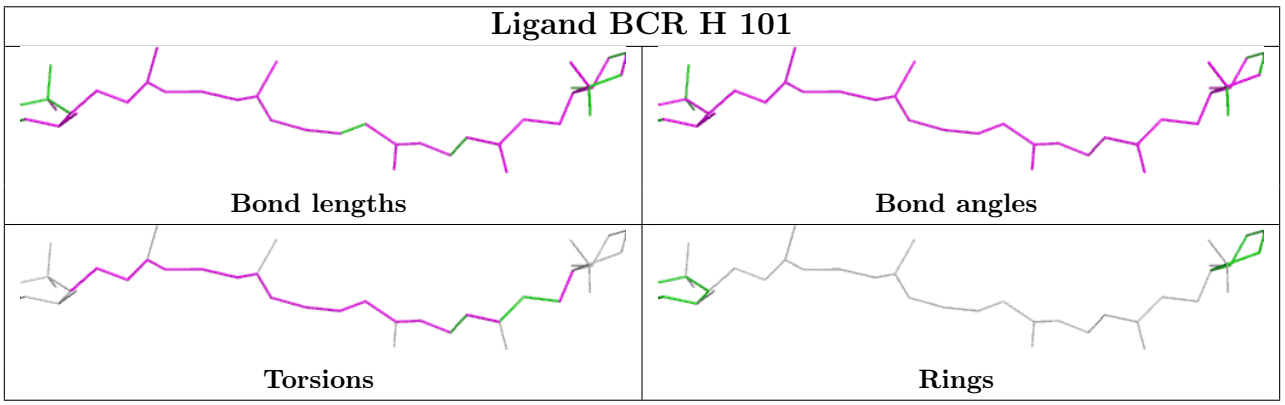
Ligand LHG d 406



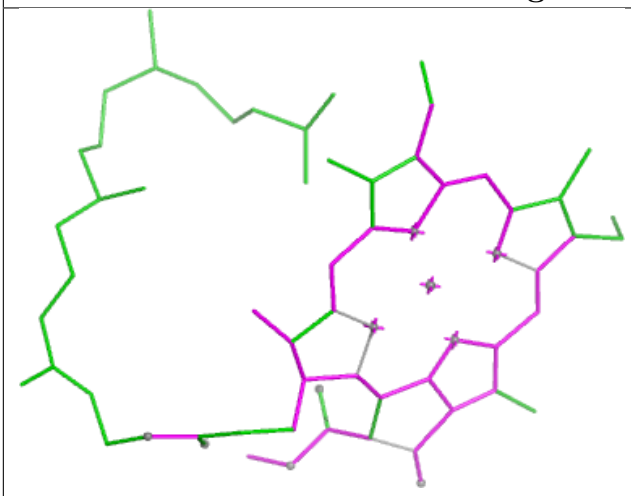
Ligand BCR B 619



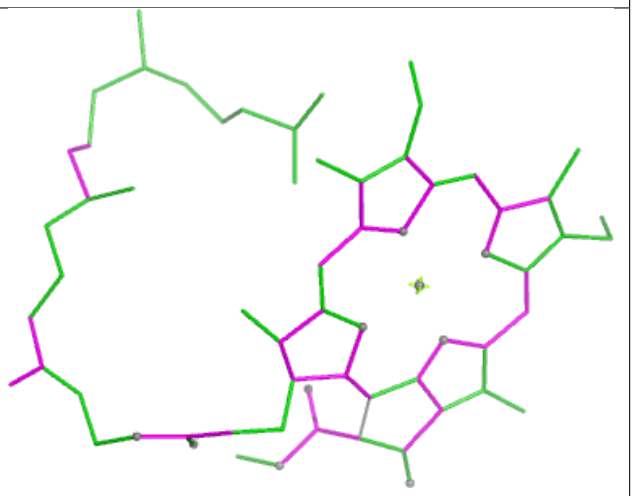
Ligand BCR H 101



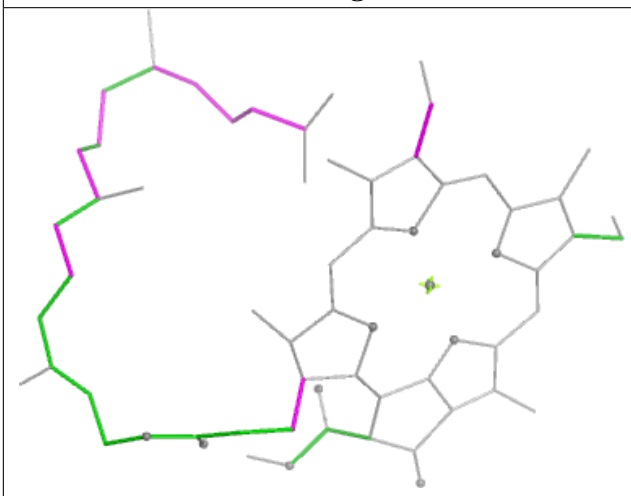
Ligand CLA b 617



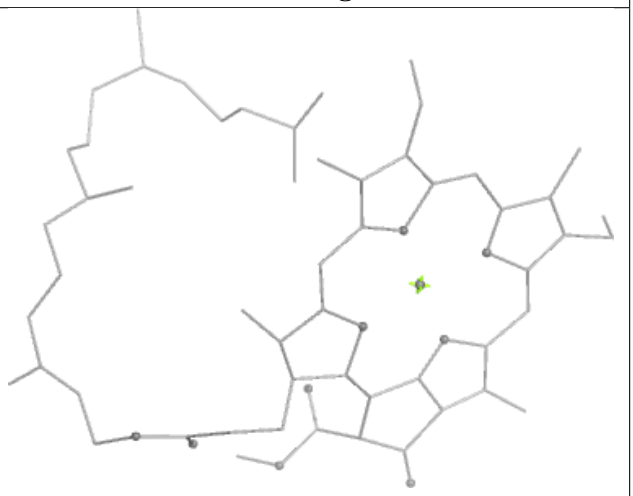
Bond lengths



Bond angles

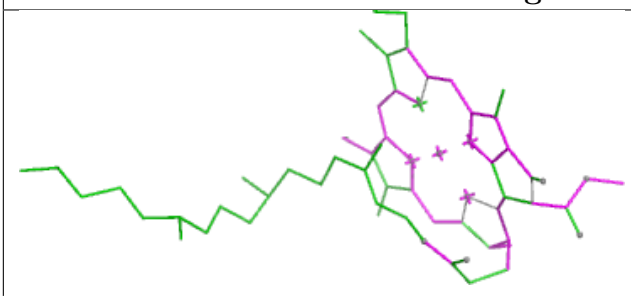


Torsions

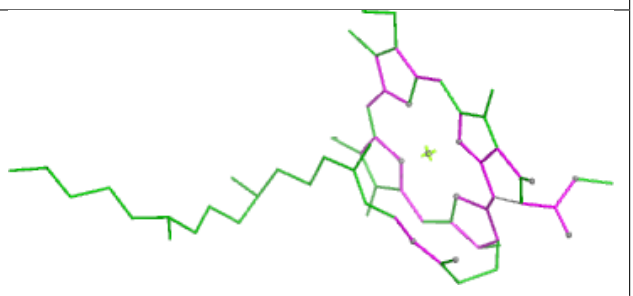


Rings

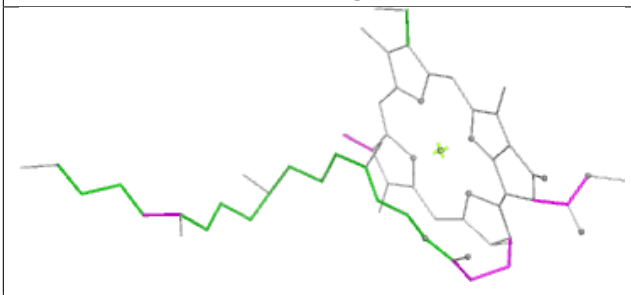
Ligand CLA C 505



Bond lengths



Bond angles

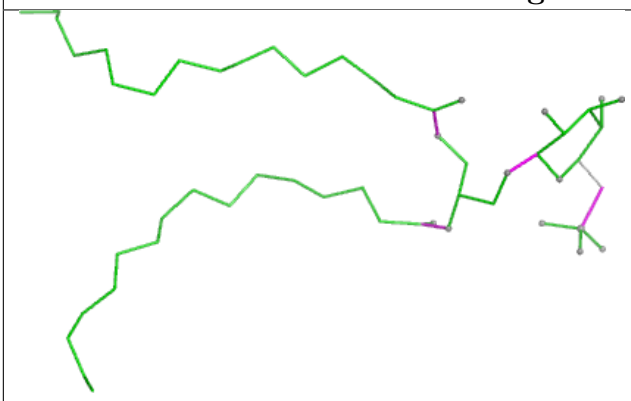


Torsions

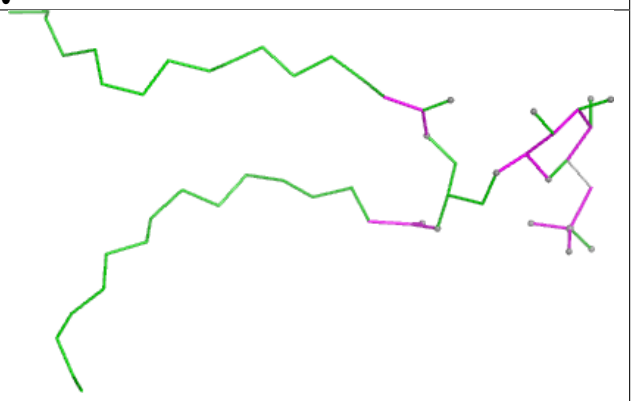


Rings

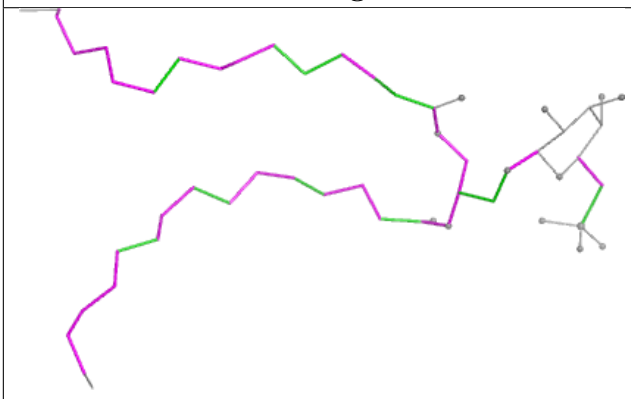
Ligand SQD b 601



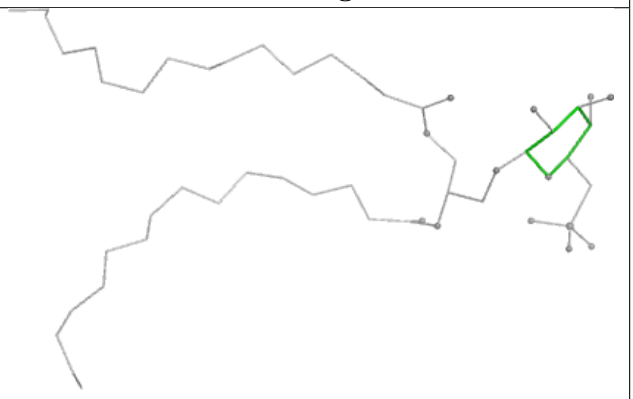
Bond lengths



Bond angles

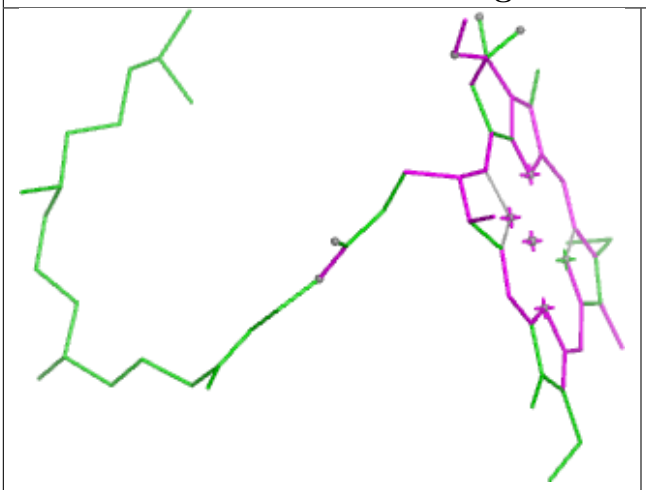


Torsions

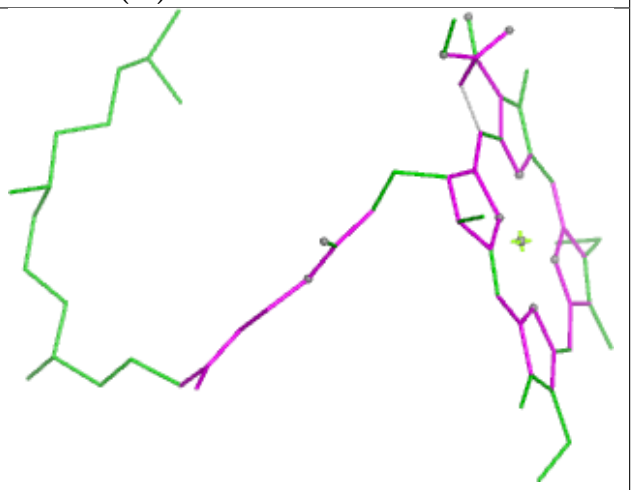


Rings

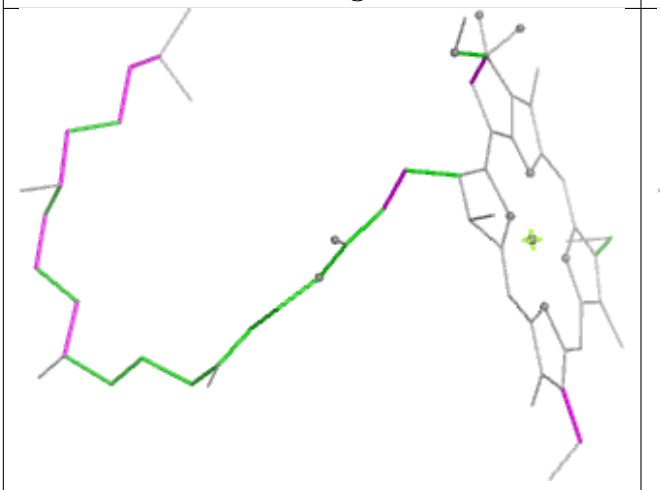
Ligand CLA b 608 (B)



Bond lengths



Bond angles

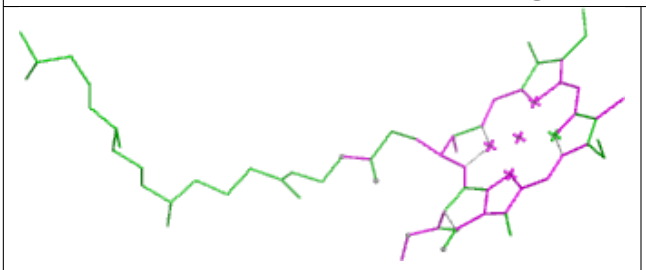


Torsions

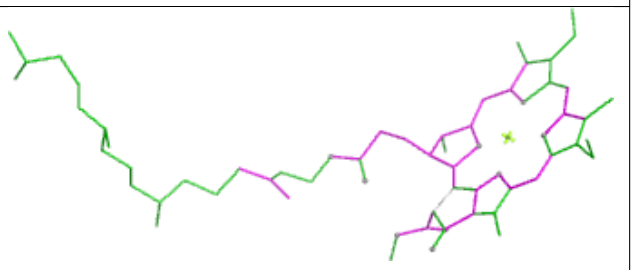


Rings

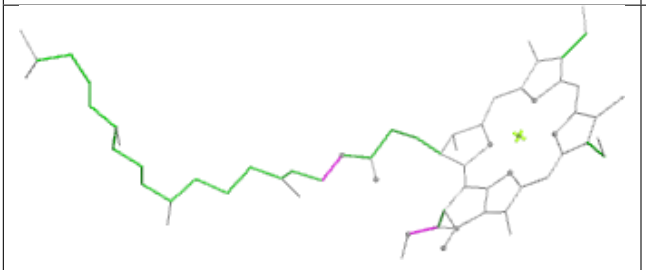
Ligand CLA a 606



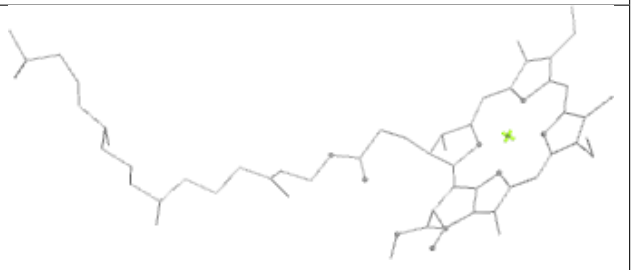
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/334 (100%)	1.45	69 (20%) 2 3	39, 63, 84, 93	4 (1%)
1	a	334/334 (100%)	1.74	110 (32%) 1 1	52, 84, 104, 114	4 (1%)
2	B	504/504 (100%)	1.29	96 (19%) 3 3	41, 68, 89, 111	10 (1%)
2	b	504/504 (100%)	1.73	160 (31%) 1 1	53, 88, 110, 131	10 (1%)
3	C	451/451 (100%)	1.31	89 (19%) 3 3	43, 72, 84, 97	5 (1%)
3	c	451/451 (100%)	1.74	154 (34%) 1 1	57, 92, 105, 118	5 (1%)
4	D	342/342 (100%)	1.32	71 (20%) 2 3	57, 64, 80, 102	0
4	d	342/342 (100%)	1.72	111 (32%) 1 1	78, 85, 101, 123	0
5	E	81/81 (100%)	1.53	20 (24%) 2 2	47, 80, 98, 104	2 (2%)
5	e	81/81 (100%)	1.93	37 (45%) 0 1	61, 101, 119, 125	2 (2%)
6	F	34/34 (100%)	1.39	6 (17%) 4 4	68, 74, 99, 102	0
6	f	34/34 (100%)	1.62	11 (32%) 1 1	89, 95, 120, 122	0
7	H	65/65 (100%)	1.43	16 (24%) 2 2	43, 74, 81, 99	2 (3%)
7	h	65/65 (100%)	1.99	25 (38%) 1 1	55, 95, 101, 120	2 (3%)
8	I	38/38 (100%)	1.76	13 (34%) 1 1	36, 74, 105, 109	1 (2%)
8	i	38/38 (100%)	2.13	16 (42%) 0 1	45, 95, 126, 130	1 (2%)
9	J	38/38 (100%)	1.65	9 (23%) 2 2	66, 78, 109, 112	0
9	j	38/38 (100%)	1.83	14 (36%) 1 1	87, 99, 129, 133	0
10	K	37/37 (100%)	1.06	3 (8%) 18 12	74, 79, 86, 88	0
10	k	37/37 (100%)	1.87	11 (29%) 1 1	94, 100, 107, 108	0
11	L	37/37 (100%)	1.34	8 (21%) 2 3	37, 62, 90, 99	1 (2%)
11	l	37/37 (100%)	1.76	12 (32%) 1 1	49, 83, 111, 120	1 (2%)
12	M	34/34 (100%)	1.66	10 (29%) 1 1	39, 64, 77, 93	1 (2%)
12	m	34/34 (100%)	2.36	12 (35%) 1 1	51, 84, 98, 114	1 (2%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	1.42	56 (23%) 2 2	40, 73, 95, 111	4 (1%)
13	o	243/243 (100%)	1.98	95 (39%) 1 1	53, 94, 116, 132	4 (1%)
14	T	30/30 (100%)	1.08	4 (13%) 7 6	32, 64, 85, 93	2 (6%)
14	t	30/30 (100%)	1.72	7 (23%) 2 2	43, 84, 105, 114	2 (6%)
15	U	97/97 (100%)	1.17	15 (15%) 5 5	64, 71, 89, 90	0
15	u	97/97 (100%)	1.64	30 (30%) 1 1	84, 92, 110, 111	0
16	V	137/137 (100%)	1.24	28 (20%) 3 3	39, 69, 80, 88	1 (0%)
16	v	137/137 (100%)	1.53	36 (26%) 1 2	51, 89, 101, 109	1 (0%)
17	Y	29/29 (100%)	1.43	7 (24%) 2 2	82, 89, 115, 118	0
17	y	29/29 (100%)	1.95	11 (37%) 1 1	103, 110, 136, 138	0
18	X	39/39 (100%)	1.32	6 (15%) 5 5	48, 80, 107, 108	1 (2%)
18	x	39/39 (100%)	1.71	11 (28%) 1 1	61, 101, 127, 129	1 (2%)
19	Z	62/62 (100%)	1.50	18 (29%) 1 1	80, 89, 109, 112	0
19	z	62/62 (100%)	2.04	29 (46%) 0 1	101, 110, 129, 133	0
All	All	5264/5264 (100%)	1.57	1436 (27%) 1 2	32, 83, 107, 138	68 (1%)

The worst 5 of 1436 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	11	GLU	12.1
12	m	5	GLN	11.3
8	i	38	GLU	10.2
2	b	485	GLU	10.0
9	j	3	SER	8.4

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CL	u	201	1/1	0.10	0.94	112,112,112,112	0
28	SQD	B	622	54/54	0.31	0.29	119,127,141,142	0
28	SQD	L	102	54/54	0.35	0.30	119,131,146,147	0
22	CL	U	201	1/1	0.36	0.58	91,91,91,91	0
28	SQD	b	601	54/54	0.36	0.27	99,107,121,121	0
31	CA	o	301	1/1	0.39	0.28	110,110,110,110	0
28	SQD	l	101	54/54	0.53	0.24	98,110,125,126	0
22	CL	a	604	1/1	0.65	0.43	83,83,83,83	0
31	CA	b	602	1/1	0.70	0.41	137,137,137,137	0
29	LMG	c	520	51/55	0.71	0.45	104,137,142,143	0
29	LMG	Z	101	37/55	0.72	0.41	96,124,129,129	0
28	SQD	x	101	43/54	0.72	0.39	128,136,140,140	0
31	CA	O	301	1/1	0.74	0.17	90,90,90,90	0
31	CA	F	102	1/1	0.75	0.20	97,97,97,97	0
28	SQD	a	614	54/54	0.75	0.39	111,124,129,130	0
32	DGD	d	405	62/66	0.75	0.38	138,151,164,165	0
30	LHG	E	102	42/49	0.76	0.41	110,124,127,127	0
28	SQD	X	101	43/54	0.76	0.34	108,115,119,119	0
28	SQD	a	612	54/54	0.76	0.35	110,119,128,128	0
32	DGD	E	101	62/66	0.77	0.38	118,130,143,144	0
29	LMG	C	519	51/55	0.78	0.35	83,117,122,123	0
24	CLA	c	513	65/65	0.78	0.32	101,106,125,126	0
27	PL9	a	611	55/55	0.79	0.41	113,130,139,140	0
29	LMG	c	519	51/55	0.79	0.39	92,118,134,135	0
29	LMG	C	518	51/55	0.80	0.35	72,98,113,114	0
28	SQD	A	614	54/54	0.80	0.32	91,103,109,109	0
30	LHG	e	101	42/49	0.80	0.35	131,145,147,148	0
27	PL9	A	611	55/55	0.81	0.38	93,109,118,119	0
26	BCR	f	101	40/40	0.82	0.32	87,91,109,110	0
32	DGD	c	516	62/66	0.82	0.30	84,94,122,124	0
29	LMG	b	622	51/55	0.82	0.34	91,100,112,116	0
24	CLA	B	602	65/65	0.83	0.27	73,82,107,107	0
29	LMG	j	101	51/55	0.83	0.31	87,96,126,129	0
29	LMG	z	101	37/55	0.83	0.30	117,145,149,150	0
26	BCR	H	101	40/40	0.83	0.31	67,74,83,83	0
24	CLA	b	603	65/65	0.83	0.28	94,102,127,128	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	k	101	40/40	0.83	0.29	95,99,100,100	0
24	CLA	C	513	65/65	0.84	0.26	80,85,105,105	0
26	BCR	h	101	40/40	0.84	0.30	87,94,103,104	0
26	BCR	B	619	40/40	0.84	0.28	62,69,81,81	0
29	LMG	a	613	51/55	0.84	0.32	114,121,126,126	0
24	CLA	c	512	65/65	0.84	0.27	99,102,124,124	0
26	BCR	I	101	40/40	0.84	0.29	71,78,81,82	0
26	BCR	T	101	40/40	0.84	0.29	65,78,85,86	0
26	BCR	c	515	40/40	0.84	0.31	92,98,102,102	0
29	LMG	A	613	51/55	0.84	0.28	94,100,105,105	0
24	CLA	c	506	65/65	0.85	0.26	93,100,136,136	0
24	CLA	b	608[A]	65/65	0.85	0.27	85,90,102,103	65
29	LMG	D	408	51/55	0.85	0.29	66,76,106,108	0
26	BCR	c	521	40/40	0.85	0.30	91,95,98,99	0
24	CLA	b	608[B]	65/65	0.85	0.27	83,87,93,95	65
30	LHG	a	616	49/49	0.85	0.31	87,94,124,125	0
28	SQD	A	612	54/54	0.85	0.33	90,98,107,108	0
29	LMG	B	621	51/55	0.86	0.29	70,80,92,95	0
24	CLA	B	617	65/65	0.86	0.23	63,69,118,119	0
24	CLA	c	501	65/65	0.86	0.25	90,93,106,108	0
23	BCT	A	605	4/4	0.86	0.38	79,80,81,82	0
26	BCR	b	620	40/40	0.86	0.29	83,89,101,101	0
26	BCR	t	101	40/40	0.86	0.34	86,99,106,106	0
26	BCR	C	514	40/40	0.86	0.28	78,84,87,88	0
27	PL9	d	404	55/55	0.87	0.26	80,84,91,93	0
30	LHG	D	407	49/49	0.87	0.27	64,69,78,81	0
26	BCR	b	621	40/40	0.87	0.26	89,94,100,101	0
26	BCR	c	514	40/40	0.87	0.28	99,105,108,108	0
24	CLA	b	609	65/65	0.87	0.24	79,82,94,95	0
26	BCR	B	620	40/40	0.87	0.24	68,74,80,80	0
24	CLA	B	607[A]	65/65	0.87	0.22	65,69,81,82	65
24	CLA	B	607[B]	65/65	0.87	0.22	63,67,72,75	65
24	CLA	c	509	65/65	0.87	0.24	91,93,108,108	0
26	BCR	K	102	40/40	0.87	0.27	70,74,78,78	0
24	CLA	B	606	65/65	0.87	0.23	59,64,75,76	0
24	CLA	C	506	65/65	0.87	0.24	72,79,115,115	0
26	BCR	K	101	40/40	0.88	0.26	75,78,79,80	0
24	CLA	c	503	65/65	0.88	0.22	89,93,96,97	0
24	CLA	C	501	65/65	0.88	0.22	69,73,85,87	0
24	CLA	c	508	65/65	0.88	0.22	87,90,115,119	0
31	CA	f	102	1/1	0.88	0.14	118,118,118,118	0
24	CLA	b	618	65/65	0.88	0.23	83,90,139,139	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	F	101	40/40	0.88	0.23	66,71,88,90	0
24	CLA	c	511	65/65	0.88	0.24	90,95,99,99	0
32	DGD	c	517	62/66	0.88	0.25	84,96,124,124	0
24	CLA	C	507	65/65	0.88	0.23	70,74,92,94	0
24	CLA	b	606	65/65	0.89	0.22	81,84,111,112	0
24	CLA	B	616	65/65	0.89	0.20	65,68,86,87	0
30	LHG	d	406	49/49	0.89	0.26	91,96,102,102	0
24	CLA	C	505	65/65	0.89	0.20	69,71,85,85	0
31	CA	B	601	1/1	0.89	0.25	117,117,117,117	0
24	CLA	a	607	65/65	0.89	0.23	80,83,124,126	0
24	CLA	c	510	65/65	0.89	0.22	86,90,96,99	0
24	CLA	b	610	65/65	0.89	0.21	82,86,92,93	0
24	CLA	b	617	65/65	0.89	0.22	86,89,107,108	0
24	CLA	a	609	65/65	0.89	0.21	83,85,133,133	0
32	DGD	C	515	62/66	0.89	0.23	64,73,102,103	0
32	DGD	C	516	62/66	0.89	0.25	63,75,103,104	0
26	BCR	b	619	40/40	0.89	0.29	84,88,90,90	0
25	PHO	d	401	64/64	0.89	0.21	80,84,90,94	0
30	LHG	D	406	49/49	0.89	0.23	70,75,81,82	0
32	DGD	c	518	62/66	0.89	0.24	83,93,113,117	0
24	CLA	B	609	65/65	0.89	0.19	61,65,71,72	0
24	CLA	C	504	65/65	0.90	0.21	66,68,95,95	0
24	CLA	b	607	65/65	0.90	0.21	80,84,95,97	0
26	BCR	a	610	40/40	0.90	0.25	83,89,93,94	0
24	CLA	d	402	65/65	0.90	0.21	75,80,95,96	0
30	LHG	l	102	49/49	0.90	0.27	84,92,104,106	0
32	DGD	H	102	62/66	0.90	0.23	66,72,79,81	0
24	CLA	d	403	65/65	0.90	0.20	86,89,126,128	0
24	CLA	b	605	65/65	0.90	0.20	79,84,92,96	0
26	BCR	A	610	40/40	0.90	0.23	63,68,73,73	0
26	BCR	B	618	40/40	0.90	0.25	63,68,69,70	0
32	DGD	h	102	62/66	0.90	0.25	87,93,99,101	0
22	CL	A	603	1/1	0.91	0.24	65,65,65,65	0
24	CLA	C	509	65/65	0.91	0.21	70,72,87,88	0
24	CLA	C	512	65/65	0.91	0.20	78,82,103,104	0
24	CLA	B	608	65/65	0.91	0.20	58,61,73,74	0
24	CLA	b	611	65/65	0.91	0.19	85,90,92,93	0
24	CLA	b	612	65/65	0.91	0.20	82,86,94,98	0
24	CLA	b	615	65/65	0.91	0.20	80,84,106,108	0
24	CLA	B	603	65/65	0.91	0.19	64,67,72,73	0
24	CLA	C	502	65/65	0.91	0.17	65,67,80,83	0
24	CLA	C	503	65/65	0.91	0.18	68,72,76,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	LHG	A	615	49/49	0.91	0.23	67,74,103,104	0
24	CLA	B	610	65/65	0.91	0.17	64,69,72,73	0
24	CLA	c	504	65/65	0.91	0.21	86,89,115,116	0
24	CLA	c	505	65/65	0.91	0.19	89,92,106,106	0
24	CLA	B	611	65/65	0.91	0.21	62,65,73,77	0
24	CLA	B	613	65/65	0.91	0.20	61,64,71,72	0
30	LHG	d	407	49/49	0.91	0.23	85,89,98,102	0
24	CLA	c	502	65/65	0.92	0.17	85,87,101,103	0
25	PHO	D	401	64/64	0.92	0.18	59,63,69,73	0
24	CLA	C	508	65/65	0.92	0.18	66,70,95,99	0
24	CLA	A	609	65/65	0.92	0.20	62,65,112,113	0
24	CLA	b	604	65/65	0.92	0.18	85,88,93,94	0
24	CLA	C	511	65/65	0.92	0.18	70,75,78,79	0
24	CLA	c	507	65/65	0.92	0.19	91,94,113,115	0
24	CLA	b	613	65/65	0.92	0.20	80,83,94,96	0
24	CLA	b	614	65/65	0.92	0.21	81,85,91,92	0
32	DGD	C	517	62/66	0.92	0.20	62,72,93,97	0
24	CLA	B	604	65/65	0.92	0.18	58,63,72,76	0
24	CLA	b	616	65/65	0.92	0.22	82,86,121,122	0
30	LHG	L	101	49/49	0.92	0.22	63,72,83,85	0
24	CLA	B	605	65/65	0.92	0.20	60,63,91,91	0
27	PL9	D	405	55/55	0.92	0.22	60,64,70,72	0
24	CLA	D	402	65/65	0.92	0.21	54,59,70,76	0
22	CL	a	603	1/1	0.92	0.26	86,86,86,86	0
24	CLA	C	510	65/65	0.93	0.17	65,69,76,78	0
24	CLA	D	403	65/65	0.93	0.20	54,59,75,76	0
24	CLA	D	404	65/65	0.93	0.18	65,68,106,107	0
25	PHO	A	608	64/64	0.93	0.18	57,62,65,67	0
24	CLA	a	606	65/65	0.93	0.20	77,80,87,95	0
24	CLA	B	615	65/65	0.93	0.18	61,65,101,102	0
24	CLA	A	607	65/65	0.93	0.19	60,62,104,106	0
24	CLA	B	614	65/65	0.93	0.18	60,63,85,87	0
34	MG	J	101	1/1	0.93	0.23	68,68,68,68	0
24	CLA	a	615	65/65	0.94	0.22	75,79,91,96	0
24	CLA	A	606	65/65	0.94	0.18	56,59,66,75	0
23	BCT	a	605	4/4	0.94	0.22	100,101,101,103	0
25	PHO	a	608	64/64	0.94	0.19	78,83,86,87	0
33	HEM	e	102	43/43	0.94	0.21	101,103,107,108	0
33	HEM	v	201	43/43	0.94	0.19	84,86,88,90	0
24	CLA	B	612	65/65	0.94	0.17	60,62,73,75	0
33	HEM	V	201	43/43	0.95	0.17	63,65,68,69	0
33	HEM	E	103	43/43	0.95	0.20	80,82,86,87	0

Continued on next page...

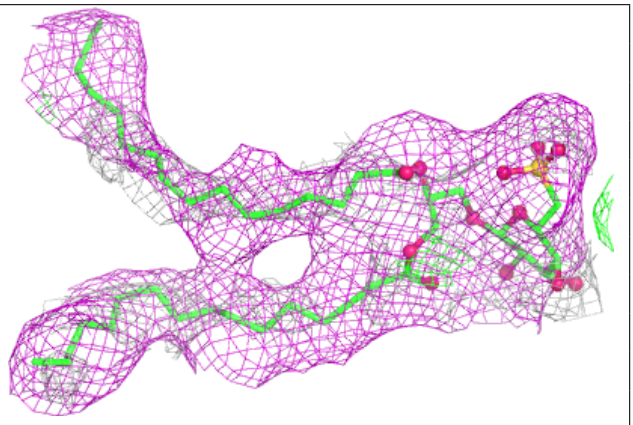
Continued from previous page...

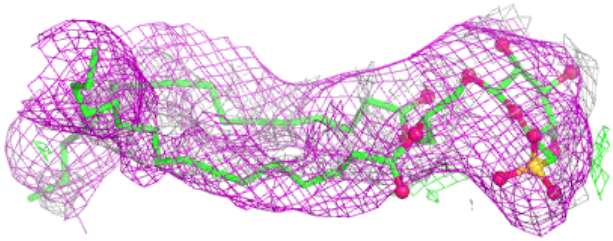
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	CL	A	604	1/1	0.96	0.15	62,62,62,62	0
20	OEX	a	601	10/10	0.96	0.16	83,84,87,88	0
34	MG	j	102	1/1	0.96	0.11	89,89,89,89	0
20	OEX	A	601	10/10	0.98	0.14	63,64,67,67	0
21	FE2	A	602	1/1	0.98	0.07	67,67,67,67	0
21	FE2	a	602	1/1	0.99	0.10	88,88,88,88	0

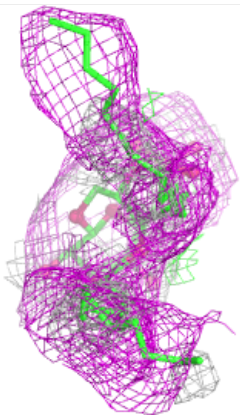
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SQD B 622:

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

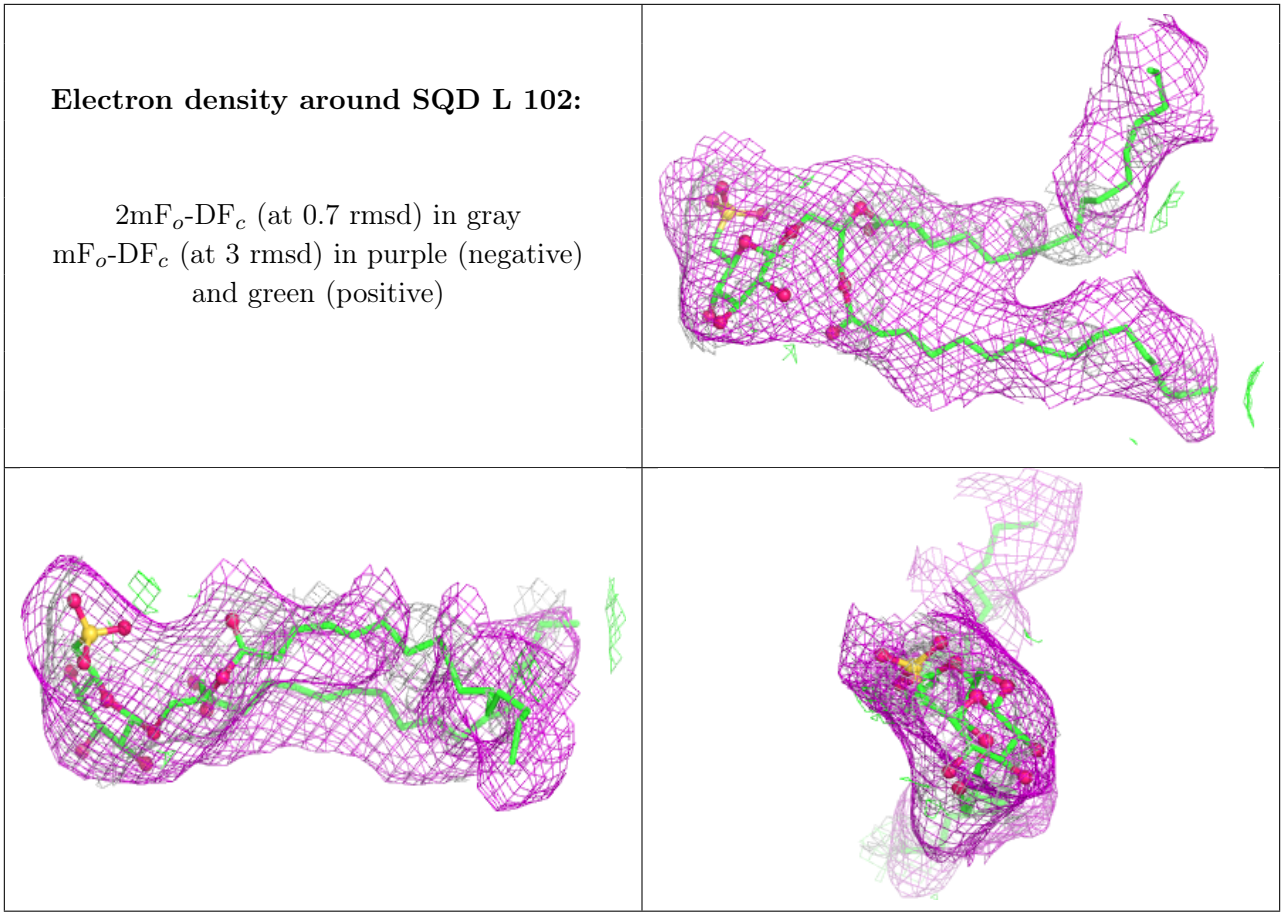






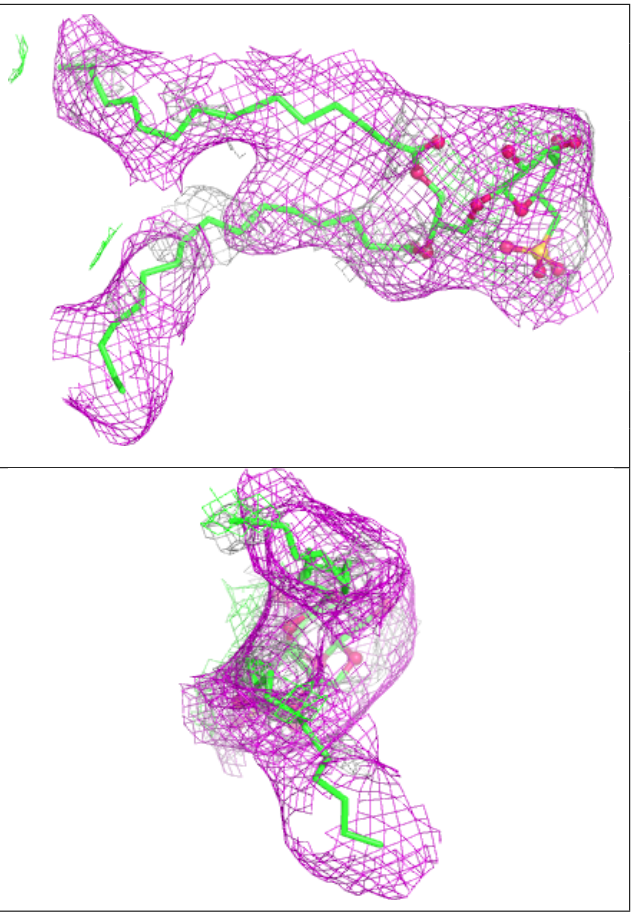
Electron density around SQD L 102:

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



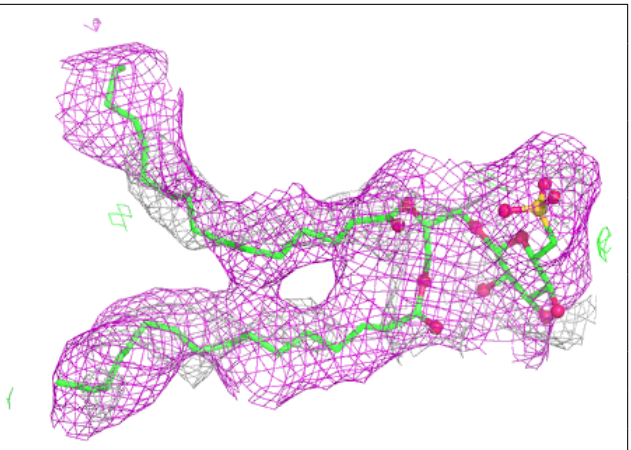
Electron density around SQD b 601:

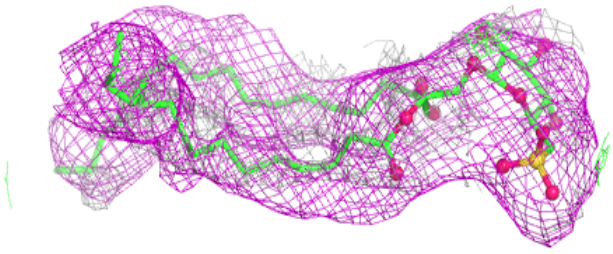
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

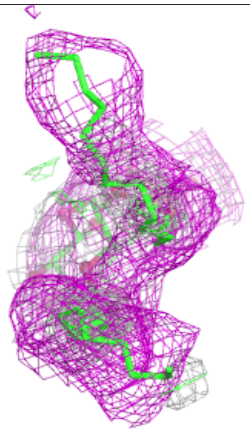


Electron density around SQD l 101:

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

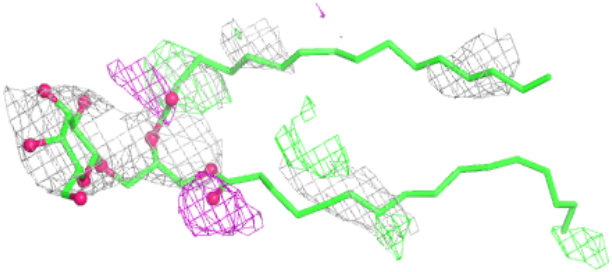


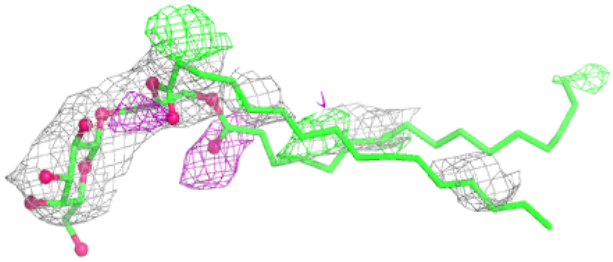


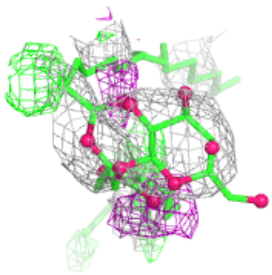


Electron density around LMG c 520:

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

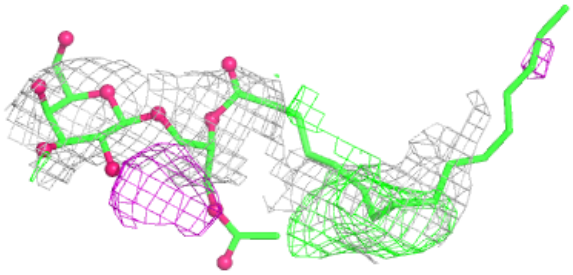


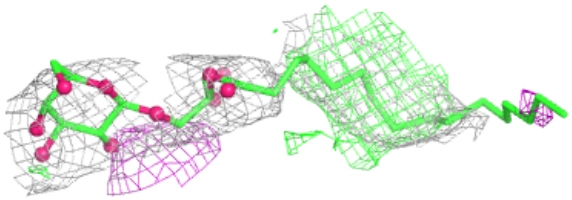


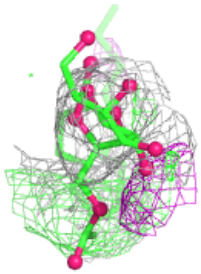


Electron density around LMG Z 101:

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

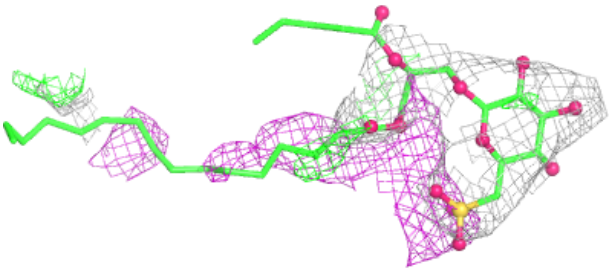


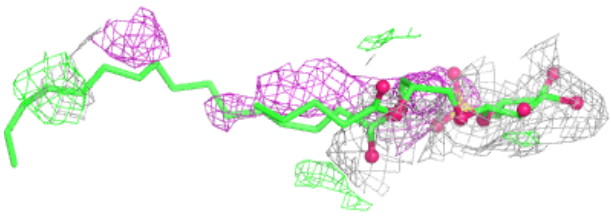


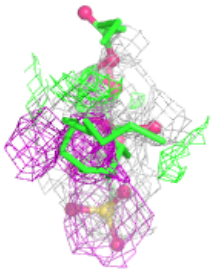


Electron density around SQD x 101:

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

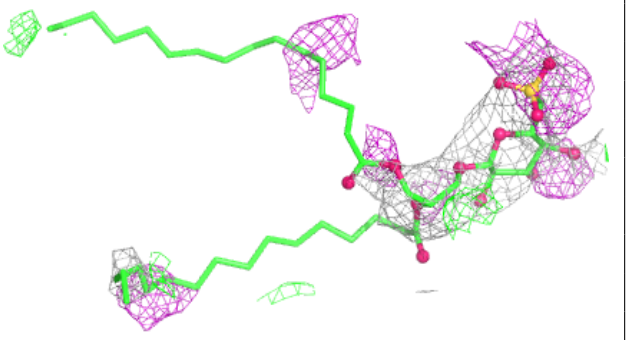


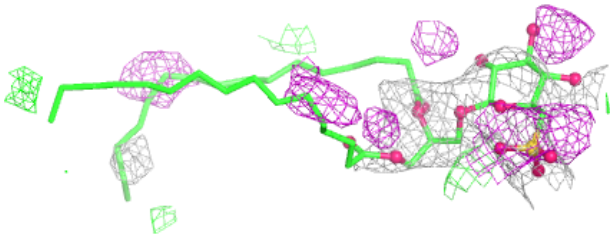




Electron density around SQD a 614:

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

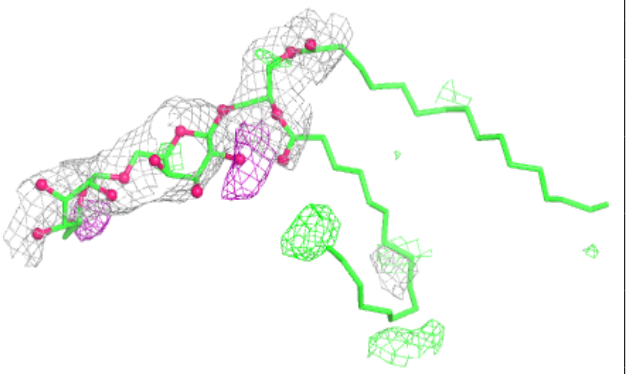


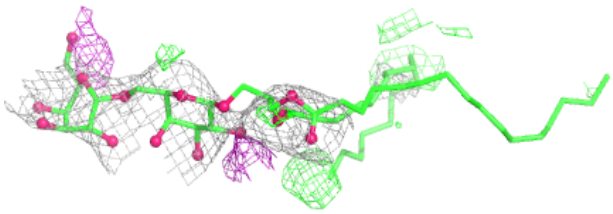




Electron density around DGD d 405:

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

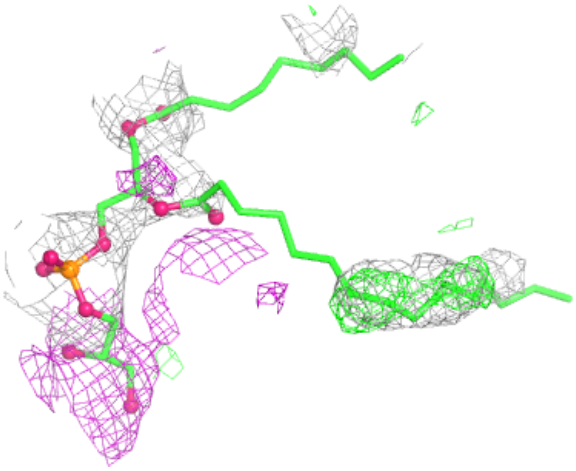


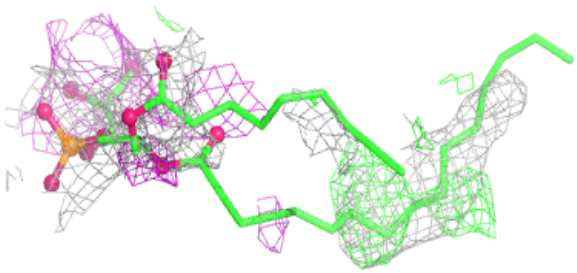


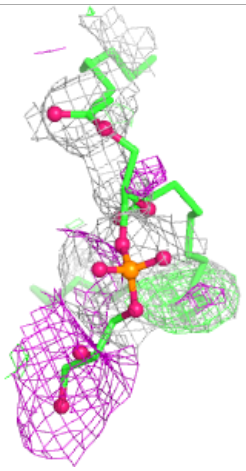


Electron density around LHG E 102:

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

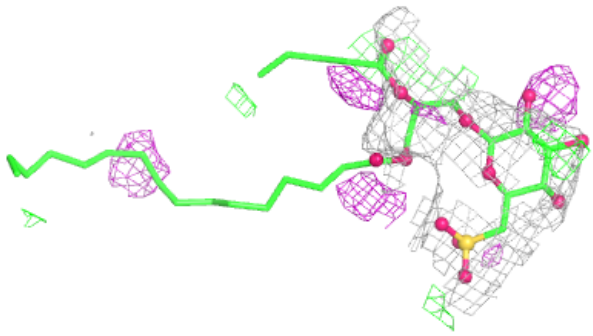


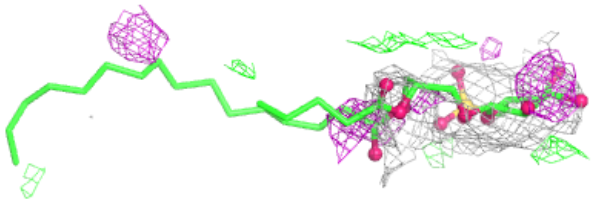




Electron density around SQD X 101:

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

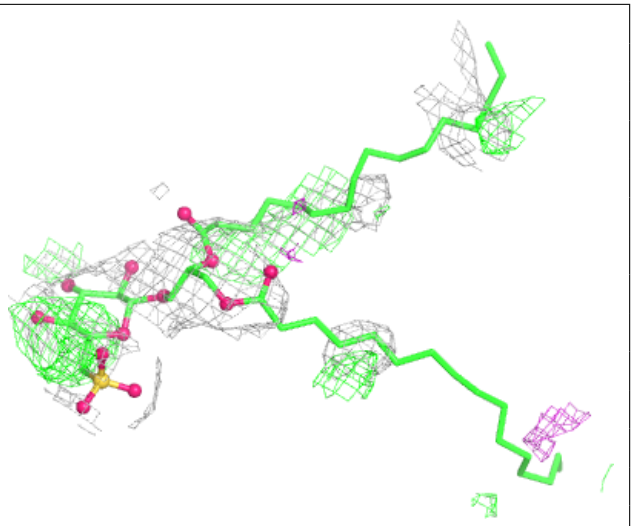


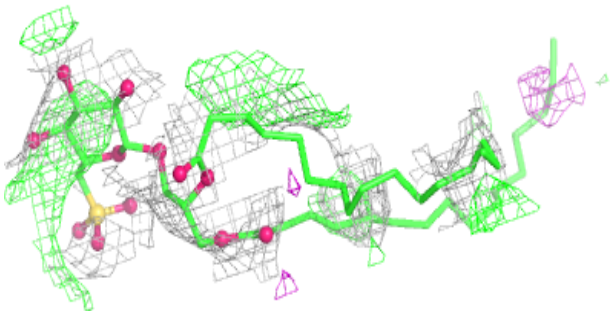




Electron density around SQD a 612:

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

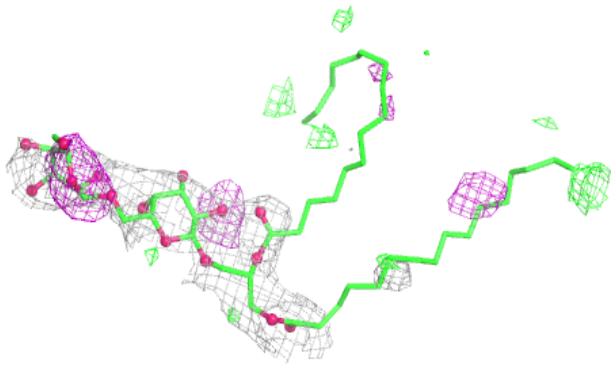


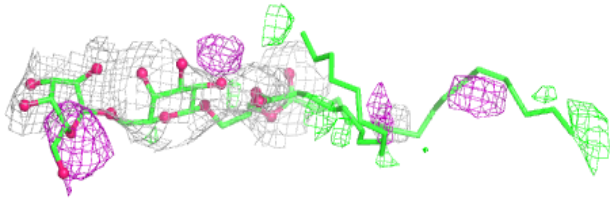


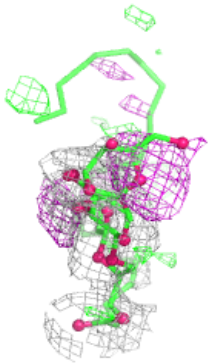


Electron density around DGD E 101:

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

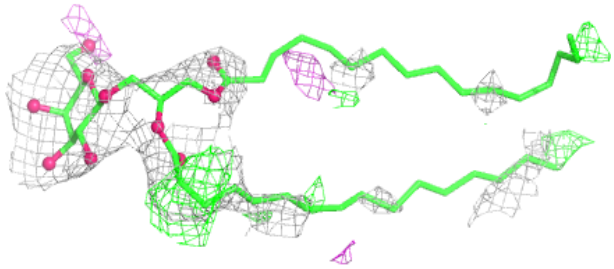


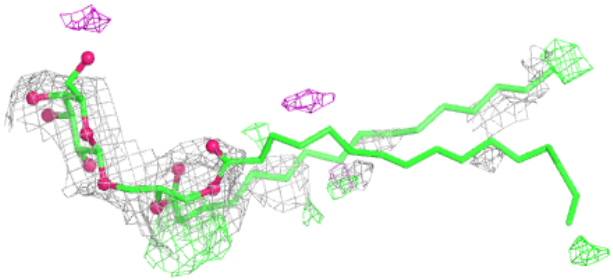


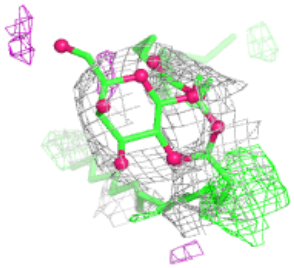


Electron density around LMG C 519:

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

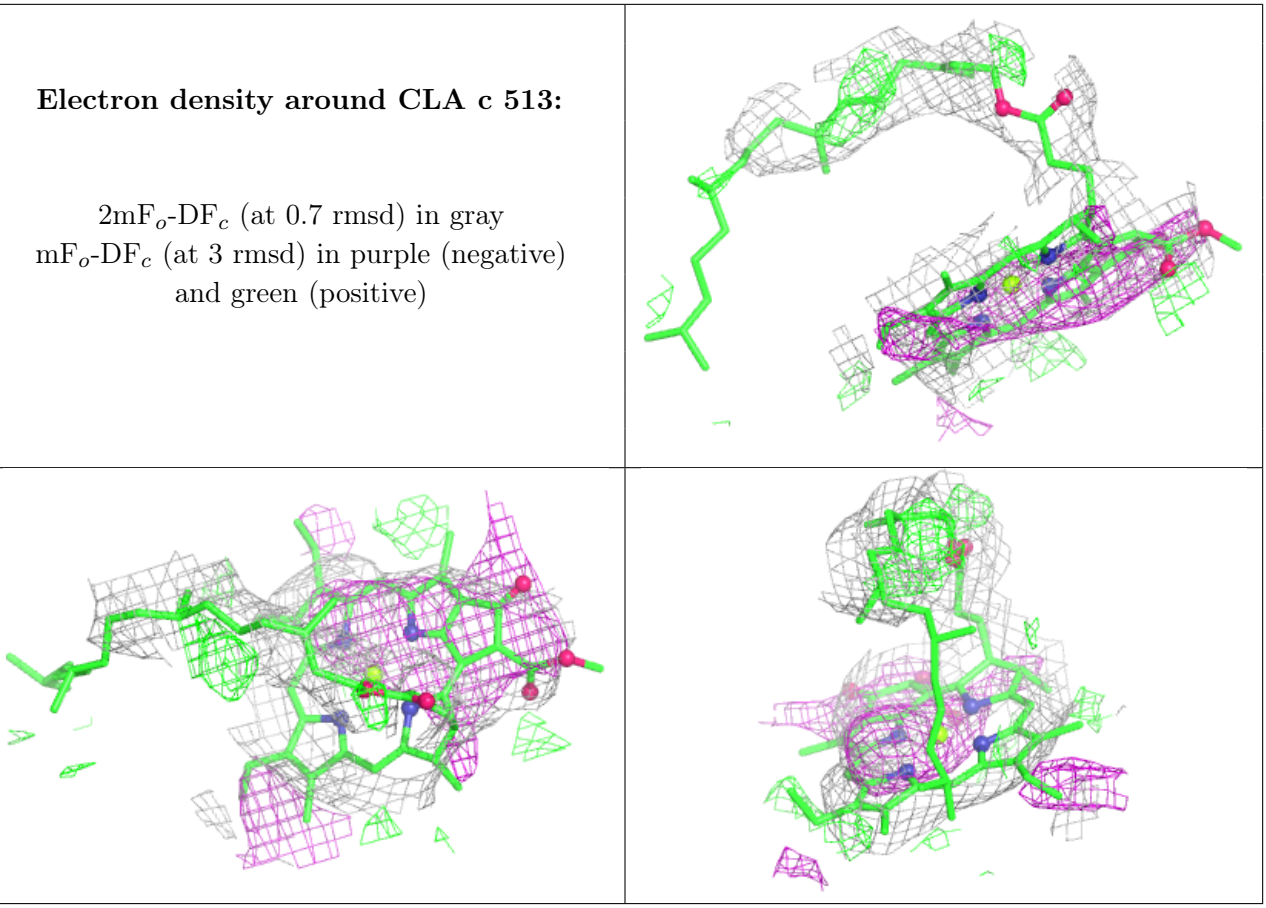






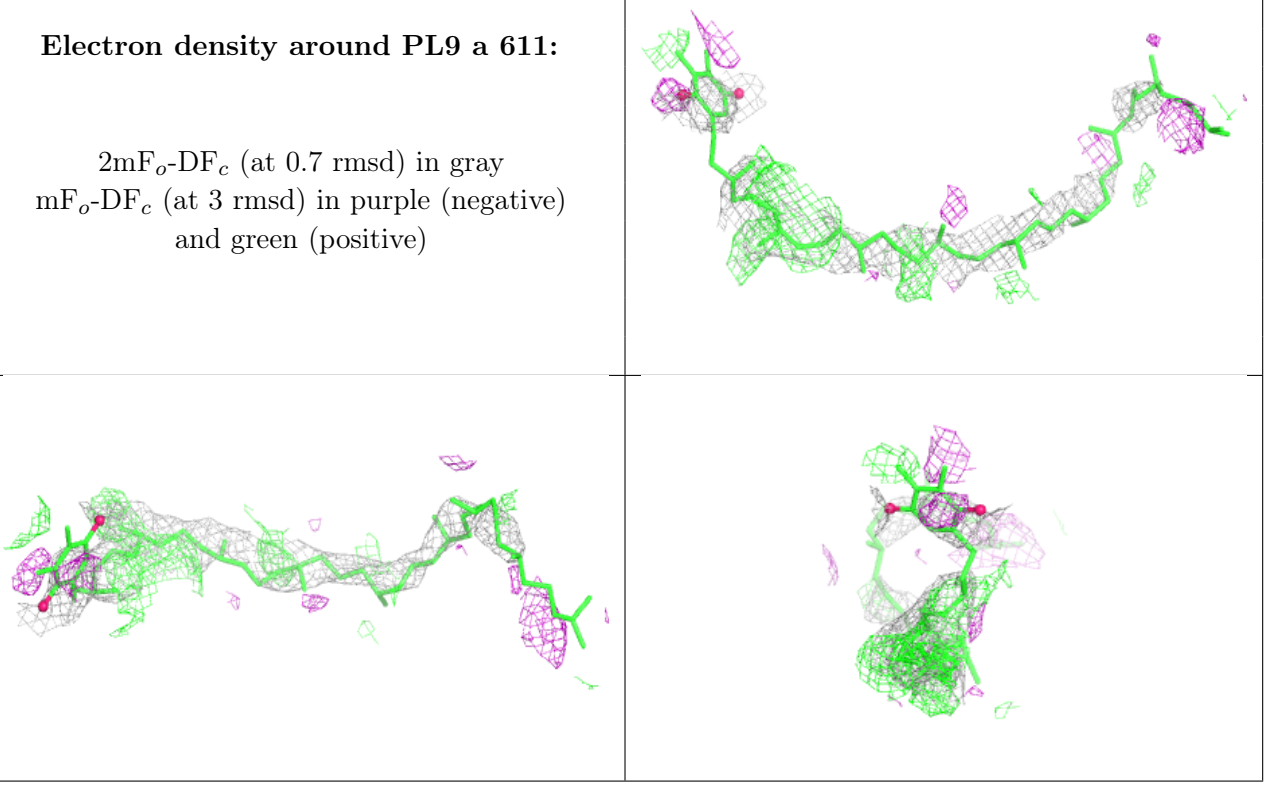
Electron density around CLA c 513:

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



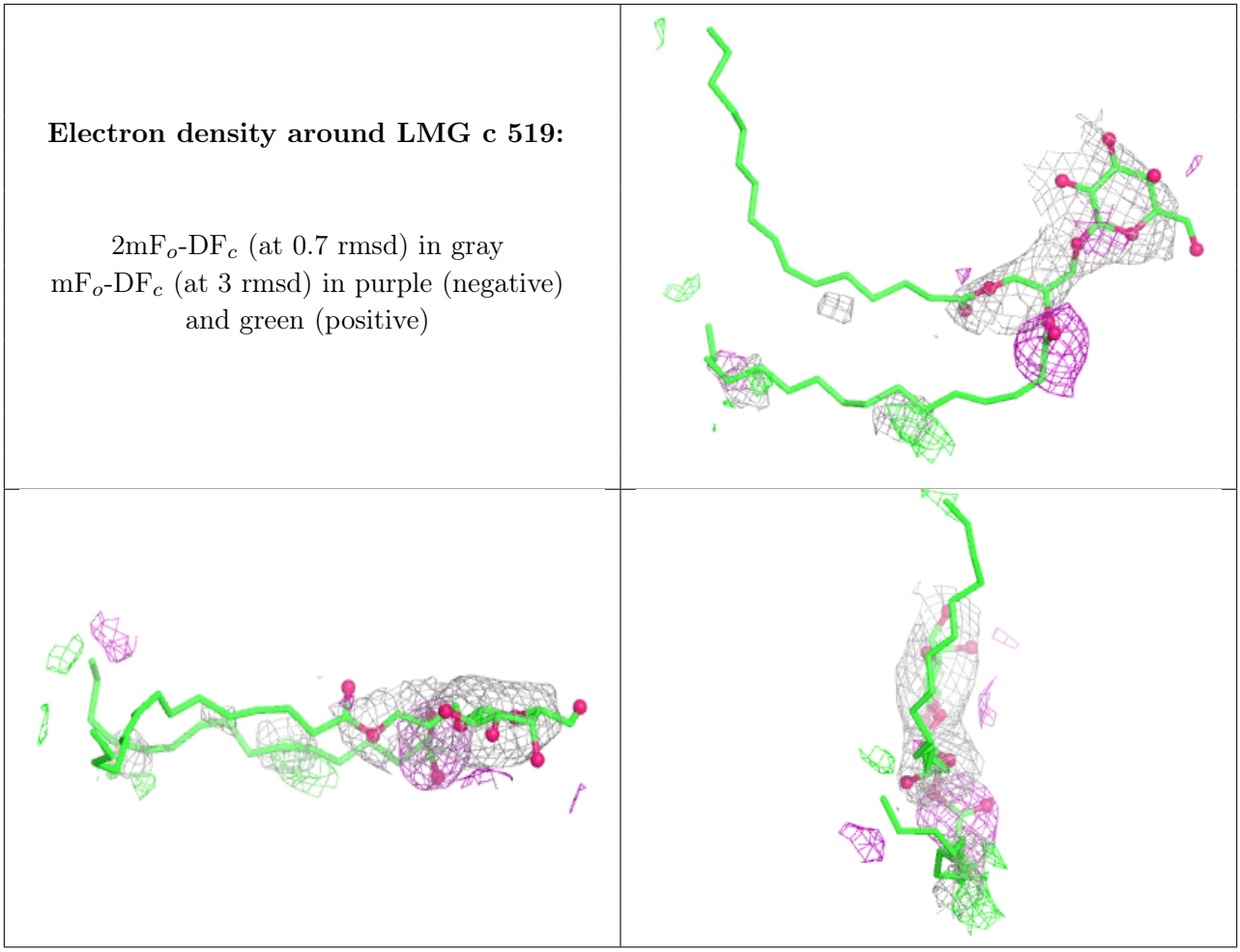
Electron density around PL9 a 611:

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



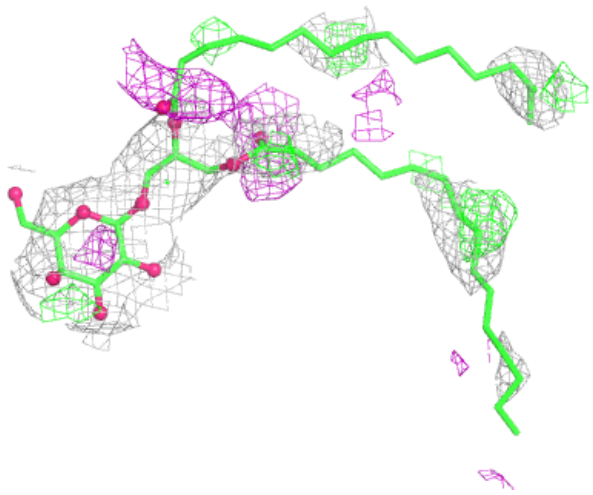
Electron density around LMG c 519:

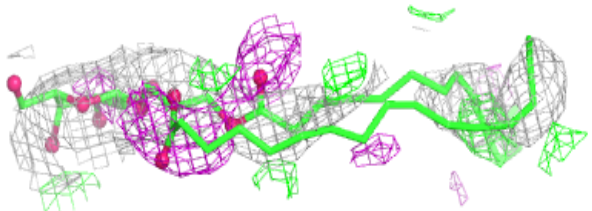
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG C 518:

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

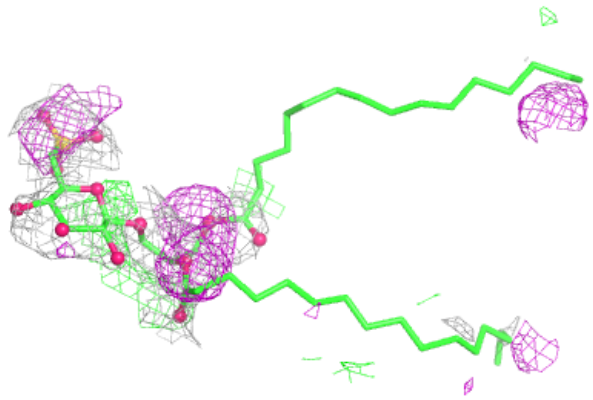


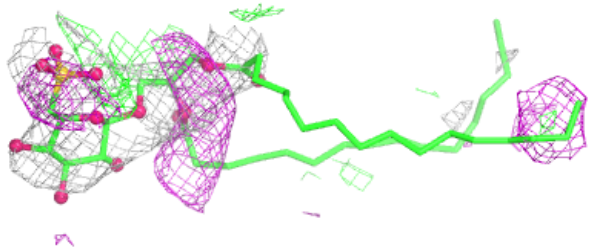


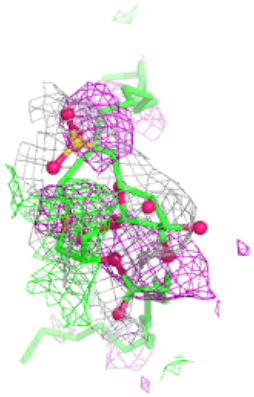


Electron density around SQD A 614:

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

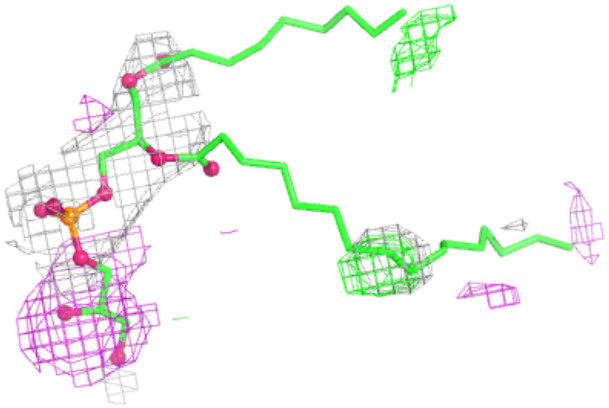


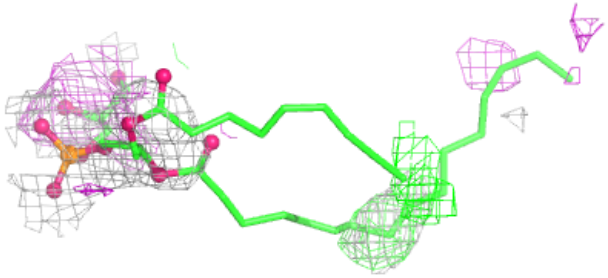




Electron density around LHG e 101:

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

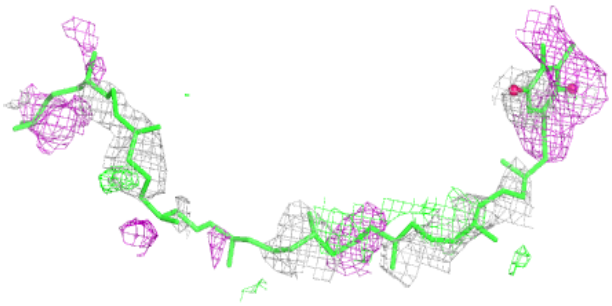


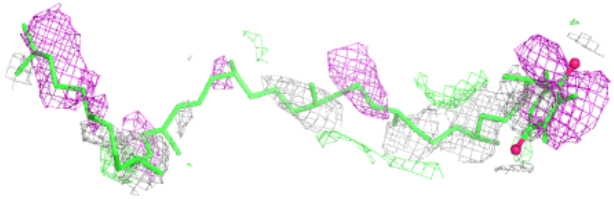


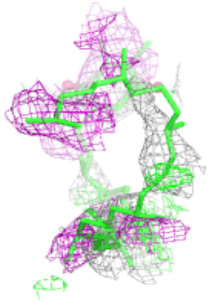


Electron density around PL9 A 611:

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

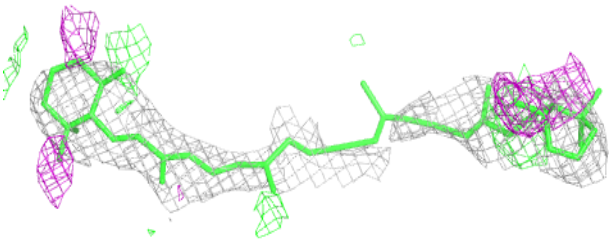


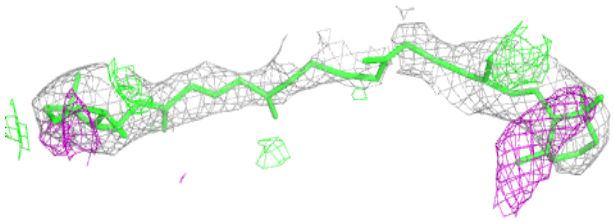


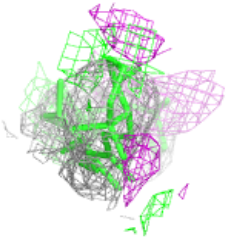


Electron density around BCR f 101:

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

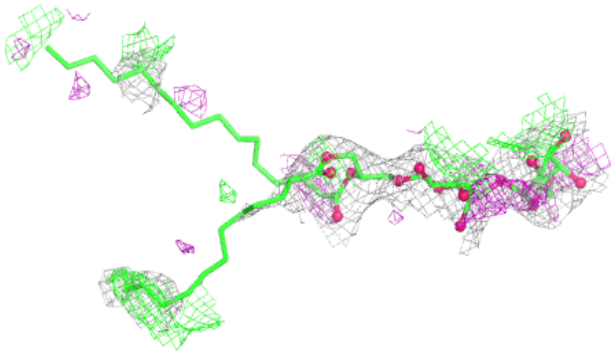


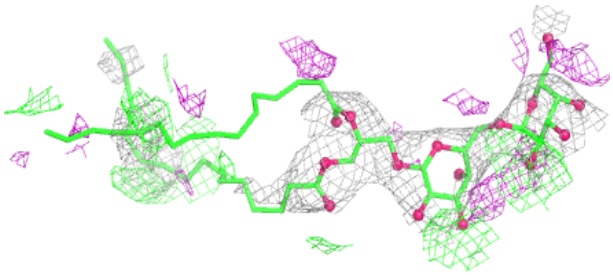


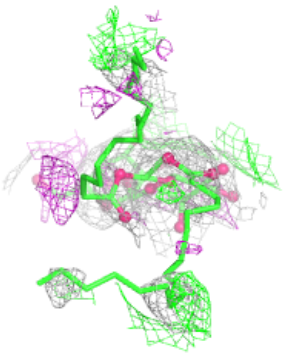


Electron density around DGD c 516:

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

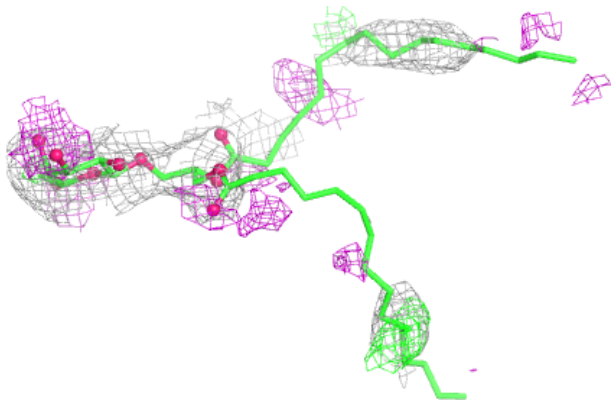


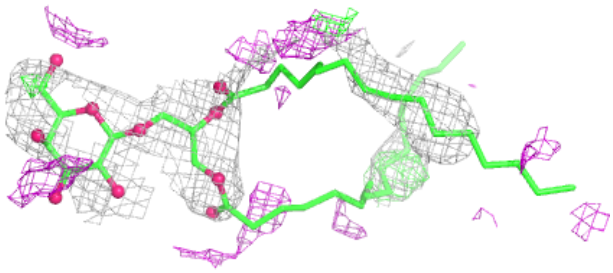


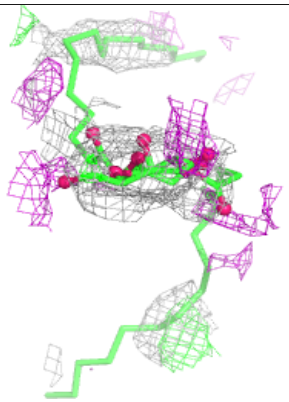


Electron density around LMG b 622:

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

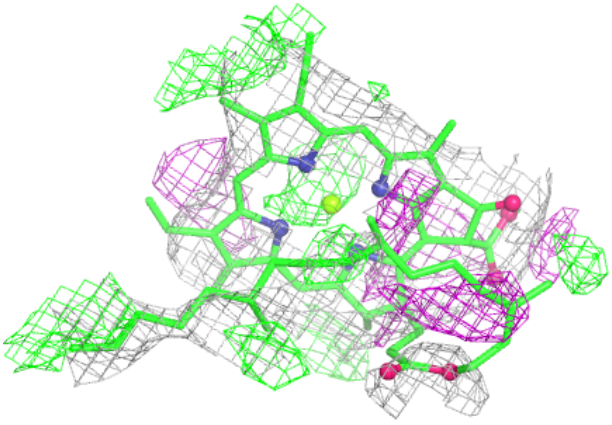


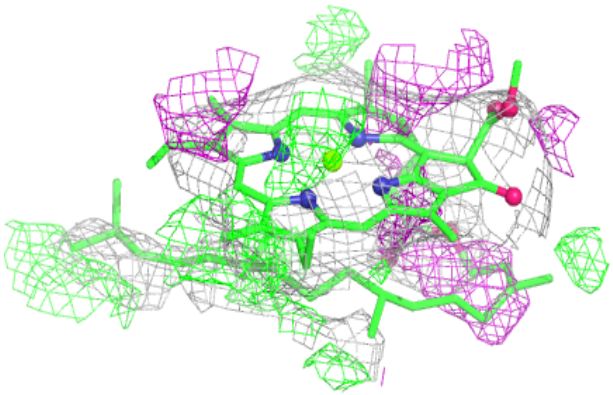


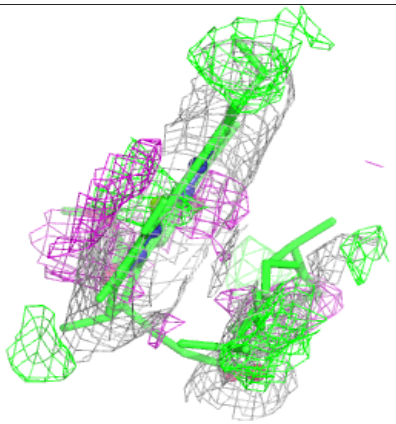


Electron density around CLA B 602:

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

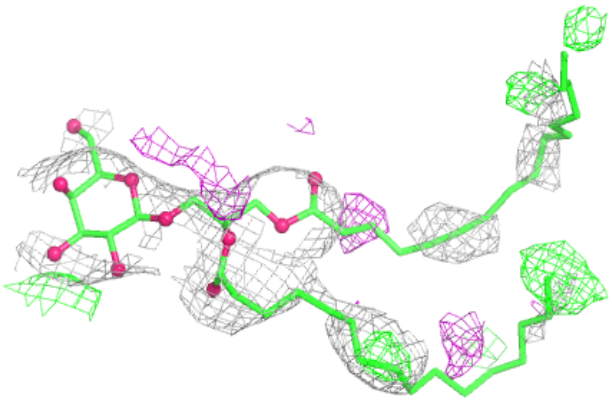


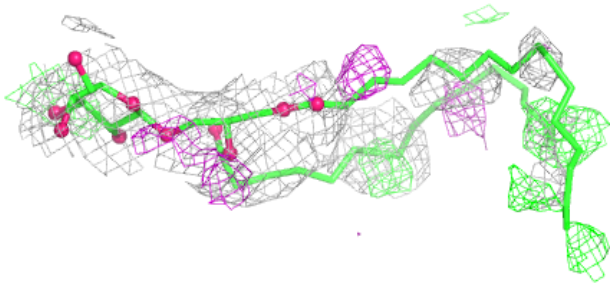


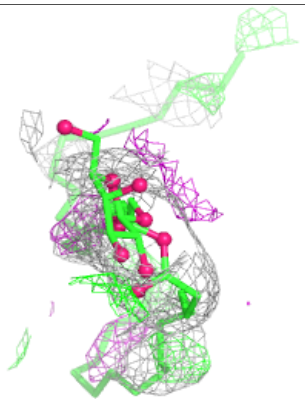


Electron density around LMG j 101:

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

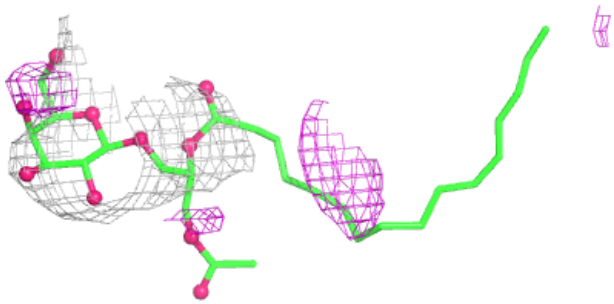


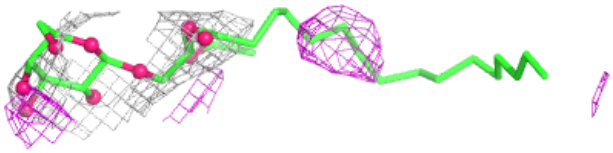


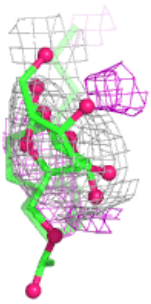


Electron density around LMG z 101:

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

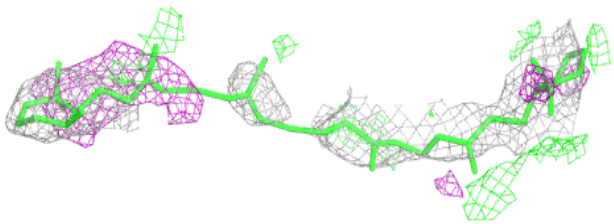


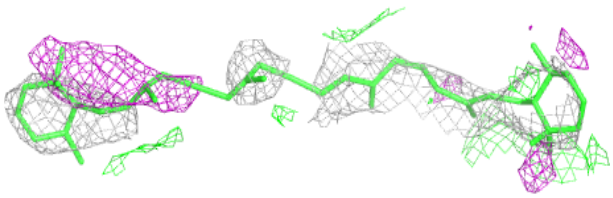


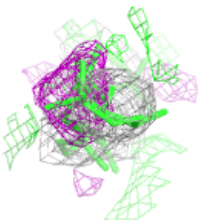


Electron density around BCR H 101:

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

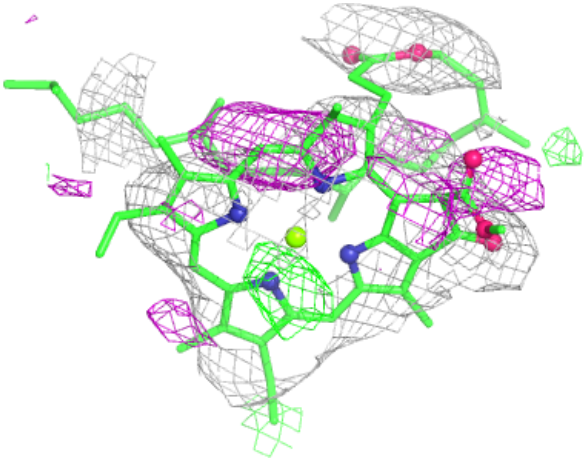


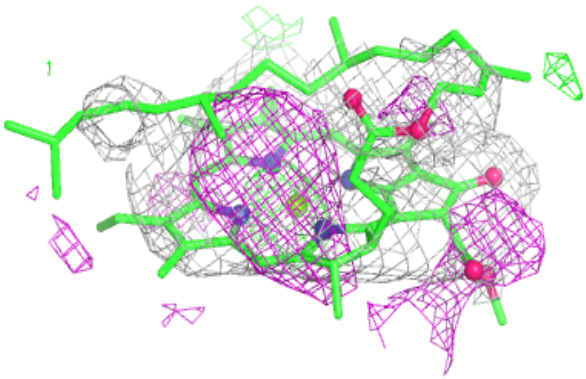


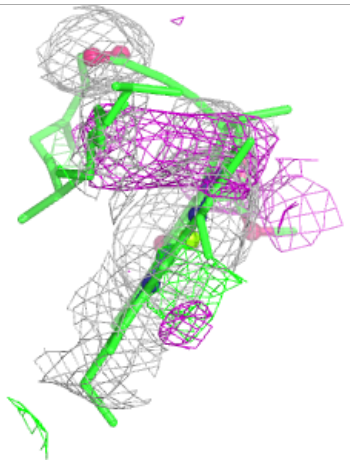


Electron density around CLA b 603:

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

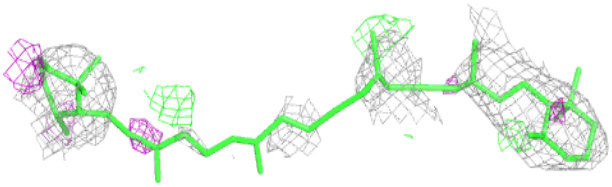


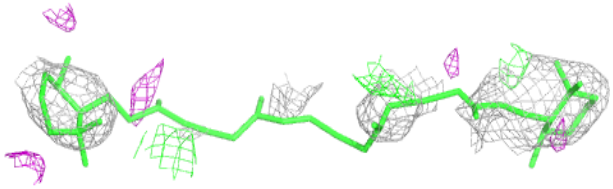


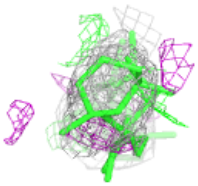


Electron density around BCR k 101:

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

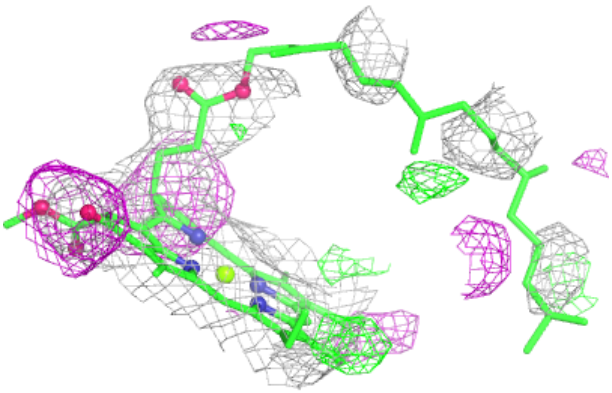


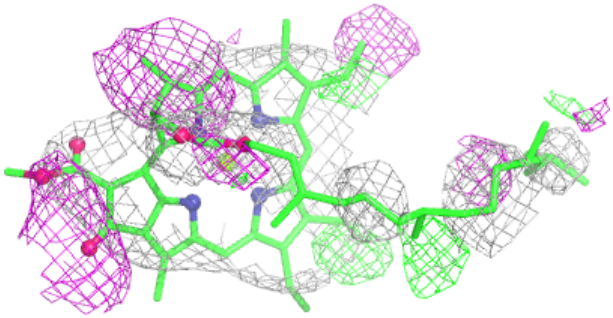


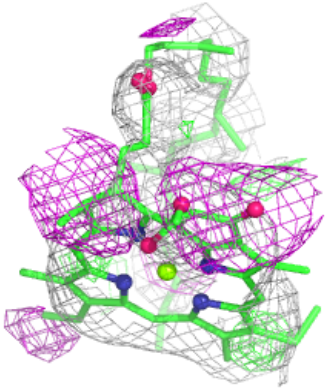


Electron density around CLA C 513:

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

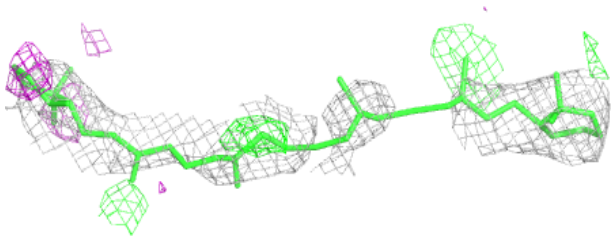


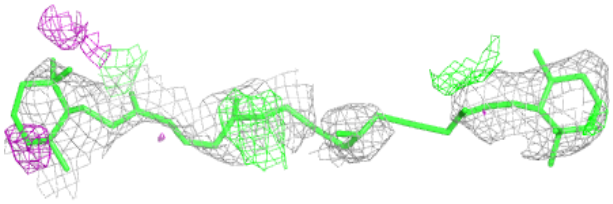


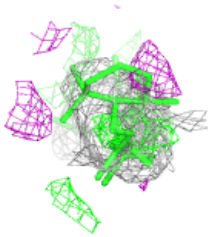


Electron density around BCR h 101:

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

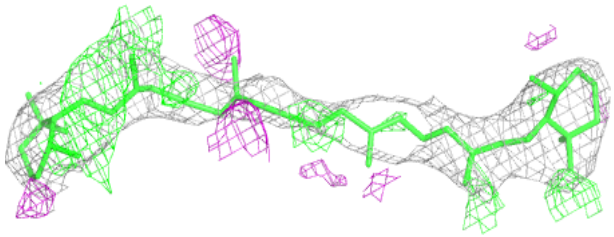


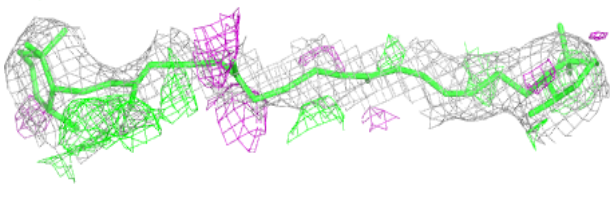


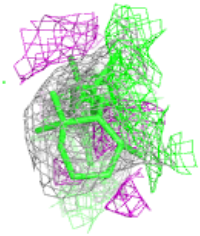


Electron density around BCR B 619:

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

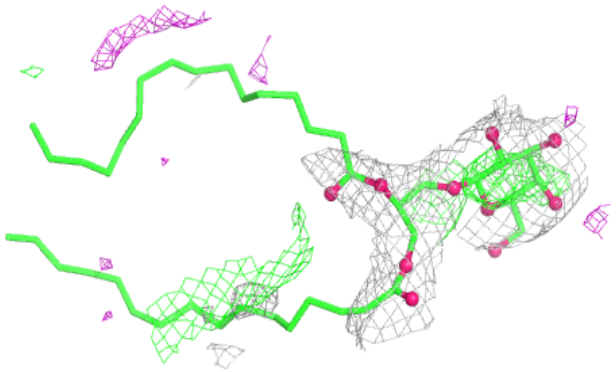


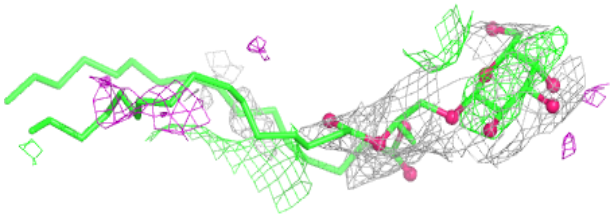


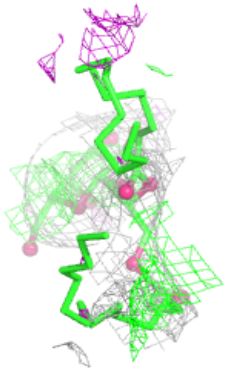


Electron density around LMG a 613:

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

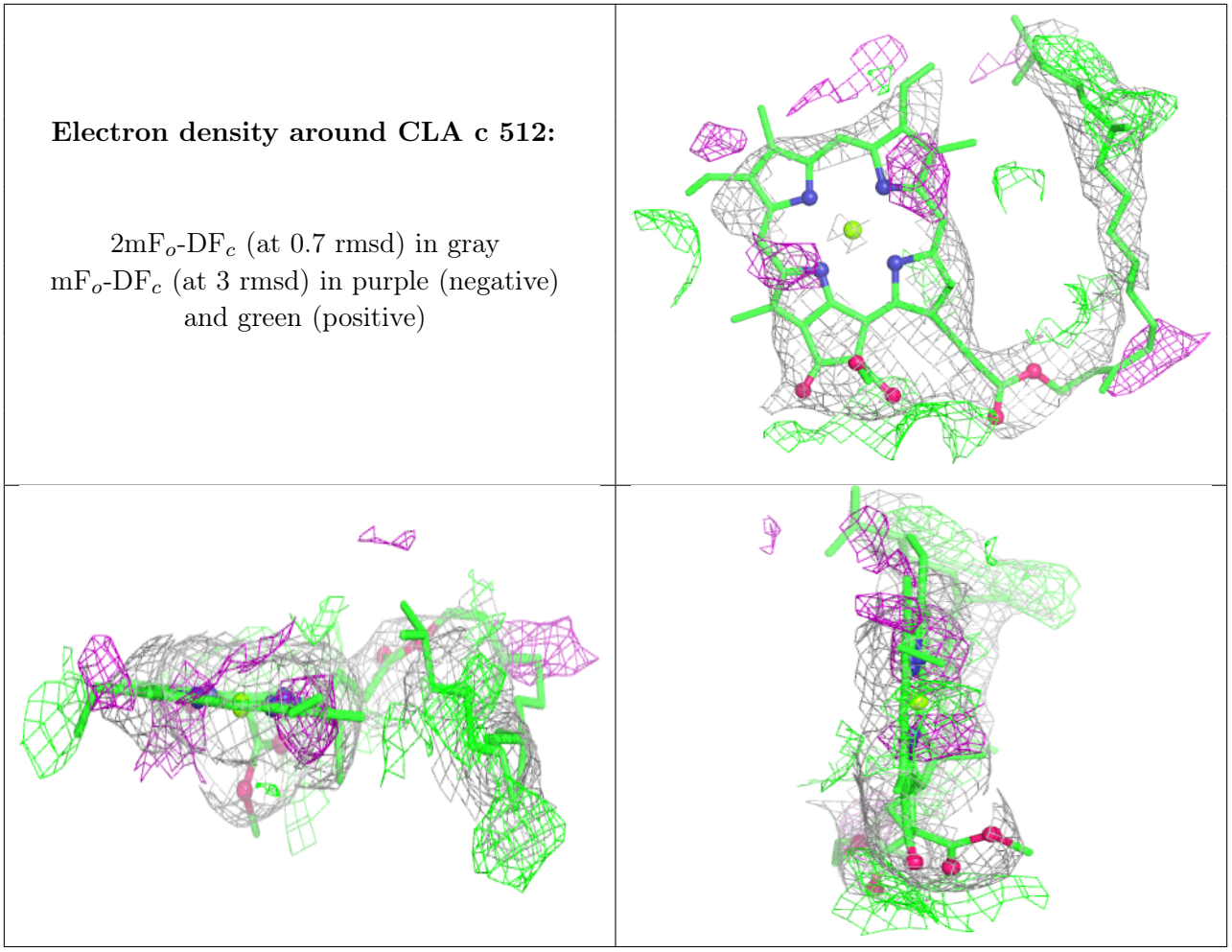






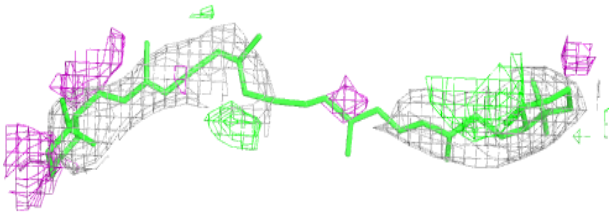
Electron density around CLA c 512:

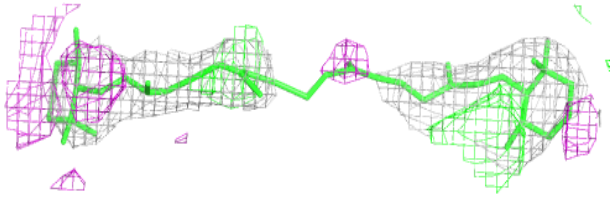
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

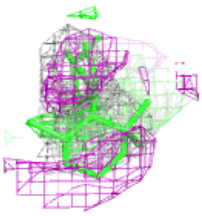


Electron density around BCR I 101:

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

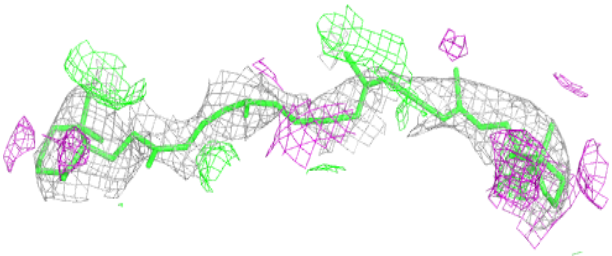


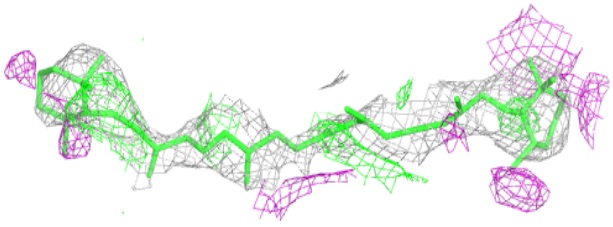


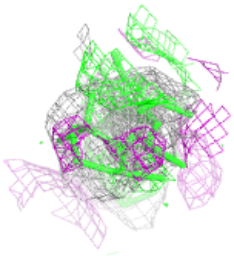


Electron density around BCR T 101:

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

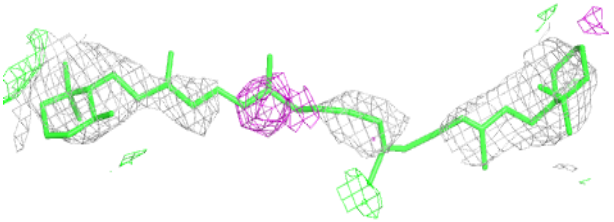


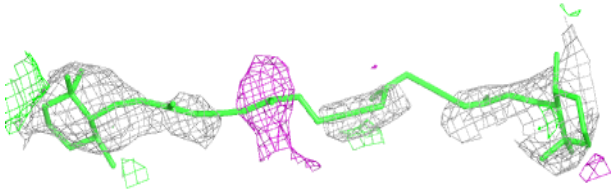


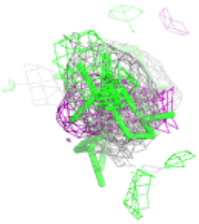


Electron density around BCR c 515:

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

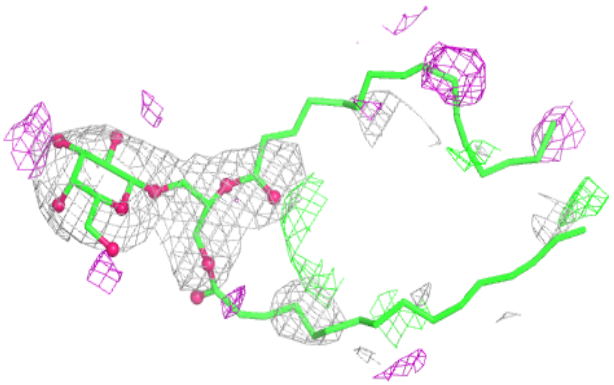


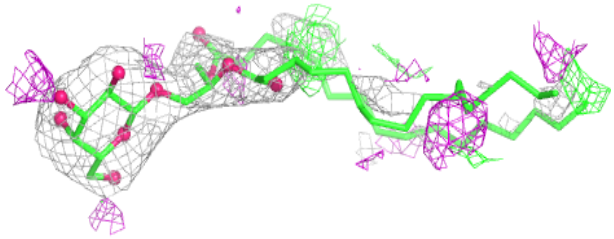


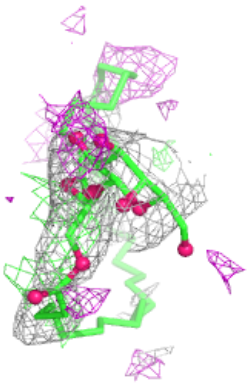


Electron density around LMG A 613:

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

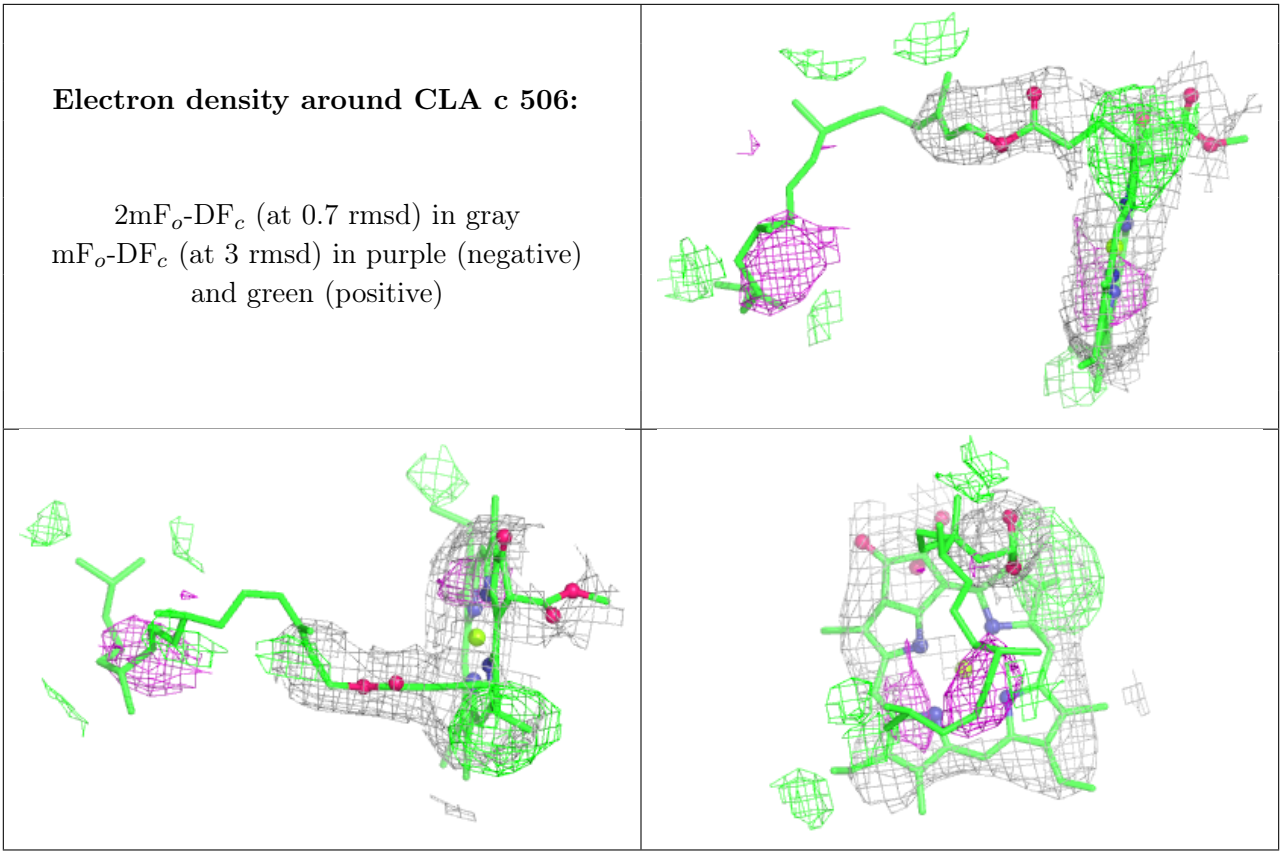






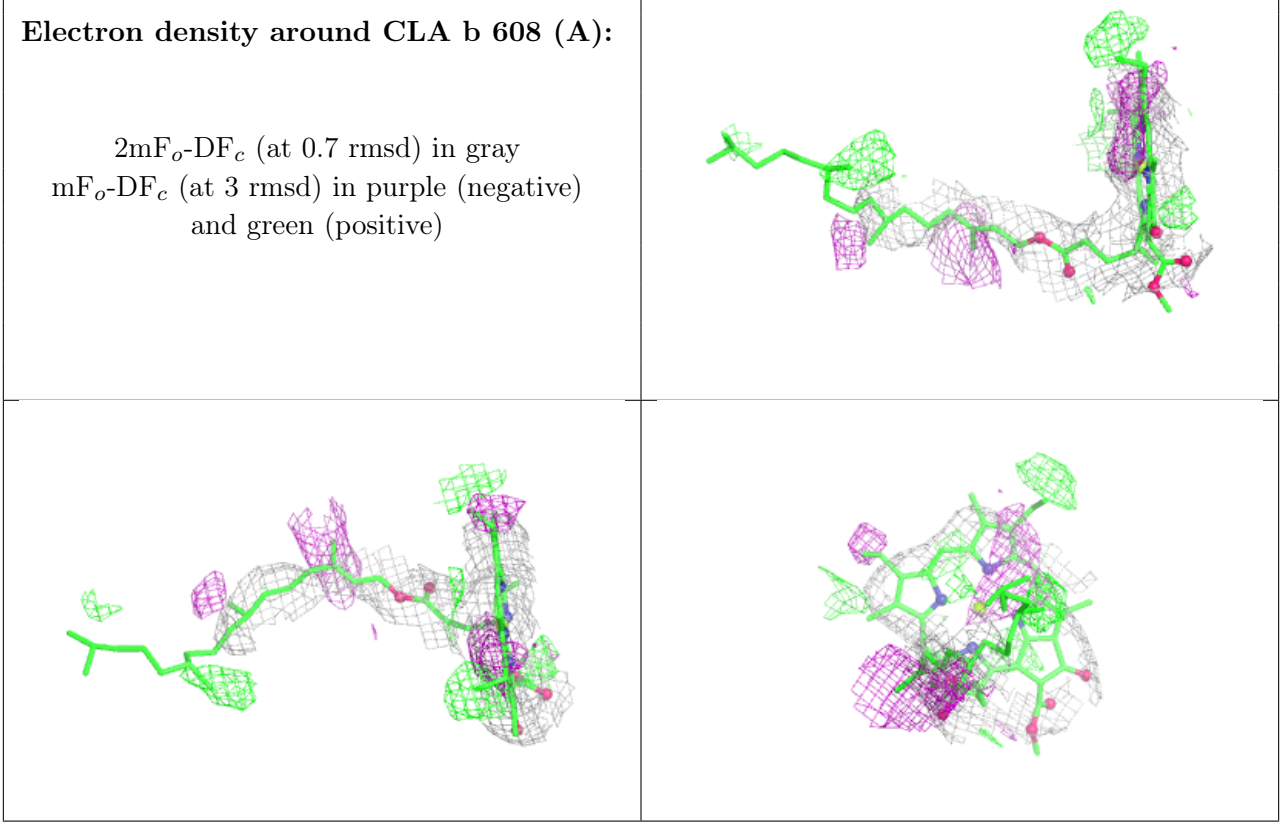
Electron density around CLA c 506:

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



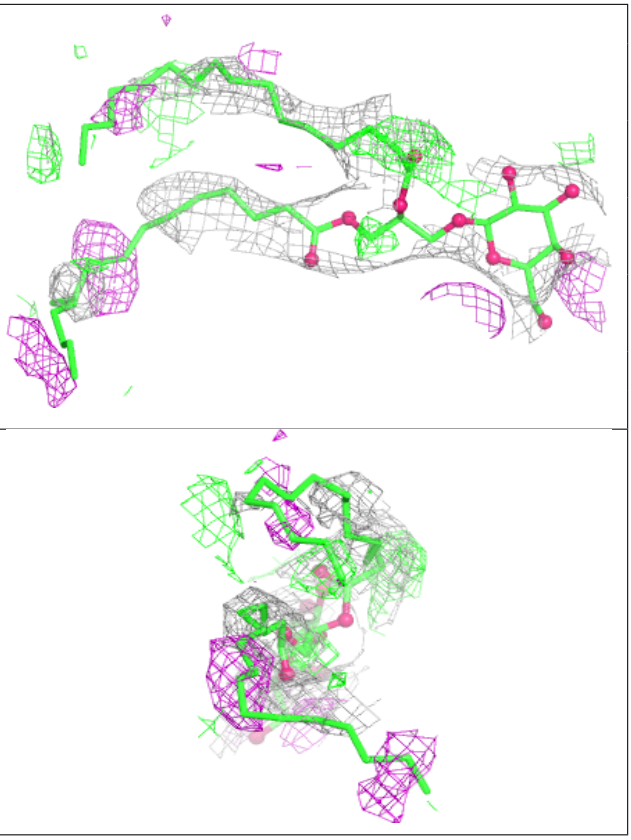
Electron density around CLA b 608 (A):

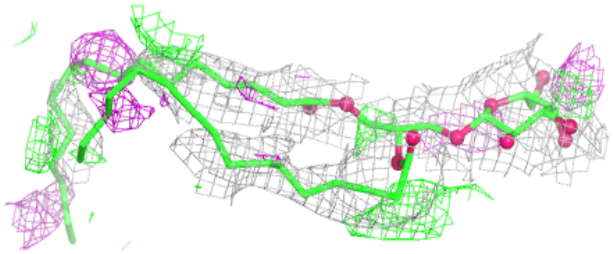
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG D 408:

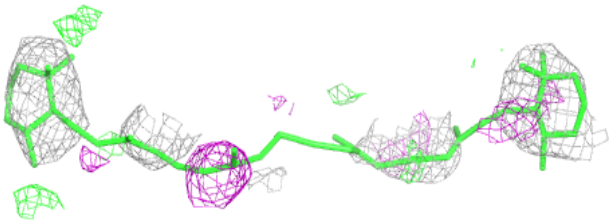
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

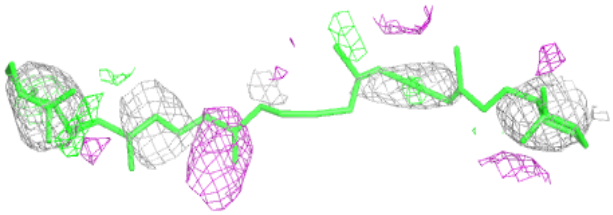


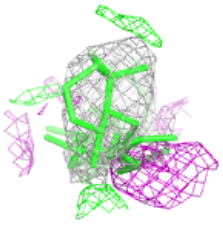


Electron density around BCR c 521:

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

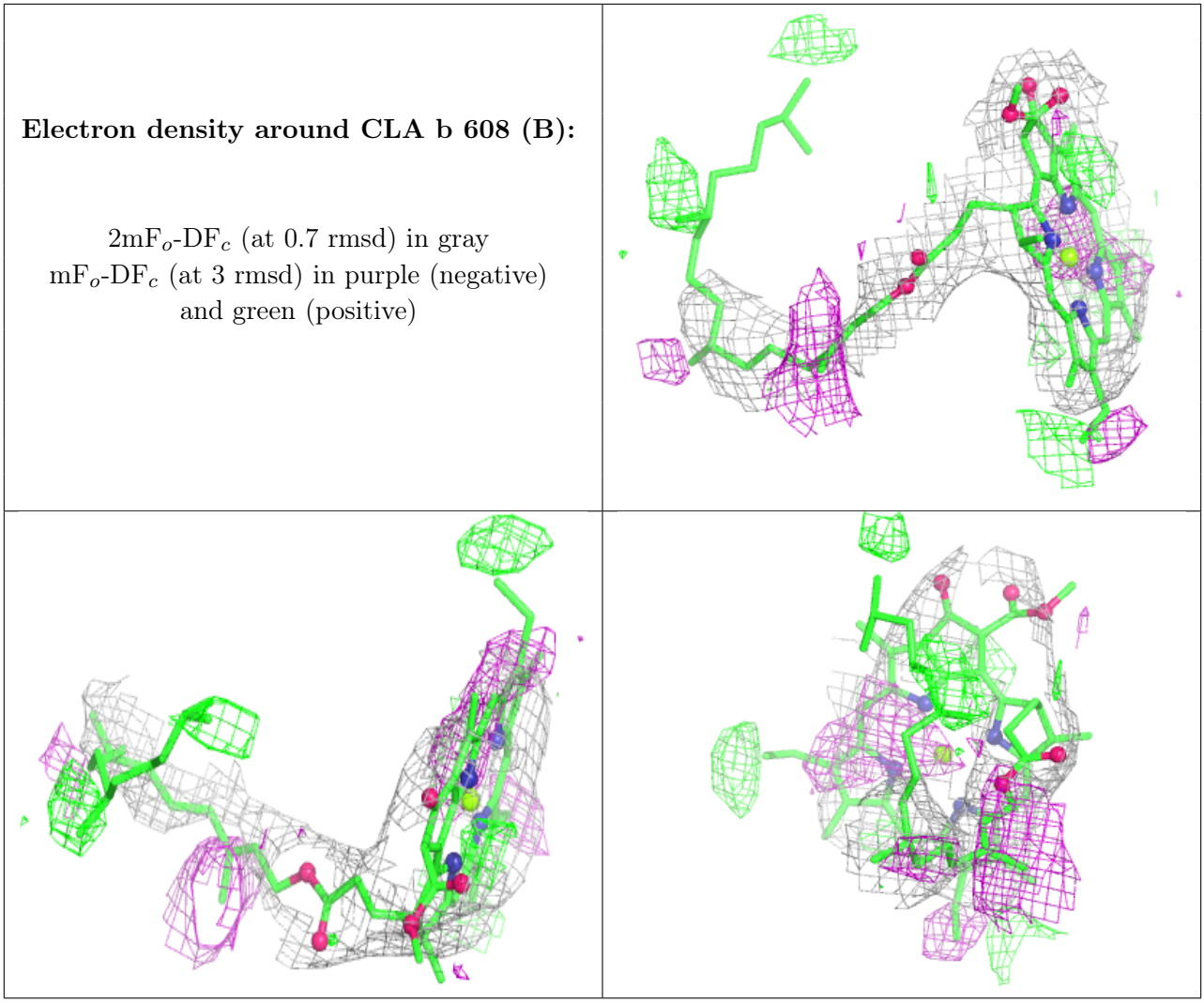






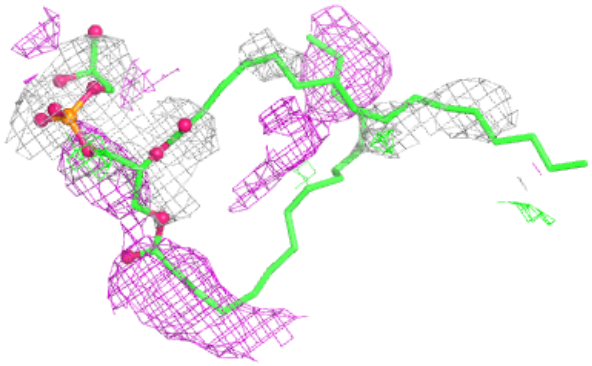
Electron density around CLA b 608 (B):

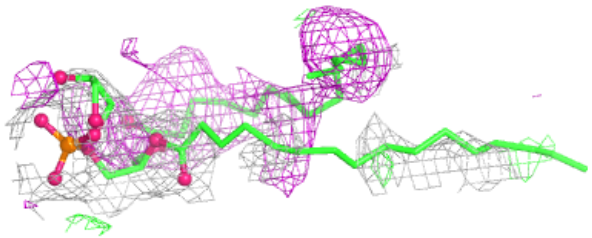
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

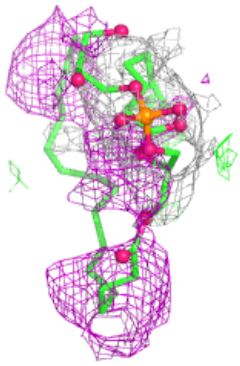


Electron density around LHG a 616:

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

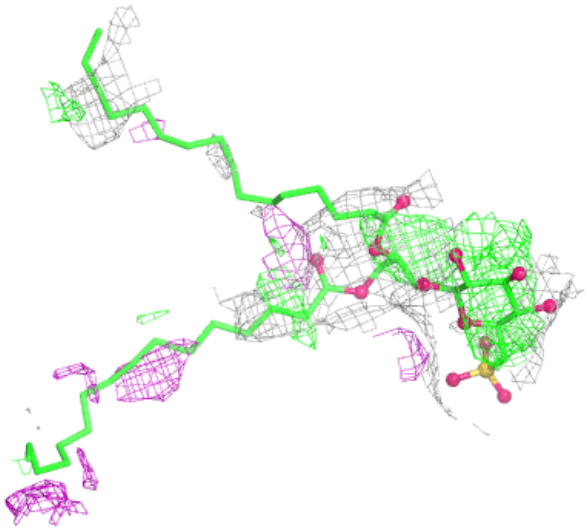


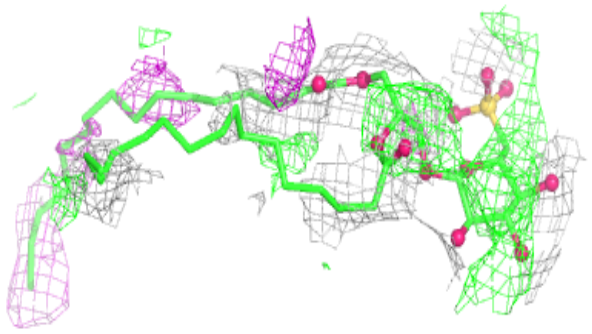


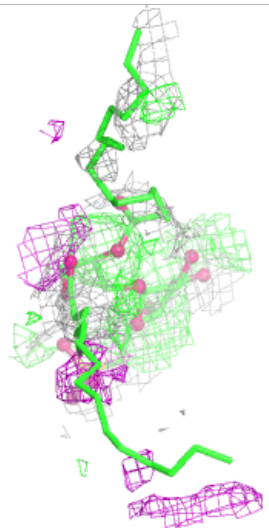


Electron density around SQD A 612:

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

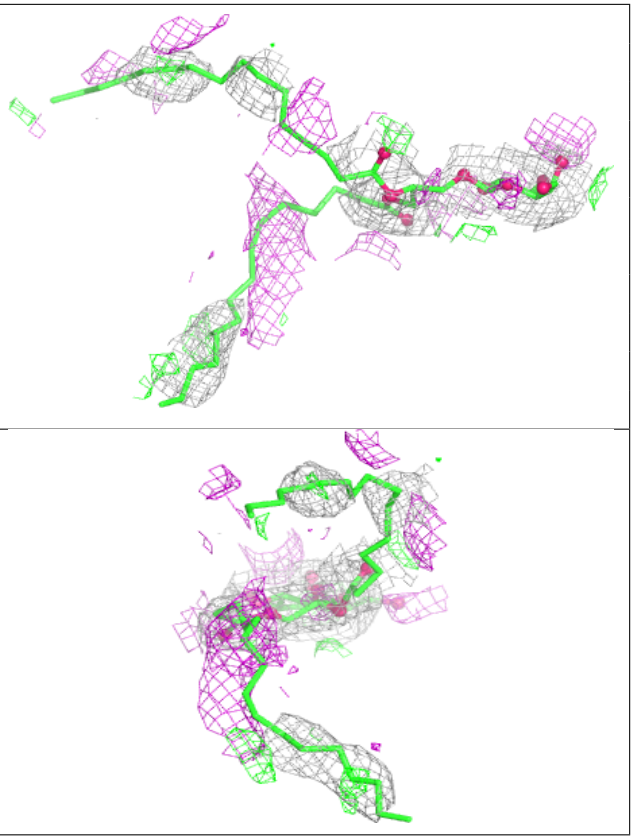


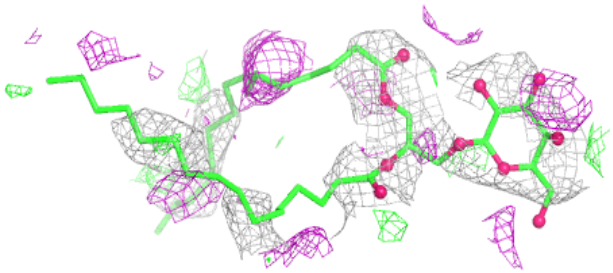




Electron density around LMG B 621:

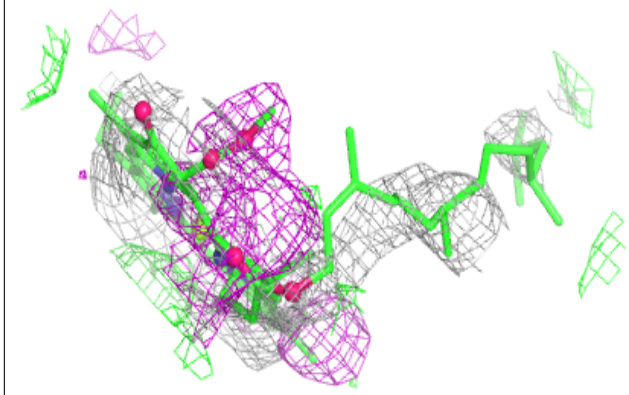
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

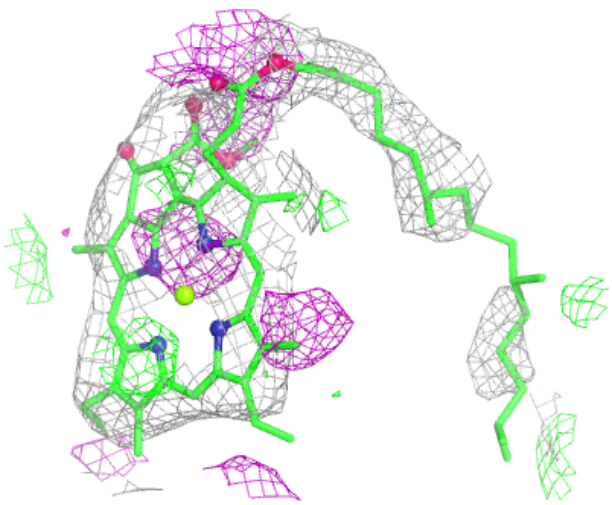


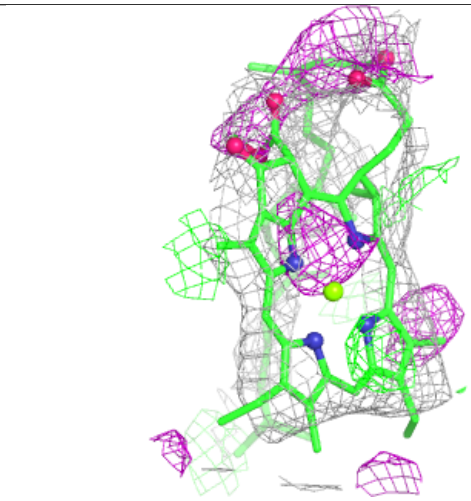


Electron density around CLA B 617:

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

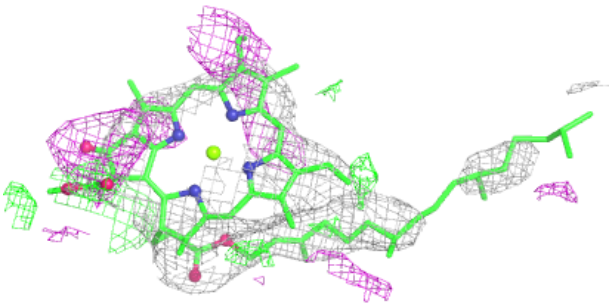


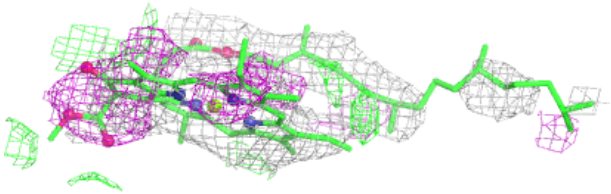


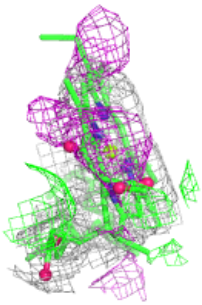


Electron density around CLA c 501:

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

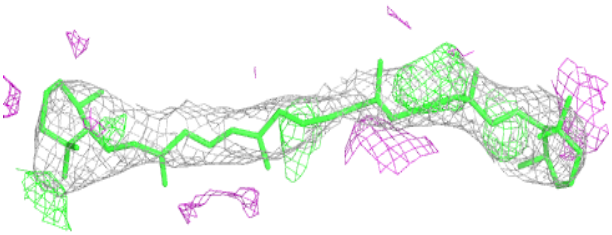


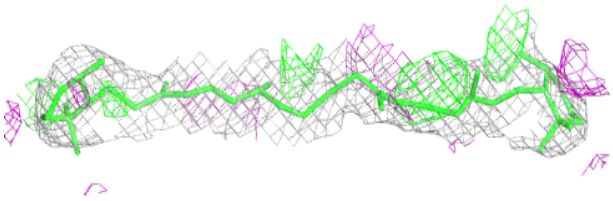


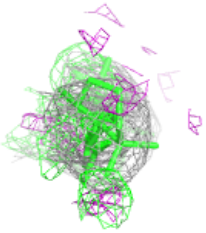


Electron density around BCR b 620:

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

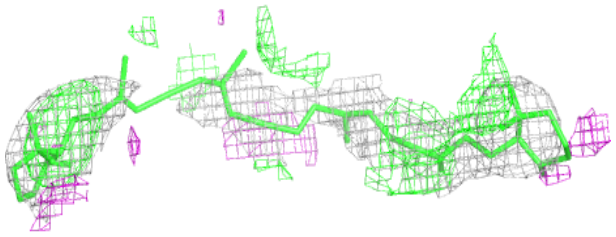


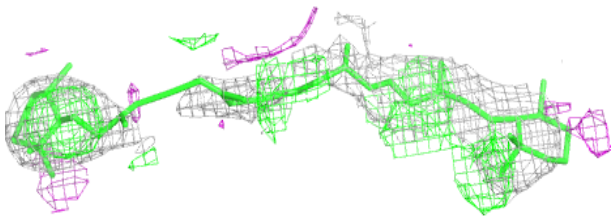


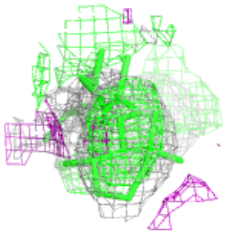


Electron density around BCR t 101:

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

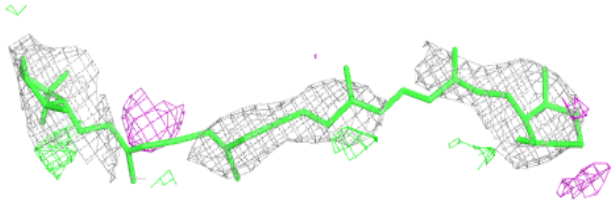


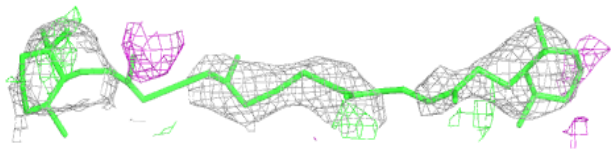


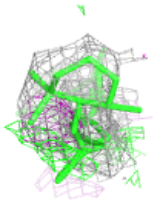


Electron density around BCR C 514:

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

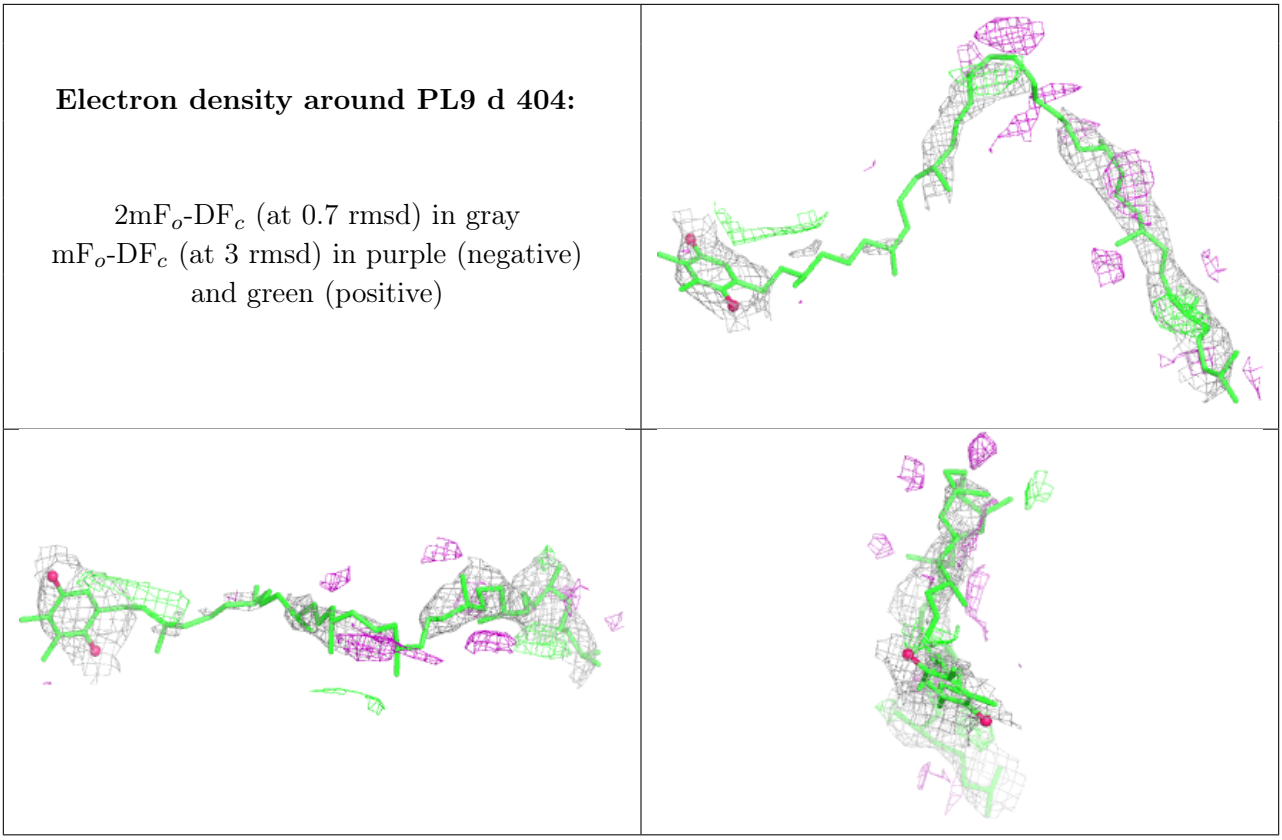






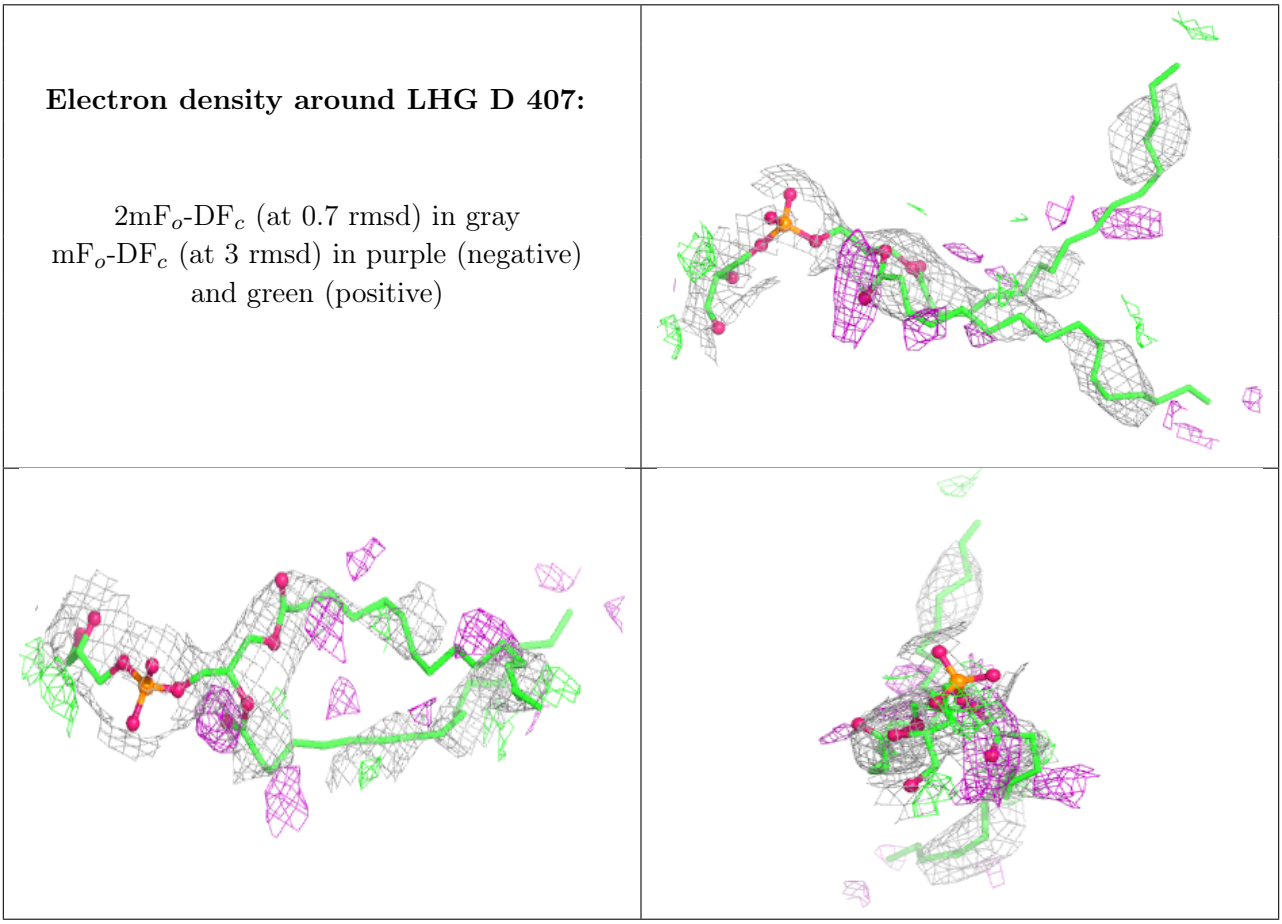
Electron density around PL9 d 404:

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



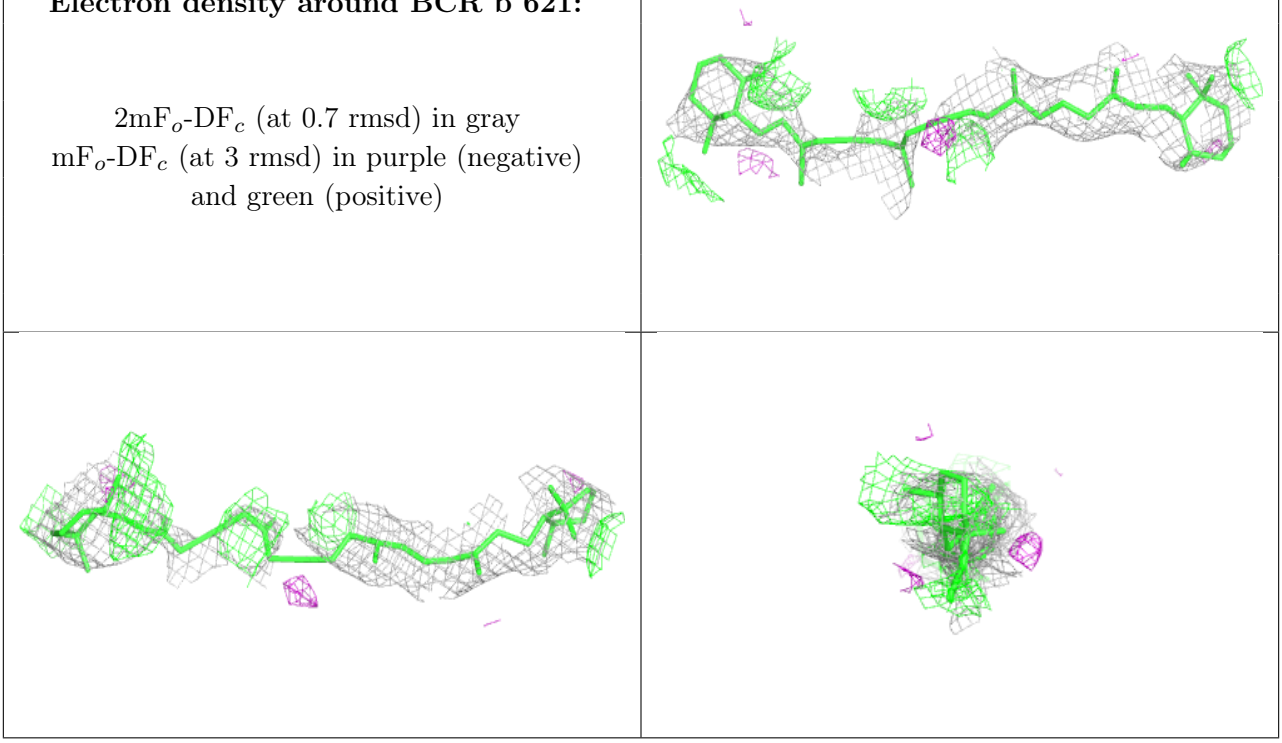
Electron density around LHG D 407:

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



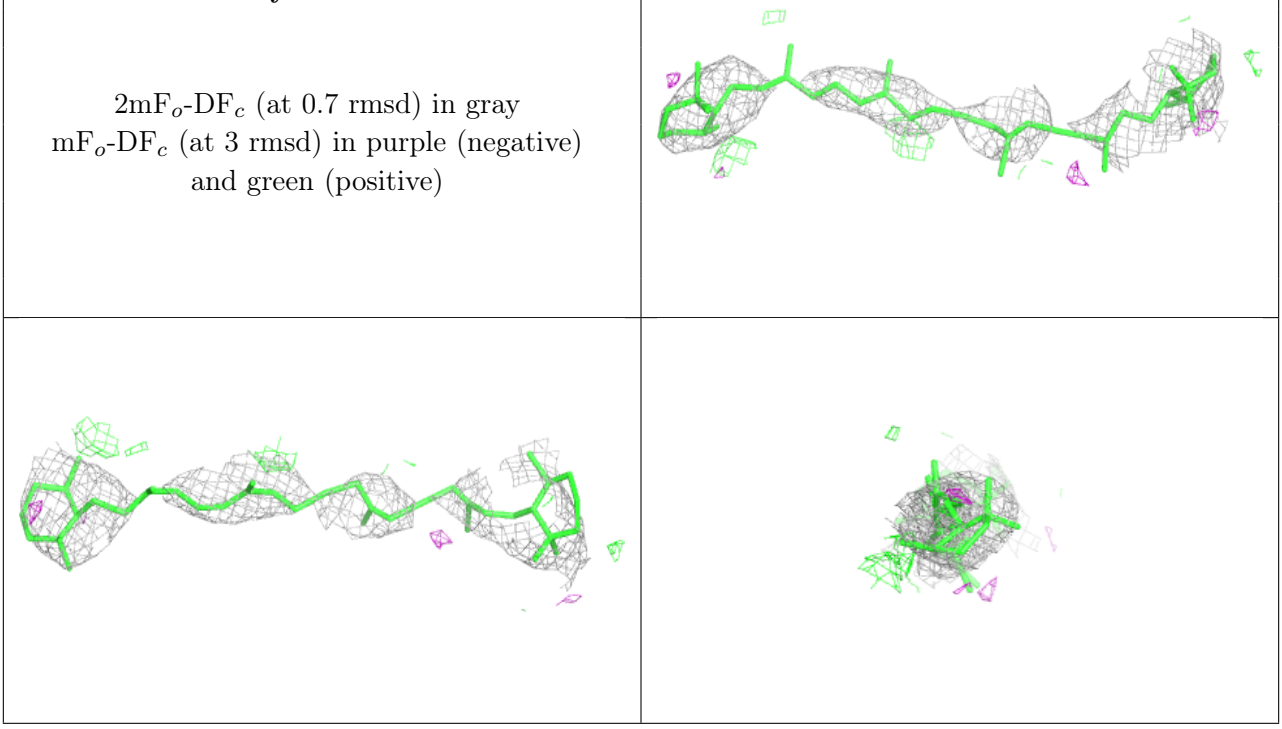
Electron density around BCR b 621:

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



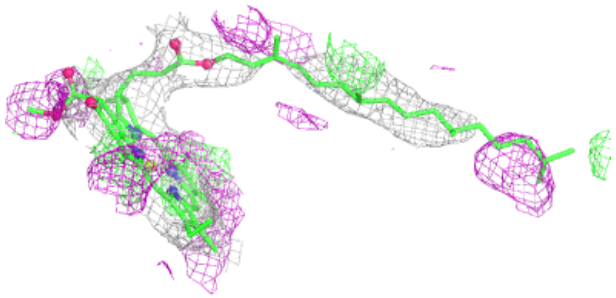
Electron density around BCR c 514:

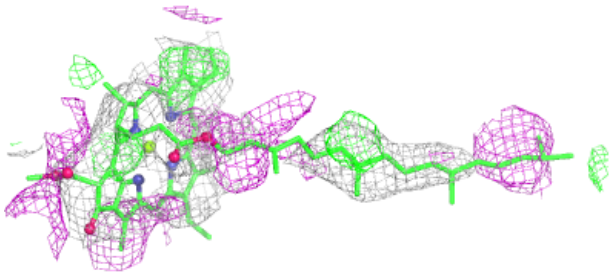
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

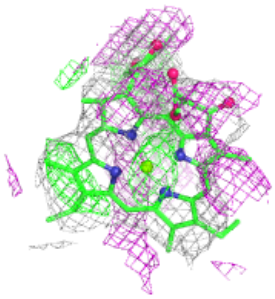


Electron density around CLA b 609:

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

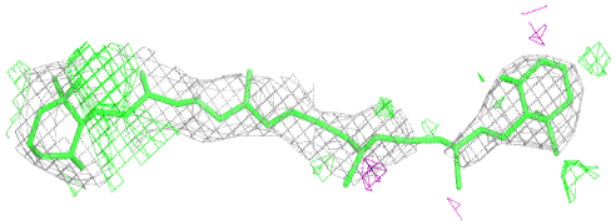


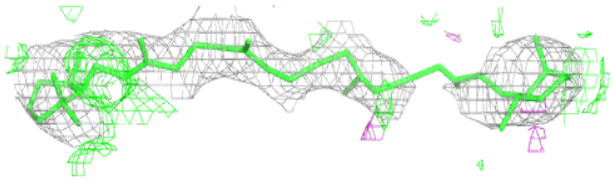


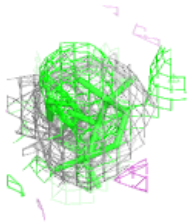


Electron density around BCR B 620:

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

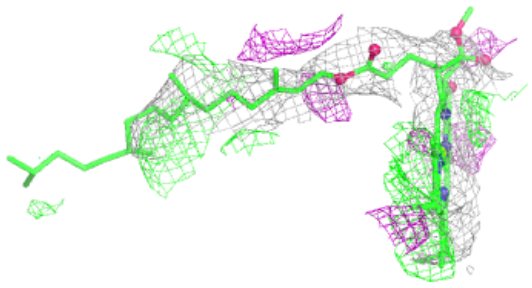


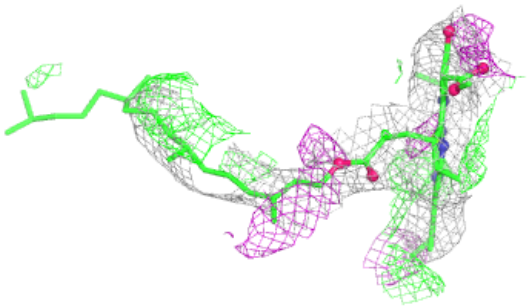


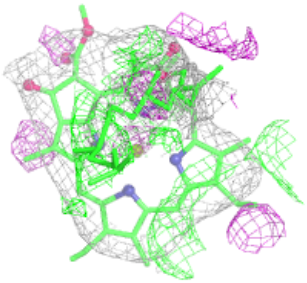


Electron density around CLA B 607 (A):

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

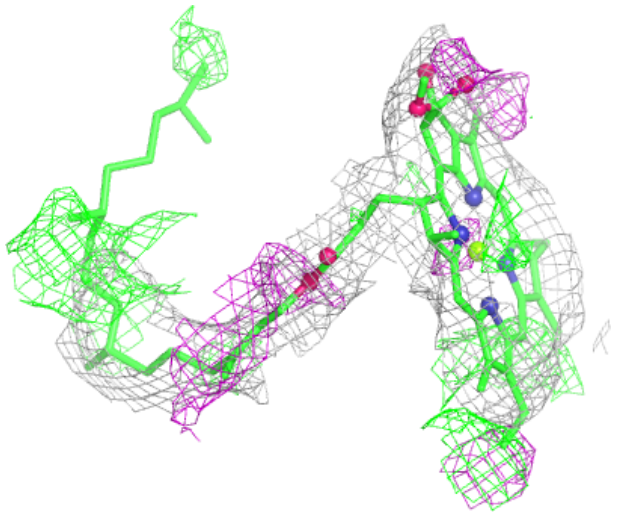


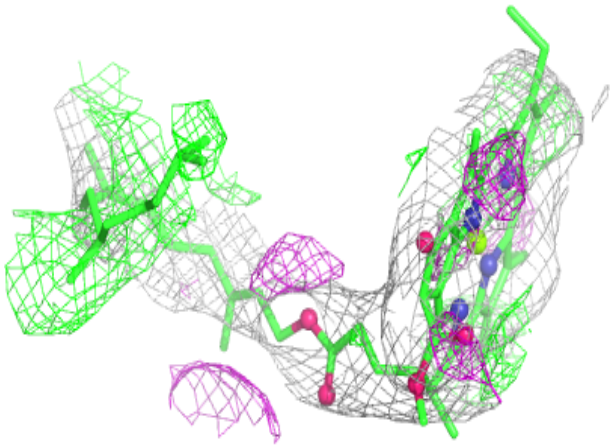


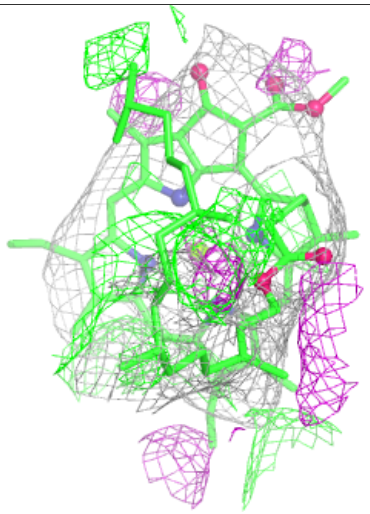


Electron density around CLA B 607 (B):

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

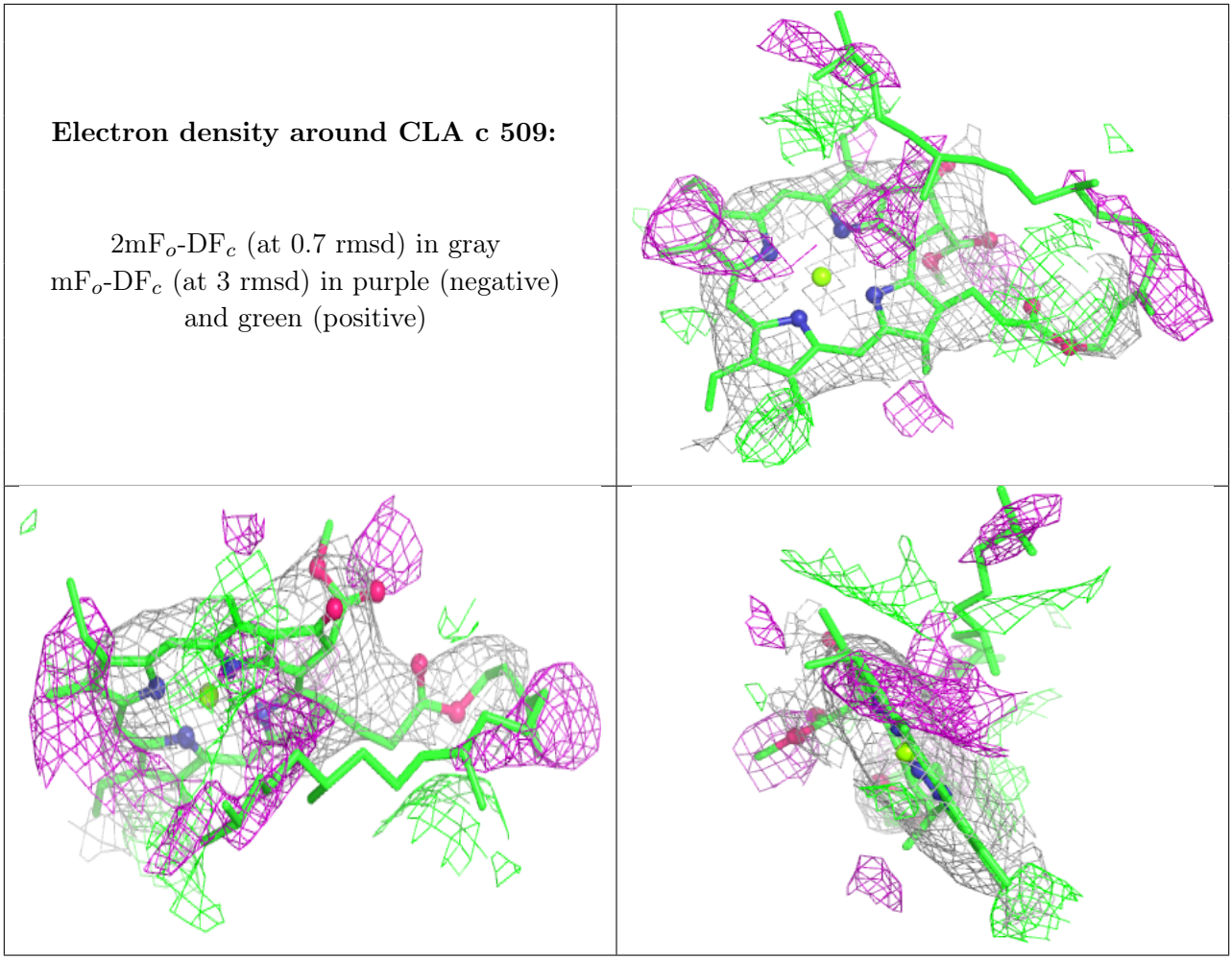






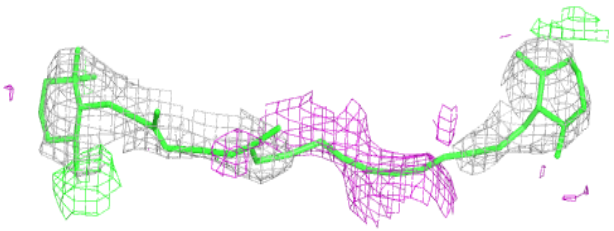
Electron density around CLA c 509:

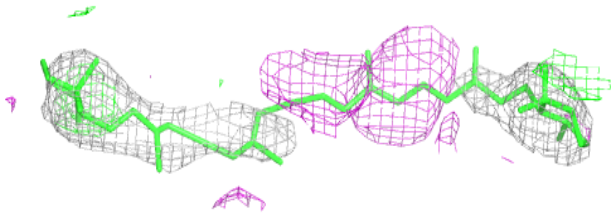
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

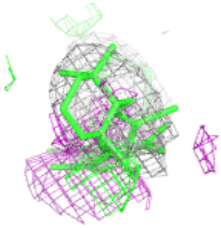


Electron density around BCR K 102:

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

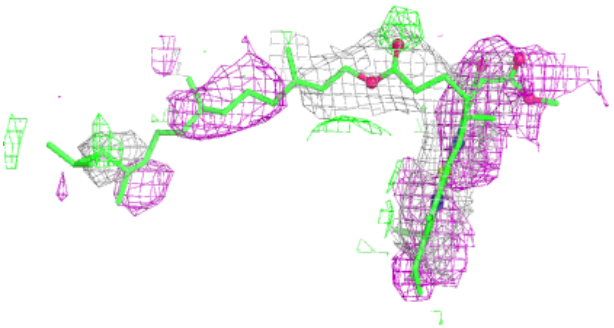


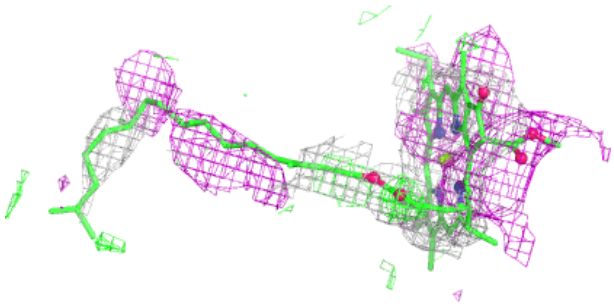


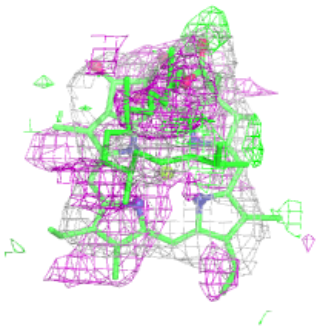


Electron density around CLA B 606:

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

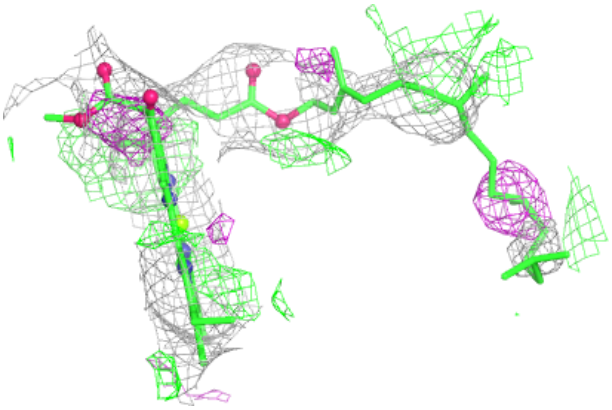


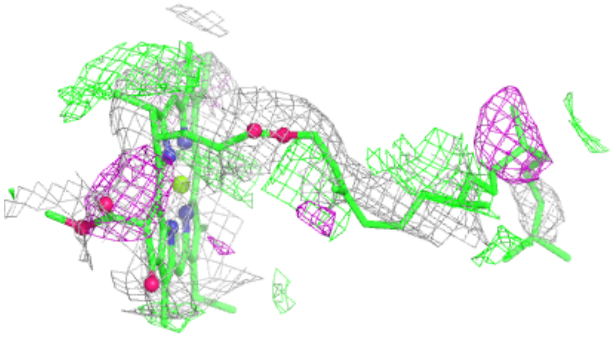


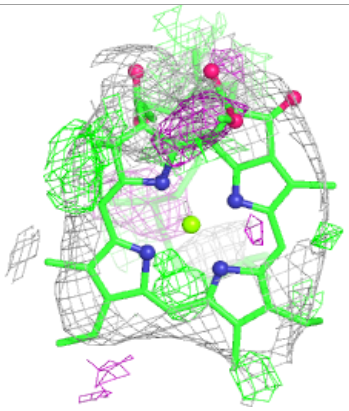


Electron density around CLA C 506:

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

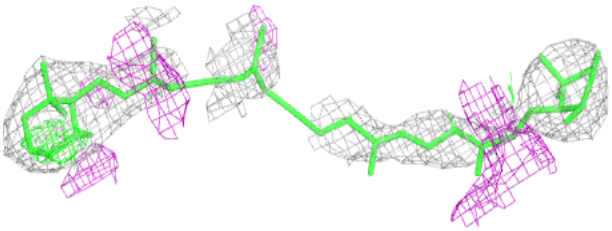


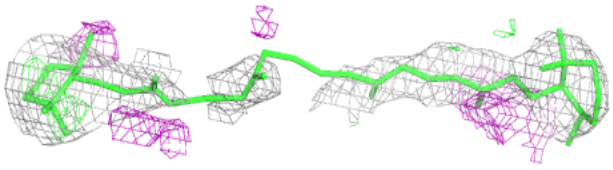


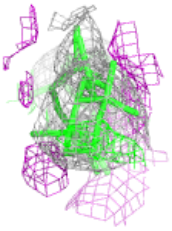


Electron density around BCR K 101:

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

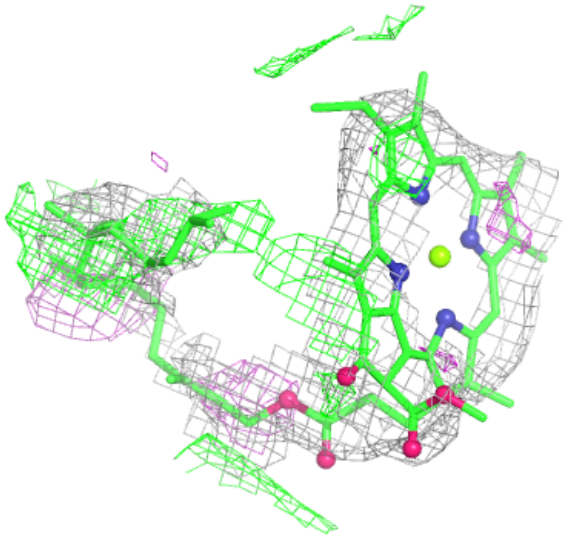


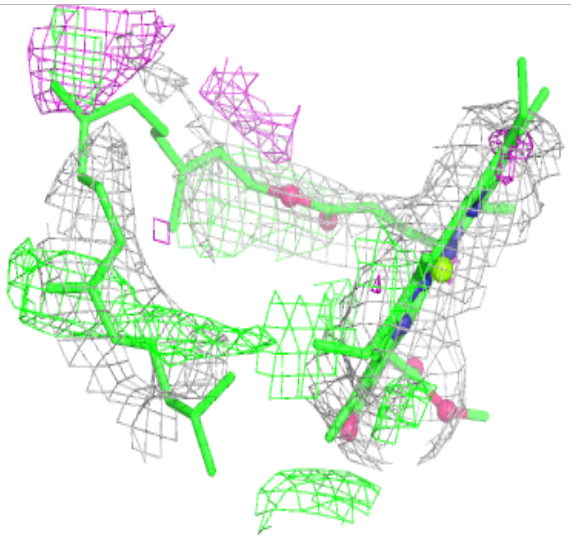


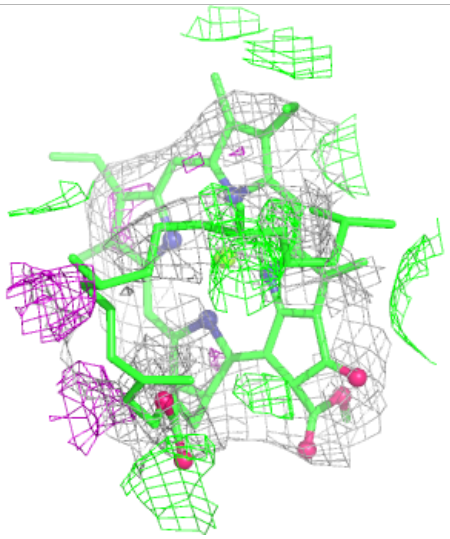


Electron density around CLA c 503:

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

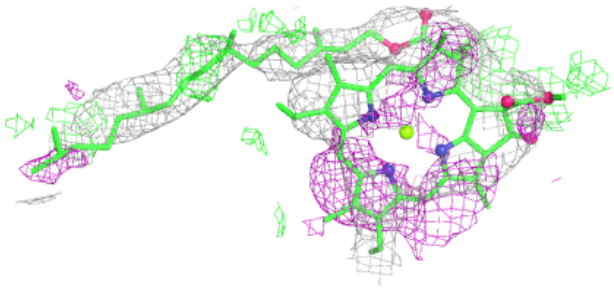


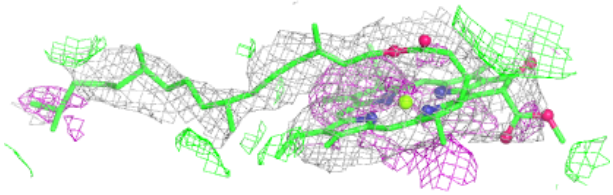


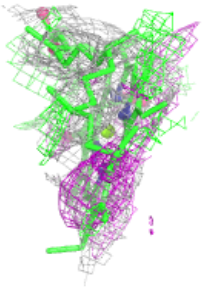


Electron density around CLA C 501:

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

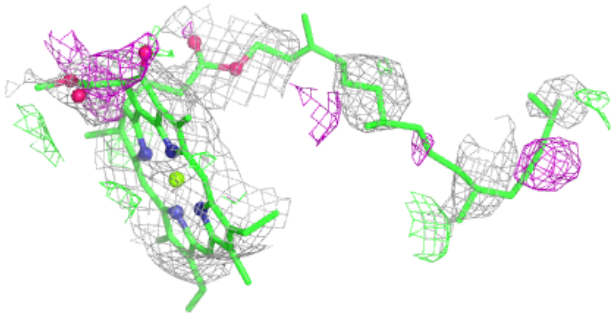


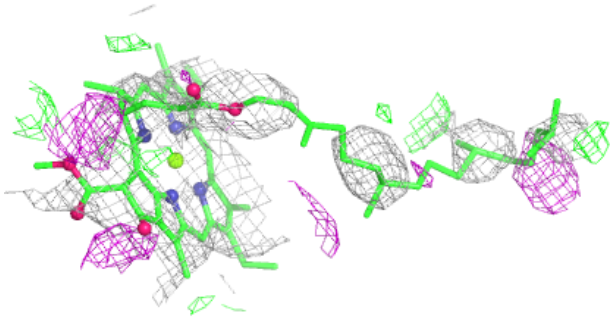


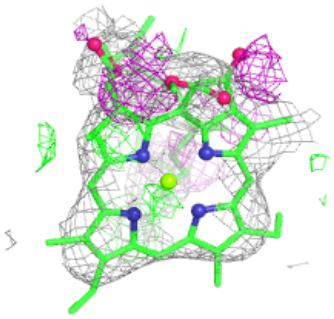


Electron density around CLA c 508:

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

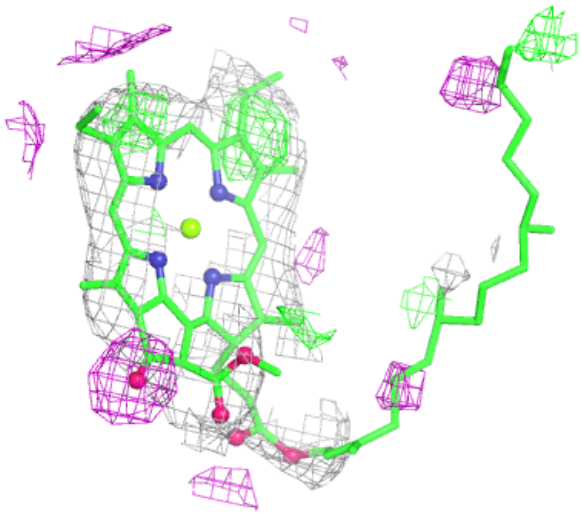


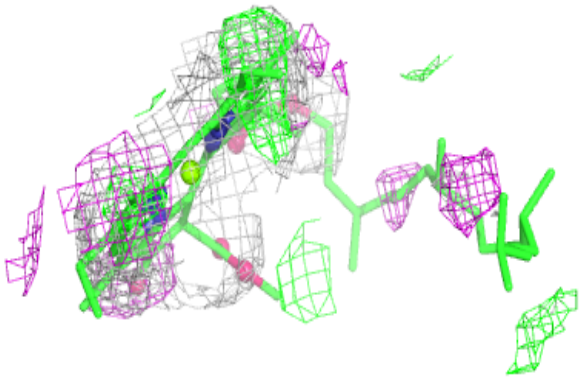


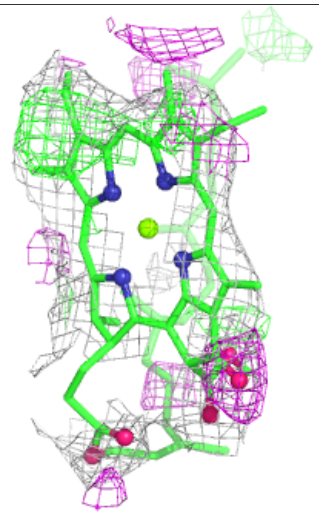


Electron density around CLA b 618:

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

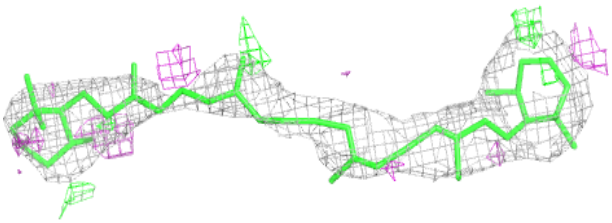


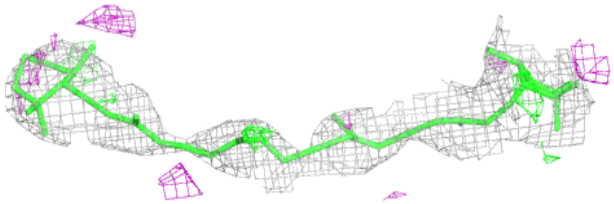


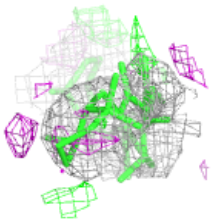


Electron density around BCR F 101:

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

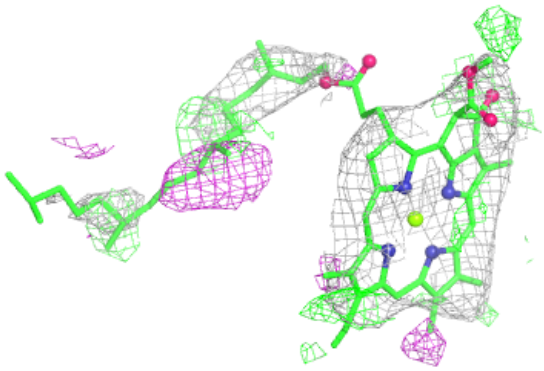


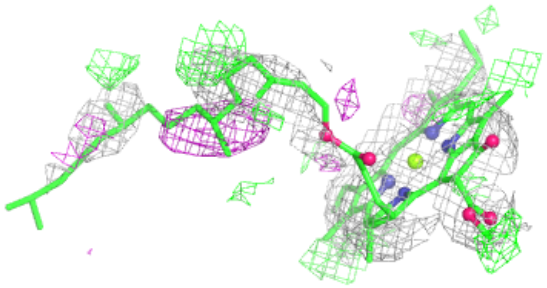


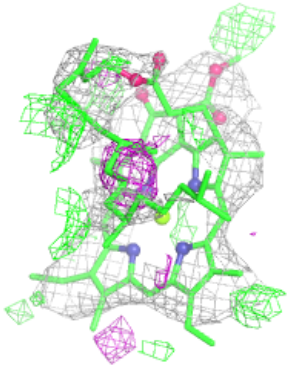


Electron density around CLA c 511:

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

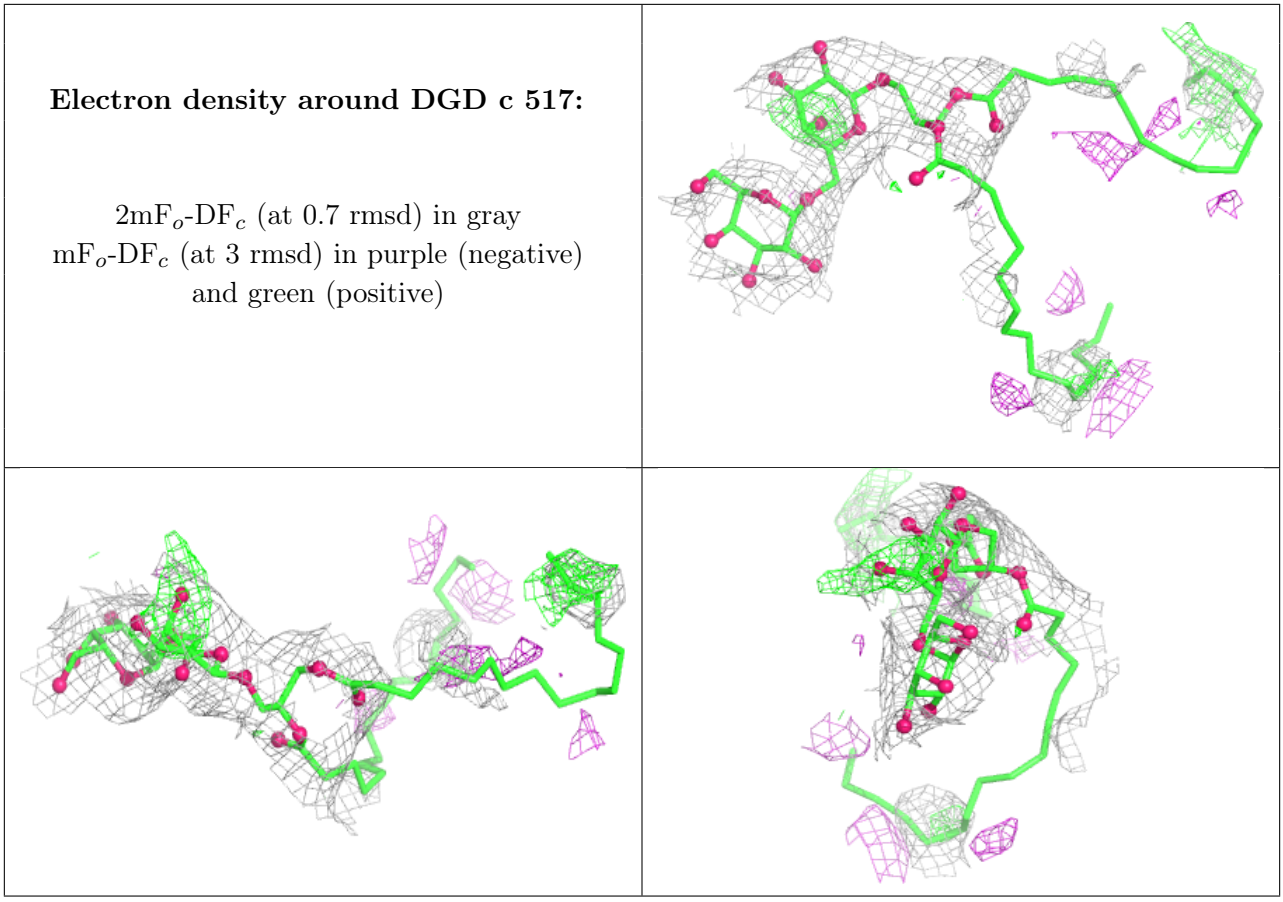






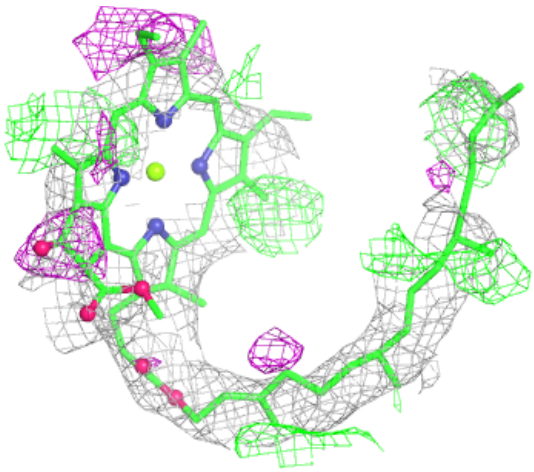
Electron density around DGD c 517:

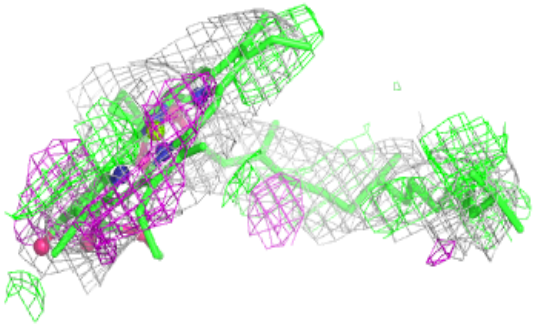
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

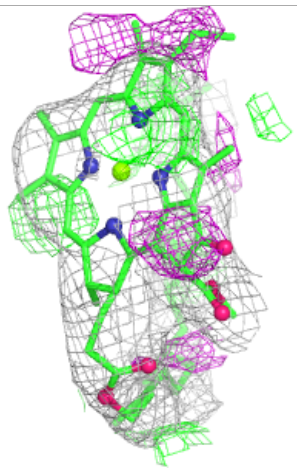


Electron density around CLA C 507:

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

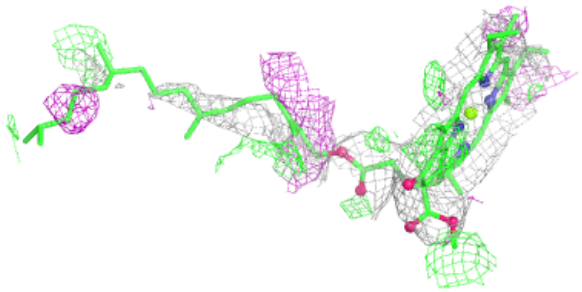


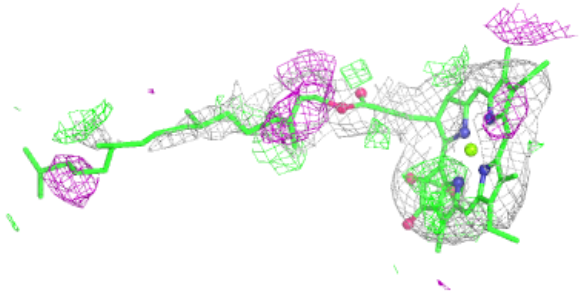


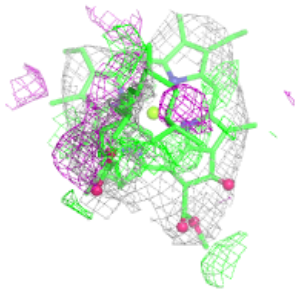


Electron density around CLA b 606:

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

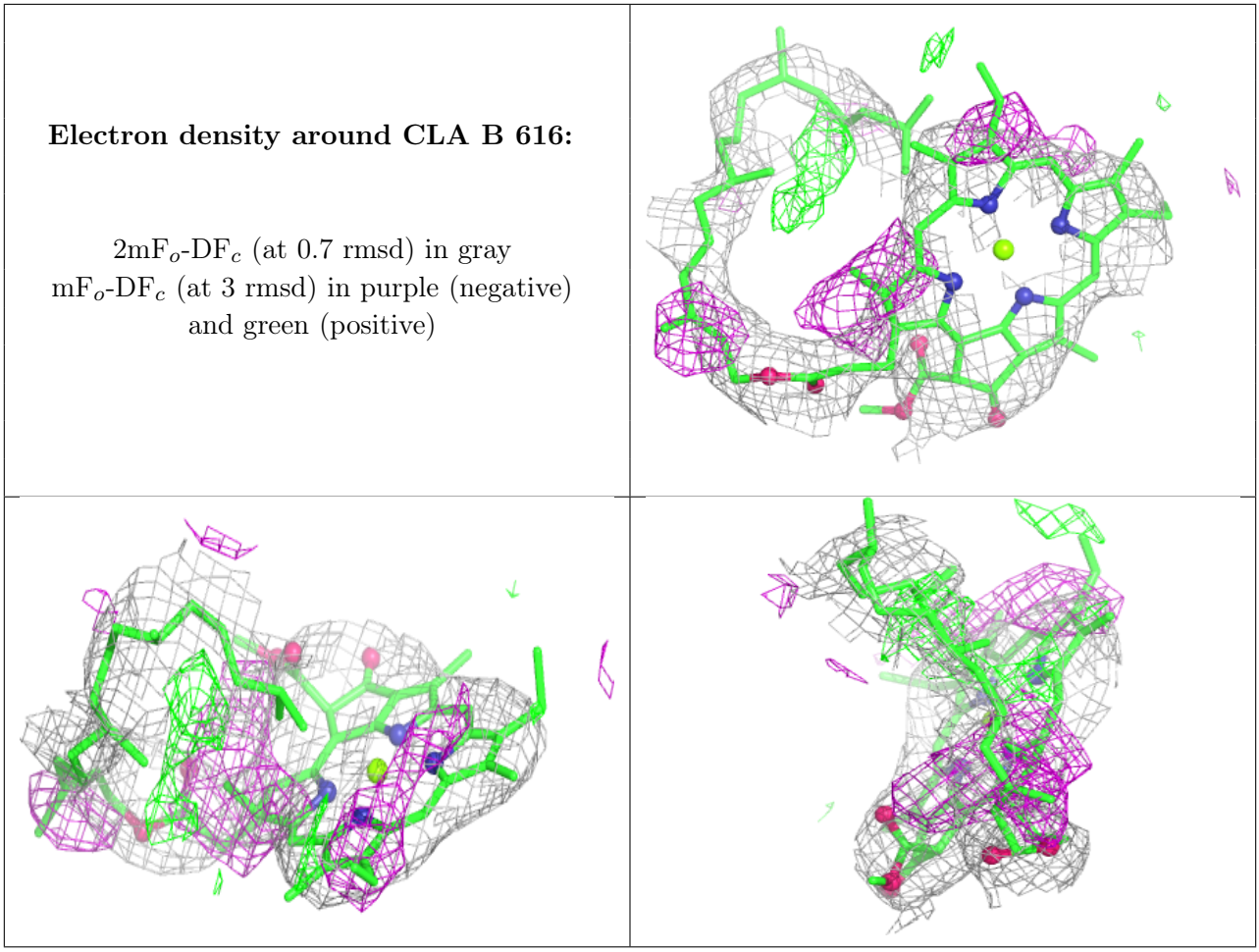






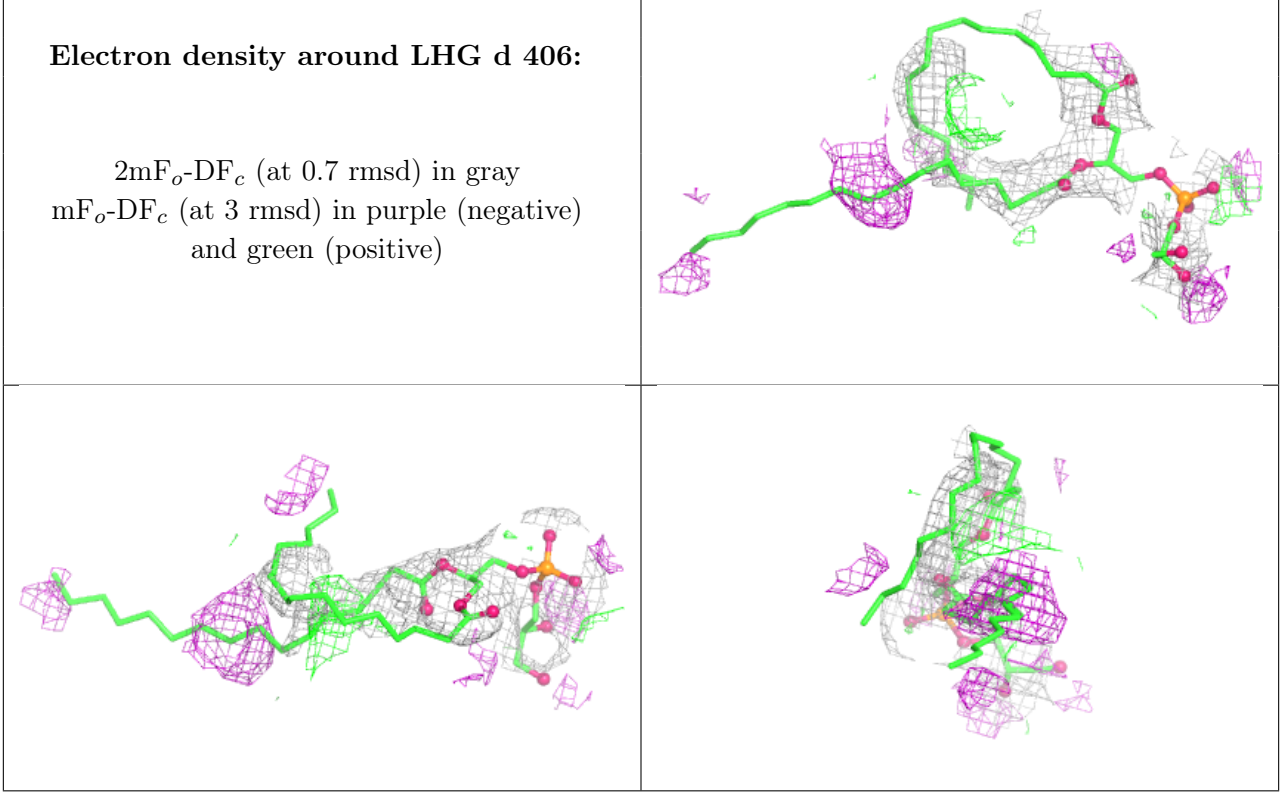
Electron density around CLA B 616:

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



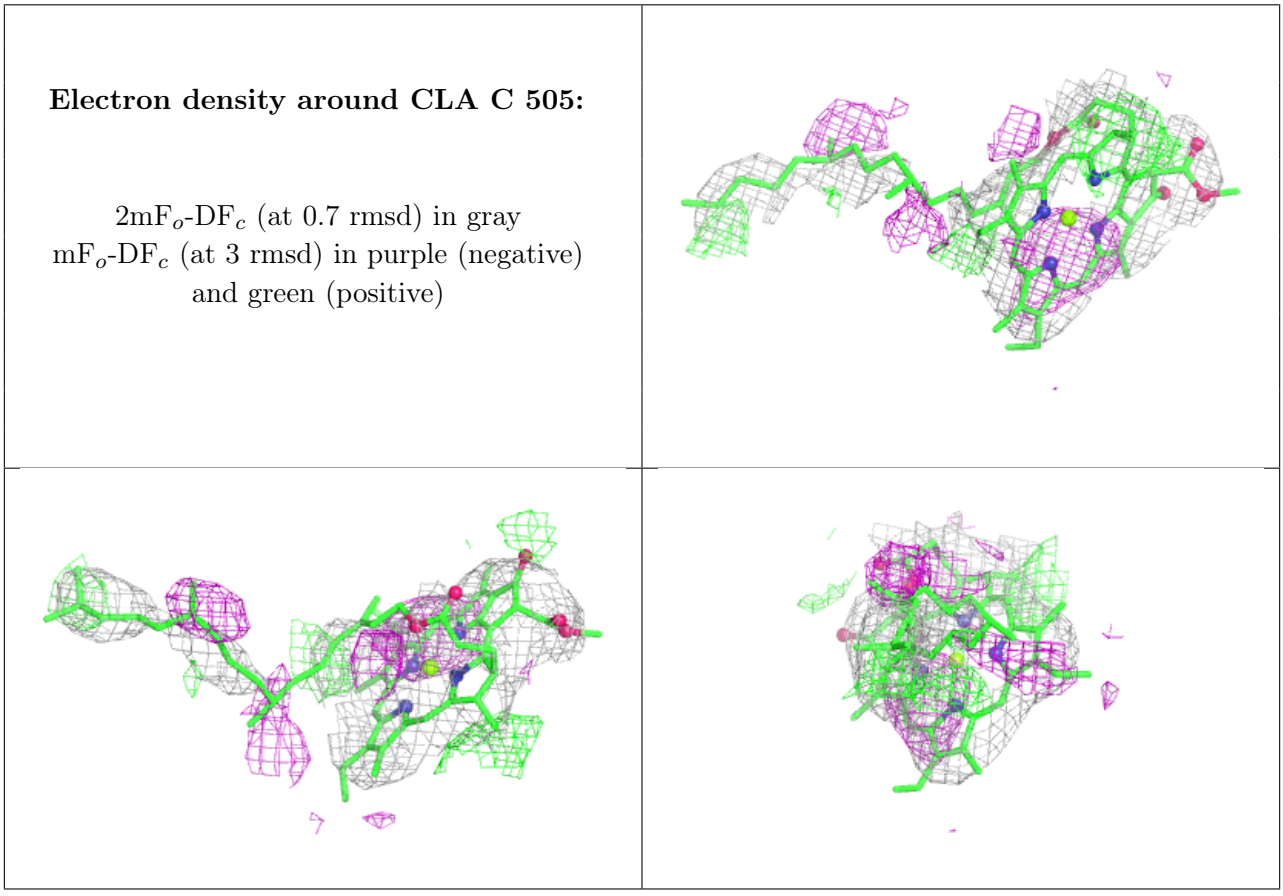
Electron density around LHG d 406:

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



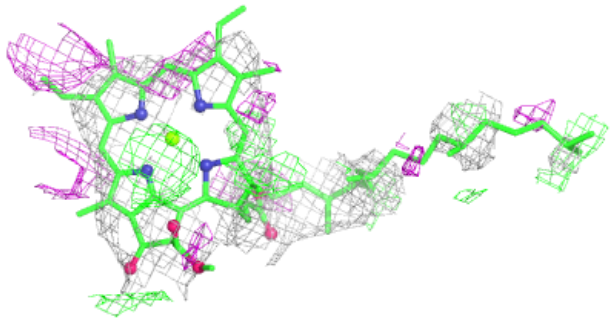
Electron density around CLA C 505:

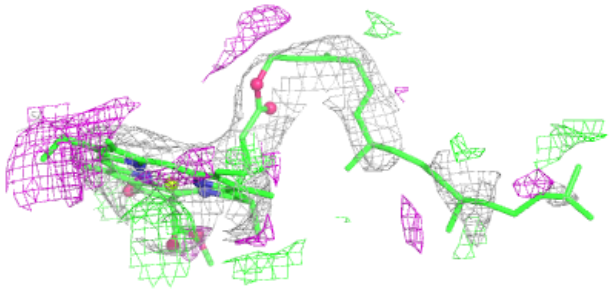
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

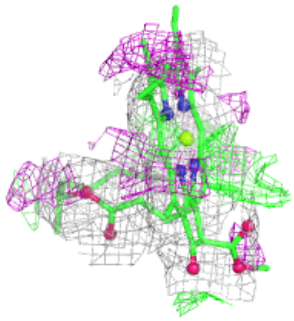


Electron density around CLA a 607:

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

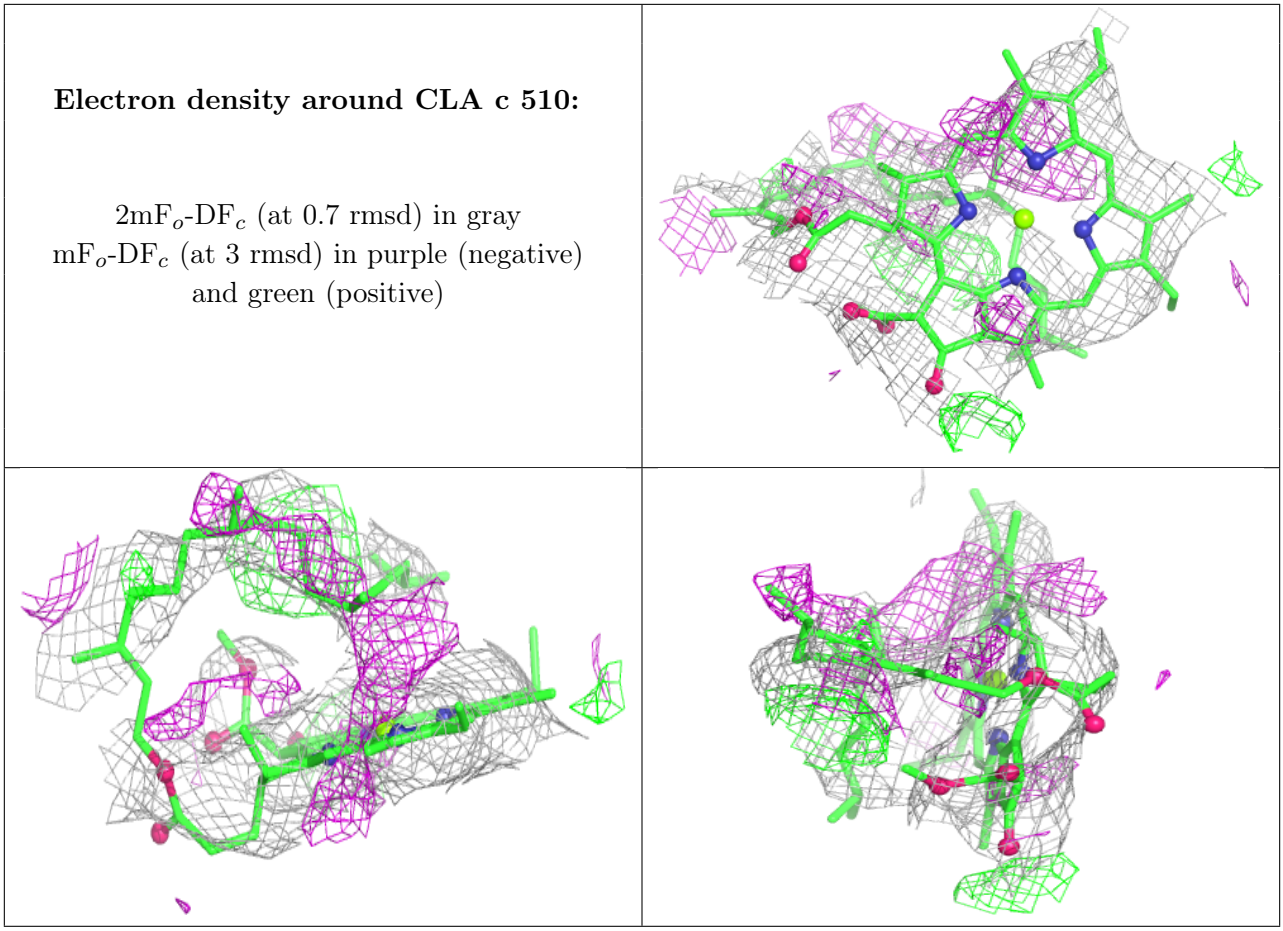






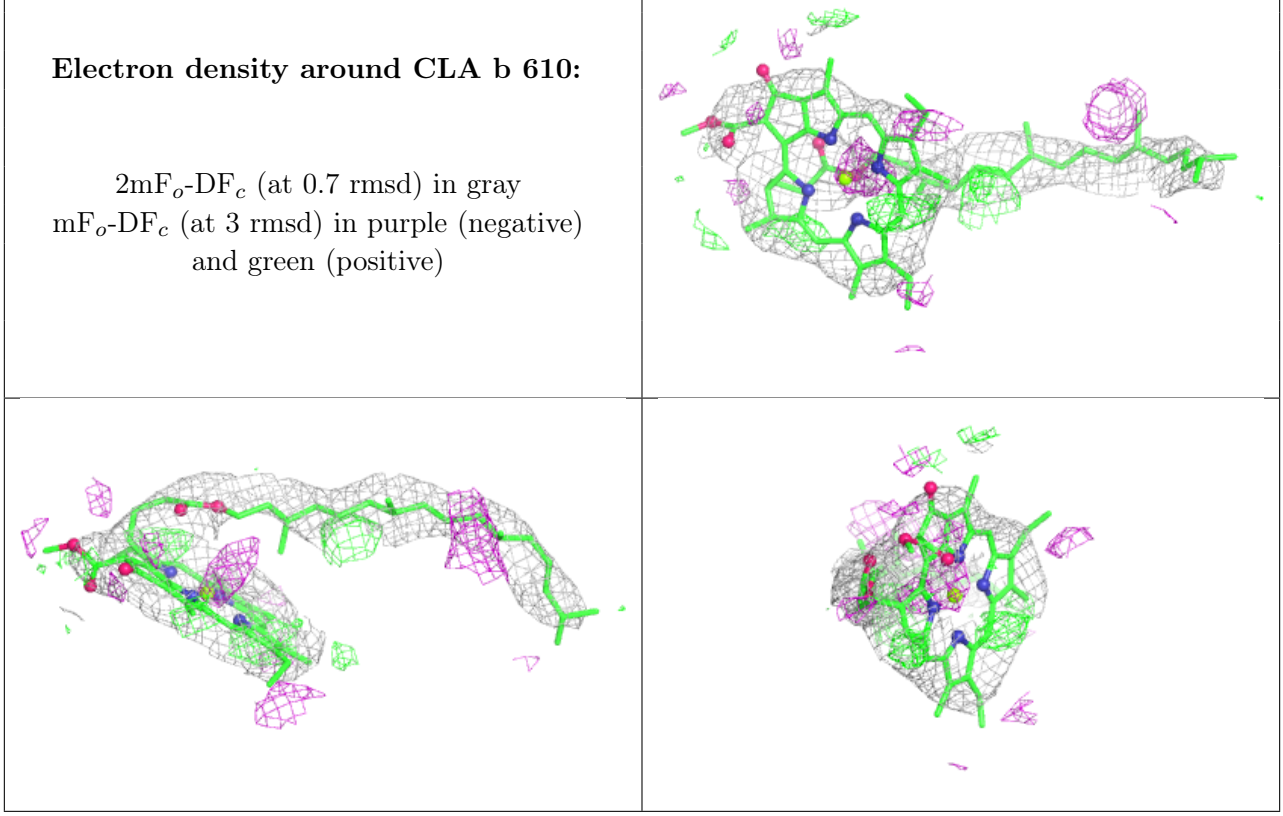
Electron density around CLA c 510:

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



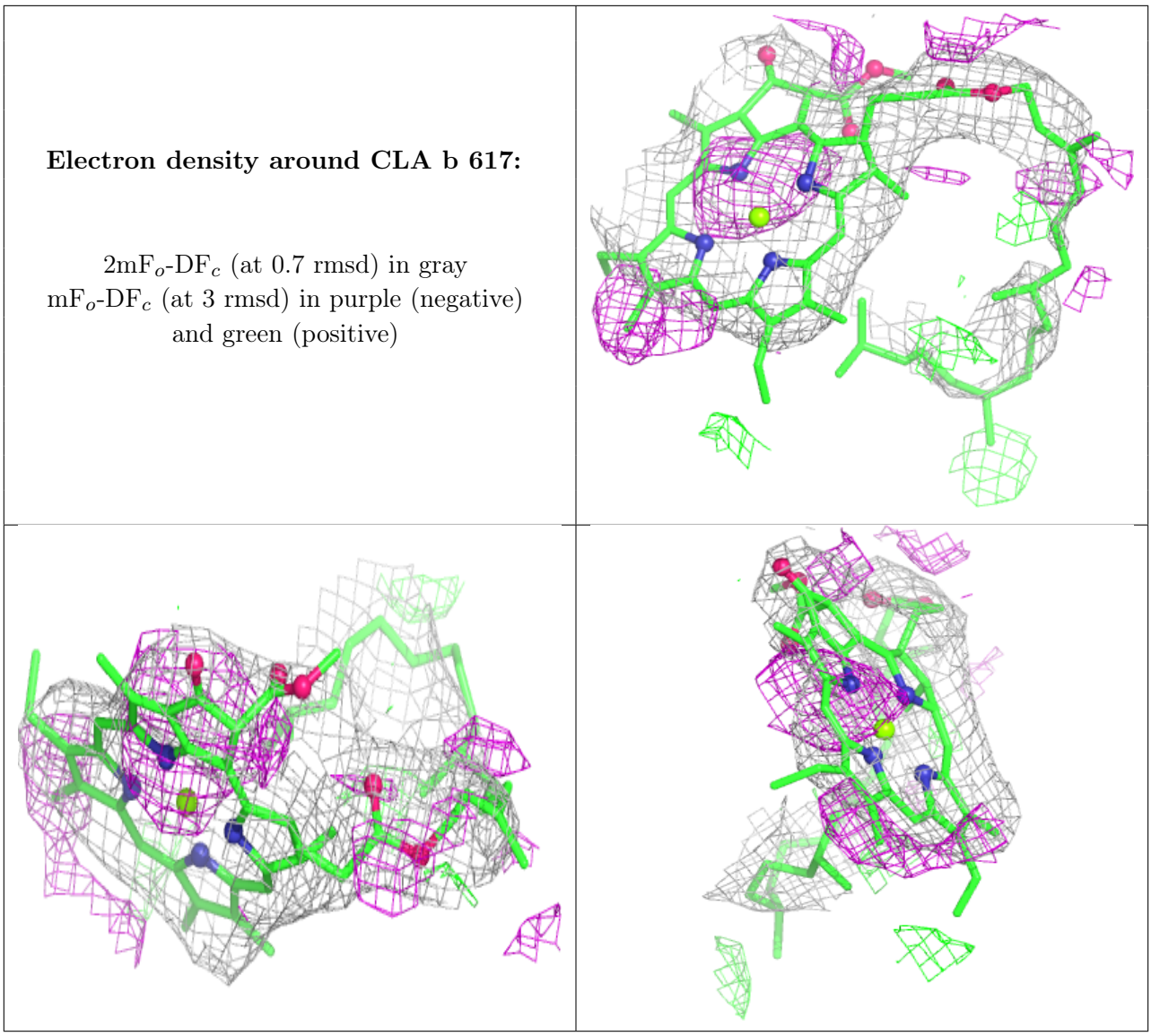
Electron density around CLA b 610:

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



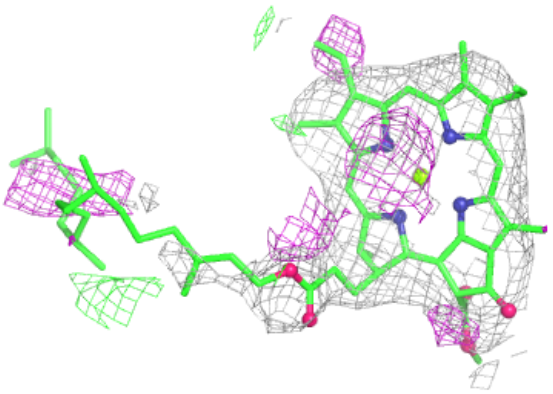
Electron density around CLA b 617:

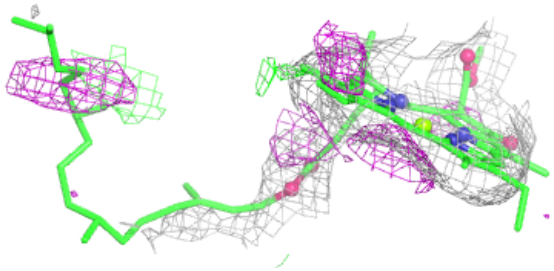
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA a 609:

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

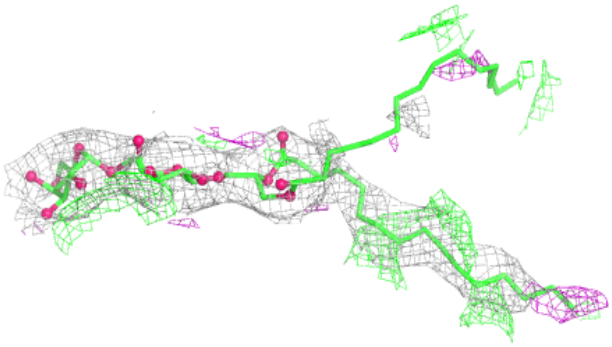


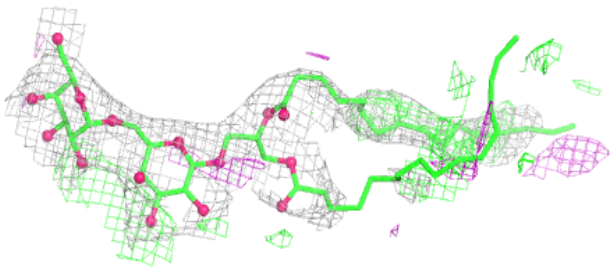


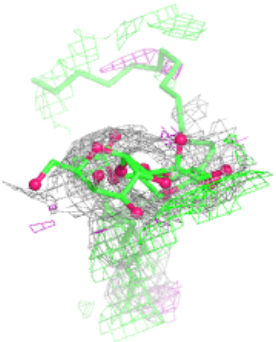


Electron density around DGD C 515:

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

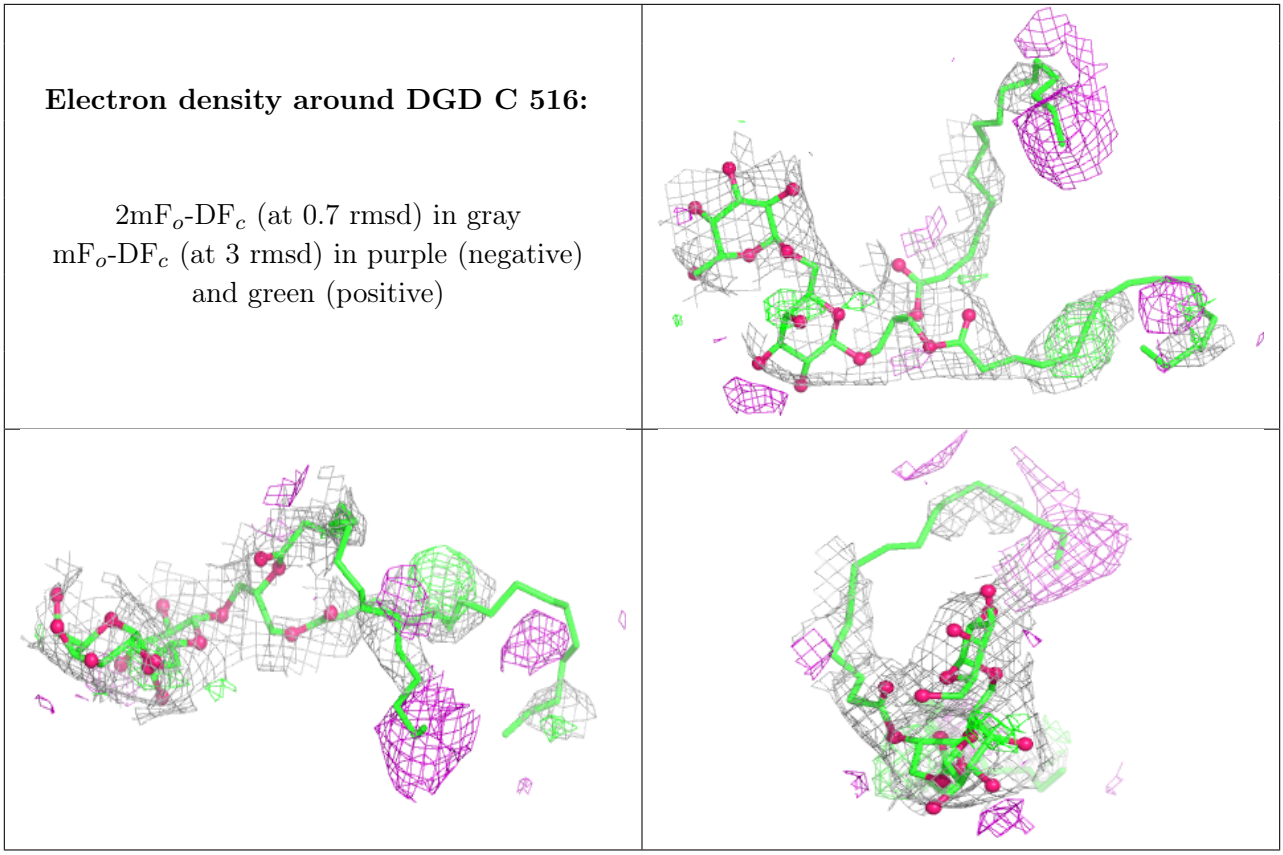






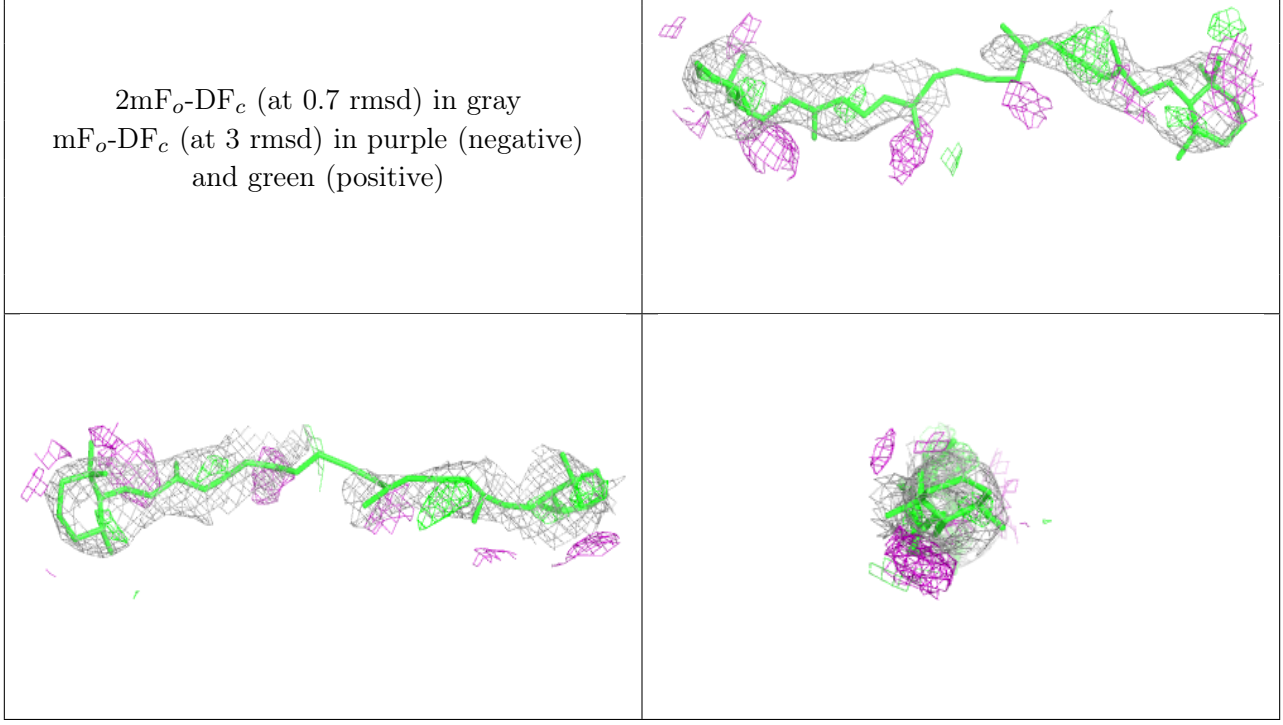
Electron density around DGD C 516:

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



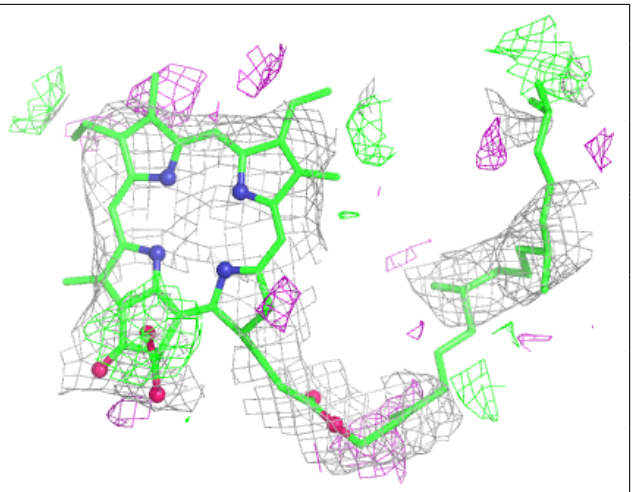
Electron density around BCR b 619:

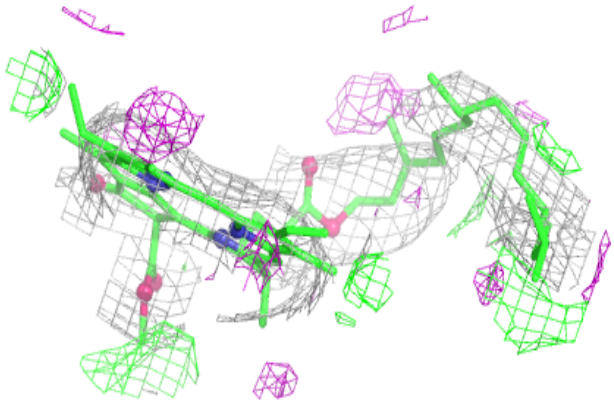
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

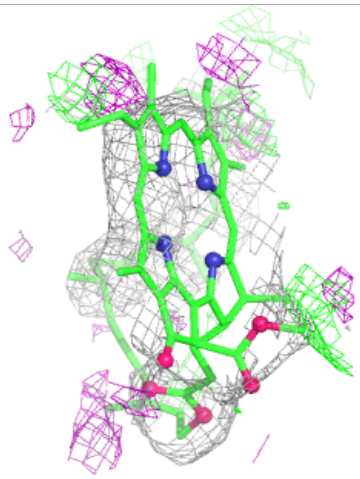


Electron density around PHO d 401:

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

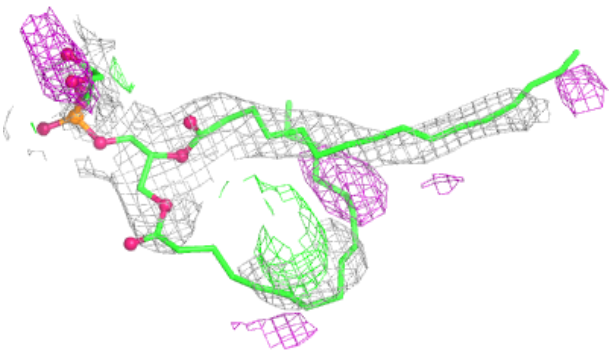


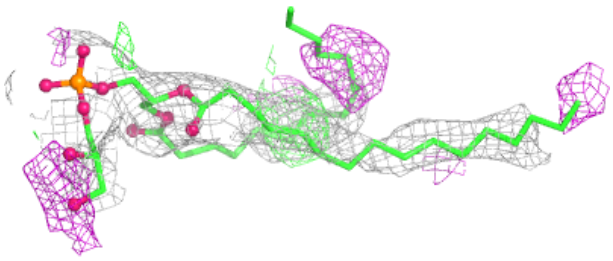


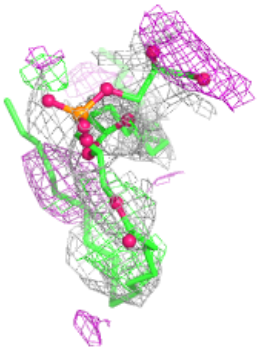


Electron density around LHG D 406:

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

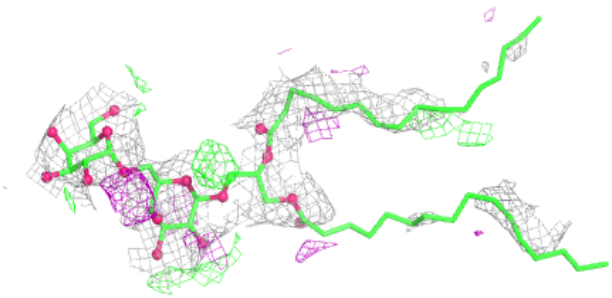


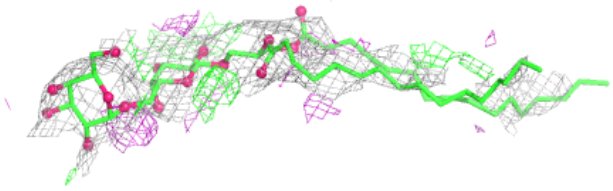


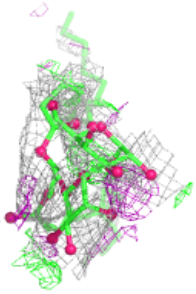


Electron density around DGD c 518:

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

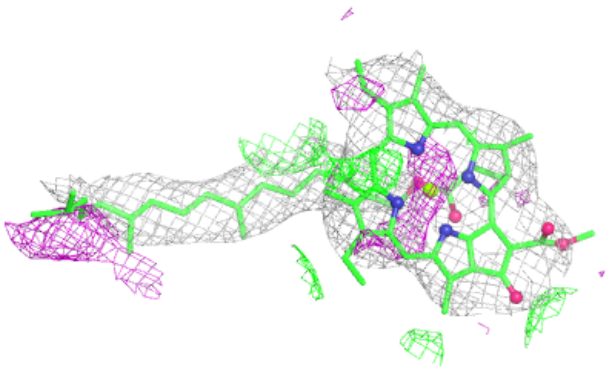


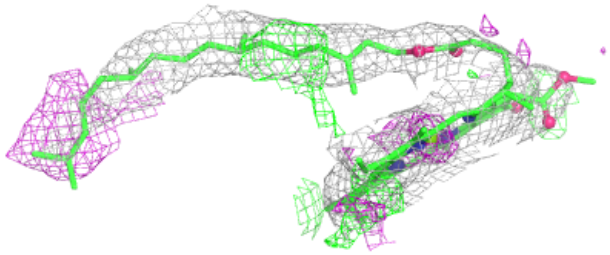


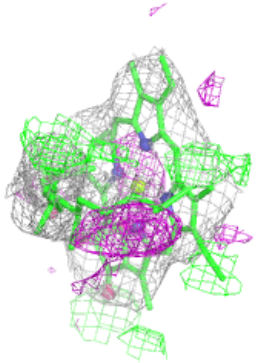


Electron density around CLA B 609:

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

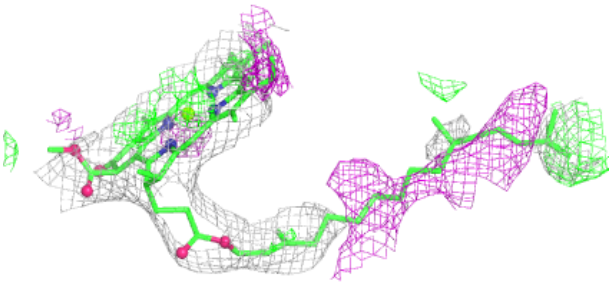


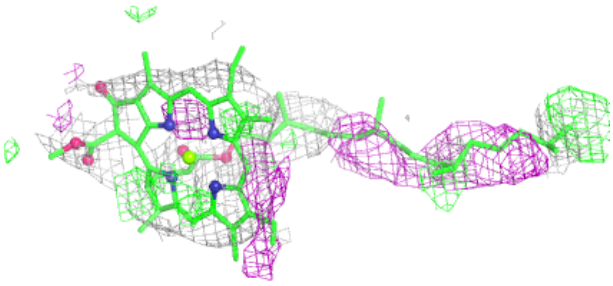


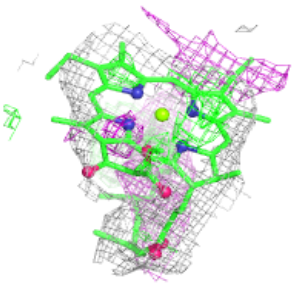


Electron density around CLA C 504:

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

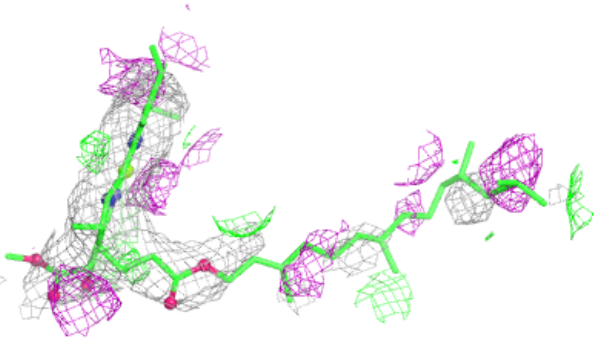


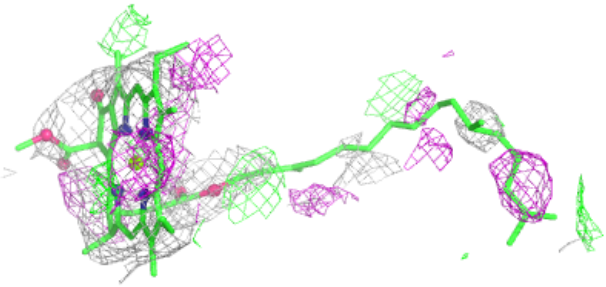


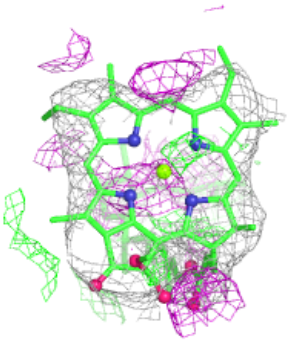


Electron density around CLA b 607:

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

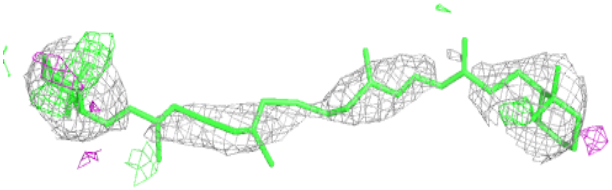


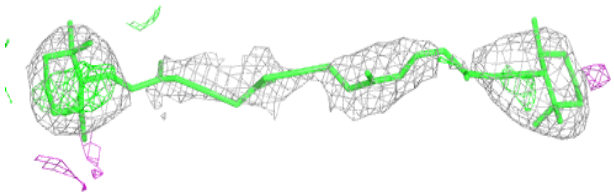


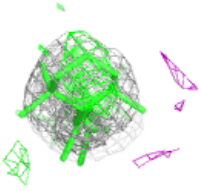


Electron density around BCR a 610:

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

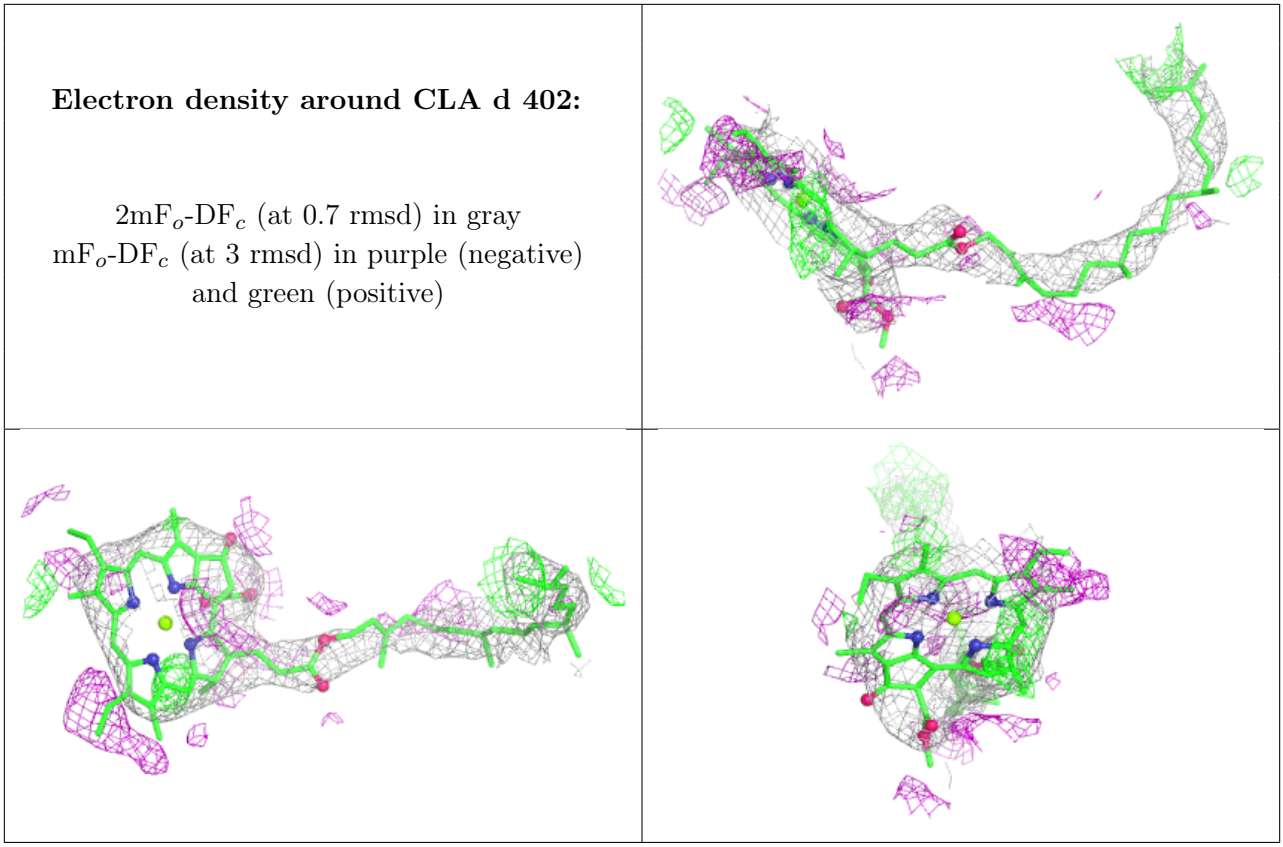






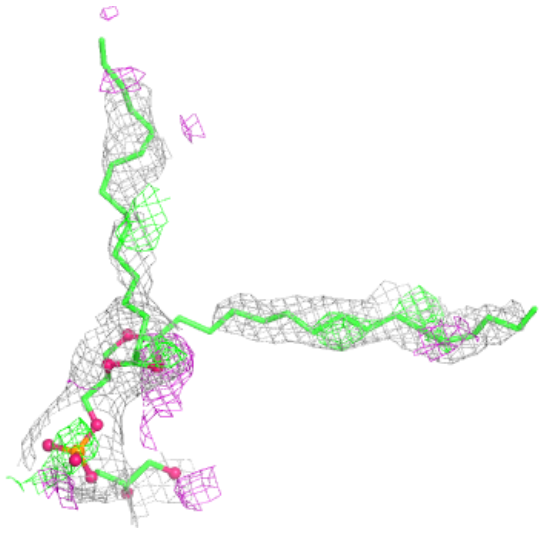
Electron density around CLA d 402:

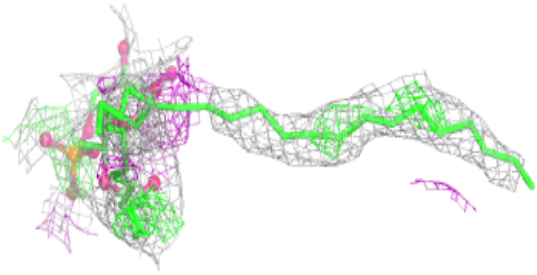
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

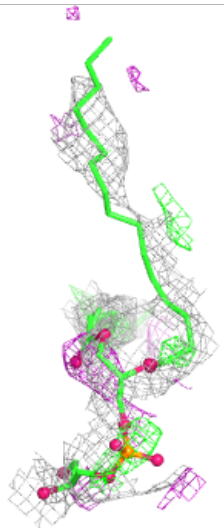


Electron density around LHG l 102:

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

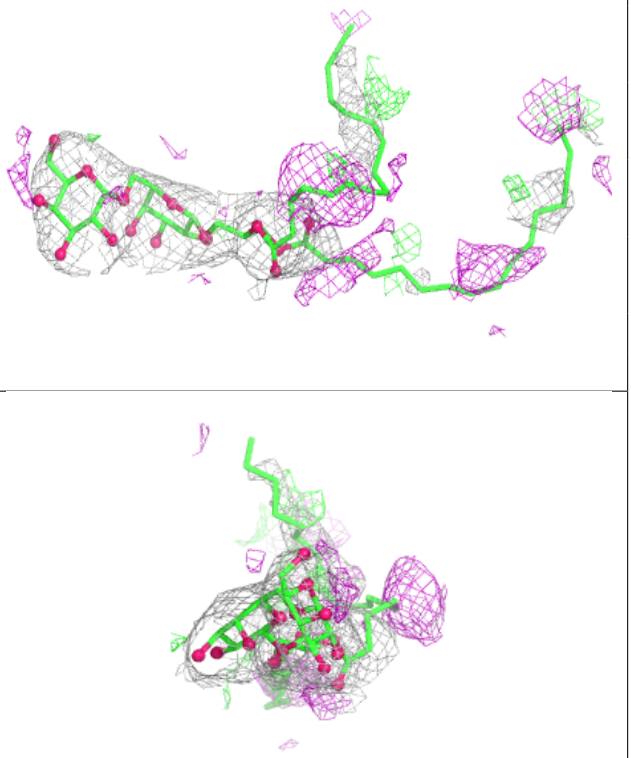


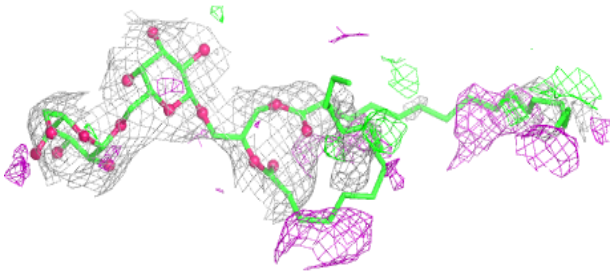




Electron density around DGD H 102:

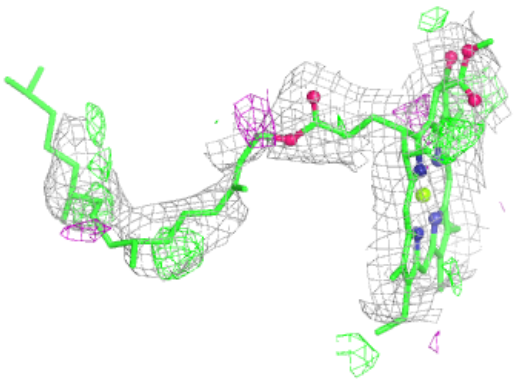
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

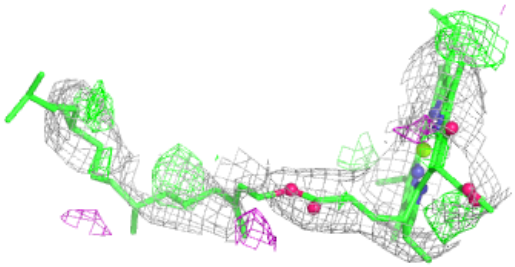


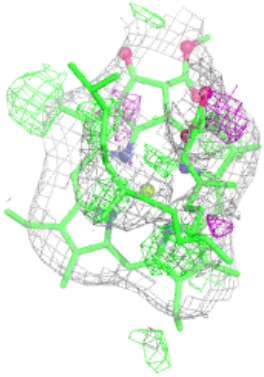


Electron density around CLA d 403:

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

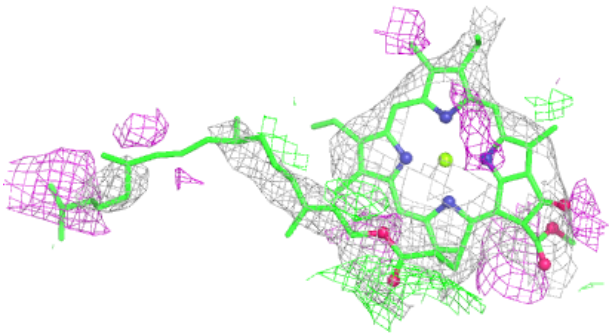


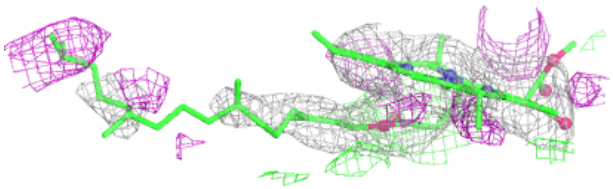


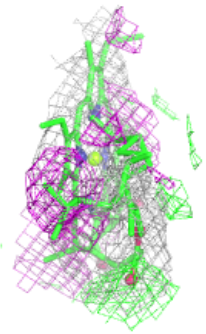


Electron density around CLA b 605:

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

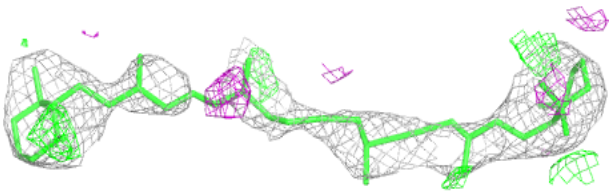


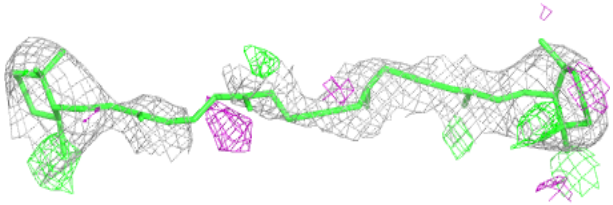


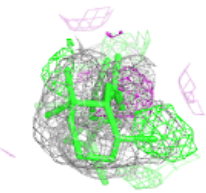


Electron density around BCR A 610:

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

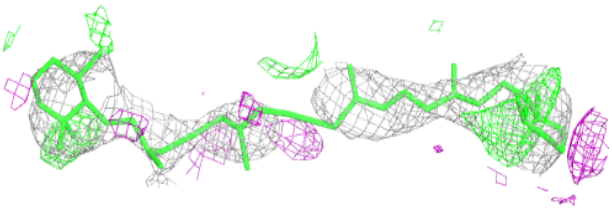


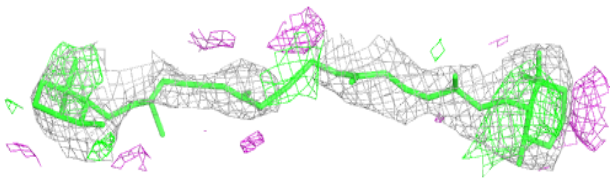


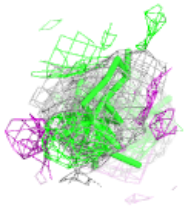


Electron density around BCR B 618:

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

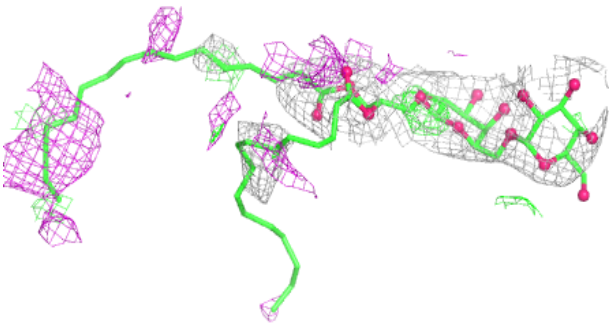


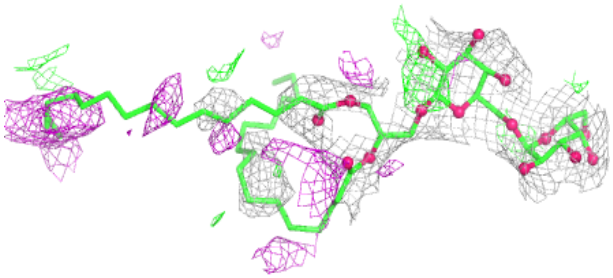


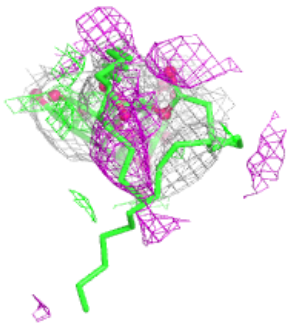


Electron density around DGD h 102:

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

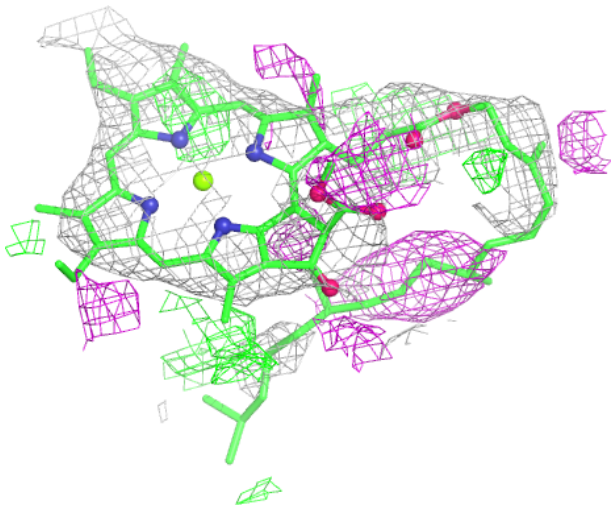


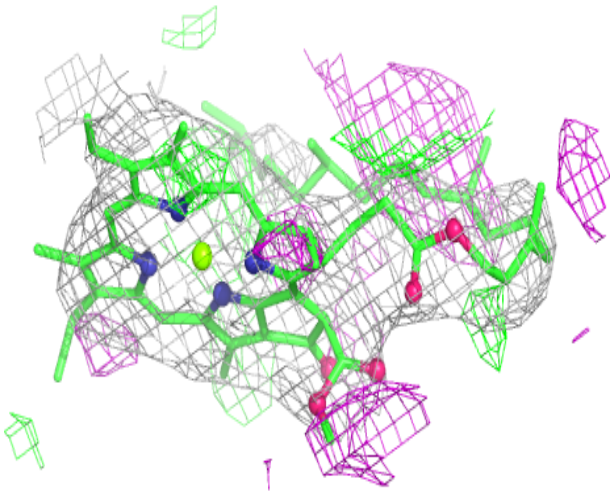


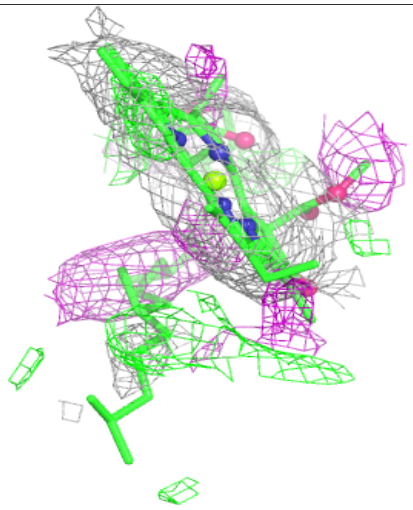


Electron density around CLA C 509:

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

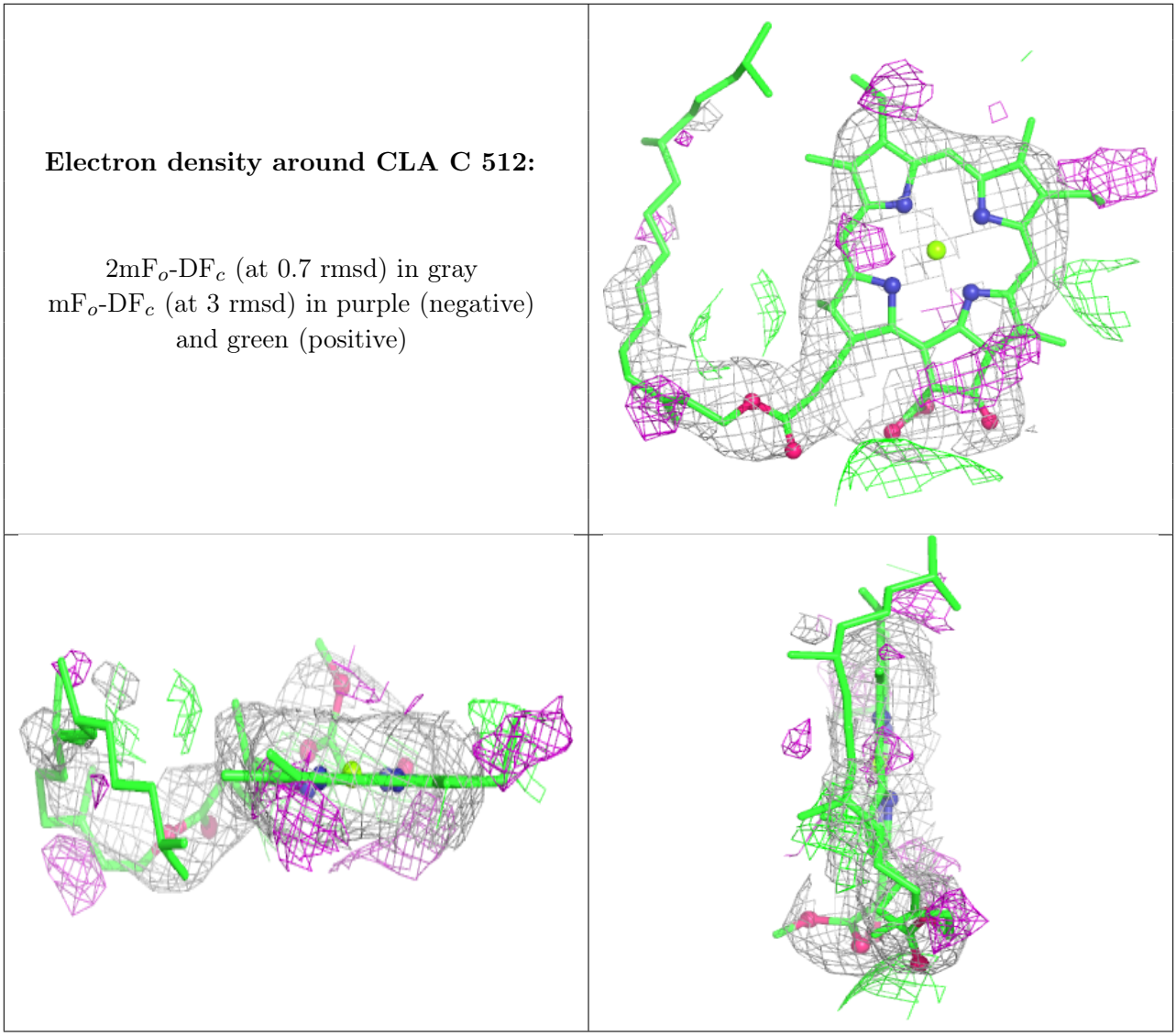






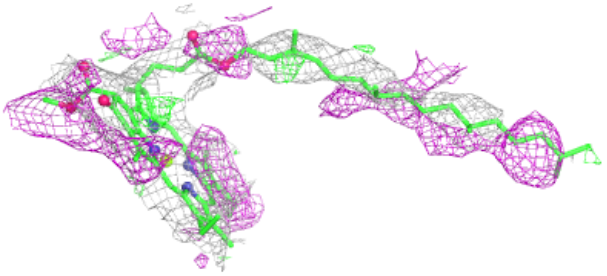
Electron density around CLA C 512:

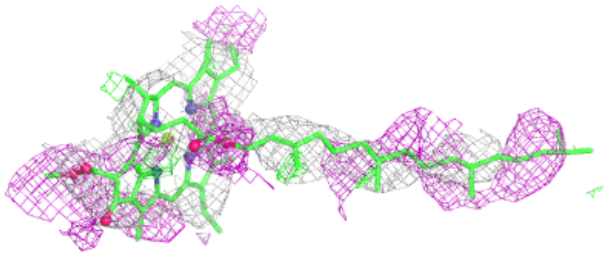
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

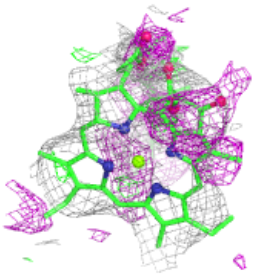


Electron density around CLA B 608:

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

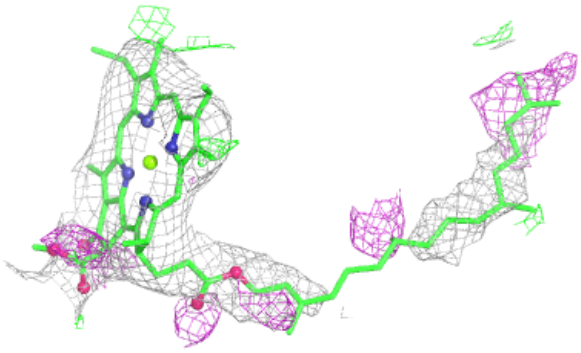


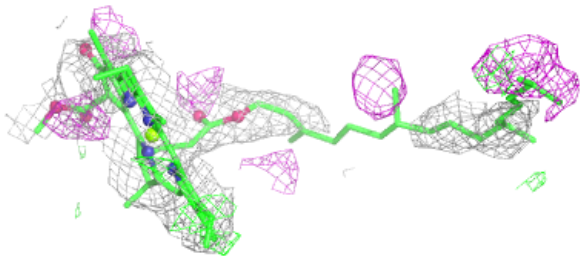


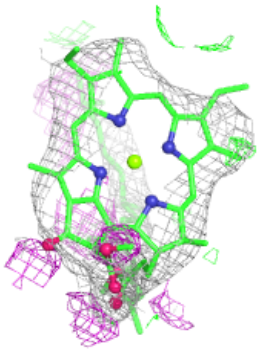


Electron density around CLA b 611:

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

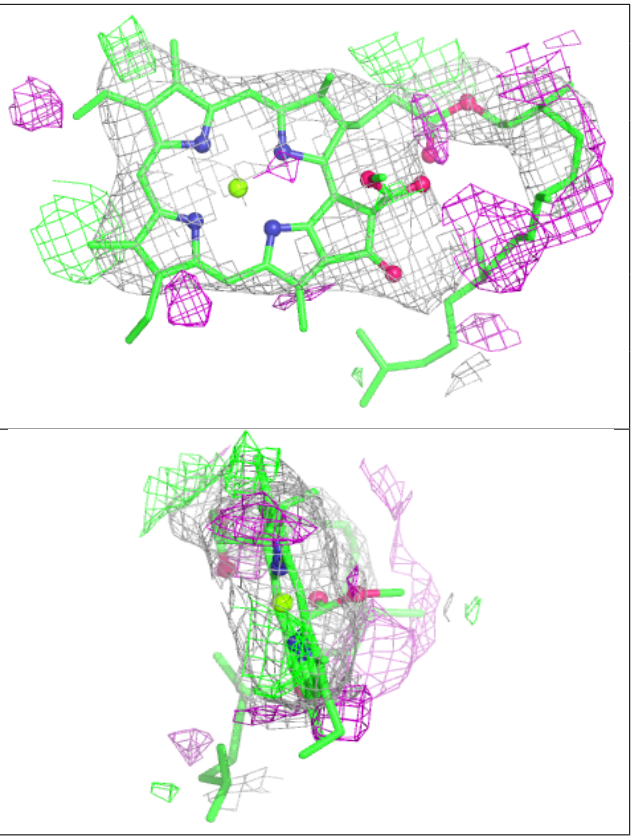


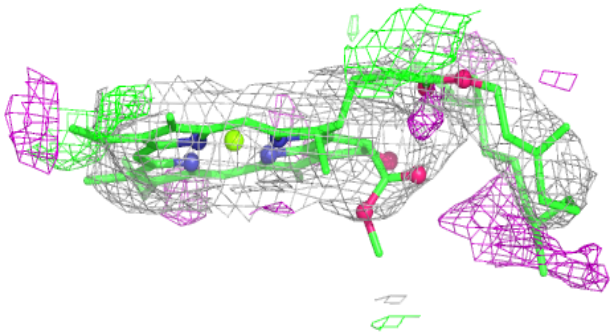




Electron density around CLA b 612:

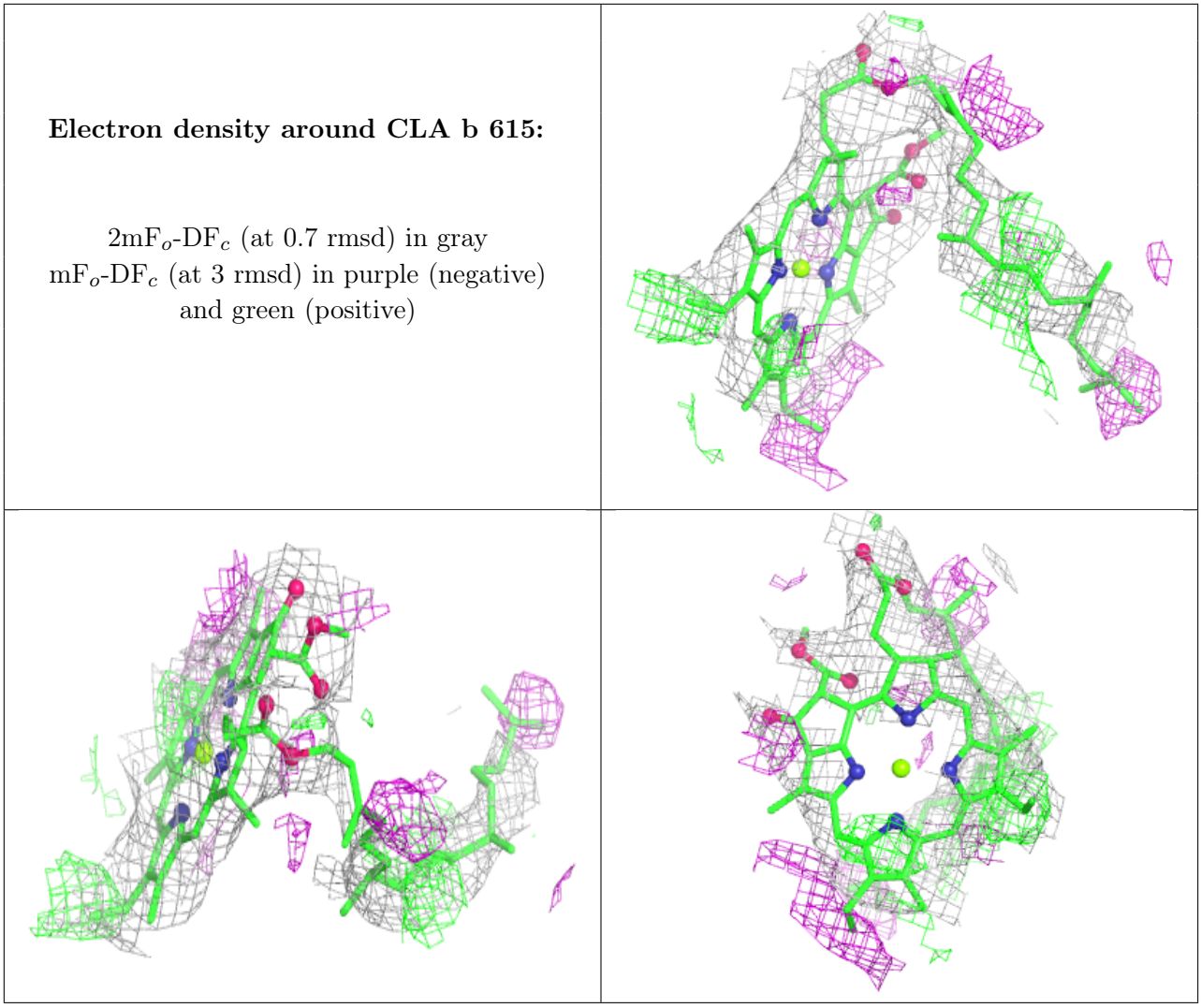
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





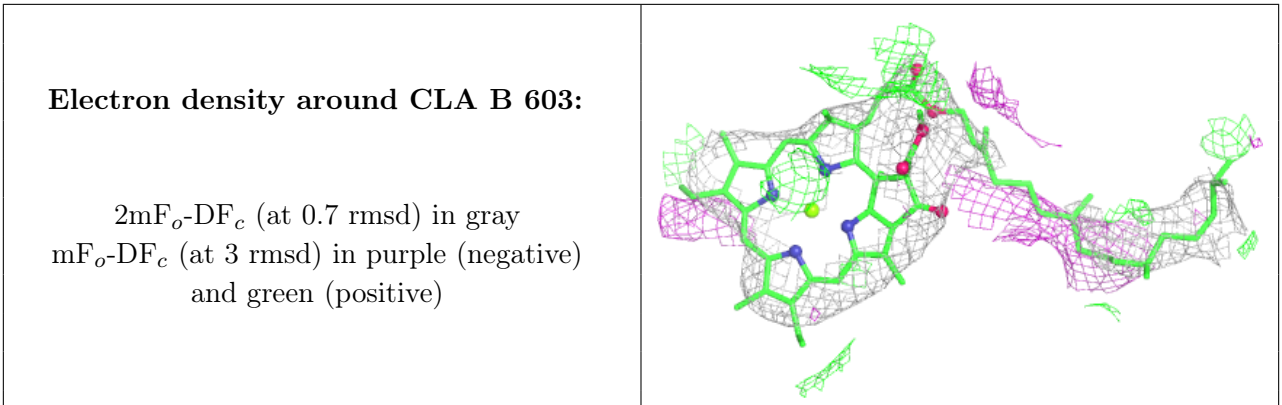
Electron density around CLA b 615:

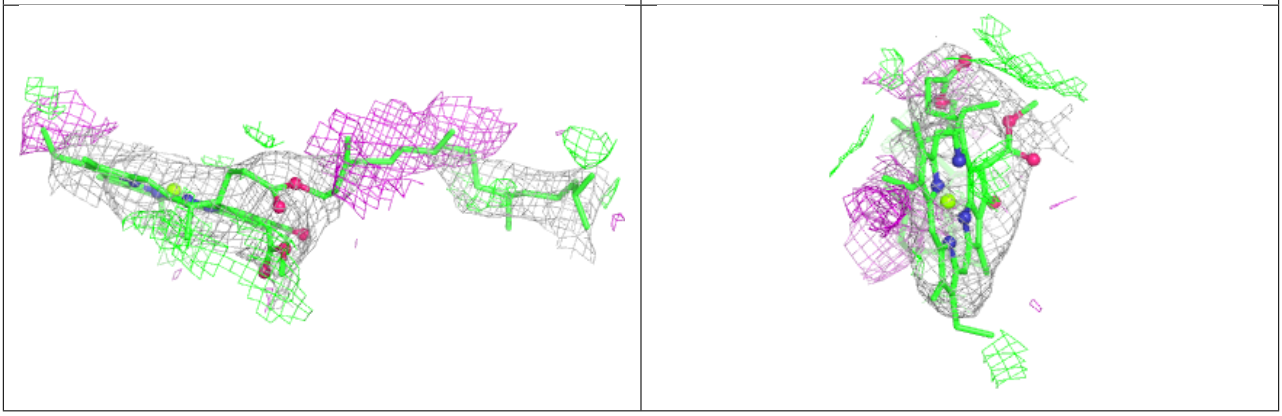
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 603:

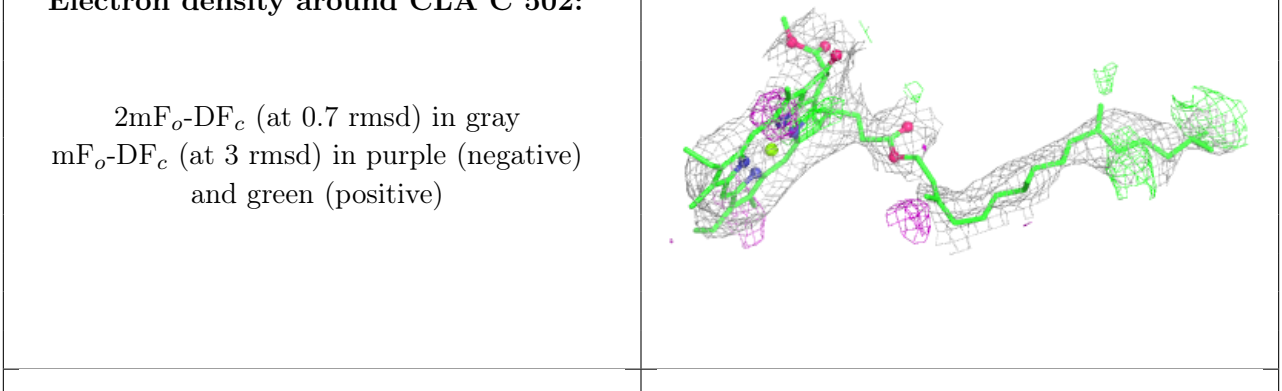
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

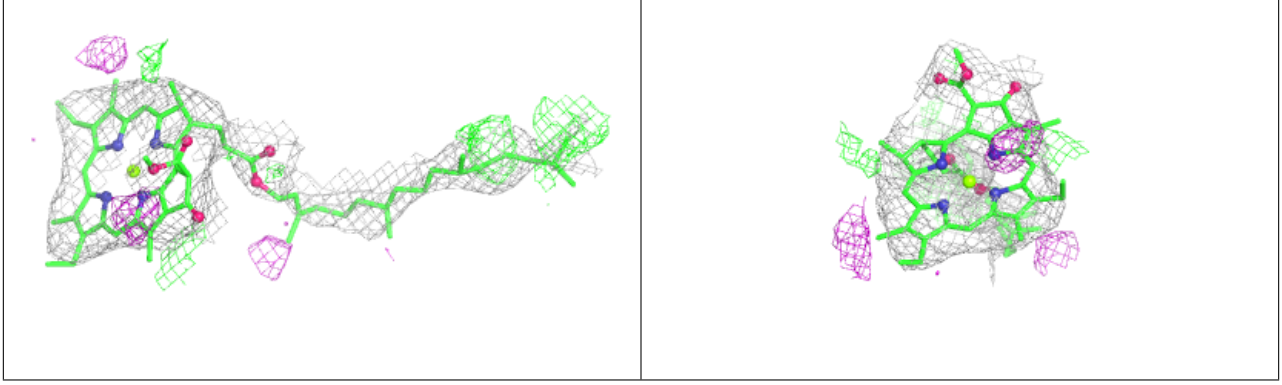




Electron density around CLA C 502:

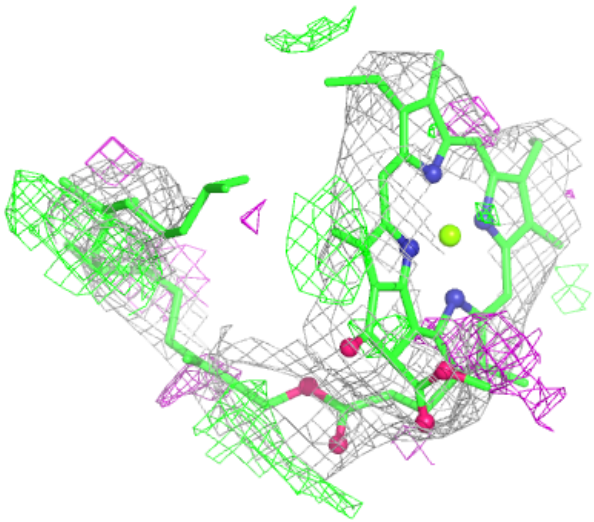
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

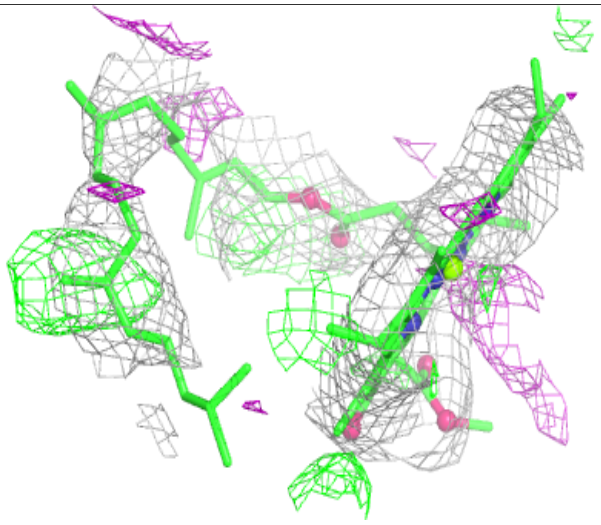


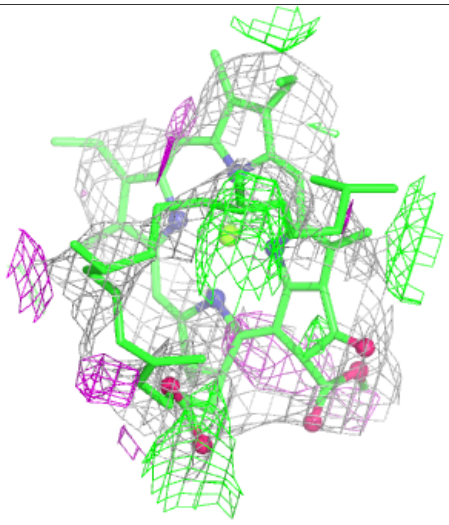


Electron density around CLA C 503:

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

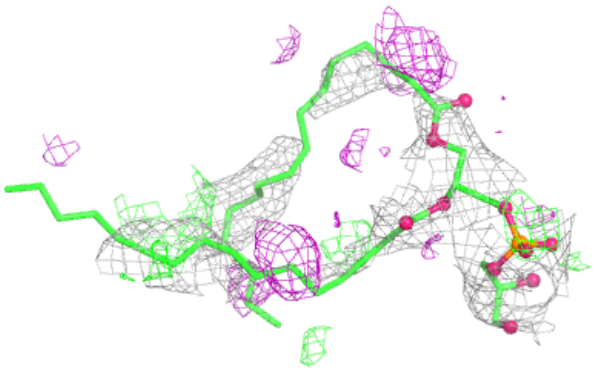


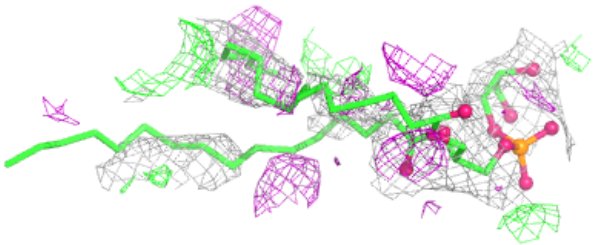


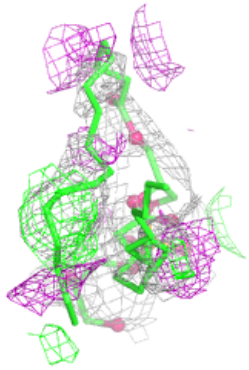


Electron density around LHG A 615:

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

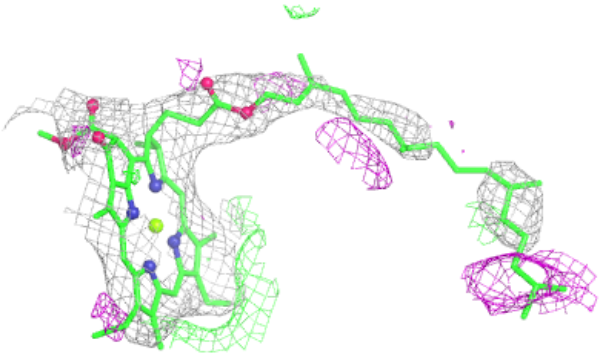


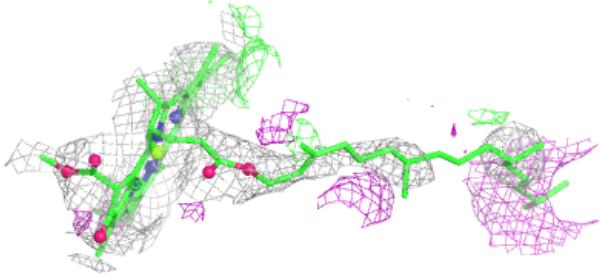


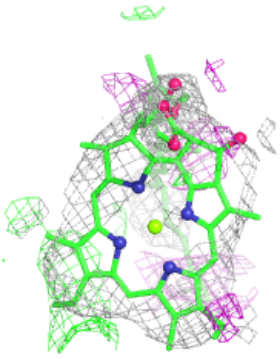


Electron density around CLA B 610:

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

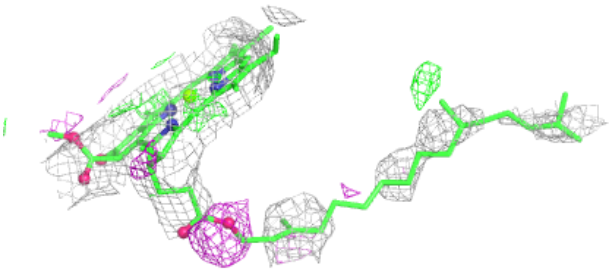


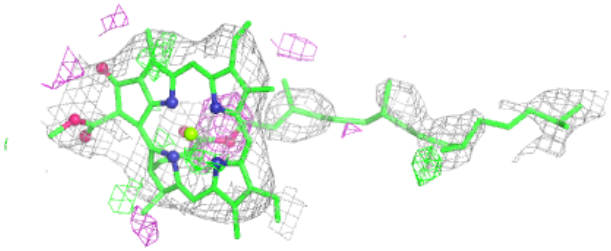


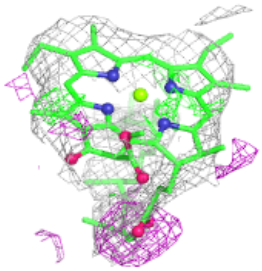


Electron density around CLA c 504:

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

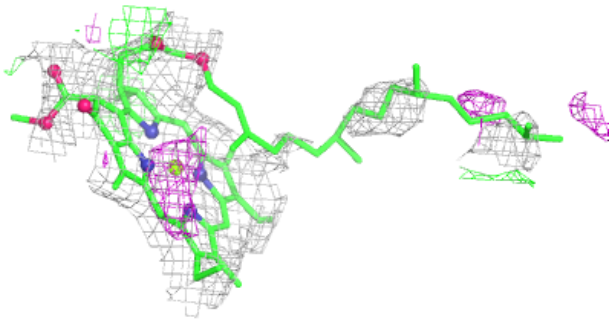


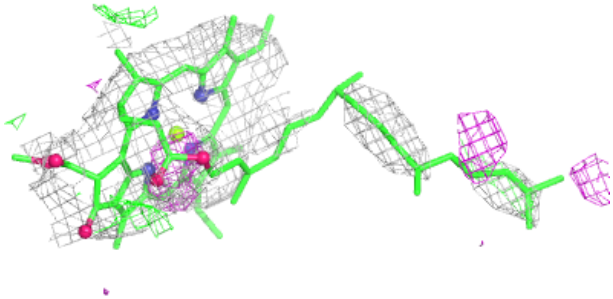


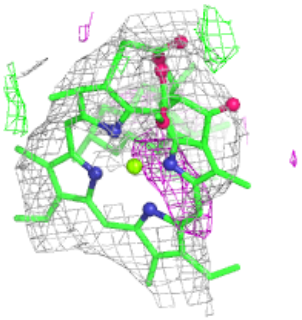


Electron density around CLA c 505:

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

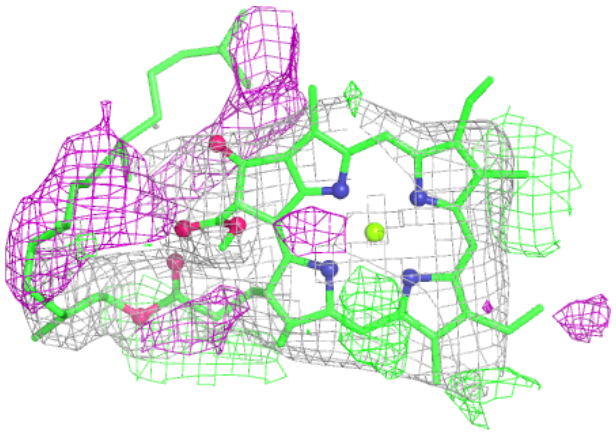


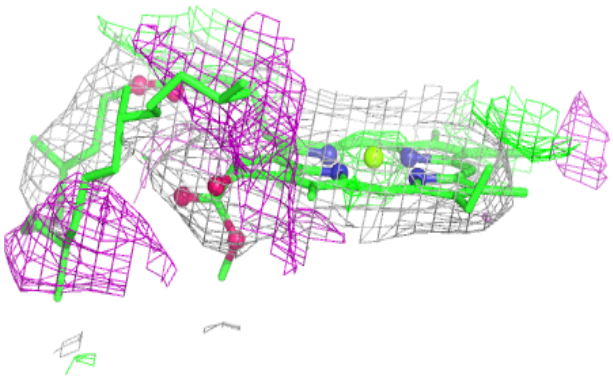


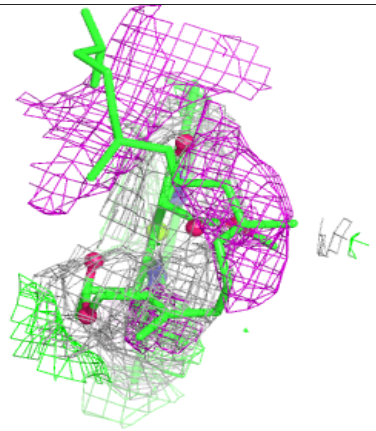


Electron density around CLA B 611:

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

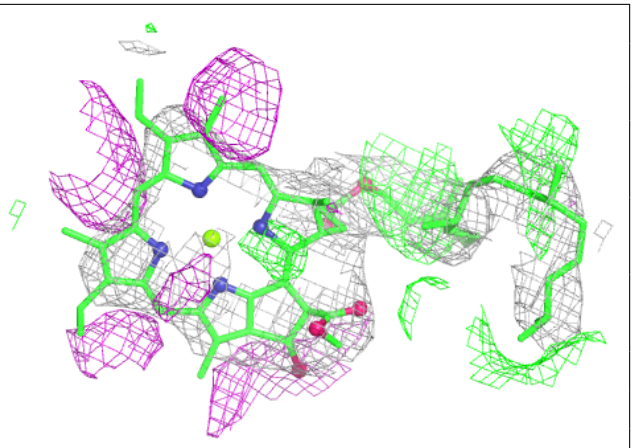


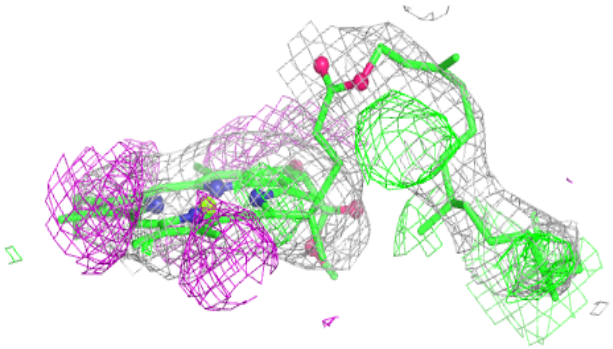


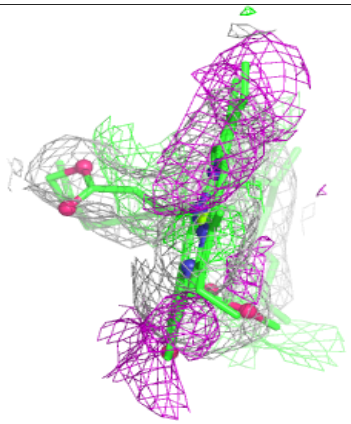


Electron density around CLA B 613:

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

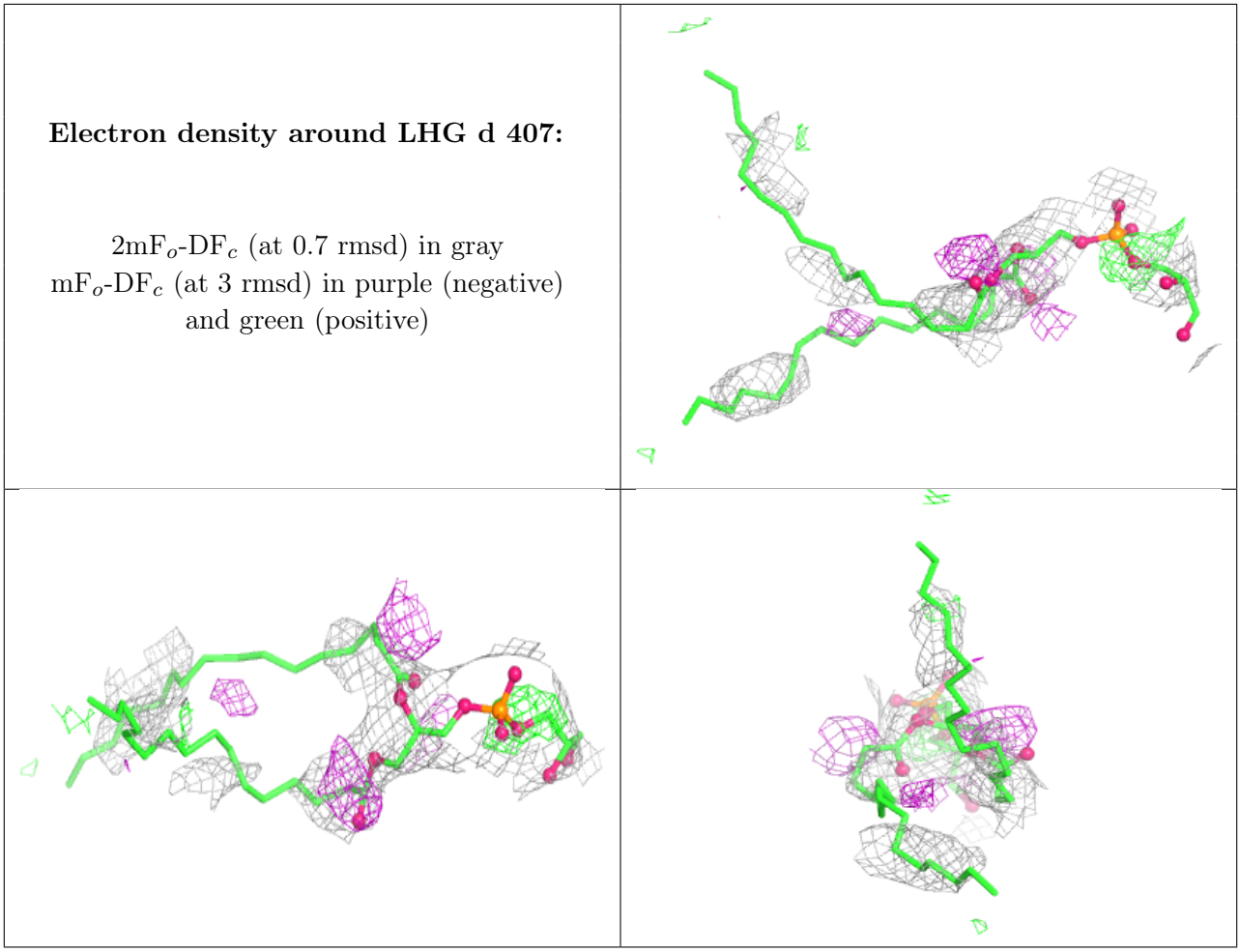






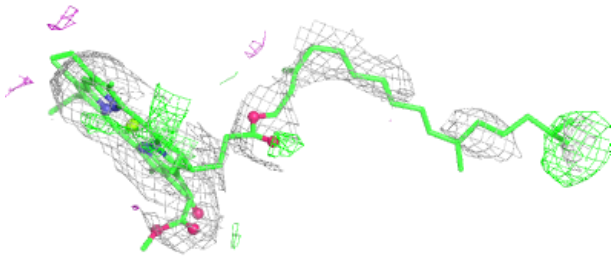
Electron density around LHG d 407:

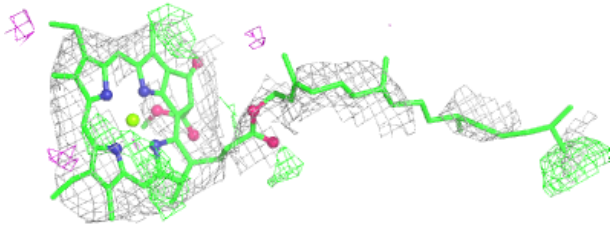
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

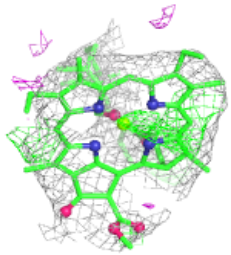


Electron density around CLA c 502:

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

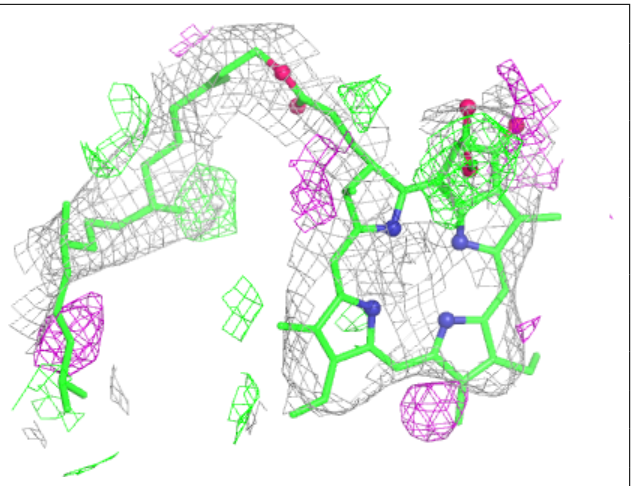


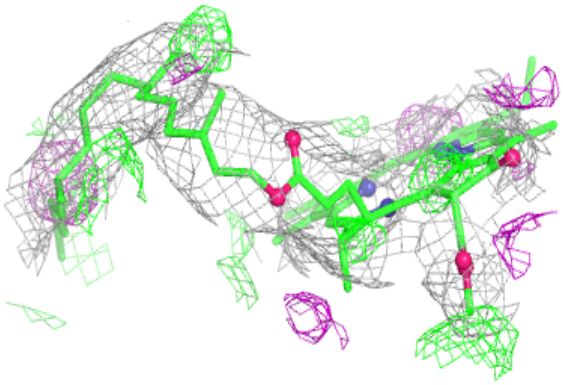


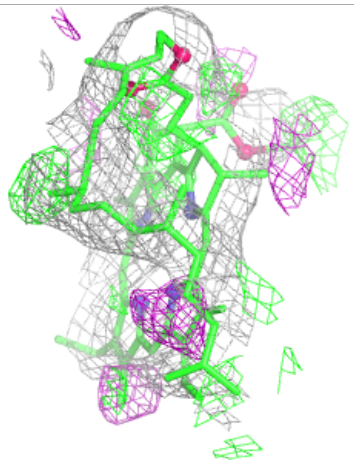


Electron density around PHO D 401:

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

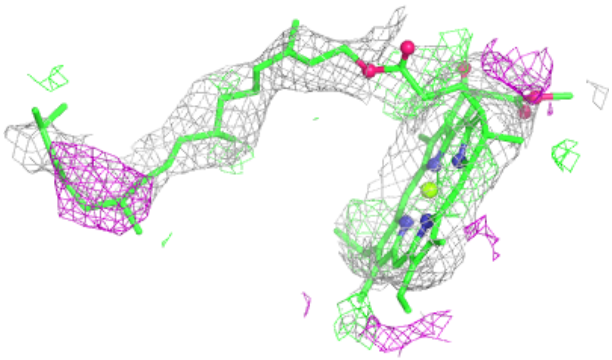


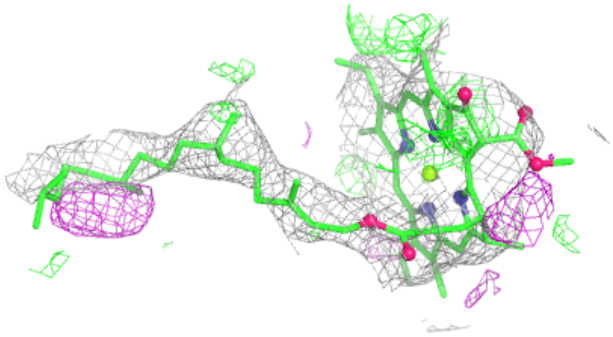


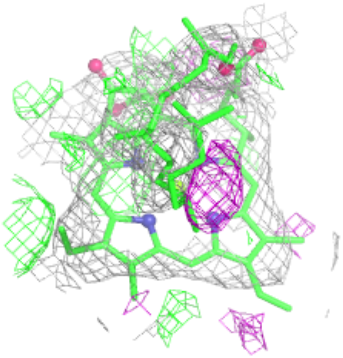


Electron density around CLA C 508:

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

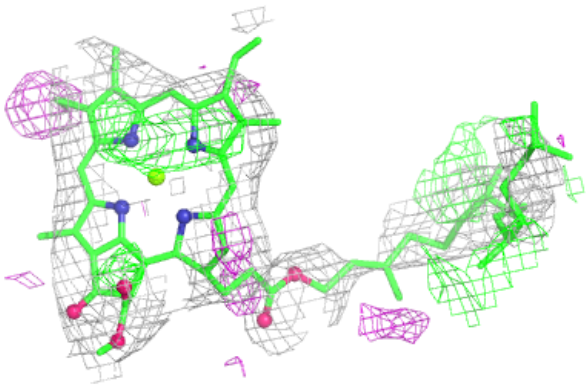


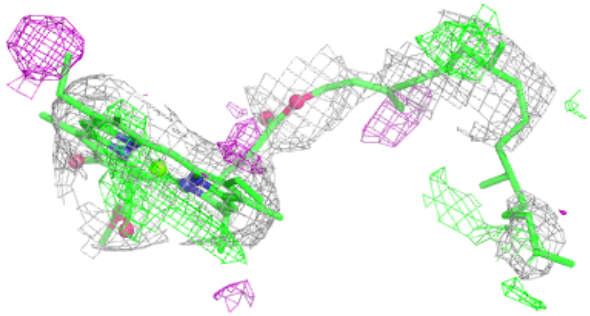


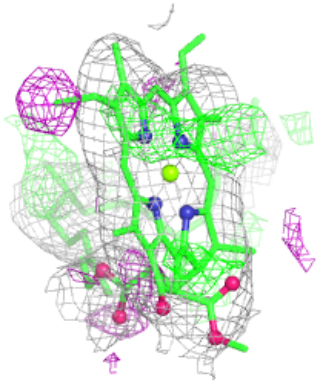


Electron density around CLA A 609:

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

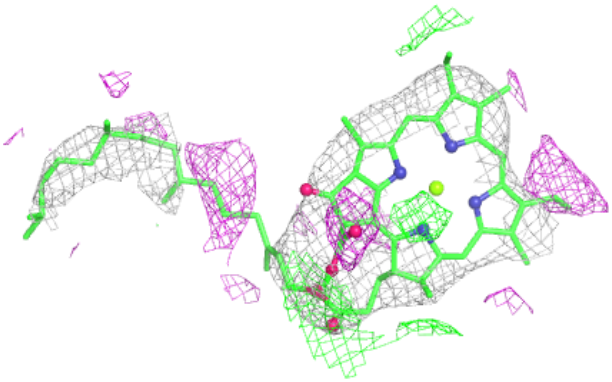


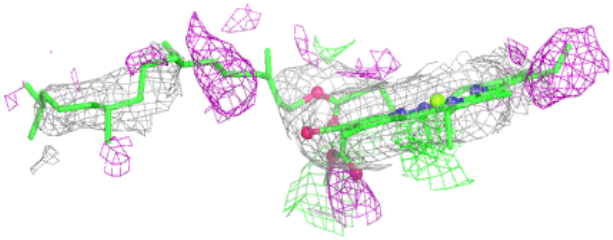


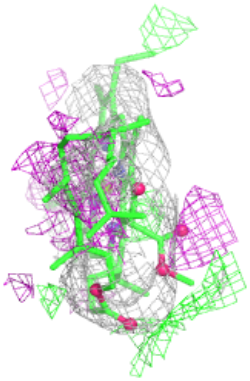


Electron density around CLA b 604:

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

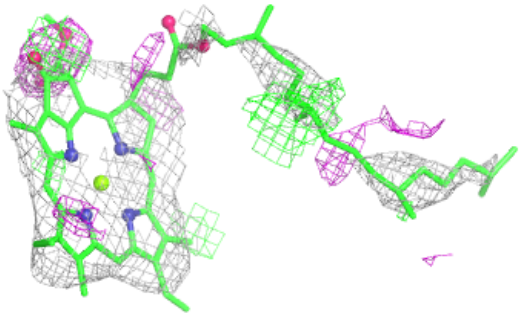


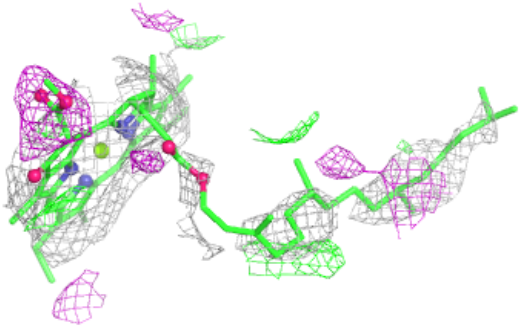


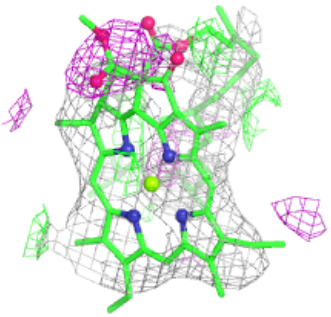


Electron density around CLA C 511:

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

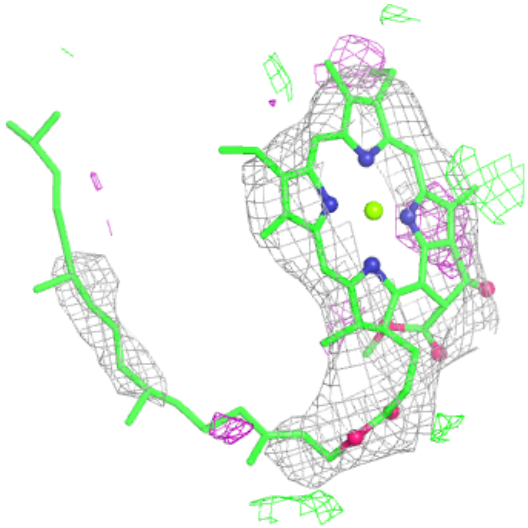


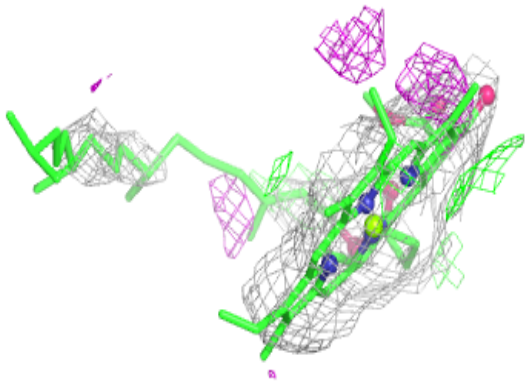


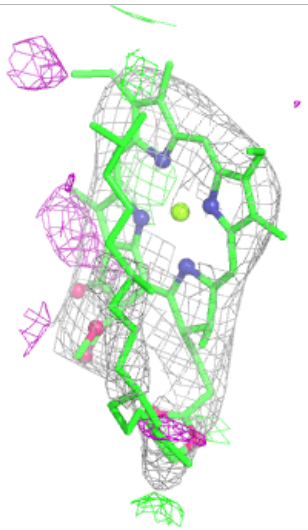


Electron density around CLA c 507:

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

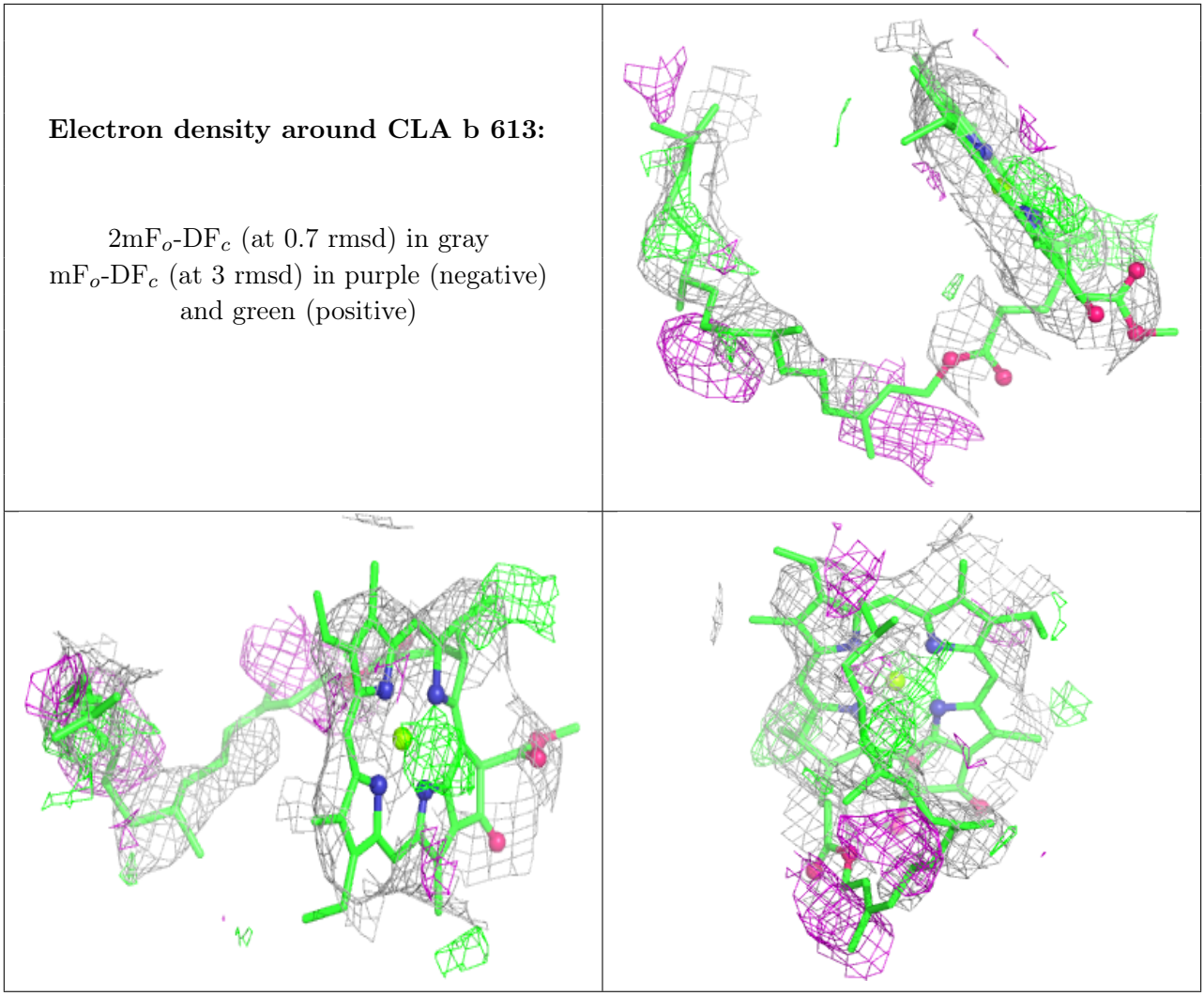






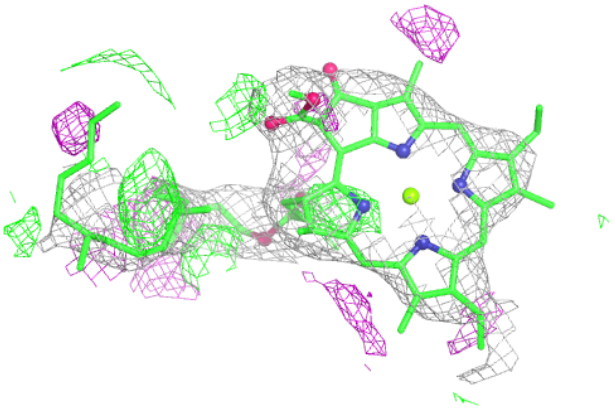
Electron density around CLA b 613:

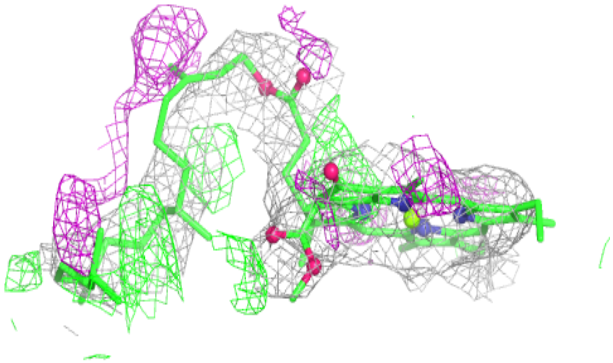
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

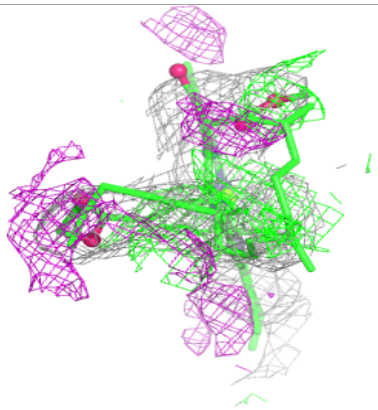


Electron density around CLA b 614:

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

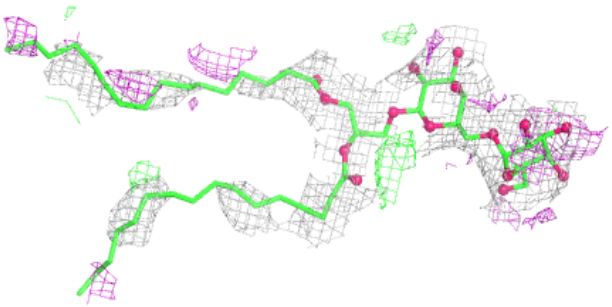


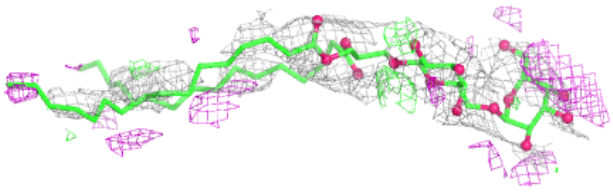


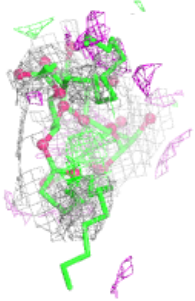


Electron density around DGD C 517:

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

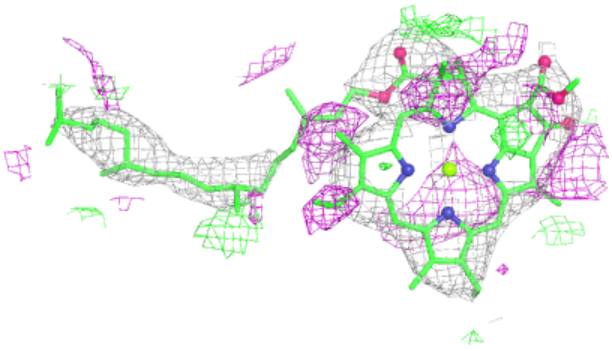


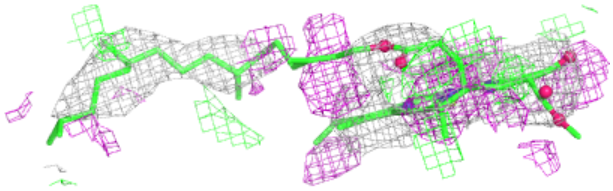


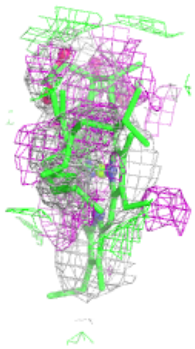


Electron density around CLA B 604:

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

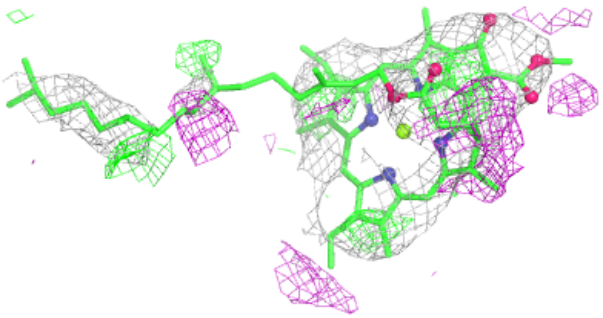


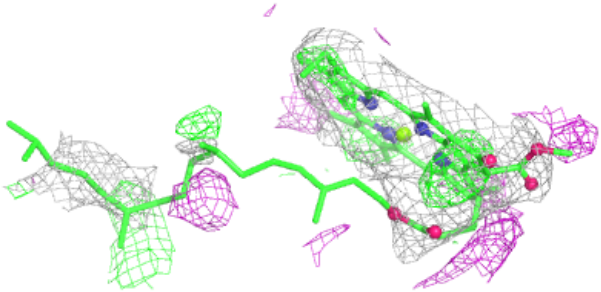


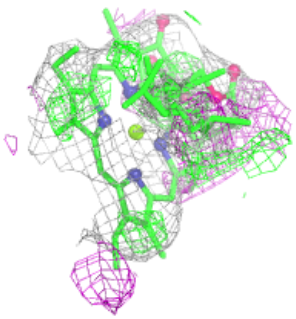


Electron density around CLA b 616:

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

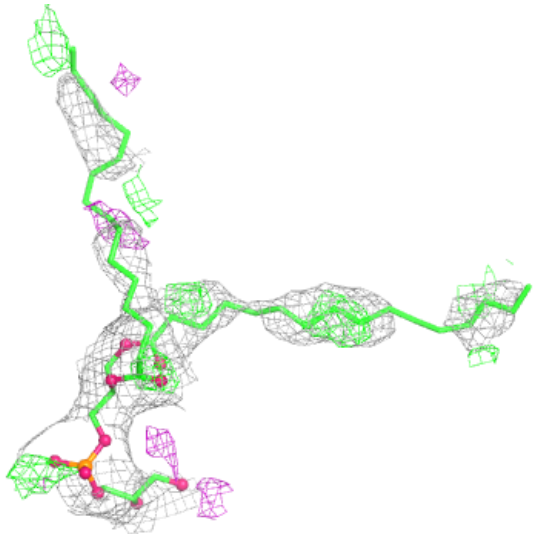


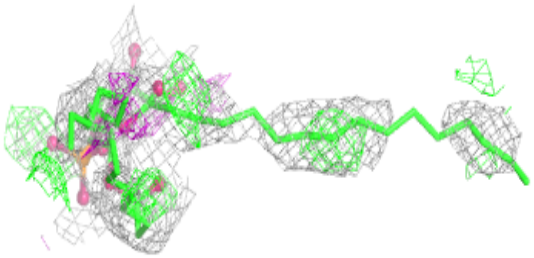


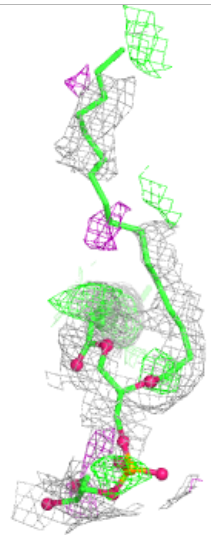


Electron density around LHG L 101:

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

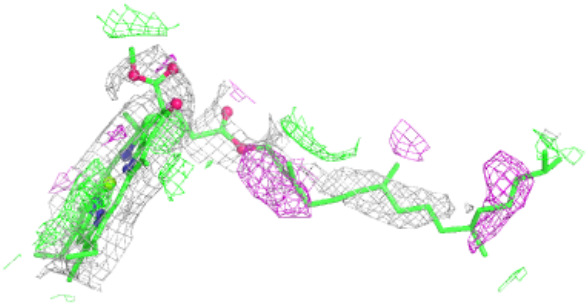


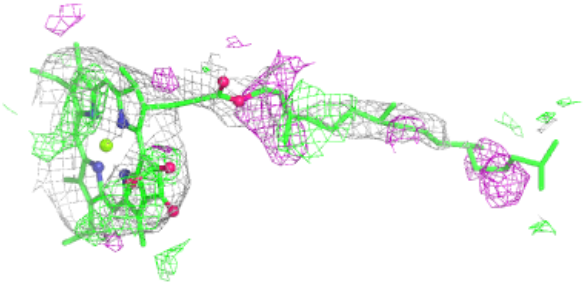


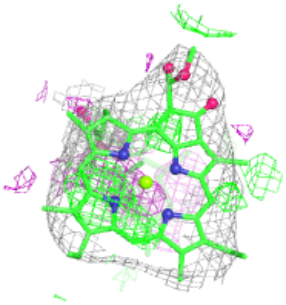


Electron density around CLA B 605:

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

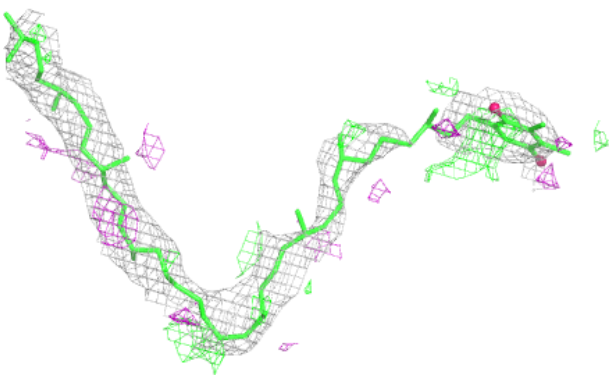


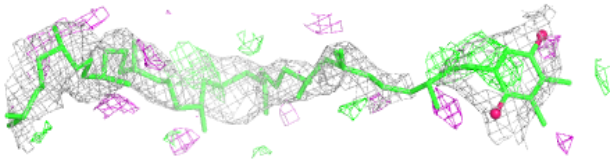


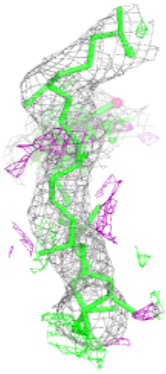


Electron density around PL9 D 405:

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

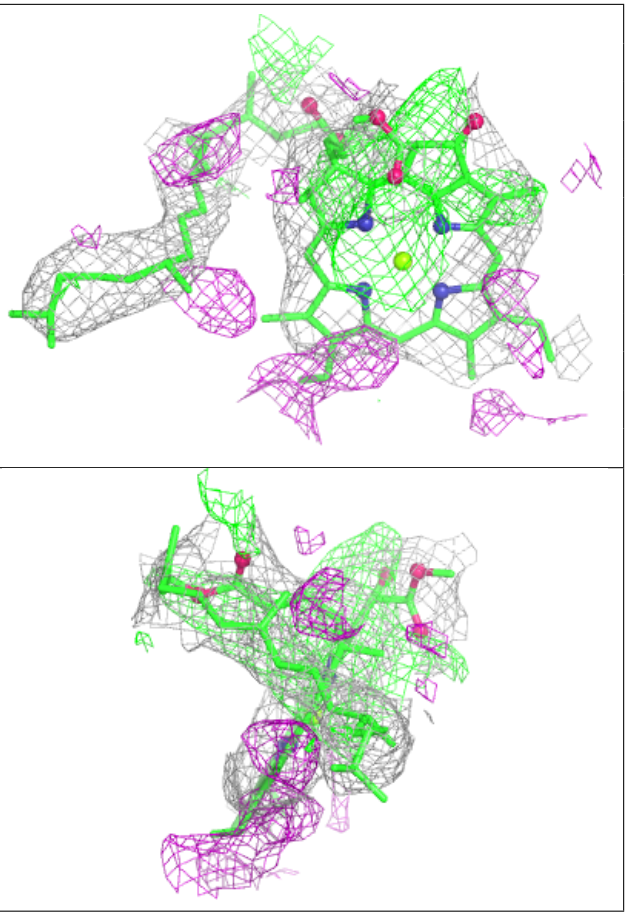






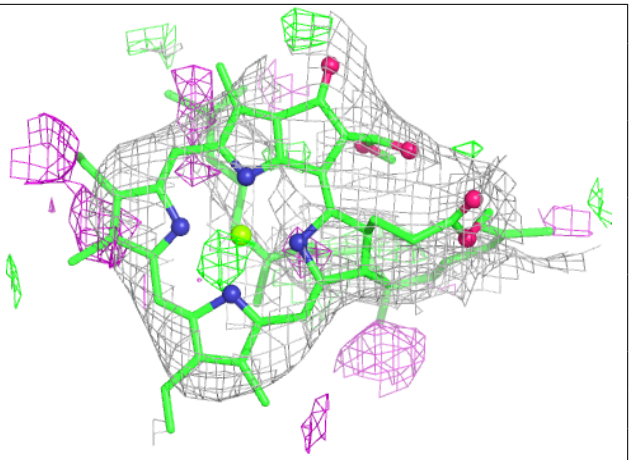
Electron density around CLA D 402:

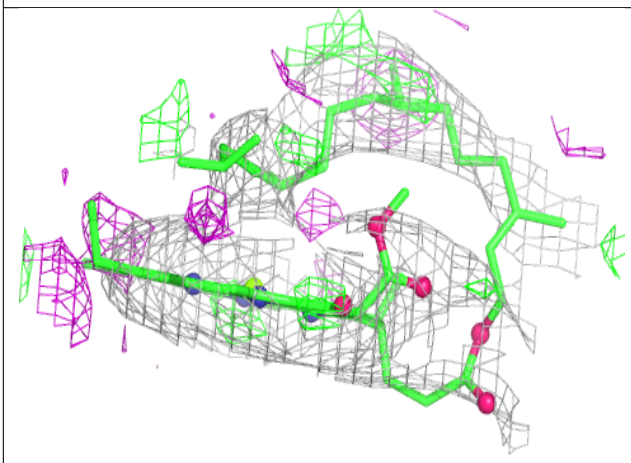
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

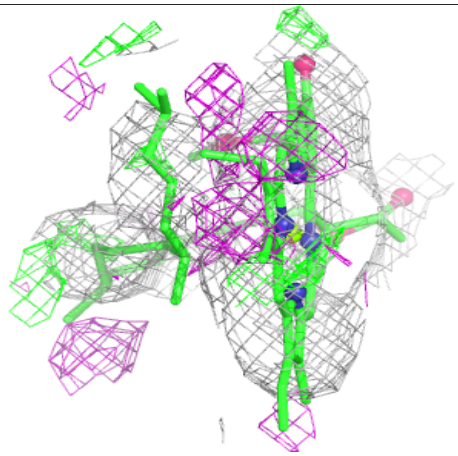


Electron density around CLA C 510:

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

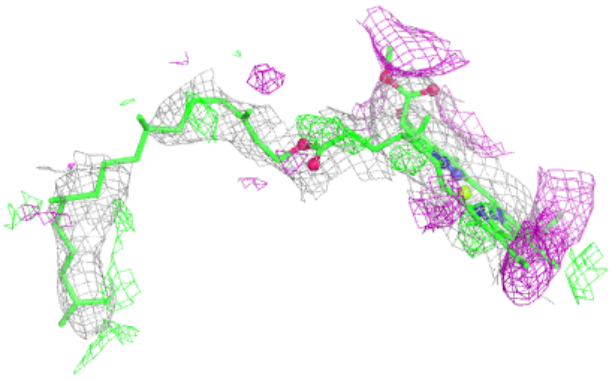


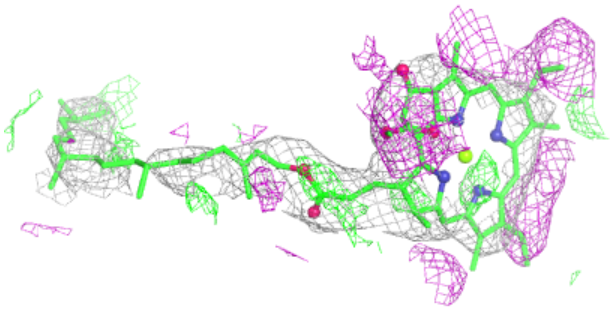




Electron density around CLA D 403:

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

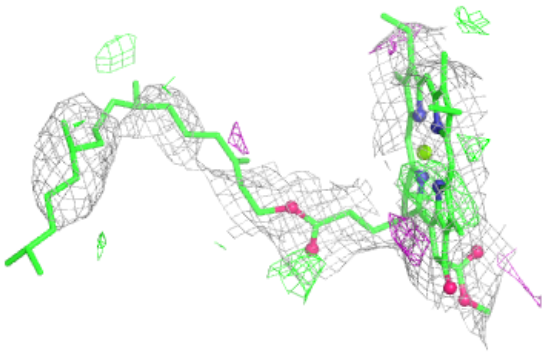


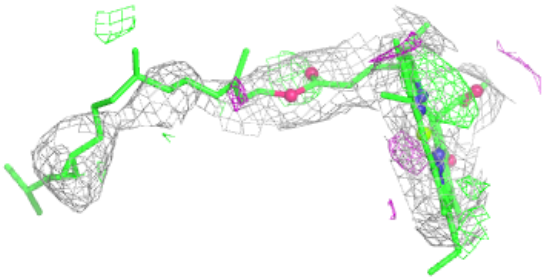


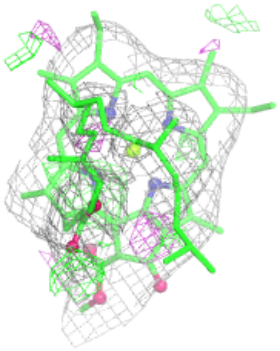


Electron density around CLA D 404:

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

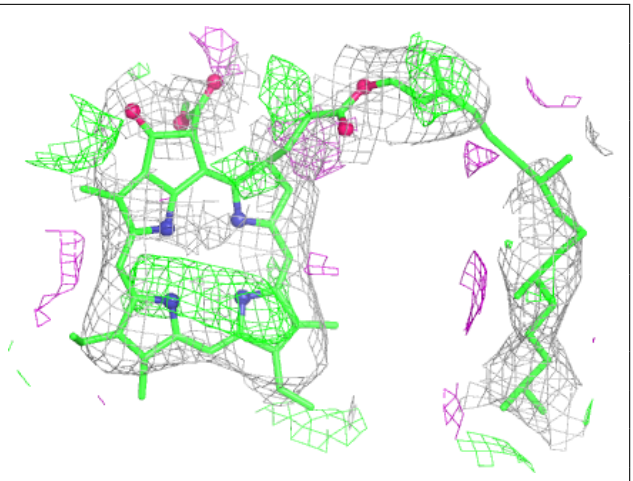


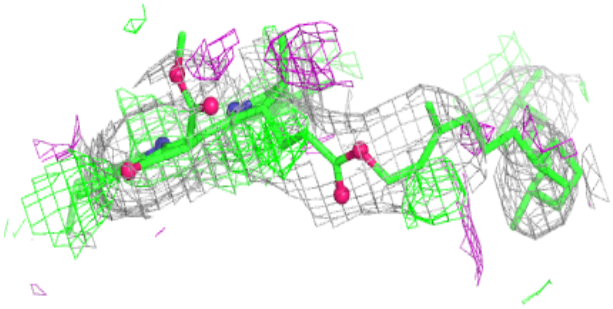


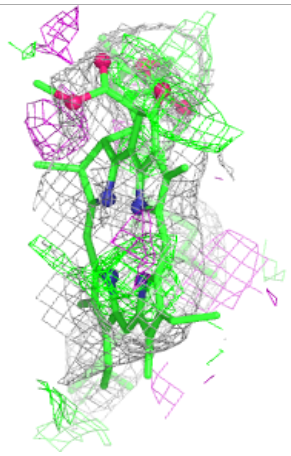


Electron density around PHO A 608:

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

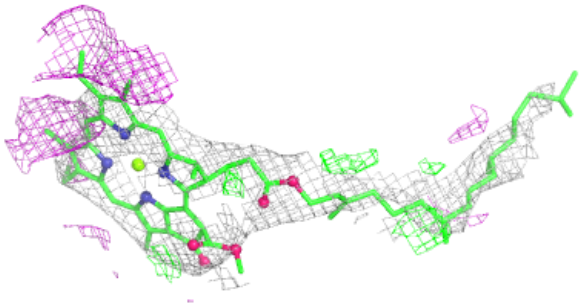


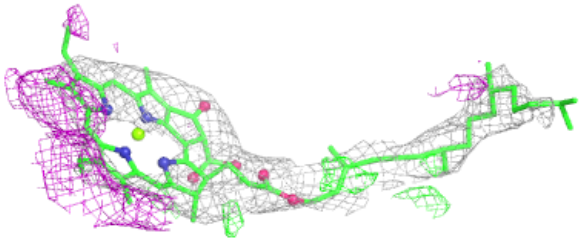


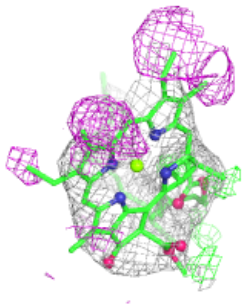


Electron density around CLA a 606:

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

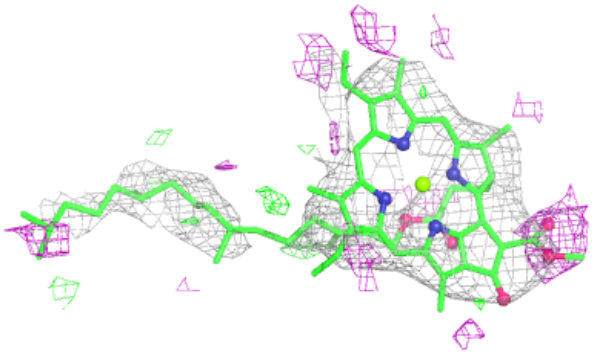


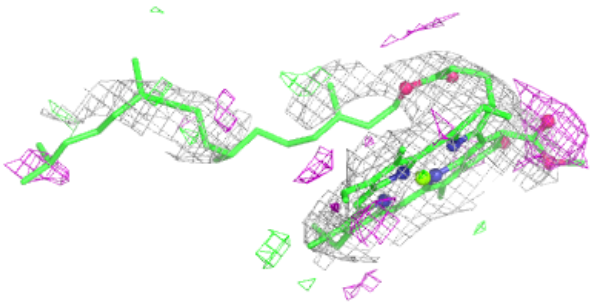


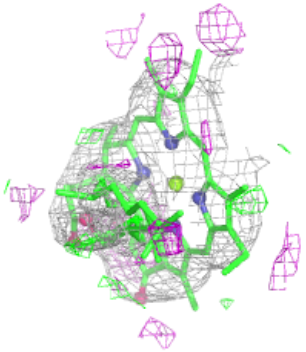


Electron density around CLA B 615:

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

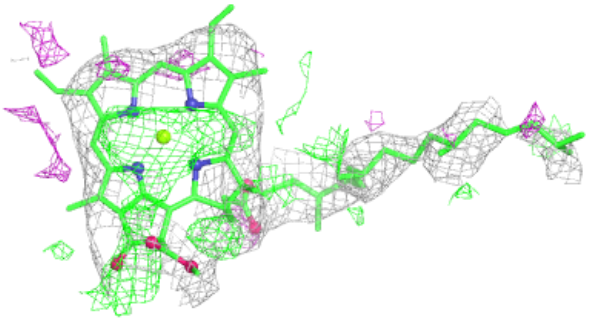


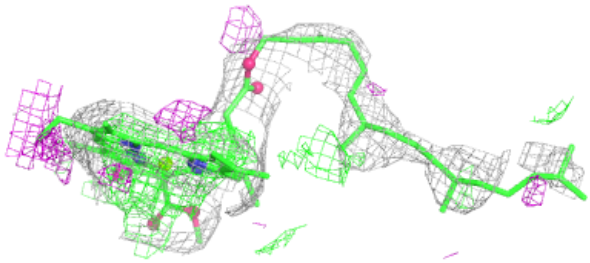


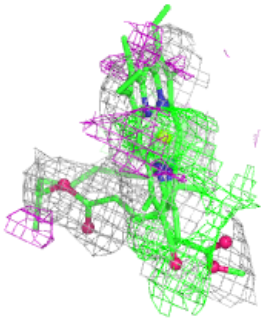


Electron density around CLA A 607:

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

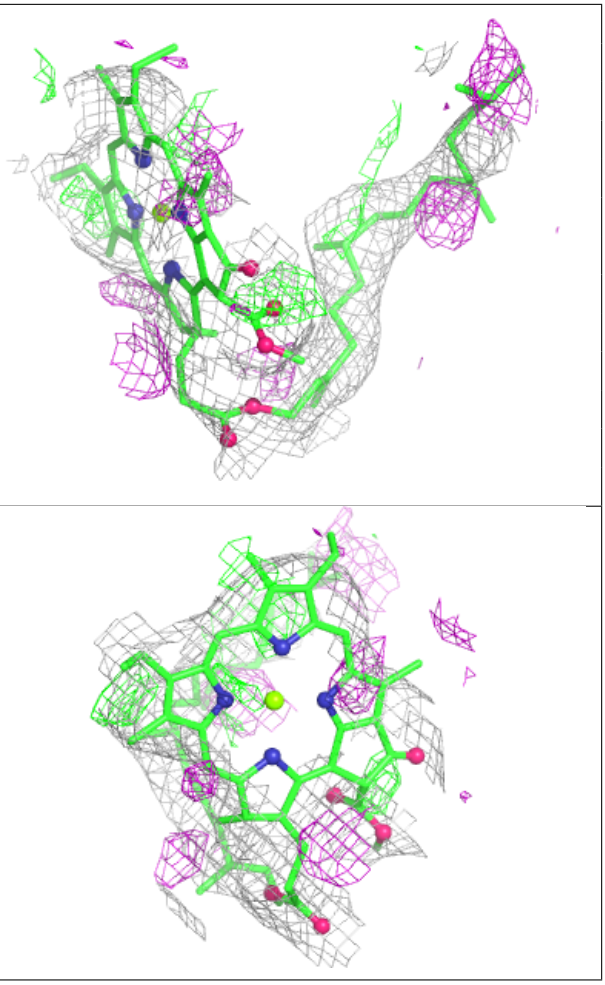






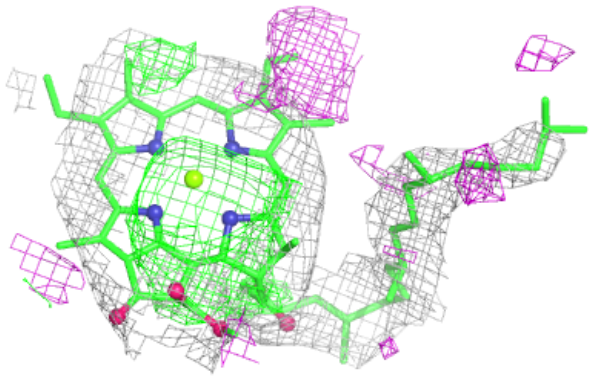
Electron density around CLA B 614:

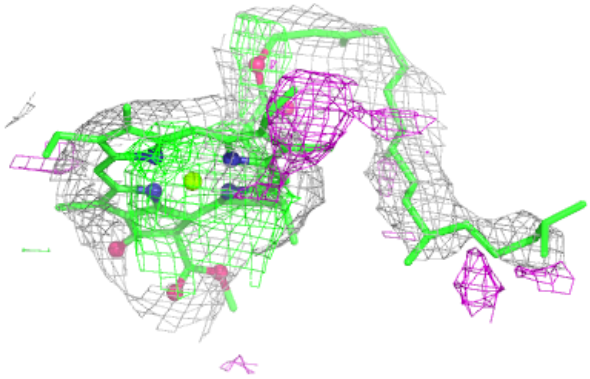
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

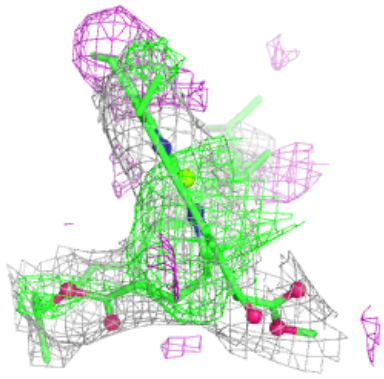


Electron density around CLA a 615:

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

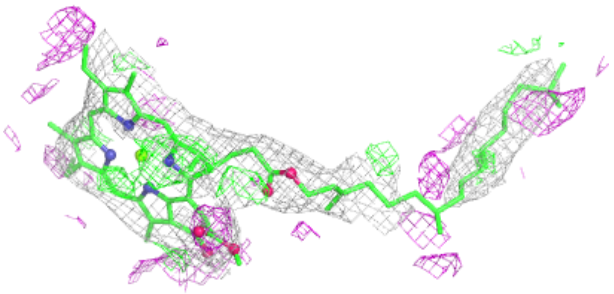


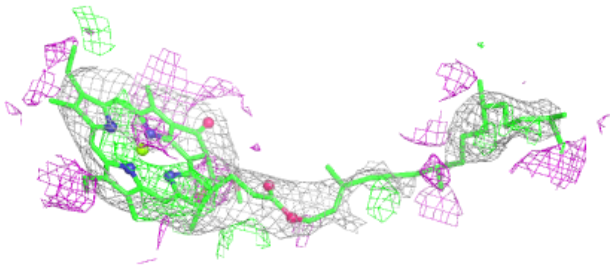


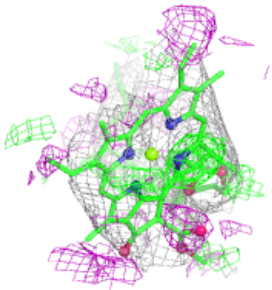


Electron density around CLA A 606:

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

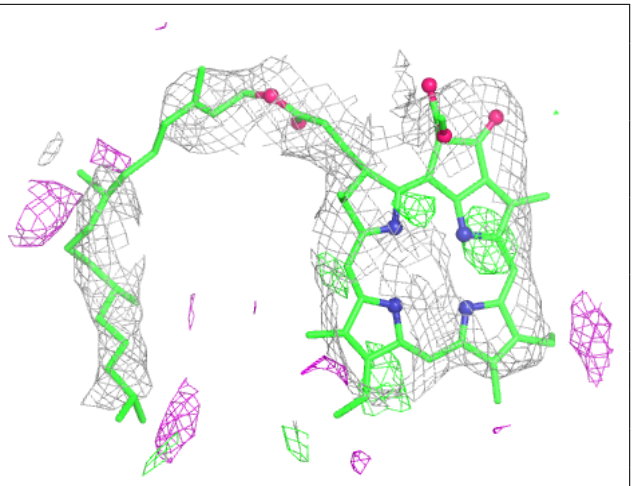


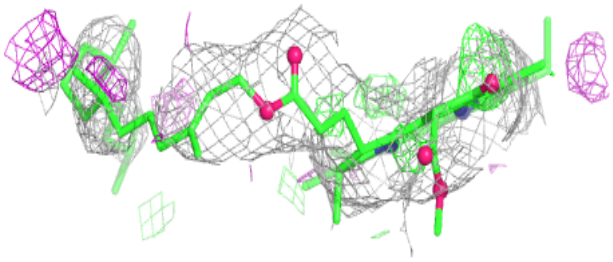


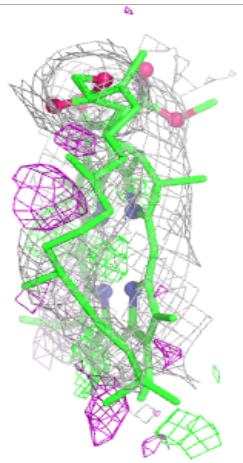


Electron density around PHO a 608:

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

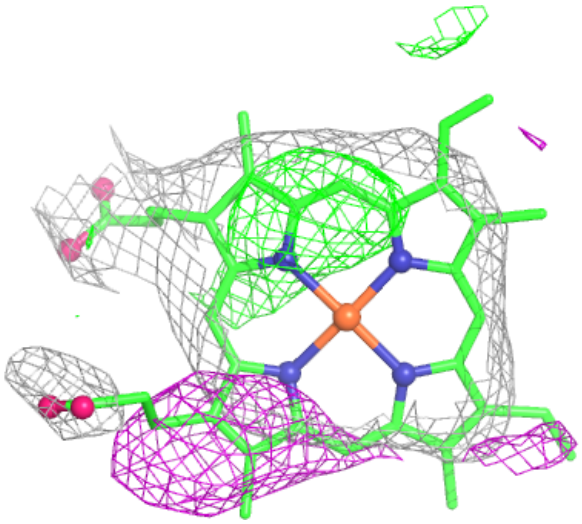


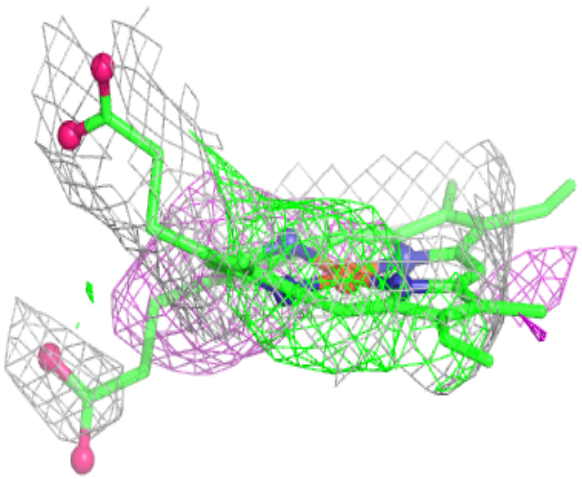


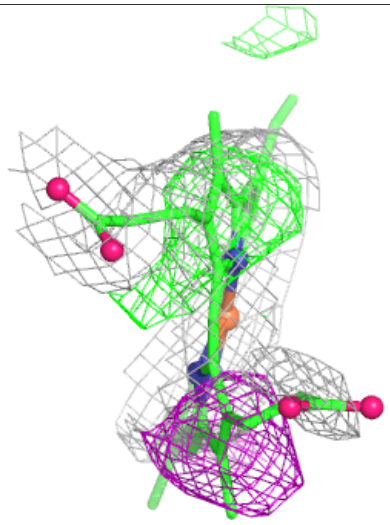


Electron density around HEM e 102:

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

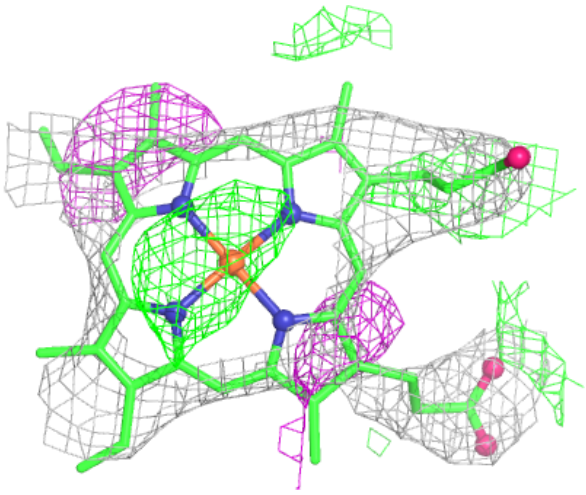


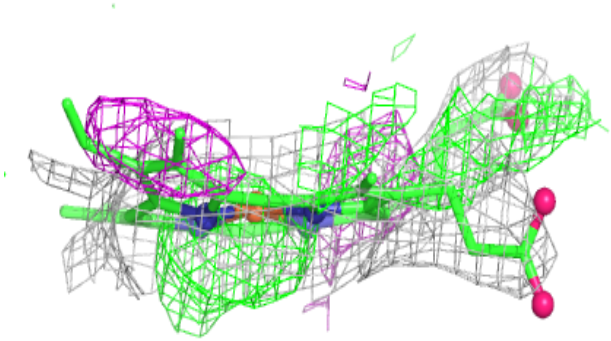


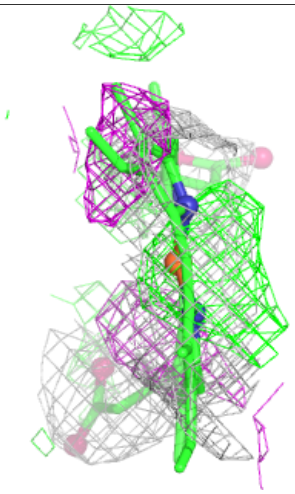


Electron density around HEM v 201:

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

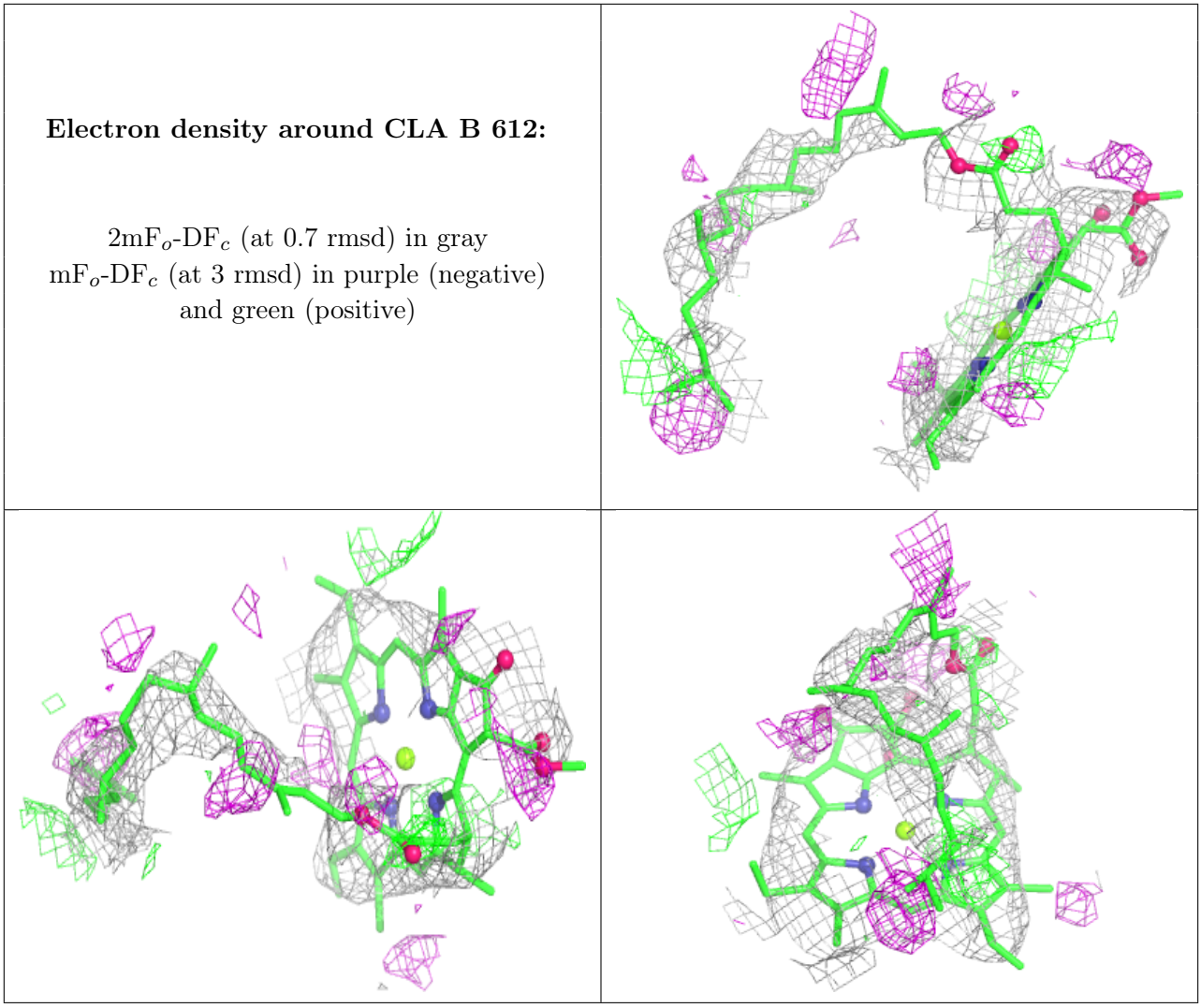






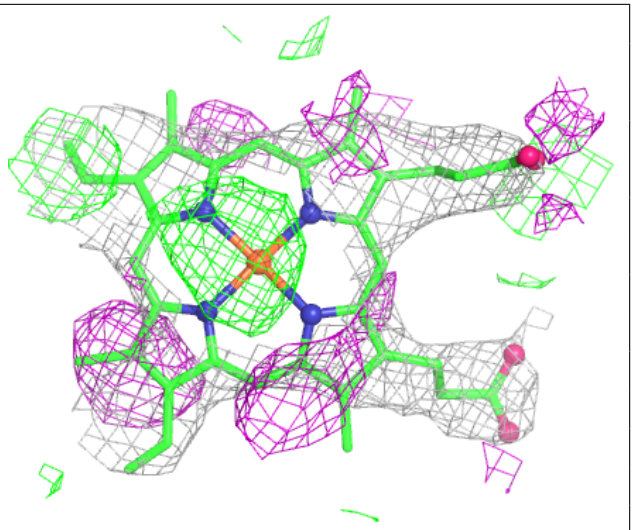
Electron density around CLA B 612:

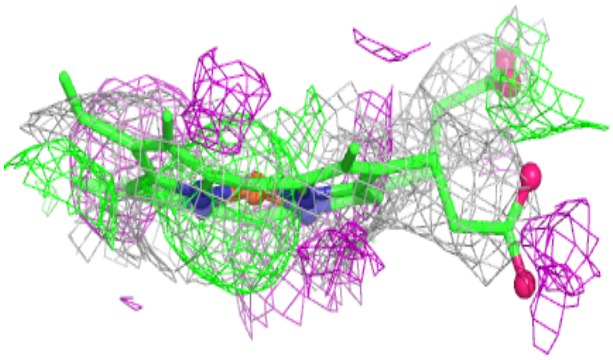
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

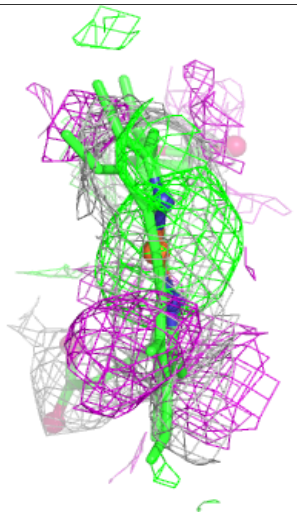


Electron density around HEM V 201:

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

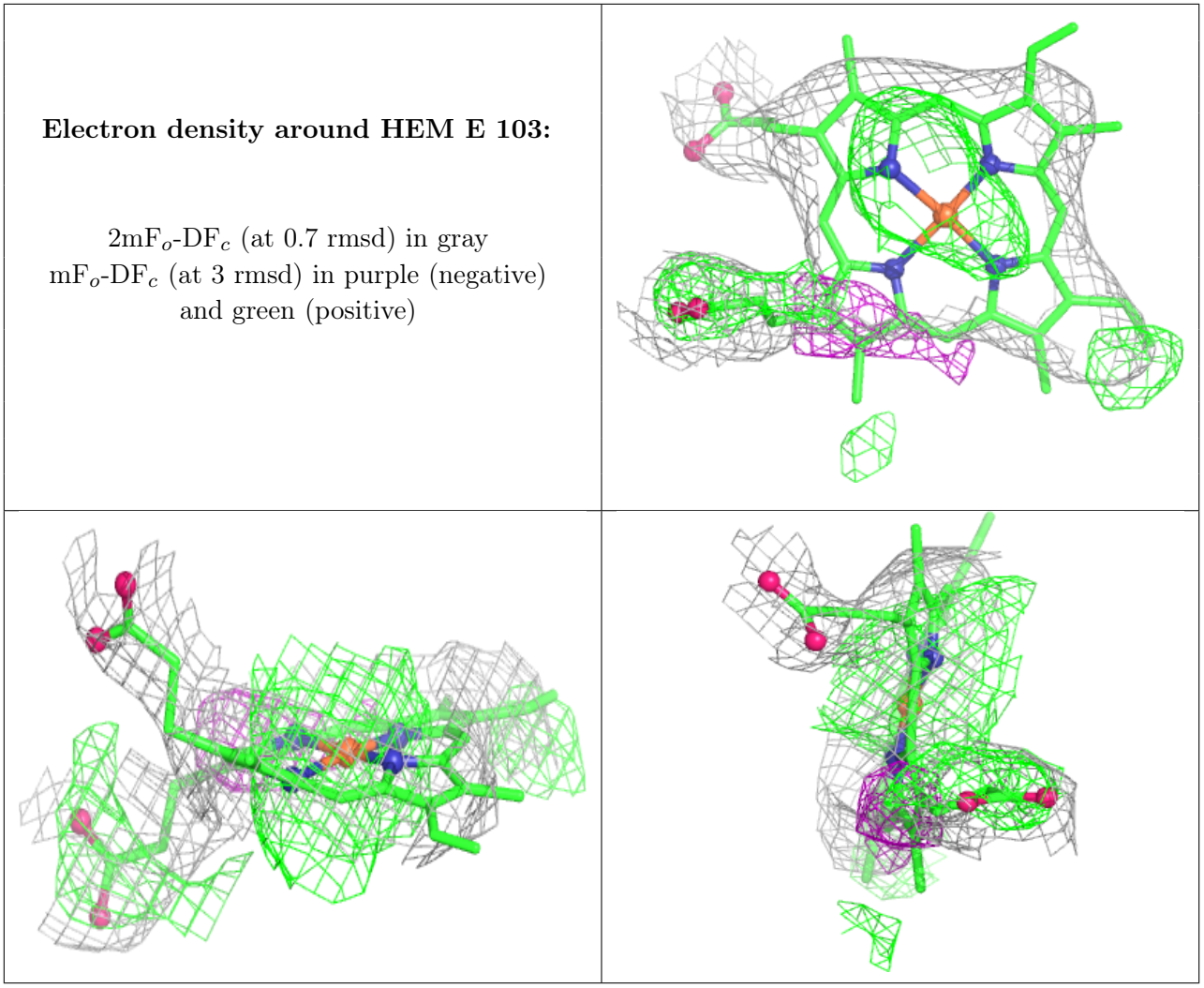






Electron density around HEM E 103:

$2mF_o$-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.