Full wwPDB X-ray Structure Validation Report (i)

Jul 11, 2021 – 12:33 AM JST

PDB ID	:	7DKZ
Title	:	Structure of plant photosystem I-light harvesting complex I supercomplex
Authors	:	Wang, J.; Yu, L.J.; Wang, W.
Deposited on	:	2020-11-25
Resolution	:	2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references (i)) were used in the production of this report:

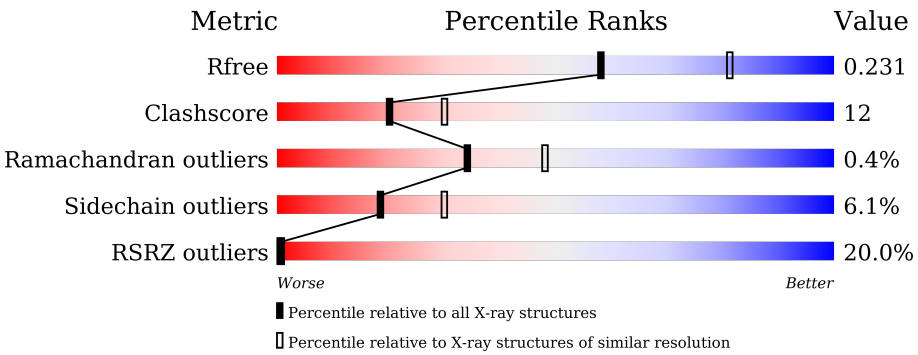
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

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 2.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	1	195	18% 75% 22% • •
2	2	269	21% 54% 19% • 24%
3	3	275	35% 65% 13% • 21%
4	4	198	10% 78% 18% • •
5	A	758	24% 77% 19% • •
6	B	734	10% 81% 17% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	C	81	6% 69% 25%
8	D	143	13% 73% 20%
9	E	66	18% 86% 9% 5%
10	F	154	3% 78% 20%
11	G	97	5% 77% 18%
12	H	88	57% 82% 16%
13	I	40	5% 62% 12% 25%
14	J	42	7% 74% 17% 7%
15	L	157	20% 72% 24%
16	K	80	54% 84% 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	1	301	X	-	-	-
17	CLA	1	302	X	-	-	-
17	CLA	1	303	X	-	-	-
17	CLA	1	304	X	-	-	-
17	CLA	1	306	X	-	-	-
17	CLA	1	307	X	-	-	-
17	CLA	1	308	X	-	-	-
17	CLA	1	309	X	-	-	-
17	CLA	1	310	X	-	-	-
17	CLA	1	311	X	-	-	-
17	CLA	1	312	X	-	-	-
17	CLA	1	313	X	-	-	-
17	CLA	2	301	X	-	-	-
17	CLA	2	302	X	-	-	-
17	CLA	2	303	X	-	-	-
17	CLA	2	307	X	-	-	-
17	CLA	2	308	X	-	-	-
17	CLA	2	309	X	-	-	-
17	CLA	2	310	X	-	-	-
17	CLA	2	311	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	2	312	X	-	-	-
17	CLA	2	319	X	-	-	-
17	CLA	3	602	X	-	-	-
17	CLA	3	603	X	-	-	-
17	CLA	3	604	X	-	-	-
17	CLA	3	605	X	-	-	-
17	CLA	3	606	X	-	-	-
17	CLA	3	608	X	-	-	-
17	CLA	3	609	X	-	-	-
17	CLA	3	610	X	-	-	-
17	CLA	3	611	X	-	-	-
17	CLA	3	612	X	-	-	-
17	CLA	3	613	X	-	-	-
17	CLA	4	302	X	-	-	-
17	CLA	4	304	X	-	-	-
17	CLA	4	308	X	-	-	-
17	CLA	4	309	X	-	-	-
17	CLA	4	310	X	-	-	-
17	CLA	4	312	X	-	-	-
17	CLA	4	313	X	-	-	-
17	CLA	4	314	X	-	-	-
17	CLA	A	801	X	-	-	-
17	CLA	A	802	X	-	-	-
17	CLA	A	803	X	-	-	-
17	CLA	A	804	X	-	-	-
17	CLA	A	805	X	-	-	-
17	CLA	A	806	X	-	-	-
17	CLA	A	807	X	-	-	-
17	CLA	A	808	X	-	-	-
17	CLA	A	809	X	-	-	-
17	CLA	A	810	X	-	-	-
17	CLA	A	811	X	-	-	-
17	CLA	A	812	X	-	-	-
17	CLA	A	813	X	-	-	-
17	CLA	A	814	X	-	-	-
17	CLA	A	815	X	-	-	-
17	CLA	A	816	X	-	-	-
17	CLA	A	817	X	-	-	-
17	CLA	A	818	X	-	-	-
17	CLA	A	819	X	-	-	-
17	CLA	A	820	X	-	-	-
17	CLA	A	821	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	A	822	X	-	-	-
17	CLA	A	823	X	-	-	-
17	CLA	A	824	X	-	-	-
17	CLA	A	825	X	-	-	-
17	CLA	A	826	X	-	-	-
17	CLA	A	827	X	-	-	-
17	CLA	A	828	X	-	-	-
17	CLA	A	829	X	-	-	-
17	CLA	A	830	X	-	-	-
17	CLA	A	831	X	-	-	-
17	CLA	A	832	X	-	-	-
17	CLA	A	833	X	-	-	-
17	CLA	A	834	X	-	-	-
17	CLA	A	835	X	-	-	-
17	CLA	A	836	X	-	-	-
17	CLA	A	837	X	-	-	-
17	CLA	A	838	X	-	-	-
17	CLA	A	839	X	-	-	-
17	CLA	A	840	X	-	-	-
17	CLA	A	841	X	-	-	-
17	CLA	A	843	X	-	-	-
17	CLA	A	853	X	-	-	-
17	CLA	B	802	X	-	-	-
17	CLA	B	803	X	-	-	-
17	CLA	B	804	X	-	-	-
17	CLA	B	805	X	-	-	-
17	CLA	B	806	X	-	-	-
17	CLA	B	807	X	-	-	-
17	CLA	B	808	X	-	-	-
17	CLA	B	809	X	-	-	-
17	CLA	B	810	X	-	-	-
17	CLA	B	811	X	-	-	-
17	CLA	B	813	X	-	-	-
17	CLA	B	814	X	-	-	-
17	CLA	B	815	X	-	-	-
17	CLA	B	816	X	-	-	-
17	CLA	B	817	X	-	-	-
17	CLA	B	818	X	-	-	-
17	CLA	B	819	X	-	-	-
17	CLA	B	820	X	-	-	-
17	CLA	B	821	X	-	-	-
17	CLA	B	822	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	CLA	B	823	X	-	-	-
17	CLA	B	824	X	-	-	-
17	CLA	B	825	X	-	-	-
17	CLA	B	826	X	-	-	-
17	CLA	B	827	X	-	-	-
17	CLA	B	828	X	-	-	-
17	CLA	B	829	X	-	-	-
17	CLA	B	830	X	-	-	-
17	CLA	B	831	X	-	-	-
17	CLA	B	832	X	-	-	-
17	CLA	B	833	X	-	-	-
17	CLA	B	834	X	-	-	-
17	CLA	B	835	X	-	-	-
17	CLA	B	836	X	-	-	-
17	CLA	B	837	X	-	-	-
17	CLA	B	838	X	-	-	-
17	CLA	B	839	X	-	-	-
17	CLA	B	840	X	-	-	-
17	CLA	B	841	X	-	-	-
17	CLA	B	842	X	-	-	-
17	CLA	F	304	X	-	-	-
17	CLA	F	306	X	-	-	-
17	CLA	F	307	X	-	-	-
17	CLA	G	103	X	-	-	-
17	CLA	G	104	X	-	-	-
17	CLA	G	105	X	-	-	-
17	CLA	J	101	X	-	-	-
17	CLA	J	103	X	-	-	-
17	CLA	K	201	X	-	-	-
17	CLA	K	202	X	-	-	-
17	CLA	L	202	X	-	-	-
17	CLA	L	203	X	-	-	-
18	CHL	1	305	X	-	-	-
18	CHL	2	304	X	-	-	-
18	CHL	2	305	X	-	-	-
18	CHL	2	306	X	-	-	-
18	CHL	2	313	X	-	-	-
18	CHL	3	601	X	-	-	-
18	CHL	3	607	X	-	-	-
18	CHL	4	301	X	-	-	-
18	CHL	4	305	X	-	-	-
18	CHL	4	306	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CHL	4	307	X	-	-	-
18	CHL	4	315	X	-	-	-
19	LUT	4	316	-	X	-	-
20	XAT	4	317	X	-	-	-
21	BCR	2	316	-	-	-	X
21	BCR	3	616	-	-	-	X
21	BCR	K	203	-	-	-	X
22	LHG	G	102	-	-	-	X
24	LMG	G	101	-	-	-	X
26	DGD	4	323	-	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 36093 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 Lhca1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	195	1507	979	252	271	5	0	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	204	1592	1042	261	285	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	216	1661	1088	268	300	5	0	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	195	1535	1006	249	277	3	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	A	742	5852	3835	997	1002	18	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ILE	VAL	conflict	UNP A0A0F6NFW5

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	B	733	5856	3848	998	996	14	0	0	0

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	C	80	611	379	107	114	11	0	0	0

- Molecule 8 is a protein called PsaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	D	140	1110	716	191	200	3	0	0	0

- Molecule 9 is a protein called PsaE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	E	63	505	320	89	96	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	PRO	-	expression tag	UNP E1C9K6
E	0	PRO	-	expression tag	UNP E1C9K6
E	14	GLN	LYS	conflict	UNP E1C9K6
E	60	VAL	-	expression tag	UNP E1C9K6
E	61	GLU	-	expression tag	UNP E1C9K6
E	62	GLU	-	expression tag	UNP E1C9K6
E	63	VAL	-	expression tag	UNP E1C9K6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	64	LYS	-	expression tag	UNP E1C9K6

- Molecule 10 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	F	152	1198	777	208	211	2	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	79	ALA	SER	conflict	UNP A0A0M3KL12
F	86	ASP	GLU	conflict	UNP A0A0M3KL12
F	107	LEU	ILE	conflict	UNP A0A0M3KL12
F	110	PRO	ALA	conflict	UNP A0A0M3KL12
F	133	GLY	ALA	conflict	UNP A0A0M3KL12
F	187	ASP	GLU	conflict	UNP A0A0M3KL12
F	203	THR	SER	conflict	UNP A0A0M3KL12

- Molecule 11 is a protein called PsaG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	G	95	737	477	122	138	0	0	0

- Molecule 12 is a protein called PsaH.

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

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	I	30	226	156	34	35	1	0	0	0

- Molecule 14 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	J	39	309	208	48	52	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is a protein called PsaL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	L	151	1122	737	182	202	1	0	0	0

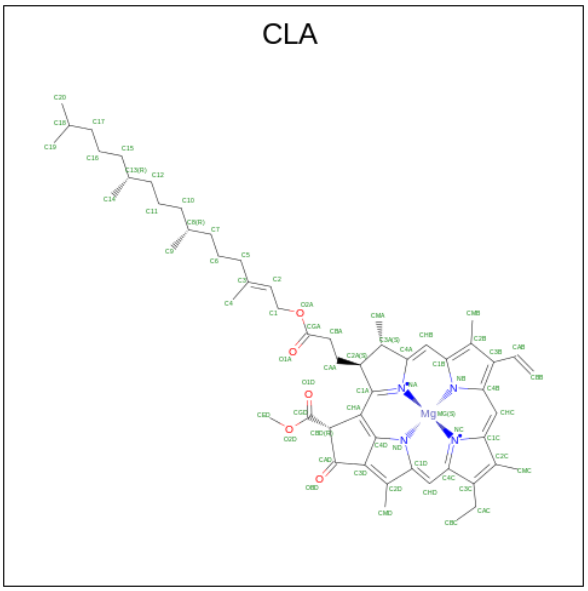
- Molecule 16 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	K	77	515	326	86	100	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	85	ALA	VAL	conflict	UNP E1C9L3

- Molecule 17 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	1	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	42	34	1	4	3	0	0
			Total	C	Mg	N	O		
17	1	1	46	36	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	52	42	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	1	1	46	36	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
17	2	1	52	42	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	2	1	43	35	1	4	3	0	0
			Total	C	Mg	N	O		
17	2	1	46	36	1	4	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	3	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	42	34	1	4	3	0	0
			Total	C	Mg	N	O		
17	3	1	47	37	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	52	42	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	3	1	46	36	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	52	42	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	56	46	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	4	1	47	37	1	4	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	49	39	1	4	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	A	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	51	41	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	A	1	52	42	1	4	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	A	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	54	44	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	59	49	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0

Continued on next page...

Continued from previous page...

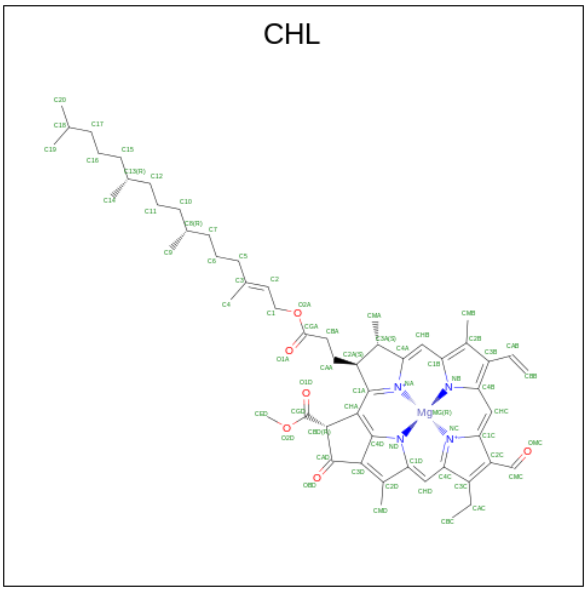
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	B	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	58	48	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	60	50	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	47	37	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	B	1	65	55	1	4	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
17	F	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	F	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	F	1	55	45	1	4	5	0	0
			Total	C	Mg	N	O		
17	G	1	41	33	1	4	3	0	0
			Total	C	Mg	N	O		
17	G	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	G	1	46	36	1	4	5	0	0
			Total	C	Mg	N	O		
17	J	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	J	1	42	34	1	4	3	0	0
			Total	C	Mg	N	O		
17	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	L	1	65	55	1	4	5	0	0
			Total	C	Mg	N	O		
17	L	1	50	40	1	4	5	0	0
			Total	C	Mg	N	O		
17	K	1	45	35	1	4	5	0	0
			Total	C	Mg	N	O		
17	K	1	60	50	1	4	5	0	0

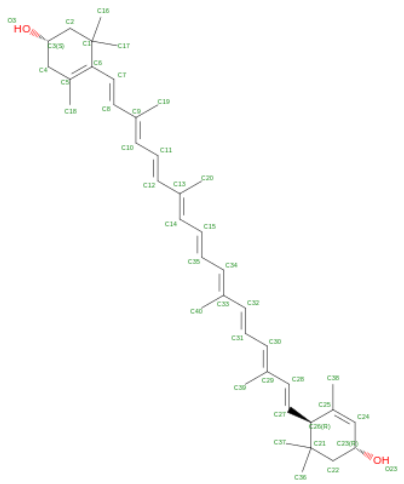
- Molecule 18 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
18	1	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
18	2	1	43	34	1	4	4	0	0
			Total	C	Mg	N	O		
18	2	1	48	37	1	4	6	0	0
			Total	C	Mg	N	O		
18	2	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
18	2	1	43	34	1	4	4	0	0
			Total	C	Mg	N	O		
18	3	1	56	45	1	4	6	0	0
			Total	C	Mg	N	O		
18	3	1	47	36	1	4	6	0	0
			Total	C	Mg	N	O		
18	4	1	61	50	1	4	6	0	0
			Total	C	Mg	N	O		
18	4	1	56	45	1	4	6	0	0
			Total	C	Mg	N	O		
18	4	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
18	4	1	51	40	1	4	6	0	0
			Total	C	Mg	N	O		
18	4	1	43	34	1	4	4	0	0

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).

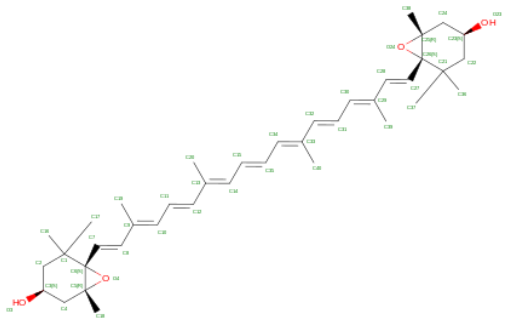
LUT



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	1	1	42	40	2	0	0
19	2	1	42	40	2	0	0
19	3	1	42	40	2	0	0
19	4	1	42	40	2	0	0

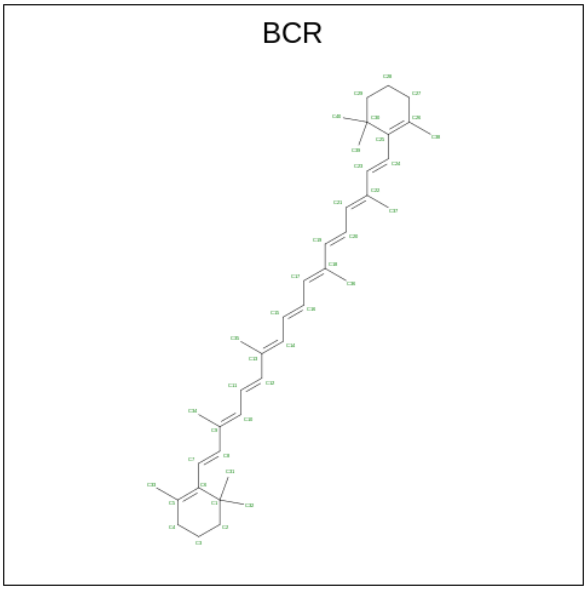
- Molecule 20 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).

XAT



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	1	1	44	40	4	0	0
20	2	1	44	40	4	0	0
20	3	1	44	40	4	0	0
20	4	1	44	40	4	0	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



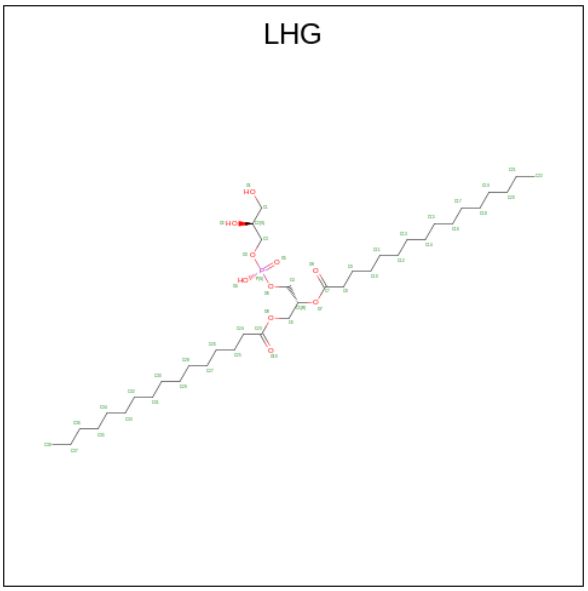
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
21	1	1	40	40	0	0
21	2	1	40	40	0	0
21	3	1	40	40	0	0
21	4	1	40	40	0	0
21	A	1	40	40	0	0
21	A	1	40	40	0	0
21	A	1	40	40	0	0
21	A	1	40	40	0	0

Continued on next page...

Continued from previous page...

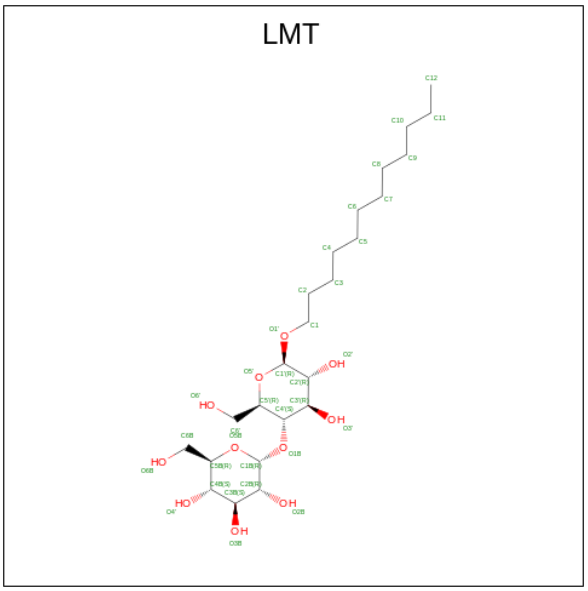
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
21	A	1	40	40	0	0
			Total	C		
21	A	1	40	40	0	0
			Total	C		
21	B	1	40	40	0	0
			Total	C		
21	B	1	40	40	0	0
			Total	C		
21	B	1	40	40	0	0
			Total	C		
21	B	1	40	40	0	0
			Total	C		
21	B	1	40	40	0	0
			Total	C		
21	B	1	40	40	0	0
			Total	C		
21	F	1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

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



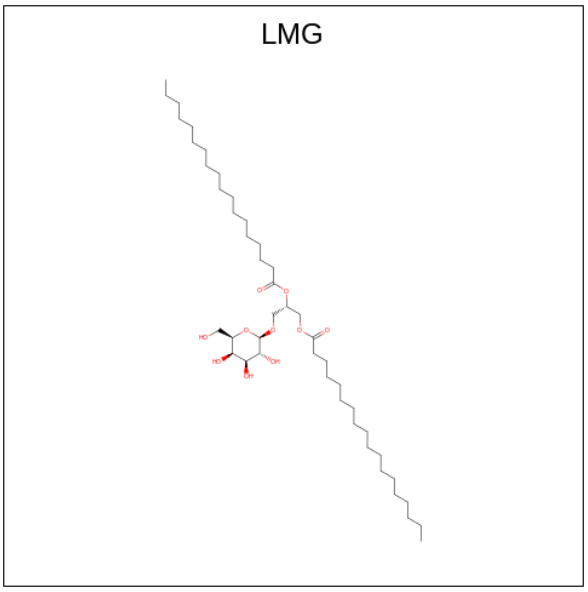
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
22	1	1	49	38	10	1	0	0
			Total	C	O	P		
22	2	1	37	26	10	1	0	0
			Total	C	O	P		
22	A	1	49	38	10	1	0	0
			Total	C	O	P		
22	A	1	27	16	10	1	0	0
			Total	C	O	P		
22	B	1	23	12	10	1	0	0
			Total	C	O	P		
22	F	1	40	29	10	1	0	0
			Total	C	O	P		
22	G	1	49	38	10	1	0	0

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
23	2	1	35	24	11	0	0
			Total	C	O		
23	A	1	35	24	11	0	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



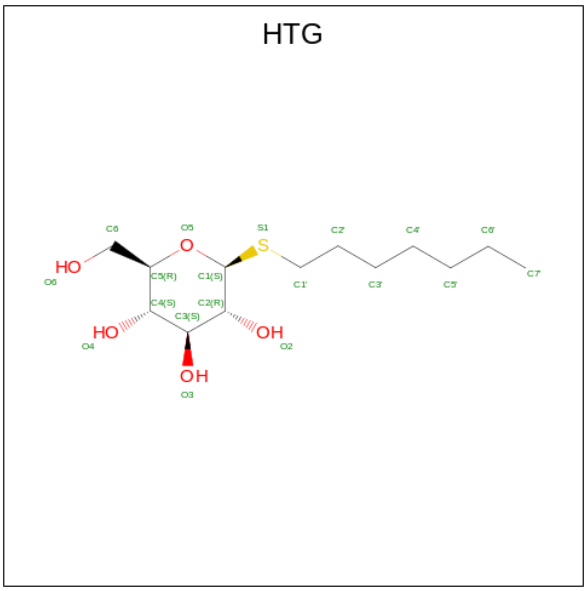
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
24	4	1	50	40	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
24	4	1	49	39	10		0	0
			Total	C	O			
24	B	1	52	42	10		0	0
			Total	C	O			
24	F	1	55	45	10		0	0
			Total	C	O			
24	G	1	40	30	10		0	0

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



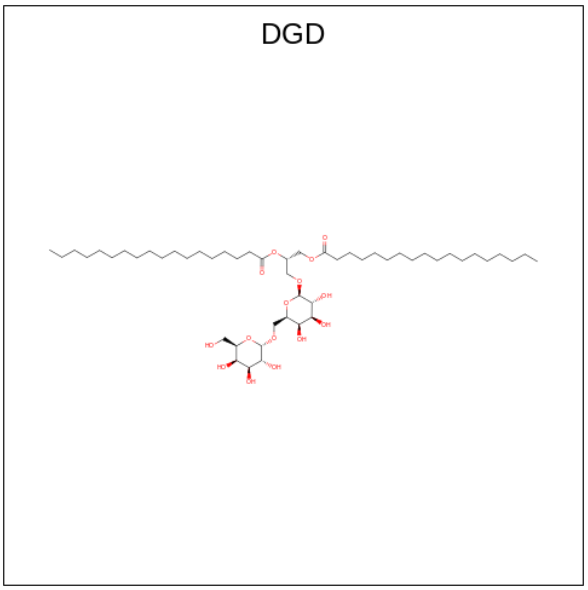
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
25	4	1	19	13	5	1	0	0
			Total	C	O	S		
25	4	1	19	13	5	1	0	0
			Total	C	O	S		
25	A	1	19	13	5	1	0	0
			Total	C	O	S		
25	B	1	19	13	5	1	0	0
			Total	C	O	S		
25	F	1	17	11	5	1	0	0
			Total	C	O	S		
25	F	1	19	13	5	1	0	0
			Total	C	O	S		
25	F	1	16	10	5	1	0	0

Continued on next page...

Continued from previous page...

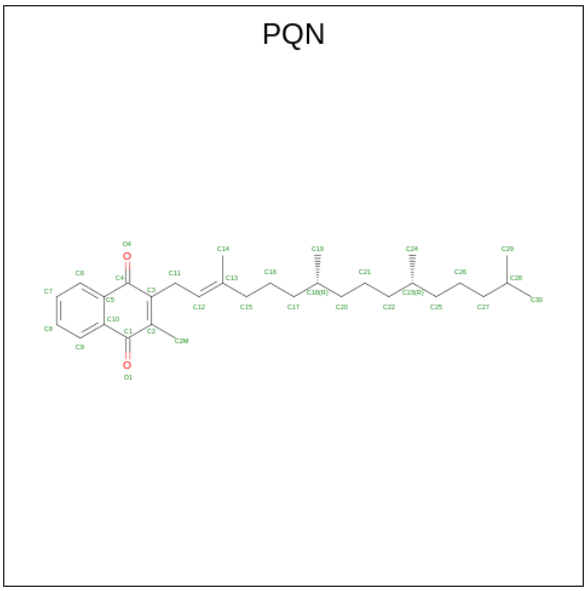
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
25	J	1	19	13	5	1	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



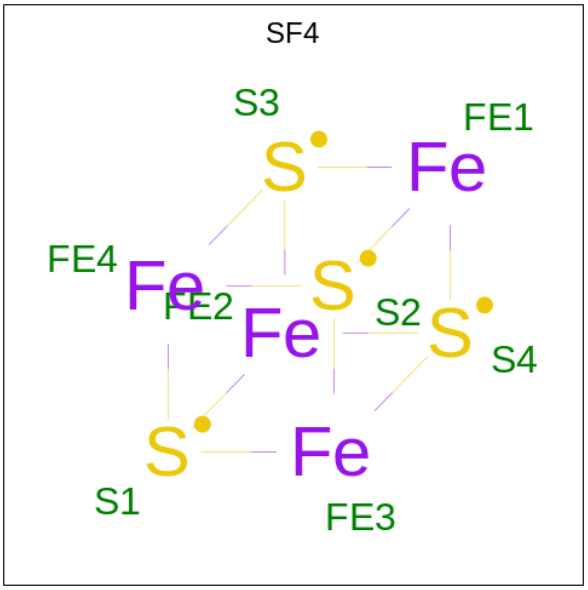
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
26	4	1	60	45	15	0	0
			Total	C	O		
26	B	1	66	51	15	0	0

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

Continued on next page...

Continued from previous page...

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

- Molecule 29 is water.

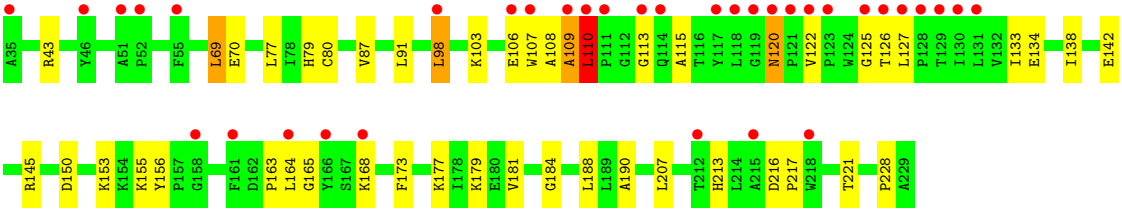
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
29	1	3	3	3	0	0
29	2	5	5	5	0	0
29	3	3	3	3	0	0
29	4	7	7	7	0	0
29	A	25	25	25	0	0
29	B	39	39	39	0	0
29	C	3	3	3	0	0
29	F	5	5	5	0	0
29	G	1	1	1	0	0
29	J	1	1	1	0	0
29	L	1	1	1	0	0

3 Residue-property plots (i)

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

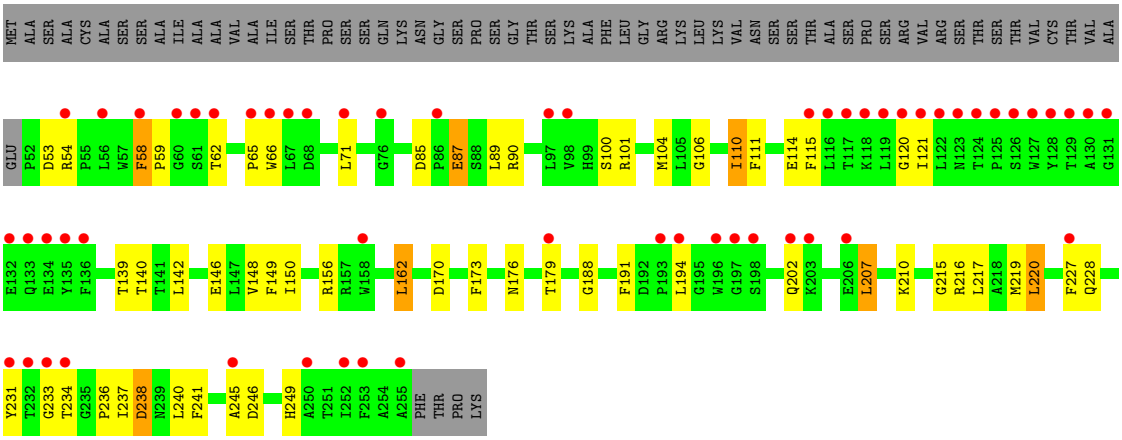
- Molecule 1: Lhca1

Chain 1:



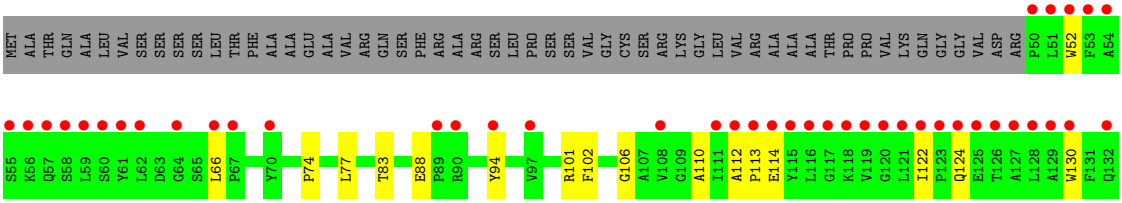
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

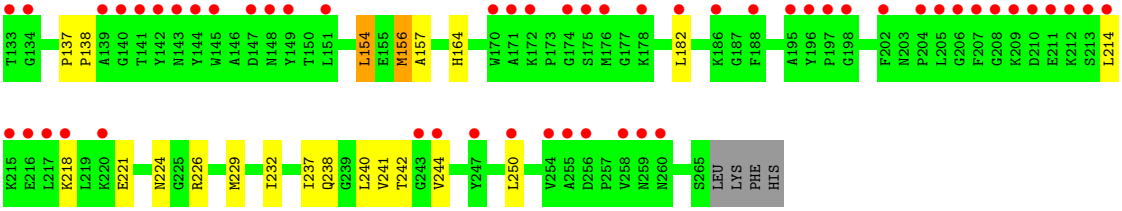
Chain 2:



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

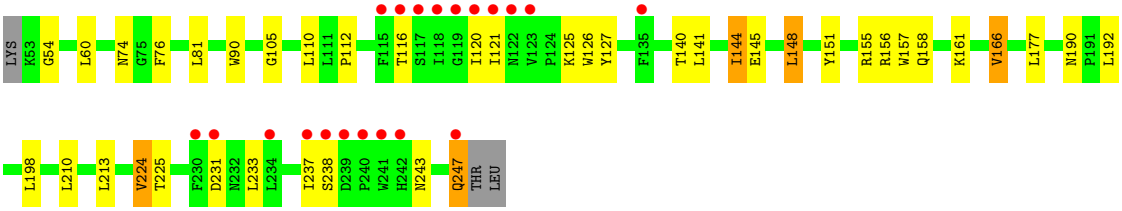
Chain 3:





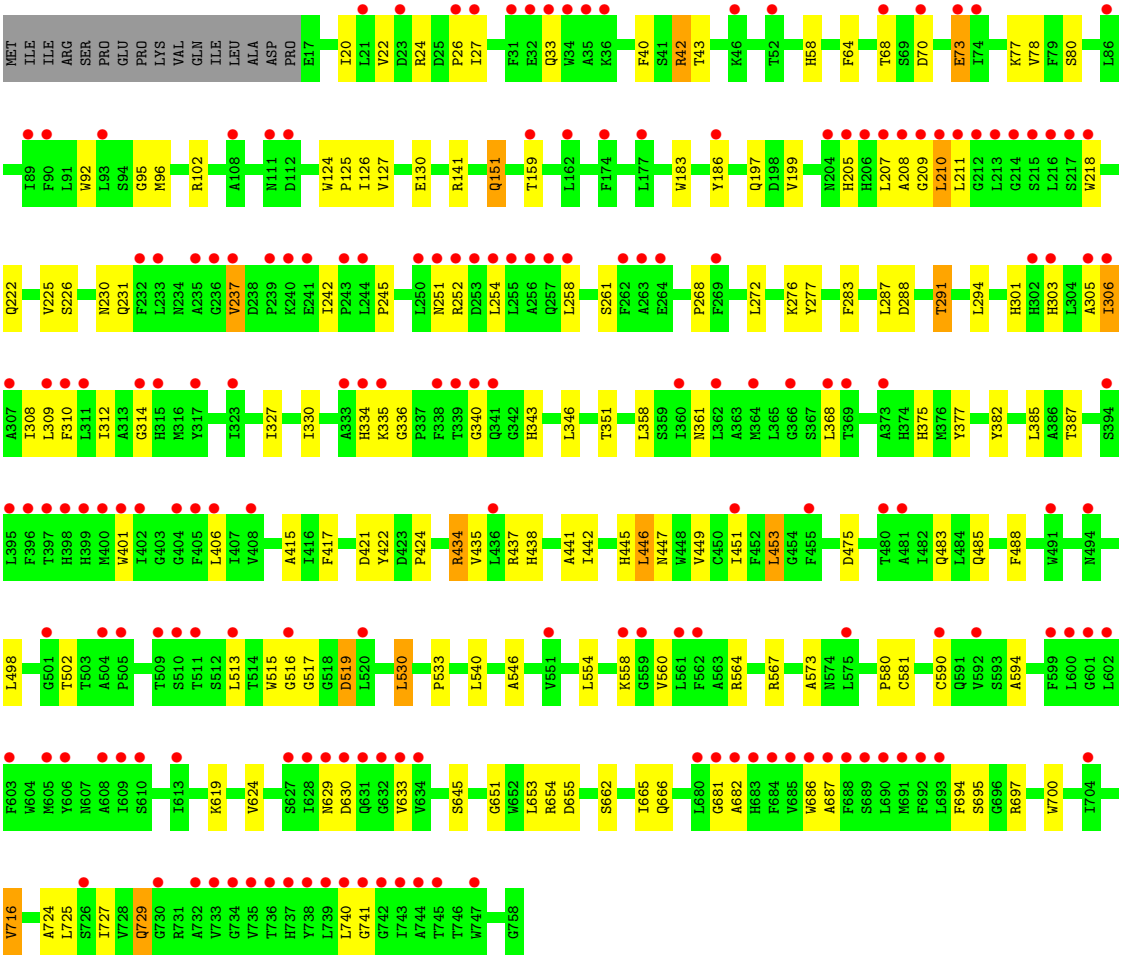
- Molecule 4: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:



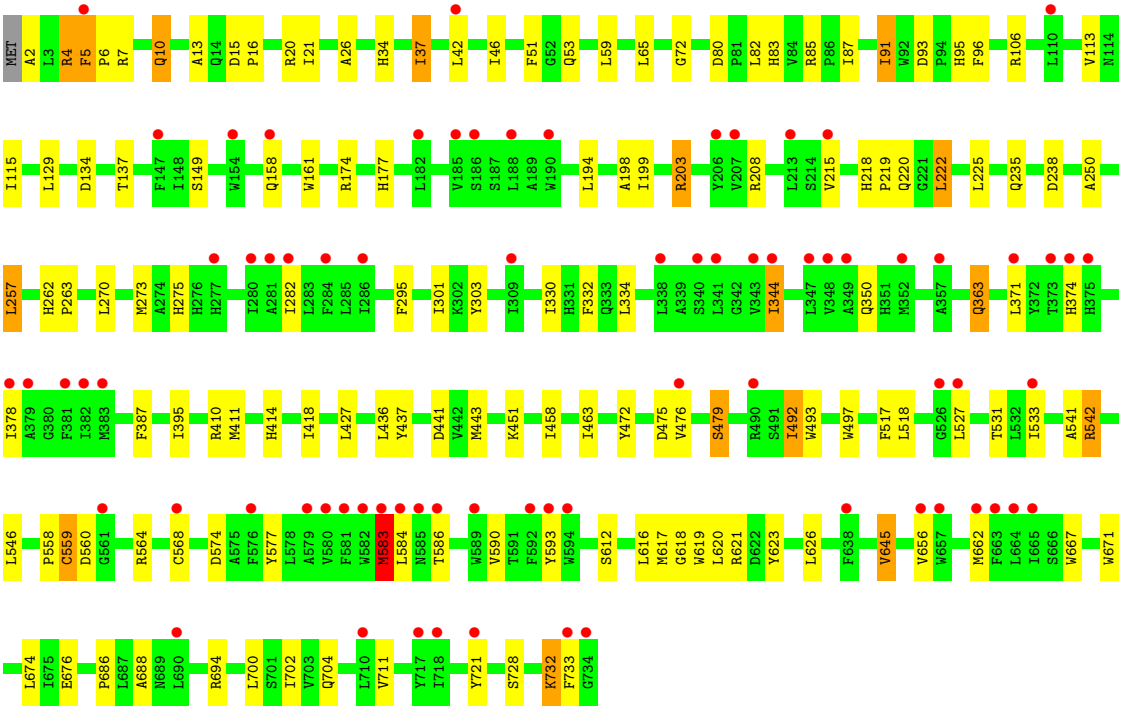
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:



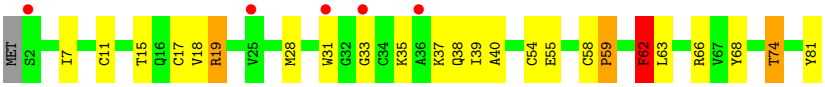
• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:



• Molecule 7: Photosystem I iron-sulfur center

Chain C:



• Molecule 8: PsaD

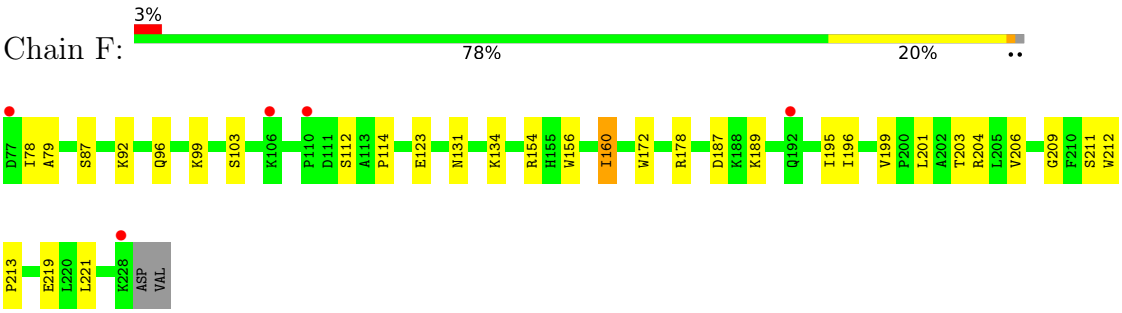
Chain D:

• Molecule 9: PsaE

Chain E:

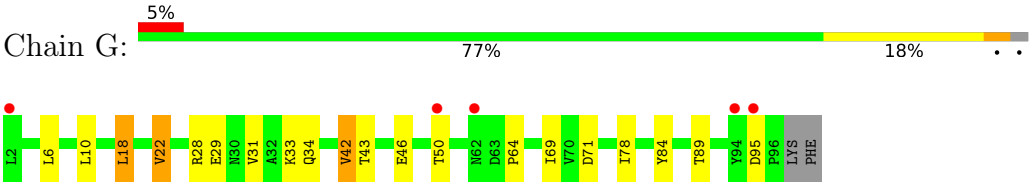
• Molecule 10: PSI-F

Chain F:



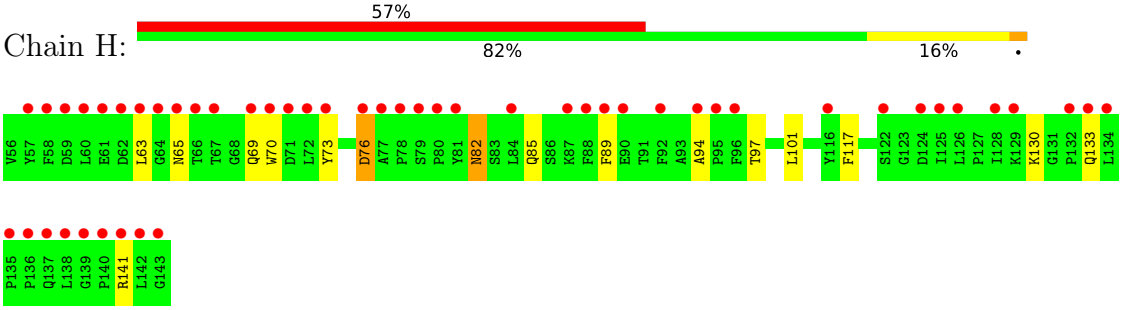
• Molecule 11: PsaG

Chain G:



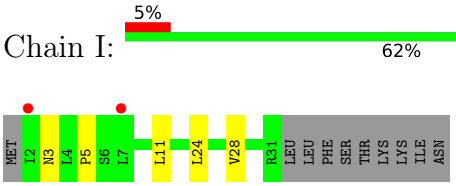
• Molecule 12: PsaH

Chain H:



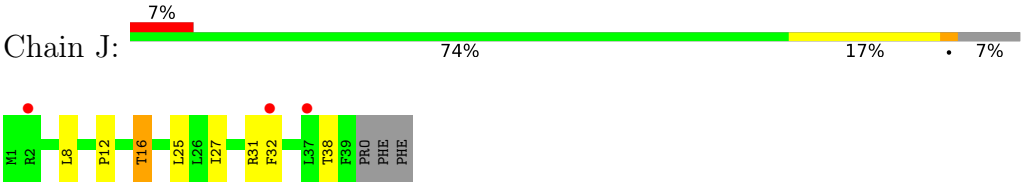
• Molecule 13: Photosystem I reaction center subunit VIII

Chain I:



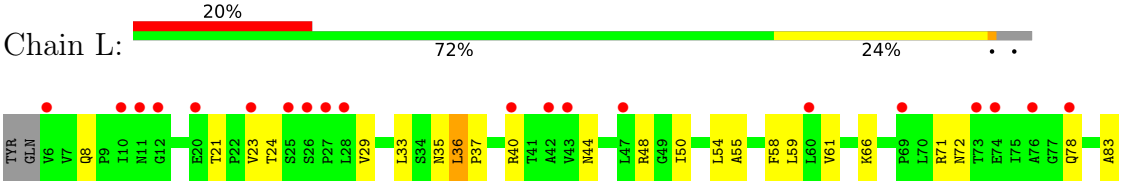
• Molecule 14: Photosystem I reaction center subunit IX

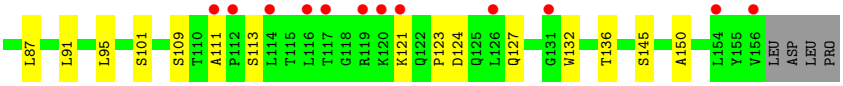
Chain J:



• Molecule 15: PsaL

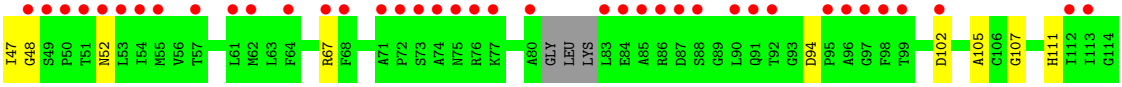
Chain L:





- Molecule 16: PSI-K

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.65Å 168.95Å 185.22Å 90.00° 121.39° 90.00°	Depositor
Resolution (Å)	44.41 – 2.39 44.41 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.41-2.39) 99.0 (44.41-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.189 , 0.227 0.194 , 0.231	Depositor DCC
R_{free} test set	11616 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 80.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36093	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]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: CHL, SF4, LUT, CLA, LMG, PQN, DGD, LMT, HTG, BCR, XAT, 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	1	0.37	0/1557	0.53	1/2127 (0.0%)
2	2	0.30	0/1651	0.46	0/2262
3	3	0.28	0/1713	0.42	0/2326
4	4	0.49	0/1584	0.62	0/2159
5	A	0.37	0/6050	0.50	0/8254
6	B	0.50	0/6068	0.65	2/8286 (0.0%)
7	C	0.79	2/624 (0.3%)	0.91	3/846 (0.4%)
8	D	0.41	0/1140	0.58	0/1540
9	E	0.47	0/515	0.57	0/700
10	F	0.47	0/1226	0.66	0/1658
11	G	0.49	0/755	0.54	0/1027
12	H	0.30	0/693	0.43	0/942
13	I	0.33	0/232	0.47	0/317
14	J	0.43	0/317	0.58	0/432
15	L	0.30	0/1153	0.45	0/1576
16	K	0.26	0/520	0.45	0/707
All	All	0.42	2/25798 (0.0%)	0.56	6/35159 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	1	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	59	PRO	N-CA	13.00	1.69	1.47
7	C	58	CYS	C-N	5.11	1.44	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	62	PHE	CB-CA-C	11.16	132.72	110.40
6	B	542	ARG	NE-CZ-NH2	-7.77	116.42	120.30
6	B	583	MET	CG-SD-CE	7.34	111.94	100.20
1	1	110	LEU	CA-CB-CG	7.14	131.73	115.30
7	C	59	PRO	CA-N-CD	-6.16	102.88	111.50
7	C	62	PHE	N-CA-CB	5.57	120.63	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	62	PHE	CA

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	1	1507	0	1468	35	0
2	2	1592	0	1531	50	0
3	3	1661	0	1620	31	0
4	4	1535	0	1496	40	0
5	A	5852	0	5713	109	0
6	B	5856	0	5653	111	0
7	C	611	0	591	18	0
8	D	1110	0	1123	18	0
9	E	505	0	503	3	0
10	F	1198	0	1228	19	0
11	G	737	0	721	14	0
12	H	673	0	667	12	0
13	I	226	0	242	3	0
14	J	309	0	320	8	0
15	L	1122	0	1133	27	0
16	K	515	0	513	5	0
17	1	672	0	636	39	0
17	2	533	0	480	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	3	542	0	433	23	0
17	4	540	0	476	28	0
17	A	2582	0	2646	146	0
17	B	2493	0	2566	130	0
17	F	165	0	154	8	0
17	G	137	0	101	10	0
17	J	107	0	103	9	0
17	K	105	0	92	4	0
17	L	180	0	183	14	0
18	1	48	0	33	6	0
18	2	185	0	128	12	0
18	3	103	0	72	19	0
18	4	262	0	207	31	0
19	1	42	0	56	9	0
19	2	42	0	56	4	0
19	3	42	0	56	4	0
19	4	42	0	56	4	0
20	1	44	0	56	3	0
20	2	44	0	56	10	0
20	3	44	0	56	13	0
20	4	44	0	56	10	0
21	1	40	0	56	0	0
21	2	40	0	56	8	0
21	3	40	0	56	4	0
21	4	40	0	56	14	0
21	A	240	0	336	26	0
21	B	240	0	336	24	0
21	F	80	0	112	4	0
21	G	40	0	56	2	0
21	I	40	0	56	4	0
21	J	80	0	112	8	0
21	K	40	0	56	4	0
21	L	120	0	168	11	0
22	1	49	0	74	6	0
22	2	37	0	44	7	0
22	A	76	0	98	3	0
22	B	23	0	16	1	0
22	F	40	0	53	2	0
22	G	49	0	74	2	0
23	2	35	0	46	3	0
23	A	35	0	45	2	0
24	4	99	0	143	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	52	0	77	6	0
24	F	55	0	86	1	0
24	G	40	0	53	3	0
25	4	38	0	52	4	0
25	A	19	0	26	0	0
25	B	19	0	26	1	0
25	F	52	0	62	2	0
25	J	19	0	26	3	0
26	4	60	0	81	29	0
26	B	66	0	96	7	0
27	A	33	0	46	6	0
27	B	33	0	46	3	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	1	3	0	0	0	0
29	2	5	0	0	0	0
29	3	3	0	0	0	0
29	4	7	0	0	0	0
29	A	25	0	0	1	0
29	B	39	0	0	2	0
29	C	3	0	0	0	0
29	F	5	0	0	0	0
29	G	1	0	0	0	0
29	J	1	0	0	0	0
29	L	1	0	0	0	0
All	All	36093	0	36006	898	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 12.

All (898) 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)
7:C:59:PRO:N	7:C:59:PRO:CA	1.69	1.32
6:B:303:TYR:CD2	11:G:34:GLN:HB3	1.94	1.03
3:3:74:PRO:HD2	20:3:615:XAT:O23	1.57	1.02
3:3:229:MET:HB3	20:3:615:XAT:H402	1.42	1.02
17:3:602:CLA:HAB	20:3:615:XAT:H32	1.44	0.99
26:4:323:DGD:C6B	26:4:323:DGD:HBE1	1.96	0.96
26:4:323:DGD:HBE1	26:4:323:DGD:HB61	1.48	0.95
2:2:219:MET:HB3	20:2:315:XAT:H402	1.46	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:303:TYR:CG	11:G:34:GLN:HB3	2.03	0.94
18:3:601:CHL:C10	18:3:601:CHL:C7	2.49	0.91
26:4:323:DGD:HBT1	26:4:323:DGD:HBF1	1.50	0.91
26:4:323:DGD:HD1	26:4:323:DGD:HG12	1.53	0.90
3:3:101:ARG:NH1	3:3:221:GLU:OE2	2.07	0.88
18:3:601:CHL:C7	18:3:601:CHL:C9	2.52	0.88
21:A:851:BCR:H362	17:A:853:CLA:H42	1.58	0.86
6:B:5:PHE:HB3	6:B:6:PRO:HD3	1.58	0.86
24:4:320:LMG:H191	24:4:320:LMG:H331	1.56	0.85
18:3:601:CHL:C10	18:3:601:CHL:C9	2.54	0.85
4:4:155:ARG:HG3	18:4:301:CHL:HED3	1.58	0.85
5:A:725:LEU:HB2	27:A:842:PQN:H6	1.59	0.83
16:K:117:VAL:HG22	17:K:202:CLA:HAB	1.62	0.82
4:4:156:ARG:NH1	17:4:308:CLA:O1D	2.13	0.81
17:A:803:CLA:HAB	17:A:810:CLA:H142	1.62	0.81
6:B:583:MET:HE1	6:B:584:LEU:HD23	1.61	0.81
6:B:574:ASP:OD2	29:B:901:HOH:O	1.96	0.81
26:4:323:DGD:O5E	26:4:323:DGD:O4E	1.93	0.80
7:C:66:ARG:HG2	7:C:68:TYR:CZ	2.16	0.80
26:4:323:DGD:HBT1	26:4:323:DGD:CEB	2.12	0.80
17:A:840:CLA:H42	17:B:802:CLA:H193	1.64	0.79
17:3:603:CLA:HBB1	20:3:615:XAT:H35	1.64	0.79
18:3:607:CHL:HHC	18:3:607:CHL:HBB1	1.64	0.78
17:4:302:CLA:H72	20:4:317:XAT:H30	1.65	0.77
17:B:823:CLA:HMD2	21:B:844:BCR:HC7	1.67	0.77
18:2:306:CHL:HMB3	21:2:316:BCR:H16C	1.66	0.76
18:4:306:CHL:H12	24:4:320:LMG:H212	1.67	0.76
17:A:838:CLA:H111	17:A:838:CLA:HAB	1.67	0.76
6:B:517:PHE:HA	17:B:838:CLA:HED1	1.67	0.75
5:A:222:GLN:HA	5:A:226:SER:HB3	1.66	0.75
18:4:301:CHL:H71	21:4:318:BCR:HC7	1.69	0.74
17:A:804:CLA:H61	21:A:848:BCR:HC8	1.70	0.74
17:B:830:CLA:HHC	17:B:830:CLA:HBB1	1.67	0.74
17:A:815:CLA:HHC	17:A:815:CLA:HBB1	1.70	0.73
14:J:31:ARG:HD3	21:J:105:BCR:H312	1.71	0.73
17:1:303:CLA:H2A	17:1:303:CLA:HED3	1.71	0.73
5:A:725:LEU:HB3	5:A:729:GLN:HG2	1.71	0.72
26:4:323:DGD:HBE2	26:4:323:DGD:HBN1	1.71	0.72
10:F:160:ILE:HD11	21:F:308:BCR:H282	1.71	0.72
5:A:533:PRO:O	5:A:619:LYS:NZ	2.23	0.71
17:B:809:CLA:HHC	17:B:809:CLA:HBB1	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1:311:CLA:HAB	17:1:311:CLA:H122	1.70	0.71
4:4:144:ILE:HD12	4:4:148:LEU:HD22	1.72	0.71
6:B:16:PRO:HG3	7:C:74:THR:HG22	1.72	0.71
6:B:531:THR:HG21	17:B:827:CLA:HAB	1.73	0.71
12:H:89:PHE:HB3	15:L:50:ILE:HD13	1.73	0.71
17:A:853:CLA:H11	6:B:616:LEU:HD12	1.72	0.70
5:A:42:ARG:H	5:A:42:ARG:HD2	1.56	0.70
3:3:74:PRO:CD	20:3:615:XAT:O23	2.39	0.70
17:B:837:CLA:HBB1	17:B:837:CLA:HMB1	1.72	0.70
1:1:98:LEU:HD13	1:1:103:LYS:HE2	1.73	0.70
2:2:87:GLU:OE1	2:2:90:ARG:NH2	2.23	0.70
6:B:645:VAL:HG11	17:B:811:CLA:HMD2	1.74	0.70
18:3:601:CHL:HMD2	21:3:616:BCR:H323	1.73	0.70
10:F:178:ARG:NH2	10:F:219:GLU:OE1	2.23	0.69
17:A:803:CLA:H43	17:A:810:CLA:HMC2	1.74	0.69
5:A:488:PHE:HB3	17:A:835:CLA:H11	1.74	0.69
17:B:838:CLA:HBB1	17:B:838:CLA:HMB1	1.74	0.69
17:A:825:CLA:HMB2	17:A:837:CLA:HBA1	1.74	0.69
5:A:401:TRP:HB3	17:A:827:CLA:HMC3	1.75	0.69
17:A:834:CLA:HMB1	21:A:850:BCR:H281	1.74	0.69
6:B:711:VAL:HG22	26:B:850:DGD:HBW2	1.76	0.68
18:3:601:CHL:C9	18:3:601:CHL:C6	2.71	0.68
6:B:463:ILE:HD11	17:B:837:CLA:H2	1.75	0.68
6:B:546:LEU:O	6:B:564:ARG:NH1	2.27	0.68
17:A:829:CLA:HBB1	17:A:829:CLA:HMB1	1.76	0.68
6:B:158:GLN:HB2	6:B:161:TRP:HD1	1.58	0.68
15:L:35:ASN:HB3	17:L:202:CLA:HAC1	1.77	0.67
5:A:64:PHE:CD2	17:A:804:CLA:HMC2	2.30	0.67
22:1:317:LHG:HC81	21:4:318:BCR:HC42	1.76	0.67
5:A:26:PRO:HB2	5:A:27:ILE:HD12	1.76	0.67
17:A:805:CLA:H151	17:A:828:CLA:HBB2	1.77	0.67
6:B:700:LEU:HD22	6:B:704:GLN:NE2	2.10	0.67
2:2:110:ILE:HG22	20:2:315:XAT:H41	1.76	0.66
6:B:129:LEU:HD12	6:B:134:ASP:HB3	1.76	0.66
17:A:821:CLA:HMD2	21:A:846:BCR:H23C	1.77	0.66
17:4:304:CLA:HMB1	17:4:304:CLA:HBB1	1.76	0.66
11:G:78:ILE:HG12	24:G:101:LMG:H262	1.76	0.66
17:A:828:CLA:H61	21:A:848:BCR:H342	1.77	0.66
17:B:810:CLA:H92	21:B:849:BCR:HC7	1.77	0.66
1:1:87:VAL:HG11	19:1:314:LUT:H10	1.77	0.66
26:4:323:DGD:HBN2	26:4:323:DGD:HB91	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:148:VAL:HG23	2:2:149:PHE:HD1	1.59	0.66
17:2:301:CLA:H72	20:2:315:XAT:H28	1.78	0.65
11:G:42:VAL:HG13	11:G:46:GLU:HB2	1.79	0.65
24:B:852:LMG:H111	24:B:852:LMG:H182	1.77	0.65
22:2:317:LHG:HC82	22:2:317:LHG:H262	1.78	0.65
21:A:846:BCR:H353	21:K:203:BCR:H323	1.77	0.65
1:1:79:HIS:HD2	20:1:315:XAT:H15	1.62	0.65
17:B:839:CLA:HBB1	17:B:839:CLA:HMB1	1.78	0.65
4:4:166:VAL:HG13	18:4:307:CHL:HMC	1.78	0.64
11:G:64:PRO:HG2	17:G:105:CLA:HBC2	1.79	0.64
16:K:67:ARG:NH1	16:K:94:ASP:OD2	2.31	0.64
26:4:323:DGD:HBE1	26:4:323:DGD:C7B	2.28	0.64
22:2:317:LHG:H132	18:3:601:CHL:H2	1.80	0.64
17:4:302:CLA:HBB1	17:4:302:CLA:HMB1	1.79	0.64
5:A:33:GLN:HB2	17:A:810:CLA:HAA2	1.80	0.64
17:A:839:CLA:HHC	17:A:839:CLA:HBB1	1.81	0.63
6:B:222:LEU:HB2	24:B:852:LMG:HC4	1.80	0.63
6:B:5:PHE:CB	6:B:6:PRO:HD3	2.29	0.63
17:3:609:CLA:HAB	19:3:614:LUT:H32	1.80	0.63
8:D:210:LEU:HD22	8:D:210:LEU:H	1.63	0.63
5:A:231:GLN:HG2	5:A:258:LEU:HD22	1.81	0.62
17:B:835:CLA:H18	17:B:836:CLA:HBC3	1.81	0.62
22:1:317:LHG:HC42	18:4:301:CHL:HAC2	1.82	0.62
14:J:8:LEU:HB3	25:J:102:HTG:H7'2	1.81	0.62
1:1:109:ALA:HB2	18:1:305:CHL:HMD1	1.80	0.62
6:B:527:LEU:O	6:B:531:THR:HG23	2.00	0.62
17:F:306:CLA:HHC	17:F:306:CLA:HBB1	1.80	0.62
1:1:179:LYS:HD3	17:1:310:CLA:HBA1	1.79	0.62
2:2:149:PHE:CD2	21:2:316:BCR:H15C	2.35	0.62
24:4:320:LMG:O5	24:4:320:LMG:O4	2.18	0.62
18:2:306:CHL:HBB2	18:2:313:CHL:C2C	2.30	0.62
4:4:60:LEU:HD21	25:4:321:HTG:S1	2.40	0.62
17:A:835:CLA:HBB1	17:A:835:CLA:HMB1	1.82	0.62
1:1:145:ARG:NH1	17:1:307:CLA:O1D	2.26	0.62
17:1:304:CLA:H2A	17:1:304:CLA:HED3	1.82	0.61
5:A:335:LYS:H	17:A:843:CLA:HBC3	1.64	0.61
17:A:838:CLA:H91	17:F:306:CLA:HAC2	1.82	0.61
6:B:208:ARG:NE	17:B:816:CLA:HED2	2.15	0.61
18:4:301:CHL:H8	21:4:318:BCR:H311	1.82	0.61
6:B:656:VAL:HG22	17:B:841:CLA:HMB3	1.82	0.61
4:4:247:GLN:HE21	4:4:247:GLN:N	1.98	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:716:VAL:HG13	10:F:178:ARG:HG3	1.82	0.61
6:B:411:MET:HE3	21:B:847:BCR:H292	1.82	0.61
2:2:149:PHE:HB3	21:2:316:BCR:H17C	1.82	0.61
26:4:323:DGD:HD5	26:4:323:DGD:O2E	2.01	0.61
2:2:106:GLY:HA2	20:2:315:XAT:H181	1.82	0.61
5:A:564:ARG:HA	5:A:573:ALA:HB2	1.82	0.61
22:2:317:LHG:H141	18:3:601:CHL:H52	1.82	0.61
17:A:853:CLA:HHB	17:B:804:CLA:H202	1.82	0.61
2:2:149:PHE:HA	21:2:316:BCR:H351	1.83	0.60
18:2:305:CHL:HBB1	18:2:305:CHL:HHC	1.82	0.60
4:4:155:ARG:CG	18:4:301:CHL:HED3	2.29	0.60
24:4:320:LMG:H171	24:4:320:LMG:H311	1.83	0.60
26:4:323:DGD:O2D	26:4:323:DGD:HG2	2.01	0.60
5:A:346:LEU:HD13	17:A:823:CLA:HMD3	1.83	0.60
1:1:77:LEU:HD12	1:1:155:LYS:HB2	1.84	0.60
3:3:77:LEU:HD23	17:3:602:CLA:H11	1.83	0.60
18:2:306:CHL:H12	17:2:308:CLA:HBC2	1.83	0.59
26:4:323:DGD:O1B	26:4:323:DGD:HA32	2.01	0.59
17:B:836:CLA:HBB1	17:B:836:CLA:HMB1	1.83	0.59
12:H:73:TYR:OH	15:L:24:THR:O	2.17	0.59
17:B:809:CLA:H2	21:I:101:BCR:HC42	1.83	0.59
5:A:662:SER:O	5:A:666:GLN:HG2	2.02	0.59
6:B:91:ILE:HD11	6:B:96:PHE:CE2	2.38	0.59
1:1:120:ASN:N	1:1:120:ASN:OD1	2.36	0.59
11:G:43:THR:OG1	11:G:46:GLU:HG3	2.02	0.59
21:L:205:BCR:H403	21:L:205:BCR:H23C	1.83	0.59
17:A:837:CLA:H111	21:A:849:BCR:H10C	1.85	0.59
6:B:560:ASP:OD2	6:B:564:ARG:NH2	2.36	0.59
17:B:822:CLA:HBC3	21:B:845:BCR:H332	1.85	0.59
4:4:192:LEU:HD12	19:4:316:LUT:H222	1.84	0.58
17:B:803:CLA:HAA1	15:L:24:THR:HG22	1.85	0.58
17:J:101:CLA:HBB1	17:J:101:CLA:HMB1	1.83	0.58
5:A:558:LYS:HE3	6:B:674:LEU:HB2	1.84	0.58
17:G:104:CLA:HHC	17:G:104:CLA:HBB1	1.83	0.58
26:4:323:DGD:HD1	26:4:323:DGD:C1G	2.24	0.58
15:L:54:LEU:HB3	17:L:202:CLA:HMA2	1.85	0.58
18:2:313:CHL:HHC	18:2:313:CHL:HBB1	1.86	0.58
10:F:172:TRP:CD1	10:F:209:GLY:HA3	2.38	0.58
18:4:315:CHL:HHC	18:4:315:CHL:HBB1	1.84	0.58
13:I:24:LEU:HD13	21:L:205:BCR:HC8	1.85	0.58
17:2:302:CLA:HMB1	17:2:302:CLA:HBB1	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:65:LEU:HD11	21:B:846:BCR:HC42	1.85	0.58
17:4:303:CLA:HBB1	20:4:317:XAT:H35	1.85	0.58
17:A:841:CLA:H161	15:L:91:LEU:HD21	1.86	0.58
15:L:109:SER:HB3	15:L:123:PRO:HB2	1.85	0.58
12:H:76:ASP:OD1	12:H:76:ASP:N	2.36	0.57
5:A:141:ARG:HG3	10:F:114:PRO:HB3	1.85	0.57
6:B:667:TRP:HA	27:B:843:PQN:H8	1.86	0.57
5:A:124:TRP:CD2	17:A:808:CLA:HED3	2.40	0.57
2:2:110:ILE:HG22	20:2:315:XAT:C4	2.33	0.57
5:A:375:HIS:ND1	17:A:817:CLA:OBD	2.38	0.57
6:B:177:HIS:CG	17:B:815:CLA:HMC2	2.40	0.57
10:F:204:ARG:HD3	22:F:302:LHG:H272	1.87	0.57
3:3:232:ILE:HG21	20:3:615:XAT:H14	1.87	0.57
1:1:138:ILE:HG21	17:1:307:CLA:HMC3	1.86	0.57
4:4:233:LEU:O	4:4:237:ILE:HG13	2.05	0.57
17:A:819:CLA:HBB2	21:A:847:BCR:H333	1.87	0.57
26:4:323:DGD:O1B	26:4:323:DGD:HA41	2.05	0.57
6:B:733:PHE:HD2	12:H:141:ARG:HH21	1.52	0.57
17:A:802:CLA:HBB1	17:A:802:CLA:HMB1	1.86	0.57
17:A:805:CLA:H92	22:A:844:LHG:H351	1.87	0.57
18:4:305:CHL:H2	21:4:318:BCR:H19C	1.86	0.56
17:B:812:CLA:H52	15:L:83:ALA:HB2	1.86	0.56
17:B:822:CLA:HBB1	17:B:822:CLA:HMB1	1.87	0.56
18:4:305:CHL:C2	21:4:318:BCR:H19C	2.35	0.56
17:A:825:CLA:H51	17:A:835:CLA:H51	1.86	0.56
17:B:809:CLA:H111	21:I:101:BCR:HC31	1.87	0.56
17:1:302:CLA:HMB1	17:1:302:CLA:HBB1	1.87	0.56
17:B:828:CLA:H122	21:B:847:BCR:H373	1.87	0.56
17:B:842:CLA:HMB1	17:B:842:CLA:HBB1	1.88	0.56
8:D:173:TYR:HB3	8:D:175:GLU:OE2	2.04	0.56
17:B:827:CLA:H43	17:B:835:CLA:HBB2	1.87	0.56
17:1:303:CLA:H2	17:1:304:CLA:HBD	1.87	0.56
17:4:303:CLA:C2C	20:4:317:XAT:H203	2.36	0.56
5:A:268:PRO:HB3	5:A:276:LYS:HD2	1.88	0.56
17:A:801:CLA:HED1	29:A:923:HOH:O	2.04	0.56
8:D:144:LEU:HB3	8:D:150:ILE:HG12	1.88	0.56
17:G:104:CLA:H3A	21:G:106:BCR:H363	1.87	0.56
17:B:828:CLA:HED1	17:B:835:CLA:HAB	1.88	0.56
7:C:35:LYS:O	7:C:37:LYS:HD3	2.06	0.56
17:B:806:CLA:HBC1	26:B:850:DGD:HAT1	1.87	0.56
17:B:836:CLA:HBA2	17:G:103:CLA:HMB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:317:LHG:H372	22:1:317:LHG:H192	1.88	0.56
5:A:40:PHE:HB3	17:A:803:CLA:HED2	1.86	0.56
5:A:251:ASN:HB3	5:A:254:LEU:HD13	1.87	0.56
6:B:26:ALA:HB2	26:B:850:DGD:HA32	1.88	0.56
6:B:374:HIS:HB2	17:B:829:CLA:C1B	2.36	0.56
17:B:806:CLA:HBC3	17:B:831:CLA:H41	1.88	0.56
8:D:76:PRO:HG2	8:D:78:THR:HG22	1.87	0.56
5:A:312:ILE:HG22	21:A:846:BCR:H17C	1.87	0.55
17:B:805:CLA:H111	21:B:849:BCR:H362	1.88	0.55
1:1:115:ALA:HB3	1:1:125:GLY:HA3	1.89	0.55
17:3:608:CLA:H12	17:3:613:CLA:HAB	1.88	0.55
4:4:125:LYS:HD2	4:4:127:TYR:OH	2.07	0.55
5:A:475:ASP:OD1	15:L:71:ARG:NH2	2.40	0.55
26:4:323:DGD:CBB	26:4:323:DGD:CFB	2.85	0.55
6:B:295:PHE:HB2	17:B:822:CLA:HED1	1.88	0.55
5:A:700:TRP:CZ2	27:A:842:PQN:H2M3	2.42	0.55
15:L:111:ALA:HB2	15:L:127:GLN:HG3	1.88	0.55
5:A:261:SER:HB3	5:A:277:TYR:HD1	1.71	0.55
26:4:323:DGD:CFB	26:4:323:DGD:CAB	2.85	0.54
17:B:834:CLA:HHB	25:F:305:HTG:H61	1.88	0.54
24:B:852:LMG:H222	24:B:852:LMG:H291	1.88	0.54
5:A:368:LEU:HD11	17:A:818:CLA:H71	1.89	0.54
6:B:203:ARG:HD2	6:B:250:ALA:HB1	1.89	0.54
17:4:311:CLA:HED3	17:4:311:CLA:H51	1.89	0.54
5:A:209:GLY:HA2	17:A:819:CLA:HBC1	1.88	0.54
17:B:809:CLA:H102	21:I:101:BCR:HC41	1.90	0.54
2:2:100:SER:HB3	2:2:215:GLY:HA3	1.89	0.54
17:2:301:CLA:HAB	20:2:315:XAT:H32	1.90	0.54
17:A:820:CLA:HMB2	17:A:824:CLA:HMA3	1.89	0.54
17:B:811:CLA:HMB1	17:B:811:CLA:HBB1	1.89	0.54
1:1:142:GLU:OE2	1:1:145:ARG:NH2	2.41	0.54
26:4:323:DGD:HBN2	26:4:323:DGD:C9B	2.38	0.54
6:B:671:TRP:CZ2	27:B:843:PQN:H2M3	2.43	0.54
17:2:303:CLA:HMB1	17:2:303:CLA:HBB1	1.89	0.53
5:A:645:SER:O	5:A:651:GLY:HA3	2.07	0.53
4:4:125:LYS:HE3	4:4:231:ASP:OD2	2.07	0.53
4:4:151:TYR:HB2	18:4:301:CHL:H11	1.89	0.53
4:4:190:ASN:HA	19:4:316:LUT:H24	1.89	0.53
16:K:107:GLY:O	16:K:111:HIS:ND1	2.41	0.53
17:1:301:CLA:HMB1	17:1:301:CLA:HBB1	1.89	0.53
6:B:303:TYR:CG	11:G:34:GLN:CB	2.87	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:823:CLA:HMB2	17:B:824:CLA:H52	1.89	0.53
7:C:17:CYS:HB2	7:C:54:CYS:HB2	1.89	0.53
2:2:101:ARG:NH1	18:2:306:CHL:OBD	2.35	0.53
2:2:146:GLU:OE2	18:2:305:CHL:HMC	2.09	0.53
5:A:406:LEU:HD21	17:A:805:CLA:H142	1.90	0.53
5:A:441:ALA:O	5:A:445:HIS:ND1	2.41	0.53
21:A:851:BCR:H382	21:A:851:BCR:H23C	1.90	0.53
14:J:32:PHE:CE2	17:J:103:CLA:HMA3	2.43	0.53
6:B:443:MET:SD	6:B:451:LYS:HE3	2.49	0.53
15:L:33:LEU:HA	15:L:36:LEU:HD22	1.91	0.53
17:A:818:CLA:H112	17:A:820:CLA:HBB2	1.91	0.53
6:B:15:ASP:HB3	6:B:20:ARG:HB2	1.90	0.53
15:L:95:LEU:HD21	21:L:205:BCR:H383	1.91	0.53
17:1:304:CLA:HBB2	18:1:305:CHL:HBB2	1.91	0.53
4:4:155:ARG:CG	18:4:301:CHL:CED	2.87	0.53
24:4:320:LMG:H162	24:4:320:LMG:H292	1.89	0.53
6:B:350:GLN:HG3	17:B:827:CLA:HED1	1.90	0.53
17:2:311:CLA:HMC2	17:2:311:CLA:H92	1.91	0.53
17:2:312:CLA:HAA2	3:3:154:LEU:HG	1.91	0.53
4:4:144:ILE:HG13	4:4:145:GLU:N	2.23	0.53
22:1:317:LHG:H132	18:4:301:CHL:H2	1.90	0.52
4:4:247:GLN:N	4:4:247:GLN:NE2	2.57	0.52
5:A:124:TRP:HD1	23:A:855:LMT:H6'2	1.75	0.52
2:2:58:PHE:HE1	18:3:601:CHL:HED3	1.74	0.52
4:4:247:GLN:HE21	4:4:247:GLN:CA	2.21	0.52
5:A:654:ARG:HD2	5:A:655:ASP:OD1	2.10	0.52
17:A:827:CLA:HBB1	17:A:827:CLA:HMB1	1.91	0.52
17:B:838:CLA:H152	21:F:308:BCR:H23C	1.91	0.52
17:1:304:CLA:HBB2	18:1:305:CHL:CBB	2.39	0.52
17:4:303:CLA:C1C	20:4:317:XAT:H203	2.40	0.52
6:B:497:TRP:CE3	17:B:819:CLA:H11	2.44	0.52
1:1:216:ASP:OD1	1:1:216:ASP:N	2.43	0.52
5:A:530:LEU:HD11	5:A:624:VAL:HA	1.91	0.52
5:A:483:GLN:HB3	5:A:485:GLN:HE21	1.74	0.52
17:A:805:CLA:CBB	17:A:828:CLA:HMC2	2.39	0.52
10:F:195:ILE:HG13	10:F:196:ILE:HG13	1.91	0.52
2:2:71:LEU:HD11	2:2:89:LEU:HD11	1.91	0.52
3:3:74:PRO:HD2	20:3:615:XAT:C23	2.40	0.52
4:4:145:GLU:OE1	18:4:306:CHL:HMC	2.10	0.52
26:4:323:DGD:HBE2	26:4:323:DGD:CFB	2.39	0.52
4:4:112:PRO:O	4:4:116:THR:HG23	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:4:321:HTG:H7'3	22:F:302:LHG:H141	1.92	0.52
17:A:823:CLA:HHB	17:A:843:CLA:CBB	2.40	0.52
17:4:302:CLA:HAB	20:4:317:XAT:H32	1.91	0.51
5:A:205:HIS:CG	17:A:812:CLA:HMC2	2.46	0.51
17:A:816:CLA:CHD	17:A:817:CLA:HBB2	2.40	0.51
17:B:827:CLA:CHB	17:B:839:CLA:HBA2	2.40	0.51
1:1:70:GLU:OE2	1:1:155:LYS:NZ	2.33	0.51
5:A:434:ARG:HH11	5:A:437:ARG:HH12	1.56	0.51
17:A:837:CLA:HBB1	17:A:837:CLA:HMB1	1.91	0.51
6:B:2:ALA:N	6:B:10:GLN:HB2	2.24	0.51
17:B:803:CLA:H92	21:L:206:BCR:H402	1.92	0.51
17:B:837:CLA:C4	17:F:307:CLA:HBB2	2.39	0.51
8:D:188:PHE:HB3	9:E:35:ARG:HH12	1.75	0.51
11:G:89:THR:HG22	24:G:101:LMG:HC72	1.91	0.51
2:2:150:ILE:HG21	17:2:307:CLA:HMC3	1.93	0.51
5:A:519:ASP:N	5:A:519:ASP:OD1	2.43	0.51
17:A:814:CLA:H43	21:A:846:BCR:HC41	1.93	0.51
17:A:836:CLA:HBB1	17:A:836:CLA:HMB1	1.93	0.51
17:K:201:CLA:H3A	21:K:203:BCR:H363	1.92	0.51
2:2:219:MET:HB3	20:2:315:XAT:C40	2.30	0.51
17:B:836:CLA:HMD2	17:G:103:CLA:HBB1	1.93	0.51
11:G:34:GLN:O	11:G:34:GLN:HG3	2.10	0.51
5:A:68:THR:HG22	5:A:70:ASP:H	1.76	0.51
6:B:282:ILE:HG21	17:B:818:CLA:H92	1.93	0.51
24:B:852:LMG:H341	17:G:104:CLA:HMC3	1.93	0.51
2:2:176:ASN:HB3	18:2:313:CHL:C2D	2.41	0.51
11:G:18:LEU:HA	11:G:22:VAL:HG13	1.93	0.51
5:A:446:LEU:HD13	5:A:554:LEU:HA	1.92	0.51
21:A:851:BCR:H21C	17:A:853:CLA:H143	1.93	0.51
4:4:155:ARG:NH1	18:4:315:CHL:HMC	2.26	0.50
17:K:201:CLA:H3A	21:K:203:BCR:C36	2.41	0.50
2:2:114:GLU:HG2	2:2:236:PRO:HD2	1.93	0.50
26:4:323:DGD:HBN2	26:4:323:DGD:CAB	2.41	0.50
26:4:323:DGD:C7B	26:4:323:DGD:CBB	2.85	0.50
17:B:825:CLA:HAB	17:B:832:CLA:HMD2	1.92	0.50
15:L:71:ARG:NH1	15:L:72:ASN:OD1	2.44	0.50
17:2:309:CLA:HMA3	22:2:317:LHG:HC32	1.93	0.50
4:4:90:TRP:NE1	26:4:323:DGD:HE4	2.26	0.50
10:F:199:VAL:O	10:F:203:THR:HG23	2.12	0.50
1:1:91:LEU:HD21	19:1:314:LUT:H173	1.93	0.50
17:1:310:CLA:HMC2	19:1:314:LUT:C11	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1:317:LHG:H301	17:4:314:CLA:HED1	1.94	0.50
17:4:304:CLA:H2	21:4:318:BCR:H272	1.94	0.50
17:1:308:CLA:HHC	19:1:314:LUT:H32	1.93	0.50
17:A:839:CLA:HBB2	27:A:842:PQN:H141	1.94	0.50
17:A:808:CLA:HMA1	14:J:27:ILE:HD13	1.94	0.50
17:A:824:CLA:HMB1	17:A:824:CLA:HBB1	1.93	0.50
6:B:82:LEU:HD22	6:B:363:GLN:HG3	1.94	0.50
21:B:844:BCR:H362	21:G:106:BCR:H312	1.94	0.50
1:1:188:LEU:HB3	20:1:315:XAT:H402	1.94	0.49
5:A:335:LYS:O	17:A:843:CLA:HBC3	2.11	0.49
6:B:411:MET:HG3	21:B:847:BCR:H402	1.94	0.49
17:B:810:CLA:HMC3	17:B:811:CLA:C3D	2.41	0.49
17:1:310:CLA:HMC2	19:1:314:LUT:H11	1.94	0.49
6:B:194:LEU:HA	6:B:198:ALA:HB3	1.94	0.49
6:B:593:TYR:CE1	17:B:837:CLA:HBC2	2.47	0.49
14:J:31:ARG:HD3	21:J:105:BCR:C31	2.41	0.49
1:1:190:ALA:HA	17:1:311:CLA:HBB1	1.95	0.49
17:A:806:CLA:H102	17:A:808:CLA:H92	1.94	0.49
6:B:617:MET:HE3	6:B:620:LEU:HB3	1.93	0.49
17:3:612:CLA:HBB1	17:3:612:CLA:HMB1	1.95	0.49
5:A:358:LEU:HB2	17:A:804:CLA:HMD3	1.94	0.49
6:B:5:PHE:CD1	6:B:5:PHE:C	2.83	0.49
1:1:165:GLY:HA3	1:1:168:LYS:HE3	1.93	0.49
2:2:207:LEU:HD22	17:2:308:CLA:HHB	1.93	0.49
26:4:323:DGD:HBT1	26:4:323:DGD:CFB	2.41	0.49
1:1:107:TRP:CZ2	1:1:115:ALA:HB2	2.47	0.49
1:1:177:LYS:O	1:1:181:VAL:HG23	2.13	0.49
3:3:238:GLN:OE1	19:3:614:LUT:H42	2.12	0.49
5:A:125:PRO:HA	5:A:130:GLU:HG3	1.94	0.49
17:B:819:CLA:HAC2	17:B:826:CLA:H202	1.94	0.49
17:1:302:CLA:HMD2	17:1:307:CLA:C1D	2.43	0.49
17:A:853:CLA:HBB1	17:A:853:CLA:HMB1	1.93	0.49
2:2:148:VAL:HG23	2:2:149:PHE:CD1	2.45	0.49
5:A:415:ALA:HB1	5:A:594:ALA:HB1	1.95	0.49
6:B:344:ILE:HD11	17:B:830:CLA:HBC1	1.95	0.49
17:B:837:CLA:H41	17:F:307:CLA:HBB2	1.94	0.49
17:1:304:CLA:HMC3	18:1:305:CHL:C2C	2.43	0.49
4:4:140:THR:O	4:4:144:ILE:HG23	2.13	0.49
4:4:155:ARG:NH1	4:4:166:VAL:HG22	2.28	0.49
5:A:183:TRP:HB2	17:A:810:CLA:HMC3	1.94	0.49
5:A:665:ILE:HD12	6:B:621:ARG:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:832:CLA:H191	17:B:803:CLA:H93	1.93	0.49
17:4:314:CLA:HBC2	26:4:323:DGD:HA81	1.95	0.49
17:B:811:CLA:H102	17:B:829:CLA:H193	1.93	0.49
17:B:838:CLA:HMB2	17:B:839:CLA:C2D	2.43	0.49
7:C:15:THR:HG22	7:C:28:MET:HG3	1.95	0.49
18:4:307:CHL:CGA	17:4:309:CLA:HMD2	2.43	0.48
5:A:80:SER:OG	5:A:186:TYR:HB2	2.12	0.48
17:A:819:CLA:HBB1	21:A:846:BCR:H14C	1.94	0.48
7:C:31:TRP:HB2	7:C:39:ILE:HG22	1.94	0.48
8:D:200:VAL:HG11	8:D:210:LEU:HD21	1.94	0.48
1:1:155:LYS:HG3	1:1:156:TYR:CD2	2.48	0.48
18:3:601:CHL:HHC	18:3:601:CHL:HBB1	1.95	0.48
5:A:208:ALA:HB2	5:A:314:GLY:HA3	1.95	0.48
17:A:841:CLA:H151	21:L:201:BCR:H351	1.95	0.48
17:3:602:CLA:CAB	20:3:615:XAT:H32	2.30	0.48
6:B:34:HIS:O	6:B:37:ILE:HG13	2.13	0.48
18:4:306:CHL:H3A	18:4:306:CHL:HBA2	1.55	0.48
6:B:218:HIS:HE1	6:B:220:GLN:HG3	1.79	0.48
17:B:821:CLA:H203	17:B:826:CLA:H171	1.95	0.48
21:B:847:BCR:H393	21:B:848:BCR:H383	1.93	0.48
12:H:130:LYS:HE3	12:H:133:GLN:NE2	2.29	0.48
15:L:66:LYS:HE3	17:L:204:CLA:H11	1.96	0.48
17:3:603:CLA:HMC2	20:3:615:XAT:H12	1.94	0.48
5:A:336:GLY:N	22:A:845:LHG:HC32	2.29	0.48
17:A:802:CLA:OBD	17:B:804:CLA:HMB3	2.13	0.48
17:A:825:CLA:HBB1	17:A:825:CLA:HMB1	1.95	0.48
17:B:816:CLA:H141	21:B:845:BCR:H16C	1.95	0.48
5:A:308:ILE:HD12	21:K:203:BCR:HC31	1.94	0.48
17:B:825:CLA:H42	17:B:826:CLA:H112	1.94	0.48
17:B:832:CLA:HBA2	17:B:842:CLA:H41	1.96	0.48
11:G:28:ARG:NH2	11:G:71:ASP:OD2	2.46	0.48
17:1:308:CLA:H92	17:1:308:CLA:H61	1.66	0.48
2:2:106:GLY:O	2:2:110:ILE:HG23	2.13	0.48
17:A:807:CLA:HBA2	17:A:807:CLA:H3A	1.44	0.48
14:J:32:PHE:HE2	17:J:103:CLA:HMA3	1.79	0.48
1:1:164:LEU:HD12	19:1:314:LUT:H222	1.94	0.48
17:2:311:CLA:CHB	17:2:312:CLA:HMD3	2.44	0.48
3:3:250:LEU:HB2	19:3:614:LUT:H22	1.96	0.48
6:B:542:ARG:NH2	29:B:906:HOH:O	2.47	0.48
24:B:852:LMG:HO2	24:B:852:LMG:HC71	1.77	0.48
17:J:103:CLA:HMD3	21:J:105:BCR:H333	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:139:THR:HA	2:2:142:LEU:HD12	1.96	0.48
4:4:224:VAL:HG12	4:4:225:THR:HG23	1.96	0.48
17:A:811:CLA:HHC	17:A:811:CLA:HBB1	1.95	0.48
6:B:106:ARG:NH2	6:B:113:VAL:O	2.41	0.48
17:B:824:CLA:HMB1	17:B:824:CLA:HBB1	1.96	0.48
17:2:311:CLA:H101	22:2:317:LHG:H311	1.96	0.47
17:A:825:CLA:H3A	17:A:837:CLA:O1A	2.14	0.47
17:A:830:CLA:HMA2	15:L:21:THR:HG21	1.95	0.47
2:2:110:ILE:HG22	20:2:315:XAT:C5	2.44	0.47
17:4:303:CLA:HMD2	17:4:308:CLA:CHD	2.44	0.47
12:H:65:ASN:OD1	12:H:70:TRP:NE1	2.42	0.47
12:H:82:ASN:HD22	12:H:82:ASN:HA	1.52	0.47
17:1:309:CLA:HBB2	21:4:318:BCR:H322	1.95	0.47
3:3:229:MET:HB3	20:3:615:XAT:C40	2.30	0.47
18:4:306:CHL:HBB1	20:4:317:XAT:H161	1.97	0.47
17:A:809:CLA:H12	17:A:811:CLA:H43	1.95	0.47
17:A:823:CLA:C2	21:A:849:BCR:H16C	2.44	0.47
3:3:112:ALA:HB3	3:3:113:PRO:HD3	1.96	0.47
4:4:157:TRP:CE2	4:4:161:LYS:HD2	2.50	0.47
11:G:69:ILE:HD12	11:G:69:ILE:H	1.79	0.47
12:H:85:GLN:HE22	17:L:202:CLA:H202	1.79	0.47
4:4:151:TYR:HE2	18:4:307:CHL:CBB	2.27	0.47
17:A:831:CLA:C3B	17:A:832:CLA:HMB2	2.45	0.47
6:B:80:ASP:OD2	6:B:83:HIS:HB2	2.13	0.47
17:B:808:CLA:H52	26:B:850:DGD:HB71	1.97	0.47
17:L:203:CLA:HMA1	17:L:204:CLA:HBC1	1.96	0.47
17:1:304:CLA:HMC3	18:1:305:CHL:C3C	2.45	0.47
17:A:831:CLA:HMC2	17:L:204:CLA:HBB2	1.96	0.47
25:J:102:HTG:H4'2	25:J:102:HTG:H1'1	1.60	0.47
17:1:309:CLA:HBC2	17:1:311:CLA:H141	1.96	0.47
2:2:111:PHE:CE2	19:2:314:LUT:H8	2.50	0.47
23:2:318:LMT:O6B	23:2:318:LMT:O4'	2.18	0.47
3:3:106:GLY:HA2	20:3:615:XAT:H181	1.96	0.47
4:4:76:PHE:HB3	17:4:302:CLA:CAD	2.45	0.47
17:A:817:CLA:H3A	17:A:817:CLA:HBA2	1.52	0.47
6:B:174:ARG:HD2	17:B:826:CLA:OBD	2.13	0.47
8:D:111:ILE:HG12	8:D:121:ILE:HG12	1.96	0.47
12:H:94:ALA:O	12:H:97:THR:OG1	2.23	0.47
16:K:47:ILE:HG23	16:K:48:GLY:H	1.79	0.47
2:2:104:MET:SD	17:2:308:CLA:HAB	2.55	0.47
4:4:105:GLY:HA3	20:4:317:XAT:C9	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:810:CLA:H102	17:A:810:CLA:H61	1.76	0.47
17:A:828:CLA:HBB1	17:A:828:CLA:HMB1	1.96	0.47
17:A:831:CLA:HMD2	17:A:832:CLA:H143	1.97	0.47
17:A:834:CLA:H3A	17:A:834:CLA:HBA2	1.67	0.47
6:B:662:MET:HB2	17:B:805:CLA:C1C	2.44	0.47
17:B:836:CLA:HAA1	17:G:103:CLA:HMA1	1.96	0.47
1:1:134:GLU:O	1:1:138:ILE:HB	2.15	0.47
17:4:308:CLA:HMB1	17:4:308:CLA:HBB1	1.97	0.47
6:B:59:LEU:HD21	17:B:809:CLA:H112	1.95	0.47
17:A:829:CLA:H62	17:A:829:CLA:H41	1.69	0.47
8:D:102:ILE:HG23	8:D:104:TRP:HZ3	1.80	0.47
17:1:309:CLA:CBB	21:4:318:BCR:H322	2.45	0.46
22:2:317:LHG:H142	22:2:317:LHG:H112	1.72	0.46
10:F:112:SER:HB2	10:F:114:PRO:HD2	1.97	0.46
17:A:804:CLA:HMB1	17:A:804:CLA:HBB1	1.97	0.46
17:B:838:CLA:C1A	17:B:838:CLA:CGA	2.93	0.46
3:3:113:PRO:HA	3:3:122:ILE:HD11	1.97	0.46
17:A:814:CLA:H12	21:A:846:BCR:HC31	1.97	0.46
7:C:7:ILE:HG12	7:C:40:ALA:HB3	1.97	0.46
10:F:78:ILE:HD11	10:F:154:ARG:NH1	2.30	0.46
10:F:99:LYS:HA	10:F:99:LYS:HD3	1.69	0.46
17:1:312:CLA:H3A	17:1:312:CLA:HBA2	1.50	0.46
2:2:194:LEU:HD12	19:2:314:LUT:H222	1.97	0.46
17:2:301:CLA:CAB	20:2:315:XAT:H32	2.45	0.46
6:B:676:GLU:HG2	7:C:81:TYR:HE2	1.80	0.46
17:B:833:CLA:HMB1	17:B:833:CLA:HBB1	1.97	0.46
17:1:302:CLA:H12	17:B:842:CLA:HMC3	1.97	0.46
17:1:307:CLA:H51	21:B:847:BCR:HC31	1.97	0.46
17:3:605:CLA:H3A	21:3:616:BCR:C21	2.45	0.46
17:B:832:CLA:HMB2	17:B:833:CLA:C2D	2.46	0.46
21:2:316:BCR:HC31	17:4:310:CLA:CAB	2.45	0.46
17:4:304:CLA:HBA2	25:4:322:HTG:S1	2.56	0.46
5:A:567:ARG:NH2	8:D:89:GLY:O	2.42	0.46
17:A:820:CLA:H2	17:A:820:CLA:H62	1.68	0.46
6:B:531:THR:HG22	17:B:827:CLA:HMC2	1.96	0.46
6:B:593:TYR:CZ	17:B:837:CLA:HBC2	2.50	0.46
17:B:827:CLA:HMB2	17:B:839:CLA:H3A	1.97	0.46
17:B:831:CLA:H13	26:B:850:DGD:HAF1	1.96	0.46
17:K:202:CLA:H41	17:K:202:CLA:H61	1.50	0.46
17:4:309:CLA:HBB1	17:4:309:CLA:HMB1	1.97	0.46
5:A:92:TRP:CZ2	17:A:827:CLA:HED2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:820:CLA:H192	17:A:820:CLA:H162	1.71	0.46
17:A:831:CLA:H111	17:A:831:CLA:H72	1.54	0.46
6:B:437:TYR:CZ	6:B:518:LEU:HB3	2.51	0.46
2:2:241:PHE:O	2:2:245:ALA:N	2.45	0.46
17:2:307:CLA:HHC	17:2:307:CLA:HBB1	1.96	0.46
3:3:110:ALA:HB1	3:3:130:TRP:HB3	1.97	0.46
18:4:305:CHL:HBB2	18:4:306:CHL:CBB	2.45	0.46
18:4:315:CHL:HBB2	21:4:318:BCR:HC8	1.98	0.46
17:B:825:CLA:H51	17:B:826:CLA:H142	1.97	0.46
8:D:189:ARG:HG2	8:D:190:SER:O	2.15	0.46
17:L:202:CLA:H151	17:L:202:CLA:H18	1.77	0.46
2:2:121:ILE:HD12	2:2:121:ILE:H	1.80	0.46
6:B:218:HIS:CD2	6:B:219:PRO:HD2	2.50	0.46
6:B:275:HIS:CD2	17:B:819:CLA:HAB	2.51	0.46
17:B:809:CLA:HED2	13:I:5:PRO:HB3	1.97	0.46
7:C:62:PHE:HD2	8:D:191:ILE:HG21	1.81	0.46
21:J:104:BCR:H20C	21:J:104:BCR:H361	1.75	0.46
15:L:95:LEU:HB3	15:L:136:THR:CG2	2.46	0.46
17:1:307:CLA:HBA2	17:1:307:CLA:H12	1.72	0.46
17:1:308:CLA:H92	19:1:314:LUT:H371	1.97	0.46
2:2:228:GLN:OE1	19:2:314:LUT:H42	2.16	0.46
4:4:81:LEU:HD13	17:4:302:CLA:H42	1.98	0.46
5:A:199:VAL:HG23	5:A:327:ILE:HD12	1.97	0.46
5:A:218:TRP:HD1	5:A:303:HIS:CD2	2.34	0.46
21:A:846:BCR:H20C	21:A:846:BCR:H361	1.74	0.46
10:F:212:TRP:CG	10:F:213:PRO:HD3	2.50	0.46
5:A:449:VAL:HG22	5:A:453:LEU:HD22	1.98	0.45
17:A:803:CLA:H2	17:A:810:CLA:H71	1.97	0.45
6:B:533:ILE:HD12	17:B:802:CLA:CMD	2.46	0.45
17:B:824:CLA:H43	22:G:102:LHG:H112	1.98	0.45
18:4:315:CHL:H2A	18:4:315:CHL:HED3	1.99	0.45
6:B:303:TYR:HE2	17:B:824:CLA:HED2	1.80	0.45
21:B:844:BCR:H15C	21:B:844:BCR:H351	1.81	0.45
17:1:302:CLA:H142	17:1:302:CLA:H111	1.81	0.45
17:B:810:CLA:H8	17:B:810:CLA:HBB1	1.99	0.45
17:B:834:CLA:H41	17:B:834:CLA:H61	1.81	0.45
3:3:66:LEU:HG	17:3:602:CLA:HED2	1.97	0.45
5:A:422:TYR:CE1	5:A:424:PRO:HD3	2.52	0.45
23:A:855:LMT:H6E	21:J:105:BCR:HC42	1.98	0.45
6:B:218:HIS:CG	6:B:219:PRO:HD2	2.52	0.45
17:2:311:CLA:H61	17:2:311:CLA:H2	1.62	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:832:CLA:HBC3	17:A:832:CLA:HHD	1.98	0.45
6:B:612:SER:O	6:B:618:GLY:HA3	2.17	0.45
17:B:827:CLA:H142	17:B:842:CLA:H203	1.98	0.45
10:F:156:TRP:CZ3	25:F:310:HTG:H2'1	2.51	0.45
17:L:202:CLA:HBA2	17:L:202:CLA:H3A	1.42	0.45
17:3:602:CLA:H71	20:3:615:XAT:H28	1.99	0.45
5:A:446:LEU:HB3	5:A:554:LEU:HD13	1.99	0.45
17:A:820:CLA:H122	17:A:823:CLA:H93	1.98	0.45
21:A:851:BCR:H371	21:A:851:BCR:H24C	1.72	0.45
6:B:4:ARG:HD3	6:B:13:ALA:O	2.16	0.45
17:B:810:CLA:H62	17:B:810:CLA:H102	1.74	0.45
18:2:313:CHL:HBB2	21:2:316:BCR:C8	2.47	0.45
26:4:323:DGD:HBN1	26:4:323:DGD:CBB	2.39	0.45
5:A:92:TRP:O	5:A:96:MET:HG2	2.17	0.45
5:A:151:GLN:H	5:A:151:GLN:HG2	1.44	0.45
5:A:417:PHE:CD1	5:A:421:ASP:HB2	2.52	0.45
17:A:824:CLA:HMB3	17:A:826:CLA:H93	1.99	0.45
6:B:257:LEU:HD22	6:B:493:TRP:HB3	1.99	0.45
11:G:84:TYR:OH	17:G:104:CLA:HMD2	2.17	0.45
2:2:101:ARG:HA	2:2:104:MET:HE3	1.98	0.45
2:2:202:GLN:N	2:2:202:GLN:OE1	2.47	0.45
3:3:83:THR:OG1	5:A:24:ARG:NH2	2.40	0.45
6:B:374:HIS:HB2	17:B:829:CLA:CHB	2.47	0.45
17:B:823:CLA:H92	17:B:823:CLA:H62	1.79	0.45
7:C:38:GLN:OE1	8:D:177:VAL:HG22	2.17	0.45
4:4:156:ARG:HG3	18:4:307:CHL:C1D	2.47	0.45
17:A:818:CLA:HBB1	17:A:818:CLA:HMB1	1.98	0.45
17:A:839:CLA:HMC2	21:F:303:BCR:H381	1.99	0.45
6:B:301:ILE:HG21	17:B:826:CLA:HAC1	1.99	0.45
6:B:694:ARG:NH2	15:L:101:SER:O	2.50	0.45
8:D:101:VAL:HB	8:D:128:LEU:HD11	1.97	0.45
6:B:531:THR:CG2	17:B:827:CLA:HAB	2.46	0.44
3:3:164:HIS:ND1	18:3:601:CHL:HBA1	2.32	0.44
17:3:603:CLA:HMD2	17:3:608:CLA:CHD	2.47	0.44
17:4:311:CLA:H51	17:4:311:CLA:H12	1.80	0.44
5:A:225:VAL:HG13	5:A:245:PRO:HB3	1.99	0.44
5:A:740:LEU:HD11	21:A:851:BCR:HC8	2.00	0.44
17:A:836:CLA:H41	17:A:836:CLA:H62	1.58	0.44
17:A:836:CLA:H91	17:L:203:CLA:H201	1.98	0.44
17:A:840:CLA:H41	17:A:840:CLA:H61	1.25	0.44
21:A:848:BCR:H20C	21:A:848:BCR:H361	1.74	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:170:ASP:HB3	2:2:173:PHE:O	2.17	0.44
17:2:309:CLA:C1D	17:2:310:CLA:HMD2	2.48	0.44
5:A:208:ALA:HB1	17:A:819:CLA:HBC3	1.99	0.44
5:A:237:VAL:HG22	5:A:242:ILE:HG12	1.99	0.44
5:A:546:ALA:HB1	17:A:836:CLA:HMB3	2.00	0.44
17:A:817:CLA:H91	17:A:817:CLA:H111	1.74	0.44
17:B:826:CLA:H161	17:B:826:CLA:H122	1.65	0.44
17:B:829:CLA:H142	17:B:829:CLA:H111	1.76	0.44
8:D:95:GLN:OE1	12:H:69:GLN:HG3	2.17	0.44
15:L:48:ARG:NH2	15:L:124:ASP:OD1	2.36	0.44
5:A:309:LEU:HG	17:A:820:CLA:HMC1	1.99	0.44
6:B:93:ASP:OD1	6:B:95:HIS:ND1	2.24	0.44
17:B:803:CLA:C4B	17:L:203:CLA:H93	2.47	0.44
17:B:821:CLA:HMC2	17:B:826:CLA:H151	1.99	0.44
24:F:309:LMG:H142	24:F:309:LMG:H171	1.60	0.44
21:L:206:BCR:H11C	21:L:206:BCR:H341	1.88	0.44
18:1:305:CHL:HMD2	17:G:103:CLA:HBC1	1.99	0.44
4:4:116:THR:HA	4:4:121:ILE:O	2.18	0.44
21:4:318:BCR:H20C	21:4:318:BCR:H361	1.79	0.44
5:A:580:PRO:HB3	5:A:727:ILE:HB	2.00	0.44
5:A:697:ARG:HB3	27:A:842:PQN:H7	1.99	0.44
17:A:841:CLA:H101	17:A:841:CLA:H13	1.77	0.44
27:A:842:PQN:H143	27:A:842:PQN:H112	1.91	0.44
22:B:801:LHG:HC62	17:B:842:CLA:HBA1	1.98	0.44
1:1:80:CYS:HB3	1:1:184:GLY:HA3	2.00	0.44
17:1:309:CLA:C1D	17:1:310:CLA:HMD2	2.48	0.44
22:2:317:LHG:HC2	18:3:601:CHL:HBC1	1.99	0.44
18:3:601:CHL:HBA2	17:3:613:CLA:O1D	2.18	0.44
4:4:155:ARG:CZ	4:4:166:VAL:HG22	2.47	0.44
17:4:311:CLA:HMC2	19:4:316:LUT:C11	2.48	0.44
5:A:288:ASP:HB3	5:A:291:THR:HG22	1.99	0.44
17:A:803:CLA:HBA2	17:A:803:CLA:H3A	1.73	0.44
17:B:803:CLA:H112	17:B:803:CLA:H91	1.73	0.44
7:C:31:TRP:CH2	7:C:33:GLY:HA3	2.53	0.44
6:B:475:ASP:HA	6:B:479:SER:HB3	1.99	0.44
17:B:841:CLA:H111	17:B:841:CLA:H152	1.73	0.44
8:D:103:THR:HA	8:D:127:ASN:O	2.18	0.44
8:D:156:ARG:HB2	8:D:166:LEU:HD11	1.99	0.44
1:1:173:PHE:CZ	17:1:308:CLA:HED3	2.53	0.44
1:1:217:PRO:O	1:1:221:THR:HG22	2.18	0.44
17:3:608:CLA:HMB2	17:3:613:CLA:C4B	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:197:GLN:NE2	5:A:351:THR:O	2.44	0.44
6:B:199:ILE:O	6:B:203:ARG:HG3	2.18	0.44
6:B:218:HIS:CE1	6:B:220:GLN:HG3	2.53	0.44
6:B:350:GLN:HG3	17:B:827:CLA:CED	2.48	0.44
6:B:395:ILE:HD11	6:B:541:ALA:HB1	1.99	0.44
17:J:101:CLA:H62	17:J:101:CLA:H102	1.53	0.44
2:2:227:PHE:O	2:2:231:TYR:HD2	2.01	0.44
17:2:302:CLA:HMD2	17:2:307:CLA:CHD	2.47	0.44
4:4:81:LEU:HD22	10:F:211:SER:HB3	1.99	0.44
5:A:515:TRP:O	5:A:517:GLY:N	2.51	0.44
17:A:838:CLA:H2	17:A:838:CLA:H61	1.82	0.44
6:B:619:TRP:O	6:B:623:TYR:HB3	2.17	0.44
6:B:645:VAL:CG1	17:B:811:CLA:HHD	2.48	0.44
17:L:203:CLA:H62	17:L:203:CLA:H41	1.71	0.44
5:A:334:HIS:HA	17:A:843:CLA:HBC2	2.00	0.43
17:A:838:CLA:C9	17:F:306:CLA:HAC2	2.47	0.43
6:B:330:ILE:HG22	17:B:807:CLA:HHD	2.00	0.43
6:B:410:ARG:HD3	17:B:832:CLA:OBD	2.17	0.43
17:B:810:CLA:H192	17:B:810:CLA:H162	1.79	0.43
15:L:61:VAL:HG21	15:L:150:ALA:HB3	1.99	0.43
2:2:156:ARG:NE	18:2:306:CHL:OMC	2.43	0.43
3:3:250:LEU:HD13	19:3:614:LUT:H163	2.00	0.43
17:4:304:CLA:C4B	20:4:317:XAT:H183	2.48	0.43
26:4:323:DGD:HBT2	26:4:323:DGD:HB72	1.61	0.43
5:A:210:LEU:HD11	17:A:812:CLA:H3A	2.00	0.43
5:A:305:ALA:HB1	17:A:816:CLA:HBC2	1.99	0.43
6:B:721:TYR:HB2	17:B:804:CLA:HED2	2.00	0.43
17:B:821:CLA:HBA2	17:B:825:CLA:H43	2.00	0.43
17:1:301:CLA:HAB	20:1:315:XAT:H32	2.01	0.43
17:3:605:CLA:HMB1	17:3:608:CLA:HBC2	1.98	0.43
5:A:58:HIS:HB2	22:A:844:LHG:H102	2.01	0.43
5:A:697:ARG:NH1	5:A:724:ALA:HB3	2.33	0.43
17:A:816:CLA:CED	17:A:816:CLA:H2A	2.48	0.43
17:A:837:CLA:H91	17:A:837:CLA:H112	1.82	0.43
17:B:815:CLA:H143	17:B:830:CLA:HMD2	1.99	0.43
17:2:308:CLA:H61	17:2:308:CLA:H101	1.69	0.43
3:3:214:LEU:HG	3:3:218:LYS:HE3	2.00	0.43
5:A:207:LEU:O	5:A:310:PHE:HB3	2.18	0.43
17:A:810:CLA:H121	17:J:101:CLA:HBB2	2.01	0.43
17:A:839:CLA:H92	17:A:839:CLA:H61	1.75	0.43
15:L:58:PHE:CD1	15:L:150:ALA:HB2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:226:ARG:HH22	17:3:602:CLA:HED3	1.83	0.43
5:A:343:HIS:HB3	5:A:346:LEU:HD12	2.00	0.43
17:A:840:CLA:H101	17:J:101:CLA:H43	2.00	0.43
6:B:387:PHE:CZ	21:B:848:BCR:H373	2.53	0.43
6:B:527:LEU:HD23	6:B:586:THR:HG21	2.00	0.43
17:B:810:CLA:C1A	17:B:810:CLA:CGA	2.96	0.43
2:2:115:PHE:HA	2:2:237:ILE:HG13	1.99	0.43
17:2:302:CLA:HMC2	20:2:315:XAT:C14	2.48	0.43
5:A:694:PHE:HB2	17:B:802:CLA:HBC2	2.00	0.43
21:A:849:BCR:H24C	21:A:849:BCR:H371	1.82	0.43
6:B:334:LEU:HB2	17:B:807:CLA:HMD3	2.01	0.43
21:B:845:BCR:H361	21:B:845:BCR:H20C	1.72	0.43
1:1:108:ALA:O	1:1:110:LEU:N	2.52	0.43
1:1:213:HIS:CG	17:1:311:CLA:HAA2	2.54	0.43
17:1:309:CLA:NA	22:1:317:LHG:O4	2.51	0.43
17:1:311:CLA:H2	17:1:312:CLA:OBD	2.19	0.43
2:2:59:PRO:HD2	18:3:601:CHL:O1D	2.19	0.43
2:2:162:LEU:HD21	23:2:318:LMT:H22	2.00	0.43
2:2:210:LYS:HD3	17:2:310:CLA:HBD	2.01	0.43
3:3:157:ALA:HA	18:3:601:CHL:H12	2.00	0.43
21:I:101:BCR:H20C	21:I:101:BCR:H361	1.85	0.43
14:J:16:THR:HG21	21:J:105:BCR:H403	2.00	0.43
2:2:220:LEU:HD21	17:2:301:CLA:HAC1	2.01	0.43
2:2:246:ASP:OD2	2:2:249:HIS:HB2	2.17	0.43
17:3:603:CLA:HMD2	17:3:608:CLA:C1D	2.49	0.43
17:3:608:CLA:HMB1	17:3:608:CLA:HBB1	2.01	0.43
5:A:335:LYS:HB2	5:A:340:GLY:O	2.18	0.43
17:A:805:CLA:HBB2	17:A:828:CLA:HMC2	2.01	0.43
17:A:808:CLA:HBB1	17:A:808:CLA:HMB1	2.00	0.43
17:A:811:CLA:H2	17:A:811:CLA:H61	1.77	0.43
6:B:472:TYR:HB3	10:F:79:ALA:HA	2.01	0.43
17:B:811:CLA:H143	17:B:811:CLA:H162	1.76	0.43
8:D:205:LYS:HD2	8:D:209:ASP:HB3	2.01	0.43
10:F:199:VAL:HB	25:J:102:HTG:H1'2	2.01	0.43
2:2:65:PRO:HD2	2:2:66:TRP:CZ3	2.53	0.43
17:2:302:CLA:HMD2	17:2:307:CLA:C1D	2.49	0.43
4:4:155:ARG:HG3	18:4:301:CHL:CED	2.36	0.43
17:A:803:CLA:H61	17:A:803:CLA:H93	1.73	0.43
17:A:807:CLA:H93	17:A:807:CLA:H61	1.80	0.43
17:A:818:CLA:H122	17:A:818:CLA:H162	1.43	0.43
6:B:72:GLY:HA2	6:B:87:ILE:HB	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:31:TRP:CZ2	7:C:33:GLY:HA3	2.54	0.43
15:L:55:ALA:HA	21:L:206:BCR:H16C	2.00	0.43
1:1:150:ASP:OD2	1:1:153:LYS:HG2	2.19	0.43
3:3:240:LEU:HG	17:A:814:CLA:HBA1	2.00	0.43
17:4:303:CLA:H101	17:4:303:CLA:H61	1.72	0.43
17:A:831:CLA:H61	17:A:831:CLA:H41	1.75	0.43
6:B:378:ILE:HD11	17:B:829:CLA:C3C	2.48	0.43
6:B:704:GLN:HG3	26:B:850:DGD:HA22	2.01	0.43
17:1:308:CLA:HBB1	17:1:310:CLA:H3A	2.01	0.42
17:2:312:CLA:HMB1	17:2:312:CLA:HBB1	2.01	0.42
17:4:302:CLA:HMC2	20:4:317:XAT:C31	2.49	0.42
5:A:126:ILE:HG13	5:A:127:VAL:HG13	2.01	0.42
5:A:306:ILE:HD13	5:A:306:ILE:HA	1.90	0.42
5:A:442:ILE:HG23	17:A:837:CLA:HBB2	2.01	0.42
17:A:822:CLA:HAB	17:A:843:CLA:CAB	2.49	0.42
6:B:671:TRP:CE2	27:B:843:PQN:H2M3	2.54	0.42
21:L:201:BCR:H333	17:L:203:CLA:NB	2.34	0.42
5:A:127:VAL:HB	17:B:834:CLA:HMD1	2.00	0.42
21:A:846:BCR:H372	16:K:105:ALA:HA	2.01	0.42
6:B:21:ILE:HG12	13:I:28:VAL:CG1	2.49	0.42
17:B:807:CLA:HBA1	17:B:807:CLA:H3A	1.87	0.42
17:B:823:CLA:H41	17:B:823:CLA:H61	1.46	0.42
1:1:69:LEU:HD23	1:1:69:LEU:HA	1.88	0.42
17:4:304:CLA:CAD	25:4:322:HTG:H1'1	2.49	0.42
6:B:85:ARG:HD2	6:B:115:ILE:HD13	2.02	0.42
17:B:803:CLA:H122	17:L:203:CLA:H172	2.01	0.42
26:B:850:DGD:HAH1	26:B:850:DGD:HAS2	1.67	0.42
7:C:15:THR:O	7:C:19:ARG:HG2	2.18	0.42
17:1:302:CLA:H11	17:1:302:CLA:H51	1.83	0.42
3:3:101:ARG:HD3	17:3:609:CLA:C4C	2.49	0.42
26:4:323:DGD:HBF2	26:4:323:DGD:HBV1	1.70	0.42
5:A:513:LEU:HD13	5:A:513:LEU:HA	1.92	0.42
17:A:820:CLA:H61	17:A:823:CLA:H2	2.01	0.42
18:4:301:CHL:C8	21:4:318:BCR:H311	2.48	0.42
17:4:302:CLA:H3A	17:4:302:CLA:CGA	2.50	0.42
21:B:847:BCR:H24C	21:B:847:BCR:H371	1.88	0.42
7:C:62:PHE:HB3	9:E:15:GLU:HG3	2.01	0.42
1:1:110:LEU:HD23	1:1:110:LEU:O	2.20	0.42
21:3:616:BCR:H15C	21:3:616:BCR:H351	1.88	0.42
17:A:810:CLA:H121	17:J:101:CLA:CBB	2.49	0.42
17:A:841:CLA:HMC2	17:B:840:CLA:H11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:411:MET:CE	21:B:847:BCR:H292	2.49	0.42
2:2:179:THR:HG23	2:2:188:GLY:HA2	2.01	0.42
17:4:304:CLA:HMB1	18:4:305:CHL:HBB1	2.01	0.42
5:A:218:TRP:HA	17:A:813:CLA:HAB	2.01	0.42
5:A:515:TRP:HA	5:A:515:TRP:CE3	2.54	0.42
17:A:819:CLA:HMA3	21:A:846:BCR:H373	2.01	0.42
17:B:815:CLA:H192	17:B:815:CLA:H161	1.83	0.42
17:B:837:CLA:H92	25:B:851:HTG:H6'2	2.02	0.42
17:1:308:CLA:CAB	19:1:314:LUT:H32	2.50	0.42
2:2:191:PHE:HB3	17:2:308:CLA:HMD1	2.01	0.42
26:4:323:DGD:HB22	10:F:221:LEU:CD2	2.50	0.42
5:A:301:HIS:CE1	17:A:817:CLA:HAB	2.54	0.42
5:A:330:ILE:O	5:A:334:HIS:ND1	2.53	0.42
5:A:435:VAL:HA	5:A:438:HIS:CE1	2.55	0.42
17:A:820:CLA:C4C	17:A:826:CLA:H152	2.50	0.42
17:A:825:CLA:H141	17:A:825:CLA:H161	1.86	0.42
21:A:850:BCR:H20C	21:A:850:BCR:H361	1.79	0.42
15:L:37:PRO:O	15:L:48:ARG:HD3	2.20	0.42
15:L:132:TRP:O	15:L:136:THR:HG23	2.19	0.42
24:4:320:LMG:H141	24:4:320:LMG:H111	1.48	0.42
17:A:804:CLA:H3A	17:A:804:CLA:HBA1	1.77	0.42
17:B:815:CLA:HMB1	17:B:815:CLA:HBB1	2.00	0.42
17:B:818:CLA:C1D	17:B:819:CLA:HBB2	2.50	0.42
17:B:828:CLA:HBB1	17:B:828:CLA:HMB1	2.00	0.42
7:C:17:CYS:SG	7:C:18:VAL:N	2.93	0.42
9:E:45:VAL:HB	9:E:49:ASN:HA	2.02	0.42
10:F:92:LYS:HE2	10:F:92:LYS:HB3	1.53	0.42
17:F:304:CLA:H112	17:F:304:CLA:H152	1.69	0.42
17:L:204:CLA:H3A	17:L:204:CLA:HBA1	1.22	0.42
4:4:54:GLY:HA3	4:4:74:ASN:OD1	2.20	0.42
5:A:629:ASN:HD22	5:A:633:VAL:HB	1.83	0.42
6:B:558:PRO:HB3	6:B:702:ILE:HB	2.02	0.42
17:B:812:CLA:H161	17:B:812:CLA:H141	1.78	0.42
21:B:846:BCR:H361	21:B:846:BCR:H20C	1.75	0.42
1:1:108:ALA:HB1	1:1:127:LEU:HD12	2.01	0.41
3:3:156:MET:HG3	17:3:608:CLA:HBB2	2.01	0.41
3:3:237:ILE:HG22	17:3:611:CLA:HMD3	2.02	0.41
3:3:241:VAL:HG13	3:3:242:THR:HG23	2.02	0.41
17:3:603:CLA:HBB1	20:3:615:XAT:C35	2.43	0.41
4:4:158:GLN:OE1	4:4:161:LYS:HE2	2.20	0.41
5:A:382:TYR:HD2	5:A:385:LEU:HD22	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:A:814:CLA:C3B	21:A:846:BCR:H333	2.50	0.41
17:B:820:CLA:H62	17:B:820:CLA:H41	1.71	0.41
18:2:304:CHL:H3A	21:2:316:BCR:H21C	2.02	0.41
18:4:305:CHL:HBB2	18:4:306:CHL:HBB1	2.02	0.41
21:4:318:BCR:H24C	21:4:318:BCR:H371	1.88	0.41
5:A:73:GLU:O	5:A:77:LYS:HG3	2.20	0.41
6:B:203:ARG:HD3	6:B:238:ASP:OD1	2.20	0.41
6:B:583:MET:HE2	6:B:583:MET:O	2.19	0.41
15:L:44:ASN:O	15:L:48:ARG:HG3	2.19	0.41
1:1:133:ILE:HD13	1:1:133:ILE:HA	1.93	0.41
2:2:104:MET:HB3	19:2:314:LUT:H402	2.02	0.41
5:A:20:ILE:HD13	17:A:809:CLA:HAA2	2.01	0.41
5:A:498:LEU:O	5:A:502:THR:OG1	2.29	0.41
5:A:682:ALA:HB1	5:A:741:GLY:O	2.19	0.41
17:A:841:CLA:H62	17:A:841:CLA:H41	1.55	0.41
6:B:51:PHE:HB3	6:B:149:SER:O	2.20	0.41
21:L:205:BCR:H20C	21:L:205:BCR:H361	1.85	0.41
18:4:305:CHL:H2	21:4:318:BCR:H17C	2.02	0.41
5:A:361:ASN:ND2	17:A:804:CLA:OBD	2.48	0.41
6:B:262:HIS:HA	6:B:263:PRO:HD3	1.91	0.41
17:B:827:CLA:H141	17:B:827:CLA:H161	1.83	0.41
21:F:308:BCR:H361	21:F:308:BCR:H20C	1.83	0.41
2:2:217:LEU:HD13	17:2:309:CLA:HBC1	2.02	0.41
4:4:213:LEU:HD23	4:4:213:LEU:HA	1.80	0.41
18:4:305:CHL:H71	18:4:307:CHL:HMB2	2.02	0.41
19:4:316:LUT:H31	19:4:316:LUT:H391	1.81	0.41
5:A:287:LEU:HD23	5:A:294:LEU:HD23	2.02	0.41
17:A:816:CLA:H143	17:A:816:CLA:H111	1.77	0.41
17:B:805:CLA:H111	17:B:805:CLA:H143	1.80	0.41
17:B:823:CLA:H143	17:B:823:CLA:H161	1.76	0.41
11:G:42:VAL:HG13	11:G:46:GLU:CB	2.49	0.41
2:2:58:PHE:CE1	18:3:601:CHL:HED3	2.55	0.41
2:2:100:SER:CB	2:2:215:GLY:HA3	2.49	0.41
23:2:318:LMT:H4O1	23:2:318:LMT:H6B	1.64	0.41
5:A:434:ARG:NH1	5:A:437:ARG:HH12	2.17	0.41
17:A:831:CLA:HMB2	21:L:201:BCR:C36	2.51	0.41
6:B:82:LEU:CD2	6:B:363:GLN:HG3	2.49	0.41
3:3:137:PRO:N	3:3:138:PRO:HD2	2.36	0.41
4:4:126:TRP:HB2	20:4:317:XAT:H3	2.03	0.41
5:A:95:GLY:N	17:A:806:CLA:HMC3	2.36	0.41
5:A:687:ALA:HB2	17:A:853:CLA:C3D	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:695:SER:OG	27:A:842:PQN:H9	2.21	0.41
17:A:804:CLA:H61	17:A:804:CLA:H101	1.88	0.41
17:A:808:CLA:H102	21:J:104:BCR:H332	2.01	0.41
17:A:824:CLA:HBA1	17:A:828:CLA:H193	2.01	0.41
6:B:270:LEU:HD23	6:B:273:MET:HE3	2.02	0.41
6:B:728:SER:O	6:B:732:LYS:HD3	2.21	0.41
17:B:810:CLA:H193	17:B:829:CLA:H18	2.03	0.41
7:C:55:GLU:HB3	7:C:63:LEU:HD13	2.03	0.41
8:D:168:PRO:HG3	8:D:173:TYR:CE1	2.55	0.41
12:H:130:LYS:HE3	12:H:133:GLN:HE21	1.85	0.41
2:2:238:ASP:OD1	2:2:238:ASP:N	2.54	0.41
17:A:840:CLA:H12	17:A:840:CLA:NA	2.35	0.41
10:F:92:LYS:O	10:F:96:GLN:HG2	2.21	0.41
1:1:103:LYS:HG3	1:1:106:GLU:OE2	2.21	0.41
1:1:163:PRO:HD2	19:1:314:LUT:H23	2.03	0.41
2:2:170:ASP:HB2	2:2:176:ASN:HB2	2.03	0.41
4:4:116:THR:HG22	4:4:121:ILE:HD12	2.03	0.41
4:4:155:ARG:CD	18:4:301:CHL:CED	2.98	0.41
18:4:306:CHL:HBC2	24:4:320:LMG:H312	2.03	0.41
21:4:318:BCR:H15C	21:4:318:BCR:H351	1.93	0.41
26:4:323:DGD:O2D	26:4:323:DGD:C3G	2.69	0.41
5:A:335:LYS:H	17:A:843:CLA:CBC	2.32	0.41
5:A:681:GLY:HA2	17:A:853:CLA:H41	2.03	0.41
17:A:803:CLA:H2	17:A:803:CLA:H62	1.71	0.41
17:A:804:CLA:H141	17:A:804:CLA:H161	1.69	0.41
6:B:42:LEU:O	6:B:46:ILE:HG13	2.21	0.41
6:B:53:GLN:HG2	17:B:807:CLA:H3A	2.03	0.41
6:B:129:LEU:HD13	17:B:816:CLA:HED3	2.03	0.41
6:B:387:PHE:CE2	21:B:848:BCR:H373	2.56	0.41
21:B:844:BCR:H20C	21:B:844:BCR:H361	1.85	0.41
21:B:848:BCR:H15C	21:B:848:BCR:H351	1.88	0.41
21:B:849:BCR:H361	21:B:849:BCR:H20C	1.78	0.41
7:C:19:ARG:HG2	7:C:19:ARG:H	1.55	0.41
24:G:101:LMG:H132	24:G:101:LMG:H161	1.83	0.41
5:A:77:LYS:HE2	5:A:186:TYR:OH	2.21	0.41
5:A:686:TRP:HZ3	17:A:853:CLA:HMD1	1.86	0.41
17:A:837:CLA:H112	17:A:837:CLA:H143	1.89	0.41
17:F:304:CLA:H161	17:F:304:CLA:H193	1.80	0.41
17:F:306:CLA:O1A	17:F:306:CLA:H2A	2.21	0.41
17:J:101:CLA:H193	17:J:101:CLA:H161	1.81	0.41
21:J:105:BCR:H20C	21:J:105:BCR:H361	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:113:SER:OG	15:L:123:PRO:HG3	2.21	0.41
15:L:145:SER:HB2	21:L:206:BCR:C5	2.51	0.41
2:2:216:ARG:O	2:2:220:LEU:HD22	2.21	0.40
3:3:164:HIS:HB3	18:3:601:CHL:HED1	2.03	0.40
3:3:182:LEU:HD21	21:3:616:BCR:H343	2.02	0.40
6:B:414:HIS:CE1	6:B:418:ILE:HD11	2.56	0.40
15:L:23:VAL:O	15:L:29:VAL:HG11	2.21	0.40
1:1:179:LYS:HD3	17:1:310:CLA:CBA	2.46	0.40
6:B:686:PRO:O	6:B:688:ALA:N	2.52	0.40
17:B:812:CLA:H101	12:H:117:PHE:HD2	1.86	0.40
17:1:309:CLA:CBC	17:1:311:CLA:H141	2.51	0.40
18:2:313:CHL:CBB	21:2:316:BCR:H10C	2.52	0.40
3:3:102:PHE:CZ	18:3:607:CHL:HED2	2.55	0.40
17:3:610:CLA:H62	17:3:610:CLA:H41	1.77	0.40
5:A:447:ASN:O	5:A:451:ILE:HG13	2.22	0.40
17:A:809:CLA:H8	17:A:812:CLA:H202	2.02	0.40
6:B:558:PRO:O	6:B:559:CYS:HB3	2.22	0.40
17:B:815:CLA:H122	21:B:845:BCR:H381	2.04	0.40
17:B:832:CLA:HBA1	17:B:832:CLA:C4A	2.52	0.40
14:J:12:PRO:O	14:J:16:THR:HG23	2.21	0.40
18:3:601:CHL:C9	18:3:601:CHL:H62	2.51	0.40
17:A:808:CLA:H122	17:A:808:CLA:H8	1.83	0.40
21:A:846:BCR:H15C	21:A:846:BCR:H351	1.76	0.40
17:A:853:CLA:H41	17:A:853:CLA:H61	1.14	0.40
24:B:852:LMG:H251	17:G:104:CLA:C1B	2.52	0.40
26:4:323:DGD:HBT1	26:4:323:DGD:HBN2	2.03	0.40
21:A:850:BCR:H15C	21:A:850:BCR:H351	1.92	0.40
6:B:531:THR:HG22	17:B:827:CLA:HHC	2.03	0.40
21:B:847:BCR:H332	22:G:102:LHG:H341	2.04	0.40

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	1	193/195 (99%)	178 (92%)	12 (6%)	3 (2%)	9	13
2	2	202/269 (75%)	191 (95%)	9 (4%)	2 (1%)	15	23
3	3	214/275 (78%)	197 (92%)	17 (8%)	0	100	100
4	4	193/198 (98%)	179 (93%)	13 (7%)	1 (0%)	29	41
5	A	740/758 (98%)	707 (96%)	30 (4%)	3 (0%)	34	48
6	B	731/734 (100%)	709 (97%)	19 (3%)	3 (0%)	34	48
7	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
8	D	138/143 (96%)	127 (92%)	9 (6%)	2 (1%)	11	15
9	E	61/66 (92%)	59 (97%)	2 (3%)	0	100	100
10	F	150/154 (97%)	148 (99%)	2 (1%)	0	100	100
11	G	93/97 (96%)	88 (95%)	5 (5%)	0	100	100
12	H	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
13	I	28/40 (70%)	26 (93%)	2 (7%)	0	100	100
14	J	37/42 (88%)	37 (100%)	0	0	100	100
15	L	149/157 (95%)	145 (97%)	4 (3%)	0	100	100
16	K	73/80 (91%)	67 (92%)	6 (8%)	0	100	100
All	All	3166/3377 (94%)	3012 (95%)	140 (4%)	14 (0%)	34	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	516	GLY
6	B	5	PHE
8	D	76	PRO
1	1	109	ALA
6	B	559	CYS
1	1	113	GLY
1	1	228	PRO
5	A	581	CYS
2	2	120	GLY
4	4	238	SER
5	A	519	ASP
8	D	169	LYS
6	B	492	ILE
2	2	233	GLY

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	1	155/158 (98%)	147 (95%)	8 (5%)	23	38
2	2	164/216 (76%)	150 (92%)	14 (8%)	10	16
3	3	167/213 (78%)	158 (95%)	9 (5%)	22	36
4	4	161/164 (98%)	149 (92%)	12 (8%)	13	21
5	A	603/618 (98%)	573 (95%)	30 (5%)	24	40
6	B	598/599 (100%)	568 (95%)	30 (5%)	24	40
7	C	69/70 (99%)	65 (94%)	4 (6%)	20	32
8	D	120/122 (98%)	109 (91%)	11 (9%)	9	13
9	E	55/58 (95%)	53 (96%)	2 (4%)	35	54
10	F	124/127 (98%)	114 (92%)	10 (8%)	11	18
11	G	80/82 (98%)	70 (88%)	10 (12%)	4	5
12	H	71/71 (100%)	67 (94%)	4 (6%)	21	34
13	I	25/36 (69%)	23 (92%)	2 (8%)	12	18
14	J	32/35 (91%)	29 (91%)	3 (9%)	8	13
15	L	118/124 (95%)	111 (94%)	7 (6%)	19	32
16	K	51/58 (88%)	49 (96%)	2 (4%)	32	50
All	All	2593/2751 (94%)	2435 (94%)	158 (6%)	18	30

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	43	ARG
1	1	69	LEU
1	1	98	LEU
1	1	110	LEU
1	1	120	ASN
1	1	122	VAL
1	1	126	THR
1	1	207	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	53	ASP
2	2	54	ARG
2	2	58	PHE
2	2	62	THR
2	2	85	ASP
2	2	87	GLU
2	2	110	ILE
2	2	140	THR
2	2	162	LEU
2	2	207	LEU
2	2	220	LEU
2	2	234	THR
2	2	238	ASP
2	2	240	LEU
3	3	52	TRP
3	3	88	GLU
3	3	94	TYR
3	3	114	GLU
3	3	124	GLN
3	3	154	LEU
3	3	156	MET
3	3	224	ASN
3	3	244	VAL
4	4	110	LEU
4	4	120	ILE
4	4	141	LEU
4	4	144	ILE
4	4	148	LEU
4	4	166	VAL
4	4	177	LEU
4	4	198	LEU
4	4	210	LEU
4	4	224	VAL
4	4	243	ASN
4	4	247	GLN
5	A	22	VAL
5	A	42	ARG
5	A	43	THR
5	A	73	GLU
5	A	78	VAL
5	A	102	ARG
5	A	151	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	159	THR
5	A	210	LEU
5	A	211	LEU
5	A	230	ASN
5	A	237	VAL
5	A	252	ARG
5	A	272	LEU
5	A	283	PHE
5	A	291	THR
5	A	306	ILE
5	A	377	TYR
5	A	387	THR
5	A	434	ARG
5	A	446	LEU
5	A	453	LEU
5	A	530	LEU
5	A	540	LEU
5	A	560	VAL
5	A	590	CYS
5	A	630	ASP
5	A	653	LEU
5	A	716	VAL
5	A	729	GLN
6	B	4	ARG
6	B	7	ARG
6	B	10	GLN
6	B	37	ILE
6	B	91	ILE
6	B	137	THR
6	B	203	ARG
6	B	215	VAL
6	B	222	LEU
6	B	225	LEU
6	B	235	GLN
6	B	257	LEU
6	B	332	PHE
6	B	344	ILE
6	B	363	GLN
6	B	371	LEU
6	B	427	LEU
6	B	436	LEU
6	B	441	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	458	ILE
6	B	476	VAL
6	B	479	SER
6	B	492	ILE
6	B	568	CYS
6	B	577	TYR
6	B	583	MET
6	B	590	VAL
6	B	626	LEU
6	B	645	VAL
6	B	732	LYS
7	C	11	CYS
7	C	19	ARG
7	C	62	PHE
7	C	74	THR
8	D	73	GLU
8	D	74	LEU
8	D	78	THR
8	D	96	VAL
8	D	105	GLU
8	D	150	ILE
8	D	151	LYS
8	D	177	VAL
8	D	189	ARG
8	D	190	SER
8	D	201	LYS
9	E	1	ILE
9	E	62	GLU
10	F	87	SER
10	F	103	SER
10	F	123	GLU
10	F	131	ASN
10	F	134	LYS
10	F	160	ILE
10	F	187	ASP
10	F	189	LYS
10	F	201	LEU
10	F	206	VAL
11	G	6	LEU
11	G	10	LEU
11	G	18	LEU
11	G	22	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	G	29	GLU
11	G	31	VAL
11	G	33	LYS
11	G	42	VAL
11	G	50	THR
11	G	95	ASP
12	H	63	LEU
12	H	76	ASP
12	H	82	ASN
12	H	101	LEU
13	I	3	ASN
13	I	11	LEU
14	J	16	THR
14	J	25	LEU
14	J	38	THR
15	L	8	GLN
15	L	36	LEU
15	L	40	ARG
15	L	59	LEU
15	L	78	GLN
15	L	87	LEU
15	L	121	LYS
16	K	52	ASN
16	K	102	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	247	GLN
6	B	218	HIS
12	H	82	ASN
12	H	85	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

215 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
17	CLA	B	826	29	56,73,73	1.66	6 (10%)	55,113,113	1.66	11 (20%)
28	SF4	C	101	7	0,12,12	0.00	-	-		
17	CLA	B	819	-	50,67,73	1.67	6 (12%)	47,105,113	1.72	13 (27%)
21	BCR	1	316	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)
17	CLA	4	310	-	51,68,73	1.57	5 (9%)	49,107,113	1.96	15 (30%)
17	CLA	A	806	-	56,73,73	1.59	5 (8%)	55,113,113	1.52	9 (16%)
17	CLA	A	831	-	56,73,73	1.58	4 (7%)	55,113,113	1.72	14 (25%)
18	CHL	1	305	1	42,56,74	2.32	13 (30%)	42,92,114	2.18	13 (30%)
17	CLA	L	203	-	56,73,73	1.57	5 (8%)	55,113,113	1.65	8 (14%)
22	LHG	B	801	17	22,22,48	1.09	2 (9%)	25,28,54	1.10	2 (8%)
17	CLA	K	202	-	51,68,73	1.69	6 (11%)	49,107,113	1.63	8 (16%)
24	LMG	4	319	-	50,50,55	0.88	3 (6%)	58,58,63	1.46	8 (13%)
25	HTG	4	322	-	19,19,19	1.07	2 (10%)	23,24,24	1.23	3 (13%)
26	DGD	4	323	-	61,61,67	0.89	2 (3%)	75,75,81	1.76	21 (28%)
17	CLA	B	833	-	51,68,73	1.54	8 (15%)	49,107,113	1.73	12 (24%)
17	CLA	3	613	-	37,54,73	1.93	5 (13%)	32,90,113	1.90	7 (21%)
17	CLA	4	311	4	43,60,73	1.82	4 (9%)	39,97,113	1.73	8 (20%)
17	CLA	B	830	-	56,73,73	1.66	8 (14%)	55,113,113	1.69	13 (23%)
17	CLA	A	853	29	56,73,73	1.54	6 (10%)	55,113,113	2.33	21 (38%)
17	CLA	A	829	-	56,73,73	1.55	8 (14%)	55,113,113	1.71	8 (14%)
17	CLA	A	822	-	42,59,73	1.83	5 (11%)	38,96,113	1.78	9 (23%)
17	CLA	B	836	29	33,53,73	1.94	4 (12%)	27,89,113	2.33	14 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
17	CLA	B	842	22	56,73,73	1.52	5 (8%)	55,113,113	1.78	15 (27%)
17	CLA	A	810	17	56,73,73	1.56	5 (8%)	55,113,113	1.63	11 (20%)
23	LMT	A	855	-	36,36,36	1.11	4 (11%)	47,47,47	0.92	1 (2%)
18	CHL	4	306	29	45,59,74	2.23	13 (28%)	46,96,114	2.41	15 (32%)
21	BCR	A	851	-	41,41,41	0.89	2 (4%)	56,56,56	1.21	6 (10%)
17	CLA	2	308	2	51,68,73	1.65	6 (11%)	49,107,113	1.56	7 (14%)
19	LUT	3	614	-	42,43,43	5.66	20 (47%)	51,60,60	5.51	31 (60%)
17	CLA	B	816	-	56,73,73	1.58	6 (10%)	55,113,113	1.62	9 (16%)
17	CLA	B	841	-	56,73,73	1.69	6 (10%)	55,113,113	1.54	10 (18%)
17	CLA	A	826	-	56,73,73	1.51	5 (8%)	55,113,113	1.55	8 (14%)
17	CLA	A	840	-	56,73,73	1.57	8 (14%)	55,113,113	1.68	14 (25%)
17	CLA	1	310	1	43,60,73	1.82	7 (16%)	39,97,113	1.65	10 (25%)
20	XAT	2	315	-	39,47,47	4.99	17 (43%)	54,74,74	5.48	32 (59%)
17	CLA	A	839	29	56,73,73	1.71	8 (14%)	55,113,113	1.36	7 (12%)
21	BCR	G	106	-	41,41,41	1.06	2 (4%)	56,56,56	1.13	5 (8%)
21	BCR	A	847	-	41,41,41	1.08	3 (7%)	56,56,56	1.22	5 (8%)
20	XAT	4	317	-	39,47,47	5.05	17 (43%)	54,74,74	5.30	32 (59%)
17	CLA	J	101	-	56,73,73	1.59	6 (10%)	55,113,113	1.69	11 (20%)
17	CLA	2	307	2	41,58,73	1.86	5 (12%)	37,95,113	1.88	10 (27%)
17	CLA	4	302	4	51,68,73	1.72	8 (15%)	49,107,113	1.61	9 (18%)
17	CLA	A	814	-	41,58,73	1.83	5 (12%)	37,95,113	1.82	9 (24%)
18	CHL	4	301	1	55,69,74	1.69	14 (25%)	58,108,114	2.32	20 (34%)
17	CLA	B	840	29	56,73,73	1.50	4 (7%)	55,113,113	1.63	9 (16%)
21	BCR	L	206	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	7 (12%)
17	CLA	1	311	1	51,68,73	1.57	6 (11%)	49,107,113	1.65	11 (22%)
17	CLA	B	827	29	56,73,73	1.49	6 (10%)	55,113,113	1.73	12 (21%)
26	DGD	B	850	-	67,67,67	1.13	6 (8%)	81,81,81	1.50	10 (12%)
18	CHL	4	315	4	37,51,74	2.22	10 (27%)	36,86,114	2.24	9 (25%)
24	LMG	B	852	-	52,52,55	1.09	4 (7%)	60,60,63	1.49	7 (11%)
21	BCR	K	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.21	6 (10%)
23	LMT	2	318	-	36,36,36	1.09	5 (13%)	47,47,47	1.11	3 (6%)
21	BCR	B	847	-	41,41,41	1.10	2 (4%)	56,56,56	1.45	10 (17%)
17	CLA	B	805	-	56,73,73	1.50	4 (7%)	55,113,113	1.58	10 (18%)
17	CLA	2	301	2	56,73,73	1.62	7 (12%)	55,113,113	1.63	10 (18%)
18	CHL	2	305	29	42,56,74	2.25	13 (30%)	42,92,114	2.33	13 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	CLA	A	825	29	56,73,73	1.59	5 (8%)	55,113,113	1.56	9 (16%)
17	CLA	A	820	29	56,73,73	1.61	5 (8%)	55,113,113	1.52	10 (18%)
17	CLA	L	204	-	41,58,73	1.91	5 (12%)	37,95,113	1.78	11 (29%)
20	XAT	1	315	-	39,47,47	5.00	17 (43%)	54,74,74	5.48	32 (59%)
25	HTG	F	305	-	19,19,19	1.05	2 (10%)	23,24,24	1.73	4 (17%)
17	CLA	B	811	6	56,73,73	1.58	4 (7%)	55,113,113	1.73	11 (20%)
20	XAT	3	615	-	39,47,47	4.99	17 (43%)	54,74,74	5.48	32 (59%)
17	CLA	1	309	22	56,73,73	1.67	4 (7%)	55,113,113	1.52	12 (21%)
17	CLA	B	808	6	56,73,73	1.41	8 (14%)	55,113,113	1.67	11 (20%)
21	BCR	I	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.21	4 (7%)
17	CLA	A	811	-	45,62,73	1.78	5 (11%)	41,99,113	1.64	7 (17%)
17	CLA	4	313	-	33,53,73	2.02	5 (15%)	27,89,113	2.21	12 (44%)
17	CLA	A	809	-	56,73,73	1.56	5 (8%)	55,113,113	1.59	9 (16%)
17	CLA	2	302	-	42,59,73	1.80	6 (14%)	38,96,113	1.88	10 (26%)
17	CLA	B	809	-	56,73,73	1.62	6 (10%)	55,113,113	1.54	10 (18%)
22	LHG	2	317	-	36,36,48	0.71	1 (2%)	39,42,54	1.23	4 (10%)
17	CLA	A	801	-	56,73,73	1.44	3 (5%)	55,113,113	2.27	15 (27%)
17	CLA	A	824	29	56,73,73	1.63	5 (8%)	55,113,113	1.58	9 (16%)
17	CLA	B	839	-	38,55,73	1.77	4 (10%)	33,91,113	2.56	18 (54%)
21	BCR	F	303	-	41,41,41	0.92	2 (4%)	56,56,56	1.43	11 (19%)
22	LHG	G	102	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	6 (11%)
24	LMG	F	309	-	55,55,55	0.85	2 (3%)	63,63,63	1.45	8 (12%)
17	CLA	A	828	-	56,73,73	1.56	5 (8%)	55,113,113	1.63	11 (20%)
17	CLA	1	303	29	42,59,73	1.78	5 (11%)	38,96,113	1.81	10 (26%)
17	CLA	B	820	-	51,68,73	1.57	5 (9%)	49,107,113	1.76	14 (28%)
18	CHL	3	607	29	41,55,74	2.25	11 (26%)	41,91,114	2.24	12 (29%)
25	HTG	4	321	-	19,19,19	1.14	2 (10%)	23,24,24	1.14	1 (4%)
17	CLA	A	823	-	46,63,73	1.78	5 (10%)	43,101,113	1.70	8 (18%)
17	CLA	4	312	4	47,64,73	1.68	7 (14%)	44,102,113	1.72	7 (15%)
17	CLA	B	804	-	56,73,73	1.68	5 (8%)	55,113,113	1.47	9 (16%)
17	CLA	B	806	-	33,53,73	1.85	4 (12%)	27,89,113	2.49	10 (37%)
17	CLA	G	103	29	32,49,73	2.13	6 (18%)	26,84,113	2.07	6 (23%)
21	BCR	A	846	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
17	CLA	1	301	1	56,73,73	1.71	5 (8%)	55,113,113	1.36	8 (14%)
17	CLA	1	313	1	37,54,73	1.86	7 (18%)	32,90,113	1.92	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	BCR	L	205	-	41,41,41	0.98	1 (2%)	56,56,56	1.10	4 (7%)
17	CLA	3	602	3	51,68,73	1.69	6 (11%)	49,107,113	1.59	9 (18%)
17	CLA	B	807	-	56,73,73	1.54	7 (12%)	55,113,113	1.62	8 (14%)
17	CLA	A	815	29	33,53,73	2.07	6 (18%)	27,89,113	2.05	9 (33%)
17	CLA	A	841	29	56,73,73	1.54	5 (8%)	55,113,113	1.63	12 (21%)
21	BCR	A	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	8 (14%)
25	HTG	A	854	-	19,19,19	0.84	1 (5%)	23,24,24	0.92	0
17	CLA	3	608	3	41,58,73	1.86	5 (12%)	37,95,113	1.82	9 (24%)
17	CLA	2	319	4	37,54,73	1.94	5 (13%)	32,90,113	1.95	11 (34%)
17	CLA	B	838	-	56,73,73	1.50	6 (10%)	55,113,113	1.82	12 (21%)
19	LUT	1	314	-	42,43,43	5.53	20 (47%)	51,60,60	5.67	33 (64%)
17	CLA	4	309	4	51,68,73	1.69	4 (7%)	49,107,113	1.55	11 (22%)
17	CLA	B	814	-	46,63,73	1.69	8 (17%)	43,101,113	1.89	10 (23%)
17	CLA	A	802	29	56,73,73	1.53	7 (12%)	55,113,113	1.90	12 (21%)
17	CLA	A	816	-	56,73,73	1.59	6 (10%)	55,113,113	1.53	10 (18%)
17	CLA	A	812	-	56,73,73	1.66	5 (8%)	55,113,113	1.57	11 (20%)
17	CLA	A	838	-	56,73,73	1.65	5 (8%)	55,113,113	1.81	15 (27%)
21	BCR	B	844	-	41,41,41	0.99	2 (4%)	56,56,56	1.28	7 (12%)
17	CLA	B	823	-	56,73,73	1.41	5 (8%)	55,113,113	1.83	10 (18%)
21	BCR	A	849	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
17	CLA	1	304	-	33,50,73	2.05	6 (18%)	27,85,113	2.03	8 (29%)
21	BCR	L	201	-	41,41,41	1.02	2 (4%)	56,56,56	1.20	6 (10%)
17	CLA	J	103	14	33,50,73	1.90	5 (15%)	27,85,113	2.17	8 (29%)
17	CLA	B	810	-	56,73,73	1.62	6 (10%)	55,113,113	1.49	11 (20%)
17	CLA	B	822	-	41,58,73	1.77	4 (9%)	37,95,113	2.05	13 (35%)
17	CLA	3	612	-	33,53,73	2.04	6 (18%)	27,89,113	2.10	7 (25%)
21	BCR	3	616	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	5 (8%)
17	CLA	1	302	-	56,73,73	1.60	4 (7%)	55,113,113	1.62	9 (16%)
22	LHG	A	845	17	26,26,48	0.87	1 (3%)	29,32,54	1.32	3 (10%)
21	BCR	2	316	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	8 (14%)
17	CLA	B	802	-	56,73,73	1.52	6 (10%)	55,113,113	1.53	13 (23%)
17	CLA	A	821	-	40,57,73	1.81	5 (12%)	34,93,113	2.04	10 (29%)
17	CLA	B	834	-	49,66,73	1.62	9 (18%)	46,104,113	1.91	16 (34%)
17	CLA	B	812	-	56,73,73	1.61	6 (10%)	55,113,113	1.41	10 (18%)
18	CHL	2	304	29	37,51,74	2.22	11 (29%)	36,86,114	2.47	13 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
21	BCR	J	104	-	41,41,41	1.00	3 (7%)	56,56,56	1.23	4 (7%)
17	CLA	2	312	-	34,51,73	2.07	5 (14%)	28,86,113	2.02	8 (28%)
18	CHL	4	305	29	50,64,74	1.90	11 (22%)	52,102,114	2.31	13 (25%)
19	LUT	4	316	-	42,43,43	5.53	22 (52%)	51,60,60	5.74	35 (68%)
17	CLA	3	609	3	41,58,73	1.82	4 (9%)	37,95,113	1.86	11 (29%)
17	CLA	B	818	-	46,63,73	1.75	4 (8%)	43,101,113	1.87	10 (23%)
21	BCR	B	848	-	41,41,41	1.06	2 (4%)	56,56,56	1.20	7 (12%)
21	BCR	B	845	-	41,41,41	0.92	1 (2%)	56,56,56	1.36	9 (16%)
17	CLA	4	304	29	41,58,73	1.64	7 (17%)	37,95,113	2.15	14 (37%)
17	CLA	G	105	11	37,54,73	1.97	7 (18%)	32,90,113	1.99	11 (34%)
17	CLA	2	309	-	32,49,73	2.09	5 (15%)	26,84,113	2.19	9 (34%)
17	CLA	A	808	5	56,73,73	1.42	7 (12%)	55,113,113	1.85	12 (21%)
18	CHL	4	307	29	45,59,74	2.21	12 (26%)	46,96,114	2.18	14 (30%)
17	CLA	1	308	1	51,68,73	1.66	6 (11%)	49,107,113	1.57	8 (16%)
17	CLA	A	813	-	33,53,73	2.05	7 (21%)	27,89,113	1.88	9 (33%)
17	CLA	B	821	29	56,73,73	1.45	6 (10%)	55,113,113	1.72	10 (18%)
17	CLA	K	201	-	33,53,73	2.01	5 (15%)	27,89,113	2.14	7 (25%)
17	CLA	F	307	10	46,63,73	1.65	6 (13%)	43,101,113	1.65	9 (20%)
21	BCR	B	846	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	8 (14%)
17	CLA	F	306	29	33,53,73	2.02	5 (15%)	27,89,113	2.10	9 (33%)
27	PQN	A	842	-	34,34,34	4.59	16 (47%)	42,45,45	4.02	17 (40%)
17	CLA	B	831	-	56,73,73	1.48	8 (14%)	55,113,113	1.92	13 (23%)
17	CLA	4	303	4	51,68,73	1.86	6 (11%)	49,107,113	1.74	10 (20%)
17	CLA	A	832	-	56,73,73	1.66	4 (7%)	55,113,113	1.61	9 (16%)
17	CLA	B	825	-	51,68,73	1.51	5 (9%)	49,107,113	1.95	11 (22%)
17	CLA	B	835	-	56,73,73	1.67	6 (10%)	55,113,113	1.42	10 (18%)
28	SF4	C	102	7	0,12,12	0.00	-	-		
25	HTG	F	310	-	16,16,19	1.15	2 (12%)	20,21,24	1.41	4 (20%)
17	CLA	A	807	5	56,73,73	1.56	7 (12%)	55,113,113	1.46	6 (10%)
17	CLA	3	611	3	46,63,73	1.76	5 (10%)	43,101,113	1.72	7 (16%)
17	CLA	1	312	-	46,63,73	1.79	4 (8%)	43,101,113	1.73	11 (25%)
17	CLA	A	830	-	41,58,73	1.87	5 (12%)	37,95,113	1.89	9 (24%)
17	CLA	L	202	15	56,73,73	1.58	5 (8%)	55,113,113	1.60	10 (18%)
18	CHL	2	306	29	45,59,74	2.15	14 (31%)	46,96,114	2.26	13 (28%)
21	BCR	4	318	-	41,41,41	0.97	1 (2%)	56,56,56	1.26	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
24	LMG	4	320	-	49,49,55	1.04	4 (8%)	57,57,63	1.46	5 (8%)
17	CLA	4	308	4	41,58,73	1.73	5 (12%)	37,95,113	2.12	11 (29%)
17	CLA	A	805	5	56,73,73	1.54	7 (12%)	55,113,113	1.63	13 (23%)
17	CLA	B	824	-	46,63,73	1.60	5 (10%)	43,101,113	1.78	8 (18%)
27	PQN	B	843	-	34,34,34	4.45	14 (41%)	42,45,45	4.44	23 (54%)
17	CLA	B	837	-	51,68,73	1.38	4 (7%)	49,107,113	2.04	12 (24%)
17	CLA	A	803	17	46,63,73	1.76	6 (13%)	43,101,113	1.63	8 (18%)
17	CLA	2	311	2	56,73,73	1.62	5 (8%)	55,113,113	1.63	9 (16%)
17	CLA	3	606	3	38,55,73	1.96	5 (13%)	33,91,113	1.96	11 (33%)
17	CLA	B	832	-	41,58,73	1.70	6 (14%)	37,95,113	1.88	10 (27%)
22	LHG	A	844	-	48,48,48	0.67	1 (2%)	51,54,54	1.29	6 (11%)
17	CLA	A	836	-	56,73,73	1.53	5 (8%)	55,113,113	1.77	11 (20%)
17	CLA	A	818	-	56,73,73	1.58	5 (8%)	55,113,113	1.66	10 (18%)
17	CLA	F	304	-	56,73,73	1.60	7 (12%)	55,113,113	1.66	9 (16%)
17	CLA	3	603	3	41,58,73	1.86	7 (17%)	37,95,113	1.85	9 (24%)
25	HTG	J	102	-	19,19,19	1.20	2 (10%)	23,24,24	1.30	3 (13%)
28	SF4	A	852	6,5	0,12,12	0.00	-	-		
17	CLA	A	834	5	33,53,73	2.03	5 (15%)	27,89,113	2.06	7 (25%)
17	CLA	B	817	-	46,63,73	1.66	6 (13%)	43,101,113	1.92	10 (23%)
19	LUT	2	314	-	42,43,43	5.62	20 (47%)	51,60,60	5.61	32 (62%)
17	CLA	A	804	-	56,73,73	1.59	6 (10%)	55,113,113	1.54	8 (14%)
17	CLA	B	803	-	56,73,73	1.60	7 (12%)	55,113,113	1.51	8 (14%)
17	CLA	A	827	-	56,73,73	1.57	5 (8%)	55,113,113	1.79	12 (21%)
24	LMG	G	101	-	40,40,55	0.87	2 (5%)	48,48,63	1.28	3 (6%)
17	CLA	B	813	-	45,62,73	1.68	7 (15%)	46,100,113	1.77	8 (17%)
18	CHL	2	313	2	37,51,74	2.28	11 (29%)	36,86,114	2.51	13 (36%)
17	CLA	A	833	-	41,58,73	1.83	6 (14%)	37,95,113	1.86	10 (27%)
17	CLA	B	829	-	56,73,73	1.60	7 (12%)	55,113,113	1.55	11 (20%)
18	CHL	3	601	2	47,61,74	2.10	12 (25%)	48,98,114	2.52	17 (35%)
17	CLA	A	835	-	42,59,73	1.85	5 (11%)	38,96,113	1.83	10 (26%)
17	CLA	3	604	-	33,53,73	2.08	5 (15%)	27,89,113	2.07	10 (37%)
17	CLA	B	828	-	56,73,73	1.65	5 (8%)	55,113,113	1.68	11 (20%)
17	CLA	2	310	2	43,60,73	1.96	6 (13%)	39,97,113	1.67	7 (17%)
17	CLA	A	817	-	56,73,73	1.64	8 (14%)	55,113,113	1.60	11 (20%)
17	CLA	A	837	-	56,73,73	1.61	4 (7%)	55,113,113	1.63	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	LHG	1	317	17	48,48,48	0.68	1 (2%)	51,54,54	1.23	6 (11%)
21	BCR	A	848	-	41,41,41	1.05	2 (4%)	56,56,56	1.22	6 (10%)
17	CLA	4	314	-	38,55,73	1.94	4 (10%)	33,91,113	2.21	14 (42%)
17	CLA	B	815	-	56,73,73	1.54	4 (7%)	55,113,113	1.55	11 (20%)
25	HTG	F	301	-	17,17,19	0.96	2 (11%)	21,22,24	0.69	0
17	CLA	G	104	-	41,58,73	1.96	5 (12%)	37,95,113	1.90	9 (24%)
17	CLA	2	303	-	51,68,73	1.67	5 (9%)	49,107,113	1.63	10 (20%)
25	HTG	B	851	-	19,19,19	1.06	1 (5%)	23,24,24	1.87	7 (30%)
17	CLA	A	819	-	33,53,73	2.03	5 (15%)	27,89,113	2.09	9 (33%)
17	CLA	A	843	22	43,60,73	1.88	6 (13%)	39,97,113	1.85	10 (25%)
21	BCR	F	308	-	41,41,41	1.05	2 (4%)	56,56,56	1.27	8 (14%)
21	BCR	B	849	-	41,41,41	0.96	2 (4%)	56,56,56	1.19	3 (5%)
17	CLA	1	307	1	56,73,73	1.64	5 (8%)	55,113,113	1.57	10 (18%)
22	LHG	F	302	-	39,39,48	0.65	0	42,45,54	1.25	6 (14%)
17	CLA	3	605	-	33,50,73	2.17	6 (18%)	27,85,113	1.86	8 (29%)
21	BCR	J	105	-	41,41,41	1.16	2 (4%)	56,56,56	1.43	9 (16%)
17	CLA	3	610	-	43,60,73	1.86	6 (13%)	39,97,113	1.92	10 (25%)
17	CLA	1	306	29	37,54,73	1.99	5 (13%)	32,90,113	1.89	9 (28%)

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
17	CLA	B	826	29	1/1/15/20	16/37/115/115	-
28	SF4	C	101	7	-	-	0/6/5/5
17	CLA	B	819	-	1/1/13/20	5/30/108/115	-
21	BCR	1	316	-	-	12/29/63/63	0/2/2/2
17	CLA	4	310	-	1/1/14/20	15/31/109/115	-
17	CLA	A	806	-	1/1/15/20	10/37/115/115	-
17	CLA	A	831	-	1/1/15/20	16/37/115/115	-
18	CHL	1	305	1	3/3/16/26	7/18/116/137	-
17	CLA	L	203	-	1/1/15/20	10/37/115/115	-
22	LHG	B	801	17	-	10/26/26/53	-
17	CLA	K	202	-	1/1/14/20	16/31/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMG	4	319	-	-	15/45/65/70	0/1/1/1
25	HTG	4	322	-	-	1/10/30/30	0/1/1/1
26	DGD	4	323	-	-	27/49/89/95	0/2/2/2
17	CLA	B	833	-	1/1/14/20	6/31/109/115	-
17	CLA	3	613	-	1/1/11/20	2/15/93/115	-
17	CLA	B	830	-	1/1/15/20	5/37/115/115	-
17	CLA	4	311	4	-	4/22/100/115	-
17	CLA	A	853	29	1/1/15/20	16/37/115/115	-
17	CLA	A	829	-	1/1/15/20	14/37/115/115	-
17	CLA	A	822	-	1/1/12/20	11/21/99/115	-
17	CLA	B	836	29	1/1/11/20	2/11/91/115	-
17	CLA	B	842	22	1/1/15/20	7/37/115/115	-
17	CLA	A	810	17	1/1/15/20	13/37/115/115	-
23	LMT	A	855	-	-	14/21/61/61	0/2/2/2
18	CHL	4	306	29	3/3/17/26	7/21/119/137	-
21	BCR	A	851	-	-	7/29/63/63	0/2/2/2
17	CLA	2	308	2	1/1/14/20	11/31/109/115	-
19	LUT	3	614	-	-	12/29/67/67	0/2/2/2
17	CLA	B	816	-	1/1/15/20	9/37/115/115	-
17	CLA	B	841	-	1/1/15/20	11/37/115/115	-
17	CLA	A	826	-	1/1/15/20	11/37/115/115	-
17	CLA	A	840	-	1/1/15/20	14/37/115/115	-
17	CLA	1	310	1	1/1/12/20	8/22/100/115	-
20	XAT	2	315	-	-	13/31/93/93	0/4/4/4
17	CLA	A	839	29	1/1/15/20	16/37/115/115	-
21	BCR	G	106	-	-	6/29/63/63	0/2/2/2
21	BCR	A	847	-	-	6/29/63/63	0/2/2/2
20	XAT	4	317	-	3/3/12/26	11/31/93/93	0/4/4/4
17	CLA	J	101	-	1/1/15/20	8/37/115/115	-
17	CLA	2	307	2	1/1/12/20	1/19/97/115	-
17	CLA	4	302	4	1/1/14/20	4/31/109/115	-
17	CLA	A	814	-	1/1/12/20	9/19/97/115	-
18	CHL	4	301	1	4/4/19/26	15/33/131/137	-
17	CLA	B	840	29	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	L	206	-	-	4/29/63/63	0/2/2/2
17	CLA	1	311	1	1/1/14/20	6/31/109/115	-
17	CLA	B	827	29	1/1/15/20	11/37/115/115	-
26	DGD	B	850	-	-	24/55/95/95	0/2/2/2
18	CHL	4	315	4	3/3/15/26	2/12/110/137	-
24	LMG	B	852	-	-	21/47/67/70	0/1/1/1
21	BCR	K	203	-	-	15/29/63/63	0/2/2/2
23	LMT	2	318	-	-	11/21/61/61	0/2/2/2
21	BCR	B	847	-	-	3/29/63/63	0/2/2/2
17	CLA	B	805	-	1/1/15/20	11/37/115/115	-
17	CLA	2	301	2	1/1/15/20	5/37/115/115	-
18	CHL	2	305	29	3/3/16/26	2/18/116/137	-
17	CLA	A	825	29	1/1/15/20	8/37/115/115	-
17	CLA	A	820	29	1/1/15/20	8/37/115/115	-
17	CLA	L	204	-	-	6/19/97/115	-
20	XAT	1	315	-	-	13/31/93/93	0/4/4/4
25	HTG	F	305	-	-	3/10/30/30	0/1/1/1
17	CLA	B	811	6	1/1/15/20	9/37/115/115	-
20	XAT	3	615	-	-	13/31/93/93	0/4/4/4
17	CLA	1	309	22	1/1/15/20	17/37/115/115	-
17	CLA	B	808	6	1/1/15/20	15/37/115/115	-
21	BCR	I	101	-	-	5/29/63/63	0/2/2/2
17	CLA	A	811	-	1/1/12/20	5/24/102/115	-
17	CLA	4	313	-	1/1/11/20	7/11/91/115	-
17	CLA	A	809	-	1/1/15/20	16/37/115/115	-
17	CLA	2	302	-	1/1/12/20	2/21/99/115	-
17	CLA	B	809	-	1/1/15/20	14/37/115/115	-
22	LHG	2	317	-	-	19/41/41/53	-
17	CLA	A	801	-	2/2/15/20	9/37/115/115	-
17	CLA	A	824	29	1/1/15/20	11/37/115/115	-
17	CLA	B	839	-	1/1/11/20	4/16/94/115	-
21	BCR	F	303	-	-	5/29/63/63	0/2/2/2
22	LHG	G	102	-	-	26/53/53/53	-
24	LMG	F	309	-	-	20/50/70/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	A	828	-	1/1/15/20	8/37/115/115	-
17	CLA	1	303	29	1/1/12/20	8/21/99/115	-
17	CLA	B	820	-	1/1/14/20	14/31/109/115	-
18	CHL	3	607	29	3/3/16/26	4/17/115/137	-
17	CLA	A	823	-	1/1/13/20	6/25/103/115	-
17	CLA	4	312	4	1/1/13/20	5/27/105/115	-
17	CLA	B	804	-	1/1/15/20	6/37/115/115	-
17	CLA	B	806	-	1/1/11/20	2/11/91/115	-
17	CLA	G	103	29	1/1/10/20	2/8/86/115	-
21	BCR	A	846	-	-	2/29/63/63	0/2/2/2
17	CLA	1	301	1	1/1/15/20	9/37/115/115	-
17	CLA	1	313	1	1/1/11/20	4/15/93/115	-
21	BCR	L	205	-	-	10/29/63/63	0/2/2/2
17	CLA	3	602	3	1/1/14/20	5/31/109/115	-
17	CLA	B	807	-	1/1/15/20	13/37/115/115	-
17	CLA	A	815	29	1/1/11/20	2/11/91/115	-
17	CLA	A	841	29	1/1/15/20	13/37/115/115	-
21	BCR	A	850	-	-	8/29/63/63	0/2/2/2
25	HTG	A	854	-	-	2/10/30/30	0/1/1/1
17	CLA	3	608	3	1/1/12/20	4/19/97/115	-
17	CLA	2	319	4	1/1/11/20	3/15/93/115	-
17	CLA	B	838	-	1/1/15/20	11/37/115/115	-
19	LUT	1	314	-	-	12/29/67/67	0/2/2/2
17	CLA	4	309	4	1/1/14/20	8/31/109/115	-
17	CLA	B	814	-	1/1/13/20	7/25/103/115	-
17	CLA	A	802	29	1/1/15/20	6/37/115/115	-
17	CLA	A	816	-	1/1/15/20	15/37/115/115	-
17	CLA	A	812	-	1/1/15/20	11/37/115/115	-
17	CLA	A	838	-	1/1/15/20	15/37/115/115	-
21	BCR	B	844	-	-	7/29/63/63	0/2/2/2
17	CLA	B	823	-	1/1/15/20	13/37/115/115	-
21	BCR	A	849	-	-	7/29/63/63	0/2/2/2
17	CLA	1	304	-	1/1/10/20	5/10/88/115	-
21	BCR	L	201	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	J	103	14	1/1/10/20	5/10/88/115	-
17	CLA	B	810	-	1/1/15/20	8/37/115/115	-
17	CLA	B	822	-	1/1/12/20	6/19/97/115	-
17	CLA	3	612	-	1/1/11/20	3/11/91/115	-
21	BCR	3	616	-	-	8/29/63/63	0/2/2/2
17	CLA	1	302	-	1/1/15/20	18/37/115/115	-
22	LHG	A	845	17	-	14/31/31/53	-
21	BCR	2	316	-	-	17/29/63/63	0/2/2/2
17	CLA	B	802	-	1/1/15/20	2/37/115/115	-
17	CLA	A	821	-	1/1/11/20	8/18/96/115	-
17	CLA	B	834	-	1/1/13/20	11/29/107/115	-
17	CLA	B	812	-	-	16/37/115/115	-
18	CHL	2	304	29	3/3/15/26	5/12/110/137	-
21	BCR	J	104	-	-	2/29/63/63	0/2/2/2
17	CLA	2	312	-	1/1/10/20	0/11/89/115	-
18	CHL	4	305	29	4/4/18/26	10/27/125/137	-
19	LUT	4	316	-	-	13/29/67/67	0/2/2/2
17	CLA	3	609	3	1/1/12/20	4/19/97/115	-
17	CLA	B	818	-	1/1/13/20	5/25/103/115	-
21	BCR	B	848	-	-	3/29/63/63	0/2/2/2
21	BCR	B	845	-	-	5/29/63/63	0/2/2/2
17	CLA	4	304	29	1/1/12/20	7/19/97/115	-
17	CLA	G	105	11	1/1/11/20	5/15/93/115	-
17	CLA	2	309	-	1/1/10/20	2/8/86/115	-
17	CLA	A	808	5	1/1/15/20	8/37/115/115	-
18	CHL	4	307	29	3/3/17/26	2/21/119/137	-
17	CLA	1	308	1	1/1/14/20	9/31/109/115	-
17	CLA	A	813	-	1/1/11/20	1/11/91/115	-
17	CLA	B	821	29	1/1/15/20	3/37/115/115	-
17	CLA	K	201	-	1/1/11/20	4/11/91/115	-
17	CLA	F	307	10	1/1/13/20	9/25/103/115	-
21	BCR	B	846	-	-	7/29/63/63	0/2/2/2
17	CLA	F	306	29	1/1/11/20	0/11/91/115	-
27	PQN	A	842	-	-	6/23/43/43	0/2/2/2
17	CLA	B	831	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	4	303	4	-	13/31/109/115	-
17	CLA	A	832	-	1/1/15/20	13/37/115/115	-
17	CLA	B	825	-	1/1/14/20	10/31/109/115	-
17	CLA	B	835	-	1/1/15/20	11/37/115/115	-
28	SF4	C	102	7	-	-	0/6/5/5
25	HTG	F	310	-	-	3/7/27/30	0/1/1/1
17	CLA	A	807	5	1/1/15/20	19/37/115/115	-
17	CLA	3	611	3	1/1/13/20	9/25/103/115	-
17	CLA	1	312	-	1/1/13/20	9/25/103/115	-
17	CLA	A	830	-	1/1/12/20	5/19/97/115	-
17	CLA	L	202	15	1/1/15/20	15/37/115/115	-
18	CHL	2	306	29	3/3/17/26	5/21/119/137	-
21	BCR	4	318	-	-	7/29/63/63	0/2/2/2
24	LMG	4	320	-	-	20/44/64/70	0/1/1/1
17	CLA	4	308	4	1/1/12/20	3/19/97/115	-
17	CLA	A	805	5	1/1/15/20	19/37/115/115	-
17	CLA	B	824	-	1/1/13/20	10/25/103/115	-
27	PQN	B	843	-	-	3/23/43/43	0/2/2/2
17	CLA	B	837	-	1/1/14/20	11/31/109/115	-
17	CLA	A	803	17	1/1/13/20	10/25/103/115	-
17	CLA	2	311	2	1/1/15/20	16/37/115/115	-
17	CLA	3	606	3	1/1/11/20	7/16/94/115	-
17	CLA	B	832	-	1/1/12/20	3/19/97/115	-
22	LHG	A	844	-	-	26/53/53/53	-
17	CLA	A	836	-	1/1/15/20	14/37/115/115	-
17	CLA	A	818	-	1/1/15/20	16/37/115/115	-
17	CLA	F	304	-	1/1/15/20	7/37/115/115	-
17	CLA	3	603	3	1/1/12/20	2/19/97/115	-
25	HTG	J	102	-	-	6/10/30/30	0/1/1/1
28	SF4	A	852	6,5	-	-	0/6/5/5
17	CLA	A	834	5	1/1/11/20	7/11/91/115	-
17	CLA	B	817	-	1/1/13/20	10/25/103/115	-
19	LUT	2	314	-	-	12/29/67/67	0/2/2/2
17	CLA	A	804	-	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CLA	B	803	-	1/1/15/20	14/37/115/115	-
17	CLA	A	827	-	1/1/15/20	9/37/115/115	-
24	LMG	G	101	-	-	15/35/55/70	0/1/1/1
17	CLA	B	813	-	1/1/13/20	11/25/101/115	-
18	CHL	2	313	2	3/3/15/26	5/12/110/137	-
17	CLA	A	833	-	1/1/12/20	3/19/97/115	-
17	CLA	B	829	-	1/1/15/20	14/37/115/115	-
18	CHL	3	601	2	3/3/17/26	3/24/122/137	-
17	CLA	A	835	-	1/1/12/20	9/21/99/115	-
17	CLA	3	604	-	1/1/11/20	3/11/91/115	-
17	CLA	B	828	-	1/1/15/20	8/37/115/115	-
17	CLA	2	310	2	1/1/12/20	7/22/100/115	-
17	CLA	A	817	-	1/1/15/20	11/37/115/115	-
17	CLA	A	837	-	1/1/15/20	15/37/115/115	-
22	LHG	1	317	17	-	23/53/53/53	-
21	BCR	A	848	-	-	7/29/63/63	0/2/2/2
17	CLA	4	314	-	1/1/11/20	2/16/94/115	-
17	CLA	B	815	-	1/1/15/20	16/37/115/115	-
25	HTG	F	301	-	-	4/8/28/30	0/1/1/1
17	CLA	G	104	-	1/1/12/20	4/19/97/115	-
17	CLA	2	303	-	1/1/14/20	17/31/109/115	-
25	HTG	B	851	-	-	7/10/30/30	0/1/1/1
17	CLA	A	819	-	1/1/11/20	3/11/91/115	-
17	CLA	A	843	22	1/1/12/20	9/22/100/115	-
21	BCR	F	308	-	-	3/29/63/63	0/2/2/2
21	BCR	B	849	-	-	8/29/63/63	0/2/2/2
17	CLA	1	307	1	1/1/15/20	13/37/115/115	-
22	LHG	F	302	-	-	30/44/44/53	-
17	CLA	3	605	-	1/1/10/20	3/10/88/115	-
21	BCR	J	105	-	-	7/29/63/63	0/2/2/2
17	CLA	3	610	-	1/1/12/20	8/22/100/115	-
17	CLA	1	306	29	1/1/11/20	1/15/93/115	-

All (1212) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	314	LUT	C24-C25	15.75	1.52	1.33
19	2	314	LUT	C24-C25	15.50	1.52	1.33
19	3	614	LUT	C24-C25	15.40	1.52	1.33
19	4	316	LUT	C24-C25	15.00	1.51	1.33
19	3	614	LUT	C14-C13	12.92	1.52	1.35
20	4	317	XAT	C34-C33	12.84	1.52	1.35
19	2	314	LUT	C34-C33	12.79	1.52	1.35
19	3	614	LUT	C10-C9	12.76	1.52	1.35
19	2	314	LUT	C10-C9	12.72	1.52	1.35
19	4	316	LUT	C10-C9	12.68	1.52	1.35
19	4	316	LUT	C14-C13	12.53	1.52	1.35
20	1	315	XAT	C14-C13	12.52	1.52	1.35
20	2	315	XAT	C14-C13	12.52	1.52	1.35
19	1	314	LUT	C14-C13	12.51	1.52	1.35
19	3	614	LUT	C30-C29	12.51	1.52	1.35
20	2	315	XAT	C34-C33	12.50	1.52	1.35
20	1	315	XAT	C34-C33	12.49	1.52	1.35
19	2	314	LUT	C14-C13	12.49	1.52	1.35
20	3	615	XAT	C34-C33	12.48	1.52	1.35
20	3	615	XAT	C14-C13	12.46	1.52	1.35
19	3	614	LUT	C34-C33	12.45	1.52	1.35
19	2	314	LUT	C30-C29	12.29	1.52	1.35
20	2	315	XAT	C10-C9	12.28	1.52	1.35
19	1	314	LUT	C30-C29	12.27	1.52	1.35
20	1	315	XAT	C10-C9	12.26	1.52	1.35
20	3	615	XAT	C10-C9	12.24	1.52	1.35
19	4	316	LUT	C30-C29	12.23	1.52	1.35
19	1	314	LUT	C34-C33	12.19	1.51	1.35
19	4	316	LUT	C34-C33	12.14	1.51	1.35
19	1	314	LUT	C10-C9	12.08	1.51	1.35
20	4	317	XAT	C10-C9	12.06	1.51	1.35
20	4	317	XAT	C30-C29	11.90	1.51	1.35
20	4	317	XAT	C14-C13	11.89	1.51	1.35
20	1	315	XAT	C30-C29	11.75	1.51	1.35
20	2	315	XAT	C30-C29	11.74	1.51	1.35
20	3	615	XAT	C30-C29	11.74	1.51	1.35
19	3	614	LUT	C5-C6	10.99	1.53	1.34
19	4	316	LUT	C5-C6	10.87	1.53	1.34
19	2	314	LUT	C5-C6	10.81	1.53	1.34
19	1	314	LUT	C5-C6	10.60	1.52	1.34
27	B	843	PQN	C3-C2	10.43	1.54	1.35
27	A	842	PQN	C3-C2	10.31	1.54	1.35
27	A	842	PQN	O4-C4	9.96	1.44	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	842	PQN	O1-C1	9.78	1.43	1.23
27	B	843	PQN	O1-C1	9.63	1.43	1.23
20	4	317	XAT	C8-C7	9.30	1.52	1.32
20	3	615	XAT	C28-C27	9.26	1.52	1.32
20	1	315	XAT	C28-C27	9.22	1.52	1.32
20	2	315	XAT	C28-C27	9.20	1.52	1.32
27	B	843	PQN	O4-C4	9.14	1.42	1.23
20	4	317	XAT	C28-C27	9.14	1.52	1.32
20	1	315	XAT	C8-C7	9.07	1.52	1.32
20	3	615	XAT	C8-C7	9.06	1.52	1.32
20	2	315	XAT	C8-C7	9.04	1.52	1.32
17	B	828	CLA	C4B-NB	8.93	1.43	1.35
17	4	303	CLA	C4B-NB	8.76	1.43	1.35
19	1	314	LUT	C28-C27	8.63	1.52	1.32
19	3	614	LUT	C28-C27	8.63	1.52	1.32
19	2	314	LUT	C28-C27	8.49	1.52	1.32
17	2	310	CLA	C4B-NB	8.48	1.42	1.35
27	B	843	PQN	C9-C10	8.44	1.53	1.39
17	B	810	CLA	C4B-NB	8.43	1.42	1.35
17	B	804	CLA	C4B-NB	8.43	1.42	1.35
17	B	835	CLA	C4B-NB	8.43	1.42	1.35
27	A	842	PQN	C12-C13	8.36	1.53	1.33
19	4	316	LUT	C28-C27	8.35	1.52	1.32
17	1	301	CLA	C4B-NB	8.33	1.42	1.35
17	2	301	CLA	C4B-NB	8.26	1.42	1.35
17	1	309	CLA	C4B-NB	8.22	1.42	1.35
17	4	302	CLA	C4B-NB	8.17	1.42	1.35
17	B	812	CLA	C4B-NB	8.17	1.42	1.35
27	A	842	PQN	C9-C10	8.17	1.52	1.39
17	F	306	CLA	C4B-NB	8.15	1.42	1.35
17	1	312	CLA	C4B-NB	8.12	1.42	1.35
17	A	817	CLA	C4B-NB	8.10	1.42	1.35
17	B	826	CLA	C4B-NB	8.09	1.42	1.35
17	A	843	CLA	C4B-NB	8.08	1.42	1.35
17	A	804	CLA	C4B-NB	8.03	1.42	1.35
17	G	103	CLA	C4B-NB	8.02	1.42	1.35
17	4	309	CLA	C4B-NB	8.01	1.42	1.35
17	3	605	CLA	C4B-NB	8.00	1.42	1.35
17	B	841	CLA	C4B-NB	7.98	1.42	1.35
17	L	204	CLA	C4B-NB	7.97	1.42	1.35
17	G	104	CLA	C4B-NB	7.95	1.42	1.35
17	A	810	CLA	C4B-NB	7.94	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	811	CLA	C4B-NB	7.93	1.42	1.35
17	1	304	CLA	C4B-NB	7.93	1.42	1.35
17	B	809	CLA	C4B-NB	7.89	1.42	1.35
17	4	313	CLA	C4B-NB	7.88	1.42	1.35
27	B	843	PQN	C12-C13	7.86	1.51	1.33
17	A	838	CLA	C4B-NB	7.85	1.42	1.35
17	2	312	CLA	C4B-NB	7.84	1.42	1.35
17	A	837	CLA	C4B-NB	7.83	1.42	1.35
17	B	830	CLA	C4B-NB	7.82	1.42	1.35
17	2	311	CLA	C4B-NB	7.81	1.42	1.35
17	A	825	CLA	C4B-NB	7.81	1.42	1.35
17	A	830	CLA	C4B-NB	7.81	1.42	1.35
17	B	802	CLA	C4B-NB	7.79	1.42	1.35
17	A	832	CLA	C4B-NB	7.78	1.42	1.35
17	3	610	CLA	C4B-NB	7.77	1.42	1.35
17	1	302	CLA	C4B-NB	7.76	1.42	1.35
17	A	840	CLA	C4B-NB	7.74	1.42	1.35
17	3	608	CLA	C4B-NB	7.72	1.42	1.35
17	A	816	CLA	C4B-NB	7.72	1.42	1.35
17	1	307	CLA	C4B-NB	7.71	1.42	1.35
17	3	606	CLA	C4B-NB	7.70	1.42	1.35
17	A	812	CLA	C4B-NB	7.70	1.42	1.35
17	2	309	CLA	C4B-NB	7.70	1.42	1.35
17	A	819	CLA	C4B-NB	7.66	1.42	1.35
17	2	303	CLA	C4B-NB	7.65	1.42	1.35
17	B	816	CLA	C4B-NB	7.63	1.42	1.35
17	A	820	CLA	C4B-NB	7.63	1.42	1.35
17	3	604	CLA	C4B-NB	7.63	1.42	1.35
17	3	611	CLA	C4B-NB	7.62	1.42	1.35
17	K	202	CLA	C4B-NB	7.62	1.42	1.35
17	A	815	CLA	C4B-NB	7.62	1.42	1.35
17	1	308	CLA	C4B-NB	7.62	1.42	1.35
27	B	843	PQN	C6-C5	7.62	1.52	1.39
17	A	822	CLA	C4B-NB	7.62	1.42	1.35
17	A	823	CLA	C4B-NB	7.61	1.42	1.35
17	A	831	CLA	C4B-NB	7.61	1.42	1.35
17	2	307	CLA	C4B-NB	7.60	1.42	1.35
17	3	612	CLA	C4B-NB	7.59	1.42	1.35
17	B	815	CLA	C4B-NB	7.59	1.42	1.35
17	3	603	CLA	C4B-NB	7.58	1.42	1.35
17	A	803	CLA	C4B-NB	7.58	1.42	1.35
17	A	824	CLA	C4B-NB	7.57	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	L	203	CLA	C4B-NB	7.56	1.42	1.35
17	A	834	CLA	C4B-NB	7.56	1.42	1.35
17	B	803	CLA	C4B-NB	7.56	1.42	1.35
17	L	202	CLA	C4B-NB	7.55	1.41	1.35
17	G	105	CLA	C4B-NB	7.54	1.41	1.35
17	3	602	CLA	C4B-NB	7.53	1.41	1.35
17	2	319	CLA	C4B-NB	7.53	1.41	1.35
17	A	853	CLA	C4B-NB	7.53	1.41	1.35
17	B	818	CLA	C4B-NB	7.50	1.41	1.35
17	B	829	CLA	C4B-NB	7.46	1.41	1.35
17	A	813	CLA	C4B-NB	7.44	1.41	1.35
17	K	201	CLA	C4B-NB	7.41	1.41	1.35
17	2	308	CLA	C4B-NB	7.40	1.41	1.35
17	4	311	CLA	C4B-NB	7.39	1.41	1.35
17	A	835	CLA	C4B-NB	7.38	1.41	1.35
17	A	839	CLA	C4B-NB	7.36	1.41	1.35
17	A	829	CLA	C4B-NB	7.35	1.41	1.35
17	3	609	CLA	C4B-NB	7.35	1.41	1.35
17	B	842	CLA	C4B-NB	7.35	1.41	1.35
27	A	842	PQN	C6-C5	7.34	1.51	1.39
17	1	306	CLA	C4B-NB	7.32	1.41	1.35
17	B	836	CLA	C4B-NB	7.29	1.41	1.35
17	B	819	CLA	C4B-NB	7.28	1.41	1.35
17	A	811	CLA	C4B-NB	7.28	1.41	1.35
17	A	814	CLA	C4B-NB	7.27	1.41	1.35
17	3	613	CLA	C4B-NB	7.26	1.41	1.35
17	A	821	CLA	C4B-NB	7.26	1.41	1.35
17	A	841	CLA	C4B-NB	7.26	1.41	1.35
20	4	317	XAT	C11-C12	7.24	1.53	1.34
17	A	836	CLA	C4B-NB	7.23	1.41	1.35
17	2	302	CLA	C4B-NB	7.23	1.41	1.35
17	A	818	CLA	C4B-NB	7.21	1.41	1.35
17	1	303	CLA	C4B-NB	7.21	1.41	1.35
17	A	806	CLA	C4B-NB	7.20	1.41	1.35
17	J	101	CLA	C4B-NB	7.19	1.41	1.35
17	A	801	CLA	C4B-NB	7.17	1.41	1.35
17	1	310	CLA	C4B-NB	7.16	1.41	1.35
17	4	314	CLA	C4B-NB	7.15	1.41	1.35
17	A	802	CLA	C4B-NB	7.12	1.41	1.35
17	4	310	CLA	C4B-NB	7.11	1.41	1.35
17	A	828	CLA	C4B-NB	7.09	1.41	1.35
17	A	833	CLA	C4B-NB	7.07	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	614	LUT	C11-C12	7.06	1.52	1.34
17	B	817	CLA	C4B-NB	7.00	1.41	1.35
17	A	809	CLA	C4B-NB	6.95	1.41	1.35
17	A	826	CLA	C4B-NB	6.92	1.41	1.35
19	2	314	LUT	C11-C12	6.91	1.52	1.34
20	4	317	XAT	C31-C32	6.89	1.52	1.34
19	3	614	LUT	C31-C32	6.88	1.52	1.34
27	A	842	PQN	C8-C9	6.86	1.53	1.38
17	F	304	CLA	C4B-NB	6.84	1.41	1.35
17	F	307	CLA	C4B-NB	6.79	1.41	1.35
27	A	842	PQN	C7-C6	6.77	1.53	1.38
19	2	314	LUT	C31-C32	6.76	1.52	1.34
20	3	615	XAT	C11-C12	6.76	1.52	1.34
20	1	315	XAT	C11-C12	6.75	1.52	1.34
17	B	805	CLA	C4B-NB	6.75	1.41	1.35
20	2	315	XAT	C11-C12	6.72	1.51	1.34
17	A	807	CLA	C4B-NB	6.71	1.41	1.35
20	1	315	XAT	C31-C32	6.71	1.51	1.34
20	2	315	XAT	C31-C32	6.71	1.51	1.34
20	3	615	XAT	C31-C32	6.70	1.51	1.34
17	A	827	CLA	C4B-NB	6.70	1.41	1.35
19	4	316	LUT	C31-C32	6.69	1.51	1.34
19	1	314	LUT	C11-C12	6.68	1.51	1.34
19	4	316	LUT	C11-C12	6.68	1.51	1.34
17	J	103	CLA	C4B-NB	6.67	1.41	1.35
19	1	314	LUT	C31-C32	6.66	1.51	1.34
17	1	313	CLA	C4B-NB	6.65	1.41	1.35
17	B	814	CLA	C4B-NB	6.65	1.41	1.35
17	4	303	CLA	C4C-NC	6.63	1.41	1.35
17	B	834	CLA	C4B-NB	6.62	1.41	1.35
27	B	843	PQN	C10-C5	6.62	1.51	1.40
17	B	825	CLA	C4B-NB	6.60	1.41	1.35
17	4	308	CLA	C4B-NB	6.59	1.41	1.35
17	B	823	CLA	C4B-NB	6.58	1.41	1.35
17	4	304	CLA	C4B-NB	6.55	1.41	1.35
17	B	822	CLA	C4B-NB	6.55	1.41	1.35
17	A	805	CLA	C4B-NB	6.53	1.41	1.35
17	A	839	CLA	C4C-NC	6.49	1.41	1.35
17	B	824	CLA	C4B-NB	6.49	1.41	1.35
17	1	311	CLA	C4B-NB	6.48	1.41	1.35
17	B	808	CLA	C4B-NB	6.48	1.41	1.35
27	B	843	PQN	C8-C9	6.46	1.52	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	837	CLA	C4B-NB	6.44	1.41	1.35
19	3	614	LUT	C8-C7	6.42	1.52	1.33
19	1	314	LUT	C35-C15	6.42	1.52	1.36
19	4	316	LUT	C8-C7	6.40	1.52	1.33
17	4	312	CLA	C4B-NB	6.39	1.40	1.35
19	3	614	LUT	C35-C15	6.37	1.52	1.36
27	B	843	PQN	C7-C6	6.37	1.52	1.38
19	2	314	LUT	C35-C15	6.34	1.52	1.36
27	A	842	PQN	C10-C5	6.34	1.51	1.40
17	G	104	CLA	C4C-NC	6.33	1.40	1.35
17	4	314	CLA	C4C-NC	6.33	1.40	1.35
19	2	314	LUT	C8-C7	6.33	1.52	1.33
17	B	820	CLA	C4B-NB	6.31	1.40	1.35
17	B	838	CLA	C4B-NB	6.30	1.40	1.35
17	3	605	CLA	C4C-NC	6.30	1.40	1.35
17	A	827	CLA	C4C-NC	6.30	1.40	1.35
17	1	301	CLA	C4C-NC	6.25	1.40	1.35
17	2	310	CLA	C4C-NC	6.23	1.40	1.35
20	3	615	XAT	C35-C15	6.21	1.52	1.36
20	1	315	XAT	C35-C15	6.21	1.52	1.36
20	2	315	XAT	C35-C15	6.21	1.52	1.36
17	1	306	CLA	C4C-NC	6.20	1.40	1.35
17	B	813	CLA	C4B-NB	6.18	1.40	1.35
17	B	813	CLA	C4C-NC	6.17	1.40	1.35
17	A	812	CLA	C4C-NC	6.17	1.40	1.35
19	1	314	LUT	C8-C7	6.17	1.51	1.33
19	4	316	LUT	C35-C15	6.16	1.52	1.36
17	B	833	CLA	C4B-NB	6.15	1.40	1.35
17	B	839	CLA	C4C-NC	6.13	1.40	1.35
17	B	806	CLA	C4C-NC	6.12	1.40	1.35
17	B	818	CLA	C4C-NC	6.12	1.40	1.35
17	A	835	CLA	C4C-NC	6.11	1.40	1.35
17	B	840	CLA	C4B-NB	6.08	1.40	1.35
17	A	824	CLA	C4C-NC	6.05	1.40	1.35
17	B	807	CLA	C4B-NB	6.05	1.40	1.35
17	2	312	CLA	C4C-NC	6.05	1.40	1.35
20	4	317	XAT	C35-C15	6.04	1.51	1.36
17	B	830	CLA	C4C-NC	6.04	1.40	1.35
17	A	832	CLA	C4C-NC	6.03	1.40	1.35
17	3	606	CLA	C4C-NC	6.03	1.40	1.35
17	A	806	CLA	C4C-NC	6.01	1.40	1.35
17	B	831	CLA	C4B-NB	6.00	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	832	CLA	C4B-NB	5.98	1.40	1.35
17	3	610	CLA	C4C-NC	5.97	1.40	1.35
17	A	811	CLA	C4C-NC	5.95	1.40	1.35
17	B	827	CLA	C4C-NC	5.94	1.40	1.35
17	4	312	CLA	C4C-NC	5.94	1.40	1.35
17	3	604	CLA	C4C-NC	5.93	1.40	1.35
17	G	105	CLA	C4C-NC	5.91	1.40	1.35
17	L	204	CLA	C4C-NC	5.91	1.40	1.35
17	B	827	CLA	C4B-NB	5.90	1.40	1.35
17	A	815	CLA	C4C-NC	5.88	1.40	1.35
17	1	313	CLA	C4C-NC	5.87	1.40	1.35
17	2	309	CLA	C4C-NC	5.85	1.40	1.35
17	B	839	CLA	C4B-NB	5.84	1.40	1.35
17	1	309	CLA	C4C-NC	5.82	1.40	1.35
17	1	307	CLA	C4C-NC	5.82	1.40	1.35
17	3	602	CLA	C4C-NC	5.82	1.40	1.35
17	K	202	CLA	C4C-NC	5.81	1.40	1.35
17	B	807	CLA	C4C-NC	5.80	1.40	1.35
17	2	311	CLA	C4C-NC	5.79	1.40	1.35
17	4	308	CLA	C4C-NC	5.77	1.40	1.35
17	2	302	CLA	C4C-NC	5.76	1.40	1.35
17	2	303	CLA	C4C-NC	5.76	1.40	1.35
17	A	823	CLA	C4C-NC	5.76	1.40	1.35
17	B	814	CLA	C4C-NC	5.75	1.40	1.35
17	A	834	CLA	C4C-NC	5.75	1.40	1.35
17	1	310	CLA	C4C-NC	5.74	1.40	1.35
17	A	820	CLA	C4C-NC	5.73	1.40	1.35
17	B	840	CLA	C4C-NC	5.73	1.40	1.35
17	A	809	CLA	C4C-NC	5.71	1.40	1.35
17	B	829	CLA	C4C-NC	5.71	1.40	1.35
17	A	828	CLA	C4C-NC	5.70	1.40	1.35
17	B	838	CLA	C4C-NC	5.69	1.40	1.35
17	A	808	CLA	C4C-NC	5.69	1.40	1.35
17	A	833	CLA	C4C-NC	5.69	1.40	1.35
17	B	803	CLA	C4C-NC	5.68	1.40	1.35
17	3	612	CLA	C4C-NC	5.67	1.40	1.35
17	A	838	CLA	C4C-NC	5.67	1.40	1.35
17	K	201	CLA	C4C-NC	5.67	1.40	1.35
17	B	826	CLA	C4C-NC	5.67	1.40	1.35
17	A	818	CLA	C4C-NC	5.66	1.40	1.35
17	B	822	CLA	C4C-NC	5.65	1.40	1.35
17	A	814	CLA	C4C-NC	5.65	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	843	CLA	C4C-NC	5.64	1.40	1.35
27	B	843	PQN	C8-C7	5.62	1.52	1.38
17	A	813	CLA	C4C-NC	5.62	1.40	1.35
17	4	302	CLA	C4C-NC	5.61	1.40	1.35
17	A	805	CLA	C4C-NC	5.60	1.40	1.35
17	A	837	CLA	C4C-NC	5.60	1.40	1.35
17	B	841	CLA	C4C-NC	5.60	1.40	1.35
17	B	806	CLA	C4B-NB	5.59	1.40	1.35
17	4	311	CLA	C4C-NC	5.59	1.40	1.35
17	A	830	CLA	C4C-NC	5.58	1.40	1.35
17	1	302	CLA	C4C-NC	5.58	1.40	1.35
17	3	611	CLA	C4C-NC	5.57	1.40	1.35
17	J	101	CLA	C4C-NC	5.53	1.40	1.35
27	A	842	PQN	C8-C7	5.52	1.52	1.38
17	L	202	CLA	C4C-NC	5.52	1.40	1.35
17	3	609	CLA	C4C-NC	5.52	1.40	1.35
17	2	307	CLA	C4C-NC	5.50	1.40	1.35
17	A	821	CLA	C4C-NC	5.50	1.40	1.35
17	3	603	CLA	C4C-NC	5.50	1.40	1.35
17	3	613	CLA	C4C-NC	5.49	1.40	1.35
17	A	816	CLA	C4C-NC	5.49	1.40	1.35
17	A	802	CLA	C4C-NC	5.48	1.40	1.35
17	B	821	CLA	C4C-NC	5.46	1.40	1.35
17	1	312	CLA	C4C-NC	5.46	1.40	1.35
17	2	319	CLA	C4C-NC	5.46	1.40	1.35
17	J	103	CLA	C4C-NC	5.45	1.40	1.35
18	2	313	CHL	O2D-CGD	5.44	1.46	1.33
18	1	305	CHL	O2D-CGD	5.44	1.46	1.33
17	A	836	CLA	C4C-NC	5.43	1.40	1.35
17	2	308	CLA	C4C-NC	5.43	1.40	1.35
17	B	821	CLA	C4B-NB	5.42	1.40	1.35
17	B	835	CLA	C4C-NC	5.40	1.40	1.35
17	G	103	CLA	C4C-NC	5.40	1.40	1.35
17	A	817	CLA	C4C-NC	5.40	1.40	1.35
17	4	309	CLA	C4C-NC	5.39	1.40	1.35
17	1	303	CLA	C4C-NC	5.39	1.40	1.35
17	A	822	CLA	C4C-NC	5.39	1.40	1.35
17	A	831	CLA	C4C-NC	5.38	1.40	1.35
18	1	305	CHL	CHC-C1C	5.38	1.48	1.35
18	4	307	CHL	C3D-C2D	5.37	1.49	1.39
18	4	307	CHL	CHC-C1C	5.37	1.48	1.35
17	B	805	CLA	C4C-NC	5.37	1.40	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	809	CLA	C4C-NC	5.36	1.40	1.35
17	2	301	CLA	C4C-NC	5.36	1.40	1.35
17	3	608	CLA	C4C-NC	5.35	1.40	1.35
17	L	203	CLA	C4C-NC	5.35	1.40	1.35
18	4	306	CHL	CHC-C1C	5.34	1.48	1.35
17	A	803	CLA	C4C-NC	5.33	1.40	1.35
17	B	832	CLA	C4C-NC	5.32	1.40	1.35
17	1	308	CLA	C4C-NC	5.29	1.39	1.35
18	3	607	CHL	O2D-CGD	5.29	1.46	1.33
17	B	833	CLA	C4C-NC	5.28	1.39	1.35
17	A	819	CLA	C4C-NC	5.26	1.39	1.35
17	A	807	CLA	C4C-NC	5.25	1.39	1.35
17	1	311	CLA	C4C-NC	5.25	1.39	1.35
17	B	819	CLA	C4C-NC	5.24	1.39	1.35
17	B	820	CLA	C4C-NC	5.23	1.39	1.35
17	4	310	CLA	C4C-NC	5.21	1.39	1.35
17	A	841	CLA	C4C-NC	5.20	1.39	1.35
17	B	831	CLA	C4C-NC	5.20	1.39	1.35
17	1	304	CLA	C4C-NC	5.18	1.39	1.35
17	B	804	CLA	C4C-NC	5.18	1.39	1.35
18	4	306	CHL	O2D-CGD	5.16	1.45	1.33
17	B	816	CLA	C4C-NC	5.15	1.39	1.35
17	F	306	CLA	C4C-NC	5.15	1.39	1.35
17	A	826	CLA	C4C-NC	5.15	1.39	1.35
18	2	304	CHL	CHC-C1C	5.14	1.48	1.35
18	2	305	CHL	O2D-CGD	5.13	1.45	1.33
17	A	825	CLA	C4C-NC	5.12	1.39	1.35
18	4	315	CHL	CHC-C1C	5.12	1.48	1.35
18	4	315	CHL	O2D-CGD	5.09	1.45	1.33
17	A	804	CLA	C4C-NC	5.07	1.39	1.35
18	2	304	CHL	OBD-CAD	5.06	1.29	1.22
18	2	313	CHL	CHC-C1C	5.05	1.47	1.35
18	2	305	CHL	CHC-C1C	5.04	1.47	1.35
17	B	836	CLA	C4C-NC	5.02	1.39	1.35
17	A	829	CLA	C4C-NC	5.00	1.39	1.35
17	B	828	CLA	C4C-NC	4.99	1.39	1.35
18	2	306	CHL	O2D-CGD	4.98	1.45	1.33
17	4	313	CLA	C4C-NC	4.96	1.39	1.35
17	F	304	CLA	C4C-NC	4.94	1.39	1.35
17	B	812	CLA	C4C-NC	4.92	1.39	1.35
18	2	306	CHL	OBD-CAD	4.88	1.29	1.22
17	A	810	CLA	C4C-NC	4.88	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	306	CHL	CHC-C1C	4.88	1.47	1.35
18	3	601	CHL	CHC-C1C	4.88	1.47	1.35
18	2	304	CHL	O2D-CGD	4.86	1.45	1.33
17	B	810	CLA	C4C-NC	4.86	1.39	1.35
17	B	817	CLA	C4C-NC	4.85	1.39	1.35
18	3	601	CHL	C3B-C2B	4.84	1.47	1.40
18	3	607	CHL	CHC-C1C	4.83	1.47	1.35
18	4	307	CHL	C2C-C3C	4.79	1.47	1.36
18	4	305	CHL	O2D-CGD	4.79	1.44	1.33
18	4	307	CHL	O2D-CGD	4.78	1.44	1.33
18	3	607	CHL	C3B-C2B	4.78	1.47	1.40
18	1	305	CHL	C3B-C2B	4.78	1.47	1.40
18	1	305	CHL	C3D-C2D	4.77	1.48	1.39
18	1	305	CHL	C2C-C3C	4.76	1.46	1.36
18	4	315	CHL	C3D-C2D	4.75	1.48	1.39
18	2	305	CHL	C3B-C2B	4.75	1.47	1.40
17	F	307	CLA	C4C-NC	4.75	1.39	1.35
17	B	815	CLA	C4C-NC	4.74	1.39	1.35
18	3	601	CHL	O2D-CGD	4.74	1.44	1.33
18	4	306	CHL	C2C-C3C	4.70	1.46	1.36
17	B	824	CLA	C4C-NC	4.69	1.39	1.35
18	3	601	CHL	OBD-CAD	4.69	1.28	1.22
17	B	811	CLA	C4C-NC	4.69	1.39	1.35
18	3	607	CHL	OBD-CAD	4.66	1.28	1.22
18	4	307	CHL	OBD-CAD	4.65	1.28	1.22
17	B	842	CLA	C4C-NC	4.65	1.39	1.35
18	4	306	CHL	O2A-CGA	4.64	1.46	1.33
18	3	601	CHL	C2C-C3C	4.63	1.46	1.36
18	4	306	CHL	C3B-C2B	4.63	1.46	1.40
18	4	305	CHL	CHC-C1C	4.61	1.46	1.35
17	A	808	CLA	C4B-NB	4.59	1.39	1.35
18	3	607	CHL	C3D-C2D	4.59	1.47	1.39
17	A	853	CLA	C4C-NC	4.59	1.39	1.35
18	2	313	CHL	C3B-C2B	4.58	1.46	1.40
18	2	305	CHL	OBD-CAD	4.58	1.28	1.22
17	B	834	CLA	C4C-NC	4.56	1.39	1.35
18	2	313	CHL	C2C-C3C	4.56	1.46	1.36
17	4	304	CLA	C4C-NC	4.54	1.39	1.35
18	2	305	CHL	O2A-CGA	4.51	1.46	1.33
17	B	823	CLA	C4C-NC	4.51	1.39	1.35
18	1	305	CHL	O2A-CGA	4.51	1.46	1.33
18	2	313	CHL	C3D-C2D	4.51	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	306	CHL	C3D-C2D	4.50	1.47	1.39
18	2	306	CHL	C2C-C3C	4.49	1.46	1.36
18	2	313	CHL	OBD-CAD	4.48	1.28	1.22
18	3	607	CHL	C2C-C3C	4.47	1.46	1.36
18	2	305	CHL	C2C-C3C	4.44	1.46	1.36
18	4	305	CHL	C3B-C2B	4.44	1.46	1.40
18	4	315	CHL	OBD-CAD	4.41	1.28	1.22
18	2	305	CHL	C3D-C2D	4.41	1.47	1.39
17	B	808	CLA	C4C-NC	4.39	1.39	1.35
18	4	305	CHL	O2A-CGA	4.38	1.46	1.33
18	4	315	CHL	C2C-C3C	4.38	1.46	1.36
18	4	301	CHL	CHC-C1C	4.36	1.46	1.35
18	4	306	CHL	C3D-C2D	4.32	1.47	1.39
17	B	802	CLA	C4C-NC	4.32	1.39	1.35
18	2	306	CHL	O2A-CGA	4.31	1.45	1.33
18	3	601	CHL	O2A-CGA	4.31	1.45	1.33
18	3	601	CHL	C3D-C2D	4.30	1.47	1.39
18	4	307	CHL	O2A-CGA	4.29	1.45	1.33
18	2	304	CHL	C2C-C3C	4.29	1.46	1.36
18	1	305	CHL	OBD-CAD	4.28	1.28	1.22
18	4	306	CHL	OBD-CAD	4.17	1.28	1.22
21	J	105	BCR	C1-C6	-4.17	1.48	1.53
26	4	323	DGD	O2G-C1B	4.16	1.46	1.34
20	4	317	XAT	C8-C9	4.16	1.54	1.45
18	4	315	CHL	C3B-C2B	4.13	1.46	1.40
17	A	801	CLA	C4C-NC	4.12	1.38	1.35
18	4	305	CHL	C3D-C2D	4.10	1.46	1.39
18	4	305	CHL	C1D-C2D	4.10	1.51	1.42
18	2	304	CHL	C3D-C2D	4.09	1.46	1.39
21	2	316	BCR	C1-C6	-4.06	1.48	1.53
18	4	307	CHL	C3B-C2B	4.06	1.46	1.40
18	2	304	CHL	C3B-C2B	4.05	1.46	1.40
17	B	825	CLA	C4C-NC	4.02	1.38	1.35
18	3	607	CHL	O2A-CGA	4.01	1.45	1.33
25	4	321	HTG	C1'-S1	-3.98	1.76	1.81
18	2	306	CHL	C3B-C2B	3.91	1.45	1.40
25	J	102	HTG	C1'-S1	-3.90	1.76	1.81
17	A	840	CLA	C4C-NC	3.87	1.38	1.35
18	2	305	CHL	C1D-C2D	3.82	1.51	1.42
17	B	837	CLA	C4C-NC	3.82	1.38	1.35
25	4	322	HTG	C1'-S1	-3.80	1.76	1.81
18	3	601	CHL	C1D-C2D	3.75	1.51	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	320	LMG	C4-C5	3.74	1.60	1.53
18	4	306	CHL	C1D-C2D	3.74	1.51	1.42
18	4	305	CHL	C2C-C3C	3.73	1.44	1.36
18	2	313	CHL	C1D-C2D	3.72	1.51	1.42
18	4	307	CHL	C1D-C2D	3.68	1.50	1.42
18	2	304	CHL	C1D-C2D	3.67	1.50	1.42
25	B	851	HTG	C1'-S1	-3.65	1.76	1.81
18	3	607	CHL	C1D-C2D	3.65	1.50	1.42
18	1	305	CHL	C1D-C2D	3.62	1.50	1.42
21	B	847	BCR	C1-C6	-3.62	1.48	1.53
21	A	850	BCR	C30-C25	-3.62	1.48	1.53
27	A	842	PQN	C3-C4	3.62	1.56	1.47
18	2	306	CHL	C1D-C2D	3.61	1.50	1.42
18	4	305	CHL	OBD-CAD	3.61	1.27	1.22
20	4	317	XAT	C28-C29	3.58	1.53	1.45
17	A	840	CLA	C1D-C2D	3.55	1.50	1.42
24	B	852	LMG	C4-C3	3.54	1.61	1.52
21	B	848	BCR	C30-C25	-3.52	1.48	1.53
26	B	850	DGD	C3D-C2D	3.52	1.61	1.52
26	4	323	DGD	O1G-C1A	3.48	1.43	1.33
25	F	310	HTG	C1'-S1	-3.47	1.77	1.81
20	4	317	XAT	C12-C13	3.46	1.53	1.45
27	A	842	PQN	C2-C1	3.45	1.55	1.48
17	B	811	CLA	CMB-C2B	-3.41	1.44	1.51
21	B	846	BCR	C30-C25	-3.40	1.49	1.53
17	B	839	CLA	C1D-C2D	3.39	1.50	1.42
21	F	308	BCR	C30-C25	-3.39	1.49	1.53
18	4	315	CHL	C1D-C2D	3.32	1.50	1.42
18	4	301	CHL	C4B-NB	-3.32	1.32	1.35
17	B	841	CLA	C1D-C2D	3.30	1.50	1.42
21	A	850	BCR	C1-C6	-3.30	1.49	1.53
21	G	106	BCR	C1-C6	-3.25	1.49	1.53
17	F	304	CLA	C1B-NB	3.24	1.38	1.35
17	1	307	CLA	C1D-C2D	3.24	1.49	1.42
27	B	843	PQN	C10-C1	3.24	1.54	1.48
21	2	316	BCR	C30-C25	-3.22	1.49	1.53
21	A	849	BCR	C30-C25	-3.21	1.49	1.53
21	L	205	BCR	C1-C6	-3.19	1.49	1.53
19	2	314	LUT	C12-C13	3.19	1.52	1.45
20	4	317	XAT	C32-C33	3.19	1.52	1.45
21	L	201	BCR	C1-C6	-3.18	1.49	1.53
21	I	101	BCR	C1-C6	-3.17	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	302	CLA	C1D-C2D	3.17	1.49	1.42
21	J	104	BCR	C1-C6	-3.15	1.49	1.53
19	4	316	LUT	C28-C29	3.15	1.52	1.45
17	F	304	CLA	C1D-C2D	3.14	1.49	1.42
21	B	847	BCR	C38-C26	-3.13	1.45	1.50
21	F	308	BCR	C1-C6	-3.13	1.49	1.53
17	B	835	CLA	C1D-C2D	3.12	1.49	1.42
25	F	301	HTG	C1'-S1	-3.12	1.77	1.81
27	A	842	PQN	C5-C4	3.12	1.54	1.48
18	4	301	CHL	C1C-NC	-3.12	1.33	1.37
27	A	842	PQN	C10-C1	3.12	1.54	1.48
21	L	206	BCR	C30-C25	-3.10	1.49	1.53
17	A	827	CLA	C1D-C2D	3.09	1.49	1.42
21	1	316	BCR	C1-C6	-3.09	1.49	1.53
17	A	807	CLA	C1D-C2D	3.09	1.49	1.42
17	B	838	CLA	C1D-C2D	3.09	1.49	1.42
18	4	301	CHL	C1B-NB	-3.09	1.32	1.35
21	A	849	BCR	C1-C6	-3.07	1.49	1.53
20	3	615	XAT	C32-C33	3.07	1.52	1.45
21	L	206	BCR	C1-C6	-3.06	1.49	1.53
17	A	825	CLA	C1D-C2D	3.06	1.49	1.42
17	A	811	CLA	C1D-C2D	3.06	1.49	1.42
17	A	818	CLA	C1D-C2D	3.06	1.49	1.42
21	A	847	BCR	C1-C6	-3.05	1.49	1.53
20	1	315	XAT	C32-C33	3.05	1.52	1.45
21	A	848	BCR	C30-C25	-3.04	1.49	1.53
17	B	834	CLA	CMB-C2B	-3.04	1.45	1.51
17	B	809	CLA	C1D-C2D	3.03	1.49	1.42
19	3	614	LUT	C28-C29	3.03	1.52	1.45
17	A	835	CLA	C1D-C2D	3.03	1.49	1.42
25	A	854	HTG	C1'-S1	-3.03	1.77	1.81
20	2	315	XAT	C32-C33	3.02	1.52	1.45
17	B	821	CLA	C1D-C2D	3.02	1.49	1.42
19	3	614	LUT	C12-C13	3.01	1.52	1.45
18	4	301	CHL	MG-NA	-3.00	1.99	2.06
21	K	203	BCR	C30-C25	-3.00	1.49	1.53
17	A	837	CLA	C1D-C2D	2.99	1.49	1.42
17	4	311	CLA	C1D-C2D	2.99	1.49	1.42
19	3	614	LUT	C11-C10	2.98	1.52	1.43
17	B	804	CLA	C1B-NB	2.97	1.37	1.35
17	A	839	CLA	C3B-C2B	-2.97	1.36	1.40
20	1	315	XAT	C28-C29	2.97	1.52	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	314	LUT	C35-C34	2.97	1.52	1.43
26	B	850	DGD	O5D-C6D	-2.97	1.38	1.43
19	3	614	LUT	C31-C30	2.97	1.52	1.43
20	2	315	XAT	C28-C29	2.96	1.52	1.45
17	B	829	CLA	C1D-C2D	2.96	1.49	1.42
21	B	848	BCR	C1-C6	-2.95	1.49	1.53
17	B	830	CLA	C3B-C2B	-2.95	1.36	1.40
19	1	314	LUT	C31-C30	2.95	1.52	1.43
18	4	301	CHL	C2C-C3C	2.94	1.43	1.36
19	1	314	LUT	C28-C29	2.94	1.52	1.45
20	3	615	XAT	C28-C29	2.94	1.52	1.45
25	J	102	HTG	C1-S1	-2.94	1.76	1.80
27	B	843	PQN	C2-C1	2.92	1.54	1.48
21	1	316	BCR	C30-C25	-2.92	1.49	1.53
17	A	841	CLA	C1D-C2D	2.92	1.49	1.42
17	B	828	CLA	C1D-C2D	2.92	1.49	1.42
17	B	842	CLA	CMB-C2B	-2.92	1.45	1.51
21	3	616	BCR	C1-C6	-2.91	1.49	1.53
19	4	316	LUT	C15-C14	2.91	1.52	1.43
19	2	314	LUT	C11-C10	2.91	1.52	1.43
24	4	320	LMG	O1-C1	2.91	1.45	1.40
21	A	848	BCR	C1-C6	-2.91	1.49	1.53
17	1	306	CLA	C1D-C2D	2.90	1.49	1.42
17	1	301	CLA	C1D-C2D	2.90	1.49	1.42
17	A	803	CLA	C1D-C2D	2.90	1.49	1.42
19	3	614	LUT	C15-C14	2.90	1.52	1.43
19	4	316	LUT	C32-C33	2.90	1.52	1.45
17	A	812	CLA	C1D-C2D	2.90	1.49	1.42
17	2	309	CLA	C1D-C2D	2.89	1.49	1.42
17	B	804	CLA	C1D-C2D	2.89	1.49	1.42
17	A	832	CLA	C1D-C2D	2.88	1.49	1.42
19	2	314	LUT	C8-C9	2.88	1.52	1.45
17	B	825	CLA	C1D-C2D	2.88	1.49	1.42
17	B	807	CLA	C1D-C2D	2.88	1.49	1.42
21	J	105	BCR	C30-C25	-2.88	1.49	1.53
17	B	812	CLA	C1D-C2D	2.87	1.49	1.42
21	K	203	BCR	C1-C6	-2.87	1.49	1.53
17	J	101	CLA	C1D-C2D	2.87	1.49	1.42
19	2	314	LUT	C28-C29	2.87	1.52	1.45
17	B	814	CLA	C1D-C2D	2.86	1.49	1.42
19	3	614	LUT	C35-C34	2.86	1.52	1.43
17	B	834	CLA	C3B-C2B	-2.86	1.36	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	846	BCR	C1-C6	-2.85	1.49	1.53
26	B	850	DGD	O6D-C5D	-2.85	1.37	1.44
19	4	316	LUT	C31-C30	2.84	1.52	1.43
17	B	807	CLA	MG-NA	2.84	2.13	2.06
17	B	842	CLA	C1D-C2D	2.84	1.49	1.42
18	4	301	CHL	O2A-CGA	2.84	1.41	1.33
17	B	831	CLA	C1D-C2D	2.84	1.49	1.42
20	1	315	XAT	C11-C10	2.83	1.52	1.43
17	2	312	CLA	C1D-C2D	2.83	1.49	1.42
20	3	615	XAT	C11-C10	2.83	1.52	1.43
17	A	813	CLA	C1D-C2D	2.83	1.49	1.42
17	A	824	CLA	C1D-C2D	2.83	1.49	1.42
17	1	309	CLA	C1D-C2D	2.82	1.49	1.42
27	B	843	PQN	C3-C4	2.82	1.54	1.47
17	A	804	CLA	C1D-C2D	2.82	1.48	1.42
17	4	303	CLA	C1D-C2D	2.82	1.48	1.42
17	4	309	CLA	C1D-C2D	2.82	1.48	1.42
17	B	827	CLA	C1D-C2D	2.81	1.48	1.42
19	2	314	LUT	C32-C33	2.81	1.52	1.45
19	4	316	LUT	C8-C9	2.81	1.52	1.45
19	3	614	LUT	C32-C33	2.81	1.52	1.45
17	B	824	CLA	C1D-C2D	2.81	1.48	1.42
17	1	303	CLA	C1D-C2D	2.81	1.48	1.42
20	2	315	XAT	C11-C10	2.80	1.52	1.43
19	1	314	LUT	C8-C9	2.80	1.52	1.45
17	2	307	CLA	C1D-C2D	2.80	1.48	1.42
19	4	316	LUT	C12-C13	2.80	1.52	1.45
17	A	839	CLA	C1D-C2D	2.80	1.48	1.42
20	3	615	XAT	C31-C30	2.80	1.52	1.43
17	3	609	CLA	C1D-C2D	2.80	1.48	1.42
20	2	315	XAT	C31-C30	2.80	1.52	1.43
20	1	315	XAT	C31-C30	2.80	1.52	1.43
17	B	819	CLA	C1D-C2D	2.79	1.48	1.42
17	2	311	CLA	C1D-C2D	2.79	1.48	1.42
17	A	831	CLA	C1D-C2D	2.79	1.48	1.42
17	B	826	CLA	MG-NA	2.78	2.12	2.06
25	F	305	HTG	C1'-S1	-2.78	1.77	1.81
21	A	847	BCR	C30-C25	-2.78	1.49	1.53
17	A	809	CLA	C1D-C2D	2.77	1.48	1.42
17	A	823	CLA	C1D-C2D	2.77	1.48	1.42
19	1	314	LUT	C15-C14	2.77	1.52	1.43
17	3	608	CLA	C1D-C2D	2.76	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	315	XAT	C8-C9	2.76	1.51	1.45
20	2	315	XAT	C8-C9	2.76	1.51	1.45
20	3	615	XAT	C8-C9	2.76	1.51	1.45
17	3	611	CLA	C1D-C2D	2.76	1.48	1.42
21	I	101	BCR	C30-C25	-2.76	1.50	1.53
24	B	852	LMG	C4-C5	2.76	1.58	1.53
17	A	817	CLA	C1D-C2D	2.76	1.48	1.42
21	3	616	BCR	C30-C25	-2.76	1.50	1.53
20	2	315	XAT	C15-C14	2.76	1.52	1.43
20	3	615	XAT	C15-C14	2.75	1.52	1.43
20	2	315	XAT	C35-C34	2.75	1.52	1.43
20	4	317	XAT	C11-C10	2.75	1.52	1.43
20	1	315	XAT	C15-C14	2.75	1.52	1.43
19	3	614	LUT	C8-C9	2.75	1.51	1.45
17	4	312	CLA	C1D-C2D	2.75	1.48	1.42
17	L	203	CLA	C1D-C2D	2.74	1.48	1.42
21	F	303	BCR	C30-C25	-2.74	1.50	1.53
20	1	315	XAT	C35-C34	2.74	1.51	1.43
19	2	314	LUT	C15-C14	2.74	1.51	1.43
18	1	305	CHL	C1B-CHB	2.74	1.48	1.41
17	B	815	CLA	C1D-C2D	2.74	1.48	1.42
17	A	822	CLA	C1D-C2D	2.74	1.48	1.42
21	B	849	BCR	C30-C25	-2.73	1.50	1.53
17	B	820	CLA	C1D-C2D	2.73	1.48	1.42
17	A	833	CLA	C1D-C2D	2.73	1.48	1.42
20	3	615	XAT	C35-C34	2.73	1.51	1.43
19	1	314	LUT	C12-C13	2.73	1.51	1.45
17	3	612	CLA	C1D-C2D	2.72	1.48	1.42
23	A	855	LMT	O4'-C4B	-2.72	1.36	1.43
17	3	605	CLA	C1D-C2D	2.72	1.48	1.42
17	B	818	CLA	C1D-C2D	2.72	1.48	1.42
19	2	314	LUT	C31-C30	2.72	1.51	1.43
19	1	314	LUT	C35-C34	2.72	1.51	1.43
17	4	313	CLA	C1D-C2D	2.71	1.48	1.42
17	A	829	CLA	C1D-C2D	2.71	1.48	1.42
17	L	202	CLA	C1D-C2D	2.71	1.48	1.42
26	B	850	DGD	C3G-C2G	2.70	1.59	1.50
25	4	321	HTG	C1-S1	-2.70	1.76	1.80
17	A	806	CLA	C1D-C2D	2.70	1.48	1.42
17	L	204	CLA	C1D-C2D	2.69	1.48	1.42
21	A	851	BCR	C1-C6	-2.69	1.50	1.53
17	3	602	CLA	C1D-C2D	2.69	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	801	LHG	P-O6	2.69	1.70	1.59
17	A	836	CLA	C1D-C2D	2.68	1.48	1.42
21	B	844	BCR	C1-C6	-2.68	1.50	1.53
17	B	820	CLA	CMD-C2D	-2.68	1.45	1.51
17	A	838	CLA	C1D-C2D	2.67	1.48	1.42
17	G	103	CLA	C1D-C2D	2.67	1.48	1.42
17	2	303	CLA	C1D-C2D	2.67	1.48	1.42
17	3	604	CLA	C1D-C2D	2.67	1.48	1.42
27	B	843	PQN	C5-C4	2.67	1.53	1.48
18	4	306	CHL	C2C-C1C	2.66	1.50	1.44
18	4	301	CHL	C2A-C1A	-2.66	1.46	1.52
17	1	304	CLA	C1D-C2D	2.66	1.48	1.42
17	A	828	CLA	C1D-C2D	2.65	1.48	1.42
18	1	305	CHL	C4B-CHC	2.65	1.48	1.41
17	A	815	CLA	C1D-C2D	2.65	1.48	1.42
18	4	306	CHL	C4B-CHC	2.64	1.48	1.41
17	4	302	CLA	C1D-C2D	2.64	1.48	1.42
17	1	312	CLA	C1D-C2D	2.64	1.48	1.42
17	3	610	CLA	C1D-C2D	2.64	1.48	1.42
17	B	806	CLA	C1B-NB	2.63	1.37	1.35
18	4	306	CHL	CHD-C4C	2.63	1.48	1.41
17	A	843	CLA	C1D-C2D	2.63	1.48	1.42
20	4	317	XAT	C31-C30	2.63	1.51	1.43
17	A	829	CLA	CMB-C2B	-2.63	1.46	1.51
25	F	305	HTG	C1-S1	-2.63	1.76	1.80
17	B	803	CLA	C1D-C2D	2.63	1.48	1.42
17	3	606	CLA	C1D-C2D	2.63	1.48	1.42
21	G	106	BCR	C30-C25	-2.63	1.50	1.53
17	B	819	CLA	CMB-C2B	-2.62	1.46	1.51
17	A	810	CLA	C1D-C2D	2.62	1.48	1.42
17	K	202	CLA	C1D-C2D	2.62	1.48	1.42
21	B	846	BCR	C1-C6	-2.62	1.50	1.53
17	G	104	CLA	CMB-C2B	-2.61	1.46	1.51
19	1	314	LUT	C32-C33	2.61	1.51	1.45
17	B	803	CLA	CMB-C2B	-2.61	1.46	1.51
17	3	613	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	820	CLA	CMB-C2B	-2.61	1.46	1.51
17	A	820	CLA	C1D-C2D	2.61	1.48	1.42
17	2	319	CLA	C1D-C2D	2.61	1.48	1.42
17	3	603	CLA	C1D-C2D	2.59	1.48	1.42
17	4	312	CLA	CMB-C2B	-2.59	1.46	1.51
17	A	826	CLA	CMB-C2B	-2.59	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	852	LMG	C3-C2	2.59	1.58	1.52
18	2	306	CHL	C2C-C1C	2.59	1.50	1.44
17	A	833	CLA	CMB-C2B	-2.58	1.46	1.51
17	A	835	CLA	CMB-C2B	-2.58	1.46	1.51
17	B	841	CLA	CMB-C2B	-2.58	1.46	1.51
17	A	807	CLA	CMB-C2B	-2.58	1.46	1.51
20	3	615	XAT	C12-C13	2.57	1.51	1.45
17	B	817	CLA	C1D-C2D	2.57	1.48	1.42
18	2	306	CHL	CHD-C4C	2.57	1.48	1.41
17	B	811	CLA	C1D-C2D	2.57	1.48	1.42
17	B	840	CLA	C1D-C2D	2.57	1.48	1.42
17	A	815	CLA	CMB-C2B	-2.57	1.46	1.51
17	A	802	CLA	C1D-C2D	2.57	1.48	1.42
17	3	613	CLA	C1D-C2D	2.56	1.48	1.42
17	A	808	CLA	C3B-CAB	-2.56	1.42	1.47
17	A	830	CLA	CMB-C2B	-2.56	1.46	1.51
20	2	315	XAT	C12-C13	2.56	1.51	1.45
17	3	605	CLA	CMB-C2B	-2.55	1.46	1.51
17	4	314	CLA	C1D-C2D	2.55	1.48	1.42
17	B	810	CLA	CMB-C2B	-2.55	1.46	1.51
17	A	816	CLA	C1D-C2D	2.55	1.48	1.42
17	2	310	CLA	CMB-C2B	-2.55	1.46	1.51
17	B	825	CLA	CMB-C2B	-2.55	1.46	1.51
18	4	315	CHL	C4B-CHC	2.55	1.48	1.41
17	1	308	CLA	C1D-C2D	2.55	1.48	1.42
17	1	304	CLA	CMB-C2B	-2.55	1.46	1.51
17	B	805	CLA	CMB-C2B	-2.54	1.46	1.51
17	A	853	CLA	C1D-C2D	2.54	1.48	1.42
20	1	315	XAT	C12-C13	2.54	1.51	1.45
17	2	308	CLA	C1D-C2D	2.54	1.48	1.42
17	2	302	CLA	C1D-C2D	2.54	1.48	1.42
17	A	818	CLA	CMB-C2B	-2.54	1.46	1.51
17	A	821	CLA	C1D-C2D	2.53	1.48	1.42
18	4	315	CHL	CHD-C4C	2.53	1.48	1.41
17	A	841	CLA	CMB-C2B	-2.53	1.46	1.51
17	A	834	CLA	C1D-C2D	2.53	1.48	1.42
17	B	816	CLA	C1D-C2D	2.53	1.48	1.42
17	B	832	CLA	C1D-C2D	2.52	1.48	1.42
24	F	309	LMG	C7-C8	2.52	1.58	1.50
17	B	836	CLA	C1D-C2D	2.52	1.48	1.42
17	1	309	CLA	CMB-C2B	-2.52	1.46	1.51
24	B	852	LMG	O1-C1	2.52	1.44	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	838	CLA	CMB-C2B	-2.51	1.46	1.51
17	B	804	CLA	CMB-C2B	-2.51	1.46	1.51
17	1	311	CLA	CMB-C2B	-2.51	1.46	1.51
18	4	307	CHL	C4B-CHC	2.51	1.48	1.41
17	A	803	CLA	CMB-C2B	-2.51	1.46	1.51
17	3	602	CLA	CMB-C2B	-2.51	1.46	1.51
19	4	316	LUT	C11-C10	2.51	1.51	1.43
17	B	826	CLA	CMB-C2B	-2.50	1.46	1.51
17	F	304	CLA	C3B-C2B	-2.50	1.36	1.40
20	4	317	XAT	C35-C34	2.50	1.51	1.43
17	A	812	CLA	CMB-C2B	-2.50	1.46	1.51
21	B	844	BCR	C30-C25	-2.50	1.50	1.53
17	G	104	CLA	C1D-C2D	2.50	1.48	1.42
17	3	606	CLA	CMB-C2B	-2.50	1.46	1.51
18	2	313	CHL	C4B-CHC	2.50	1.47	1.41
17	A	805	CLA	C1D-C2D	2.49	1.48	1.42
17	B	807	CLA	CMB-C2B	-2.49	1.46	1.51
23	2	318	LMT	O3B-C3B	-2.49	1.37	1.43
17	A	806	CLA	CMB-C2B	-2.49	1.46	1.51
17	B	813	CLA	C1D-C2D	2.49	1.48	1.42
17	1	310	CLA	C1D-C2D	2.49	1.48	1.42
17	G	103	CLA	CMB-C2B	-2.49	1.46	1.51
18	2	304	CHL	CHD-C4C	2.48	1.48	1.41
18	4	307	CHL	C2C-C1C	2.48	1.49	1.44
17	K	201	CLA	C1D-C2D	2.48	1.48	1.42
17	4	310	CLA	C1D-C2D	2.48	1.48	1.42
21	4	318	BCR	C1-C6	-2.48	1.50	1.53
17	1	307	CLA	CMB-C2B	-2.48	1.46	1.51
17	A	817	CLA	CMB-C2B	-2.48	1.46	1.51
23	2	318	LMT	O3'-C3'	-2.47	1.37	1.43
17	1	310	CLA	CMB-C2B	-2.47	1.46	1.51
17	B	823	CLA	C1D-C2D	2.47	1.48	1.42
17	3	610	CLA	CMB-C2B	-2.47	1.46	1.51
17	A	838	CLA	CMC-C2C	-2.46	1.45	1.51
17	B	808	CLA	CMB-C2B	-2.46	1.46	1.51
17	G	105	CLA	C1D-C2D	2.46	1.48	1.42
17	A	814	CLA	C1D-C2D	2.46	1.48	1.42
17	B	822	CLA	C1D-C2D	2.46	1.48	1.42
17	F	304	CLA	MG-NA	2.46	2.12	2.06
17	A	834	CLA	CMB-C2B	-2.45	1.46	1.51
17	B	831	CLA	CMB-C2B	-2.45	1.46	1.51
17	A	819	CLA	C1D-C2D	2.45	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	306	CLA	CMB-C2B	-2.45	1.46	1.51
17	4	302	CLA	CMD-C2D	-2.45	1.45	1.51
17	2	310	CLA	C1D-C2D	2.45	1.48	1.42
18	4	307	CHL	CHD-C4C	2.45	1.48	1.41
17	A	830	CLA	C1D-C2D	2.45	1.48	1.42
17	B	802	CLA	C1D-C2D	2.45	1.48	1.42
17	A	807	CLA	C3B-C2B	-2.44	1.37	1.40
17	B	829	CLA	C1C-C2C	2.44	1.48	1.42
17	1	303	CLA	CMB-C2B	-2.44	1.46	1.51
17	B	828	CLA	CMC-C2C	-2.44	1.45	1.51
17	B	812	CLA	CMB-C2B	-2.44	1.46	1.51
17	F	307	CLA	CMB-C2B	-2.43	1.46	1.51
17	2	311	CLA	CMB-C2B	-2.43	1.46	1.51
17	3	604	CLA	CMB-C2B	-2.43	1.46	1.51
17	B	805	CLA	C1D-C2D	2.42	1.48	1.42
17	2	307	CLA	CMB-C2B	-2.42	1.46	1.51
17	3	608	CLA	CMB-C2B	-2.42	1.46	1.51
17	A	821	CLA	CMB-C2B	-2.42	1.46	1.51
22	G	102	LHG	P-O6	2.42	1.69	1.59
17	1	311	CLA	C3B-C2B	-2.42	1.37	1.40
17	A	829	CLA	C3B-C2B	-2.42	1.37	1.40
21	L	201	BCR	C30-C25	-2.42	1.50	1.53
17	B	810	CLA	C3B-C2B	-2.42	1.37	1.40
17	2	301	CLA	C1D-C2D	2.42	1.48	1.42
17	B	830	CLA	C1D-C2D	2.42	1.48	1.42
17	J	101	CLA	MG-NA	2.41	2.12	2.06
18	2	305	CHL	CHD-C4C	2.41	1.48	1.41
17	B	828	CLA	CMB-C2B	-2.41	1.46	1.51
17	2	302	CLA	CMC-C2C	-2.41	1.45	1.51
17	2	301	CLA	CMB-C2B	-2.41	1.46	1.51
22	1	317	LHG	O7-C5	-2.40	1.40	1.46
17	A	831	CLA	CMB-C2B	-2.40	1.46	1.51
17	A	832	CLA	CMB-C2B	-2.40	1.46	1.51
24	4	320	LMG	C4-C3	2.40	1.58	1.52
17	B	807	CLA	CMD-C2D	-2.40	1.45	1.51
18	2	306	CHL	C4C-C3C	2.40	1.49	1.45
17	K	202	CLA	CMB-C2B	-2.40	1.46	1.51
25	4	322	HTG	C1-S1	-2.39	1.77	1.80
17	2	303	CLA	CMB-C2B	-2.39	1.46	1.51
17	J	103	CLA	CMB-C2B	-2.39	1.46	1.51
17	3	611	CLA	CMB-C2B	-2.39	1.46	1.51
17	A	809	CLA	CMB-C2B	-2.39	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	822	CLA	CMB-C2B	-2.38	1.46	1.51
20	4	317	XAT	C15-C14	2.38	1.50	1.43
17	4	310	CLA	CMB-C2B	-2.38	1.46	1.51
17	A	843	CLA	CMB-C2B	-2.38	1.46	1.51
17	A	853	CLA	CMC-C2C	-2.38	1.45	1.51
17	B	821	CLA	C3B-C2B	-2.38	1.37	1.40
17	J	101	CLA	CAC-C3C	-2.38	1.46	1.52
17	B	825	CLA	C1C-C2C	2.37	1.47	1.42
17	A	819	CLA	CMB-C2B	-2.37	1.46	1.51
17	B	838	CLA	C1B-NB	2.37	1.37	1.35
17	B	806	CLA	C1D-C2D	2.37	1.47	1.42
18	3	607	CHL	CHD-C4C	2.37	1.47	1.41
17	3	612	CLA	CMB-C2B	-2.37	1.46	1.51
17	2	309	CLA	CMB-C2B	-2.37	1.46	1.51
17	B	834	CLA	C1D-C2D	2.37	1.47	1.42
25	F	310	HTG	C1-S1	-2.37	1.77	1.80
21	A	846	BCR	C30-C25	-2.36	1.50	1.53
18	2	305	CHL	C4B-CHC	2.36	1.47	1.41
21	B	845	BCR	C30-C25	-2.36	1.50	1.53
17	F	307	CLA	C1D-C2D	2.36	1.47	1.42
17	L	202	CLA	CMB-C2B	-2.36	1.46	1.51
17	3	613	CLA	CMD-C2D	-2.36	1.45	1.51
17	B	830	CLA	C2-C3	2.36	1.38	1.33
17	B	831	CLA	C3B-C2B	-2.35	1.37	1.40
22	A	844	LHG	O7-C5	-2.35	1.40	1.46
17	B	836	CLA	CMB-C2B	-2.35	1.46	1.51
18	4	301	CHL	C3B-C2B	2.35	1.43	1.40
17	A	840	CLA	CMD-C2D	-2.35	1.46	1.51
17	2	308	CLA	CMB-C2B	-2.35	1.46	1.51
17	2	312	CLA	CMB-C2B	-2.35	1.46	1.51
17	B	816	CLA	CMB-C2B	-2.35	1.46	1.51
17	B	835	CLA	C3B-C2B	-2.35	1.37	1.40
19	3	614	LUT	C7-C6	2.34	1.53	1.45
22	A	845	LHG	P-O6	2.34	1.68	1.59
17	A	826	CLA	C1D-C2D	2.34	1.47	1.42
17	A	801	CLA	C1D-C2D	2.34	1.47	1.42
17	A	837	CLA	CMB-C2B	-2.34	1.46	1.51
17	B	809	CLA	CMB-C2B	-2.34	1.46	1.51
18	3	601	CHL	CHD-C4C	2.33	1.47	1.41
18	1	305	CHL	C2C-C1C	2.33	1.49	1.44
17	1	308	CLA	CMB-C2B	-2.33	1.46	1.51
17	F	307	CLA	CMD-C2D	-2.33	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	839	CLA	CMC-C2C	-2.33	1.46	1.51
17	1	312	CLA	CMB-C2B	-2.33	1.46	1.51
17	A	814	CLA	CMB-C2B	-2.33	1.46	1.51
17	B	802	CLA	CMB-C2B	-2.33	1.46	1.51
18	3	601	CHL	C4B-CHC	2.33	1.47	1.41
17	4	303	CLA	CMB-C2B	-2.33	1.46	1.51
17	4	308	CLA	C1C-C2C	2.32	1.47	1.42
18	4	301	CHL	OBD-CAD	2.32	1.25	1.22
18	4	301	CHL	C3A-C2A	-2.32	1.48	1.54
21	A	851	BCR	C30-C25	-2.32	1.50	1.53
17	L	203	CLA	CMB-C2B	-2.32	1.46	1.51
18	2	304	CHL	C4B-CHC	2.32	1.47	1.41
18	1	305	CHL	CHD-C4C	2.32	1.47	1.41
17	L	204	CLA	CMB-C2B	-2.31	1.46	1.51
17	K	201	CLA	CMB-C2B	-2.31	1.46	1.51
17	B	823	CLA	CMB-C2B	-2.31	1.46	1.51
17	B	838	CLA	CAC-C3C	-2.31	1.46	1.52
17	3	609	CLA	CMB-C2B	-2.31	1.46	1.51
17	B	824	CLA	CMD-C2D	-2.31	1.46	1.51
17	3	603	CLA	CMB-C2B	-2.31	1.46	1.51
17	A	823	CLA	CMB-C2B	-2.31	1.46	1.51
23	A	855	LMT	O3'-C3'	-2.30	1.37	1.43
17	A	805	CLA	CMB-C2B	-2.30	1.46	1.51
17	A	811	CLA	CMB-C2B	-2.30	1.46	1.51
18	1	305	CHL	MG-NA	-2.30	2.00	2.06
17	B	808	CLA	C3B-C2B	-2.30	1.37	1.40
18	2	305	CHL	C4C-C3C	2.30	1.49	1.45
17	B	840	CLA	CMD-C2D	-2.29	1.46	1.51
17	A	853	CLA	CMB-C2B	-2.29	1.46	1.51
17	B	832	CLA	CMD-C2D	-2.29	1.46	1.51
18	4	305	CHL	C4B-CHC	2.29	1.47	1.41
17	A	808	CLA	CMC-C2C	-2.29	1.46	1.51
17	B	813	CLA	CMC-C2C	-2.28	1.46	1.51
17	J	103	CLA	C1D-C2D	2.28	1.47	1.42
17	B	824	CLA	CMB-C2B	-2.28	1.46	1.51
17	B	814	CLA	C1C-C2C	2.28	1.47	1.42
17	B	831	CLA	CAC-C3C	-2.28	1.46	1.52
17	B	835	CLA	C1C-C2C	2.28	1.47	1.42
17	F	304	CLA	CMB-C2B	-2.28	1.46	1.51
17	B	809	CLA	CMD-C2D	-2.27	1.46	1.51
17	A	808	CLA	CMB-C2B	-2.27	1.46	1.51
17	2	310	CLA	CMC-C2C	-2.27	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	853	CLA	CAC-C3C	-2.27	1.46	1.52
17	G	105	CLA	CMB-C2B	-2.26	1.46	1.51
17	G	104	CLA	CAC-C3C	-2.26	1.46	1.52
17	1	313	CLA	C1D-C2D	2.26	1.47	1.42
19	4	316	LUT	C35-C34	2.26	1.50	1.43
18	2	313	CHL	C4C-C3C	2.26	1.48	1.45
17	A	808	CLA	C1D-C2D	2.26	1.47	1.42
18	2	306	CHL	C4B-CHC	2.26	1.47	1.41
17	4	314	CLA	C3B-CAB	-2.26	1.43	1.47
17	B	822	CLA	CMB-C2B	-2.25	1.47	1.51
17	4	311	CLA	CMB-C2B	-2.25	1.47	1.51
17	A	836	CLA	CMB-C2B	-2.25	1.47	1.51
17	1	310	CLA	C3B-C2B	-2.25	1.37	1.40
18	2	313	CHL	C1B-CHB	2.25	1.47	1.41
17	2	302	CLA	CMD-C2D	-2.25	1.46	1.51
17	G	103	CLA	CMD-C2D	-2.25	1.46	1.51
17	B	833	CLA	CMB-C2B	-2.24	1.47	1.51
17	A	807	CLA	CMC-C2C	-2.24	1.46	1.51
17	A	840	CLA	C3B-C2B	-2.24	1.37	1.40
18	2	306	CHL	C1B-CHB	2.24	1.47	1.41
17	4	312	CLA	CAC-C3C	-2.24	1.46	1.52
17	4	313	CLA	CMB-C2B	-2.24	1.47	1.51
17	A	810	CLA	CMB-C2B	-2.24	1.47	1.51
27	A	842	PQN	C11-C3	2.24	1.55	1.51
17	1	311	CLA	C1D-C2D	2.24	1.47	1.42
17	A	824	CLA	CMB-C2B	-2.24	1.47	1.51
23	2	318	LMT	O2'-C2'	-2.24	1.37	1.43
17	B	813	CLA	CMB-C2B	-2.24	1.47	1.51
17	K	202	CLA	CMD-C2D	-2.24	1.46	1.51
17	B	803	CLA	C3B-C2B	-2.23	1.37	1.40
17	B	832	CLA	C3B-C2B	-2.23	1.37	1.40
17	B	841	CLA	C1B-NB	2.23	1.37	1.35
17	B	833	CLA	MG-NA	2.23	2.11	2.06
17	A	813	CLA	CMB-C2B	-2.23	1.47	1.51
18	2	313	CHL	CHD-C4C	2.22	1.47	1.41
17	B	817	CLA	CMB-C2B	-2.22	1.47	1.51
17	A	806	CLA	CMC-C2C	-2.22	1.46	1.51
17	B	826	CLA	CAC-C3C	-2.22	1.46	1.52
17	A	827	CLA	CMD-C2D	-2.22	1.46	1.51
17	A	816	CLA	CMB-C2B	-2.21	1.47	1.51
17	B	819	CLA	C3B-C2B	-2.21	1.37	1.40
17	2	319	CLA	CMB-C2B	-2.21	1.47	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	302	CLA	CMB-C2B	-2.21	1.47	1.51
23	2	318	LMT	O2B-C2B	-2.21	1.37	1.43
17	4	302	CLA	CMB-C2B	-2.20	1.47	1.51
17	B	823	CLA	CAC-C3C	-2.20	1.46	1.52
19	1	314	LUT	C11-C10	2.20	1.50	1.43
24	4	319	LMG	O6-C5	-2.20	1.39	1.44
17	B	830	CLA	CMB-C2B	-2.20	1.47	1.51
17	2	308	CLA	CMD-C2D	-2.20	1.46	1.51
17	A	825	CLA	CMB-C2B	-2.20	1.47	1.51
17	A	829	CLA	CMD-C2D	-2.20	1.46	1.51
17	A	816	CLA	CMD-C2D	-2.20	1.46	1.51
19	4	316	LUT	C7-C6	2.20	1.52	1.45
17	4	304	CLA	C1D-C2D	2.20	1.47	1.42
19	2	314	LUT	C7-C6	2.20	1.52	1.45
17	A	809	CLA	CMD-C2D	-2.19	1.46	1.51
17	A	839	CLA	C3B-CAB	-2.19	1.43	1.47
17	B	814	CLA	CMB-C2B	-2.19	1.47	1.51
17	A	818	CLA	CMD-C2D	-2.19	1.46	1.51
17	1	313	CLA	CAC-C3C	-2.19	1.46	1.52
17	2	312	CLA	CMD-C2D	-2.19	1.46	1.51
17	A	804	CLA	CMB-C2B	-2.19	1.47	1.51
17	2	319	CLA	CMD-C2D	-2.19	1.46	1.51
17	G	105	CLA	CMC-C2C	-2.19	1.46	1.51
17	F	306	CLA	C3B-C2B	-2.18	1.37	1.40
17	B	833	CLA	C4B-CHC	-2.18	1.34	1.41
21	J	104	BCR	C38-C26	-2.18	1.47	1.50
18	2	305	CHL	C1B-CHB	2.18	1.47	1.41
17	B	833	CLA	CAC-C3C	-2.18	1.46	1.52
17	A	815	CLA	CMD-C2D	-2.18	1.46	1.51
17	A	826	CLA	CMD-C2D	-2.18	1.46	1.51
17	4	309	CLA	CAC-C3C	-2.18	1.46	1.52
18	3	601	CHL	C1B-CHB	2.17	1.47	1.41
17	2	301	CLA	CMD-C2D	-2.17	1.46	1.51
17	A	805	CLA	C3B-C2B	-2.17	1.37	1.40
21	J	104	BCR	C30-C25	-2.17	1.50	1.53
17	F	306	CLA	C1D-C2D	2.17	1.47	1.42
17	B	809	CLA	CAC-C3C	-2.16	1.46	1.52
17	B	832	CLA	CMB-C2B	-2.16	1.47	1.51
21	2	316	BCR	C33-C5	-2.16	1.47	1.50
17	A	805	CLA	CAC-C3C	-2.16	1.46	1.52
17	B	817	CLA	CMC-C2C	-2.16	1.46	1.51
24	4	319	LMG	C7-C8	2.16	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	837	CLA	C1D-C2D	2.16	1.47	1.42
17	A	827	CLA	C1C-C2C	2.16	1.47	1.42
17	1	302	CLA	CMD-C2D	-2.15	1.46	1.51
25	F	301	HTG	C1-S1	-2.15	1.77	1.80
17	B	802	CLA	C1C-C2C	2.15	1.47	1.42
18	4	306	CHL	C1B-CHB	2.15	1.47	1.41
17	1	313	CLA	CMC-C2C	-2.15	1.46	1.51
17	A	803	CLA	CMD-C2D	-2.15	1.46	1.51
17	G	103	CLA	C3B-C2B	-2.15	1.37	1.40
17	B	814	CLA	MG-NA	2.15	2.11	2.06
17	B	826	CLA	C1D-C2D	2.15	1.47	1.42
17	1	310	CLA	CMD-C2D	-2.15	1.46	1.51
17	1	307	CLA	CMC-C2C	-2.15	1.46	1.51
17	J	101	CLA	C1C-C2C	2.14	1.47	1.42
18	4	315	CHL	C4C-C3C	2.14	1.48	1.45
18	4	301	CHL	O2D-CGD	2.14	1.38	1.33
17	1	308	CLA	CMD-C2D	-2.14	1.46	1.51
17	3	608	CLA	CMD-C2D	-2.14	1.46	1.51
17	A	840	CLA	C3B-CAB	-2.14	1.43	1.47
17	B	816	CLA	CAC-C3C	-2.13	1.46	1.52
17	L	202	CLA	CMD-C2D	-2.13	1.46	1.51
17	A	824	CLA	CMD-C2D	-2.13	1.46	1.51
18	3	607	CHL	C4B-CHC	2.13	1.46	1.41
17	F	306	CLA	CMB-C2B	-2.13	1.47	1.51
17	4	308	CLA	CMD-C2D	-2.13	1.46	1.51
17	L	203	CLA	CMD-C2D	-2.13	1.46	1.51
19	4	316	LUT	C26-C27	2.13	1.53	1.50
17	B	831	CLA	C3B-CAB	-2.13	1.43	1.47
17	A	829	CLA	CMC-C2C	-2.13	1.46	1.51
18	3	601	CHL	C2C-C1C	2.13	1.49	1.44
17	A	841	CLA	CMC-C2C	-2.13	1.46	1.51
24	G	101	LMG	C4-C5	2.13	1.57	1.53
17	1	301	CLA	CMB-C2B	-2.12	1.47	1.51
17	B	827	CLA	C1B-NB	2.12	1.37	1.35
17	A	822	CLA	CMD-C2D	-2.12	1.46	1.51
18	4	301	CHL	CBD-CGD	-2.12	1.45	1.52
26	B	850	DGD	C1E-C2E	2.12	1.58	1.52
17	B	830	CLA	CMD-C2D	-2.12	1.46	1.51
17	1	308	CLA	CAC-C3C	-2.12	1.47	1.52
17	B	834	CLA	CAC-C3C	-2.12	1.47	1.52
17	4	308	CLA	C1D-C2D	2.12	1.47	1.42
17	B	821	CLA	C1C-C2C	2.11	1.47	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	842	PQN	C2M-C2	2.11	1.55	1.50
17	B	827	CLA	C1C-C2C	2.11	1.47	1.42
17	A	805	CLA	C1C-C2C	2.11	1.47	1.42
17	A	823	CLA	CMD-C2D	-2.11	1.46	1.51
17	A	828	CLA	C1C-C2C	2.11	1.47	1.42
18	2	304	CHL	C4C-C3C	2.11	1.48	1.45
17	4	304	CLA	C4B-CHC	-2.11	1.35	1.41
17	B	833	CLA	C1D-C2D	2.11	1.47	1.42
17	B	841	CLA	CMD-C2D	-2.11	1.46	1.51
17	3	606	CLA	CMD-C2D	-2.11	1.46	1.51
17	2	310	CLA	CMD-C2D	-2.11	1.46	1.51
17	B	815	CLA	CMB-C2B	-2.11	1.47	1.51
17	3	604	CLA	CMD-C2D	-2.10	1.46	1.51
21	F	303	BCR	C1-C6	-2.10	1.50	1.53
17	A	840	CLA	MG-NA	2.10	2.11	2.06
17	B	808	CLA	C1D-C2D	2.10	1.47	1.42
17	1	304	CLA	CMD-C2D	-2.10	1.46	1.51
24	4	320	LMG	C3-C2	2.10	1.57	1.52
17	K	201	CLA	CMD-C2D	-2.10	1.46	1.51
17	2	308	CLA	CMC-C2C	-2.10	1.46	1.51
17	A	839	CLA	C1C-C2C	2.10	1.47	1.42
17	A	828	CLA	CAC-C3C	-2.10	1.47	1.52
17	3	611	CLA	CMD-C2D	-2.09	1.46	1.51
17	3	610	CLA	CMC-C2C	-2.09	1.46	1.51
17	B	821	CLA	CMB-C2B	-2.09	1.47	1.51
17	B	813	CLA	CMD-C2D	-2.09	1.46	1.51
17	4	310	CLA	CMC-C2C	-2.09	1.46	1.51
17	4	304	CLA	CAC-C3C	-2.09	1.47	1.52
17	1	303	CLA	CMD-C2D	-2.09	1.46	1.51
17	A	839	CLA	CMB-C2B	-2.09	1.47	1.51
17	4	303	CLA	C3B-C2B	-2.09	1.37	1.40
17	B	808	CLA	CMD-C2D	-2.09	1.46	1.51
17	A	825	CLA	C1C-C2C	2.09	1.47	1.42
17	B	834	CLA	CMC-C2C	-2.09	1.46	1.51
17	A	815	CLA	CMC-C2C	-2.09	1.46	1.51
17	B	820	CLA	C3B-CAB	-2.09	1.43	1.47
17	1	306	CLA	CMD-C2D	-2.08	1.46	1.51
17	2	301	CLA	CMC-C2C	-2.08	1.46	1.51
17	A	817	CLA	CMC-C2C	-2.08	1.46	1.51
17	A	834	CLA	CMD-C2D	-2.08	1.46	1.51
17	3	603	CLA	CAC-C3C	-2.08	1.47	1.52
17	A	813	CLA	C3B-CAB	-2.08	1.43	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	304	CHL	C1B-CHB	2.08	1.46	1.41
17	B	810	CLA	CMC-C2C	-2.08	1.46	1.51
17	4	302	CLA	MG-NA	2.08	2.11	2.06
17	A	817	CLA	C3B-C2B	-2.08	1.37	1.40
17	2	307	CLA	CMD-C2D	-2.08	1.46	1.51
17	B	802	CLA	CMD-C2D	-2.08	1.46	1.51
17	B	842	CLA	C3B-C2B	-2.08	1.37	1.40
17	2	303	CLA	CMD-C2D	-2.08	1.46	1.51
17	B	839	CLA	CMB-C2B	-2.08	1.47	1.51
17	B	814	CLA	O2A-CGA	2.08	1.39	1.33
17	A	829	CLA	CAC-C3C	-2.08	1.47	1.52
23	2	318	LMT	O4'-C4B	-2.07	1.38	1.43
17	B	835	CLA	CMB-C2B	-2.07	1.47	1.51
17	B	817	CLA	CAC-C3C	-2.07	1.47	1.52
19	4	316	LUT	C22-C21	-2.07	1.52	1.54
17	A	803	CLA	C3B-C2B	-2.07	1.37	1.40
17	B	803	CLA	CAC-C3C	-2.07	1.47	1.52
24	G	101	LMG	O7-C8	-2.07	1.41	1.46
18	4	301	CHL	C1D-C2D	2.07	1.47	1.42
18	3	607	CHL	C4C-C3C	2.07	1.48	1.45
17	A	812	CLA	CMD-C2D	-2.07	1.46	1.51
17	1	311	CLA	CMD-C2D	-2.07	1.46	1.51
17	B	831	CLA	C1C-C2C	2.07	1.47	1.42
17	F	307	CLA	C3B-C2B	-2.07	1.37	1.40
17	B	807	CLA	C1C-C2C	2.07	1.47	1.42
17	B	816	CLA	O1D-CGD	2.07	1.26	1.21
17	1	301	CLA	MG-NA	2.07	2.11	2.06
17	A	802	CLA	CMB-C2B	-2.06	1.47	1.51
17	A	802	CLA	CMC-C2C	-2.06	1.46	1.51
18	4	306	CHL	CMC-C2C	2.06	1.49	1.45
17	A	816	CLA	CMC-C2C	-2.06	1.46	1.51
17	J	103	CLA	C1C-C2C	2.06	1.47	1.42
17	A	804	CLA	C1C-C2C	2.06	1.47	1.42
17	B	808	CLA	C1C-C2C	2.06	1.47	1.42
17	A	821	CLA	CMD-C2D	-2.06	1.46	1.51
19	1	314	LUT	C7-C6	2.06	1.52	1.45
17	A	817	CLA	CAC-C3C	-2.06	1.47	1.52
17	1	310	CLA	CMC-C2C	-2.06	1.46	1.51
17	B	829	CLA	CMB-C2B	-2.06	1.47	1.51
21	B	849	BCR	C38-C26	-2.05	1.47	1.50
21	A	847	BCR	C33-C5	-2.05	1.47	1.50
17	3	602	CLA	CMD-C2D	-2.05	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	813	CLA	CAB-C3B	-2.05	1.47	1.51
17	3	602	CLA	CMC-C2C	-2.05	1.46	1.51
17	A	843	CLA	CMD-C2D	-2.05	1.46	1.51
17	3	612	CLA	CMC-C2C	-2.05	1.46	1.51
17	A	830	CLA	CMC-C2C	-2.05	1.46	1.51
17	B	808	CLA	CAC-C3C	-2.05	1.47	1.52
17	4	304	CLA	CMB-C2B	-2.05	1.47	1.51
24	F	309	LMG	C4-C5	2.05	1.57	1.53
17	A	804	CLA	CMD-C2D	-2.05	1.46	1.51
17	B	829	CLA	O2D-CGD	2.05	1.38	1.33
17	B	814	CLA	CMD-C2D	-2.05	1.46	1.51
17	B	837	CLA	C3B-CAB	-2.05	1.43	1.47
18	4	305	CHL	C1B-CHB	2.05	1.46	1.41
17	1	313	CLA	CMD-C2D	-2.05	1.46	1.51
17	A	836	CLA	CMC-C2C	-2.04	1.46	1.51
17	B	818	CLA	CMD-C2D	-2.04	1.46	1.51
23	A	855	LMT	O2B-C2B	-2.04	1.38	1.43
17	A	813	CLA	CAC-C3C	-2.04	1.47	1.52
18	2	306	CHL	CMC-C2C	2.04	1.49	1.45
17	A	820	CLA	CMD-C2D	-2.04	1.46	1.51
17	A	807	CLA	CAC-C3C	-2.04	1.47	1.52
17	3	605	CLA	CMC-C2C	-2.04	1.46	1.51
17	3	612	CLA	CMD-C2D	-2.04	1.46	1.51
17	A	833	CLA	CMD-C2D	-2.04	1.46	1.51
17	B	834	CLA	O2D-CGD	2.04	1.38	1.33
17	2	309	CLA	CMD-C2D	-2.04	1.46	1.51
18	4	305	CHL	C2C-C1C	2.03	1.48	1.44
17	A	808	CLA	CMD-C2D	-2.03	1.46	1.51
17	3	610	CLA	CMD-C2D	-2.03	1.46	1.51
17	4	312	CLA	O2A-CGA	2.03	1.39	1.33
18	4	307	CHL	C4C-C3C	2.03	1.48	1.45
17	B	803	CLA	CMD-C2D	-2.03	1.46	1.51
17	1	313	CLA	CMB-C2B	-2.03	1.47	1.51
17	B	810	CLA	CMD-C2D	-2.03	1.46	1.51
17	A	817	CLA	CMD-C2D	-2.03	1.46	1.51
22	B	801	LHG	O7-C7	2.03	1.40	1.34
17	B	829	CLA	C3B-C2B	-2.02	1.37	1.40
17	4	303	CLA	CAC-C3C	-2.02	1.47	1.52
17	4	302	CLA	CAC-C3C	-2.02	1.47	1.52
17	4	304	CLA	CMD-C2D	-2.02	1.46	1.51
17	B	812	CLA	C3B-CAB	-2.02	1.43	1.47
17	3	603	CLA	CMC-C2C	-2.02	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	834	CLA	CMD-C2D	-2.02	1.46	1.51
17	A	802	CLA	CAC-C3C	-2.02	1.47	1.52
17	1	304	CLA	CMC-C2C	-2.02	1.46	1.51
17	B	819	CLA	CMD-C2D	-2.02	1.46	1.51
17	4	313	CLA	CMD-C2D	-2.02	1.46	1.51
17	G	105	CLA	CMD-C2D	-2.02	1.46	1.51
17	A	813	CLA	CMC-C2C	-2.02	1.46	1.51
17	G	105	CLA	C3B-CAB	-2.02	1.43	1.47
17	B	838	CLA	C1C-C2C	2.02	1.47	1.42
17	K	202	CLA	CMC-C2C	-2.01	1.46	1.51
17	3	605	CLA	CMD-C2D	-2.01	1.46	1.51
17	B	830	CLA	C1C-C2C	2.01	1.47	1.42
17	B	827	CLA	O1D-CGD	2.01	1.26	1.21
17	A	819	CLA	CMD-C2D	-2.01	1.46	1.51
17	2	311	CLA	CAC-C3C	-2.01	1.47	1.52
17	2	301	CLA	MG-NA	2.01	2.11	2.06
17	A	840	CLA	CMC-C2C	-2.01	1.46	1.51
17	B	812	CLA	CMD-C2D	-2.01	1.46	1.51
17	L	204	CLA	CMC-C2C	-2.01	1.46	1.51
17	3	603	CLA	CMD-C2D	-2.01	1.46	1.51
17	4	312	CLA	C1C-C2C	2.01	1.47	1.42
17	B	833	CLA	CMD-C2D	-2.01	1.46	1.51
17	A	843	CLA	C3B-C2B	-2.01	1.37	1.40
17	A	814	CLA	CMD-C2D	-2.01	1.46	1.51
22	2	317	LHG	O7-C5	-2.01	1.41	1.46
17	4	302	CLA	C1C-C2C	2.01	1.47	1.42
17	A	802	CLA	C1B-NB	2.01	1.37	1.35
17	A	811	CLA	CMD-C2D	-2.01	1.46	1.51
17	A	833	CLA	CMC-C2C	-2.01	1.46	1.51
23	A	855	LMT	O3B-C3B	-2.01	1.38	1.43
24	4	319	LMG	O8-C9	-2.01	1.40	1.45
26	B	850	DGD	C4E-C3E	2.00	1.57	1.52
18	2	305	CHL	MG-NA	-2.00	2.01	2.06
17	A	835	CLA	CMC-C2C	-2.00	1.46	1.51
17	A	810	CLA	CAC-C3C	-2.00	1.47	1.52

All (2188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	842	PQN	C6-C5-C10	-13.60	104.14	119.26
27	A	842	PQN	C9-C10-C5	-12.36	105.51	119.26
19	4	316	LUT	C31-C30-C29	-11.83	110.43	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	4	316	LUT	C11-C10-C9	-11.79	110.48	127.31
19	2	314	LUT	C35-C34-C33	-11.70	110.62	127.31
19	1	314	LUT	C31-C30-C29	-11.69	110.62	127.31
19	1	314	LUT	C15-C14-C13	-11.64	110.70	127.31
19	3	614	LUT	C15-C14-C13	-11.62	110.73	127.31
20	3	615	XAT	C35-C34-C33	-11.45	110.97	127.31
20	1	315	XAT	C35-C34-C33	-11.44	110.98	127.31
20	2	315	XAT	C35-C34-C33	-11.43	111.00	127.31
19	4	316	LUT	C18-C5-C6	-11.33	111.81	124.53
20	4	317	XAT	C31-C30-C29	-11.18	111.36	127.31
19	4	316	LUT	C32-C33-C34	-11.07	101.96	118.94
19	3	614	LUT	C31-C30-C29	-11.04	111.55	127.31
19	2	314	LUT	C15-C14-C13	-11.01	111.60	127.31
19	3	614	LUT	C35-C34-C33	-10.99	111.63	127.31
19	2	314	LUT	C18-C5-C6	-10.97	112.21	124.53
20	3	615	XAT	C31-C30-C29	-10.95	111.68	127.31
20	1	315	XAT	C31-C30-C29	-10.95	111.69	127.31
20	2	315	XAT	C31-C30-C29	-10.92	111.72	127.31
19	4	316	LUT	C15-C14-C13	-10.90	111.75	127.31
19	1	314	LUT	C11-C10-C9	-10.59	112.19	127.31
20	1	315	XAT	C15-C14-C13	-10.50	112.33	127.31
20	2	315	XAT	C15-C14-C13	-10.49	112.33	127.31
20	3	615	XAT	C15-C14-C13	-10.48	112.36	127.31
19	1	314	LUT	C35-C34-C33	-10.34	112.55	127.31
19	3	614	LUT	C18-C5-C6	-10.19	113.08	124.53
20	4	317	XAT	C35-C34-C33	-10.11	112.88	127.31
19	2	314	LUT	C31-C30-C29	-9.96	113.09	127.31
20	1	315	XAT	C8-C9-C10	-9.80	103.90	118.94
20	3	615	XAT	C8-C9-C10	-9.80	103.91	118.94
20	2	315	XAT	C8-C9-C10	-9.79	103.92	118.94
20	4	317	XAT	C27-C28-C29	-9.74	110.42	125.53
19	1	314	LUT	C18-C5-C6	-9.65	113.69	124.53
20	4	317	XAT	C15-C14-C13	-9.51	113.74	127.31
19	1	314	LUT	C8-C9-C10	-9.45	104.44	118.94
27	B	843	PQN	C6-C5-C10	-9.42	108.79	119.26
19	4	316	LUT	C35-C34-C33	-9.38	113.92	127.31
20	4	317	XAT	C12-C13-C14	-9.33	104.63	118.94
19	4	316	LUT	C8-C9-C10	-9.23	104.78	118.94
19	2	314	LUT	C11-C10-C9	-9.22	114.15	127.31
18	4	306	CHL	C2C-C3C-C4C	-9.21	99.92	106.49
20	1	315	XAT	C27-C28-C29	-9.21	111.24	125.53
20	2	315	XAT	C27-C28-C29	-9.19	111.26	125.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	615	XAT	C27-C28-C29	-9.19	111.27	125.53
19	2	314	LUT	C28-C29-C30	-9.08	105.01	118.94
19	1	314	LUT	C32-C33-C34	-8.97	105.18	118.94
20	1	315	XAT	C12-C13-C14	-8.95	105.20	118.94
20	2	315	XAT	C12-C13-C14	-8.95	105.21	118.94
20	3	615	XAT	C12-C13-C14	-8.94	105.22	118.94
20	2	315	XAT	C40-C33-C34	-8.84	110.54	122.92
20	1	315	XAT	C40-C33-C34	-8.83	110.56	122.92
20	3	615	XAT	C40-C33-C34	-8.83	110.56	122.92
20	4	317	XAT	C39-C29-C30	-8.79	110.61	122.92
20	4	317	XAT	C11-C10-C9	-8.77	114.79	127.31
20	4	317	XAT	C20-C13-C14	-8.75	110.66	122.92
19	3	614	LUT	C8-C9-C10	-8.69	105.61	118.94
19	3	614	LUT	C11-C10-C9	-8.68	114.92	127.31
19	1	314	LUT	C7-C8-C9	-8.68	113.12	126.23
19	2	314	LUT	C8-C9-C10	-8.66	105.66	118.94
27	B	843	PQN	C9-C10-C5	-8.54	109.77	119.26
19	2	314	LUT	C7-C8-C9	-8.53	113.35	126.23
19	1	314	LUT	C39-C29-C30	-8.49	111.04	122.92
19	4	316	LUT	C35-C15-C14	-8.48	106.10	123.47
20	3	615	XAT	C11-C10-C9	-8.47	115.22	127.31
20	1	315	XAT	C11-C10-C9	-8.46	115.23	127.31
20	2	315	XAT	C39-C29-C30	-8.45	111.08	122.92
20	1	315	XAT	C39-C29-C30	-8.43	111.11	122.92
20	3	615	XAT	C39-C29-C30	-8.42	111.13	122.92
20	2	315	XAT	C11-C10-C9	-8.42	115.29	127.31
27	B	843	PQN	C2M-C2-C3	-8.37	110.74	124.40
27	B	843	PQN	C11-C3-C4	-8.32	109.60	118.50
19	2	314	LUT	C12-C13-C14	-8.27	106.25	118.94
20	2	315	XAT	C32-C33-C34	-8.22	106.33	118.94
20	1	315	XAT	C32-C33-C34	-8.21	106.34	118.94
27	B	843	PQN	C11-C12-C13	-8.20	113.14	126.79
20	3	615	XAT	C32-C33-C34	-8.18	106.38	118.94
19	4	316	LUT	C8-C7-C6	-8.17	104.25	127.20
19	4	316	LUT	C15-C35-C34	-8.16	106.77	123.47
19	1	314	LUT	C12-C13-C14	-8.08	106.55	118.94
20	1	315	XAT	C28-C29-C30	-8.04	106.60	118.94
20	3	615	XAT	C28-C29-C30	-8.03	106.61	118.94
20	2	315	XAT	C28-C29-C30	-8.03	106.62	118.94
20	4	317	XAT	C8-C9-C10	-8.02	106.64	118.94
19	2	314	LUT	C35-C15-C14	-8.01	107.06	123.47
20	4	317	XAT	C35-C15-C14	-7.98	107.13	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	3	614	LUT	C32-C33-C34	-7.95	106.75	118.94
27	B	843	PQN	C6-C5-C4	-7.95	108.45	120.10
20	2	315	XAT	C20-C13-C14	-7.92	111.83	122.92
20	1	315	XAT	C20-C13-C14	-7.91	111.84	122.92
20	3	615	XAT	C20-C13-C14	-7.91	111.84	122.92
19	3	614	LUT	C7-C8-C9	-7.87	114.34	126.23
19	4	316	LUT	C28-C29-C30	-7.87	106.86	118.94
19	2	314	LUT	C39-C29-C30	-7.83	111.96	122.92
20	4	317	XAT	C7-C8-C9	-7.75	113.51	125.53
19	4	316	LUT	C39-C29-C30	-7.73	112.09	122.92
18	2	305	CHL	C2C-C3C-C4C	-7.72	100.99	106.49
19	3	614	LUT	C40-C33-C34	-7.70	112.14	122.92
19	2	314	LUT	C32-C33-C34	-7.70	107.13	118.94
18	2	313	CHL	C2C-C3C-C4C	-7.69	101.01	106.49
19	3	614	LUT	C39-C29-C30	-7.69	112.15	122.92
18	4	301	CHL	C2C-C3C-C4C	-7.64	101.04	106.49
17	B	821	CLA	C4A-NA-C1A	7.62	110.13	106.71
20	2	315	XAT	C19-C9-C10	-7.61	112.26	122.92
20	1	315	XAT	C19-C9-C10	-7.59	112.28	122.92
20	3	615	XAT	C19-C9-C10	-7.57	112.32	122.92
19	4	316	LUT	C12-C13-C14	-7.57	107.33	118.94
19	2	314	LUT	C20-C13-C14	-7.56	112.33	122.92
18	4	307	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
18	2	304	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
20	4	317	XAT	O24-C25-C24	-7.48	107.77	113.38
20	2	315	XAT	C6-C7-C8	-7.44	110.26	125.99
20	4	317	XAT	C26-C27-C28	-7.44	110.26	125.99
20	1	315	XAT	C6-C7-C8	-7.44	110.27	125.99
20	3	615	XAT	C6-C7-C8	-7.44	110.27	125.99
19	1	314	LUT	C28-C29-C30	-7.42	107.56	118.94
18	3	601	CHL	O2D-CGD-CBD	7.42	124.45	111.27
18	2	306	CHL	C2C-C3C-C4C	-7.39	101.22	106.49
19	3	614	LUT	C15-C35-C34	-7.38	108.36	123.47
20	4	317	XAT	C19-C9-C10	-7.35	112.62	122.92
20	3	615	XAT	C15-C35-C34	-7.35	108.42	123.47
20	2	315	XAT	C15-C35-C34	-7.34	108.44	123.47
20	1	315	XAT	C15-C35-C34	-7.33	108.46	123.47
18	3	601	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
17	L	203	CLA	C4A-NA-C1A	7.24	109.96	106.71
17	B	840	CLA	C4A-NA-C1A	7.22	109.95	106.71
19	1	314	LUT	C8-C7-C6	-7.19	107.01	127.20
20	1	315	XAT	C26-C27-C28	-7.19	110.80	125.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	615	XAT	C26-C27-C28	-7.18	110.81	125.99
20	2	315	XAT	C7-C8-C9	-7.18	114.39	125.53
20	2	315	XAT	C26-C27-C28	-7.17	110.83	125.99
20	1	315	XAT	C7-C8-C9	-7.17	114.41	125.53
19	1	314	LUT	C1-C6-C5	-7.16	112.52	122.61
20	4	317	XAT	C32-C33-C34	-7.15	107.97	118.94
20	3	615	XAT	C7-C8-C9	-7.15	114.44	125.53
19	3	614	LUT	C28-C29-C30	-7.11	108.04	118.94
19	1	314	LUT	C35-C15-C14	-7.09	108.95	123.47
19	3	614	LUT	C1-C6-C5	-7.06	112.67	122.61
17	A	831	CLA	C4A-NA-C1A	7.05	109.87	106.71
19	3	614	LUT	C20-C13-C14	-7.04	113.06	122.92
19	3	614	LUT	C19-C9-C10	-7.03	113.07	122.92
20	4	317	XAT	C28-C29-C30	-7.01	108.19	118.94
17	3	610	CLA	C4A-NA-C1A	6.98	109.84	106.71
19	1	314	LUT	C40-C33-C34	-6.98	113.15	122.92
19	2	314	LUT	C40-C33-C34	-6.97	113.15	122.92
18	1	305	CHL	C2C-C3C-C4C	-6.96	101.53	106.49
19	3	614	LUT	C12-C13-C14	-6.93	108.30	118.94
18	4	315	CHL	C2C-C3C-C4C	-6.92	101.55	106.49
18	3	607	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
17	B	806	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	2	314	LUT	C15-C35-C34	-6.89	109.35	123.47
19	2	314	LUT	C1-C6-C5	-6.87	112.94	122.61
18	4	305	CHL	C2C-C3C-C4C	-6.87	101.59	106.49
19	1	314	LUT	C15-C35-C34	-6.84	109.47	123.47
17	B	831	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	1	314	LUT	C19-C9-C10	-6.78	113.42	122.92
19	3	614	LUT	C8-C7-C6	-6.78	108.17	127.20
19	2	314	LUT	C38-C25-C24	-6.74	109.14	123.56
19	1	314	LUT	C20-C13-C14	-6.72	113.51	122.92
17	B	808	CLA	C4A-NA-C1A	6.72	109.73	106.71
17	B	822	CLA	C4A-NA-C1A	6.70	109.72	106.71
17	3	613	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	4	316	LUT	C7-C8-C9	-6.68	116.14	126.23
19	4	316	LUT	C40-C33-C34	-6.67	113.58	122.92
27	B	843	PQN	C9-C10-C1	-6.64	110.37	120.10
20	4	317	XAT	C15-C35-C34	-6.63	109.89	123.47
17	B	811	CLA	C4A-NA-C1A	6.62	109.68	106.71
17	3	611	CLA	C4A-NA-C1A	6.61	109.68	106.71
20	2	315	XAT	C35-C15-C14	-6.60	109.95	123.47
20	1	315	XAT	C35-C15-C14	-6.59	109.97	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	615	XAT	C35-C15-C14	-6.59	109.98	123.47
18	4	306	CHL	C3C-C4C-NC	6.58	117.95	110.57
17	A	826	CLA	C4A-NA-C1A	6.57	109.66	106.71
17	G	104	CLA	C4A-NA-C1A	6.55	109.65	106.71
27	B	843	PQN	O4-C4-C5	-6.52	111.00	121.56
17	A	801	CLA	C3D-CAD-CBD	-6.52	99.02	107.61
17	K	202	CLA	C4A-NA-C1A	6.52	109.64	106.71
17	1	307	CLA	C4A-NA-C1A	6.49	109.62	106.71
17	4	304	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	3	614	LUT	C38-C25-C24	-6.48	109.71	123.56
17	A	829	CLA	C4A-NA-C1A	6.44	109.60	106.71
17	3	612	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	3	614	LUT	C35-C15-C14	-6.41	110.35	123.47
17	L	202	CLA	C4A-NA-C1A	6.41	109.59	106.71
20	4	317	XAT	O24-C25-C38	-6.39	107.39	115.06
27	B	843	PQN	O1-C1-C2	-6.39	111.95	120.25
17	G	103	CLA	C4A-NA-C1A	6.38	109.58	106.71
17	A	814	CLA	C4A-NA-C1A	6.38	109.58	106.71
17	A	819	CLA	C4A-NA-C1A	6.37	109.57	106.71
17	K	201	CLA	C4A-NA-C1A	6.36	109.57	106.71
19	2	314	LUT	C8-C7-C6	-6.36	109.34	127.20
17	A	822	CLA	C4A-NA-C1A	6.36	109.56	106.71
17	A	843	CLA	C4A-NA-C1A	6.36	109.56	106.71
17	A	836	CLA	C4A-NA-C1A	6.36	109.56	106.71
17	B	823	CLA	C4A-NA-C1A	6.35	109.56	106.71
17	A	828	CLA	C4A-NA-C1A	6.33	109.55	106.71
17	3	603	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	4	316	LUT	C20-C13-C14	-6.32	114.07	122.92
17	A	824	CLA	C4A-NA-C1A	6.31	109.55	106.71
19	2	314	LUT	C19-C9-C10	-6.25	114.16	122.92
17	A	853	CLA	C4A-NA-C1A	6.22	109.50	106.71
27	A	842	PQN	C15-C13-C12	-6.22	108.53	121.12
17	B	825	CLA	C4A-NA-C1A	6.21	109.50	106.71
17	2	302	CLA	C4A-NA-C1A	6.20	109.49	106.71
17	1	308	CLA	C4A-NA-C1A	6.19	109.49	106.71
17	A	830	CLA	C4A-NA-C1A	6.18	109.49	106.71
27	A	842	PQN	C11-C3-C4	-6.18	111.89	118.50
19	4	316	LUT	C38-C25-C24	-6.17	110.37	123.56
17	2	312	CLA	C4A-NA-C1A	6.16	109.48	106.71
27	A	842	PQN	C11-C12-C13	-6.16	116.54	126.79
27	B	843	PQN	C15-C13-C12	-6.16	108.66	121.12
17	3	604	CLA	C4A-NA-C1A	6.15	109.47	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	808	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	4	316	LUT	C1-C6-C5	-6.15	113.95	122.61
17	B	803	CLA	C4A-NA-C1A	6.14	109.47	106.71
17	J	103	CLA	C4A-NA-C1A	6.11	109.45	106.71
17	A	837	CLA	C4A-NA-C1A	6.08	109.44	106.71
17	G	105	CLA	C4A-NA-C1A	6.08	109.44	106.71
17	A	801	CLA	O2D-CGD-CBD	6.08	122.07	111.27
17	2	311	CLA	C4A-NA-C1A	6.06	109.43	106.71
17	A	823	CLA	C4A-NA-C1A	6.06	109.43	106.71
17	4	313	CLA	C4A-NA-C1A	6.06	109.43	106.71
17	2	309	CLA	C4A-NA-C1A	6.01	109.41	106.71
17	A	821	CLA	C4A-NA-C1A	6.01	109.41	106.71
17	B	841	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	F	305	HTG	O5-C1-C2	-5.96	102.81	110.31
17	A	833	CLA	C4A-NA-C1A	5.96	109.39	106.71
17	A	801	CLA	C4A-NA-C1A	5.93	109.37	106.71
17	1	303	CLA	C4A-NA-C1A	5.92	109.37	106.71
17	A	818	CLA	C4A-NA-C1A	5.88	109.35	106.71
17	A	841	CLA	C4A-NA-C1A	5.88	109.35	106.71
17	B	837	CLA	C4A-NA-C1A	5.86	109.34	106.71
17	B	813	CLA	C4A-NA-C1A	5.86	109.34	106.71
17	A	817	CLA	C4A-NA-C1A	5.85	109.34	106.71
17	B	842	CLA	C4A-NA-C1A	5.83	109.33	106.71
20	3	615	XAT	C10-C11-C12	-5.81	105.07	123.22
20	1	315	XAT	C10-C11-C12	-5.81	105.09	123.22
17	A	802	CLA	C4A-NA-C1A	5.81	109.32	106.71
20	2	315	XAT	C10-C11-C12	-5.79	105.14	123.22
17	L	204	CLA	C4A-NA-C1A	5.79	109.31	106.71
17	2	303	CLA	C4A-NA-C1A	5.79	109.31	106.71
17	1	304	CLA	C4A-NA-C1A	5.78	109.31	106.71
20	4	317	XAT	C6-C7-C8	-5.77	113.78	125.99
17	A	815	CLA	C4A-NA-C1A	5.77	109.30	106.71
19	1	314	LUT	C38-C25-C24	-5.77	111.22	123.56
19	4	316	LUT	C19-C9-C10	-5.74	114.88	122.92
17	B	828	CLA	C4A-NA-C1A	5.73	109.28	106.71
17	A	805	CLA	C4A-NA-C1A	5.73	109.28	106.71
18	4	301	CHL	C3C-C4C-NC	5.73	116.99	110.57
19	1	314	LUT	C30-C31-C32	-5.72	105.37	123.22
17	3	609	CLA	C4A-NA-C1A	5.72	109.28	106.71
19	2	314	LUT	C30-C31-C32	-5.71	105.39	123.22
17	3	606	CLA	C4A-NA-C1A	5.69	109.27	106.71
17	A	834	CLA	C4A-NA-C1A	5.68	109.26	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	304	CLA	C4A-NA-C1A	5.67	109.25	106.71
17	3	605	CLA	C4A-NA-C1A	5.65	109.25	106.71
17	4	311	CLA	C4A-NA-C1A	5.64	109.24	106.71
17	A	827	CLA	C4A-NA-C1A	5.64	109.24	106.71
17	B	815	CLA	C4A-NA-C1A	5.62	109.23	106.71
17	A	853	CLA	C1-C2-C3	-5.62	116.33	126.04
26	4	323	DGD	C1D-O6D-C5D	-5.61	102.68	113.69
27	A	842	PQN	O4-C4-C5	-5.59	112.51	121.56
17	B	824	CLA	C4A-NA-C1A	5.59	109.22	106.71
17	A	825	CLA	C4A-NA-C1A	5.59	109.22	106.71
17	A	832	CLA	C4A-NA-C1A	5.58	109.21	106.71
19	1	314	LUT	C10-C11-C12	-5.58	105.82	123.22
19	4	316	LUT	C30-C31-C32	-5.56	105.86	123.22
17	A	810	CLA	C4A-NA-C1A	5.55	109.20	106.71
18	2	313	CHL	C3C-C4C-NC	5.54	116.79	110.57
27	B	843	PQN	O1-C1-C10	-5.54	112.59	121.56
18	2	306	CHL	C3C-C4C-NC	5.53	116.77	110.57
17	3	608	CLA	C4A-NA-C1A	5.52	109.19	106.71
18	4	306	CHL	CHD-C4C-C3C	-5.52	116.72	124.84
19	4	316	LUT	C11-C12-C13	-5.51	110.93	126.42
17	B	814	CLA	C4A-NA-C1A	5.50	109.18	106.71
20	4	317	XAT	C40-C33-C34	-5.50	115.22	122.92
27	A	842	PQN	C2M-C2-C3	-5.49	115.44	124.40
17	A	809	CLA	C4A-NA-C1A	5.49	109.17	106.71
17	1	310	CLA	C4A-NA-C1A	5.49	109.17	106.71
17	2	308	CLA	C4A-NA-C1A	5.49	109.17	106.71
17	A	812	CLA	C4A-NA-C1A	5.47	109.17	106.71
18	4	305	CHL	O2D-CGD-CBD	5.46	120.97	111.27
17	1	313	CLA	C4A-NA-C1A	5.45	109.16	106.71
17	2	310	CLA	C4A-NA-C1A	5.41	109.14	106.71
17	B	827	CLA	C4A-NA-C1A	5.40	109.13	106.71
17	B	833	CLA	CMB-C2B-C1B	-5.36	120.22	128.46
18	4	307	CHL	C3C-C4C-NC	5.35	116.58	110.57
17	A	811	CLA	C4A-NA-C1A	5.35	109.11	106.71
17	4	312	CLA	C4A-NA-C1A	5.34	109.11	106.71
19	1	314	LUT	C11-C12-C13	-5.34	111.42	126.42
18	4	305	CHL	C3C-C4C-NC	5.33	116.55	110.57
17	A	816	CLA	C4A-NA-C1A	5.33	109.10	106.71
18	2	313	CHL	O2D-CGD-CBD	5.33	120.73	111.27
27	A	842	PQN	C7-C6-C5	-5.32	109.75	119.81
17	A	835	CLA	C4A-NA-C1A	5.31	109.09	106.71
19	2	314	LUT	C31-C32-C33	-5.30	111.53	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	817	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
17	B	834	CLA	C4A-NA-C1A	5.28	109.08	106.71
17	B	818	CLA	O2D-CGD-O1D	-5.28	113.51	123.84
17	4	308	CLA	C4A-NA-C1A	5.27	109.08	106.71
17	1	302	CLA	C4A-NA-C1A	5.27	109.08	106.71
17	B	823	CLA	CMB-C2B-C1B	-5.26	120.38	128.46
18	2	305	CHL	C3C-C4C-NC	5.26	116.47	110.57
19	3	614	LUT	C30-C31-C32	-5.25	106.84	123.22
18	3	601	CHL	C3C-C4C-NC	5.25	116.45	110.57
18	2	304	CHL	C3C-C4C-NC	5.24	116.45	110.57
17	3	602	CLA	C4A-NA-C1A	5.24	109.06	106.71
17	4	314	CLA	C4A-NA-C1A	5.22	109.06	106.71
17	1	311	CLA	C4A-NA-C1A	5.22	109.05	106.71
19	3	614	LUT	C31-C32-C33	-5.22	111.75	126.42
20	4	317	XAT	C10-C11-C12	-5.22	106.93	123.22
20	4	317	XAT	C31-C32-C33	-5.20	111.81	126.42
19	3	614	LUT	C11-C12-C13	-5.18	111.85	126.42
17	A	806	CLA	C4A-NA-C1A	5.14	109.02	106.71
17	A	813	CLA	C4A-NA-C1A	5.14	109.02	106.71
27	B	843	PQN	C14-C13-C12	-5.13	110.51	123.68
20	3	615	XAT	C18-C5-C4	5.13	120.05	114.28
20	1	315	XAT	C18-C5-C4	5.12	120.04	114.28
20	2	315	XAT	C18-C5-C4	5.11	120.03	114.28
17	A	820	CLA	C4A-NA-C1A	5.10	109.00	106.71
19	2	314	LUT	C11-C12-C13	-5.10	112.09	126.42
19	3	614	LUT	C10-C11-C12	-5.10	107.31	123.22
17	2	319	CLA	C4A-NA-C1A	5.09	108.99	106.71
27	A	842	PQN	C8-C9-C10	-5.07	110.23	119.81
19	4	316	LUT	C10-C11-C12	-5.07	107.41	123.22
18	3	607	CHL	C3C-C4C-NC	5.05	116.23	110.57
18	3	601	CHL	CHD-C4C-C3C	-5.04	117.43	124.84
17	B	814	CLA	CMB-C2B-C1B	-5.03	120.73	128.46
17	4	310	CLA	C4A-NA-C1A	5.00	108.96	106.71
18	4	301	CHL	CHD-C4C-C3C	-5.00	117.49	124.84
17	J	101	CLA	O2D-CGD-O1D	-4.99	114.08	123.84
17	F	306	CLA	C4A-NA-C1A	4.99	108.95	106.71
17	B	836	CLA	C4A-NA-C1A	4.98	108.94	106.71
20	3	615	XAT	C20-C13-C12	-4.97	110.24	118.08
20	1	315	XAT	C20-C13-C12	-4.97	110.25	118.08
20	2	315	XAT	C20-C13-C12	-4.97	110.25	118.08
17	B	805	CLA	C4A-NA-C1A	4.95	108.93	106.71
17	1	306	CLA	C4A-NA-C1A	4.94	108.93	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	B	843	PQN	C5-C10-C1	-4.94	115.33	120.68
17	B	820	CLA	CMB-C2B-C1B	-4.93	120.88	128.46
17	2	301	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
17	A	802	CLA	C4D-C3D-CAD	-4.92	105.72	108.47
17	A	818	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
17	A	853	CLA	O2D-CGD-O1D	-4.91	114.25	123.84
18	2	313	CHL	CHD-C4C-C3C	-4.90	117.64	124.84
19	2	314	LUT	C10-C11-C12	-4.90	107.94	123.22
17	A	801	CLA	OBD-CAD-C3D	4.89	136.10	127.98
17	A	804	CLA	C4A-NA-C1A	4.88	108.90	106.71
18	1	305	CHL	C3C-C4C-NC	4.88	116.04	110.57
18	4	307	CHL	CHD-C4C-C3C	-4.87	117.68	124.84
17	1	309	CLA	C4A-NA-C1A	4.87	108.89	106.71
17	B	817	CLA	C4A-NA-C1A	4.86	108.89	106.71
19	3	614	LUT	C4-C5-C6	-4.85	110.04	120.85
26	4	323	DGD	O2G-C1B-C2B	4.83	121.91	111.50
17	B	827	CLA	O1D-CGD-CBD	4.82	134.36	124.48
17	F	307	CLA	C4A-NA-C1A	4.82	108.87	106.71
17	B	825	CLA	CMB-C2B-C1B	-4.81	121.06	128.46
19	3	614	LUT	C19-C9-C8	-4.80	110.52	118.08
27	B	843	PQN	C7-C8-C9	-4.79	112.90	120.19
17	B	804	CLA	C4A-NA-C1A	4.78	108.86	106.71
17	B	811	CLA	CMB-C2B-C1B	-4.77	121.12	128.46
17	1	312	CLA	C4A-NA-C1A	4.77	108.85	106.71
27	A	842	PQN	C7-C8-C9	-4.76	112.94	120.19
17	B	838	CLA	O2D-CGD-O1D	-4.76	114.54	123.84
17	B	820	CLA	CMB-C2B-C3B	4.75	133.56	124.68
26	B	850	DGD	O5D-C6D-C5D	-4.75	100.26	109.05
17	A	801	CLA	C4D-C3D-CAD	-4.74	105.83	108.47
17	A	853	CLA	O2A-CGA-O1A	-4.74	111.62	123.59
18	2	304	CHL	O2D-CGD-CBD	4.74	119.69	111.27
27	B	843	PQN	C2M-C2-C1	-4.73	108.43	116.27
17	B	806	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
17	4	312	CLA	CMB-C2B-C1B	-4.71	121.23	128.46
20	2	315	XAT	C31-C32-C33	-4.71	113.19	126.42
18	4	315	CHL	C3C-C4C-NC	4.70	115.85	110.57
17	B	807	CLA	CMB-C2B-C1B	-4.70	121.23	128.46
20	1	315	XAT	C31-C32-C33	-4.70	113.21	126.42
17	B	816	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
19	1	314	LUT	C31-C32-C33	-4.69	113.23	126.42
20	3	615	XAT	C31-C32-C33	-4.69	113.23	126.42
19	2	314	LUT	C4-C5-C6	-4.67	110.43	120.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	1	314	LUT	C4-C5-C6	-4.67	110.45	120.85
17	4	310	CLA	O2D-CGD-O1D	-4.66	114.72	123.84
20	3	615	XAT	C30-C31-C32	-4.66	108.68	123.22
17	A	803	CLA	C4A-NA-C1A	4.66	108.80	106.71
17	B	832	CLA	C4A-NA-C1A	4.66	108.80	106.71
20	1	315	XAT	C30-C31-C32	-4.65	108.69	123.22
17	B	817	CLA	CMB-C2B-C3B	4.65	133.38	124.68
18	2	305	CHL	O2D-CGD-CBD	4.65	119.53	111.27
20	2	315	XAT	C30-C31-C32	-4.65	108.72	123.22
17	B	838	CLA	O1D-CGD-CBD	4.64	133.99	124.48
17	B	812	CLA	C4A-NA-C1A	4.64	108.79	106.71
17	A	837	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
20	4	317	XAT	C38-C25-C24	4.63	119.49	114.28
17	A	853	CLA	CED-O2D-CGD	-4.63	105.46	115.94
17	B	824	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
18	2	304	CHL	CHD-C4C-C3C	-4.61	118.06	124.84
17	B	839	CLA	O2D-CGD-O1D	-4.60	114.84	123.84
17	4	303	CLA	C1-C2-C3	-4.60	118.09	126.04
19	1	314	LUT	C7-C6-C5	-4.59	110.34	121.46
18	2	306	CHL	CHD-C4C-C3C	-4.57	118.12	124.84
17	B	823	CLA	CMB-C2B-C3B	4.54	133.18	124.68
17	A	807	CLA	C4A-NA-C1A	4.54	108.75	106.71
18	3	607	CHL	O2D-CGD-CBD	4.53	119.32	111.27
18	4	305	CHL	C4-C3-C5	4.52	122.87	115.27
17	B	838	CLA	C4A-NA-C1A	4.51	108.73	106.71
19	1	314	LUT	C20-C13-C12	-4.50	110.99	118.08
17	A	804	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
25	B	851	HTG	O5-C1-C2	4.49	115.96	110.31
17	B	831	CLA	O2D-CGD-CBD	4.48	119.24	111.27
17	B	809	CLA	C4A-NA-C1A	4.48	108.72	106.71
17	B	805	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
17	B	819	CLA	O2D-CGD-O1D	-4.48	115.08	123.84
17	B	830	CLA	C4A-NA-C1A	4.48	108.72	106.71
17	2	311	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
17	B	827	CLA	O2D-CGD-O1D	-4.47	115.10	123.84
19	4	316	LUT	C7-C6-C5	-4.47	110.64	121.46
17	B	833	CLA	CMB-C2B-C3B	4.45	133.00	124.68
17	4	302	CLA	C4A-NA-C1A	4.43	108.70	106.71
17	A	838	CLA	C4A-NA-C1A	4.42	108.69	106.71
17	B	806	CLA	CMB-C2B-C3B	4.42	132.94	124.68
17	2	301	CLA	C4A-NA-C1A	4.42	108.69	106.71
18	3	607	CHL	CHD-C4C-C3C	-4.40	118.37	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	851	HTG	C1'-S1-C1	4.40	108.32	100.09
17	A	827	CLA	C1-C2-C3	-4.40	118.44	126.04
20	3	615	XAT	C39-C29-C28	-4.39	111.16	118.08
20	1	315	XAT	C39-C29-C28	-4.38	111.17	118.08
17	B	828	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
17	F	304	CLA	O2A-CGA-O1A	-4.38	112.54	123.59
20	2	315	XAT	C38-C25-C24	4.37	119.20	114.28
20	3	615	XAT	C38-C25-C24	4.37	119.20	114.28
20	1	315	XAT	C38-C25-C24	4.37	119.19	114.28
17	2	307	CLA	C4A-NA-C1A	4.36	108.67	106.71
20	2	315	XAT	C39-C29-C28	-4.36	111.21	118.08
17	B	839	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
18	4	305	CHL	CHD-C4C-C3C	-4.35	118.45	124.84
20	1	315	XAT	C19-C9-C8	-4.34	111.24	118.08
17	A	821	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
20	3	615	XAT	C19-C9-C8	-4.33	111.25	118.08
17	3	608	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
20	2	315	XAT	C19-C9-C8	-4.33	111.26	118.08
17	B	839	CLA	O2A-CGA-O1A	-4.32	112.70	123.59
17	A	827	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
18	1	305	CHL	O2D-CGD-CBD	4.30	118.91	111.27
17	B	837	CLA	C1-C2-C3	-4.30	118.61	126.04
19	2	314	LUT	C19-C9-C8	-4.29	111.32	118.08
27	B	843	PQN	C8-C7-C6	-4.28	113.66	120.19
17	A	834	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
20	1	315	XAT	C11-C12-C13	-4.26	114.46	126.42
17	B	802	CLA	CMB-C2B-C1B	-4.25	121.93	128.46
17	A	838	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
20	3	615	XAT	C11-C12-C13	-4.25	114.48	126.42
20	2	315	XAT	C11-C12-C13	-4.25	114.48	126.42
17	4	314	CLA	O2D-CGD-O1D	-4.24	115.56	123.84
17	A	824	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
20	2	315	XAT	C18-C5-C6	-4.23	115.17	122.26
17	A	835	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
17	2	309	CLA	CMB-C2B-C1B	-4.22	121.97	128.46
17	A	801	CLA	CMD-C2D-C3D	4.22	132.57	124.68
17	4	309	CLA	C4A-NA-C1A	4.22	108.60	106.71
17	4	303	CLA	C4A-NA-C1A	4.22	108.60	106.71
17	1	302	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
22	A	844	LHG	O4-P-O5	4.21	133.05	112.24
20	3	615	XAT	C18-C5-C6	-4.21	115.21	122.26
19	3	614	LUT	C40-C33-C32	-4.21	111.45	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	809	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
22	2	317	LHG	O4-P-O5	4.20	133.01	112.24
20	1	315	XAT	C18-C5-C6	-4.20	115.22	122.26
19	4	316	LUT	C31-C32-C33	-4.20	114.63	126.42
20	4	317	XAT	C30-C31-C32	-4.19	110.14	123.22
18	2	305	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
17	B	807	CLA	C4A-NA-C1A	4.19	108.59	106.71
18	4	305	CHL	CAC-C3C-C4C	4.18	130.24	124.81
18	4	315	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
19	2	314	LUT	C7-C6-C5	-4.17	111.37	121.46
17	2	307	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
17	A	803	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
17	B	830	CLA	O2A-C1-C2	4.16	119.56	108.64
24	4	320	LMG	O6-C5-C4	4.15	117.23	109.69
17	B	814	CLA	CMB-C2B-C3B	4.15	132.44	124.68
22	G	102	LHG	O4-P-O5	4.15	132.76	112.24
22	F	302	LHG	O4-P-O5	4.15	132.75	112.24
24	B	852	LMG	O1-C1-C2	4.14	114.77	108.30
18	2	305	CHL	CAC-C3C-C4C	4.14	130.18	124.81
17	B	831	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
17	B	829	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
17	B	839	CLA	C4A-NA-C1A	4.11	108.56	106.71
17	A	836	CLA	O2D-CGD-O1D	-4.10	115.82	123.84
18	3	601	CHL	O2D-CGD-O1D	-4.10	115.83	123.84
22	A	845	LHG	O4-P-O5	4.09	132.47	112.24
17	B	810	CLA	C4A-NA-C1A	4.09	108.55	106.71
17	A	840	CLA	C1-C2-C3	-4.09	118.97	126.04
27	B	843	PQN	O4-C4-C3	-4.09	113.99	120.56
17	1	313	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
17	J	101	CLA	C4A-NA-C1A	4.07	108.54	106.71
17	4	308	CLA	O2D-CGD-CBD	4.07	118.51	111.27
18	4	301	CHL	O2D-CGD-O1D	-4.07	115.89	123.84
17	A	825	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
17	B	837	CLA	CMD-C2D-C3D	4.05	132.26	124.68
17	B	816	CLA	C4A-NA-C1A	4.05	108.53	106.71
17	K	201	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
19	1	314	LUT	C19-C9-C8	-4.04	111.71	118.08
17	B	819	CLA	C4A-NA-C1A	4.03	108.52	106.71
17	B	826	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
17	A	830	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
17	A	817	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
17	A	827	CLA	CMB-C2B-C3B	4.03	132.22	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	853	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
17	A	838	CLA	C1-C2-C3	-4.03	119.08	126.04
19	3	614	LUT	C20-C13-C12	-4.02	111.74	118.08
17	A	839	CLA	C4A-NA-C1A	4.02	108.51	106.71
17	B	816	CLA	O1D-CGD-CBD	4.02	132.70	124.48
21	J	105	BCR	C2-C1-C6	4.02	116.66	110.48
18	4	301	CHL	O2A-CGA-CBA	4.02	124.51	111.91
18	4	315	CHL	O2D-CGD-CBD	4.01	118.40	111.27
26	4	323	DGD	O6D-C5D-C6D	4.01	114.75	106.67
27	B	843	PQN	C7-C6-C5	-4.01	112.24	119.81
22	1	317	LHG	O4-P-O5	4.01	132.04	112.24
17	2	301	CLA	CMB-C2B-C3B	4.00	132.17	124.68
17	B	831	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
17	F	306	CLA	CMD-C2D-C3D	3.99	132.15	124.68
17	A	818	CLA	CMB-C2B-C3B	3.99	132.15	124.68
22	B	801	LHG	O4-P-O5	3.98	131.93	112.24
17	A	808	CLA	CMB-C2B-C3B	3.98	132.12	124.68
17	B	824	CLA	CMB-C2B-C3B	3.98	132.12	124.68
17	2	308	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
17	1	312	CLA	C4D-C3D-CAD	-3.98	106.25	108.47
17	F	307	CLA	CAA-C2A-C3A	-3.97	101.92	112.78
17	1	301	CLA	C4A-NA-C1A	3.96	108.49	106.71
17	B	818	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
17	B	832	CLA	O2D-CGD-O1D	-3.95	116.11	123.84
17	A	832	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
19	2	314	LUT	C39-C29-C28	-3.95	111.86	118.08
17	B	826	CLA	C4D-C3D-CAD	-3.95	106.27	108.47
17	A	836	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
17	3	612	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
17	A	853	CLA	OBD-CAD-CBD	-3.94	120.27	125.89
17	2	312	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
17	B	816	CLA	CMB-C2B-C3B	3.93	132.04	124.68
18	2	306	CHL	O2D-CGD-CBD	3.93	118.26	111.27
17	B	839	CLA	CMB-C2B-C3B	3.93	132.03	124.68
17	B	837	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
17	4	304	CLA	C4D-C3D-CAD	-3.92	106.28	108.47
17	F	307	CLA	CMB-C2B-C1B	-3.92	122.45	128.46
17	J	101	CLA	O2D-CGD-CBD	3.91	118.22	111.27
17	A	807	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
21	B	847	BCR	C27-C26-C25	3.88	128.36	122.73
17	B	825	CLA	CMB-C2B-C3B	3.87	131.93	124.68
17	B	837	CLA	CMB-C2B-C3B	3.87	131.93	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	829	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
17	A	841	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
17	3	602	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
17	4	304	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
27	B	843	PQN	C10-C5-C4	-3.86	116.51	120.68
19	3	614	LUT	C39-C29-C28	-3.85	112.01	118.08
17	1	306	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
17	A	804	CLA	CMB-C2B-C3B	3.85	131.87	124.68
17	A	825	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
17	B	806	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
25	F	310	HTG	C3-C4-C5	3.83	117.07	110.24
17	3	609	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
27	A	842	PQN	O1-C1-C10	-3.83	115.37	121.56
20	4	317	XAT	C18-C5-C4	3.83	118.58	114.28
17	A	802	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
17	1	313	CLA	CMB-C2B-C3B	3.82	131.83	124.68
17	B	818	CLA	CMB-C2B-C3B	3.82	131.82	124.68
18	3	601	CHL	C6-C5-C3	-3.81	108.39	114.62
17	B	818	CLA	O2D-CGD-CBD	3.81	118.03	111.27
17	B	839	CLA	CAA-C2A-C1A	-3.80	99.51	111.97
18	4	315	CHL	CAC-C3C-C4C	3.80	129.74	124.81
17	A	838	CLA	O2D-CGD-CBD	3.80	118.02	111.27
17	B	835	CLA	C4A-NA-C1A	3.80	108.41	106.71
19	4	316	LUT	C4-C5-C6	-3.80	112.38	120.85
18	4	301	CHL	C4D-C3D-CAD	3.80	110.59	108.47
17	4	303	CLA	CMD-C2D-C3D	3.80	131.78	124.68
17	L	202	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
17	2	302	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
17	B	842	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
17	B	807	CLA	O2D-CGD-O1D	-3.79	116.43	123.84
21	3	616	BCR	C2-C1-C6	3.79	116.31	110.48
17	A	832	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
24	F	309	LMG	O1-C1-C2	-3.77	102.41	108.30
17	A	816	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
17	1	303	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
17	B	828	CLA	CMB-C2B-C3B	3.77	131.73	124.68
17	A	815	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
17	1	302	CLA	CMB-C2B-C3B	3.76	131.72	124.68
17	4	310	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
18	4	315	CHL	C3B-C4B-NB	3.76	114.07	109.21
18	4	301	CHL	C1-C2-C3	-3.76	119.55	126.04
17	3	604	CLA	CMB-C2B-C1B	-3.75	122.70	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	837	CLA	CMB-C2B-C3B	3.75	131.69	124.68
17	4	308	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
25	4	321	HTG	C1'-S1-C1	3.74	107.08	100.09
17	B	809	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
18	1	305	CHL	CHD-C4C-C3C	-3.74	119.35	124.84
17	A	829	CLA	CMB-C2B-C1B	-3.73	122.72	128.46
17	2	319	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
17	A	802	CLA	OBD-CAD-CBD	-3.72	120.58	125.89
24	4	320	LMG	O6-C1-O1	-3.71	101.19	109.97
19	4	316	LUT	C20-C13-C12	-3.71	112.23	118.08
18	3	607	CHL	C3B-C4B-NB	3.71	114.00	109.21
17	B	803	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
18	2	304	CHL	C3B-C4B-NB	3.70	113.99	109.21
17	B	830	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
17	A	838	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
17	3	613	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
17	B	825	CLA	CAA-C2A-C3A	-3.68	102.69	112.78
17	4	310	CLA	C4D-C3D-CAD	-3.68	106.42	108.47
24	F	309	LMG	O6-C1-O1	-3.68	101.26	109.97
19	1	314	LUT	C40-C33-C32	-3.67	112.30	118.08
17	B	838	CLA	CMB-C2B-C3B	3.66	131.53	124.68
19	4	316	LUT	C18-C5-C4	-3.66	107.58	114.36
17	G	105	CLA	CMB-C2B-C1B	-3.66	122.85	128.46
17	3	610	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
17	G	104	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
17	4	308	CLA	CMB-C2B-C3B	3.65	131.50	124.68
17	A	839	CLA	C1-C2-C3	-3.65	119.73	126.04
17	A	840	CLA	C4A-NA-C1A	3.65	108.34	106.71
17	A	802	CLA	CMB-C2B-C3B	3.64	131.49	124.68
17	2	303	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
17	1	312	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
17	J	101	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	B	850	DGD	O6D-C1D-O3G	-3.63	101.39	109.97
17	B	807	CLA	CMB-C2B-C3B	3.62	131.46	124.68
17	2	311	CLA	CMB-C2B-C3B	3.62	131.46	124.68
17	B	827	CLA	CED-O2D-CGD	-3.62	107.75	115.94
17	B	836	CLA	CMC-C2C-C3C	3.61	131.75	124.94
19	1	314	LUT	C39-C29-C28	-3.61	112.39	118.08
18	2	306	CHL	C1-C2-C3	-3.61	120.92	126.75
19	4	316	LUT	C22-C23-C24	-3.60	107.64	111.74
17	B	829	CLA	C4A-NA-C1A	3.60	108.33	106.71
17	4	310	CLA	CAA-C2A-C3A	-3.60	102.92	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	806	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
21	L	201	BCR	C15-C16-C17	-3.60	116.11	123.47
17	B	836	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
17	A	809	CLA	CMB-C2B-C3B	3.59	131.40	124.68
17	A	828	CLA	C4D-C3D-CAD	-3.59	106.47	108.47
17	A	808	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
17	J	103	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
17	4	304	CLA	CMD-C2D-C3D	3.58	131.38	124.68
21	J	105	BCR	C29-C30-C25	3.58	115.99	110.48
17	A	812	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
18	4	301	CHL	O2A-CGA-O1A	-3.57	114.57	123.59
17	1	308	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
25	B	851	HTG	C1-C2-C3	3.57	117.63	110.59
17	B	808	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
18	4	301	CHL	C2A-C1A-CHA	-3.56	117.64	123.86
18	4	306	CHL	O2D-CGD-CBD	3.56	117.59	111.27
17	B	837	CLA	CMC-C2C-C3C	3.56	131.65	124.94
17	4	302	CLA	O2A-CGA-O1A	-3.56	114.62	123.59
17	4	308	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
17	A	853	CLA	CMB-C2B-C3B	3.55	131.32	124.68
17	A	802	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
17	B	837	CLA	C4D-C3D-CAD	-3.55	106.49	108.47
17	3	603	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
17	G	105	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
26	4	323	DGD	C1E-O6E-C5E	3.54	120.64	113.69
17	2	310	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
17	A	823	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
17	B	822	CLA	O1D-CGD-CBD	3.53	131.71	124.48
17	B	821	CLA	C4D-C3D-CAD	-3.53	106.50	108.47
17	A	802	CLA	CMD-C2D-C3D	3.53	131.28	124.68
19	3	614	LUT	C7-C6-C5	-3.53	112.92	121.46
17	K	202	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
17	3	606	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
17	L	203	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
17	B	833	CLA	C4A-NA-C1A	3.52	108.29	106.71
17	G	103	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
17	L	204	CLA	O2D-CGD-O1D	-3.52	116.97	123.84
17	4	312	CLA	CMB-C2B-C3B	3.51	131.25	124.68
20	4	317	XAT	C11-C12-C13	-3.51	116.54	126.42
21	4	318	BCR	C2-C1-C6	3.51	115.89	110.48
17	F	304	CLA	C1-O2A-CGA	-3.51	107.23	116.44
27	A	842	PQN	C14-C13-C12	-3.51	114.67	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	2	311	CLA	O2D-CGD-O1D	-3.51	116.97	123.84
18	4	301	CHL	CAC-C3C-C4C	3.51	129.36	124.81
17	A	820	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
17	B	834	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
17	4	311	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
17	4	314	CLA	OBD-CAD-CBD	-3.50	120.89	125.89
17	A	838	CLA	C4D-C3D-CAD	-3.50	106.52	108.47
21	A	846	BCR	C15-C14-C13	-3.50	122.32	127.31
17	A	833	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
17	B	834	CLA	CHB-C4A-NA	3.49	129.34	124.51
17	2	309	CLA	CMB-C2B-C3B	3.49	131.21	124.68
17	A	832	CLA	CMB-C2B-C3B	3.49	131.20	124.68
17	A	825	CLA	CMB-C2B-C3B	3.48	131.20	124.68
17	A	811	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
17	3	608	CLA	CMB-C2B-C3B	3.48	131.19	124.68
17	B	805	CLA	CMB-C2B-C3B	3.48	131.19	124.68
17	J	101	CLA	CMB-C2B-C3B	3.48	131.18	124.68
17	B	825	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
17	A	836	CLA	CMB-C2B-C3B	3.47	131.18	124.68
17	A	816	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
17	A	824	CLA	CMB-C2B-C3B	3.47	131.17	124.68
25	J	102	HTG	C1'-S1-C1	3.46	106.57	100.09
17	A	821	CLA	CMB-C2B-C3B	3.46	131.15	124.68
17	1	309	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
17	A	802	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
17	B	836	CLA	C4D-C3D-CAD	-3.46	106.54	108.47
17	A	831	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
17	B	813	CLA	C4D-C3D-CAD	-3.45	106.54	108.47
17	1	304	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
18	3	601	CHL	C3B-C4B-NB	3.44	113.66	109.21
17	A	829	CLA	O2D-CGD-CBD	3.44	117.38	111.27
17	A	821	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
18	4	307	CHL	C1-C2-C3	-3.44	121.19	126.75
17	4	314	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
17	A	835	CLA	CMB-C2B-C3B	3.44	131.11	124.68
17	B	802	CLA	CMB-C2B-C3B	3.44	131.11	124.68
17	B	810	CLA	CMD-C2D-C3D	3.44	131.11	124.68
24	F	309	LMG	O1-C7-C8	-3.43	102.62	110.90
17	A	838	CLA	O2A-CGA-O1A	-3.43	114.93	123.59
17	A	806	CLA	C4D-C3D-CAD	-3.43	106.56	108.47
17	A	808	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
17	A	840	CLA	O2D-CGD-O1D	-3.43	117.13	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	4	319	LMG	O1-C1-C2	-3.43	102.95	108.30
17	4	308	CLA	C4D-C3D-CAD	-3.43	106.56	108.47
17	A	810	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
17	B	839	CLA	CHB-C4A-NA	3.42	129.24	124.51
17	K	201	CLA	CMB-C2B-C3B	3.42	131.08	124.68
17	B	826	CLA	OBD-CAD-CBD	-3.41	121.02	125.89
17	B	838	CLA	OBD-CAD-CBD	-3.41	121.02	125.89
17	F	306	CLA	C4D-C3D-CAD	-3.41	106.57	108.47
17	B	831	CLA	C1B-CHB-C4A	-3.41	123.37	130.12
17	B	842	CLA	O2A-CGA-O1A	-3.41	114.99	123.59
18	2	305	CHL	C3B-C4B-NB	3.40	113.61	109.21
17	2	308	CLA	CMB-C2B-C3B	3.40	131.04	124.68
21	A	850	BCR	C33-C5-C6	-3.40	120.71	124.53
17	B	812	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
17	1	311	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
17	A	808	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
17	B	832	CLA	C4D-C3D-CAD	-3.39	106.58	108.47
17	4	303	CLA	OBD-CAD-CBD	-3.39	121.06	125.89
17	4	302	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
18	2	304	CHL	CAC-C3C-C4C	3.38	129.20	124.81
22	A	845	LHG	O8-C23-C24	3.38	120.24	111.38
17	3	612	CLA	CMB-C2B-C3B	3.38	131.00	124.68
18	4	305	CHL	C3B-C4B-NB	3.37	113.57	109.21
17	A	836	CLA	OBD-CAD-CBD	-3.37	121.08	125.89
18	4	301	CHL	C3B-C4B-NB	3.37	113.57	109.21
17	B	809	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
17	A	841	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
18	2	313	CHL	C3B-C4B-NB	3.37	113.56	109.21
17	3	611	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
17	A	814	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
17	A	805	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
17	A	822	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
18	4	305	CHL	CBC-CAC-C3C	-3.35	103.19	112.43
17	A	810	CLA	C4D-C3D-CAD	-3.35	106.60	108.47
17	4	313	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
17	A	803	CLA	O1D-CGD-CBD	3.34	131.32	124.48
17	2	307	CLA	CMB-C2B-C3B	3.34	130.93	124.68
21	J	104	BCR	C27-C26-C25	3.34	127.58	122.73
17	A	826	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
27	B	843	PQN	C8-C9-C10	-3.34	113.51	119.81
17	J	103	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
24	4	319	LMG	O2-C2-C1	-3.33	101.95	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	304	CLA	C1-C2-C3	-3.33	120.28	126.04
17	A	810	CLA	CMD-C2D-C3D	3.32	130.90	124.68
17	2	312	CLA	CMB-C2B-C3B	3.32	130.90	124.68
17	B	813	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
17	A	835	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
17	B	829	CLA	CMB-C2B-C3B	3.31	130.87	124.68
18	4	307	CHL	CAC-C3C-C4C	3.31	129.10	124.81
17	A	805	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
17	B	808	CLA	C11-C12-C13	-3.30	105.24	115.92
17	B	834	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
17	B	822	CLA	CMC-C2C-C3C	3.30	131.16	124.94
17	B	808	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
17	A	827	CLA	O1D-CGD-CBD	3.30	131.24	124.48
17	B	833	CLA	CMC-C2C-C3C	3.30	131.16	124.94
17	K	202	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
17	B	838	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
17	B	819	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
17	4	308	CLA	O2A-CGA-O1A	-3.29	115.30	123.59
17	B	806	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
17	A	840	CLA	OBD-CAD-CBD	-3.28	121.20	125.89
17	A	834	CLA	CMB-C2B-C3B	3.28	130.82	124.68
17	B	836	CLA	CMB-C2B-C3B	3.28	130.82	124.68
17	2	307	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
17	B	814	CLA	O2D-CGD-CBD	3.28	117.09	111.27
17	B	832	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
17	1	312	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
27	A	842	PQN	C6-C5-C4	-3.27	115.31	120.10
17	1	306	CLA	CMB-C2B-C3B	3.27	130.79	124.68
20	3	615	XAT	C40-C33-C32	-3.26	112.94	118.08
17	A	808	CLA	O2A-CGA-O1A	-3.26	115.36	123.59
17	B	839	CLA	C4D-C3D-CAD	-3.26	106.65	108.47
17	A	819	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
17	B	813	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
17	4	303	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
17	B	839	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
26	4	323	DGD	O5D-C1E-C2E	3.24	113.37	108.30
17	4	310	CLA	CMB-C2B-C3B	3.24	130.75	124.68
17	A	830	CLA	CMB-C2B-C3B	3.24	130.75	124.68
20	1	315	XAT	C40-C33-C32	-3.24	112.97	118.08
17	B	839	CLA	CBC-CAC-C3C	-3.24	104.01	112.27
17	A	840	CLA	O2A-CGA-O1A	-3.24	115.41	123.59
20	2	315	XAT	C40-C33-C32	-3.24	112.97	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	609	CLA	CMB-C2B-C3B	3.24	130.73	124.68
17	B	813	CLA	OBD-CAD-CBD	-3.23	121.28	125.89
17	1	303	CLA	CMB-C2B-C3B	3.23	130.72	124.68
17	4	314	CLA	O2A-CGA-O1A	-3.23	115.44	123.59
17	4	308	CLA	OBD-CAD-CBD	-3.23	121.28	125.89
21	A	850	BCR	C24-C23-C22	-3.23	121.36	126.23
20	3	615	XAT	C38-C25-C26	-3.23	116.85	122.26
18	2	306	CHL	C3B-C4B-NB	3.23	113.38	109.21
17	A	823	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
17	4	304	CLA	O1D-CGD-CBD	3.23	131.08	124.48
17	4	304	CLA	CMC-C2C-C3C	3.22	131.02	124.94
17	A	810	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
17	B	826	CLA	O2A-CGA-O1A	-3.22	115.46	123.59
17	A	836	CLA	CMD-C2D-C3D	3.22	130.71	124.68
17	A	843	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
17	B	825	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
17	2	303	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
17	3	602	CLA	CMB-C2B-C3B	3.21	130.69	124.68
21	B	847	BCR	C15-C14-C13	-3.21	122.72	127.31
17	B	825	CLA	CHB-C4A-NA	3.21	128.95	124.51
20	4	317	XAT	O4-C5-C18	-3.21	111.21	115.06
20	1	315	XAT	C38-C25-C26	-3.21	116.88	122.26
17	4	309	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
18	4	305	CHL	O2D-CGD-O1D	-3.21	117.56	123.84
17	B	835	CLA	OBD-CAD-CBD	-3.21	121.31	125.89
17	2	307	CLA	C4D-C3D-CAD	-3.21	106.68	108.47
17	G	105	CLA	CMB-C2B-C3B	3.21	130.68	124.68
17	A	807	CLA	CMB-C2B-C3B	3.20	130.66	124.68
20	2	315	XAT	C38-C25-C26	-3.20	116.91	122.26
17	A	836	CLA	C4D-C3D-CAD	-3.19	106.69	108.47
17	A	834	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
17	B	826	CLA	C4A-NA-C1A	3.19	108.14	106.71
17	A	817	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
17	J	103	CLA	CHB-C4A-NA	3.18	128.91	124.51
19	2	314	LUT	C40-C33-C32	-3.18	113.06	118.08
17	B	814	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
17	A	829	CLA	CMD-C2D-C3D	3.18	130.63	124.68
17	2	302	CLA	CMB-C2B-C3B	3.18	130.63	124.68
21	B	847	BCR	C38-C26-C27	-3.18	107.50	113.62
17	A	801	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
17	F	304	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
26	4	323	DGD	O6E-C5E-C4E	3.16	115.44	109.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	309	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
17	B	821	CLA	CHB-C4A-NA	3.16	128.88	124.51
17	A	816	CLA	CMB-C2B-C3B	3.16	130.59	124.68
17	B	836	CLA	CMD-C2D-C3D	3.16	130.58	124.68
17	B	821	CLA	CED-O2D-CGD	3.15	123.06	115.94
17	A	853	CLA	C1-O2A-CGA	-3.14	108.20	116.44
17	B	826	CLA	C1-C2-C3	-3.14	120.61	126.04
25	F	305	HTG	C1'-S1-C1	3.14	105.96	100.09
17	B	820	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
21	F	303	BCR	C35-C13-C14	-3.14	118.53	122.92
17	A	805	CLA	CMB-C2B-C3B	3.14	130.54	124.68
21	B	847	BCR	C40-C30-C39	-3.14	98.91	108.53
17	B	832	CLA	CMD-C2D-C3D	3.13	130.54	124.68
17	A	833	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	B	826	CLA	CMD-C2D-C3D	3.13	130.53	124.68
26	4	323	DGD	C6D-O5D-C1E	3.13	119.85	113.74
17	A	827	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	2	312	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
17	A	819	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
17	B	839	CLA	CBA-CAA-C2A	3.12	123.07	113.86
17	B	811	CLA	CMB-C2B-C3B	3.12	130.51	124.68
17	B	832	CLA	O2A-CGA-O1A	-3.12	115.73	123.59
17	B	822	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
17	F	307	CLA	CMB-C2B-C3B	3.11	130.50	124.68
17	B	823	CLA	C1-C2-C3	-3.11	120.67	126.04
17	1	311	CLA	CMD-C2D-C3D	3.10	130.49	124.68
17	A	801	CLA	CGD-CBD-CAD	3.10	120.78	110.73
17	L	202	CLA	CMB-C2B-C3B	3.10	130.48	124.68
18	2	306	CHL	CAC-C3C-C4C	3.10	128.83	124.81
17	1	308	CLA	CMB-C2B-C3B	3.10	130.48	124.68
17	B	830	CLA	C4-C3-C5	-3.10	110.06	115.27
17	B	831	CLA	CMB-C2B-C3B	3.10	130.47	124.68
18	3	607	CHL	CAC-C3C-C4C	3.10	128.83	124.81
17	2	307	CLA	OBD-CAD-CBD	-3.08	121.49	125.89
17	A	831	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
25	4	322	HTG	C1'-S1-C1	3.08	105.86	100.09
18	4	306	CHL	O2A-CGA-CBA	3.07	121.56	111.91
18	4	301	CHL	O2D-CGD-CBD	3.07	116.73	111.27
17	B	807	CLA	CAA-C2A-C1A	-3.07	101.92	111.97
17	2	301	CLA	CMD-C2D-C3D	3.07	130.42	124.68
21	B	849	BCR	C27-C26-C25	3.07	127.18	122.73
18	4	305	CHL	C2A-C1A-CHA	-3.07	118.50	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	844	BCR	C35-C13-C14	-3.06	118.63	122.92
17	2	301	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
17	A	805	CLA	CMD-C2D-C3D	3.06	130.41	124.68
17	1	311	CLA	OBD-CAD-CBD	-3.06	121.52	125.89
17	3	613	CLA	CMB-C2B-C3B	3.06	130.40	124.68
17	L	202	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
19	4	316	LUT	C37-C21-C22	-3.05	103.65	109.44
21	4	318	BCR	C3-C4-C5	-3.05	108.63	114.08
17	3	610	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
17	B	842	CLA	CMB-C2B-C3B	3.05	130.38	124.68
17	A	812	CLA	OBD-CAD-CBD	-3.04	121.55	125.89
17	2	308	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	L	203	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
17	A	812	CLA	CMB-C2B-C3B	3.04	130.36	124.68
21	J	104	BCR	C2-C1-C6	3.04	115.16	110.48
21	A	850	BCR	C2-C1-C6	3.04	115.16	110.48
17	A	853	CLA	CMD-C2D-C3D	3.04	130.36	124.68
17	B	804	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
17	F	306	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
17	B	809	CLA	CHB-C4A-NA	3.03	128.71	124.51
17	3	602	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
17	B	810	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
17	B	823	CLA	O2A-CGA-O1A	-3.02	115.96	123.59
21	K	203	BCR	C2-C1-C6	3.02	115.13	110.48
17	2	319	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
17	J	103	CLA	CMB-C2B-C3B	3.02	130.33	124.68
17	B	828	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
17	A	841	CLA	CMB-C2B-C3B	3.01	130.31	124.68
17	B	815	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
18	2	306	CHL	O2A-CGA-CBA	3.01	121.35	111.91
17	B	809	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
17	3	603	CLA	CMB-C2B-C3B	3.01	130.31	124.68
21	1	316	BCR	C15-C16-C17	-3.01	117.31	123.47
17	3	604	CLA	CMB-C2B-C3B	3.01	130.30	124.68
17	A	828	CLA	CMB-C2B-C3B	3.00	130.30	124.68
17	4	308	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
17	2	303	CLA	CMB-C2B-C3B	3.00	130.29	124.68
17	A	833	CLA	CMB-C2B-C3B	3.00	130.29	124.68
17	A	807	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
17	F	306	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
21	A	846	BCR	C24-C23-C22	-2.99	121.72	126.23
27	A	842	PQN	C8-C7-C6	-2.99	115.64	120.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	310	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
17	3	609	CLA	C4D-C3D-CAD	-2.99	106.80	108.47
21	3	616	BCR	C15-C16-C17	-2.99	117.36	123.47
17	A	808	CLA	CHB-C4A-NA	2.98	128.64	124.51
17	4	311	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
18	2	313	CHL	CAC-C3C-C4C	2.98	128.68	124.81
17	3	606	CLA	OBD-CAD-CBD	-2.98	121.64	125.89
18	4	306	CHL	CAC-C3C-C4C	2.98	128.67	124.81
21	J	105	BCR	C33-C5-C6	-2.98	121.18	124.53
21	F	303	BCR	C16-C17-C18	-2.98	123.06	127.31
17	A	811	CLA	CMB-C2B-C3B	2.98	130.25	124.68
17	A	843	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
17	A	803	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
17	4	302	CLA	CMB-C2B-C3B	2.97	130.24	124.68
17	K	202	CLA	CMB-C2B-C3B	2.97	130.24	124.68
21	F	308	BCR	C8-C7-C6	-2.97	118.85	127.20
17	A	814	CLA	CMB-C2B-C3B	2.97	130.24	124.68
17	A	823	CLA	CMB-C2B-C3B	2.97	130.23	124.68
17	B	810	CLA	O2D-CGD-CBD	2.97	116.54	111.27
17	3	611	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
25	4	322	HTG	O5-C1-C2	-2.97	106.58	110.31
17	B	842	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
18	3	607	CHL	C1C-C2C-C3C	-2.96	104.76	107.11
17	B	826	CLA	CMB-C2B-C3B	2.96	130.21	124.68
17	B	819	CLA	CMD-C2D-C3D	2.96	130.21	124.68
17	B	838	CLA	CMD-C2D-C3D	2.96	130.21	124.68
24	B	852	LMG	O6-C1-O1	-2.95	102.98	109.97
17	A	810	CLA	CMB-C2B-C3B	2.95	130.20	124.68
17	2	309	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
17	3	605	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
17	B	822	CLA	CHB-C4A-NA	2.95	128.59	124.51
17	4	312	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
21	B	844	BCR	C15-C14-C13	-2.95	123.11	127.31
18	4	305	CHL	CHB-C4A-NA	2.95	128.59	124.51
17	B	817	CLA	C1B-CHB-C4A	-2.94	124.28	130.12
17	A	828	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
17	L	203	CLA	CMB-C2B-C3B	2.94	130.19	124.68
17	A	821	CLA	CMD-C2D-C3D	2.94	130.18	124.68
17	A	853	CLA	OBD-CAD-C3D	2.93	132.85	127.98
17	B	805	CLA	C4D-C3D-CAD	-2.93	106.83	108.47
17	B	810	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
17	A	801	CLA	C1B-CHB-C4A	-2.93	124.31	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	4	310	CLA	CMD-C2D-C3D	2.93	130.16	124.68
17	1	312	CLA	CMB-C2B-C3B	2.92	130.15	124.68
17	1	307	CLA	CHB-C4A-NA	2.92	128.55	124.51
17	2	310	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
17	B	817	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
17	B	827	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	4	323	DGD	O1G-C1A-C2A	2.92	121.07	111.91
17	A	830	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
24	4	319	LMG	O3-C3-C2	-2.91	103.61	110.35
17	B	831	CLA	O2A-CGA-O1A	-2.91	116.24	123.59
17	A	806	CLA	CMB-C2B-C3B	2.91	130.13	124.68
17	3	610	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	B	852	LMG	O6-C1-C2	-2.91	104.19	110.35
17	4	309	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
17	B	829	CLA	C4D-C3D-CAD	-2.91	106.85	108.47
17	4	312	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
17	1	304	CLA	CMD-C2D-C3D	2.91	130.11	124.68
17	A	820	CLA	CMB-C2B-C3B	2.90	130.11	124.68
17	B	818	CLA	CMD-C2D-C3D	2.90	130.11	124.68
17	L	204	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
17	4	310	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
17	B	814	CLA	CHB-C4A-NA	2.90	128.52	124.51
17	A	818	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
17	3	604	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
17	1	310	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
17	B	829	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
17	B	811	CLA	OBD-CAD-CBD	-2.89	121.76	125.89
18	1	305	CHL	C1B-CHB-C4A	-2.89	124.39	130.12
17	B	840	CLA	CMD-C2D-C3D	2.89	130.09	124.68
17	J	103	CLA	CMD-C2D-C3D	2.89	130.08	124.68
17	B	808	CLA	CMB-C2B-C3B	2.89	130.08	124.68
17	A	840	CLA	O2D-CGD-CBD	2.88	116.39	111.27
17	1	311	CLA	C4D-C3D-CAD	-2.88	106.86	108.47
18	1	305	CHL	O2A-CGA-CBA	2.88	120.96	111.91
17	A	815	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
17	B	821	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
17	B	830	CLA	C1B-CHB-C4A	-2.88	124.41	130.12
17	A	843	CLA	CMC-C2C-C3C	2.88	130.37	124.94
17	A	801	CLA	CMB-C2B-C3B	2.88	130.06	124.68
18	1	305	CHL	CAC-C3C-C4C	2.88	128.54	124.81
17	B	814	CLA	C4D-C3D-CAD	-2.88	106.87	108.47
21	F	303	BCR	C39-C30-C25	-2.88	105.63	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	808	CLA	CHB-C4A-NA	2.87	128.49	124.51
17	A	837	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
17	1	307	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
17	B	813	CLA	CMD-C2D-C3D	2.87	130.05	124.68
17	A	822	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
17	B	841	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
18	3	601	CHL	O2A-CGA-CBA	2.87	120.90	111.91
17	B	821	CLA	CMB-C2B-C3B	2.86	130.04	124.68
17	B	815	CLA	CHB-C4A-NA	2.86	128.47	124.51
17	A	828	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
17	B	802	CLA	C4A-NA-C1A	2.86	107.99	106.71
17	1	302	CLA	OBD-CAD-CBD	-2.86	121.81	125.89
18	4	306	CHL	C2A-C1A-CHA	-2.86	118.86	123.86
19	4	316	LUT	C21-C26-C27	-2.86	109.08	112.70
17	B	836	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
18	3	601	CHL	CMB-C2B-C3B	2.86	130.02	124.68
17	1	313	CLA	CMD-C2D-C3D	2.86	130.02	124.68
21	2	316	BCR	C15-C14-C13	-2.85	123.24	127.31
17	1	304	CLA	CMB-C2B-C3B	2.85	130.02	124.68
17	1	302	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
17	B	842	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
17	1	307	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
17	1	304	CLA	CHB-C4A-NA	2.84	128.45	124.51
21	A	846	BCR	C11-C10-C9	-2.84	123.25	127.31
17	G	104	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
17	4	309	CLA	CMB-C2B-C3B	2.84	130.00	124.68
18	3	601	CHL	C2A-C1A-CHA	-2.84	118.89	123.86
17	B	802	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
26	B	850	DGD	CDB-CCB-CBB	-2.84	100.01	114.42
17	4	302	CLA	CED-O2D-CGD	2.84	122.36	115.94
17	A	838	CLA	CMB-C2B-C3B	2.84	129.99	124.68
17	B	830	CLA	C1-C2-C3	-2.84	121.14	126.04
17	B	824	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
17	4	310	CLA	CHB-C4A-NA	2.84	128.43	124.51
17	B	841	CLA	OBD-CAD-CBD	-2.83	121.84	125.89
17	B	834	CLA	O2D-CGD-CBD	2.83	116.30	111.27
17	3	606	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
21	B	846	BCR	C15-C14-C13	-2.83	123.27	127.31
17	A	826	CLA	CMB-C2B-C3B	2.83	129.98	124.68
21	B	844	BCR	C7-C8-C9	-2.83	121.96	126.23
18	3	601	CHL	C4-C3-C5	2.83	120.03	115.27
17	B	834	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	610	CLA	CHB-C4A-NA	2.83	128.43	124.51
17	B	804	CLA	OBD-CAD-C3D	2.83	132.68	127.98
17	4	304	CLA	CMB-C2B-C3B	2.83	129.97	124.68
17	4	302	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
17	B	819	CLA	O1D-CGD-CBD	2.83	130.27	124.48
21	F	308	BCR	C2-C1-C6	2.83	114.83	110.48
20	1	315	XAT	O24-C25-C24	2.83	115.50	113.38
17	A	829	CLA	CMB-C2B-C3B	2.83	129.97	124.68
17	4	304	CLA	CHB-C4A-NA	2.82	128.42	124.51
17	4	303	CLA	C4D-C3D-CAD	-2.82	106.89	108.47
17	B	809	CLA	CMB-C2B-C3B	2.82	129.96	124.68
17	A	808	CLA	CMD-C2D-C3D	2.82	129.96	124.68
17	4	310	CLA	O2D-CGD-CBD	2.82	116.28	111.27
20	3	615	XAT	O24-C25-C24	2.82	115.50	113.38
17	B	834	CLA	C4-C3-C5	2.82	120.02	115.27
17	A	826	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
27	B	843	PQN	C17-C16-C15	-2.82	105.70	113.36
21	2	316	BCR	C33-C5-C6	-2.82	121.36	124.53
19	2	314	LUT	C18-C5-C4	-2.82	109.13	114.36
17	B	835	CLA	C4-C3-C5	2.82	120.01	115.27
17	B	824	CLA	CHB-C4A-NA	2.82	128.41	124.51
17	B	805	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
17	A	820	CLA	CMD-C2D-C3D	2.81	129.94	124.68
17	B	830	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
17	B	834	CLA	CMD-C2D-C3D	2.81	129.94	124.68
17	B	809	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
17	B	826	CLA	CHA-C1A-NA	-2.81	119.96	126.40
24	4	319	LMG	O7-C10-O9	-2.81	116.91	123.70
17	B	819	CLA	CAA-C2A-C1A	-2.81	102.77	111.97
17	A	809	CLA	C1-C2-C3	-2.81	121.19	126.04
17	B	837	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
17	1	303	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
17	K	201	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
18	4	307	CHL	O2D-CGD-CBD	2.80	116.25	111.27
19	4	316	LUT	C37-C21-C36	2.80	112.02	107.89
17	3	606	CLA	CMB-C2B-C3B	2.80	129.91	124.68
17	A	838	CLA	CMD-C2D-C3D	2.80	129.91	124.68
17	3	612	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
17	2	307	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
17	3	611	CLA	CMB-C2B-C3B	2.80	129.91	124.68
17	B	830	CLA	CAA-CBA-CGA	-2.80	105.08	113.25
17	4	303	CLA	O1D-CGD-CBD	2.80	130.20	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	317	XAT	C39-C29-C28	-2.79	113.67	118.08
17	B	806	CLA	O2D-CGD-CBD	2.79	116.23	111.27
18	2	313	CHL	C2A-C1A-CHA	-2.79	118.98	123.86
17	B	828	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
17	B	831	CLA	C1-C2-C3	-2.79	121.22	126.04
17	A	813	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
23	2	318	LMT	C3'-C4'-C5'	-2.79	104.54	110.93
17	B	809	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
17	B	816	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
17	B	827	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
17	B	838	CLA	CED-O2D-CGD	-2.78	109.65	115.94
17	B	822	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
17	1	309	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
17	A	815	CLA	CMB-C2B-C3B	2.78	129.87	124.68
17	4	313	CLA	CAA-CBA-CGA	-2.78	107.62	113.59
17	B	839	CLA	OBD-CAD-CBD	-2.78	121.93	125.89
17	A	817	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
17	A	822	CLA	CMB-C2B-C3B	2.77	129.86	124.68
17	A	820	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
18	1	305	CHL	CED-O2D-CGD	2.77	122.20	115.94
20	2	315	XAT	O24-C25-C24	2.77	115.46	113.38
17	B	839	CLA	O2D-CGD-CBD	2.77	116.19	111.27
17	1	301	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
17	A	853	CLA	O2D-CGD-CBD	2.77	116.18	111.27
17	F	304	CLA	CHB-C4A-NA	2.77	128.34	124.51
17	B	842	CLA	C7-C6-C5	-2.76	105.85	113.36
22	1	317	LHG	C11-C10-C9	-2.76	100.39	114.42
17	A	807	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
17	A	828	CLA	CMD-C2D-C3D	2.76	129.85	124.68
22	A	844	LHG	C11-C10-C9	-2.76	100.40	114.42
17	3	608	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
21	J	104	BCR	C15-C16-C17	-2.76	117.82	123.47
17	2	319	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
24	G	101	LMG	C1-C2-C3	-2.76	104.25	110.00
17	A	836	CLA	O1D-CGD-CBD	2.76	130.12	124.48
21	2	316	BCR	C24-C23-C22	-2.76	122.07	126.23
17	B	838	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	B	852	LMG	C7-O1-C1	2.75	119.12	113.74
17	B	841	CLA	CMC-C2C-C3C	2.75	130.13	124.94
21	A	851	BCR	C24-C23-C22	-2.75	122.07	126.23
21	G	106	BCR	C24-C23-C22	-2.75	122.08	126.23
17	B	811	CLA	CMC-C2C-C3C	2.75	130.13	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	823	CLA	CHB-C4A-NA	2.75	128.32	124.51
26	4	323	DGD	O1G-C1A-O1A	-2.75	116.65	123.59
17	B	807	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
17	B	822	CLA	CMB-C2B-C3B	2.75	129.82	124.68
17	4	314	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
17	A	809	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
17	A	828	CLA	OBD-CAD-CBD	-2.74	121.98	125.89
18	2	304	CHL	C4D-C3D-CAD	2.74	110.00	108.47
18	2	313	CHL	O1D-CGD-CBD	-2.74	118.88	124.48
17	A	817	CLA	OBD-CAD-CBD	-2.74	121.98	125.89
17	B	833	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
18	4	307	CHL	O2A-CGA-CBA	2.74	120.49	111.91
17	B	820	CLA	OBD-CAD-CBD	-2.74	121.99	125.89
17	B	804	CLA	CBC-CAC-C3C	-2.74	105.30	112.27
17	B	823	CLA	CMD-C2D-C3D	2.73	129.79	124.68
17	B	805	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
17	A	853	CLA	C4D-C3D-CAD	-2.73	106.95	108.47
17	A	831	CLA	O2D-CGD-CBD	2.73	116.12	111.27
17	B	817	CLA	CMC-C2C-C3C	2.73	130.08	124.94
17	A	818	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
18	1	305	CHL	C3B-C4B-NB	2.72	112.73	109.21
17	B	833	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
17	B	840	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
21	B	848	BCR	C15-C14-C13	-2.72	123.43	127.31
18	3	601	CHL	C1-C2-C3	-2.72	121.34	126.04
18	2	304	CHL	O2D-CGD-O1D	-2.72	118.53	123.84
17	1	311	CLA	O2A-CGA-O1A	-2.71	116.74	123.59
21	J	105	BCR	C37-C22-C21	-2.71	119.12	122.92
17	B	824	CLA	C1-C2-C3	-2.71	121.35	126.04
17	A	832	CLA	O2D-CGD-CBD	2.71	116.09	111.27
18	4	301	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
17	B	817	CLA	CMD-C2D-C3D	2.71	129.75	124.68
17	4	313	CLA	C4D-C3D-CAD	-2.71	106.96	108.47
17	A	811	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
17	B	828	CLA	C1-C2-C3	-2.71	121.36	126.04
17	J	101	CLA	CMD-C2D-C3D	2.71	129.75	124.68
18	4	306	CHL	CHB-C4A-NA	2.71	128.26	124.51
17	A	830	CLA	CMD-C2D-C3D	2.71	129.74	124.68
17	B	842	CLA	CHB-C4A-NA	2.70	128.25	124.51
17	1	306	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
23	2	318	LMT	C3B-C4B-C5B	-2.70	105.42	110.24
17	2	308	CLA	C1B-CHB-C4A	-2.70	124.77	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	105	CLA	CMD-C2D-C3D	2.70	129.73	124.68
21	2	316	BCR	C27-C26-C25	2.70	126.65	122.73
17	B	804	CLA	OBD-CAD-CBD	-2.70	122.04	125.89
17	B	819	CLA	C4D-C3D-CAD	-2.70	106.97	108.47
17	1	309	CLA	CMB-C2B-C3B	2.69	129.72	124.68
17	A	819	CLA	CMD-C2D-C3D	2.69	129.72	124.68
17	2	309	CLA	CAA-C2A-C3A	-2.69	109.81	116.10
17	B	811	CLA	CMD-C2D-C3D	2.69	129.71	124.68
17	B	831	CLA	CHB-C4A-NA	2.69	128.23	124.51
17	A	802	CLA	CHB-C4A-NA	2.69	128.23	124.51
17	A	806	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
21	L	206	BCR	C33-C5-C6	-2.69	121.51	124.53
17	B	828	CLA	O1D-CGD-CBD	2.69	129.98	124.48
17	3	609	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
17	B	820	CLA	C4A-NA-C1A	2.68	107.91	106.71
21	B	845	BCR	C39-C30-C25	2.68	114.65	110.30
22	A	844	LHG	O8-C23-C24	2.68	120.32	111.91
17	A	843	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	1	310	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
21	A	851	BCR	C7-C8-C9	-2.68	122.19	126.23
17	1	311	CLA	CHB-C4A-NA	2.68	128.22	124.51
17	A	821	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	B	821	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
17	A	829	CLA	CHB-C4A-NA	2.68	128.21	124.51
17	B	825	CLA	O2A-CGA-O1A	-2.68	116.84	123.59
17	B	818	CLA	C1-O2A-CGA	2.67	123.46	116.44
17	A	840	CLA	C5-C3-C2	2.67	126.53	121.12
17	B	825	CLA	CMD-C2D-C3D	2.67	129.68	124.68
17	B	841	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
19	4	316	LUT	C40-C33-C32	-2.67	113.87	118.08
17	1	311	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
18	4	307	CHL	C5-C3-C4	2.67	120.50	114.60
21	L	206	BCR	C11-C10-C9	-2.67	123.50	127.31
17	4	308	CLA	CMD-C2D-C3D	2.67	129.67	124.68
17	B	829	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
17	2	302	CLA	C4D-C3D-CAD	-2.67	106.98	108.47
25	F	310	HTG	C4-C3-C2	2.67	115.48	110.82
17	B	803	CLA	CMB-C2B-C1B	-2.67	124.37	128.46
17	4	313	CLA	CMB-C2B-C1B	-2.67	124.37	128.46
21	A	846	BCR	C15-C16-C17	-2.67	118.01	123.47
21	G	106	BCR	C16-C15-C14	-2.67	118.01	123.47
17	B	816	CLA	C1B-CHB-C4A	-2.67	124.84	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	818	CLA	OBD-CAD-CBD	-2.66	122.09	125.89
17	A	831	CLA	CMB-C2B-C3B	2.66	129.66	124.68
17	B	830	CLA	CMD-C2D-C3D	2.66	129.66	124.68
22	G	102	LHG	C11-C10-C9	-2.66	100.90	114.42
17	A	802	CLA	CMC-C2C-C3C	2.66	129.96	124.94
17	3	604	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
17	4	314	CLA	CMD-C2D-C3D	2.66	129.66	124.68
17	B	834	CLA	CMB-C2B-C3B	2.66	129.66	124.68
17	1	312	CLA	CMD-C2D-C3D	2.66	129.66	124.68
17	4	302	CLA	O2D-CGD-CBD	2.66	116.00	111.27
17	A	833	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	B	836	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	A	822	CLA	CHB-C4A-NA	2.66	128.19	124.51
17	1	306	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
17	2	319	CLA	CMC-C2C-C3C	2.66	129.95	124.94
22	F	302	LHG	O8-C23-C24	2.66	120.24	111.91
18	2	305	CHL	OMC-CMC-C2C	-2.65	119.69	125.69
17	G	104	CLA	C4D-C3D-CAD	-2.65	106.99	108.47
18	2	305	CHL	CMB-C2B-C3B	2.65	129.64	124.68
17	B	824	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
17	A	853	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
27	A	842	PQN	C2M-C2-C1	-2.65	111.87	116.27
17	2	301	CLA	OBD-CAD-CBD	-2.65	122.11	125.89
18	3	607	CHL	CMB-C2B-C3B	2.65	129.64	124.68
21	A	847	BCR	C27-C26-C25	2.65	126.58	122.73
17	A	815	CLA	CHB-C4A-NA	2.65	128.18	124.51
17	A	810	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
17	A	805	CLA	O2D-CGD-CBD	2.65	115.97	111.27
19	2	314	LUT	C20-C13-C12	-2.65	113.91	118.08
17	G	104	CLA	CMB-C2B-C3B	2.64	129.63	124.68
17	B	806	CLA	CHB-C4A-NA	2.64	128.17	124.51
17	A	827	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
17	B	840	CLA	CHB-C4A-NA	2.64	128.16	124.51
18	4	315	CHL	CHB-C4A-NA	2.64	128.16	124.51
17	B	820	CLA	CMC-C2C-C3C	2.64	129.92	124.94
17	1	312	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
22	G	102	LHG	O8-C23-C24	2.64	120.19	111.91
17	A	835	CLA	C1-C2-C3	-2.64	121.48	126.04
17	G	104	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	3	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
17	4	313	CLA	CHB-C4A-NA	2.64	128.16	124.51
17	B	830	CLA	O2A-CGA-O1A	-2.64	116.94	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	803	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
17	B	807	CLA	O1D-CGD-CBD	2.64	129.88	124.48
18	4	305	CHL	O2A-CGA-CBA	2.64	120.18	111.91
17	1	308	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
17	3	603	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
26	4	323	DGD	O2E-C2E-C3E	-2.63	104.26	110.35
17	B	810	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
17	1	301	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
17	A	801	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
19	3	614	LUT	C22-C23-C24	-2.63	108.75	111.74
17	2	319	CLA	CHB-C4A-NA	2.63	128.15	124.51
17	A	843	CLA	CMB-C2B-C3B	2.63	129.60	124.68
17	A	802	CLA	O2D-CGD-CBD	2.63	115.94	111.27
17	A	839	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
17	B	842	CLA	CMD-C2D-C3D	2.63	129.60	124.68
17	4	309	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
17	3	606	CLA	CHB-C4A-NA	2.62	128.14	124.51
17	G	104	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
21	L	206	BCR	C27-C26-C25	2.62	126.54	122.73
17	A	820	CLA	C4D-C3D-CAD	-2.62	107.01	108.47
17	2	310	CLA	CMD-C2D-C3D	2.62	129.58	124.68
17	A	819	CLA	CMB-C2B-C3B	2.62	129.58	124.68
17	B	832	CLA	CMB-C2B-C3B	2.62	129.58	124.68
17	A	831	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
17	A	819	CLA	CHB-C4A-NA	2.62	128.13	124.51
17	B	809	CLA	O2D-CGD-CBD	2.62	115.92	111.27
17	2	302	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
17	J	103	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
17	B	835	CLA	C4D-C3D-CAD	-2.61	107.01	108.47
17	A	801	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
17	A	806	CLA	O2A-CGA-O1A	-2.61	117.00	123.59
17	A	809	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	B	820	CLA	C1-C2-C3	-2.61	121.53	126.04
17	A	814	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
17	A	841	CLA	C4D-C3D-CAD	-2.61	107.02	108.47
17	A	806	CLA	CMD-C2D-C3D	2.61	129.56	124.68
17	A	803	CLA	CHB-C4A-NA	2.61	128.12	124.51
17	1	307	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
17	B	840	CLA	CMB-C2B-C3B	2.61	129.55	124.68
17	1	303	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
17	B	836	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
17	L	202	CLA	CMD-C2D-C3D	2.60	129.55	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
17	1	308	CLA	CHB-C4A-NA	2.60	128.10	124.51
17	1	304	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
17	B	809	CLA	OBD-CAD-CBD	-2.59	122.19	125.89
17	B	808	CLA	CMD-C2D-C3D	2.59	129.53	124.68
18	4	307	CHL	C2A-C1A-CHA	-2.59	119.32	123.86
18	3	607	CHL	CHB-C4A-NA	2.59	128.10	124.51
17	B	827	CLA	C4D-C3D-CAD	-2.59	107.02	108.47
17	B	803	CLA	CHB-C4A-NA	2.59	128.09	124.51
21	F	303	BCR	C37-C22-C21	-2.59	119.30	122.92
17	B	836	CLA	C2A-C1A-CHA	2.59	128.39	123.86
17	B	833	CLA	O2A-C1-C2	-2.59	101.83	108.64
17	B	812	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
17	A	832	CLA	CHB-C4A-NA	2.59	128.09	124.51
17	L	203	CLA	CHB-C4A-NA	2.59	128.09	124.51
18	2	305	CHL	C2A-C1A-CHA	-2.58	119.34	123.86
17	B	835	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
21	3	616	BCR	C24-C23-C22	-2.58	122.33	126.23
21	B	846	BCR	C24-C23-C22	-2.58	122.34	126.23
17	4	309	CLA	C4D-C3D-CAD	-2.58	107.03	108.47
25	J	102	HTG	O5-C5-C6	2.58	112.84	106.44
17	A	836	CLA	CHB-C4A-NA	2.58	128.07	124.51
18	3	601	CHL	CAC-C3C-C4C	2.57	128.15	124.81
21	A	848	BCR	C15-C14-C13	-2.57	123.64	127.31
17	B	820	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
18	2	305	CHL	O2A-CGA-CBA	2.57	119.97	111.91
17	4	313	CLA	O2D-CGD-CBD	2.57	115.83	111.27
17	B	802	CLA	CAA-C2A-C1A	-2.57	103.56	111.97
21	J	105	BCR	C38-C26-C25	-2.57	121.64	124.53
17	4	309	CLA	CHB-C4A-NA	2.56	128.06	124.51
17	K	201	CLA	CMD-C2D-C3D	2.56	129.47	124.68
27	A	842	PQN	C9-C10-C1	-2.56	116.34	120.10
21	A	850	BCR	C27-C26-C25	2.56	126.45	122.73
17	A	853	CLA	C5-C3-C2	2.56	126.30	121.12
17	B	835	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
17	2	309	CLA	CHB-C4A-NA	2.56	128.05	124.51
17	A	838	CLA	C1-O2A-CGA	-2.56	109.73	116.44
21	A	848	BCR	C33-C5-C6	-2.56	121.66	124.53
17	A	813	CLA	CMD-C2D-C3D	2.56	129.46	124.68
18	4	301	CHL	CBC-CAC-C3C	-2.55	105.39	112.43
17	B	802	CLA	C1-C2-C3	-2.55	121.63	126.04
18	2	306	CHL	C2A-C1A-CHA	-2.55	119.39	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	845	BCR	C7-C8-C9	-2.55	122.38	126.23
17	K	202	CLA	CHB-C4A-NA	2.55	128.04	124.51
21	L	201	BCR	C27-C26-C25	2.55	126.44	122.73
17	2	319	CLA	O2A-CGA-O1A	-2.55	115.14	123.14
18	4	305	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
17	2	312	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
17	A	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
17	A	814	CLA	CMD-C2D-C3D	2.55	129.45	124.68
17	B	811	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
17	A	807	CLA	CHB-C4A-NA	2.55	128.03	124.51
17	A	827	CLA	CHB-C4A-NA	2.55	128.03	124.51
17	B	816	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
17	B	823	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
17	J	101	CLA	CED-O2D-CGD	-2.55	110.17	115.94
17	2	301	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
17	1	302	CLA	CMC-C2C-C3C	2.55	129.74	124.94
17	B	830	CLA	CHB-C4A-NA	2.55	128.03	124.51
21	F	308	BCR	C33-C5-C6	-2.55	121.67	124.53
17	G	104	CLA	CMC-C2C-C3C	2.54	129.74	124.94
17	A	820	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
17	4	313	CLA	CMD-C2D-C3D	2.54	129.44	124.68
26	4	323	DGD	O2D-C2D-C3D	-2.54	104.47	110.35
21	B	846	BCR	C7-C8-C9	-2.54	122.39	126.23
21	A	847	BCR	C15-C16-C17	-2.54	118.27	123.47
17	A	832	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
21	L	206	BCR	C24-C23-C22	-2.54	122.39	126.23
18	2	305	CHL	CHB-C4A-NA	2.54	128.03	124.51
21	B	846	BCR	C15-C16-C17	-2.54	118.27	123.47
17	3	602	CLA	CMD-C2D-C3D	2.54	129.43	124.68
20	3	615	XAT	C37-C21-C36	2.54	111.11	107.37
17	3	606	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
17	B	820	CLA	O2A-C1-C2	2.53	115.30	108.64
17	A	820	CLA	OBD-CAD-CBD	-2.53	122.28	125.89
21	A	847	BCR	C33-C5-C6	-2.53	121.68	124.53
18	3	601	CHL	C1C-C2C-C3C	-2.53	105.10	107.11
18	2	304	CHL	C2A-C1A-CHA	-2.53	119.43	123.86
17	B	828	CLA	CHB-C4A-NA	2.53	128.01	124.51
17	B	833	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
17	3	606	CLA	CMD-C2D-C3D	2.53	129.41	124.68
17	A	821	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	1	305	CHL	C1C-C2C-C3C	-2.53	105.11	107.11
21	B	845	BCR	C33-C5-C6	-2.53	121.69	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	804	CLA	O2A-C1-C2	-2.53	101.99	108.64
25	F	310	HTG	O5-C1-C2	-2.53	107.13	110.31
21	B	848	BCR	C27-C26-C25	2.53	126.40	122.73
22	A	845	LHG	C11-C10-C9	-2.53	101.59	114.42
24	4	320	LMG	C4-C3-C2	2.53	115.24	110.82
18	4	306	CHL	C3B-C4B-NB	2.53	112.48	109.21
17	3	609	CLA	CMD-C2D-C3D	2.53	129.41	124.68
20	2	315	XAT	C37-C21-C36	2.53	111.10	107.37
17	B	834	CLA	CED-O2D-CGD	2.52	121.64	115.94
24	4	320	LMG	C7-O1-C1	2.52	118.67	113.74
21	A	846	BCR	C2-C1-C6	2.52	114.36	110.48
17	A	826	CLA	CMC-C2C-C3C	2.52	129.70	124.94
17	1	306	CLA	CHB-C4A-NA	2.52	128.00	124.51
17	A	825	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
21	L	206	BCR	C15-C14-C13	-2.52	123.71	127.31
17	A	833	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
17	2	302	CLA	CMC-C2C-C3C	2.52	129.69	124.94
17	1	309	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
19	2	314	LUT	C21-C26-C27	-2.52	109.52	112.70
17	B	827	CLA	CAA-C2A-C1A	-2.52	103.73	111.97
17	A	853	CLA	CHA-C1A-NA	-2.52	120.64	126.40
17	A	840	CLA	CGD-CBD-CAD	-2.52	102.58	110.73
17	A	838	CLA	OBD-CAD-CBD	-2.52	122.30	125.89
17	3	603	CLA	CMD-C2D-C3D	2.51	129.38	124.68
17	B	817	CLA	CHB-C4A-NA	2.51	127.99	124.51
20	1	315	XAT	C37-C21-C36	2.51	111.08	107.37
22	A	844	LHG	C20-C19-C18	-2.51	101.67	114.42
17	2	310	CLA	CMB-C2B-C3B	2.51	129.38	124.68
17	B	820	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	3	607	CHL	CED-O2D-CGD	2.51	121.62	115.94
17	L	202	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	L	206	BCR	C7-C8-C9	-2.51	122.44	126.23
17	2	307	CLA	CHB-C4A-NA	2.51	127.98	124.51
17	A	832	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
17	2	308	CLA	CHB-C4A-NA	2.51	127.98	124.51
18	4	307	CHL	C3B-C4B-NB	2.51	112.45	109.21
17	B	822	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
17	B	819	CLA	CMB-C2B-C3B	2.50	129.36	124.68
17	A	802	CLA	C1-C2-C3	-2.50	121.71	126.04
17	A	813	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
17	B	805	CLA	CMD-C2D-C3D	2.50	129.36	124.68
17	A	831	CLA	CHB-C4A-NA	2.50	127.97	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	830	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
26	B	850	DGD	O2D-C2D-C1D	-2.50	103.97	110.05
17	B	841	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
17	F	306	CLA	CMC-C2C-C3C	2.50	129.65	124.94
17	3	606	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
17	3	613	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
17	A	841	CLA	CMD-C2D-C3D	2.50	129.35	124.68
17	3	610	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
21	B	846	BCR	C2-C1-C6	2.49	114.32	110.48
21	2	316	BCR	C7-C8-C9	-2.49	122.47	126.23
21	L	201	BCR	C33-C5-C6	-2.49	121.73	124.53
17	1	311	CLA	CMB-C2B-C3B	2.49	129.34	124.68
17	B	839	CLA	CMD-C2D-C3D	2.49	129.34	124.68
17	F	307	CLA	CHB-C4A-NA	2.49	127.96	124.51
21	F	303	BCR	C27-C26-C25	2.49	126.35	122.73
17	1	309	CLA	CHB-C4A-NA	2.49	127.96	124.51
18	4	306	CHL	CMB-C2B-C3B	2.49	129.34	124.68
17	B	842	CLA	O2A-C1-C2	-2.49	102.09	108.64
17	B	842	CLA	C4-C3-C5	2.49	119.46	115.27
17	A	817	CLA	O1D-CGD-CBD	2.49	129.58	124.48
17	4	314	CLA	CMB-C2B-C3B	2.49	129.33	124.68
21	F	308	BCR	C11-C10-C9	-2.49	123.76	127.31
17	B	830	CLA	CMB-C2B-C3B	2.49	129.33	124.68
17	B	831	CLA	C3A-C2A-C1A	2.49	105.06	101.34
17	A	843	CLA	CMD-C2D-C3D	2.49	129.33	124.68
17	B	827	CLA	CMC-C2C-C3C	2.48	129.63	124.94
17	B	802	CLA	CMC-C2C-C3C	2.48	129.62	124.94
22	2	317	LHG	O8-C23-C24	2.48	119.69	111.91
17	4	308	CLA	CHB-C4A-NA	2.48	127.94	124.51
17	3	605	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
21	A	848	BCR	C11-C10-C9	-2.48	123.77	127.31
17	L	204	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
17	A	825	CLA	O2D-CGD-CBD	2.47	115.67	111.27
17	A	837	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
21	4	318	BCR	C7-C8-C9	-2.47	122.50	126.23
17	G	103	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
17	A	821	CLA	C4D-C3D-CAD	-2.47	107.09	108.47
17	A	828	CLA	CHB-C4A-NA	2.47	127.93	124.51
18	2	305	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
18	2	306	CHL	C1C-C2C-C3C	-2.47	105.16	107.11
17	A	830	CLA	CHB-C4A-NA	2.47	127.92	124.51
17	B	806	CLA	C3A-C2A-C1A	2.46	105.03	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	1	312	CLA	OBD-CAD-CBD	-2.46	122.37	125.89
21	F	308	BCR	C27-C26-C25	2.46	126.31	122.73
21	A	850	BCR	C15-C14-C13	-2.46	123.80	127.31
17	K	201	CLA	CHB-C4A-NA	2.46	127.92	124.51
17	A	853	CLA	O1D-CGD-CBD	2.46	129.52	124.48
17	4	302	CLA	C4-C3-C5	2.46	119.41	115.27
17	1	309	CLA	CMD-C2D-C3D	2.46	129.28	124.68
17	A	824	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
17	2	303	CLA	C1-C2-C3	-2.46	121.79	126.04
18	4	307	CHL	O2A-CGA-O1A	-2.46	117.39	123.59
17	1	310	CLA	CHB-C4A-NA	2.46	127.91	124.51
17	2	319	CLA	CMB-C2B-C3B	2.46	129.27	124.68
17	A	840	CLA	C4D-C3D-CAD	-2.45	107.10	108.47
17	A	841	CLA	OBD-CAD-CBD	-2.45	122.39	125.89
17	B	817	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
17	4	310	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
21	A	851	BCR	C2-C1-C6	2.45	114.26	110.48
17	A	843	CLA	CHB-C4A-NA	2.45	127.90	124.51
18	2	313	CHL	CHB-C4A-NA	2.45	127.90	124.51
21	K	203	BCR	C27-C26-C25	2.45	126.29	122.73
17	4	314	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
17	A	803	CLA	CMB-C2B-C3B	2.45	129.26	124.68
17	A	816	CLA	O2D-CGD-CBD	2.45	115.62	111.27
17	B	840	CLA	OBD-CAD-CBD	-2.45	122.40	125.89
19	2	314	LUT	C22-C23-C24	-2.45	108.96	111.74
17	1	302	CLA	C4D-C3D-CAD	-2.44	107.11	108.47
21	F	308	BCR	C16-C15-C14	-2.44	118.47	123.47
17	B	803	CLA	CMD-C2D-C3D	2.44	129.25	124.68
17	B	802	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
18	2	306	CHL	CHB-C4A-NA	2.44	127.89	124.51
17	B	833	CLA	CBC-CAC-C3C	-2.44	106.05	112.27
17	2	311	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
17	A	809	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
17	B	806	CLA	CMD-C2D-C3D	2.44	129.24	124.68
22	2	317	LHG	C11-C10-C9	-2.44	102.05	114.42
17	4	311	CLA	CMB-C2B-C3B	2.44	129.24	124.68
17	B	822	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
17	3	612	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	3	616	BCR	C15-C14-C13	-2.44	123.83	127.31
17	A	805	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
18	3	601	CHL	CHB-C4A-NA	2.44	127.88	124.51
21	F	303	BCR	C38-C26-C27	-2.43	108.94	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	F	306	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
17	B	814	CLA	CMD-C2D-C3D	2.43	129.23	124.68
26	4	323	DGD	C3G-O3G-C1D	2.43	118.49	113.74
21	A	848	BCR	C8-C7-C6	-2.43	120.38	127.20
17	2	311	CLA	C4D-C3D-CAD	-2.43	107.12	108.47
17	B	831	CLA	CGD-CBD-CAD	2.43	118.60	110.73
17	B	804	CLA	CMD-C2D-C3D	2.43	129.22	124.68
17	B	834	CLA	OBD-CAD-CBD	-2.43	122.43	125.89
26	4	323	DGD	O4D-C4D-C5D	-2.42	103.28	109.30
17	1	301	CLA	CMB-C2B-C3B	2.42	129.21	124.68
18	4	306	CHL	C1-O2A-CGA	2.42	122.79	116.44
17	B	818	CLA	C4A-NA-C1A	2.42	107.79	106.71
17	3	613	CLA	CHB-C4A-NA	2.42	127.85	124.51
17	3	609	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
17	A	840	CLA	CHB-C4A-NA	2.41	127.85	124.51
17	A	808	CLA	C4D-C3D-CAD	-2.41	107.12	108.47
17	A	853	CLA	C6-C5-C3	-2.41	107.13	113.45
17	A	813	CLA	CMB-C2B-C3B	2.41	129.19	124.68
17	B	840	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
17	B	821	CLA	CMC-C2C-C3C	2.41	129.49	124.94
17	2	302	CLA	CMD-C2D-C3D	2.41	129.19	124.68
26	4	323	DGD	O3G-C3G-C2G	2.41	116.71	110.90
17	A	811	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	J	103	CLA	C4D-C3D-CAD	-2.41	107.13	108.47
17	A	823	CLA	CHB-C4A-NA	2.41	127.84	124.51
17	A	809	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
19	3	614	LUT	C18-C5-C4	-2.41	109.90	114.36
17	A	811	CLA	C1B-CHB-C4A	-2.40	125.35	130.12
17	4	314	CLA	CHB-C4A-NA	2.40	127.84	124.51
17	1	301	CLA	OBD-CAD-CBD	-2.40	122.46	125.89
17	B	805	CLA	O1D-CGD-CBD	2.40	129.40	124.48
17	3	610	CLA	CMD-C2D-C3D	2.40	129.17	124.68
21	A	850	BCR	C15-C16-C17	-2.40	118.55	123.47
17	4	313	CLA	OBD-CAD-CBD	-2.40	122.46	125.89
18	3	607	CHL	C2A-C1A-CHA	-2.40	119.66	123.86
17	B	811	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
17	3	612	CLA	CMD-C2D-C3D	2.40	129.17	124.68
17	A	801	CLA	CHB-C4A-NA	2.40	127.83	124.51
17	A	837	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	4	317	XAT	O23-C23-C22	-2.40	105.04	109.80
21	I	101	BCR	C33-C5-C6	-2.40	121.84	124.53
17	B	827	CLA	O2A-CGA-O1A	-2.40	117.55	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	203	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
17	B	840	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
17	A	817	CLA	CMD-C2D-C3D	2.39	129.16	124.68
17	A	816	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
17	B	814	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
17	1	303	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	4	317	XAT	C20-C13-C12	-2.39	114.31	118.08
17	2	309	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
25	J	102	HTG	O4-C4-C3	-2.39	104.82	110.35
17	B	805	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
17	4	309	CLA	CMD-C2D-C3D	2.39	129.15	124.68
17	3	602	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
17	B	820	CLA	CAA-CBA-CGA	-2.39	106.27	113.25
17	A	834	CLA	CMD-C2D-C3D	2.39	129.15	124.68
17	A	835	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
17	B	842	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
21	B	848	BCR	C38-C26-C25	-2.39	121.85	124.53
17	G	105	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
17	B	806	CLA	CED-O2D-CGD	2.39	121.34	115.94
21	B	844	BCR	C27-C26-C25	2.39	126.20	122.73
17	1	312	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
18	4	307	CHL	C4A-NA-C1A	-2.38	105.63	106.71
17	A	829	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
17	3	603	CLA	C1-C2-C3	-2.38	122.90	126.75
17	3	612	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
17	4	314	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
21	A	847	BCR	C15-C14-C13	-2.38	123.92	127.31
17	B	819	CLA	CMC-C2C-C3C	2.38	129.42	124.94
17	2	303	CLA	CMD-C2D-C3D	2.38	129.12	124.68
17	A	806	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
21	A	849	BCR	C27-C26-C25	2.37	126.18	122.73
26	4	323	DGD	O6D-C1D-C2D	-2.37	105.33	110.35
23	A	855	LMT	C1'-O5'-C5'	-2.37	109.03	113.69
17	B	823	CLA	OBD-CAD-CBD	-2.37	122.50	125.89
21	A	849	BCR	C16-C15-C14	-2.37	118.61	123.47
21	F	303	BCR	C29-C30-C25	2.37	114.13	110.48
17	L	203	CLA	CMD-C2D-C3D	2.37	129.12	124.68
17	2	307	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
17	L	204	CLA	CMD-C2D-C3D	2.37	129.10	124.68
21	J	105	BCR	C7-C8-C9	-2.36	122.66	126.23
17	1	307	CLA	CMC-C2C-C3C	2.36	129.40	124.94
17	1	306	CLA	OBD-CAD-CBD	-2.36	122.52	125.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	808	CLA	C1-O2A-CGA	-2.36	110.25	116.44
17	1	302	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
17	B	804	CLA	C1-O2A-CGA	2.36	122.63	116.44
17	B	836	CLA	CAA-CBA-CGA	-2.36	108.52	113.59
17	1	309	CLA	OBD-CAD-CBD	-2.36	122.53	125.89
17	2	311	CLA	CHB-C4A-NA	2.35	127.77	124.51
17	B	819	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	B	802	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
17	1	310	CLA	CMB-C2B-C3B	2.35	129.08	124.68
17	B	812	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	A	838	CLA	CMA-C3A-C4A	-2.35	105.46	111.77
17	B	810	CLA	CHB-C4A-NA	2.35	127.76	124.51
17	B	808	CLA	O1D-CGD-CBD	2.35	129.29	124.48
21	B	848	BCR	C29-C30-C25	2.35	114.09	110.48
17	A	841	CLA	O2D-CGD-CBD	2.35	115.44	111.27
21	B	848	BCR	C2-C1-C6	2.35	114.09	110.48
21	K	203	BCR	C24-C23-C22	-2.35	122.69	126.23
17	A	817	CLA	CMB-C2B-C3B	2.35	129.07	124.68
17	B	838	CLA	CMC-C2C-C3C	2.35	129.36	124.94
17	A	818	CLA	CHB-C4A-NA	2.34	127.75	124.51
17	B	812	CLA	CMB-C2B-C3B	2.34	129.06	124.68
21	A	849	BCR	C33-C5-C6	-2.34	121.90	124.53
17	B	830	CLA	C5-C3-C2	2.34	125.86	121.12
17	B	815	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
17	A	821	CLA	O2D-CGD-CBD	2.34	115.43	111.27
17	3	605	CLA	CMB-C2B-C3B	2.34	129.06	124.68
18	2	313	CHL	C1C-C2C-C3C	-2.34	105.26	107.11
17	A	812	CLA	OBD-CAD-C3D	2.34	131.86	127.98
21	F	303	BCR	C15-C14-C13	-2.34	123.97	127.31
17	A	828	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
17	B	837	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
21	F	308	BCR	C35-C13-C14	-2.34	119.65	122.92
17	3	603	CLA	CHB-C4A-NA	2.34	127.74	124.51
17	A	841	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
24	F	309	LMG	O8-C28-O10	-2.34	117.70	123.59
17	4	314	CLA	OBD-CAD-C3D	2.33	131.86	127.98
17	B	819	CLA	C1-C2-C3	-2.33	122.01	126.04
17	A	838	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
17	3	604	CLA	CMD-C2D-C3D	2.33	129.04	124.68
17	F	307	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
21	L	205	BCR	C29-C30-C25	2.33	114.07	110.48
21	L	205	BCR	C28-C27-C26	-2.33	109.91	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	804	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
17	L	204	CLA	O2D-CGD-CBD	2.33	115.41	111.27
18	3	601	CHL	O1D-CGD-CBD	-2.33	119.71	124.48
19	4	316	LUT	C19-C9-C8	-2.33	114.40	118.08
17	L	202	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
26	4	323	DGD	C3E-C4E-C5E	2.33	114.40	110.24
21	A	851	BCR	C28-C27-C26	-2.33	109.92	114.08
17	A	837	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
17	2	307	CLA	CMD-C2D-C3D	2.33	129.04	124.68
17	A	830	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	1	304	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	A	822	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	A	810	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
17	B	803	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
17	G	105	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
17	G	103	CLA	CHB-C4A-NA	2.33	127.73	124.51
17	2	312	CLA	CHB-C4A-NA	2.32	127.73	124.51
21	B	845	BCR	C27-C26-C25	2.32	126.10	122.73
17	B	832	CLA	O1D-CGD-CBD	2.32	129.24	124.48
21	3	616	BCR	C3-C4-C5	-2.32	109.93	114.08
17	A	831	CLA	CMD-C2D-C3D	2.32	129.02	124.68
17	1	312	CLA	O2D-CGD-CBD	2.32	115.39	111.27
18	2	313	CHL	CED-O2D-CGD	2.32	121.18	115.94
17	A	816	CLA	CMD-C2D-C3D	2.32	129.01	124.68
17	2	302	CLA	OBD-CAD-CBD	-2.32	122.58	125.89
17	A	804	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
17	A	840	CLA	CMD-C2D-C3D	2.32	129.01	124.68
21	B	845	BCR	C15-C16-C17	-2.32	118.73	123.47
17	A	820	CLA	O2A-CGA-O1A	-2.32	117.75	123.59
18	2	304	CHL	OMC-CMC-C2C	-2.31	120.45	125.69
17	3	605	CLA	CHB-C4A-NA	2.31	127.71	124.51
17	B	815	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
17	3	609	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
17	F	307	CLA	O1D-CGD-CBD	2.31	129.21	124.48
17	B	841	CLA	CAA-CBA-CGA	-2.31	106.50	113.25
17	B	842	CLA	C16-C15-C13	-2.31	108.45	115.92
17	A	815	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
17	1	313	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
17	4	309	CLA	OBD-CAD-CBD	-2.31	122.60	125.89
17	1	313	CLA	C4D-C3D-CAD	-2.31	107.18	108.47
17	4	309	CLA	O2D-CGD-CBD	2.31	115.36	111.27
17	1	303	CLA	C1B-CHB-C4A	-2.30	125.55	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	829	CLA	CMD-C2D-C3D	2.30	128.99	124.68
21	J	105	BCR	C27-C26-C25	2.30	126.08	122.73
17	4	304	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
17	B	802	CLA	CMD-C2D-C3D	2.30	128.99	124.68
26	4	323	DGD	O3E-C3E-C2E	-2.30	105.02	110.35
17	2	303	CLA	CHB-C4A-NA	2.30	127.70	124.51
17	A	813	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
17	B	838	CLA	C4D-C3D-CAD	-2.30	107.19	108.47
21	G	106	BCR	C27-C26-C25	2.30	126.07	122.73
17	A	808	CLA	C3A-C2A-C1A	2.30	104.79	101.34
17	B	833	CLA	CHA-C1A-NA	-2.30	121.13	126.40
17	1	311	CLA	O1D-CGD-CBD	2.30	129.19	124.48
25	F	310	HTG	O5-C5-C4	2.30	113.87	109.69
17	B	827	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
17	A	809	CLA	OBD-CAD-CBD	-2.30	122.61	125.89
17	A	819	CLA	CMC-C2C-C3C	2.30	129.28	124.94
17	B	824	CLA	CMC-C2C-C3C	2.30	129.28	124.94
17	3	613	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	A	836	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
17	B	827	CLA	CMD-C2D-C3D	2.30	128.97	124.68
17	B	839	CLA	CMC-C2C-C3C	2.30	129.27	124.94
17	4	314	CLA	O1D-CGD-CBD	2.30	129.18	124.48
17	A	825	CLA	CAA-C2A-C1A	-2.29	104.46	111.97
17	3	604	CLA	CHB-C4A-NA	2.29	127.68	124.51
21	A	848	BCR	C27-C26-C25	2.29	126.06	122.73
17	2	319	CLA	CMD-C2D-C3D	2.29	128.97	124.68
21	B	847	BCR	C37-C22-C21	-2.29	119.71	122.92
20	4	317	XAT	C16-C1-C2	-2.29	105.00	108.98
17	2	319	CLA	O2D-CGD-CBD	2.29	115.34	111.27
17	B	810	CLA	C1-O2A-CGA	-2.29	110.44	116.44
17	1	310	CLA	CMD-C2D-C3D	2.29	128.96	124.68
22	1	317	LHG	O8-C23-O10	-2.29	117.82	123.59
23	2	318	LMT	O5B-C5B-C6B	2.29	112.12	106.44
17	1	308	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
17	A	840	CLA	C7-C6-C5	-2.29	107.15	113.36
17	B	822	CLA	CED-O2D-CGD	2.29	121.11	115.94
22	F	302	LHG	C20-C19-C18	-2.29	102.82	114.42
17	1	307	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
27	A	842	PQN	C17-C16-C15	-2.28	107.15	113.36
22	G	102	LHG	C20-C19-C18	-2.28	102.83	114.42
21	L	205	BCR	C2-C1-C6	2.28	114.00	110.48
27	B	843	PQN	C10-C1-C2	-2.28	115.70	118.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	811	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
17	B	807	CLA	C3A-C2A-C1A	2.28	104.75	101.34
24	F	309	LMG	C40-C39-C38	-2.28	102.85	114.42
17	A	834	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
17	A	843	CLA	CBC-CAC-C3C	2.28	118.07	112.27
19	4	316	LUT	C2-C3-C4	-2.28	107.19	110.30
22	A	844	LHG	O8-C23-O10	-2.28	117.84	123.59
17	2	319	CLA	OBD-CAD-CBD	-2.28	122.64	125.89
18	2	313	CHL	CMB-C2B-C3B	2.28	128.94	124.68
17	B	836	CLA	OBD-CAD-CBD	-2.28	122.64	125.89
21	1	316	BCR	C33-C5-C6	-2.28	121.97	124.53
17	A	824	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
21	A	846	BCR	C27-C26-C25	2.27	126.03	122.73
17	B	816	CLA	OBD-CAD-CBD	-2.27	122.65	125.89
17	A	814	CLA	C1-C2-C3	-2.27	123.08	126.75
17	A	824	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
17	A	816	CLA	CHB-C4A-NA	2.27	127.65	124.51
17	K	201	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
17	L	204	CLA	CMB-C2B-C3B	2.27	128.92	124.68
17	B	818	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
17	B	820	CLA	OBD-CAD-C3D	2.27	131.75	127.98
26	B	850	DGD	CFB-CEB-CDB	-2.27	102.91	114.42
22	F	302	LHG	C11-C10-C9	-2.27	102.91	114.42
21	B	846	BCR	C33-C5-C6	-2.27	121.98	124.53
17	B	833	CLA	CAA-C2A-C3A	-2.27	106.57	112.78
26	B	850	DGD	CBB-CAB-C9B	-2.27	102.92	114.42
17	A	812	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	3	613	CLA	CMC-C2C-C3C	2.26	129.21	124.94
21	L	206	BCR	C15-C16-C17	-2.26	118.84	123.47
17	1	307	CLA	CMB-C2B-C3B	2.26	128.91	124.68
21	B	847	BCR	C21-C20-C19	-2.26	116.17	123.22
21	B	844	BCR	C24-C23-C22	-2.26	122.82	126.23
17	A	832	CLA	CMD-C2D-C3D	2.26	128.91	124.68
17	A	805	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	A	810	CLA	CHB-C4A-NA	2.26	127.64	124.51
17	A	817	CLA	C4D-C3D-CAD	-2.26	107.21	108.47
26	4	323	DGD	C1D-C2D-C3D	-2.26	105.29	110.00
17	A	812	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
21	B	847	BCR	C30-C25-C26	-2.26	119.44	122.61
17	B	816	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
17	B	815	CLA	CMB-C2B-C3B	2.26	128.90	124.68
18	4	306	CHL	C1-C2-C3	-2.26	123.10	126.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	314	LUT	C3-C4-C5	-2.25	107.36	111.85
17	B	803	CLA	O2D-CGD-CBD	2.25	115.27	111.27
17	B	825	CLA	C1-C2-C3	-2.25	122.14	126.04
17	B	810	CLA	CHA-C1A-NA	-2.25	121.24	126.40
17	A	834	CLA	CHB-C4A-NA	2.25	127.63	124.51
17	B	836	CLA	C3A-C2A-C1A	2.25	104.71	101.34
17	A	826	CLA	CHB-C4A-NA	2.25	127.63	124.51
17	B	820	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
17	B	832	CLA	CMC-C2C-C3C	2.25	129.18	124.94
17	B	828	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
24	F	309	LMG	O3-C3-C2	-2.25	105.15	110.35
17	B	822	CLA	CMD-C2D-C3D	2.25	128.88	124.68
17	F	304	CLA	CMC-C2C-C3C	2.25	129.18	124.94
17	2	303	CLA	OBD-CAD-CBD	-2.25	122.69	125.89
17	B	837	CLA	CED-O2D-CGD	-2.24	110.86	115.94
17	A	839	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
21	B	846	BCR	C27-C26-C25	2.24	125.99	122.73
17	A	805	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
17	B	819	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
21	A	848	BCR	C24-C23-C22	-2.24	122.85	126.23
17	L	204	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	1	317	LHG	C18-C17-C16	-2.24	103.04	114.42
17	B	829	CLA	OBD-CAD-CBD	-2.24	122.69	125.89
17	A	804	CLA	CMD-C2D-C3D	2.24	128.87	124.68
24	B	852	LMG	C40-C39-C38	-2.24	103.05	114.42
17	3	609	CLA	CHB-C4A-NA	2.24	127.61	124.51
17	B	815	CLA	O2D-CGD-CBD	2.24	115.25	111.27
24	4	319	LMG	O7-C10-C11	2.24	116.32	111.50
21	A	849	BCR	C15-C14-C13	-2.24	124.12	127.31
17	3	606	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
21	G	106	BCR	C33-C5-C6	-2.24	122.02	124.53
17	G	103	CLA	CMD-C2D-C3D	2.24	128.86	124.68
24	4	319	LMG	C38-C37-C36	-2.24	103.07	114.42
17	A	826	CLA	CMD-C2D-C3D	2.24	128.86	124.68
17	1	311	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
17	A	839	CLA	C3B-C4B-NB	-2.23	106.32	109.21
17	B	822	CLA	C1-C2-C3	-2.23	123.14	126.75
17	G	103	CLA	CAA-C2A-C3A	-2.23	110.89	116.10
17	A	833	CLA	CMD-C2D-C3D	2.23	128.85	124.68
21	B	849	BCR	C16-C15-C14	-2.23	118.91	123.47
17	2	312	CLA	CMC-C2C-C3C	2.23	129.14	124.94
17	B	834	CLA	CAA-C2A-C1A	-2.23	104.67	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	605	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
17	A	828	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
17	F	306	CLA	CHB-C4A-NA	2.23	127.59	124.51
21	B	846	BCR	C35-C13-C14	-2.23	119.80	122.92
17	3	603	CLA	C4D-C3D-CAD	-2.23	107.23	108.47
17	3	611	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
17	A	831	CLA	CAA-CBA-CGA	-2.22	106.75	113.25
17	3	602	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
21	I	101	BCR	C16-C15-C14	-2.22	118.92	123.47
17	A	837	CLA	OBD-CAD-CBD	-2.22	122.72	125.89
17	3	611	CLA	CMD-C2D-C3D	2.22	128.83	124.68
17	B	813	CLA	CAB-C3B-C2B	2.22	129.03	124.69
17	B	831	CLA	O1A-CGA-CBA	2.22	132.38	123.73
17	A	853	CLA	C2A-C1A-CHA	2.21	127.73	123.86
17	B	821	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
17	4	314	CLA	O2D-CGD-CBD	2.21	115.20	111.27
17	A	804	CLA	C1-C2-C3	-2.21	122.22	126.04
17	F	306	CLA	CMB-C2B-C3B	2.21	128.82	124.68
21	1	316	BCR	C29-C30-C25	2.21	113.89	110.48
21	B	845	BCR	C2-C1-C6	2.21	113.89	110.48
17	B	836	CLA	CHA-C1A-NA	-2.21	121.34	126.40
17	3	605	CLA	CMD-C2D-C3D	2.21	128.81	124.68
17	A	824	CLA	CHB-C4A-NA	2.21	127.57	124.51
17	B	834	CLA	C4D-C3D-CAD	-2.21	107.24	108.47
17	3	608	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	4	319	LMG	O6-C1-O1	-2.21	104.74	109.97
17	2	302	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
17	B	839	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
21	F	303	BCR	C2-C1-C6	2.21	113.88	110.48
17	2	310	CLA	CHB-C4A-NA	2.21	127.56	124.51
17	F	304	CLA	O2A-CGA-CBA	2.21	118.83	111.91
17	1	301	CLA	C6-C5-C3	-2.21	107.67	113.45
17	4	310	CLA	O1D-CGD-CBD	2.20	129.00	124.48
17	B	834	CLA	CMA-C3A-C4A	-2.20	105.85	111.77
17	F	307	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
17	3	609	CLA	C1-C2-C3	-2.20	123.19	126.75
17	1	301	CLA	CED-O2D-CGD	2.20	120.92	115.94
17	A	838	CLA	CHB-C4A-NA	2.20	127.56	124.51
21	1	316	BCR	C28-C27-C26	-2.20	110.14	114.08
17	A	815	CLA	CMD-C2D-C3D	2.20	128.79	124.68
21	A	849	BCR	C8-C7-C6	-2.20	121.02	127.20
17	A	827	CLA	CBC-CAC-C3C	2.20	117.87	112.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	811	CLA	CBA-CAA-C2A	-2.20	107.37	113.86
18	1	305	CHL	C4A-NA-C1A	2.20	107.69	106.71
17	A	805	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
17	A	818	CLA	C1-C2-C3	-2.20	122.24	126.04
17	B	813	CLA	C1-O2A-CGA	2.20	122.21	116.44
17	G	105	CLA	O2D-CGD-CBD	2.20	115.17	111.27
17	B	802	CLA	C11-C10-C8	-2.20	108.82	115.92
17	1	309	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
25	B	851	HTG	C1-O5-C5	2.20	116.63	112.58
17	B	810	CLA	CMC-C2C-C3C	2.20	129.08	124.94
17	B	815	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
17	G	104	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
17	B	833	CLA	O2D-CGD-CBD	2.19	115.17	111.27
18	2	306	CHL	C5-C3-C4	2.19	119.45	114.60
17	B	825	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
18	4	301	CHL	CMA-C3A-C4A	-2.19	105.88	111.77
17	1	307	CLA	OBD-CAD-CBD	-2.19	122.76	125.89
17	B	818	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
17	A	811	CLA	OBD-CAD-CBD	-2.19	122.77	125.89
17	B	839	CLA	O1D-CGD-CBD	2.19	128.96	124.48
17	B	839	CLA	CHA-C1A-NA	-2.19	121.39	126.40
17	3	610	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
17	B	804	CLA	CHB-C4A-NA	2.19	127.54	124.51
17	4	313	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	1	314	LUT	C22-C23-C24	-2.19	109.25	111.74
17	B	821	CLA	O2D-CGD-CBD	2.18	115.15	111.27
17	J	101	CLA	CBC-CAC-C3C	-2.18	106.70	112.27
17	1	303	CLA	CMD-C2D-C3D	2.18	128.76	124.68
17	1	310	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
21	B	847	BCR	C40-C30-C25	2.18	113.83	110.30
17	G	105	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
21	A	849	BCR	C24-C23-C22	-2.18	122.94	126.23
17	A	831	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
17	B	835	CLA	CHB-C4A-NA	2.18	127.52	124.51
17	K	202	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
17	3	606	CLA	CMC-C2C-C3C	2.18	129.05	124.94
17	1	310	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
17	B	837	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
17	A	815	CLA	CAA-CBA-CGA	-2.18	108.91	113.59
17	B	815	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
17	2	301	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
17	3	610	CLA	CMC-C2C-C3C	2.18	129.04	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	839	CLA	CMD-C2D-C3D	2.18	128.75	124.68
17	A	836	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
17	F	307	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
17	A	816	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
17	1	313	CLA	CHB-C4A-NA	2.17	127.52	124.51
19	1	314	LUT	C18-C5-C4	-2.17	110.33	114.36
17	1	302	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	A	814	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	3	608	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
17	A	808	CLA	O2D-CGD-CBD	2.17	115.12	111.27
17	1	306	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
17	B	812	CLA	CMC-C2C-C3C	2.17	129.03	124.94
17	L	202	CLA	CMC-C2C-C3C	2.17	129.03	124.94
17	A	820	CLA	CHB-C4A-NA	2.17	127.51	124.51
17	J	101	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
24	4	320	LMG	O2-C2-C3	-2.17	105.34	110.35
22	2	317	LHG	C27-C26-C25	-2.17	103.42	114.42
17	3	605	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
27	B	843	PQN	C5-C4-C3	-2.17	114.45	118.42
17	4	309	CLA	CMC-C2C-C3C	2.17	129.03	124.94
17	4	313	CLA	CMB-C2B-C3B	2.17	128.73	124.68
17	4	304	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
17	B	812	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
17	A	813	CLA	OBD-CAD-CBD	-2.16	122.81	125.89
17	B	841	CLA	CHB-C4A-NA	2.16	127.50	124.51
17	A	812	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
17	2	303	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
17	2	311	CLA	CMD-C2D-C3D	2.16	128.72	124.68
21	A	847	BCR	C38-C26-C25	-2.16	122.10	124.53
26	4	323	DGD	C4E-C3E-C2E	2.16	114.59	110.82
17	2	312	CLA	O2D-CGD-CBD	2.16	115.10	111.27
22	G	102	LHG	C18-C17-C16	-2.16	103.48	114.42
17	A	814	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
17	4	311	CLA	CHB-C4A-NA	2.16	127.49	124.51
17	4	312	CLA	CHB-C4A-NA	2.15	127.49	124.51
18	2	304	CHL	CHB-C4A-NA	2.15	127.49	124.51
24	F	309	LMG	C38-C37-C36	-2.15	103.49	114.42
21	B	847	BCR	C2-C1-C6	2.15	113.80	110.48
25	F	305	HTG	C6-C5-C4	-2.15	107.96	113.00
17	B	829	CLA	CAA-C2A-C1A	2.15	119.03	111.97
17	A	812	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
17	3	608	CLA	CMC-C2C-C3C	2.15	129.00	124.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	2	304	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
24	G	101	LMG	O3-C3-C2	-2.15	105.38	110.35
17	B	812	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
25	B	851	HTG	O5-C5-C6	2.15	111.78	106.44
17	A	835	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
17	B	840	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
17	B	837	CLA	OBD-CAD-CBD	-2.15	122.83	125.89
17	A	822	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
17	4	303	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
26	B	850	DGD	O2G-C1B-O1B	-2.15	118.51	123.70
17	3	604	CLA	CMC-C2C-C3C	2.15	128.99	124.94
17	A	831	CLA	C4D-C3D-CAD	-2.14	107.27	108.47
22	F	302	LHG	C27-C26-C25	-2.14	103.54	114.42
21	A	846	BCR	C37-C22-C21	-2.14	119.92	122.92
17	1	313	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
21	4	318	BCR	C16-C15-C14	-2.14	119.09	123.47
17	1	307	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
17	2	303	CLA	CMC-C2C-C3C	2.14	128.98	124.94
21	F	303	BCR	C16-C15-C14	-2.14	119.09	123.47
21	K	203	BCR	C15-C16-C17	-2.14	119.09	123.47
17	B	812	CLA	CMD-C2D-C3D	2.14	128.68	124.68
18	4	301	CHL	C4-C3-C5	2.14	118.87	115.27
18	4	306	CHL	CED-O2D-CGD	2.14	120.78	115.94
17	A	805	CLA	O2A-CGA-CBA	2.14	118.62	111.91
24	G	101	LMG	O6-C1-O1	-2.14	104.91	109.97
21	2	316	BCR	C38-C26-C25	-2.14	122.13	124.53
17	2	302	CLA	CHB-C4A-NA	2.14	127.47	124.51
17	3	602	CLA	CHB-C4A-NA	2.13	127.46	124.51
17	A	833	CLA	C1-C2-C3	-2.13	123.30	126.75
17	3	602	CLA	OBD-CAD-CBD	-2.13	122.85	125.89
21	4	318	BCR	C40-C30-C25	2.13	113.76	110.30
17	4	304	CLA	C2A-C1A-CHA	2.13	127.59	123.86
17	1	303	CLA	CMC-C2C-C3C	2.13	128.96	124.94
21	1	316	BCR	C15-C14-C13	-2.13	124.27	127.31
18	4	307	CHL	CHB-C4A-NA	2.13	127.46	124.51
21	A	851	BCR	C15-C16-C17	-2.13	119.11	123.47
17	B	829	CLA	CHA-C1A-NA	-2.13	121.52	126.40
17	A	801	CLA	O2A-C1-C2	-2.13	103.05	108.64
17	3	604	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
17	B	815	CLA	CMC-C2C-C3C	2.13	128.95	124.94
17	4	310	CLA	C11-C10-C8	-2.13	109.05	115.92
17	B	842	CLA	C1-C2-C3	-2.13	122.37	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	827	CLA	CMC-C2C-C3C	2.13	128.95	124.94
17	A	812	CLA	CMC-C2C-C3C	2.12	128.95	124.94
17	B	835	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
17	L	203	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
21	A	849	BCR	C16-C17-C18	-2.12	124.28	127.31
17	A	827	CLA	C4-C3-C5	2.12	118.84	115.27
17	1	306	CLA	O2A-CGA-O1A	-2.12	116.49	123.14
18	4	315	CHL	CMB-C2B-C3B	2.12	128.65	124.68
26	B	850	DGD	O6E-C5E-C6E	-2.12	101.16	106.44
21	L	201	BCR	C2-C1-C6	2.12	113.74	110.48
26	B	850	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
17	A	824	CLA	C16-C15-C13	-2.12	109.08	115.92
17	A	801	CLA	CHA-C1A-NA	-2.12	121.55	126.40
17	B	810	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
22	1	317	LHG	O8-C23-C24	2.12	118.55	111.91
17	A	833	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
21	4	318	BCR	C29-C30-C25	2.12	113.74	110.48
17	A	813	CLA	CAA-CBA-CGA	-2.12	109.04	113.59
21	K	203	BCR	C3-C4-C5	-2.12	110.30	114.08
17	1	312	CLA	CHB-C4A-NA	2.12	127.44	124.51
21	I	101	BCR	C10-C11-C12	-2.12	116.62	123.22
17	A	804	CLA	CAA-CBA-CGA	-2.11	107.07	113.25
17	A	805	CLA	C4D-C3D-CAD	-2.11	107.29	108.47
17	B	812	CLA	O2D-CGD-CBD	2.11	115.03	111.27
21	B	848	BCR	C15-C16-C17	-2.11	119.14	123.47
24	B	852	LMG	C38-C37-C36	-2.11	103.69	114.42
18	4	301	CHL	CHB-C4A-NA	2.11	127.44	124.51
21	L	201	BCR	C7-C8-C9	-2.11	123.04	126.23
18	3	607	CHL	O1D-CGD-CBD	-2.11	120.16	124.48
17	B	822	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
17	3	604	CLA	O1D-CGD-CBD	2.11	128.81	124.48
17	A	814	CLA	C4D-C3D-CAD	-2.11	107.29	108.47
17	B	819	CLA	OBD-CAD-CBD	-2.11	122.88	125.89
21	4	318	BCR	C11-C10-C9	-2.11	124.30	127.31
17	B	802	CLA	C3B-C4B-NB	-2.11	106.48	109.21
17	4	304	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
17	A	819	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
17	4	303	CLA	O2A-C1-C2	2.11	114.18	108.64
17	B	842	CLA	O2D-CGD-CBD	2.11	115.01	111.27
17	A	822	CLA	CMD-C2D-C3D	2.11	128.62	124.68
17	1	309	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
17	B	805	CLA	CHA-C1A-NA	-2.11	121.57	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	810	CLA	OBD-CAD-CBD	-2.11	122.89	125.89
17	B	802	CLA	C6-C7-C8	-2.11	109.11	115.92
17	A	823	CLA	CMD-C2D-C3D	2.10	128.62	124.68
17	A	843	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
17	A	810	CLA	O1D-CGD-CBD	2.10	128.79	124.48
17	A	835	CLA	CMD-C2D-C3D	2.10	128.61	124.68
17	A	835	CLA	CHB-C4A-NA	2.10	127.42	124.51
21	4	318	BCR	C28-C27-C26	-2.10	110.33	114.08
17	B	835	CLA	CMD-C2D-C3D	2.10	128.61	124.68
17	B	828	CLA	C16-C15-C13	-2.10	109.13	115.92
17	4	304	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
17	A	825	CLA	CHB-C4A-NA	2.10	127.42	124.51
17	B	818	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
17	B	838	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
17	1	304	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
17	A	823	CLA	CMC-C2C-C3C	2.10	128.90	124.94
17	B	834	CLA	C1-C2-C3	-2.10	122.42	126.04
17	A	826	CLA	C1-C2-C3	-2.10	122.42	126.04
19	1	314	LUT	C21-C26-C27	-2.10	110.05	112.70
21	J	105	BCR	C30-C25-C26	-2.09	119.66	122.61
17	1	308	CLA	CMD-C2D-C3D	2.09	128.60	124.68
17	4	311	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
25	F	305	HTG	C1-C2-C3	-2.09	106.45	110.59
21	B	845	BCR	C28-C27-C26	-2.09	110.34	114.08
21	2	316	BCR	C11-C10-C9	-2.09	124.32	127.31
21	B	844	BCR	C33-C5-C6	-2.09	122.18	124.53
18	2	313	CHL	OBD-CAD-C3D	-2.09	124.51	127.98
21	K	203	BCR	C33-C5-C6	-2.09	122.18	124.53
21	B	844	BCR	C2-C1-C6	2.09	113.69	110.48
21	A	851	BCR	C38-C26-C27	-2.09	109.61	113.62
17	A	817	CLA	CHB-C4A-NA	2.09	127.40	124.51
17	A	838	CLA	CHA-C1A-NA	-2.09	121.62	126.40
22	1	317	LHG	C20-C19-C18	-2.09	103.84	114.42
17	A	818	CLA	CAA-C2A-C1A	-2.09	105.14	111.97
17	A	841	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
17	B	826	CLA	C2A-C1A-CHA	2.09	127.50	123.86
18	2	304	CHL	CBC-CAC-C3C	-2.08	106.68	112.43
21	2	316	BCR	C37-C22-C21	-2.08	120.00	122.92
17	B	829	CLA	CHB-C4A-NA	2.08	127.39	124.51
17	3	608	CLA	CHB-C4A-NA	2.08	127.39	124.51
21	A	850	BCR	C20-C21-C22	-2.08	124.34	127.31
17	L	202	CLA	OBD-CAD-CBD	-2.08	122.92	125.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	4	323	DGD	O3D-C3D-C4D	2.08	115.16	110.35
17	A	818	CLA	OBD-CAD-C3D	2.08	131.44	127.98
24	4	319	LMG	C3-C4-C5	-2.08	106.53	110.24
17	B	823	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
17	K	202	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	F	309	LMG	C42-C41-C40	-2.08	103.87	114.42
17	B	814	CLA	OBD-CAD-CBD	-2.08	122.93	125.89
17	B	808	CLA	CMC-C2C-C3C	2.08	128.86	124.94
17	L	204	CLA	C4D-C3D-CAD	-2.08	107.31	108.47
18	4	301	CHL	C4-C3-C2	-2.08	118.35	123.68
21	B	849	BCR	C38-C26-C27	-2.08	109.63	113.62
17	K	202	CLA	CMD-C2D-C3D	2.08	128.56	124.68
17	A	812	CLA	CED-O2D-CGD	2.08	120.63	115.94
17	B	820	CLA	O2D-CGD-CBD	2.08	114.96	111.27
17	A	839	CLA	C3A-C2A-C1A	2.08	104.45	101.34
18	1	305	CHL	O2A-CGA-O1A	-2.07	118.36	123.59
17	L	204	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
17	A	831	CLA	C1-C2-C3	-2.07	122.46	126.04
17	A	823	CLA	O2D-CGD-CBD	2.07	114.95	111.27
17	B	828	CLA	C4D-C3D-CAD	-2.07	107.31	108.47
17	A	853	CLA	O2A-CGA-CBA	2.07	118.41	111.91
17	G	105	CLA	CHB-C4A-NA	2.07	127.37	124.51
17	A	827	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
21	F	308	BCR	C30-C25-C26	-2.07	119.70	122.61
21	I	101	BCR	C15-C14-C13	-2.07	124.36	127.31
18	4	301	CHL	CMB-C2B-C3B	2.07	128.54	124.68
17	4	313	CLA	CBC-CAC-C3C	-2.06	107.01	112.27
17	A	825	CLA	C3A-C2A-C1A	2.06	104.43	101.34
17	2	301	CLA	CMC-C2C-C3C	2.06	128.83	124.94
17	A	831	CLA	CMC-C2C-C3C	2.06	128.83	124.94
17	L	204	CLA	CMC-C2C-C3C	2.06	128.83	124.94
18	4	306	CHL	O2A-CGA-O1A	-2.06	118.39	123.59
19	4	316	LUT	C21-C26-C25	2.06	115.11	111.42
21	J	104	BCR	C24-C23-C22	-2.06	123.12	126.23
17	A	837	CLA	CMC-C2C-C3C	2.06	128.83	124.94
17	A	835	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
17	2	301	CLA	C1-C2-C3	-2.06	122.48	126.04
18	3	601	CHL	CGD-CBD-CAD	-2.06	104.07	110.73
17	4	304	CLA	CED-O2D-CGD	2.06	120.59	115.94
17	A	841	CLA	C1-C2-C3	-2.06	122.48	126.04
17	A	830	CLA	C1-C2-C3	-2.06	123.43	126.75
22	A	844	LHG	C27-C26-C25	-2.06	103.99	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	4	307	CHL	CMB-C2B-C1B	2.05	131.62	128.46
17	2	309	CLA	CMD-C2D-C3D	2.05	128.52	124.68
24	B	852	LMG	O1-C7-C8	-2.05	105.94	110.90
18	4	301	CHL	C7-C6-C5	-2.05	107.78	113.36
22	F	302	LHG	C18-C17-C16	-2.05	104.00	114.42
25	4	322	HTG	C3-C4-C5	2.05	113.90	110.24
18	1	305	CHL	CBC-CAC-C3C	-2.05	106.77	112.43
17	B	834	CLA	OBD-CAD-C3D	2.05	131.39	127.98
17	F	304	CLA	C11-C10-C8	-2.05	109.28	115.92
21	F	303	BCR	C33-C5-C6	-2.05	122.22	124.53
17	1	301	CLA	O2D-CGD-CBD	2.05	114.92	111.27
25	B	851	HTG	C2'-C1'-S1	-2.05	105.77	112.40
21	J	105	BCR	C16-C15-C14	-2.05	119.28	123.47
17	A	837	CLA	C1-C2-C3	-2.05	122.50	126.04
17	A	841	CLA	CHB-C4A-NA	2.05	127.35	124.51
17	A	815	CLA	O2D-CGD-CBD	2.05	114.91	111.27
17	G	105	CLA	C3A-C2A-C1A	2.05	104.41	101.34
17	B	832	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
25	B	851	HTG	C3-C4-C5	-2.05	106.59	110.24
26	4	323	DGD	O4D-C4D-C3D	2.04	115.07	110.35
17	3	609	CLA	OBD-CAD-CBD	-2.04	122.97	125.89
17	B	808	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
17	A	828	CLA	O1D-CGD-CBD	2.04	128.66	124.48
21	A	846	BCR	C35-C13-C14	-2.04	120.06	122.92
20	4	317	XAT	O24-C25-C26	-2.04	57.27	58.96
17	4	302	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
21	1	316	BCR	C2-C1-C6	2.04	113.62	110.48
21	A	850	BCR	C38-C26-C25	-2.04	122.24	124.53
18	2	306	CHL	C4D-C3D-CAD	2.04	109.61	108.47
17	1	308	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
18	4	315	CHL	C1C-C2C-C3C	-2.04	105.50	107.11
17	3	608	CLA	CMD-C2D-C3D	2.03	128.48	124.68
17	4	311	CLA	CMC-C2C-C3C	2.03	128.78	124.94
17	A	840	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
17	A	840	CLA	OBD-CAD-C3D	2.03	131.36	127.98
17	1	309	CLA	CHA-C1A-NA	-2.03	121.74	126.40
17	2	308	CLA	CMD-C2D-C3D	2.03	128.48	124.68
17	A	816	CLA	CMC-C2C-C3C	2.03	128.77	124.94
17	A	833	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
17	A	824	CLA	O2D-CGD-CBD	2.03	114.87	111.27
17	B	826	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
17	B	817	CLA	C3A-C2A-C1A	2.03	104.38	101.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	848	BCR	C39-C30-C25	-2.03	107.01	110.30
17	B	815	CLA	C12-C11-C10	-2.02	103.94	113.24
17	A	817	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
17	4	303	CLA	CHB-C4A-NA	2.02	127.31	124.51
17	A	805	CLA	O2A-C1-C2	2.02	113.95	108.64
17	J	101	CLA	CHB-C4A-NA	2.02	127.31	124.51
17	4	310	CLA	CAA-C2A-C1A	-2.02	105.35	111.97
17	B	811	CLA	CHB-C4A-NA	2.02	127.31	124.51
17	B	841	CLA	CAA-C2A-C1A	-2.02	105.35	111.97
17	B	841	CLA	OBD-CAD-C3D	2.02	131.34	127.98
17	L	202	CLA	O2D-CGD-CBD	2.02	114.86	111.27
18	2	305	CHL	C1C-C2C-C3C	-2.02	105.51	107.11
17	B	835	CLA	CHA-C1A-NA	-2.02	121.77	126.40
21	G	106	BCR	C8-C7-C6	-2.02	121.53	127.20
17	B	831	CLA	CMD-C2D-C3D	2.02	128.46	124.68
22	B	801	LHG	O8-C23-C24	2.02	121.19	112.38
17	2	309	CLA	CMA-C3A-C2A	-2.02	111.39	116.10
21	L	205	BCR	C33-C5-C6	-2.02	122.26	124.53
17	1	310	CLA	C4D-C3D-CAD	-2.02	107.34	108.47
17	2	310	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
17	A	822	CLA	OBD-CAD-CBD	-2.02	123.01	125.89
17	B	803	CLA	CMB-C2B-C3B	2.02	128.45	124.68
17	1	303	CLA	OBD-CAD-CBD	-2.02	123.02	125.89
17	A	831	CLA	CBA-CAA-C2A	-2.01	107.92	113.86
17	4	312	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
21	B	845	BCR	C35-C13-C14	-2.01	120.10	122.92
17	A	821	CLA	CMC-C2C-C3C	2.01	128.74	124.94
26	B	850	DGD	O6D-C5D-C6D	-2.01	102.60	106.67
17	A	813	CLA	CHB-C4A-NA	2.01	127.29	124.51
21	B	845	BCR	C31-C1-C6	2.01	113.56	110.30
17	4	311	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
22	G	102	LHG	O8-C23-O10	-2.01	118.52	123.59
17	A	803	CLA	CMD-C2D-C3D	2.01	128.44	124.68
17	J	101	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
21	L	201	BCR	C15-C14-C13	-2.01	124.44	127.31
18	4	306	CHL	OMC-CMC-C2C	-2.01	121.15	125.69
17	2	311	CLA	O1D-CGD-CBD	2.01	128.59	124.48
17	3	610	CLA	C2A-C1A-CHA	2.00	127.36	123.86
17	1	310	CLA	OBD-CAD-CBD	-2.00	123.03	125.89
17	B	808	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
21	B	847	BCR	C24-C23-C22	-2.00	123.21	126.23
17	A	853	CLA	C4-C3-C2	-2.00	118.55	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	819	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (178) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	1	301	CLA	ND
17	1	302	CLA	ND
17	1	303	CLA	ND
17	1	304	CLA	ND
17	1	306	CLA	ND
17	1	307	CLA	ND
17	1	308	CLA	ND
17	1	309	CLA	ND
17	1	310	CLA	ND
17	1	311	CLA	ND
17	1	312	CLA	ND
17	1	313	CLA	ND
17	2	301	CLA	ND
17	2	302	CLA	ND
17	2	303	CLA	ND
17	2	307	CLA	ND
17	2	308	CLA	ND
17	2	309	CLA	ND
17	2	310	CLA	ND
17	2	311	CLA	ND
17	2	312	CLA	ND
17	2	319	CLA	ND
17	3	602	CLA	ND
17	3	603	CLA	ND
17	3	604	CLA	ND
17	3	605	CLA	ND
17	3	606	CLA	ND
17	3	608	CLA	ND
17	3	609	CLA	ND
17	3	610	CLA	ND
17	3	611	CLA	ND
17	3	612	CLA	ND
17	3	613	CLA	ND
17	4	302	CLA	ND
17	4	304	CLA	ND
17	4	308	CLA	ND
17	4	309	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	4	310	CLA	ND
17	4	312	CLA	ND
17	4	313	CLA	ND
17	4	314	CLA	ND
17	A	801	CLA	CBD
17	A	801	CLA	ND
17	A	802	CLA	ND
17	A	803	CLA	ND
17	A	804	CLA	ND
17	A	805	CLA	ND
17	A	806	CLA	ND
17	A	807	CLA	ND
17	A	808	CLA	ND
17	A	809	CLA	ND
17	A	810	CLA	ND
17	A	811	CLA	ND
17	A	812	CLA	ND
17	A	813	CLA	ND
17	A	814	CLA	ND
17	A	815	CLA	ND
17	A	816	CLA	ND
17	A	817	CLA	ND
17	A	818	CLA	ND
17	A	819	CLA	ND
17	A	820	CLA	ND
17	A	821	CLA	ND
17	A	822	CLA	ND
17	A	823	CLA	ND
17	A	824	CLA	ND
17	A	825	CLA	ND
17	A	826	CLA	ND
17	A	827	CLA	ND
17	A	828	CLA	ND
17	A	829	CLA	ND
17	A	830	CLA	ND
17	A	831	CLA	ND
17	A	832	CLA	ND
17	A	833	CLA	ND
17	A	834	CLA	ND
17	A	835	CLA	ND
17	A	836	CLA	ND
17	A	837	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	A	838	CLA	ND
17	A	839	CLA	ND
17	A	840	CLA	ND
17	A	841	CLA	ND
17	A	843	CLA	ND
17	A	853	CLA	ND
17	B	802	CLA	ND
17	B	803	CLA	ND
17	B	804	CLA	ND
17	B	805	CLA	ND
17	B	806	CLA	ND
17	B	807	CLA	ND
17	B	808	CLA	ND
17	B	809	CLA	ND
17	B	810	CLA	ND
17	B	811	CLA	ND
17	B	813	CLA	ND
17	B	814	CLA	ND
17	B	815	CLA	ND
17	B	816	CLA	ND
17	B	817	CLA	ND
17	B	818	CLA	ND
17	B	819	CLA	ND
17	B	820	CLA	ND
17	B	821	CLA	ND
17	B	822	CLA	ND
17	B	823	CLA	ND
17	B	824	CLA	ND
17	B	825	CLA	ND
17	B	826	CLA	ND
17	B	827	CLA	ND
17	B	828	CLA	ND
17	B	829	CLA	ND
17	B	830	CLA	ND
17	B	831	CLA	ND
17	B	832	CLA	ND
17	B	833	CLA	ND
17	B	834	CLA	ND
17	B	835	CLA	ND
17	B	836	CLA	ND
17	B	837	CLA	ND
17	B	838	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
17	B	839	CLA	ND
17	B	840	CLA	ND
17	B	841	CLA	ND
17	B	842	CLA	ND
17	F	304	CLA	ND
17	F	306	CLA	ND
17	F	307	CLA	ND
17	G	103	CLA	ND
17	G	104	CLA	ND
17	G	105	CLA	ND
17	J	101	CLA	ND
17	J	103	CLA	ND
17	L	202	CLA	ND
17	L	203	CLA	ND
17	K	201	CLA	ND
17	K	202	CLA	ND
18	1	305	CHL	ND
18	1	305	CHL	NC
18	1	305	CHL	NA
18	2	304	CHL	ND
18	2	304	CHL	NC
18	2	304	CHL	NA
18	2	305	CHL	ND
18	2	305	CHL	NC
18	2	305	CHL	NA
18	2	306	CHL	ND
18	2	306	CHL	NC
18	2	306	CHL	NA
18	2	313	CHL	ND
18	2	313	CHL	NC
18	2	313	CHL	NA
18	3	601	CHL	ND
18	3	601	CHL	NC
18	3	601	CHL	NA
18	3	607	CHL	ND
18	3	607	CHL	NC
18	3	607	CHL	NA
18	4	301	CHL	C8
18	4	301	CHL	ND
18	4	301	CHL	NC
18	4	301	CHL	NA
18	4	305	CHL	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	4	305	CHL	ND
18	4	305	CHL	NC
18	4	305	CHL	NA
18	4	306	CHL	ND
18	4	306	CHL	NC
18	4	306	CHL	NA
18	4	307	CHL	ND
18	4	307	CHL	NC
18	4	307	CHL	NA
18	4	315	CHL	ND
18	4	315	CHL	NC
18	4	315	CHL	NA
20	4	317	XAT	C25
20	4	317	XAT	C6
20	4	317	XAT	C26

All (1918) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	304	CLA	CHA-CBD-CGD-O1D
17	1	307	CLA	CBA-CGA-O2A-C1
17	1	307	CLA	O1A-CGA-O2A-C1
17	1	309	CLA	C1A-C2A-CAA-CBA
17	1	311	CLA	CBD-CGD-O2D-CED
17	1	312	CLA	C1A-C2A-CAA-CBA
17	1	312	CLA	CHA-CBD-CGD-O1D
17	1	312	CLA	CHA-CBD-CGD-O2D
17	1	313	CLA	CBA-CGA-O2A-C1
17	2	309	CLA	CBD-CGD-O2D-CED
17	2	310	CLA	CBD-CGD-O2D-CED
17	2	310	CLA	C2-C3-C5-C6
17	2	310	CLA	C4-C3-C5-C6
17	3	602	CLA	CHA-CBD-CGD-O1D
17	3	602	CLA	CHA-CBD-CGD-O2D
17	3	604	CLA	CBD-CGD-O2D-CED
17	3	606	CLA	C1A-C2A-CAA-CBA
17	3	606	CLA	C3A-C2A-CAA-CBA
17	3	611	CLA	CHA-CBD-CGD-O1D
17	3	611	CLA	CHA-CBD-CGD-O2D
17	4	304	CLA	C1A-C2A-CAA-CBA
17	4	309	CLA	CBD-CGD-O2D-CED
17	4	310	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	4	310	CLA	CHA-CBD-CGD-O1D
17	4	310	CLA	CHA-CBD-CGD-O2D
17	A	801	CLA	CHA-CBD-CGD-O1D
17	A	801	CLA	CHA-CBD-CGD-O2D
17	A	803	CLA	C1A-C2A-CAA-CBA
17	A	803	CLA	C3A-C2A-CAA-CBA
17	A	804	CLA	CHA-CBD-CGD-O1D
17	A	804	CLA	CHA-CBD-CGD-O2D
17	A	804	CLA	CAD-CBD-CGD-O1D
17	A	805	CLA	C1A-C2A-CAA-CBA
17	A	805	CLA	CBD-CGD-O2D-CED
17	A	807	CLA	C3A-C2A-CAA-CBA
17	A	809	CLA	CHA-CBD-CGD-O1D
17	A	809	CLA	CHA-CBD-CGD-O2D
17	A	810	CLA	C1A-C2A-CAA-CBA
17	A	814	CLA	C1A-C2A-CAA-CBA
17	A	814	CLA	C3A-C2A-CAA-CBA
17	A	814	CLA	CBA-CGA-O2A-C1
17	A	814	CLA	O1A-CGA-O2A-C1
17	A	814	CLA	CHA-CBD-CGD-O1D
17	A	814	CLA	CHA-CBD-CGD-O2D
17	A	815	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	CHA-CBD-CGD-O2D
17	A	817	CLA	C3A-C2A-CAA-CBA
17	A	818	CLA	C1A-C2A-CAA-CBA
17	A	818	CLA	C3A-C2A-CAA-CBA
17	A	819	CLA	C2C-C3C-CAC-CBC
17	A	822	CLA	CBD-CGD-O2D-CED
17	A	825	CLA	C6-C7-C8-C9
17	A	828	CLA	C2A-CAA-CBA-CGA
17	A	829	CLA	CHA-CBD-CGD-O2D
17	A	831	CLA	C1A-C2A-CAA-CBA
17	A	831	CLA	C2-C3-C5-C6
17	A	831	CLA	C4-C3-C5-C6
17	A	832	CLA	CHA-CBD-CGD-O2D
17	A	834	CLA	C1A-C2A-CAA-CBA
17	A	834	CLA	C3A-C2A-CAA-CBA
17	A	834	CLA	C2A-CAA-CBA-CGA
17	A	834	CLA	CHA-CBD-CGD-O1D
17	A	834	CLA	CHA-CBD-CGD-O2D
17	A	836	CLA	C2-C3-C5-C6
17	A	836	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	837	CLA	C1A-C2A-CAA-CBA
17	A	840	CLA	C4-C3-C5-C6
17	A	843	CLA	C2C-C3C-CAC-CBC
17	A	853	CLA	C4-C3-C5-C6
17	B	807	CLA	C1A-C2A-CAA-CBA
17	B	807	CLA	C3A-C2A-CAA-CBA
17	B	810	CLA	CHA-CBD-CGD-O1D
17	B	810	CLA	CHA-CBD-CGD-O2D
17	B	812	CLA	CBD-CGD-O2D-CED
17	B	815	CLA	C2C-C3C-CAC-CBC
17	B	820	CLA	C3A-C2A-CAA-CBA
17	B	820	CLA	C2-C3-C5-C6
17	B	820	CLA	C6-C7-C8-C9
17	B	824	CLA	C1A-C2A-CAA-CBA
17	B	825	CLA	C1A-C2A-CAA-CBA
17	B	825	CLA	CHA-CBD-CGD-O1D
17	B	825	CLA	CHA-CBD-CGD-O2D
17	B	830	CLA	C1A-C2A-CAA-CBA
17	B	830	CLA	C3A-C2A-CAA-CBA
17	B	830	CLA	C2A-CAA-CBA-CGA
17	B	831	CLA	C1A-C2A-CAA-CBA
17	B	834	CLA	C4-C3-C5-C6
17	B	837	CLA	C2C-C3C-CAC-CBC
17	B	839	CLA	C1A-C2A-CAA-CBA
17	B	839	CLA	C3A-C2A-CAA-CBA
17	J	103	CLA	C1A-C2A-CAA-CBA
17	J	103	CLA	C3A-C2A-CAA-CBA
17	L	202	CLA	C1A-C2A-CAA-CBA
17	L	202	CLA	C3A-C2A-CAA-CBA
17	L	203	CLA	C4-C3-C5-C6
17	L	204	CLA	C3A-C2A-CAA-CBA
17	K	202	CLA	C2-C3-C5-C6
17	K	202	CLA	C4-C3-C5-C6
18	1	305	CHL	C1A-C2A-CAA-CBA
18	2	304	CHL	C1C-C2C-CMC-OMC
18	2	313	CHL	CHA-CBD-CGD-O1D
18	2	313	CHL	CHA-CBD-CGD-O2D
18	4	301	CHL	C1A-C2A-CAA-CBA
18	4	301	CHL	CBD-CGD-O2D-CED
18	4	305	CHL	CBA-CGA-O2A-C1
18	4	305	CHL	C1C-C2C-CMC-OMC
18	4	305	CHL	C3C-C2C-CMC-OMC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	4	305	CHL	C2-C3-C5-C6
18	4	305	CHL	C4-C3-C5-C6
18	4	306	CHL	C1A-C2A-CAA-CBA
18	4	306	CHL	C3A-C2A-CAA-CBA
18	4	306	CHL	C2A-CAA-CBA-CGA
18	4	315	CHL	CBD-CGD-O2D-CED
19	1	314	LUT	C5-C6-C7-C8
19	1	314	LUT	C11-C10-C9-C19
19	1	314	LUT	C10-C11-C12-C13
19	1	314	LUT	C20-C13-C14-C15
19	1	314	LUT	C39-C29-C30-C31
19	1	314	LUT	C40-C33-C34-C35
19	2	314	LUT	C5-C6-C7-C8
19	2	314	LUT	C11-C10-C9-C8
19	2	314	LUT	C10-C11-C12-C13
19	2	314	LUT	C20-C13-C14-C15
19	2	314	LUT	C39-C29-C30-C31
19	2	314	LUT	C31-C32-C33-C40
19	2	314	LUT	C40-C33-C34-C35
19	3	614	LUT	C5-C6-C7-C8
19	3	614	LUT	C11-C10-C9-C8
19	3	614	LUT	C10-C11-C12-C13
19	3	614	LUT	C20-C13-C14-C15
19	3	614	LUT	C39-C29-C30-C31
19	3	614	LUT	C40-C33-C34-C35
19	4	316	LUT	C5-C6-C7-C8
19	4	316	LUT	C7-C8-C9-C19
19	4	316	LUT	C11-C10-C9-C19
19	4	316	LUT	C20-C13-C14-C15
19	4	316	LUT	C39-C29-C30-C31
19	4	316	LUT	C31-C32-C33-C40
19	4	316	LUT	C40-C33-C34-C35
20	1	315	XAT	C7-C8-C9-C19
20	1	315	XAT	C11-C10-C9-C19
20	1	315	XAT	C20-C13-C14-C15
20	1	315	XAT	C39-C29-C30-C31
20	1	315	XAT	C40-C33-C34-C35
20	2	315	XAT	C7-C8-C9-C19
20	2	315	XAT	C11-C10-C9-C19
20	2	315	XAT	C20-C13-C14-C15
20	2	315	XAT	C39-C29-C30-C31
20	2	315	XAT	C40-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	3	615	XAT	C7-C8-C9-C19
20	3	615	XAT	C11-C10-C9-C19
20	3	615	XAT	C20-C13-C14-C15
20	3	615	XAT	C39-C29-C30-C31
20	3	615	XAT	C40-C33-C34-C35
20	4	317	XAT	C7-C8-C9-C19
20	4	317	XAT	C11-C10-C9-C19
20	4	317	XAT	C11-C12-C13-C20
20	4	317	XAT	C20-C13-C14-C15
20	4	317	XAT	C27-C28-C29-C39
20	4	317	XAT	C39-C29-C30-C31
20	4	317	XAT	C31-C32-C33-C40
20	4	317	XAT	C40-C33-C34-C35
21	1	316	BCR	C7-C8-C9-C34
21	1	316	BCR	C11-C12-C13-C14
21	1	316	BCR	C11-C12-C13-C35
21	1	316	BCR	C20-C21-C22-C37
21	2	316	BCR	C10-C11-C12-C13
21	2	316	BCR	C16-C17-C18-C36
21	2	316	BCR	C21-C22-C23-C24
21	2	316	BCR	C37-C22-C23-C24
21	3	616	BCR	C23-C24-C25-C30
21	A	846	BCR	C21-C22-C23-C24
21	A	847	BCR	C7-C8-C9-C10
21	A	847	BCR	C7-C8-C9-C34
21	A	848	BCR	C7-C8-C9-C34
21	A	848	BCR	C20-C21-C22-C23
21	A	848	BCR	C20-C21-C22-C37
21	A	849	BCR	C1-C6-C7-C8
21	A	849	BCR	C6-C7-C8-C9
21	A	849	BCR	C7-C8-C9-C34
21	A	850	BCR	C37-C22-C23-C24
21	A	850	BCR	C23-C24-C25-C26
21	A	851	BCR	C7-C8-C9-C34
21	B	844	BCR	C7-C8-C9-C34
21	B	844	BCR	C11-C12-C13-C35
21	B	844	BCR	C21-C22-C23-C24
21	B	844	BCR	C37-C22-C23-C24
21	B	845	BCR	C21-C22-C23-C24
21	B	845	BCR	C37-C22-C23-C24
21	B	846	BCR	C21-C22-C23-C24
21	B	846	BCR	C37-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	B	847	BCR	C23-C24-C25-C30
21	B	848	BCR	C16-C17-C18-C36
21	B	848	BCR	C23-C24-C25-C26
21	B	849	BCR	C1-C6-C7-C8
21	B	849	BCR	C7-C8-C9-C34
21	F	303	BCR	C7-C8-C9-C34
21	F	303	BCR	C35-C13-C14-C15
21	G	106	BCR	C20-C21-C22-C37
21	G	106	BCR	C22-C23-C24-C25
21	G	106	BCR	C23-C24-C25-C30
21	I	101	BCR	C20-C21-C22-C37
21	J	104	BCR	C11-C12-C13-C35
21	J	105	BCR	C1-C6-C7-C8
21	J	105	BCR	C37-C22-C23-C24
21	J	105	BCR	C23-C24-C25-C26
21	L	201	BCR	C21-C22-C23-C24
21	L	201	BCR	C37-C22-C23-C24
21	L	201	BCR	C23-C24-C25-C30
21	L	205	BCR	C21-C22-C23-C24
21	L	205	BCR	C37-C22-C23-C24
21	L	205	BCR	C23-C24-C25-C26
21	L	205	BCR	C23-C24-C25-C30
21	L	206	BCR	C23-C24-C25-C30
21	K	203	BCR	C18-C19-C20-C21
21	K	203	BCR	C20-C21-C22-C23
21	K	203	BCR	C21-C22-C23-C24
21	K	203	BCR	C37-C22-C23-C24
22	1	317	LHG	C3-O3-P-O5
22	2	317	LHG	C4-O6-P-O5
22	2	317	LHG	C24-C23-O8-C6
22	B	801	LHG	C4-O6-P-O4
22	F	302	LHG	O2-C2-C3-O3
22	F	302	LHG	C3-O3-P-O5
22	F	302	LHG	C3-O3-P-O6
22	F	302	LHG	C4-O6-P-O4
22	F	302	LHG	C5-C4-O6-P
22	G	102	LHG	O1-C1-C2-C3
22	G	102	LHG	C4-O6-P-O4
23	2	318	LMT	C2B-C1B-O1B-C4'
23	2	318	LMT	C2'-C1'-O1'-C1
23	2	318	LMT	O5'-C1'-O1'-C1
24	4	320	LMG	O6-C1-O1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	4	320	LMG	O1-C7-C8-O7
24	4	320	LMG	O9-C10-O7-C8
24	4	320	LMG	C11-C10-O7-C8
24	B	852	LMG	C2-C1-O1-C7
24	B	852	LMG	O6-C1-O1-C7
24	G	101	LMG	O7-C8-C9-O8
25	B	851	HTG	O5-C1-S1-C1'
25	F	301	HTG	C2-C1-S1-C1'
25	F	301	HTG	O5-C1-S1-C1'
25	F	310	HTG	C2-C1-S1-C1'
25	F	310	HTG	O5-C1-S1-C1'
25	J	102	HTG	O5-C1-S1-C1'
25	J	102	HTG	C2'-C1'-S1-C1
26	4	323	DGD	C2B-C1B-O2G-C2G
26	4	323	DGD	C2G-C3G-O3G-C1D
26	4	323	DGD	O6D-C1D-O3G-C3G
26	4	323	DGD	C5D-C6D-O5D-C1E
26	4	323	DGD	O6E-C1E-O5D-C6D
27	A	842	PQN	C12-C11-C3-C2
27	A	842	PQN	C11-C12-C13-C14
27	A	842	PQN	C14-C13-C15-C16
27	B	843	PQN	C12-C11-C3-C2
27	B	843	PQN	C11-C12-C13-C14
27	B	843	PQN	C14-C13-C15-C16
17	2	309	CLA	O1D-CGD-O2D-CED
17	4	304	CLA	O1D-CGD-O2D-CED
18	4	307	CHL	O1D-CGD-O2D-CED
23	2	318	LMT	O5B-C1B-O1B-C4'
17	A	815	CLA	O1D-CGD-O2D-CED
17	B	808	CLA	O1D-CGD-O2D-CED
17	1	303	CLA	CBD-CGD-O2D-CED
17	1	304	CLA	CBD-CGD-O2D-CED
17	3	602	CLA	CBD-CGD-O2D-CED
17	3	611	CLA	CBD-CGD-O2D-CED
17	4	303	CLA	CBD-CGD-O2D-CED
17	4	304	CLA	CBD-CGD-O2D-CED
17	4	311	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	CBD-CGD-O2D-CED
17	A	814	CLA	CBD-CGD-O2D-CED
17	A	821	CLA	CBD-CGD-O2D-CED
17	A	831	CLA	CBD-CGD-O2D-CED
17	B	808	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	822	CLA	CBD-CGD-O2D-CED
17	J	103	CLA	CBD-CGD-O2D-CED
17	K	201	CLA	CBD-CGD-O2D-CED
18	2	304	CHL	CBD-CGD-O2D-CED
18	4	306	CHL	CBD-CGD-O2D-CED
18	4	307	CHL	CBD-CGD-O2D-CED
17	3	608	CLA	O1A-CGA-O2A-C1
18	4	305	CHL	O1A-CGA-O2A-C1
22	2	317	LHG	O10-C23-O8-C6
17	1	313	CLA	O1A-CGA-O2A-C1
17	4	309	CLA	O1D-CGD-O2D-CED
17	K	201	CLA	O1D-CGD-O2D-CED
18	4	301	CHL	O1D-CGD-O2D-CED
18	4	315	CHL	O1D-CGD-O2D-CED
17	1	311	CLA	O1D-CGD-O2D-CED
17	2	310	CLA	O1D-CGD-O2D-CED
17	A	822	CLA	O1D-CGD-O2D-CED
17	B	822	CLA	O1D-CGD-O2D-CED
17	J	103	CLA	O1D-CGD-O2D-CED
23	2	318	LMT	C4B-C5B-C6B-O6B
17	A	817	CLA	CBD-CGD-O2D-CED
17	A	837	CLA	CBD-CGD-O2D-CED
17	B	813	CLA	CBD-CGD-O2D-CED
17	B	826	CLA	CBD-CGD-O2D-CED
17	B	831	CLA	CBD-CGD-O2D-CED
17	G	103	CLA	CBD-CGD-O2D-CED
18	1	305	CHL	CBD-CGD-O2D-CED
18	2	313	CHL	CBD-CGD-O2D-CED
18	3	607	CHL	CBD-CGD-O2D-CED
17	A	822	CLA	O1A-CGA-O2A-C1
17	A	840	CLA	O1A-CGA-O2A-C1
17	L	202	CLA	O1A-CGA-O2A-C1
17	L	204	CLA	O1A-CGA-O2A-C1
22	G	102	LHG	O10-C23-O8-C6
24	G	101	LMG	O10-C28-O8-C9
17	3	604	CLA	O1D-CGD-O2D-CED
17	B	812	CLA	O1D-CGD-O2D-CED
26	4	323	DGD	C4E-C5E-C6E-O5E
17	3	602	CLA	O1D-CGD-O2D-CED
17	A	805	CLA	O1D-CGD-O2D-CED
17	1	313	CLA	CBD-CGD-O2D-CED
18	2	306	CHL	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	821	CLA	O1D-CGD-O2D-CED
22	A	845	LHG	O9-C7-O7-C5
24	F	309	LMG	O9-C10-O7-C8
26	4	323	DGD	O1B-C1B-O2G-C2G
17	2	303	CLA	C3-C5-C6-C7
17	A	807	CLA	C3-C5-C6-C7
17	A	810	CLA	C3-C5-C6-C7
17	A	838	CLA	C3-C5-C6-C7
17	B	820	CLA	C3-C5-C6-C7
17	3	608	CLA	CBA-CGA-O2A-C1
17	A	807	CLA	CBA-CGA-O2A-C1
17	A	840	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	CBA-CGA-O2A-C1
22	G	102	LHG	C24-C23-O8-C6
22	A	845	LHG	C8-C7-O7-C5
17	4	311	CLA	O1D-CGD-O2D-CED
17	A	814	CLA	O1D-CGD-O2D-CED
26	4	323	DGD	O6E-C5E-C6E-O5E
17	A	829	CLA	C4-C3-C5-C6
17	B	820	CLA	C4-C3-C5-C6
17	B	824	CLA	C4-C3-C5-C6
24	G	101	LMG	C4-C5-C6-O5
17	A	853	CLA	C2-C3-C5-C6
17	B	834	CLA	C2-C3-C5-C6
17	L	203	CLA	C2-C3-C5-C6
17	3	610	CLA	CBD-CGD-O2D-CED
17	A	816	CLA	CBD-CGD-O2D-CED
17	J	101	CLA	CBD-CGD-O2D-CED
17	B	840	CLA	C2A-CAA-CBA-CGA
17	3	611	CLA	O1D-CGD-O2D-CED
17	2	311	CLA	C3-C5-C6-C7
17	B	808	CLA	C3-C5-C6-C7
17	B	817	CLA	C3-C5-C6-C7
17	A	822	CLA	CBA-CGA-O2A-C1
17	A	833	CLA	CBA-CGA-O2A-C1
17	B	817	CLA	CBA-CGA-O2A-C1
17	L	202	CLA	CBA-CGA-O2A-C1
17	L	204	CLA	CBA-CGA-O2A-C1
18	4	306	CHL	CBA-CGA-O2A-C1
24	G	101	LMG	C29-C28-O8-C9
26	B	850	DGD	O6E-C5E-C6E-O5E
18	2	304	CHL	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	841	CLA	CBD-CGD-O2D-CED
17	1	303	CLA	O1D-CGD-O2D-CED
17	4	303	CLA	O1D-CGD-O2D-CED
23	A	855	LMT	C4B-C5B-C6B-O6B
17	A	807	CLA	O1A-CGA-O2A-C1
17	A	833	CLA	O1A-CGA-O2A-C1
18	4	306	CHL	O1A-CGA-O2A-C1
23	A	855	LMT	O5'-C5'-C6'-O6'
17	A	827	CLA	CBD-CGD-O2D-CED
17	A	835	CLA	CBD-CGD-O2D-CED
17	A	843	CLA	CBD-CGD-O2D-CED
17	B	835	CLA	CBD-CGD-O2D-CED
17	G	104	CLA	CBD-CGD-O2D-CED
17	G	105	CLA	CBD-CGD-O2D-CED
17	A	810	CLA	O1D-CGD-O2D-CED
17	A	816	CLA	C3-C5-C6-C7
17	A	831	CLA	C3-C5-C6-C7
17	A	832	CLA	C3-C5-C6-C7
17	B	811	CLA	C3-C5-C6-C7
17	B	823	CLA	C3-C5-C6-C7
17	4	303	CLA	CBA-CGA-O2A-C1
17	A	818	CLA	CBA-CGA-O2A-C1
17	A	835	CLA	CBA-CGA-O2A-C1
17	B	812	CLA	O1A-CGA-O2A-C1
25	F	301	HTG	O5-C5-C6-O6
26	B	850	DGD	C4E-C5E-C6E-O5E
18	4	306	CHL	O1D-CGD-O2D-CED
24	F	309	LMG	C11-C10-O7-C8
17	1	302	CLA	CBD-CGD-O2D-CED
26	4	323	DGD	C7B-C8B-C9B-CAB
26	4	323	DGD	C3A-C4A-C5A-C6A
26	4	323	DGD	CEB-CFB-CGB-CHB
23	2	318	LMT	O5B-C5B-C6B-O6B
17	1	304	CLA	O1D-CGD-O2D-CED
17	B	804	CLA	CBD-CGD-O2D-CED
17	A	804	CLA	C3-C5-C6-C7
17	A	820	CLA	C3-C5-C6-C7
17	A	840	CLA	C3-C5-C6-C7
17	A	841	CLA	C3-C5-C6-C7
17	A	853	CLA	C3-C5-C6-C7
17	B	809	CLA	C3-C5-C6-C7
17	4	303	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	835	CLA	O1A-CGA-O2A-C1
17	A	841	CLA	C4-C3-C5-C6
17	B	823	CLA	C4-C3-C5-C6
17	A	840	CLA	C2-C3-C5-C6
17	A	841	CLA	C2-C3-C5-C6
17	B	823	CLA	C2-C3-C5-C6
17	B	824	CLA	C2-C3-C5-C6
17	3	612	CLA	CBD-CGD-O2D-CED
17	3	606	CLA	C2A-CAA-CBA-CGA
17	B	812	CLA	C2A-CAA-CBA-CGA
23	A	855	LMT	O5B-C5B-C6B-O6B
24	G	101	LMG	O6-C5-C6-O5
17	A	818	CLA	O1A-CGA-O2A-C1
17	B	817	CLA	O1A-CGA-O2A-C1
17	B	813	CLA	C3-C5-C6-C7
17	A	841	CLA	CBA-CGA-O2A-C1
18	2	306	CHL	CBA-CGA-O2A-C1
17	A	831	CLA	O1D-CGD-O2D-CED
17	B	813	CLA	O1D-CGD-O2D-CED
17	B	831	CLA	O1D-CGD-O2D-CED
17	A	834	CLA	CBD-CGD-O2D-CED
17	B	834	CLA	CBD-CGD-O2D-CED
22	2	317	LHG	C28-C29-C30-C31
26	4	323	DGD	CBB-CCB-CDB-CEB
17	A	803	CLA	C3-C5-C6-C7
17	A	805	CLA	C3-C5-C6-C7
17	B	815	CLA	C3-C5-C6-C7
17	B	826	CLA	C3-C5-C6-C7
17	L	202	CLA	C3-C5-C6-C7
18	1	305	CHL	O1D-CGD-O2D-CED
17	1	309	CLA	CBA-CGA-O2A-C1
17	3	606	CLA	CBA-CGA-O2A-C1
17	4	308	CLA	CBA-CGA-O2A-C1
17	A	830	CLA	CBA-CGA-O2A-C1
17	B	803	CLA	CBA-CGA-O2A-C1
17	G	104	CLA	CBA-CGA-O2A-C1
24	B	852	LMG	C29-C28-O8-C9
26	4	323	DGD	C2A-C1A-O1G-C1G
17	A	832	CLA	CBD-CGD-O2D-CED
17	B	810	CLA	C15-C16-C17-C18
25	F	301	HTG	C4-C5-C6-O6
24	4	320	LMG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	A	845	LHG	O6-C4-C5-O7
17	A	810	CLA	C13-C15-C16-C17
17	A	853	CLA	C15-C16-C17-C18
26	4	323	DGD	C2D-C1D-O3G-C3G
22	B	801	LHG	C24-C23-O8-C6
17	1	309	CLA	O1A-CGA-O2A-C1
17	B	803	CLA	O1A-CGA-O2A-C1
17	1	308	CLA	C4-C3-C5-C6
17	A	829	CLA	C2-C3-C5-C6
17	1	302	CLA	C11-C12-C13-C14
17	2	303	CLA	C11-C10-C8-C9
17	2	308	CLA	C11-C10-C8-C9
17	4	310	CLA	C6-C7-C8-C9
17	A	804	CLA	C11-C10-C8-C9
17	A	809	CLA	C11-C10-C8-C9
17	A	812	CLA	C11-C10-C8-C9
17	A	816	CLA	C11-C12-C13-C14
17	A	836	CLA	C11-C12-C13-C14
17	A	839	CLA	C6-C7-C8-C9
17	A	839	CLA	C11-C12-C13-C14
17	A	840	CLA	C11-C10-C8-C9
17	B	803	CLA	C11-C12-C13-C14
17	B	803	CLA	C14-C13-C15-C16
17	B	805	CLA	C14-C13-C15-C16
17	B	809	CLA	C6-C7-C8-C9
17	B	809	CLA	C14-C13-C15-C16
17	B	811	CLA	C14-C13-C15-C16
17	B	815	CLA	C14-C13-C15-C16
17	B	821	CLA	C11-C12-C13-C14
17	B	829	CLA	C11-C12-C13-C14
17	B	831	CLA	C14-C13-C15-C16
17	B	835	CLA	C14-C13-C15-C16
17	B	842	CLA	C11-C12-C13-C14
18	4	301	CHL	C6-C7-C8-C9
17	B	826	CLA	O1D-CGD-O2D-CED
18	3	607	CHL	O1D-CGD-O2D-CED
17	2	301	CLA	C15-C16-C17-C18
17	A	827	CLA	C15-C16-C17-C18
17	B	820	CLA	C10-C11-C12-C13
17	B	829	CLA	C8-C10-C11-C12
18	4	305	CHL	C2A-CAA-CBA-CGA
19	1	314	LUT	C7-C8-C9-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	1	314	LUT	C11-C12-C13-C20
19	1	314	LUT	C31-C32-C33-C40
19	2	314	LUT	C7-C8-C9-C19
19	2	314	LUT	C27-C28-C29-C39
19	3	614	LUT	C7-C8-C9-C19
19	3	614	LUT	C27-C28-C29-C39
19	3	614	LUT	C31-C32-C33-C40
19	4	316	LUT	C11-C12-C13-C20
20	1	315	XAT	C11-C12-C13-C20
20	1	315	XAT	C27-C28-C29-C39
20	1	315	XAT	C31-C32-C33-C40
20	2	315	XAT	C11-C12-C13-C20
20	2	315	XAT	C27-C28-C29-C39
20	2	315	XAT	C31-C32-C33-C40
20	3	615	XAT	C11-C12-C13-C20
20	3	615	XAT	C27-C28-C29-C39
20	3	615	XAT	C31-C32-C33-C40
21	2	316	BCR	C7-C8-C9-C34
21	4	318	BCR	C7-C8-C9-C34
21	A	846	BCR	C37-C22-C23-C24
21	A	850	BCR	C7-C8-C9-C34
21	F	303	BCR	C11-C12-C13-C35
21	4	318	BCR	C7-C8-C9-C10
21	A	850	BCR	C21-C22-C23-C24
21	L	205	BCR	C7-C8-C9-C10
22	2	317	LHG	O9-C7-O7-C5
24	4	320	LMG	C10-C11-C12-C13
17	3	606	CLA	O1A-CGA-O2A-C1
26	4	323	DGD	O1A-C1A-O1G-C1G
17	3	602	CLA	C10-C11-C12-C13
17	A	818	CLA	C8-C10-C11-C12
23	A	855	LMT	C4'-C5'-C6'-O6'
17	A	837	CLA	O1D-CGD-O2D-CED
17	B	803	CLA	C3-C5-C6-C7
17	2	302	CLA	CBA-CGA-O2A-C1
17	A	823	CLA	CBA-CGA-O2A-C1
17	1	307	CLA	C15-C16-C17-C18
17	2	308	CLA	C8-C10-C11-C12
17	A	804	CLA	C15-C16-C17-C18
17	A	827	CLA	C8-C10-C11-C12
17	A	829	CLA	C13-C15-C16-C17
17	B	808	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	816	CLA	C13-C15-C16-C17
17	B	823	CLA	C13-C15-C16-C17
17	B	838	CLA	C15-C16-C17-C18
27	A	842	PQN	C25-C26-C27-C28
17	G	103	CLA	O1D-CGD-O2D-CED
17	1	310	CLA	CBD-CGD-O2D-CED
17	1	312	CLA	C5-C6-C7-C8
17	4	310	CLA	C8-C10-C11-C12
17	A	806	CLA	C5-C6-C7-C8
17	A	812	CLA	C8-C10-C11-C12
17	A	812	CLA	C10-C11-C12-C13
17	A	817	CLA	C10-C11-C12-C13
17	A	853	CLA	C10-C11-C12-C13
17	B	833	CLA	C8-C10-C11-C12
22	F	302	LHG	C7-C8-C9-C10
26	4	323	DGD	C1B-C2B-C3B-C4B
17	1	302	CLA	C5-C6-C7-C8
17	B	826	CLA	C8-C10-C11-C12
17	B	840	CLA	C15-C16-C17-C18
22	G	102	LHG	C5-C4-O6-P
22	G	102	LHG	C7-C8-C9-C10
23	A	855	LMT	O1'-C1-C2-C3
17	A	803	CLA	C5-C6-C7-C8
17	A	837	CLA	C10-C11-C12-C13
17	A	817	CLA	O1D-CGD-O2D-CED
17	1	302	CLA	C6-C7-C8-C10
17	1	309	CLA	C11-C10-C8-C7
17	A	806	CLA	C11-C12-C13-C15
17	A	807	CLA	C11-C12-C13-C15
17	A	808	CLA	C6-C7-C8-C10
17	A	818	CLA	C12-C13-C15-C16
17	A	825	CLA	C6-C7-C8-C10
17	A	836	CLA	C6-C7-C8-C10
17	B	808	CLA	C11-C10-C8-C7
17	B	808	CLA	C11-C12-C13-C15
17	B	811	CLA	C12-C13-C15-C16
17	B	812	CLA	C11-C12-C13-C15
17	B	826	CLA	C12-C13-C15-C16
17	B	829	CLA	C12-C13-C15-C16
18	4	301	CHL	C6-C7-C8-C10
17	4	308	CLA	O1A-CGA-O2A-C1
17	A	830	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	841	CLA	O1A-CGA-O2A-C1
17	A	814	CLA	C2A-CAA-CBA-CGA
17	A	822	CLA	C2A-CAA-CBA-CGA
17	L	203	CLA	C2A-CAA-CBA-CGA
17	L	204	CLA	C2A-CAA-CBA-CGA
18	2	313	CHL	O1D-CGD-O2D-CED
17	1	308	CLA	C5-C6-C7-C8
17	A	804	CLA	C10-C11-C12-C13
17	A	820	CLA	C15-C16-C17-C18
17	A	825	CLA	C15-C16-C17-C18
17	A	831	CLA	C15-C16-C17-C18
17	A	838	CLA	C5-C6-C7-C8
17	B	816	CLA	C15-C16-C17-C18
21	K	203	BCR	C6-C7-C8-C9
17	4	313	CLA	CBD-CGD-O2D-CED
17	4	314	CLA	CBD-CGD-O2D-CED
17	B	823	CLA	CBD-CGD-O2D-CED
24	F	309	LMG	O6-C1-O1-C7
17	B	811	CLA	C13-C15-C16-C17
18	2	306	CHL	O1D-CGD-O2D-CED
19	4	316	LUT	C10-C11-C12-C13
19	4	316	LUT	C30-C31-C32-C33
20	1	315	XAT	C30-C31-C32-C33
20	2	315	XAT	C30-C31-C32-C33
20	3	615	XAT	C30-C31-C32-C33
20	4	317	XAT	C30-C31-C32-C33
21	1	316	BCR	C10-C11-C12-C13
21	3	616	BCR	C18-C19-C20-C21
21	A	850	BCR	C10-C11-C12-C13
21	B	847	BCR	C10-C11-C12-C13
25	B	851	HTG	S1-C1'-C2'-C3'
17	1	309	CLA	C5-C6-C7-C8
17	A	801	CLA	C15-C16-C17-C18
17	B	805	CLA	C13-C15-C16-C17
17	B	821	CLA	C13-C15-C16-C17
17	B	825	CLA	C10-C11-C12-C13
17	G	104	CLA	O1A-CGA-O2A-C1
18	2	306	CHL	O1A-CGA-O2A-C1
17	2	303	CLA	C5-C6-C7-C8
17	4	303	CLA	C10-C11-C12-C13
17	A	804	CLA	C13-C15-C16-C17
17	A	817	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	827	CLA	C10-C11-C12-C13
17	2	302	CLA	O1A-CGA-O2A-C1
17	A	823	CLA	O1A-CGA-O2A-C1
17	1	302	CLA	C13-C15-C16-C17
17	A	805	CLA	C15-C16-C17-C18
17	A	807	CLA	C8-C10-C11-C12
17	A	810	CLA	C15-C16-C17-C18
17	A	836	CLA	C15-C16-C17-C18
17	B	820	CLA	C5-C6-C7-C8
17	K	202	CLA	C8-C10-C11-C12
22	2	317	LHG	C4-O6-P-O3
22	A	844	LHG	C3-O3-P-O6
22	A	845	LHG	C3-O3-P-O6
22	A	845	LHG	C4-O6-P-O3
22	B	801	LHG	C4-O6-P-O3
22	F	302	LHG	C4-O6-P-O3
22	G	102	LHG	C4-O6-P-O3
17	B	831	CLA	CBA-CGA-O2A-C1
17	1	313	CLA	O1D-CGD-O2D-CED
17	B	805	CLA	CBD-CGD-O2D-CED
17	B	803	CLA	C15-C16-C17-C18
17	A	816	CLA	O1D-CGD-O2D-CED
22	F	302	LHG	C1-C2-C3-O3
17	B	838	CLA	C4-C3-C5-C6
17	1	311	CLA	C5-C6-C7-C8
17	B	842	CLA	C8-C10-C11-C12
18	4	301	CHL	C8-C10-C11-C12
18	4	301	CHL	C11-C12-C13-C15
20	4	317	XAT	C29-C30-C31-C32
22	F	302	LHG	C23-C24-C25-C26
24	B	852	LMG	C28-C29-C30-C31
22	2	317	LHG	C9-C10-C11-C12
22	G	102	LHG	C14-C15-C16-C17
24	G	101	LMG	C11-C10-O7-C8
19	2	314	LUT	C11-C10-C9-C19
19	3	614	LUT	C11-C10-C9-C19
21	4	318	BCR	C20-C21-C22-C37
21	A	851	BCR	C20-C21-C22-C37
21	B	846	BCR	C16-C17-C18-C36
21	B	849	BCR	C16-C17-C18-C36
21	F	303	BCR	C16-C17-C18-C36
21	L	201	BCR	C16-C17-C18-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	L	205	BCR	C20-C21-C22-C37
21	K	203	BCR	C20-C21-C22-C37
25	F	305	HTG	C1'-C2'-C3'-C4'
22	G	102	LHG	C15-C16-C17-C18
26	B	850	DGD	CCA-CDA-CEA-CFA
17	A	806	CLA	C16-C17-C18-C19
17	A	810	CLA	C16-C17-C18-C19
17	B	817	CLA	C6-C7-C8-C10
25	J	102	HTG	S1-C1'-C2'-C3'
24	F	309	LMG	C38-C39-C40-C41
26	B	850	DGD	C9A-CAA-CBA-CCA
26	4	323	DGD	C1G-C2G-O2G-C1B
17	3	610	CLA	O1D-CGD-O2D-CED
17	B	834	CLA	C5-C6-C7-C8
17	B	840	CLA	CBD-CGD-O2D-CED
17	J	101	CLA	O1D-CGD-O2D-CED
22	A	844	LHG	C32-C33-C34-C35
24	B	852	LMG	C11-C12-C13-C14
26	4	323	DGD	C2A-C3A-C4A-C5A
26	4	323	DGD	C6B-C7B-C8B-C9B
26	4	323	DGD	CDB-CEB-CFB-CGB
17	B	835	CLA	O1D-CGD-O2D-CED
19	4	316	LUT	C28-C29-C30-C31
20	1	315	XAT	C12-C13-C14-C15
20	2	315	XAT	C12-C13-C14-C15
20	3	615	XAT	C12-C13-C14-C15
21	1	316	BCR	C20-C21-C22-C23
21	2	316	BCR	C12-C13-C14-C15
21	2	316	BCR	C16-C17-C18-C19
21	4	318	BCR	C20-C21-C22-C23
21	A	848	BCR	C16-C17-C18-C19
21	B	845	BCR	C11-C10-C9-C8
21	B	849	BCR	C11-C10-C9-C8
21	B	849	BCR	C16-C17-C18-C19
21	I	101	BCR	C20-C21-C22-C23
21	L	205	BCR	C20-C21-C22-C23
21	K	203	BCR	C16-C17-C18-C19
23	A	855	LMT	C2'-C1'-O1'-C1
22	A	844	LHG	C24-C25-C26-C27
24	B	852	LMG	C12-C13-C14-C15
17	B	815	CLA	C13-C15-C16-C17
17	B	826	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	836	CLA	C16-C17-C18-C19
17	L	202	CLA	C4-C3-C5-C6
22	2	317	LHG	C11-C10-C9-C8
22	G	102	LHG	C31-C32-C33-C34
24	4	319	LMG	C32-C33-C34-C35
24	F	309	LMG	C34-C35-C36-C37
26	B	850	DGD	C8B-C9B-CAB-CBB
17	B	838	CLA	C2-C3-C5-C6
17	1	302	CLA	C6-C7-C8-C9
17	A	801	CLA	C14-C13-C15-C16
17	A	806	CLA	C14-C13-C15-C16
17	A	809	CLA	C11-C12-C13-C14
17	A	829	CLA	C14-C13-C15-C16
17	B	823	CLA	C14-C13-C15-C16
17	B	840	CLA	C6-C7-C8-C9
17	L	202	CLA	C14-C13-C15-C16
17	A	843	CLA	O1D-CGD-O2D-CED
22	1	317	LHG	C9-C10-C11-C12
22	1	317	LHG	C15-C16-C17-C18
23	A	855	LMT	C6-C7-C8-C9
24	4	320	LMG	C15-C16-C17-C18
17	B	808	CLA	C5-C6-C7-C8
17	3	610	CLA	C2A-CAA-CBA-CGA
17	A	808	CLA	C2A-CAA-CBA-CGA
19	1	314	LUT	C27-C28-C29-C39
19	2	314	LUT	C11-C12-C13-C20
19	3	614	LUT	C11-C12-C13-C20
19	4	316	LUT	C27-C28-C29-C39
21	L	205	BCR	C7-C8-C9-C34
22	2	317	LHG	C27-C28-C29-C30
22	A	844	LHG	C17-C18-C19-C20
26	B	850	DGD	CDB-CEB-CFB-CGB
22	A	845	LHG	O1-C1-C2-C3
22	B	801	LHG	O1-C1-C2-C3
22	F	302	LHG	O1-C1-C2-C3
25	J	102	HTG	C1'-C2'-C3'-C4'
21	2	316	BCR	C7-C8-C9-C10
17	K	202	CLA	C3-C5-C6-C7
22	2	317	LHG	C8-C7-O7-C5
22	G	102	LHG	C16-C17-C18-C19
23	2	318	LMT	C11-C10-C9-C8
26	4	323	DGD	C5B-C6B-C7B-C8B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	850	DGD	C3B-C4B-C5B-C6B
22	1	317	LHG	C32-C33-C34-C35
22	G	102	LHG	C17-C18-C19-C20
24	4	319	LMG	C36-C37-C38-C39
24	4	320	LMG	C13-C14-C15-C16
24	G	101	LMG	C15-C16-C17-C18
17	A	832	CLA	C16-C17-C18-C19
17	B	817	CLA	C6-C7-C8-C9
18	4	305	CHL	C6-C7-C8-C9
17	B	829	CLA	C13-C15-C16-C17
17	B	841	CLA	O1D-CGD-O2D-CED
22	1	317	LHG	C14-C15-C16-C17
22	A	844	LHG	C27-C28-C29-C30
26	B	850	DGD	CEB-CFB-CGB-CHB
17	G	104	CLA	O1D-CGD-O2D-CED
22	2	317	LHG	C10-C11-C12-C13
22	1	317	LHG	C7-C8-C9-C10
17	4	309	CLA	C10-C11-C12-C13
17	A	809	CLA	C5-C6-C7-C8
24	B	852	LMG	O10-C28-O8-C9
22	A	844	LHG	C15-C16-C17-C18
24	B	852	LMG	C14-C15-C16-C17
24	B	852	LMG	C38-C39-C40-C41
17	1	310	CLA	CBA-CGA-O2A-C1
22	A	844	LHG	C29-C30-C31-C32
17	G	105	CLA	O1D-CGD-O2D-CED
17	1	309	CLA	C3A-C2A-CAA-CBA
17	1	310	CLA	C3A-C2A-CAA-CBA
17	1	312	CLA	C3A-C2A-CAA-CBA
17	4	303	CLA	C3A-C2A-CAA-CBA
17	4	304	CLA	C3A-C2A-CAA-CBA
17	A	810	CLA	C3A-C2A-CAA-CBA
17	A	831	CLA	C3A-C2A-CAA-CBA
17	A	835	CLA	C3A-C2A-CAA-CBA
17	B	831	CLA	C3A-C2A-CAA-CBA
17	F	307	CLA	C3A-C2A-CAA-CBA
17	J	101	CLA	C3A-C2A-CAA-CBA
18	1	305	CHL	C3A-C2A-CAA-CBA
18	4	301	CHL	C3A-C2A-CAA-CBA
20	1	315	XAT	C29-C30-C31-C32
20	2	315	XAT	C29-C30-C31-C32
20	3	615	XAT	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	4	320	LMG	C20-C21-C22-C23
26	B	850	DGD	C1B-C2B-C3B-C4B
17	B	834	CLA	O1D-CGD-O2D-CED
17	1	312	CLA	C6-C7-C8-C9
22	2	317	LHG	C25-C26-C27-C28
24	G	101	LMG	C17-C18-C19-C20
26	B	850	DGD	CBA-CCA-CDA-CEA
21	3	616	BCR	C14-C15-C16-C17
22	1	317	LHG	C23-C24-C25-C26
24	F	309	LMG	C28-C29-C30-C31
22	1	317	LHG	C11-C10-C9-C8
17	A	837	CLA	C4-C3-C5-C6
17	F	307	CLA	C4-C3-C5-C6
17	1	307	CLA	C2-C3-C5-C6
17	A	803	CLA	C2-C3-C5-C6
17	A	837	CLA	C2-C3-C5-C6
17	B	813	CLA	C2-C3-C5-C6
17	F	307	CLA	C2-C3-C5-C6
17	L	202	CLA	C2-C3-C5-C6
22	A	844	LHG	C8-C7-O7-C5
22	A	845	LHG	O1-C1-C2-O2
24	F	309	LMG	C29-C30-C31-C32
17	4	303	CLA	C11-C12-C13-C14
17	2	311	CLA	C5-C6-C7-C8
17	A	831	CLA	C5-C6-C7-C8
22	1	317	LHG	C16-C17-C18-C19
22	G	102	LHG	C11-C10-C9-C8
25	A	854	HTG	C4-C5-C6-O6
22	F	302	LHG	C17-C18-C19-C20
24	B	852	LMG	C16-C17-C18-C19
24	F	309	LMG	C14-C15-C16-C17
17	B	831	CLA	O1A-CGA-O2A-C1
22	F	302	LHG	C14-C15-C16-C17
22	F	302	LHG	C15-C16-C17-C18
17	2	303	CLA	C2-C1-O2A-CGA
25	B	851	HTG	C4-C5-C6-O6
17	A	802	CLA	C10-C11-C12-C13
17	A	828	CLA	C15-C16-C17-C18
22	A	844	LHG	C11-C10-C9-C8
22	G	102	LHG	C25-C26-C27-C28
24	4	319	LMG	C35-C36-C37-C38
26	4	323	DGD	C3B-C4B-C5B-C6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	850	DGD	C8A-C9A-CAA-CBA
18	4	301	CHL	C11-C12-C13-C14
17	B	837	CLA	C3-C5-C6-C7
21	1	316	BCR	C23-C24-C25-C26
21	1	316	BCR	C23-C24-C25-C30
21	2	316	BCR	C1-C6-C7-C8
21	2	316	BCR	C5-C6-C7-C8
21	3	616	BCR	C23-C24-C25-C26
21	4	318	BCR	C23-C24-C25-C26
21	4	318	BCR	C23-C24-C25-C30
21	A	847	BCR	C1-C6-C7-C8
21	A	847	BCR	C5-C6-C7-C8
21	A	847	BCR	C23-C24-C25-C26
21	A	847	BCR	C23-C24-C25-C30
21	A	850	BCR	C23-C24-C25-C30
21	B	847	BCR	C23-C24-C25-C26
21	B	848	BCR	C23-C24-C25-C30
21	B	849	BCR	C5-C6-C7-C8
21	G	106	BCR	C23-C24-C25-C26
21	J	105	BCR	C5-C6-C7-C8
21	J	105	BCR	C23-C24-C25-C30
21	L	201	BCR	C23-C24-C25-C26
21	L	206	BCR	C23-C24-C25-C26
17	A	816	CLA	CBA-CGA-O2A-C1
17	A	821	CLA	CBA-CGA-O2A-C1
17	A	843	CLA	CBA-CGA-O2A-C1
17	4	303	CLA	C5-C6-C7-C8
17	A	816	CLA	C13-C15-C16-C17
17	A	840	CLA	C10-C11-C12-C13
17	B	835	CLA	C5-C6-C7-C8
22	1	317	LHG	C8-C7-O7-C5
17	A	832	CLA	O1D-CGD-O2D-CED
17	B	809	CLA	CBD-CGD-O2D-CED
24	B	852	LMG	C34-C35-C36-C37
17	1	307	CLA	C4-C3-C5-C6
17	A	803	CLA	C4-C3-C5-C6
17	B	813	CLA	C4-C3-C5-C6
17	A	835	CLA	O1D-CGD-O2D-CED
17	2	311	CLA	C12-C13-C15-C16
17	4	303	CLA	C6-C7-C8-C10
17	A	801	CLA	C12-C13-C15-C16
17	A	802	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	804	CLA	C11-C10-C8-C7
17	A	809	CLA	C11-C10-C8-C7
17	A	809	CLA	C11-C12-C13-C15
17	A	818	CLA	C11-C10-C8-C7
17	A	826	CLA	C2-C3-C5-C6
17	A	827	CLA	C11-C10-C8-C7
17	A	828	CLA	C2-C3-C5-C6
17	A	829	CLA	C12-C13-C15-C16
17	A	836	CLA	C11-C12-C13-C15
17	A	838	CLA	C6-C7-C8-C10
17	B	803	CLA	C12-C13-C15-C16
17	B	807	CLA	C11-C10-C8-C7
17	B	809	CLA	C11-C10-C8-C7
17	B	820	CLA	C11-C10-C8-C7
17	B	821	CLA	C11-C12-C13-C15
17	B	823	CLA	C12-C13-C15-C16
17	B	835	CLA	C12-C13-C15-C16
17	B	837	CLA	C11-C10-C8-C7
17	B	840	CLA	C2-C3-C5-C6
17	B	840	CLA	C6-C7-C8-C10
17	J	101	CLA	C11-C10-C8-C7
17	B	829	CLA	C3-C5-C6-C7
17	1	310	CLA	O1A-CGA-O2A-C1
17	A	806	CLA	C16-C17-C18-C20
17	B	809	CLA	C16-C17-C18-C19
17	L	202	CLA	C16-C17-C18-C19
17	A	827	CLA	O1D-CGD-O2D-CED
24	G	101	LMG	O9-C10-O7-C8
17	A	836	CLA	CBA-CGA-O2A-C1
17	B	824	CLA	CBA-CGA-O2A-C1
17	B	833	CLA	CBA-CGA-O2A-C1
17	3	613	CLA	C2A-CAA-CBA-CGA
17	1	302	CLA	O1D-CGD-O2D-CED
17	A	807	CLA	C5-C6-C7-C8
17	A	836	CLA	C13-C15-C16-C17
22	G	102	LHG	C9-C10-C11-C12
17	1	302	CLA	C15-C16-C17-C18
26	B	850	DGD	C6B-C7B-C8B-C9B
23	A	855	LMT	C1-C2-C3-C4
22	1	317	LHG	C24-C25-C26-C27
19	3	614	LUT	C6-C7-C8-C9
21	K	203	BCR	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	3	608	CLA	CBD-CGD-O2D-CED
17	1	308	CLA	C11-C12-C13-C15
17	2	308	CLA	C11-C12-C13-C14
23	A	855	LMT	O5'-C1'-O1'-C1
22	1	317	LHG	C17-C18-C19-C20
17	2	303	CLA	C10-C11-C12-C13
17	B	838	CLA	C13-C15-C16-C17
22	A	844	LHG	O9-C7-O7-C5
26	4	323	DGD	C2E-C1E-O5D-C6D
17	A	824	CLA	CBD-CGD-O2D-CED
17	A	853	CLA	C16-C17-C18-C20
25	B	851	HTG	C1'-C2'-C3'-C4'
24	4	319	LMG	C33-C34-C35-C36
17	3	610	CLA	C4-C3-C5-C6
17	A	826	CLA	C4-C3-C5-C6
17	A	838	CLA	C4-C3-C5-C6
17	B	840	CLA	C4-C3-C5-C6
17	1	308	CLA	C2-C3-C5-C6
17	A	838	CLA	C2-C3-C5-C6
17	1	308	CLA	C6-C7-C8-C9
17	2	311	CLA	C14-C13-C15-C16
17	A	802	CLA	C11-C10-C8-C9
17	A	806	CLA	C11-C12-C13-C14
17	A	807	CLA	C11-C12-C13-C14
17	A	818	CLA	C11-C10-C8-C9
17	A	827	CLA	C11-C10-C8-C9
17	A	829	CLA	C11-C10-C8-C9
17	A	836	CLA	C6-C7-C8-C9
17	A	837	CLA	C14-C13-C15-C16
17	A	838	CLA	C11-C12-C13-C14
17	A	839	CLA	C14-C13-C15-C16
17	B	807	CLA	C11-C10-C8-C9
17	B	808	CLA	C11-C10-C8-C9
17	B	808	CLA	C11-C12-C13-C14
17	B	809	CLA	C11-C10-C8-C9
17	B	820	CLA	C11-C10-C8-C9
17	B	828	CLA	C11-C10-C8-C9
17	B	829	CLA	C14-C13-C15-C16
17	B	837	CLA	C11-C10-C8-C9
17	J	101	CLA	C11-C10-C8-C9
17	3	612	CLA	O1D-CGD-O2D-CED
24	F	309	LMG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	811	CLA	C3-C5-C6-C7
17	2	303	CLA	C2A-CAA-CBA-CGA
17	A	802	CLA	C2A-CAA-CBA-CGA
17	A	817	CLA	C2A-CAA-CBA-CGA
17	A	853	CLA	C2A-CAA-CBA-CGA
18	1	305	CHL	C2A-CAA-CBA-CGA
24	4	319	LMG	C30-C31-C32-C33
24	4	320	LMG	O6-C5-C6-O5
21	A	851	BCR	C7-C8-C9-C10
17	A	816	CLA	O1A-CGA-O2A-C1
17	A	843	CLA	O1A-CGA-O2A-C1
17	1	306	CLA	C1A-C2A-CAA-CBA
17	1	310	CLA	C1A-C2A-CAA-CBA
17	2	303	CLA	C1A-C2A-CAA-CBA
17	2	308	CLA	C1A-C2A-CAA-CBA
17	3	609	CLA	C1A-C2A-CAA-CBA
17	4	303	CLA	C1A-C2A-CAA-CBA
17	4	313	CLA	C1A-C2A-CAA-CBA
17	A	807	CLA	C1A-C2A-CAA-CBA
17	A	808	CLA	C1A-C2A-CAA-CBA
17	A	817	CLA	C1A-C2A-CAA-CBA
17	A	835	CLA	C1A-C2A-CAA-CBA
17	B	803	CLA	C1A-C2A-CAA-CBA
17	B	806	CLA	C1A-C2A-CAA-CBA
17	B	820	CLA	C1A-C2A-CAA-CBA
17	B	822	CLA	C1A-C2A-CAA-CBA
17	B	829	CLA	C1A-C2A-CAA-CBA
17	F	304	CLA	C1A-C2A-CAA-CBA
17	F	307	CLA	C1A-C2A-CAA-CBA
17	J	101	CLA	C1A-C2A-CAA-CBA
17	L	204	CLA	C1A-C2A-CAA-CBA
17	1	301	CLA	C16-C17-C18-C19
17	1	301	CLA	C16-C17-C18-C20
17	1	308	CLA	C11-C12-C13-C14
17	B	812	CLA	C16-C17-C18-C19
17	B	825	CLA	C11-C12-C13-C15
17	L	202	CLA	C16-C17-C18-C20
17	A	804	CLA	C8-C10-C11-C12
24	4	320	LMG	C14-C15-C16-C17
17	A	821	CLA	O1A-CGA-O2A-C1
17	K	202	CLA	C10-C11-C12-C13
17	B	832	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	A	845	LHG	O6-C4-C5-C6
17	4	312	CLA	C5-C6-C7-C8
17	A	829	CLA	C5-C6-C7-C8
17	A	832	CLA	C16-C17-C18-C20
18	4	305	CHL	C6-C7-C8-C10
17	2	301	CLA	C3-C5-C6-C7
24	4	319	LMG	O6-C5-C6-O5
17	A	828	CLA	C4-C3-C5-C6
26	B	850	DGD	C4B-C5B-C6B-C7B
17	A	836	CLA	C10-C11-C12-C13
17	B	838	CLA	C8-C10-C11-C12
17	A	834	CLA	O1D-CGD-O2D-CED
17	A	836	CLA	O1A-CGA-O2A-C1
17	B	833	CLA	O1A-CGA-O2A-C1
17	1	311	CLA	C11-C12-C13-C15
27	A	842	PQN	C26-C27-C28-C29
25	B	851	HTG	O5-C5-C6-O6
22	A	845	LHG	C4-C5-C6-O8
22	F	302	LHG	C25-C26-C27-C28
24	4	320	LMG	O1-C7-C8-C9
24	F	309	LMG	O1-C7-C8-C9
17	B	837	CLA	C5-C6-C7-C8
24	4	320	LMG	C28-C29-C30-C31
19	1	314	LUT	C14-C15-C35-C34
17	1	307	CLA	C8-C10-C11-C12
17	A	839	CLA	C5-C6-C7-C8
25	F	305	HTG	S1-C1'-C2'-C3'
24	4	320	LMG	C18-C19-C20-C21
24	4	319	LMG	C31-C32-C33-C34
24	B	852	LMG	C39-C40-C41-C42
17	2	308	CLA	C11-C12-C13-C15
17	A	816	CLA	C10-C11-C12-C13
22	F	302	LHG	O1-C1-C2-O2
22	G	102	LHG	O1-C1-C2-O2
17	1	310	CLA	C3-C5-C6-C7
17	2	311	CLA	C13-C15-C16-C17
24	4	320	LMG	C21-C22-C23-C24
21	K	203	BCR	C16-C17-C18-C36
17	A	811	CLA	C6-C7-C8-C9
17	B	824	CLA	O1A-CGA-O2A-C1
17	4	310	CLA	C2-C3-C5-C6
17	1	302	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	809	CLA	C16-C17-C18-C20
17	B	830	CLA	CBA-CGA-O2A-C1
23	2	318	LMT	O5'-C5'-C6'-O6'
22	A	844	LHG	C26-C27-C28-C29
17	A	829	CLA	CBD-CGD-O2D-CED
17	A	828	CLA	C13-C15-C16-C17
17	K	202	CLA	C5-C6-C7-C8
17	1	309	CLA	C2A-CAA-CBA-CGA
17	2	311	CLA	C8-C10-C11-C12
17	A	816	CLA	C15-C16-C17-C18
17	B	829	CLA	C15-C16-C17-C18
17	4	308	CLA	C2-C1-O2A-CGA
17	B	835	CLA	C2-C1-O2A-CGA
26	B	850	DGD	CFB-CGB-CHB-CIB
17	1	310	CLA	O1D-CGD-O2D-CED
24	B	852	LMG	O6-C5-C6-O5
17	A	810	CLA	C8-C10-C11-C12
17	1	309	CLA	C16-C17-C18-C20
17	B	812	CLA	C16-C17-C18-C20
17	B	809	CLA	C5-C6-C7-C8
17	B	840	CLA	O1D-CGD-O2D-CED
17	B	830	CLA	O1A-CGA-O2A-C1
22	2	317	LHG	C23-C24-C25-C26
17	4	309	CLA	C5-C6-C7-C8
17	B	841	CLA	C15-C16-C17-C18
24	4	320	LMG	C2-C1-O1-C7
17	A	805	CLA	CAA-CBA-CGA-O2A
22	A	844	LHG	O7-C5-C6-O8
23	2	318	LMT	C4-C5-C6-C7
24	G	101	LMG	C14-C15-C16-C17
17	4	310	CLA	C4-C3-C5-C6
17	1	302	CLA	C12-C13-C15-C16
17	1	309	CLA	C11-C12-C13-C15
17	1	309	CLA	C12-C13-C15-C16
17	2	303	CLA	C11-C10-C8-C7
17	2	308	CLA	C11-C10-C8-C7
17	A	805	CLA	C11-C10-C8-C7
17	A	806	CLA	C6-C7-C8-C10
17	A	806	CLA	C12-C13-C15-C16
17	A	816	CLA	C11-C12-C13-C15
17	A	828	CLA	C12-C13-C15-C16
17	A	829	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	837	CLA	C12-C13-C15-C16
17	A	838	CLA	C11-C12-C13-C15
17	A	839	CLA	C6-C7-C8-C10
17	A	839	CLA	C12-C13-C15-C16
17	B	802	CLA	C11-C12-C13-C15
17	B	803	CLA	C6-C7-C8-C10
17	B	805	CLA	C11-C10-C8-C7
17	B	809	CLA	C6-C7-C8-C10
17	B	815	CLA	C11-C10-C8-C7
17	B	826	CLA	C11-C10-C8-C7
17	B	828	CLA	C11-C10-C8-C7
17	B	834	CLA	C6-C7-C8-C10
17	B	835	CLA	C11-C12-C13-C15
17	L	202	CLA	C11-C12-C13-C15
17	L	202	CLA	C12-C13-C15-C16
17	K	202	CLA	C6-C7-C8-C10
18	4	301	CHL	C11-C10-C8-C7
24	F	309	LMG	C18-C19-C20-C21
17	1	307	CLA	C14-C13-C15-C16
17	1	309	CLA	C11-C10-C8-C9
17	1	309	CLA	C11-C12-C13-C14
17	4	302	CLA	C11-C10-C8-C9
17	A	805	CLA	C11-C10-C8-C9
17	A	805	CLA	C11-C12-C13-C14
17	A	805	CLA	C14-C13-C15-C16
17	A	806	CLA	C6-C7-C8-C9
17	A	832	CLA	C6-C7-C8-C9
17	A	840	CLA	C6-C7-C8-C9
17	B	803	CLA	C6-C7-C8-C9
17	B	805	CLA	C11-C10-C8-C9
17	B	815	CLA	C11-C10-C8-C9
17	B	816	CLA	C6-C7-C8-C9
17	B	826	CLA	C11-C10-C8-C9
17	B	826	CLA	C14-C13-C15-C16
17	B	827	CLA	C14-C13-C15-C16
17	B	828	CLA	C11-C12-C13-C14
17	B	835	CLA	C6-C7-C8-C9
17	B	835	CLA	C11-C12-C13-C14
17	B	837	CLA	C6-C7-C8-C9
17	B	838	CLA	C14-C13-C15-C16
17	K	202	CLA	C6-C7-C8-C9
17	B	807	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	853	CLA	C16-C17-C18-C19
22	1	317	LHG	C28-C29-C30-C31
17	B	811	CLA	C15-C16-C17-C18
22	F	302	LHG	C26-C27-C28-C29
17	2	303	CLA	CBA-CGA-O2A-C1
17	B	818	CLA	CBA-CGA-O2A-C1
17	B	804	CLA	C15-C16-C17-C18
22	G	102	LHG	C27-C28-C29-C30
25	A	854	HTG	O5-C5-C6-O6
17	A	836	CLA	C16-C17-C18-C20
17	2	303	CLA	C8-C10-C11-C12
22	G	102	LHG	O6-C4-C5-C6
17	A	824	CLA	CBA-CGA-O2A-C1
21	B	849	BCR	C10-C11-C12-C13
17	1	312	CLA	CAA-CBA-CGA-O2A
17	B	804	CLA	O1D-CGD-O2D-CED
17	B	814	CLA	C4-C3-C5-C6
17	B	809	CLA	O1D-CGD-O2D-CED
17	B	812	CLA	C5-C6-C7-C8
17	B	832	CLA	O1A-CGA-O2A-C1
24	F	309	LMG	C40-C41-C42-C43
17	B	827	CLA	C16-C17-C18-C20
26	B	850	DGD	C5A-C6A-C7A-C8A
26	B	850	DGD	C2B-C3B-C4B-C5B
17	A	826	CLA	CBA-CGA-O2A-C1
17	A	805	CLA	C3A-C2A-CAA-CBA
17	A	837	CLA	C3A-C2A-CAA-CBA
17	B	823	CLA	O1D-CGD-O2D-CED
21	K	203	BCR	C15-C16-C17-C18
23	A	855	LMT	C2-C1-O1'-C1'
17	B	805	CLA	O1D-CGD-O2D-CED
17	1	309	CLA	C15-C16-C17-C18
17	B	808	CLA	C8-C10-C11-C12
17	B	813	CLA	C6-C7-C8-C10
17	1	302	CLA	CBA-CGA-O2A-C1
17	A	809	CLA	C8-C10-C11-C12
17	B	818	CLA	C5-C6-C7-C8
24	G	101	LMG	C7-C8-C9-O8
26	B	850	DGD	O1G-C1G-C2G-C3G
22	F	302	LHG	C11-C10-C9-C8
24	4	319	LMG	C17-C18-C19-C20
17	B	814	CLA	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	4	320	LMG	C29-C30-C31-C32
24	B	852	LMG	C15-C16-C17-C18
26	B	850	DGD	C9B-CAB-CBB-CCB
17	B	814	CLA	C2-C3-C5-C6
18	2	304	CHL	C3C-C2C-CMC-OMC
24	4	319	LMG	C18-C19-C20-C21
17	1	307	CLA	C3-C5-C6-C7
22	B	801	LHG	O1-C1-C2-O2
24	B	852	LMG	C29-C30-C31-C32
26	4	323	DGD	C6A-C7A-C8A-C9A
22	B	801	LHG	C7-C8-C9-C10
18	3	601	CHL	CBA-CGA-O2A-C1
22	A	844	LHG	C19-C20-C21-C22
17	4	310	CLA	C10-C11-C12-C13
22	1	317	LHG	C19-C20-C21-C22
26	4	323	DGD	O1G-C1A-C2A-C3A
22	F	302	LHG	C18-C19-C20-C21
24	G	101	LMG	C16-C17-C18-C19
17	1	302	CLA	O1A-CGA-O2A-C1
22	A	844	LHG	C10-C11-C12-C13
24	F	309	LMG	O7-C8-C9-O8
17	B	809	CLA	C15-C16-C17-C18
17	A	810	CLA	C16-C17-C18-C20
17	B	825	CLA	C11-C12-C13-C14
27	A	842	PQN	C26-C27-C28-C30
22	A	844	LHG	C1-C2-C3-O3
24	B	852	LMG	O9-C10-O7-C8
17	A	837	CLA	C2-C1-O2A-CGA
17	A	853	CLA	C2-C1-O2A-CGA
17	1	302	CLA	C14-C13-C15-C16
17	1	309	CLA	C14-C13-C15-C16
17	2	301	CLA	C6-C7-C8-C9
17	A	808	CLA	C6-C7-C8-C9
17	A	812	CLA	C11-C12-C13-C14
17	A	817	CLA	C14-C13-C15-C16
17	A	818	CLA	C14-C13-C15-C16
17	A	826	CLA	C6-C7-C8-C9
17	A	831	CLA	C14-C13-C15-C16
17	B	827	CLA	C11-C10-C8-C9
17	B	834	CLA	C11-C10-C8-C9
17	F	304	CLA	C14-C13-C15-C16
18	4	301	CHL	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	1	312	CLA	C6-C7-C8-C10
17	B	813	CLA	C6-C7-C8-C9
17	B	826	CLA	C16-C17-C18-C20
17	B	837	CLA	C11-C12-C13-C15
21	2	316	BCR	C23-C24-C25-C26
21	2	316	BCR	C23-C24-C25-C30
21	A	848	BCR	C1-C6-C7-C8
21	A	848	BCR	C5-C6-C7-C8
21	A	849	BCR	C5-C6-C7-C8
21	A	849	BCR	C23-C24-C25-C26
21	A	850	BCR	C1-C6-C7-C8
21	A	850	BCR	C5-C6-C7-C8
21	B	844	BCR	C23-C24-C25-C26
21	L	201	BCR	C1-C6-C7-C8
21	L	201	BCR	C5-C6-C7-C8
21	L	205	BCR	C5-C6-C7-C8
21	L	206	BCR	C1-C6-C7-C8
21	L	206	BCR	C5-C6-C7-C8
17	3	611	CLA	C5-C6-C7-C8
24	F	309	LMG	C35-C36-C37-C38
17	3	608	CLA	O1D-CGD-O2D-CED
17	4	313	CLA	O1D-CGD-O2D-CED
18	2	313	CHL	C1A-C2A-CAA-CBA
21	3	616	BCR	C21-C22-C23-C24
21	B	845	BCR	C7-C8-C9-C10
17	1	309	CLA	C16-C17-C18-C19
17	1	311	CLA	C11-C12-C13-C14
17	4	303	CLA	C11-C12-C13-C15
17	A	829	CLA	O1D-CGD-O2D-CED
17	J	101	CLA	C10-C11-C12-C13
17	B	818	CLA	O1A-CGA-O2A-C1
17	A	839	CLA	O1D-CGD-O2D-CED
17	A	838	CLA	C15-C16-C17-C18
17	4	302	CLA	C11-C10-C8-C7
17	A	805	CLA	C11-C12-C13-C15
17	A	805	CLA	C12-C13-C15-C16
17	A	812	CLA	C11-C10-C8-C7
17	A	812	CLA	C11-C12-C13-C15
17	A	818	CLA	C11-C12-C13-C15
17	A	826	CLA	C6-C7-C8-C10
17	A	832	CLA	C6-C7-C8-C10
17	A	839	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	840	CLA	C6-C7-C8-C10
17	A	841	CLA	C11-C12-C13-C15
17	B	805	CLA	C12-C13-C15-C16
17	B	811	CLA	C6-C7-C8-C10
17	B	816	CLA	C6-C7-C8-C10
17	B	820	CLA	C6-C7-C8-C10
17	B	828	CLA	C11-C12-C13-C15
17	B	831	CLA	C11-C12-C13-C15
17	B	834	CLA	C11-C10-C8-C7
17	B	835	CLA	C6-C7-C8-C10
17	B	837	CLA	C6-C7-C8-C10
17	B	840	CLA	C12-C13-C15-C16
17	F	304	CLA	C12-C13-C15-C16
17	L	202	CLA	C6-C7-C8-C10
17	A	805	CLA	C8-C10-C11-C12
21	1	316	BCR	C19-C20-C21-C22
21	2	316	BCR	C15-C16-C17-C18
17	1	302	CLA	C16-C17-C18-C19
17	B	810	CLA	C16-C17-C18-C19
17	B	820	CLA	C11-C12-C13-C15
17	B	807	CLA	C10-C11-C12-C13
17	B	826	CLA	C13-C15-C16-C17
17	B	829	CLA	C10-C11-C12-C13
17	2	303	CLA	O1A-CGA-O2A-C1
17	B	819	CLA	C2A-CAA-CBA-CGA
17	A	843	CLA	C4C-C3C-CAC-CBC
21	3	616	BCR	C11-C10-C9-C34
21	4	318	BCR	C16-C17-C18-C36
17	L	203	CLA	C3-C5-C6-C7
22	G	102	LHG	C10-C11-C12-C13
17	B	826	CLA	C16-C17-C18-C19
17	A	811	CLA	CBA-CGA-O2A-C1
17	A	831	CLA	CBA-CGA-O2A-C1
17	A	824	CLA	C10-C11-C12-C13
17	4	309	CLA	CAD-CBD-CGD-O2D
17	A	825	CLA	CAD-CBD-CGD-O2D
17	A	840	CLA	CAD-CBD-CGD-O2D
17	B	813	CLA	CAD-CBD-CGD-O2D
17	B	827	CLA	CAD-CBD-CGD-O2D
17	B	828	CLA	CAD-CBD-CGD-O2D
17	B	838	CLA	CAD-CBD-CGD-O2D
17	A	809	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	810	CLA	C4-C3-C5-C6
24	F	309	LMG	C39-C40-C41-C42
24	F	309	LMG	C7-C8-C9-O8
17	A	824	CLA	O1A-CGA-O2A-C1
22	B	801	LHG	O6-C4-C5-O7
17	A	810	CLA	C5-C6-C7-C8
17	B	823	CLA	C5-C6-C7-C8
24	4	319	LMG	C22-C23-C24-C25
21	L	201	BCR	C14-C15-C16-C17
17	B	827	CLA	C16-C17-C18-C19
17	1	304	CLA	CHA-CBD-CGD-O2D
17	2	301	CLA	CHA-CBD-CGD-O1D
17	2	301	CLA	CHA-CBD-CGD-O2D
17	A	807	CLA	CHA-CBD-CGD-O1D
17	A	807	CLA	CHA-CBD-CGD-O2D
17	A	816	CLA	CHA-CBD-CGD-O1D
17	A	819	CLA	CHA-CBD-CGD-O1D
17	A	822	CLA	CHA-CBD-CGD-O1D
17	A	822	CLA	CHA-CBD-CGD-O2D
17	A	823	CLA	CHA-CBD-CGD-O1D
17	A	823	CLA	CHA-CBD-CGD-O2D
17	A	829	CLA	CHA-CBD-CGD-O1D
17	A	832	CLA	CHA-CBD-CGD-O1D
17	B	807	CLA	CHA-CBD-CGD-O1D
17	B	807	CLA	CHA-CBD-CGD-O2D
17	B	815	CLA	CHA-CBD-CGD-O1D
17	B	817	CLA	CHA-CBD-CGD-O1D
17	B	826	CLA	CHA-CBD-CGD-O1D
17	B	826	CLA	CHA-CBD-CGD-O2D
17	B	828	CLA	CHA-CBD-CGD-O1D
17	B	831	CLA	CHA-CBD-CGD-O1D
17	B	838	CLA	CHA-CBD-CGD-O1D
17	G	105	CLA	CHA-CBD-CGD-O1D
17	G	105	CLA	CHA-CBD-CGD-O2D
17	K	202	CLA	CHA-CBD-CGD-O1D
17	A	808	CLA	C3-C5-C6-C7
21	2	316	BCR	C20-C21-C22-C23
22	A	845	LHG	O7-C5-C6-O8
17	A	826	CLA	O1A-CGA-O2A-C1
22	F	302	LHG	C10-C11-C12-C13
17	A	816	CLA	C16-C17-C18-C19
17	A	824	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	810	CLA	C3-C5-C6-C7
26	4	323	DGD	C4B-C5B-C6B-C7B
18	3	601	CHL	O1A-CGA-O2A-C1
17	A	825	CLA	C11-C12-C13-C14
17	A	832	CLA	C11-C12-C13-C14
17	A	838	CLA	C6-C7-C8-C9
17	A	853	CLA	C11-C12-C13-C14
17	B	840	CLA	C14-C13-C15-C16
17	B	841	CLA	C6-C7-C8-C9
17	A	811	CLA	O1A-CGA-O2A-C1
17	B	812	CLA	C13-C15-C16-C17
17	4	304	CLA	C2A-CAA-CBA-CGA
17	4	313	CLA	C2A-CAA-CBA-CGA
24	4	319	LMG	C29-C30-C31-C32
26	B	850	DGD	CDA-CEA-CFA-CGA
17	A	839	CLA	C8-C10-C11-C12
20	4	317	XAT	C7-C8-C9-C10
21	J	105	BCR	C21-C22-C23-C24
17	A	836	CLA	C3-C5-C6-C7
17	A	823	CLA	C1A-C2A-CAA-CBA
17	B	815	CLA	C1A-C2A-CAA-CBA
17	B	833	CLA	C1A-C2A-CAA-CBA
17	K	202	CLA	C1A-C2A-CAA-CBA
18	3	607	CHL	C1A-C2A-CAA-CBA
17	4	302	CLA	C10-C11-C12-C13
17	4	304	CLA	C2-C1-O2A-CGA
17	A	839	CLA	CBD-CGD-O2D-CED
17	2	311	CLA	CBA-CGA-O2A-C1
22	1	317	LHG	C3-O3-P-O6
23	2	318	LMT	O1'-C1-C2-C3
24	F	309	LMG	C37-C38-C39-C40
22	F	302	LHG	C9-C10-C11-C12
17	A	843	CLA	C4-C3-C5-C6
22	G	102	LHG	C2-C3-O3-P
17	3	610	CLA	C2-C3-C5-C6
22	B	801	LHG	O10-C23-O8-C6
23	A	855	LMT	C5-C6-C7-C8
22	2	317	LHG	C4-O6-P-O4
22	A	844	LHG	C3-O3-P-O5
22	A	845	LHG	C3-O3-P-O5
22	A	845	LHG	C4-O6-P-O5
22	G	102	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	4	309	CLA	C11-C12-C13-C14
22	A	844	LHG	C13-C14-C15-C16
17	A	838	CLA	C8-C10-C11-C12
17	3	609	CLA	CBA-CGA-O2A-C1
22	B	801	LHG	O6-C4-C5-C6
22	1	317	LHG	O9-C7-O7-C5
22	F	302	LHG	O9-C7-O7-C5
22	G	102	LHG	C33-C34-C35-C36
17	3	611	CLA	C6-C7-C8-C9
22	F	302	LHG	C13-C14-C15-C16
17	1	303	CLA	C2-C3-C5-C6
17	A	822	CLA	C2-C3-C5-C6
17	A	843	CLA	CAD-CBD-CGD-O1D
17	B	807	CLA	CAD-CBD-CGD-O1D
17	J	103	CLA	CAD-CBD-CGD-O1D
17	A	831	CLA	O1A-CGA-O2A-C1
17	4	314	CLA	O1D-CGD-O2D-CED
25	F	305	HTG	C2'-C3'-C4'-C5'
17	B	807	CLA	CBA-CGA-O2A-C1
17	B	816	CLA	CBA-CGA-O2A-C1
24	B	852	LMG	C33-C34-C35-C36
17	1	301	CLA	C11-C12-C13-C15
17	1	302	CLA	C11-C12-C13-C15
17	2	303	CLA	C6-C7-C8-C10
17	2	311	CLA	C6-C7-C8-C10
17	2	311	CLA	C11-C10-C8-C7
17	4	310	CLA	C3A-C2A-CAA-CBA
17	A	807	CLA	C11-C10-C8-C7
17	A	807	CLA	C12-C13-C15-C16
17	A	824	CLA	C11-C12-C13-C15
17	A	825	CLA	C11-C12-C13-C15
17	A	831	CLA	C12-C13-C15-C16
17	A	832	CLA	C11-C12-C13-C15
17	B	803	CLA	C11-C12-C13-C15
17	B	815	CLA	C11-C12-C13-C15
17	B	815	CLA	C12-C13-C15-C16
17	B	816	CLA	C11-C12-C13-C15
17	B	826	CLA	C11-C12-C13-C15
17	B	829	CLA	C11-C12-C13-C15
17	B	838	CLA	C12-C13-C15-C16
17	B	841	CLA	C6-C7-C8-C10
17	B	841	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	842	CLA	C11-C12-C13-C15
17	L	203	CLA	C12-C13-C15-C16
17	K	202	CLA	C11-C10-C8-C7
22	A	844	LHG	O6-C4-C5-O7
22	G	102	LHG	O6-C4-C5-O7
25	B	851	HTG	C2-C1-S1-C1'
25	J	102	HTG	C2-C1-S1-C1'
17	A	820	CLA	C13-C15-C16-C17
22	A	844	LHG	O2-C2-C3-O3
17	A	827	CLA	C16-C17-C18-C19
17	B	805	CLA	C16-C17-C18-C19
17	B	814	CLA	C6-C7-C8-C10
17	2	311	CLA	O1A-CGA-O2A-C1
24	F	309	LMG	O1-C7-C8-O7
22	1	317	LHG	C24-C23-O8-C6
17	B	816	CLA	O1A-CGA-O2A-C1
17	A	853	CLA	C8-C10-C11-C12
18	4	301	CHL	C10-C11-C12-C13
17	B	841	CLA	C3-C5-C6-C7
17	3	609	CLA	O1A-CGA-O2A-C1
17	B	828	CLA	C8-C10-C11-C12
17	B	842	CLA	CAA-CBA-CGA-O2A
17	1	307	CLA	C11-C12-C13-C14
17	2	303	CLA	C6-C7-C8-C9
17	A	807	CLA	C14-C13-C15-C16
17	A	818	CLA	C11-C12-C13-C14
17	A	826	CLA	C11-C12-C13-C14
17	A	828	CLA	C14-C13-C15-C16
17	A	838	CLA	C11-C10-C8-C9
17	A	838	CLA	C14-C13-C15-C16
17	A	841	CLA	C11-C12-C13-C14
17	B	811	CLA	C6-C7-C8-C9
17	B	819	CLA	C11-C10-C8-C9
17	B	826	CLA	C11-C12-C13-C14
17	B	831	CLA	C11-C12-C13-C14
17	B	838	CLA	C11-C12-C13-C14
17	B	807	CLA	O1A-CGA-O2A-C1
17	B	837	CLA	C11-C12-C13-C14
25	J	102	HTG	C4'-C5'-C6'-C7'
17	A	835	CLA	C2A-CAA-CBA-CGA
17	B	828	CLA	C10-C11-C12-C13
17	B	823	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	823	CLA	CBA-CGA-O2A-C1
22	F	302	LHG	C19-C20-C21-C22
23	2	318	LMT	C5-C6-C7-C8
17	A	853	CLA	CBD-CGD-O2D-CED
22	1	317	LHG	C27-C28-C29-C30
17	B	807	CLA	C15-C16-C17-C18
17	A	828	CLA	C3-C5-C6-C7
17	A	837	CLA	C3-C5-C6-C7
23	A	855	LMT	C2B-C1B-O1B-C4'
17	B	840	CLA	C13-C15-C16-C17
17	A	816	CLA	C16-C17-C18-C20
17	A	826	CLA	C16-C17-C18-C20
17	B	841	CLA	C16-C17-C18-C20
24	B	852	LMG	C36-C37-C38-C39
17	A	824	CLA	C15-C16-C17-C18
17	A	821	CLA	C1-C2-C3-C4
17	B	813	CLA	O1A-CGA-O2A-C1
24	4	320	LMG	C36-C37-C38-C39
22	F	302	LHG	C4-C5-O7-C7
17	2	311	CLA	C2A-CAA-CBA-CGA
17	A	807	CLA	C2A-CAA-CBA-CGA
17	A	805	CLA	CBA-CGA-O2A-C1
17	1	307	CLA	C2-C1-O2A-CGA
17	B	808	CLA	C2-C1-O2A-CGA
17	B	823	CLA	C2-C1-O2A-CGA
17	B	829	CLA	C2-C1-O2A-CGA
17	F	307	CLA	C2-C1-O2A-CGA
18	3	601	CHL	C2-C1-O2A-CGA
22	A	844	LHG	C16-C17-C18-C19
26	B	850	DGD	CBB-CCB-CDB-CEB
17	B	819	CLA	CAA-CBA-CGA-O2A
17	F	304	CLA	C13-C15-C16-C17
17	A	801	CLA	C3-C5-C6-C7
21	3	616	BCR	C1-C6-C7-C8
21	A	849	BCR	C23-C24-C25-C30
21	B	844	BCR	C23-C24-C25-C30
21	I	101	BCR	C1-C6-C7-C8
21	L	205	BCR	C1-C6-C7-C8
21	K	203	BCR	C1-C6-C7-C8
21	K	203	BCR	C5-C6-C7-C8
17	1	303	CLA	O1A-CGA-O2A-C1
22	F	302	LHG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	1	303	CLA	CBA-CGA-O2A-C1
17	B	829	CLA	CBA-CGA-O2A-C1
24	4	319	LMG	C37-C38-C39-C40
17	3	611	CLA	C6-C7-C8-C10
17	4	310	CLA	C11-C12-C13-C14
21	A	851	BCR	C16-C17-C18-C19
17	1	308	CLA	O1A-CGA-O2A-C1
17	B	817	CLA	C5-C6-C7-C8
17	1	308	CLA	CBA-CGA-O2A-C1
22	2	317	LHG	C3-O3-P-O6
17	A	809	CLA	C12-C13-C15-C16
17	A	843	CLA	C2-C3-C5-C6
18	4	301	CHL	C2-C3-C5-C6
24	4	319	LMG	C12-C13-C14-C15
17	1	301	CLA	C11-C12-C13-C14
17	2	311	CLA	C11-C10-C8-C9
17	A	824	CLA	C11-C12-C13-C14
17	B	815	CLA	C11-C12-C13-C14
17	B	834	CLA	C6-C7-C8-C9
17	L	202	CLA	C6-C7-C8-C9
17	L	202	CLA	C11-C12-C13-C14
17	K	202	CLA	C11-C10-C8-C9
19	1	314	LUT	C13-C14-C15-C35
21	L	201	BCR	C13-C14-C15-C16
21	K	203	BCR	C19-C20-C21-C22
17	A	839	CLA	C16-C17-C18-C19
17	B	810	CLA	C16-C17-C18-C20
22	G	102	LHG	C11-C12-C13-C14
24	4	319	LMG	C21-C22-C23-C24
17	A	841	CLA	C10-C11-C12-C13
24	F	309	LMG	C20-C21-C22-C23
17	4	312	CLA	O1A-CGA-O2A-C1
17	4	302	CLA	C8-C10-C11-C12
22	1	317	LHG	C29-C30-C31-C32
17	B	803	CLA	C4-C3-C5-C6
18	4	301	CHL	C4-C3-C5-C6
17	A	810	CLA	C2-C3-C5-C6
22	2	317	LHG	C29-C30-C31-C32
17	A	809	CLA	CBA-CGA-O2A-C1
17	B	813	CLA	CBA-CGA-O2A-C1
22	F	302	LHG	C24-C23-O8-C6
24	B	852	LMG	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	829	CLA	O1A-CGA-O2A-C1
17	4	312	CLA	CBA-CGA-O2A-C1
21	1	316	BCR	C18-C19-C20-C21
17	B	812	CLA	C4-C3-C5-C6
17	B	812	CLA	C2-C3-C5-C6
17	A	839	CLA	C13-C15-C16-C17
17	B	807	CLA	C2-C1-O2A-CGA
17	4	309	CLA	C11-C12-C13-C15
24	G	101	LMG	C21-C22-C23-C24
17	1	301	CLA	C15-C16-C17-C18
17	3	611	CLA	C2A-CAA-CBA-CGA
17	A	840	CLA	C2A-CAA-CBA-CGA
22	A	845	LHG	O10-C23-C24-C25
26	B	850	DGD	O1G-C1G-C2G-O2G
17	A	805	CLA	CAA-CBA-CGA-O1A
17	A	822	CLA	C3A-C2A-CAA-CBA
17	B	815	CLA	C3A-C2A-CAA-CBA
17	L	203	CLA	C3A-C2A-CAA-CBA
17	A	820	CLA	C16-C17-C18-C19
17	2	311	CLA	C6-C7-C8-C9
17	4	312	CLA	C6-C7-C8-C9
17	A	816	CLA	C6-C7-C8-C9
17	A	820	CLA	C6-C7-C8-C9
17	A	820	CLA	C11-C10-C8-C9
17	A	820	CLA	C14-C13-C15-C16
17	B	805	CLA	C16-C17-C18-C20
21	A	851	BCR	C11-C10-C9-C34
21	A	851	BCR	C16-C17-C18-C36
21	B	845	BCR	C11-C10-C9-C34
21	B	846	BCR	C11-C10-C9-C34
21	B	846	BCR	C20-C21-C22-C37
21	J	105	BCR	C35-C13-C14-C15
21	L	201	BCR	C11-C10-C9-C34
25	F	310	HTG	C1'-C2'-C3'-C4'
24	4	319	LMG	O9-C10-O7-C8
17	2	319	CLA	C2A-CAA-CBA-CGA
24	4	320	LMG	C33-C34-C35-C36
21	B	849	BCR	C14-C15-C16-C17
22	G	102	LHG	C28-C29-C30-C31
17	A	839	CLA	C15-C16-C17-C18
17	B	818	CLA	C4-C3-C5-C6
17	3	610	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	802	CLA	C1A-C2A-CAA-CBA
17	A	809	CLA	C1A-C2A-CAA-CBA
17	A	822	CLA	C1A-C2A-CAA-CBA
17	1	301	CLA	C6-C7-C8-C10
17	1	309	CLA	C6-C7-C8-C10
17	2	308	CLA	C6-C7-C8-C10
17	A	801	CLA	C11-C12-C13-C15
17	A	838	CLA	C11-C10-C8-C7
17	A	840	CLA	C11-C10-C8-C7
17	A	853	CLA	C12-C13-C15-C16
17	B	809	CLA	C12-C13-C15-C16
17	B	810	CLA	C6-C7-C8-C10
17	B	819	CLA	C11-C10-C8-C7
17	B	827	CLA	C11-C12-C13-C15
17	B	827	CLA	C13-C15-C16-C17
17	B	838	CLA	C5-C6-C7-C8
22	A	845	LHG	O8-C23-C24-C25
21	2	316	BCR	C9-C10-C11-C12
17	A	823	CLA	C2A-CAA-CBA-CGA
25	B	851	HTG	C4'-C5'-C6'-C7'
17	A	818	CLA	C5-C6-C7-C8
24	G	101	LMG	C19-C20-C21-C22
17	A	801	CLA	C13-C15-C16-C17
17	F	304	CLA	C15-C16-C17-C18
17	A	809	CLA	O1A-CGA-O2A-C1
23	A	855	LMT	O5B-C1B-O1B-C4'
21	A	851	BCR	C11-C10-C9-C8
21	B	846	BCR	C20-C21-C22-C23
21	G	106	BCR	C20-C21-C22-C23
21	L	201	BCR	C11-C10-C9-C8
19	4	316	LUT	C13-C14-C15-C35
24	F	309	LMG	C16-C17-C18-C19
17	A	805	CLA	O1A-CGA-O2A-C1
25	4	322	HTG	C4-C5-C6-O6
17	A	839	CLA	C4-C3-C5-C6
17	A	840	CLA	C2-C1-O2A-CGA
17	B	817	CLA	C2-C1-O2A-CGA
17	K	202	CLA	C2-C1-O2A-CGA
17	A	827	CLA	C10-C11-C12-C13
17	A	829	CLA	C6-C7-C8-C9
17	3	612	CLA	C2A-CAA-CBA-CGA
17	F	307	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	1	303	CLA	C4-C3-C5-C6
17	A	822	CLA	C4-C3-C5-C6
17	B	814	CLA	O1A-CGA-O2A-C1
17	B	819	CLA	C11-C12-C13-C14
17	A	811	CLA	C2A-CAA-CBA-CGA
17	A	841	CLA	C2A-CAA-CBA-CGA
17	B	805	CLA	C2A-CAA-CBA-CGA
17	B	822	CLA	C2A-CAA-CBA-CGA
21	3	616	BCR	C5-C6-C7-C8
21	A	848	BCR	C23-C24-C25-C30
21	G	106	BCR	C1-C6-C7-C8
21	I	101	BCR	C5-C6-C7-C8
21	K	203	BCR	C23-C24-C25-C30
22	2	317	LHG	C4-C5-C6-O8
21	I	101	BCR	C19-C20-C21-C22
17	A	818	CLA	C4-C3-C5-C6
22	A	844	LHG	C30-C31-C32-C33
17	B	825	CLA	C2-C3-C5-C6
22	G	102	LHG	C23-C24-C25-C26
17	F	304	CLA	C10-C11-C12-C13
17	A	803	CLA	C6-C7-C8-C9
17	A	826	CLA	C16-C17-C18-C19
17	B	841	CLA	C16-C17-C18-C19
17	4	303	CLA	C8-C10-C11-C12
17	A	830	CLA	C2A-CAA-CBA-CGA
17	A	831	CLA	C2A-CAA-CBA-CGA
17	4	309	CLA	C8-C10-C11-C12
17	A	817	CLA	CAA-CBA-CGA-O2A
17	A	807	CLA	C4-C3-C5-C6
26	B	850	DGD	CAA-CBA-CCA-CDA
17	A	805	CLA	C2-C3-C5-C6
17	A	817	CLA	C12-C13-C15-C16
17	A	820	CLA	C6-C7-C8-C10
17	A	826	CLA	C11-C12-C13-C15
17	A	837	CLA	C6-C7-C8-C10
26	B	850	DGD	CAB-CBB-CCB-CDB
17	B	810	CLA	C10-C11-C12-C13
17	1	312	CLA	CAA-CBA-CGA-O1A
22	B	801	LHG	C2-C3-O3-P
22	F	302	LHG	O7-C5-C6-O8
17	2	319	CLA	CAA-CBA-CGA-O2A
17	A	809	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	A	839	CLA	C16-C17-C18-C20
17	B	824	CLA	C6-C7-C8-C9
17	4	310	CLA	C4C-C3C-CAC-CBC
17	A	832	CLA	C4C-C3C-CAC-CBC
17	B	837	CLA	C4C-C3C-CAC-CBC
21	2	316	BCR	C11-C10-C9-C34
21	F	308	BCR	C35-C13-C14-C15
21	J	104	BCR	C20-C21-C22-C37
17	4	311	CLA	CAA-CBA-CGA-O2A
17	A	804	CLA	C4-C3-C5-C6
17	A	805	CLA	C4-C3-C5-C6
17	A	839	CLA	C2-C3-C5-C6
17	B	808	CLA	C2-C3-C5-C6
17	4	310	CLA	C11-C12-C13-C15
17	B	824	CLA	CAA-CBA-CGA-O2A
17	1	301	CLA	C6-C7-C8-C9
17	A	807	CLA	C11-C10-C8-C9
17	A	827	CLA	C11-C12-C13-C14
17	B	841	CLA	C14-C13-C15-C16
17	L	203	CLA	C14-C13-C15-C16
22	1	317	LHG	C31-C32-C33-C34
17	1	307	CLA	C3A-C2A-CAA-CBA
17	A	802	CLA	C3A-C2A-CAA-CBA
17	A	808	CLA	C3A-C2A-CAA-CBA
17	B	835	CLA	C3A-C2A-CAA-CBA
24	4	320	LMG	C17-C18-C19-C20
17	2	308	CLA	O1A-CGA-O2A-C1
22	A	844	LHG	O7-C7-C8-C9
17	B	836	CLA	CBD-CGD-O2D-CED
17	2	308	CLA	CAD-CBD-CGD-O2D
17	2	310	CLA	CAD-CBD-CGD-O2D
17	3	604	CLA	CAD-CBD-CGD-O2D
17	3	606	CLA	CAD-CBD-CGD-O2D
17	4	304	CLA	CAD-CBD-CGD-O2D
17	A	801	CLA	CAD-CBD-CGD-O2D
17	A	804	CLA	CAD-CBD-CGD-O2D
17	A	806	CLA	CAD-CBD-CGD-O2D
17	A	813	CLA	CAD-CBD-CGD-O2D
17	A	819	CLA	CAD-CBD-CGD-O2D
17	A	826	CLA	CAD-CBD-CGD-O2D
17	A	853	CLA	CAD-CBD-CGD-O2D
17	B	806	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	814	CLA	CAD-CBD-CGD-O2D
17	B	823	CLA	CAD-CBD-CGD-O2D
17	B	831	CLA	CAD-CBD-CGD-O2D
17	B	837	CLA	CAD-CBD-CGD-O2D
17	B	842	CLA	CAD-CBD-CGD-O2D
17	K	201	CLA	CAD-CBD-CGD-O2D
18	2	304	CHL	CAD-CBD-CGD-O2D
18	4	305	CHL	CAD-CBD-CGD-O2D
22	F	302	LHG	C6-C5-O7-C7
17	1	311	CLA	C2A-CAA-CBA-CGA
17	2	308	CLA	C2A-CAA-CBA-CGA
22	A	844	LHG	C34-C35-C36-C37
17	B	825	CLA	C4-C3-C5-C6
17	B	829	CLA	C5-C6-C7-C8
17	A	818	CLA	C2-C3-C5-C6
21	A	849	BCR	C7-C8-C9-C10
21	F	303	BCR	C7-C8-C9-C10
17	1	304	CLA	C2C-C3C-CAC-CBC
17	4	310	CLA	C2C-C3C-CAC-CBC
17	A	832	CLA	C2C-C3C-CAC-CBC
17	B	836	CLA	C2C-C3C-CAC-CBC
17	F	307	CLA	C2C-C3C-CAC-CBC
17	K	201	CLA	C2C-C3C-CAC-CBC
20	1	315	XAT	O4-C6-C7-C8
20	2	315	XAT	O4-C6-C7-C8
20	3	615	XAT	O4-C6-C7-C8
22	A	844	LHG	C4-C5-C6-O8
22	F	302	LHG	C4-C5-C6-O8
26	4	323	DGD	O1A-C1A-C2A-C3A
17	B	840	CLA	CBA-CGA-O2A-C1
17	1	302	CLA	CAA-CBA-CGA-O2A
17	K	202	CLA	CAA-CBA-CGA-O2A
17	A	824	CLA	O2A-C1-C2-C3
17	A	825	CLA	O2A-C1-C2-C3
17	A	841	CLA	O2A-C1-C2-C3
17	B	832	CLA	O2A-C1-C2-C3
23	A	855	LMT	C4-C5-C6-C7
17	2	308	CLA	CBA-CGA-O2A-C1
21	1	316	BCR	C14-C15-C16-C17
17	A	808	CLA	CAA-CBA-CGA-O2A
17	B	815	CLA	O1D-CGD-O2D-CED
17	1	301	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	1	301	CLA	CHA-CBD-CGD-O2D
17	1	303	CLA	CHA-CBD-CGD-O1D
17	1	303	CLA	CHA-CBD-CGD-O2D
17	2	303	CLA	CHA-CBD-CGD-O1D
17	2	303	CLA	CHA-CBD-CGD-O2D
17	2	311	CLA	CHA-CBD-CGD-O1D
17	2	311	CLA	CHA-CBD-CGD-O2D
17	3	605	CLA	CHA-CBD-CGD-O1D
17	3	605	CLA	CHA-CBD-CGD-O2D
17	4	313	CLA	CHA-CBD-CGD-O1D
17	4	313	CLA	CHA-CBD-CGD-O2D
17	A	818	CLA	CHA-CBD-CGD-O1D
17	A	818	CLA	CHA-CBD-CGD-O2D
17	A	821	CLA	CHA-CBD-CGD-O1D
17	A	821	CLA	CHA-CBD-CGD-O2D
17	A	830	CLA	CHA-CBD-CGD-O1D
17	A	830	CLA	CHA-CBD-CGD-O2D
17	A	837	CLA	CHA-CBD-CGD-O1D
17	A	837	CLA	CHA-CBD-CGD-O2D
17	A	838	CLA	CHA-CBD-CGD-O1D
17	A	838	CLA	CHA-CBD-CGD-O2D
17	B	804	CLA	CHA-CBD-CGD-O1D
17	B	804	CLA	CHA-CBD-CGD-O2D
17	B	809	CLA	CHA-CBD-CGD-O2D
17	B	813	CLA	CHA-CBD-CGD-O2D
17	B	815	CLA	CHA-CBD-CGD-O2D
17	B	817	CLA	CHA-CBD-CGD-O2D
17	B	822	CLA	CHA-CBD-CGD-O2D
17	B	834	CLA	CHA-CBD-CGD-O1D
17	B	834	CLA	CHA-CBD-CGD-O2D
17	K	202	CLA	CHA-CBD-CGD-O2D
18	1	305	CHL	CHA-CBD-CGD-O1D
18	1	305	CHL	CHA-CBD-CGD-O2D
21	2	316	BCR	C19-C20-C21-C22
21	F	308	BCR	C9-C10-C11-C12
17	2	310	CLA	CAA-CBA-CGA-O2A
17	B	812	CLA	CAA-CBA-CGA-O2A
17	A	807	CLA	C2-C3-C5-C6
20	1	315	XAT	C11-C10-C9-C8
20	2	315	XAT	C11-C10-C9-C8
20	3	615	XAT	C11-C10-C9-C8
21	B	846	BCR	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	F	308	BCR	C12-C13-C14-C15
17	A	841	CLA	C5-C6-C7-C8
17	B	841	CLA	C13-C15-C16-C17
24	G	101	LMG	C22-C23-C24-C25
17	3	610	CLA	CAA-CBA-CGA-O2A
17	A	803	CLA	CAA-CBA-CGA-O2A
17	B	811	CLA	CAA-CBA-CGA-O2A
17	F	307	CLA	CAA-CBA-CGA-O2A
17	G	105	CLA	CBA-CGA-O2A-C1
17	A	812	CLA	CBA-CGA-O2A-C1
24	B	852	LMG	C11-C10-O7-C8
17	1	308	CLA	C11-C10-C8-C7
17	A	841	CLA	C6-C7-C8-C10
17	A	853	CLA	C11-C10-C8-C7
17	B	818	CLA	C2-C3-C5-C6
17	B	833	CLA	C2-C3-C5-C6
22	A	844	LHG	O8-C23-C24-C25
17	4	303	CLA	C6-C7-C8-C9
17	A	809	CLA	C14-C13-C15-C16
17	A	812	CLA	C14-C13-C15-C16
17	A	831	CLA	C6-C7-C8-C9
17	A	841	CLA	C6-C7-C8-C9
17	B	812	CLA	C11-C12-C13-C14
17	B	816	CLA	C11-C12-C13-C14
17	B	825	CLA	C6-C7-C8-C9
17	B	840	CLA	O1A-CGA-O2A-C1
17	B	824	CLA	C6-C7-C8-C10
17	L	203	CLA	C16-C17-C18-C19
17	A	812	CLA	O1A-CGA-O2A-C1
22	1	317	LHG	O8-C23-C24-C25
17	B	814	CLA	CBA-CGA-O2A-C1
22	A	844	LHG	O9-C7-C8-C9
24	B	852	LMG	C23-C24-C25-C26
17	A	835	CLA	CAA-CBA-CGA-O2A
17	B	824	CLA	CAA-CBA-CGA-O1A
17	L	203	CLA	C5-C6-C7-C8
17	1	307	CLA	C1A-C2A-CAA-CBA
17	A	804	CLA	C1A-C2A-CAA-CBA
17	A	840	CLA	C1A-C2A-CAA-CBA
17	B	817	CLA	C1A-C2A-CAA-CBA
17	B	842	CLA	C1A-C2A-CAA-CBA
17	L	203	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	2	306	CHL	C1A-C2A-CAA-CBA
17	4	311	CLA	CAA-CBA-CGA-O1A
17	3	609	CLA	C2-C1-O2A-CGA
17	A	825	CLA	C2-C1-O2A-CGA
17	A	809	CLA	CAA-CBA-CGA-O1A
17	B	812	CLA	CAA-CBA-CGA-O1A
17	1	302	CLA	C10-C11-C12-C13
17	4	312	CLA	C2A-CAA-CBA-CGA
17	1	302	CLA	CAA-CBA-CGA-O1A
18	3	607	CHL	CBA-CGA-O2A-C1
18	2	305	CHL	C2-C1-O2A-CGA
17	2	310	CLA	CAA-CBA-CGA-O1A
22	2	317	LHG	C3-O3-P-O5
17	3	610	CLA	CAA-CBA-CGA-O1A
17	A	821	CLA	O2A-C1-C2-C3
17	3	613	CLA	CAA-CBA-CGA-O2A
21	K	203	BCR	C23-C24-C25-C26
17	A	808	CLA	CAA-CBA-CGA-O1A
17	1	310	CLA	CAA-CBA-CGA-O2A
17	2	311	CLA	C10-C11-C12-C13
17	B	815	CLA	C15-C16-C17-C18
17	3	606	CLA	CAA-CBA-CGA-O2A
17	B	808	CLA	C4-C3-C5-C6
17	2	319	CLA	CAD-CBD-CGD-O1D
17	3	605	CLA	CAD-CBD-CGD-O1D
17	4	313	CLA	CAD-CBD-CGD-O1D
17	A	829	CLA	CAD-CBD-CGD-O1D
17	A	837	CLA	CAD-CBD-CGD-O1D
17	B	803	CLA	CAD-CBD-CGD-O1D
17	B	812	CLA	CAD-CBD-CGD-O1D
17	B	815	CLA	CAD-CBD-CGD-O1D
17	B	822	CLA	CAD-CBD-CGD-O1D
17	B	842	CLA	CAD-CBD-CGD-O1D
18	4	301	CHL	CAD-CBD-CGD-O1D
17	F	307	CLA	CAA-CBA-CGA-O1A
17	K	202	CLA	CAA-CBA-CGA-O1A
26	B	850	DGD	C4A-C5A-C6A-C7A
17	B	808	CLA	CAA-CBA-CGA-O2A
17	B	802	CLA	C15-C16-C17-C18
17	1	309	CLA	C6-C7-C8-C9
17	A	853	CLA	C11-C10-C8-C9
17	B	827	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	B	820	CLA	O1A-CGA-O2A-C1
17	3	611	CLA	CBA-CGA-O2A-C1
17	3	603	CLA	CAA-CBA-CGA-O2A
17	2	307	CLA	O1A-CGA-O2A-C1
17	A	812	CLA	C2A-CAA-CBA-CGA
17	A	807	CLA	CAA-CBA-CGA-O2A
17	B	805	CLA	CAA-CBA-CGA-O2A
17	B	816	CLA	CAA-CBA-CGA-O2A
17	B	839	CLA	CAA-CBA-CGA-O2A
17	B	811	CLA	CAA-CBA-CGA-O1A
17	B	820	CLA	C11-C12-C13-C14
17	B	833	CLA	C4-C3-C5-C6
22	F	302	LHG	C24-C25-C26-C27
17	4	310	CLA	C6-C7-C8-C10
17	4	310	CLA	C11-C10-C8-C7
17	A	817	CLA	C11-C12-C13-C15
17	A	831	CLA	C6-C7-C8-C10
17	B	803	CLA	C2-C3-C5-C6
17	B	824	CLA	C3A-C2A-CAA-CBA
17	B	825	CLA	C6-C7-C8-C10
17	B	827	CLA	C6-C7-C8-C10
17	B	827	CLA	C11-C10-C8-C7
17	B	831	CLA	C12-C13-C15-C16
17	F	304	CLA	C3A-C2A-CAA-CBA
17	J	101	CLA	C6-C7-C8-C10
17	2	303	CLA	CAA-CBA-CGA-O1A
17	A	835	CLA	CAA-CBA-CGA-O1A
22	1	317	LHG	O9-C7-C8-C9
17	2	303	CLA	CAA-CBA-CGA-O2A
17	A	812	CLA	CAA-CBA-CGA-O2A
17	A	833	CLA	CAA-CBA-CGA-O2A
21	1	316	BCR	C7-C8-C9-C10
21	B	844	BCR	C7-C8-C9-C10
17	A	803	CLA	CAA-CBA-CGA-O1A
22	1	317	LHG	O10-C23-C24-C25
19	2	314	LUT	C13-C14-C15-C35
17	A	803	CLA	C6-C7-C8-C10
17	A	824	CLA	CAA-CBA-CGA-O2A
17	3	603	CLA	CAA-CBA-CGA-O1A
17	B	808	CLA	CAA-CBA-CGA-O1A
17	L	204	CLA	CAA-CBA-CGA-O2A
22	2	317	LHG	O8-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	2	305	CHL	C2A-CAA-CBA-CGA
17	B	804	CLA	C16-C17-C18-C20
17	1	307	CLA	C10-C11-C12-C13
17	A	824	CLA	CAA-CBA-CGA-O1A
17	B	839	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

197 monomers are involved in 630 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	826	CLA	8	0
17	B	819	CLA	4	0
17	4	310	CLA	1	0
17	A	806	CLA	2	0
17	A	831	CLA	6	0
18	1	305	CHL	6	0
17	L	203	CLA	6	0
22	B	801	LHG	1	0
17	K	202	CLA	2	0
25	4	322	HTG	2	0
26	4	323	DGD	29	0
17	B	833	CLA	2	0
17	3	613	CLA	3	0
17	4	311	CLA	3	0
17	B	830	CLA	3	0
17	A	853	CLA	9	0
17	A	829	CLA	2	0
17	A	822	CLA	1	0
17	B	836	CLA	5	0
17	B	842	CLA	5	0
17	A	810	CLA	8	0
23	A	855	LMT	2	0
18	4	306	CHL	7	0
21	A	851	BCR	5	0
17	2	308	CLA	5	0
19	3	614	LUT	4	0
17	B	816	CLA	3	0
17	B	841	CLA	2	0
17	A	826	CLA	2	0
17	A	840	CLA	4	0
17	1	310	CLA	6	0
20	2	315	XAT	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	839	CLA	4	0
21	G	106	BCR	2	0
21	A	847	BCR	1	0
20	4	317	XAT	10	0
17	J	101	CLA	6	0
17	2	307	CLA	4	0
17	4	302	CLA	7	0
17	A	814	CLA	4	0
18	4	301	CHL	11	0
17	B	840	CLA	1	0
21	L	206	BCR	4	0
17	1	311	CLA	6	0
17	B	827	CLA	11	0
26	B	850	DGD	7	0
18	4	315	CHL	4	0
24	B	852	LMG	6	0
21	K	203	BCR	4	0
23	2	318	LMT	3	0
21	B	847	BCR	8	0
17	B	805	CLA	3	0
17	2	301	CLA	4	0
18	2	305	CHL	2	0
17	A	825	CLA	5	0
17	A	820	CLA	8	0
17	L	204	CLA	4	0
20	1	315	XAT	3	0
25	F	305	HTG	1	0
17	B	811	CLA	6	0
20	3	615	XAT	13	0
17	1	309	CLA	6	0
17	B	808	CLA	1	0
21	I	101	BCR	4	0
17	A	811	CLA	3	0
17	A	809	CLA	3	0
17	2	302	CLA	4	0
17	B	809	CLA	6	0
22	2	317	LHG	7	0
17	A	801	CLA	1	0
17	A	824	CLA	4	0
17	B	839	CLA	4	0
21	F	303	BCR	1	0
22	G	102	LHG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	F	309	LMG	1	0
17	A	828	CLA	6	0
17	1	303	CLA	2	0
17	B	820	CLA	1	0
18	3	607	CHL	2	0
25	4	321	HTG	2	0
17	A	823	CLA	5	0
17	B	804	CLA	3	0
17	B	806	CLA	2	0
17	G	103	CLA	4	0
21	A	846	BCR	11	0
17	1	301	CLA	2	0
21	L	205	BCR	4	0
17	3	602	CLA	6	0
17	B	807	CLA	4	0
17	A	815	CLA	1	0
17	A	841	CLA	5	0
21	A	850	BCR	3	0
17	3	608	CLA	7	0
17	B	838	CLA	5	0
19	1	314	LUT	9	0
17	4	309	CLA	2	0
17	A	802	CLA	2	0
17	A	816	CLA	4	0
17	A	812	CLA	3	0
17	A	838	CLA	4	0
21	B	844	BCR	4	0
17	B	823	CLA	5	0
21	A	849	BCR	3	0
17	1	304	CLA	6	0
21	L	201	BCR	3	0
17	J	103	CLA	3	0
17	B	810	CLA	7	0
17	B	822	CLA	3	0
17	3	612	CLA	1	0
21	3	616	BCR	4	0
17	1	302	CLA	5	0
22	A	845	LHG	1	0
21	2	316	BCR	8	0
17	B	802	CLA	3	0
17	A	821	CLA	1	0
17	B	834	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	812	CLA	3	0
18	2	304	CHL	1	0
21	J	104	BCR	2	0
17	2	312	CLA	3	0
18	4	305	CHL	7	0
19	4	316	LUT	4	0
17	3	609	CLA	2	0
17	B	818	CLA	2	0
21	B	848	BCR	4	0
21	B	845	BCR	4	0
17	4	304	CLA	6	0
17	G	105	CLA	1	0
17	2	309	CLA	3	0
17	A	808	CLA	6	0
18	4	307	CHL	5	0
17	1	308	CLA	6	0
17	A	813	CLA	1	0
17	B	821	CLA	3	0
17	K	201	CLA	2	0
17	F	307	CLA	2	0
21	B	846	BCR	2	0
17	F	306	CLA	4	0
27	A	842	PQN	6	0
17	B	831	CLA	2	0
17	4	303	CLA	5	0
17	A	832	CLA	4	0
17	B	825	CLA	4	0
17	B	835	CLA	3	0
25	F	310	HTG	1	0
17	A	807	CLA	2	0
17	3	611	CLA	1	0
17	1	312	CLA	2	0
17	A	830	CLA	1	0
17	L	202	CLA	5	0
18	2	306	CHL	5	0
21	4	318	BCR	14	0
24	4	320	LMG	7	0
17	4	308	CLA	3	0
17	A	805	CLA	5	0
17	B	824	CLA	4	0
27	B	843	PQN	3	0
17	B	837	CLA	7	0

Continued on next page...

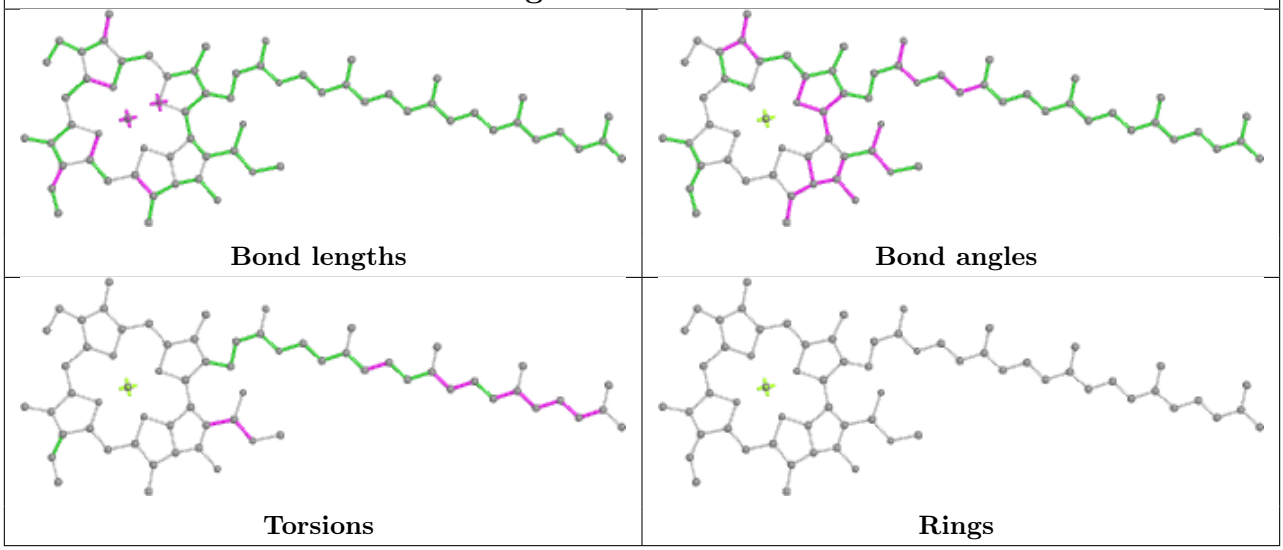
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	803	CLA	7	0
17	2	311	CLA	4	0
17	B	832	CLA	5	0
22	A	844	LHG	2	0
17	A	836	CLA	4	0
17	A	818	CLA	4	0
17	F	304	CLA	2	0
17	3	603	CLA	5	0
25	J	102	HTG	3	0
17	A	834	CLA	2	0
19	2	314	LUT	4	0
17	A	804	CLA	8	0
17	B	803	CLA	6	0
17	A	827	CLA	3	0
24	G	101	LMG	3	0
18	2	313	CHL	5	0
17	B	829	CLA	6	0
18	3	601	CHL	17	0
17	A	835	CLA	3	0
17	B	828	CLA	3	0
17	2	310	CLA	2	0
17	A	817	CLA	5	0
17	A	837	CLA	7	0
22	1	317	LHG	6	0
21	A	848	BCR	3	0
17	4	314	CLA	2	0
17	B	815	CLA	5	0
17	G	104	CLA	5	0
17	2	303	CLA	1	0
25	B	851	HTG	1	0
17	A	819	CLA	5	0
17	A	843	CLA	6	0
21	F	308	BCR	3	0
21	B	849	BCR	3	0
17	1	307	CLA	5	0
22	F	302	LHG	2	0
17	3	605	CLA	2	0
21	J	105	BCR	6	0
17	3	610	CLA	1	0

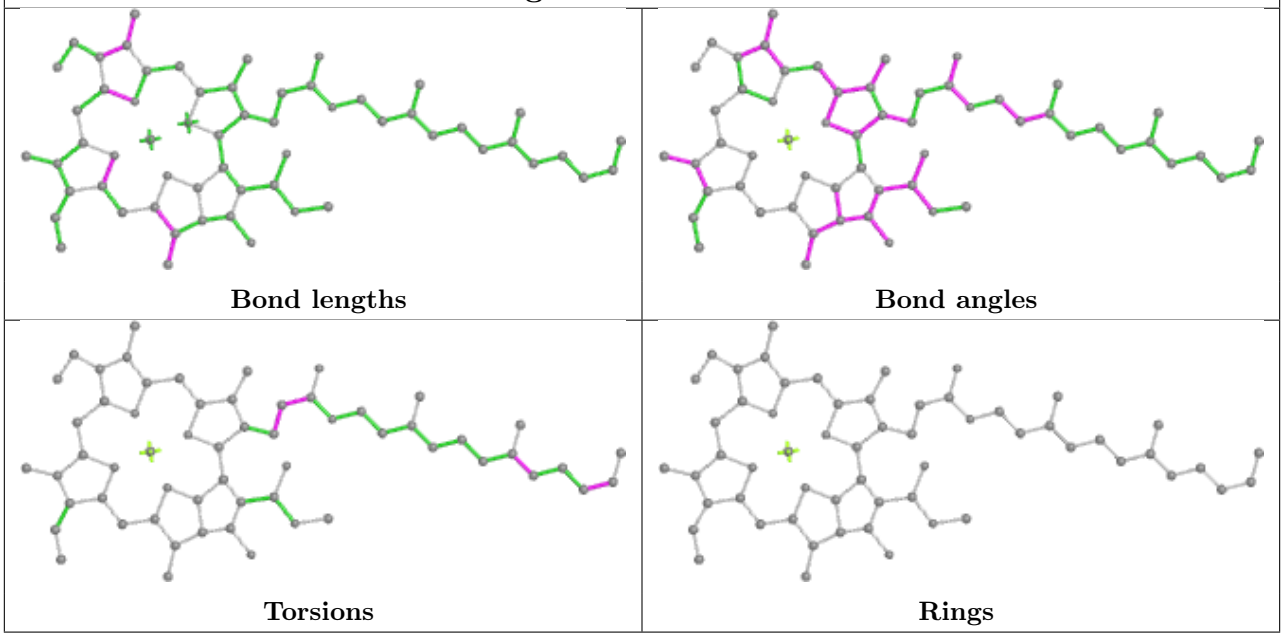
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

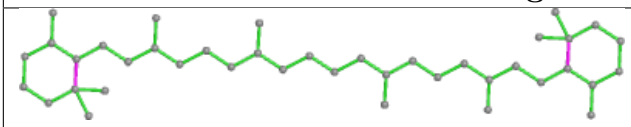
Ligand CLA B 826



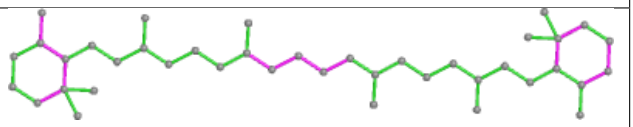
Ligand CLA B 819



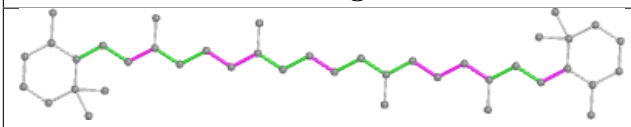
Ligand BCR 1 316



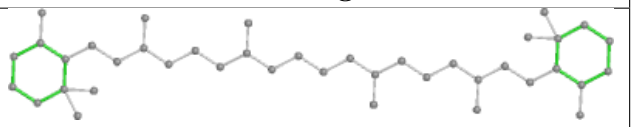
Bond lengths



Bond angles

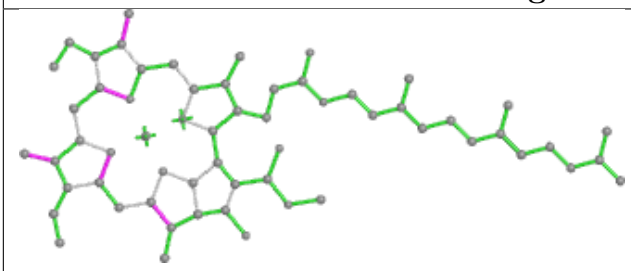


Torsions

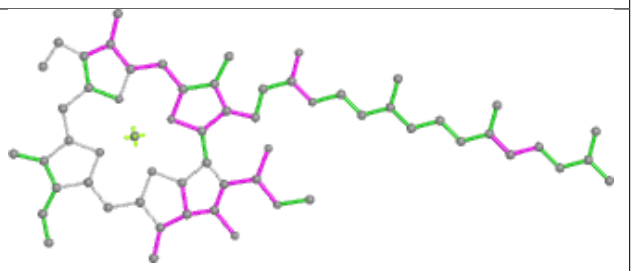


Rings

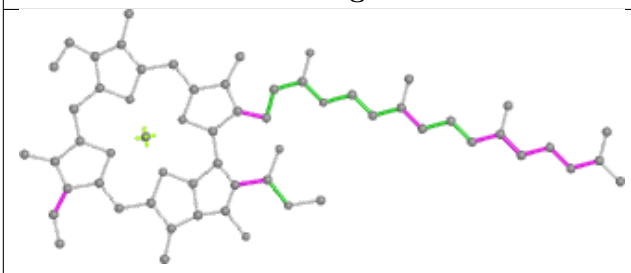
Ligand CLA 4 310



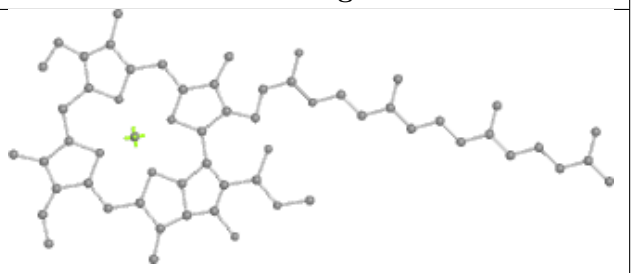
Bond lengths



Bond angles

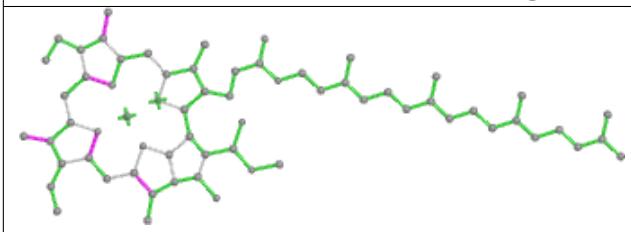


Torsions

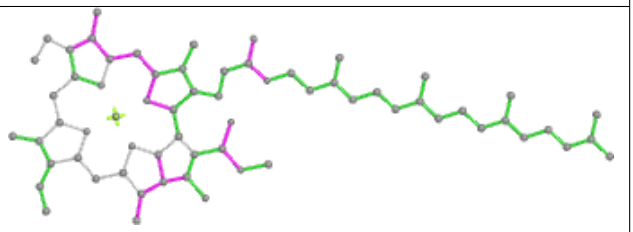


Rings

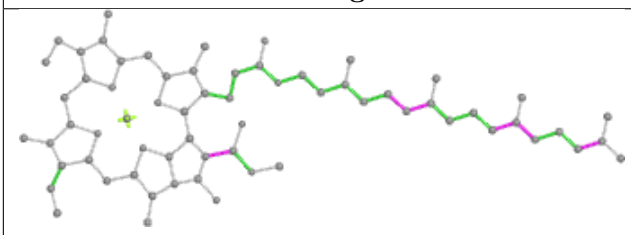
Ligand CLA A 806



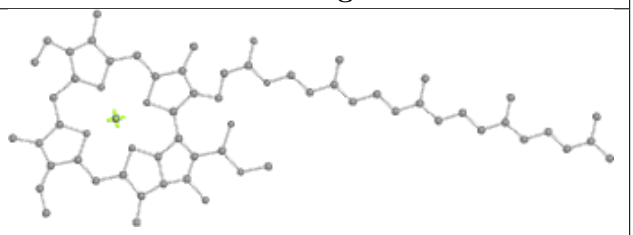
Bond lengths



Bond angles

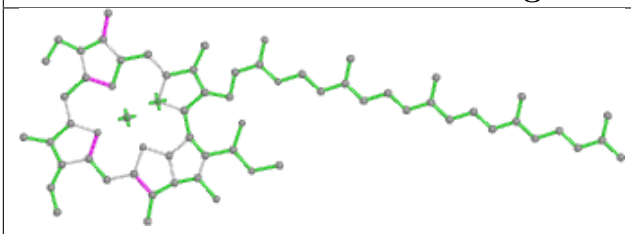


Torsions

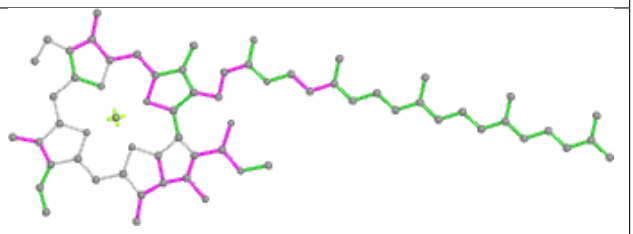


Rings

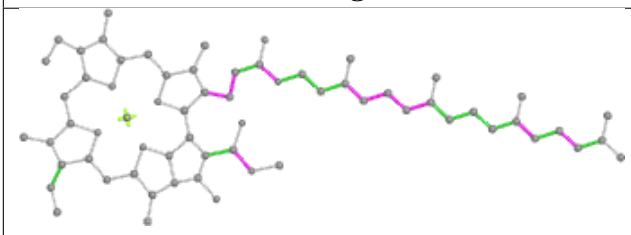
Ligand CLA A 831



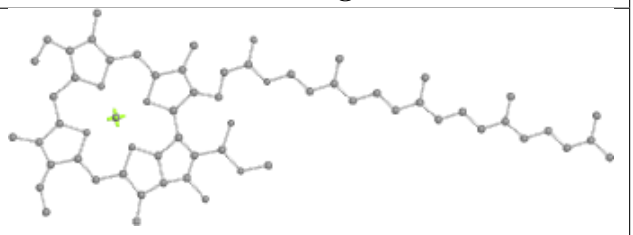
Bond lengths



Bond angles

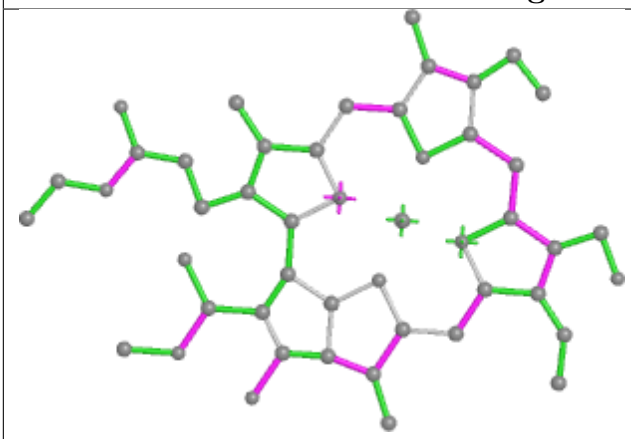


Torsions

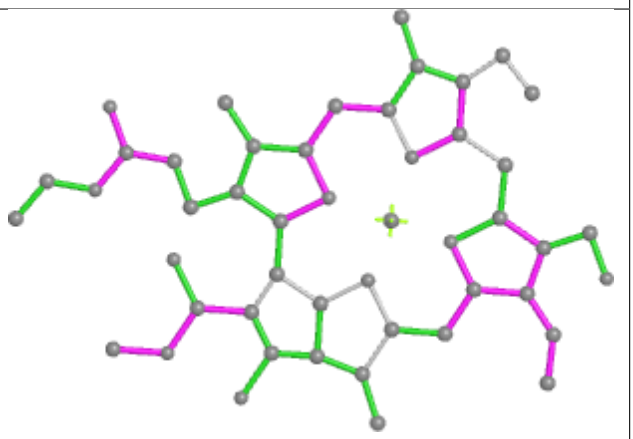


Rings

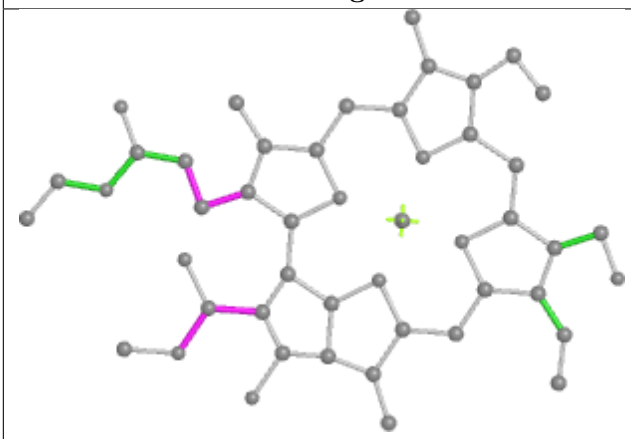
Ligand CHL 1 305



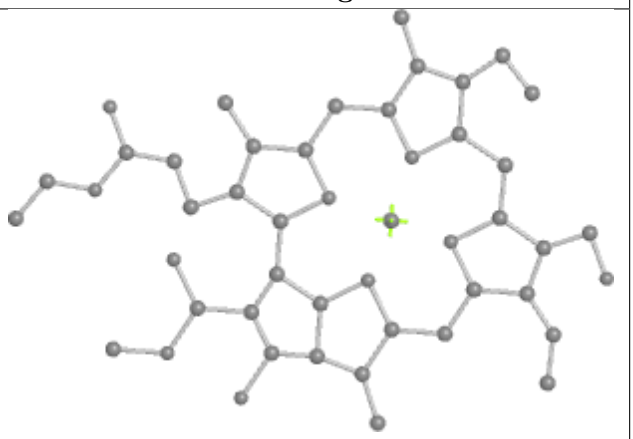
Bond lengths



Bond angles

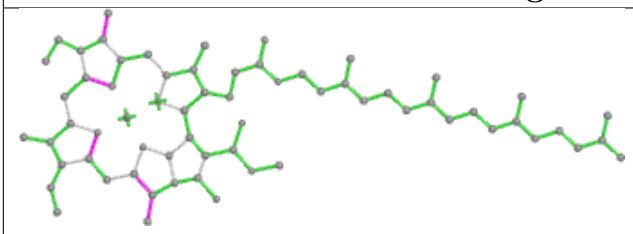


Torsions

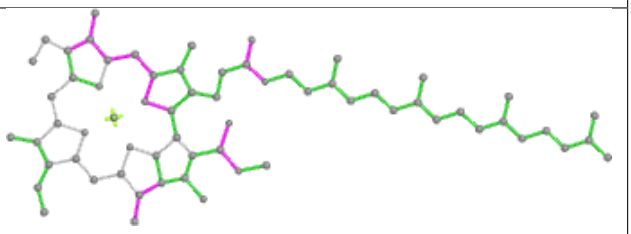


Rings

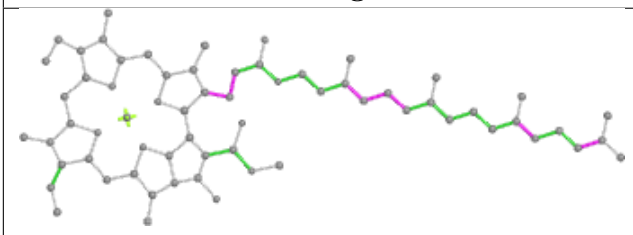
Ligand CLA L 203



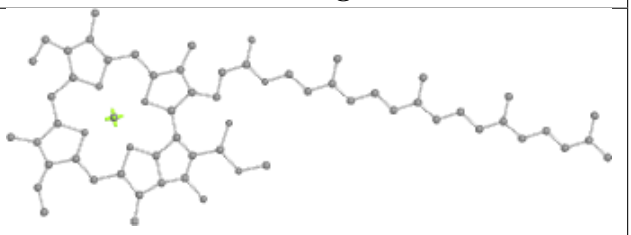
Bond lengths



Bond angles

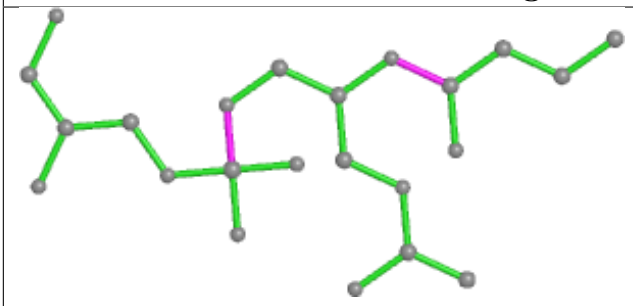


Torsions

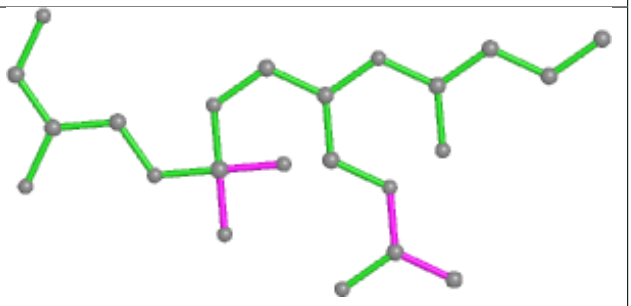


Rings

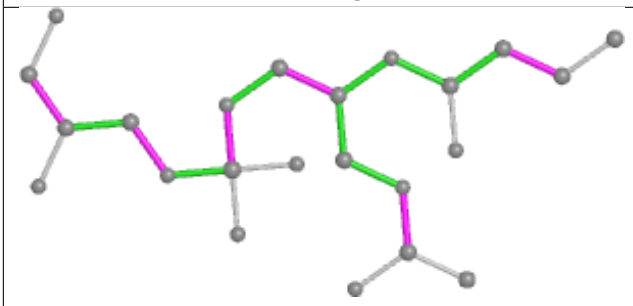
Ligand LHG B 801



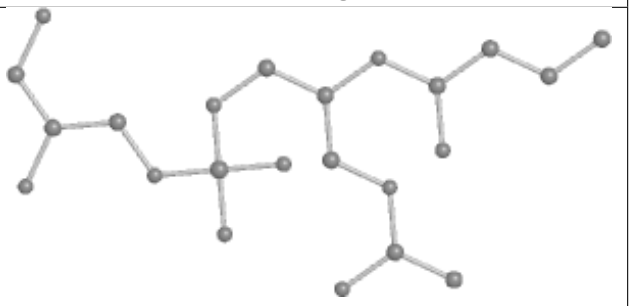
Bond lengths



Bond angles

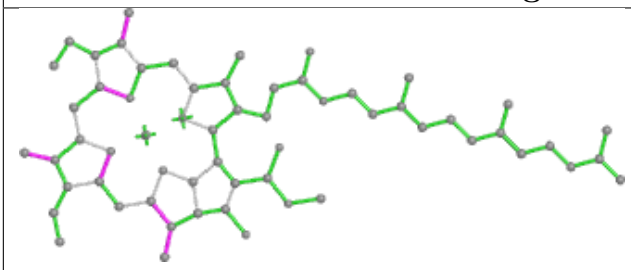


Torsions

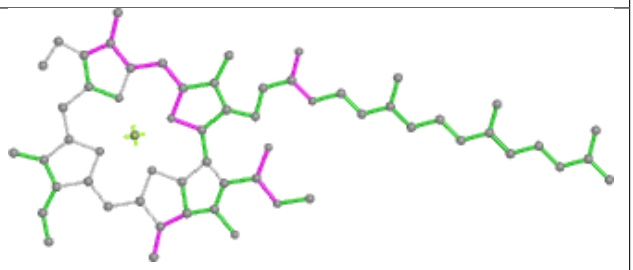


Rings

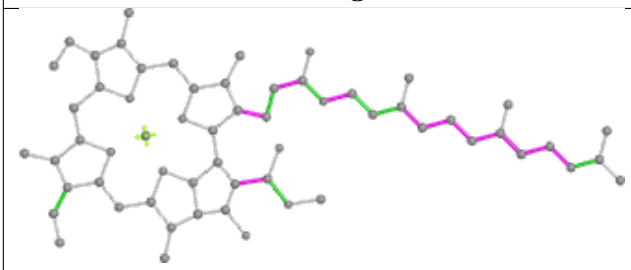
Ligand CLA K 202



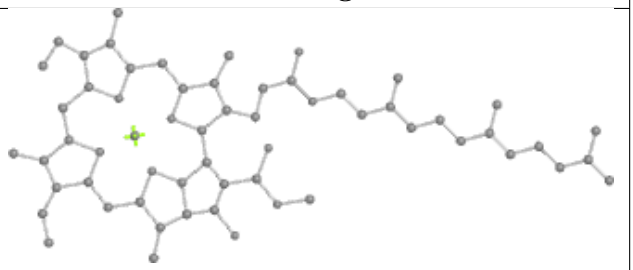
Bond lengths



Bond angles

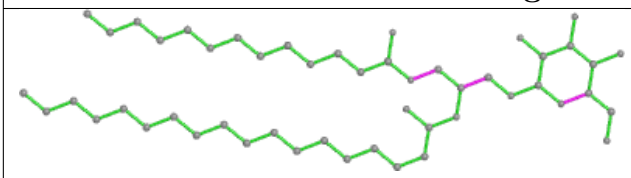


Torsions

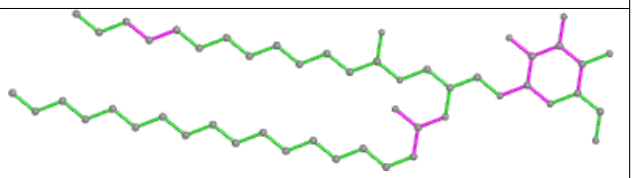


Rings

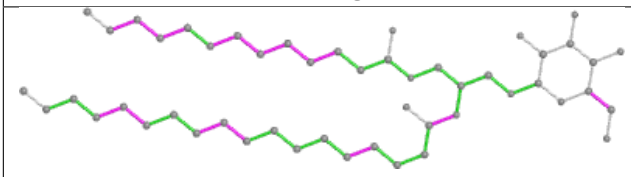
Ligand LMG 4 319



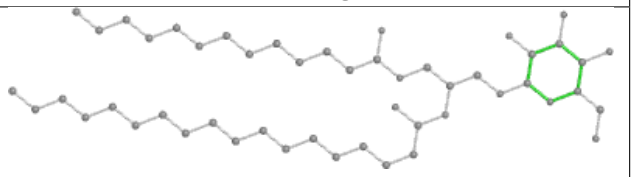
Bond lengths



Bond angles

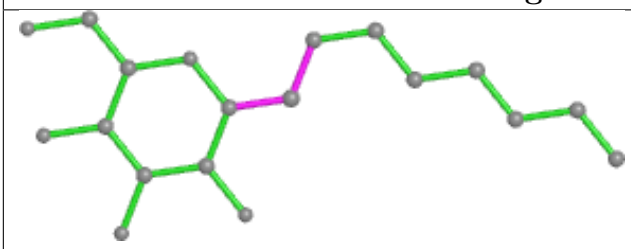


Torsions

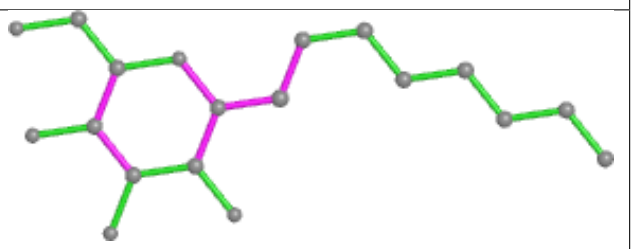


Rings

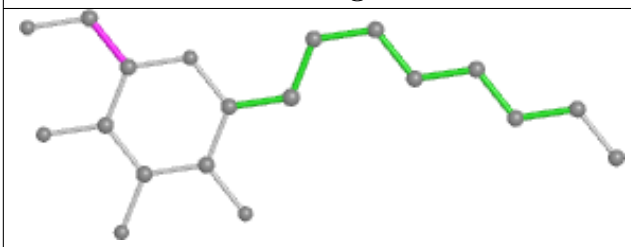
Ligand HTG 4 322



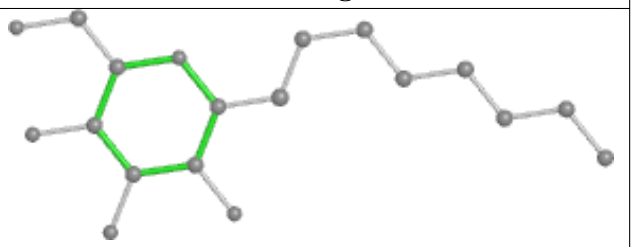
Bond lengths



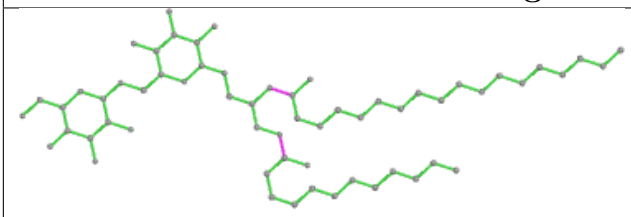
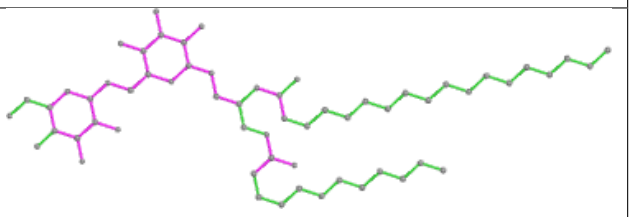
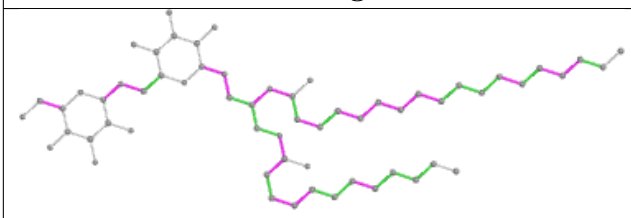
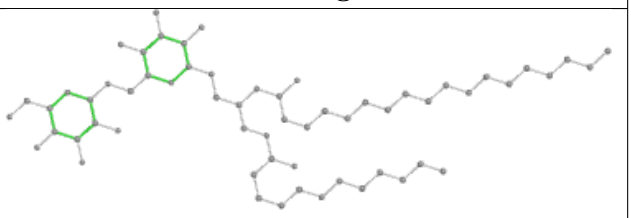
Bond angles

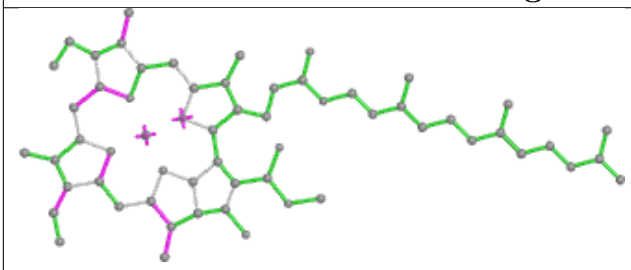
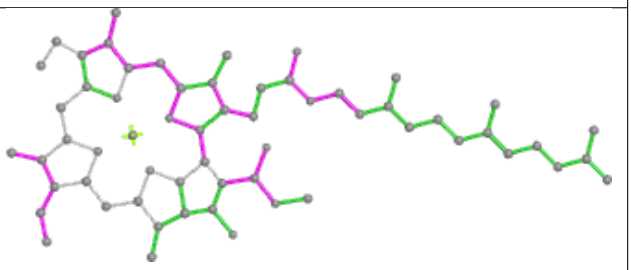
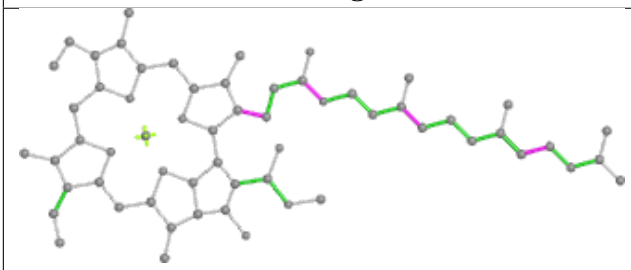
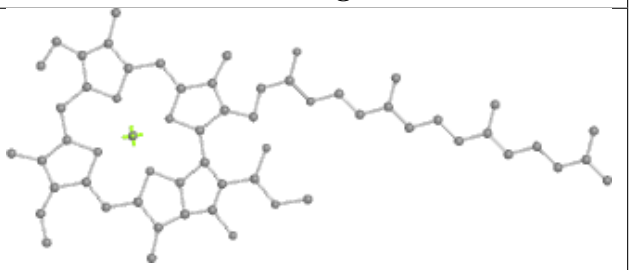


Torsions

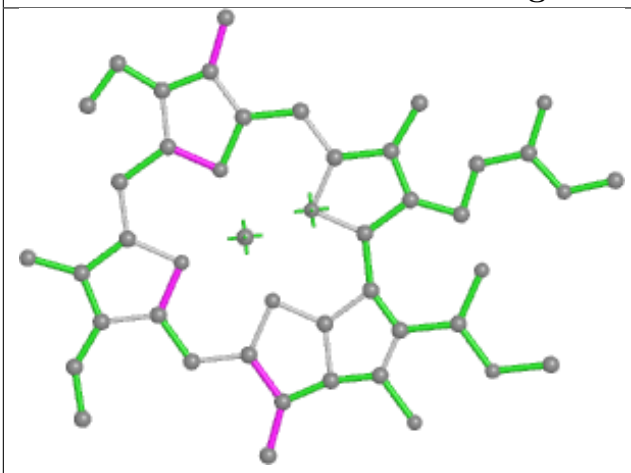


Rings

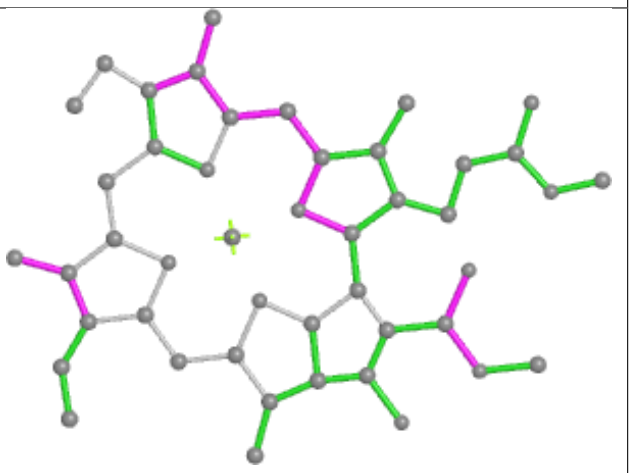
Ligand DGD 4 323	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 833	
 Bond lengths	 Bond angles
 Torsions	 Rings

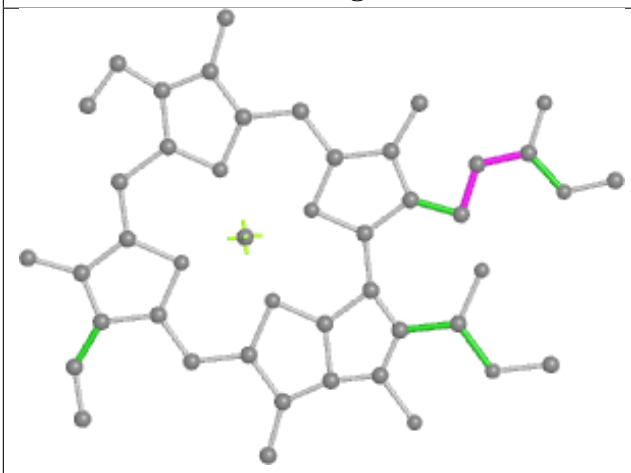
Ligand CLA 3 613



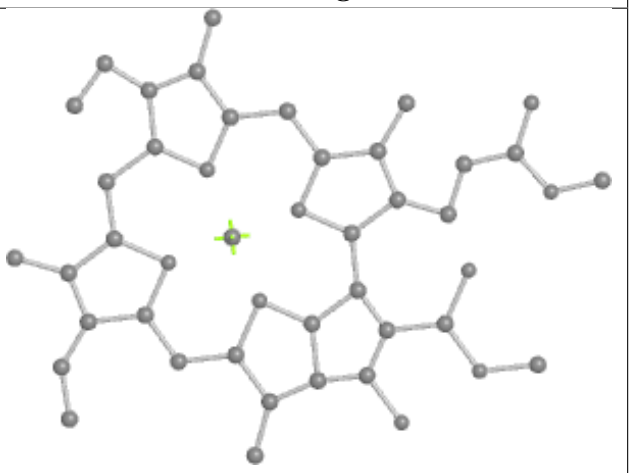
Bond lengths



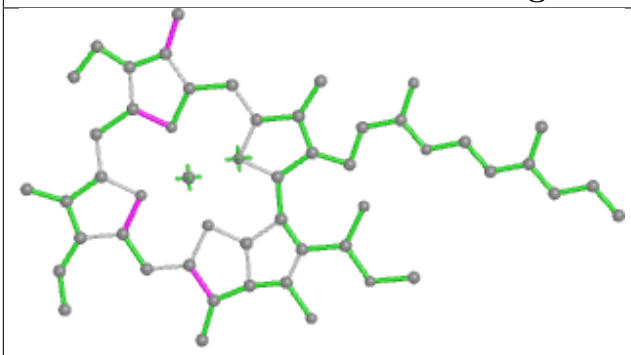
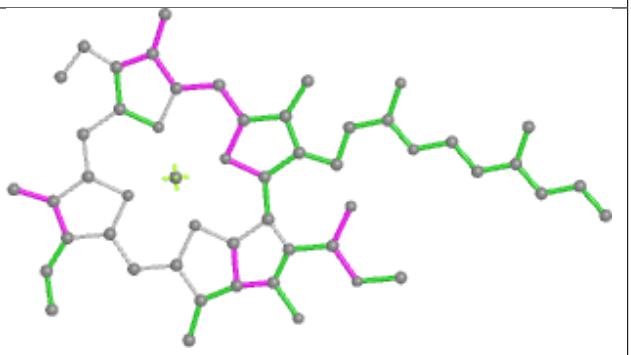
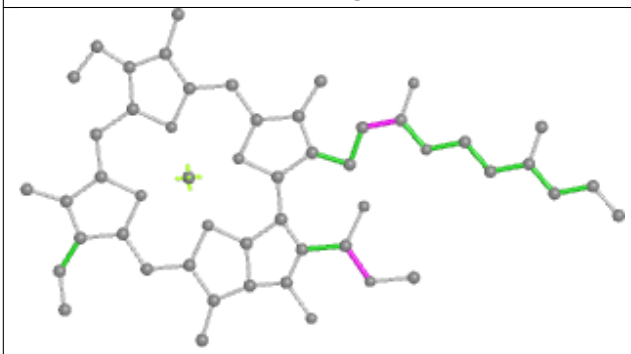
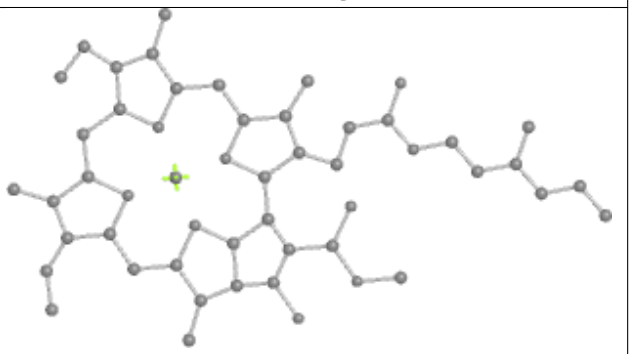
Bond angles

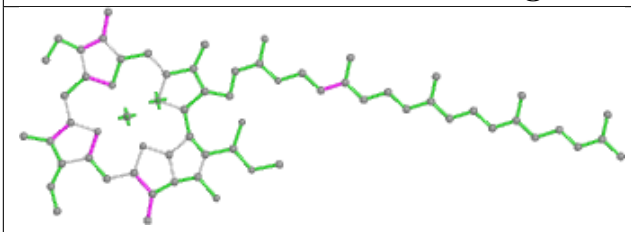
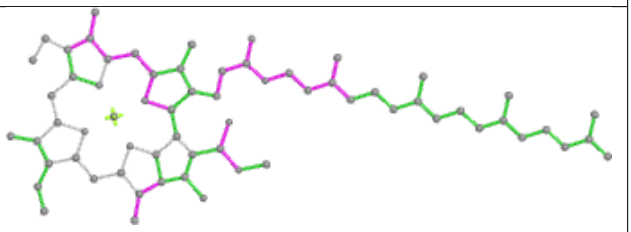
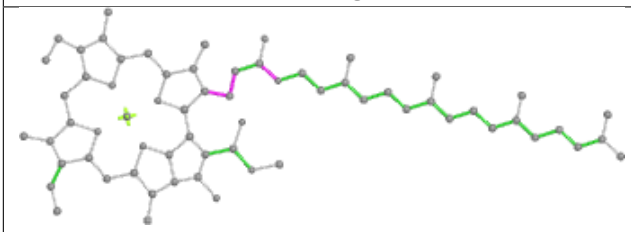
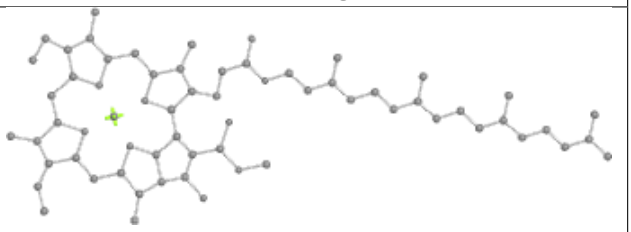


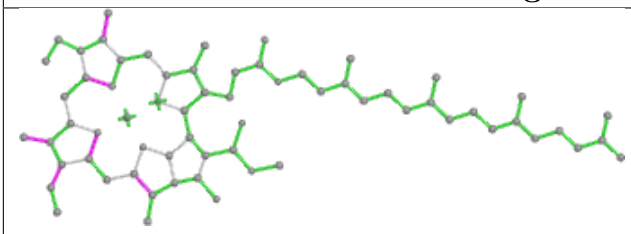
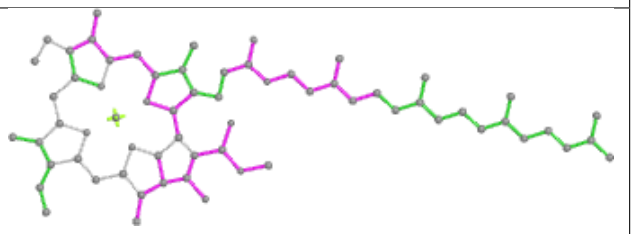
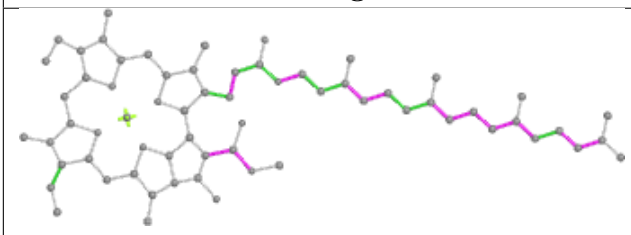
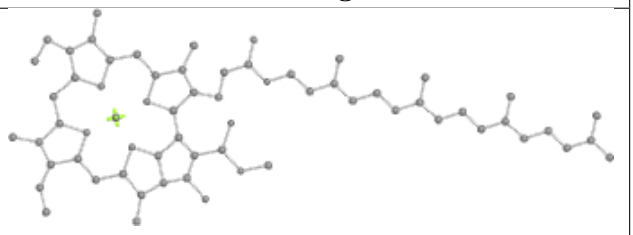
Torsions

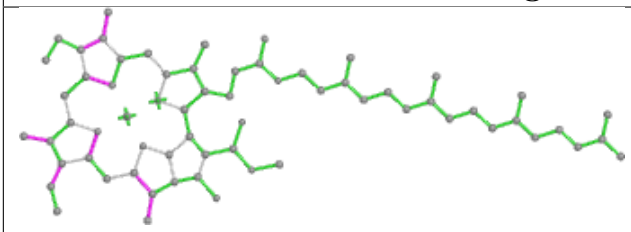
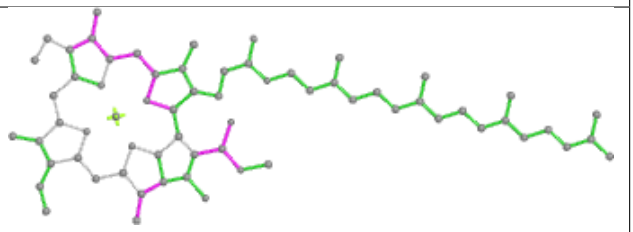
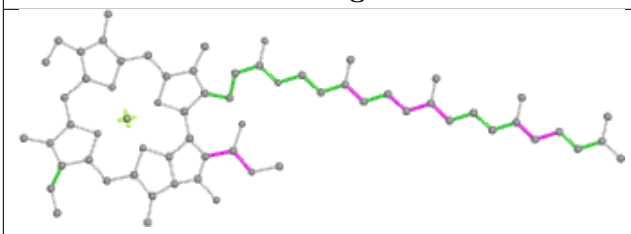
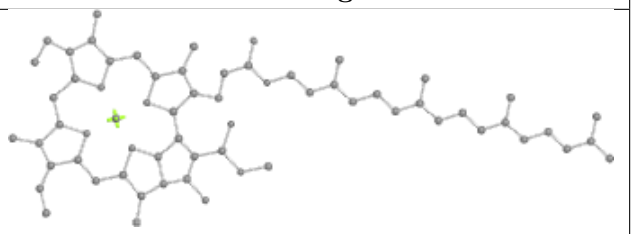


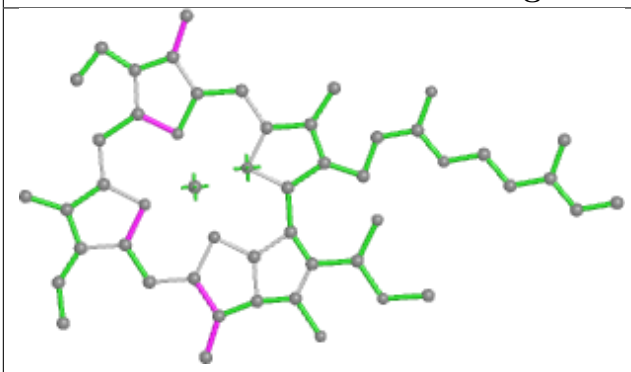
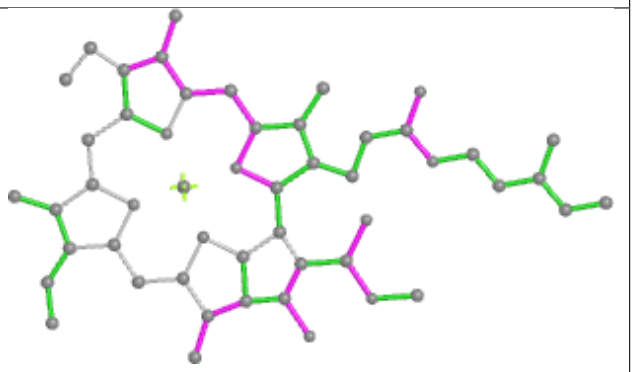
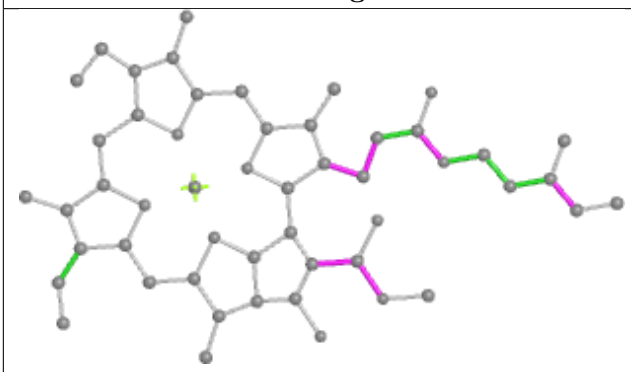
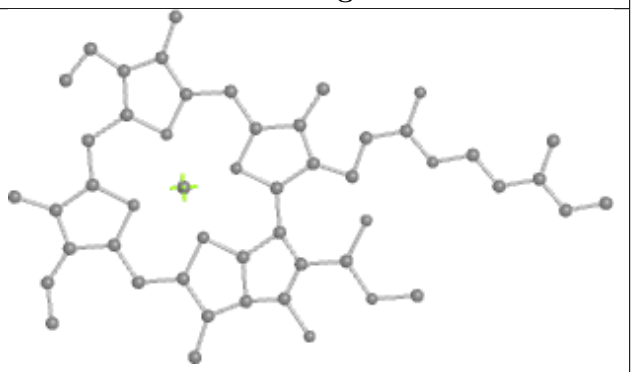
Rings

Ligand CLA 4 311	
 Bond lengths	 Bond angles
 Torsions	 Rings

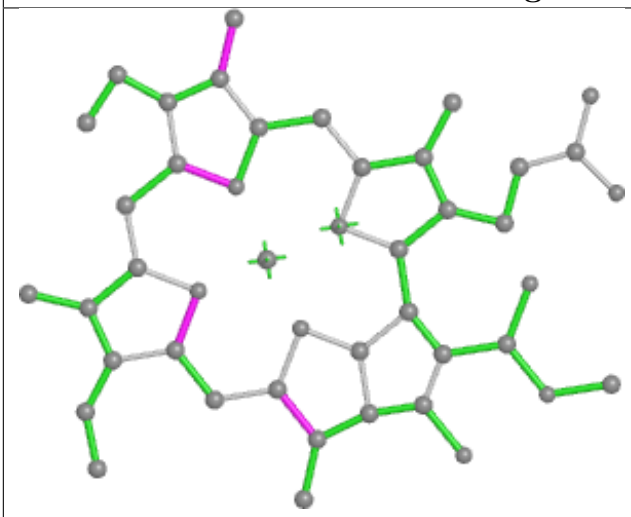
Ligand CLA B 830	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 853	
 Bond lengths	 Bond angles
 Torsions	 Rings

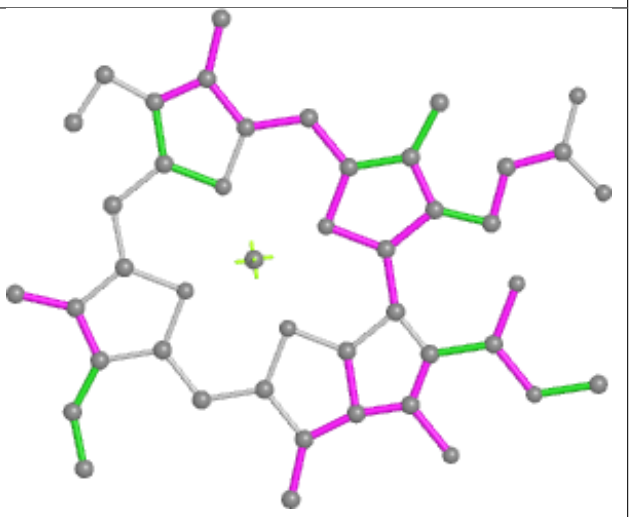
Ligand CLA A 829	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

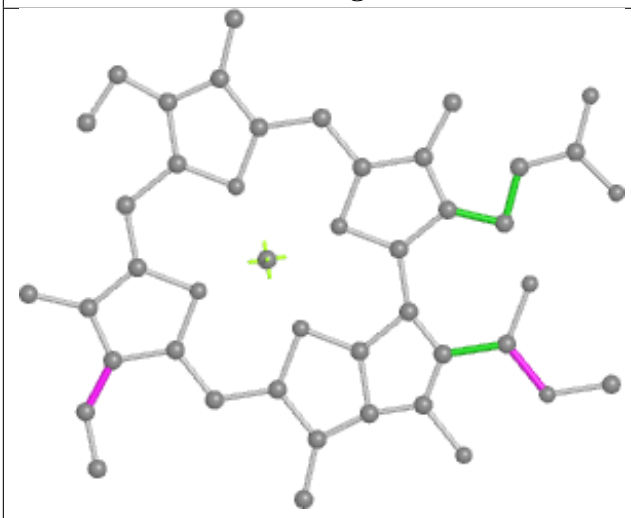
Ligand CLA B 836



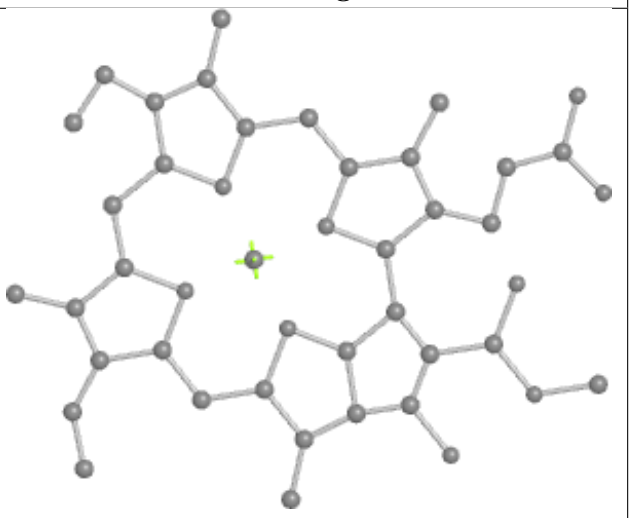
Bond lengths



Bond angles

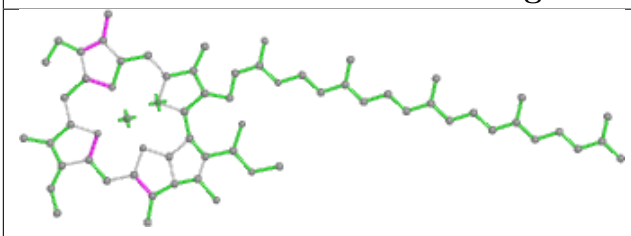


Torsions

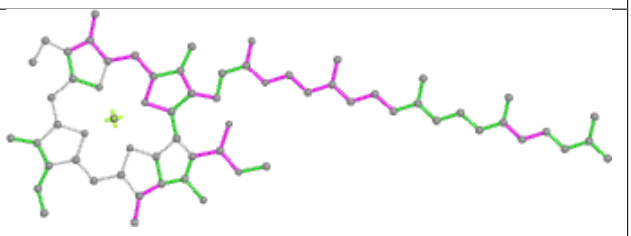


Rings

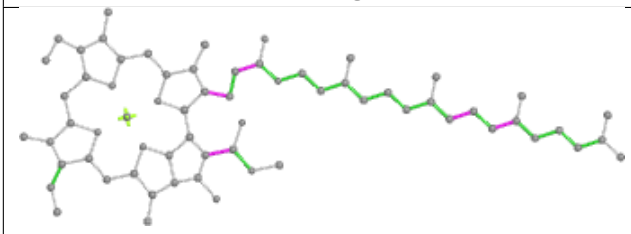
Ligand CLA B 842



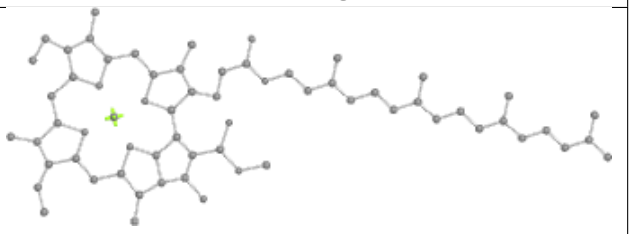
Bond lengths



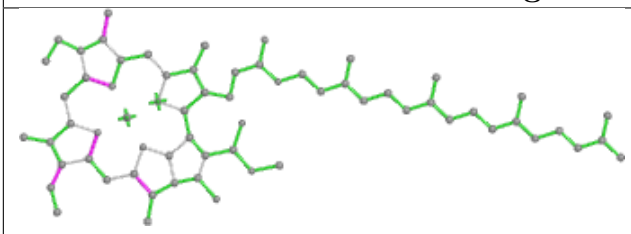
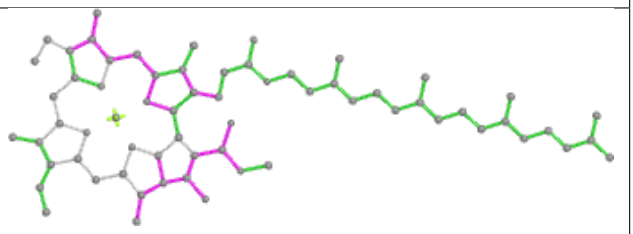
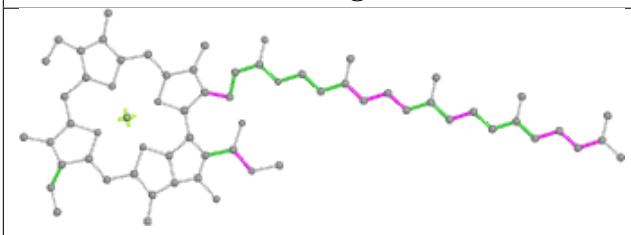
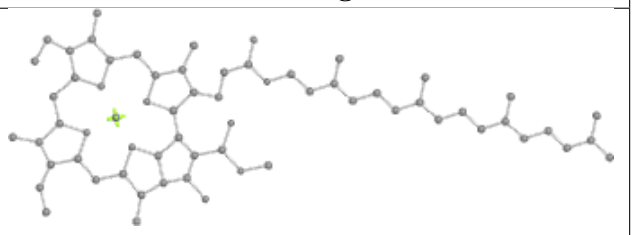
Bond angles

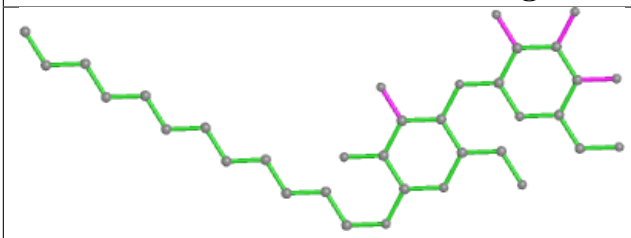
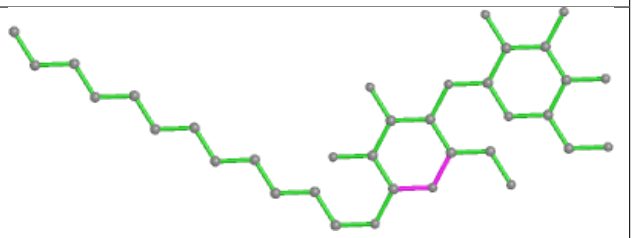
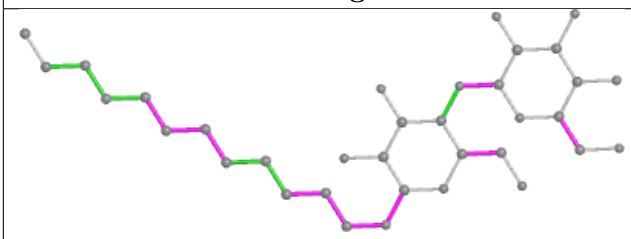
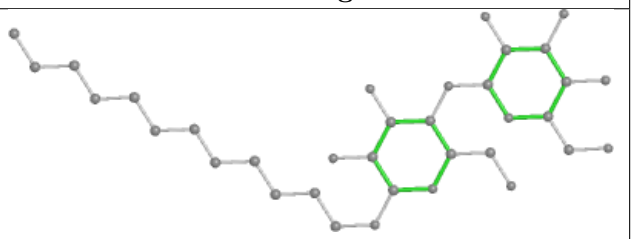


Torsions

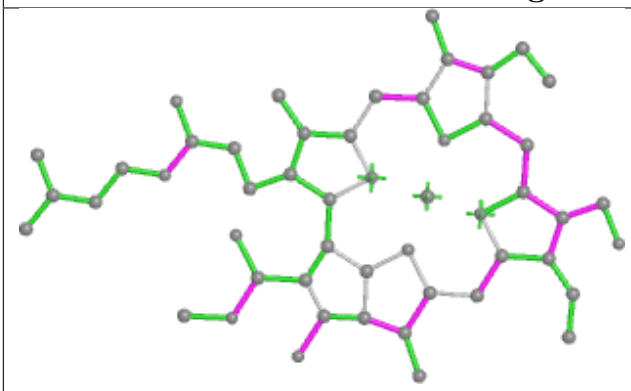


Rings

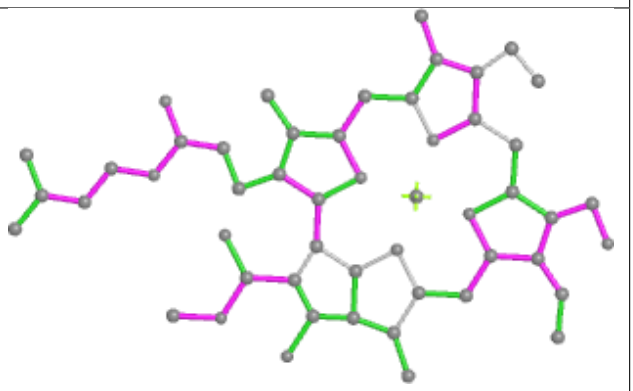
Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 855	
 Bond lengths	 Bond angles
 Torsions	 Rings

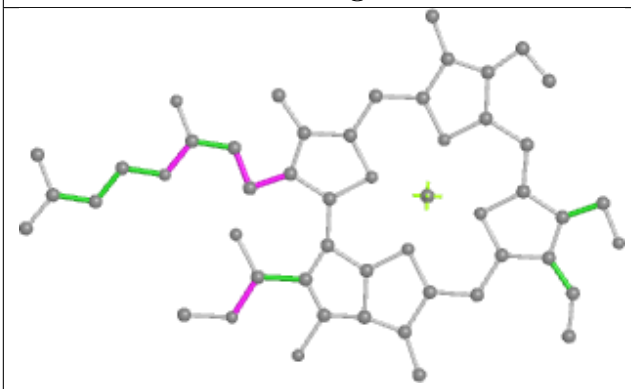
Ligand CHL 4 306



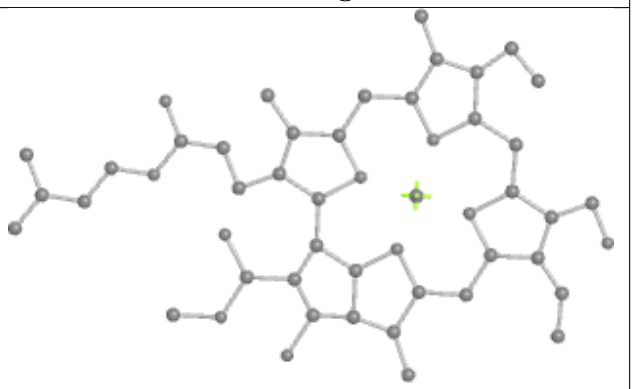
Bond lengths



Bond angles

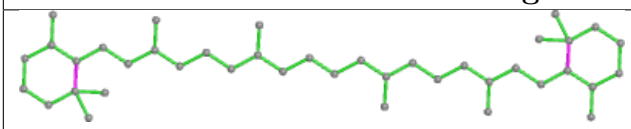


Torsions

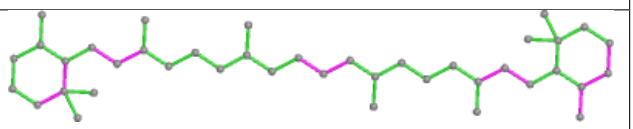


Rings

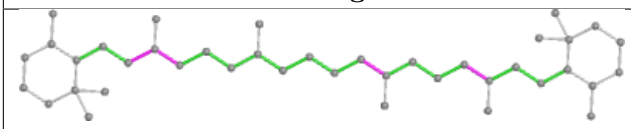
Ligand BCR A 851



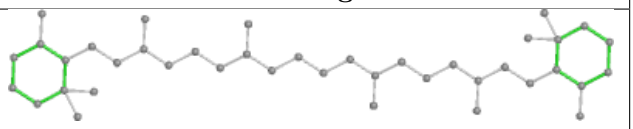
Bond lengths



Bond angles

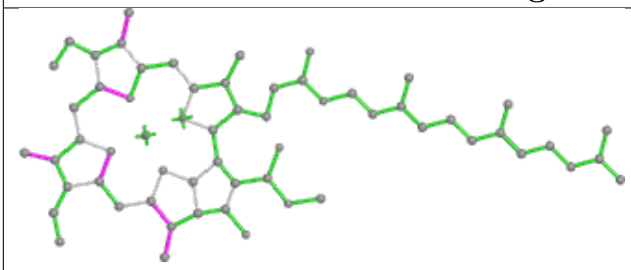


Torsions

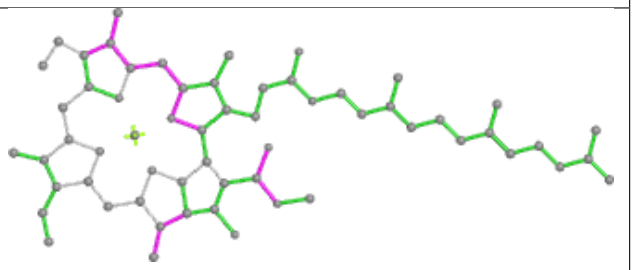


Rings

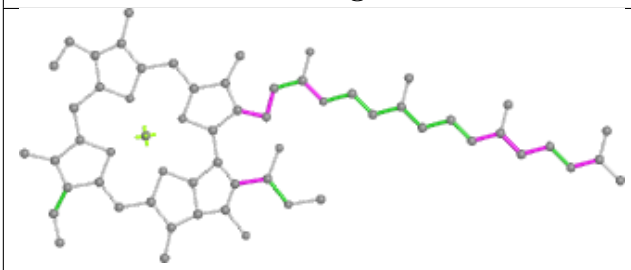
Ligand CLA 2 308



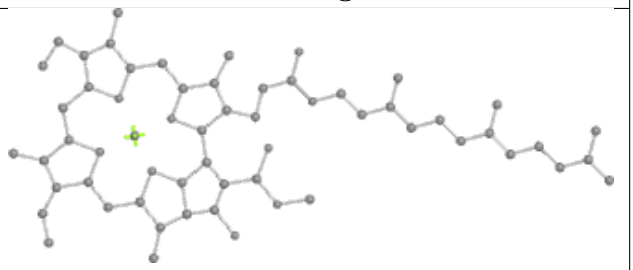
Bond lengths



Bond angles

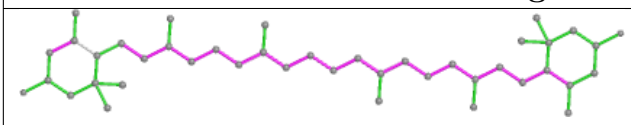


Torsions

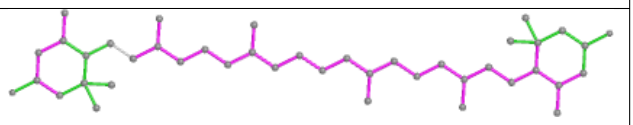


Rings

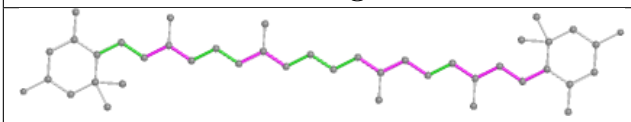
Ligand LUT 3 614



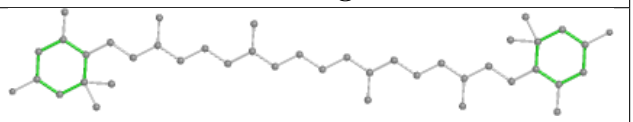
Bond lengths



Bond angles

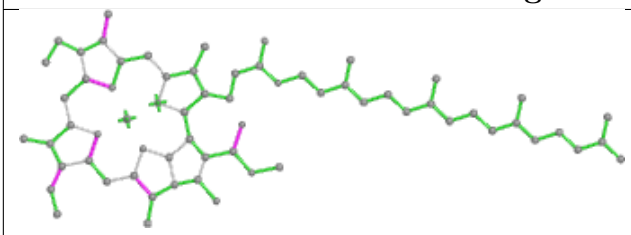


Torsions

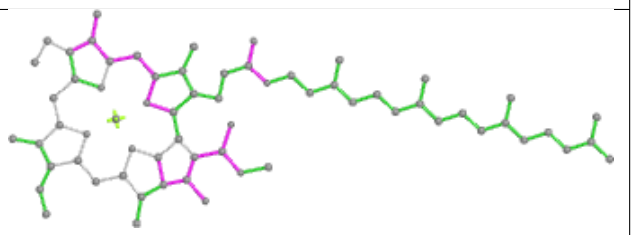


Rings

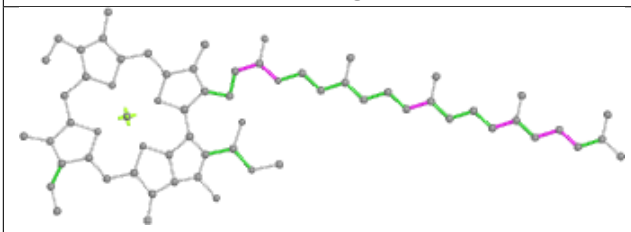
Ligand CLA B 816



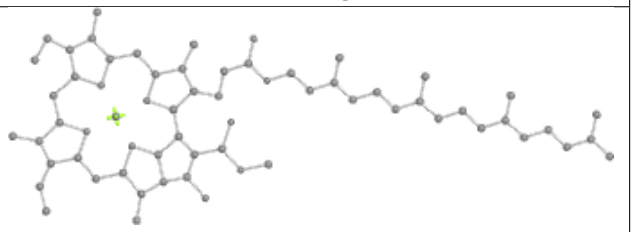
Bond lengths



Bond angles

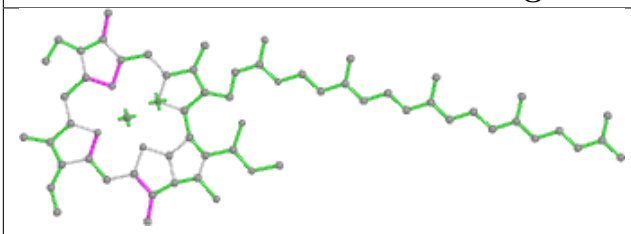


Torsions

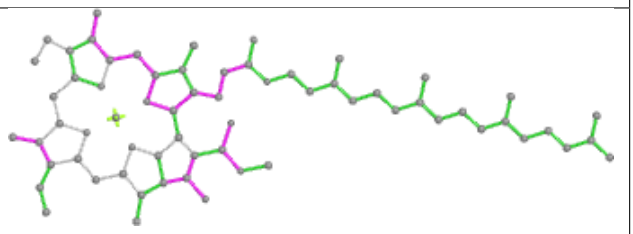


Rings

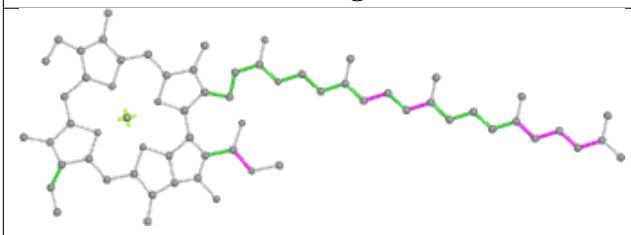
Ligand CLA B 841



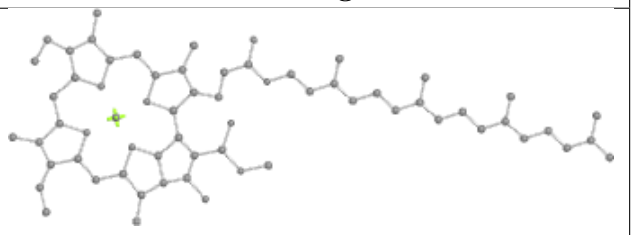
Bond lengths



Bond angles

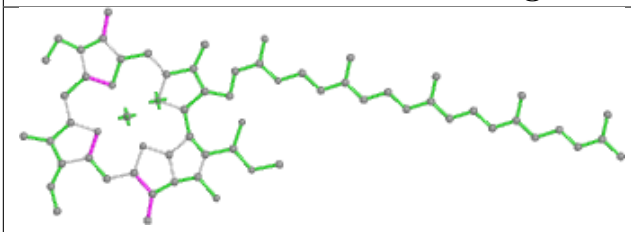


Torsions

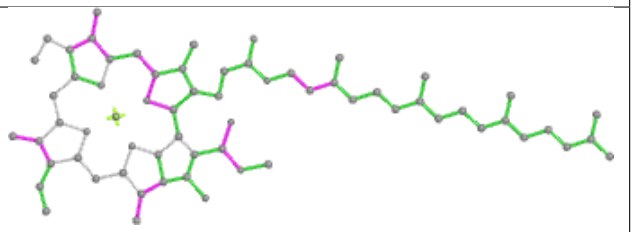


Rings

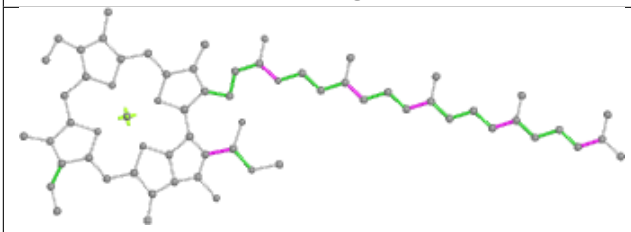
Ligand CLA A 826



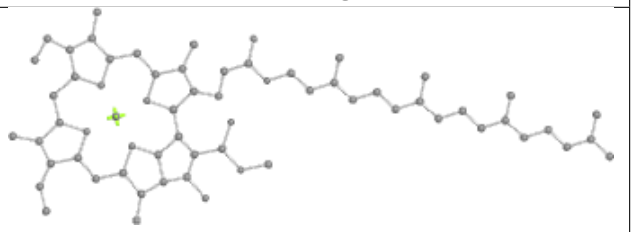
Bond lengths



Bond angles

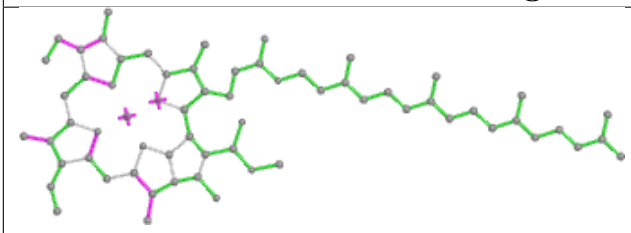


Torsions

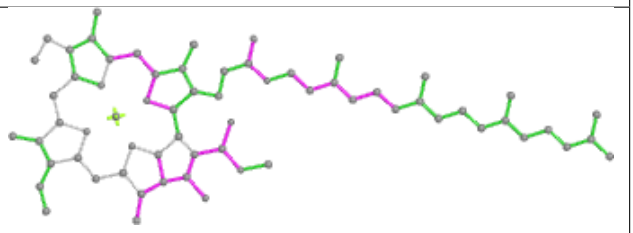


Rings

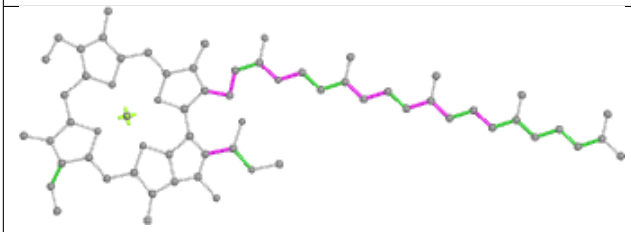
Ligand CLA A 840



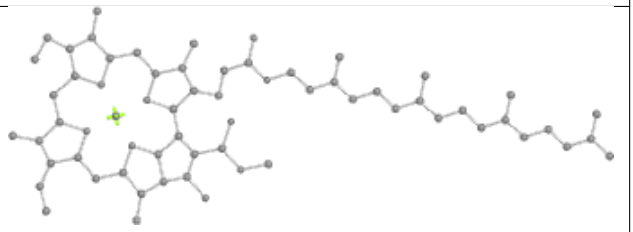
Bond lengths



Bond angles

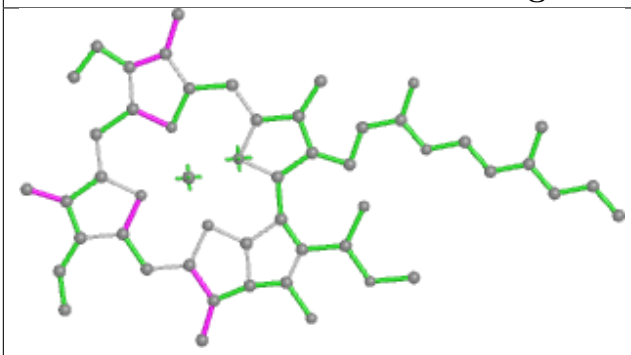


Torsions

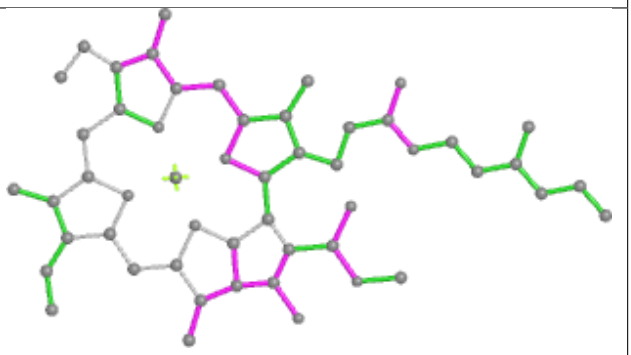


Rings

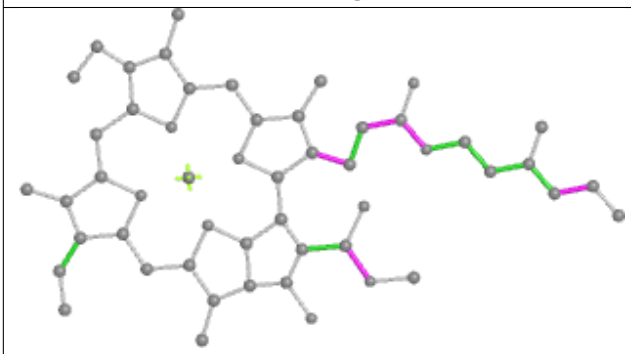
Ligand CLA 1 310



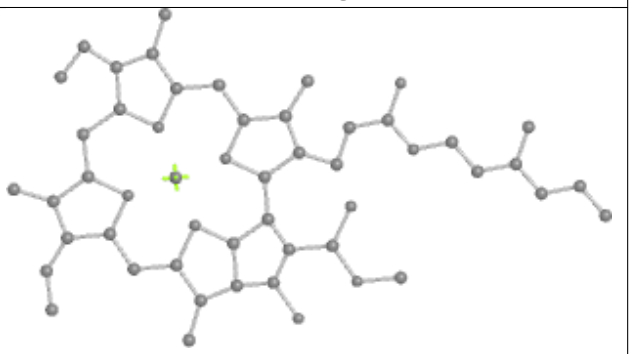
Bond lengths



Bond angles

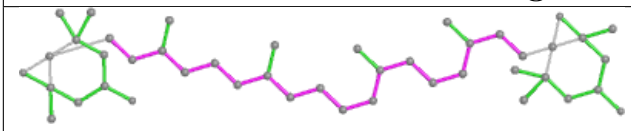


Torsions

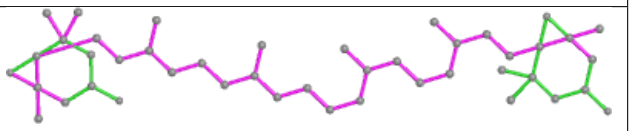


Rings

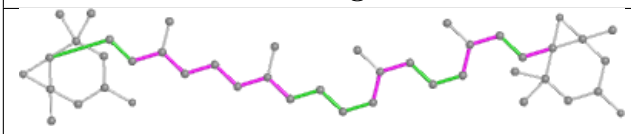
Ligand XAT 2 315



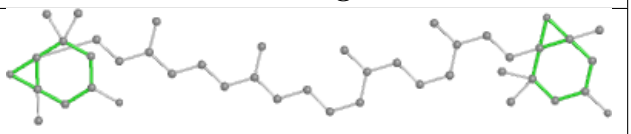
Bond lengths



Bond angles

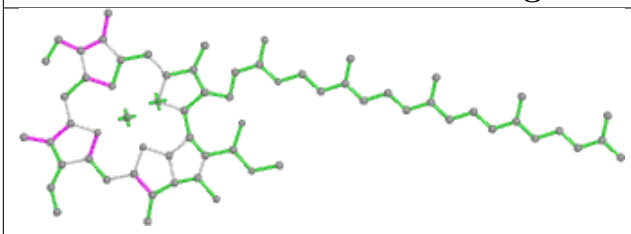


Torsions

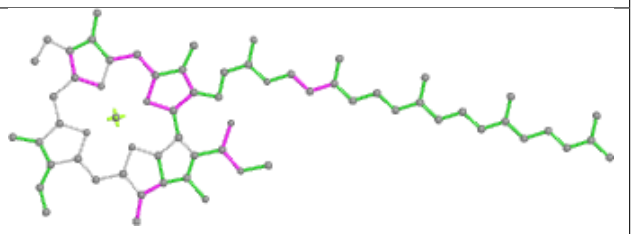


Rings

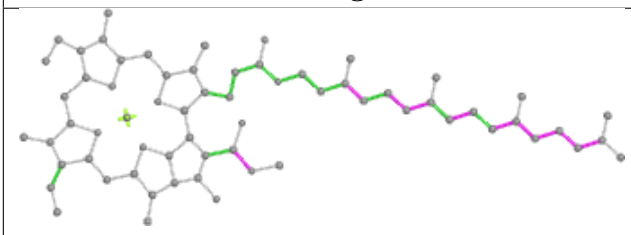
Ligand CLA A 839



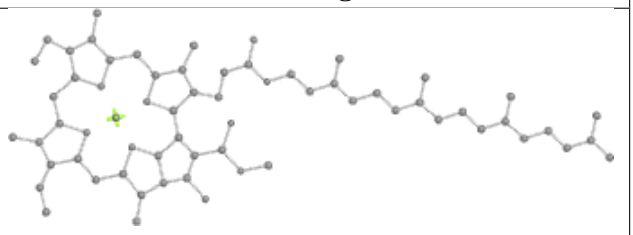
Bond lengths



Bond angles

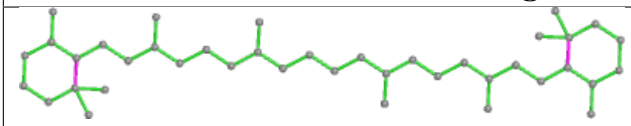


Torsions

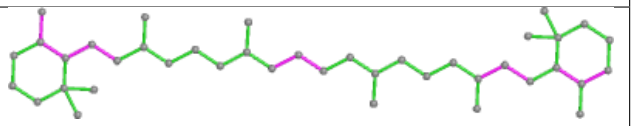


Rings

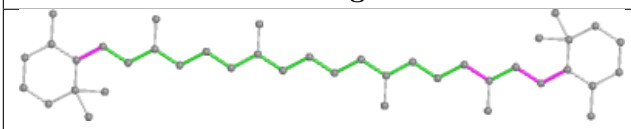
Ligand BCR G 106



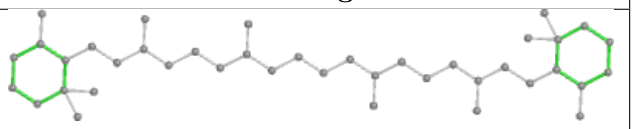
Bond lengths



Bond angles

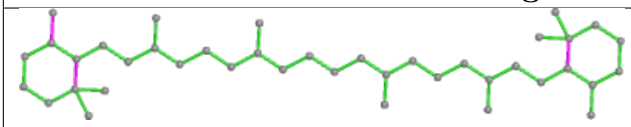


Torsions

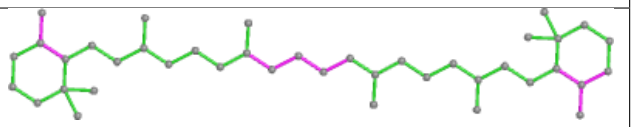


Rings

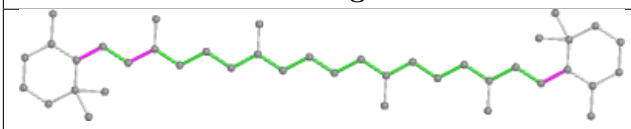
Ligand BCR A 847



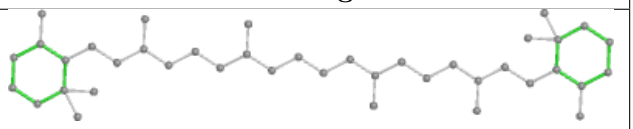
Bond lengths



Bond angles

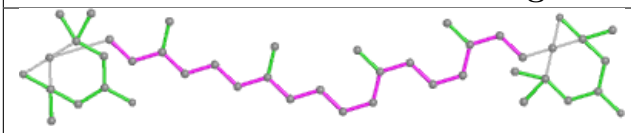


Torsions

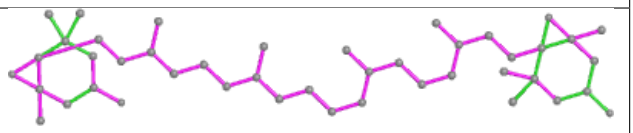


Rings

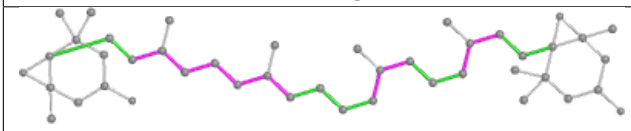
Ligand XAT 4 317



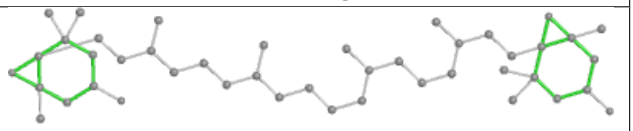
Bond lengths



Bond angles

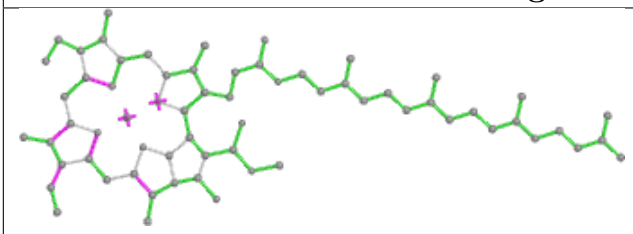


Torsions

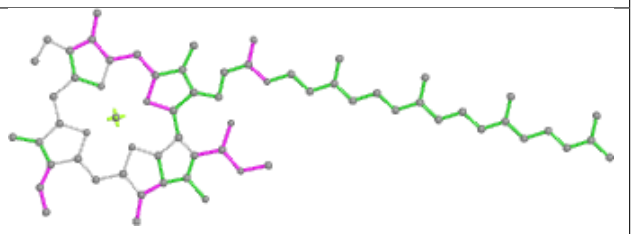


Rings

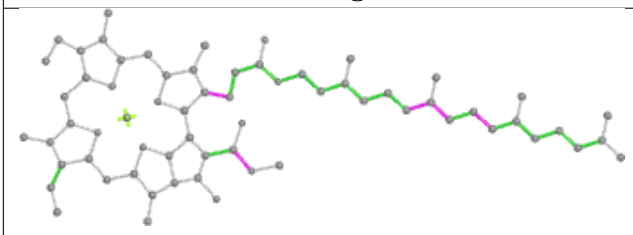
Ligand CLA J 101



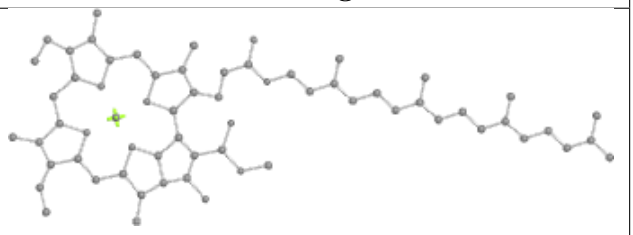
Bond lengths



Bond angles

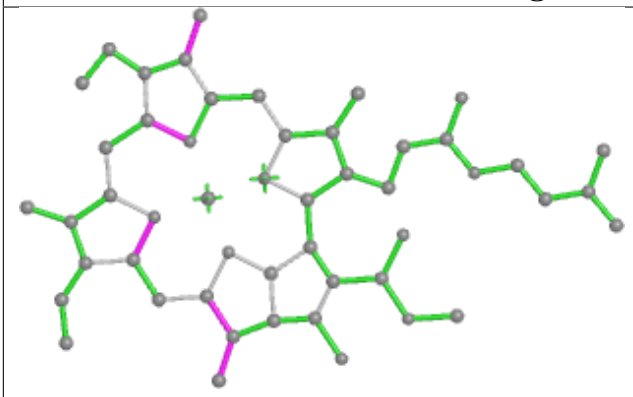


Torsions

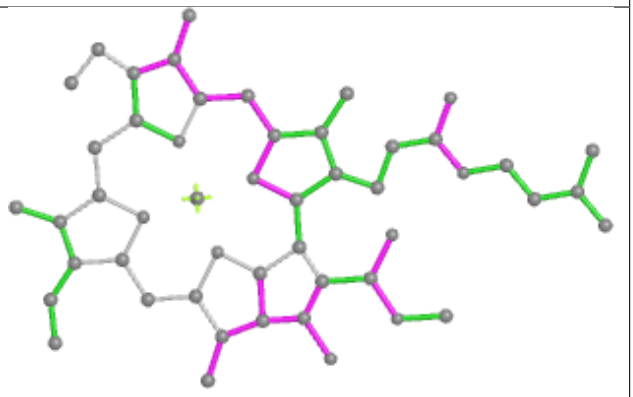


Rings

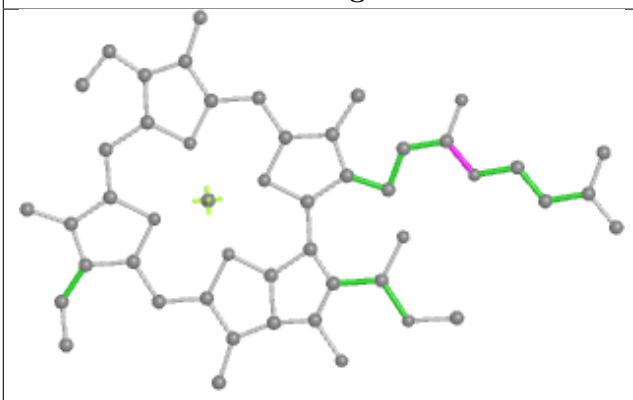
Ligand CLA 2 307



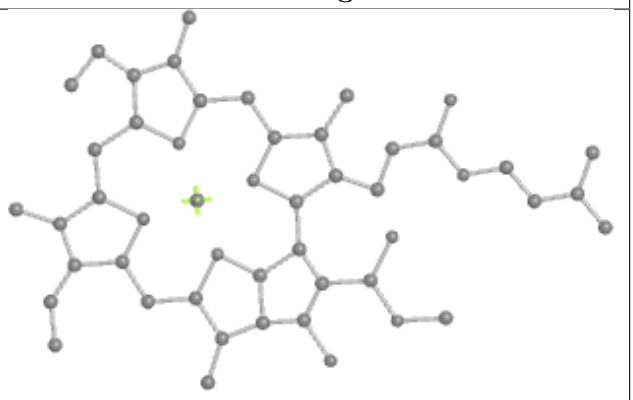
Bond lengths



Bond angles

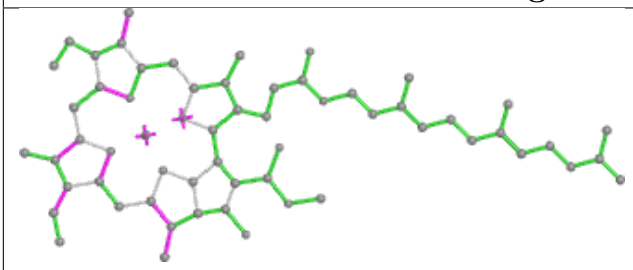


Torsions

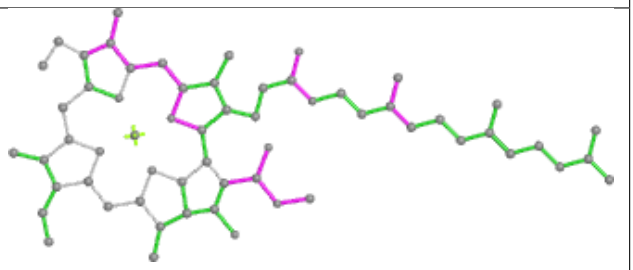


Rings

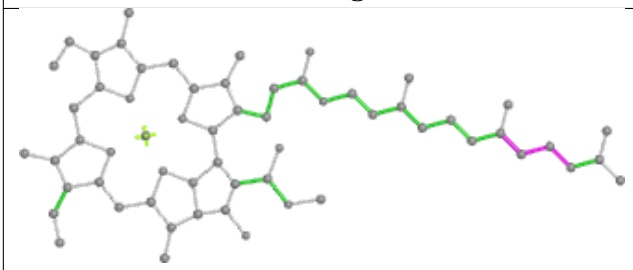
Ligand CLA 4 302



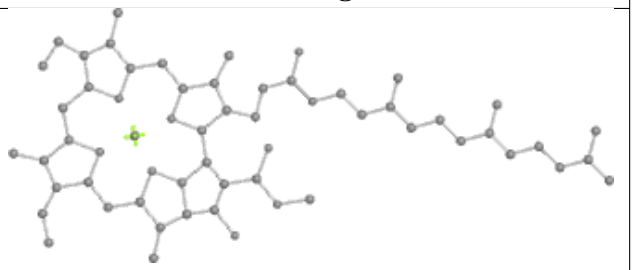
Bond lengths



Bond angles

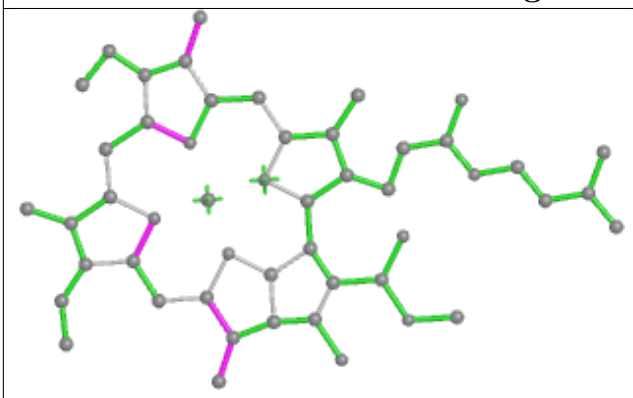


Torsions

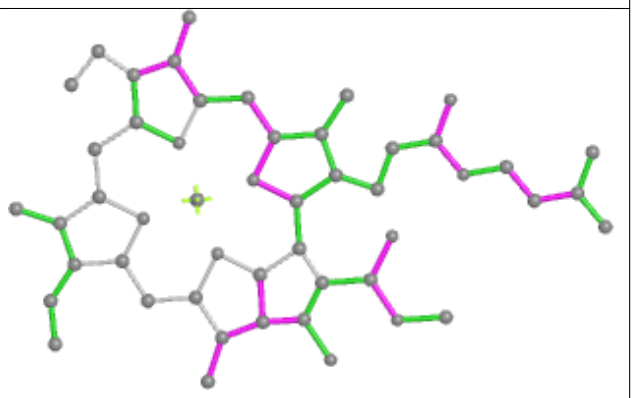


Rings

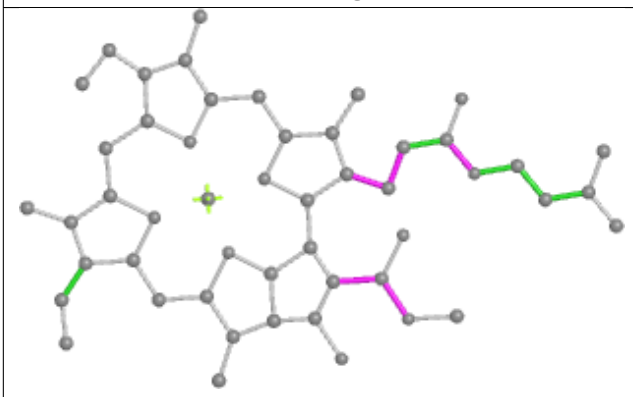
Ligand CLA A 814



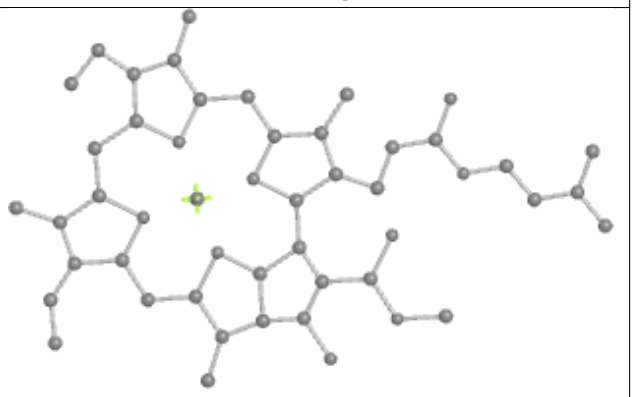
Bond lengths



Bond angles

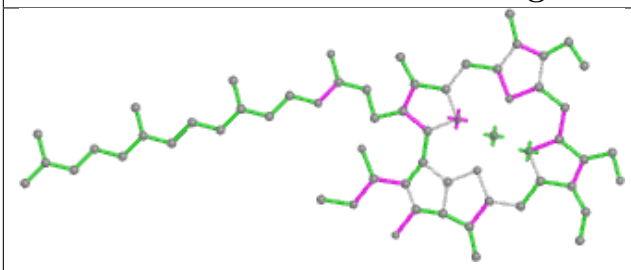


Torsions

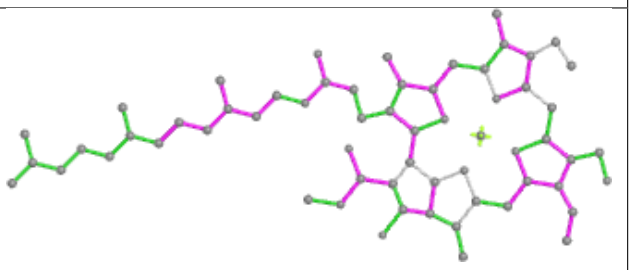


Rings

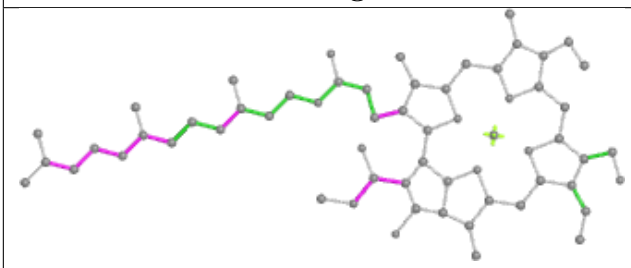
Ligand CHL 4 301



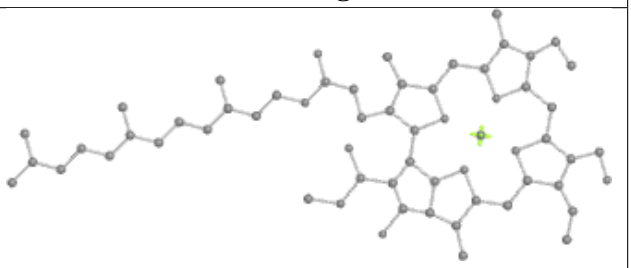
Bond lengths



Bond angles

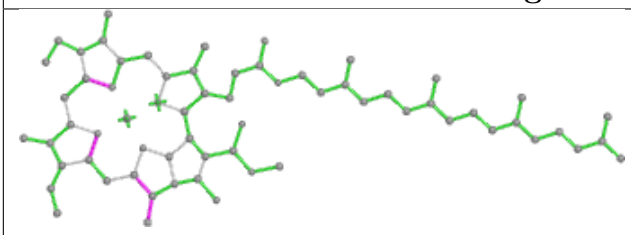


Torsions

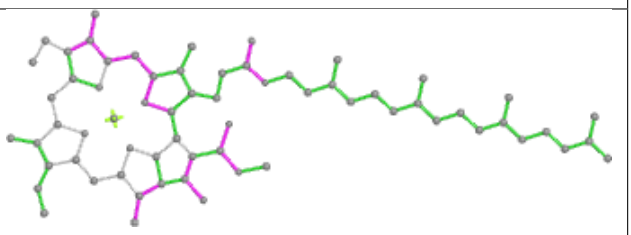


Rings

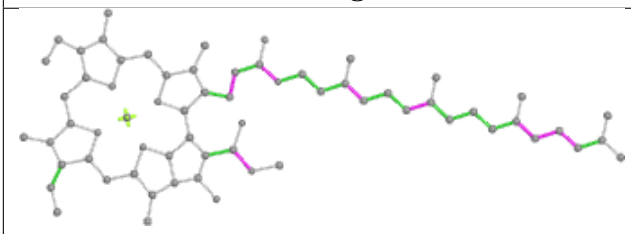
Ligand CLA B 840



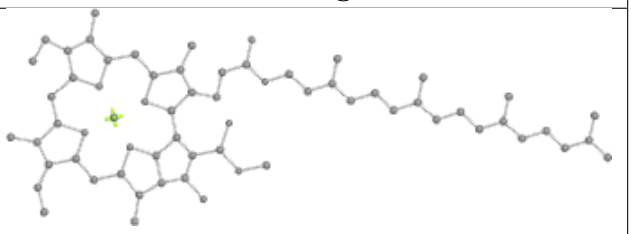
Bond lengths



Bond angles

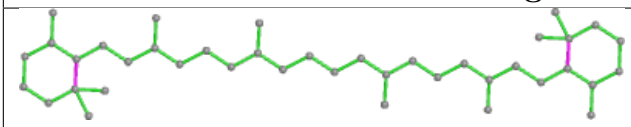


Torsions

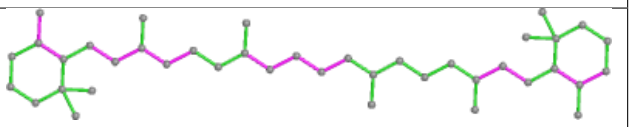


Rings

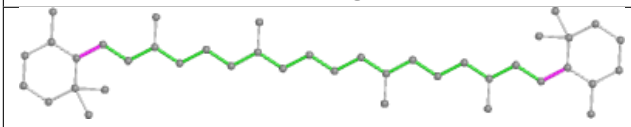
Ligand BCR L 206



Bond lengths



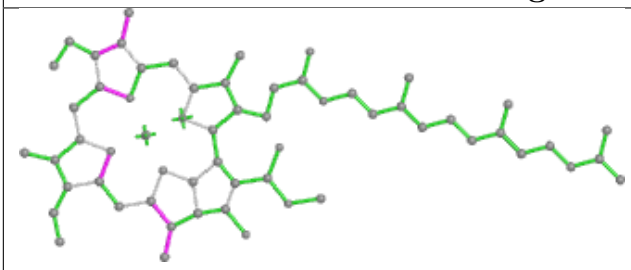
Bond angles



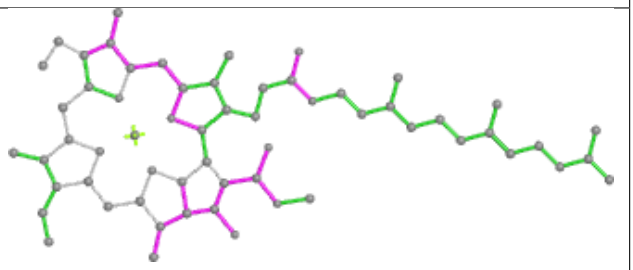
Torsions

Rings

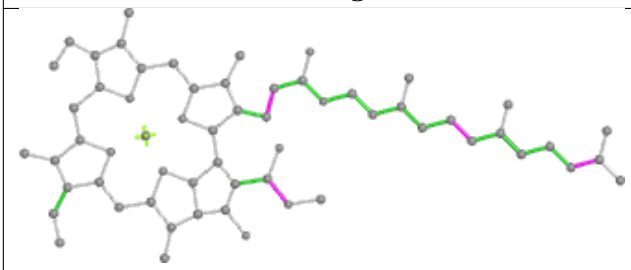
Ligand CLA 1 311



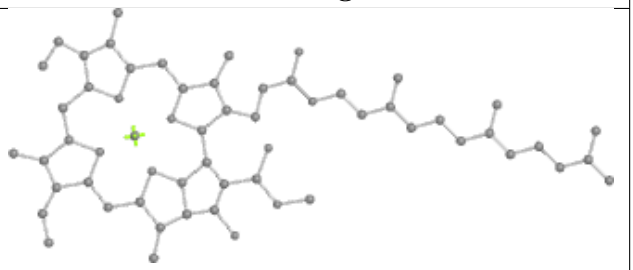
Bond lengths



Bond angles

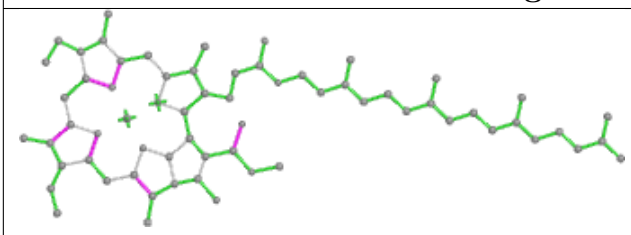


Torsions

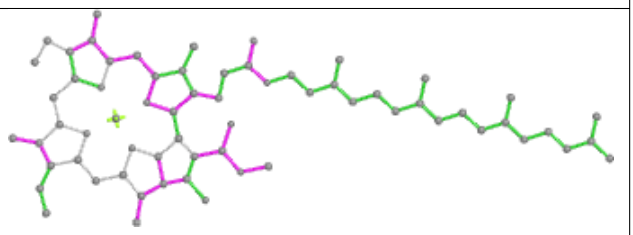


Rings

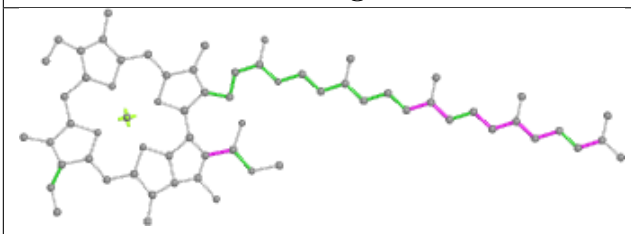
Ligand CLA B 827



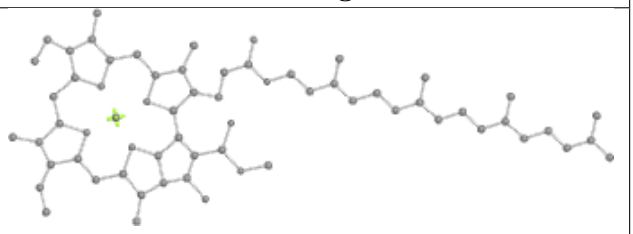
Bond lengths



Bond angles

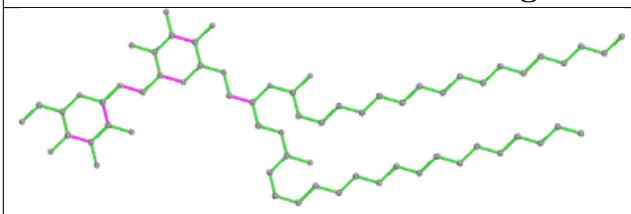


Torsions

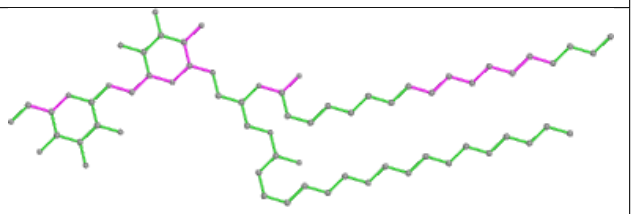


Rings

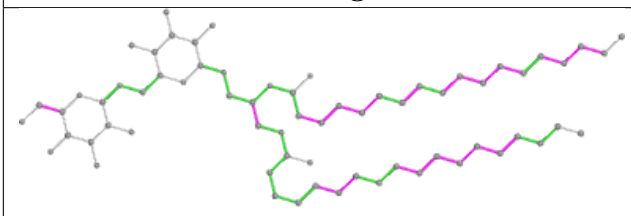
Ligand DGD B 850



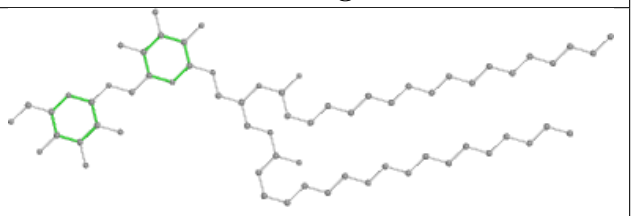
Bond lengths



Bond angles

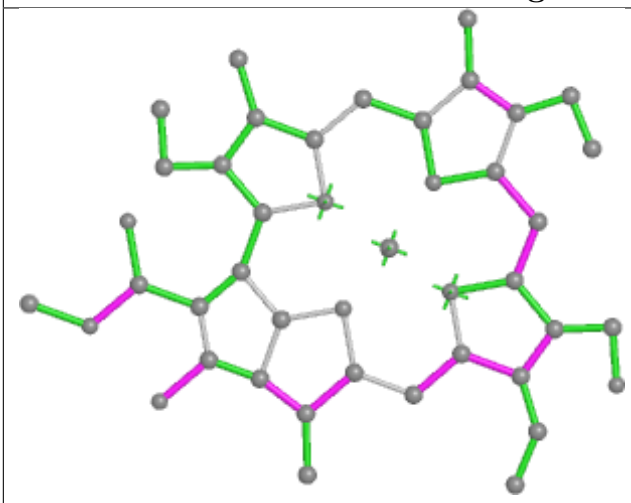


Torsions

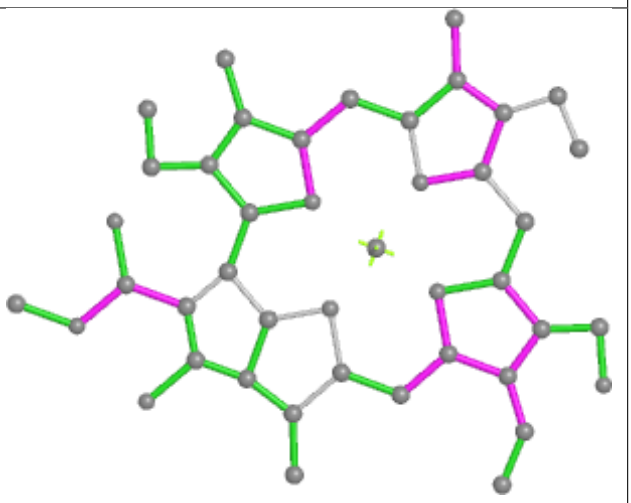


Rings

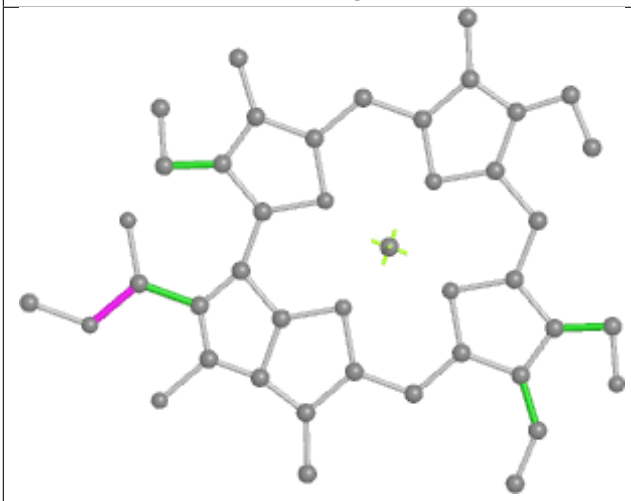
Ligand CHL 4 315



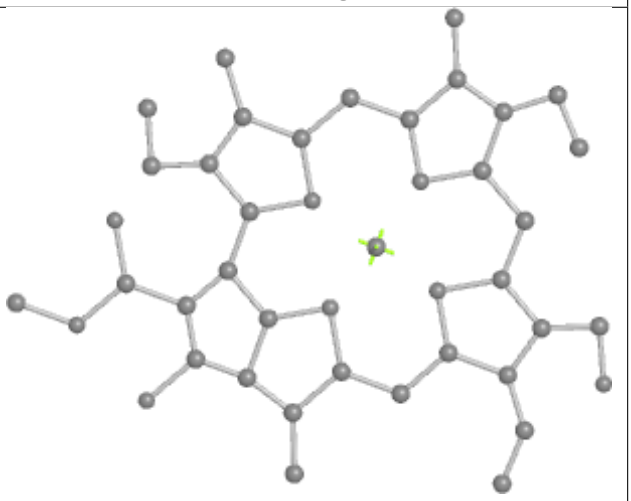
Bond lengths



Bond angles

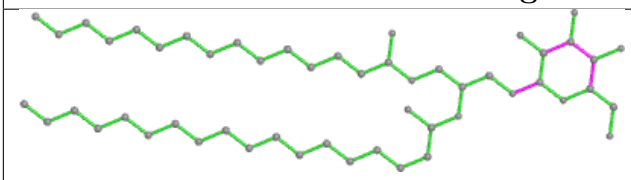


Torsions

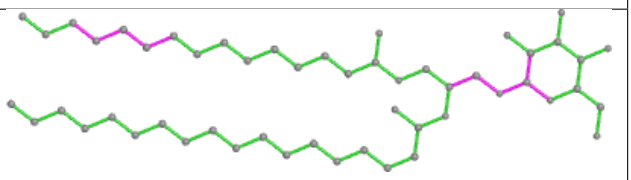


Rings

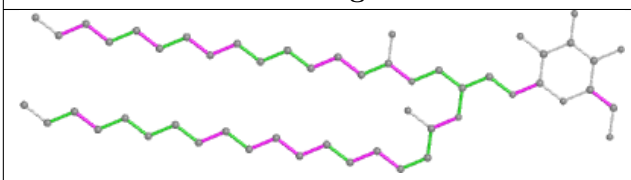
Ligand LMG B 852



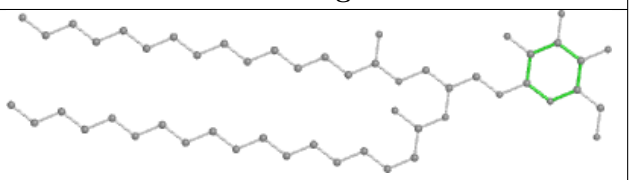
Bond lengths



Bond angles

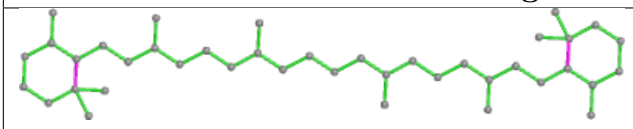


Torsions

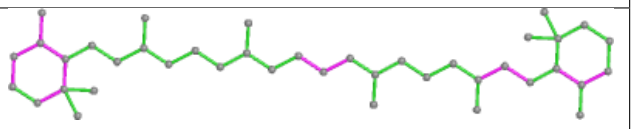


Rings

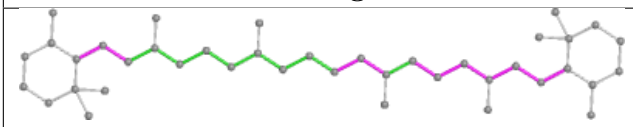
Ligand BCR K 203



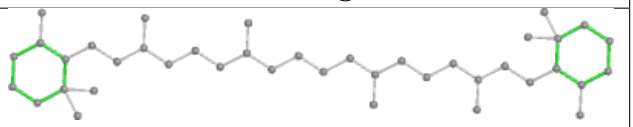
Bond lengths



Bond angles

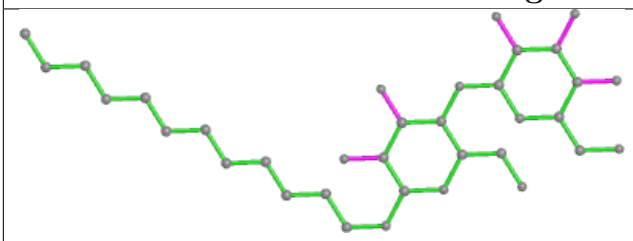


Torsions

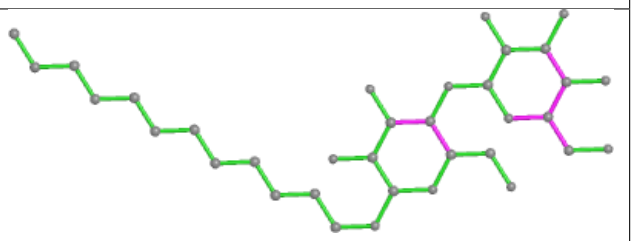


Rings

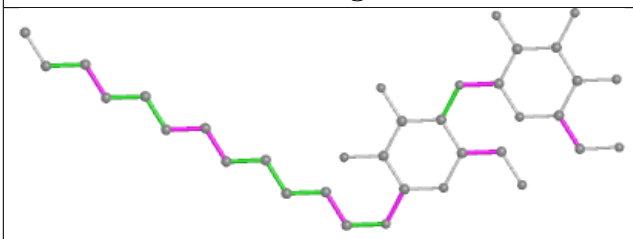
Ligand LMT 2 318



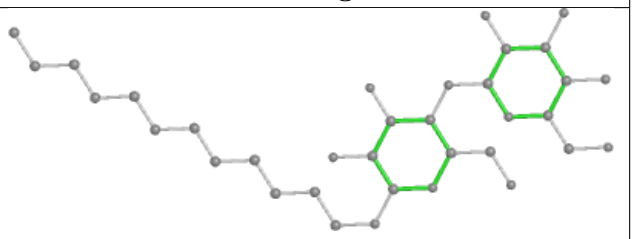
Bond lengths



Bond angles

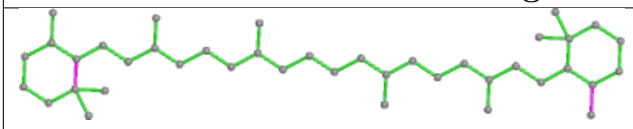


Torsions

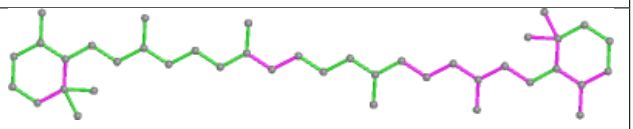


Rings

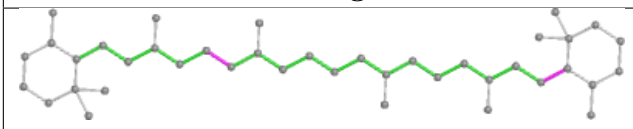
Ligand BCR B 847



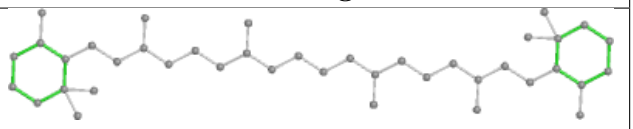
Bond lengths



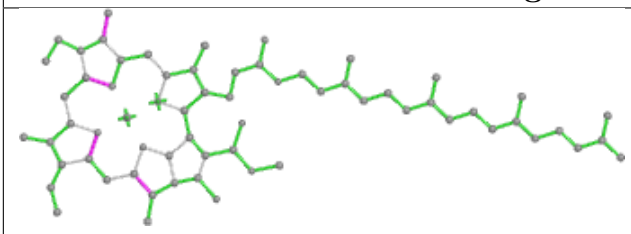
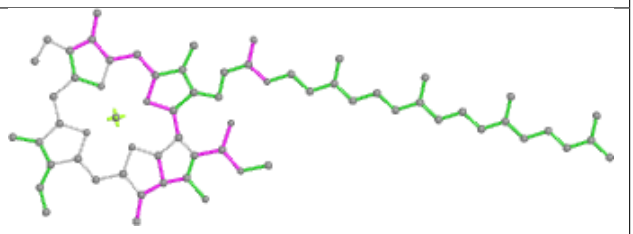
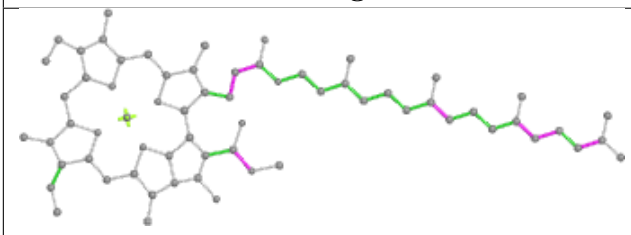
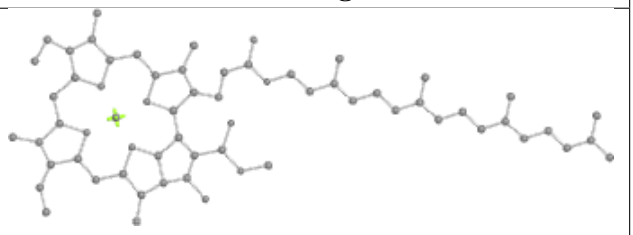
Bond angles

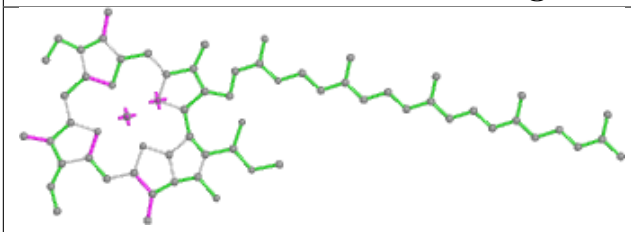
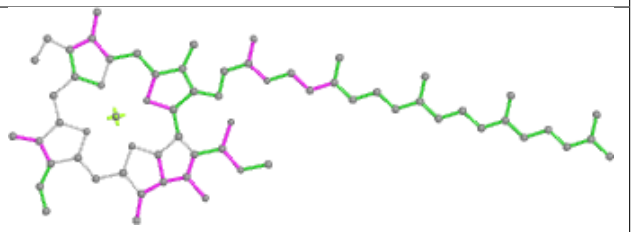
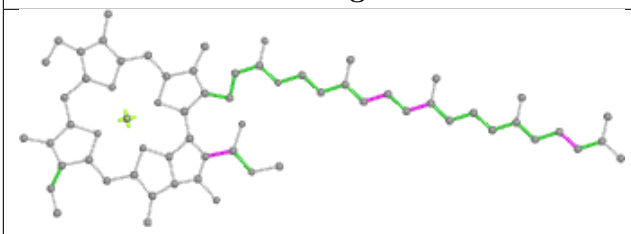
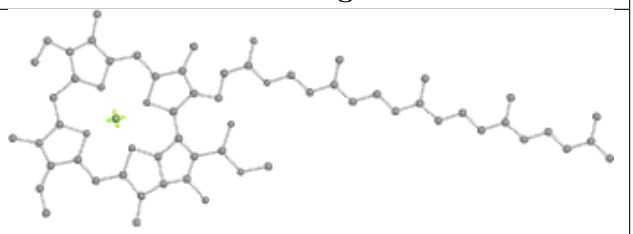


Torsions

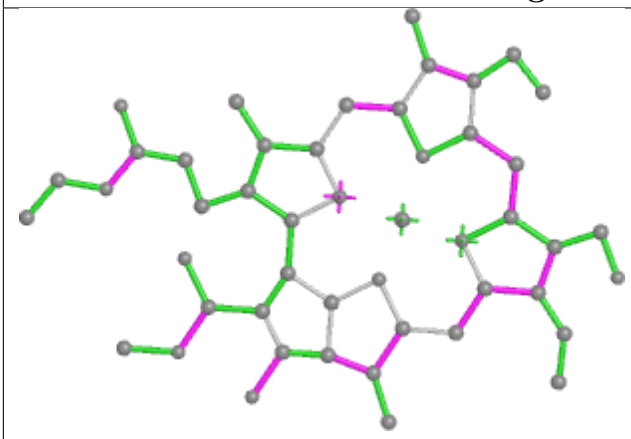


Rings

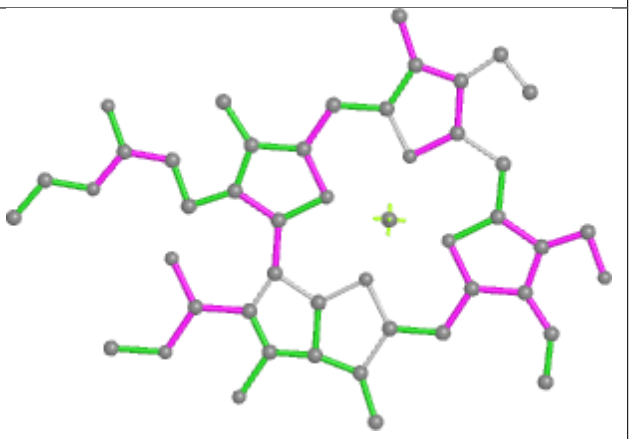
Ligand CLA B 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 2 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

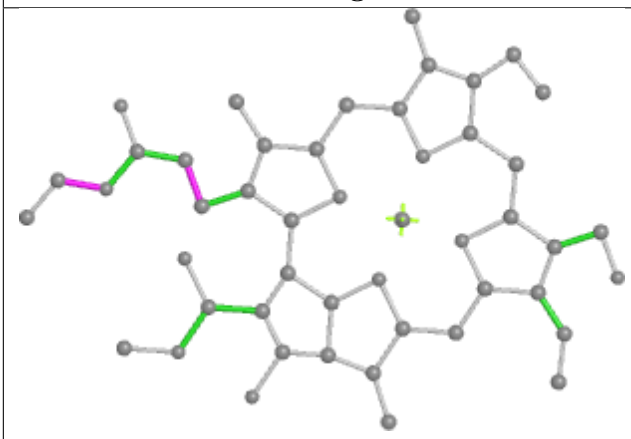
Ligand CHL 2 305



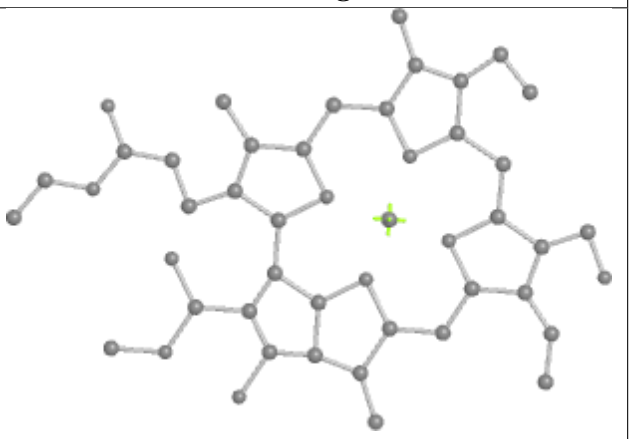
Bond lengths



Bond angles

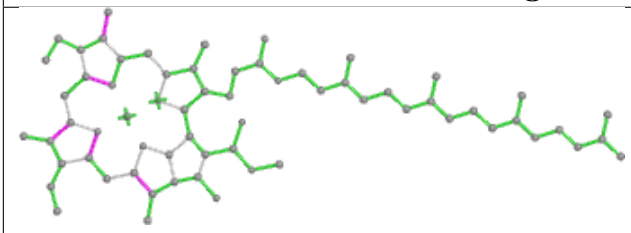


Torsions

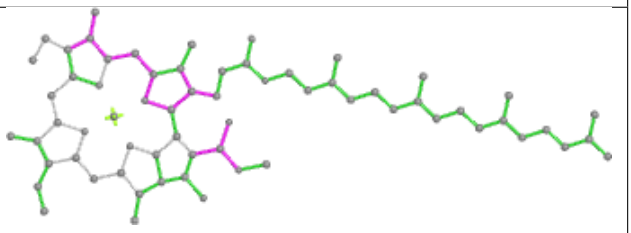


Rings

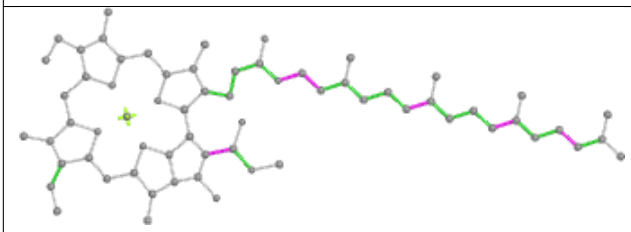
Ligand CLA A 825



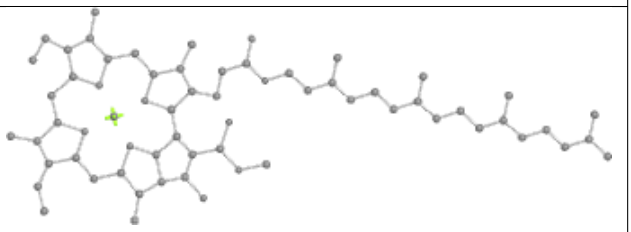
Bond lengths



Bond angles

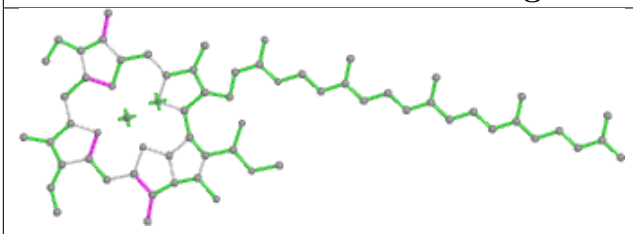


Torsions

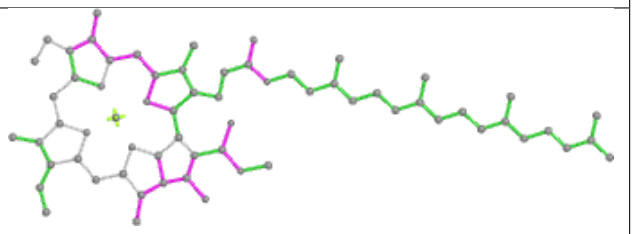


Rings

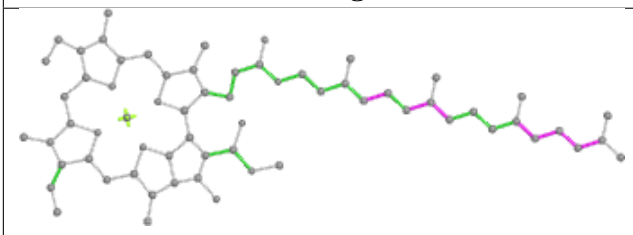
Ligand CLA A 820



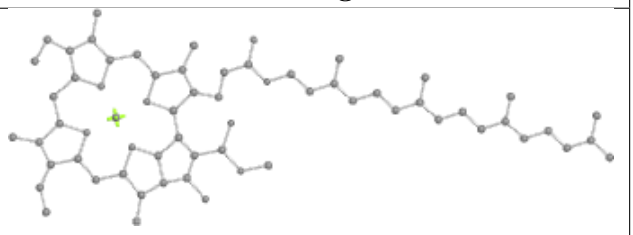
Bond lengths



Bond angles

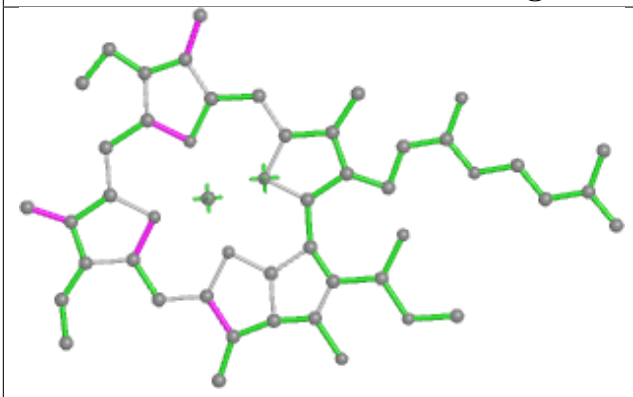


Torsions

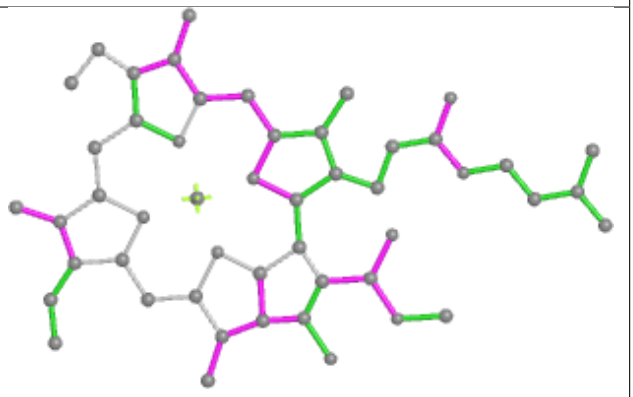


Rings

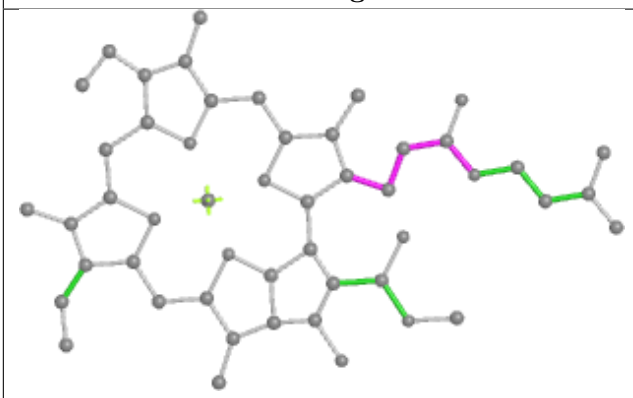
Ligand CLA L 204



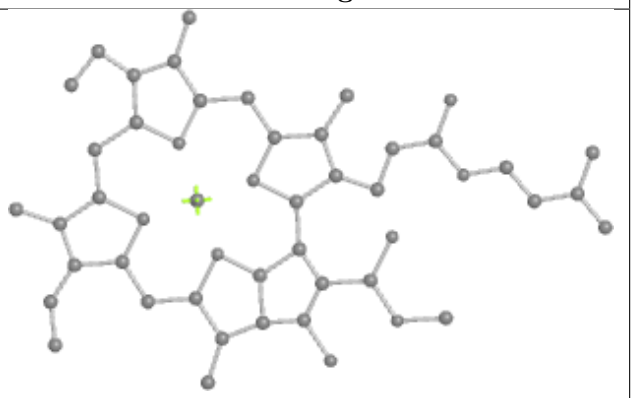
Bond lengths



Bond angles

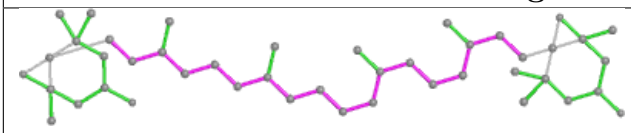


Torsions

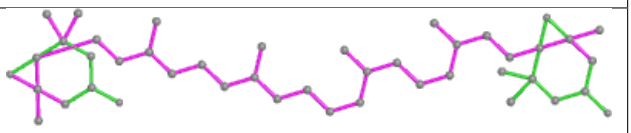


Rings

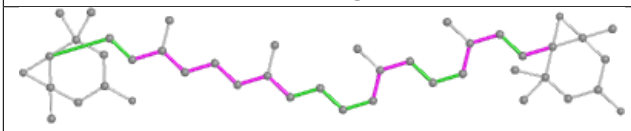
Ligand XAT 1 315



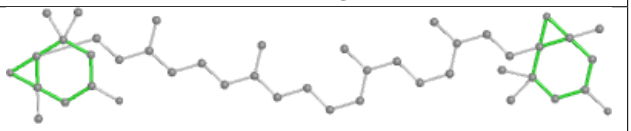
Bond lengths



Bond angles

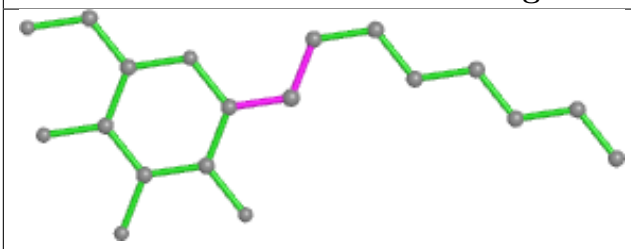


Torsions

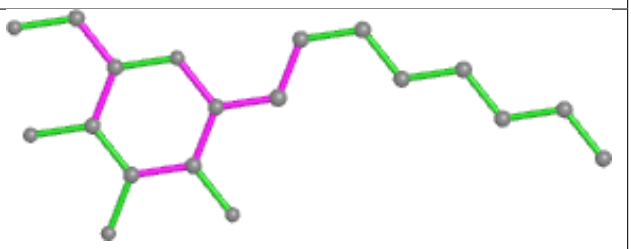


Rings

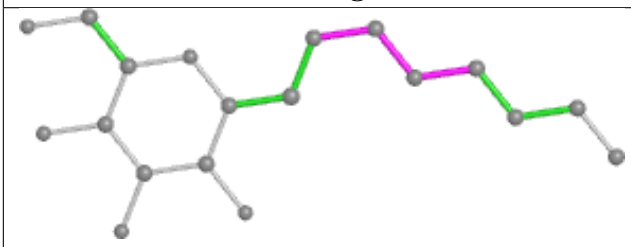
Ligand HTG F 305



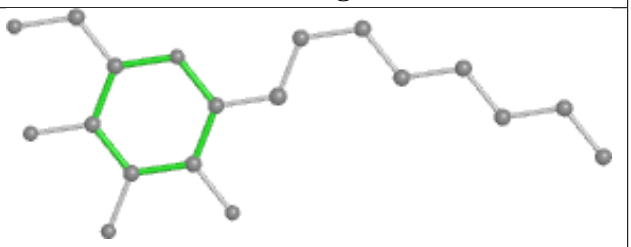
Bond lengths



Bond angles

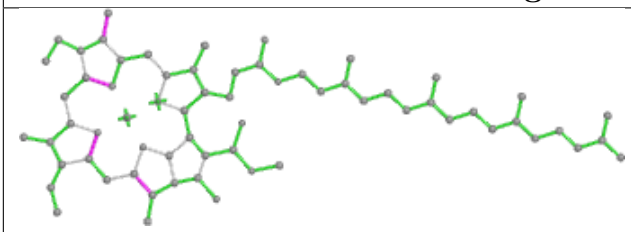


Torsions

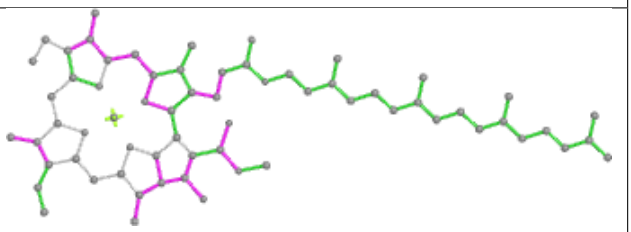


Rings

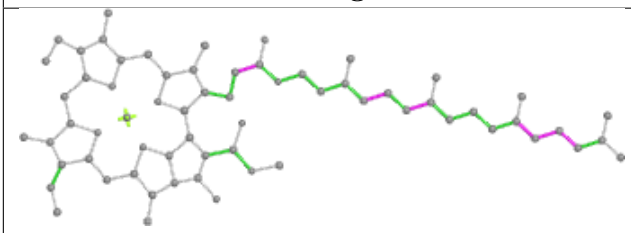
Ligand CLA B 811



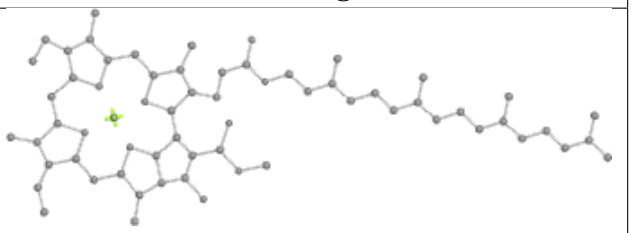
Bond lengths



Bond angles

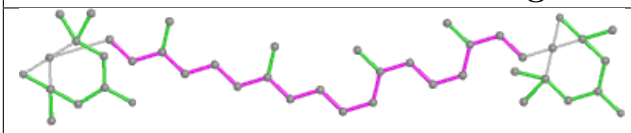


Torsions

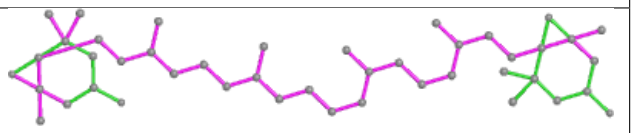


Rings

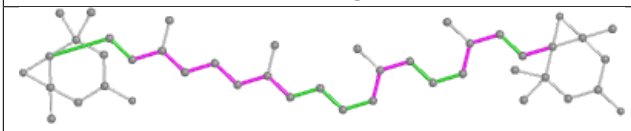
Ligand XAT 3 615



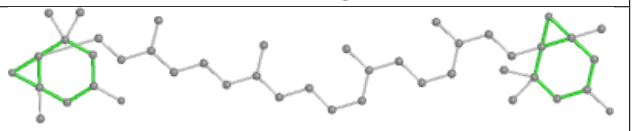
Bond lengths



Bond angles

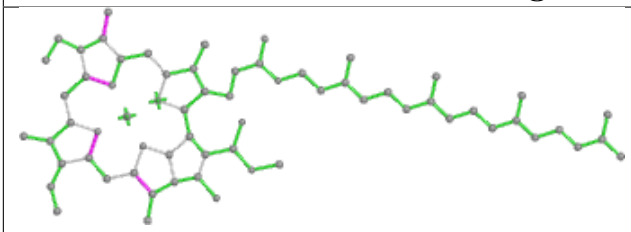


Torsions

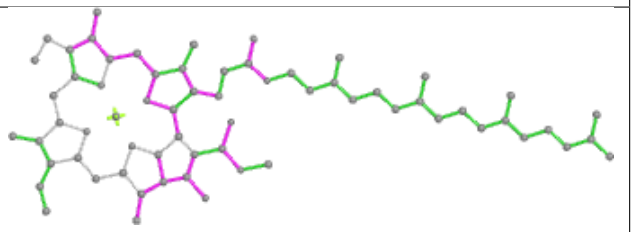


Rings

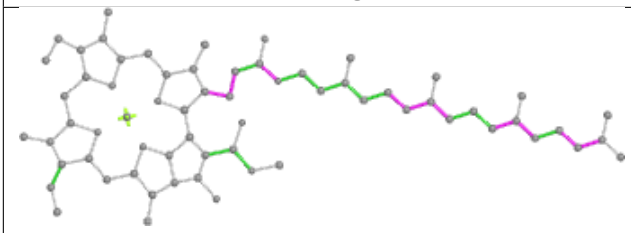
Ligand CLA 1 309



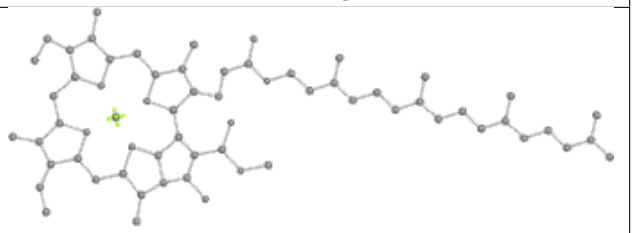
Bond lengths



Bond angles

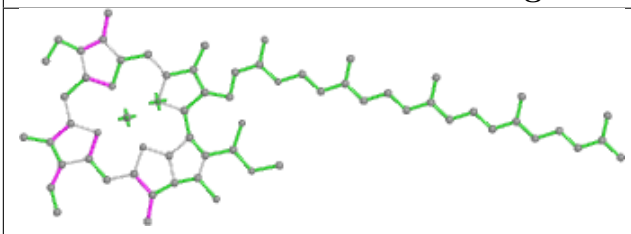


Torsions

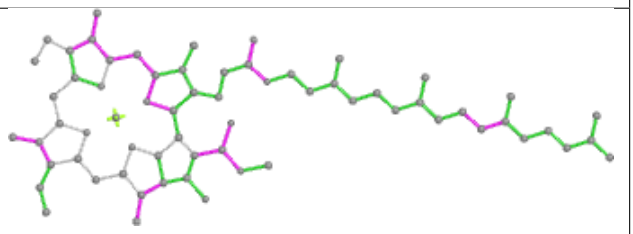


Rings

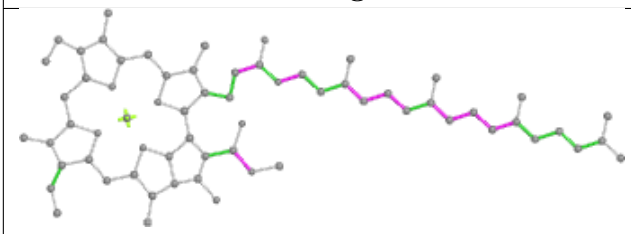
Ligand CLA B 808



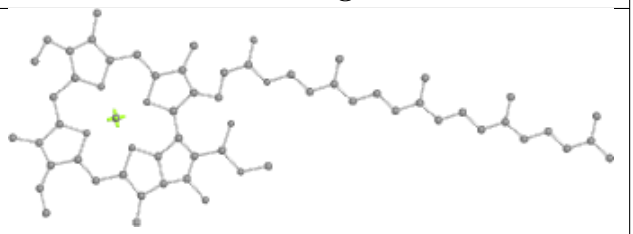
Bond lengths



Bond angles

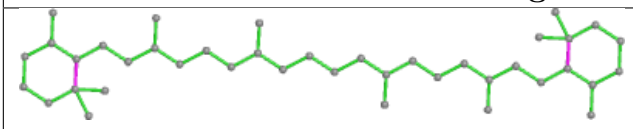


Torsions

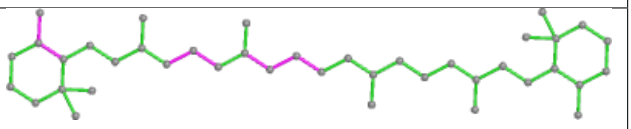


Rings

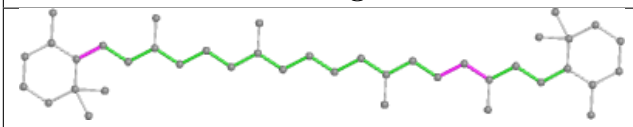
Ligand BCR I 101



Bond lengths



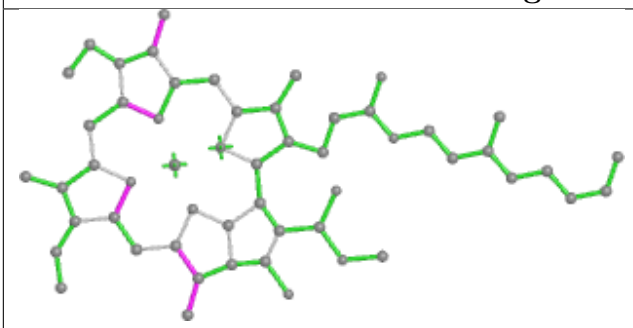
Bond angles



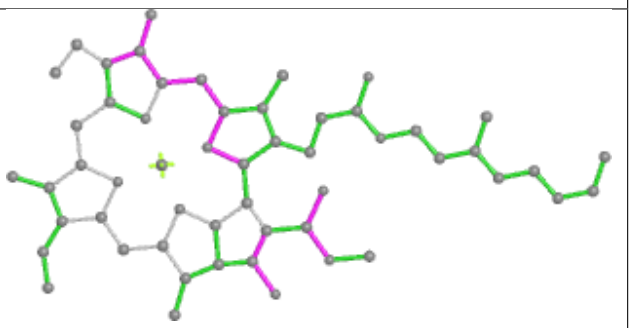
Torsions

Rings

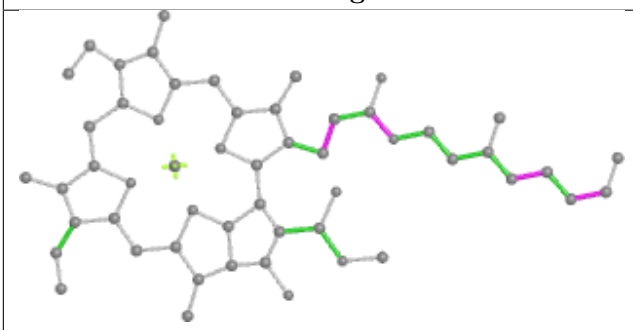
Ligand CLA A 811



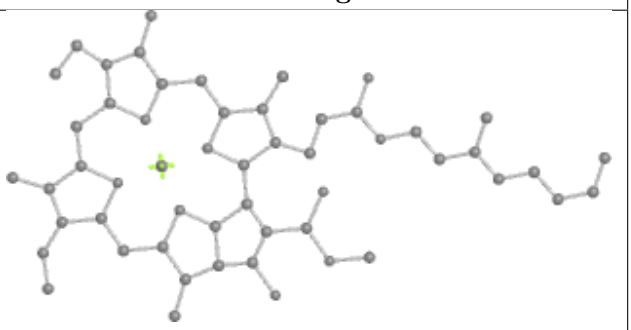
Bond lengths



Bond angles

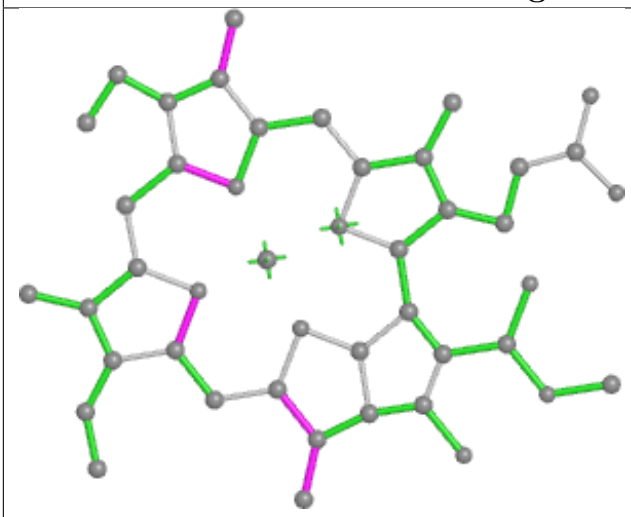


Torsions

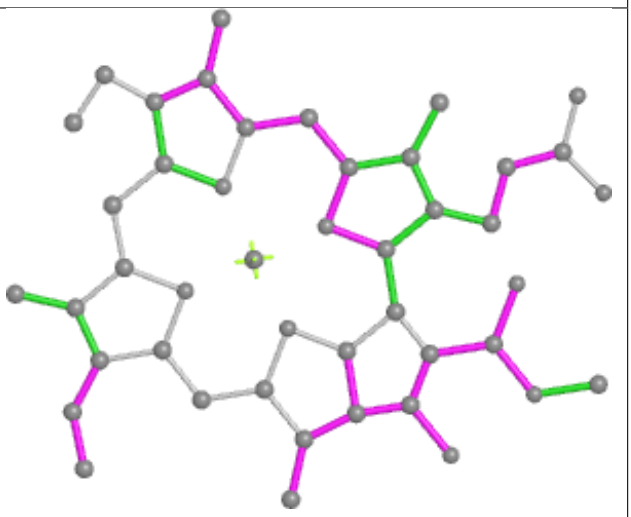


Rings

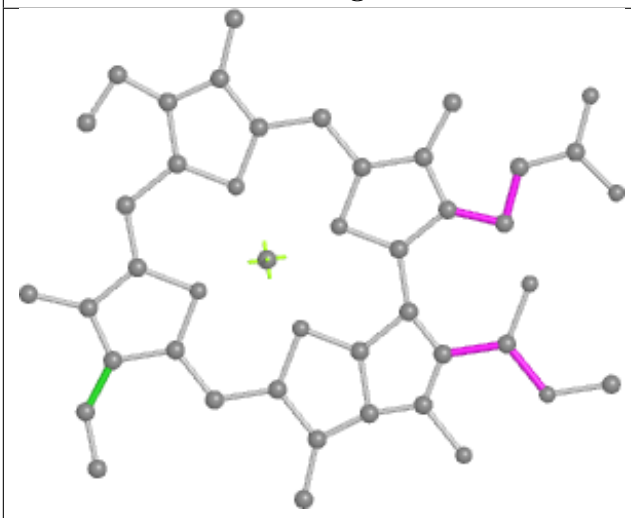
Ligand CLA 4 313



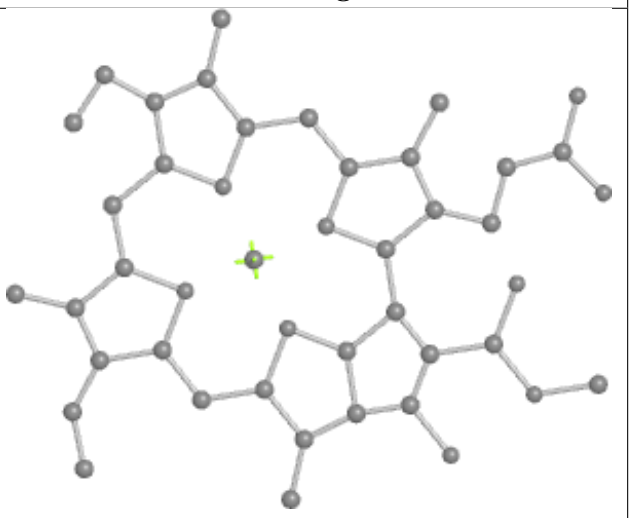
Bond lengths



Bond angles

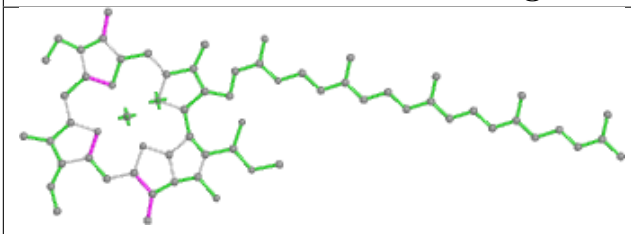


Torsions

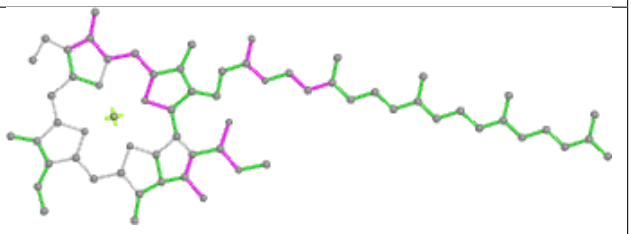


Rings

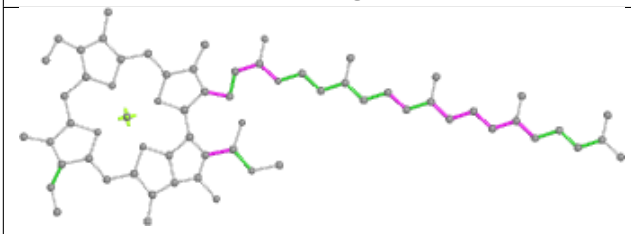
Ligand CLA A 809



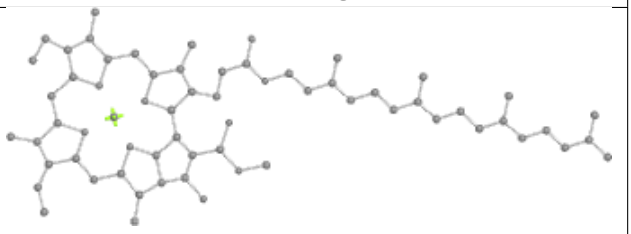
Bond lengths



Bond angles

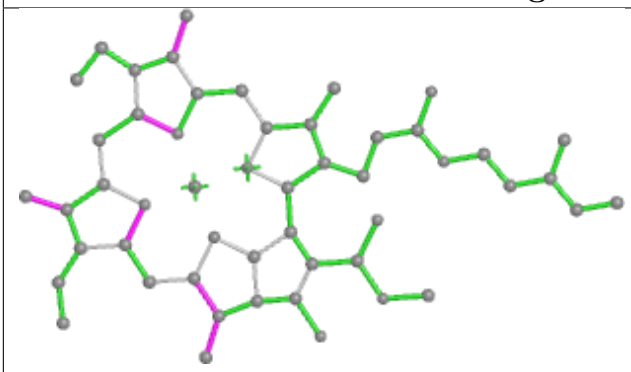


Torsions

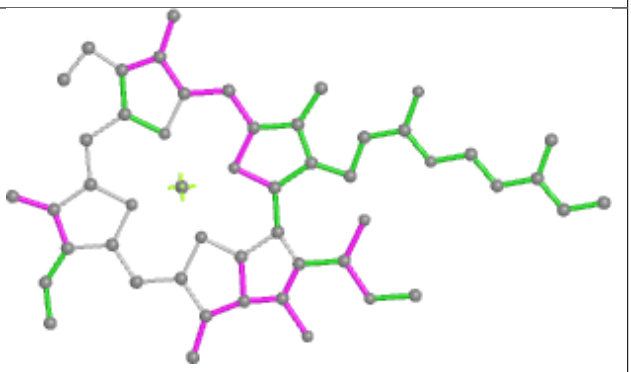


Rings

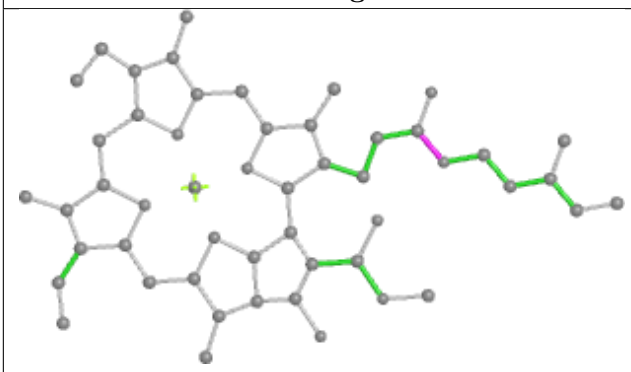
Ligand CLA 2 302



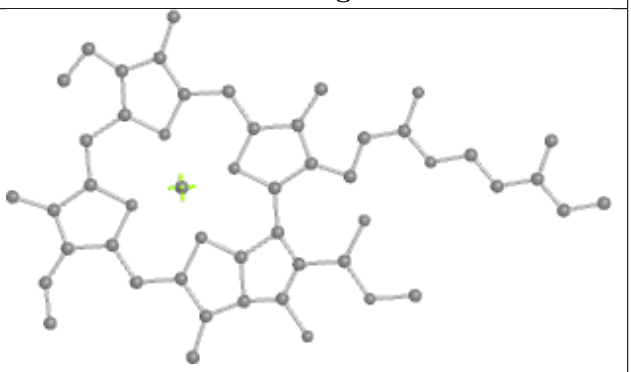
Bond lengths



Bond angles

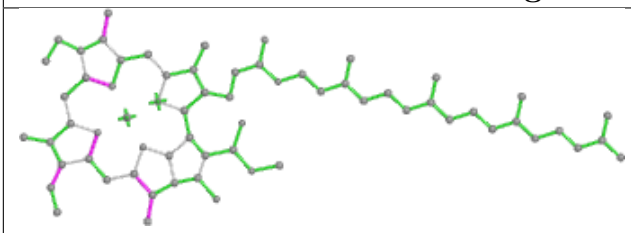


Torsions

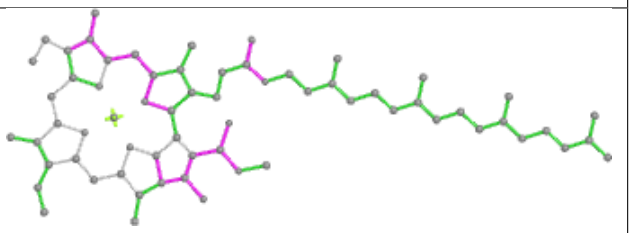


Rings

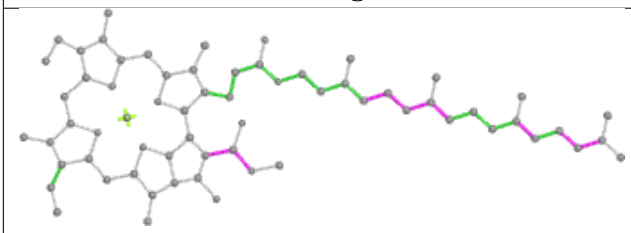
Ligand CLA B 809



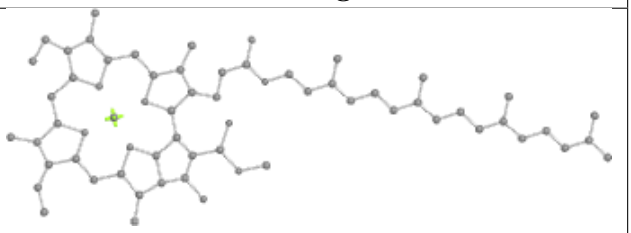
Bond lengths



Bond angles

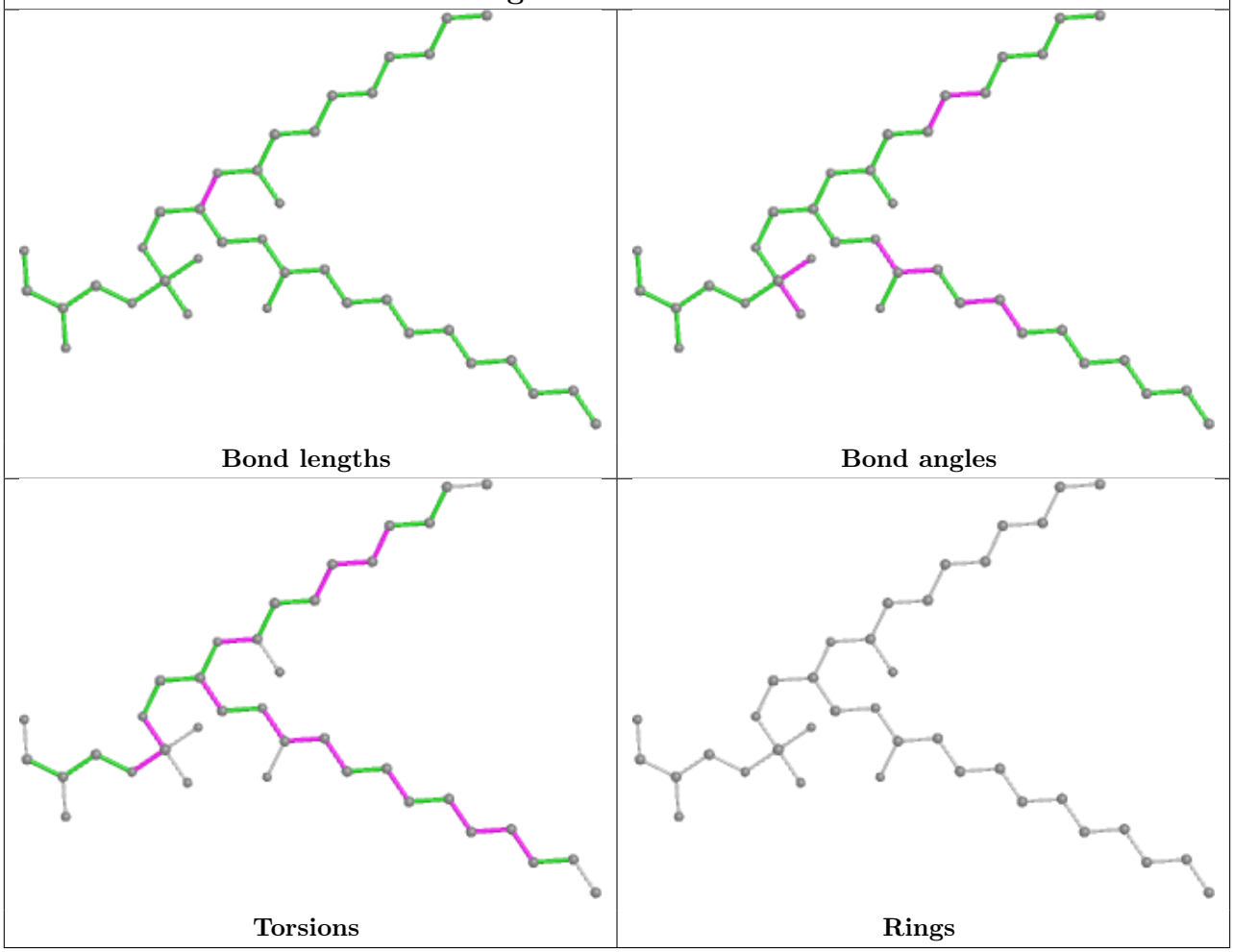


Torsions

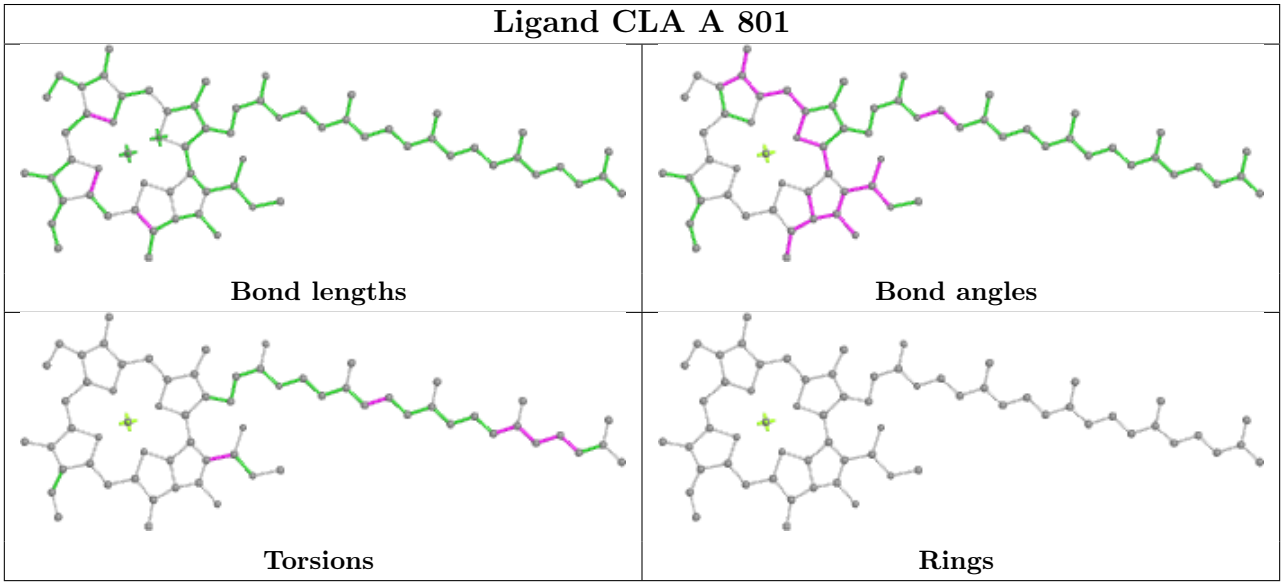


Rings

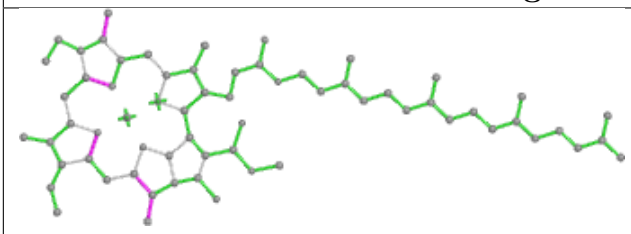
Ligand LHG 2 317



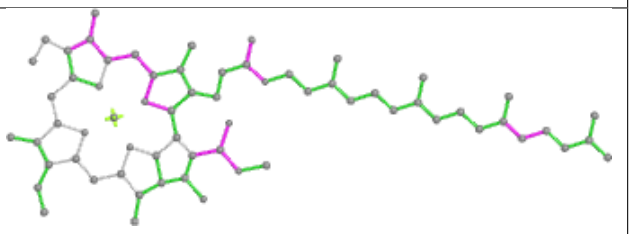
Ligand CLA A 801



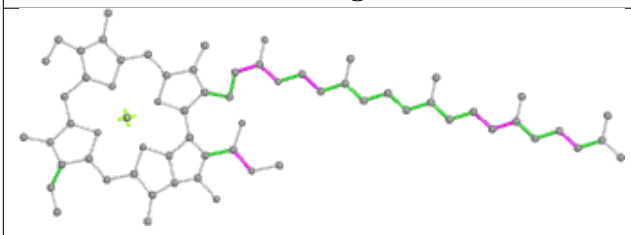
Ligand CLA A 824



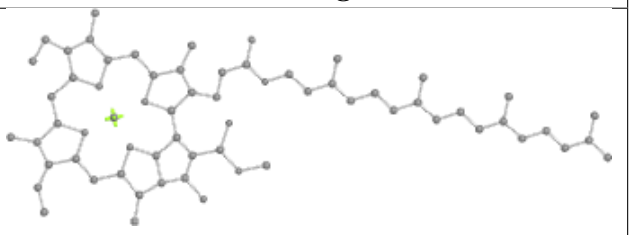
Bond lengths



Bond angles

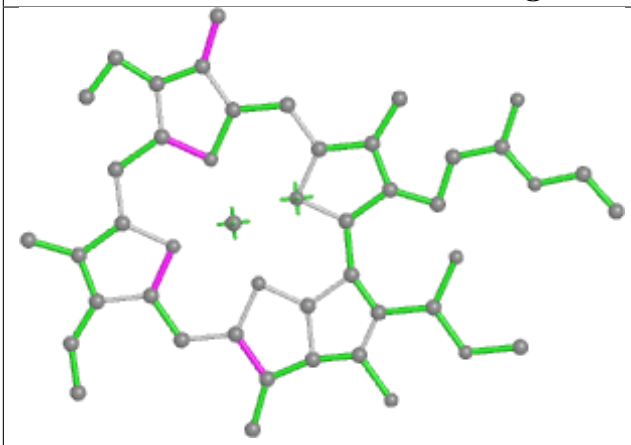


Torsions

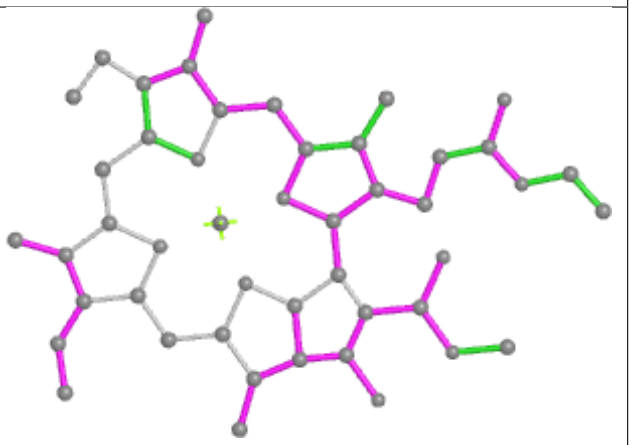


Rings

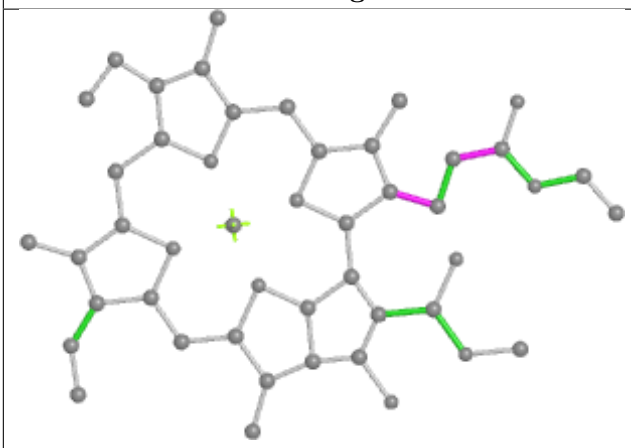
Ligand CLA B 839



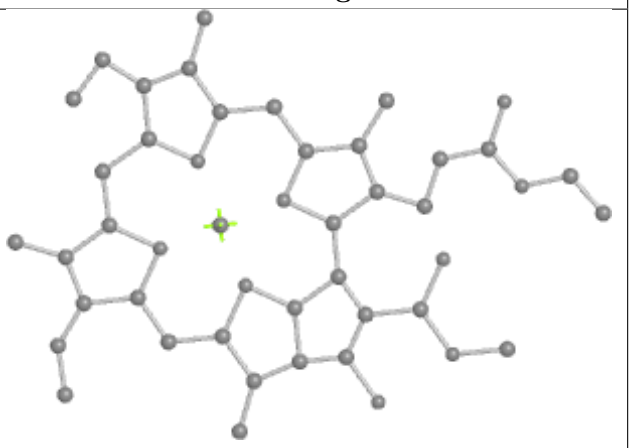
Bond lengths



Bond angles

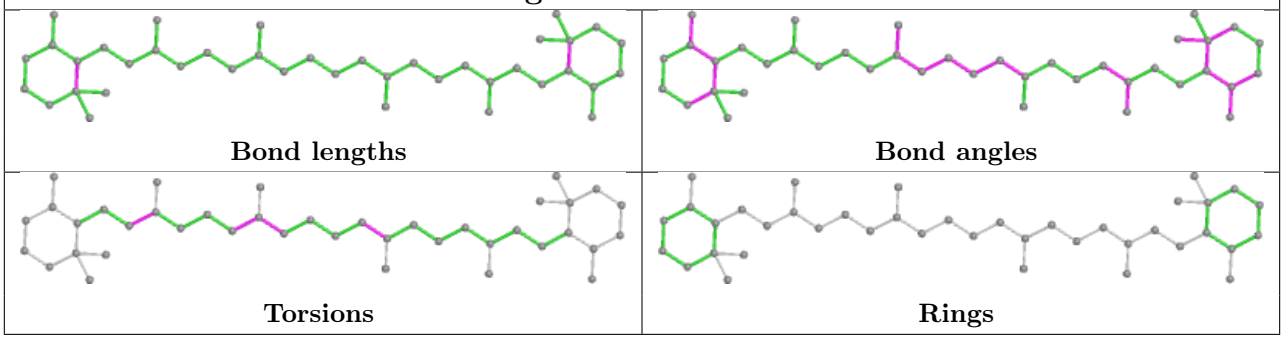


Torsions

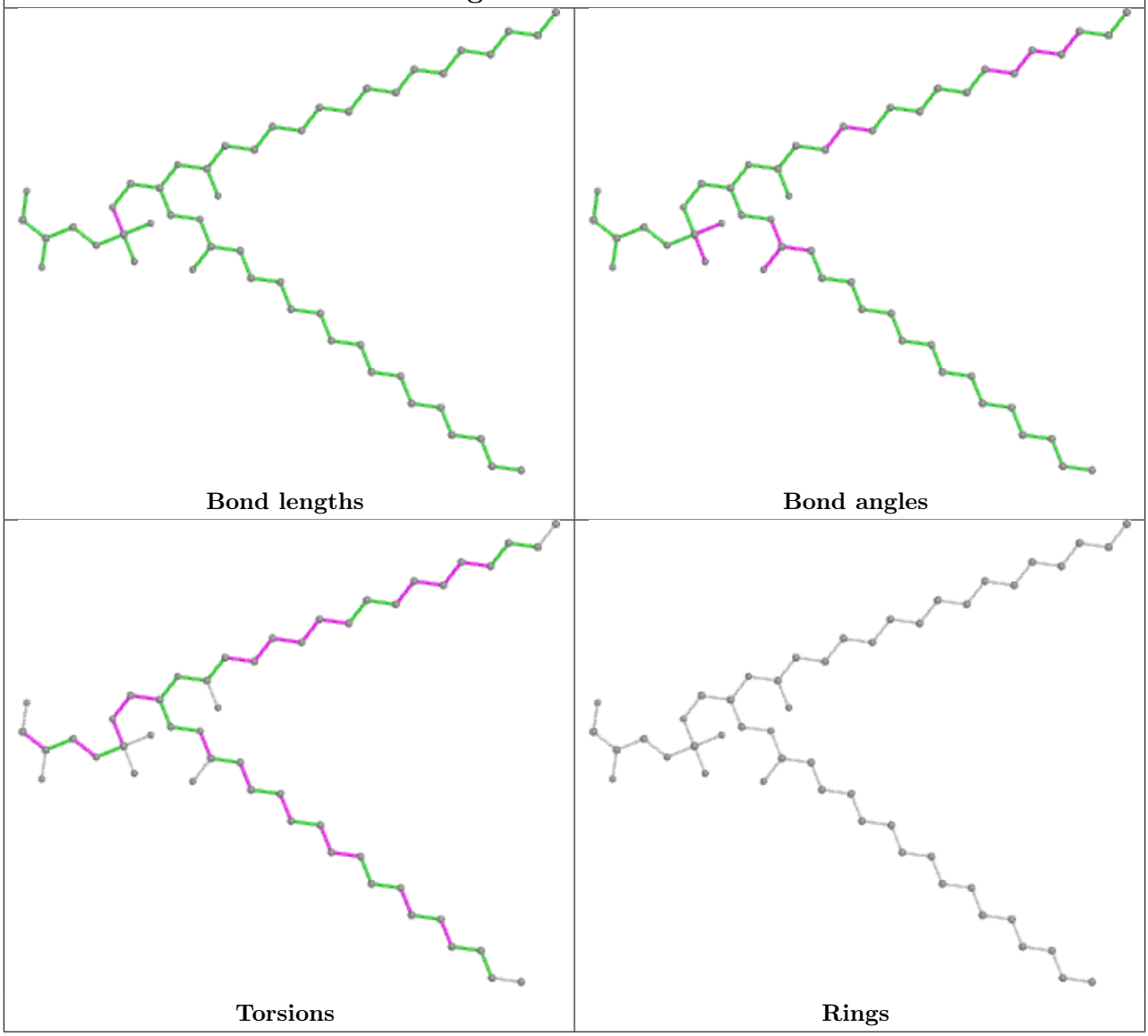


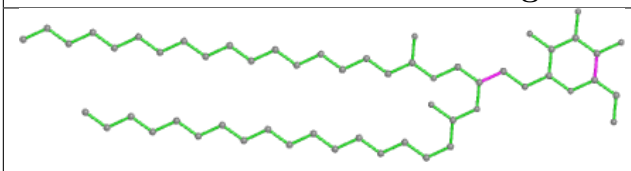
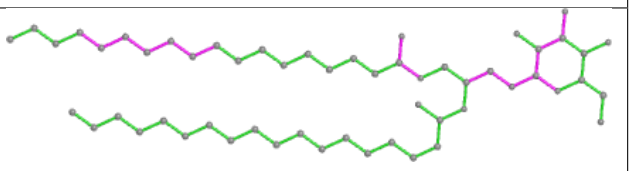
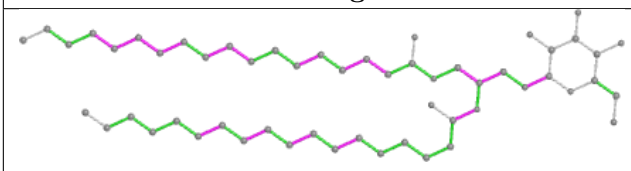
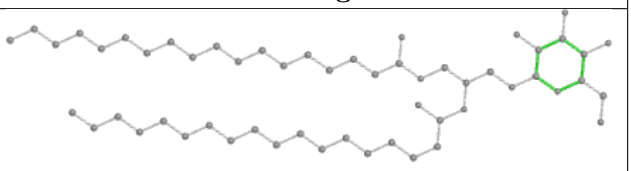
Rings

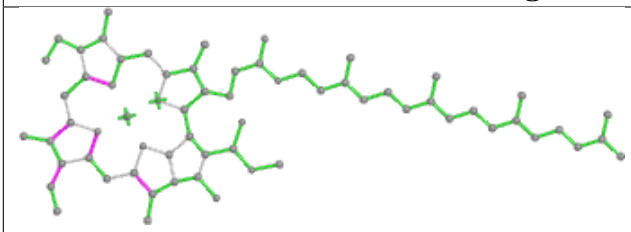
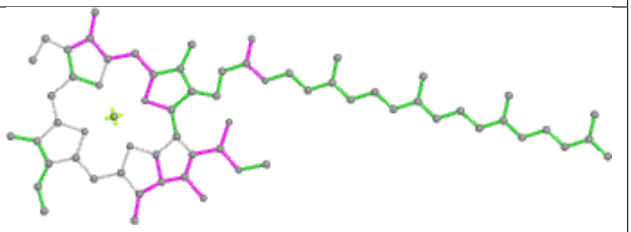
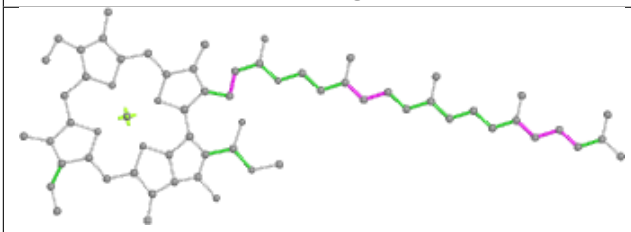
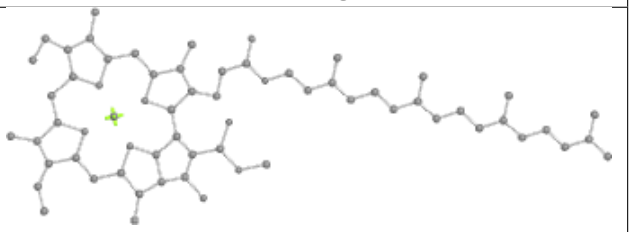
Ligand BCR F 303



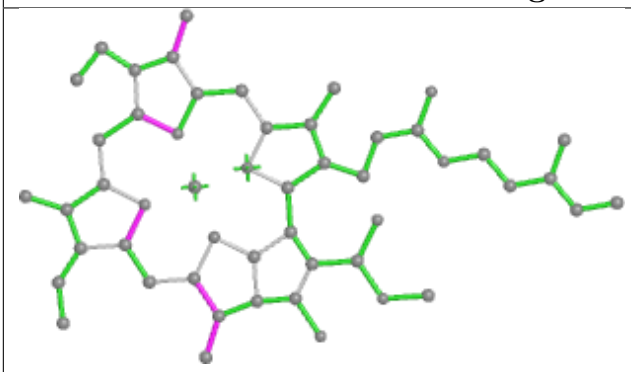
Ligand LHG G 102



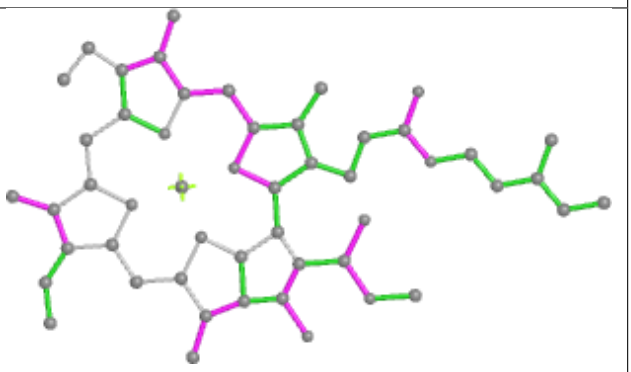
Ligand LMG F 309	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 828	
 Bond lengths	 Bond angles
 Torsions	 Rings

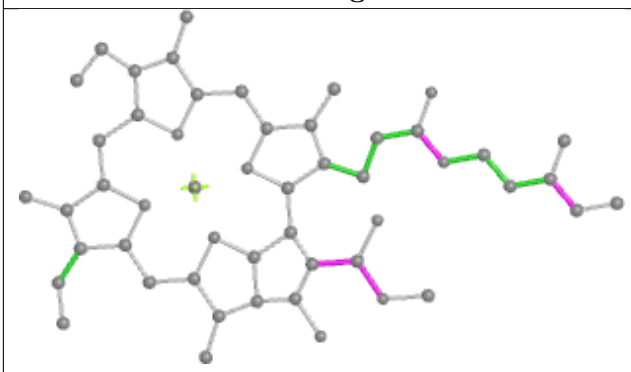
Ligand CLA 1 303



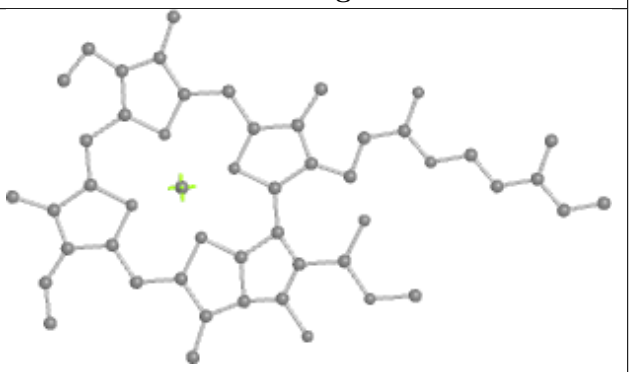
Bond lengths



Bond angles

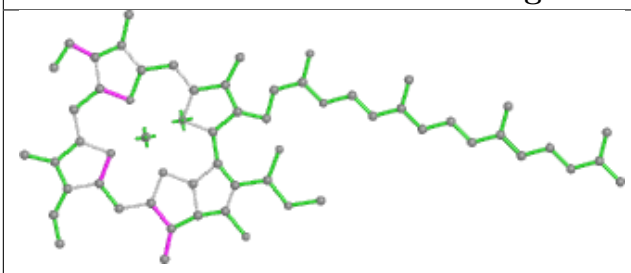


Torsions

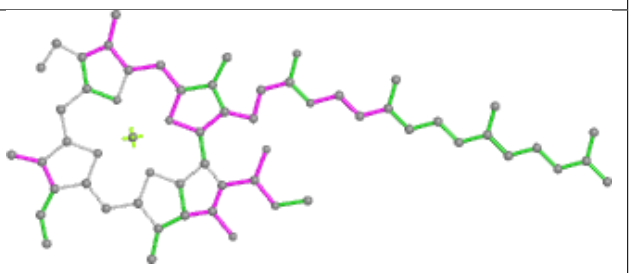


Rings

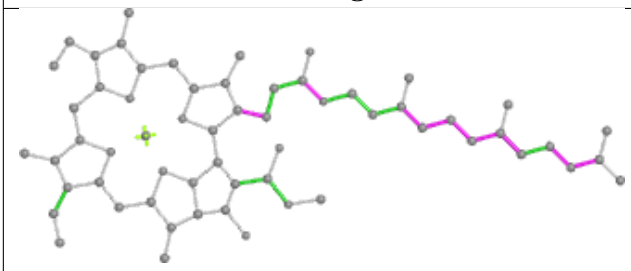
Ligand CLA B 820



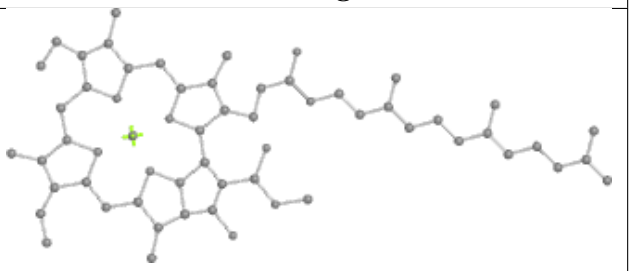
Bond lengths



Bond angles

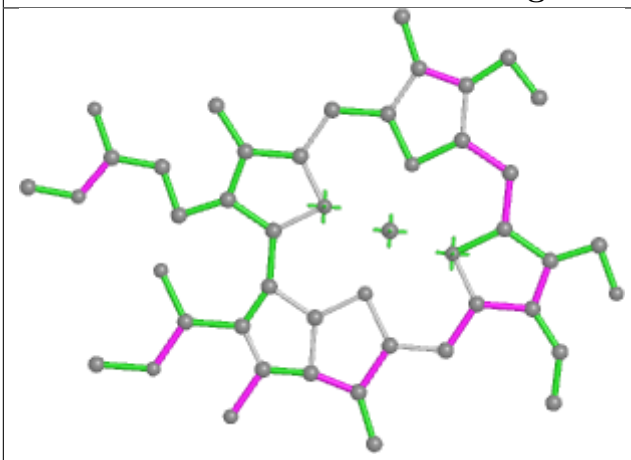


Torsions

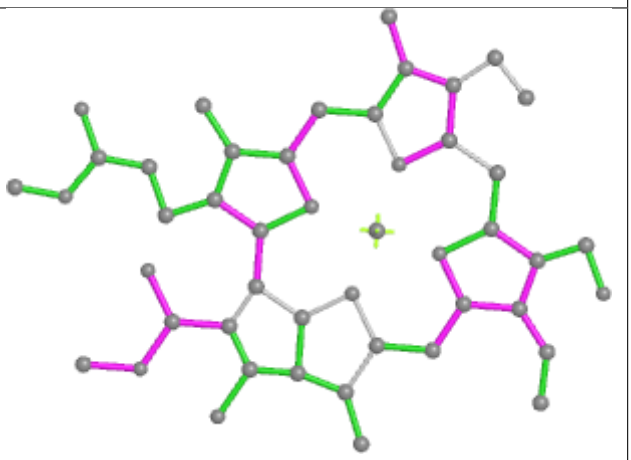


Rings

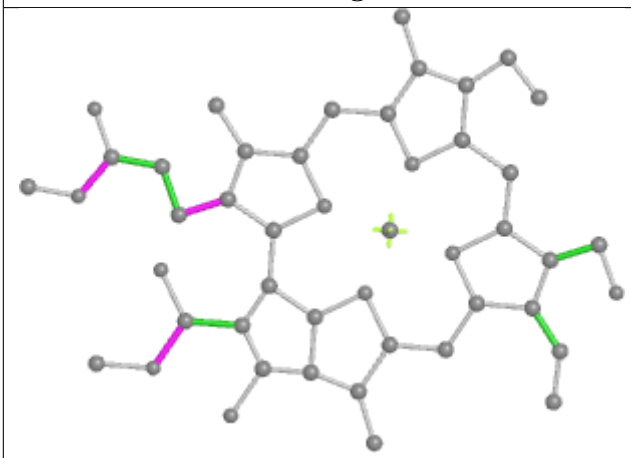
Ligand CHL 3 607



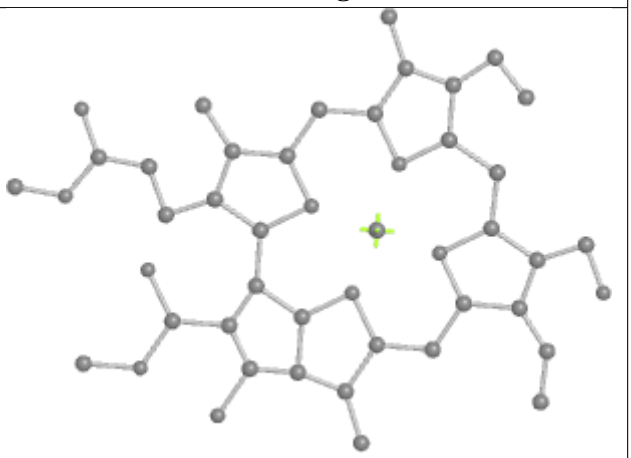
Bond lengths



Bond angles

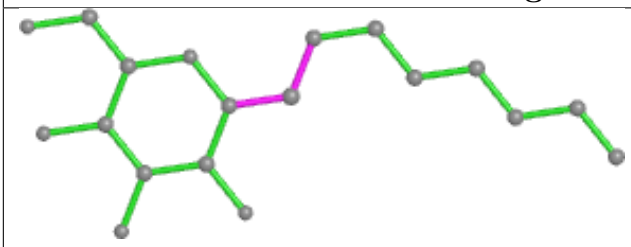


Torsions

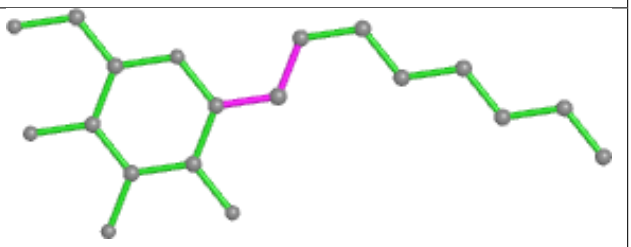


Rings

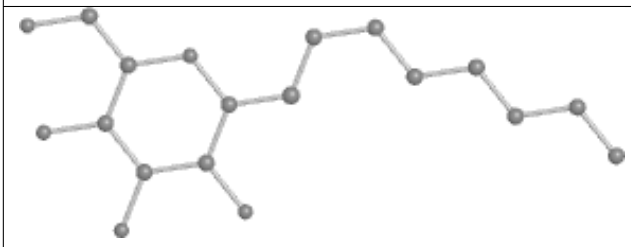
Ligand HTG 4 321



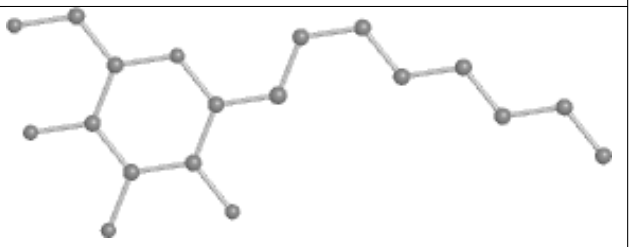
Bond lengths



Bond angles

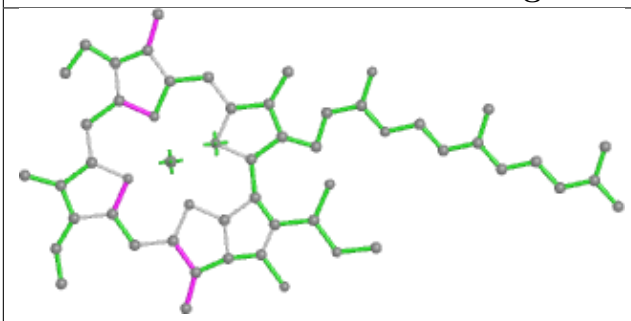


Torsions

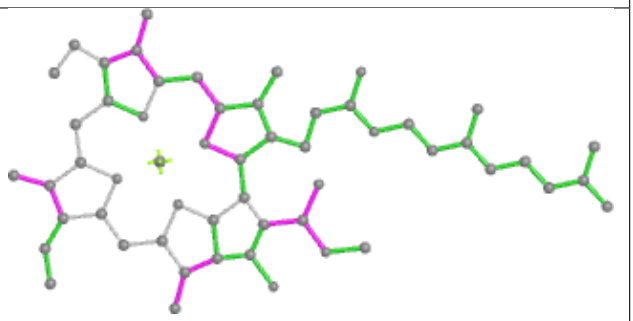


Rings

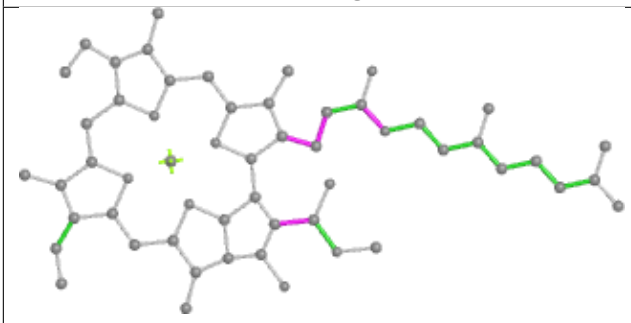
Ligand CLA A 823



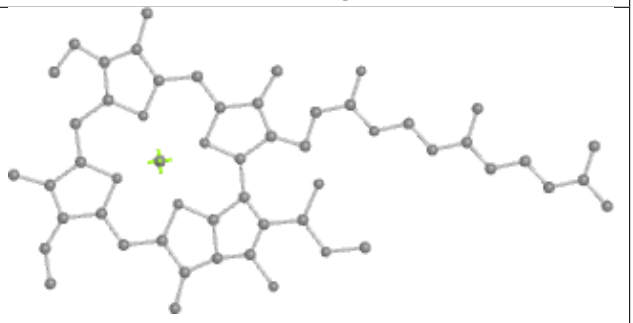
Bond lengths



Bond angles

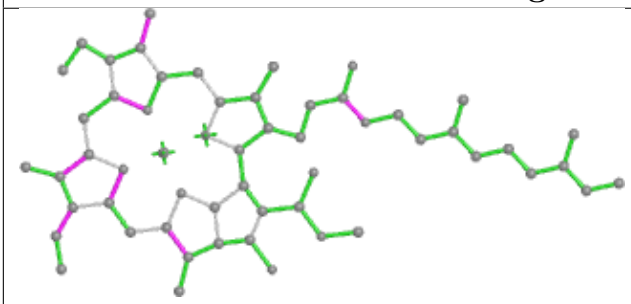


Torsions

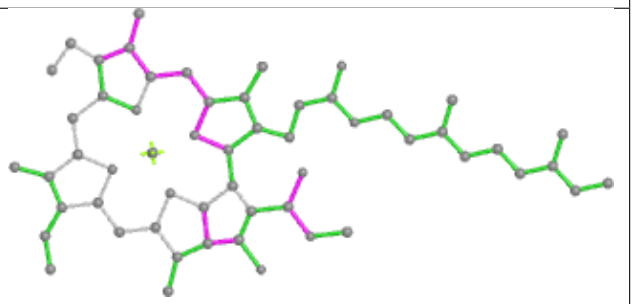


Rings

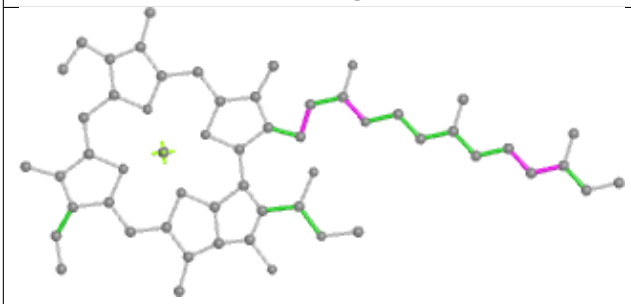
Ligand CLA 4 312



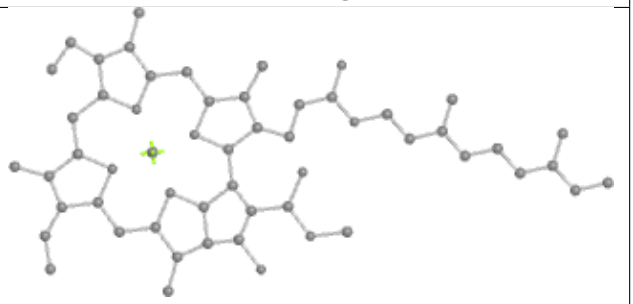
Bond lengths



Bond angles

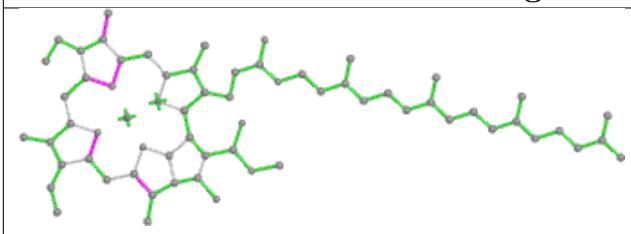


Torsions

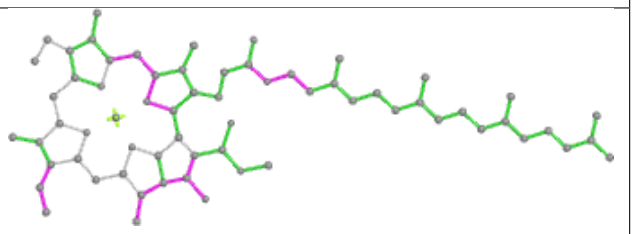


Rings

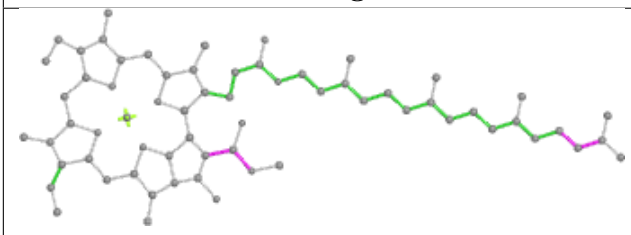
Ligand CLA B 804



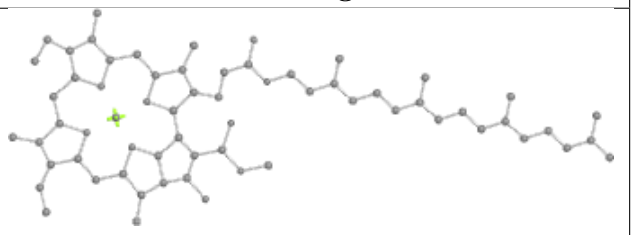
Bond lengths



Bond angles

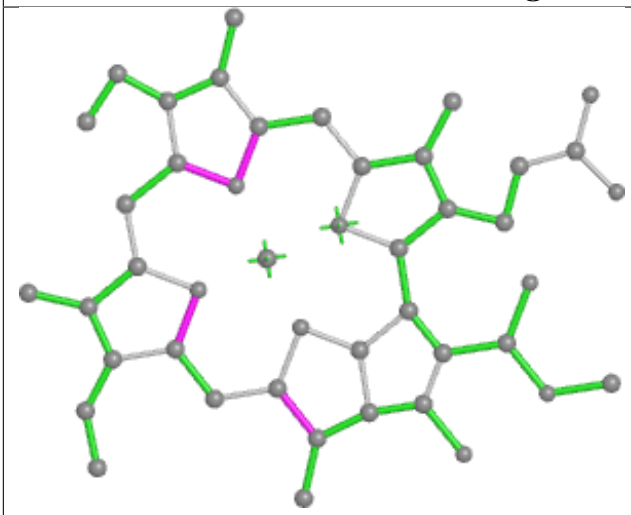


Torsions

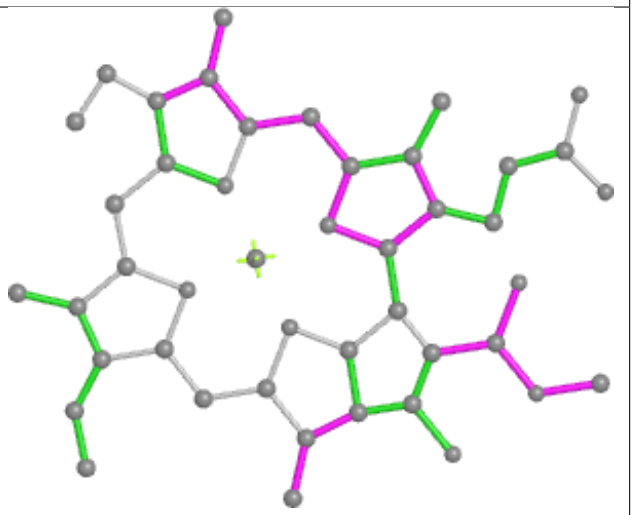


Rings

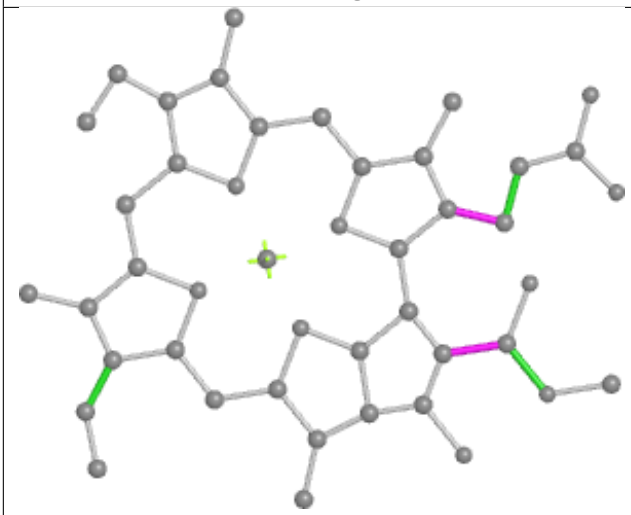
Ligand CLA B 806



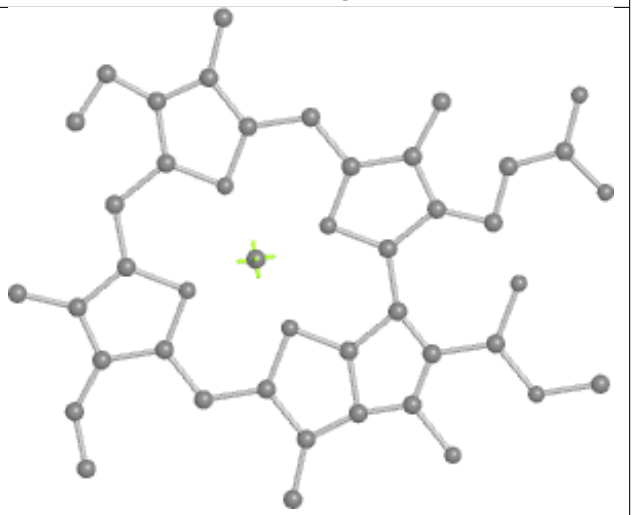
Bond lengths



Bond angles

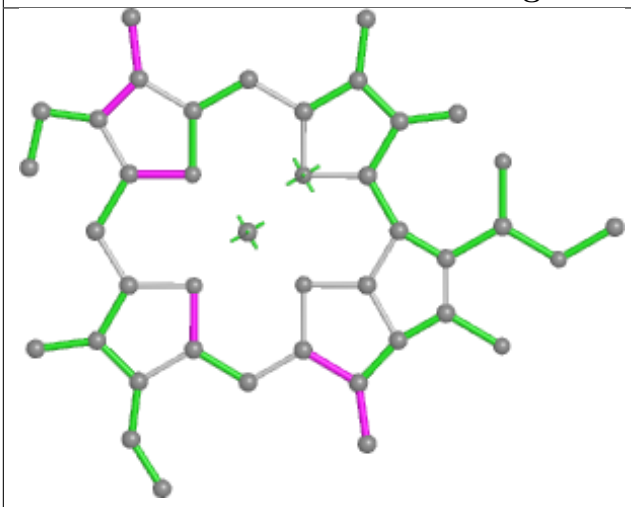


Torsions

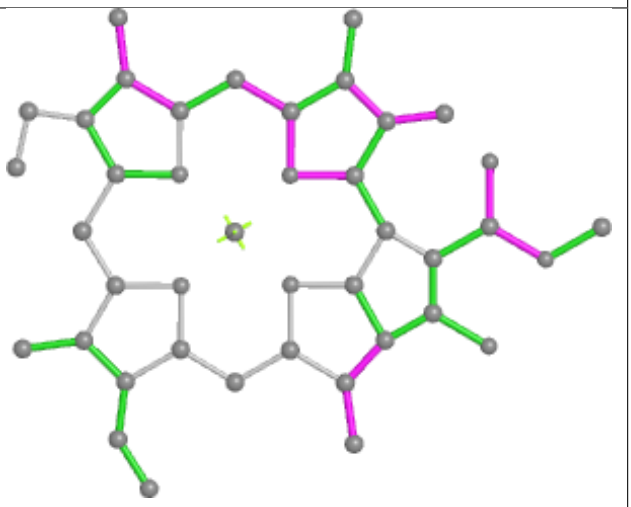


Rings

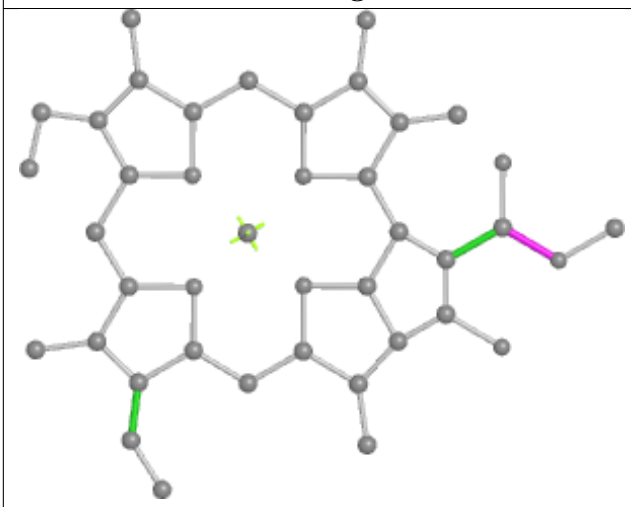
Ligand CLA G 103



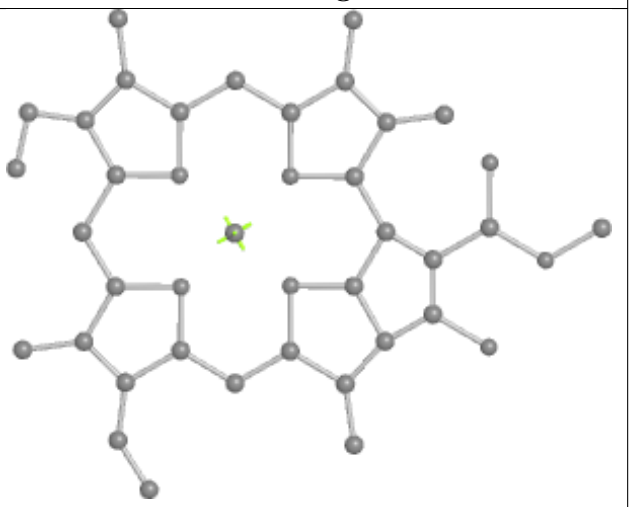
Bond lengths



Bond angles

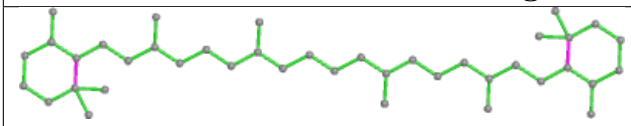


Torsions

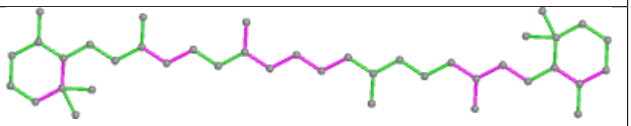


Rings

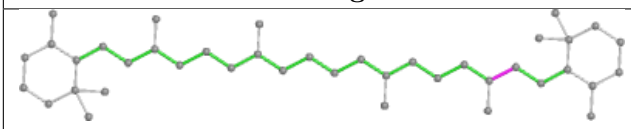
Ligand BCR A 846



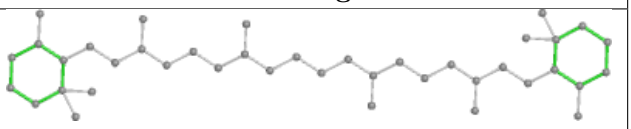
Bond lengths



Bond angles

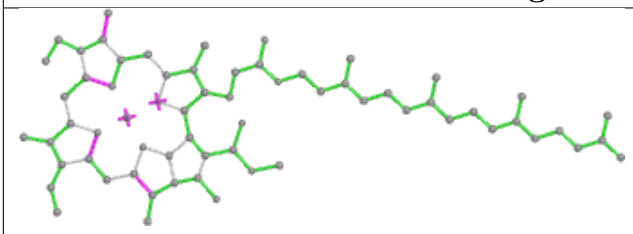


Torsions

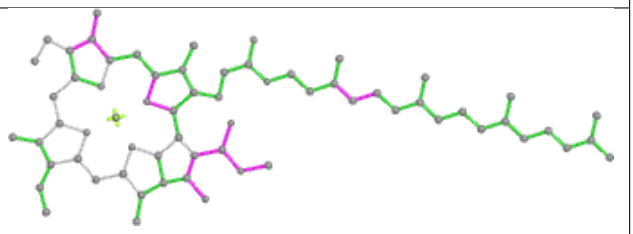


Rings

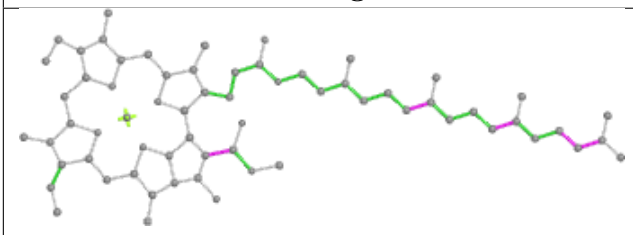
Ligand CLA 1 301



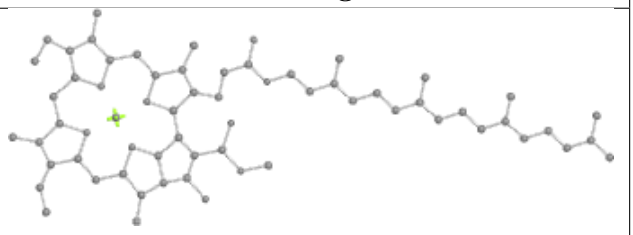
Bond lengths



Bond angles

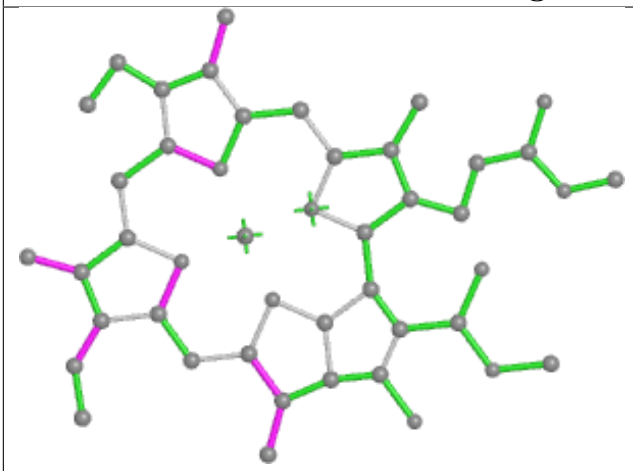


Torsions

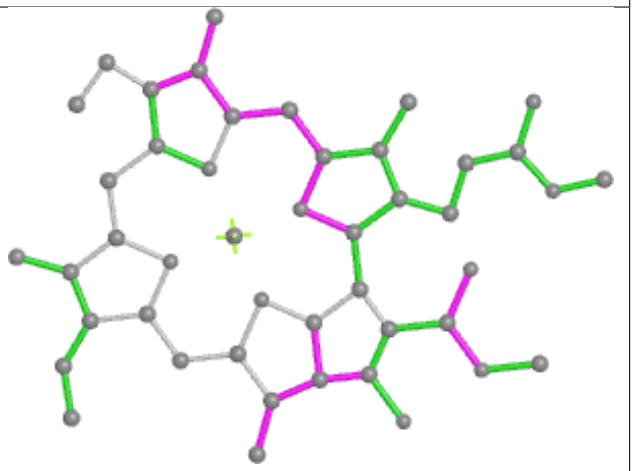


Rings

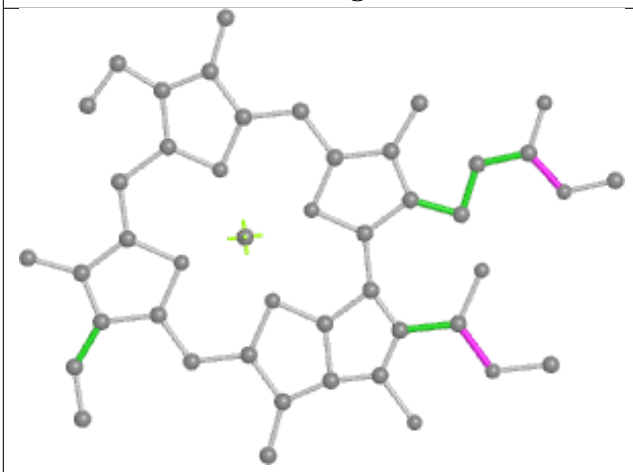
Ligand CLA 1 313



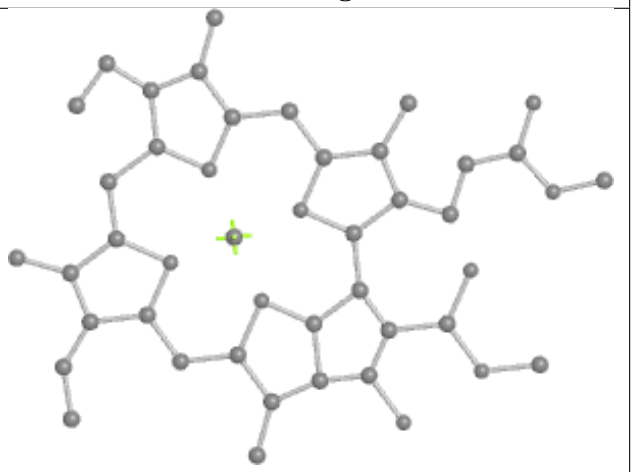
Bond lengths



Bond angles

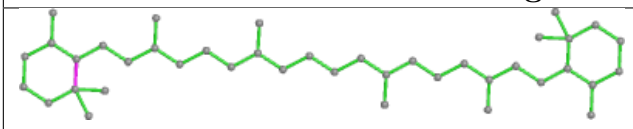


Torsions

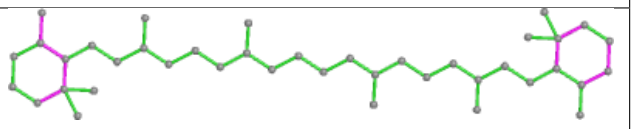


Rings

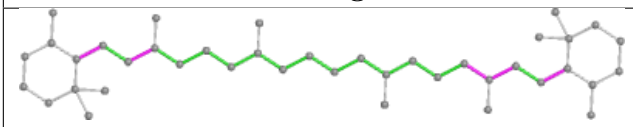
Ligand BCR L 205



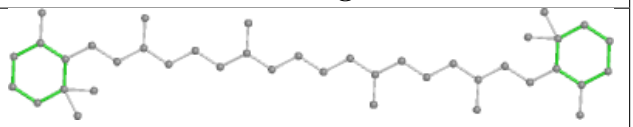
Bond lengths



Bond angles

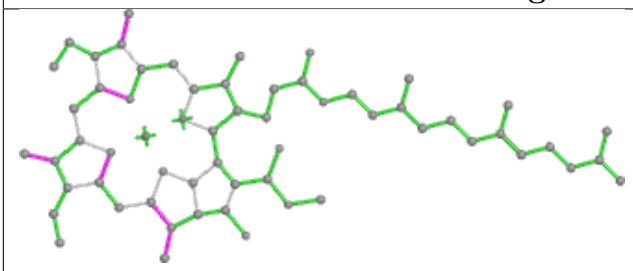


Torsions

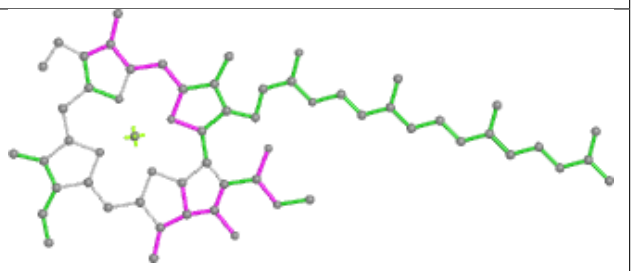


Rings

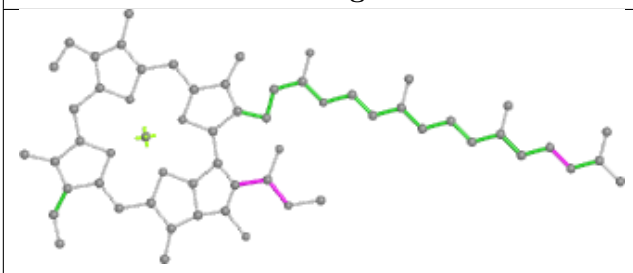
Ligand CLA 3 602



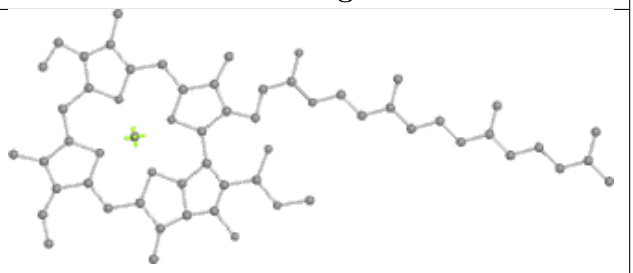
Bond lengths



Bond angles

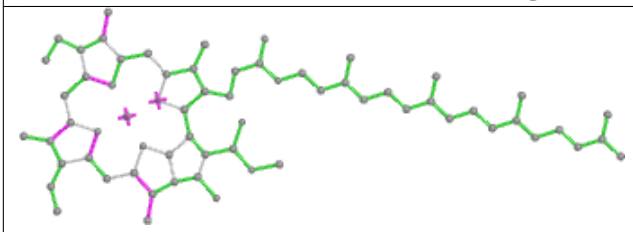


Torsions

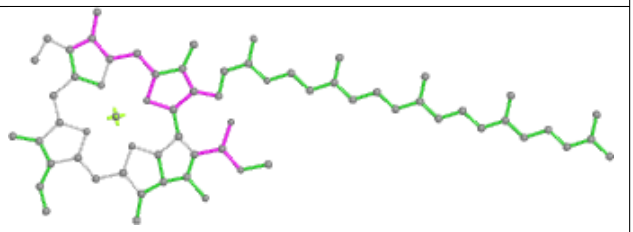


Rings

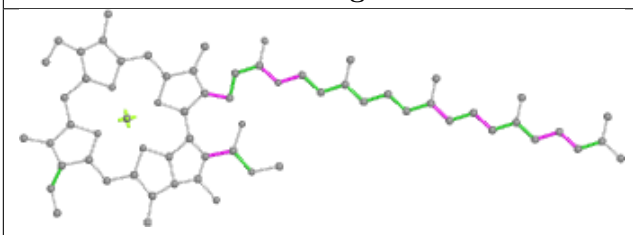
Ligand CLA B 807



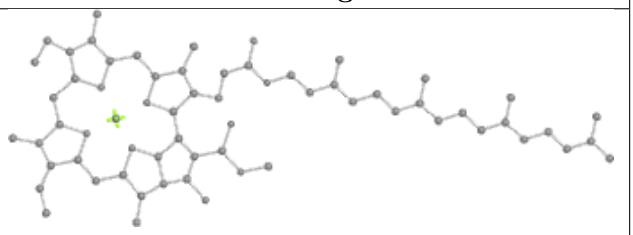
Bond lengths



Bond angles

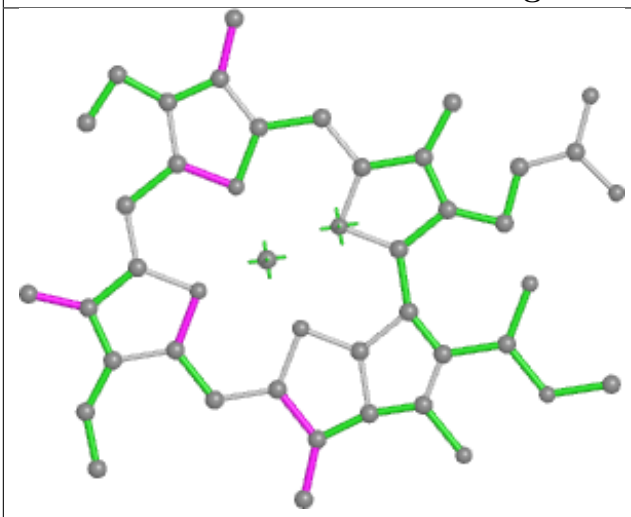


Torsions

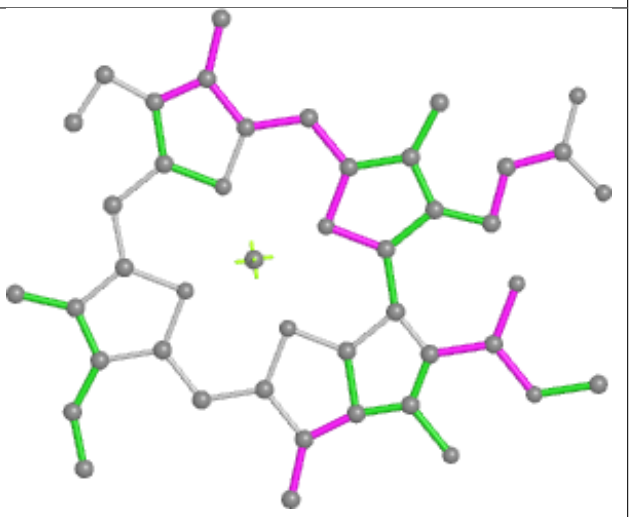


Rings

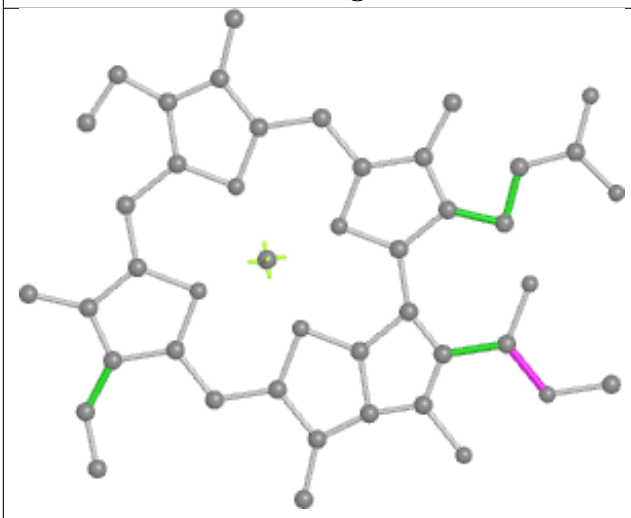
Ligand CLA A 815



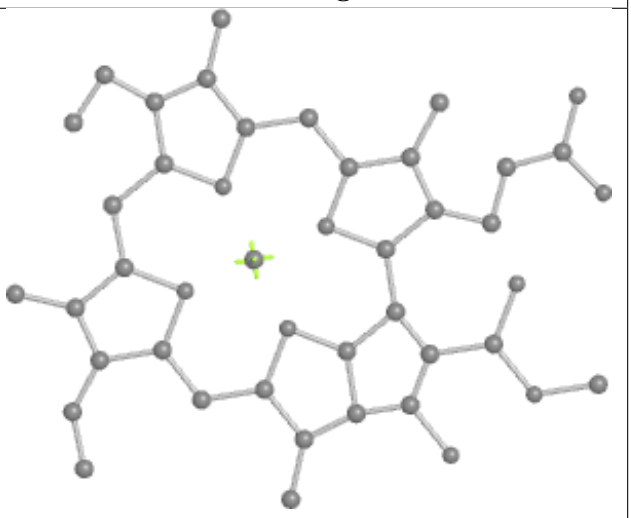
Bond lengths



Bond angles

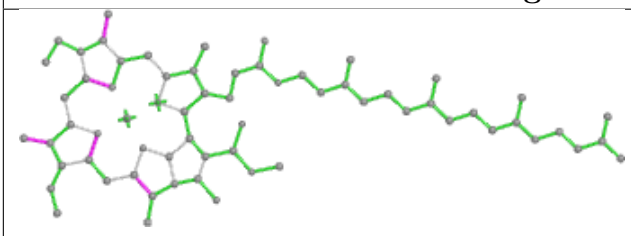


Torsions

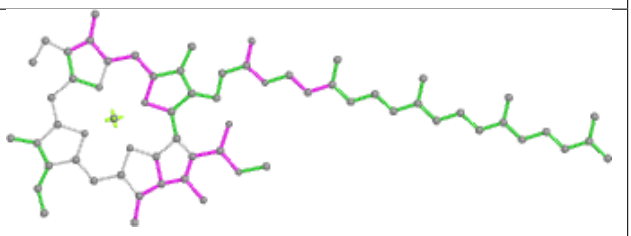


Rings

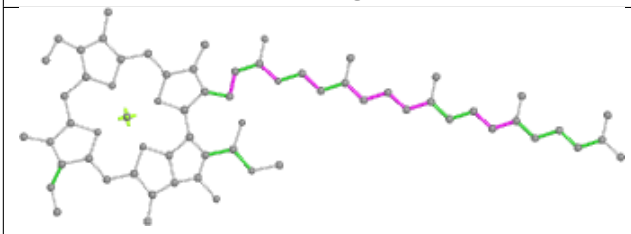
Ligand CLA A 841



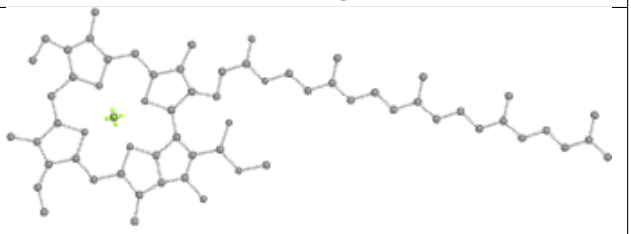
Bond lengths



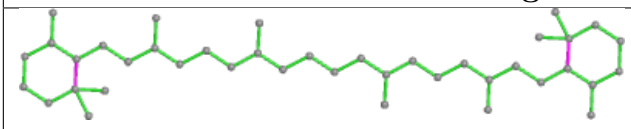
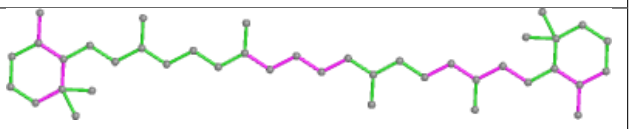
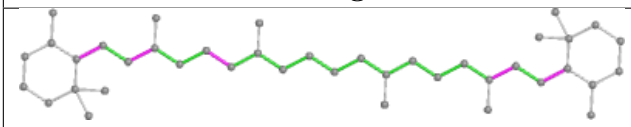
Bond angles

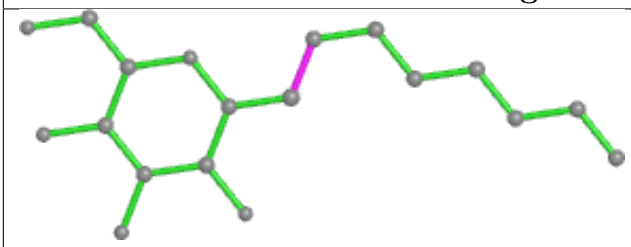
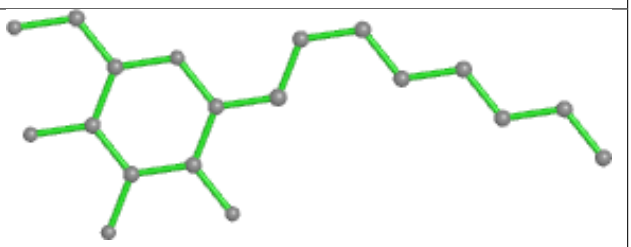
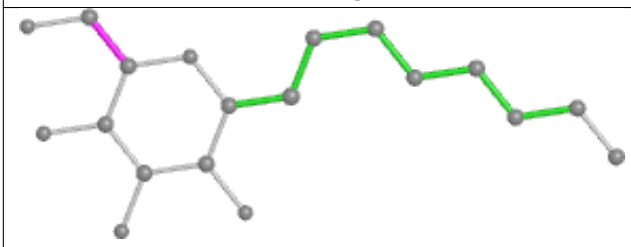
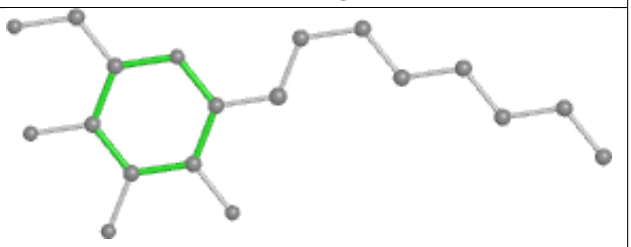


Torsions

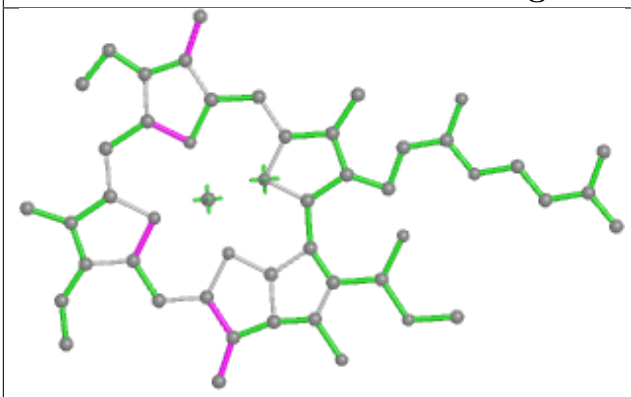


Rings

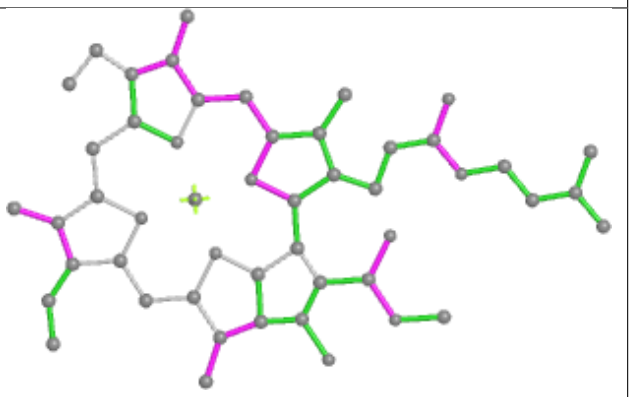
Ligand BCR A 850	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand HTG A 854	
 Bond lengths	 Bond angles
 Torsions	 Rings

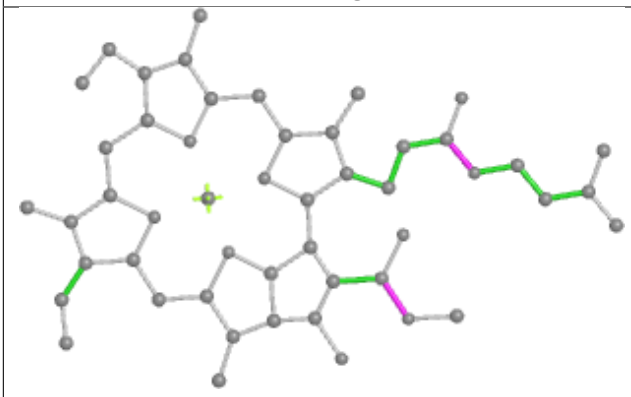
Ligand CLA 3 608



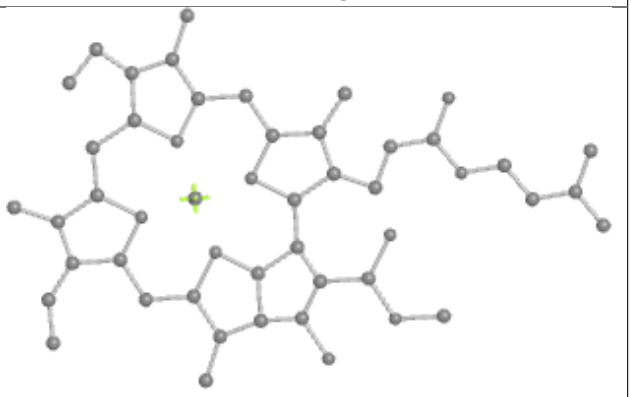
Bond lengths



Bond angles

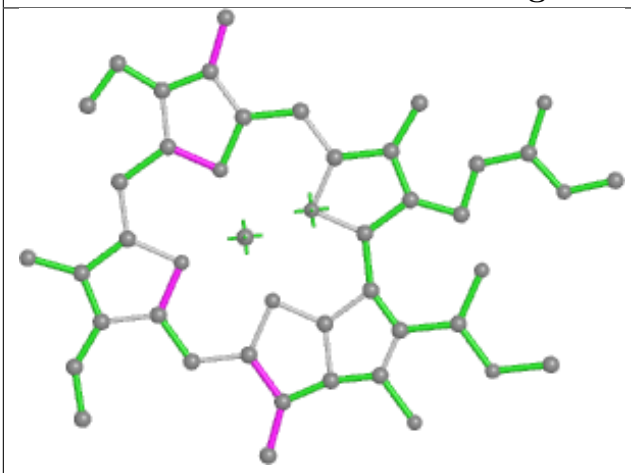


Torsions

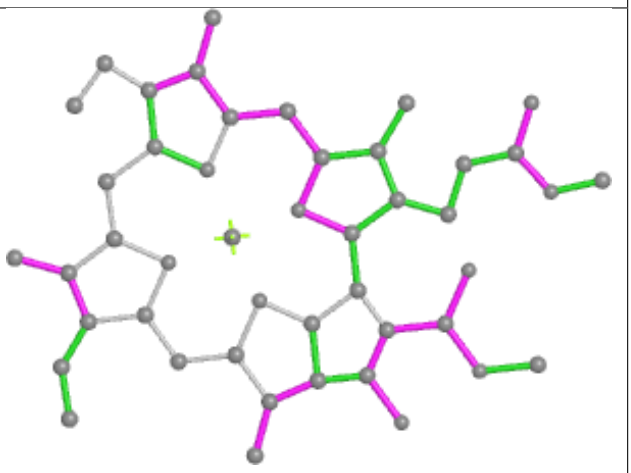


Rings

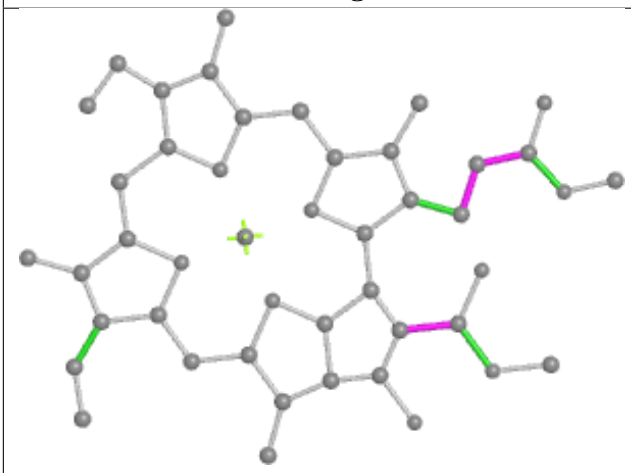
Ligand CLA 2 319



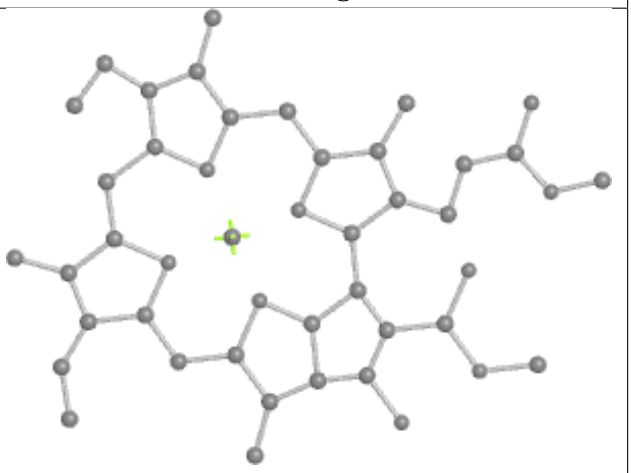
Bond lengths



Bond angles

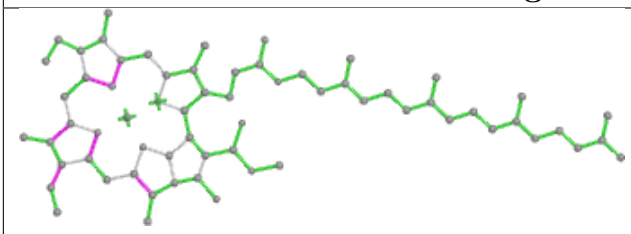


Torsions

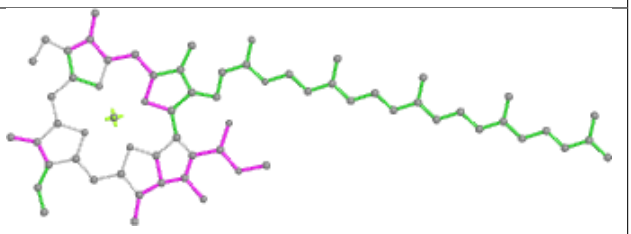


Rings

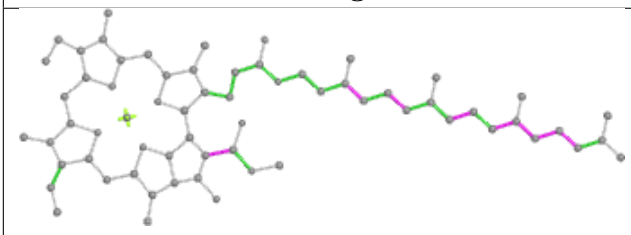
Ligand CLA B 838



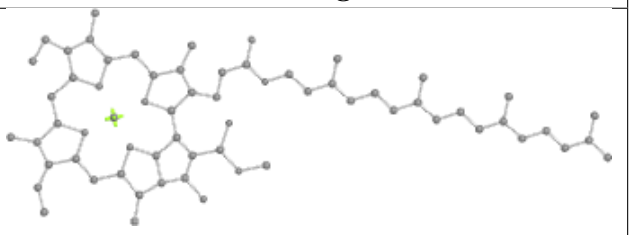
Bond lengths



Bond angles

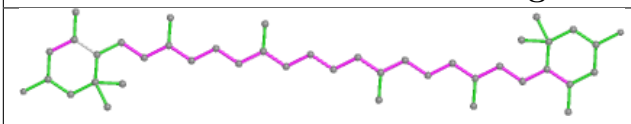


Torsions

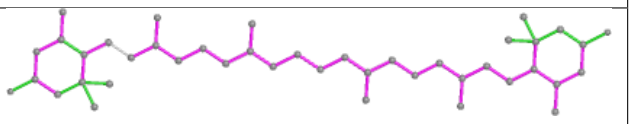


Rings

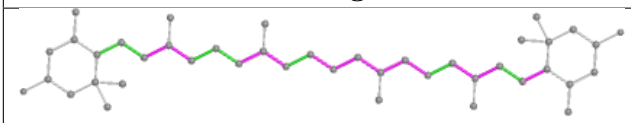
Ligand LUT 1 314



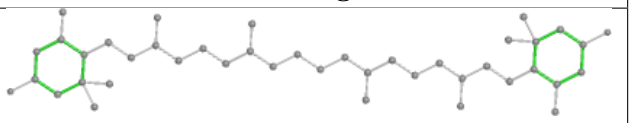
Bond lengths



Bond angles

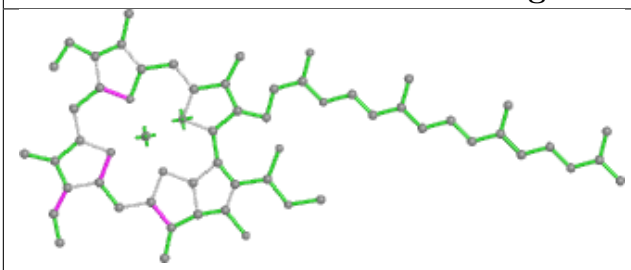


Torsions

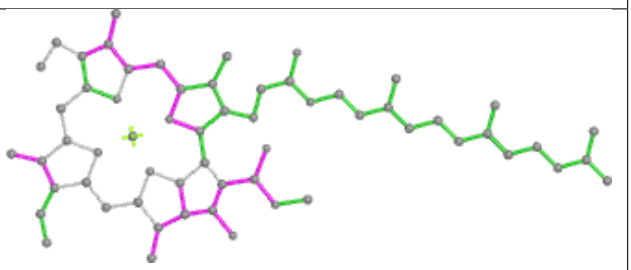


Rings

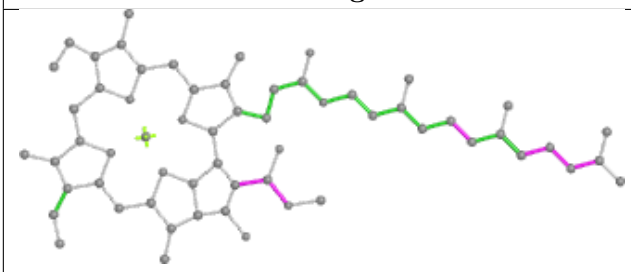
Ligand CLA 4 309



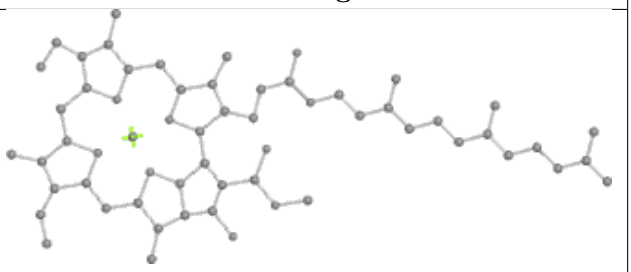
Bond lengths



Bond angles

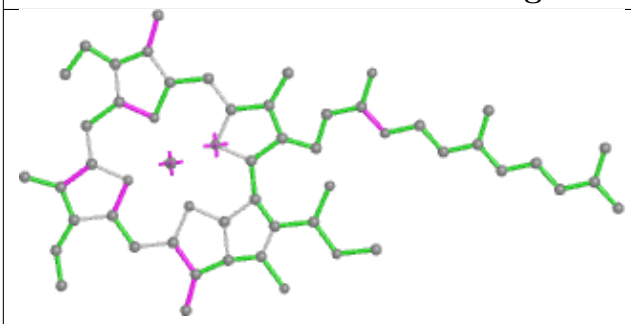


Torsions

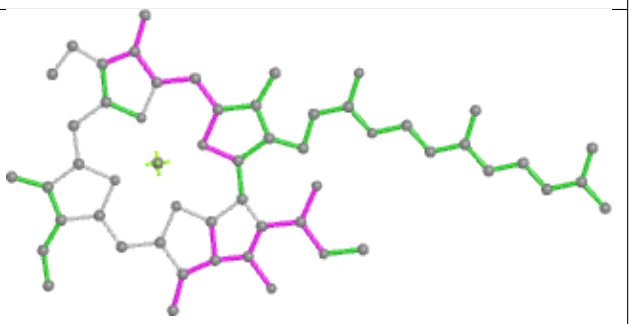


Rings

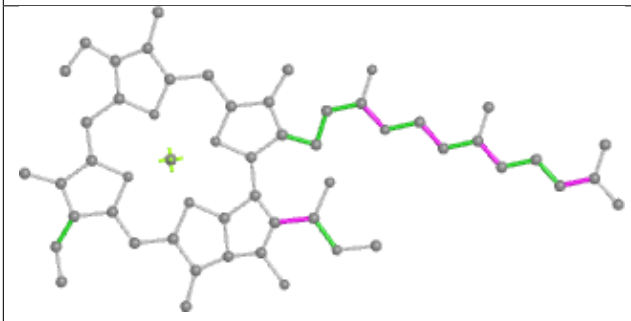
Ligand CLA B 814



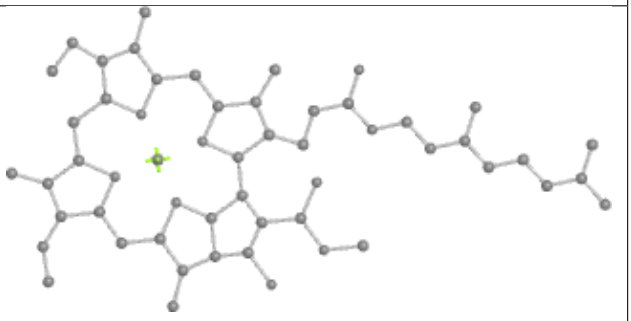
Bond lengths



Bond angles

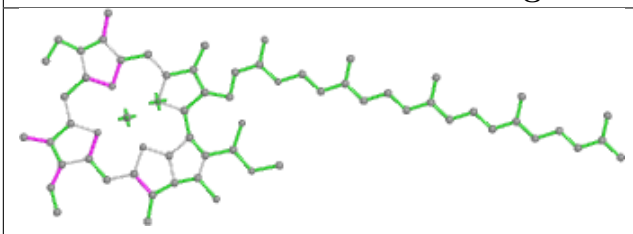


Torsions

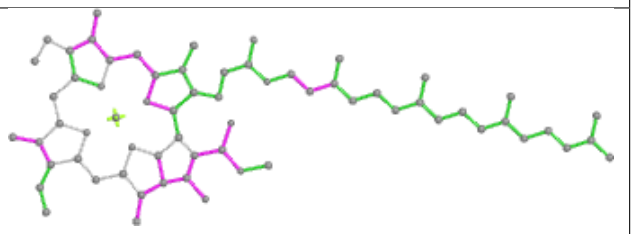


Rings

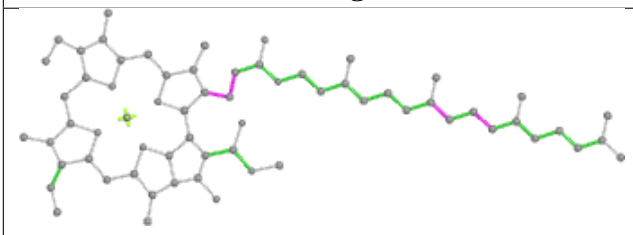
Ligand CLA A 802



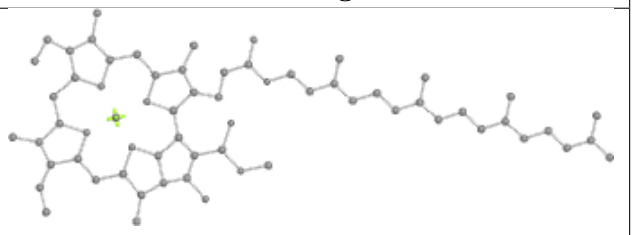
Bond lengths



Bond angles

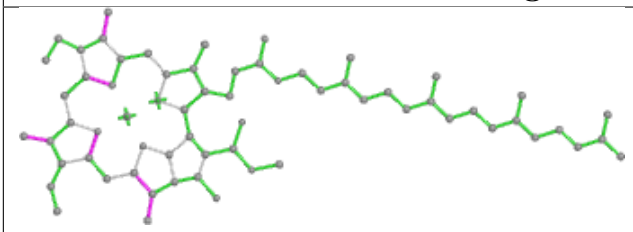


Torsions

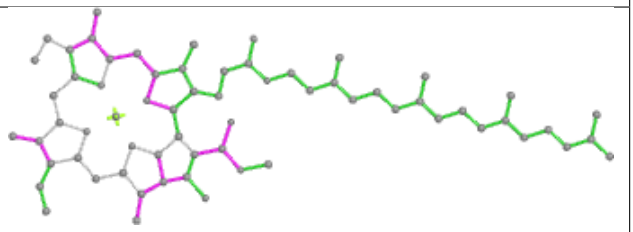


Rings

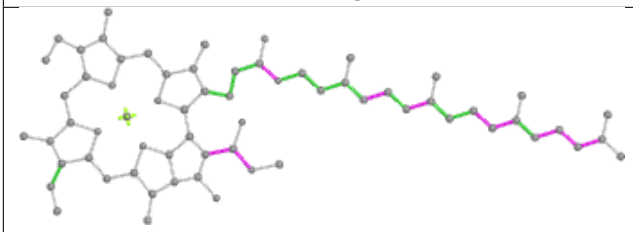
Ligand CLA A 816



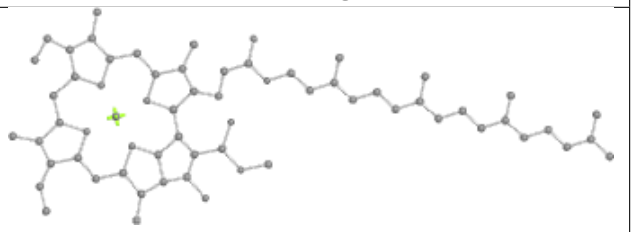
Bond lengths



Bond angles

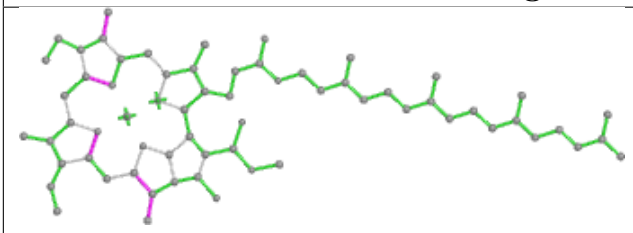


Torsions

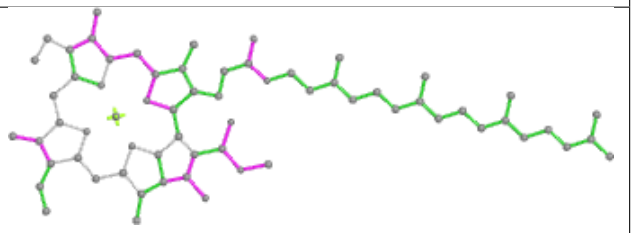


Rings

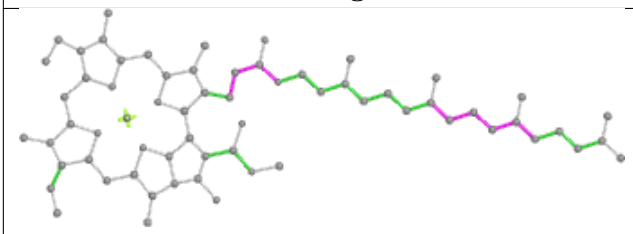
Ligand CLA A 812



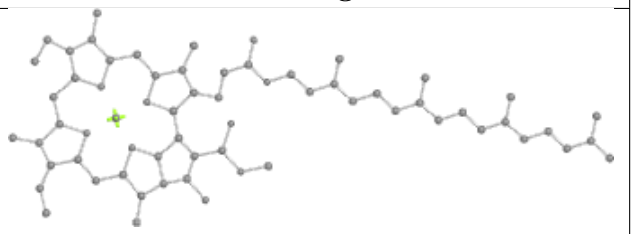
Bond lengths



Bond angles

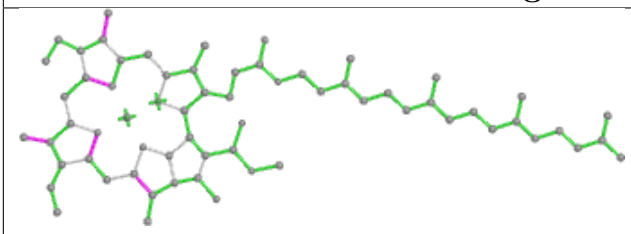


Torsions

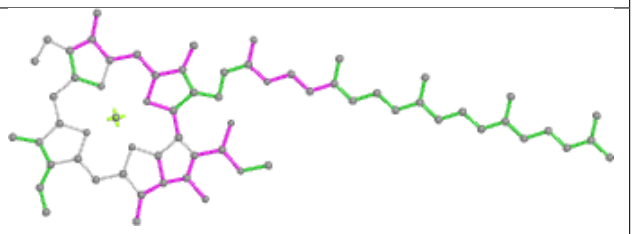


Rings

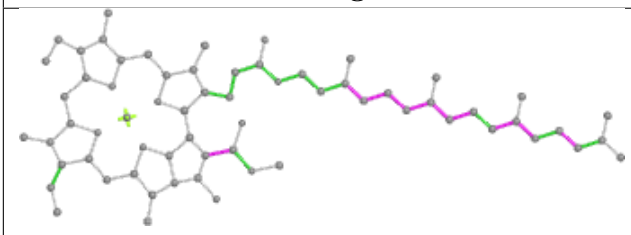
Ligand CLA A 838



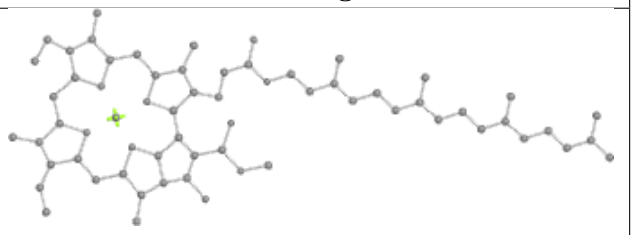
Bond lengths



Bond angles

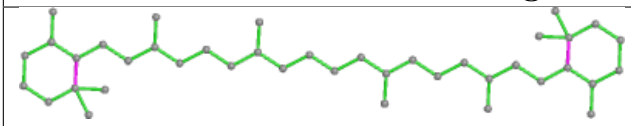


Torsions

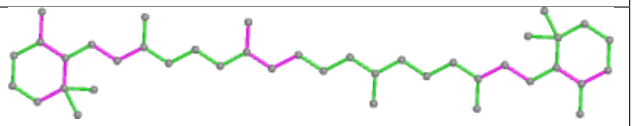


Rings

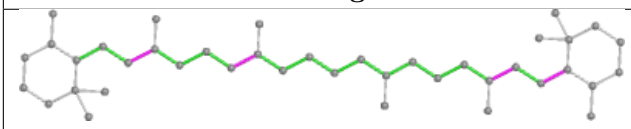
Ligand BCR B 844



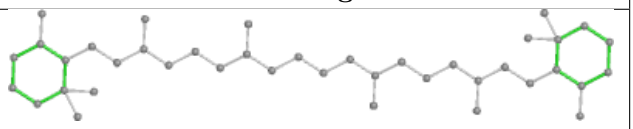
Bond lengths



Bond angles

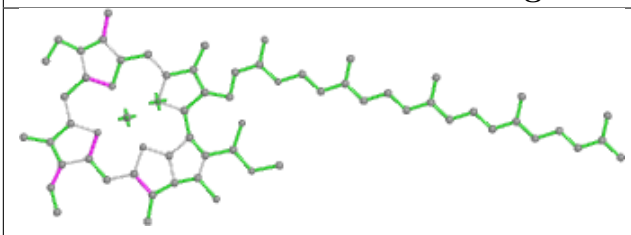


Torsions

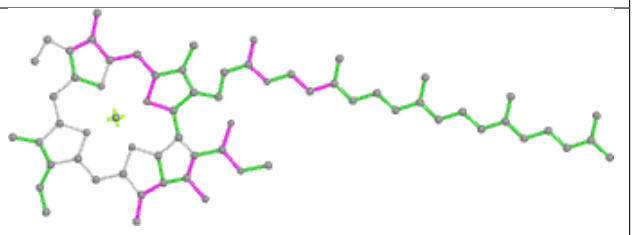


Rings

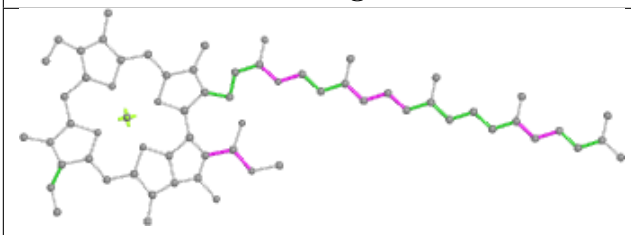
Ligand CLA B 823



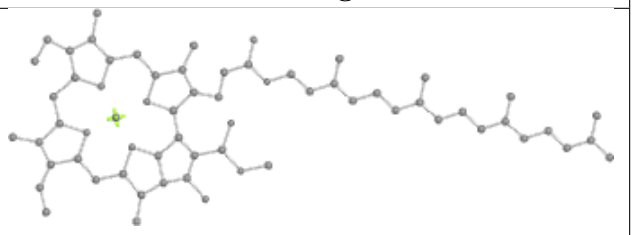
Bond lengths



Bond angles

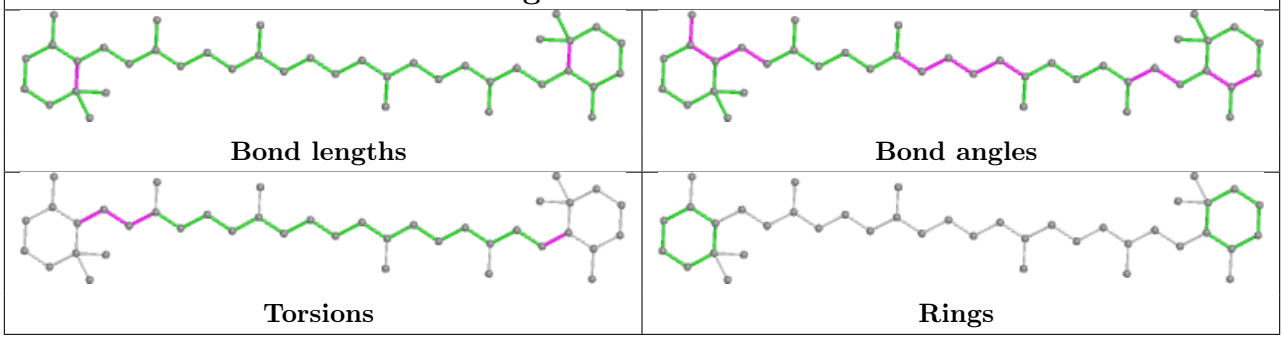


Torsions

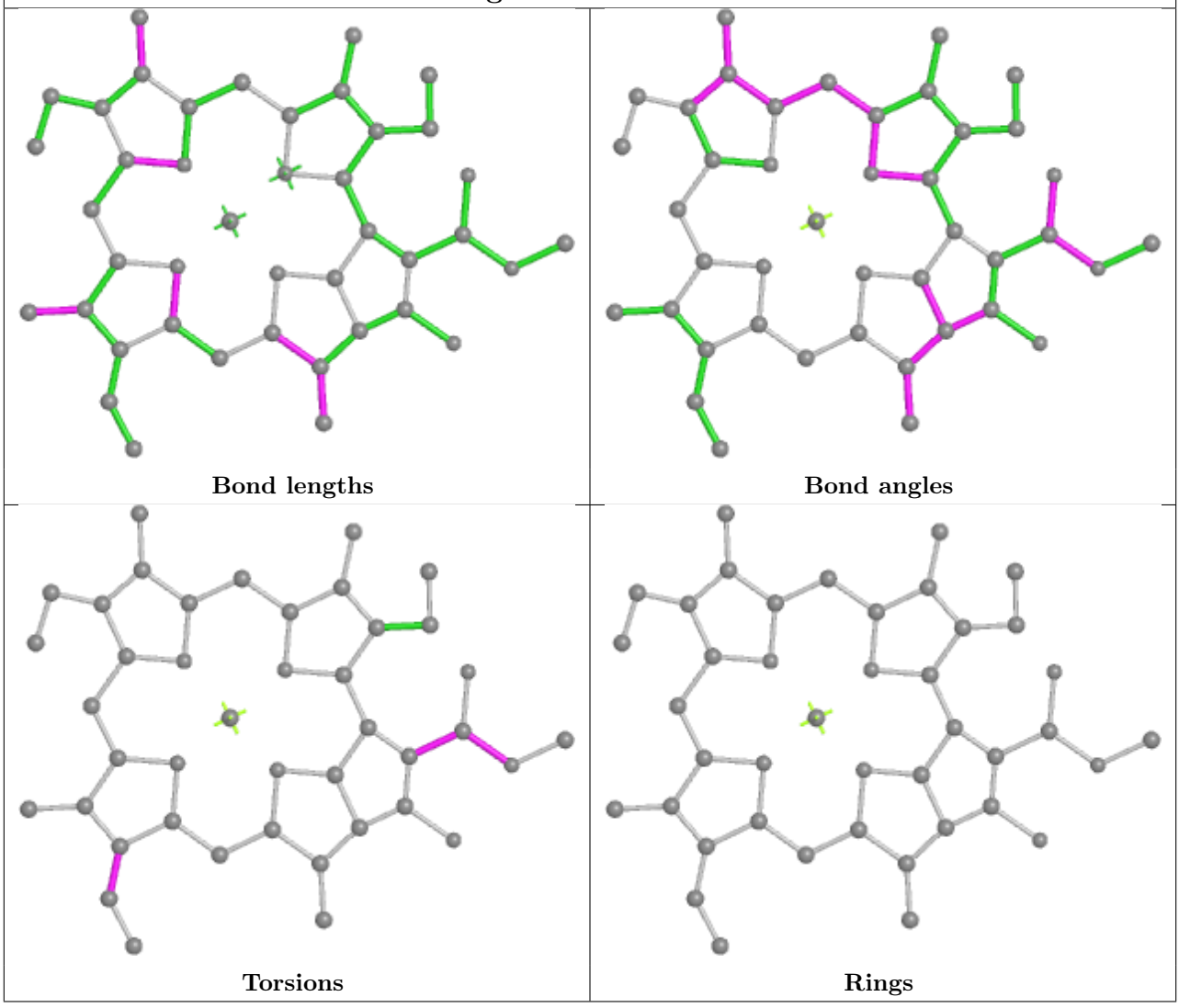


Rings

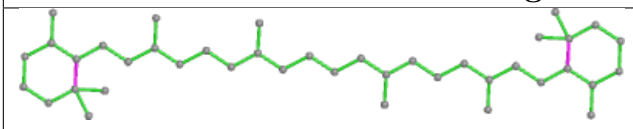
Ligand BCR A 849



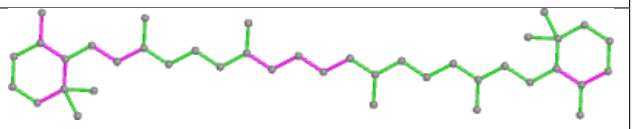
Ligand CLA 1 304



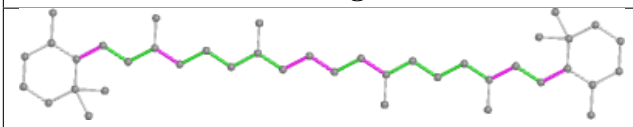
Ligand BCR L 201



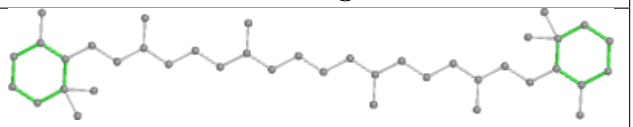
Bond lengths



Bond angles

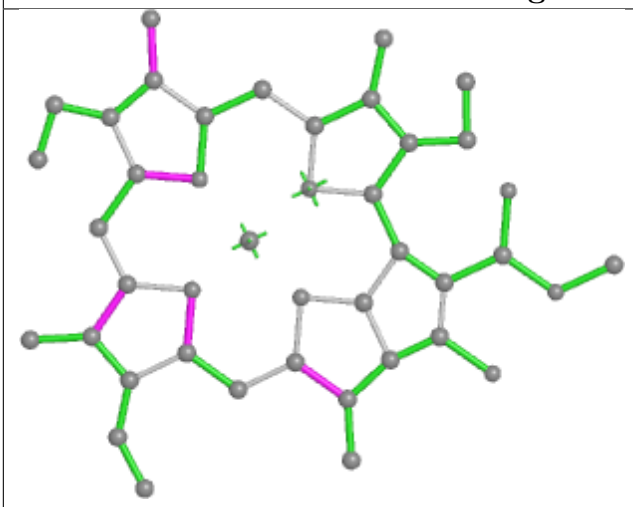


Torsions

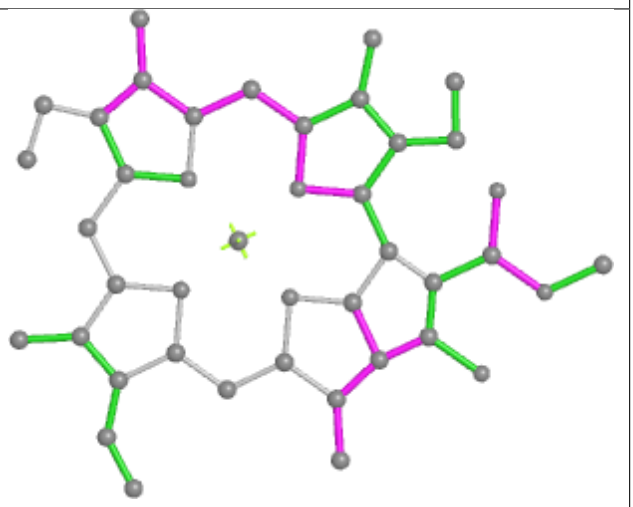


Rings

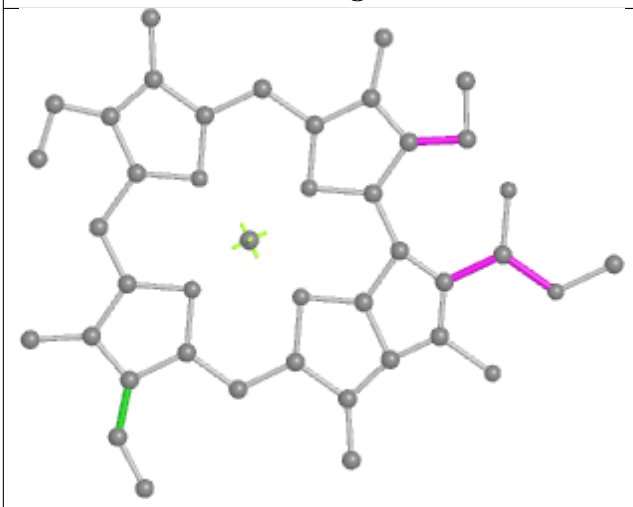
Ligand CLA J 103



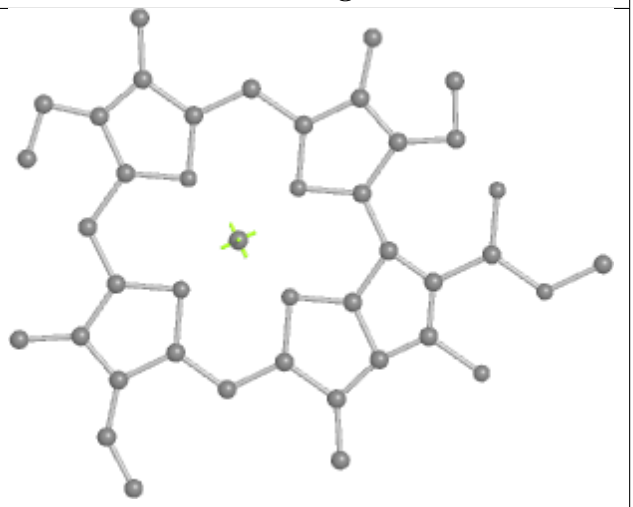
Bond lengths



Bond angles

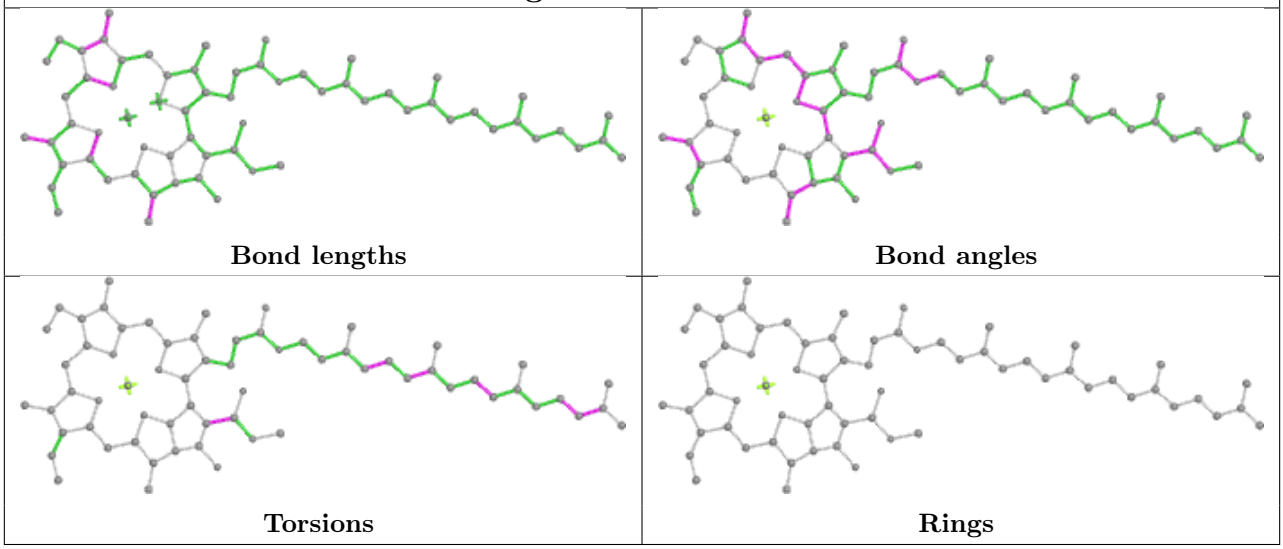


Torsions

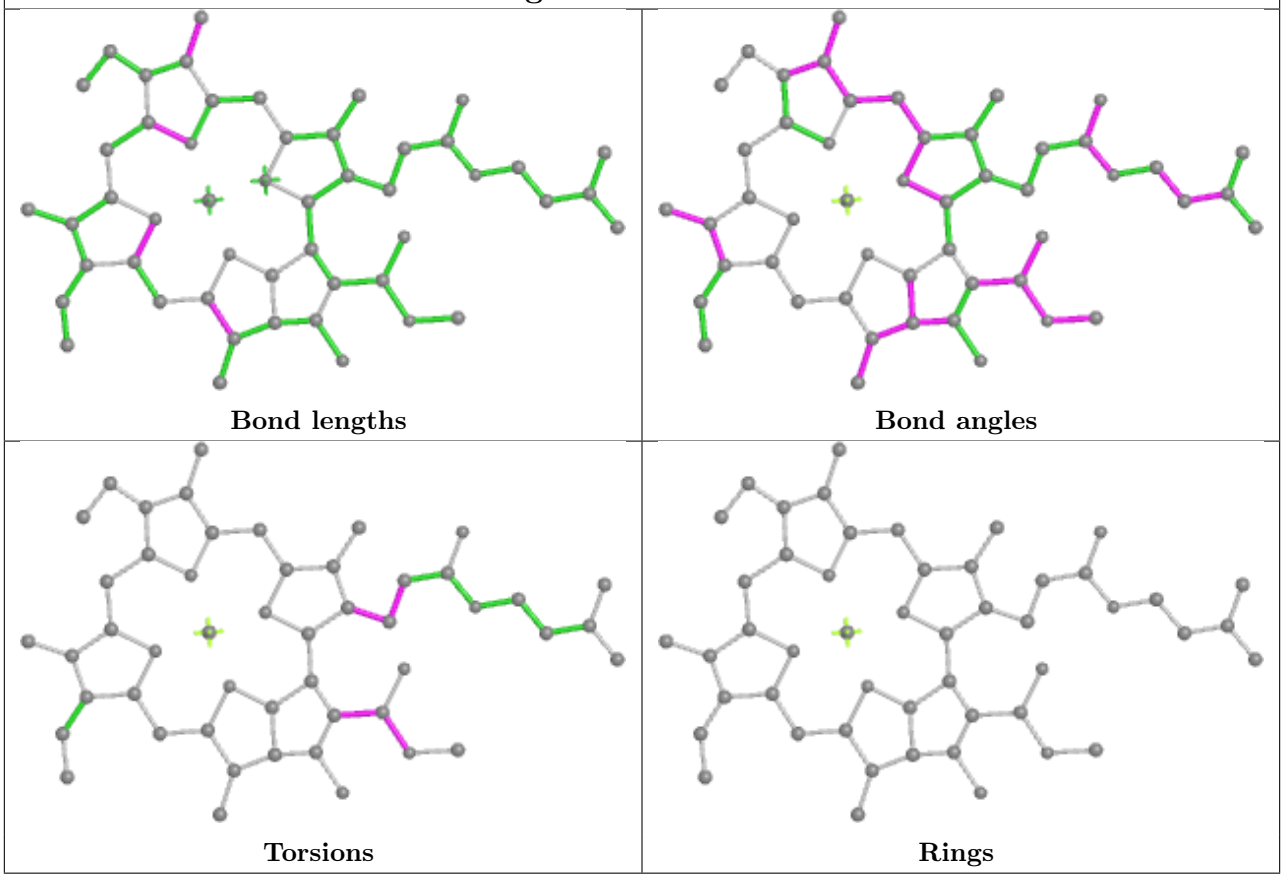


Rings

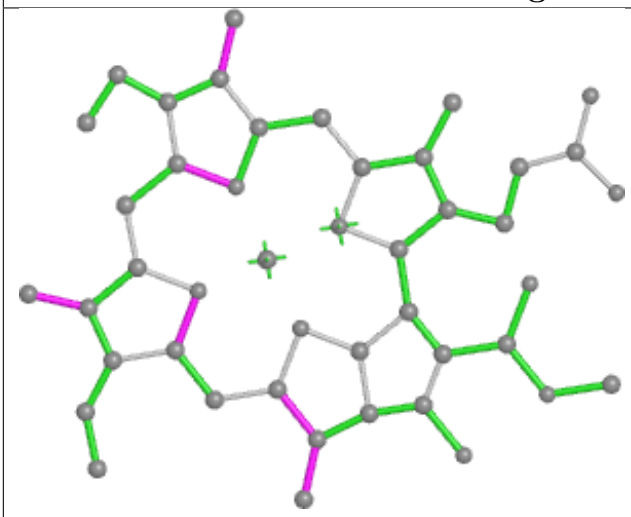
Ligand CLA B 810



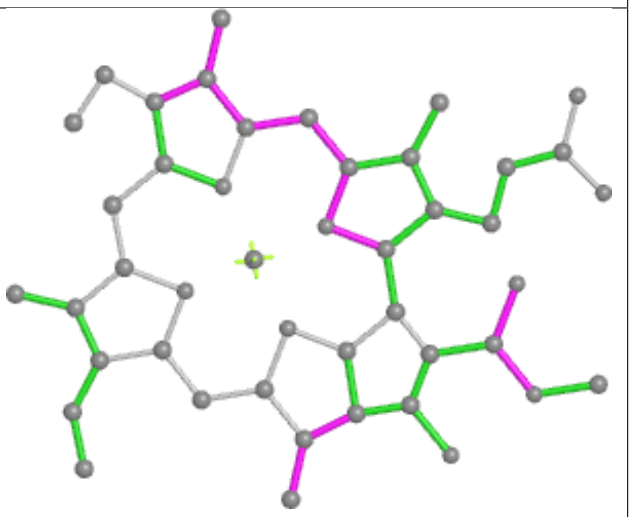
Ligand CLA B 822



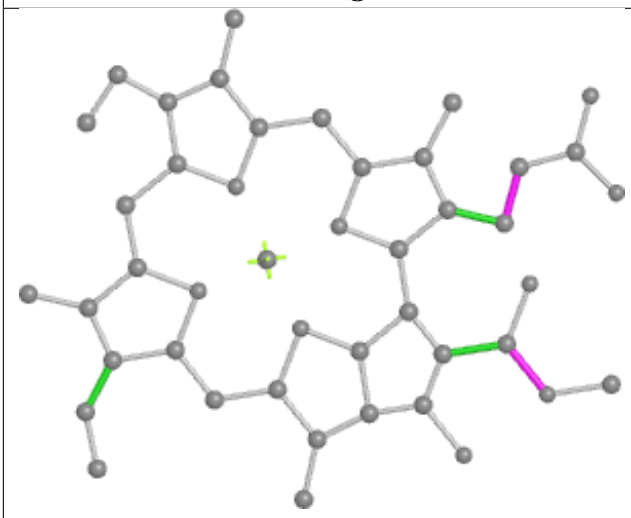
Ligand CLA 3 612



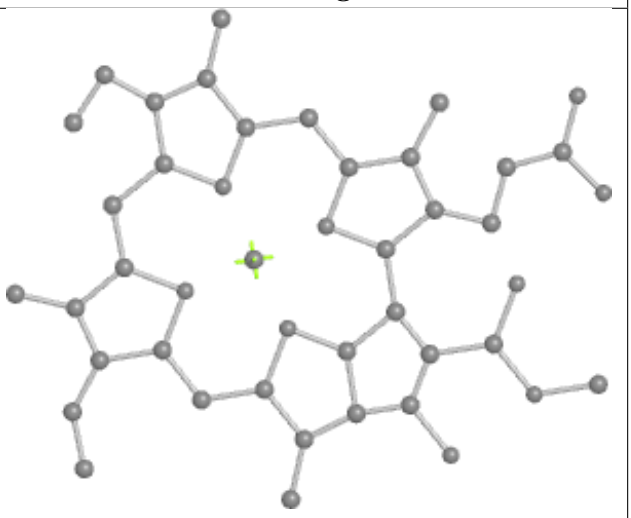
Bond lengths



Bond angles

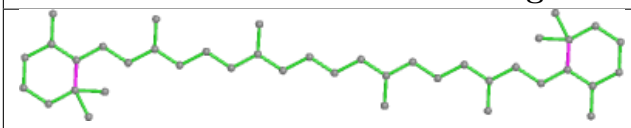


Torsions

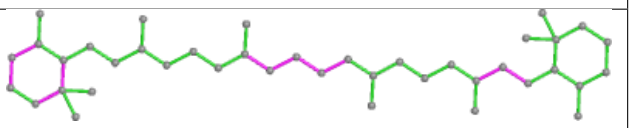


Rings

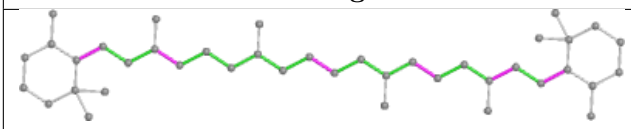
Ligand BCR 3 616



Bond lengths



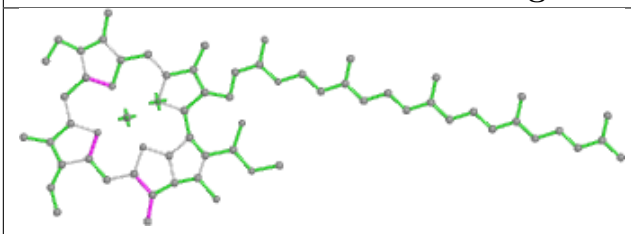
Bond angles



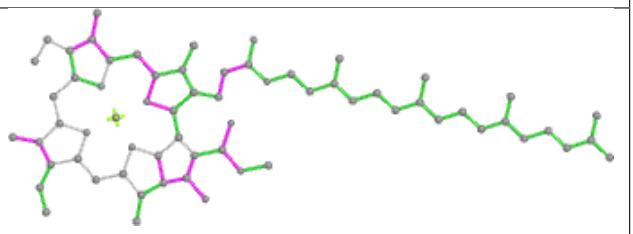
Torsions

Rings

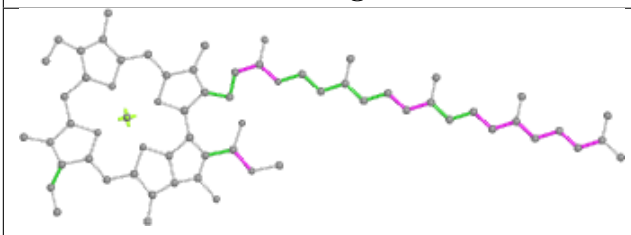
Ligand CLA 1 302



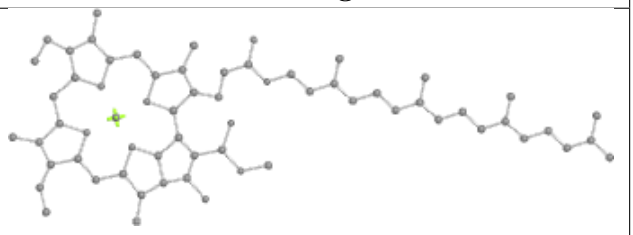
Bond lengths



Bond angles

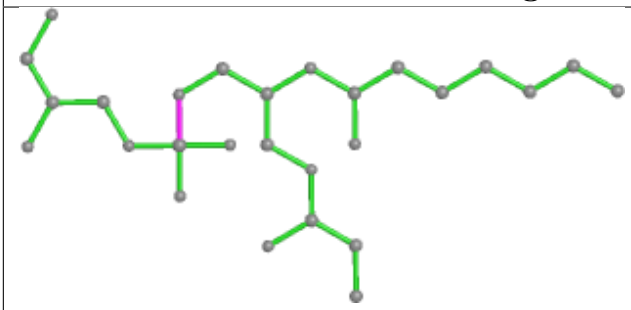


Torsions

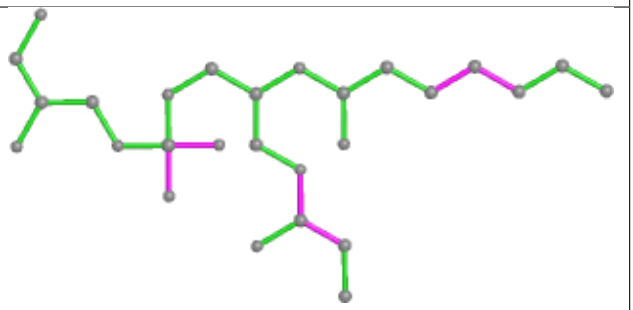


Rings

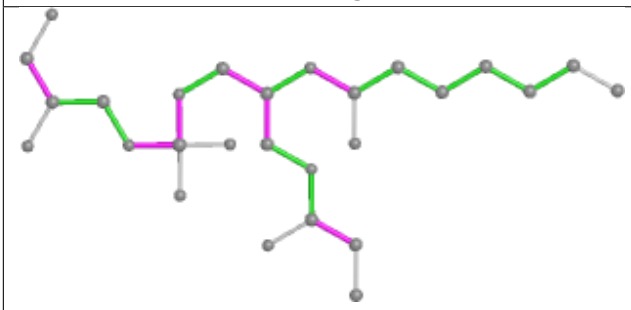
Ligand LHG A 845



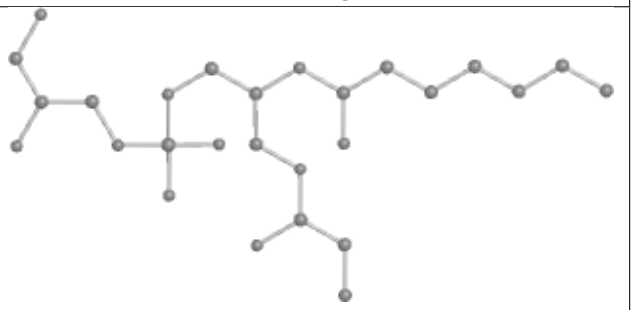
Bond lengths



Bond angles

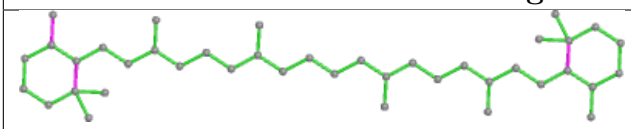


Torsions

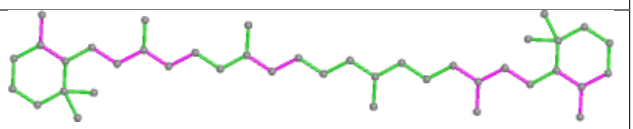


Rings

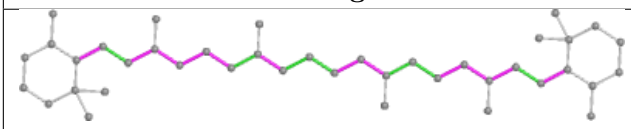
Ligand BCR 2 316



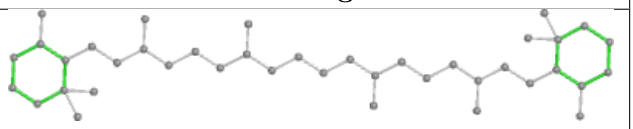
Bond lengths



Bond angles

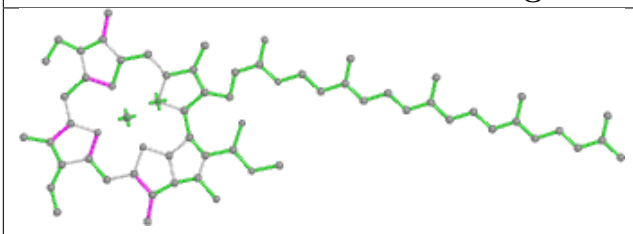


Torsions

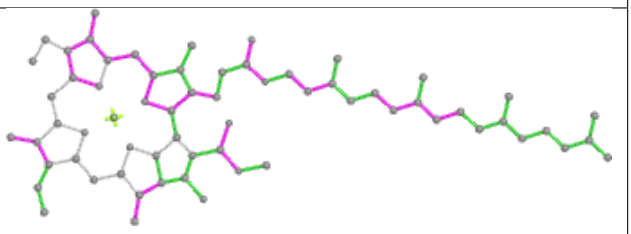


Rings

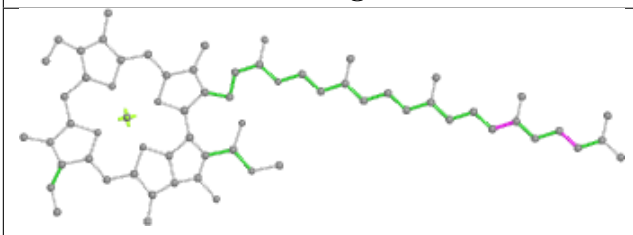
Ligand CLA B 802



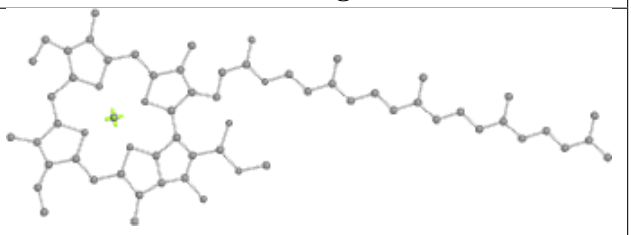
Bond lengths



Bond angles

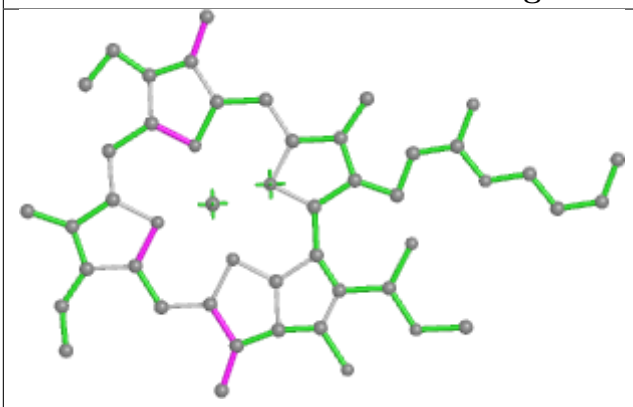


Torsions

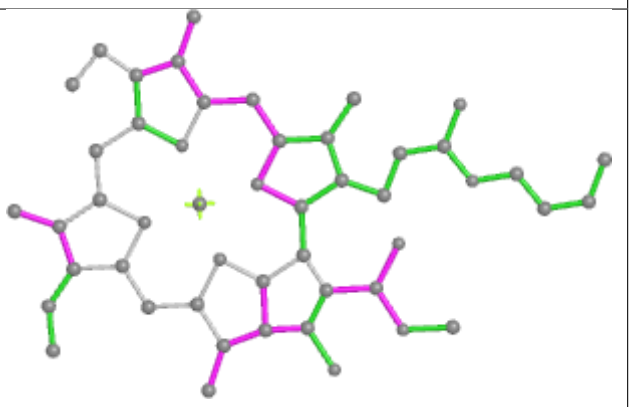


Rings

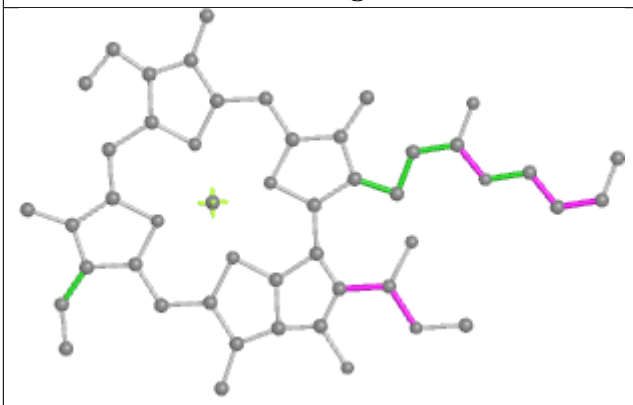
Ligand CLA A 821



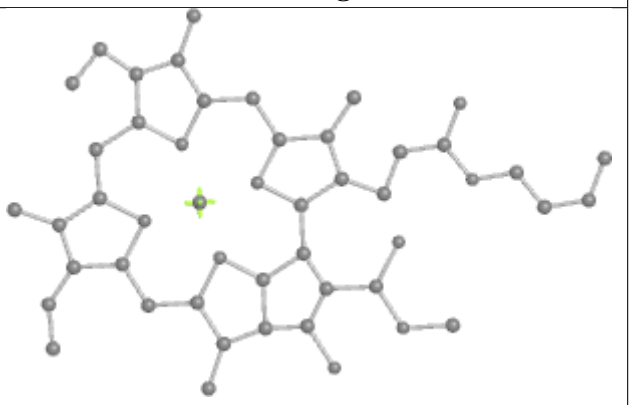
Bond lengths



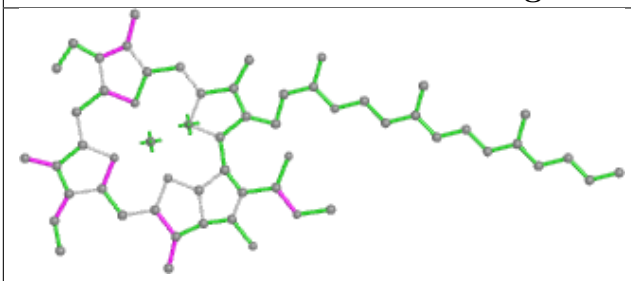
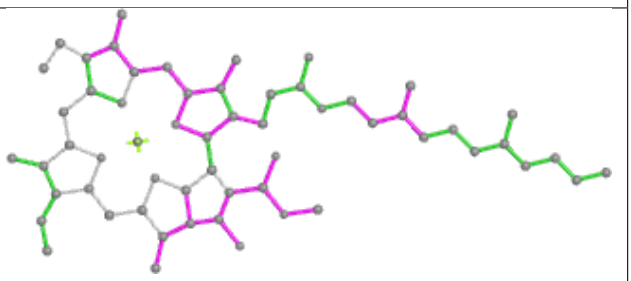
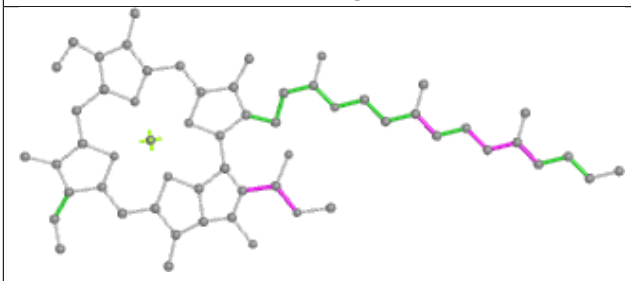
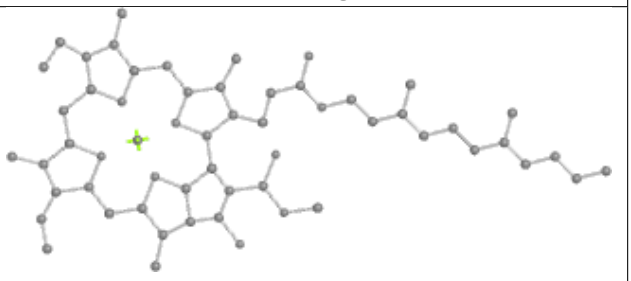
Bond angles

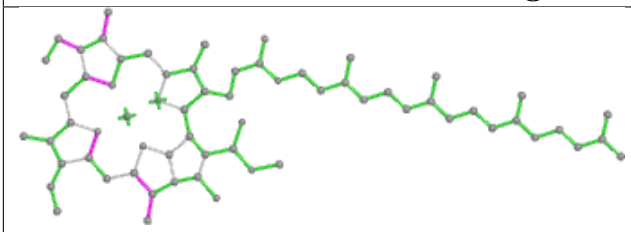
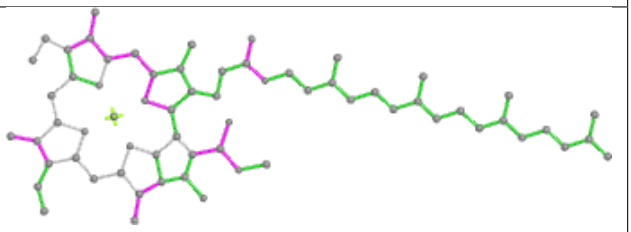
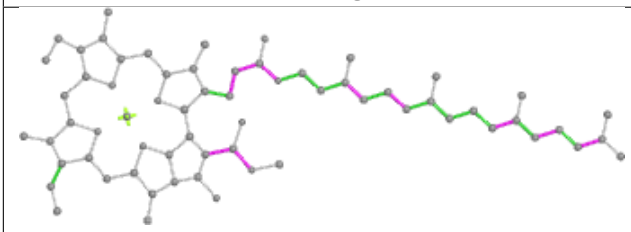
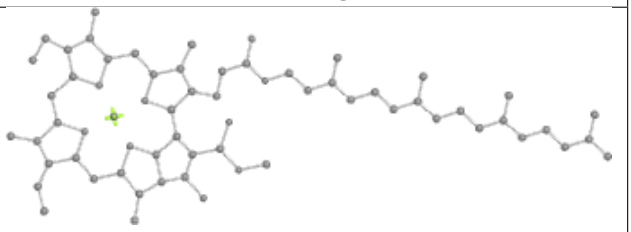


Torsions

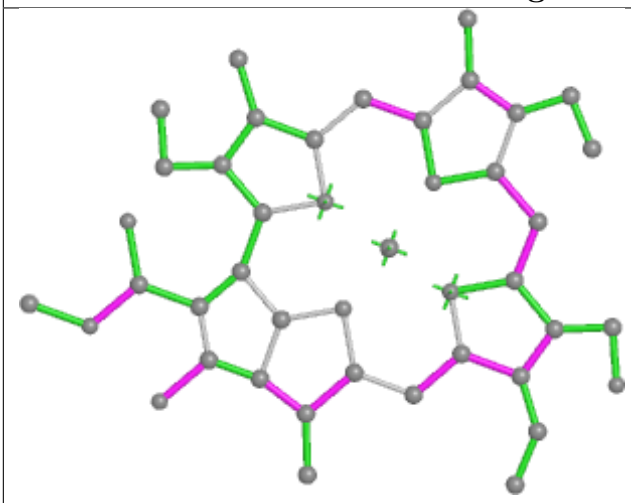


Rings

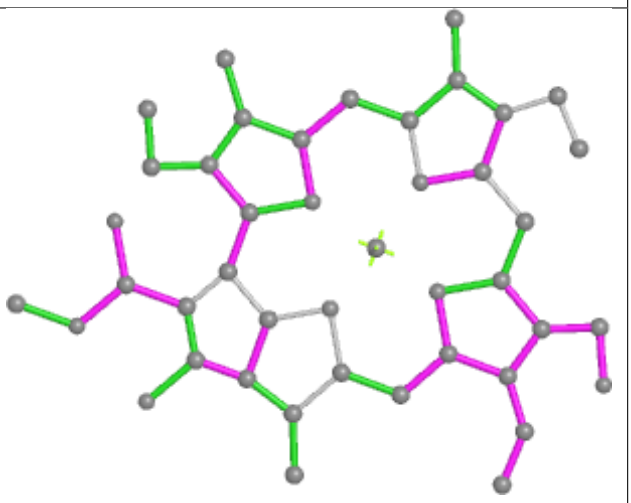
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

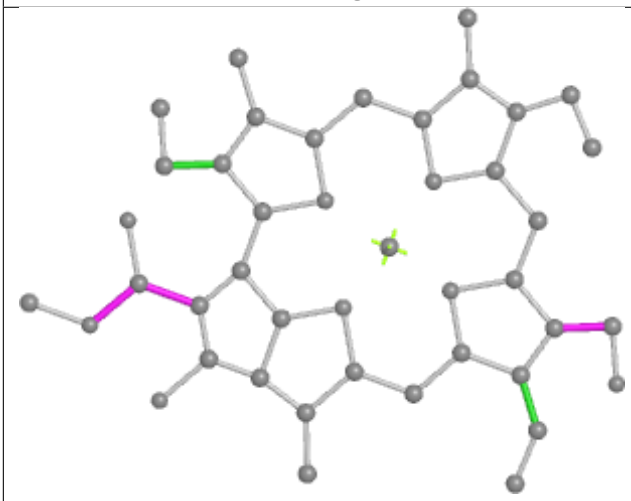
Ligand CHL 2 304



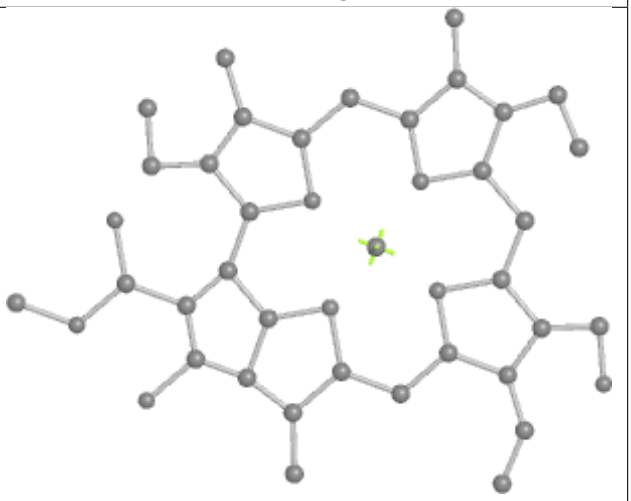
Bond lengths



Bond angles

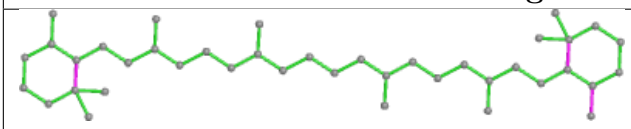


Torsions

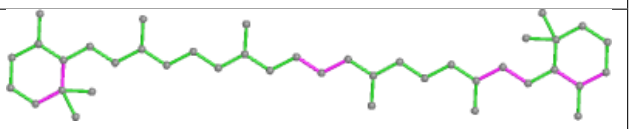


Rings

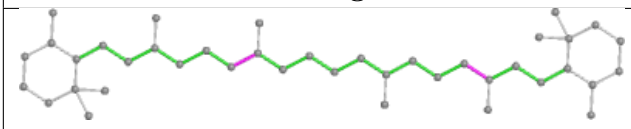
Ligand BCR J 104



Bond lengths



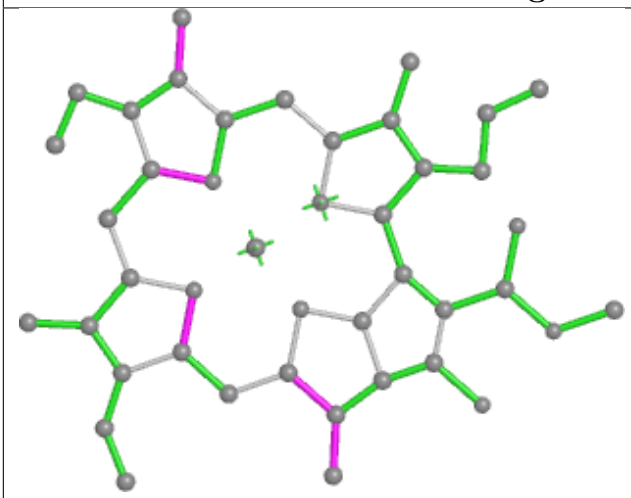
Bond angles



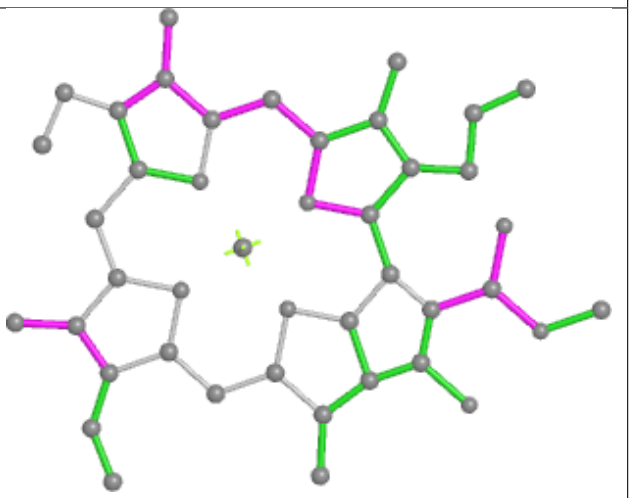
Torsions

Rings

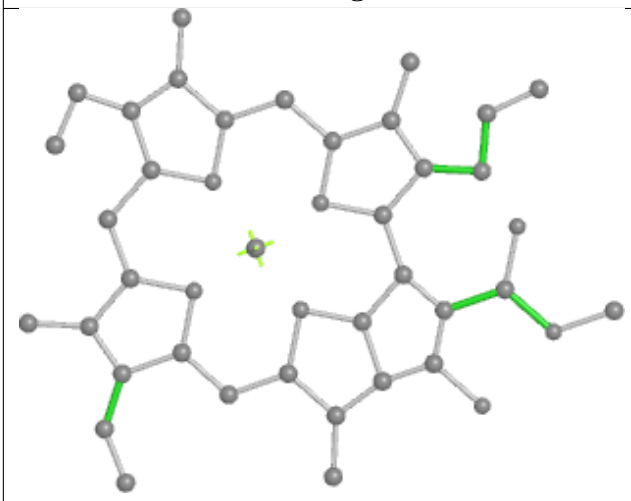
Ligand CLA 2 312



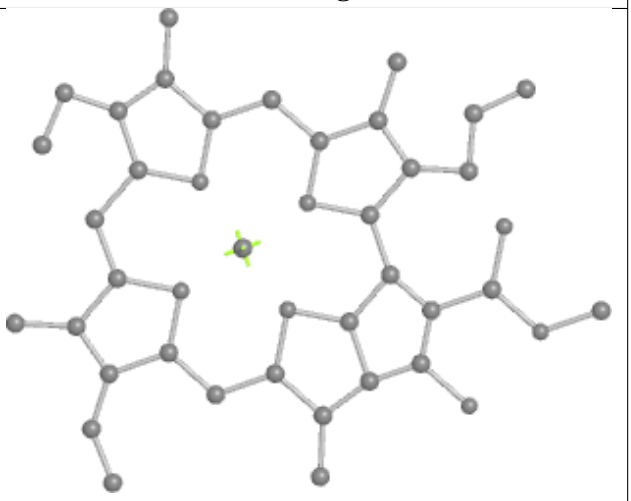
Bond lengths



Bond angles

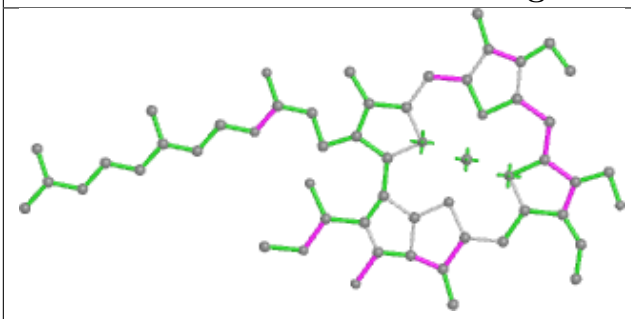


Torsions

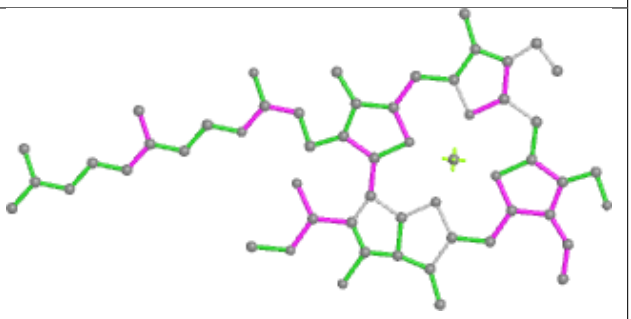


Rings

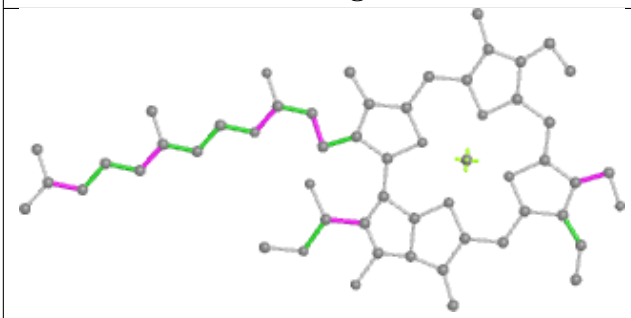
Ligand CHL 4 305



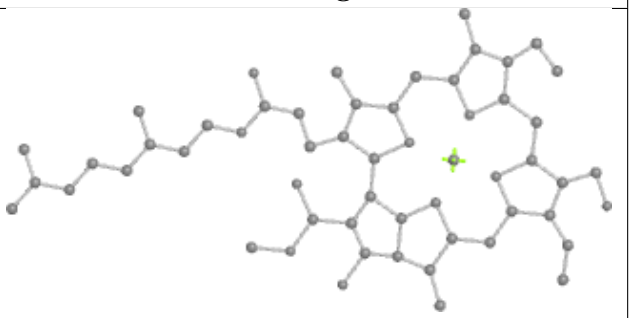
Bond lengths



Bond angles

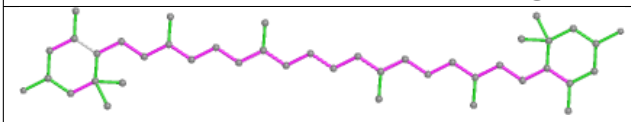


Torsions

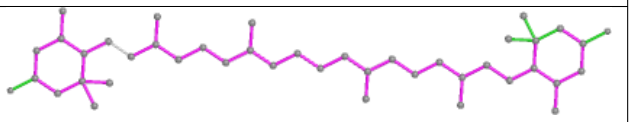


Rings

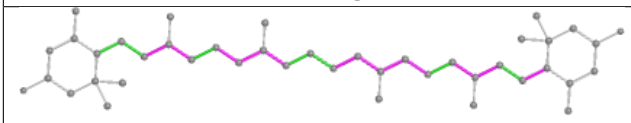
Ligand LUT 4 316



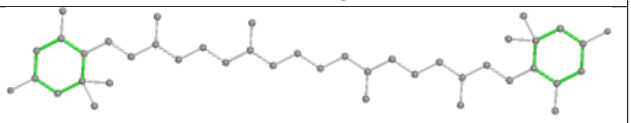
Bond lengths



Bond angles

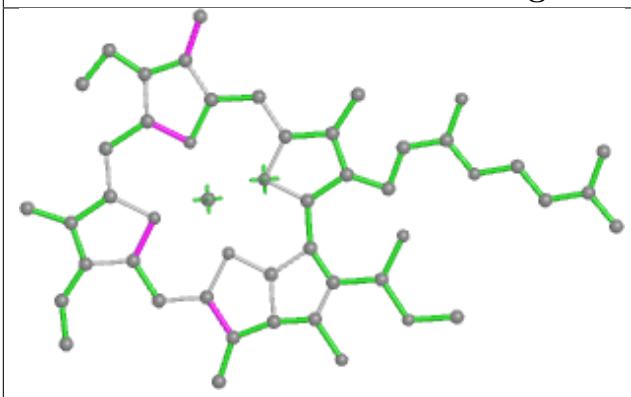


Torsions

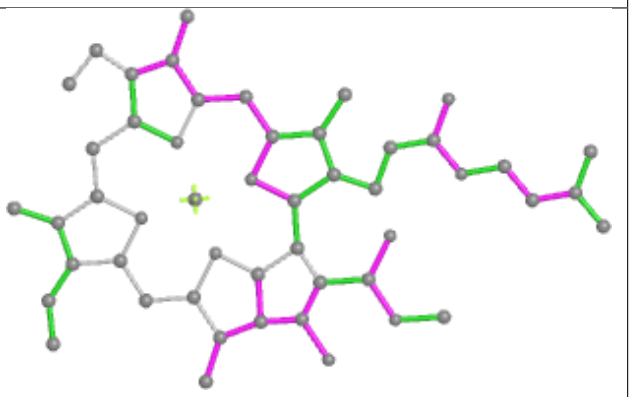


Rings

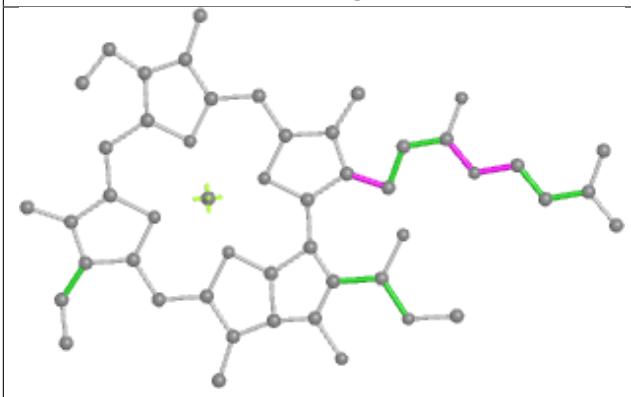
Ligand CLA 3 609



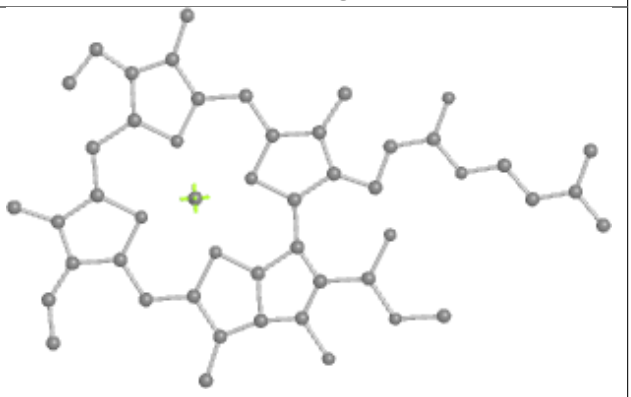
Bond lengths



Bond angles

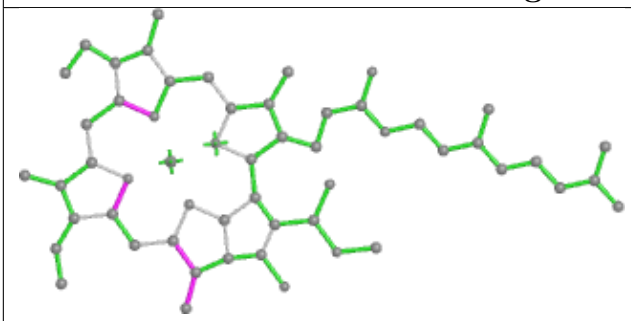


Torsions

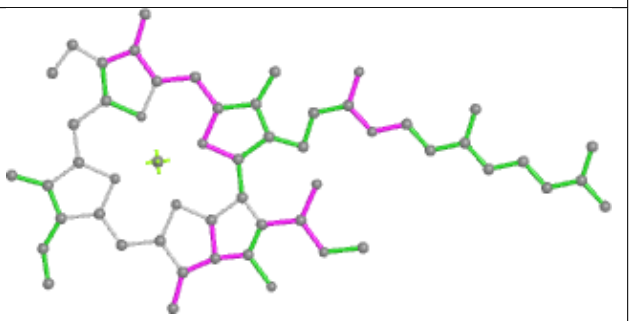


Rings

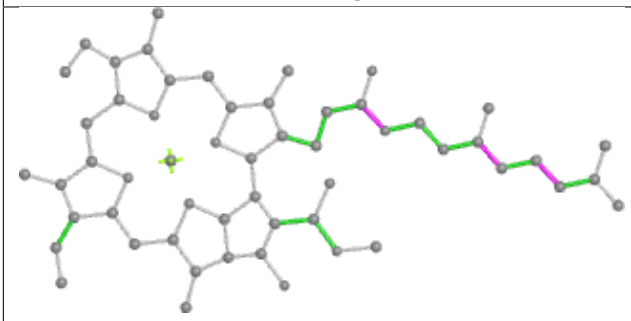
Ligand CLA B 818



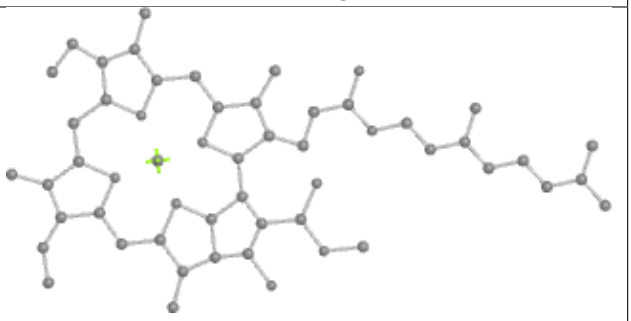
Bond lengths



Bond angles

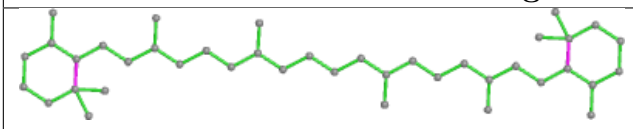


Torsions

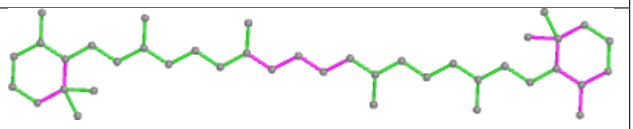


Rings

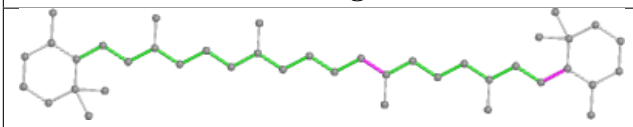
Ligand BCR B 848



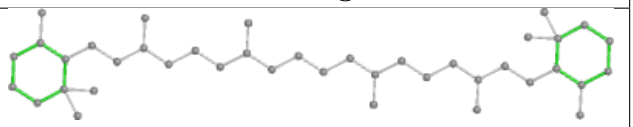
Bond lengths



Bond angles

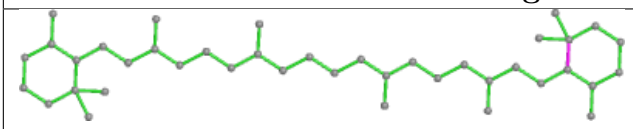


Torsions

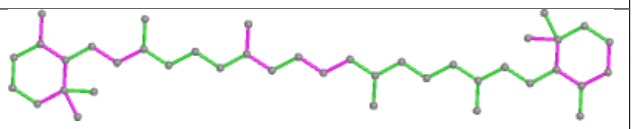


Rings

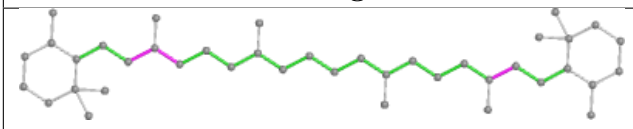
Ligand BCR B 845



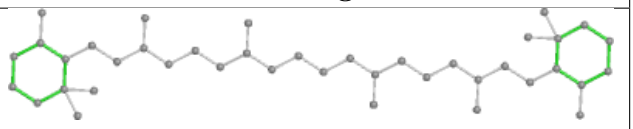
Bond lengths



Bond angles

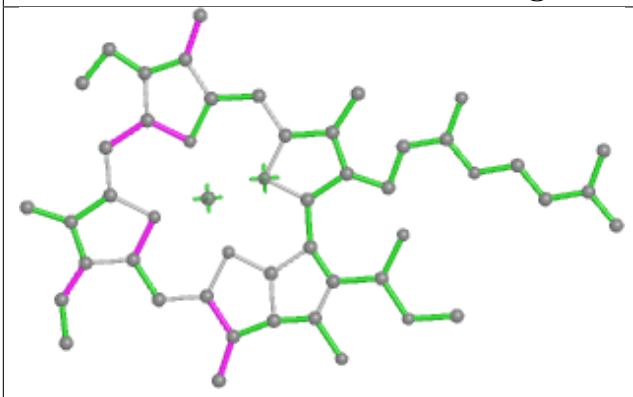


Torsions

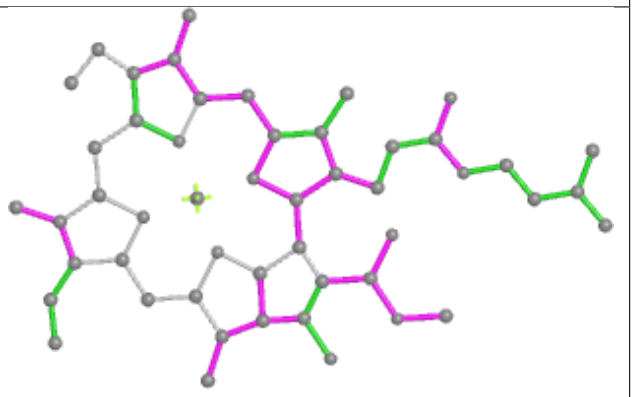


Rings

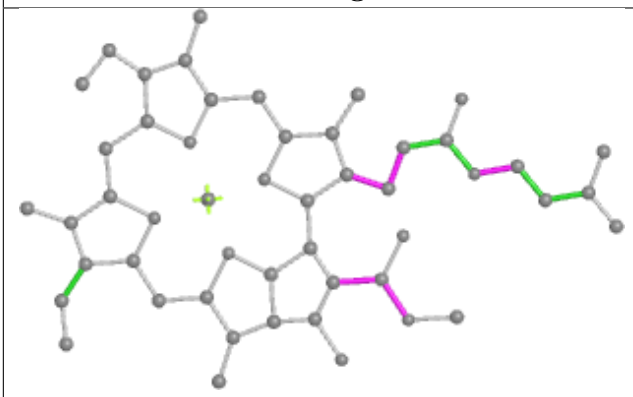
Ligand CLA 4 304



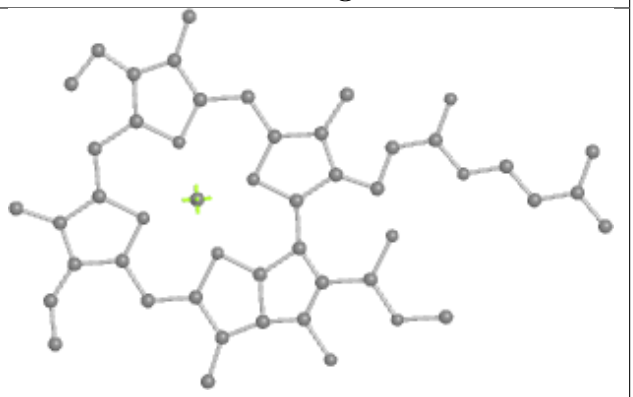
Bond lengths



Bond angles

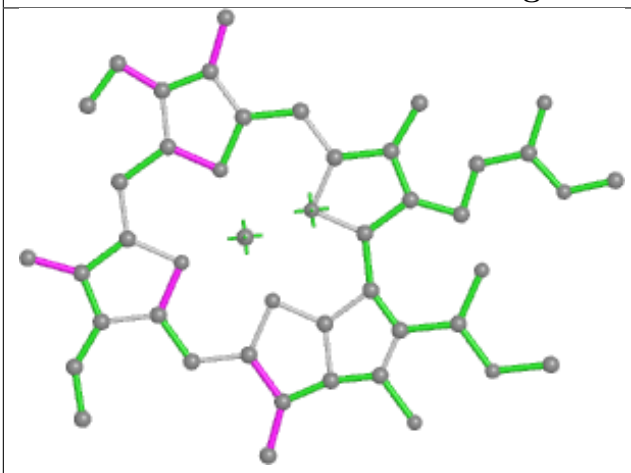


Torsions

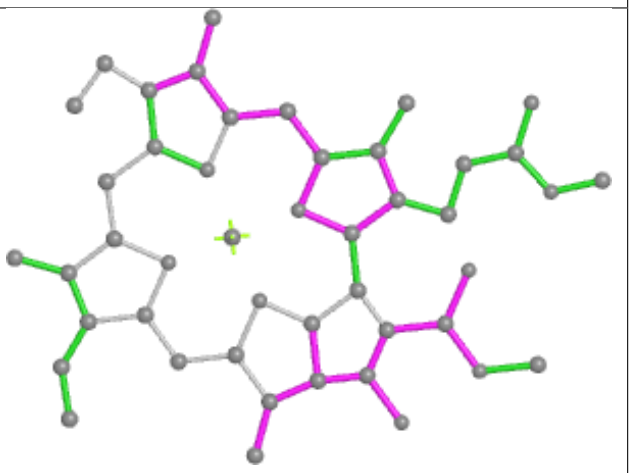


Rings

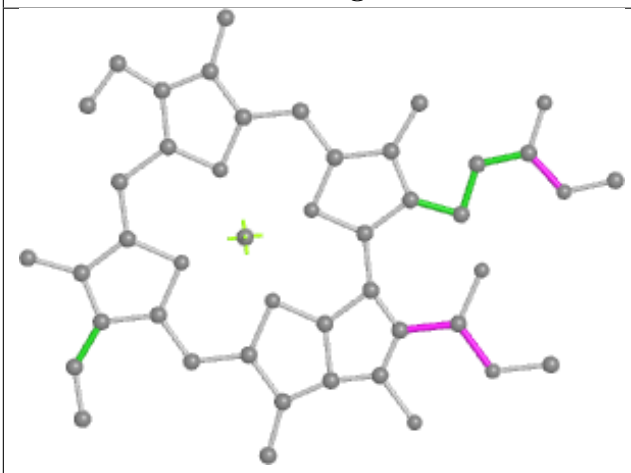
Ligand CLA G 105



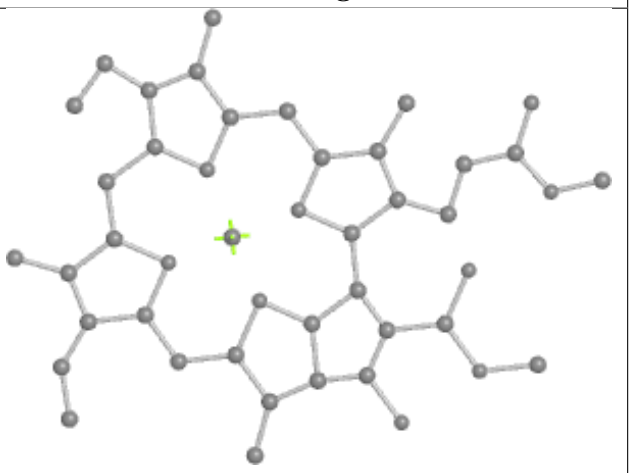
Bond lengths



Bond angles

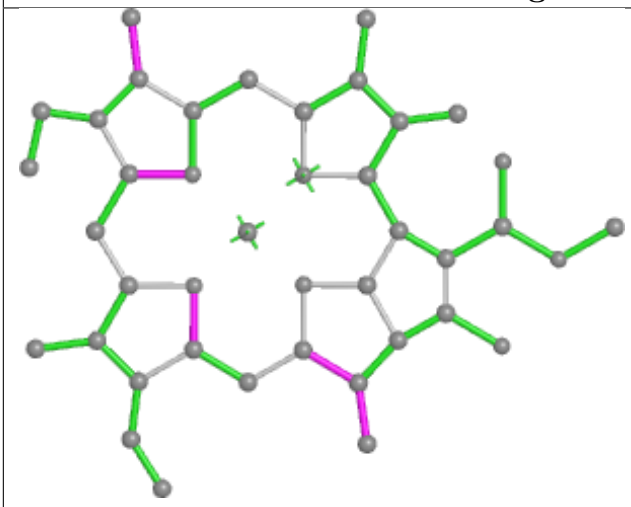


Torsions

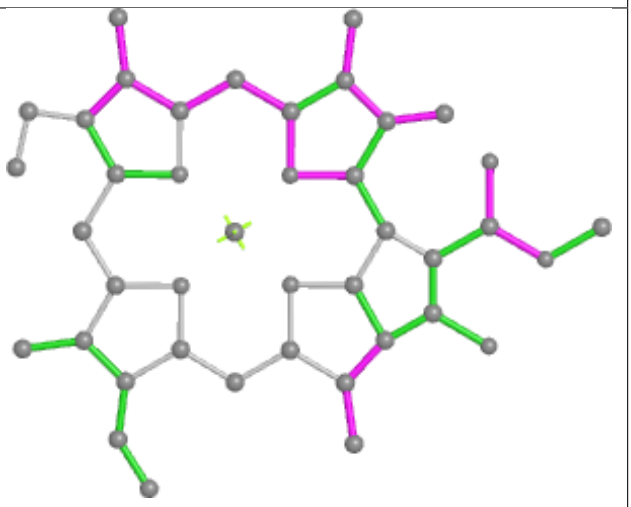


Rings

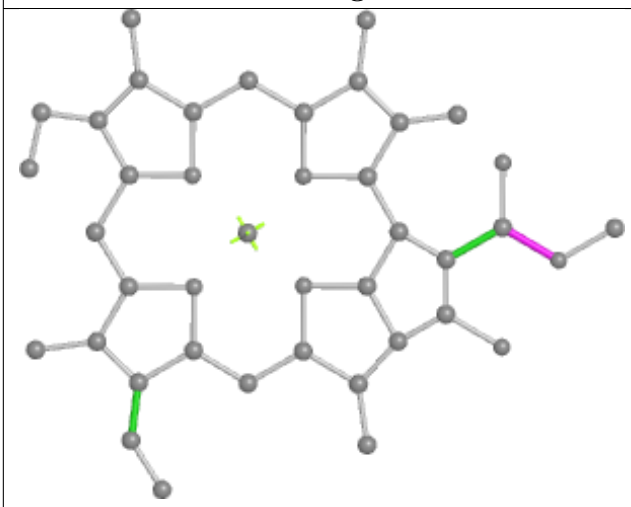
Ligand CLA 2 309



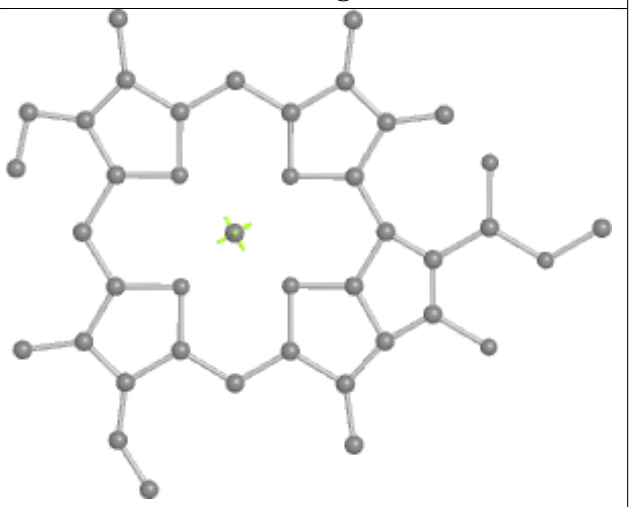
Bond lengths



Bond angles

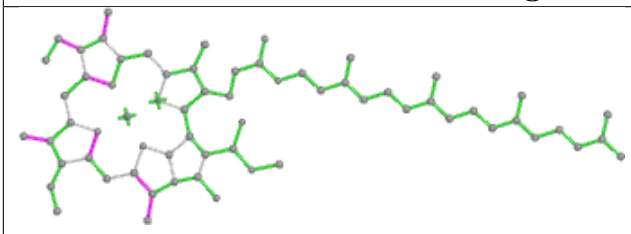


Torsions

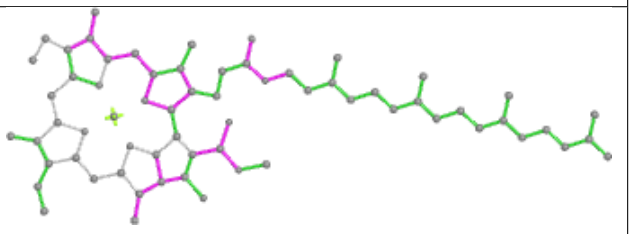


Rings

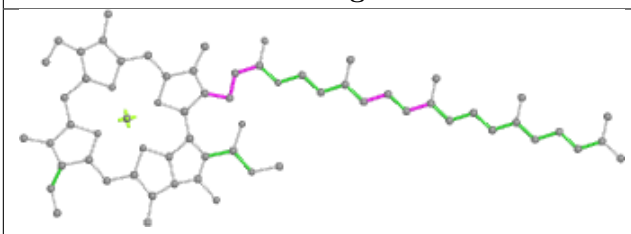
Ligand CLA A 808



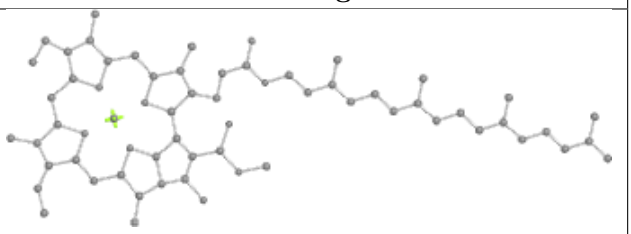
Bond lengths



Bond angles

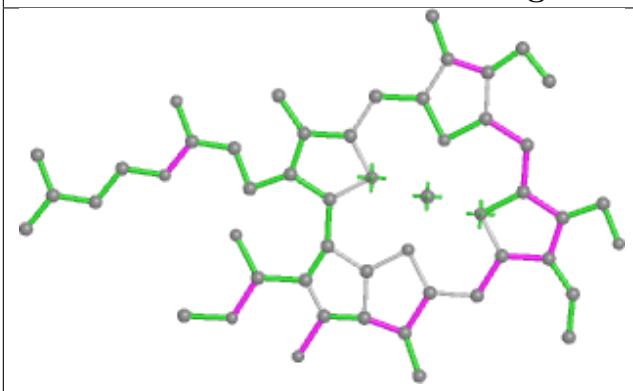


Torsions

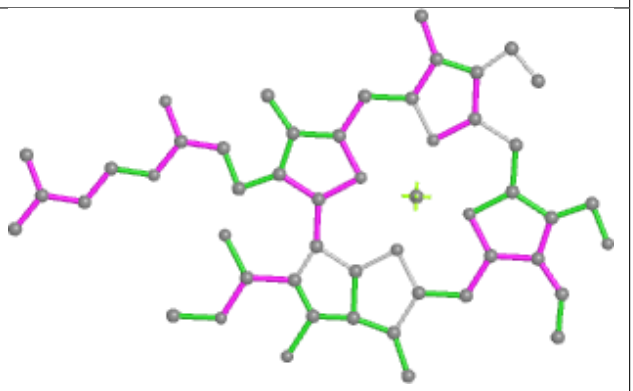


Rings

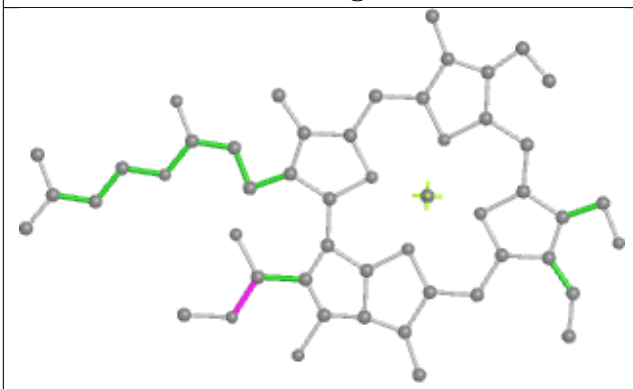
Ligand CHL 4 307



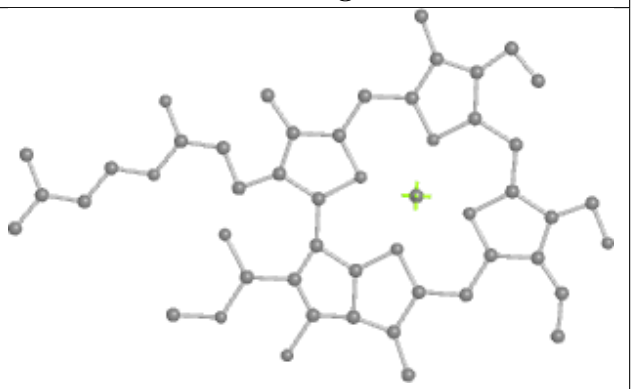
Bond lengths



Bond angles

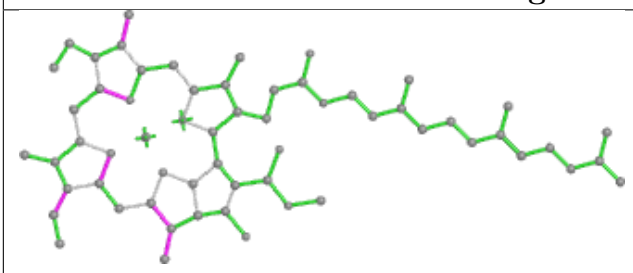


Torsions

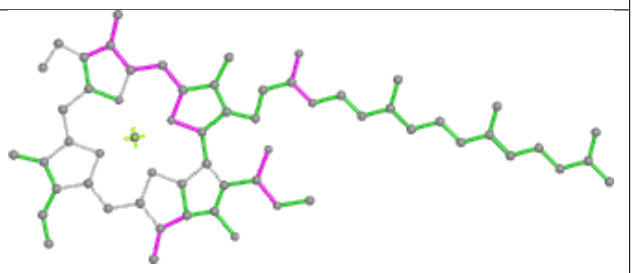


Rings

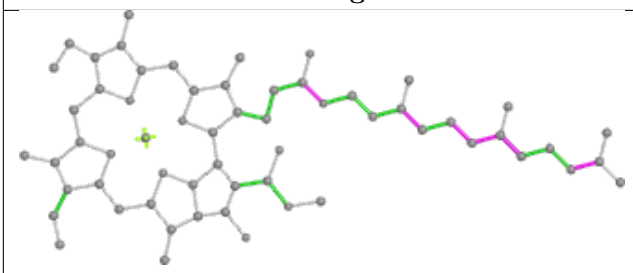
Ligand CLA 1 308



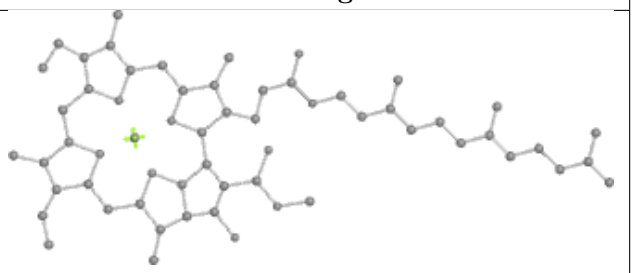
Bond lengths



Bond angles

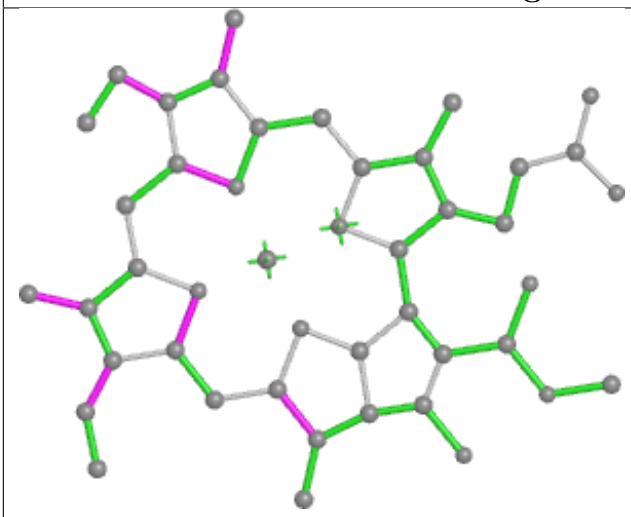


Torsions

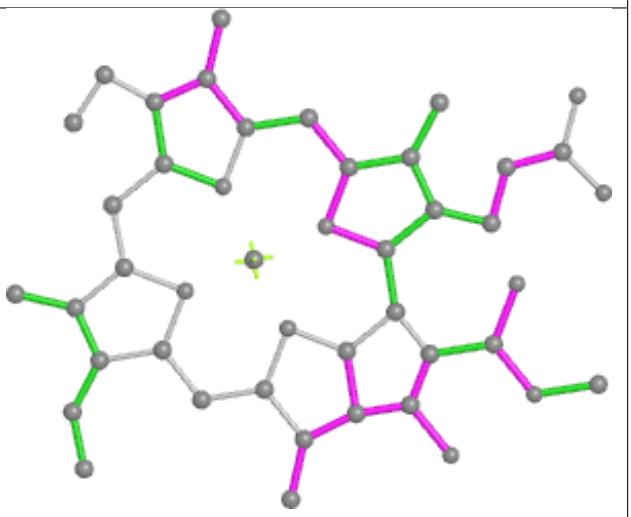


Rings

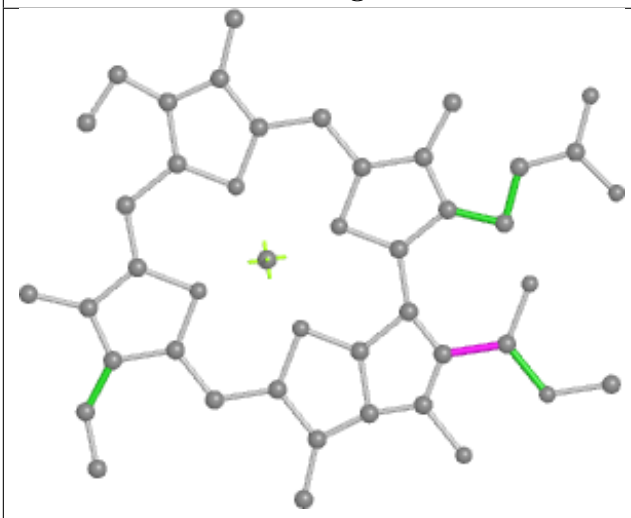
Ligand CLA A 813



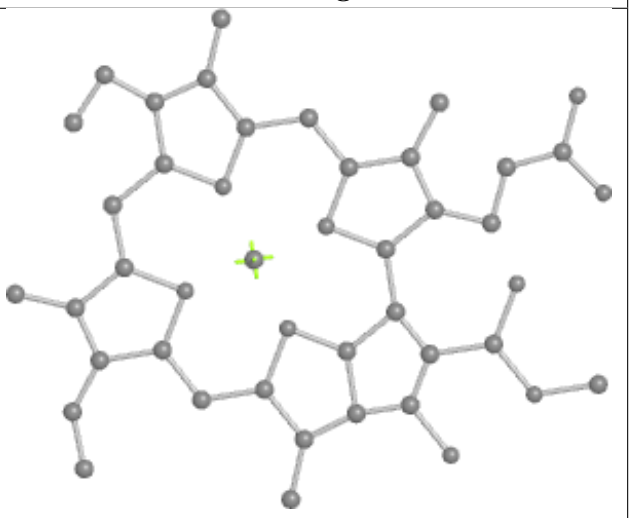
Bond lengths



Bond angles

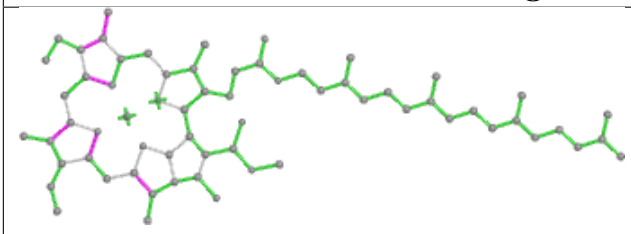


Torsions

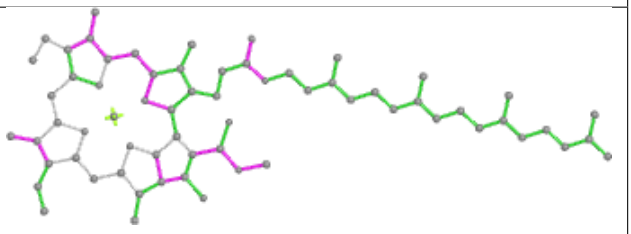


Rings

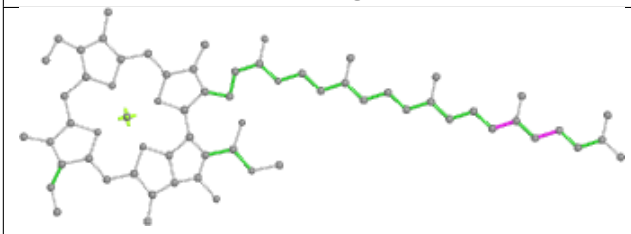
Ligand CLA B 821



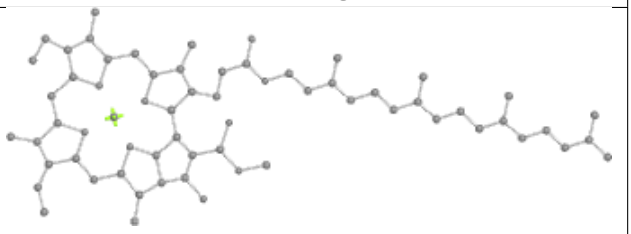
Bond lengths



Bond angles

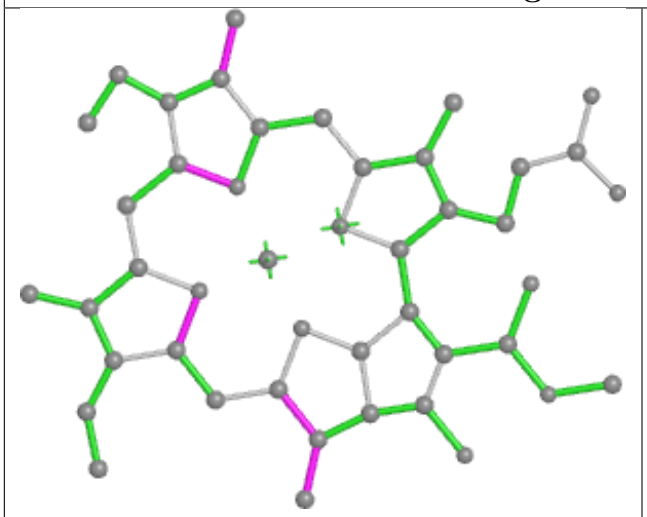


Torsions

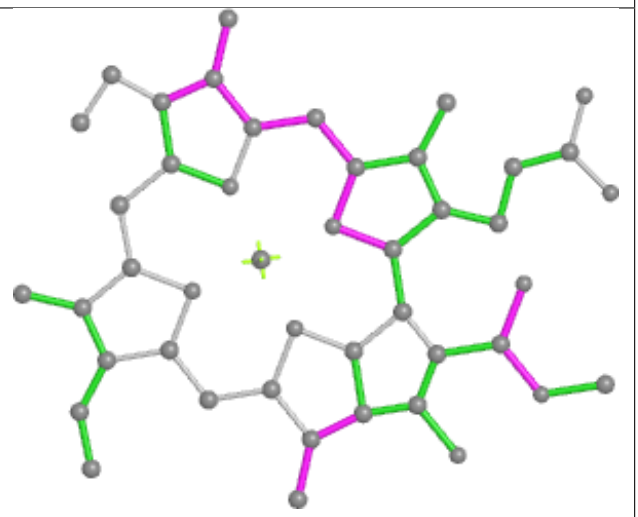


Rings

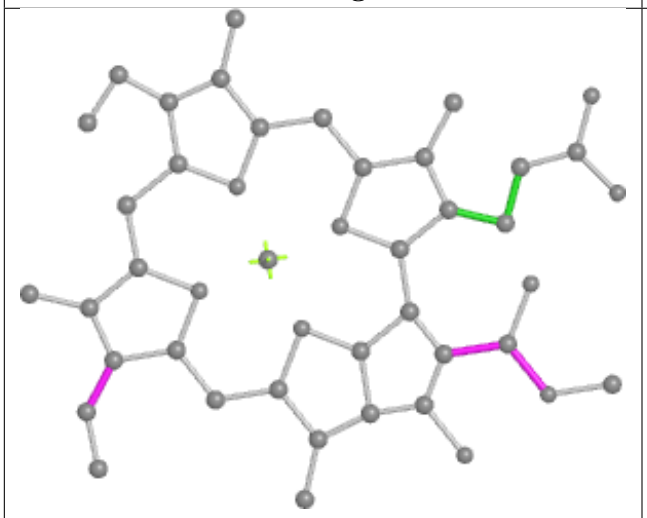
Ligand CLA K 201



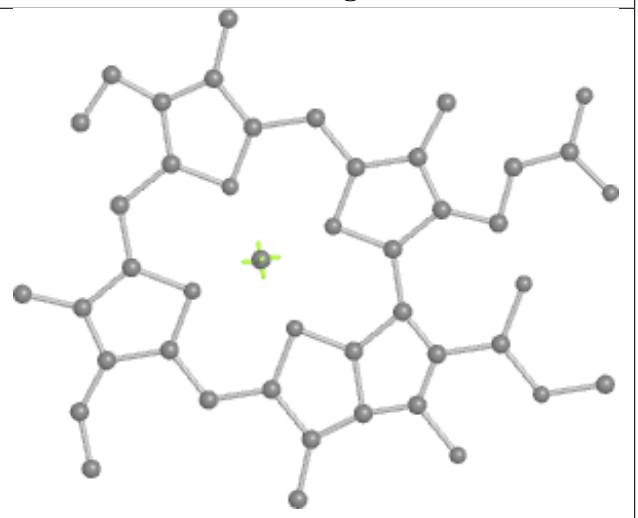
Bond lengths



Bond angles

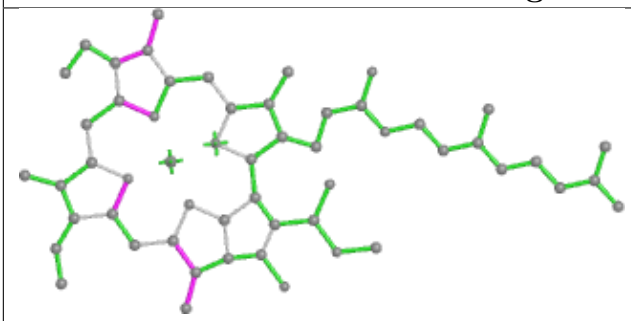


Torsions

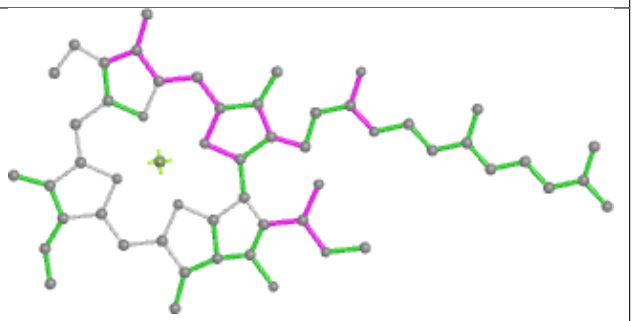


Rings

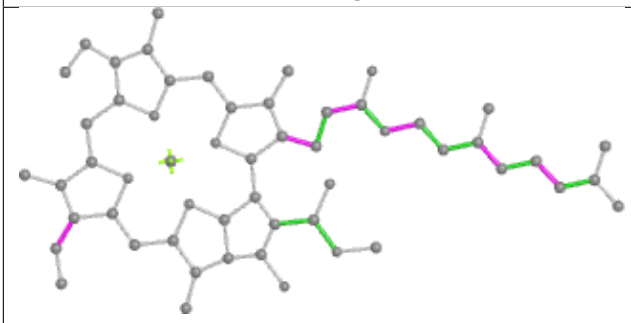
Ligand CLA F 307



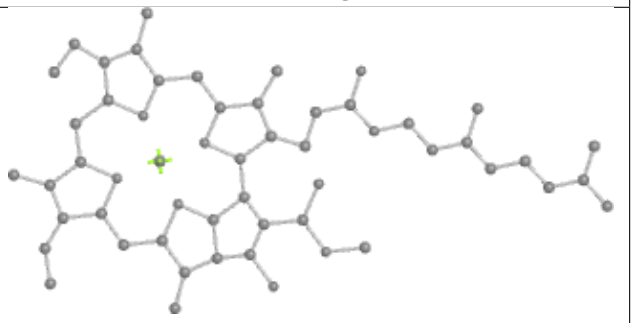
Bond lengths



Bond angles

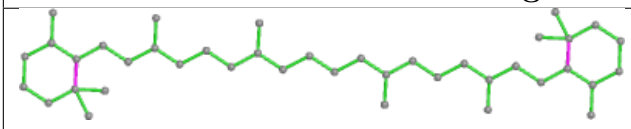


Torsions

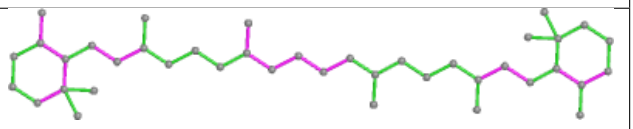


Rings

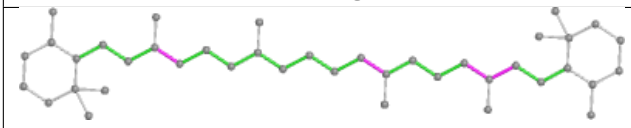
Ligand BCR B 846



Bond lengths



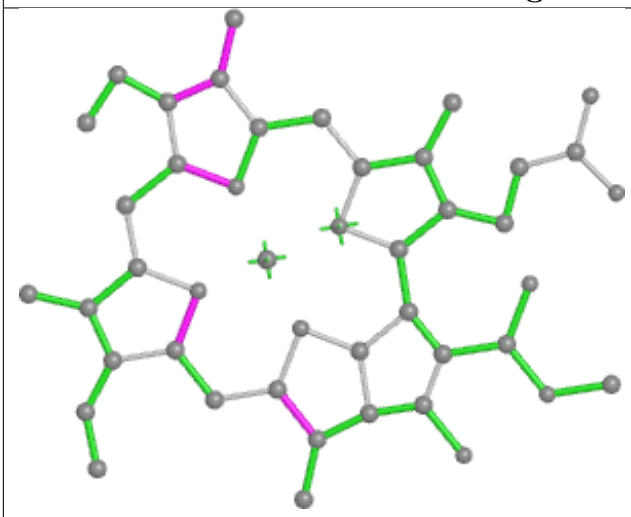
Bond angles



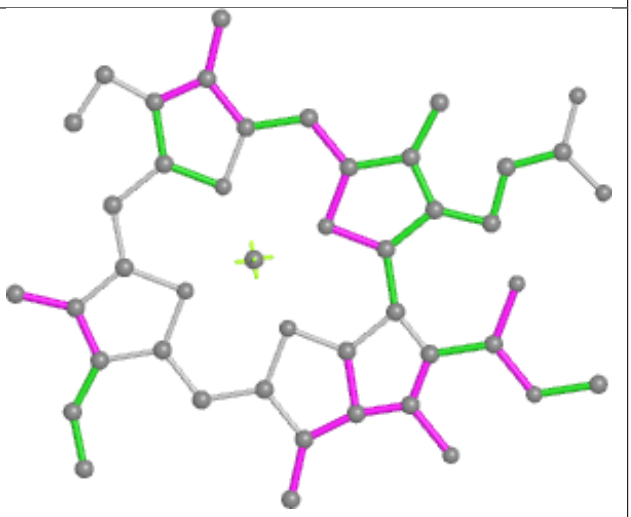
Torsions

Rings

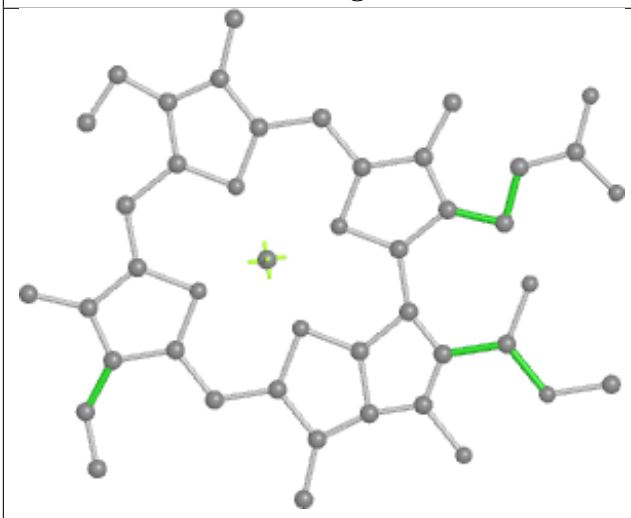
Ligand CLA F 306



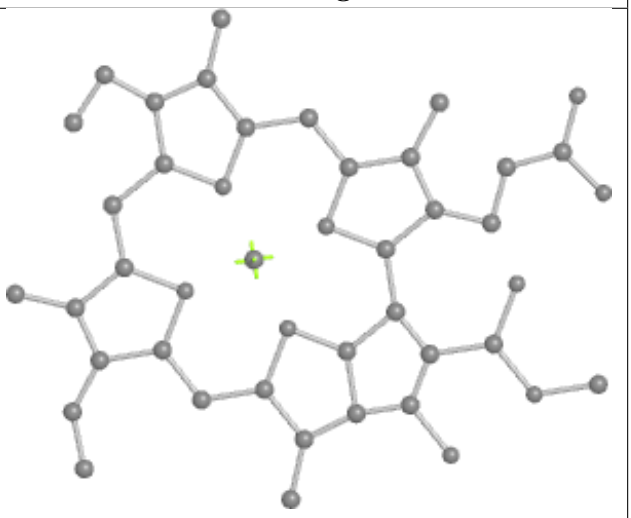
Bond lengths



Bond angles

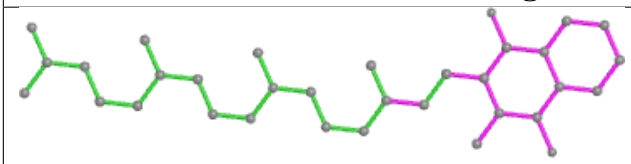


Torsions

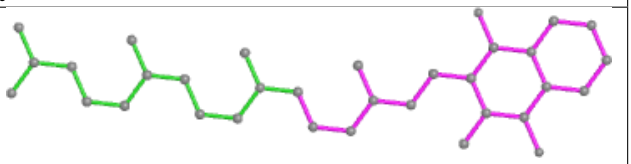


Rings

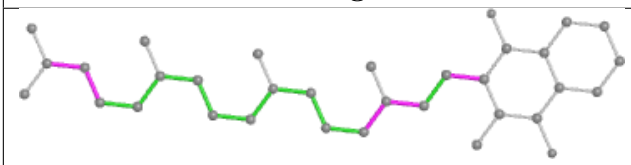
Ligand PQN A 842



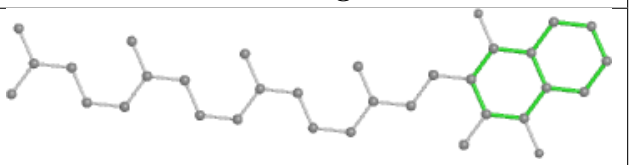
Bond lengths



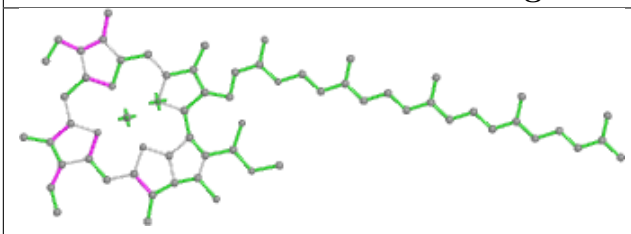
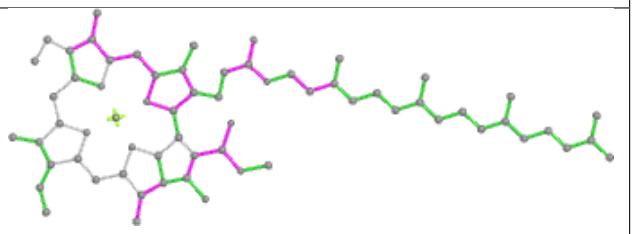
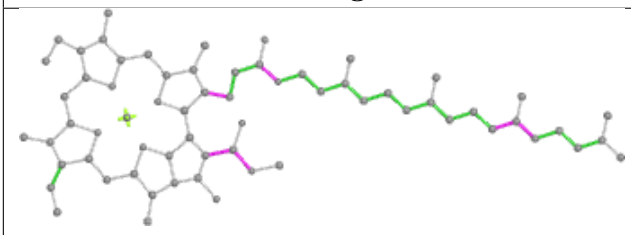
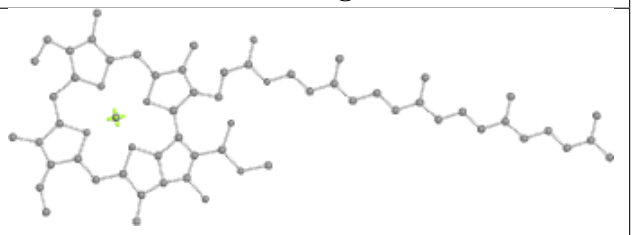
Bond angles

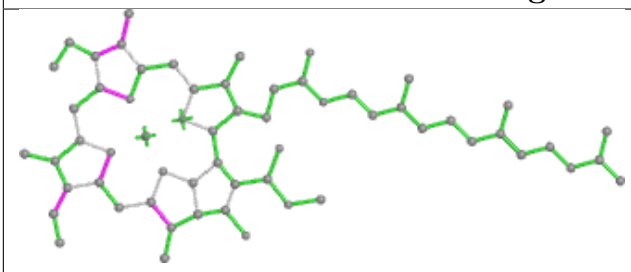
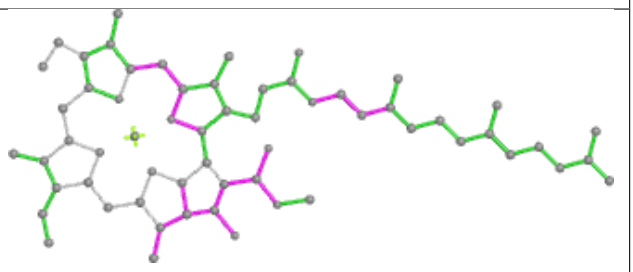
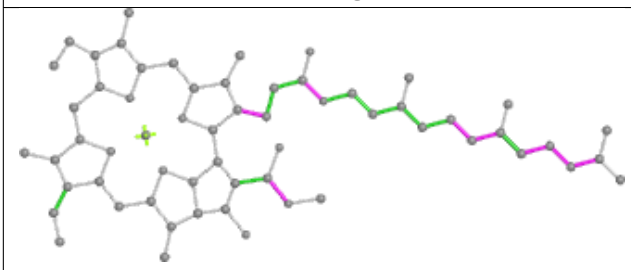
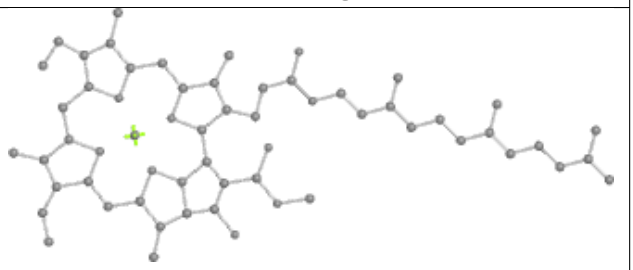


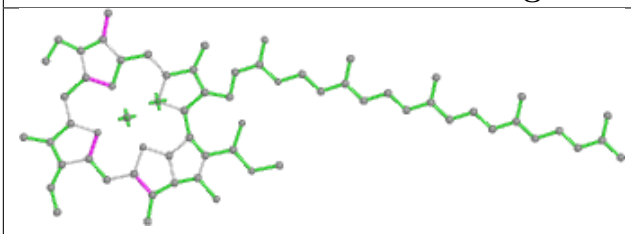
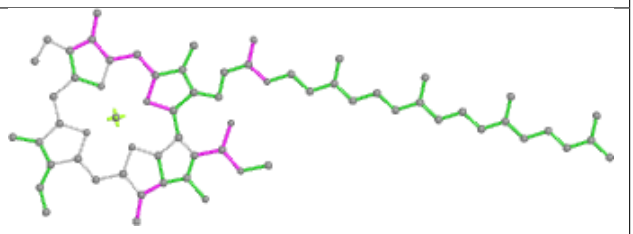
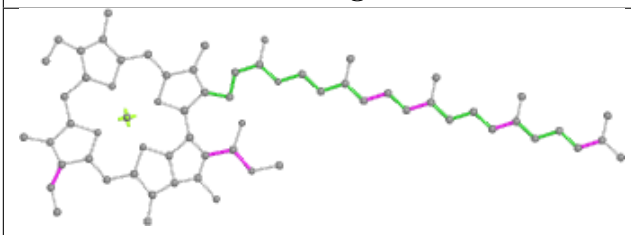
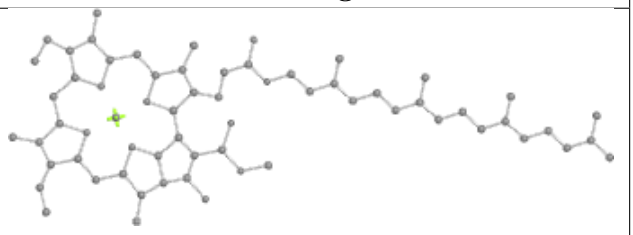
Torsions

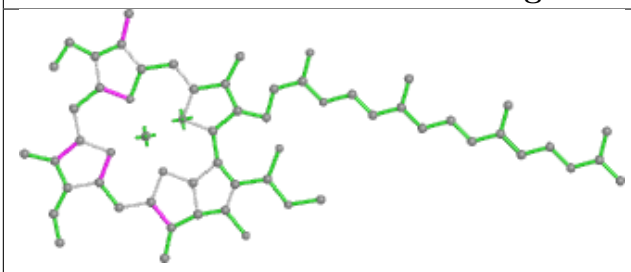
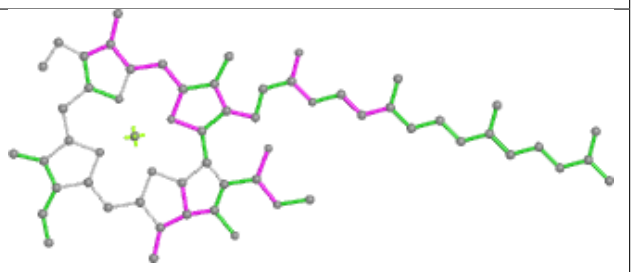
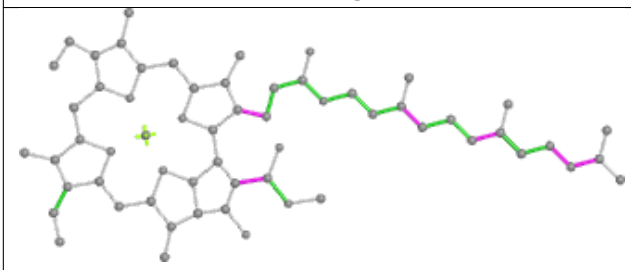
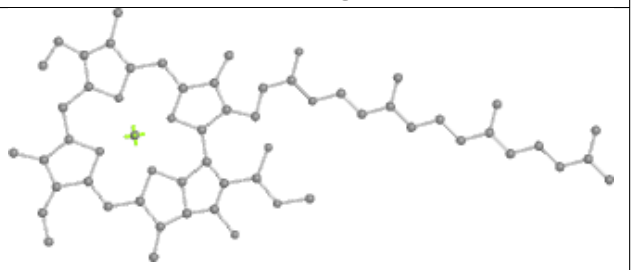


Rings

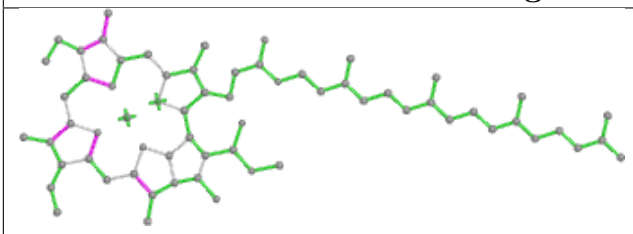
Ligand CLA B 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 4 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

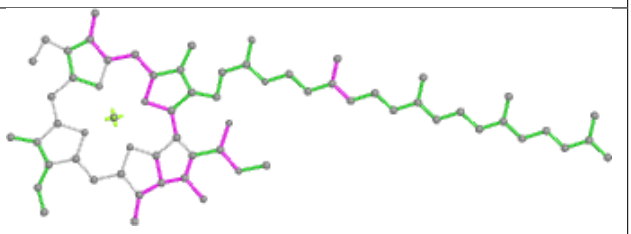
Ligand CLA A 832	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 825	
 Bond lengths	 Bond angles
 Torsions	 Rings

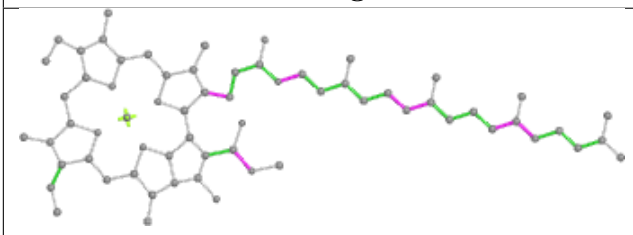
Ligand CLA B 835



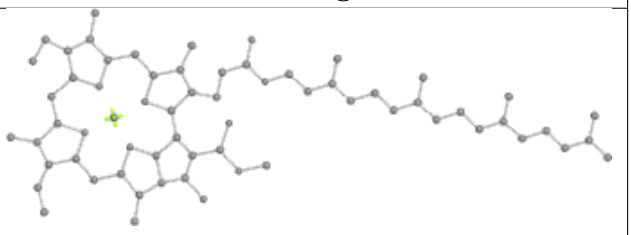
Bond lengths



Bond angles

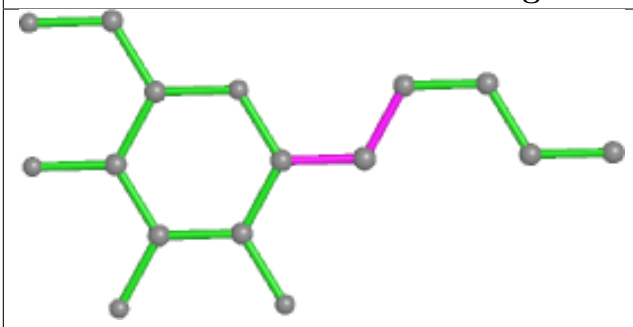


Torsions

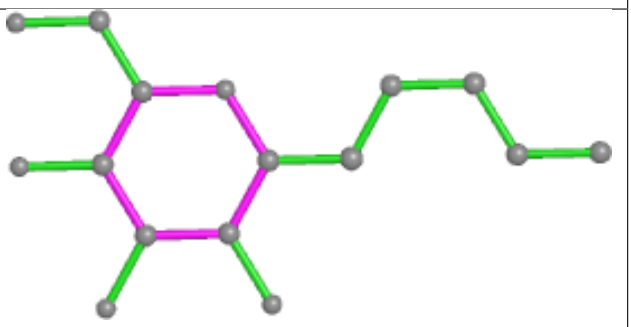


Rings

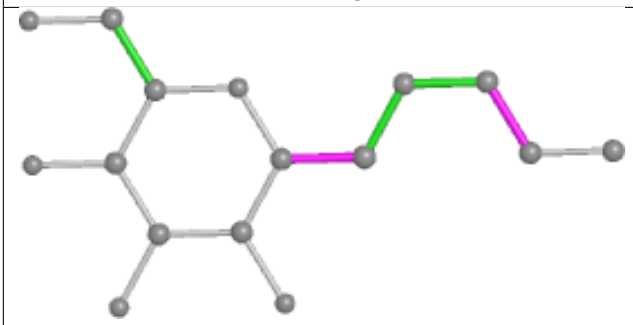
Ligand HTG F 310



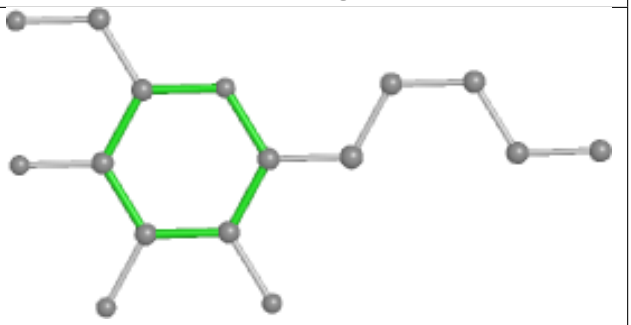
Bond lengths



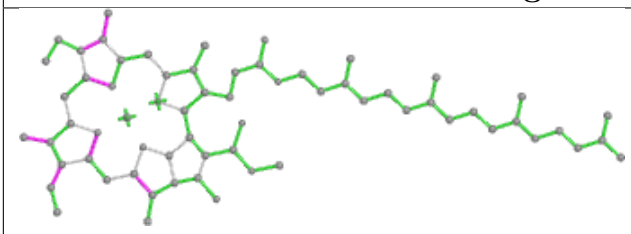
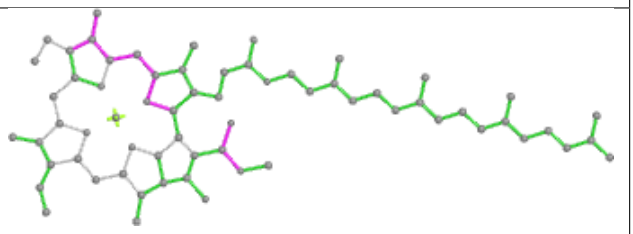
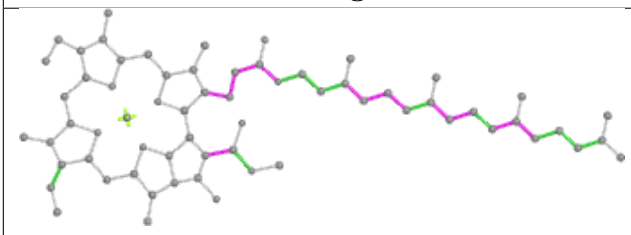
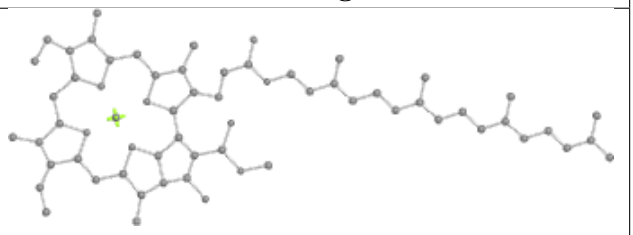
Bond angles

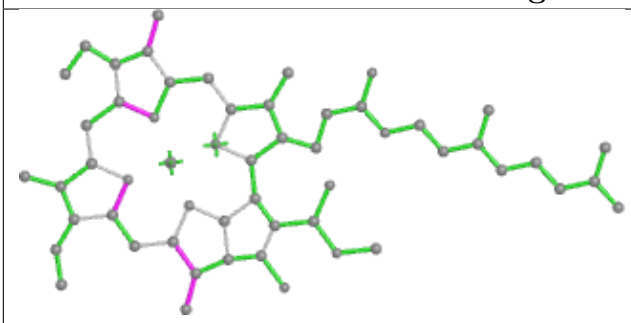
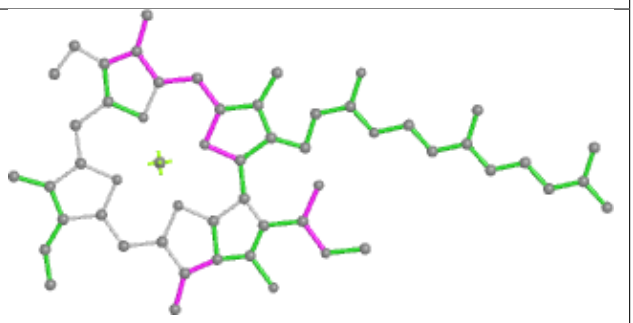
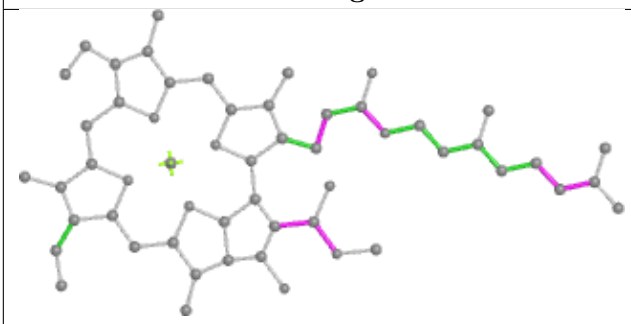
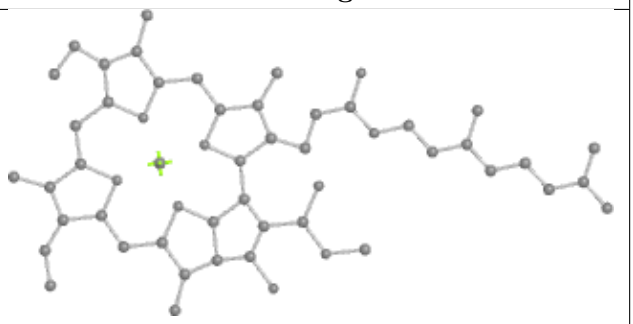


Torsions

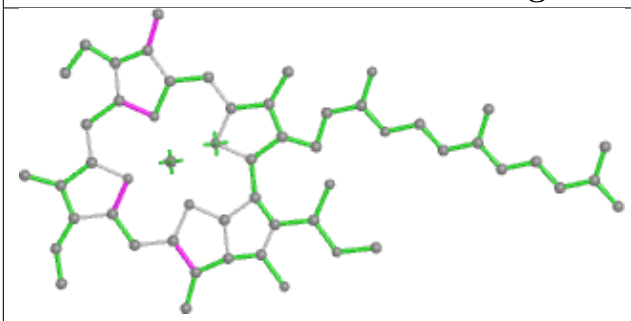


Rings

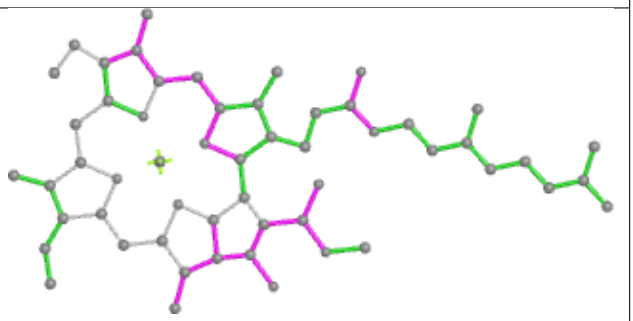
Ligand CLA A 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA 3 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

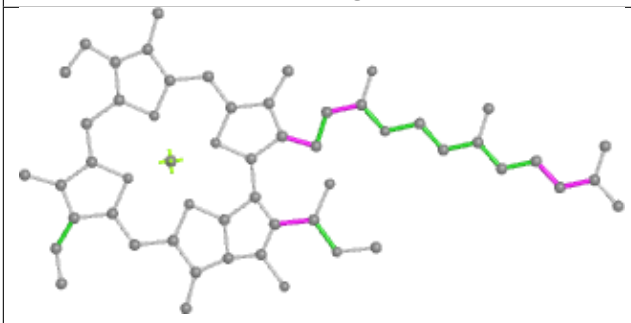
Ligand CLA 1 312



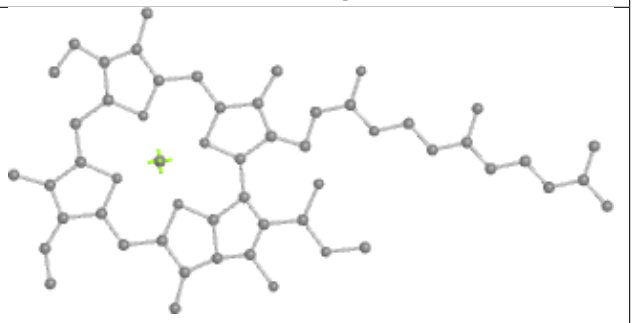
Bond lengths



Bond angles

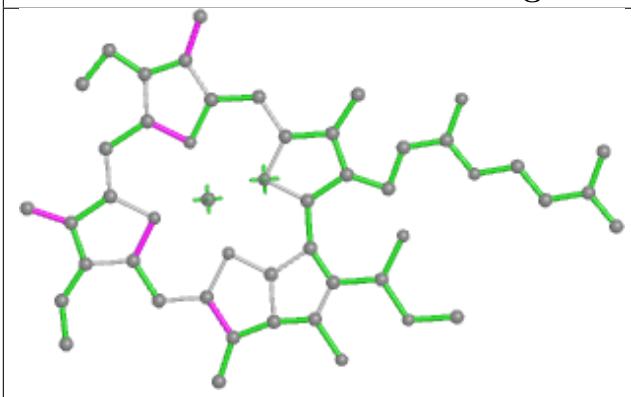


Torsions

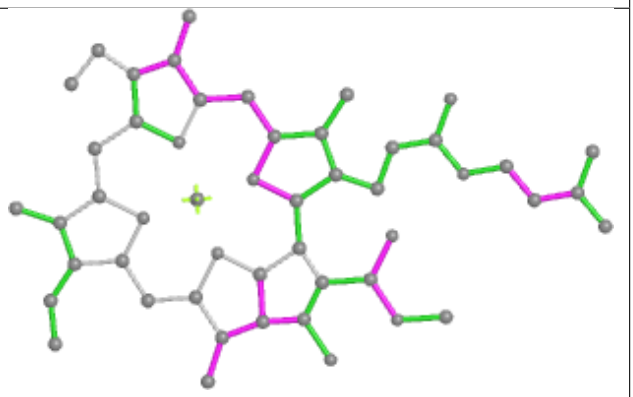


Rings

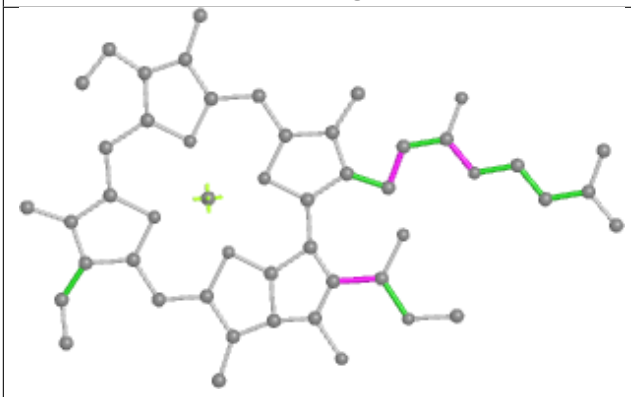
Ligand CLA A 830



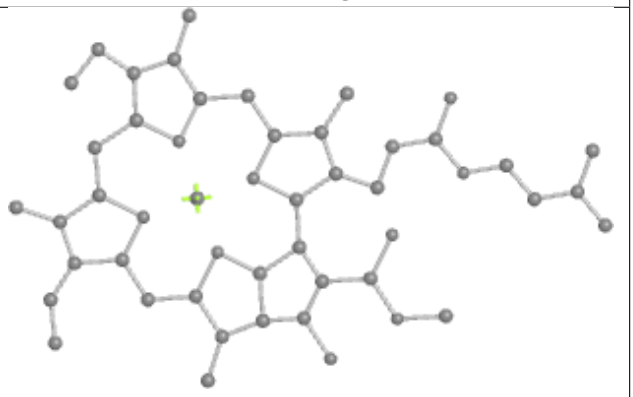
Bond lengths



Bond angles

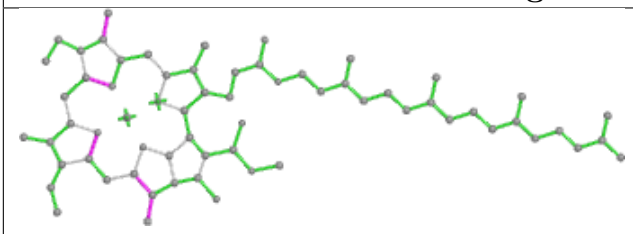


Torsions

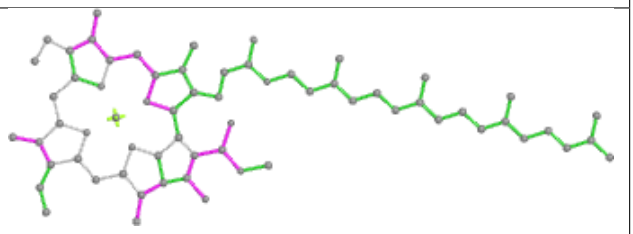


Rings

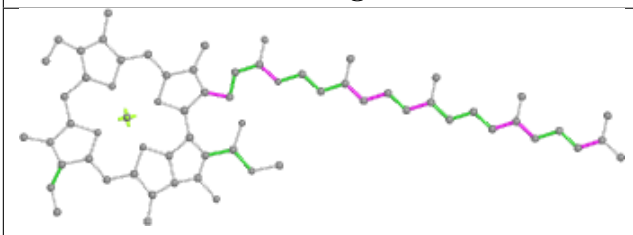
Ligand CLA L 202



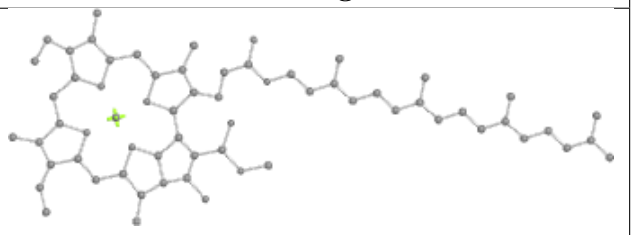
Bond lengths



Bond angles

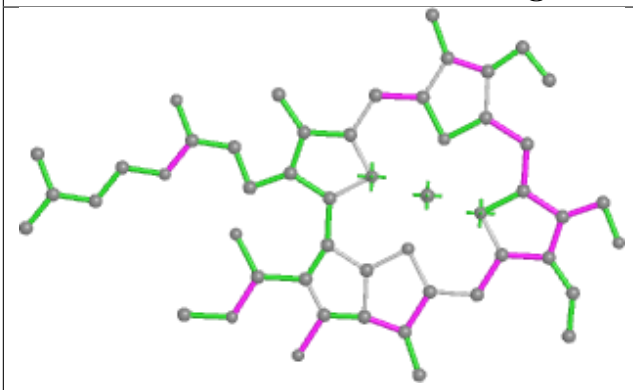


Torsions

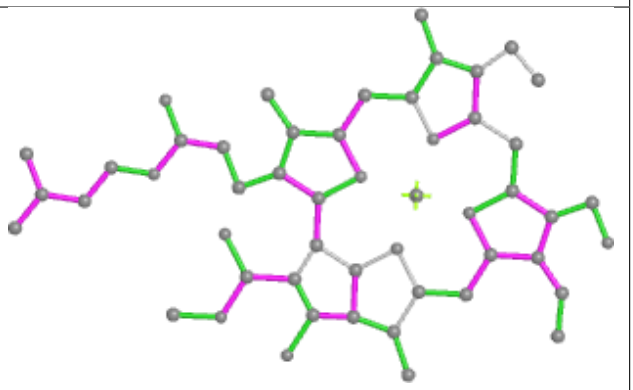


Rings

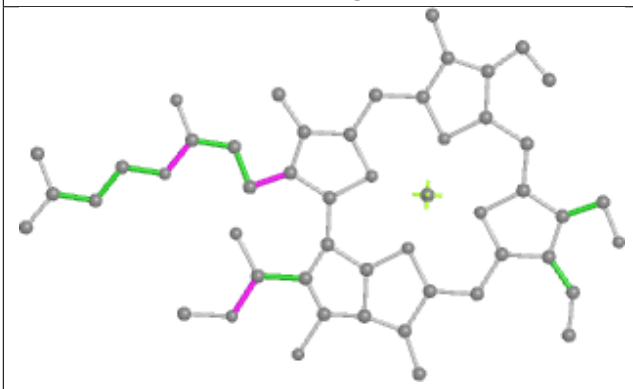
Ligand CHL 2 306



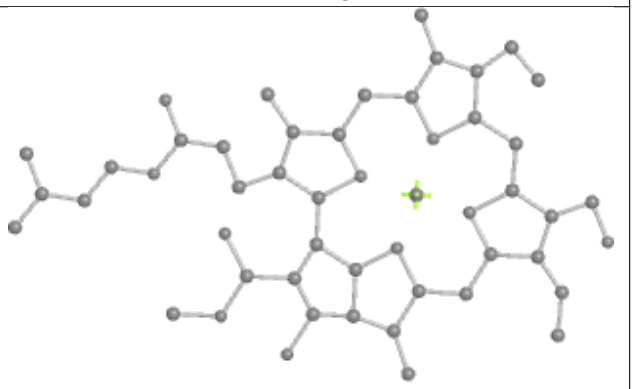
Bond lengths



Bond angles

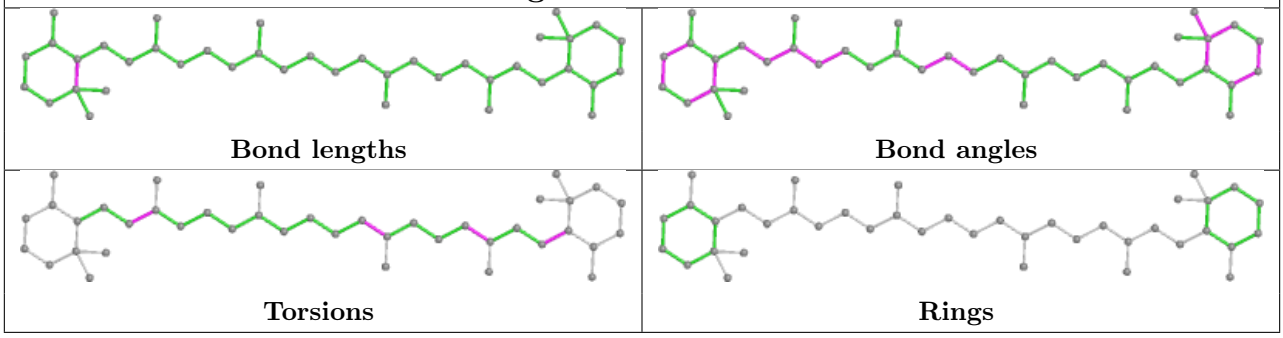


Torsions

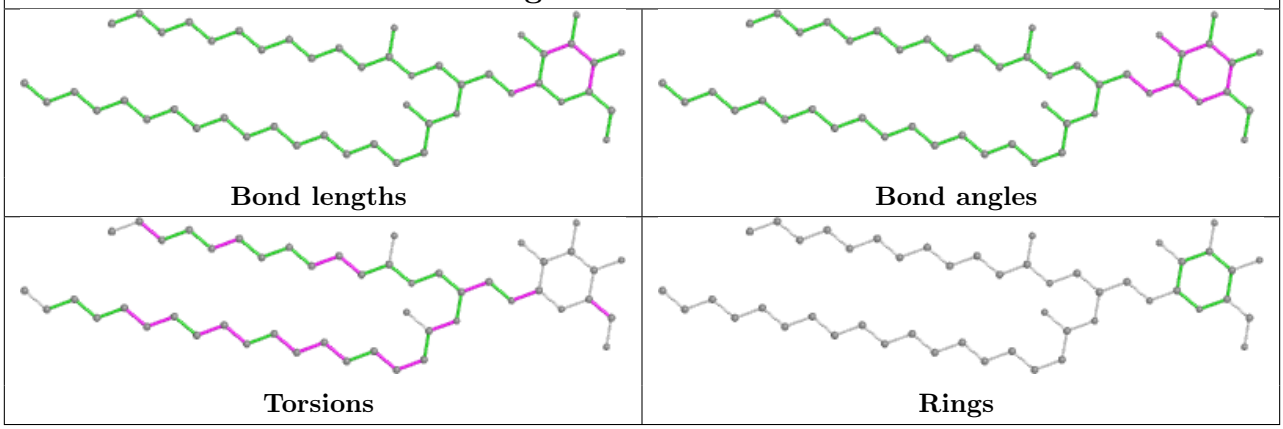


Rings

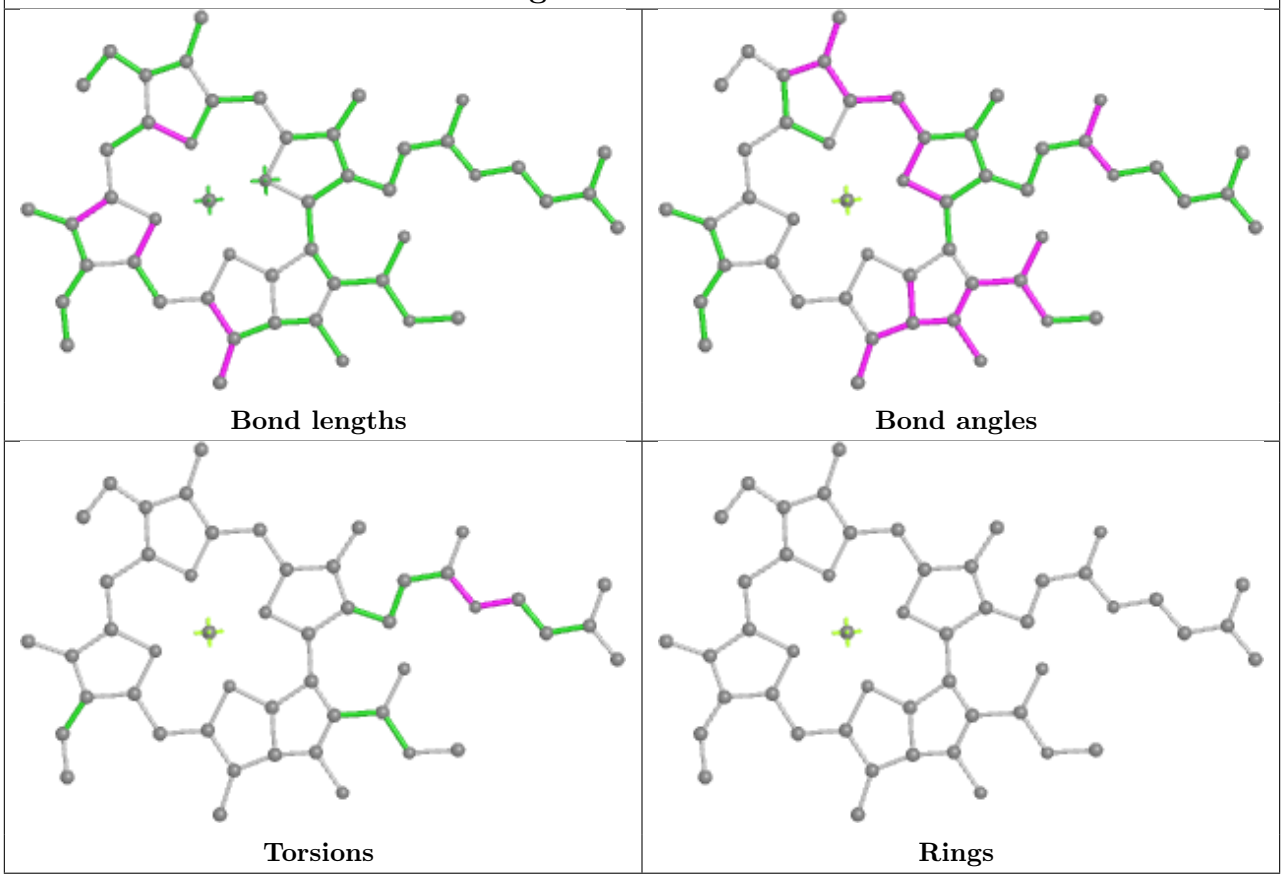
Ligand BCR 4 318

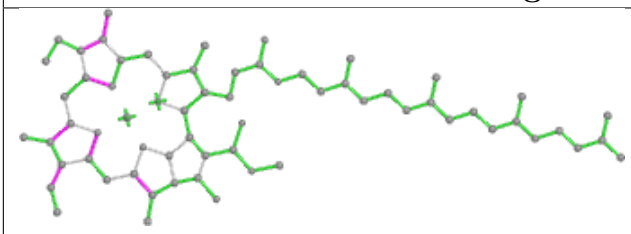
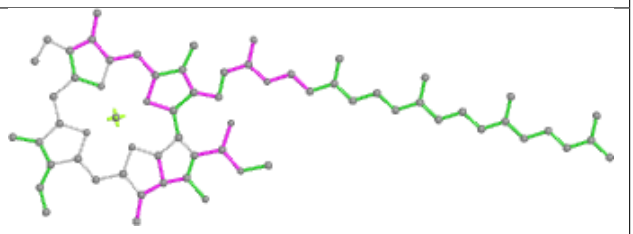
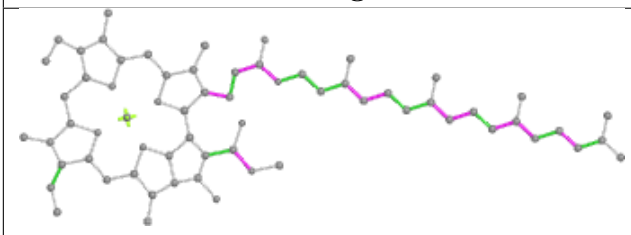
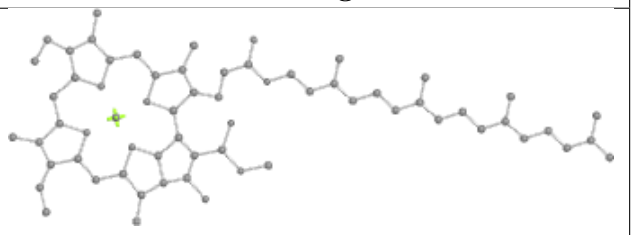


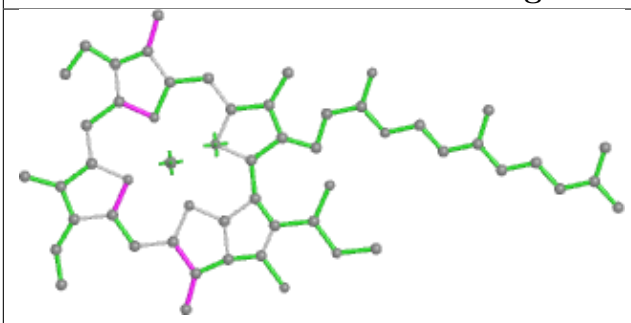
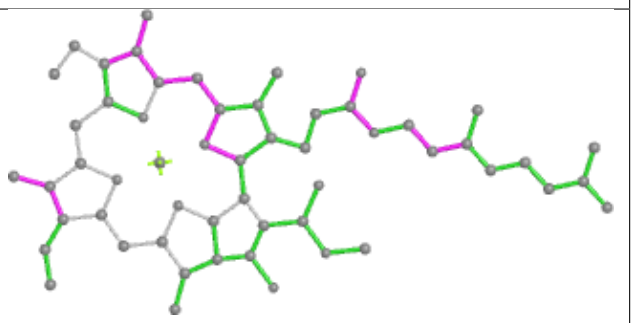
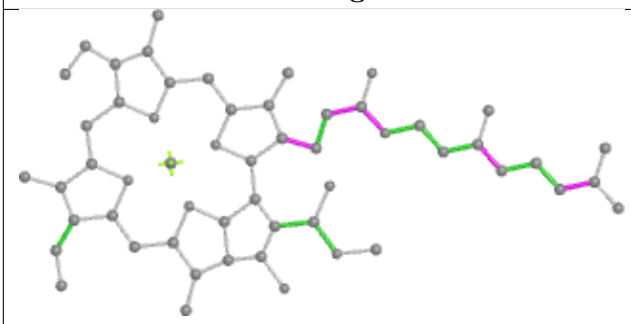
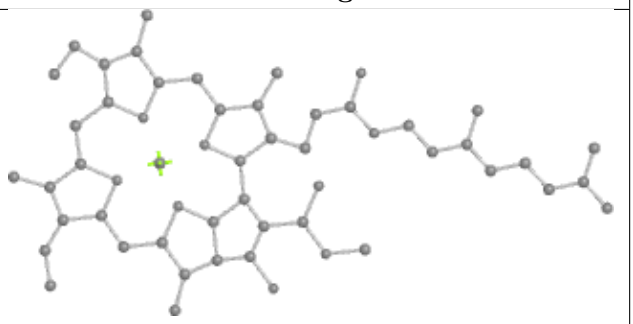
Ligand LMG 4 320



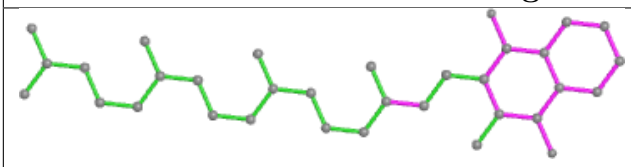
Ligand CLA 4 308



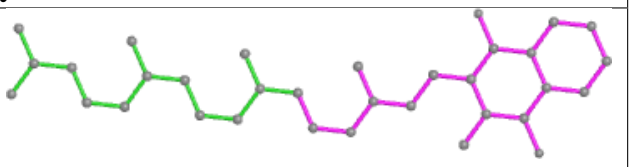
Ligand CLA A 805	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

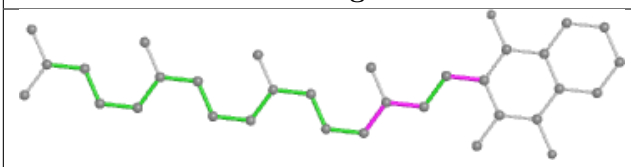
Ligand PQN B 843



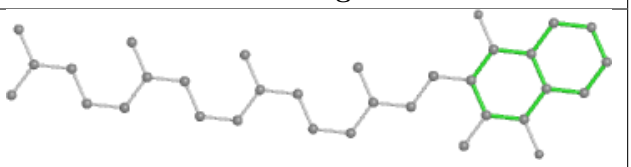
Bond lengths



Bond angles

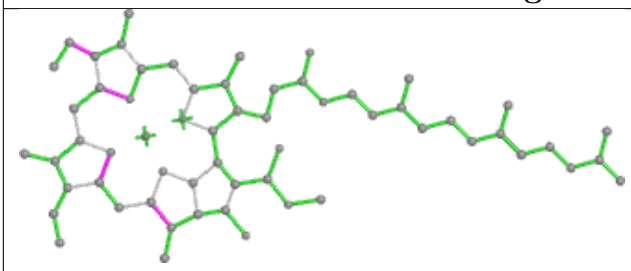


Torsions

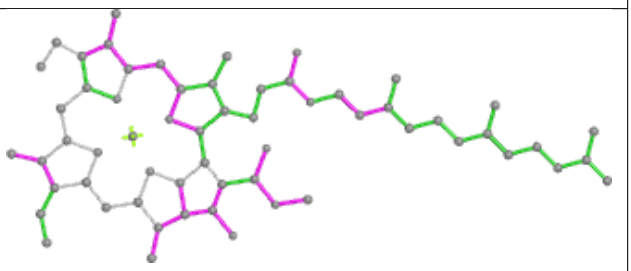


Rings

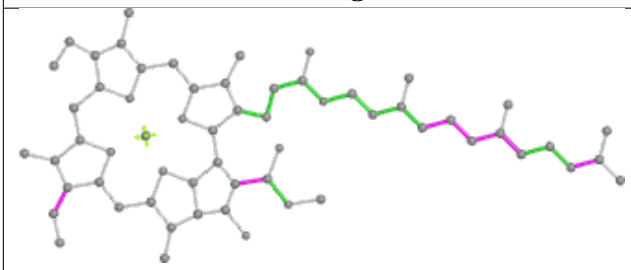
Ligand CLA B 837



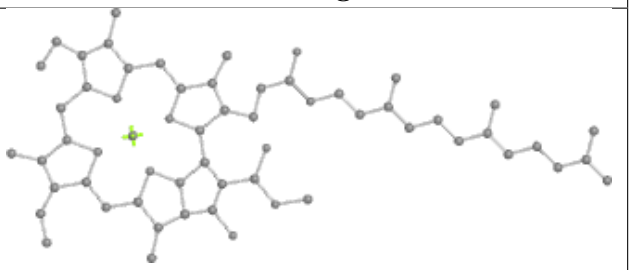
Bond lengths



Bond angles

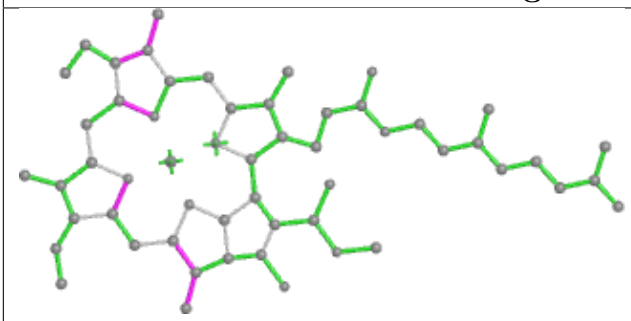


Torsions

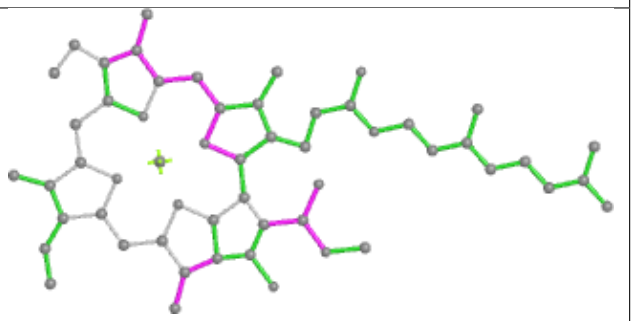


Rings

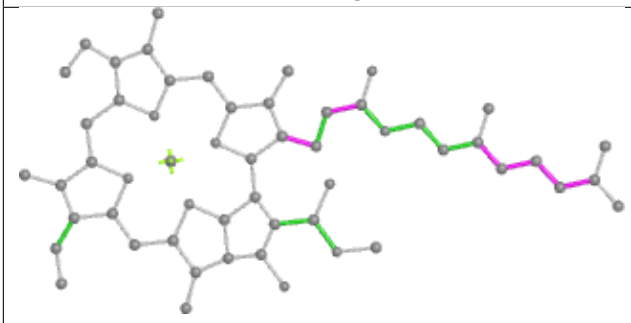
Ligand CLA A 803



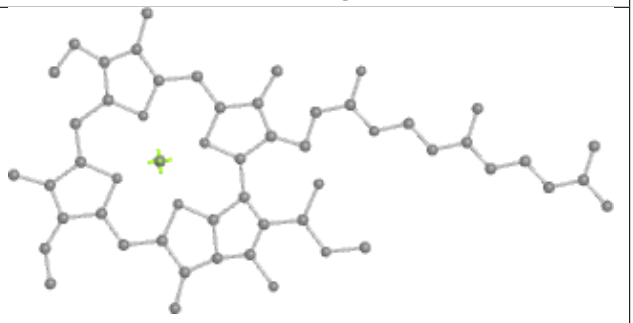
Bond lengths



Bond angles

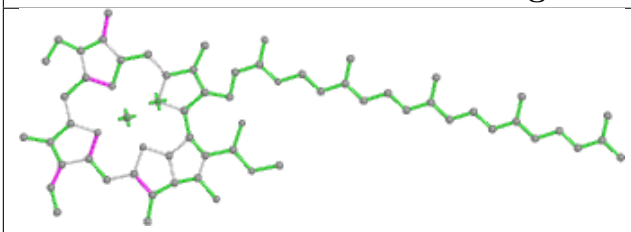


Torsions

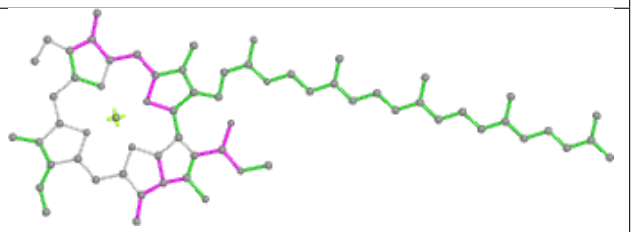


Rings

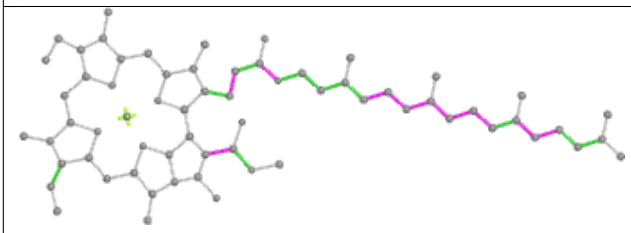
Ligand CLA 2 311



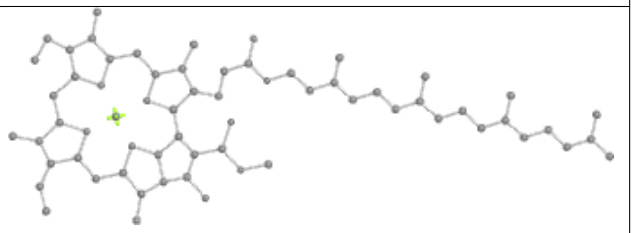
Bond lengths



Bond angles

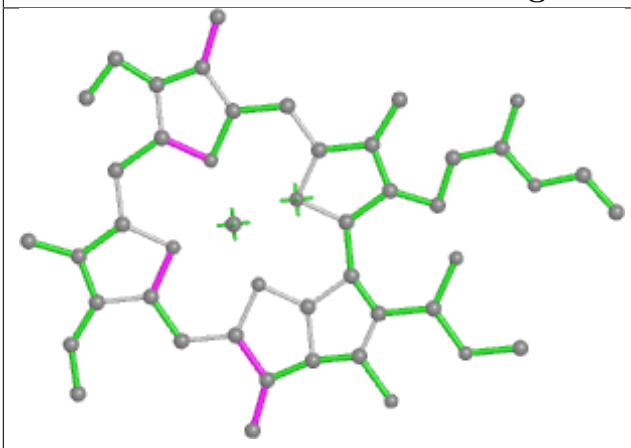


Torsions

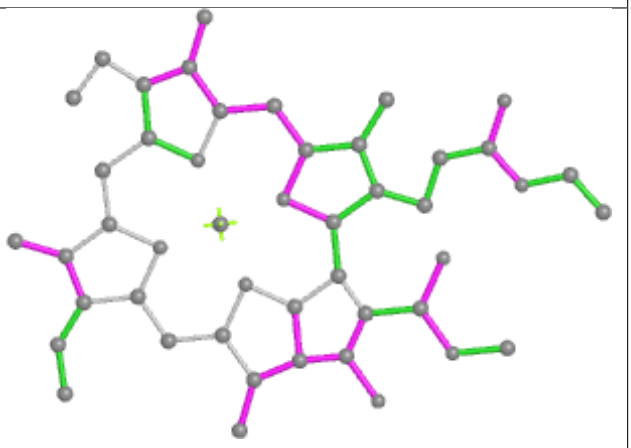


Rings

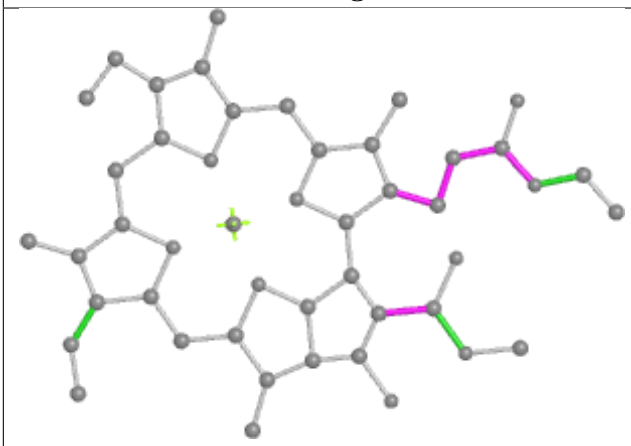
Ligand CLA 3 606



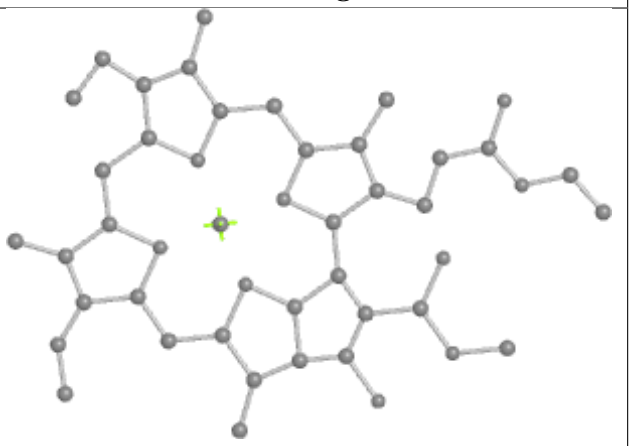
Bond lengths



Bond angles

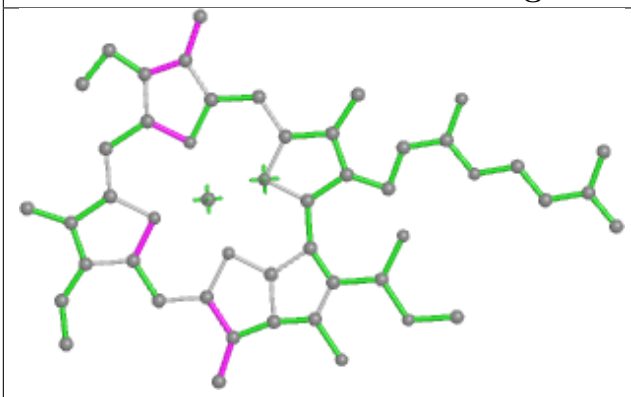


Torsions

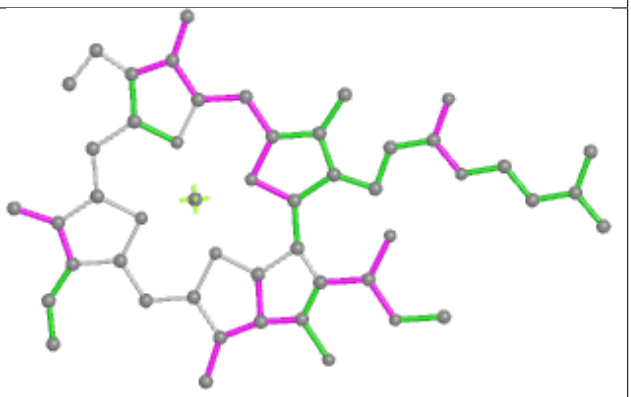


Rings

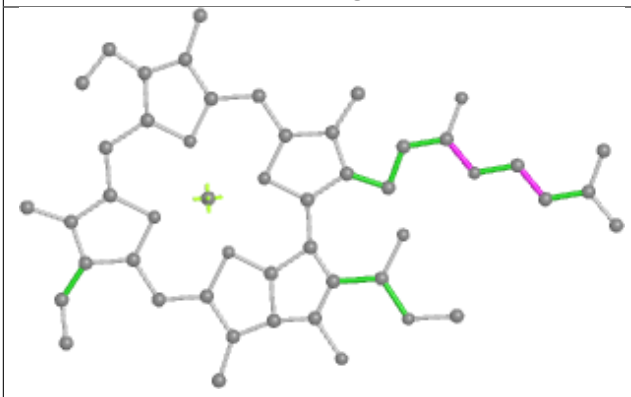
Ligand CLA B 832



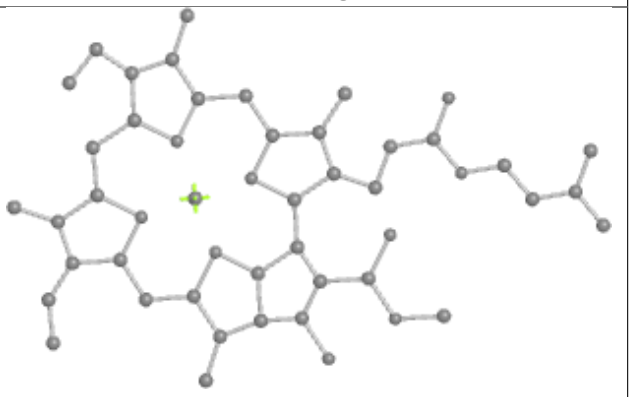
Bond lengths



Bond angles

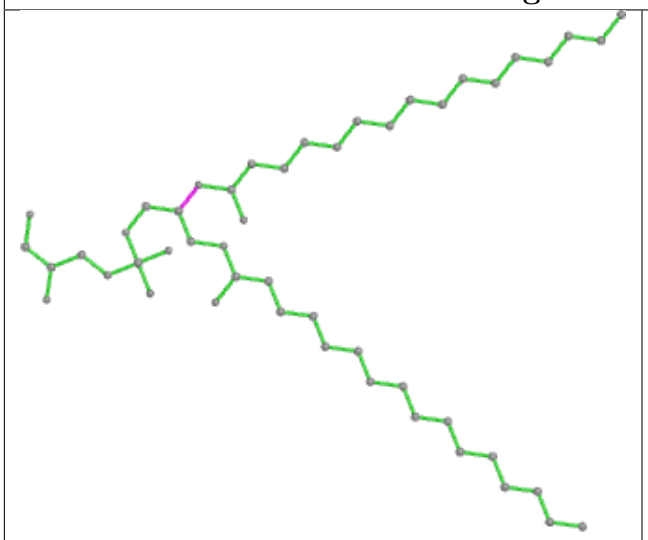


Torsions

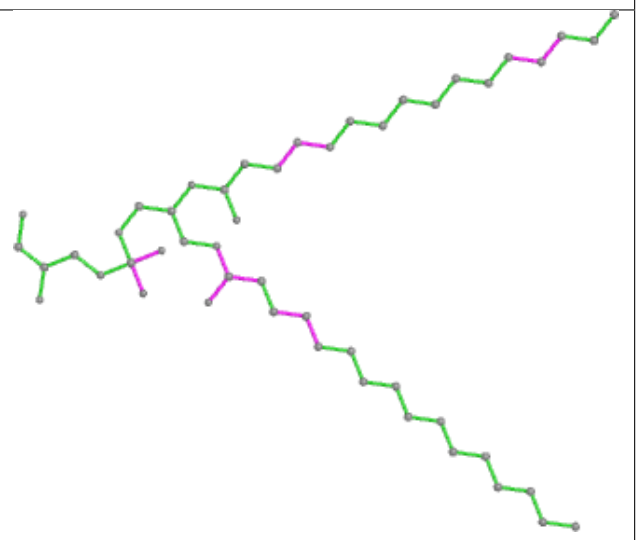


Rings

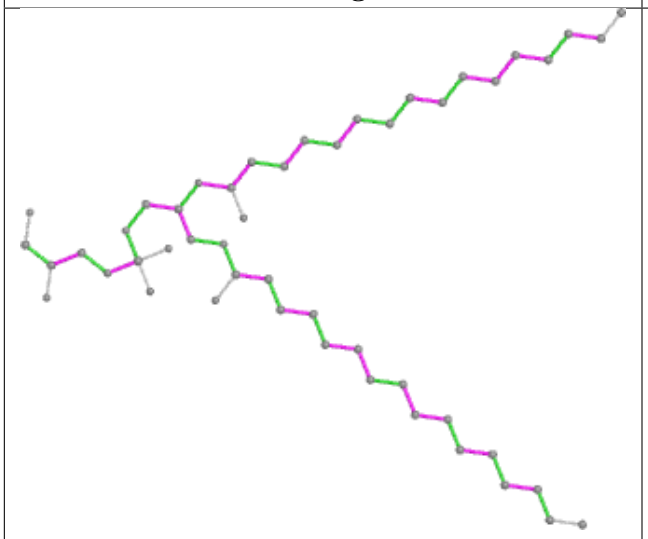
Ligand LHG A 844



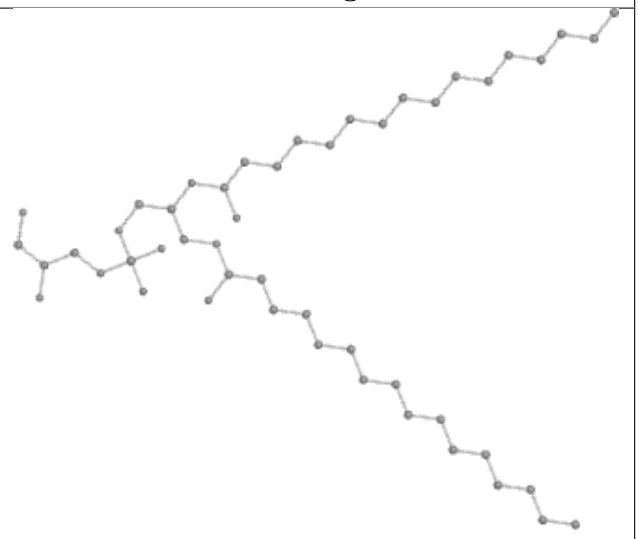
Bond lengths



Bond angles

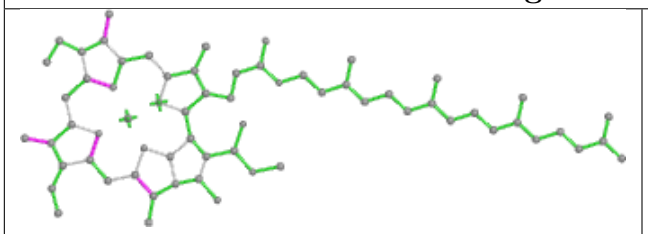


Torsions

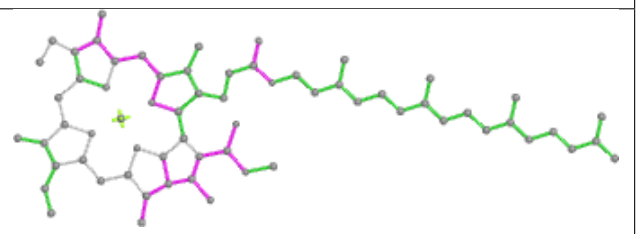


Rings

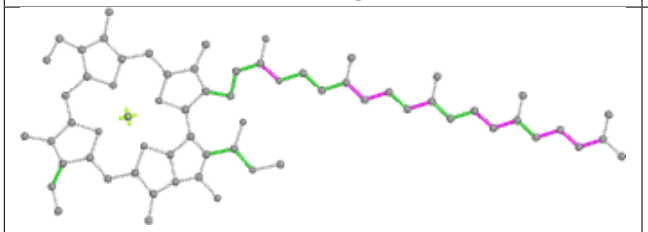
Ligand CLA A 836



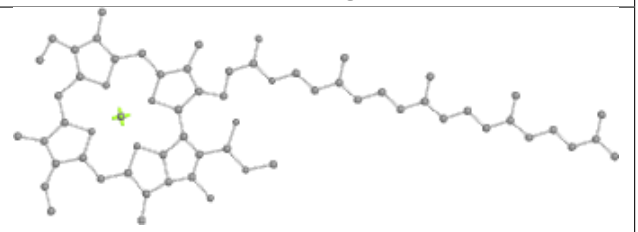
Bond lengths



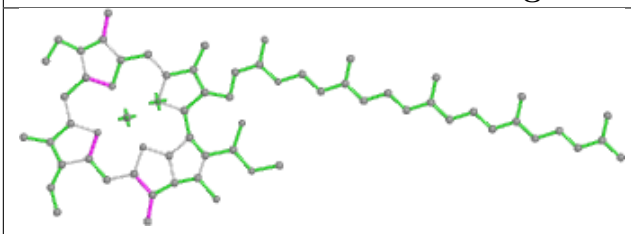
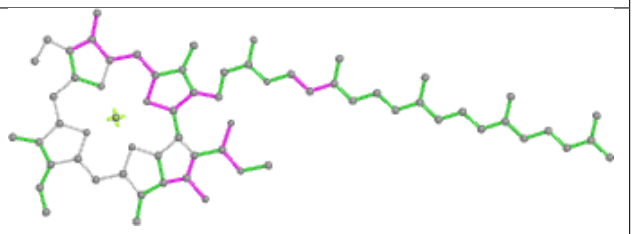
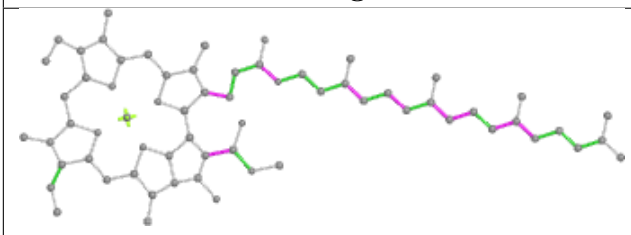
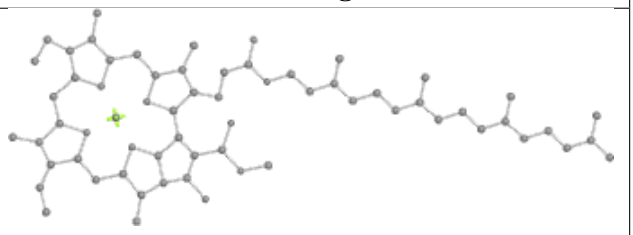
Bond angles

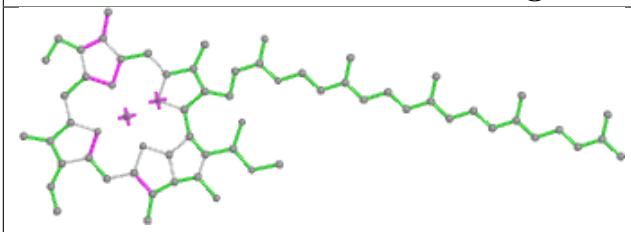
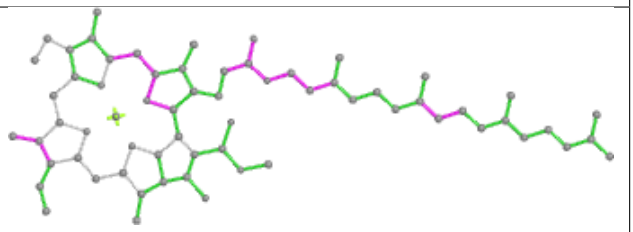
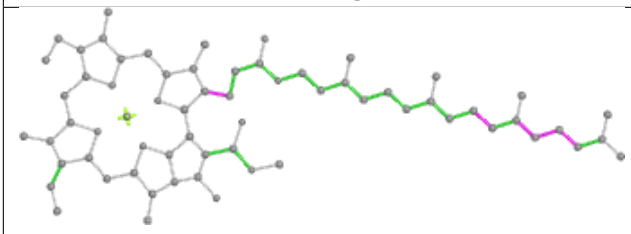
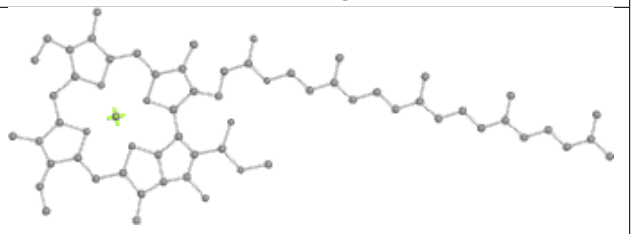


Torsions

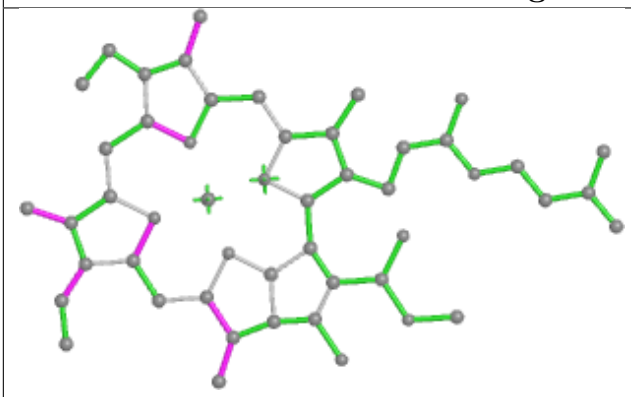


Rings

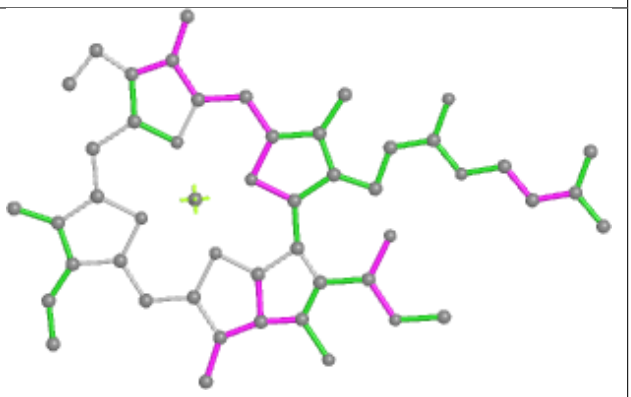
Ligand CLA A 818	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA F 304	
 Bond lengths	 Bond angles
 Torsions	 Rings

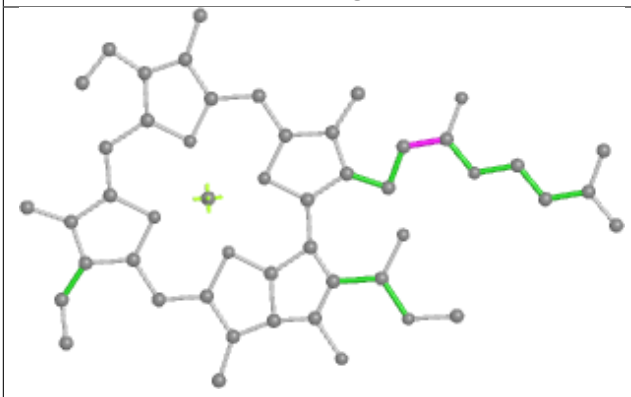
Ligand CLA 3 603



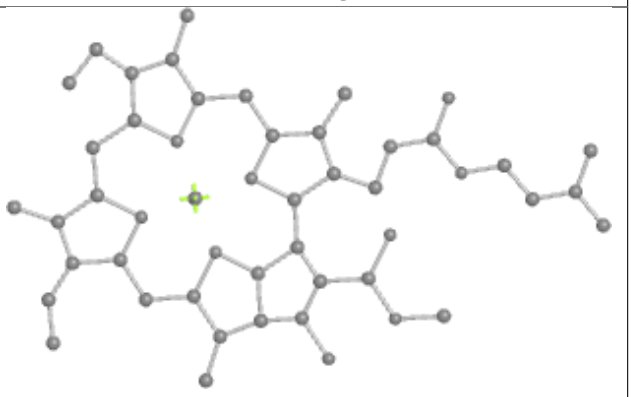
Bond lengths



Bond angles

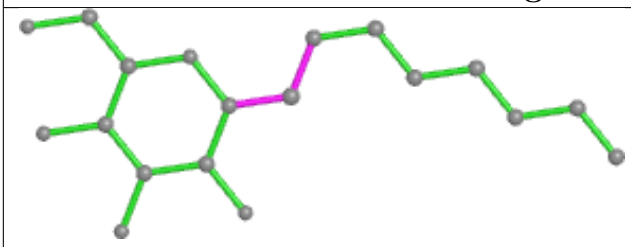


Torsions

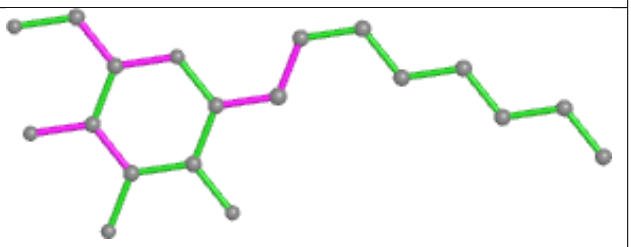


Rings

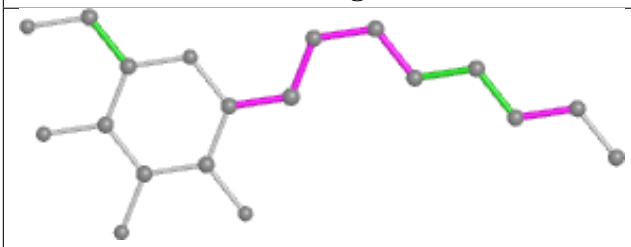
Ligand HTG J 102



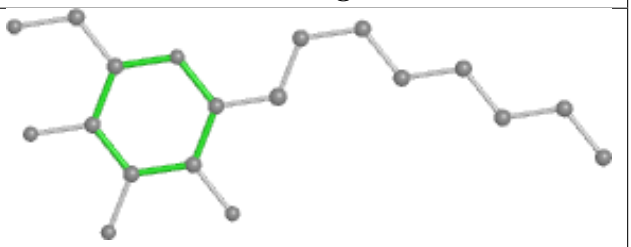
Bond lengths



Bond angles

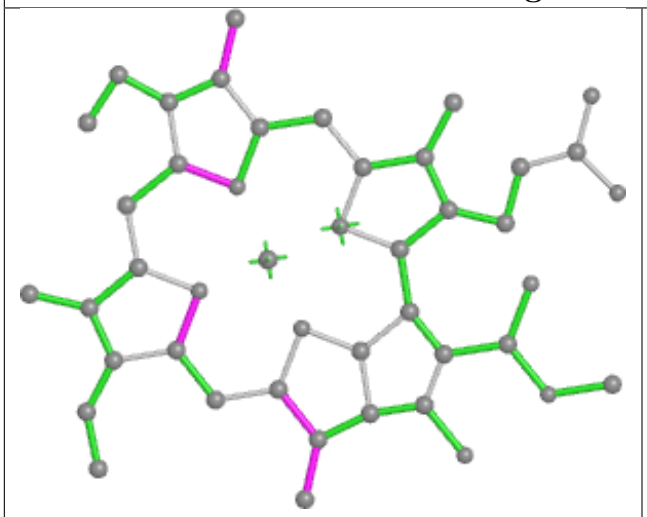


Torsions

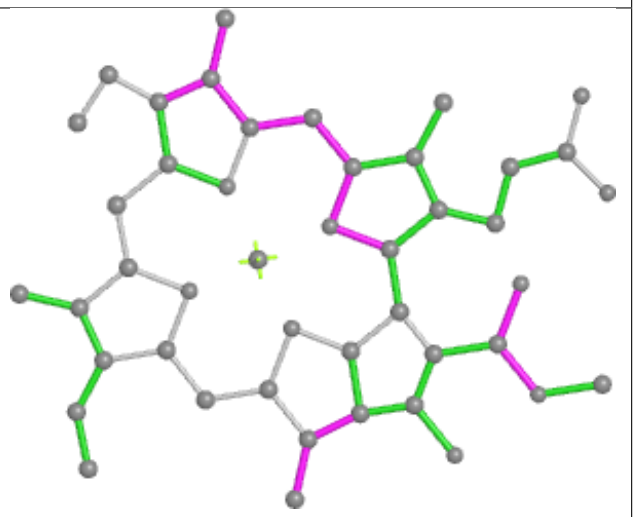


Rings

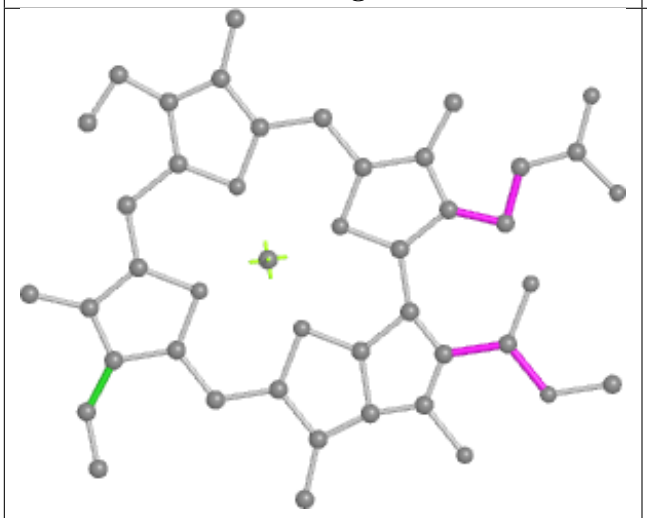
Ligand CLA A 834



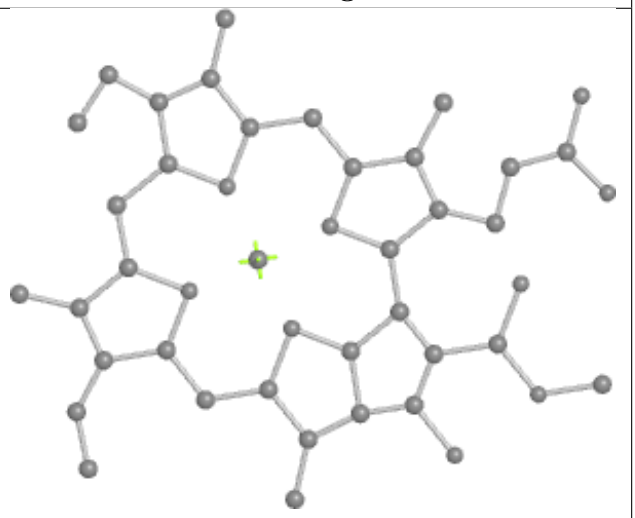
Bond lengths



Bond angles

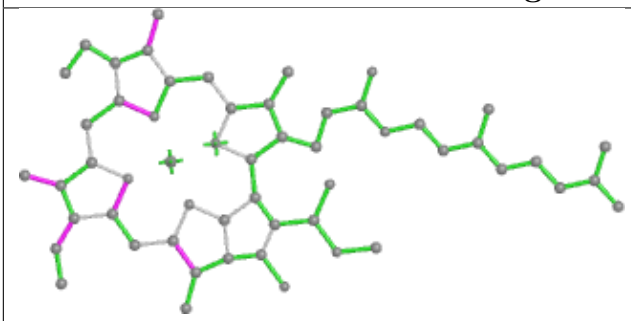


Torsions

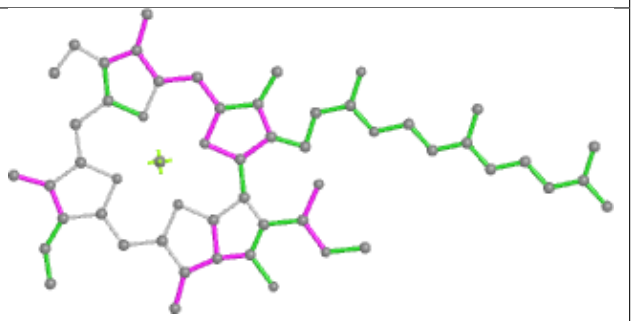


Rings

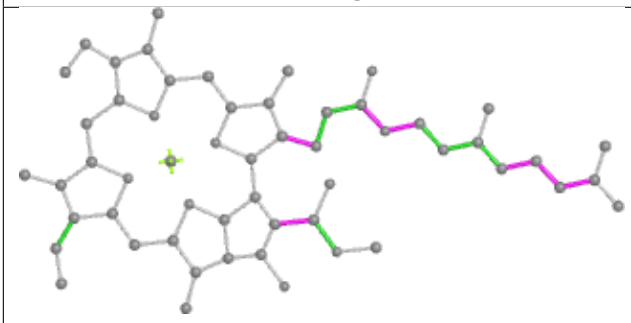
Ligand CLA B 817



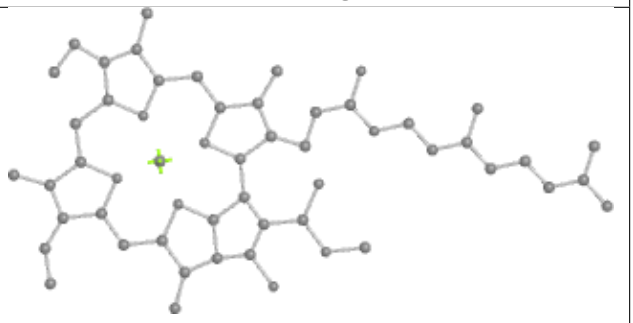
Bond lengths



Bond angles

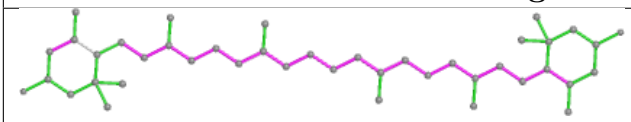


Torsions

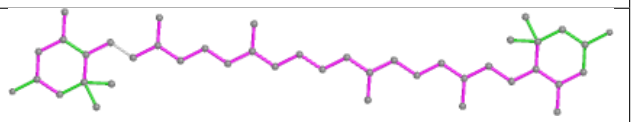


Rings

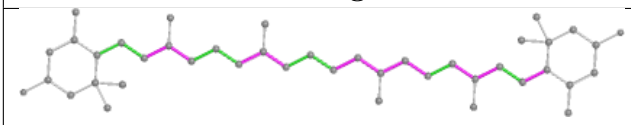
Ligand LUT 2 314



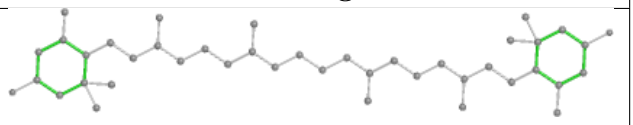
Bond lengths



Bond angles

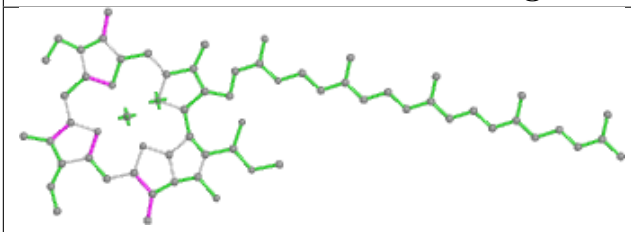


Torsions

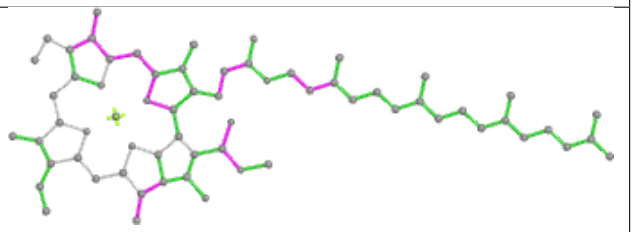


Rings

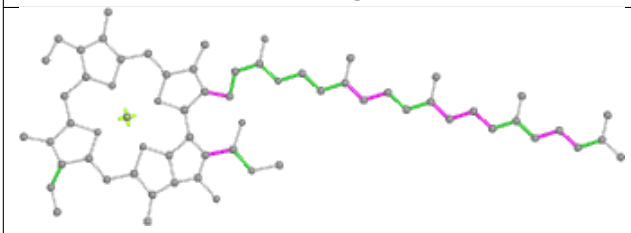
Ligand CLA A 804



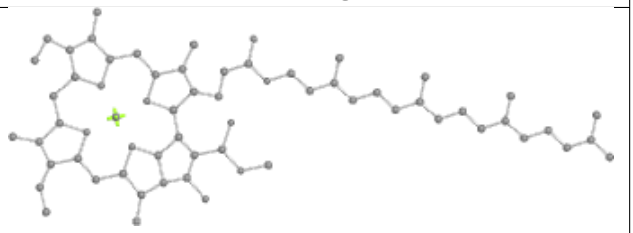
Bond lengths



Bond angles

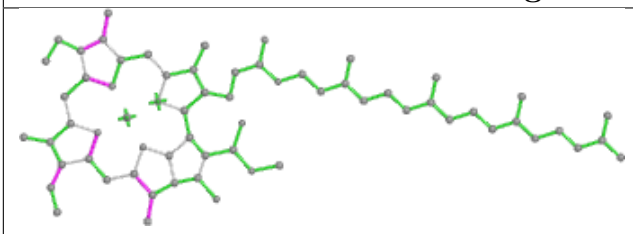


Torsions

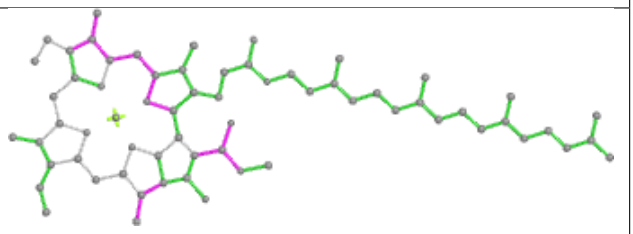


Rings

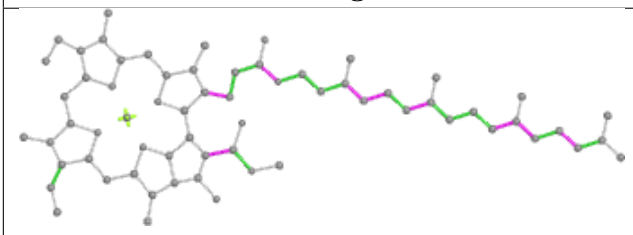
Ligand CLA B 803



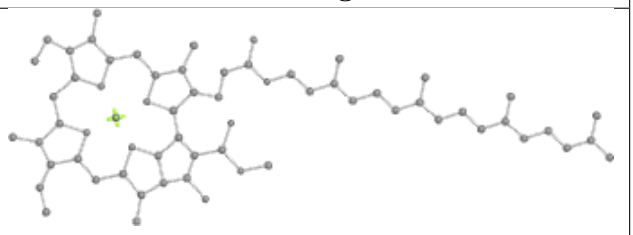
Bond lengths



Bond angles

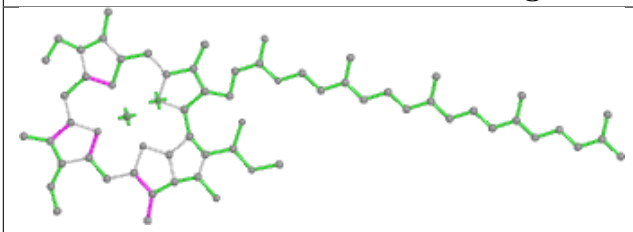


Torsions

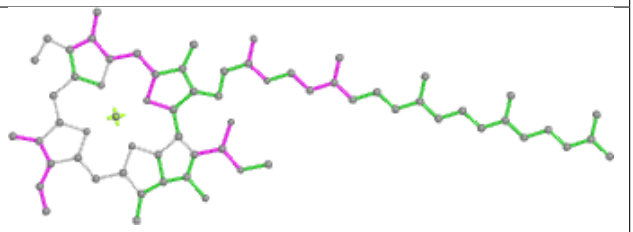


Rings

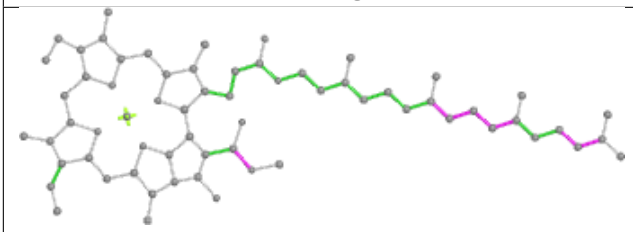
Ligand CLA A 827



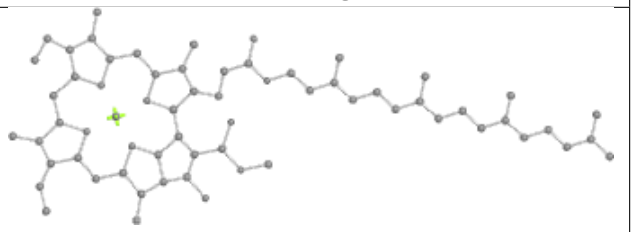
Bond lengths



Bond angles

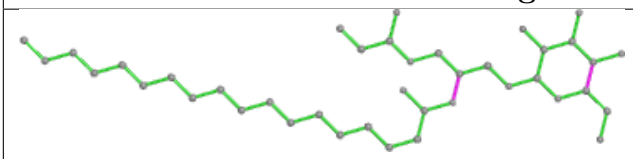


Torsions

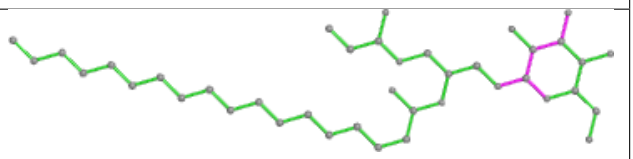


Rings

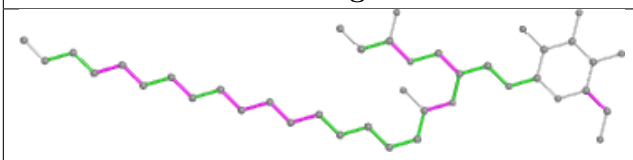
Ligand LMG G 101



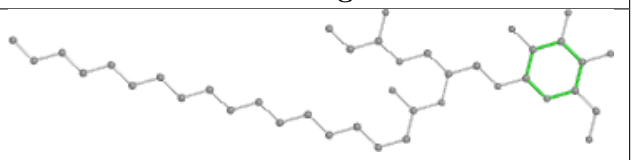
Bond lengths



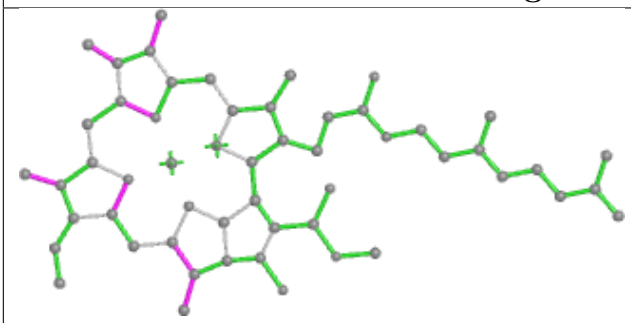
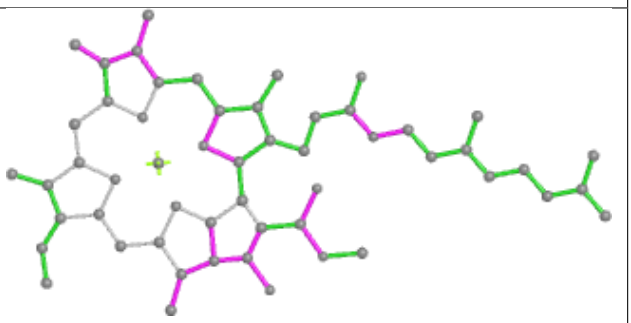
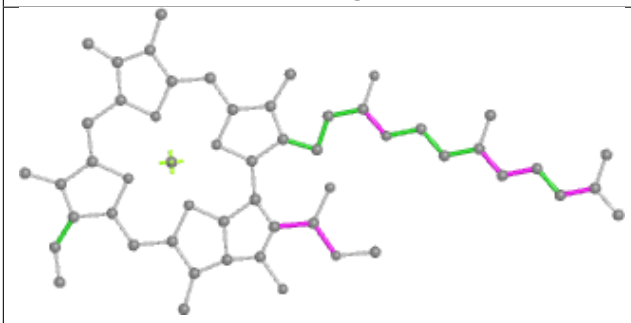
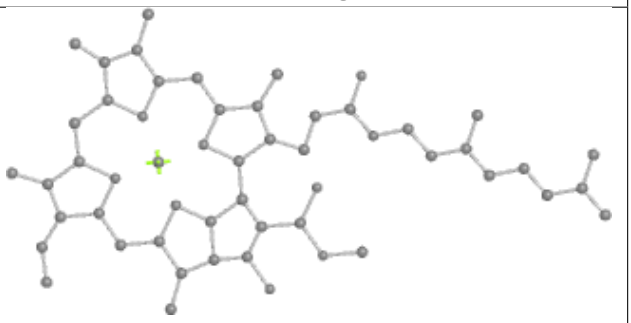
Bond angles



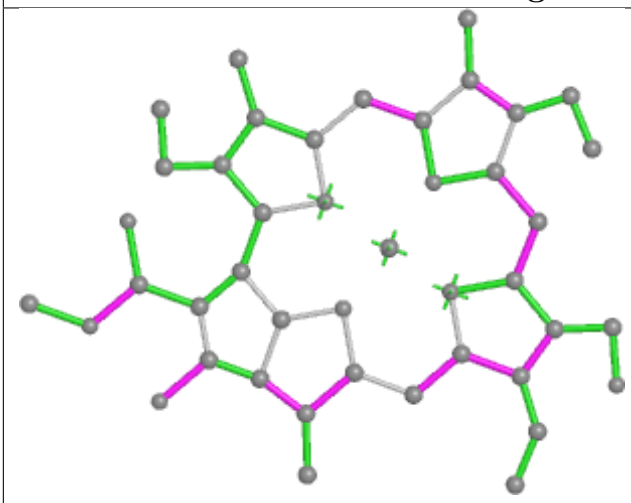
Torsions



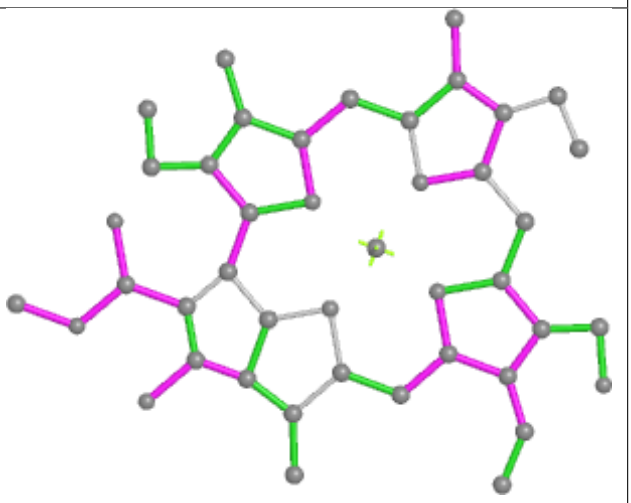
Rings

Ligand CLA B 813	
 Bond lengths	 Bond angles
 Torsions	 Rings

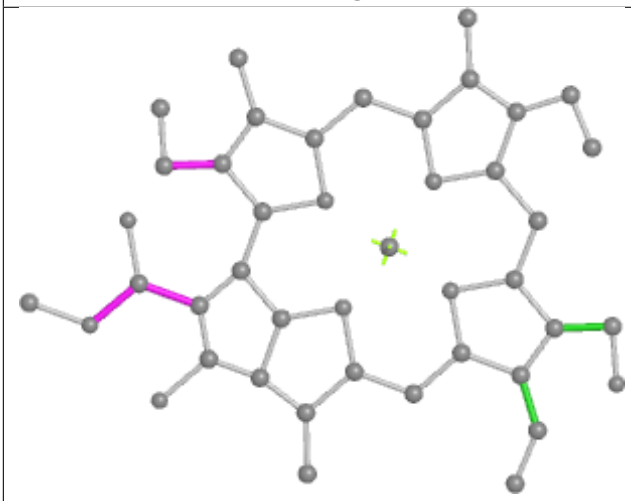
Ligand CHL 2 313



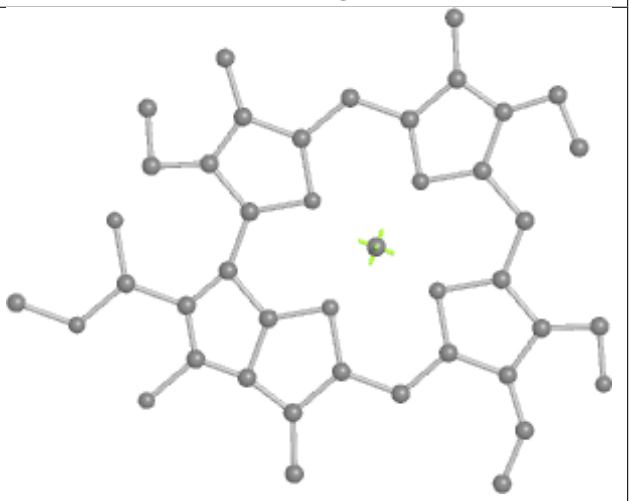
Bond lengths



Bond angles

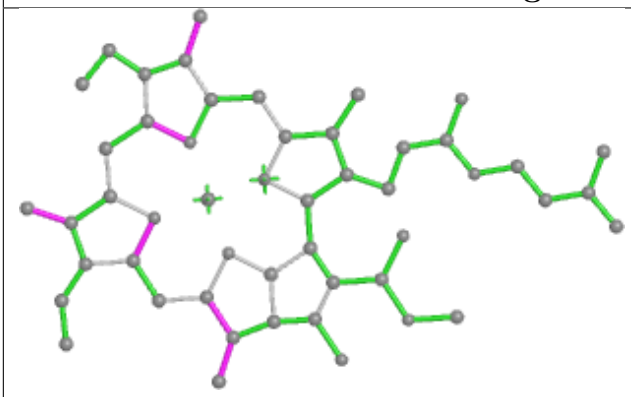


Torsions

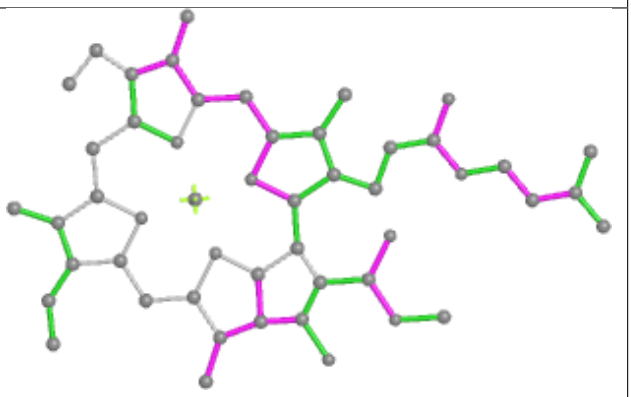


Rings

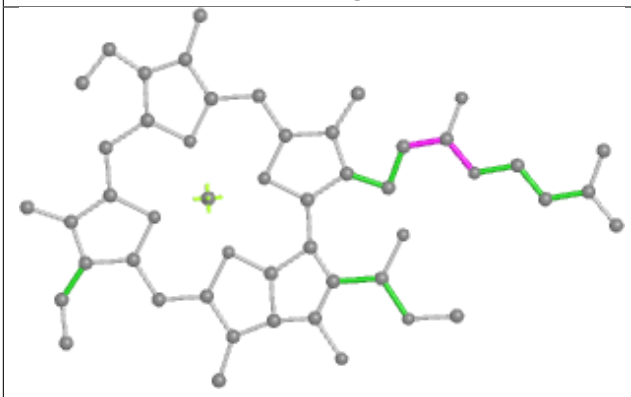
Ligand CLA A 833



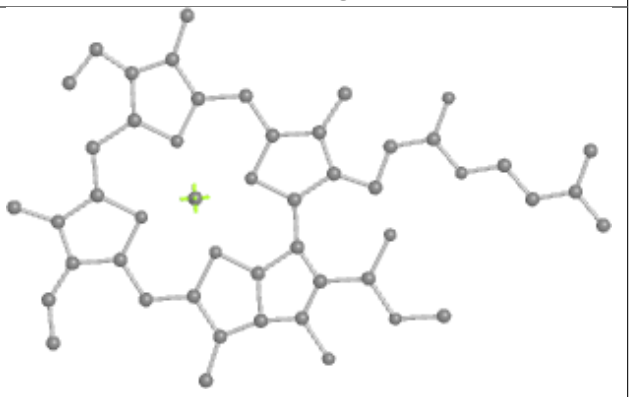
Bond lengths



Bond angles

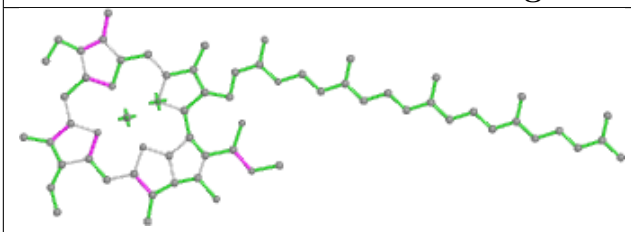


Torsions

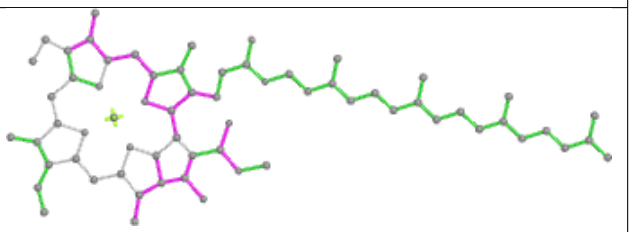


Rings

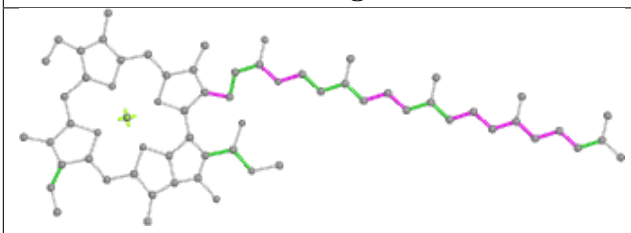
Ligand CLA B 829



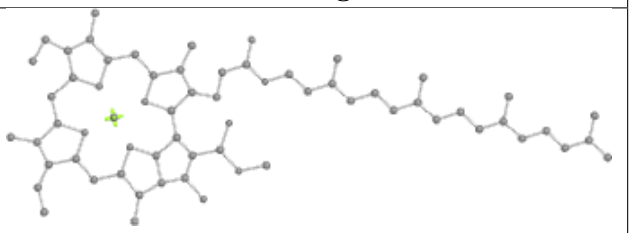
Bond lengths



Bond angles

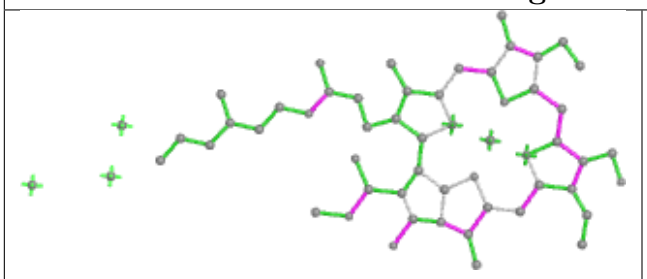


Torsions

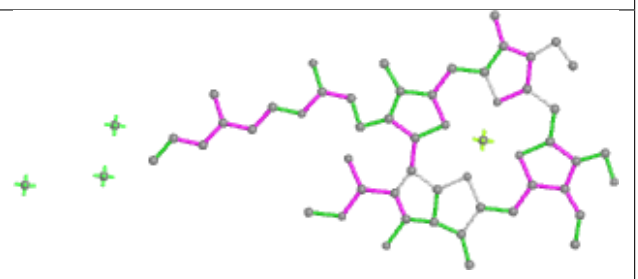


Rings

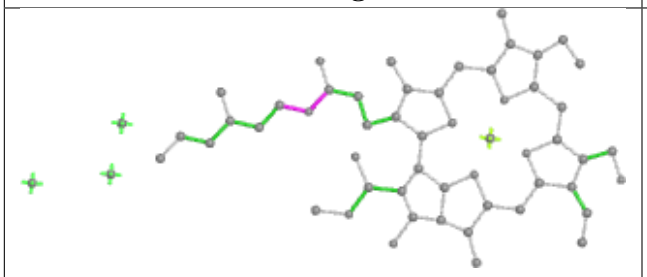
Ligand CHL 3 601



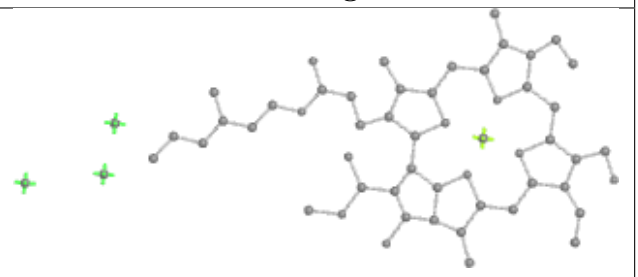
Bond lengths



Bond angles

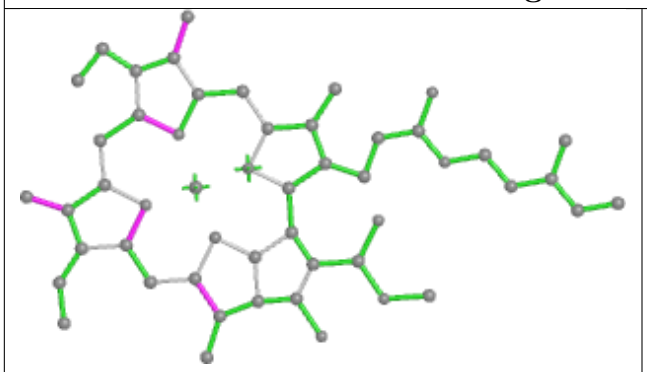


Torsions

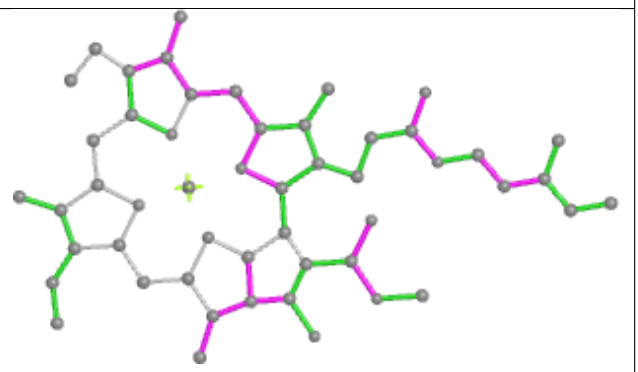


Rings

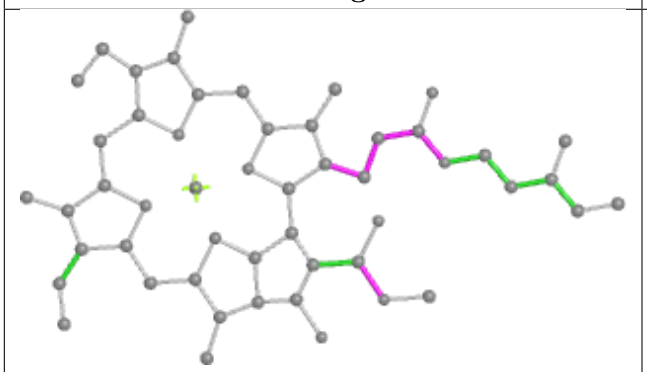
Ligand CLA A 835



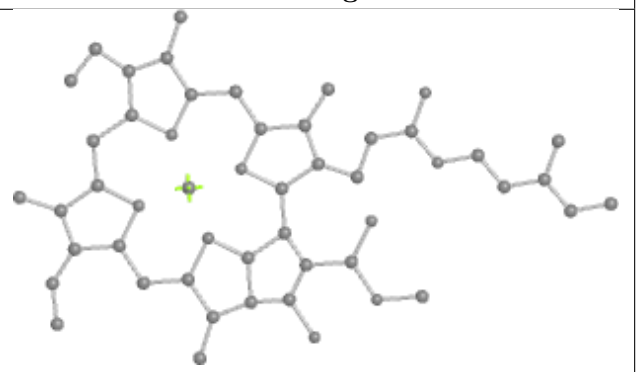
Bond lengths



Bond angles

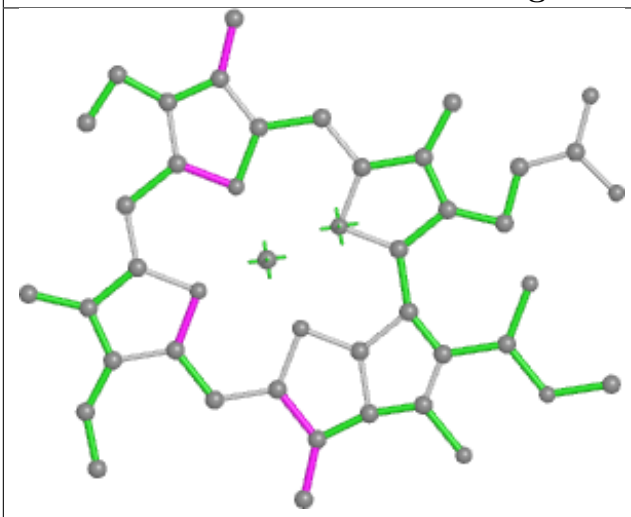


Torsions

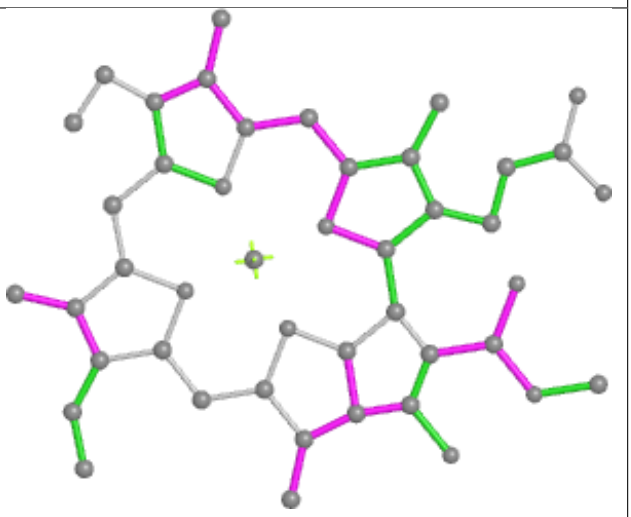


Rings

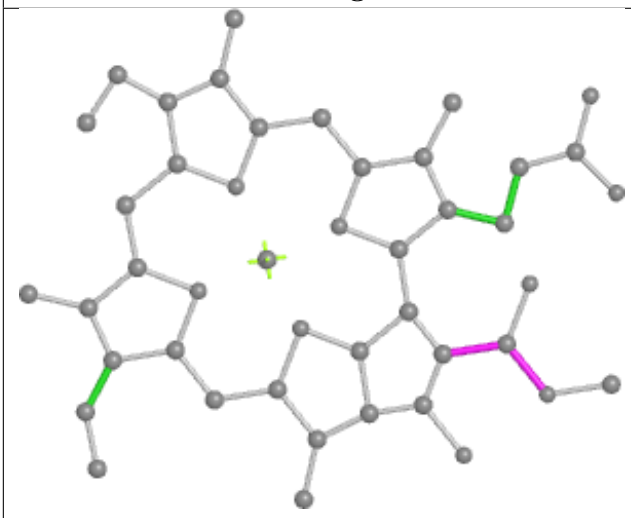
Ligand CLA 3 604



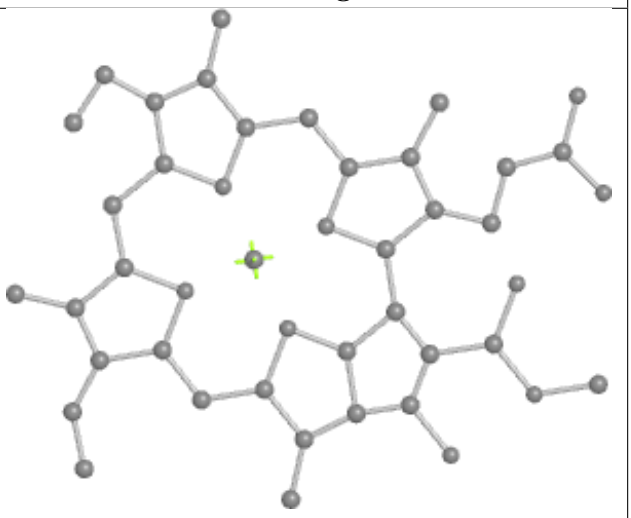
Bond lengths



Bond angles

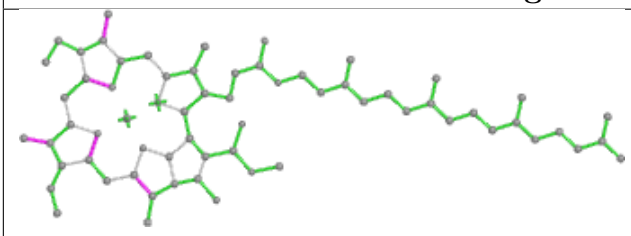


Torsions

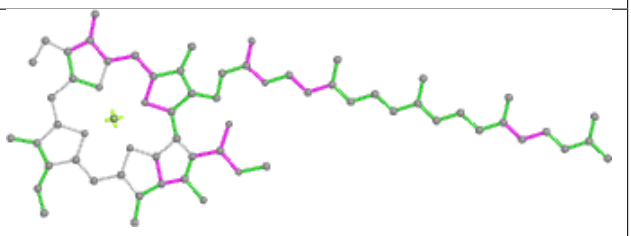


Rings

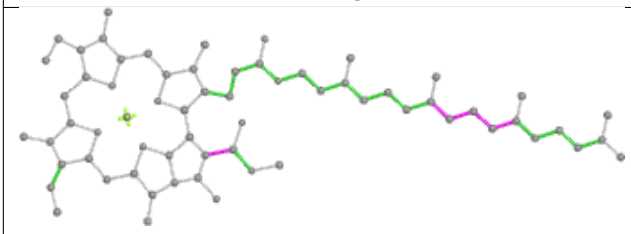
Ligand CLA B 828



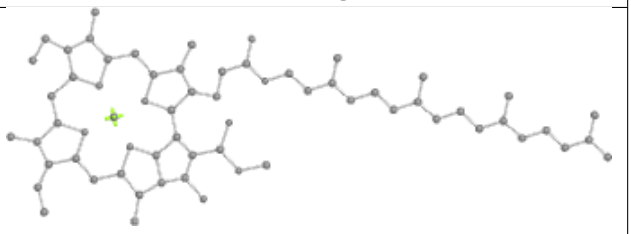
Bond lengths



Bond angles

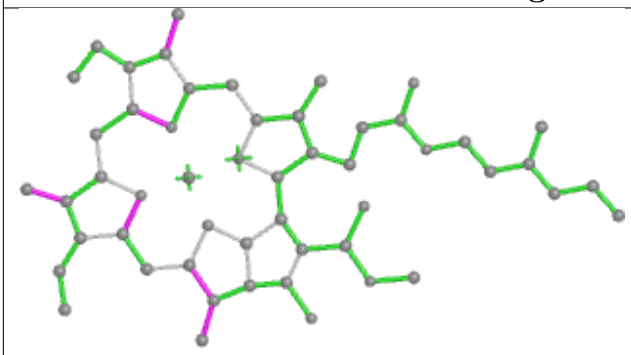


Torsions

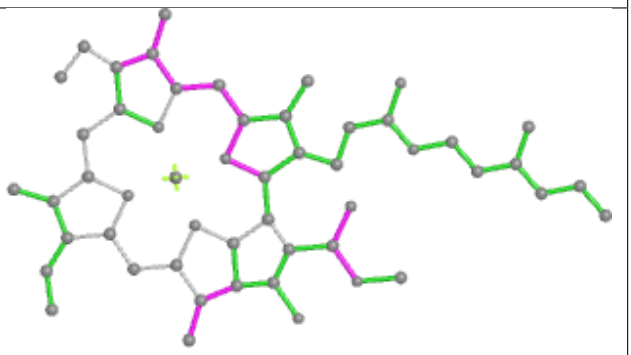


Rings

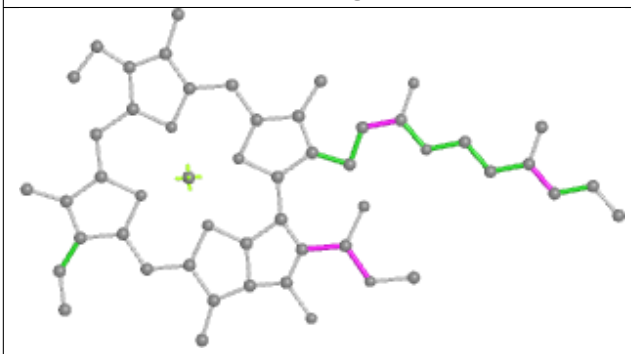
Ligand CLA 2 310



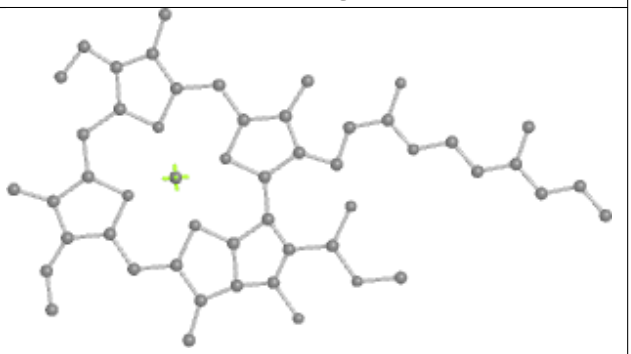
Bond lengths



Bond angles

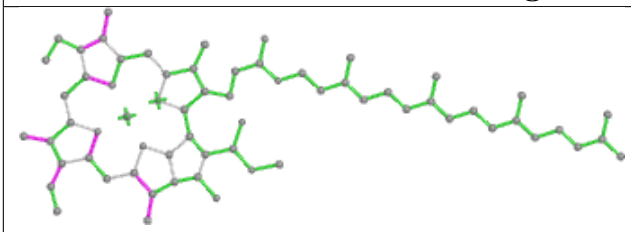


Torsions

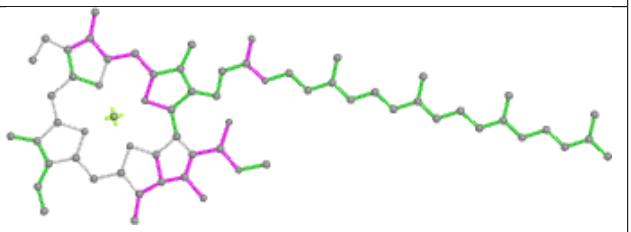


Rings

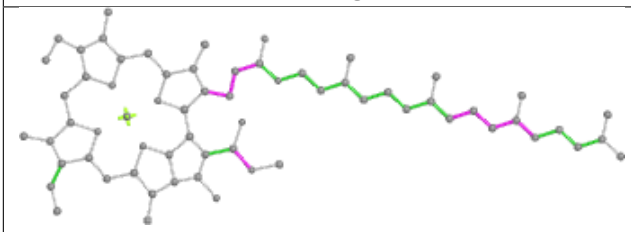
Ligand CLA A 817



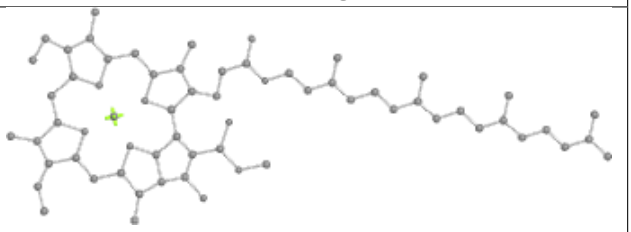
Bond lengths



Bond angles

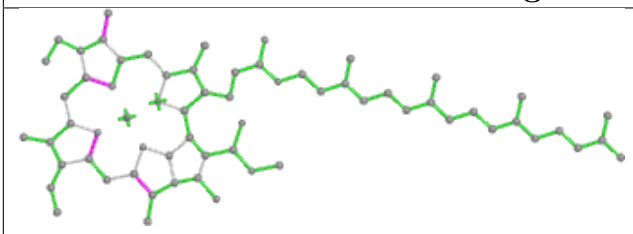


Torsions

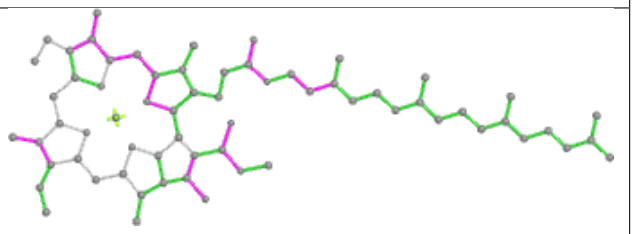


Rings

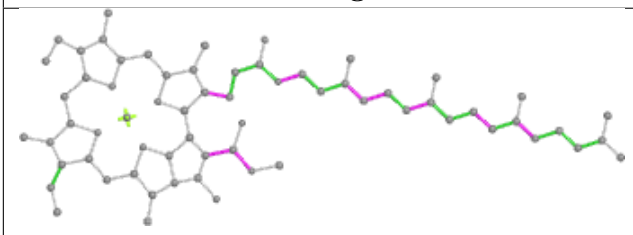
Ligand CLA A 837



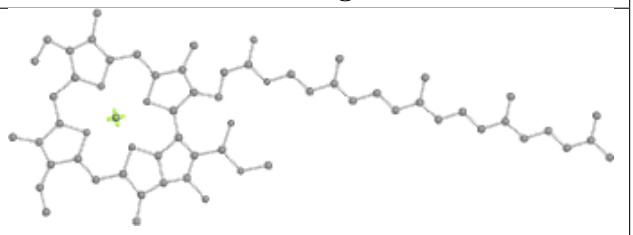
Bond lengths



Bond angles

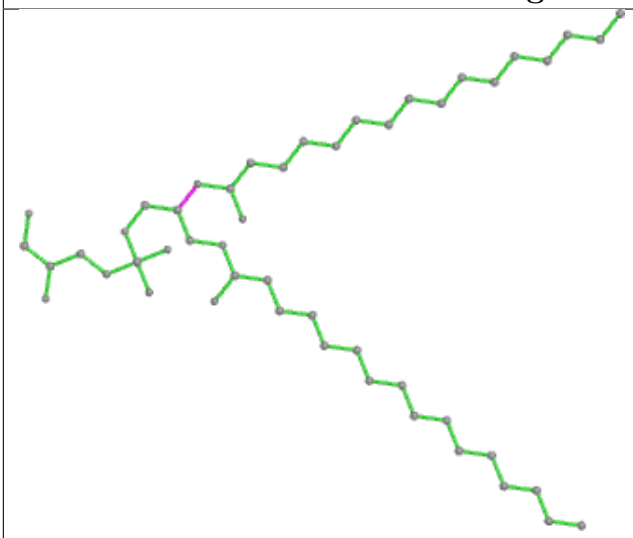


Torsions

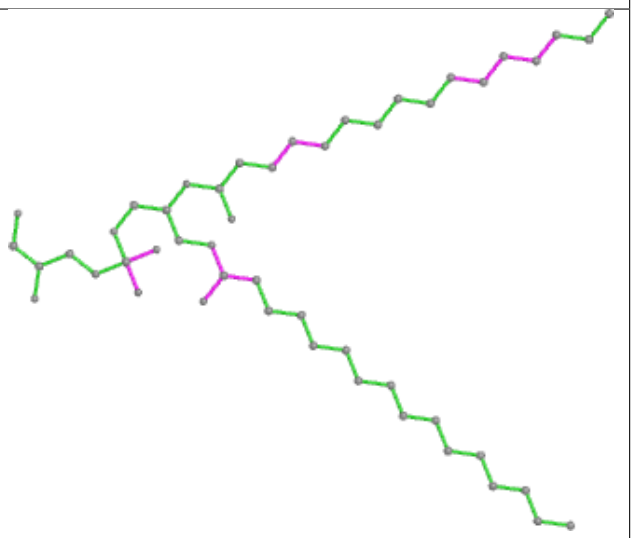


Rings

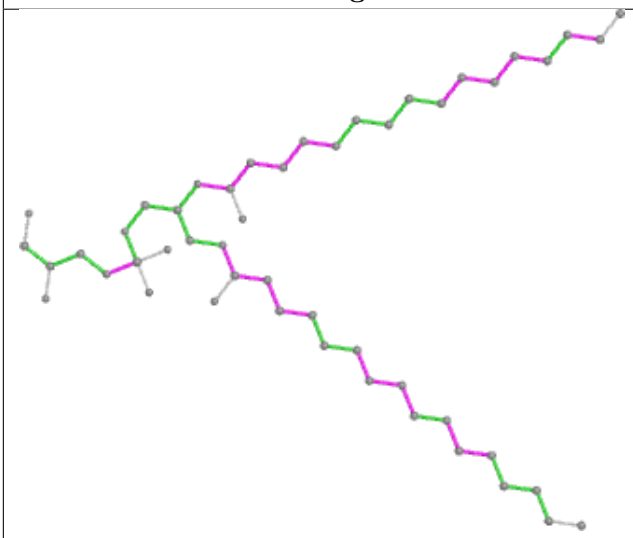
Ligand LHG 1 317



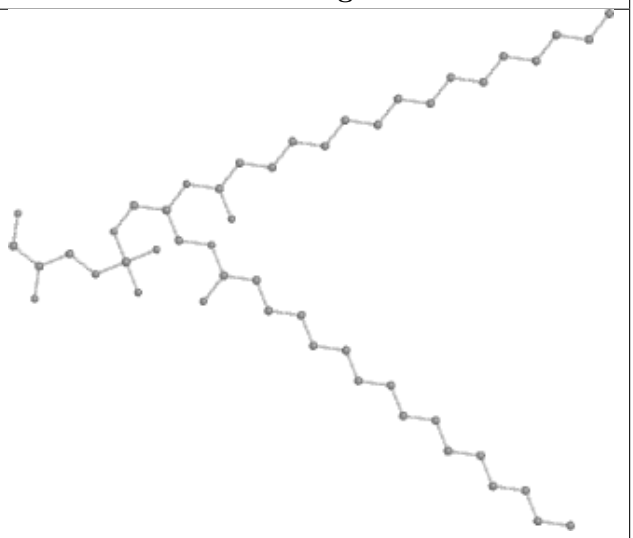
Bond lengths



Bond angles

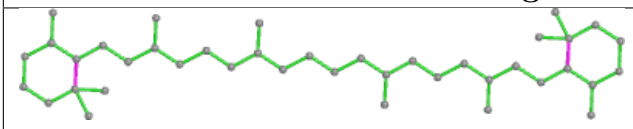


Torsions

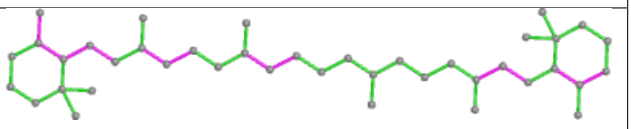


Rings

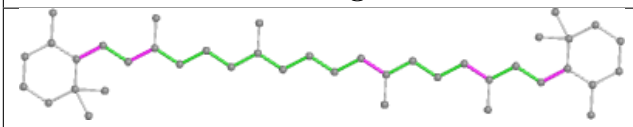
Ligand BCR A 848



Bond lengths



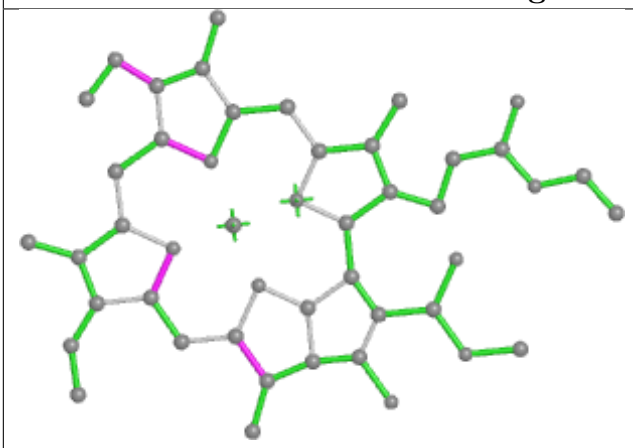
Bond angles



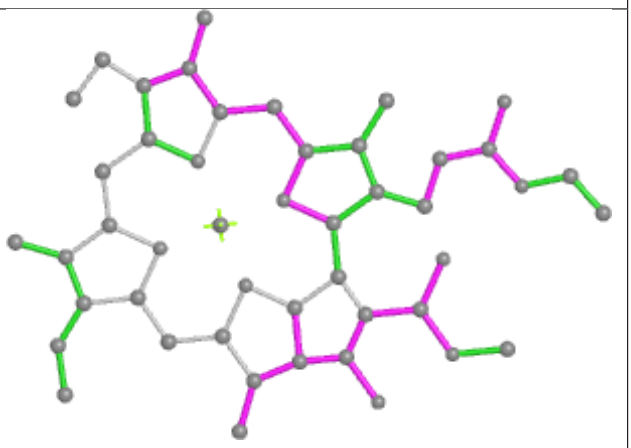
Torsions

Rings

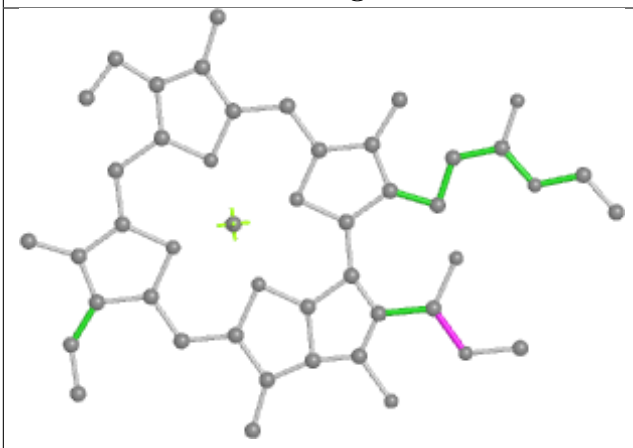
Ligand CLA 4 314



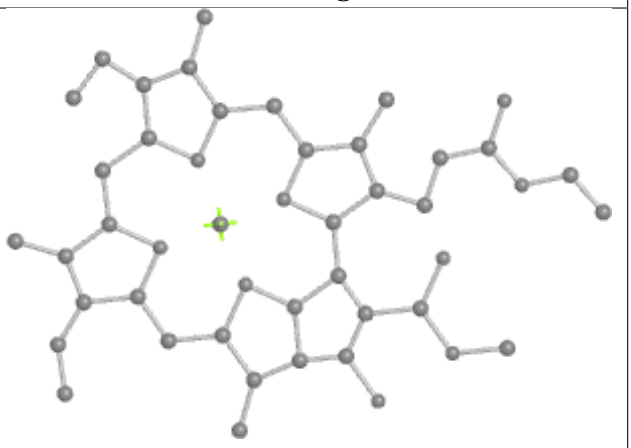
Bond lengths



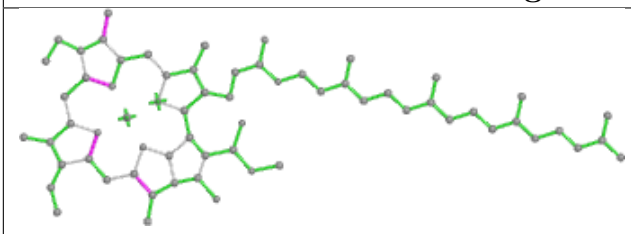
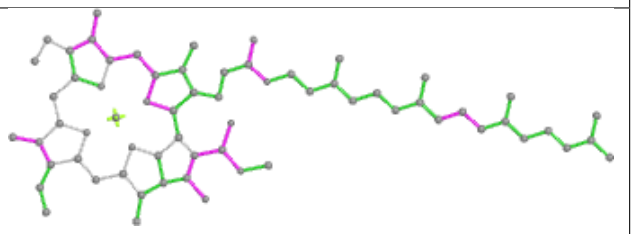
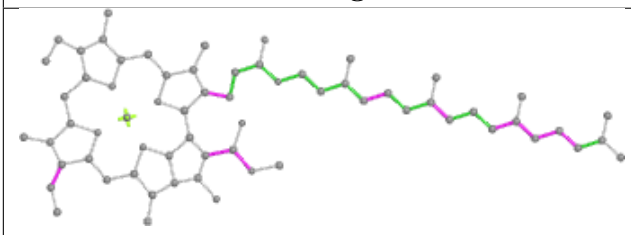
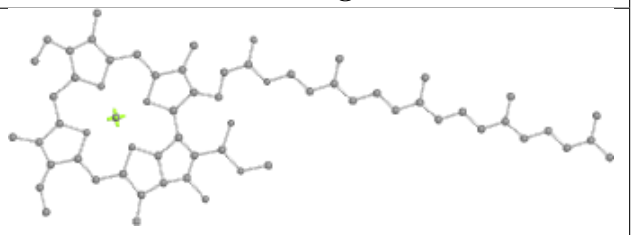
Bond angles

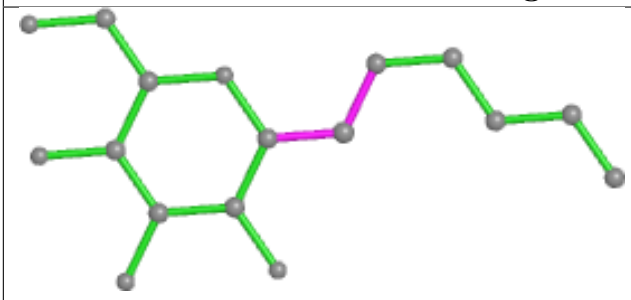
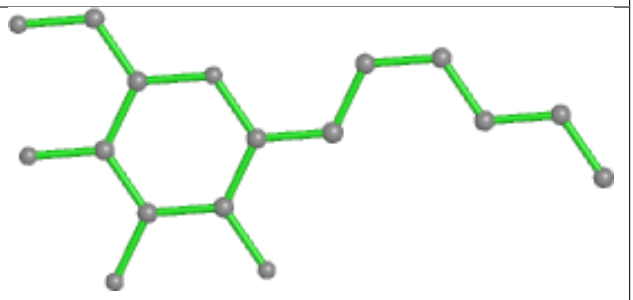
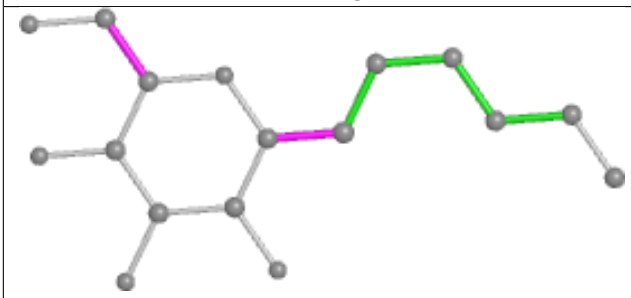
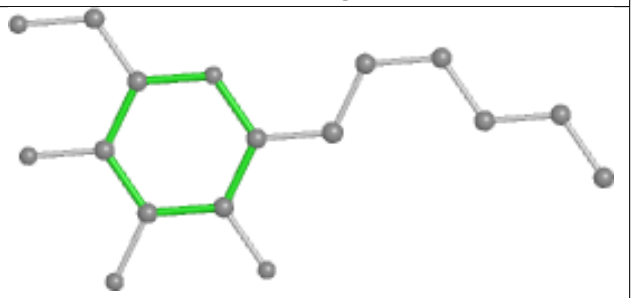


Torsions

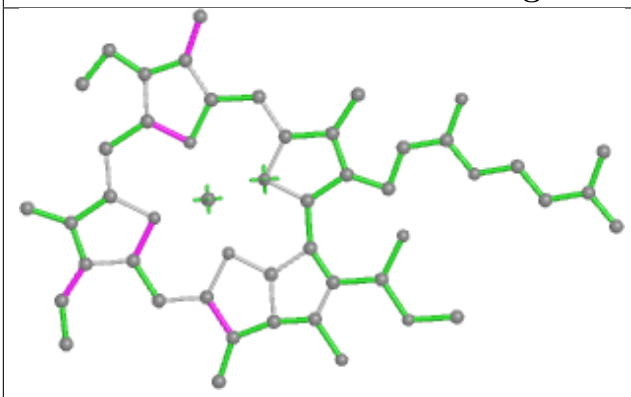


Rings

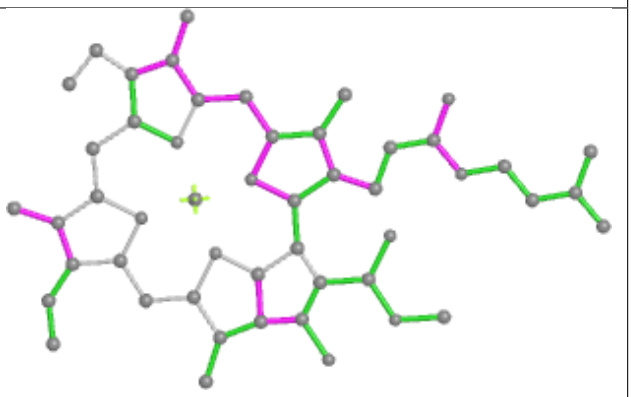
Ligand CLA B 815	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HTG F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

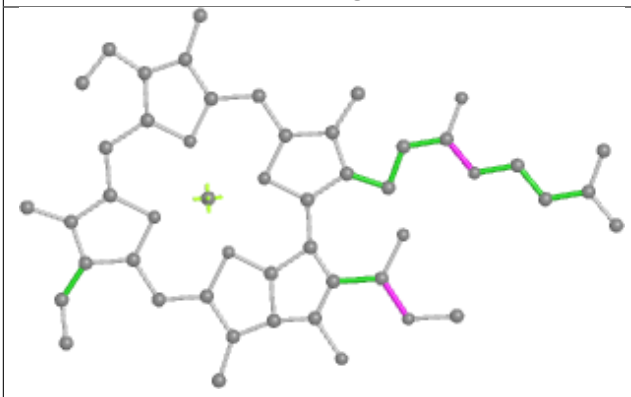
Ligand CLA G 104



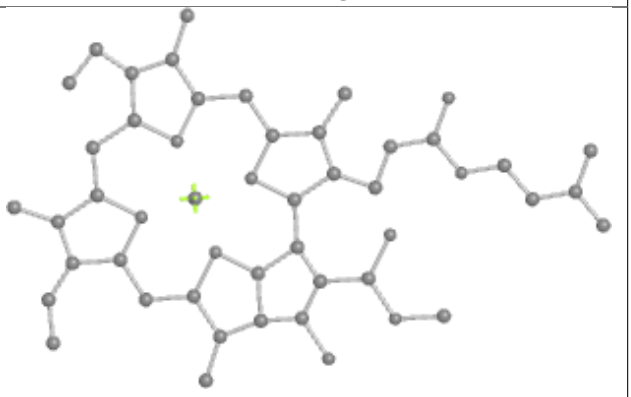
Bond lengths



Bond angles

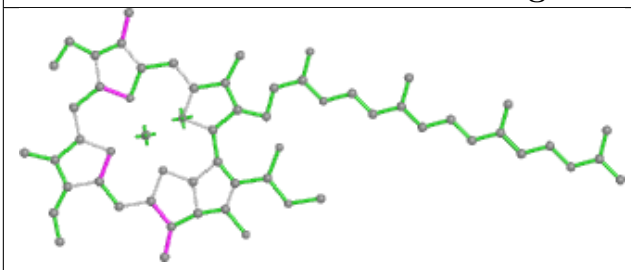


Torsions

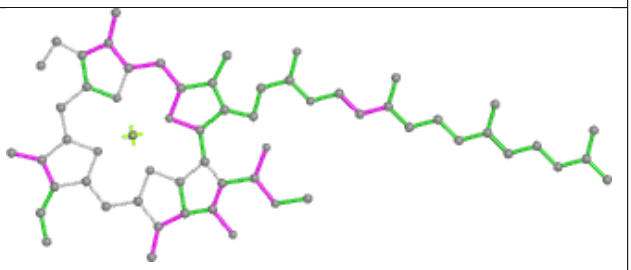


Rings

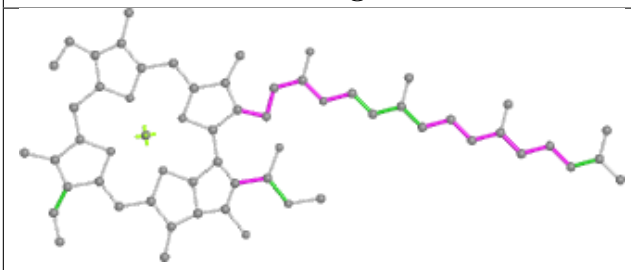
Ligand CLA 2 303



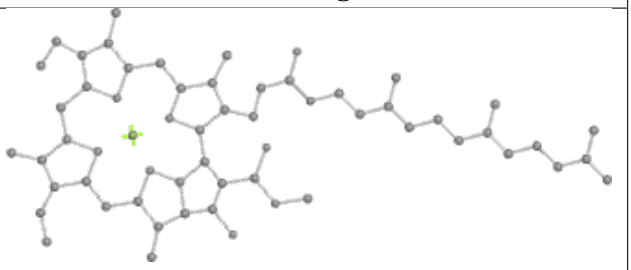
Bond lengths



Bond angles

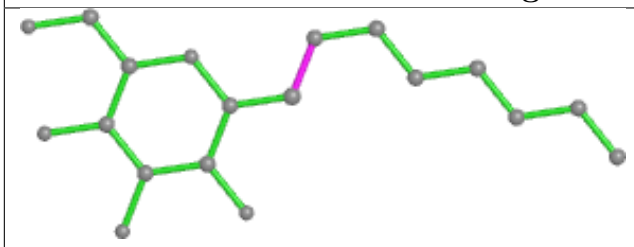


Torsions

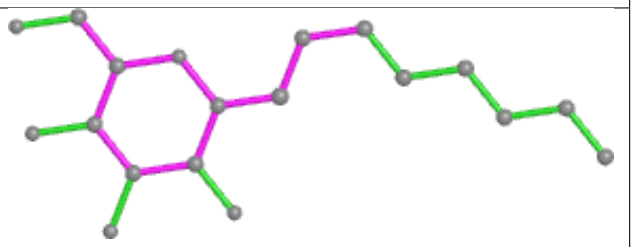


Rings

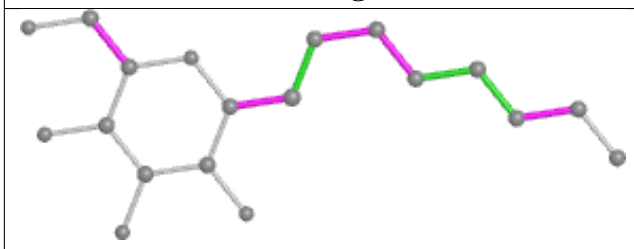
Ligand HTG B 851



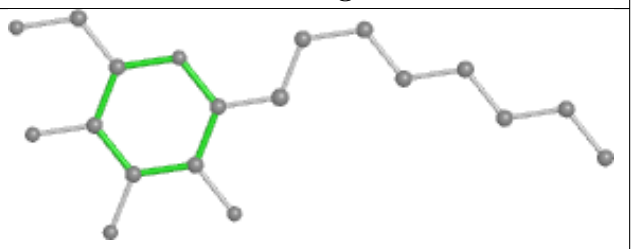
Bond lengths



Bond angles

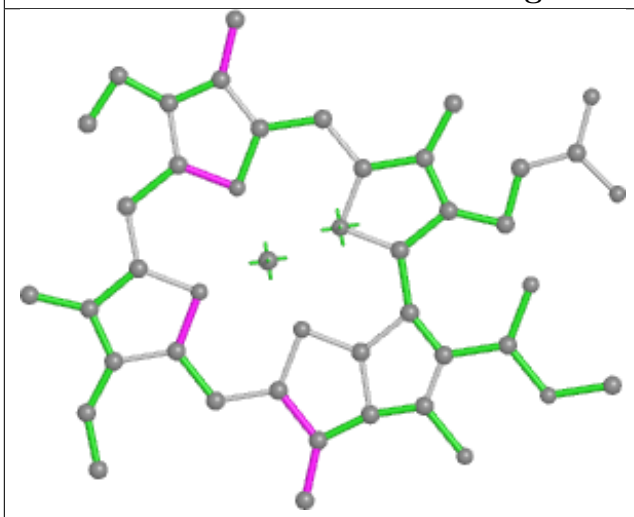


Torsions

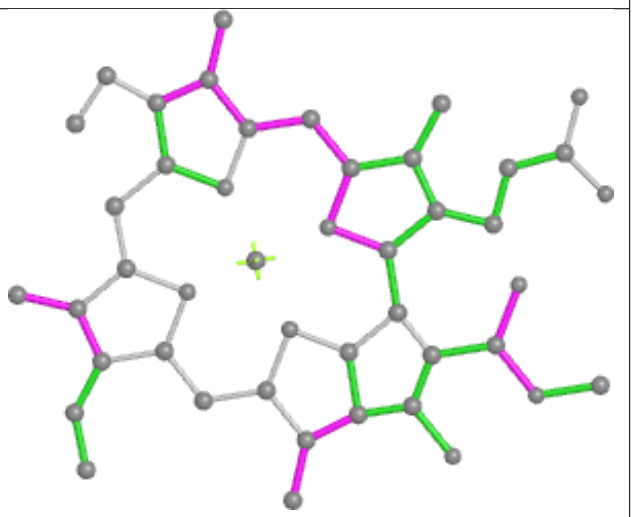


Rings

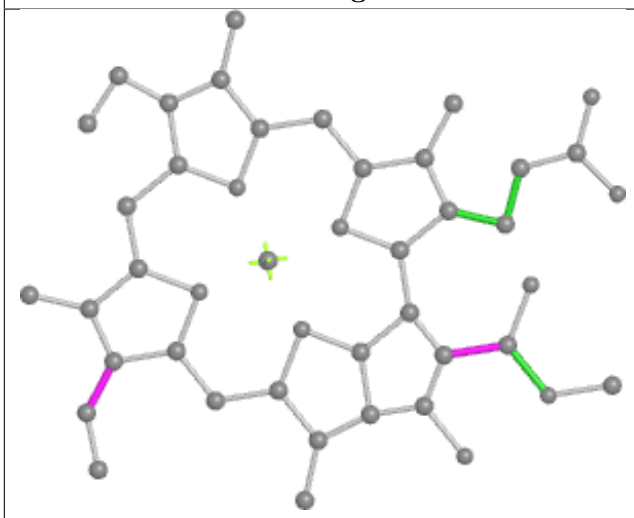
Ligand CLA A 819



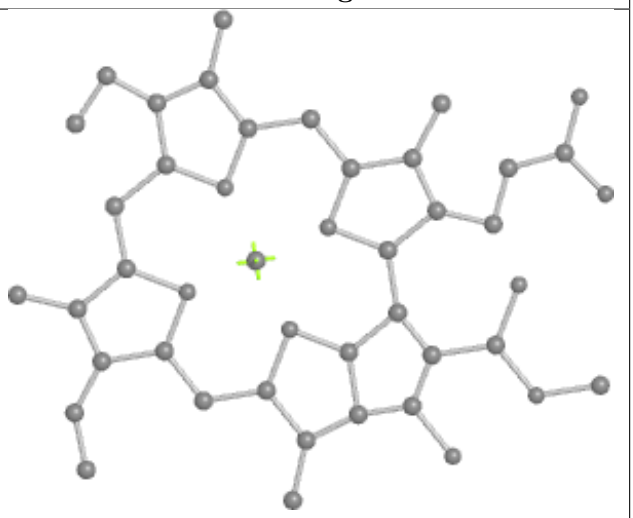
Bond lengths



Bond angles

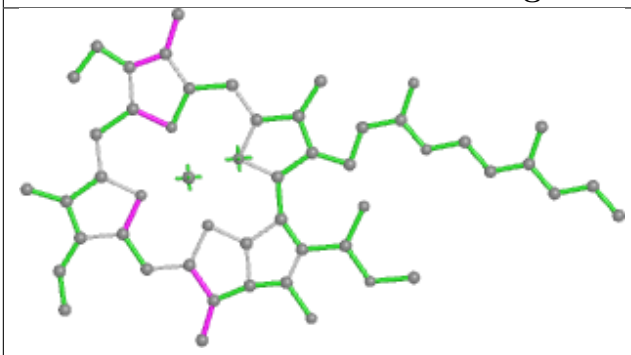


Torsions

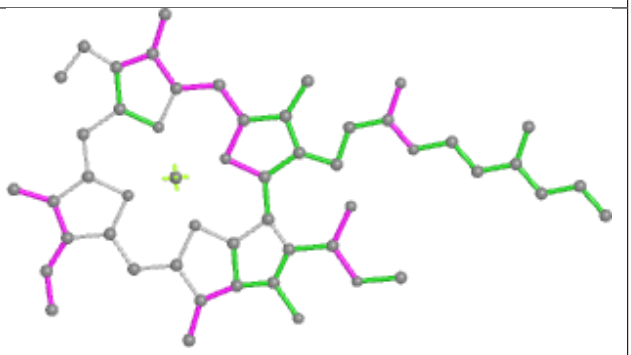


Rings

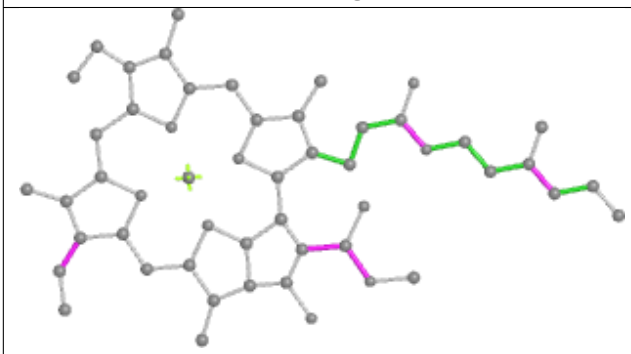
Ligand CLA A 843



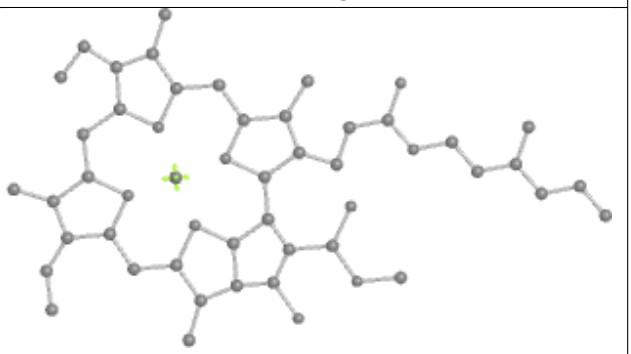
Bond lengths



Bond angles

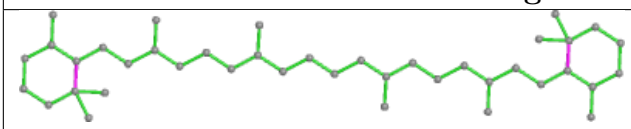


Torsions

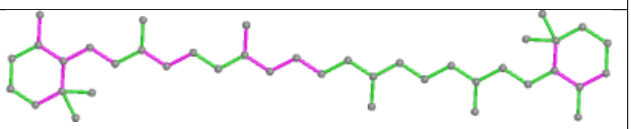


Rings

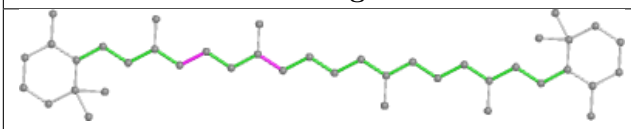
Ligand BCR F 308



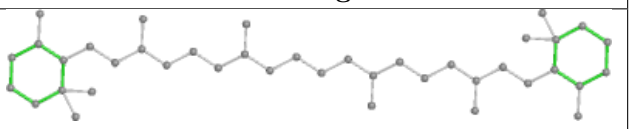
Bond lengths



Bond angles

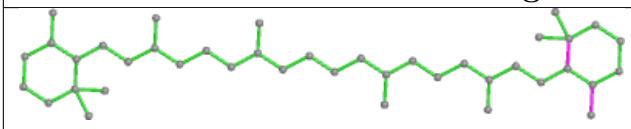


Torsions

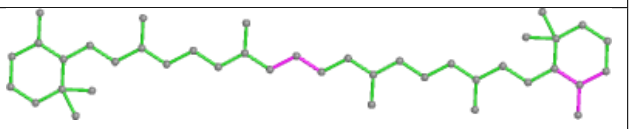


Rings

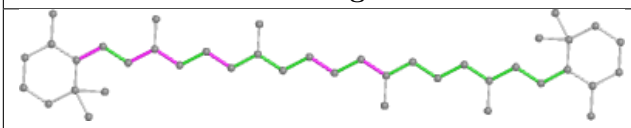
Ligand BCR B 849



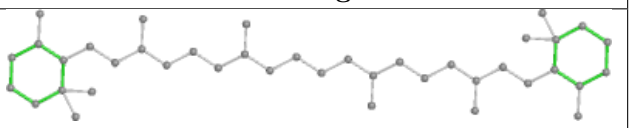
Bond lengths



Bond angles

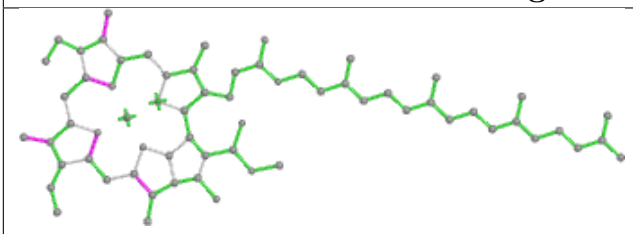


Torsions

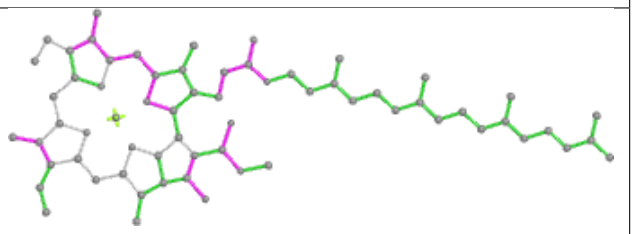


Rings

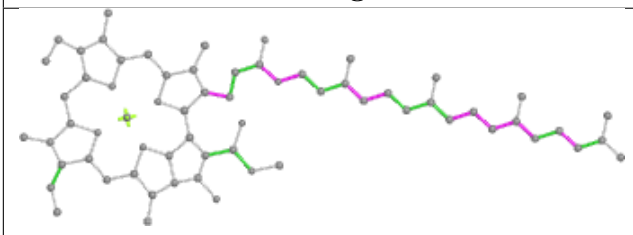
Ligand CLA 1 307



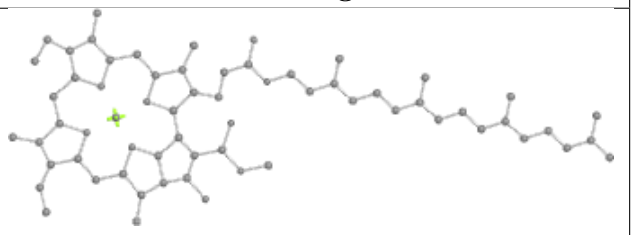
Bond lengths



Bond angles

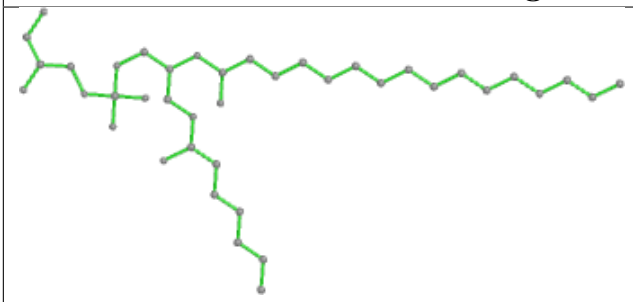


Torsions

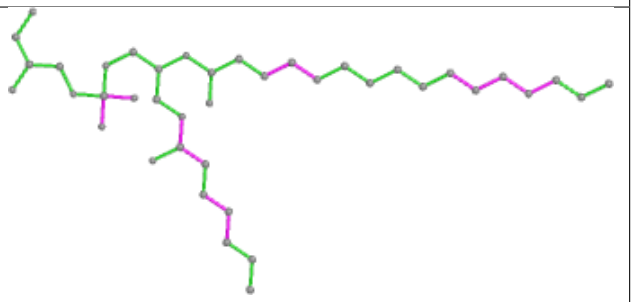


Rings

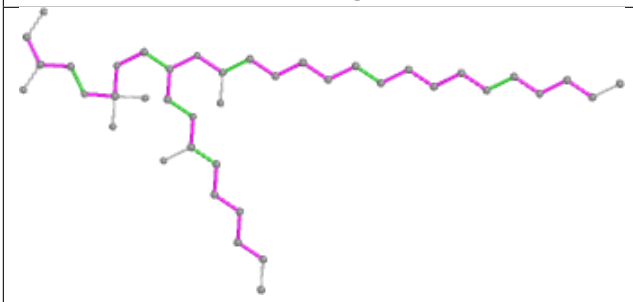
Ligand LHG F 302



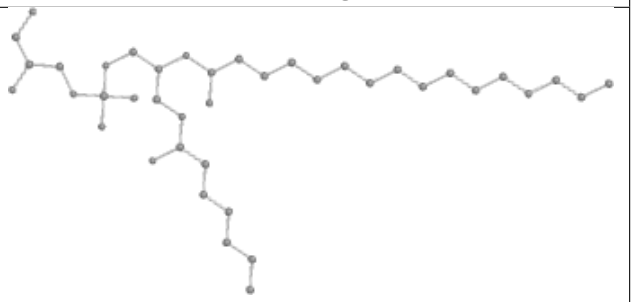
Bond lengths



Bond angles

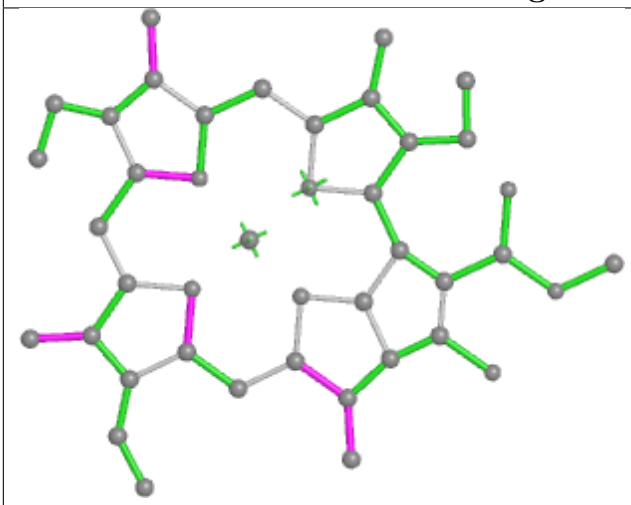


Torsions

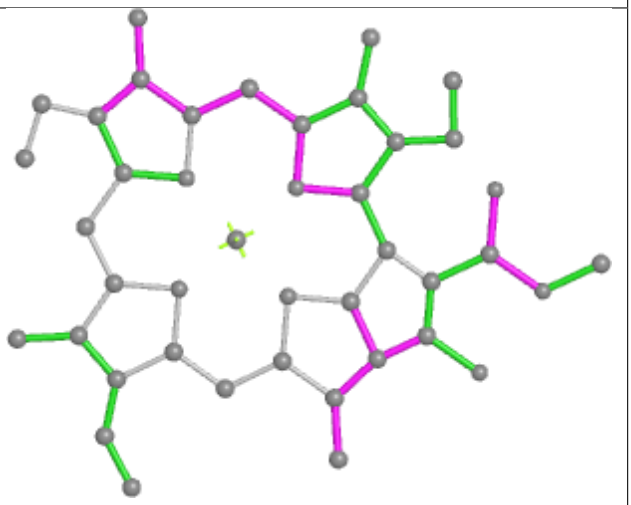


Rings

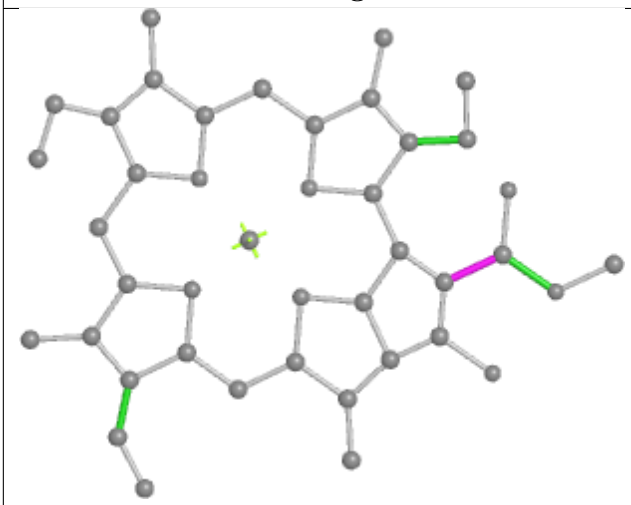
Ligand CLA 3 605



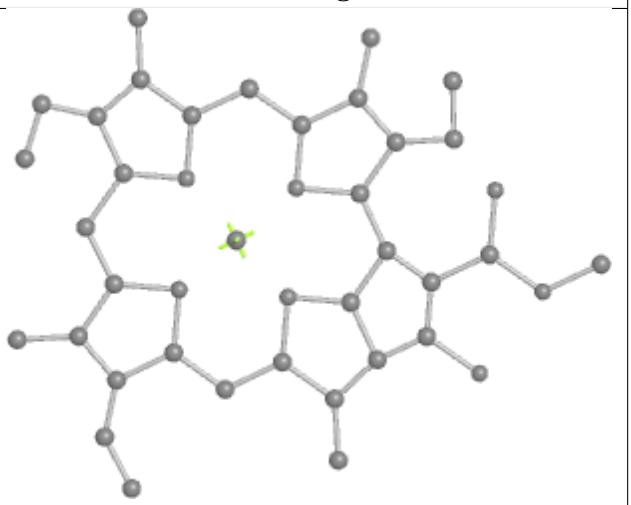
Bond lengths



Bond angles

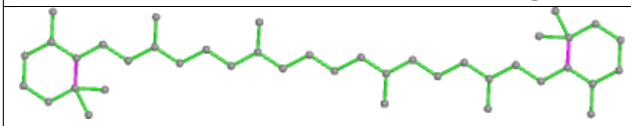


Torsions

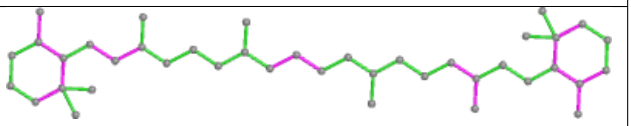


Rings

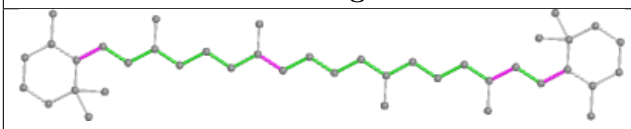
Ligand BCR J 105



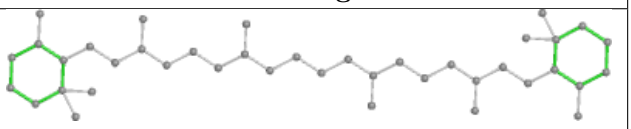
Bond lengths



Bond angles

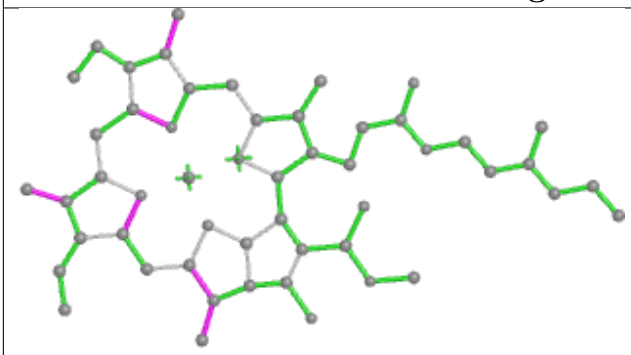


Torsions

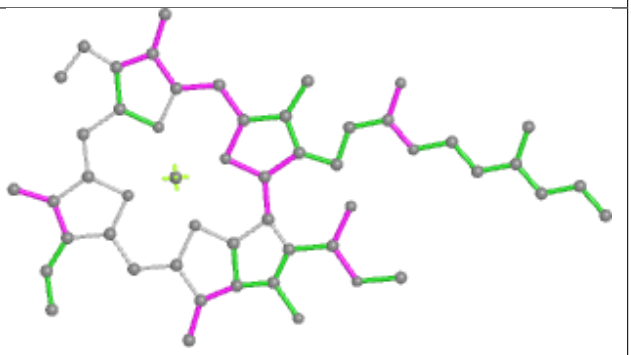


Rings

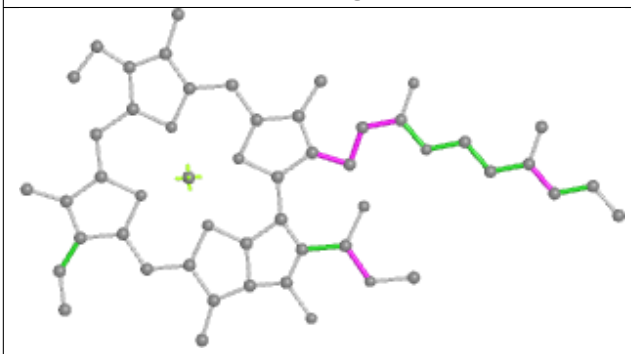
Ligand CLA 3 610



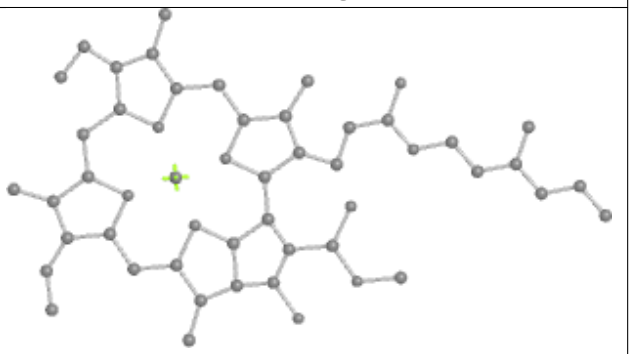
Bond lengths



Bond angles

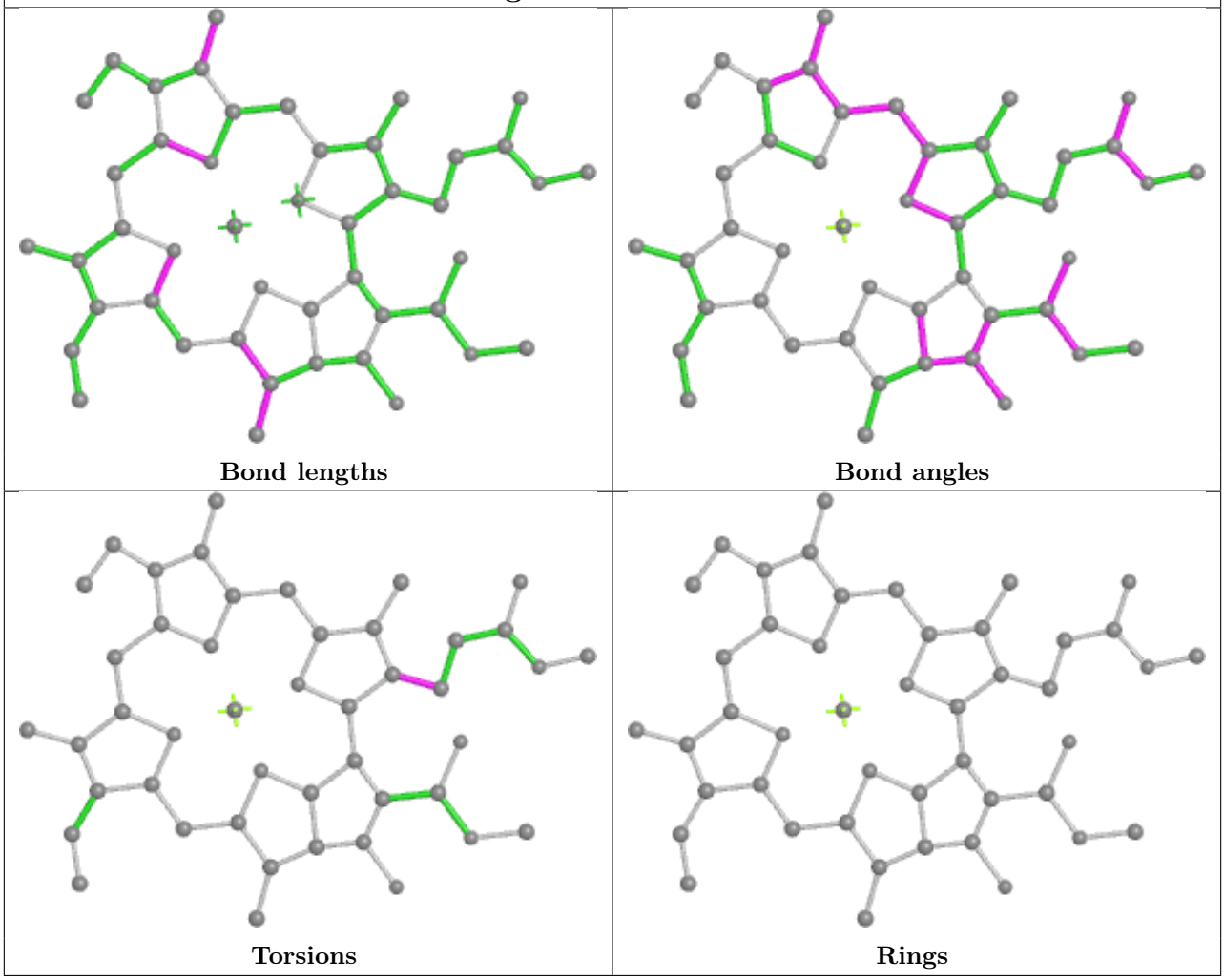


Torsions



Rings

Ligand CLA 1 306



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	1	195/195 (100%)	0.83	35 (17%)	1	1	66, 95, 152, 193	0
2	2	204/269 (75%)	1.33	57 (27%)	0	0	87, 121, 159, 212	0
3	3	216/275 (78%)	2.37	97 (44%)	0	0	114, 161, 229, 257	0
4	4	195/198 (98%)	0.27	20 (10%)	6	6	60, 74, 111, 143	0
5	A	742/758 (97%)	1.08	180 (24%)	0	0	52, 94, 150, 233	0
6	B	733/734 (99%)	0.54	75 (10%)	6	6	30, 69, 98, 132	0
7	C	80/81 (98%)	0.37	5 (6%)	20	18	30, 78, 94, 120	0
8	D	140/143 (97%)	0.61	18 (12%)	3	3	66, 101, 137, 158	0
9	E	63/66 (95%)	1.32	12 (19%)	1	1	65, 84, 111, 129	0
10	F	152/154 (98%)	0.09	5 (3%)	46	45	30, 70, 96, 138	0
11	G	95/97 (97%)	0.13	5 (5%)	26	25	30, 91, 125, 156	0
12	H	88/88 (100%)	2.26	50 (56%)	0	0	96, 132, 182, 259	0
13	I	30/40 (75%)	0.61	2 (6%)	17	16	92, 108, 146, 208	0
14	J	39/42 (92%)	0.11	3 (7%)	13	12	60, 73, 101, 112	0
15	L	151/157 (96%)	0.89	32 (21%)	0	0	102, 137, 165, 192	0
16	K	77/80 (96%)	3.11	43 (55%)	0	0	137, 198, 248, 302	0
All	All	3200/3377 (94%)	0.94	639 (19%)	1	0	30, 91, 178, 302	0

All (639) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	I	2	ILE	16.1
3	3	121	LEU	15.9
3	3	128	LEU	14.4
16	K	85	ALA	12.5
3	3	122	ILE	12.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2	231	TYR	12.4
3	3	115	TYR	11.7
3	3	51	LEU	11.5
16	K	51	THR	10.9
15	L	116	LEU	10.6
16	K	72	PRO	10.3
3	3	129	ALA	10.2
12	H	142	LEU	10.1
5	A	263	ALA	9.7
3	3	119	VAL	9.3
16	K	68	PHE	9.2
1	1	109	ALA	8.5
1	1	110	LEU	8.0
2	2	132	GLU	8.0
16	K	49	SER	7.9
16	K	73	SER	7.9
1	1	128	PRO	7.7
3	3	142	TYR	7.7
9	E	1	ILE	7.5
2	2	67	LEU	7.5
3	3	116	LEU	7.5
16	K	83	LEU	7.4
3	3	56	LYS	7.2
3	3	52	TRP	7.2
12	H	88	PHE	7.2
1	1	127	LEU	7.0
5	A	210	LEU	6.9
12	H	92	PHE	6.9
5	A	208	ALA	6.8
2	2	198	SER	6.8
1	1	111	PRO	6.8
3	3	151	LEU	6.8
3	3	113	PRO	6.8
2	2	196	TRP	6.7
3	3	62	LEU	6.7
16	K	96	ALA	6.7
15	L	156	VAL	6.6
3	3	118	LYS	6.6
2	2	128	TYR	6.6
16	K	121	LEU	6.6
3	3	207	PHE	6.6
3	3	59	LEU	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	3	205	LEU	6.5
3	3	125	GLU	6.5
2	2	234	THR	6.4
16	K	98	PHE	6.4
5	A	516	GLY	6.4
16	K	71	ALA	6.4
1	1	122	VAL	6.3
4	4	118	ILE	6.3
2	2	86	PRO	6.2
2	2	121	ILE	6.2
3	3	217	LEU	6.2
5	A	633	VAL	6.2
12	H	84	LEU	6.1
12	H	70	TRP	6.1
16	K	86	ARG	5.8
12	H	134	LEU	5.8
3	3	127	ALA	5.7
2	2	122	LEU	5.7
3	3	141	THR	5.6
15	L	23	VAL	5.6
11	G	2	LEU	5.6
2	2	60	GLY	5.6
3	3	259	ASN	5.5
16	K	64	PHE	5.5
3	3	120	GLY	5.5
2	2	129	THR	5.5
5	A	735	VAL	5.4
2	2	123	ASN	5.4
2	2	255	ALA	5.4
5	A	211	LEU	5.4
3	3	130	TRP	5.4
1	1	121	PRO	5.4
2	2	124	THR	5.3
3	3	214	LEU	5.3
3	3	123	PRO	5.3
16	K	112	ILE	5.2
5	A	209	GLY	5.2
3	3	247	TYR	5.2
2	2	194	LEU	5.2
3	3	148	ASN	5.2
3	3	50	PRO	5.2
16	K	53	LEU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	K	113	ILE	5.1
3	3	126	THR	5.1
5	A	739	LEU	5.1
2	2	61	SER	5.1
5	A	743	ILE	5.1
12	H	79	SER	5.1
16	K	124	ILE	5.1
3	3	112	ALA	5.0
5	A	250	LEU	5.0
1	1	164	LEU	5.0
5	A	207	LEU	5.0
5	A	111	ASN	5.0
5	A	335	LYS	5.0
15	L	20	GLU	5.0
3	3	54	ALA	5.0
8	D	74	LEU	5.0
5	A	631	GLN	5.0
5	A	310	PHE	4.9
9	E	57	LEU	4.9
1	1	98	LEU	4.9
5	A	687	ALA	4.8
1	1	118	LEU	4.8
5	A	216	LEU	4.8
2	2	136	PHE	4.8
3	3	57	GLN	4.8
16	K	88	SER	4.8
15	L	27	PRO	4.8
16	K	55	MET	4.8
3	3	117	GLY	4.7
5	A	264	GLU	4.7
12	H	58	PHE	4.7
5	A	257	GLN	4.7
3	3	55	SER	4.7
2	2	252	ILE	4.7
16	K	50	PRO	4.7
5	A	212	GLY	4.7
1	1	120	ASN	4.6
5	A	686	TRP	4.6
5	A	215	SER	4.6
16	K	76	ARG	4.6
4	4	239	ASP	4.6
3	3	111	ILE	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	A	401	TRP	4.6
5	A	632	GLY	4.6
5	A	323	ILE	4.6
3	3	132	GLN	4.6
3	3	258	VAL	4.5
2	2	233	GLY	4.5
8	D	111	ILE	4.5
5	A	255	LEU	4.5
12	H	135	PRO	4.5
5	A	634	VAL	4.5
3	3	195	ALA	4.5
1	1	215	ALA	4.5
1	1	114	GLN	4.4
3	3	176	MET	4.4
6	B	5	PHE	4.4
16	K	48	GLY	4.4
5	A	235	ALA	4.4
12	H	140	PRO	4.4
15	L	112	PRO	4.4
2	2	133	GLN	4.3
5	A	505	PRO	4.3
16	K	74	ALA	4.3
5	A	253	ASP	4.3
1	1	161	PHE	4.3
16	K	84	GLU	4.3
5	A	244	LEU	4.3
2	2	127	TRP	4.3
5	A	741	GLY	4.3
6	B	734	GLY	4.3
5	A	232	PHE	4.2
12	H	136	PRO	4.2
16	K	61	LEU	4.2
9	E	3	PRO	4.2
3	3	215	LYS	4.2
3	3	61	TYR	4.2
12	H	71	ASP	4.2
1	1	123	PRO	4.2
1	1	51	ALA	4.2
5	A	159	THR	4.1
1	1	166	TYR	4.1
12	H	80	PRO	4.1
1	1	119	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	3	220	LYS	4.1
5	A	685	VAL	4.1
3	3	94	TYR	4.1
6	B	206	TYR	4.1
6	B	580	VAL	4.1
12	H	81	TYR	4.1
5	A	108	ALA	4.0
4	4	123	VAL	4.0
5	A	691	MET	4.0
16	K	92	THR	4.0
2	2	71	LEU	4.0
5	A	405	PHE	4.0
5	A	481	ALA	4.0
3	3	134	GLY	4.0
5	A	682	ALA	4.0
5	A	306	ILE	4.0
1	1	107	TRP	4.0
5	A	258	LEU	3.9
5	A	688	PHE	3.9
2	2	120	GLY	3.9
12	H	132	PRO	3.9
5	A	334	HIS	3.9
12	H	61	GLU	3.9
9	E	4	LYS	3.9
15	L	10	ILE	3.9
2	2	250	ALA	3.9
2	2	253	PHE	3.9
2	2	131	GLY	3.8
9	E	2	GLY	3.8
2	2	119	LEU	3.8
16	K	115	VAL	3.8
3	3	250	LEU	3.8
12	H	69	GLN	3.8
10	F	110	PRO	3.8
12	H	122	SER	3.8
5	A	733	VAL	3.8
12	H	95	PRO	3.8
4	4	122	ASN	3.8
6	B	280	ILE	3.8
5	A	400	MET	3.8
12	H	72	LEU	3.8
3	3	213	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	A	339	THR	3.7
5	A	254	LEU	3.7
16	K	95	PRO	3.7
5	A	70	ASP	3.7
3	3	254	VAL	3.7
5	A	603	PHE	3.7
12	H	96	PHE	3.7
6	B	215	VAL	3.7
5	A	738	TYR	3.7
15	L	111	ALA	3.7
1	1	129	THR	3.7
12	H	67	THR	3.7
4	4	231	ASP	3.7
15	L	76	ALA	3.7
3	3	149	TYR	3.7
3	3	175	SER	3.7
5	A	734	GLY	3.7
12	H	139	GLY	3.7
16	K	54	ILE	3.7
5	A	737	HIS	3.6
12	H	137	GLN	3.6
5	A	692	PHE	3.6
5	A	609	ILE	3.6
9	E	35	ARG	3.6
3	3	174	GLY	3.6
4	4	115	PHE	3.6
6	B	717	TYR	3.6
5	A	251	ASN	3.6
4	4	116	THR	3.6
2	2	135	TYR	3.6
5	A	606	TYR	3.5
3	3	114	GLU	3.5
5	A	510	SER	3.5
6	B	357	ALA	3.5
6	B	154	TRP	3.5
6	B	379	ALA	3.5
5	A	455	PHE	3.5
6	B	581	PHE	3.5
2	2	56	LEU	3.5
15	L	28	LEU	3.5
5	A	689	SER	3.5
15	L	25	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	A	309	LEU	3.5
12	H	66	THR	3.4
5	A	217	SER	3.4
3	3	243	GLY	3.4
15	L	40	ARG	3.4
10	F	106	LYS	3.4
5	A	402	ILE	3.4
12	H	63	LEU	3.4
5	A	520	LEU	3.4
2	2	97	LEU	3.4
3	3	216	GLU	3.4
5	A	311	LEU	3.4
5	A	608	ALA	3.4
8	D	126	PRO	3.3
15	L	120	LYS	3.3
5	A	213	LEU	3.3
1	1	212	THR	3.3
3	3	133	THR	3.3
5	A	307	ALA	3.3
5	A	395	LEU	3.3
5	A	690	LEU	3.3
6	B	664	LEU	3.3
5	A	396	PHE	3.3
5	A	303	HIS	3.3
3	3	196	TYR	3.3
15	L	47	LEU	3.3
16	K	90	LEU	3.3
5	A	239	PRO	3.3
12	H	78	PRO	3.3
2	2	117	THR	3.3
3	3	170	TRP	3.3
5	A	34	TRP	3.3
5	A	256	ALA	3.3
3	3	70	TYR	3.3
5	A	742	GLY	3.3
10	F	228	LYS	3.3
5	A	681	GLY	3.3
15	L	78	GLN	3.3
6	B	213	LEU	3.3
8	D	154	PHE	3.3
6	B	348	VAL	3.3
2	2	62	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	K	52	ASN	3.2
5	A	269	PHE	3.2
15	L	74	GLU	3.2
15	L	131	GLY	3.2
12	H	94	ALA	3.2
5	A	26	PRO	3.2
12	H	62	ASP	3.2
4	4	241	TRP	3.2
5	A	46	LYS	3.2
5	A	397	THR	3.2
9	E	63	VAL	3.2
3	3	89	PRO	3.2
2	2	202	GLN	3.2
3	3	143	ASN	3.2
5	A	214	GLY	3.2
15	L	11	ASN	3.2
12	H	133	GLN	3.2
5	A	262	PHE	3.2
3	3	211	GLU	3.2
16	K	87	ASP	3.2
4	4	242	HIS	3.1
6	B	378	ILE	3.1
5	A	747	TRP	3.1
7	C	36	ALA	3.1
15	L	42	ALA	3.1
3	3	188	PHE	3.1
8	D	165	TYR	3.1
4	4	247	GLN	3.1
12	H	124	ASP	3.1
16	K	80	ALA	3.1
5	A	394	SER	3.1
12	H	141	ARG	3.1
5	A	732	ALA	3.1
16	K	67	ARG	3.1
11	G	95	ASP	3.1
3	3	212	LYS	3.1
2	2	130	ALA	3.1
5	A	21	LEU	3.1
5	A	205	HIS	3.0
6	B	585	ASN	3.0
5	A	740	LEU	3.0
1	1	125	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2	68	ASP	3.0
12	H	89	PHE	3.0
11	G	94	TYR	3.0
5	A	509	THR	3.0
5	A	559	GLY	3.0
15	L	60	LEU	3.0
3	3	202	PHE	3.0
3	3	208	GLY	3.0
5	A	511	THR	3.0
6	B	341	LEU	3.0
5	A	683	HIS	3.0
2	2	245	ALA	3.0
6	B	657	TRP	3.0
4	4	230	PHE	3.0
5	A	302	HIS	3.0
6	B	662	MET	3.0
4	4	117	SER	3.0
6	B	344	ILE	3.0
9	E	62	GLU	3.0
5	A	693	LEU	2.9
3	3	60	SER	2.9
3	3	210	ASP	2.9
4	4	120	ILE	2.9
3	3	67	PRO	2.9
7	C	31	TRP	2.9
5	A	206	HIS	2.9
6	B	373	THR	2.9
12	H	59	ASP	2.9
6	B	579	ALA	2.9
5	A	628	ILE	2.9
5	A	32	GLU	2.9
16	K	77	LYS	2.9
3	3	204	PRO	2.9
2	2	126	SER	2.9
5	A	86	LEU	2.9
8	D	72	PRO	2.9
16	K	117	VAL	2.9
5	A	236	GLY	2.9
3	3	255	ALA	2.9
6	B	589	TRP	2.9
14	J	2	ARG	2.9
5	A	704	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	K	91	GLN	2.8
6	B	185	VAL	2.8
15	L	114	LEU	2.8
1	1	126	THR	2.8
3	3	124	GLN	2.8
8	D	151	LYS	2.8
12	H	65	ASN	2.8
5	A	74	ILE	2.8
5	A	551	VAL	2.8
6	B	42	LEU	2.8
6	B	352	MET	2.8
6	B	584	LEU	2.8
6	B	586	THR	2.8
8	D	147	LYS	2.8
15	L	6	VAL	2.8
6	B	340	SER	2.8
5	A	480	THR	2.8
6	B	282	ILE	2.8
6	B	286	ILE	2.8
16	K	75	ASN	2.8
2	2	203	LYS	2.8
3	3	198	GLY	2.8
5	A	362	LEU	2.8
3	3	108	VAL	2.7
3	3	140	GLY	2.7
5	A	501	GLY	2.7
16	K	57	THR	2.7
2	2	206	GLU	2.7
9	E	5	ARG	2.7
5	A	243	PRO	2.7
14	J	32	PHE	2.7
4	4	121	ILE	2.7
12	H	143	GLY	2.7
6	B	583	MET	2.7
5	A	399	HIS	2.7
5	A	730	GLY	2.7
3	3	139	ALA	2.7
1	1	46	TYR	2.7
12	H	116	TYR	2.7
6	B	381	PHE	2.7
5	A	602	LEU	2.7
7	C	25	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	A	240	LYS	2.7
2	2	197	GLY	2.7
6	B	718	ILE	2.7
2	2	179	THR	2.7
5	A	333	ALA	2.6
5	A	744	ALA	2.6
4	4	234	LEU	2.6
5	A	599	PHE	2.6
5	A	241	GLU	2.6
2	2	232	THR	2.6
15	L	117	THR	2.6
8	D	182	GLN	2.6
5	A	31	PHE	2.6
5	A	610	SER	2.6
7	C	2	SER	2.6
8	D	128	LEU	2.6
5	A	73	GLU	2.6
3	3	178	LYS	2.6
6	B	582	TRP	2.6
5	A	590	CYS	2.6
15	L	73	THR	2.6
4	4	238	SER	2.6
3	3	66	LEU	2.6
3	3	256	ASP	2.6
4	4	119	GLY	2.6
5	A	745	THR	2.6
5	A	36	LYS	2.6
12	H	129	LYS	2.6
5	A	368	LEU	2.6
6	B	690	LEU	2.6
15	L	126	LEU	2.6
2	2	98	VAL	2.6
3	3	53	PHE	2.6
6	B	383	MET	2.6
6	B	733	PHE	2.6
12	H	76	ASP	2.6
16	K	102	ASP	2.6
5	A	233	LEU	2.5
5	A	406	LEU	2.5
3	3	90	ARG	2.5
3	3	197	PRO	2.5
3	3	145	TRP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	B	371	LEU	2.5
8	D	73	GLU	2.5
3	3	218	LYS	2.5
5	A	601	GLY	2.5
3	3	144	TYR	2.5
4	4	240	PRO	2.5
12	H	87	LYS	2.5
5	A	600	LEU	2.5
6	B	374	HIS	2.5
16	K	97	GLY	2.5
6	B	343	VAL	2.5
1	1	130	ILE	2.5
5	A	89	ILE	2.5
5	A	314	GLY	2.5
6	B	347	LEU	2.5
12	H	60	LEU	2.5
5	A	562	PHE	2.5
3	3	172	LYS	2.5
12	H	57	TYR	2.5
5	A	513	LEU	2.5
6	B	338	LEU	2.5
6	B	158	GLN	2.5
2	2	227	PHE	2.5
3	3	58	SER	2.5
5	A	112	ASP	2.5
6	B	186	SER	2.5
8	D	188	PHE	2.5
1	1	218	TRP	2.5
1	1	117	TYR	2.5
5	A	436	LEU	2.5
1	1	35	ALA	2.4
5	A	373	ALA	2.4
2	2	66	TRP	2.4
5	A	561	LEU	2.4
5	A	237	VAL	2.4
6	B	349	ALA	2.4
2	2	65	PRO	2.4
2	2	76	GLY	2.4
5	A	736	THR	2.4
10	F	192	GLN	2.4
8	D	75	ASP	2.4
5	A	27	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	H	125	ILE	2.4
5	A	93	LEU	2.4
5	A	162	LEU	2.4
5	A	684	PHE	2.4
6	B	207	VAL	2.4
15	L	43	VAL	2.4
5	A	52	THR	2.4
15	L	154	LEU	2.4
6	B	277	HIS	2.4
6	B	281	ALA	2.4
3	3	209	LYS	2.4
6	B	110	LEU	2.4
6	B	710	LEU	2.4
3	3	147	ASP	2.4
5	A	364	MET	2.4
2	2	58	PHE	2.4
12	H	90	GLU	2.4
8	D	169	LYS	2.4
15	L	121	LYS	2.4
3	3	64	GLY	2.4
5	A	23	ASP	2.4
5	A	252	ARG	2.4
12	H	126	LEU	2.4
2	2	193	PRO	2.4
3	3	171	ALA	2.4
9	E	26	VAL	2.4
6	B	568	CYS	2.4
3	3	206	GLY	2.3
12	H	73	TYR	2.3
5	A	504	ALA	2.3
8	D	79	PRO	2.3
1	1	106	GLU	2.3
9	E	7	ALA	2.3
4	4	135	PHE	2.3
6	B	382	ILE	2.3
5	A	630	ASP	2.3
3	3	244	VAL	2.3
15	L	12	GLY	2.3
6	B	375	HIS	2.3
3	3	260	ASN	2.3
5	A	68	THR	2.3
5	A	680	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	L	26	SER	2.3
6	B	190	TRP	2.3
5	A	90	PHE	2.3
6	B	147	PHE	2.3
6	B	476	VAL	2.3
2	2	125	PRO	2.3
8	D	155	TYR	2.3
5	A	404	GLY	2.3
5	A	398	HIS	2.3
6	B	665	ILE	2.3
11	G	50	THR	2.2
14	J	37	LEU	2.2
1	1	113	GLY	2.2
2	2	134	GLU	2.2
10	F	77	ASP	2.2
5	A	341	GLN	2.2
5	A	613	ILE	2.2
13	I	7	LEU	2.2
6	B	721	TYR	2.2
2	2	54	ARG	2.2
6	B	594	TRP	2.2
3	3	182	LEU	2.2
5	A	605	MET	2.2
6	B	284	PHE	2.2
15	L	119	ARG	2.2
6	B	593	TYR	2.2
5	A	33	GLN	2.2
12	H	77	ALA	2.2
6	B	188	LEU	2.2
3	3	97	VAL	2.2
5	A	340	GLY	2.2
5	A	592	VAL	2.2
6	B	561	GLY	2.2
6	B	638	PHE	2.2
5	A	491	TRP	2.2
16	K	62	MET	2.2
7	C	33	GLY	2.2
2	2	115	PHE	2.1
5	A	174	PHE	2.1
6	B	309	ILE	2.1
6	B	182	LEU	2.1
12	H	138	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	A	726	SER	2.1
5	A	204	ASN	2.1
12	H	64	GLY	2.1
1	1	52	PRO	2.1
5	A	177	LEU	2.1
5	A	494	ASN	2.1
1	1	168	LYS	2.1
5	A	186	TYR	2.1
1	1	131	LEU	2.1
5	A	575	LEU	2.1
1	1	55	PHE	2.1
5	A	629	ASN	2.1
5	A	627	SER	2.1
5	A	360	ILE	2.1
5	A	369	THR	2.1
6	B	656	VAL	2.1
5	A	558	LYS	2.1
6	B	576	PHE	2.1
9	E	42	PHE	2.1
15	L	69	PRO	2.1
2	2	116	LEU	2.1
5	A	408	VAL	2.1
6	B	526	GLY	2.1
5	A	317	TYR	2.1
8	D	71	PRO	2.1
4	4	237	ILE	2.0
5	A	315	HIS	2.0
5	A	451	ILE	2.0
3	3	186	LYS	2.0
5	A	35	ALA	2.0
2	2	158	TRP	2.0
6	B	490	ARG	2.0
6	B	663	PHE	2.0
6	B	533	ILE	2.0
5	A	366	GLY	2.0
16	K	99	THR	2.0
5	A	218	TRP	2.0
5	A	338	PHE	2.0
6	B	592	PHE	2.0
11	G	62	ASN	2.0
6	B	527	LEU	2.0
12	H	128	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1	158	GLY	2.0
8	D	183	GLY	2.0
2	2	118	LYS	2.0
5	A	305	ALA	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	LHG	G	102	49/49	0.50	0.45	92,119,171,174	0
24	LMG	G	101	40/55	0.59	0.42	110,157,180,181	0
21	BCR	K	203	40/40	0.67	0.42	142,185,227,229	0
20	XAT	3	615	44/44	0.70	0.33	62,89,98,100	0
25	HTG	B	851	19/19	0.70	0.37	107,134,142,143	0
25	HTG	F	301	17/19	0.72	0.32	124,149,155,159	0
25	HTG	F	310	16/19	0.72	0.38	114,141,144,146	0
23	LMT	A	855	35/35	0.73	0.23	97,154,171,172	0
24	LMG	4	320	49/55	0.74	0.33	96,119,174,176	0
21	BCR	2	316	40/40	0.77	0.60	148,157,172,173	0
21	BCR	A	846	40/40	0.77	0.32	116,137,151,153	0
25	HTG	4	322	19/19	0.78	0.25	107,129,140,145	0
21	BCR	G	106	40/40	0.78	0.26	71,90,129,130	0
21	BCR	3	616	40/40	0.78	0.44	156,164,187,189	0
21	BCR	A	849	40/40	0.78	0.38	100,137,196,199	0
26	DGD	4	323	60/66	0.78	0.24	90,115,130,138	0
22	LHG	F	302	40/49	0.79	0.28	111,140,164,167	0
17	CLA	K	201	45/65	0.82	0.24	172,184,191,193	0
17	CLA	2	303	60/65	0.82	0.31	120,132,139,142	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	DGD	B	850	66/66	0.82	0.25	80,94,119,120	0
24	LMG	F	309	55/55	0.83	0.23	91,108,120,124	0
17	CLA	3	604	45/65	0.84	0.30	137,162,170,173	0
22	LHG	2	317	37/49	0.84	0.32	155,163,179,187	0
19	LUT	3	614	42/42	0.84	0.30	127,146,163,166	0
24	LMG	B	852	52/55	0.84	0.23	100,127,143,148	0
17	CLA	A	814	50/65	0.85	0.24	119,141,161,164	0
17	CLA	3	610	52/65	0.85	0.30	177,188,210,215	0
25	HTG	4	321	19/19	0.85	0.30	125,139,147,147	0
17	CLA	A	843	52/65	0.86	0.38	173,188,196,199	0
17	CLA	G	103	41/65	0.86	0.19	105,122,131,136	0
20	XAT	2	315	44/44	0.86	0.30	62,89,98,100	0
17	CLA	L	203	65/65	0.86	0.25	119,143,157,167	0
21	BCR	B	846	40/40	0.86	0.21	62,77,125,126	0
23	LMT	2	318	35/35	0.86	0.15	120,133,143,146	0
21	BCR	A	850	40/40	0.87	0.24	72,108,147,148	0
17	CLA	L	204	50/65	0.87	0.33	122,147,157,163	0
17	CLA	A	817	65/65	0.87	0.26	103,129,169,173	0
17	CLA	A	813	45/65	0.87	0.18	89,111,120,126	0
21	BCR	1	316	40/40	0.88	0.39	98,125,149,151	0
17	CLA	3	602	60/65	0.88	0.20	132,157,174,178	0
17	CLA	3	609	50/65	0.88	0.26	147,163,173,175	0
17	CLA	A	824	65/65	0.88	0.23	90,102,108,111	0
17	CLA	A	833	50/65	0.88	0.22	120,135,146,157	0
17	CLA	K	202	60/65	0.89	0.28	146,176,193,196	0
21	BCR	B	847	40/40	0.89	0.23	49,65,85,92	0
17	CLA	L	202	65/65	0.89	0.29	142,154,170,175	0
21	BCR	L	206	40/40	0.89	0.27	156,168,177,178	0
17	CLA	A	815	45/65	0.89	0.20	114,125,135,140	0
17	CLA	B	817	55/65	0.89	0.19	72,86,123,134	0
17	CLA	A	820	65/65	0.89	0.20	103,126,143,144	0
19	LUT	2	314	42/42	0.90	0.18	97,114,124,130	0
21	BCR	J	105	40/40	0.90	0.17	73,85,100,101	0
21	BCR	L	205	40/40	0.90	0.22	101,116,137,137	0
17	CLA	A	825	65/65	0.90	0.20	76,98,163,165	0
21	BCR	A	847	40/40	0.90	0.45	87,120,171,173	0
22	LHG	1	317	49/49	0.90	0.21	85,100,127,130	0
17	CLA	3	612	45/65	0.90	0.33	197,212,229,235	0
17	CLA	A	811	54/65	0.90	0.24	107,127,140,140	0
25	HTG	F	305	19/19	0.90	0.20	62,83,100,104	0
17	CLA	2	312	43/65	0.90	0.16	122,142,146,147	0
17	CLA	3	611	55/65	0.90	0.14	143,177,193,195	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	BCR	F	303	40/40	0.90	0.23	48,60,65,66	0
18	CHL	2	305	48/66	0.91	0.25	105,129,162,162	0
22	LHG	A	845	27/49	0.91	0.41	128,174,191,196	0
19	LUT	1	314	42/42	0.91	0.15	67,95,116,120	0
17	CLA	A	803	55/65	0.91	0.19	64,82,119,124	0
17	CLA	A	809	65/65	0.91	0.24	100,120,149,151	0
21	BCR	A	848	40/40	0.91	0.56	92,116,163,164	0
17	CLA	J	103	42/65	0.91	0.21	83,101,120,125	0
17	CLA	1	304	42/65	0.91	0.13	80,107,125,133	0
18	CHL	1	305	48/66	0.91	0.16	102,114,132,134	0
21	BCR	L	201	40/40	0.92	0.27	95,107,120,123	0
17	CLA	4	304	50/65	0.92	0.15	55,78,112,117	0
17	CLA	1	303	51/65	0.92	0.17	112,124,138,143	0
17	CLA	A	837	65/65	0.92	0.24	92,103,174,177	0
17	CLA	A	821	49/65	0.92	0.18	130,142,169,175	0
21	BCR	B	845	40/40	0.92	0.24	62,73,118,122	0
17	CLA	B	816	65/65	0.92	0.19	65,78,97,99	0
17	CLA	A	822	51/65	0.92	0.20	137,148,164,169	0
17	CLA	B	824	55/65	0.92	0.18	63,74,104,112	0
17	CLA	A	812	65/65	0.92	0.29	88,112,121,122	0
18	CHL	3	601	56/66	0.92	0.17	108,134,146,147	0
24	LMG	4	319	50/55	0.92	0.20	68,89,131,132	0
17	CLA	A	804	65/65	0.93	0.20	77,91,115,117	0
17	CLA	2	310	52/65	0.93	0.17	106,113,156,164	0
17	CLA	1	307	65/65	0.93	0.18	74,93,123,129	0
17	CLA	1	312	55/65	0.93	0.17	74,88,119,123	0
17	CLA	1	301	65/65	0.93	0.14	60,72,107,115	0
18	CHL	2	313	43/66	0.93	0.10	99,119,137,139	0
17	CLA	A	801	65/65	0.93	0.23	52,67,83,87	0
17	CLA	2	308	60/65	0.93	0.19	111,122,145,151	0
17	CLA	A	834	45/65	0.93	0.36	156,170,177,185	0
17	CLA	A	835	51/65	0.93	0.19	78,102,129,135	0
17	CLA	A	829	65/65	0.94	0.20	68,82,94,98	0
17	CLA	A	830	50/65	0.94	0.20	102,117,152,156	0
17	CLA	A	831	65/65	0.94	0.25	84,103,108,110	0
21	BCR	I	101	40/40	0.94	0.21	92,99,112,114	0
17	CLA	4	312	56/65	0.94	0.14	70,84,109,112	0
17	CLA	3	606	47/65	0.94	0.15	113,124,135,138	0
17	CLA	A	816	65/65	0.94	0.19	116,134,152,155	0
18	CHL	2	304	43/66	0.94	0.18	101,117,129,137	0
17	CLA	3	608	50/65	0.94	0.17	120,130,136,139	0
18	CHL	2	306	51/66	0.94	0.17	84,101,141,144	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	A	840	65/65	0.94	0.28	52,63,76,90	0
17	CLA	A	819	45/65	0.94	0.19	126,138,151,155	0
22	LHG	B	801	23/49	0.94	0.13	67,88,119,120	0
17	CLA	B	803	65/65	0.94	0.22	106,119,153,161	0
17	CLA	B	804	65/65	0.94	0.23	50,60,68,74	0
17	CLA	B	813	54/65	0.94	0.12	61,90,114,117	0
17	CLA	B	814	55/65	0.94	0.15	61,75,121,123	0
17	CLA	B	815	65/65	0.94	0.17	57,67,75,77	0
17	CLA	1	310	52/65	0.94	0.15	88,103,145,147	0
17	CLA	1	306	46/65	0.94	0.17	91,101,117,120	0
17	CLA	B	818	55/65	0.94	0.14	63,73,95,102	0
21	BCR	4	318	40/40	0.94	0.16	61,90,99,104	0
17	CLA	B	823	65/65	0.94	0.18	62,75,131,140	0
17	CLA	1	302	65/65	0.94	0.16	70,87,125,128	0
17	CLA	B	842	65/65	0.94	0.16	57,69,84,94	0
17	CLA	3	603	50/65	0.94	0.23	116,128,132,135	0
17	CLA	G	104	50/65	0.94	0.14	76,95,125,133	0
21	BCR	B	844	40/40	0.94	0.19	69,83,97,102	0
17	CLA	G	105	46/65	0.94	0.21	92,122,136,144	0
17	CLA	1	308	60/65	0.94	0.15	89,100,129,133	0
27	PQN	B	843	33/33	0.94	0.26	65,84,91,97	0
17	CLA	1	311	60/65	0.95	0.14	64,75,111,113	0
17	CLA	B	807	65/65	0.95	0.17	57,69,79,82	0
17	CLA	B	812	65/65	0.95	0.20	76,107,137,144	0
17	CLA	A	805	65/65	0.95	0.25	69,82,91,93	0
17	CLA	A	806	65/65	0.95	0.17	72,81,131,134	0
17	CLA	2	307	50/65	0.95	0.16	90,95,110,113	0
17	CLA	A	826	65/65	0.95	0.20	90,119,149,154	0
18	CHL	4	301	61/66	0.95	0.13	66,78,116,118	0
17	CLA	A	828	65/65	0.95	0.29	73,89,106,107	0
17	CLA	A	810	65/65	0.95	0.19	80,88,102,113	0
17	CLA	B	820	60/65	0.95	0.29	46,66,85,87	0
19	LUT	4	316	42/42	0.95	0.14	63,72,86,91	0
20	XAT	1	315	44/44	0.95	0.15	62,89,98,100	0
17	CLA	1	309	65/65	0.95	0.23	84,105,142,147	0
17	CLA	3	605	42/65	0.95	0.13	125,135,143,147	0
17	CLA	B	826	65/65	0.95	0.21	50,67,87,92	0
17	CLA	B	831	65/65	0.95	0.19	48,63,105,107	0
17	CLA	B	838	65/65	0.95	0.16	43,58,72,81	0
17	CLA	B	839	47/65	0.95	0.17	52,58,84,93	0
17	CLA	A	832	65/65	0.95	0.19	89,101,142,149	0
17	CLA	4	309	60/65	0.95	0.13	61,72,98,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	4	310	60/65	0.95	0.19	68,89,116,121	0
25	HTG	A	854	19/19	0.95	0.10	63,78,85,96	0
17	CLA	4	311	52/65	0.95	0.14	72,83,118,119	0
17	CLA	J	101	65/65	0.95	0.17	62,76,93,101	0
17	CLA	2	309	41/65	0.95	0.15	126,134,143,146	0
17	CLA	A	839	65/65	0.95	0.19	47,59,97,101	0
25	HTG	J	102	19/19	0.95	0.24	75,82,115,120	0
17	CLA	4	313	45/65	0.95	0.14	73,98,120,127	0
17	CLA	2	301	65/65	0.95	0.15	86,105,122,135	0
27	PQN	A	842	33/33	0.95	0.30	49,61,85,91	0
17	CLA	2	302	51/65	0.95	0.12	89,102,120,127	0
17	CLA	4	308	50/65	0.96	0.15	52,64,103,109	0
21	BCR	B	848	40/40	0.96	0.20	48,58,74,79	0
21	BCR	B	849	40/40	0.96	0.21	60,75,82,83	0
17	CLA	2	319	46/65	0.96	0.15	68,80,109,111	0
21	BCR	F	308	40/40	0.96	0.15	53,62,72,78	0
17	CLA	A	827	65/65	0.96	0.26	64,76,89,94	0
17	CLA	B	822	50/65	0.96	0.17	70,80,109,113	0
21	BCR	J	104	40/40	0.96	0.17	63,73,87,91	0
17	CLA	A	841	65/65	0.96	0.23	82,100,138,149	0
17	CLA	2	311	65/65	0.96	0.16	109,127,142,147	0
17	CLA	B	825	60/65	0.96	0.19	51,60,107,115	0
17	CLA	A	853	65/65	0.96	0.31	48,61,88,96	0
18	CHL	3	607	47/66	0.96	0.17	124,135,160,166	0
17	CLA	B	829	65/65	0.96	0.22	54,65,124,133	0
18	CHL	4	305	56/66	0.96	0.15	68,77,116,118	0
22	LHG	A	844	49/49	0.96	0.27	69,83,92,96	0
18	CHL	4	306	51/66	0.96	0.16	66,79,130,133	0
18	CHL	4	315	43/66	0.96	0.12	67,88,102,117	0
17	CLA	3	613	46/65	0.96	0.13	106,121,156,159	0
17	CLA	B	832	50/65	0.96	0.13	53,62,96,105	0
17	CLA	B	833	60/65	0.96	0.13	44,58,104,110	0
17	CLA	B	834	58/65	0.96	0.13	46,59,102,105	0
17	CLA	B	835	65/65	0.96	0.19	53,67,106,116	0
17	CLA	B	836	45/65	0.96	0.12	62,71,94,97	0
17	CLA	4	302	60/65	0.96	0.12	50,62,94,97	0
20	XAT	4	317	44/44	0.96	0.15	58,67,81,88	0
17	CLA	B	805	65/65	0.96	0.27	62,78,101,112	0
17	CLA	B	806	45/65	0.96	0.13	62,71,90,114	0
17	CLA	F	304	65/65	0.96	0.17	44,58,76,84	0
17	CLA	F	307	55/65	0.96	0.13	49,67,123,125	0
17	CLA	4	303	60/65	0.96	0.16	52,67,108,113	0

Continued on next page...

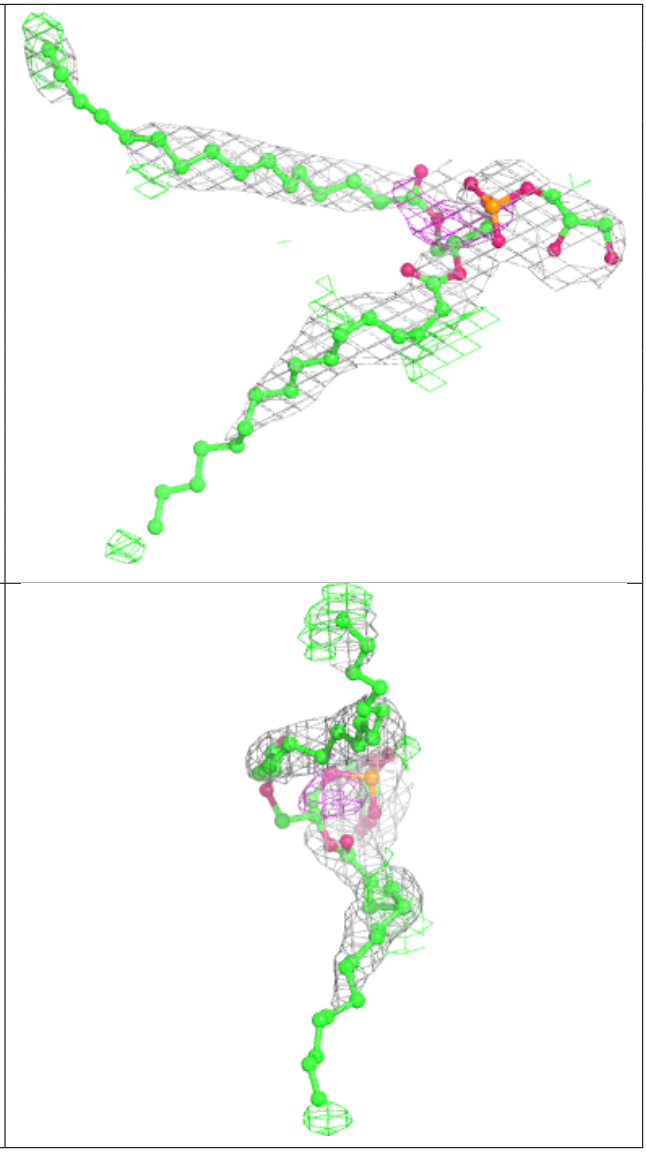
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	CLA	B	809	65/65	0.96	0.17	71,88,138,144	0
17	CLA	B	811	65/65	0.96	0.21	70,83,118,125	0
17	CLA	4	314	47/65	0.96	0.14	57,70,104,106	0
17	CLA	1	313	46/65	0.96	0.13	73,84,105,117	0
21	BCR	A	851	40/40	0.96	0.27	45,63,77,79	0
17	CLA	A	823	55/65	0.96	0.14	105,121,137,143	0
17	CLA	A	802	65/65	0.96	0.19	59,73,82,90	0
17	CLA	A	836	65/65	0.96	0.14	86,106,146,154	0
17	CLA	B	830	65/65	0.97	0.27	48,68,83,97	0
17	CLA	B	821	65/65	0.97	0.24	56,67,98,103	0
17	CLA	B	810	65/65	0.97	0.23	63,73,95,101	0
17	CLA	A	838	65/65	0.97	0.21	45,55,71,78	0
17	CLA	A	818	65/65	0.97	0.27	91,103,125,130	0
17	CLA	B	808	65/65	0.97	0.19	49,70,88,92	0
17	CLA	B	819	59/65	0.97	0.22	55,66,81,85	0
17	CLA	B	837	60/65	0.97	0.19	46,57,105,106	0
17	CLA	B	827	65/65	0.97	0.23	43,58,106,109	0
17	CLA	B	802	65/65	0.97	0.30	48,60,81,93	0
17	CLA	B	840	65/65	0.97	0.18	70,91,118,124	0
17	CLA	B	841	65/65	0.97	0.20	57,72,127,136	0
17	CLA	B	828	65/65	0.98	0.23	45,58,72,78	0
17	CLA	F	306	45/65	0.98	0.11	55,66,75,85	0
17	CLA	A	808	65/65	0.98	0.15	54,69,114,118	0
18	CHL	4	307	51/66	0.98	0.11	60,73,90,101	0
17	CLA	A	807	65/65	0.98	0.19	59,73,104,120	0
28	SF4	A	852	8/8	0.99	0.21	55,67,73,74	0
28	SF4	C	101	8/8	0.99	0.19	69,76,84,85	0
28	SF4	C	102	8/8	0.99	0.14	75,76,85,89	0

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

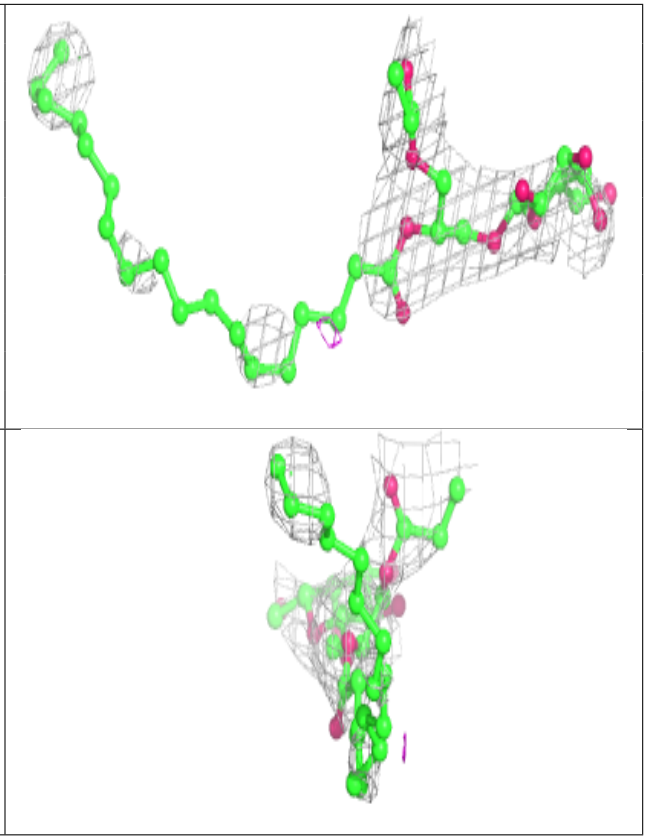
Electron density around LHG G 102:

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



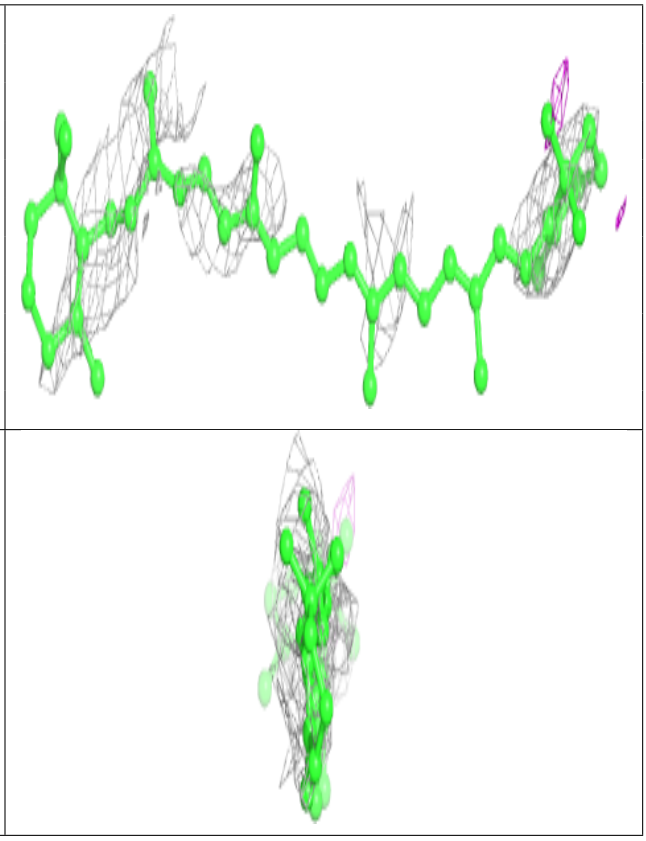
Electron density around LMG G 101:

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



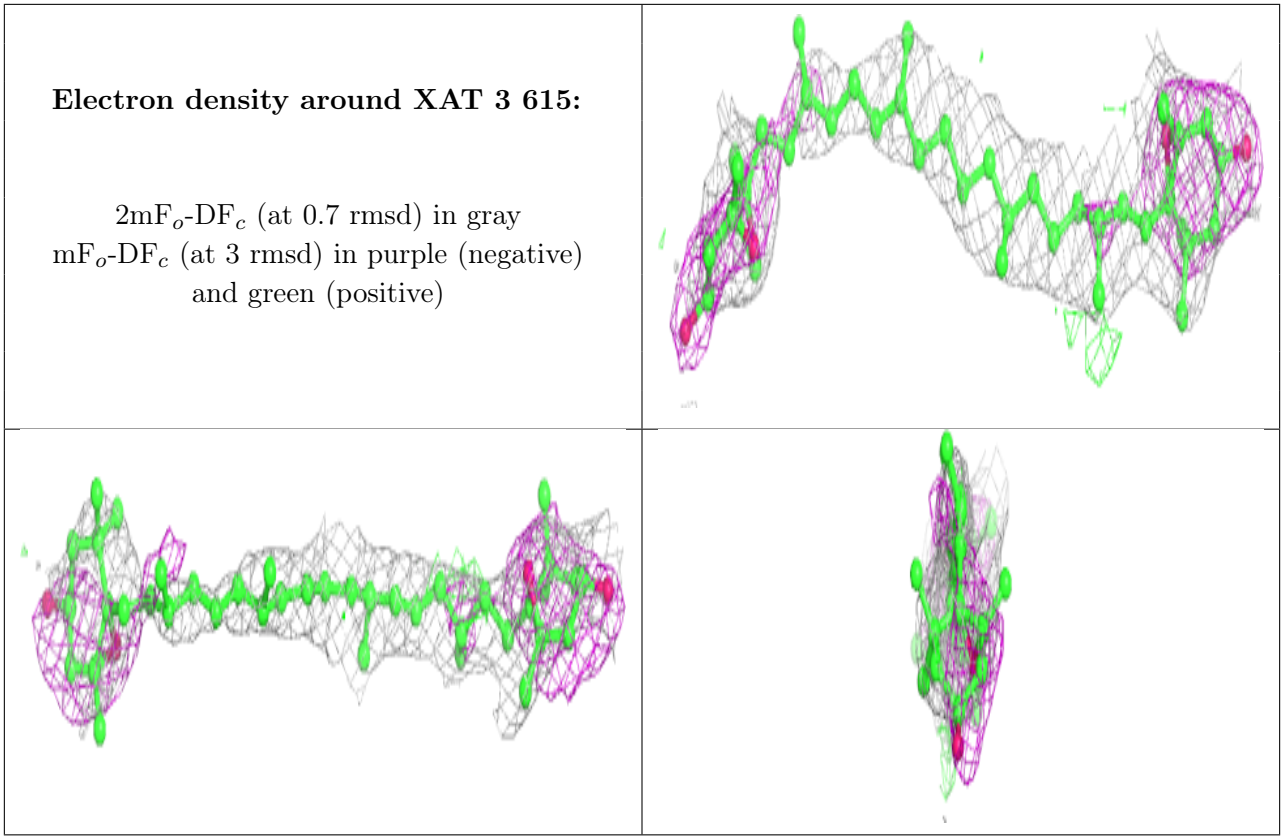
Electron density around BCR K 203:

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



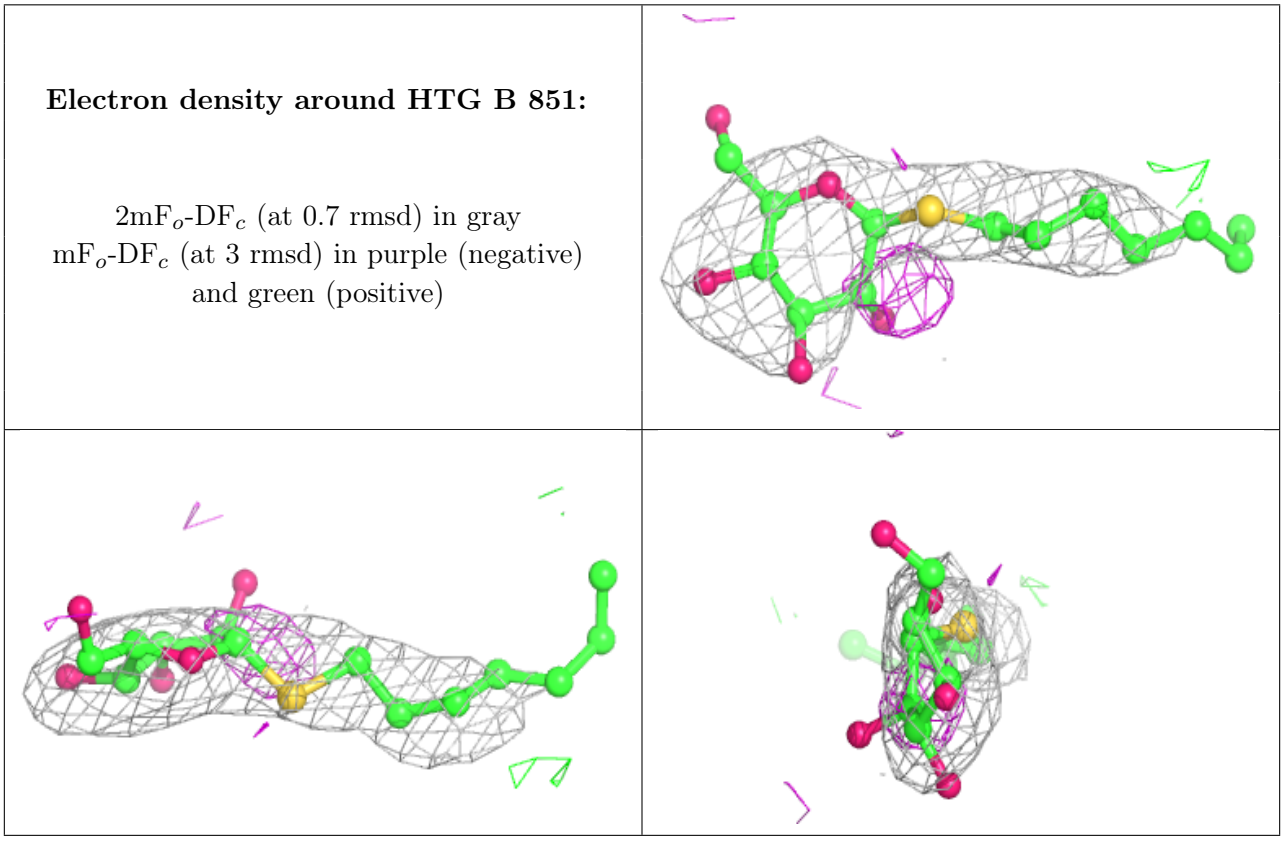
Electron density around XAT 3 615:

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



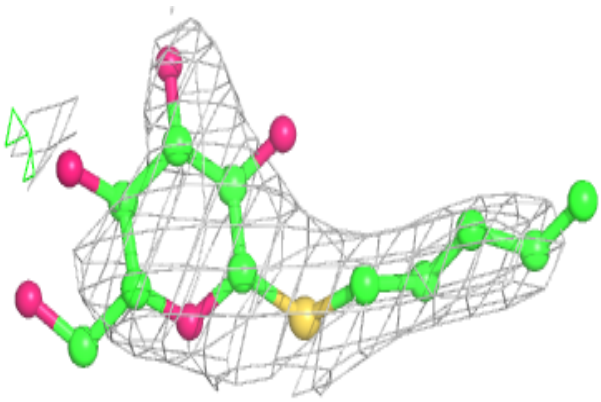
Electron density around HTG B 851:

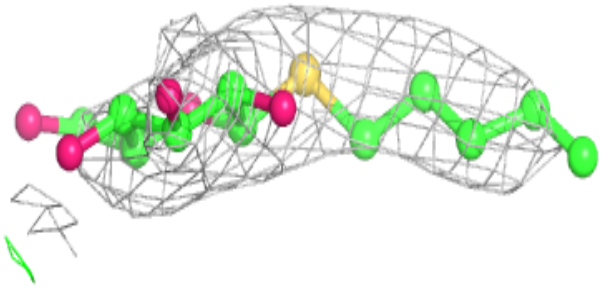
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

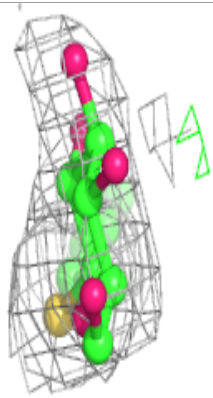


Electron density around HTG F 301:

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

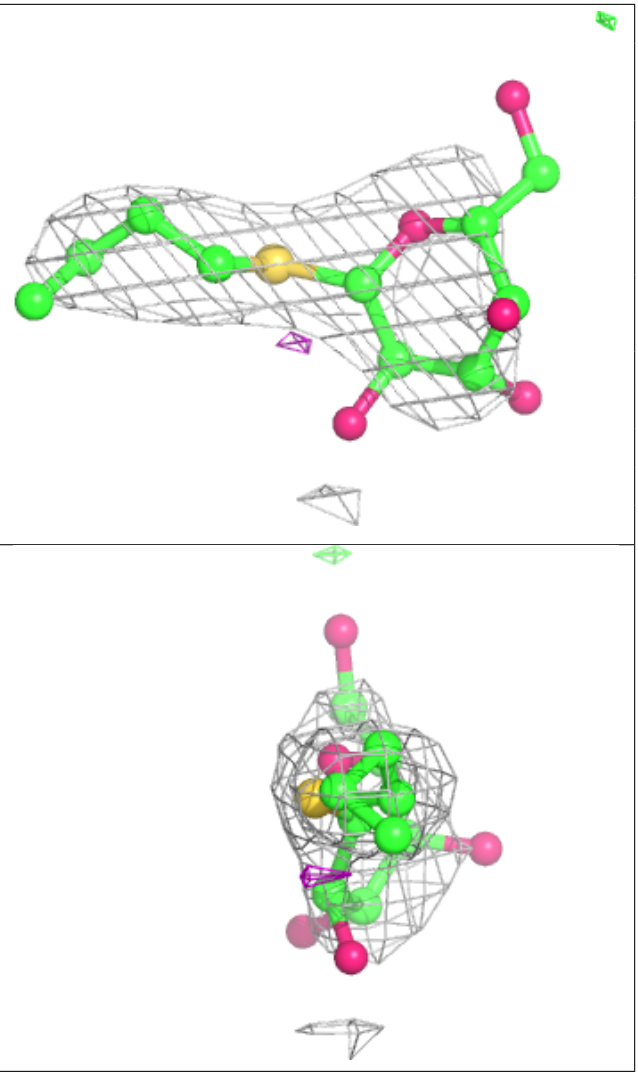






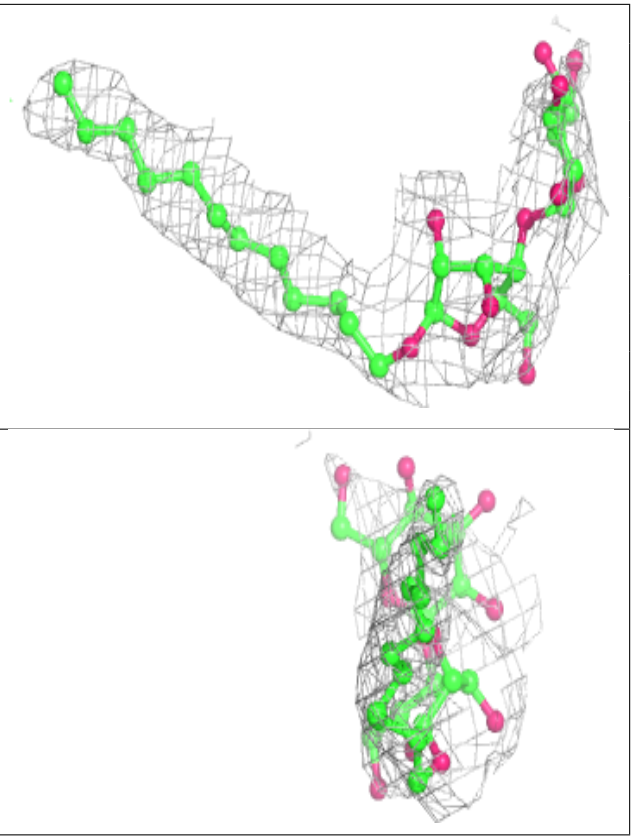
Electron density around HTG F 310:

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



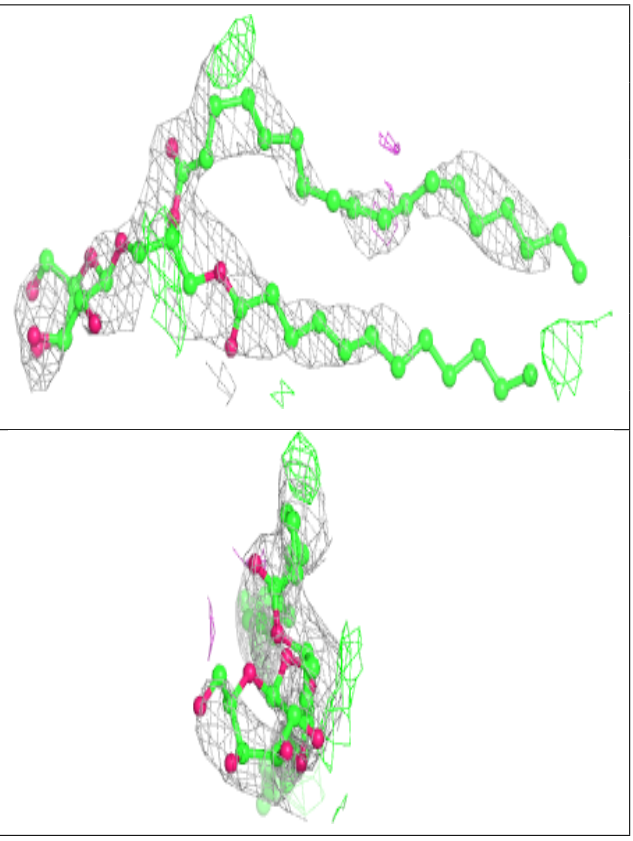
Electron density around LMT A 855:

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



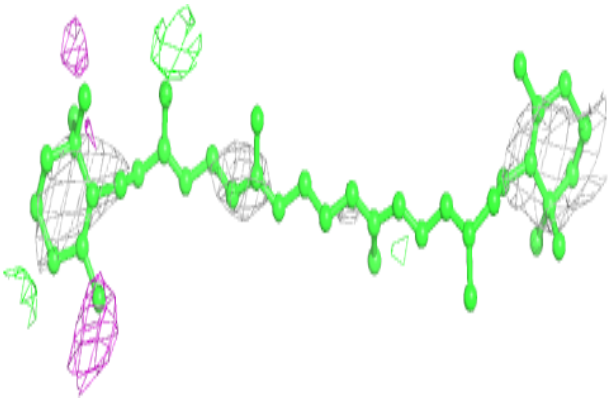
Electron density around LMG 4 320:

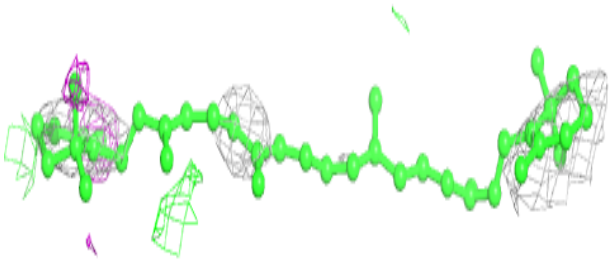
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

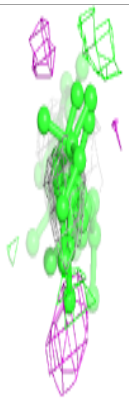


Electron density around BCR 2 316:

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

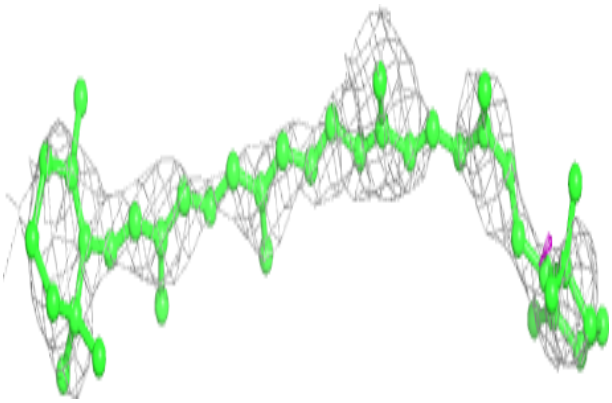


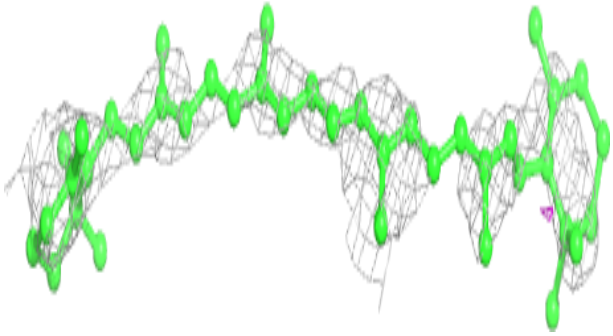


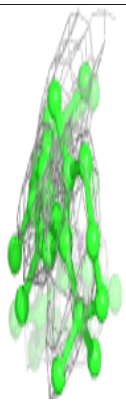


Electron density around BCR A 846:

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

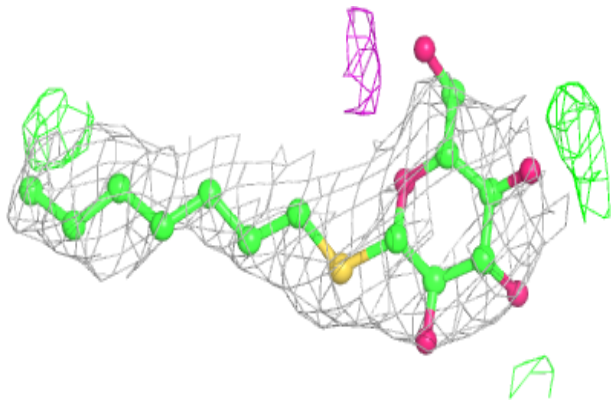


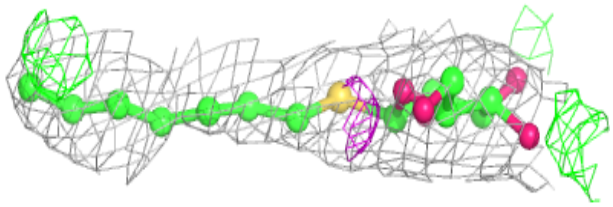


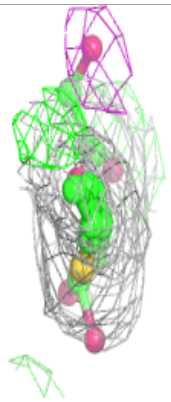


Electron density around HTG 4 322:

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

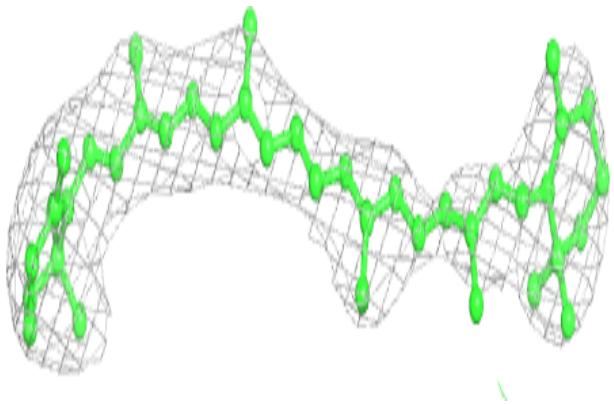


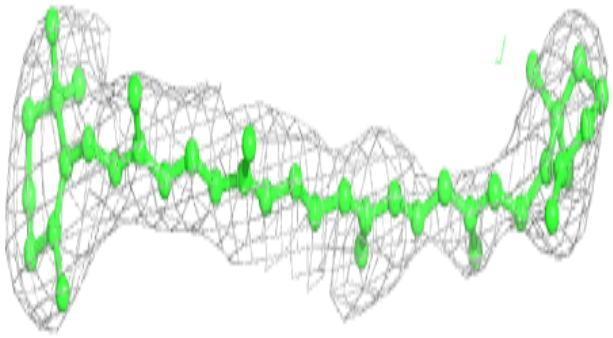


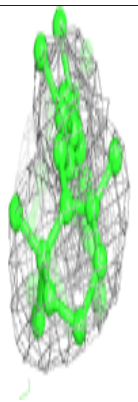


Electron density around BCR G 106:

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

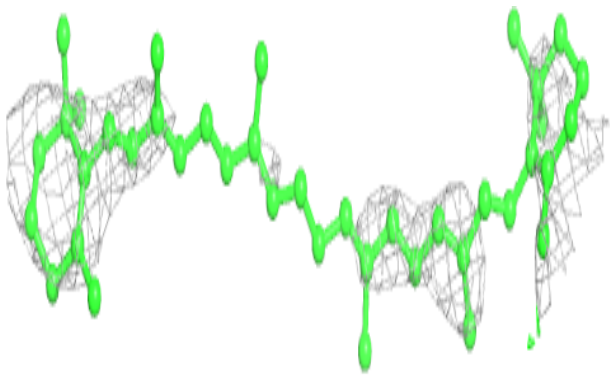


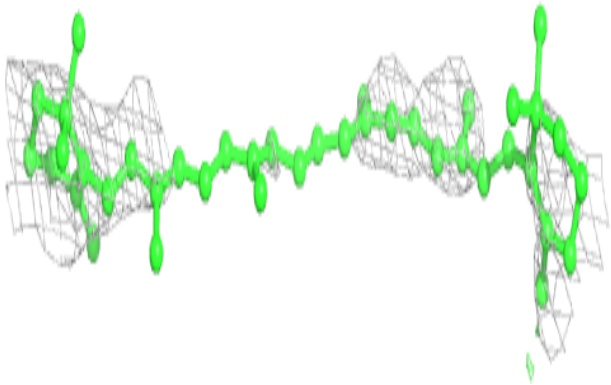


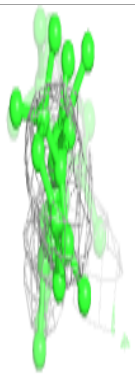


Electron density around BCR 3 616:

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

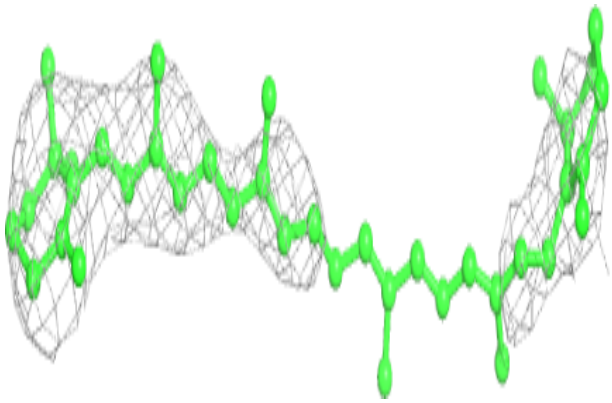


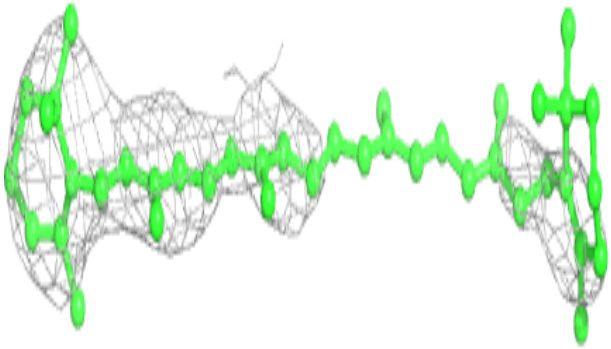


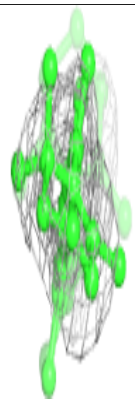


Electron density around BCR A 849:

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

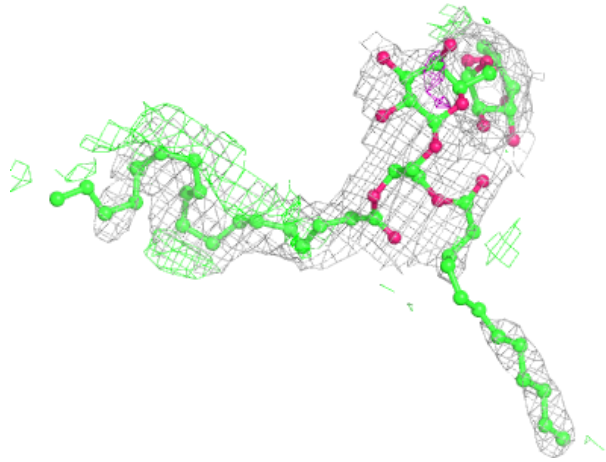


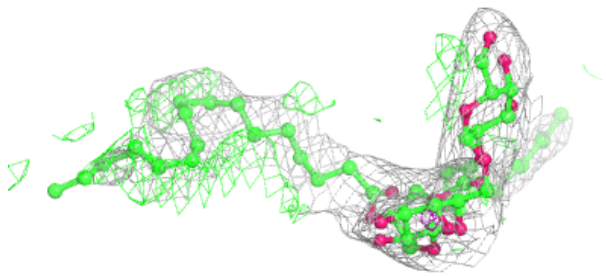


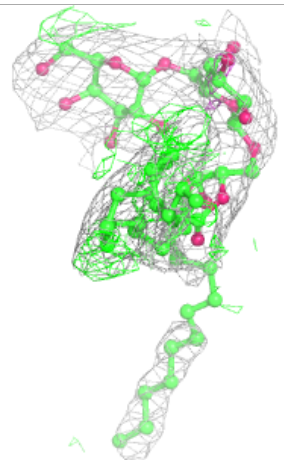


Electron density around DGD 4 323:

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

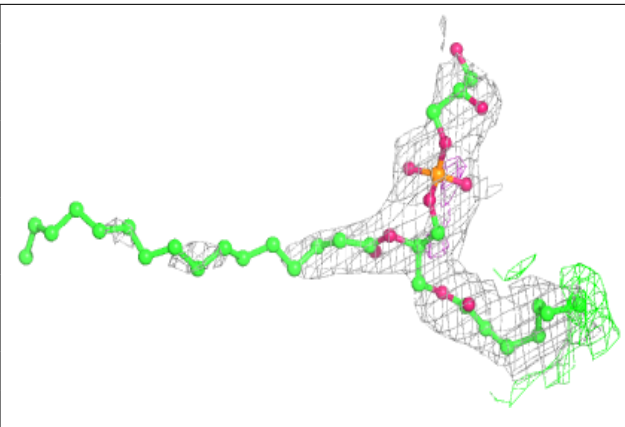


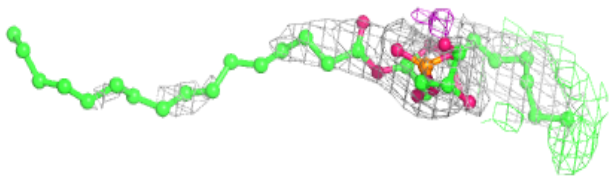


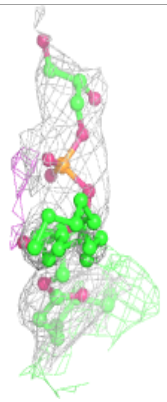


Electron density around LHG F 302:

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

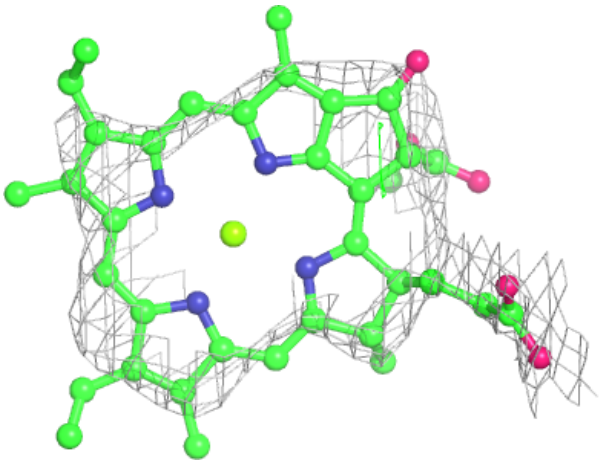


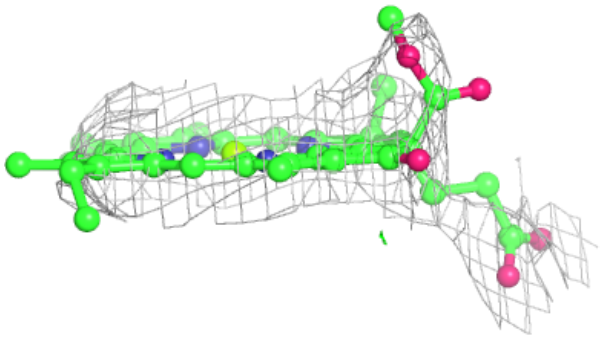


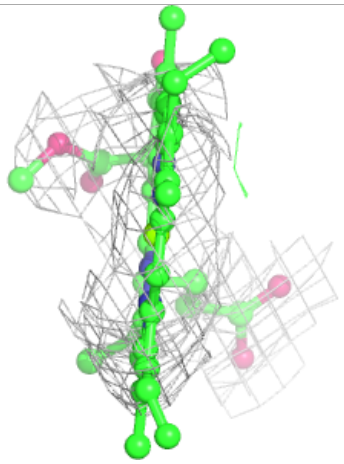


Electron density around CLA K 201:

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

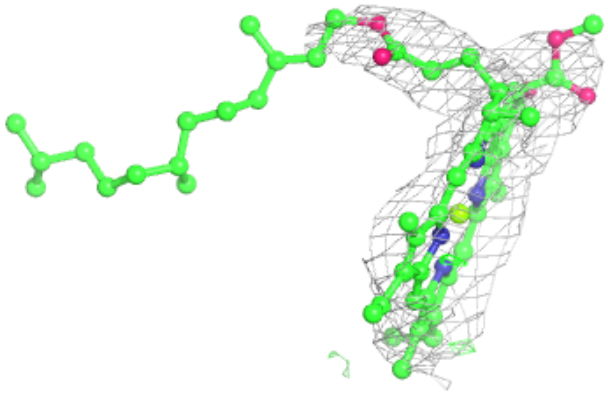


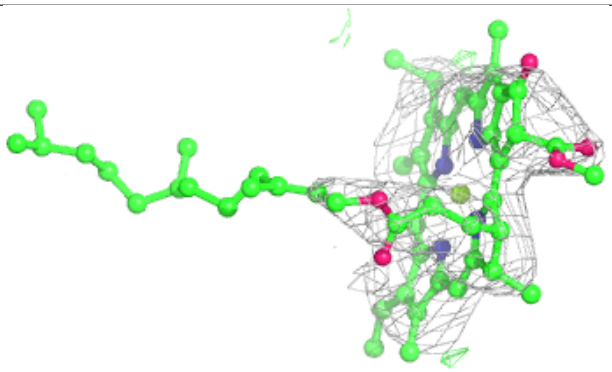


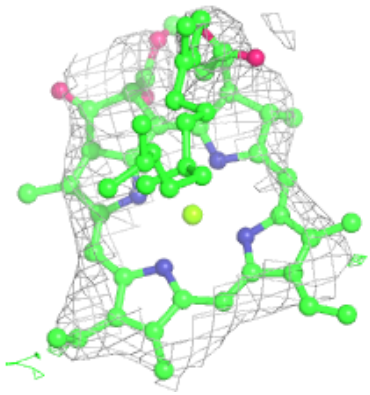


Electron density around CLA 2 303:

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

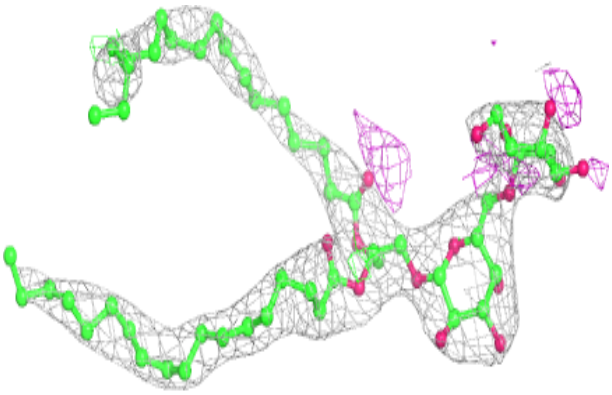


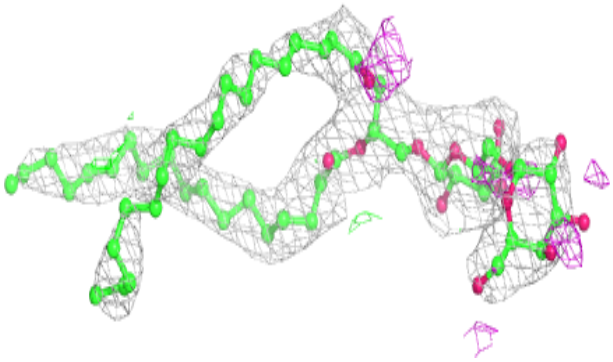


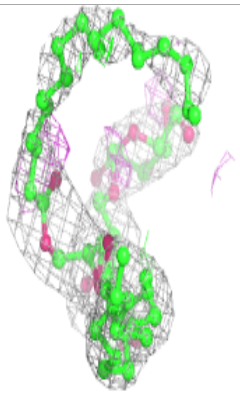


Electron density around DGD B 850:

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

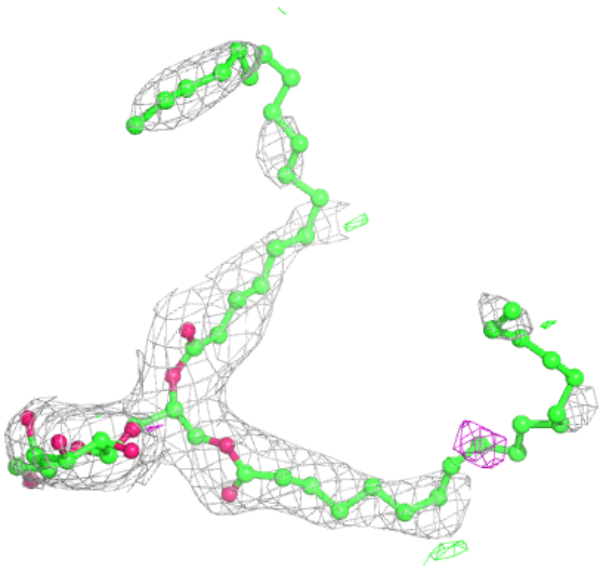


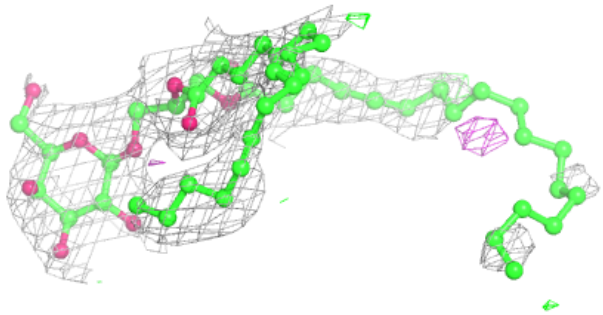


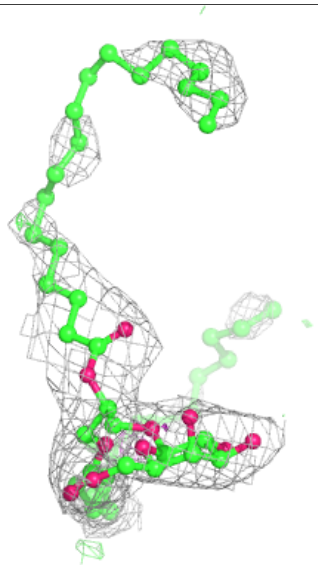


Electron density around LMG F 309:

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

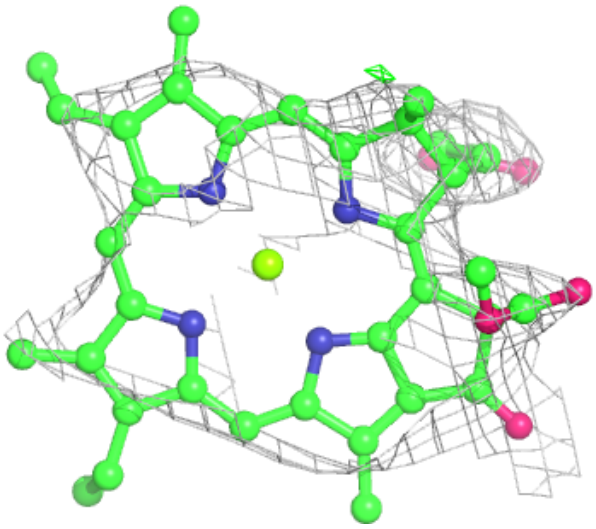


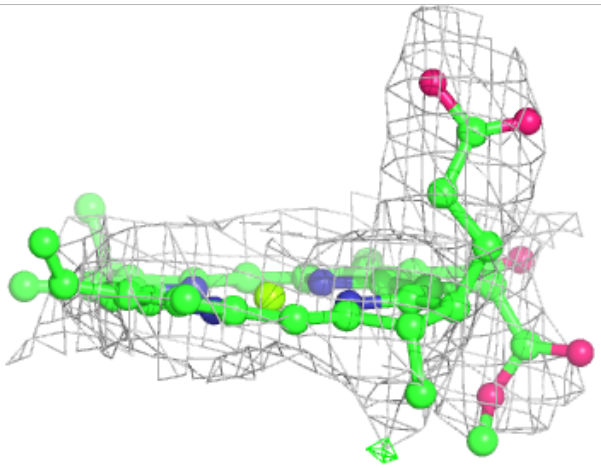


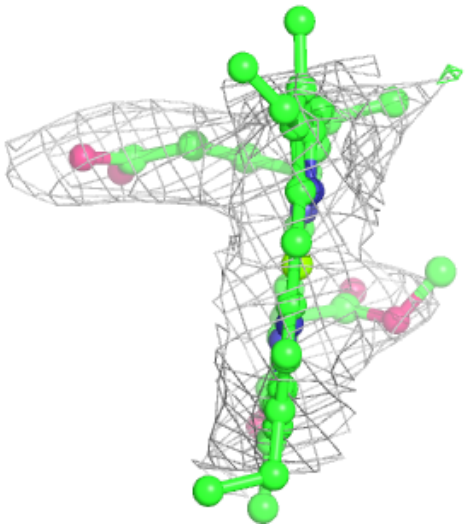


Electron density around CLA 3 604:

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

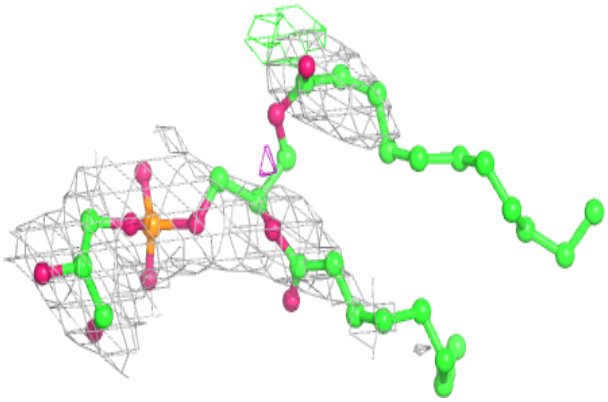


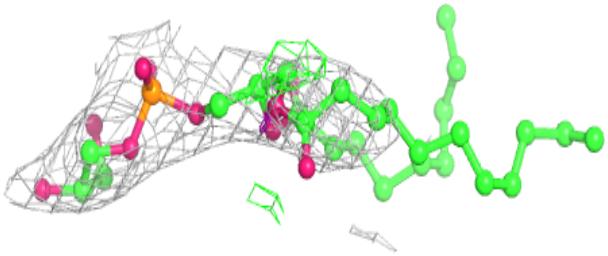




Electron density around LHG 2 317:

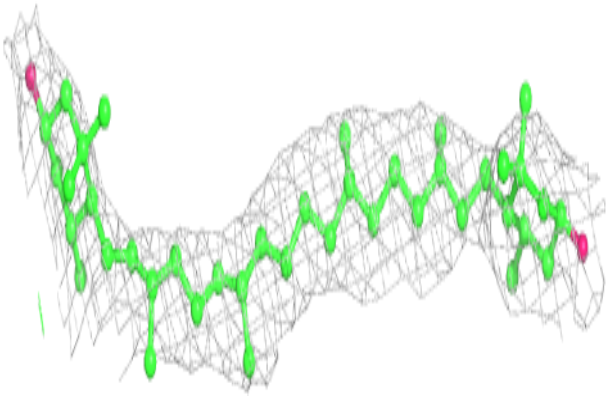
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

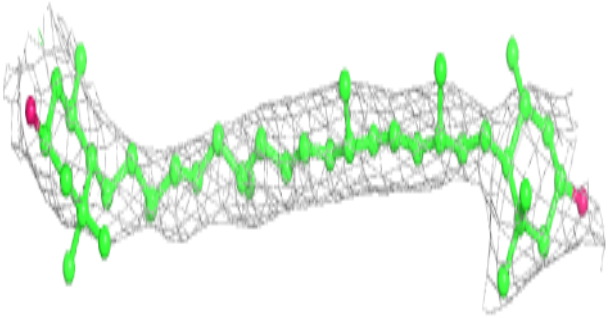


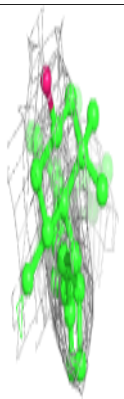


Electron density around LUT 3 614:

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

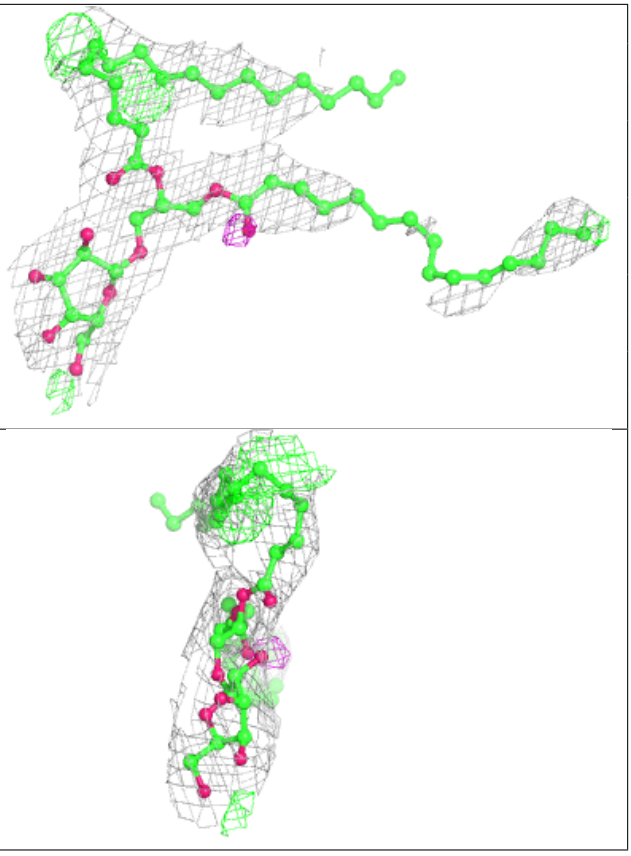


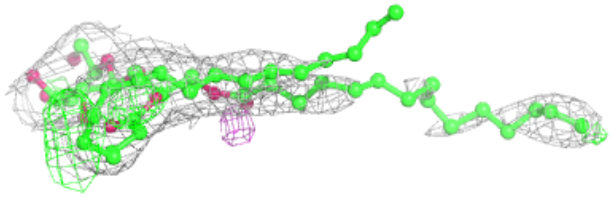




Electron density around LMG B 852:

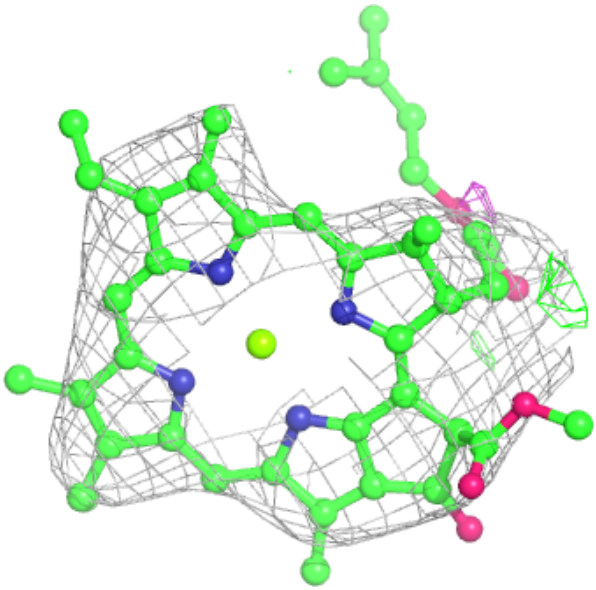
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

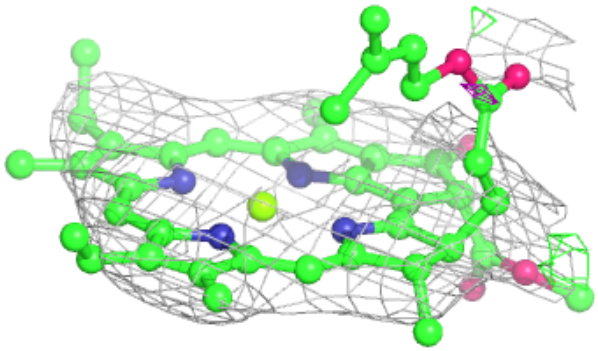


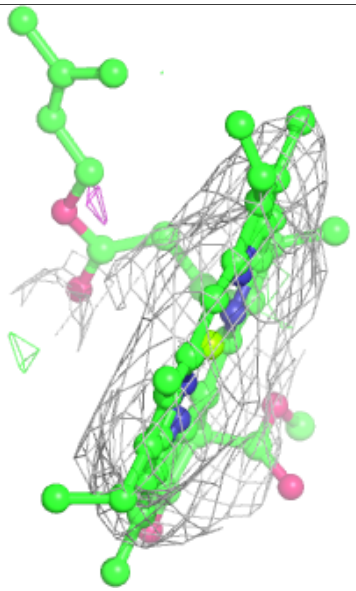


Electron density around CLA A 814:

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

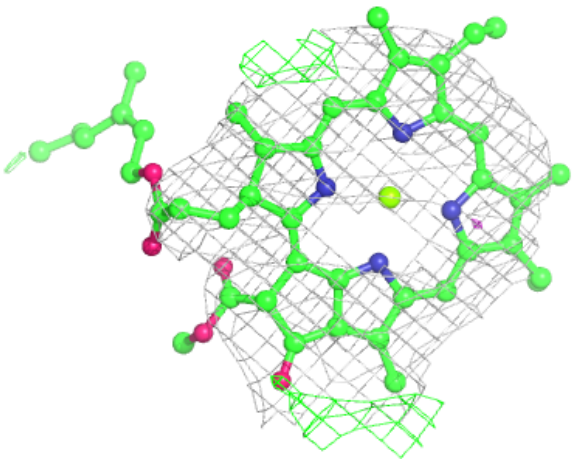


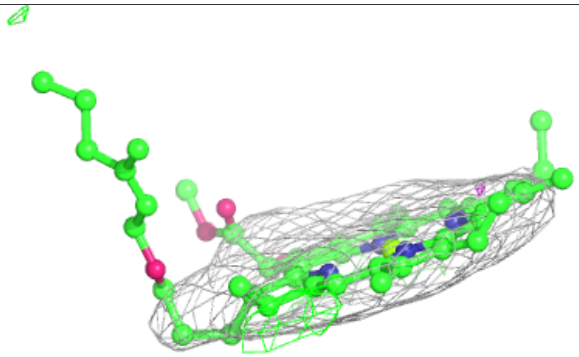


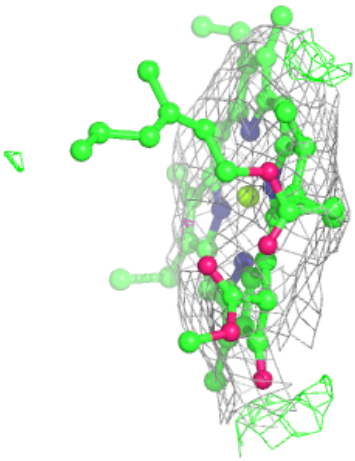


Electron density around CLA 3 610:

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

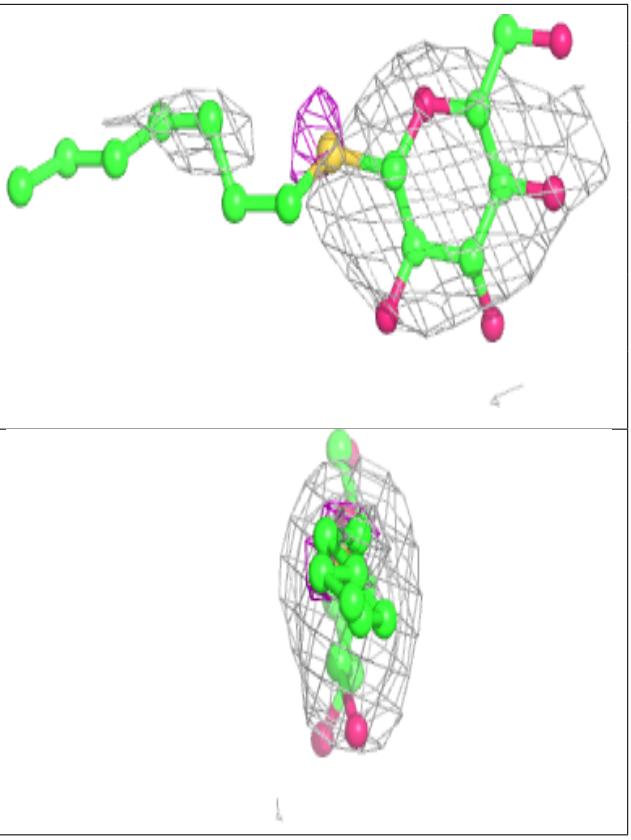


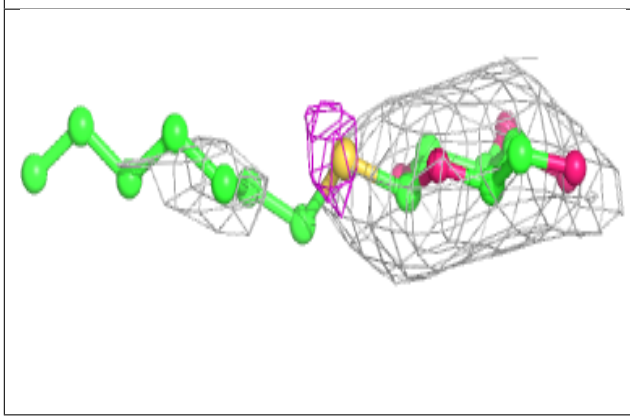




Electron density around HTG 4 321:

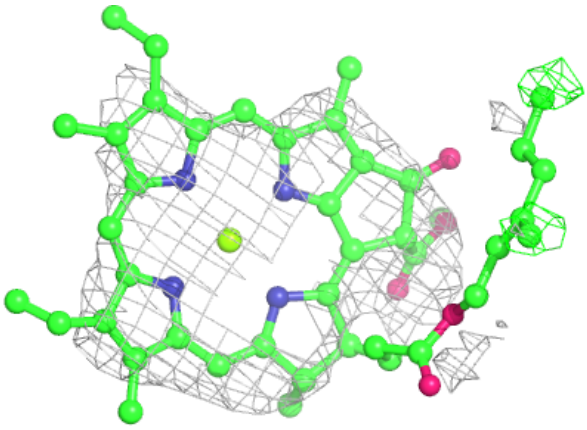
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

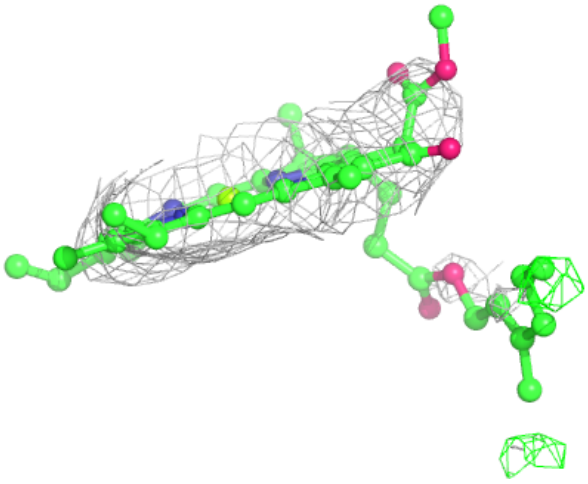


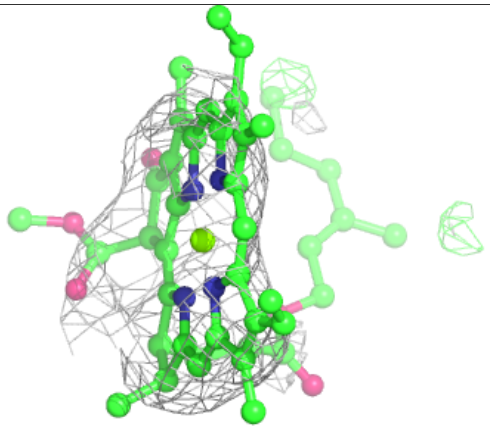


Electron density around CLA A 843:

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

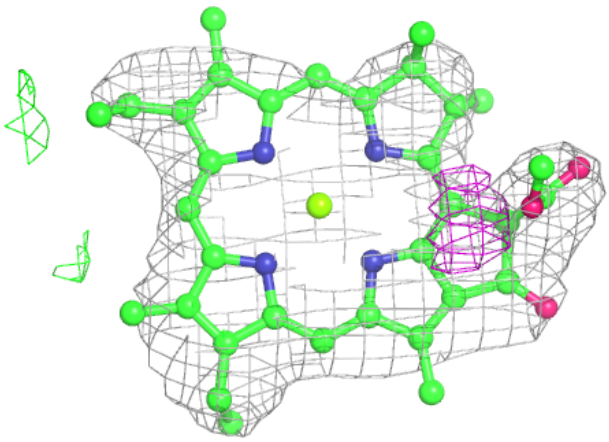


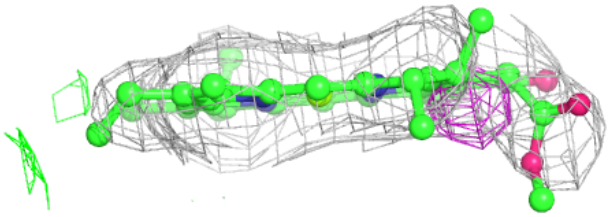


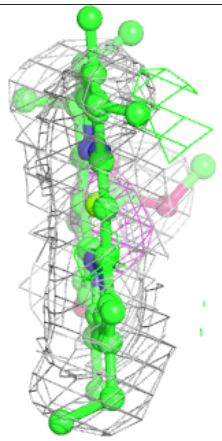


Electron density around CLA G 103:

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

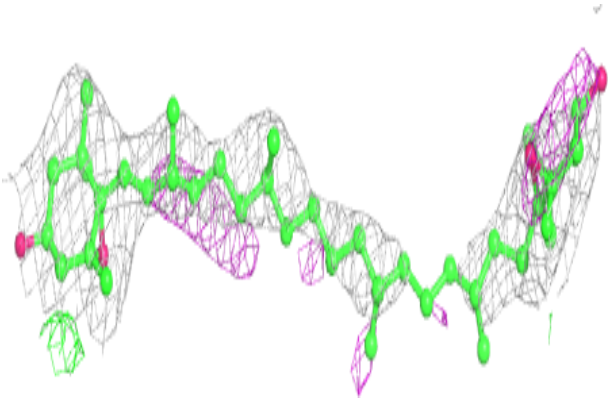


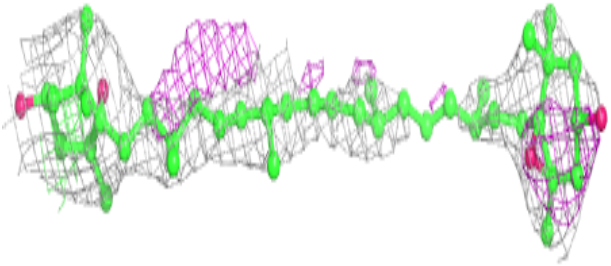


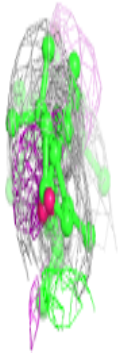


Electron density around XAT 2 315:

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

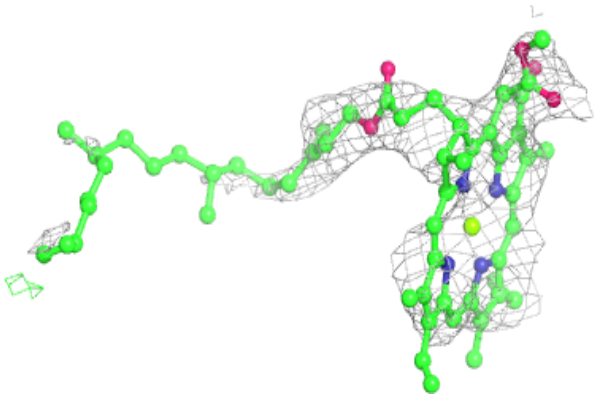


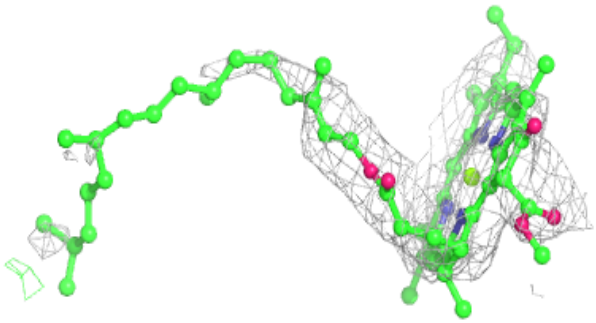


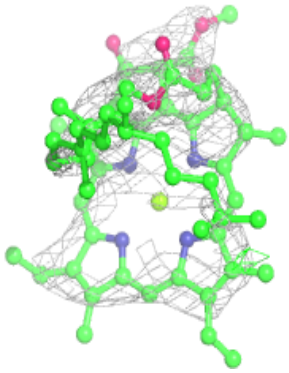


Electron density around CLA L 203:

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

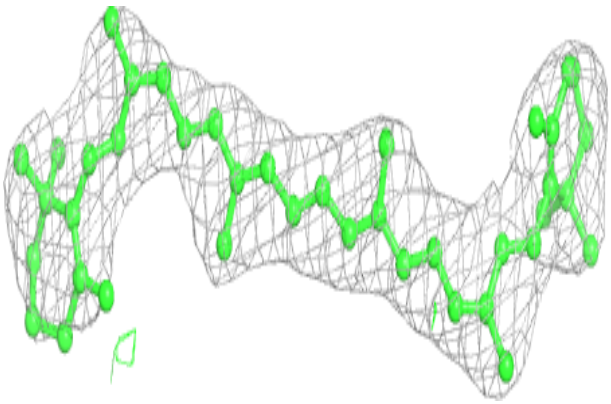


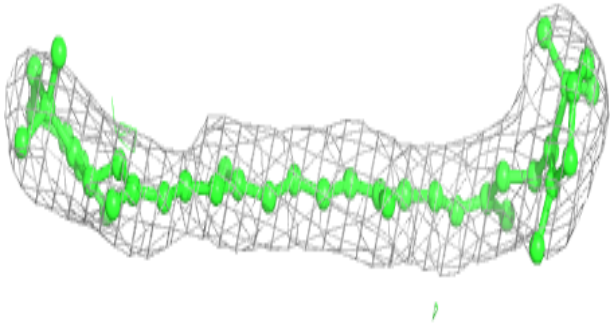


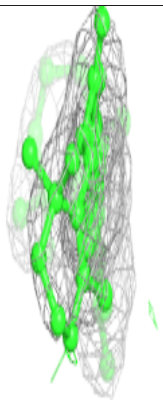


Electron density around BCR B 846:

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

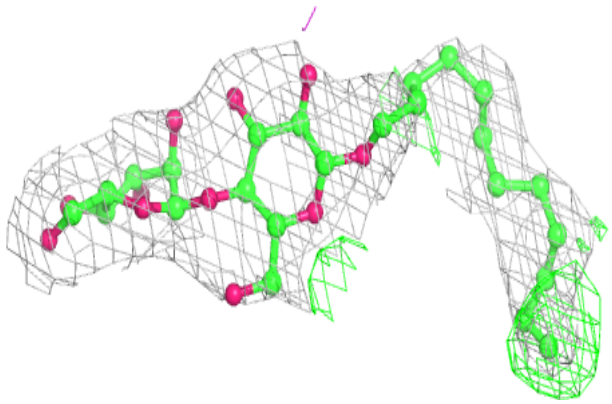


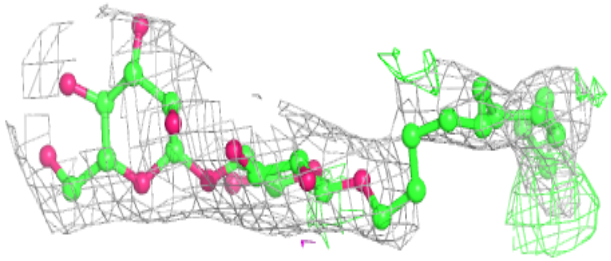


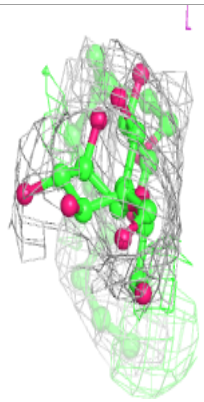


Electron density around LMT 2 318:

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

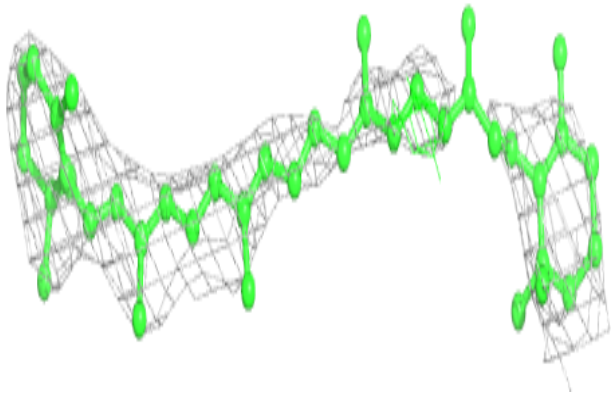


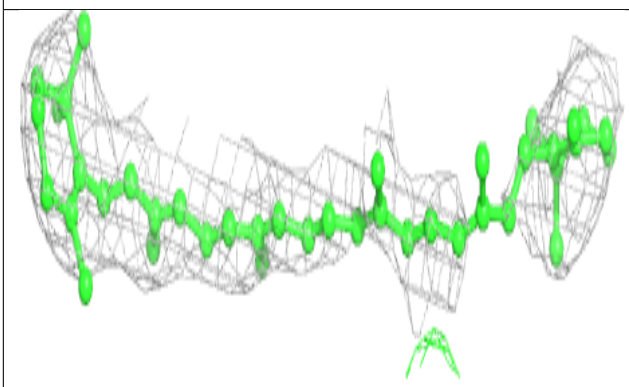


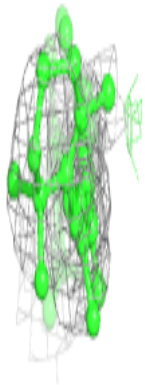


Electron density around BCR A 850:

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

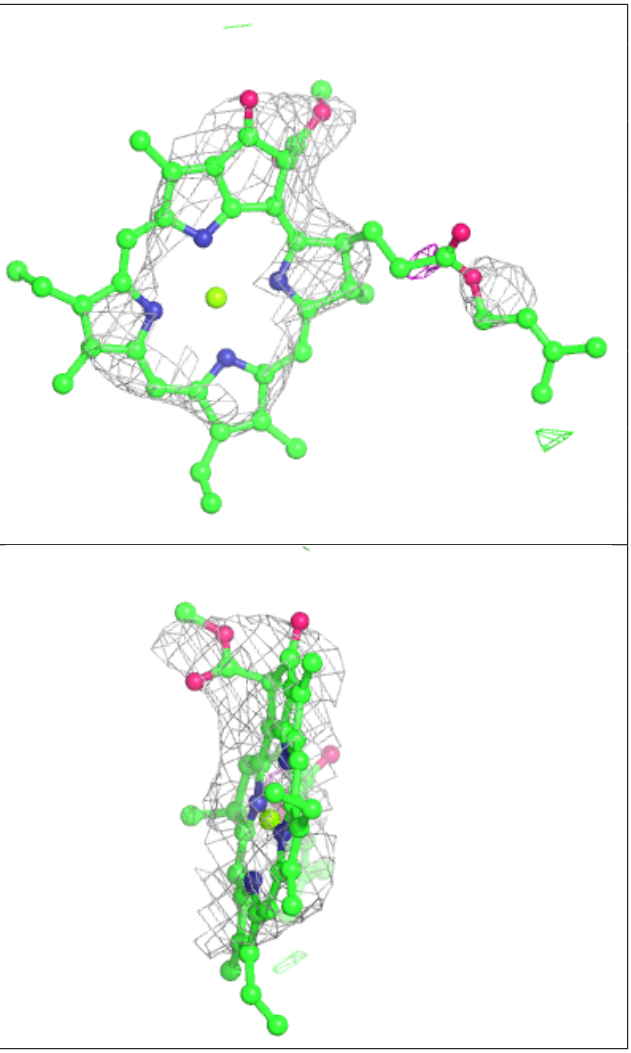






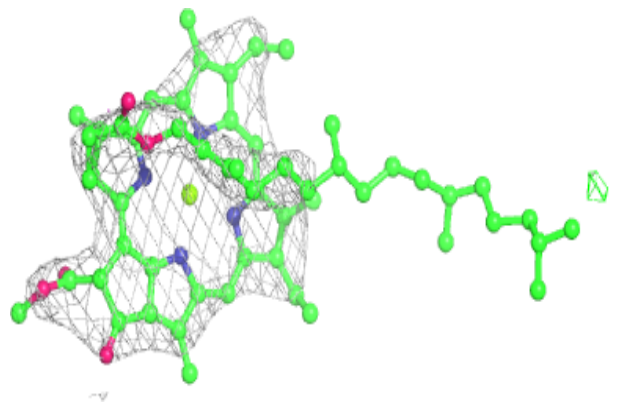
Electron density around CLA L 204:

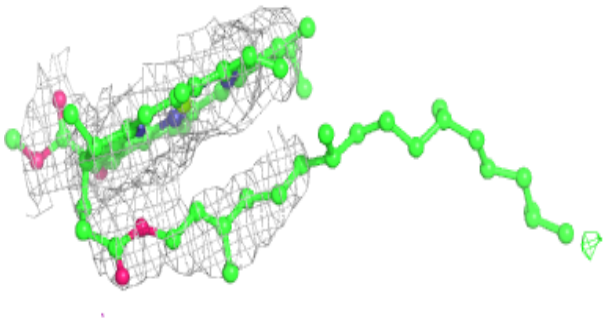
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

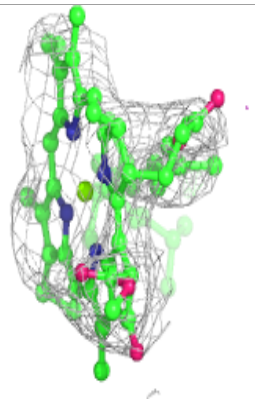


Electron density around CLA A 817:

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

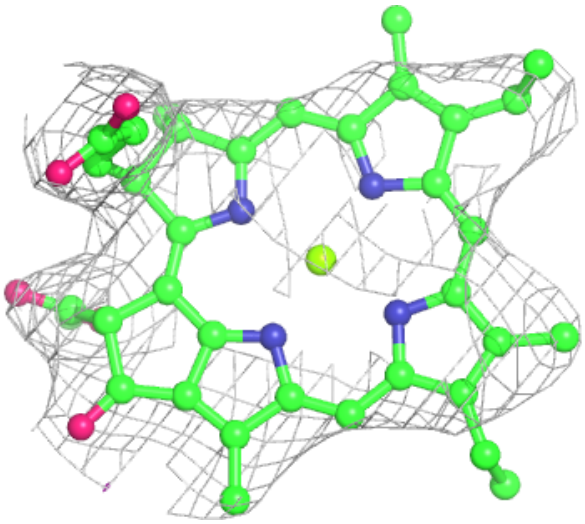


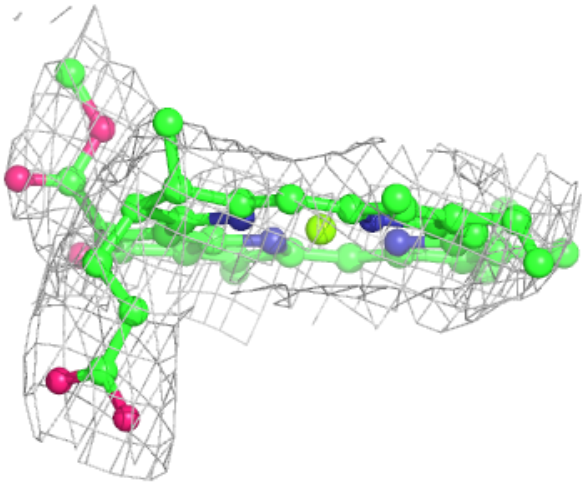


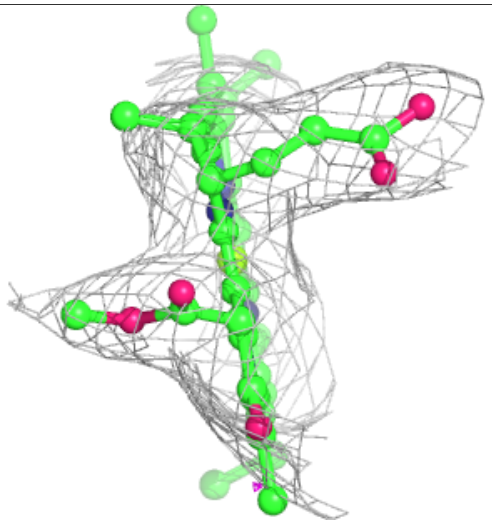


Electron density around CLA A 813:

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

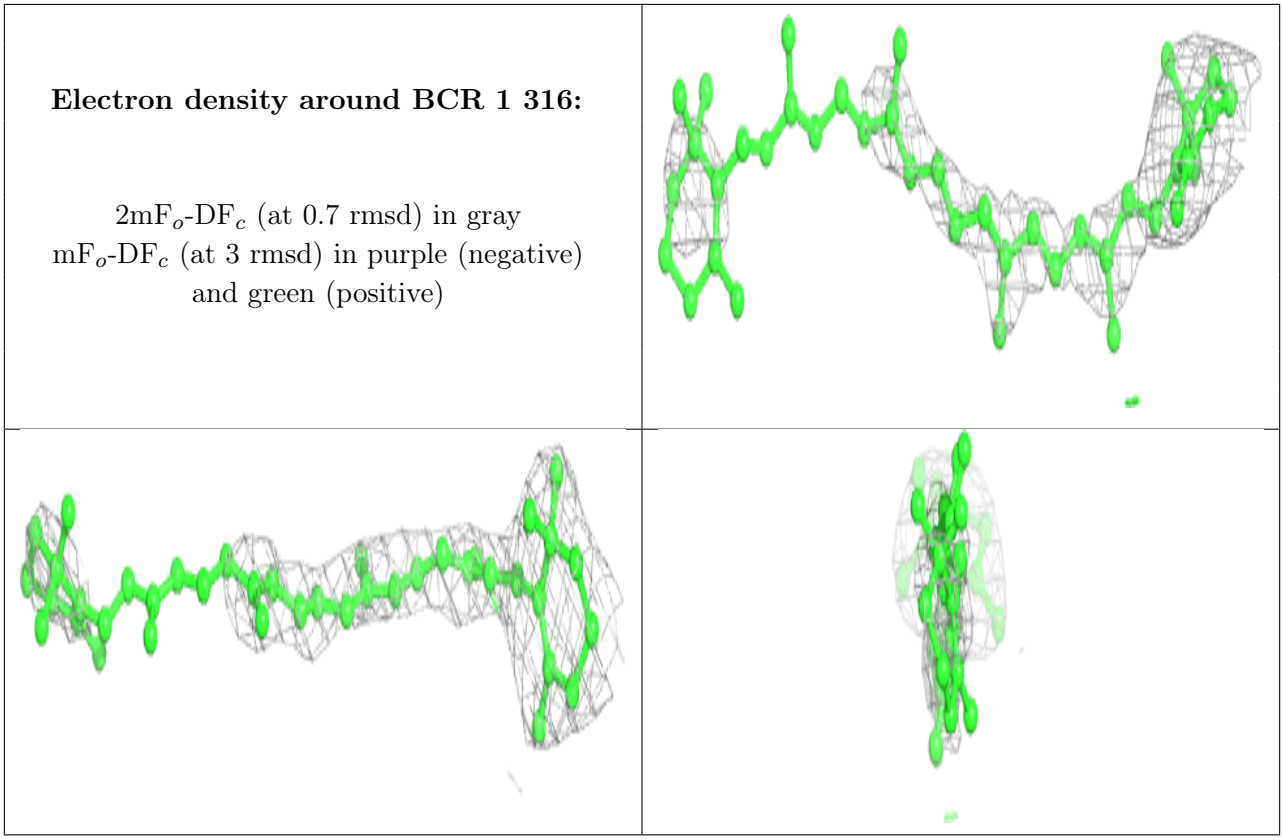






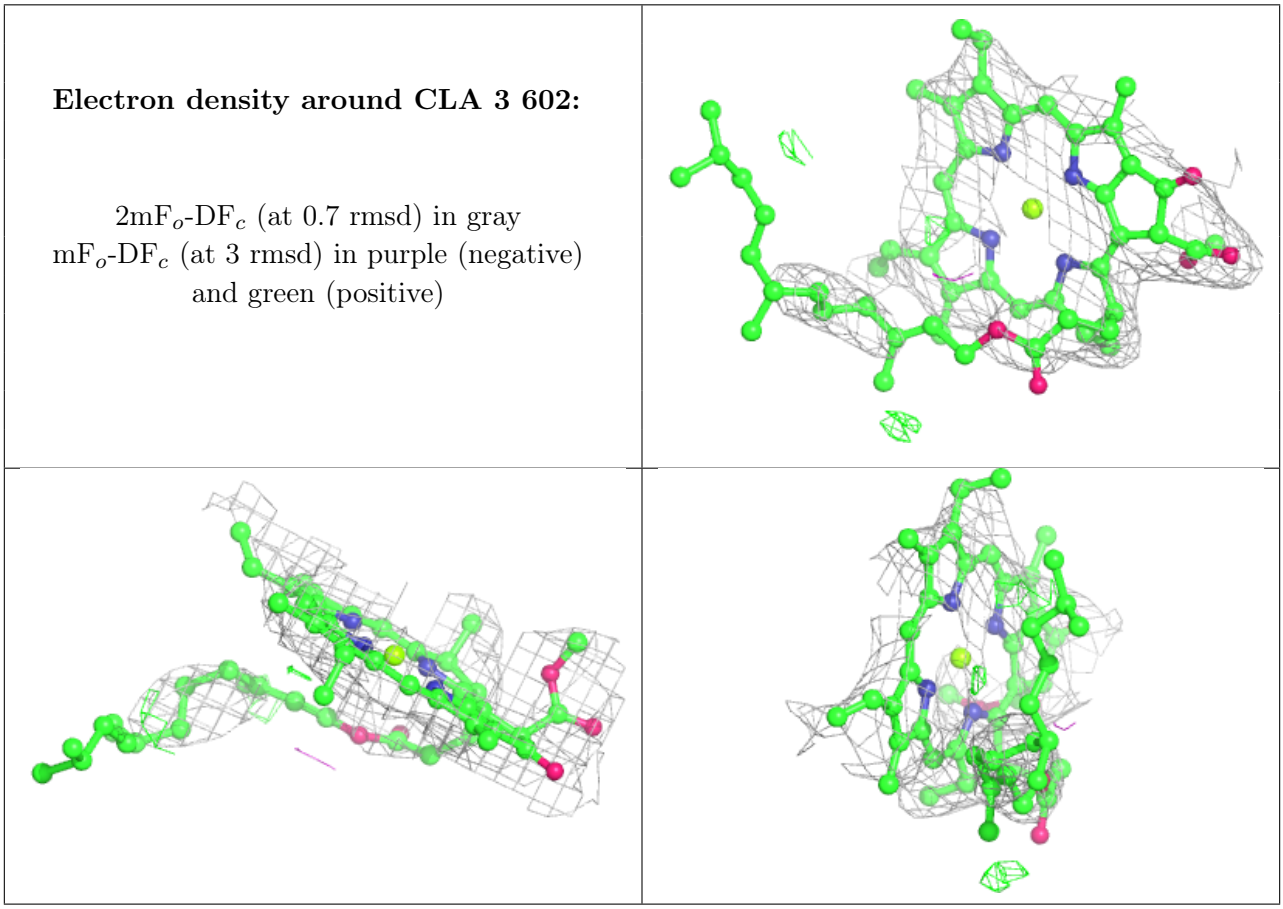
Electron density around BCR 1 316:

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



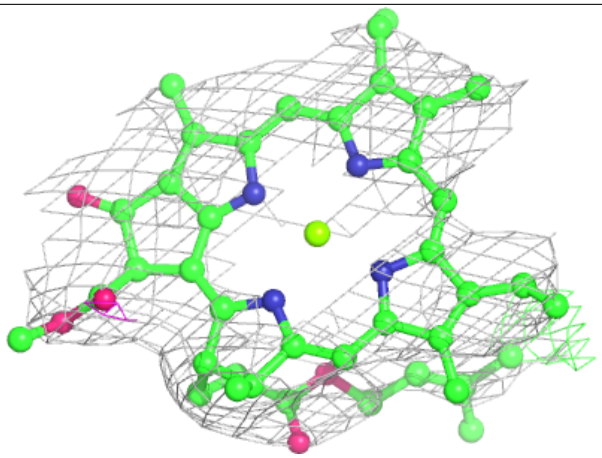
Electron density around CLA 3 602:

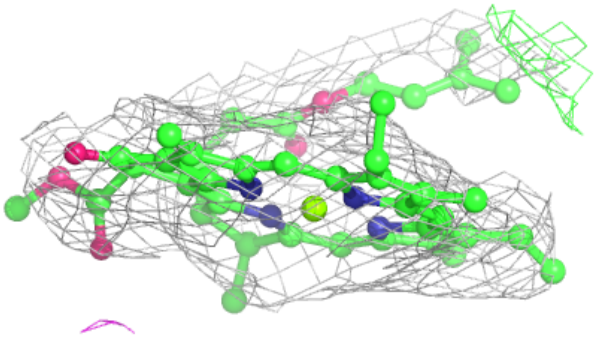
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

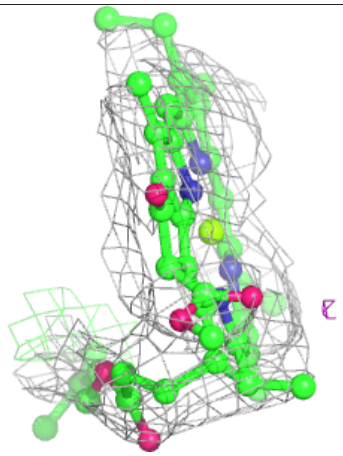


Electron density around CLA 3 609:

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

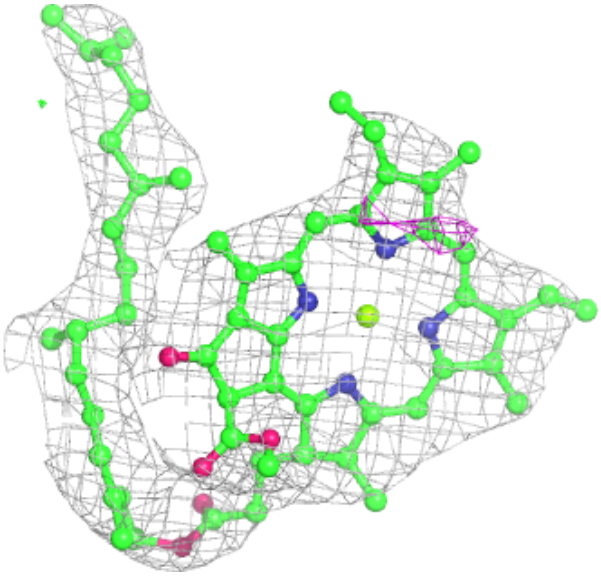


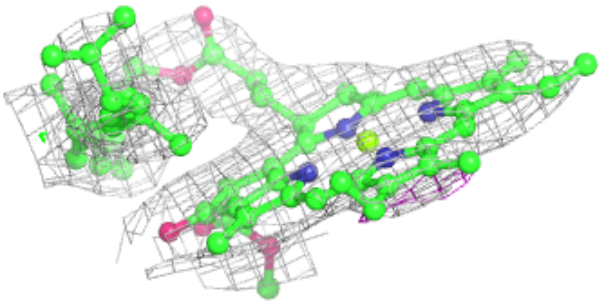


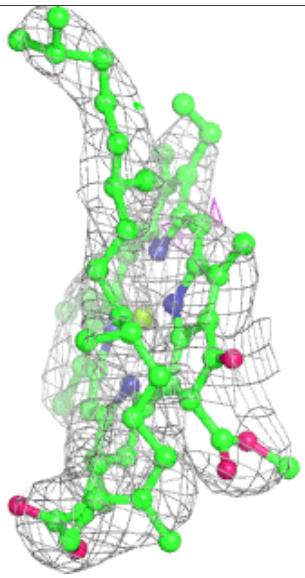


Electron density around CLA A 824:

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

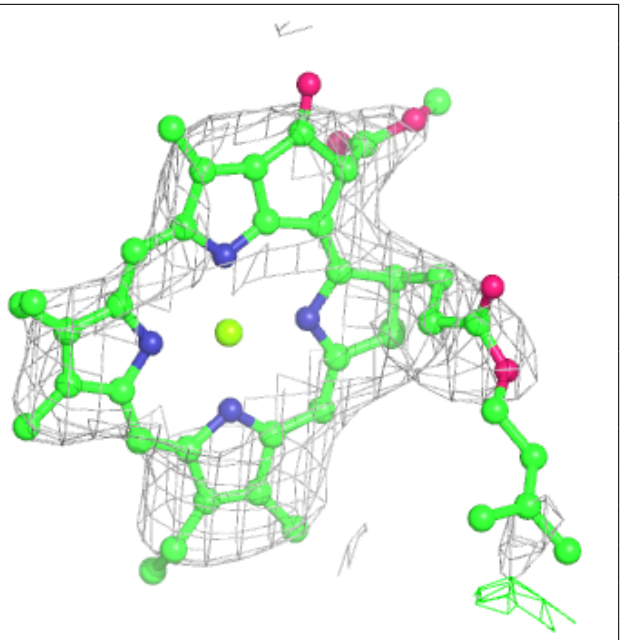


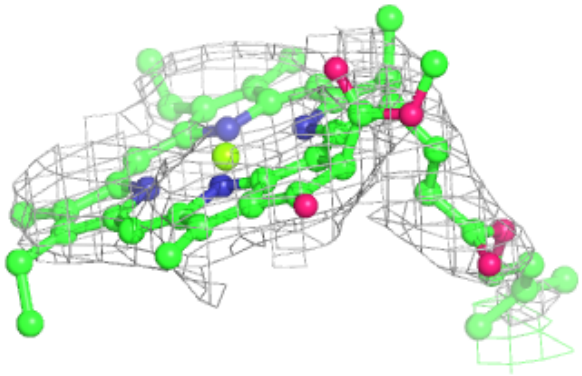


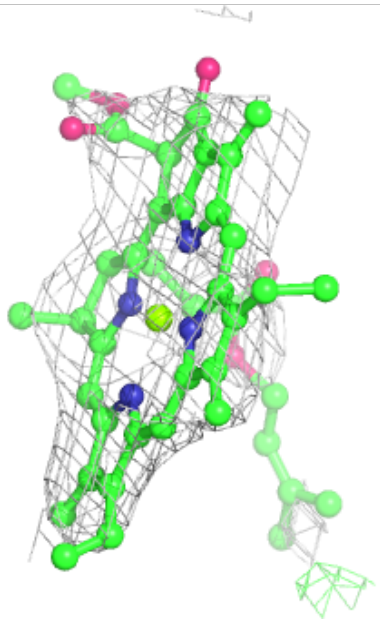


Electron density around CLA A 833:

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

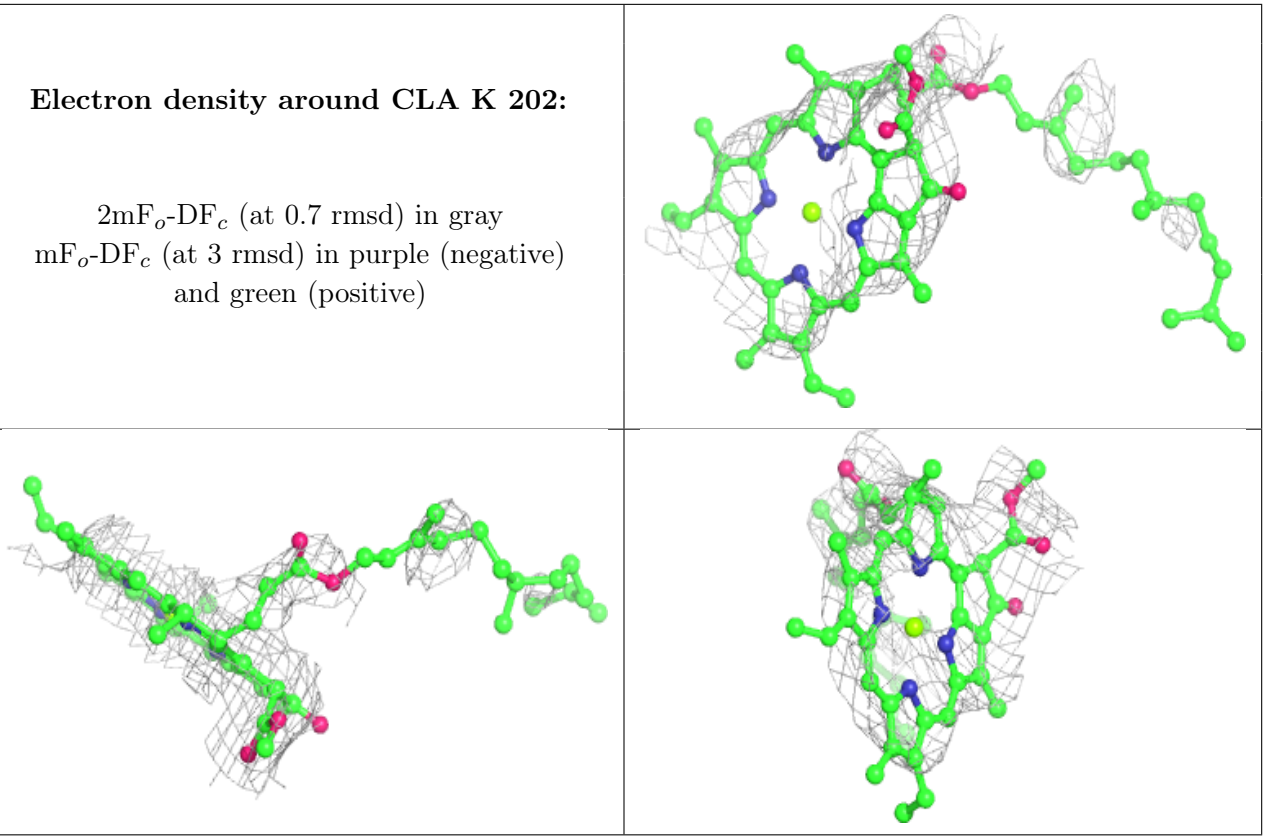






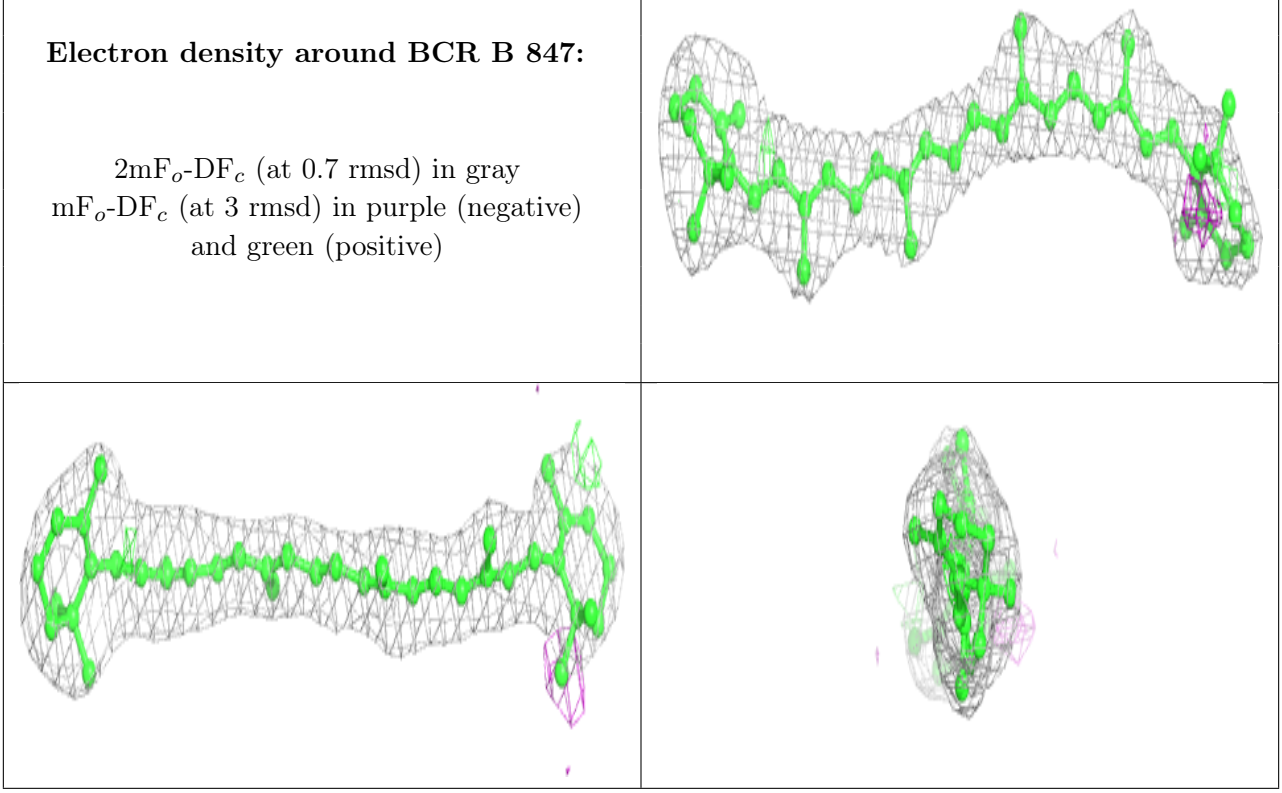
Electron density around CLA K 202:

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



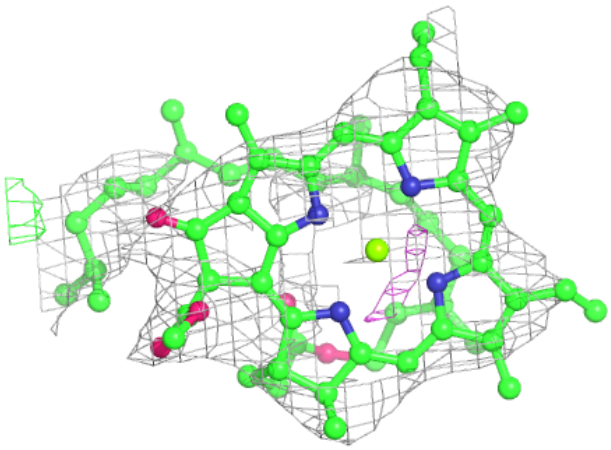
Electron density around BCR B 847:

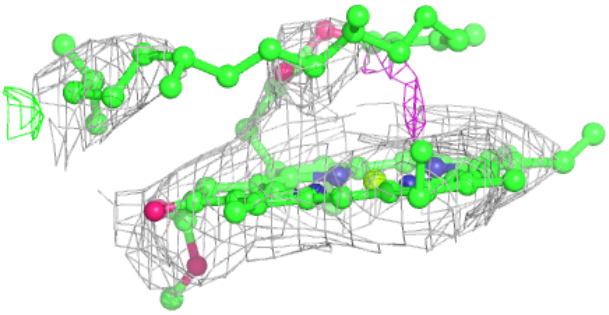
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

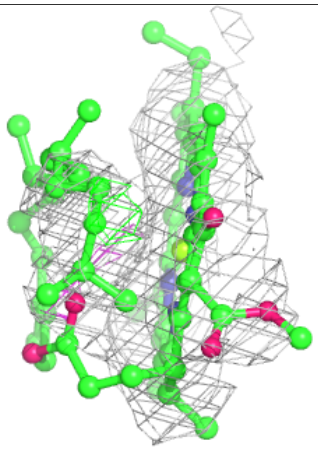


Electron density around CLA L 202:

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

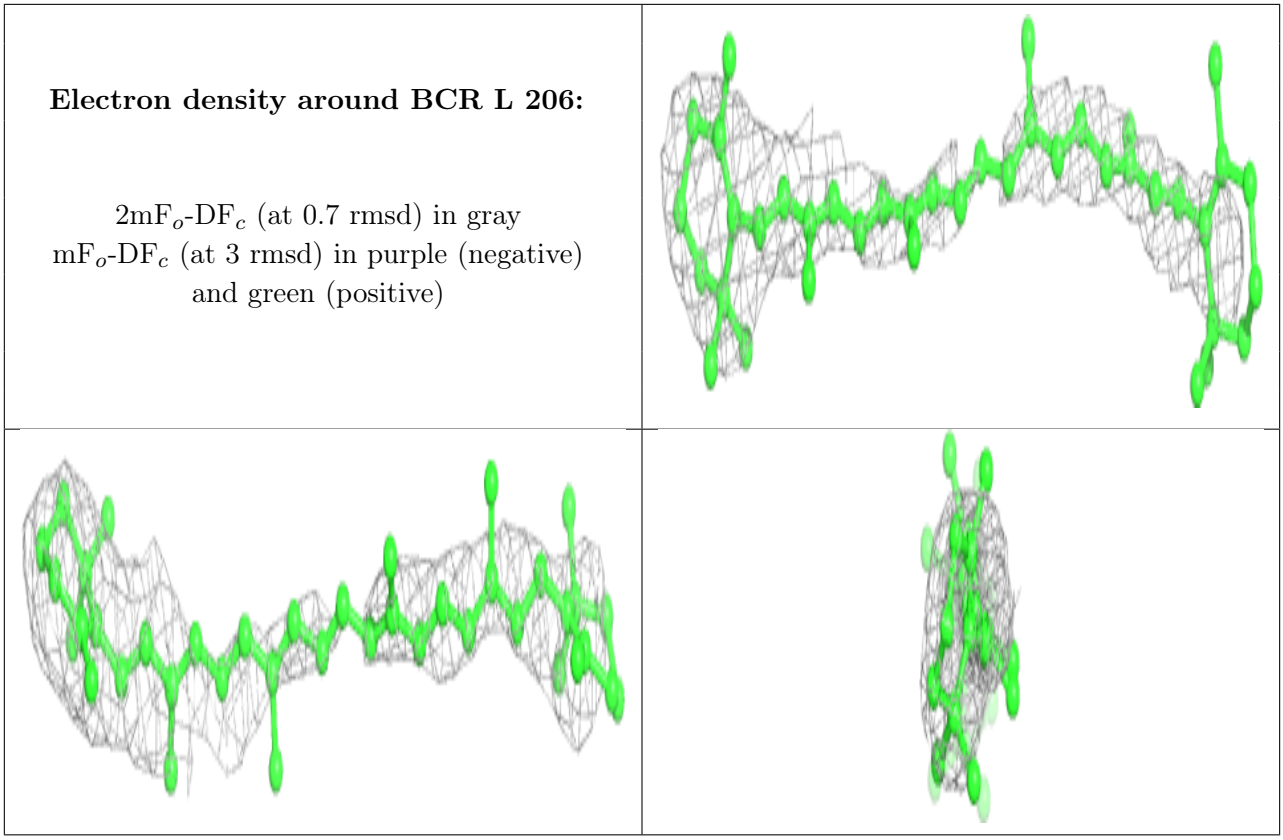






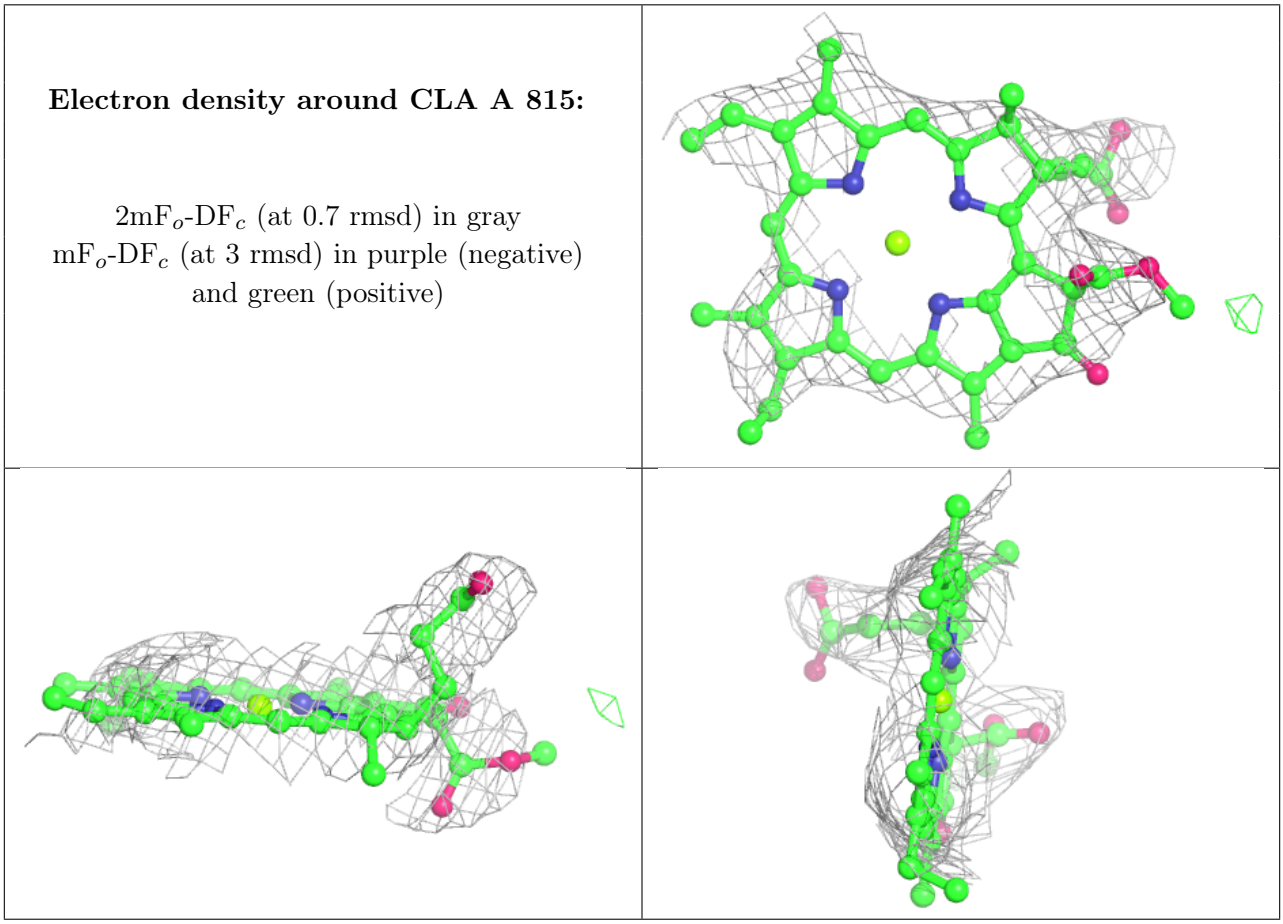
Electron density around BCR L 206:

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



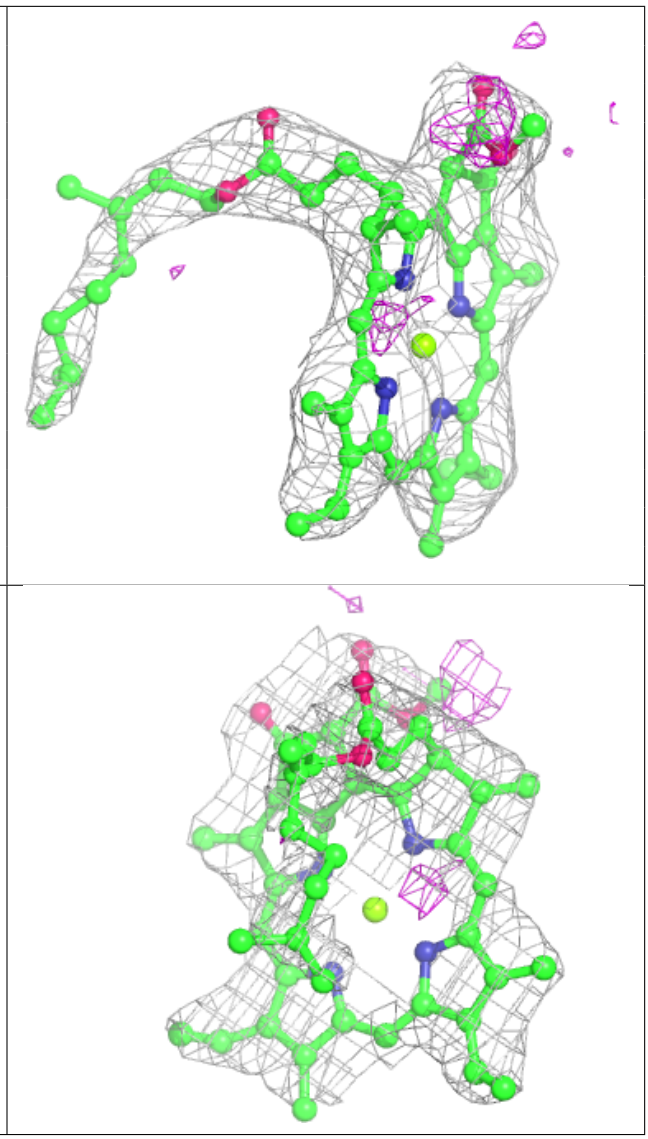
Electron density around CLA A 815:

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



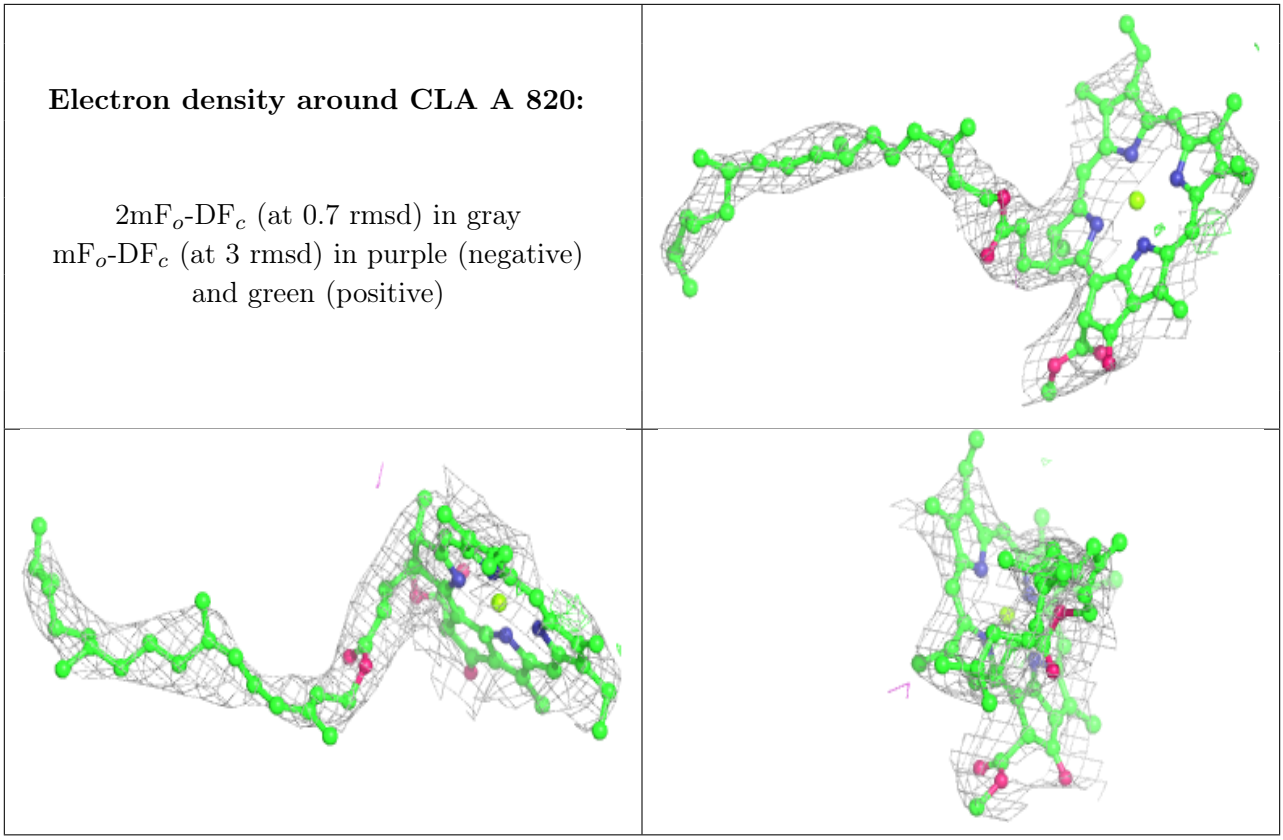
Electron density around CLA B 817:

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



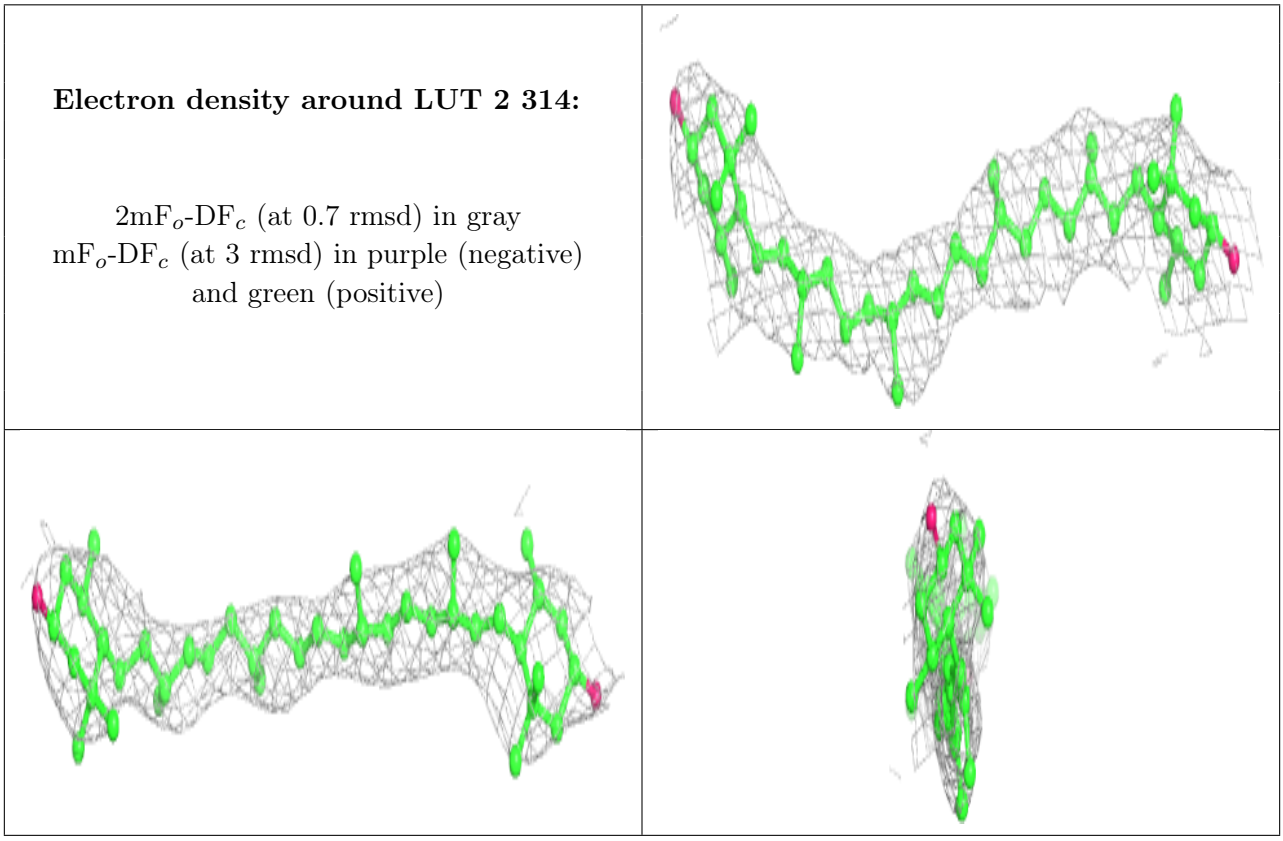
Electron density around CLA A 820:

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



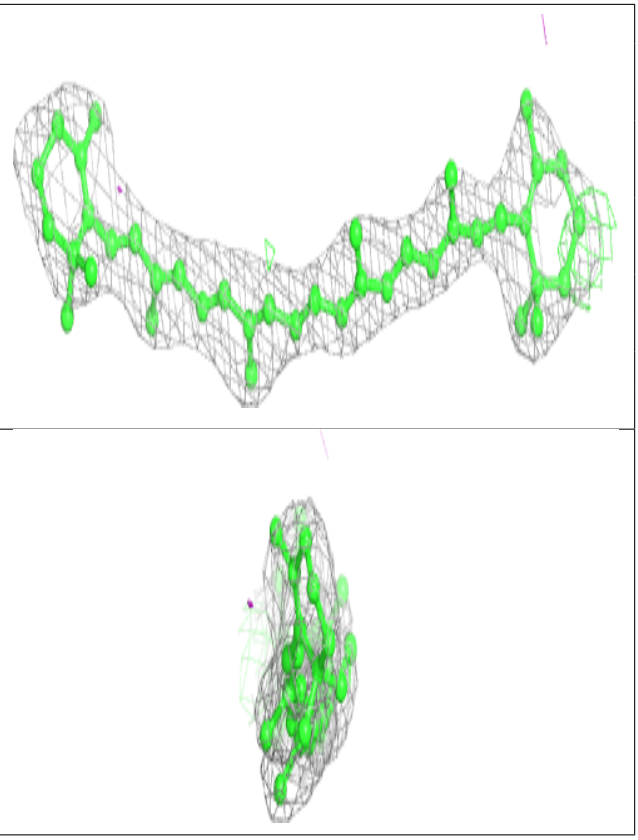
Electron density around LUT 2 314:

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



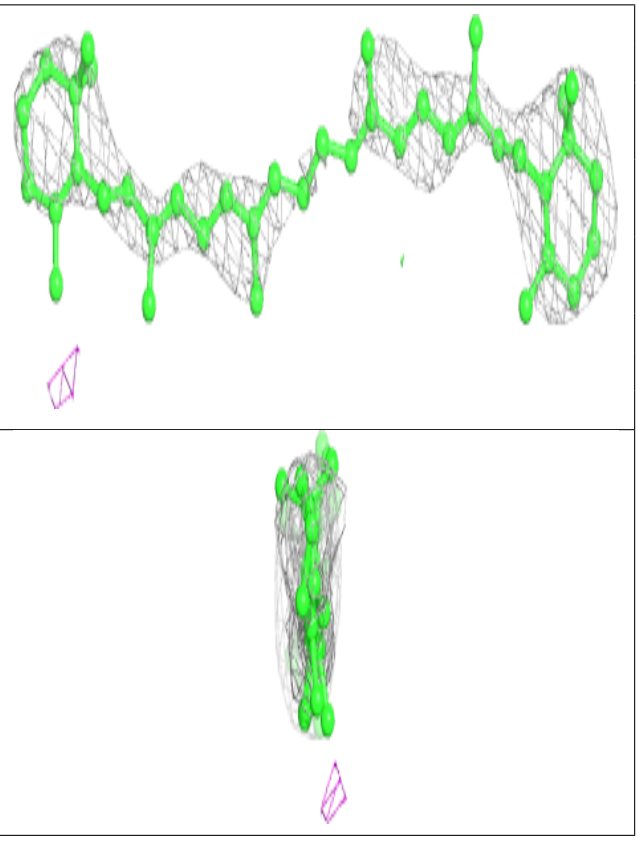
Electron density around BCR J 105:

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



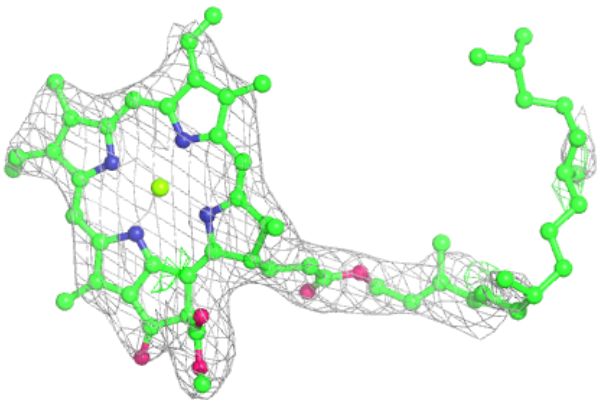
Electron density around BCR L 205:

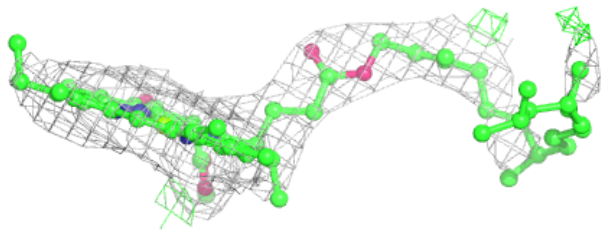
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

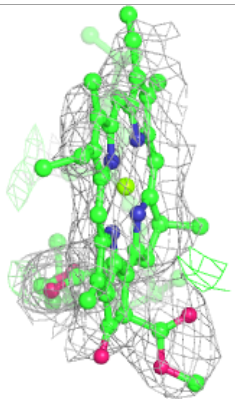


Electron density around CLA A 825:

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

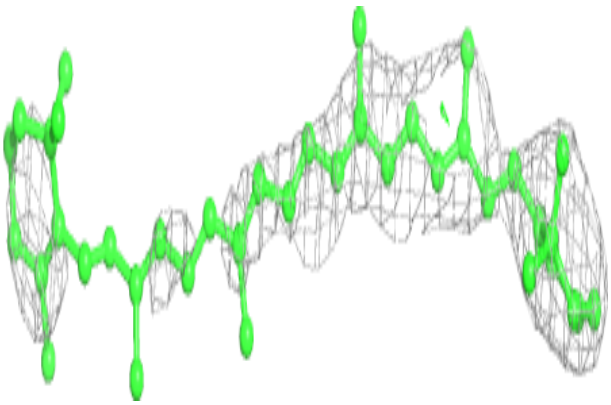


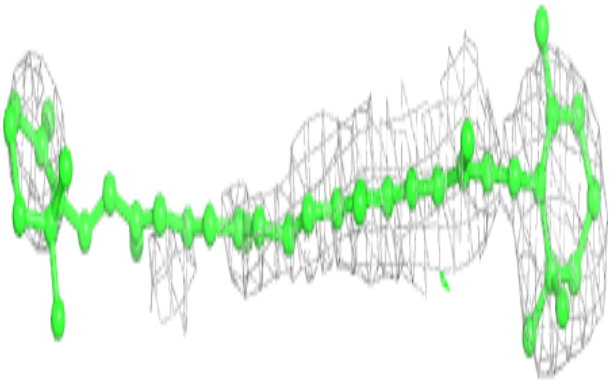


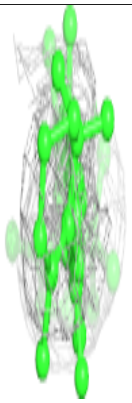


Electron density around BCR A 847:

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

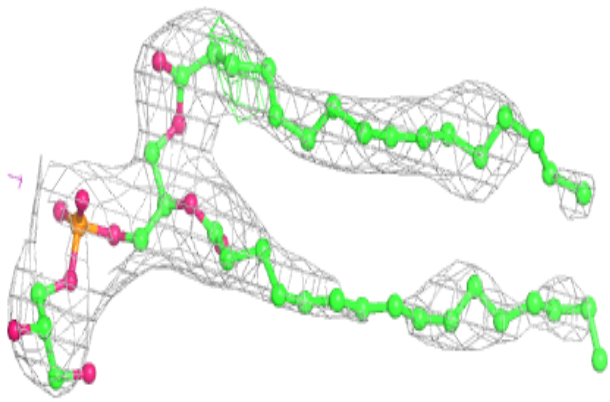


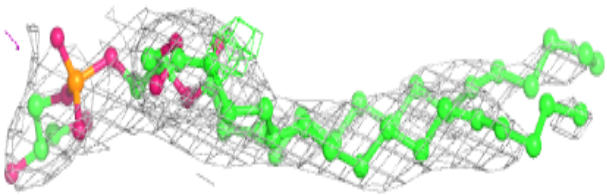


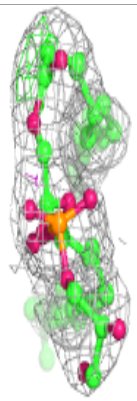


Electron density around LHG 1 317:

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

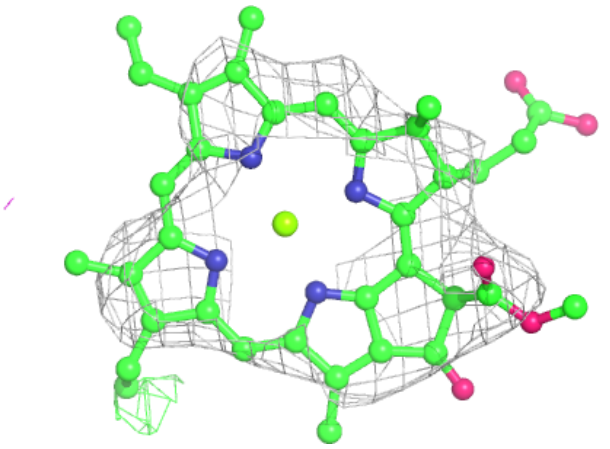


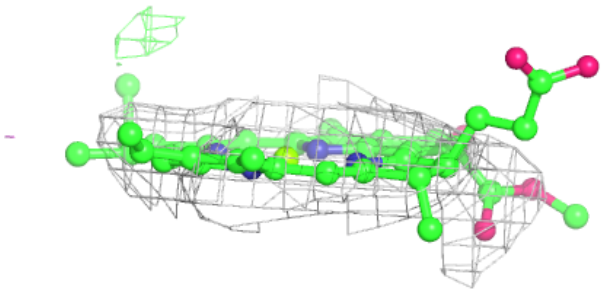


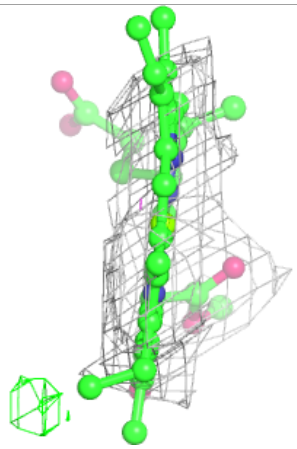


Electron density around CLA 3 612:

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

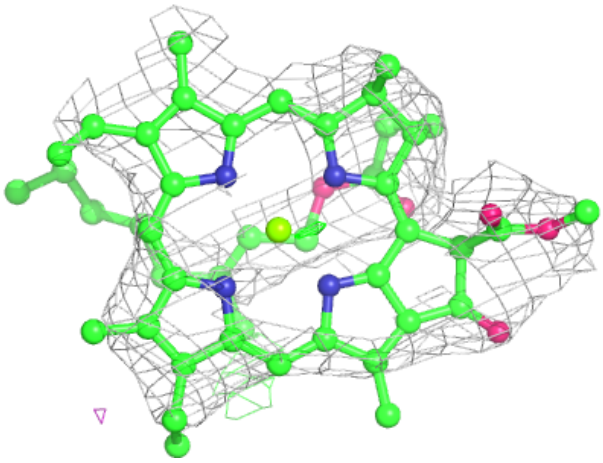


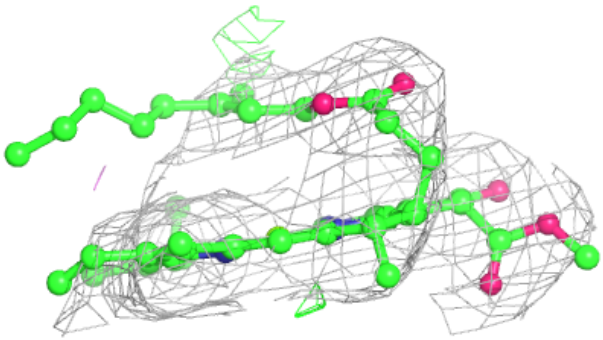


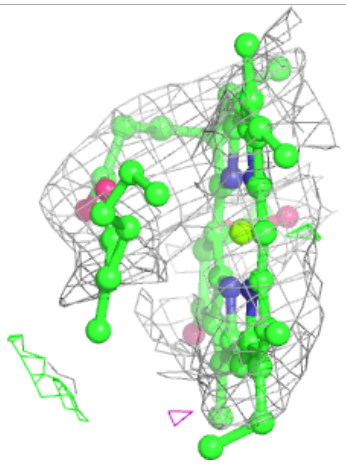


Electron density around CLA A 811:

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

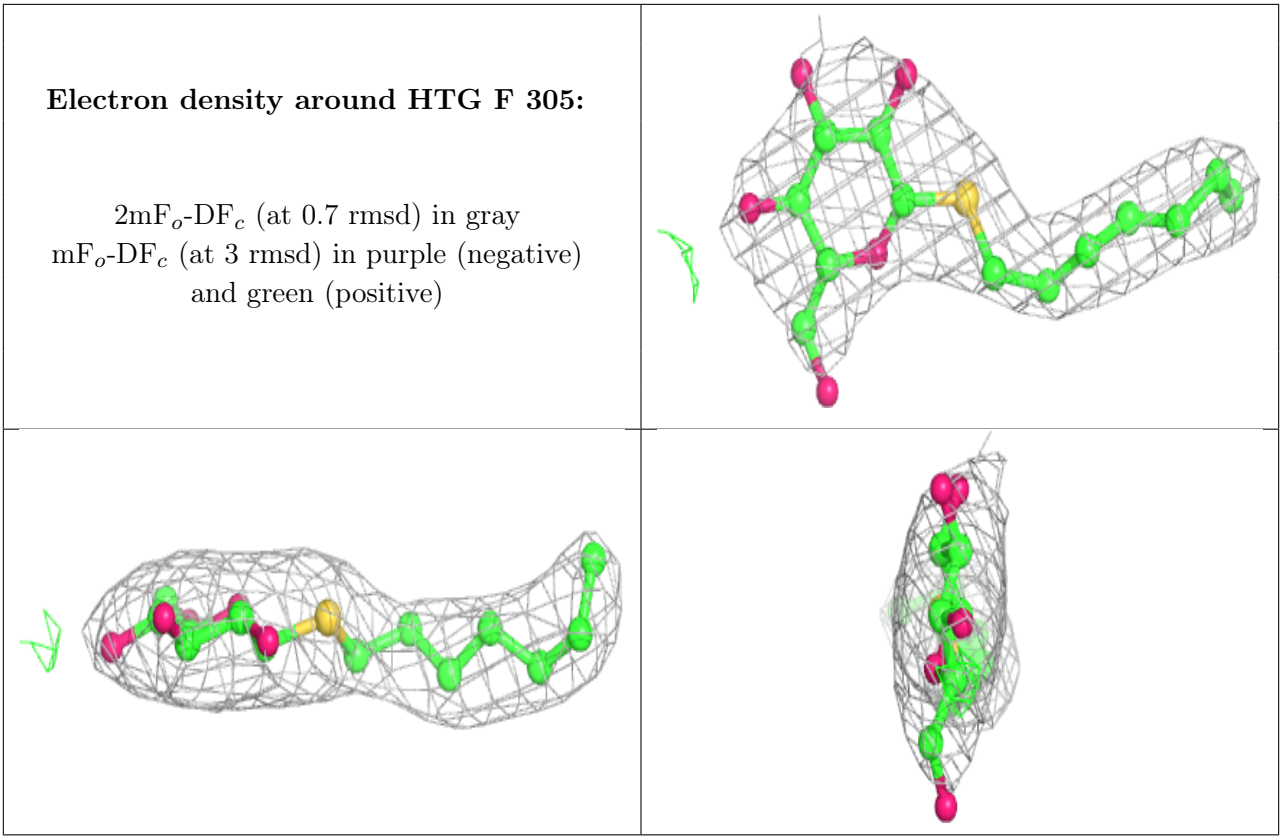






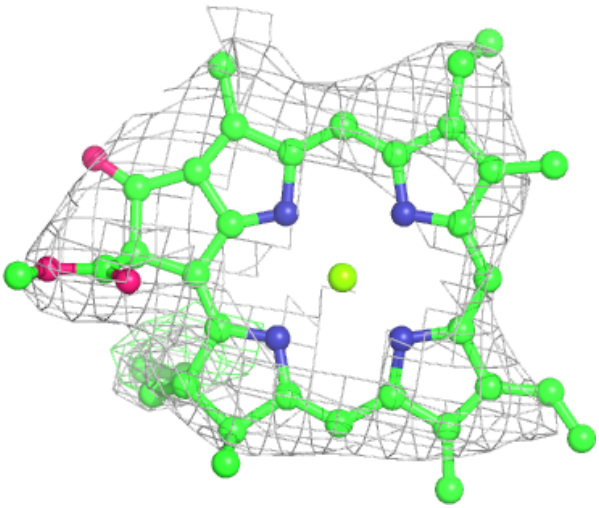
Electron density around HTG F 305:

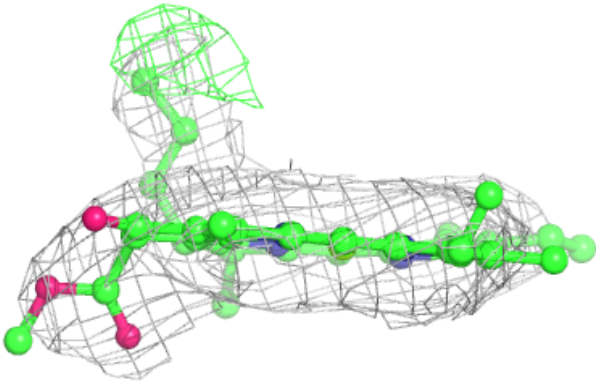
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

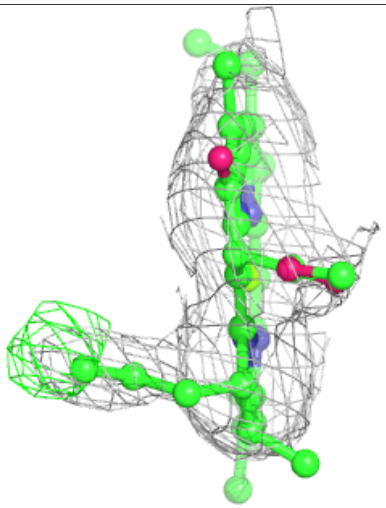


Electron density around CLA 2 312:

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

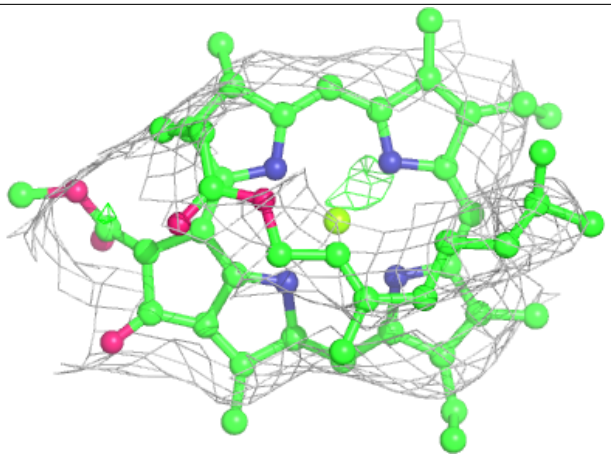


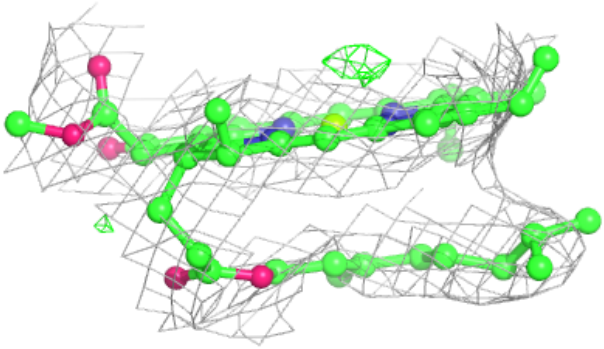


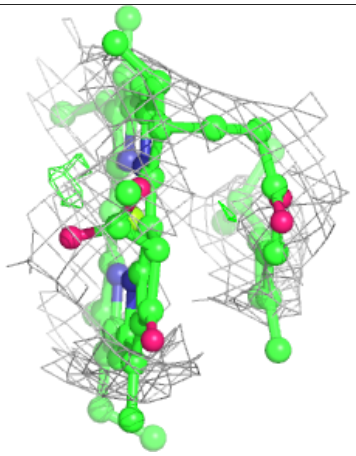


Electron density around CLA 3 611:

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

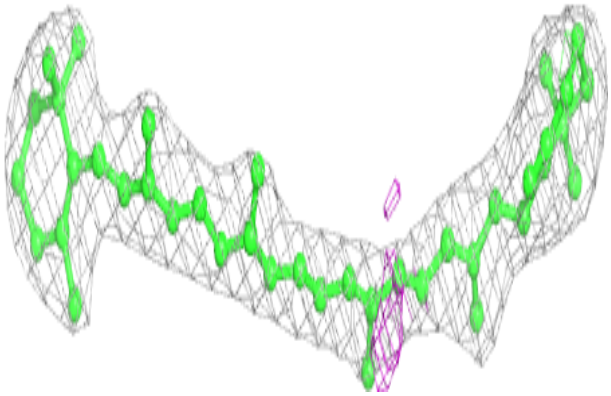


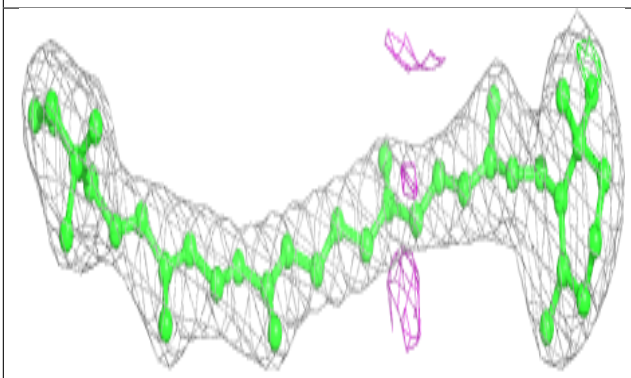


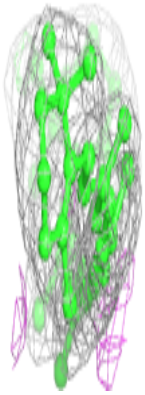


Electron density around BCR F 303:

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

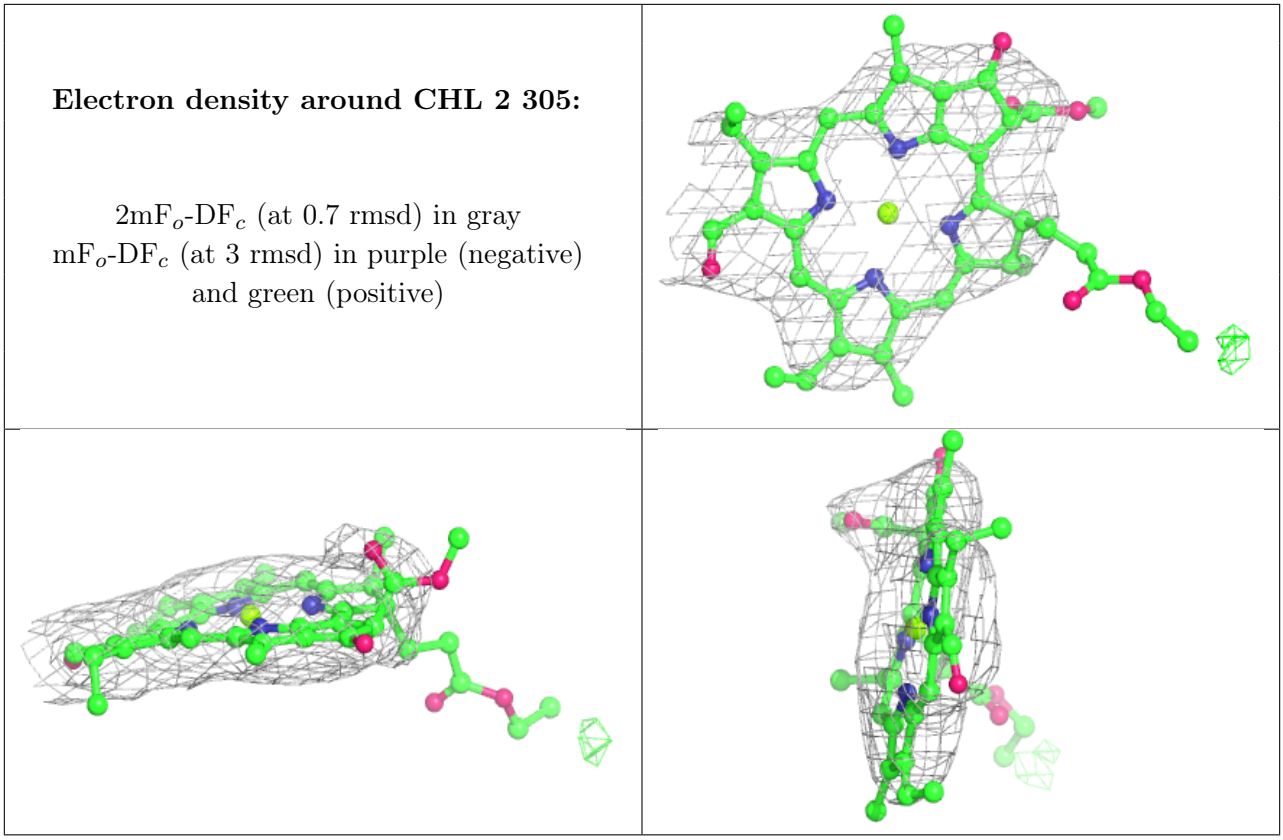






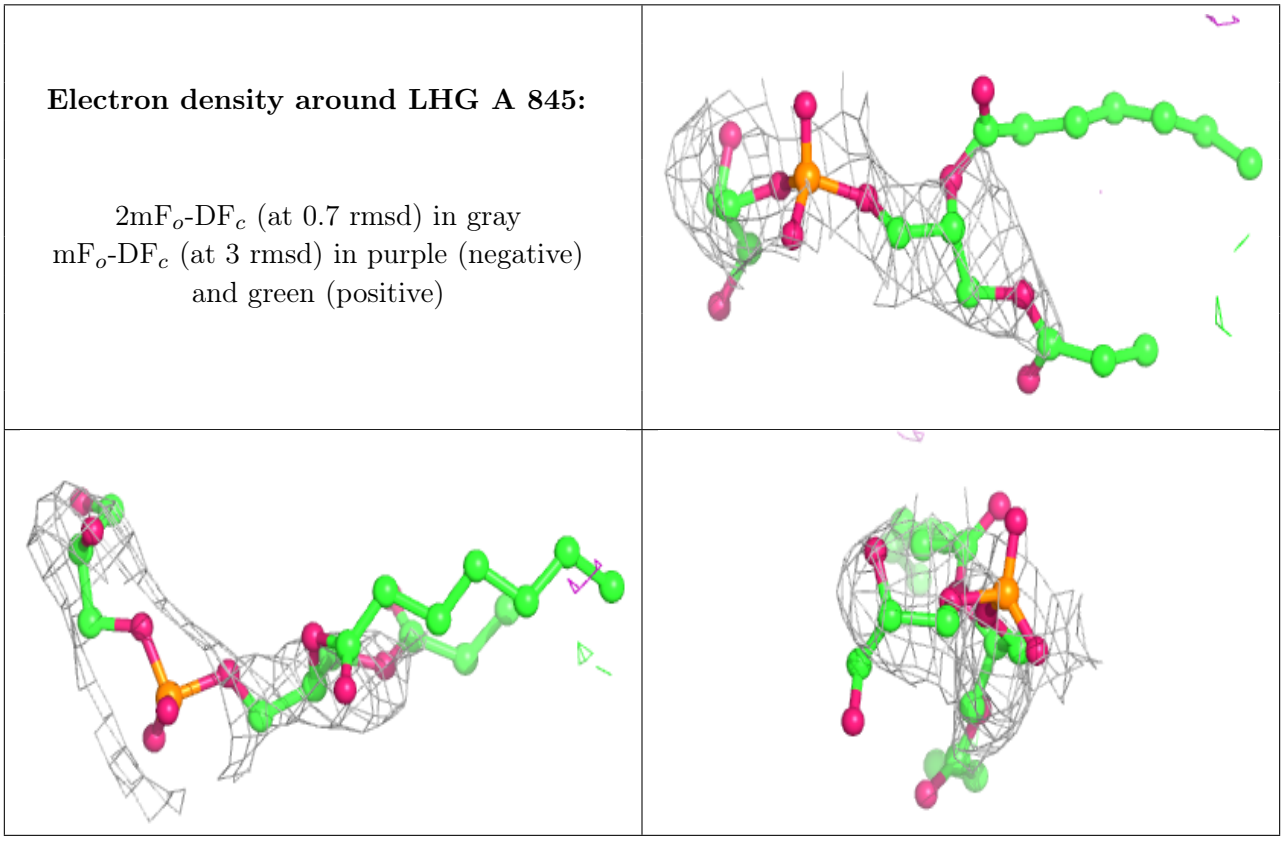
Electron density around CHL 2 305:

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



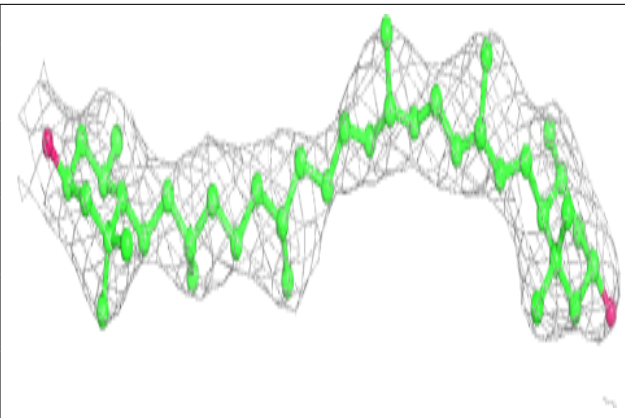
Electron density around LHG A 845:

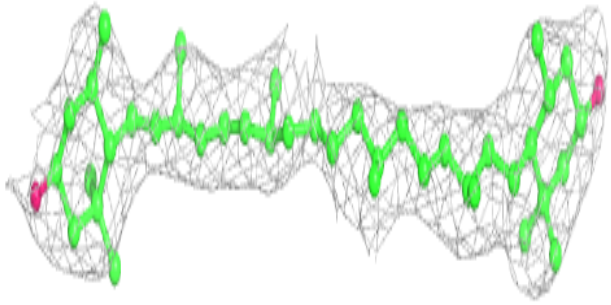
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LUT 1 314:

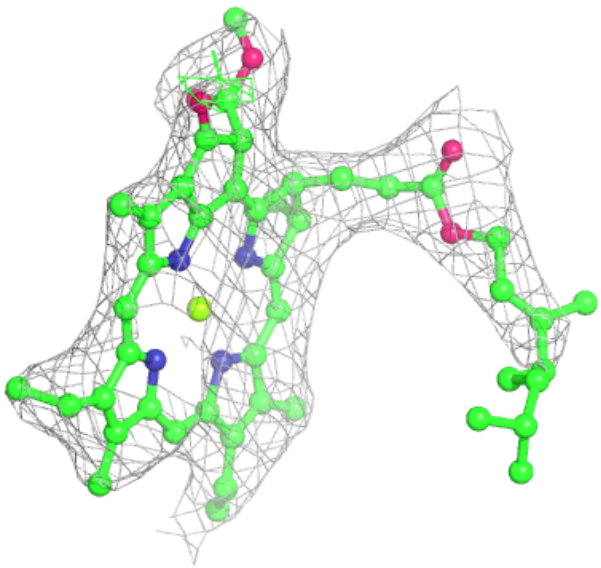
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

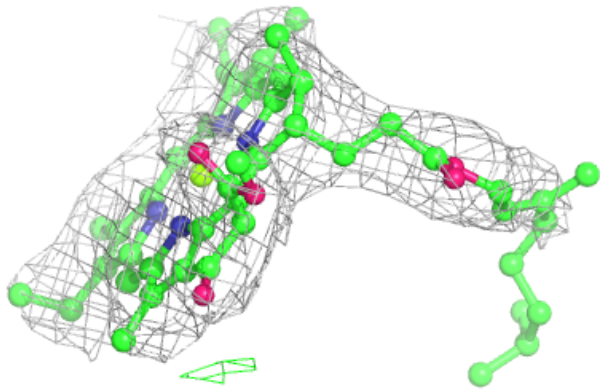


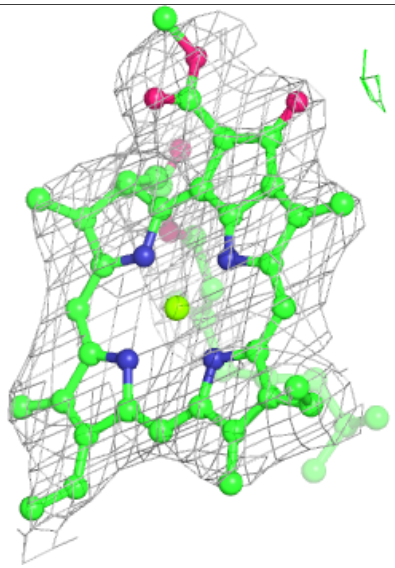


Electron density around CLA A 803:

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

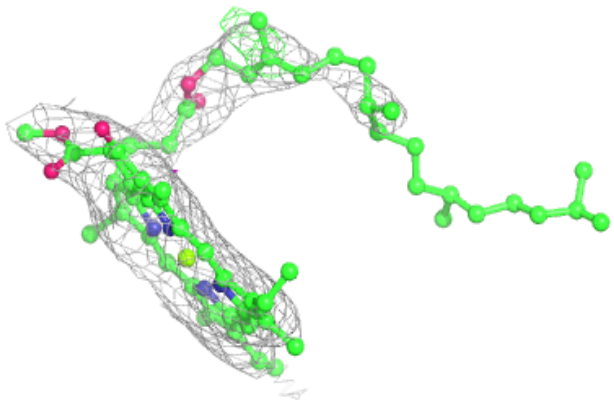


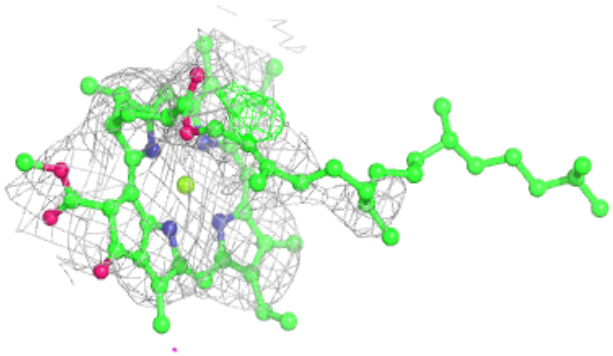


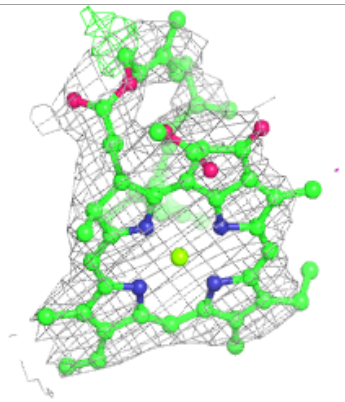


Electron density around CLA A 809:

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

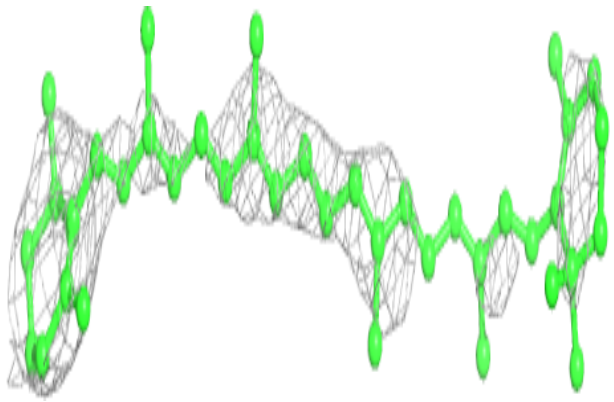


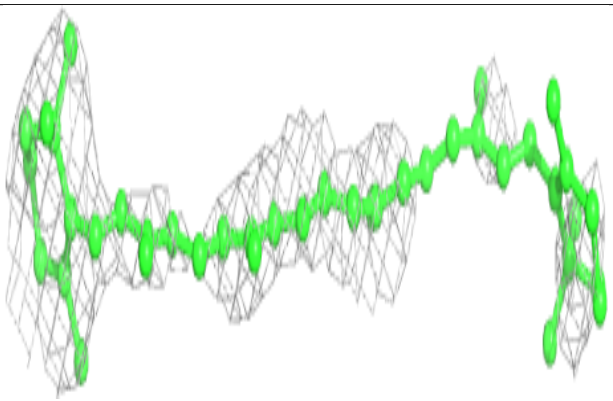


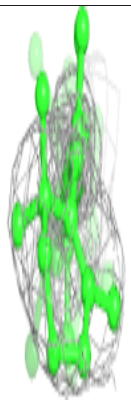


Electron density around BCR A 848:

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

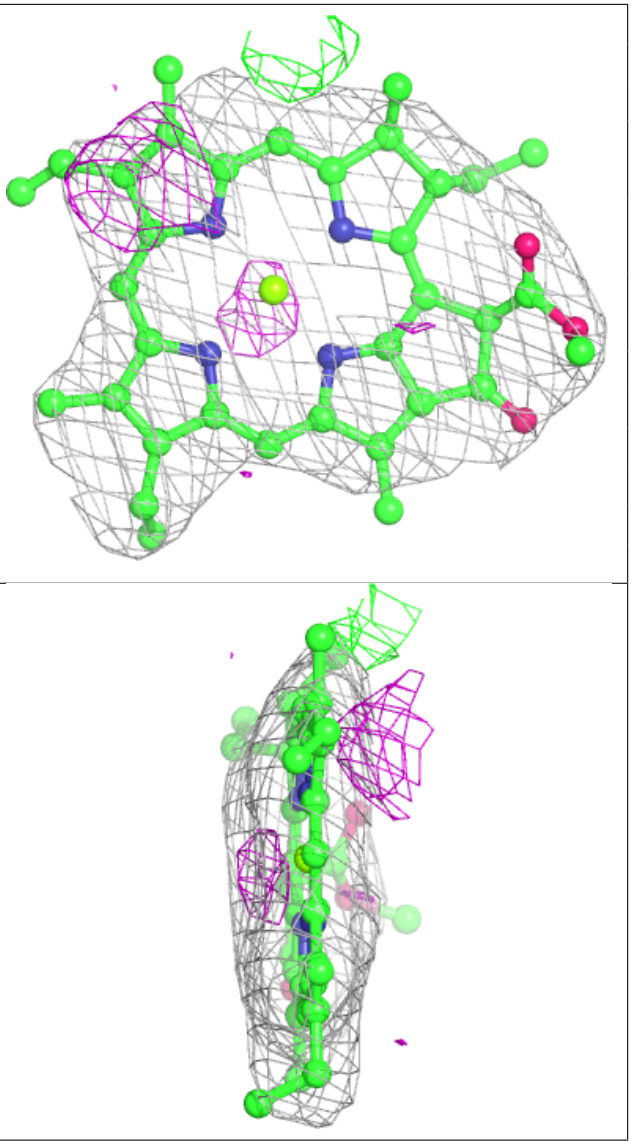






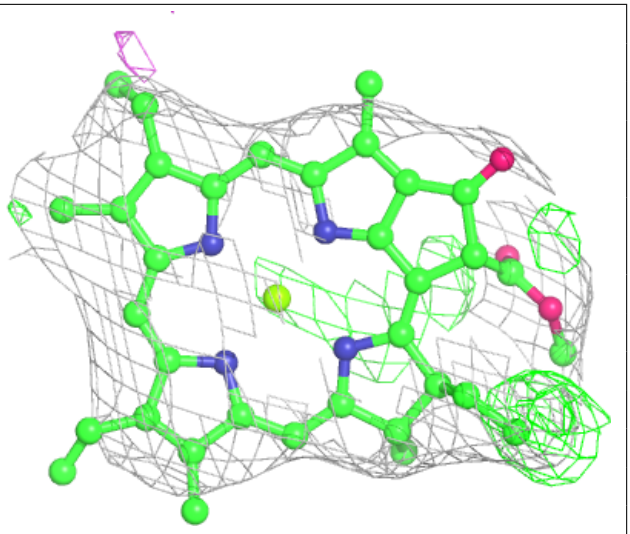
Electron density around CLA J 103:

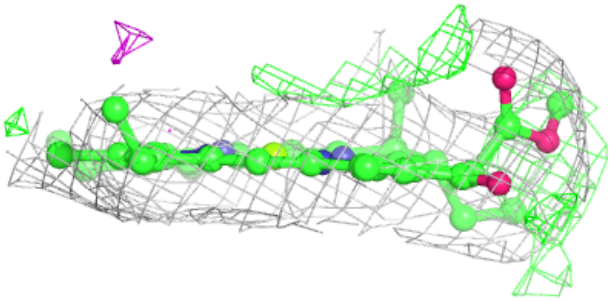
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

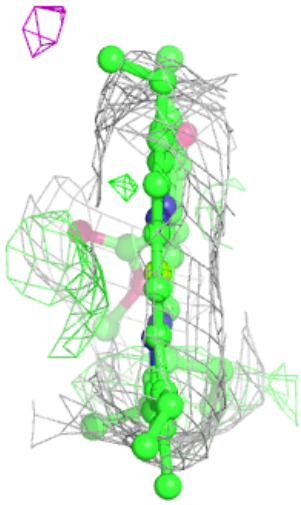


Electron density around CLA 1 304:

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

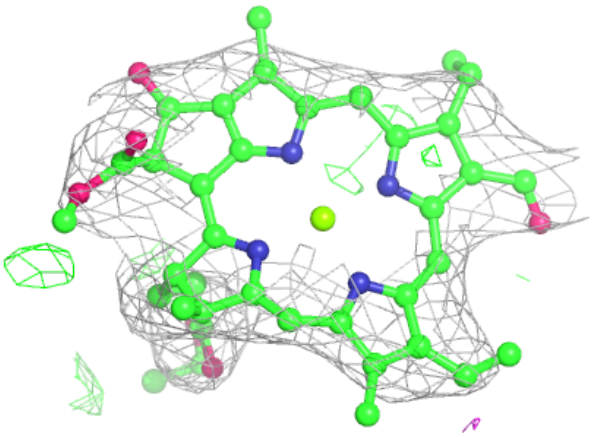


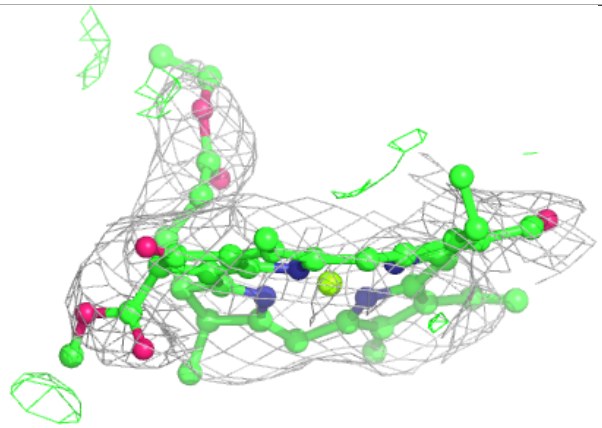


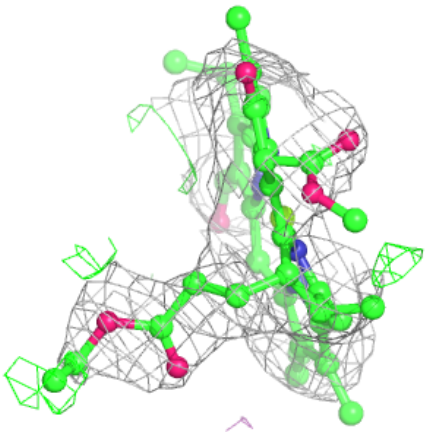


Electron density around CHL 1 305:

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

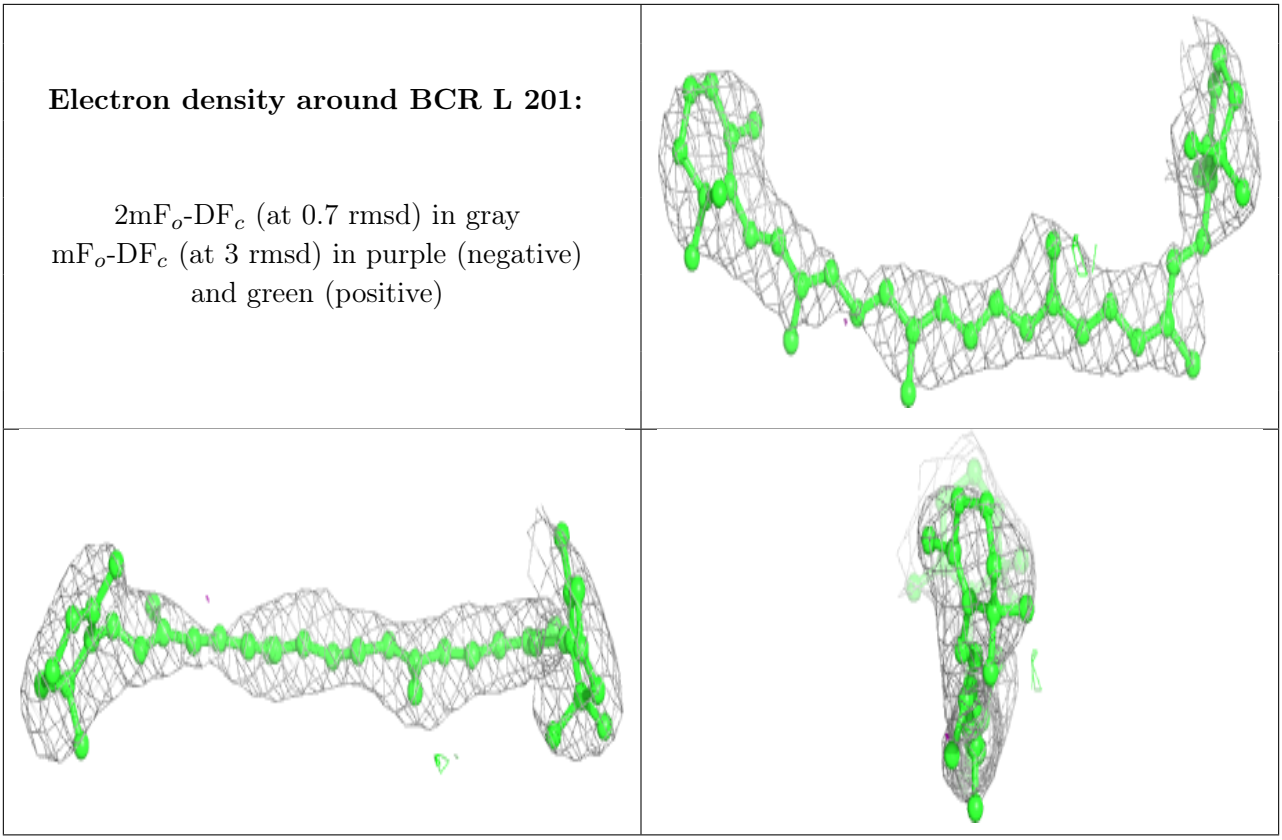






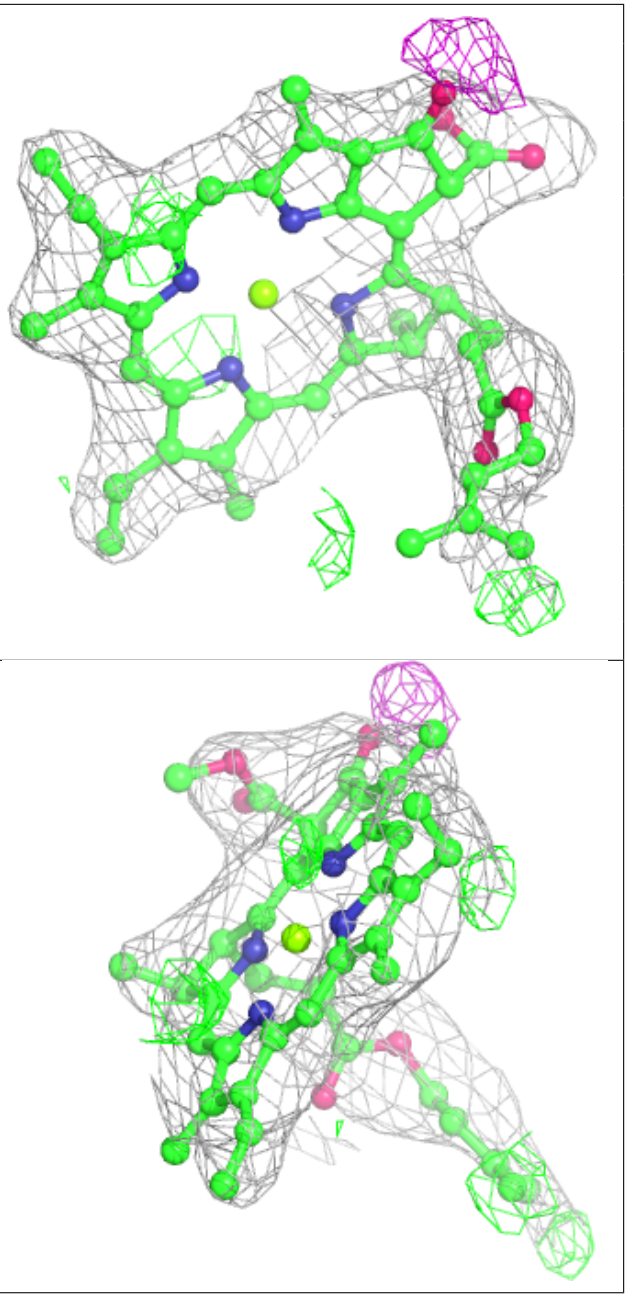
Electron density around BCR L 201:

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



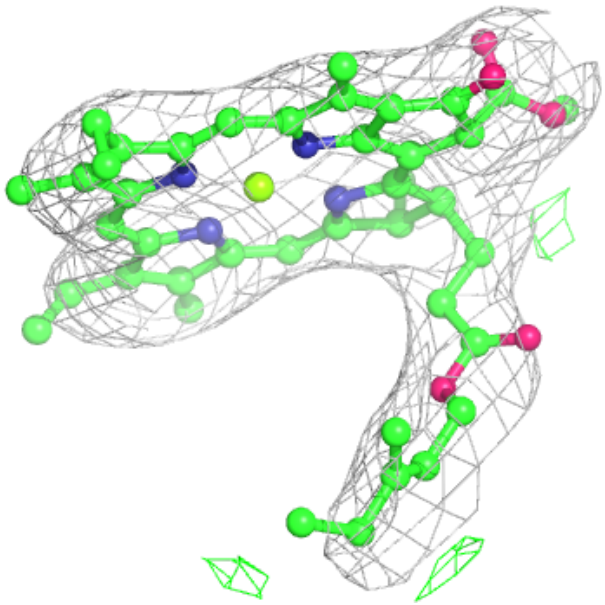
Electron density around CLA 4 304:

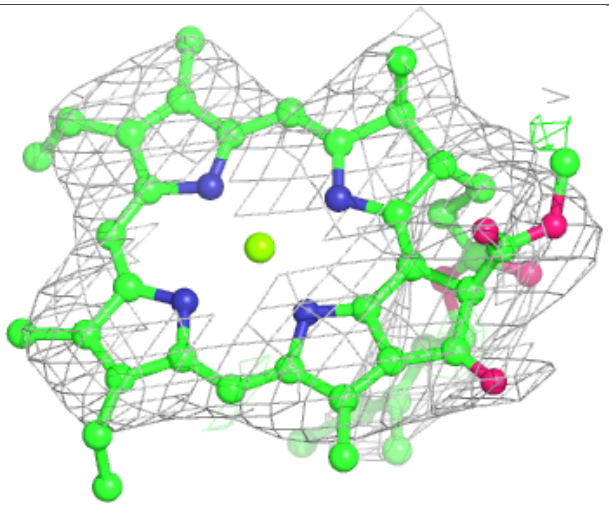
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

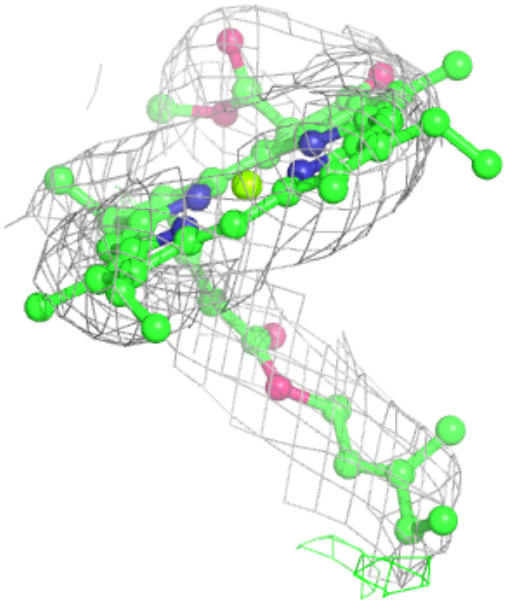


Electron density around CLA 1 303:

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

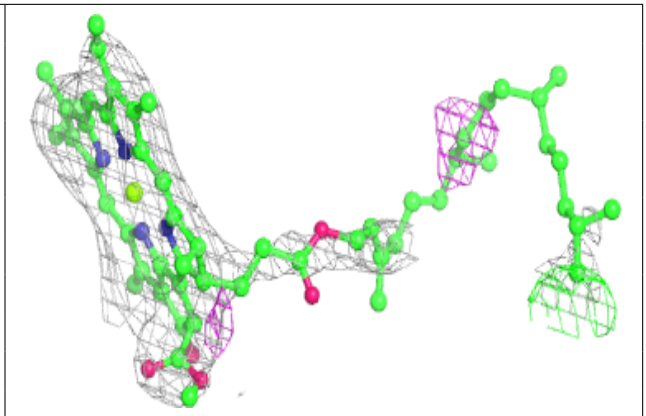


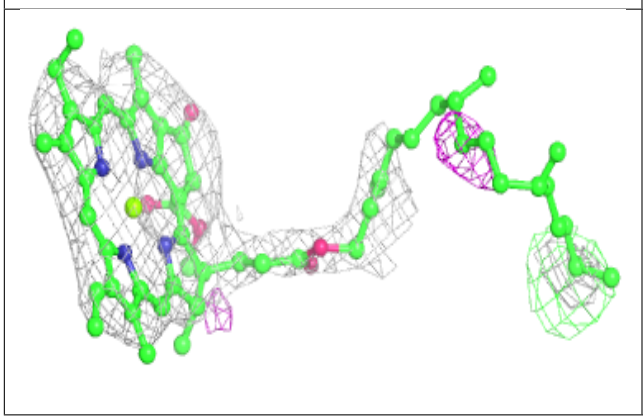


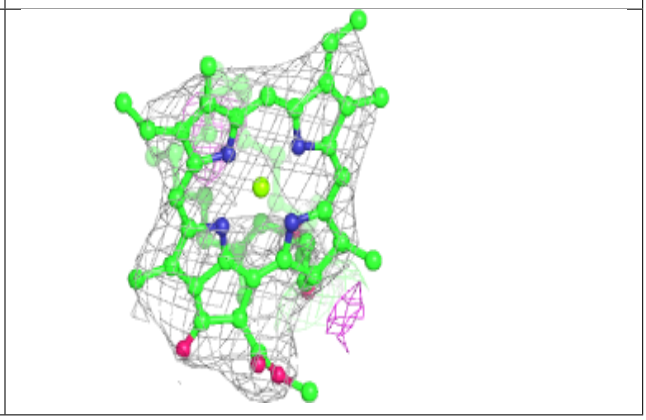


Electron density around CLA A 837:

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

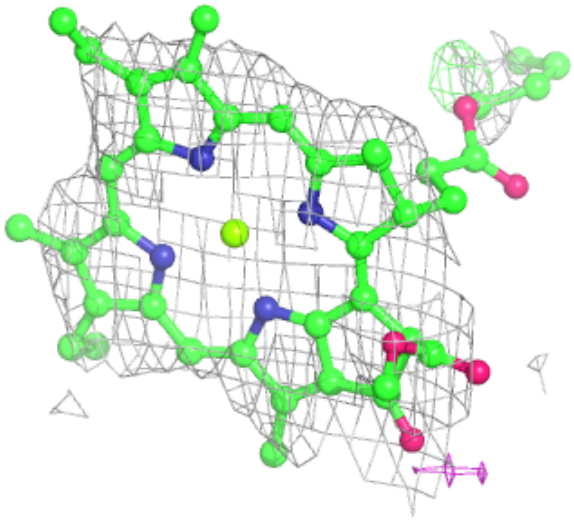


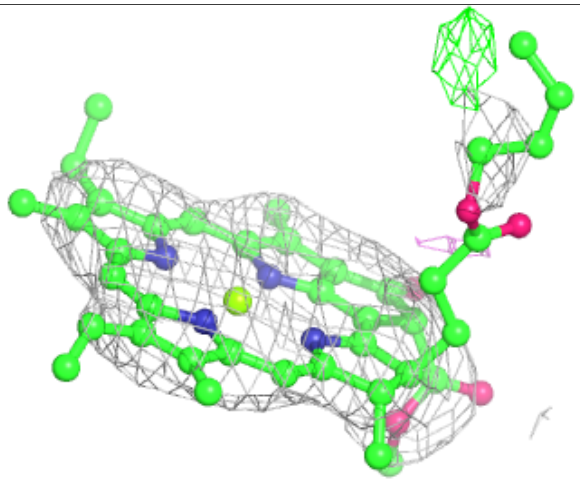


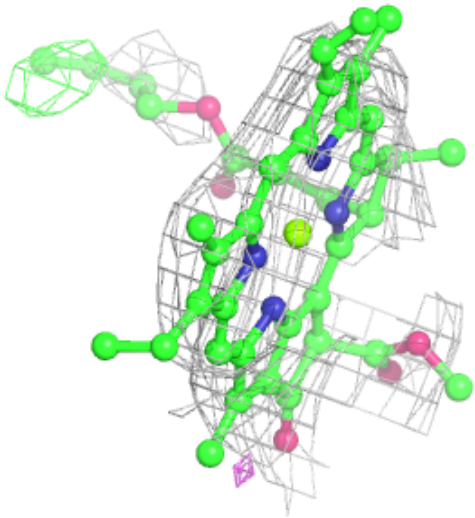


Electron density around CLA A 821:

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

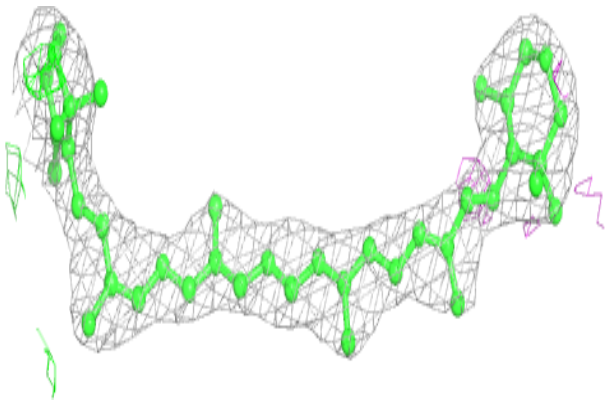


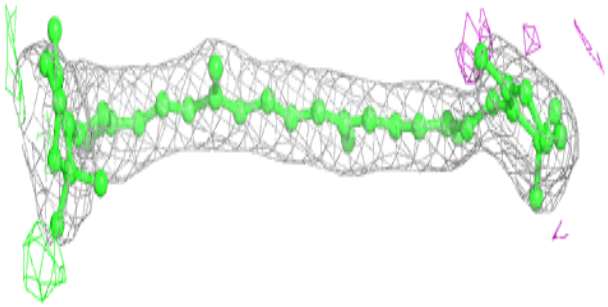


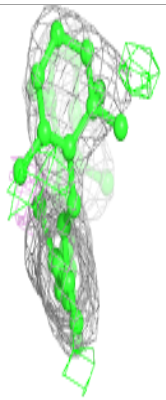


Electron density around BCR B 845:

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

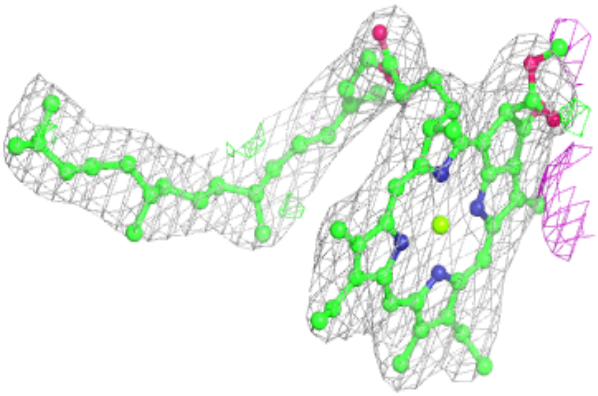


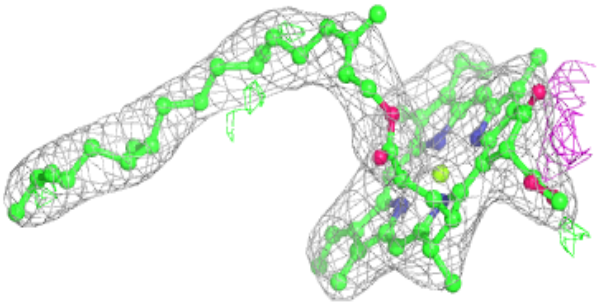


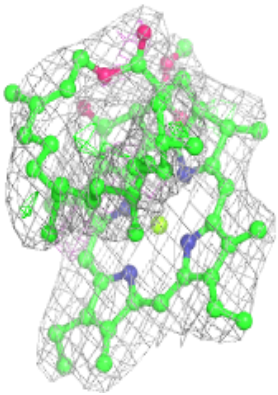


Electron density around CLA B 816:

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

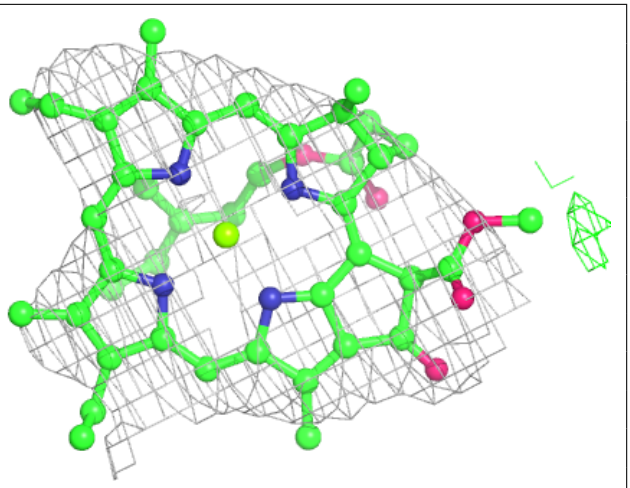


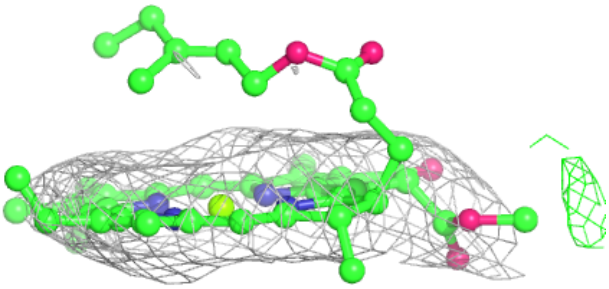


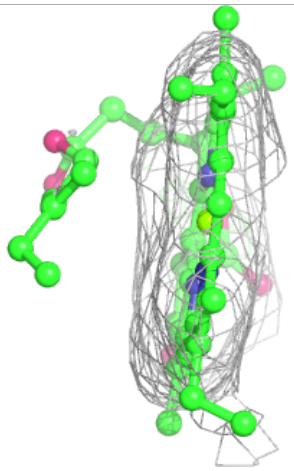


Electron density around CLA A 822:

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

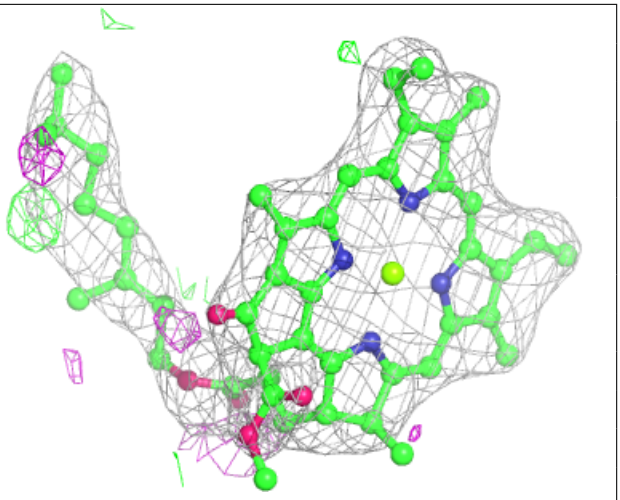


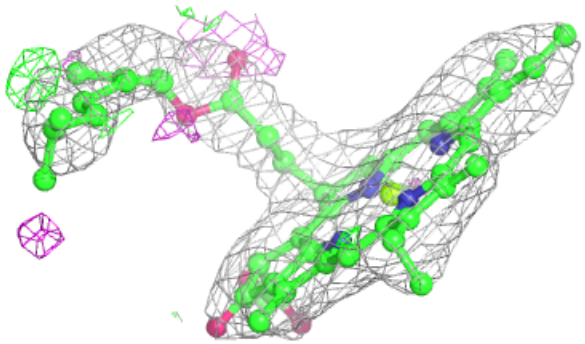


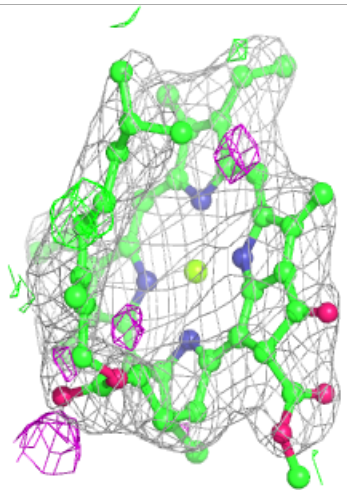


Electron density around CLA B 824:

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

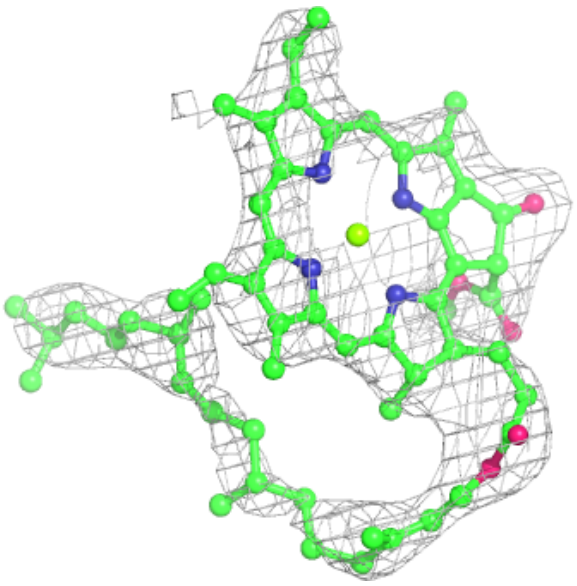


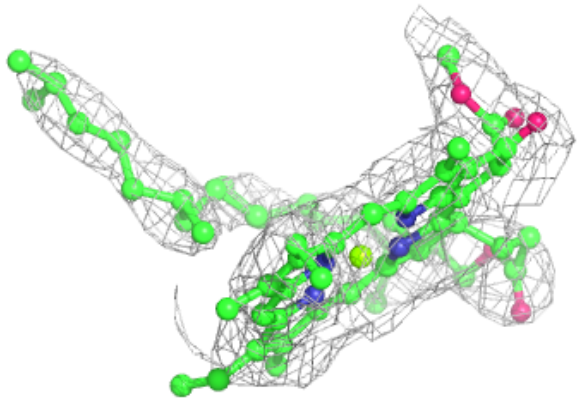


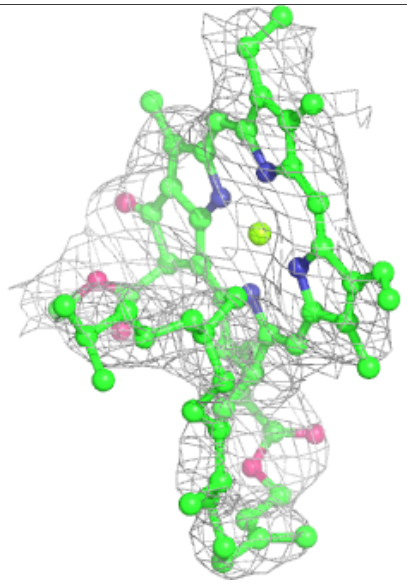


Electron density around CLA A 812:

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

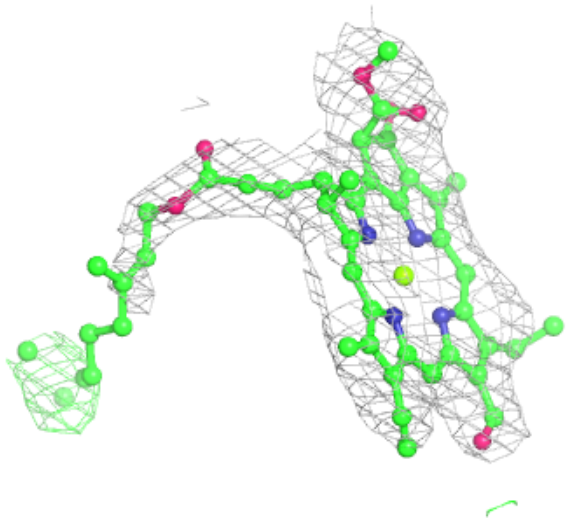


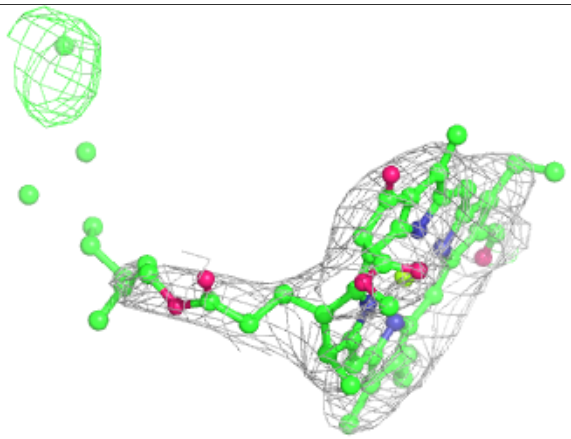


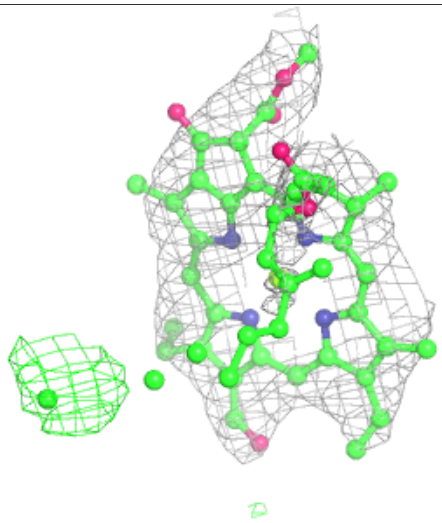


Electron density around CHL 3 601:

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

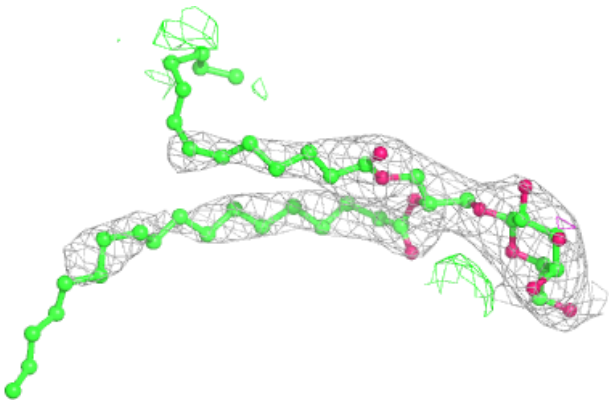


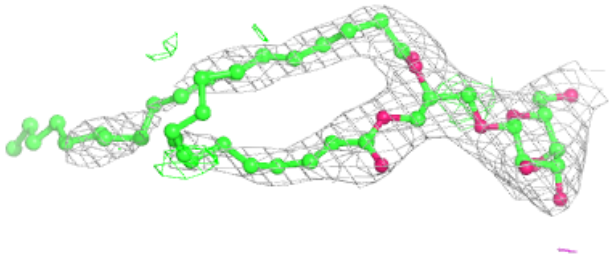


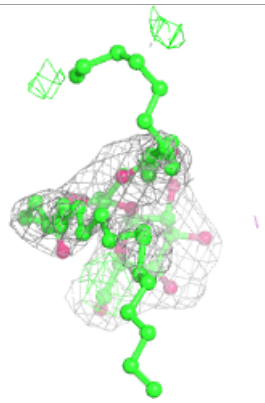


Electron density around LMG 4 319:

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

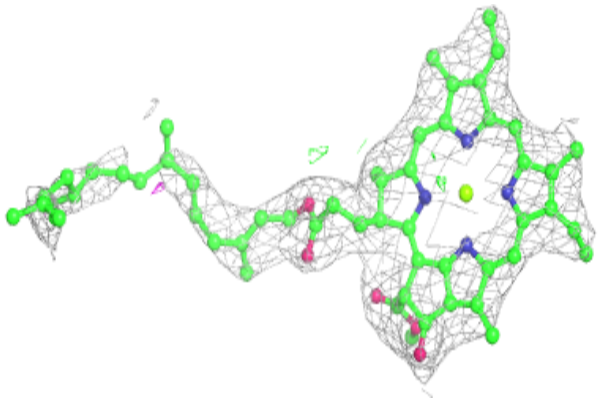


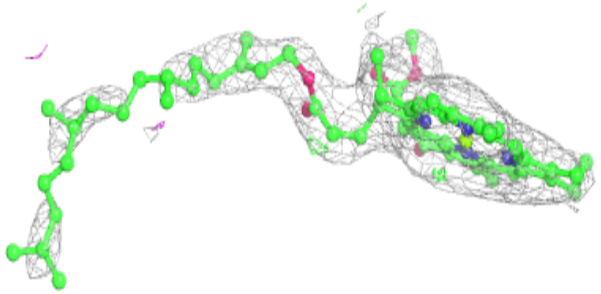


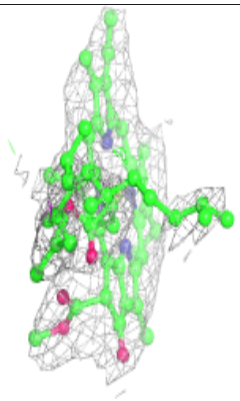


Electron density around CLA A 804:

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

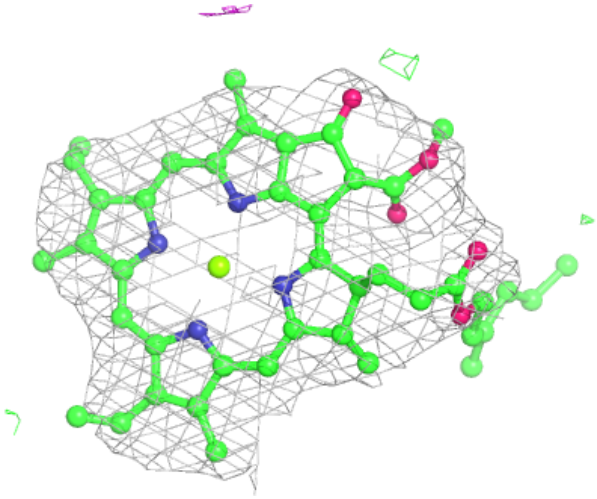


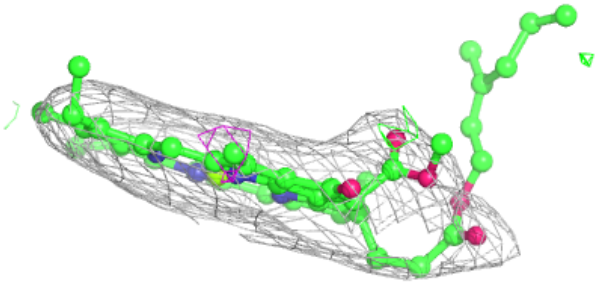


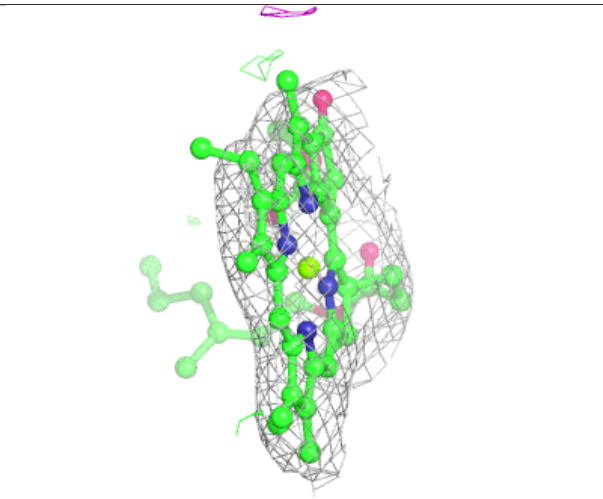


Electron density around CLA 2 310:

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

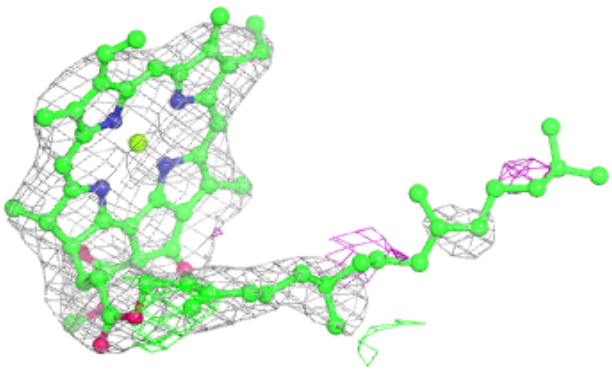


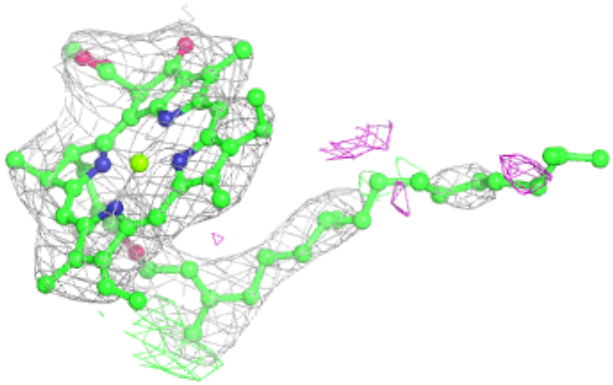


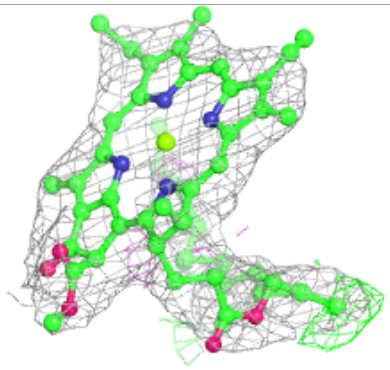


Electron density around CLA 1 307:

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

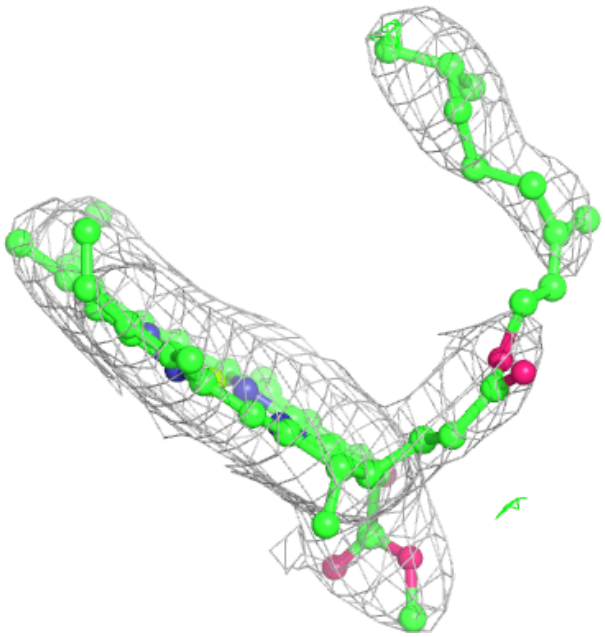


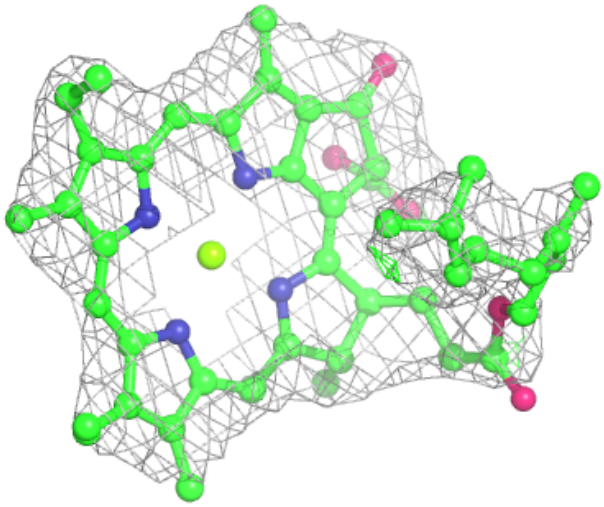


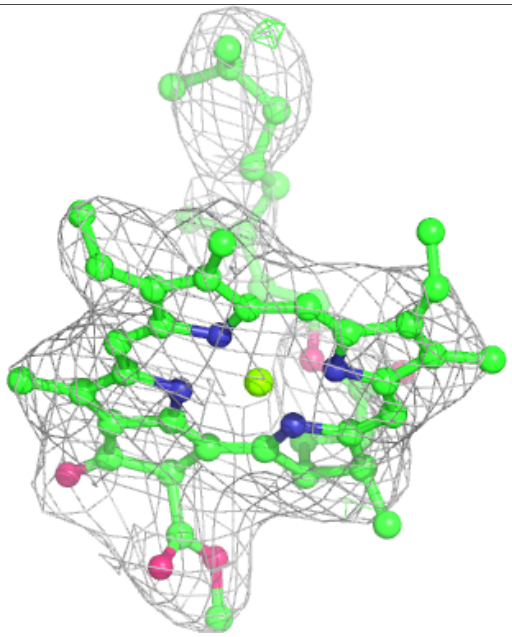


Electron density around CLA 1 312:

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

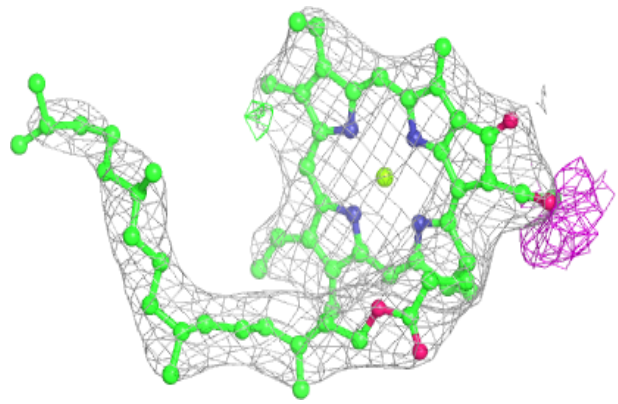


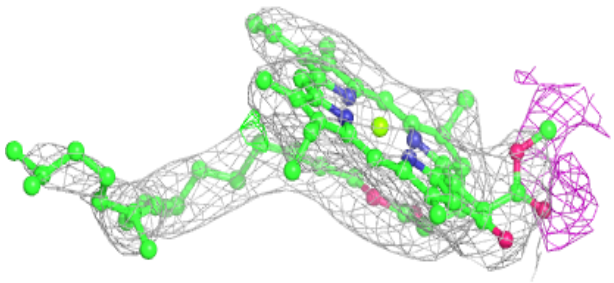


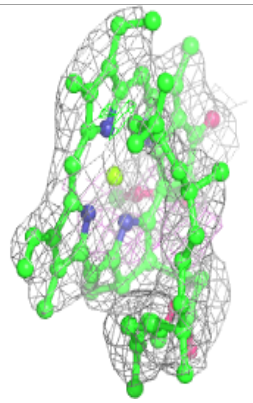


Electron density around CLA 1 301:

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

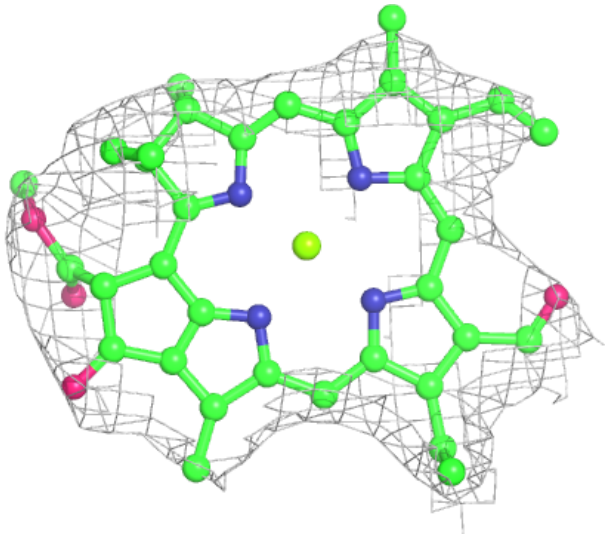


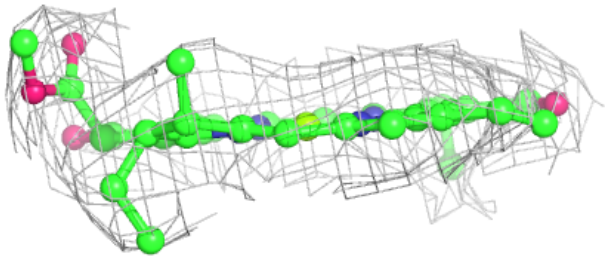


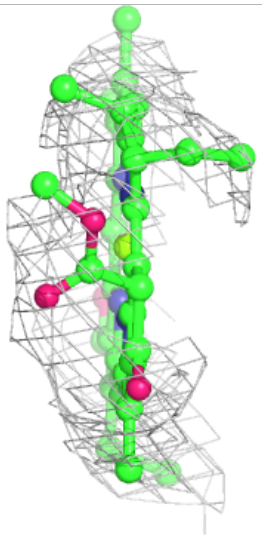


Electron density around CHL 2 313:

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

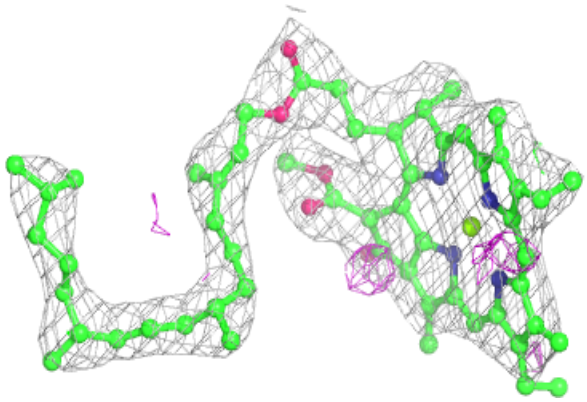


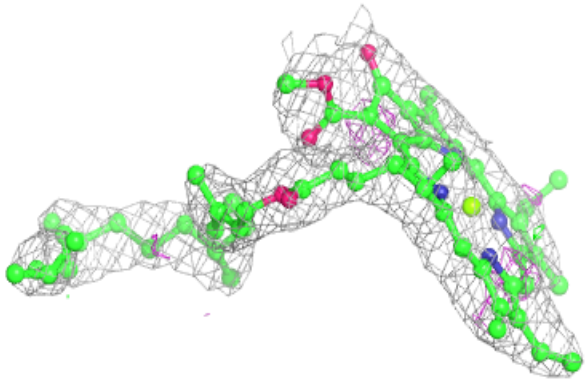


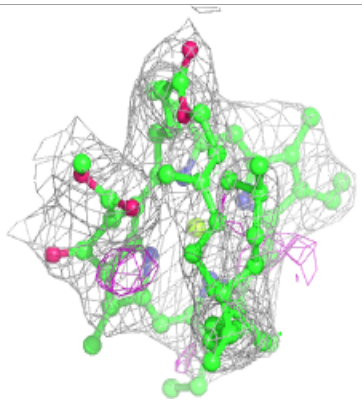


Electron density around CLA A 801:

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

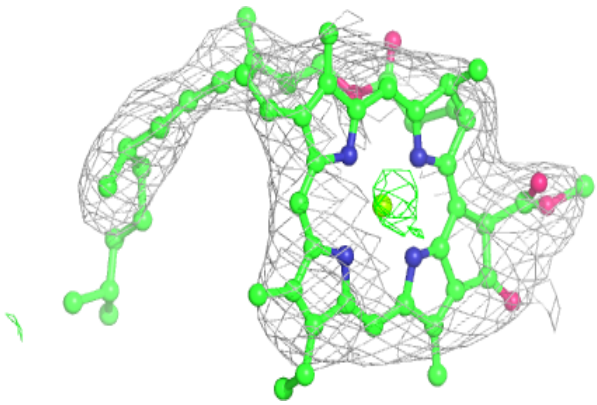


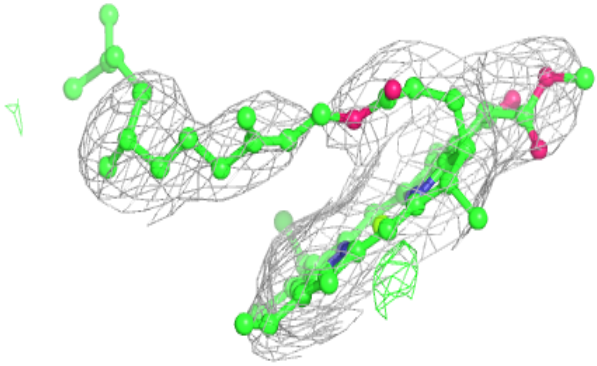


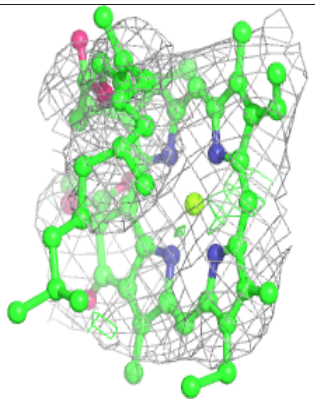


Electron density around CLA 2 308:

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

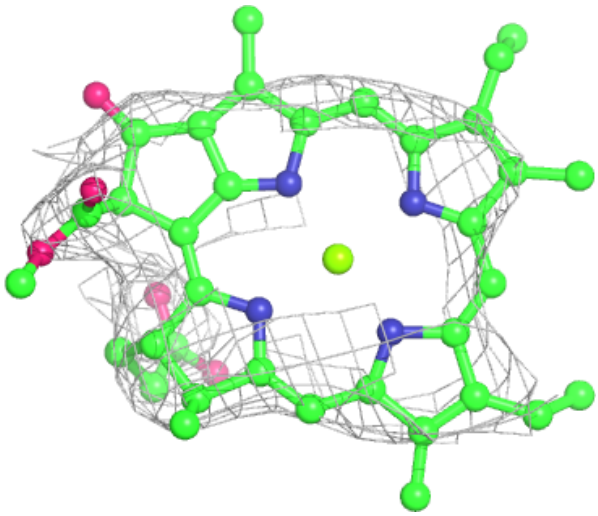


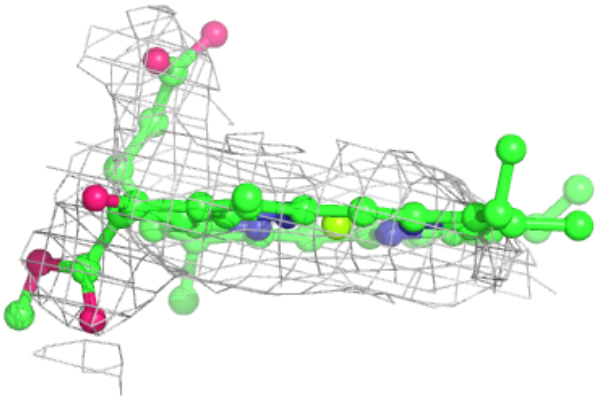


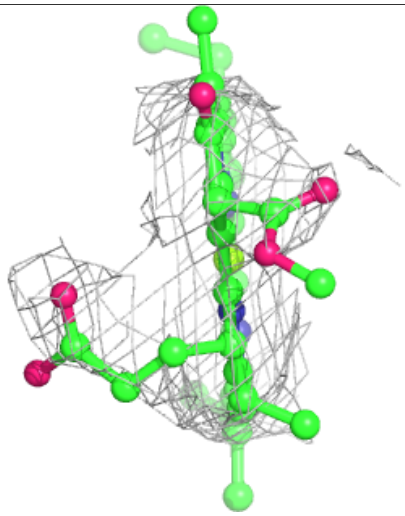


Electron density around CLA A 834:

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

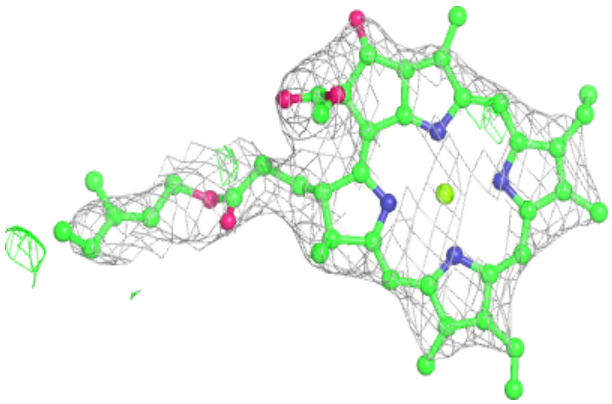


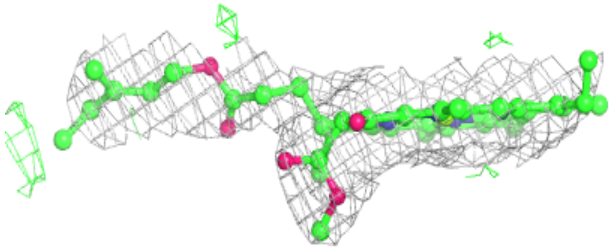


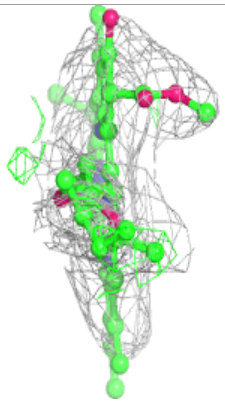


Electron density around CLA A 835:

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

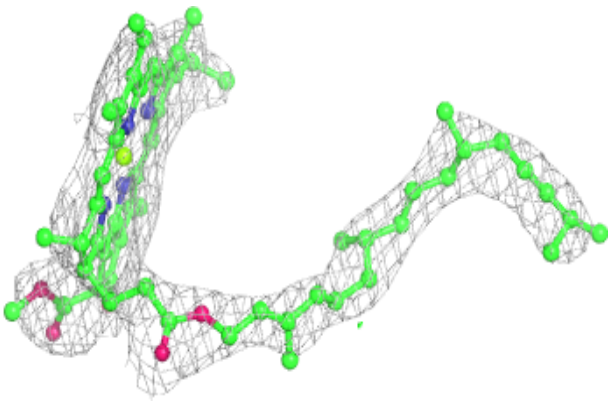


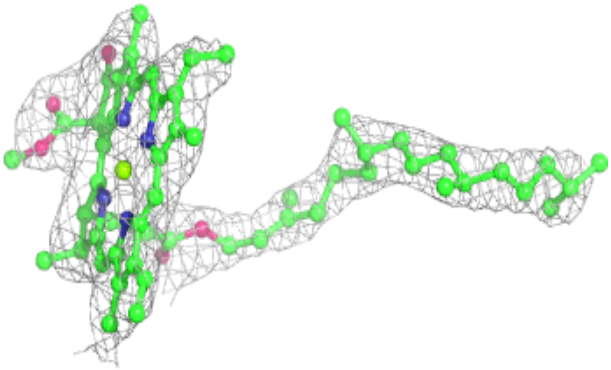


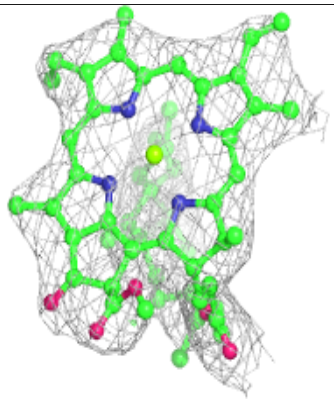


Electron density around CLA A 829:

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

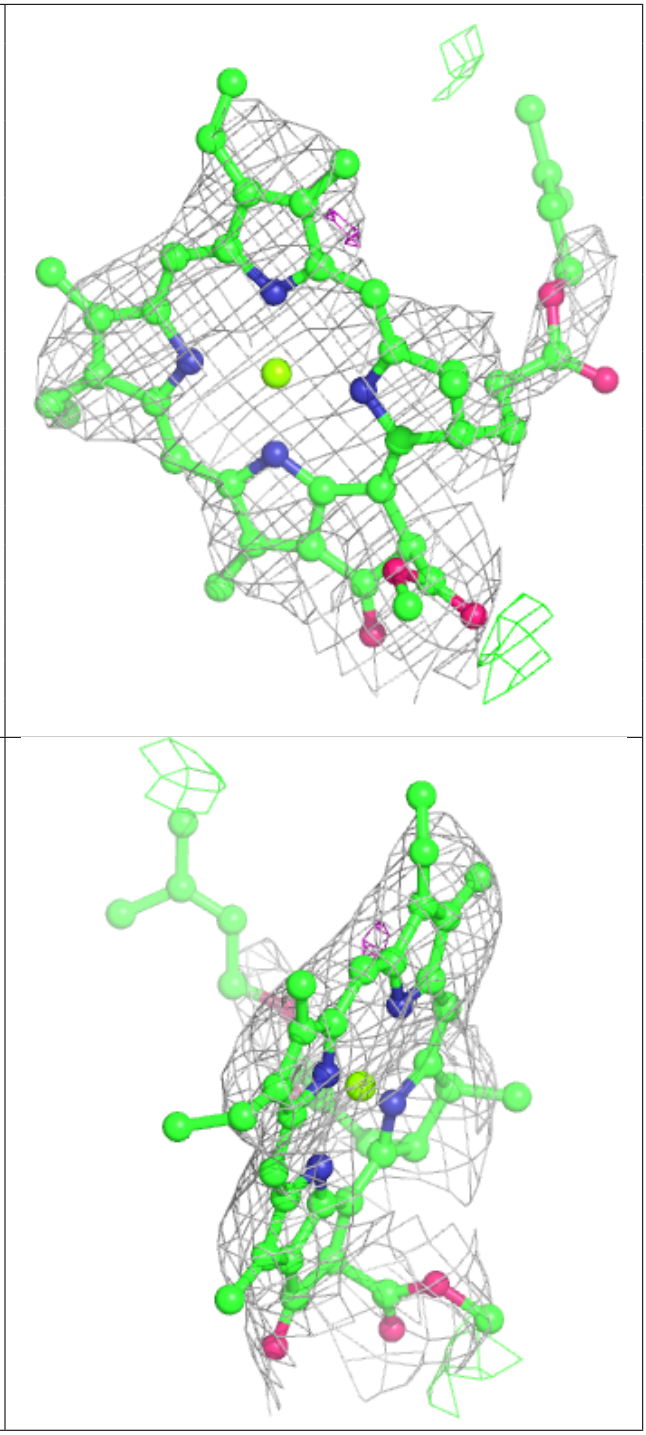






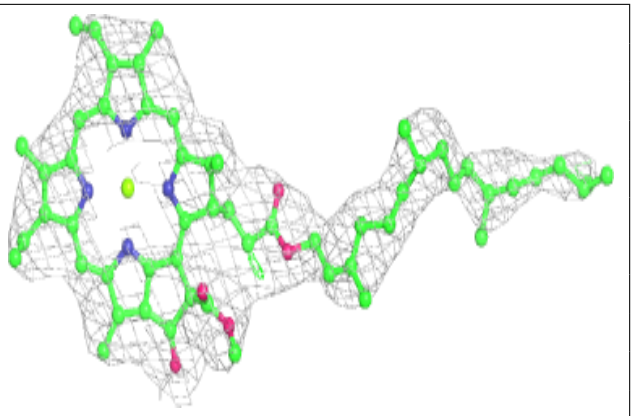
Electron density around CLA A 830:

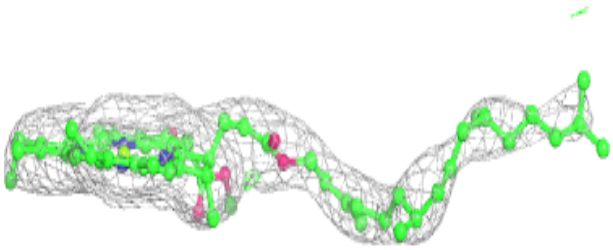
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

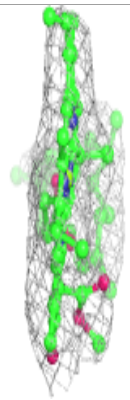


Electron density around CLA A 831:

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

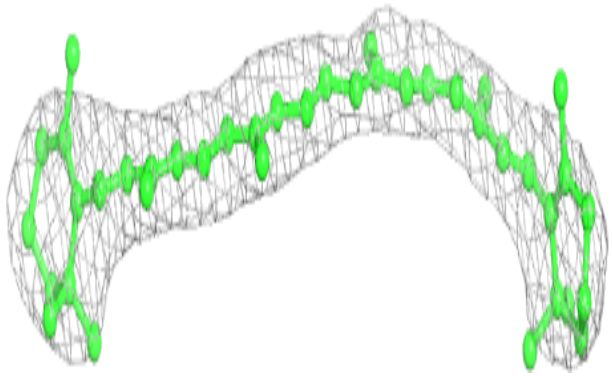


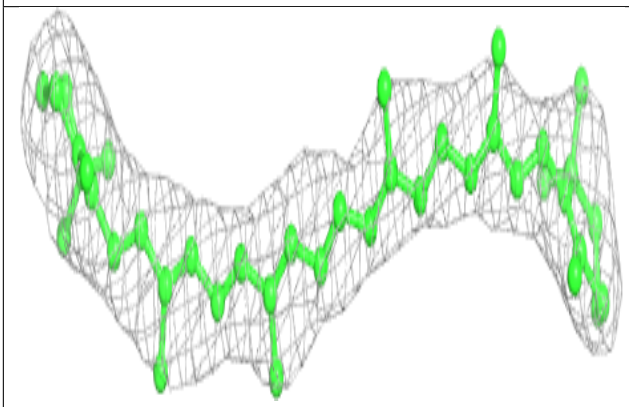


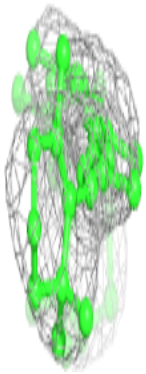


Electron density around BCR I 101:

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

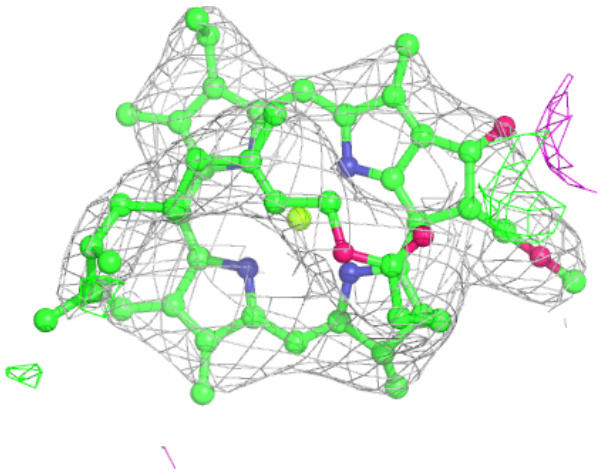


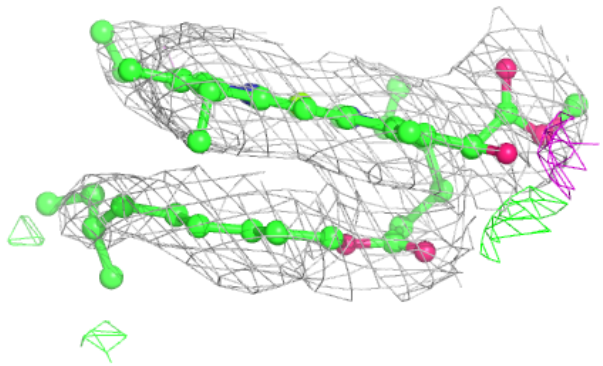


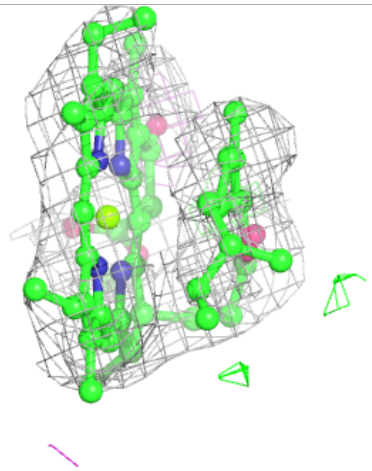


Electron density around CLA 4 312:

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

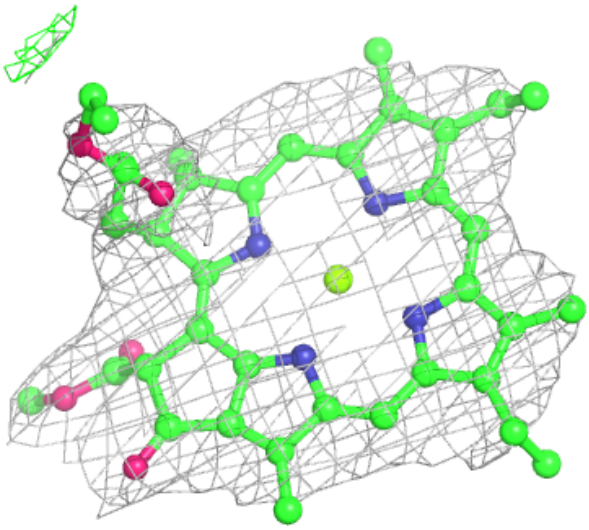


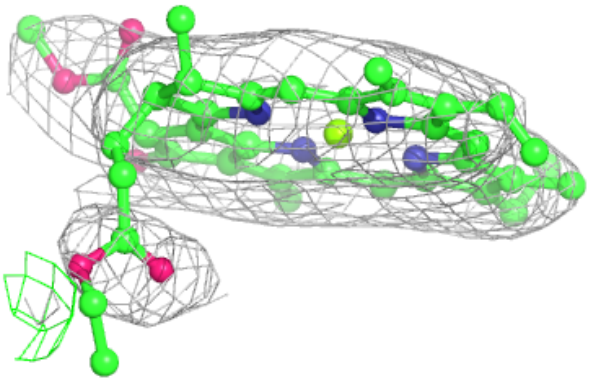


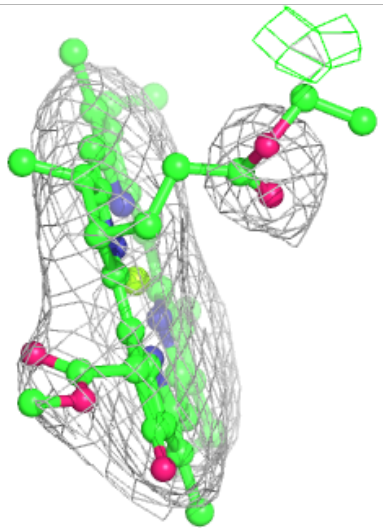


Electron density around CLA 3 606:

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

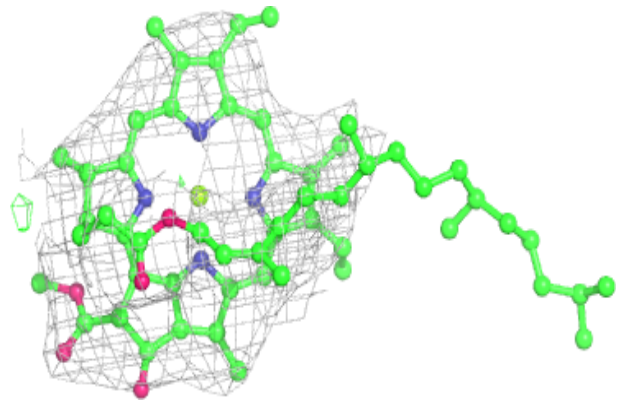


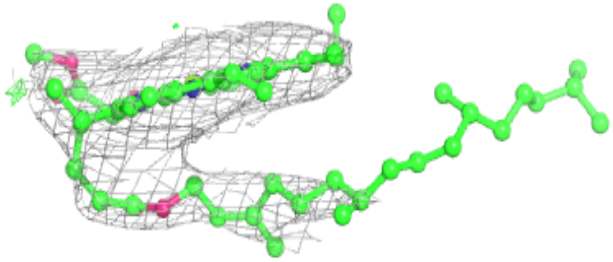


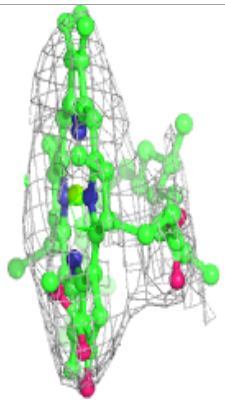


Electron density around CLA A 816:

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

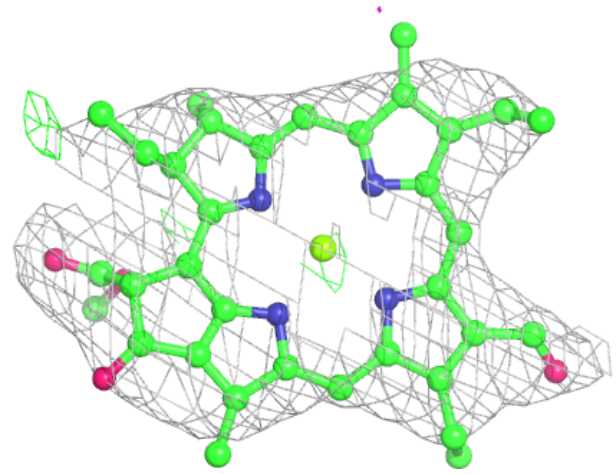


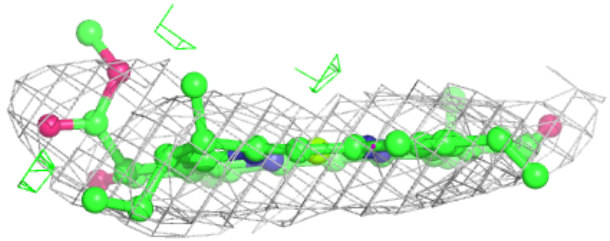


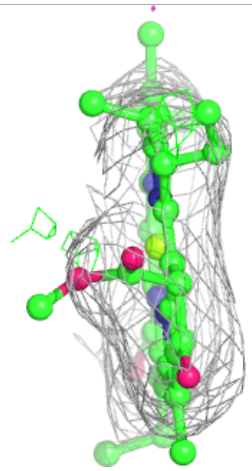


Electron density around CHL 2 304:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

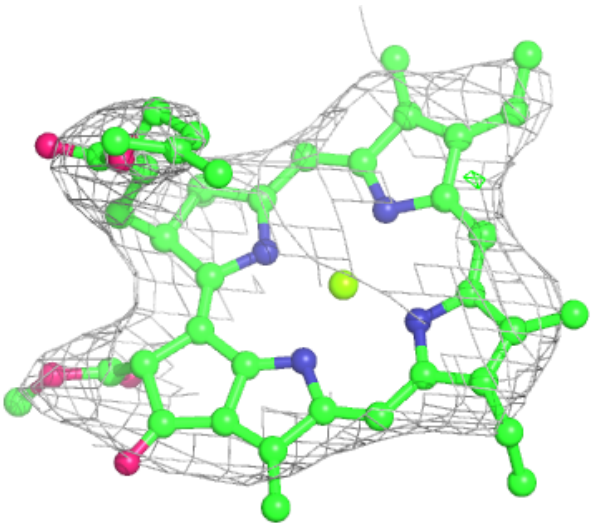


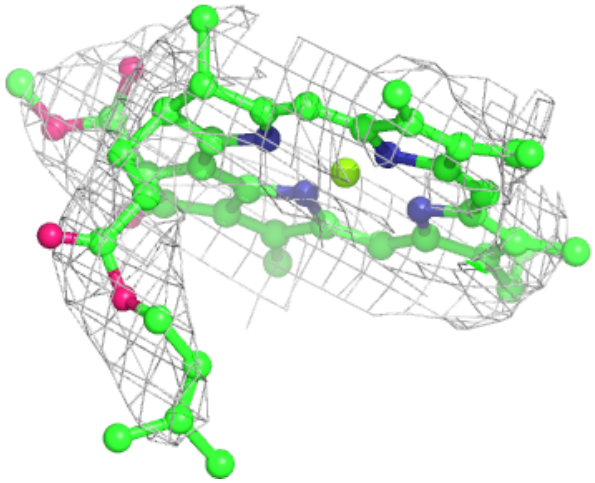


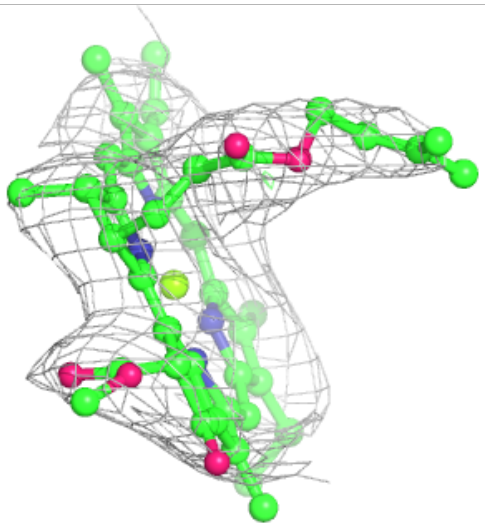


Electron density around CLA 3 608:

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

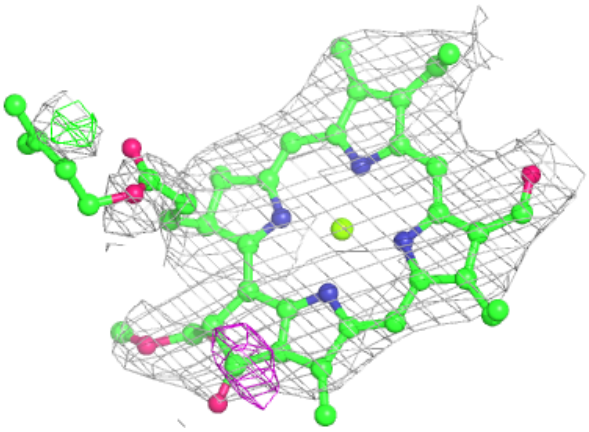


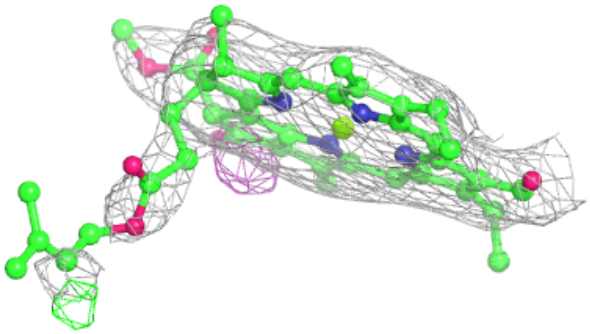


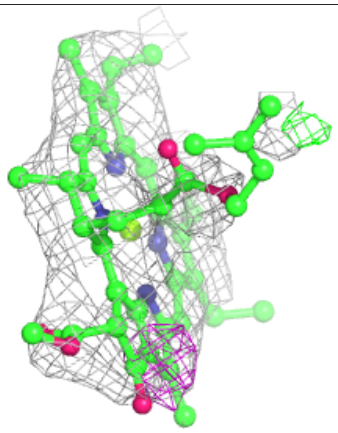


Electron density around CHL 2 306:

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

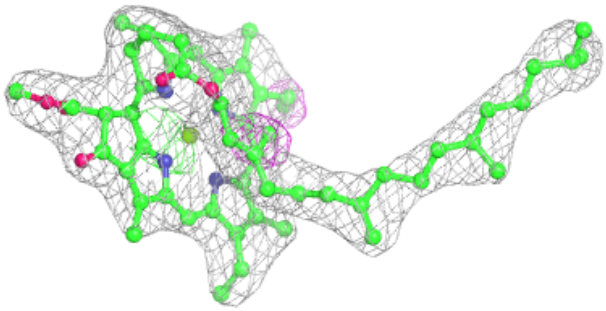


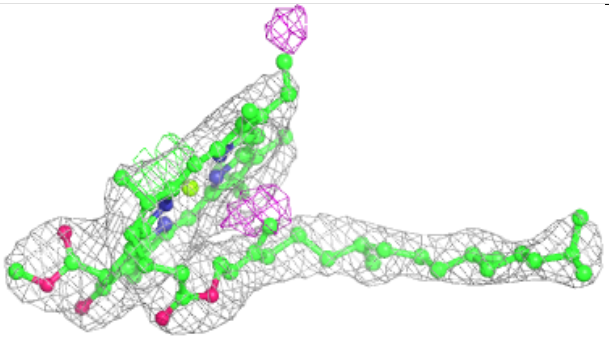


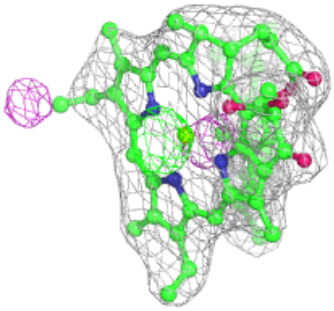


Electron density around CLA A 840:

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

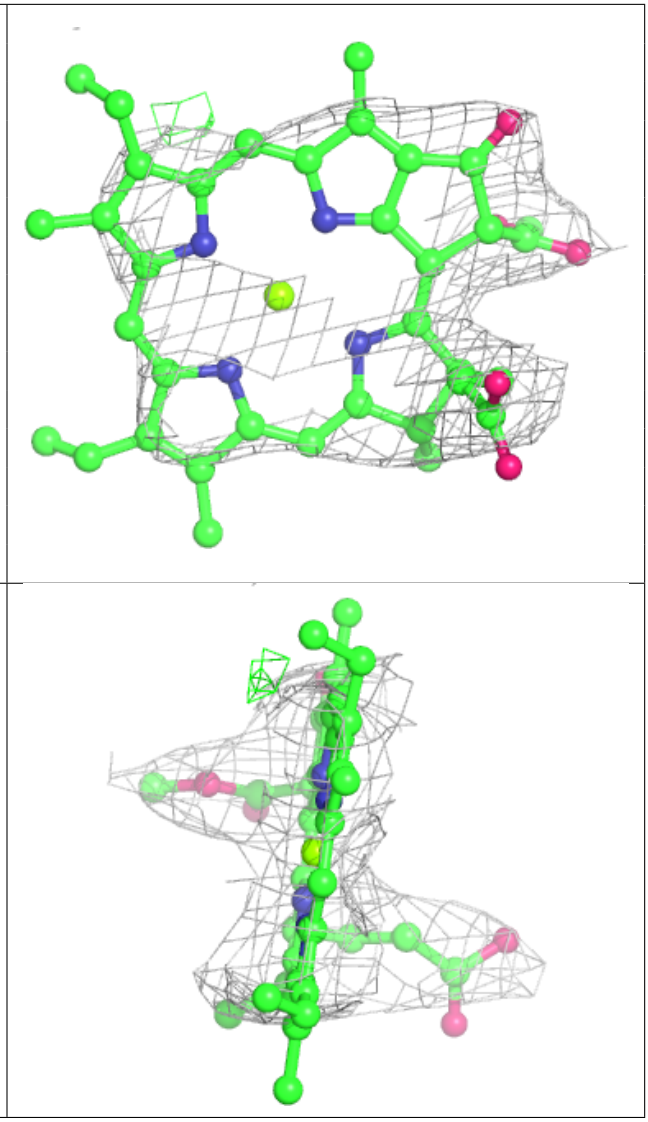






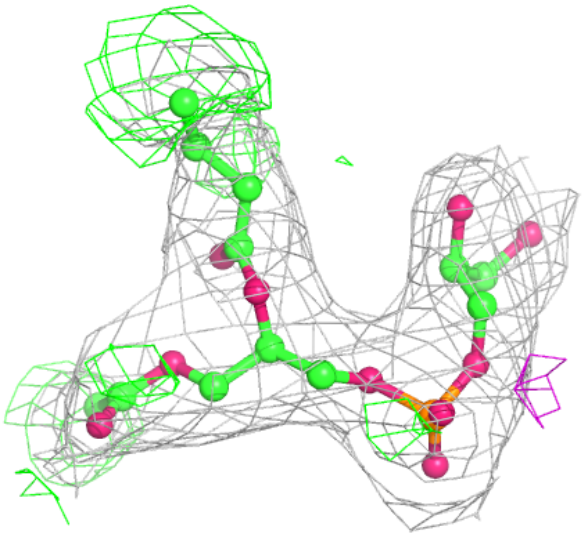
Electron density around CLA A 819:

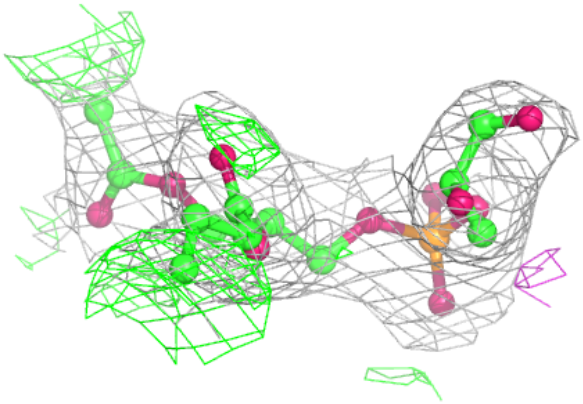
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

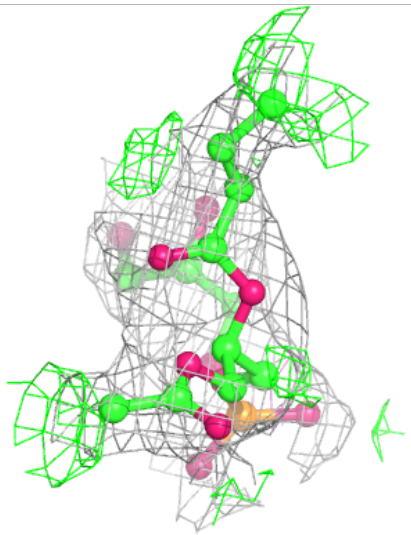


Electron density around LHG B 801:

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

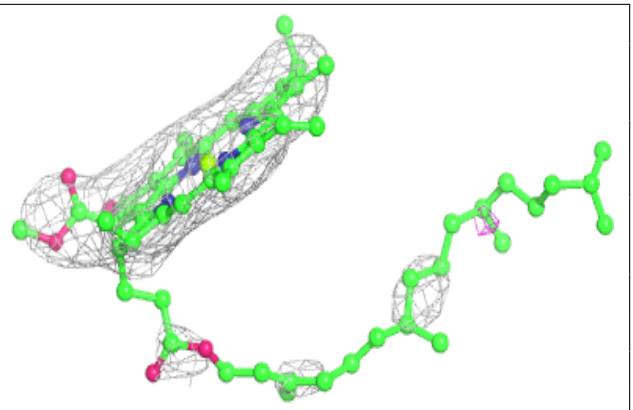


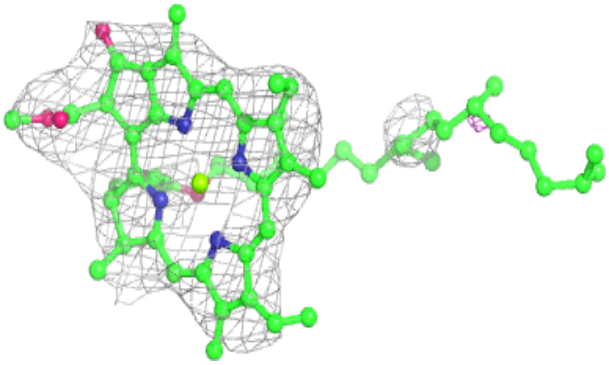


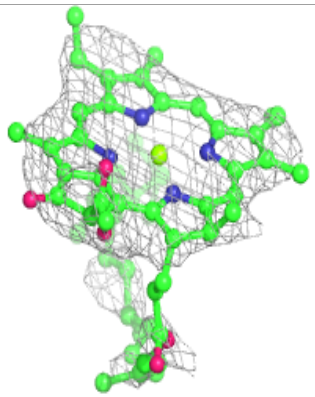


Electron density around CLA B 803:

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

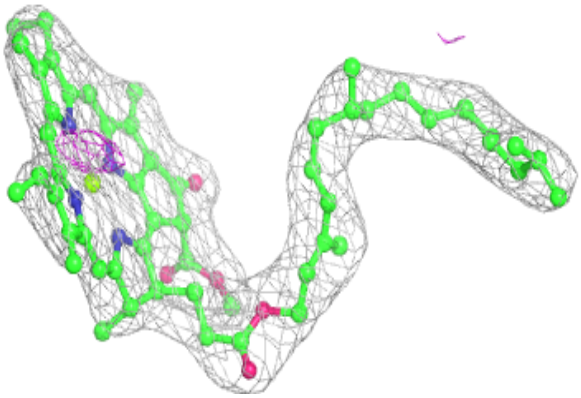


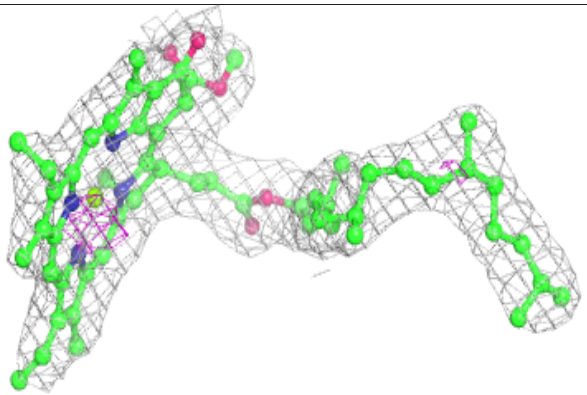


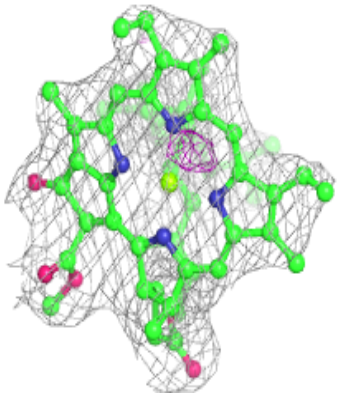


Electron density around CLA B 804:

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

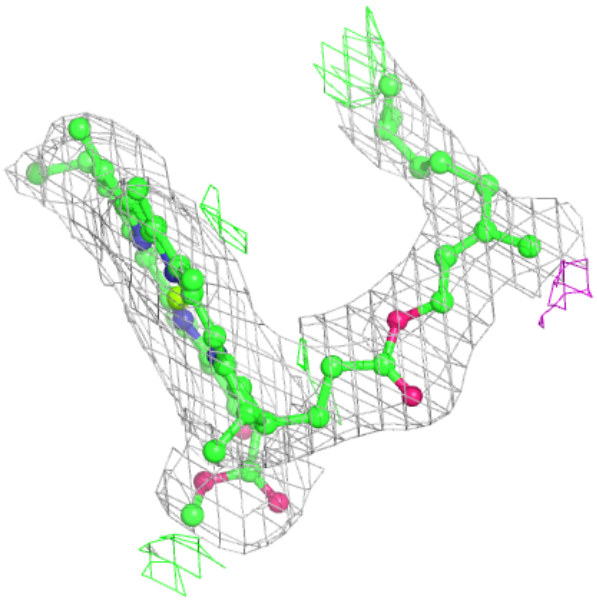


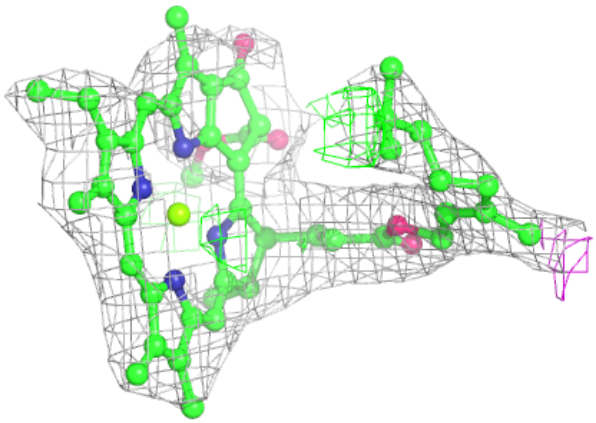


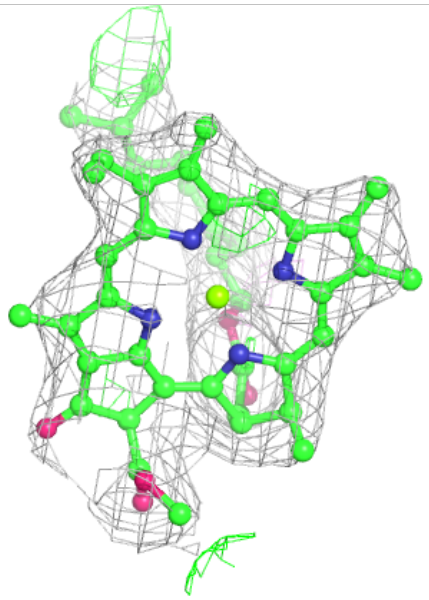


Electron density around CLA B 813:

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

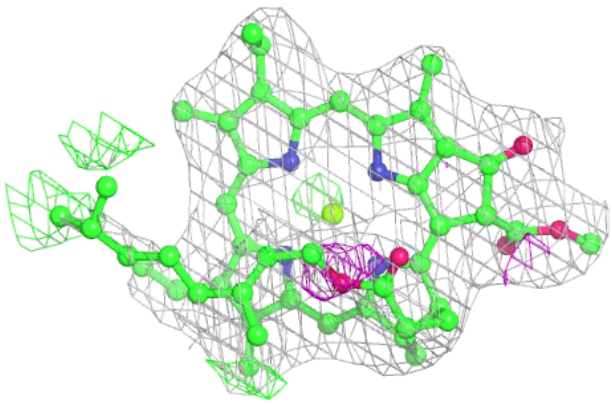


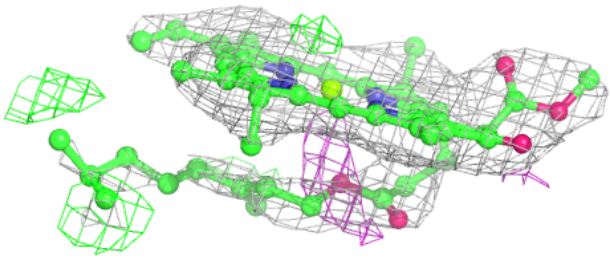


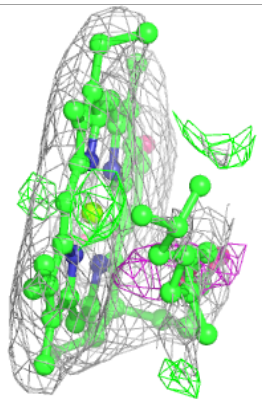


Electron density around CLA B 814:

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

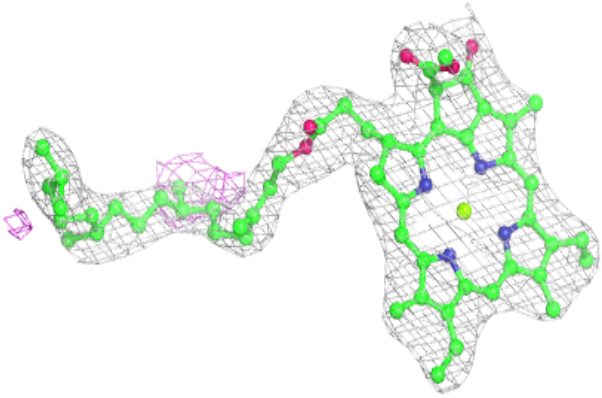


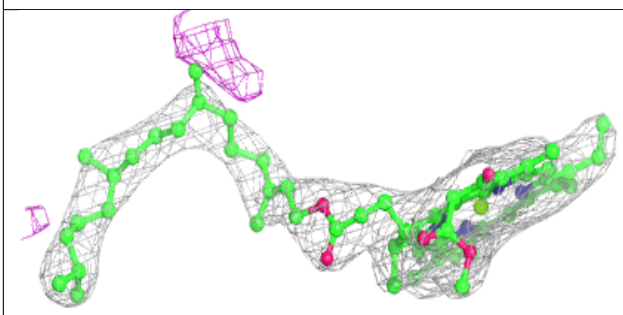


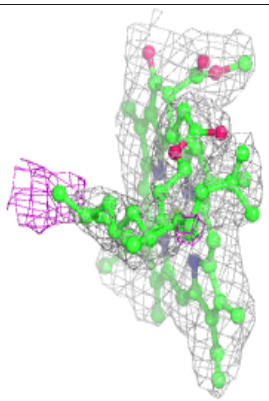


Electron density around CLA B 815:

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

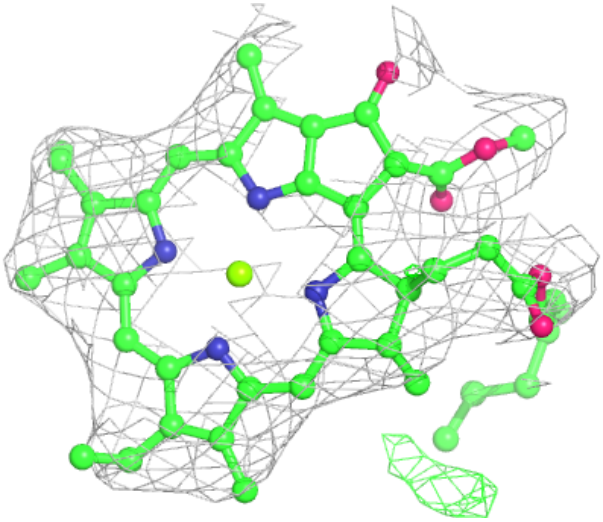


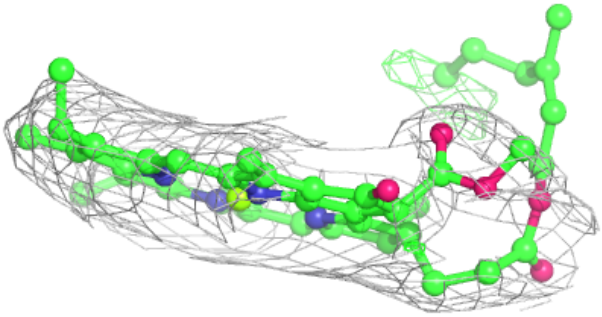


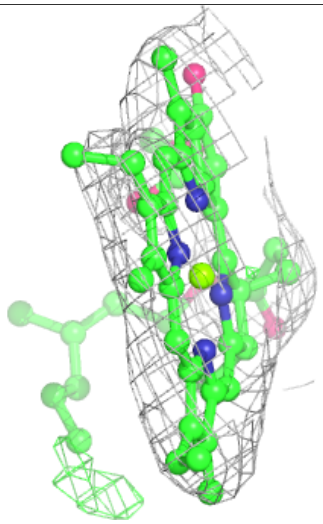


Electron density around CLA 1 310:

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

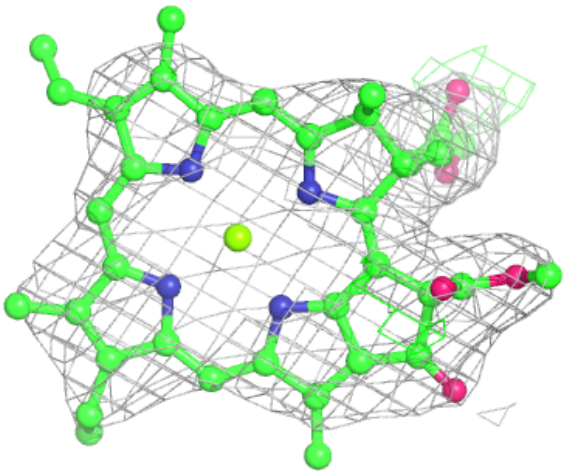


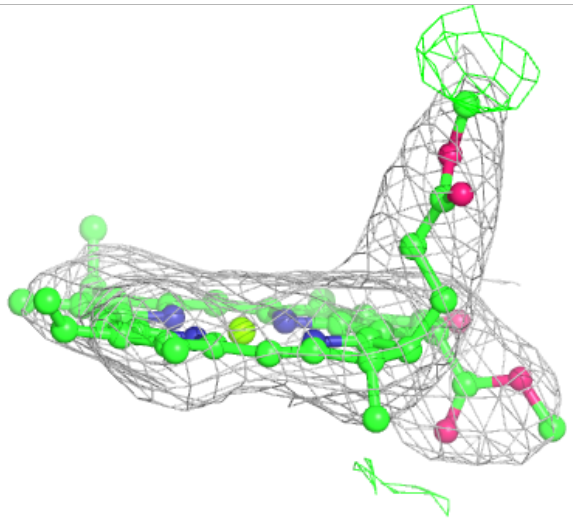


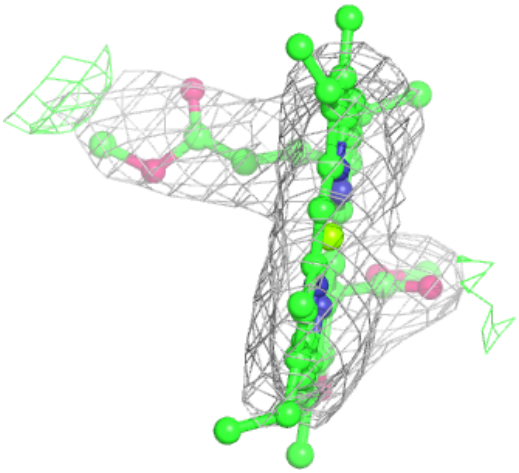


Electron density around CLA 1 306:

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

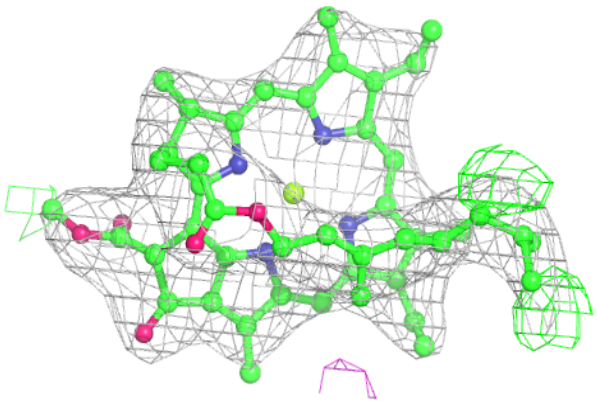


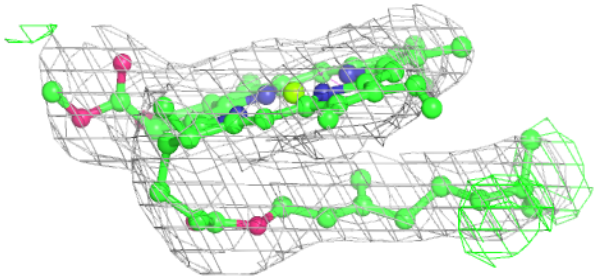


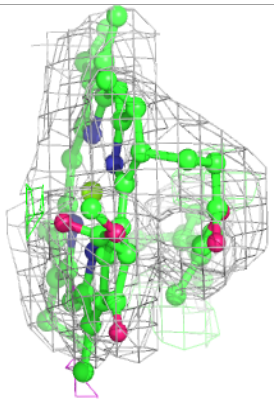


Electron density around CLA B 818:

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

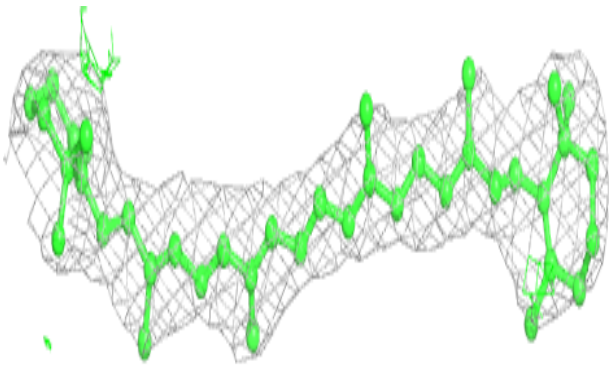


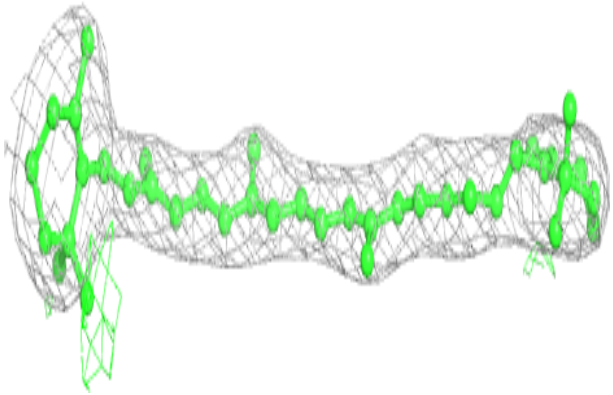


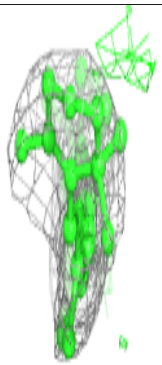


Electron density around BCR 4 318:

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

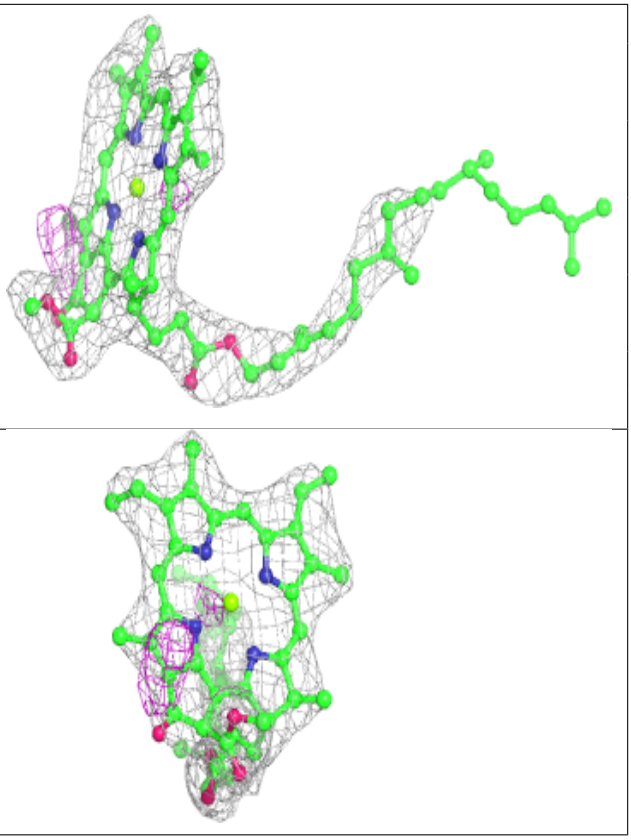


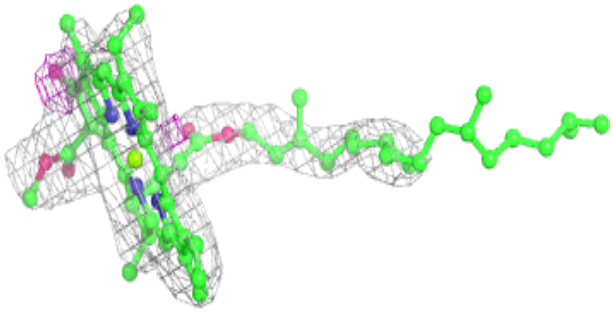




Electron density around CLA B 823:

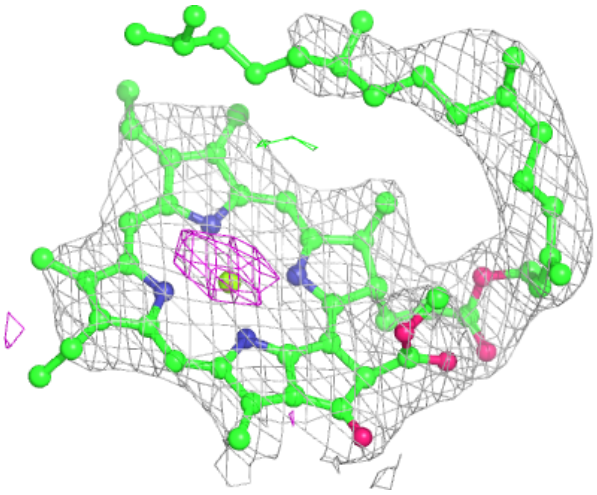
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

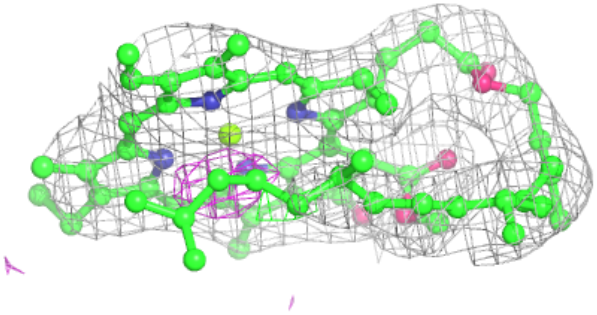


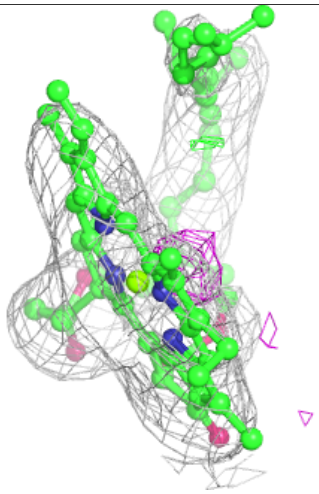


Electron density around CLA 1 302:

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

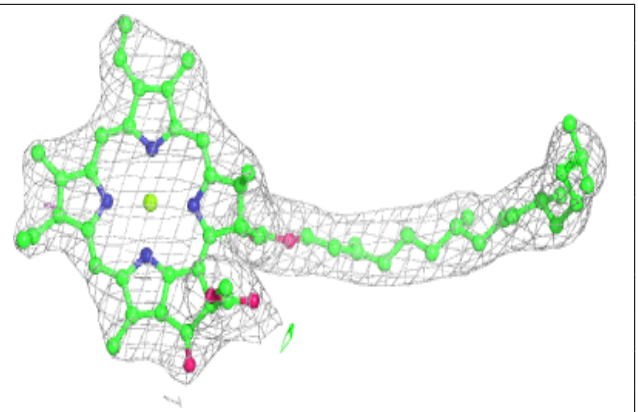


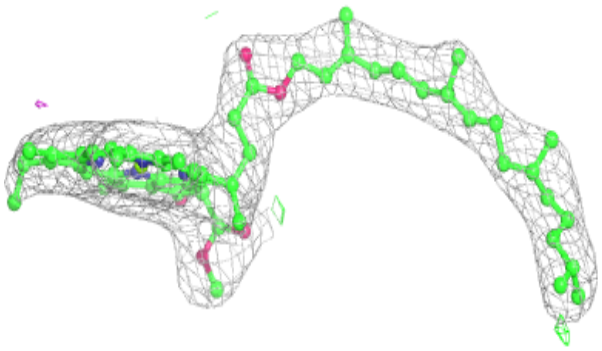


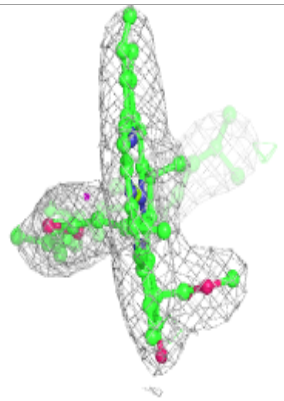


Electron density around CLA B 842:

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

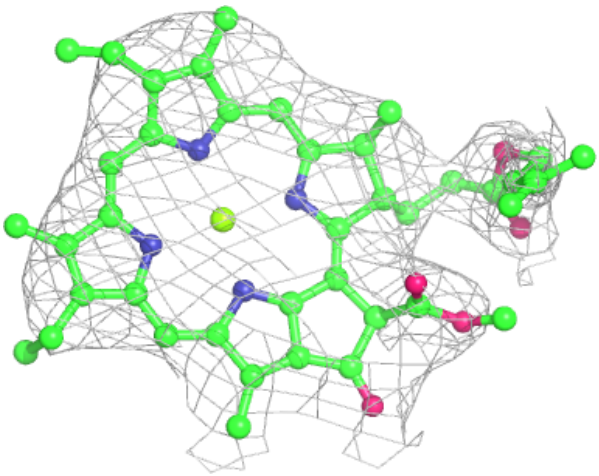


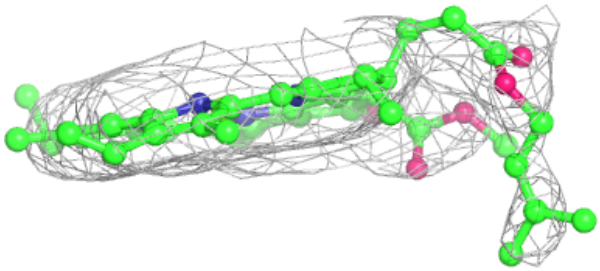


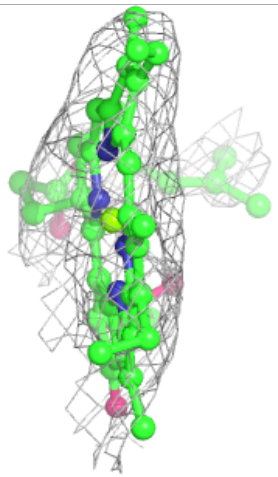


Electron density around CLA 3 603:

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

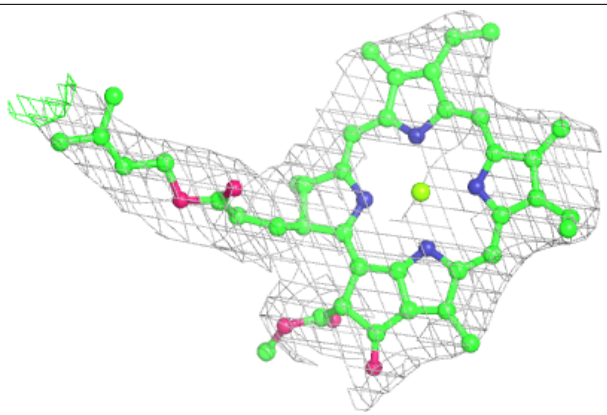


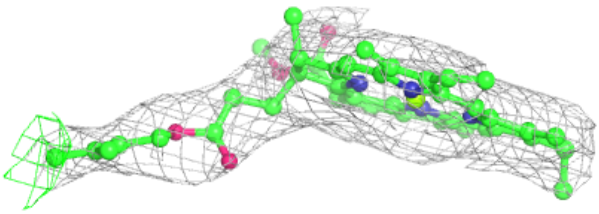


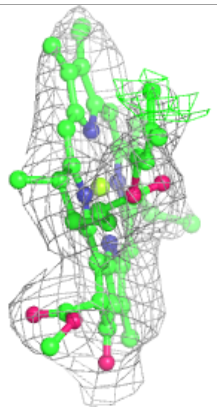


Electron density around CLA G 104:

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

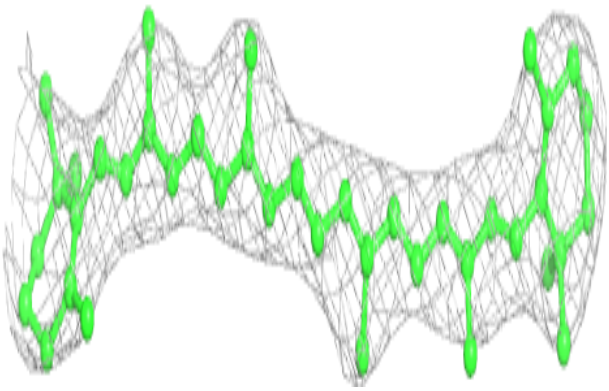


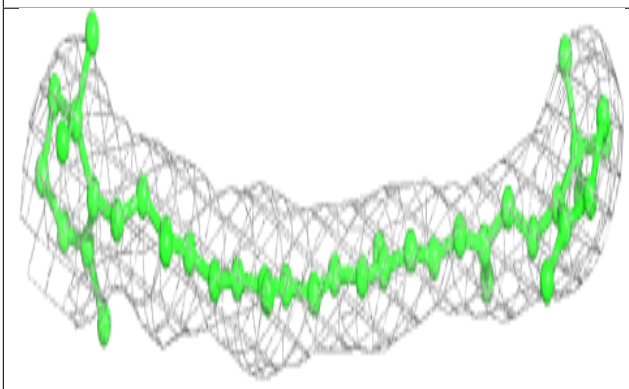


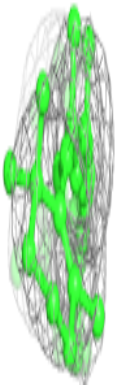


Electron density around BCR B 844:

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

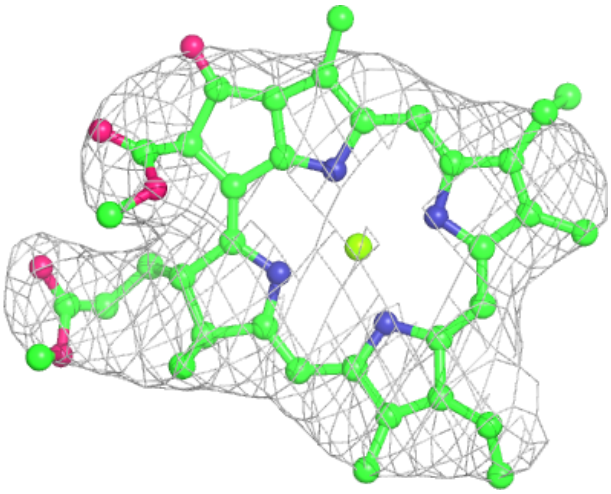


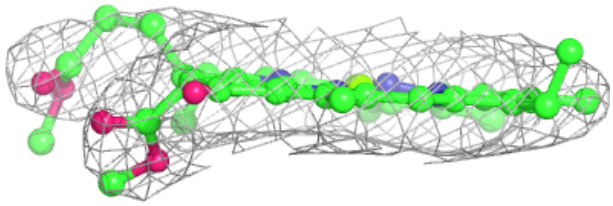


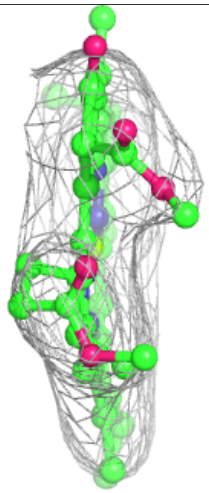


Electron density around CLA G 105:

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

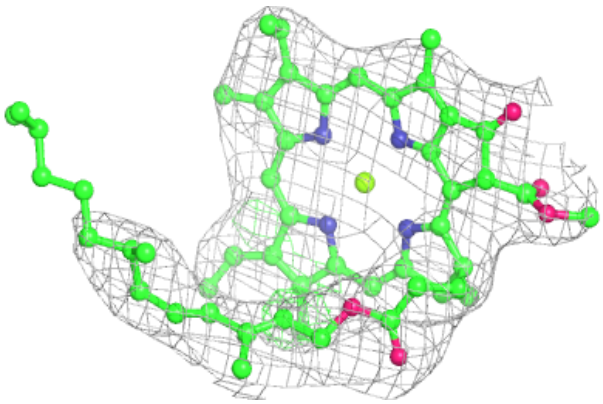


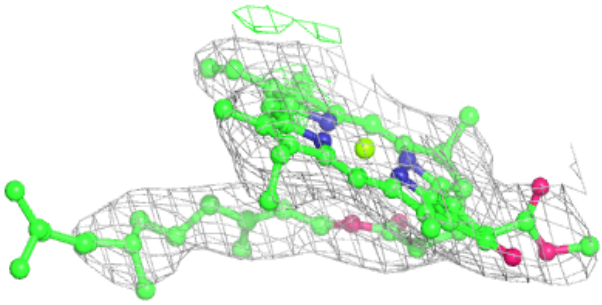


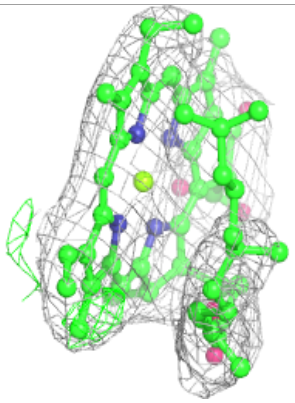


Electron density around CLA 1 308:

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

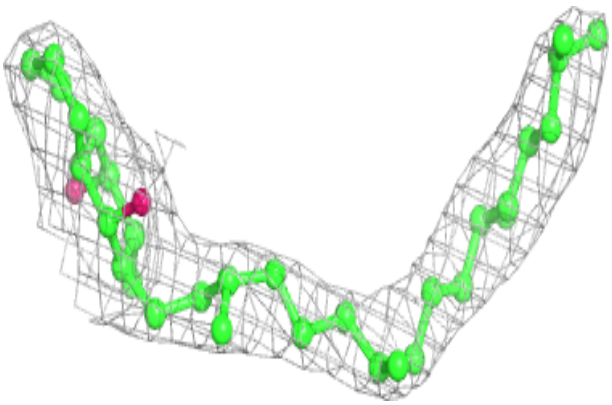


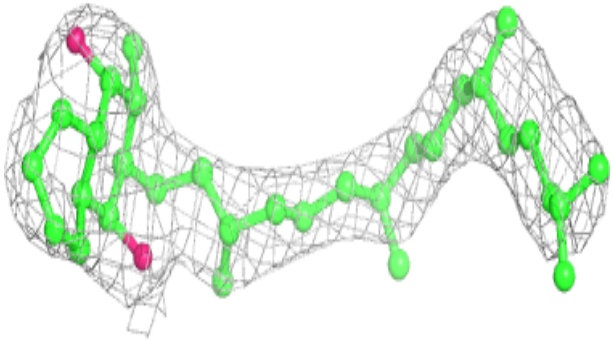


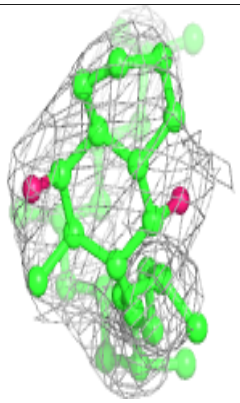


Electron density around PQN B 843:

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

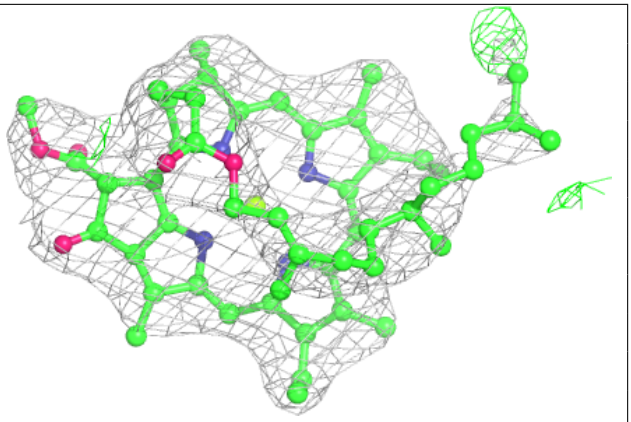


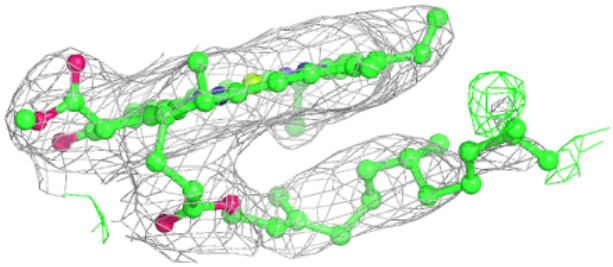


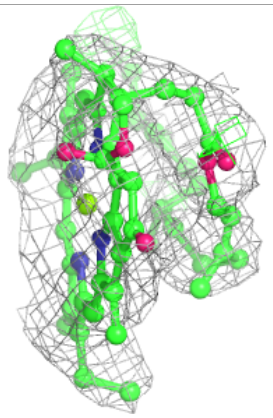


Electron density around CLA 1 311:

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

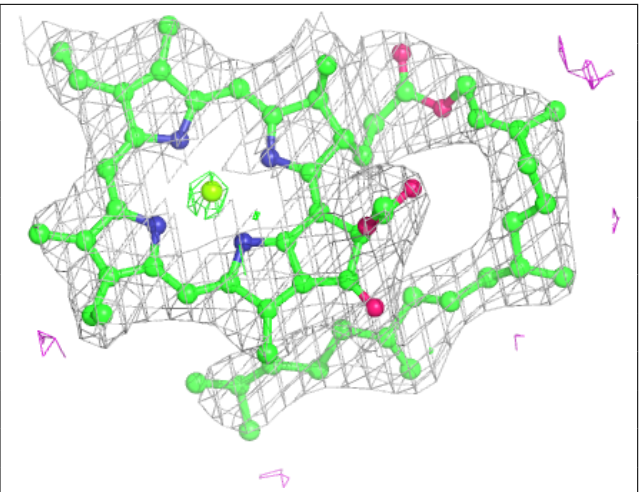


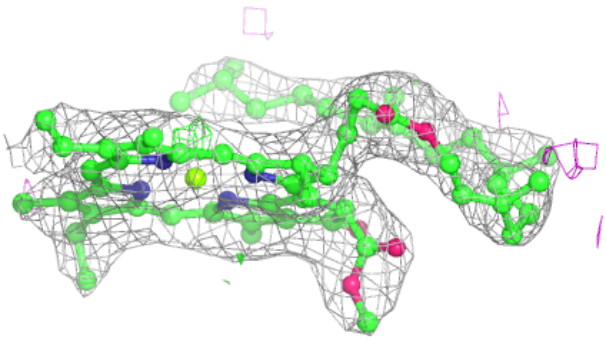




Electron density around CLA B 807:

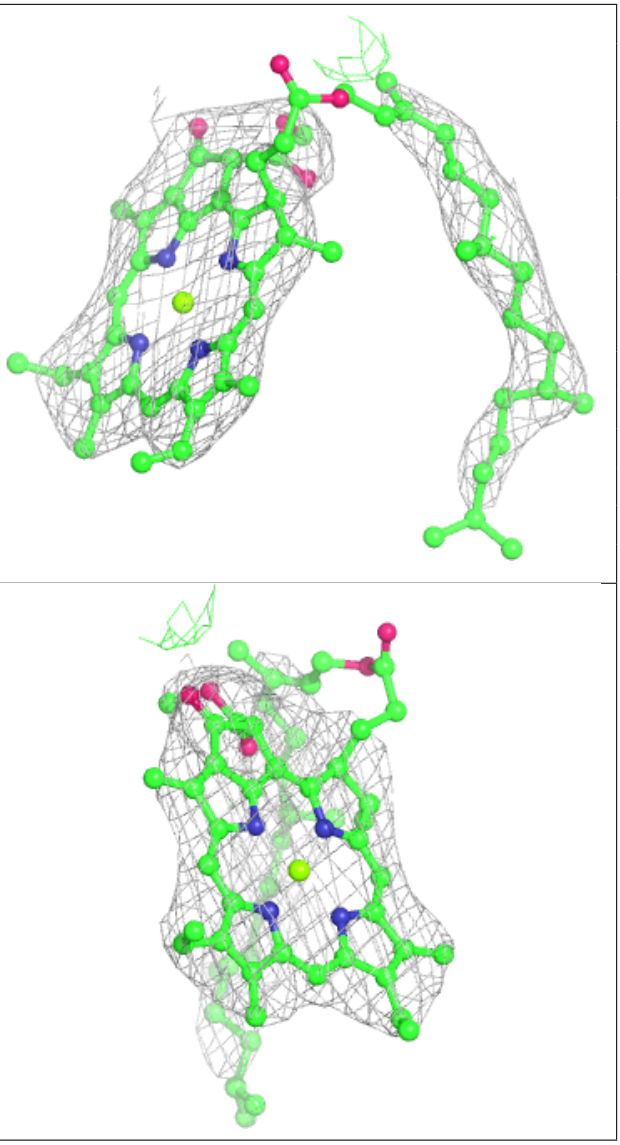
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

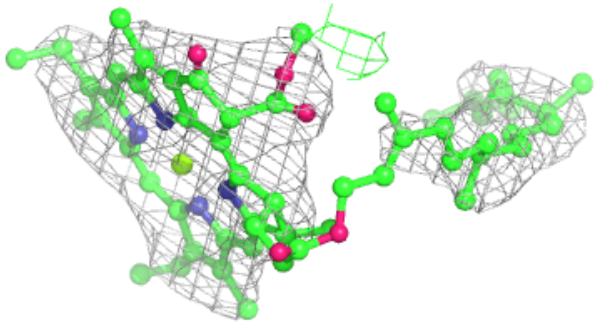




Electron density around CLA B 812:

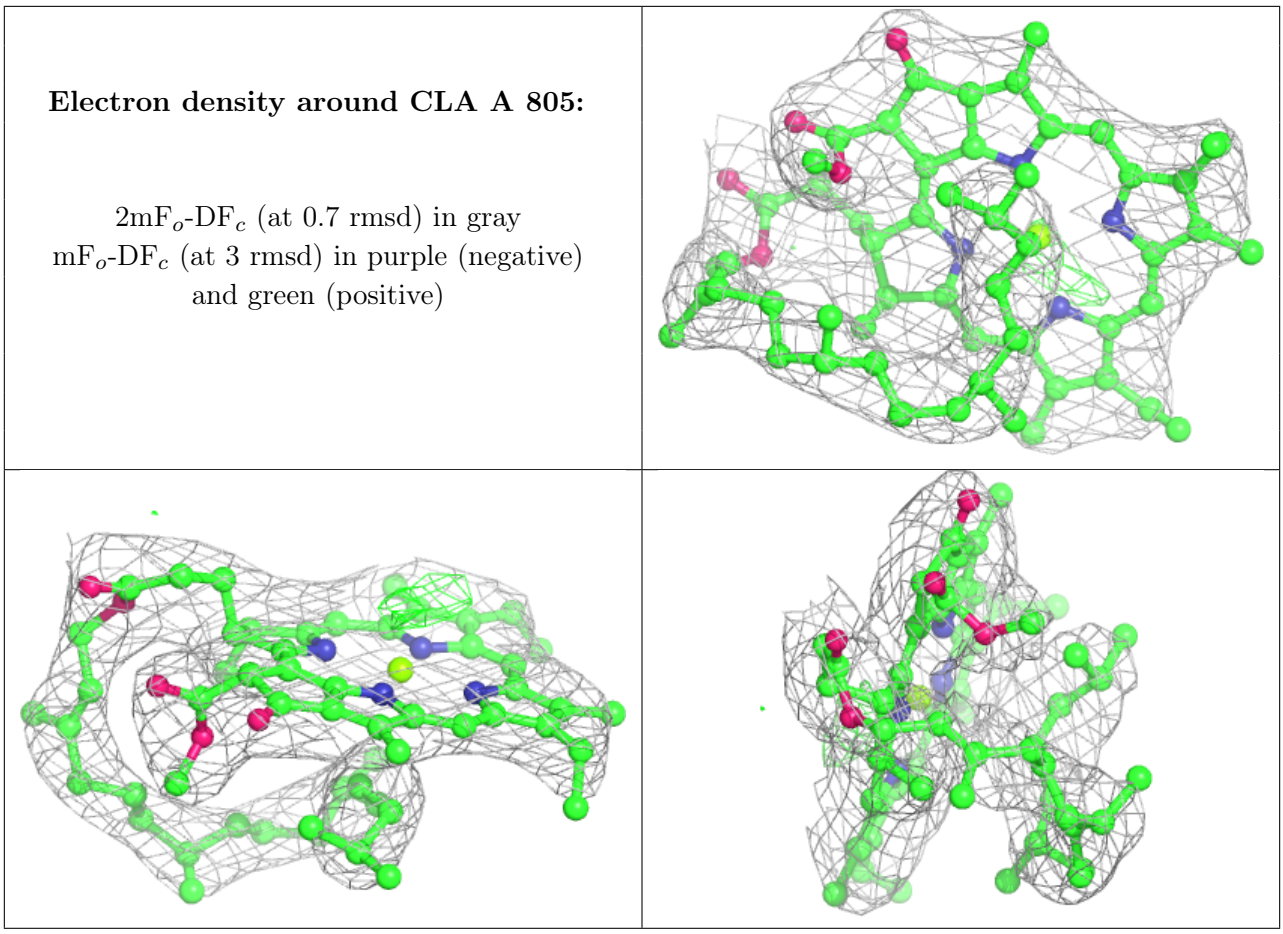
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





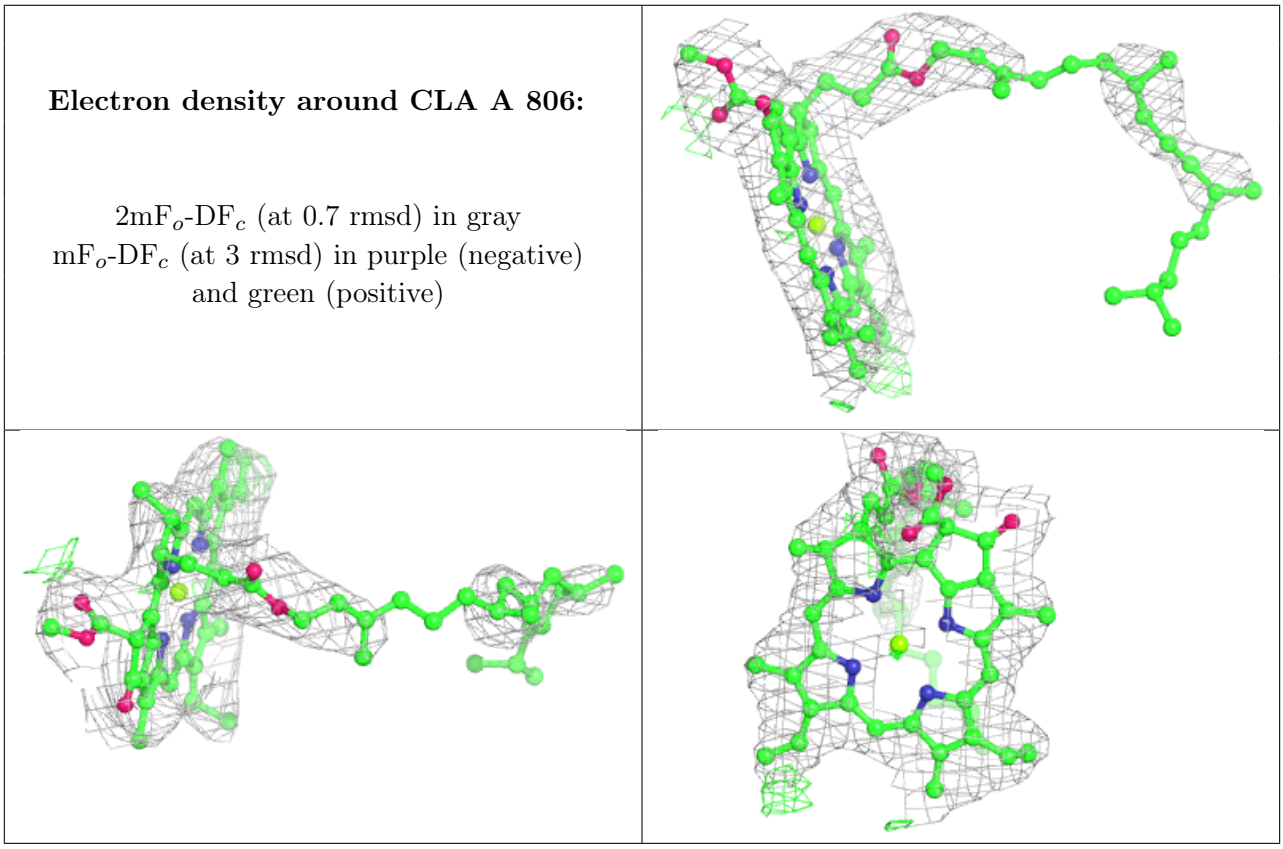
Electron density around CLA A 805:

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



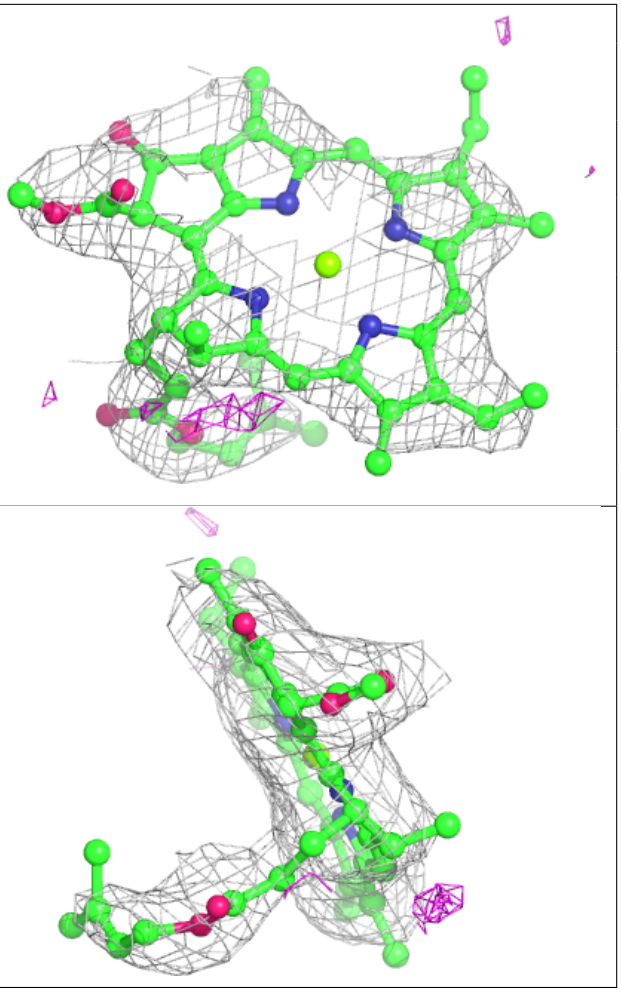
Electron density around CLA A 806:

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



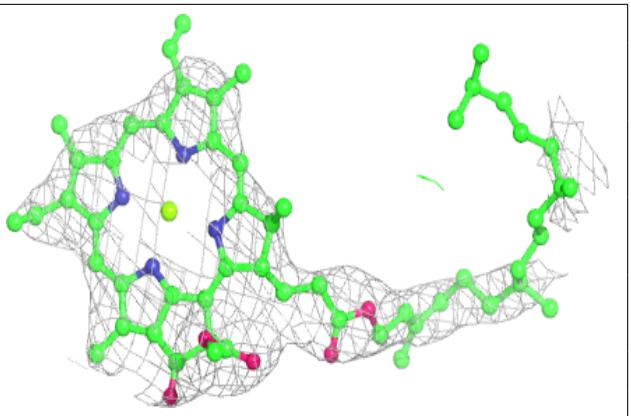
Electron density around CLA 2 307:

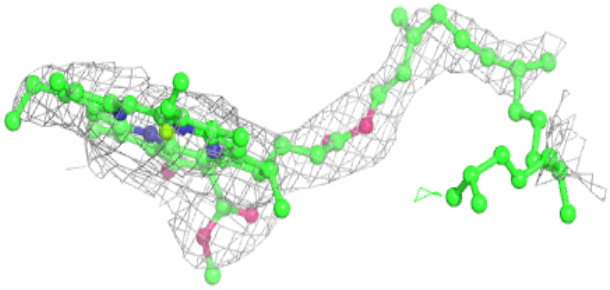
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

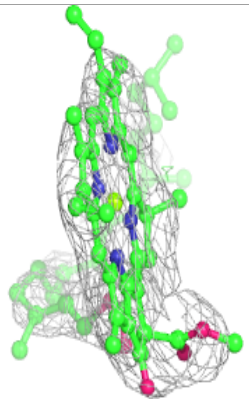


Electron density around CLA A 826:

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

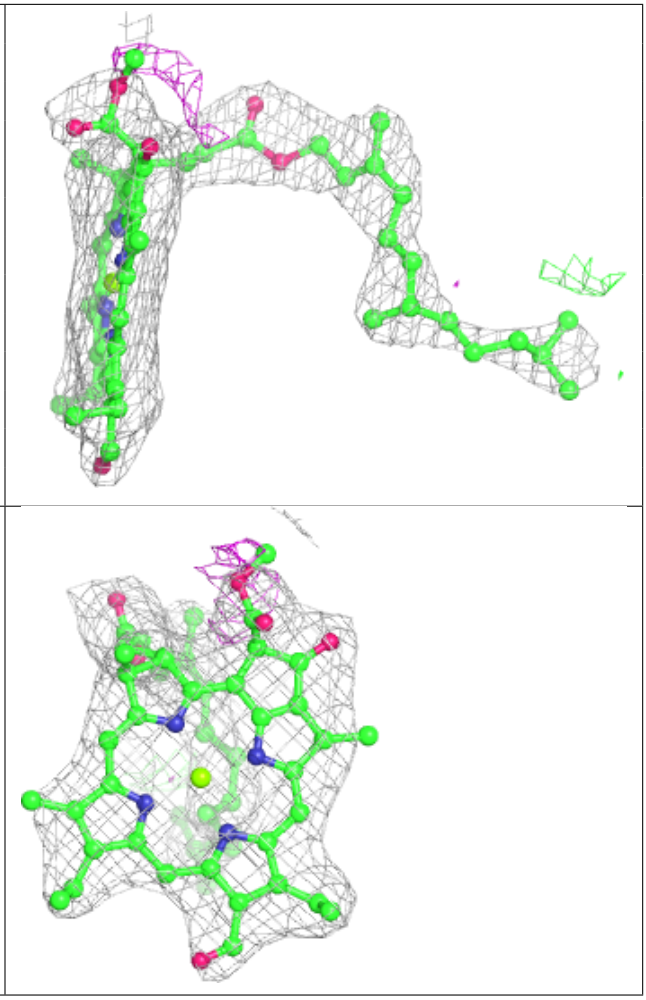






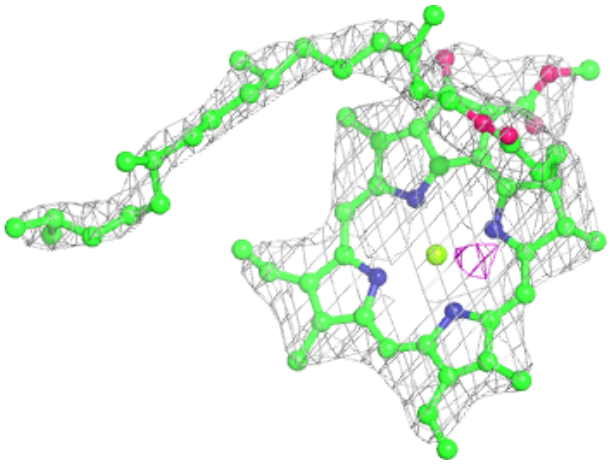
Electron density around CHL 4 301:

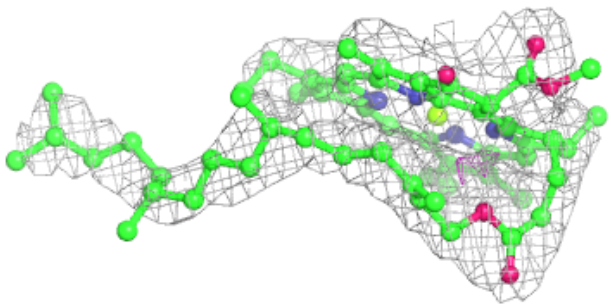
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

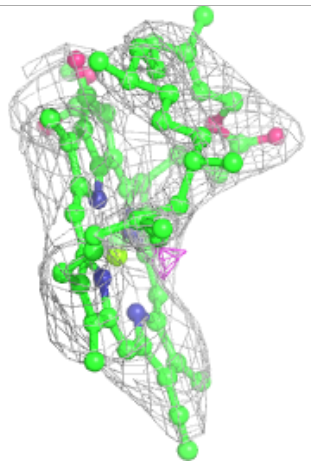


Electron density around CLA A 828:

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

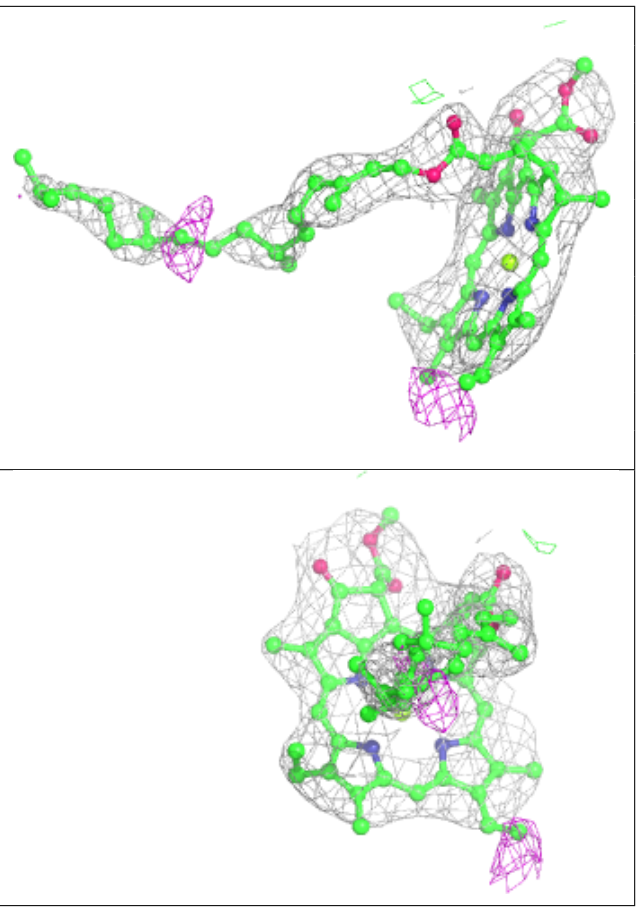






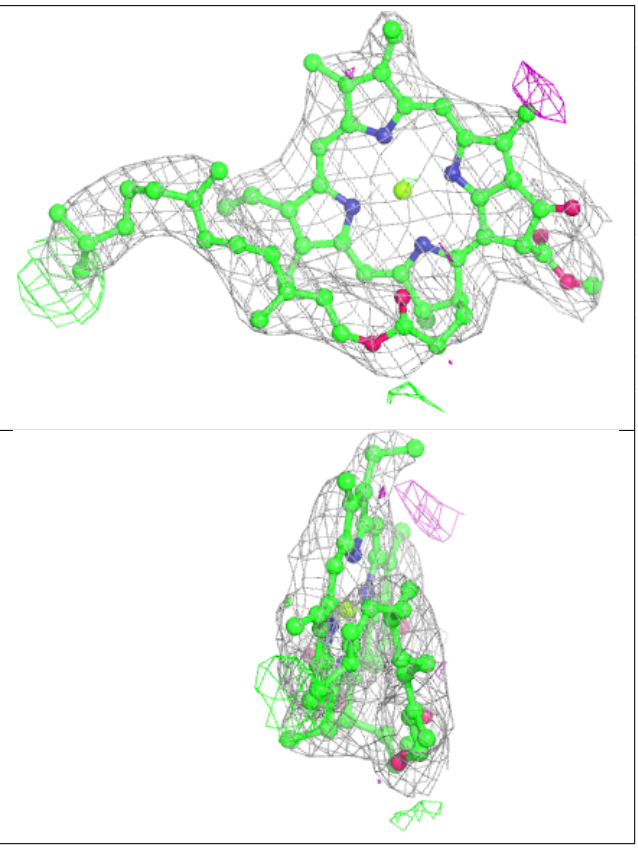
Electron density around CLA A 810:

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



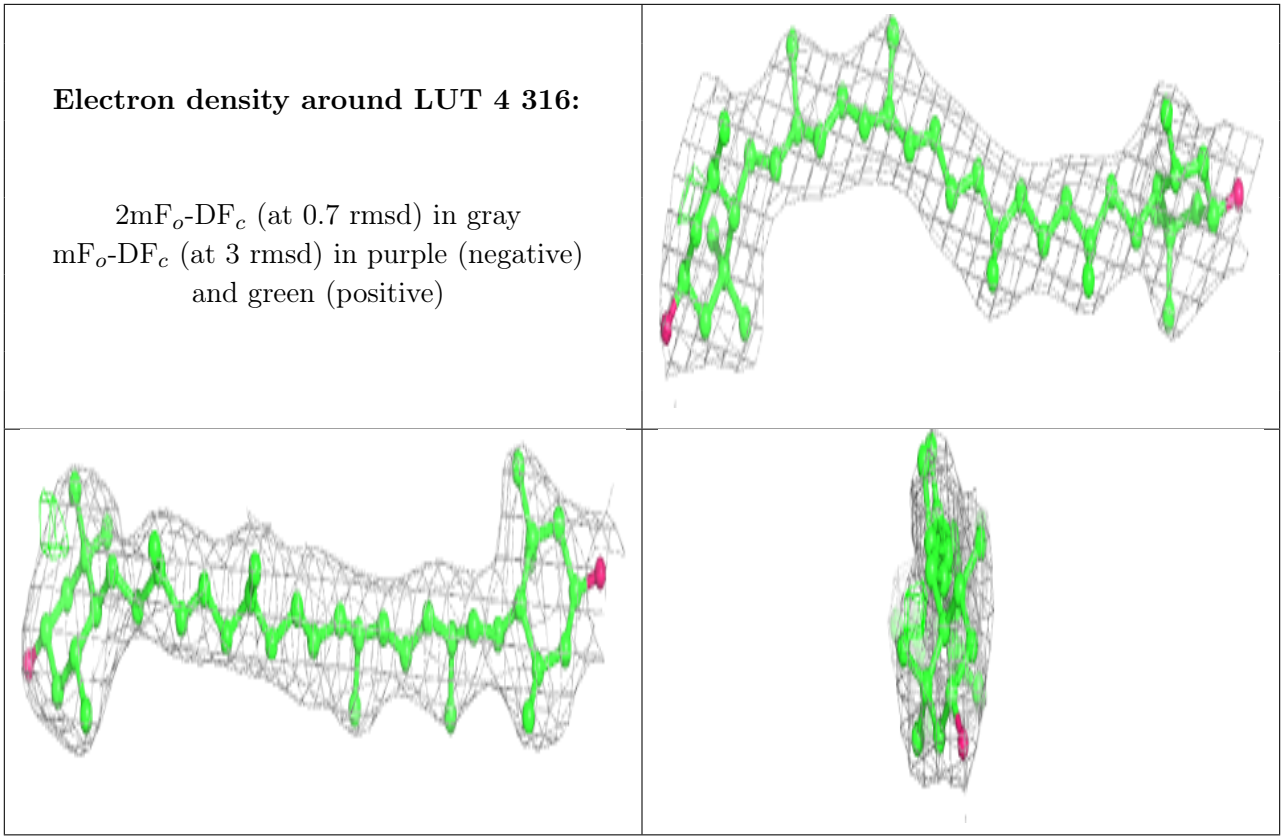
Electron density around CLA B 820:

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



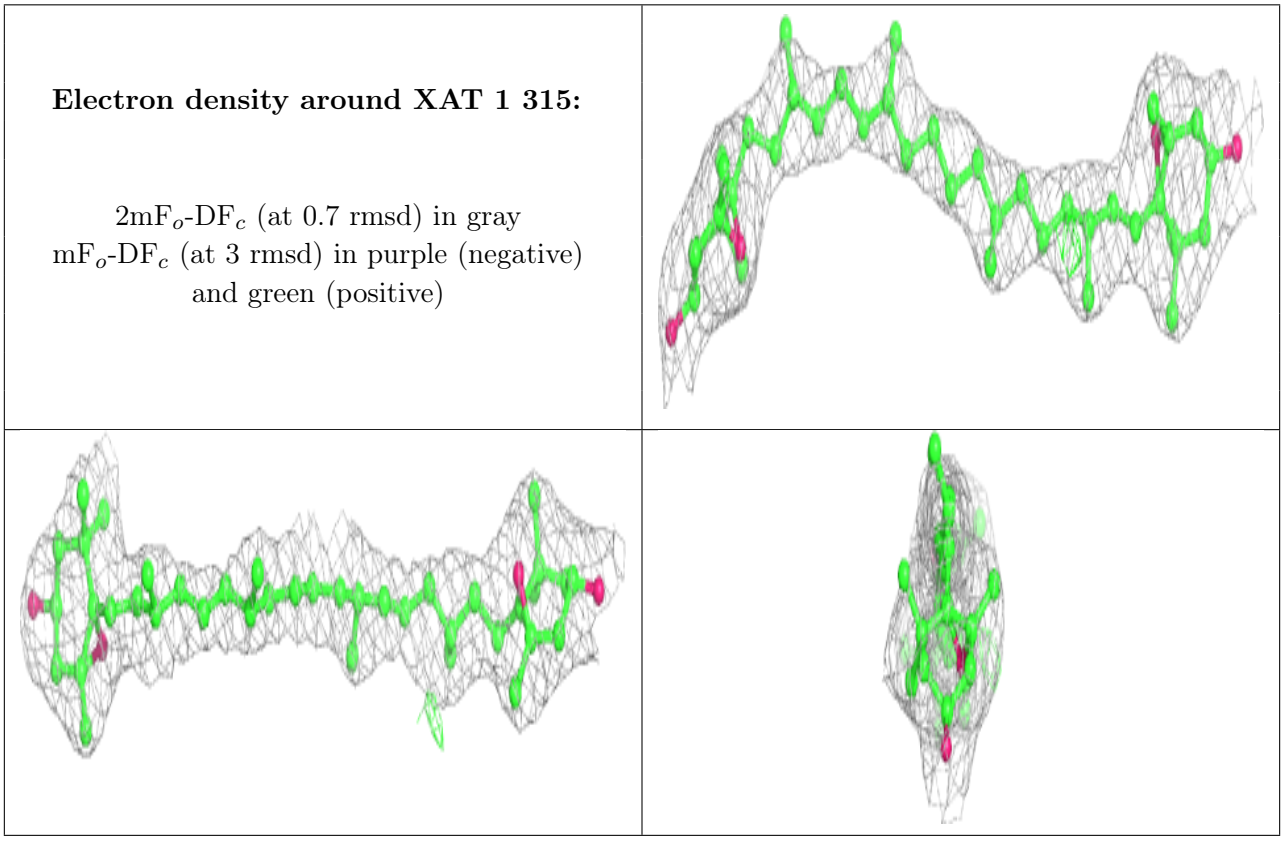
Electron density around LUT 4 316:

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



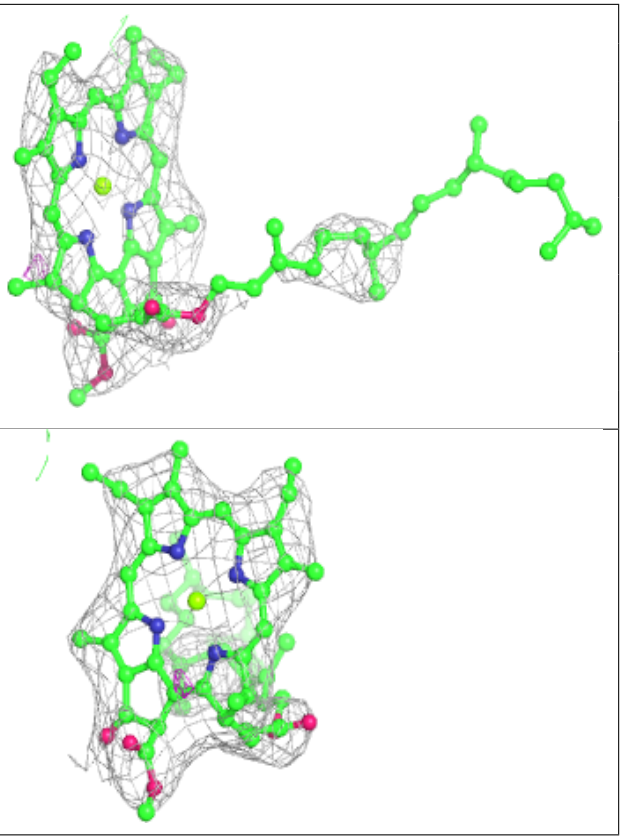
Electron density around XAT 1 315:

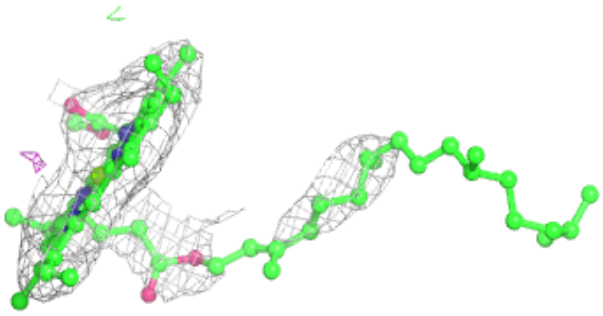
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 1 309:

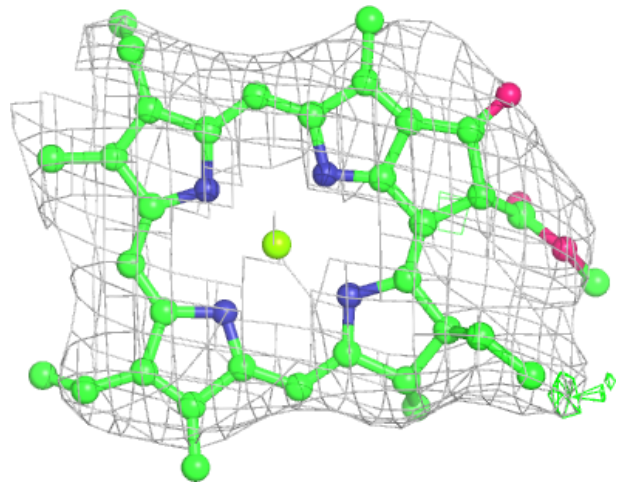
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

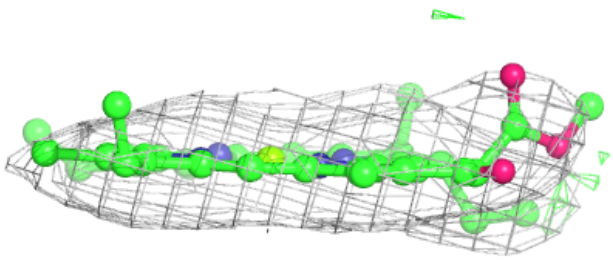


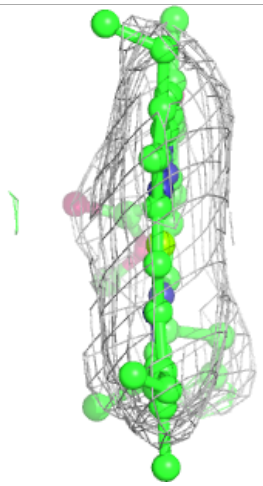


Electron density around CLA 3 605:

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

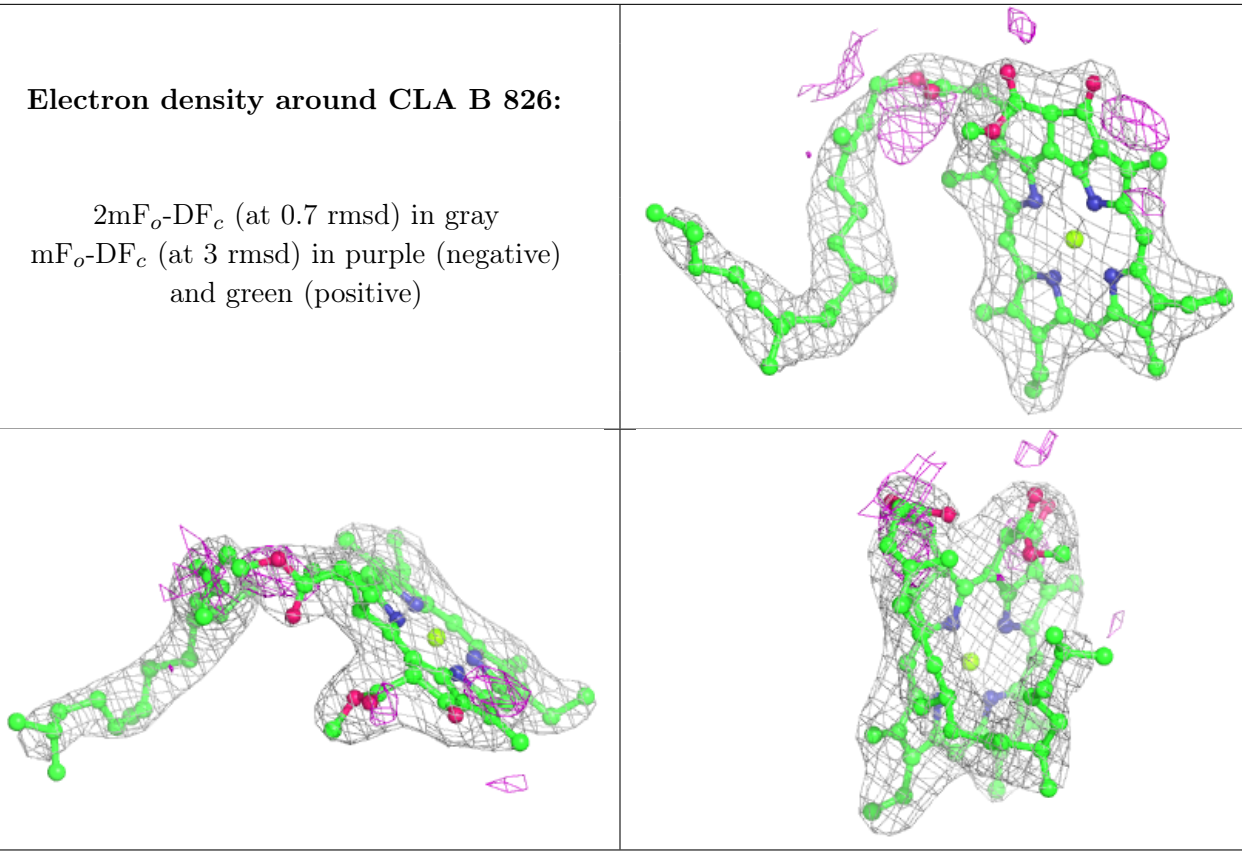






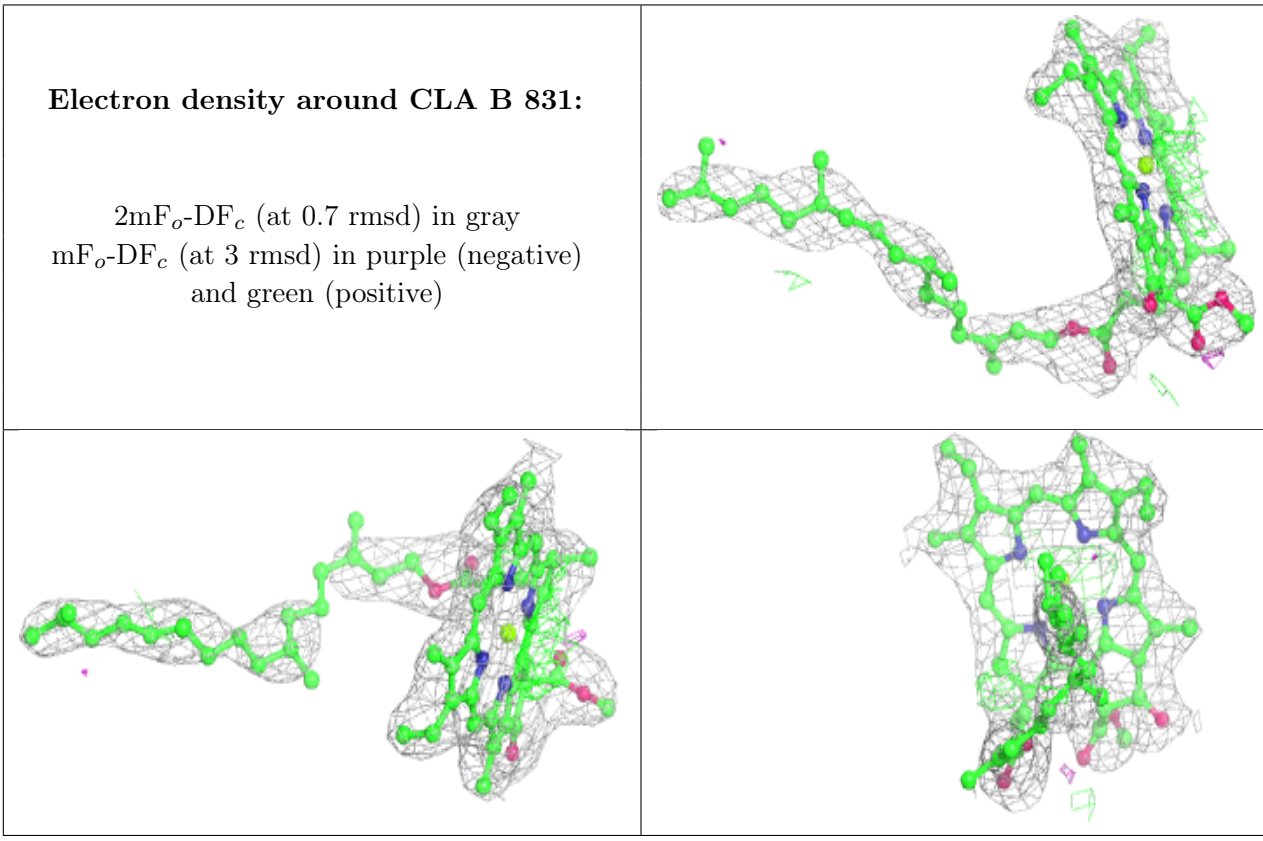
Electron density around CLA B 826:

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



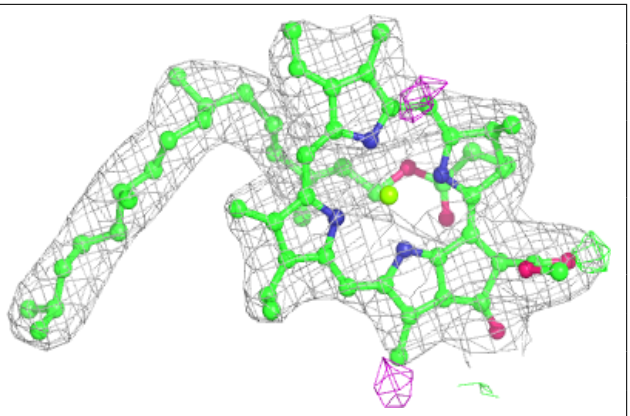
Electron density around CLA B 831:

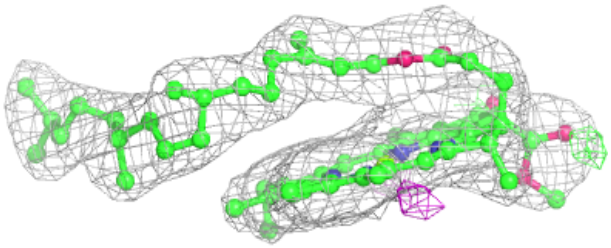
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

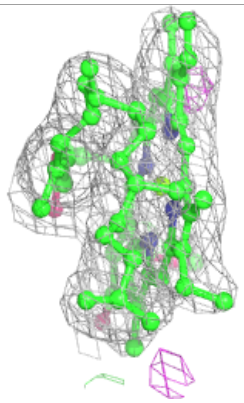


Electron density around CLA B 838:

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

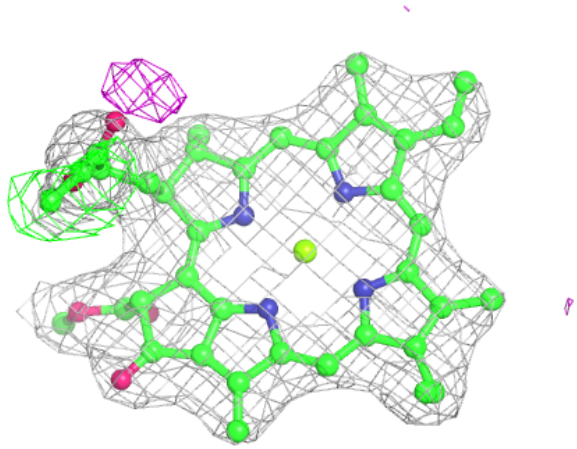


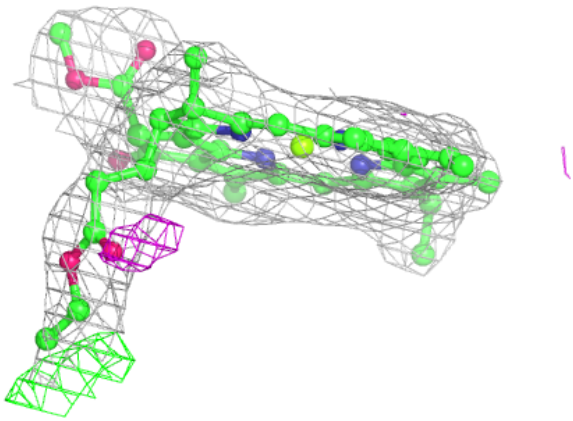


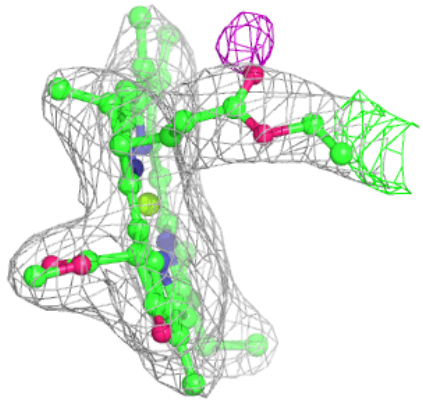


Electron density around CLA B 839:

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

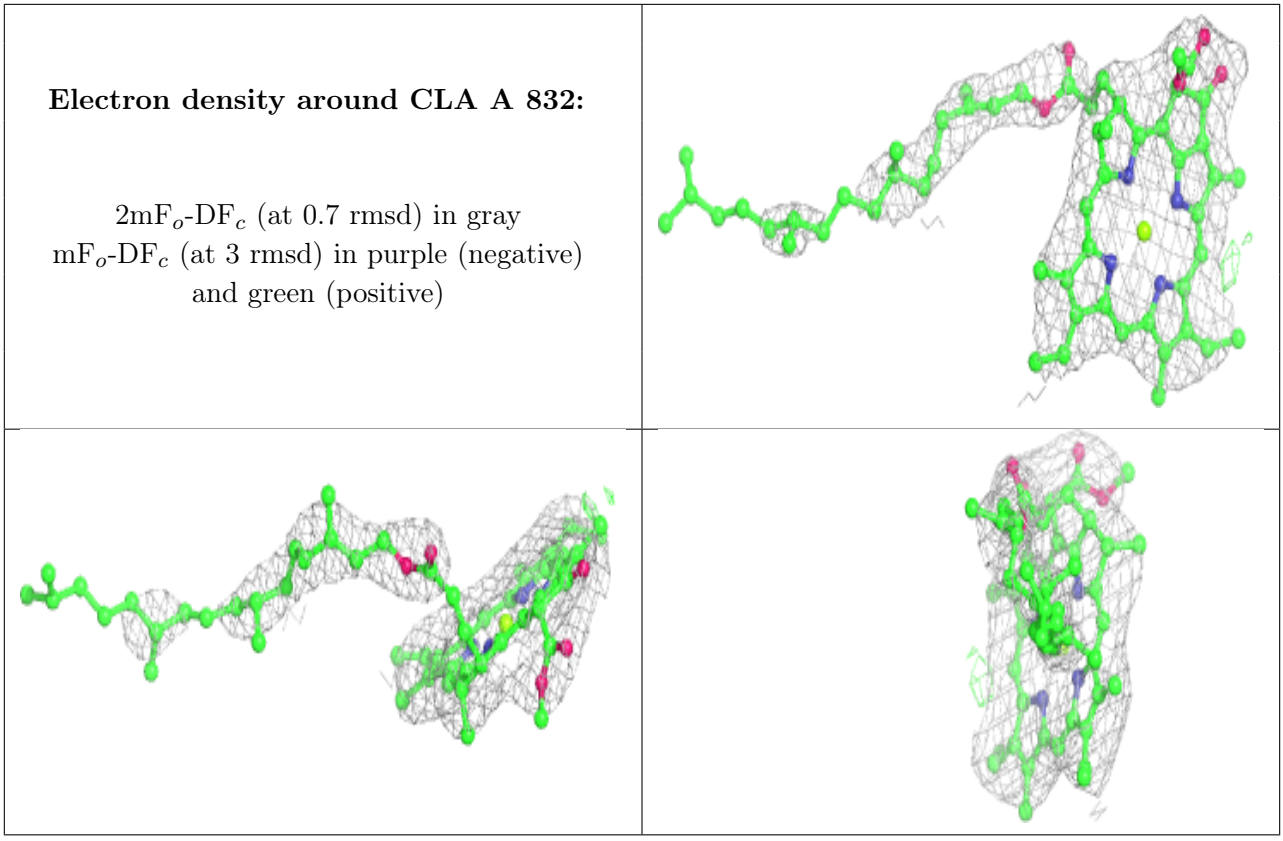






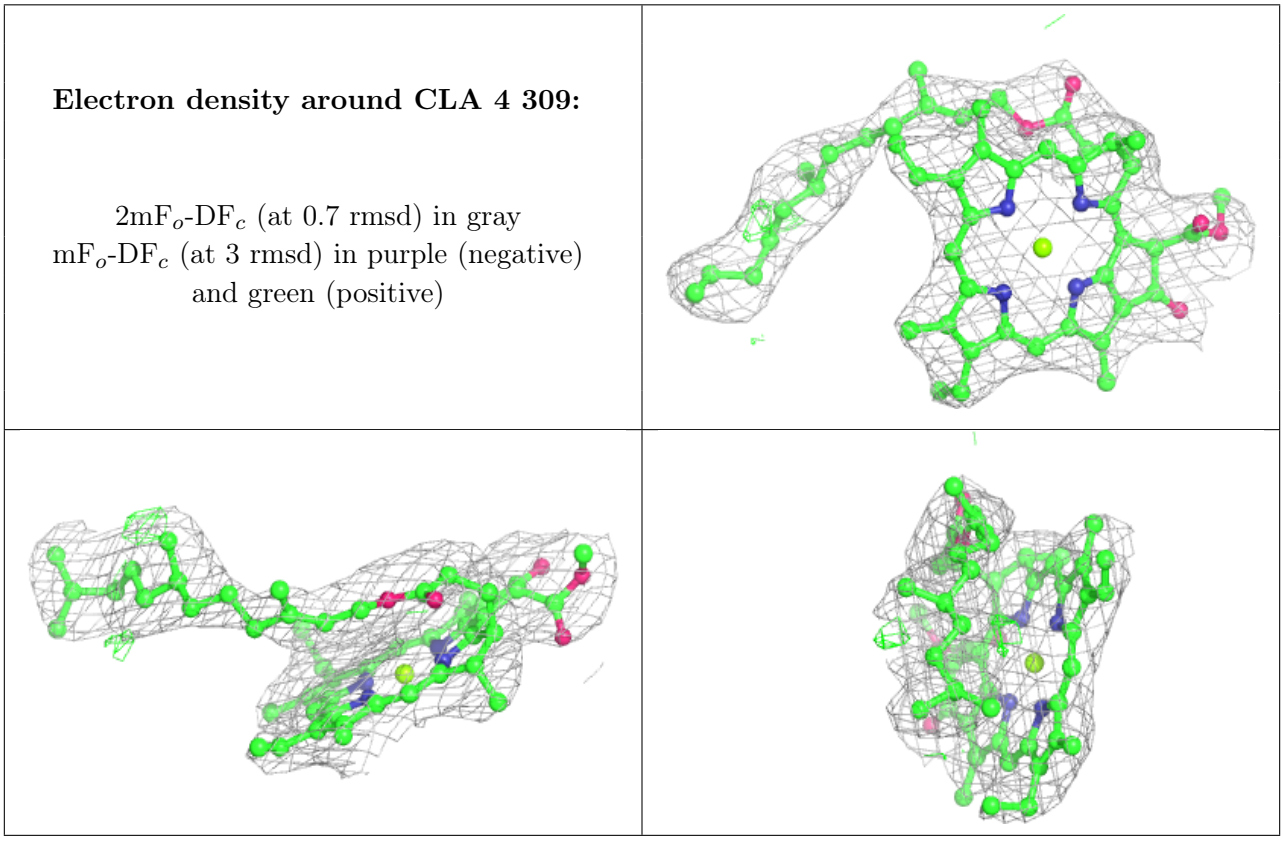
Electron density around CLA A 832:

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



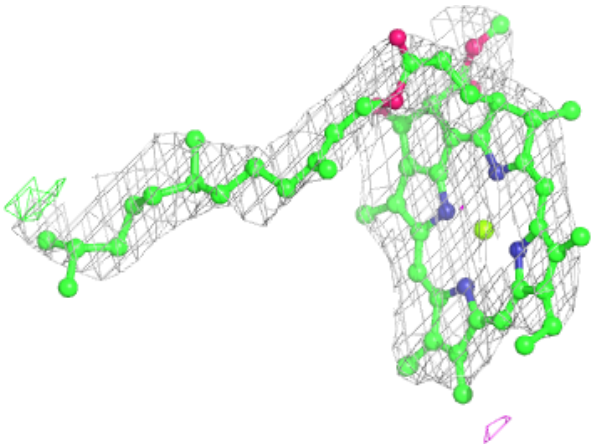
Electron density around CLA 4 309:

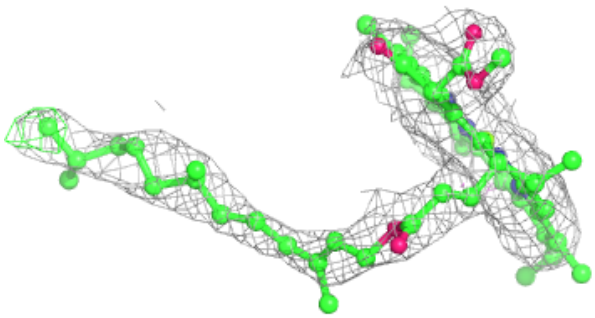
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

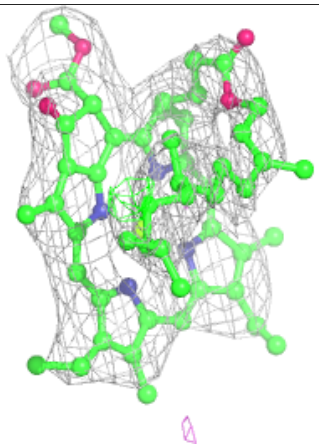


Electron density around CLA 4 310:

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

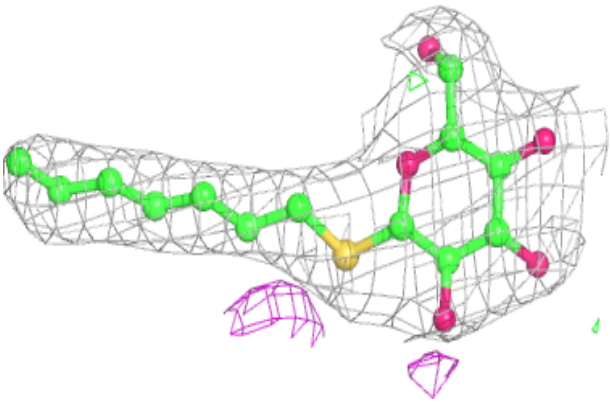


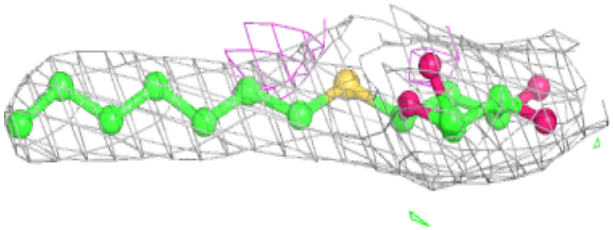


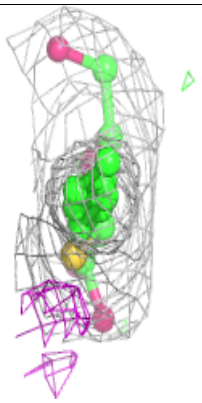


Electron density around HTG A 854:

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

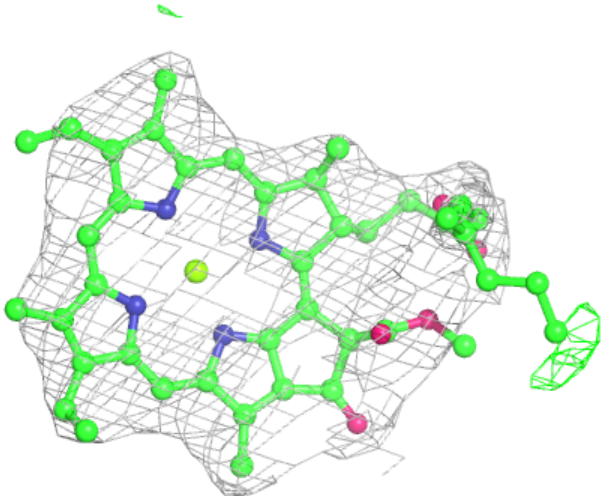


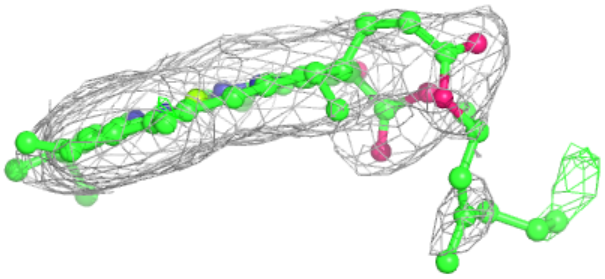


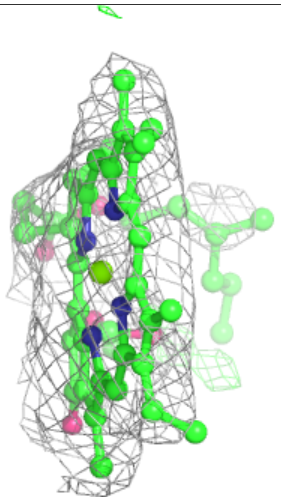


Electron density around CLA 4 311:

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

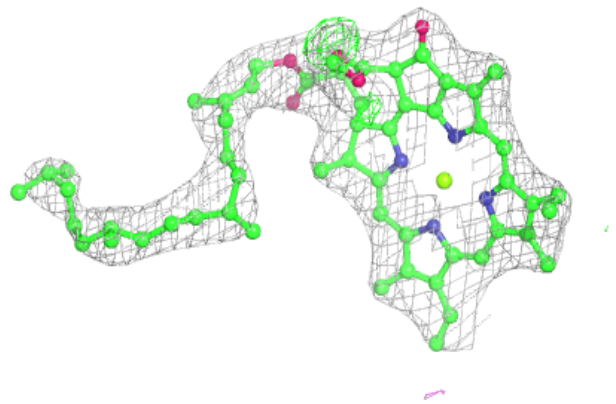


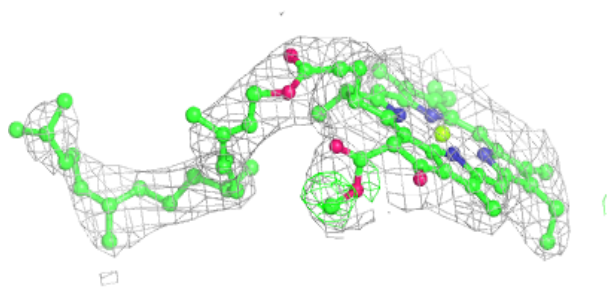


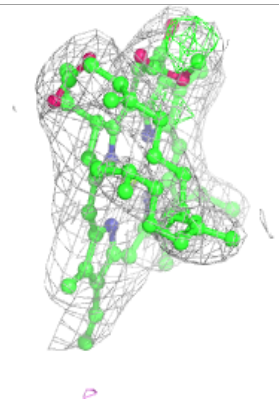


Electron density around CLA J 101:

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

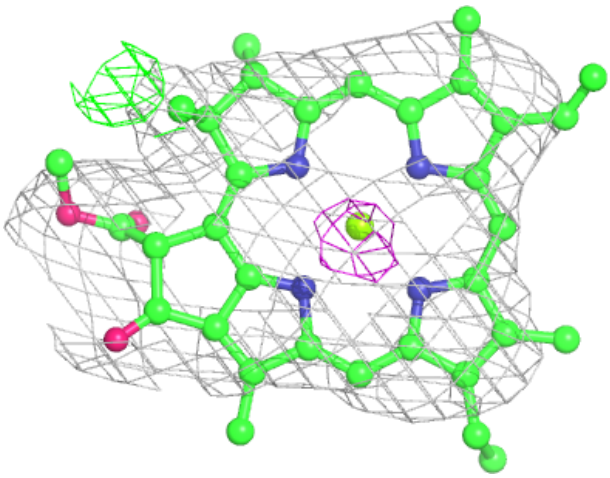


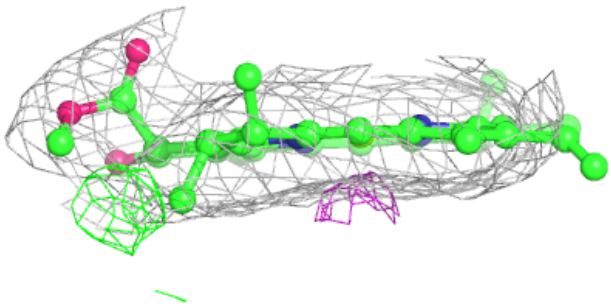


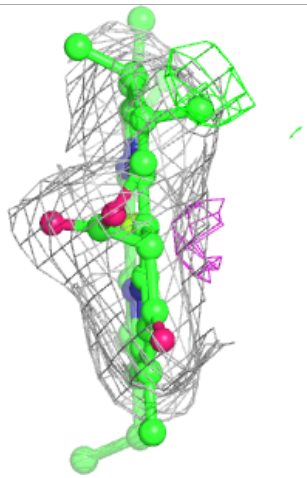


Electron density around CLA 2 309:

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

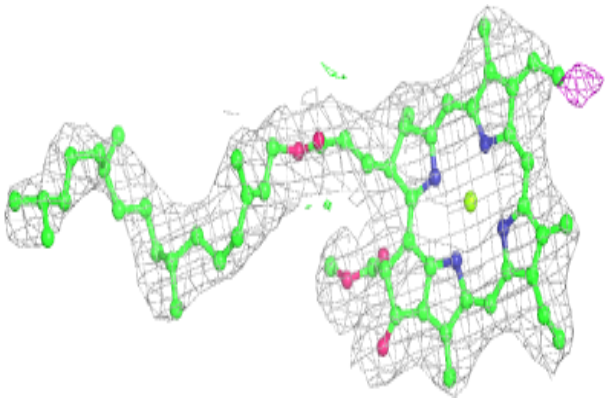


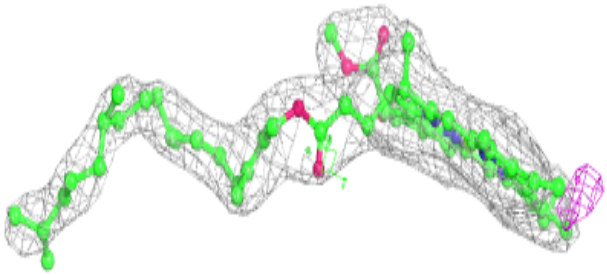


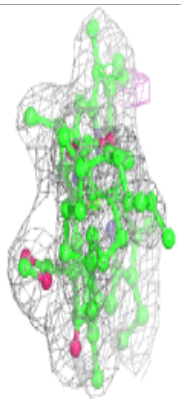


Electron density around CLA A 839:

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

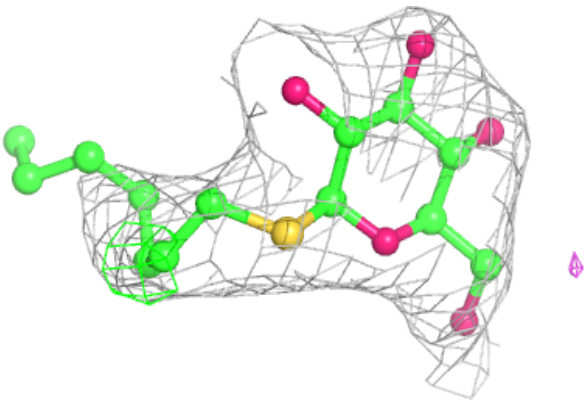


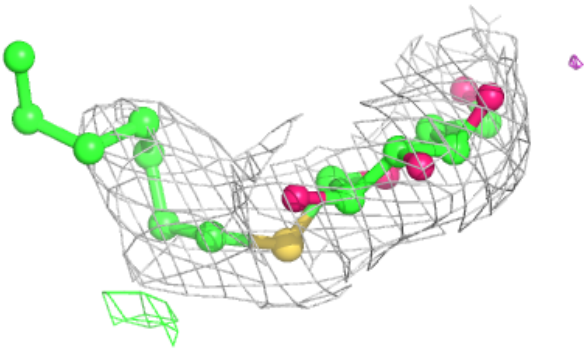


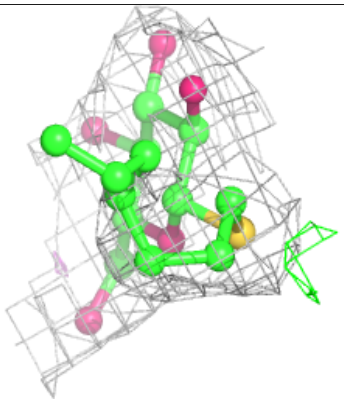


Electron density around HTG J 102:

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

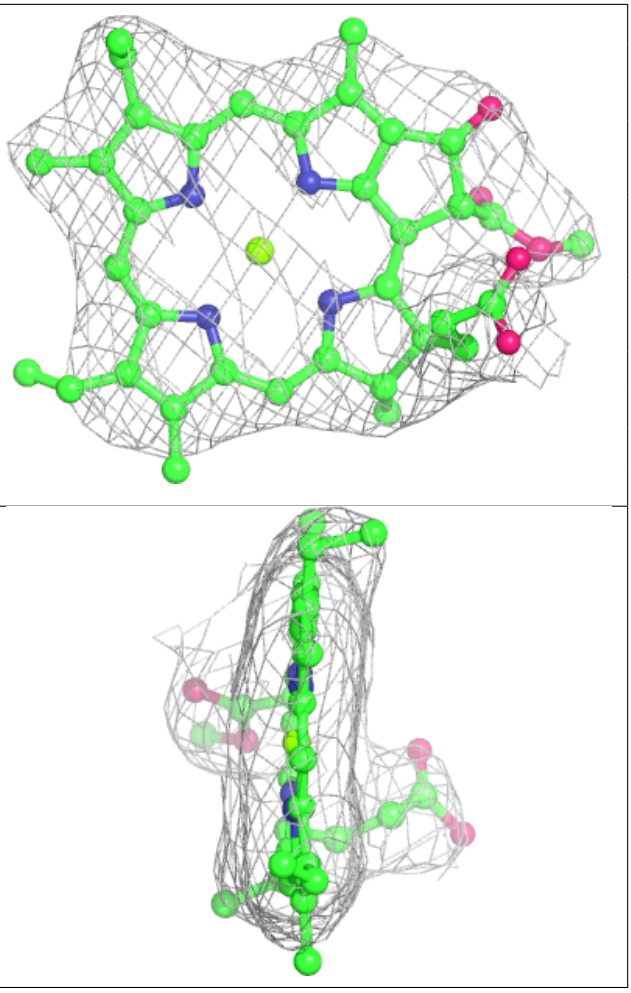






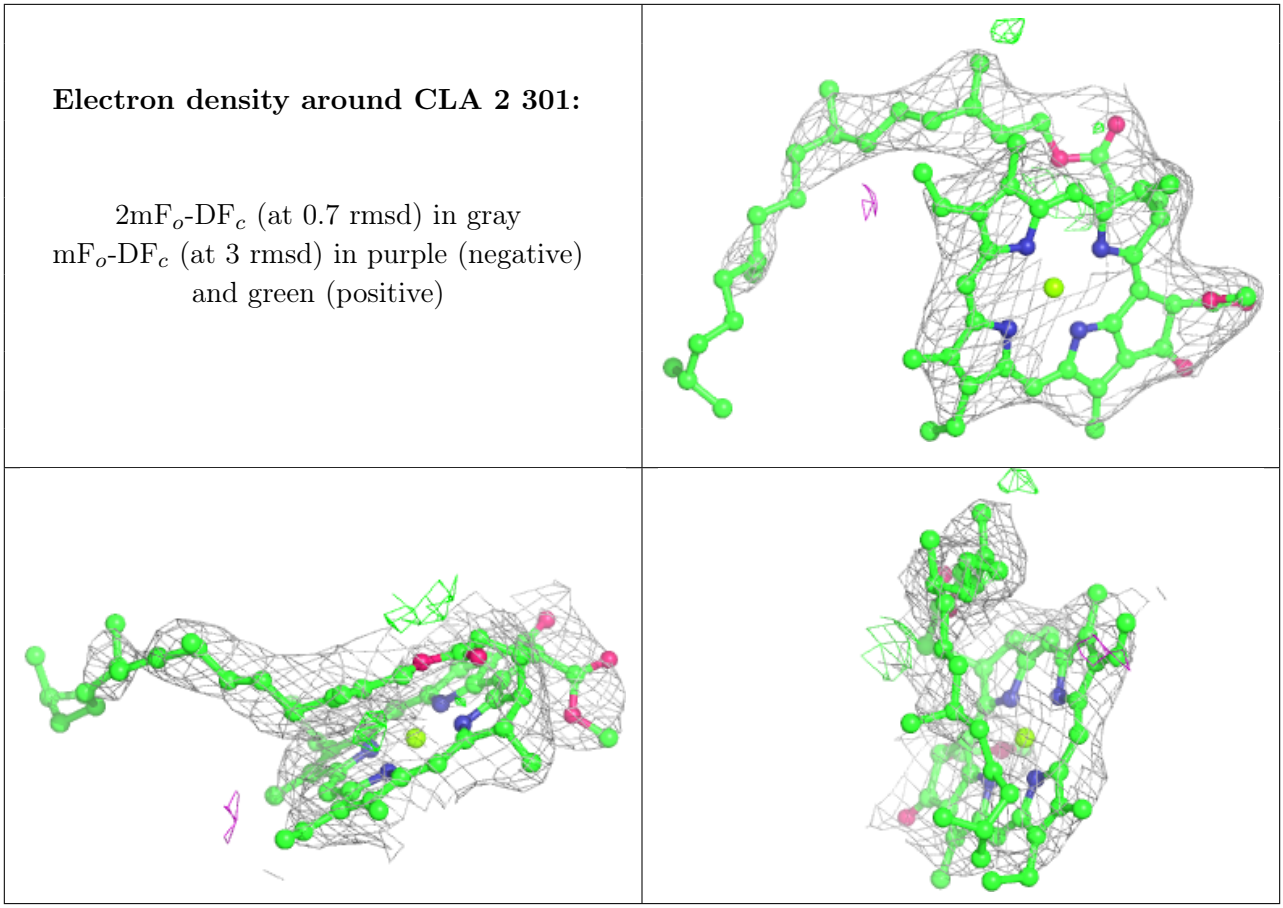
Electron density around CLA 4 313:

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



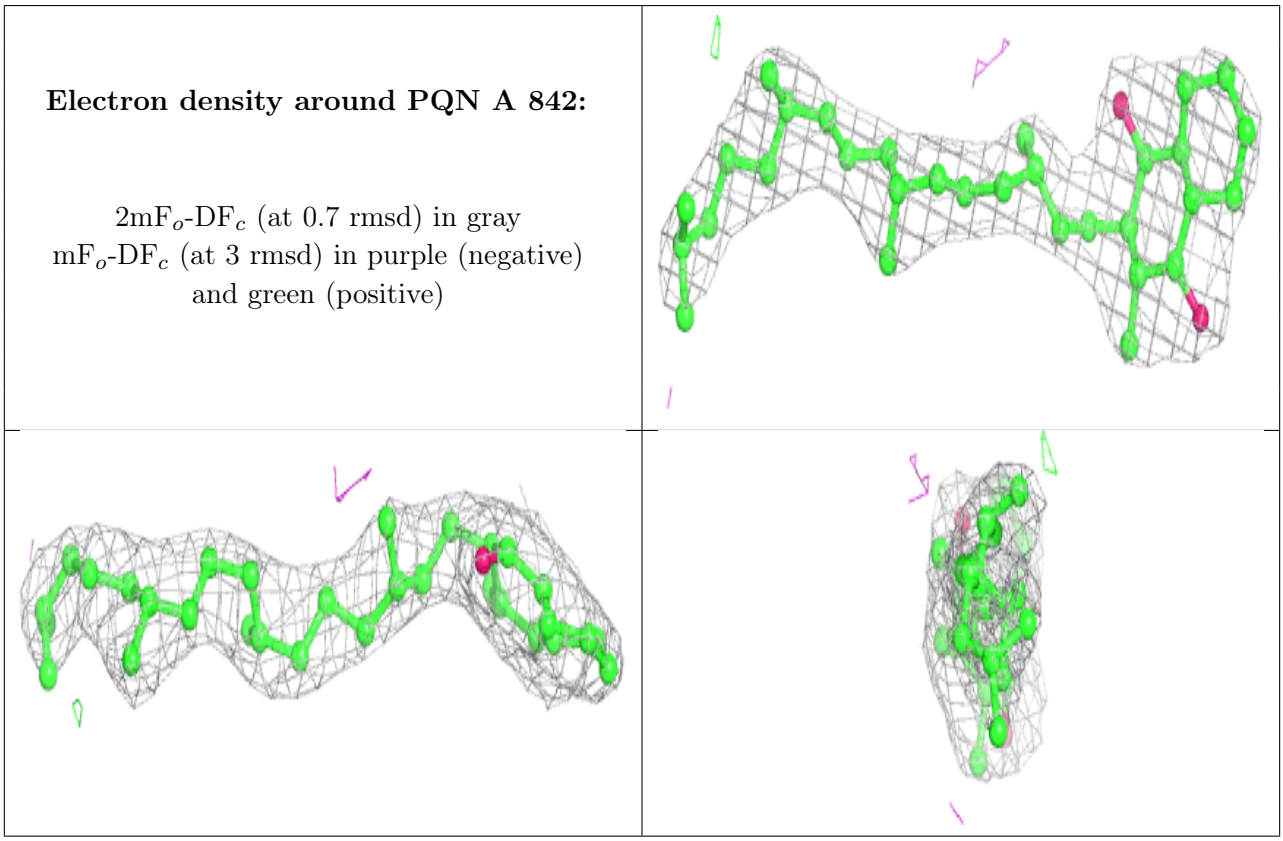
Electron density around CLA 2 301:

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



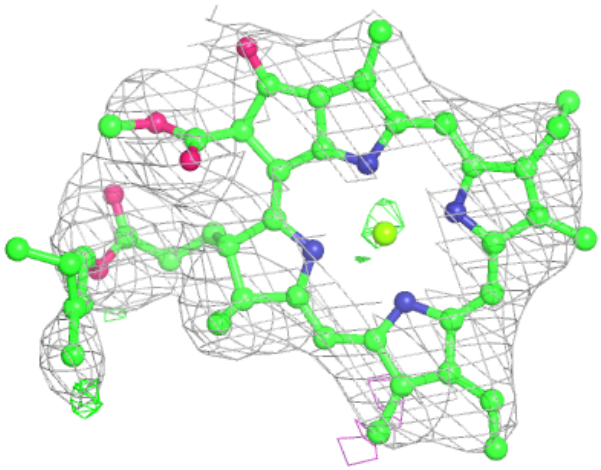
Electron density around PQN A 842:

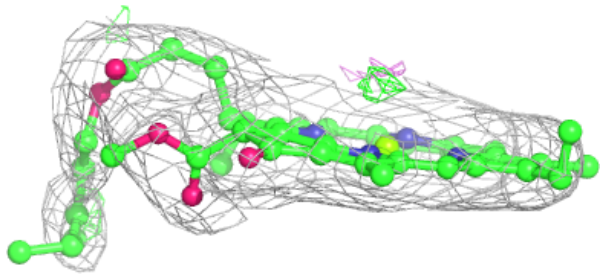
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

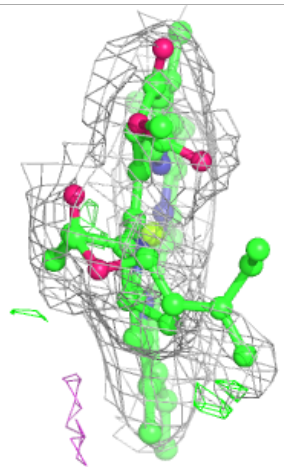


Electron density around CLA 2 302:

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

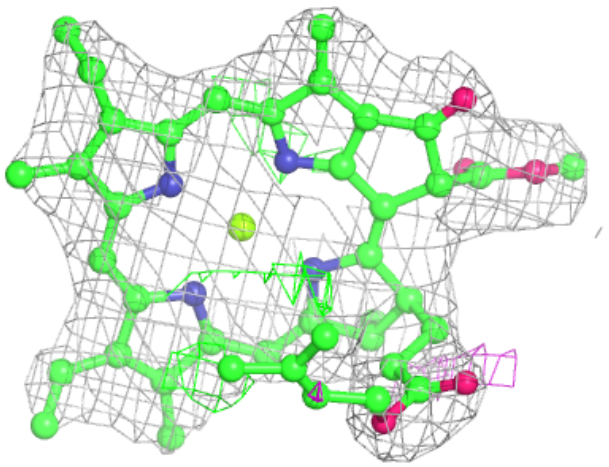


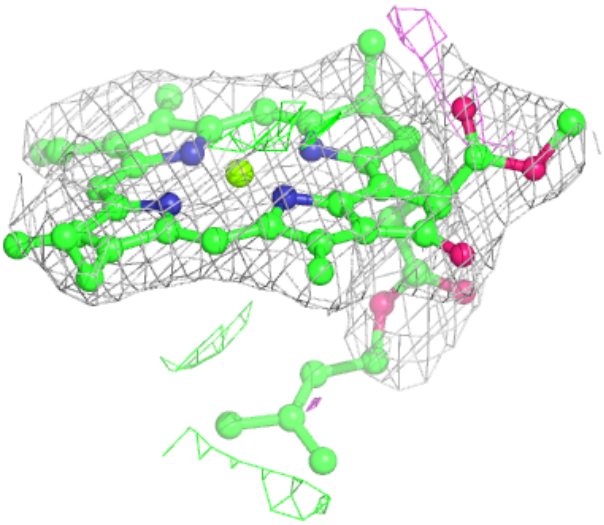


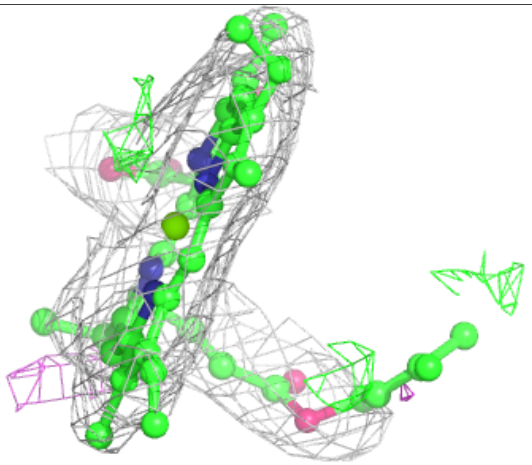


Electron density around CLA 4 308:

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

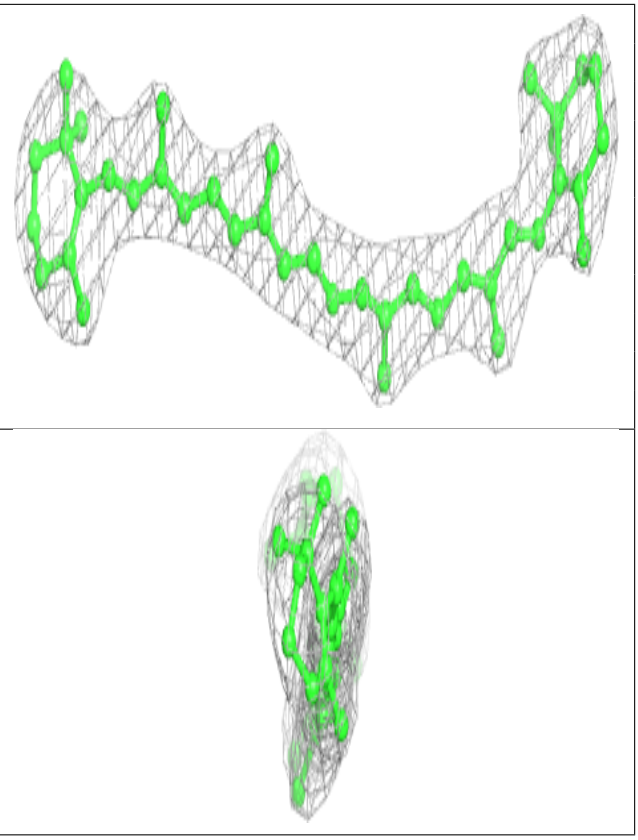






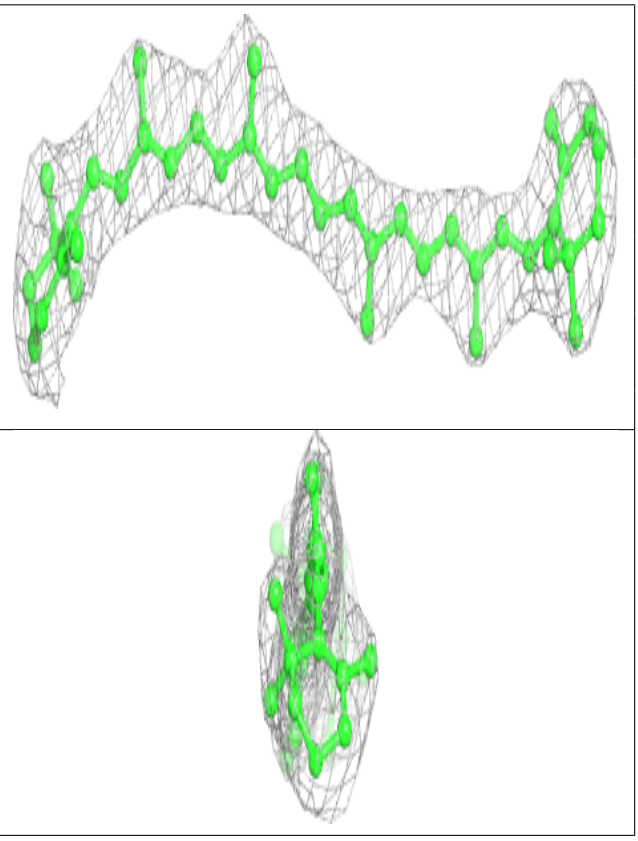
Electron density around BCR B 848:

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



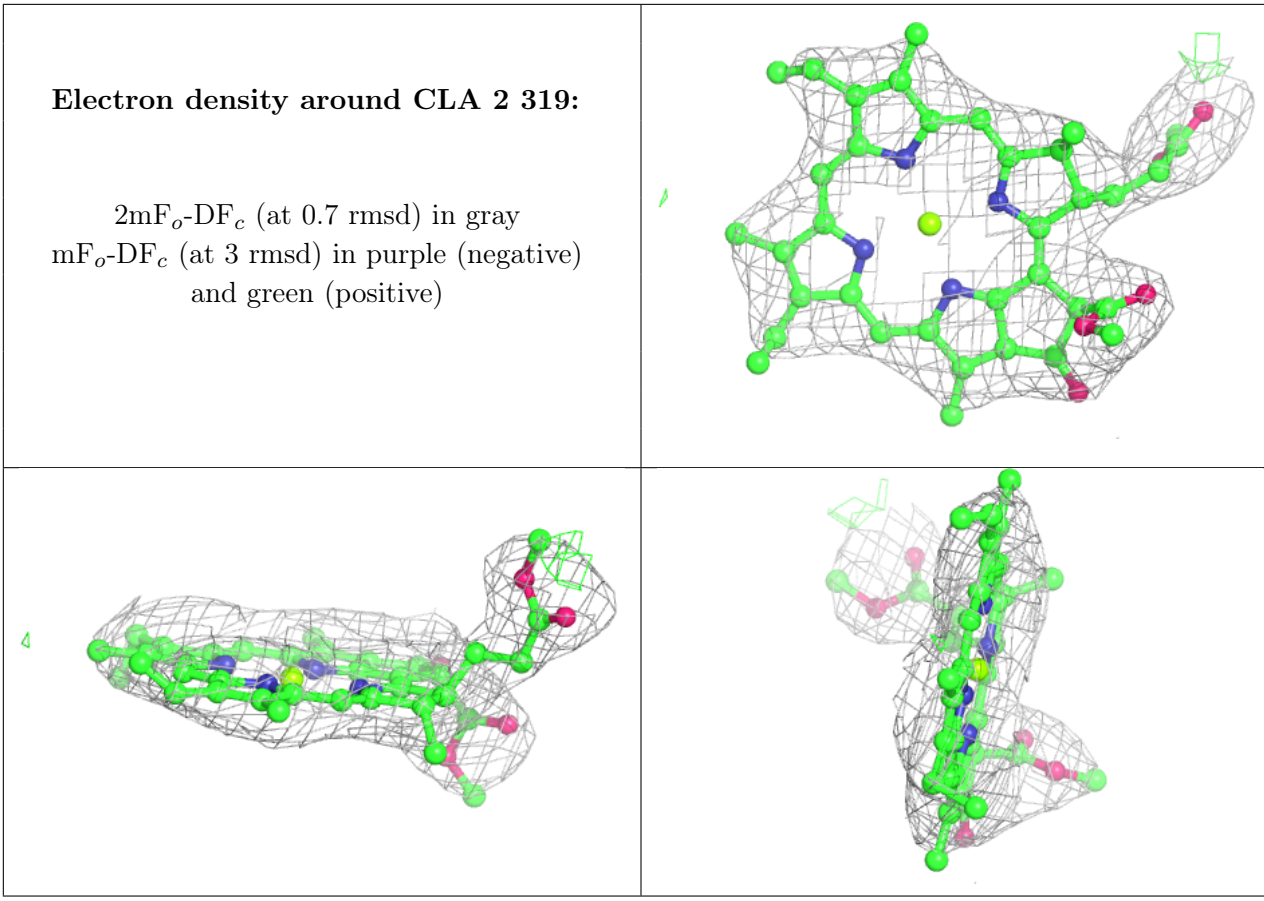
Electron density around BCR B 849:

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



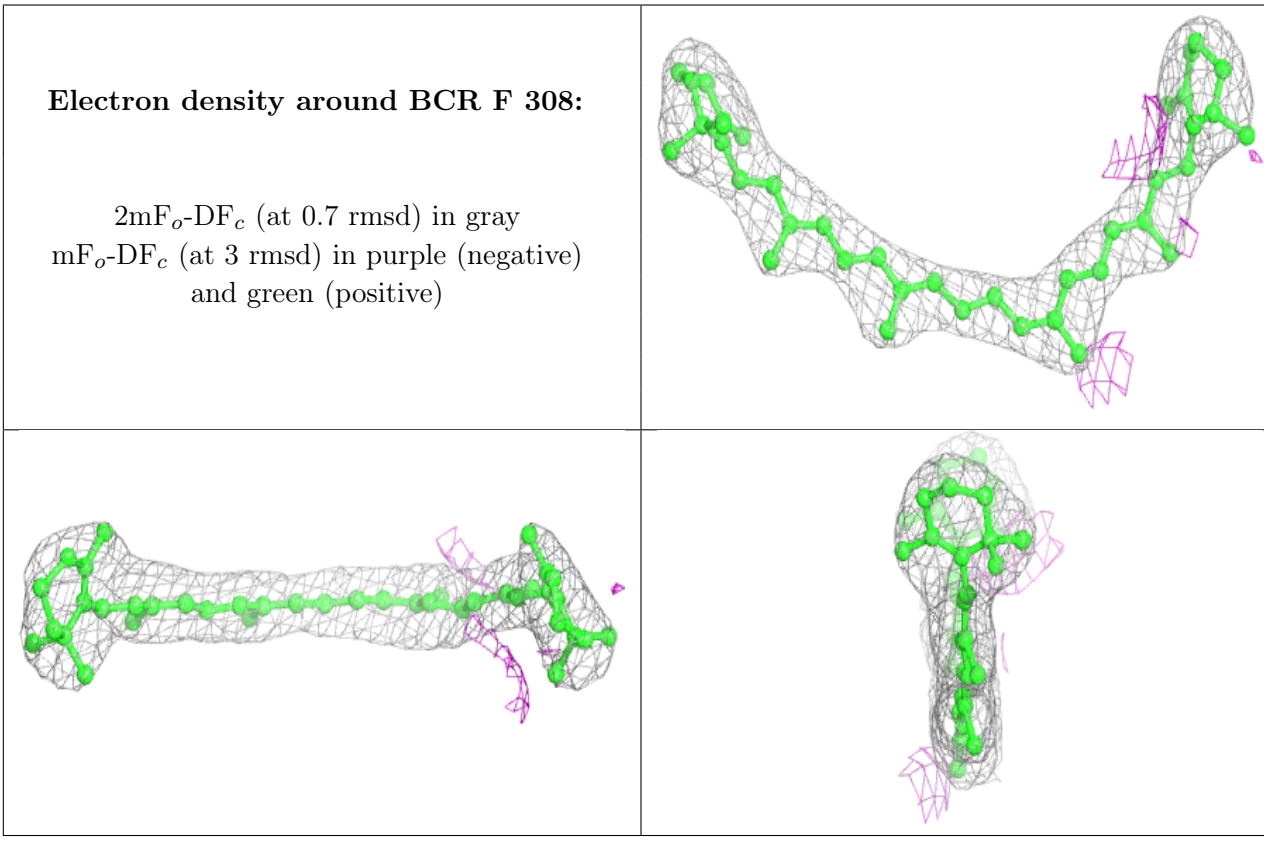
Electron density around CLA 2 319:

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



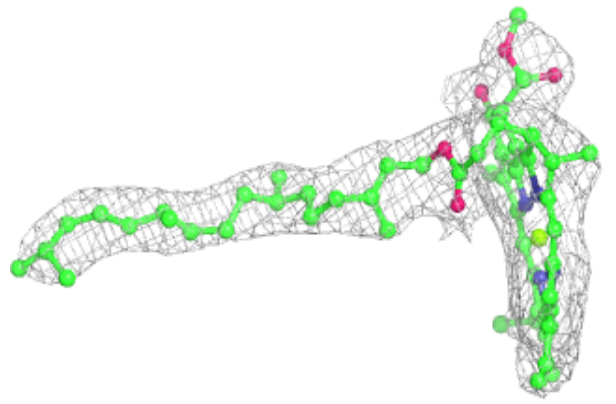
Electron density around BCR F 308:

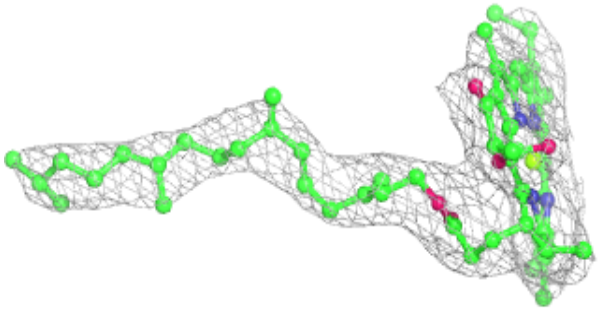
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

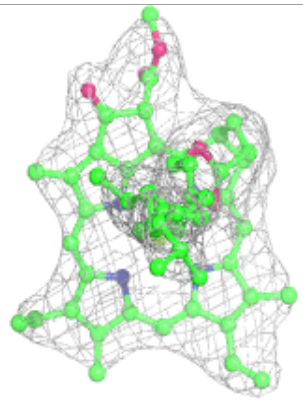


Electron density around CLA A 827:

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

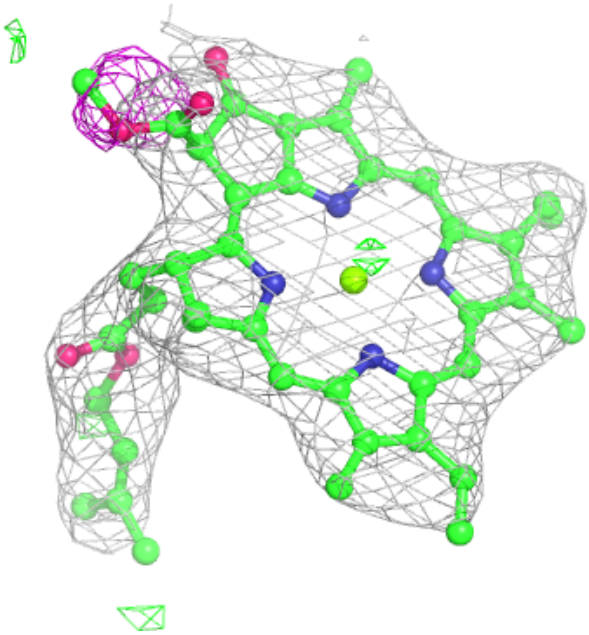


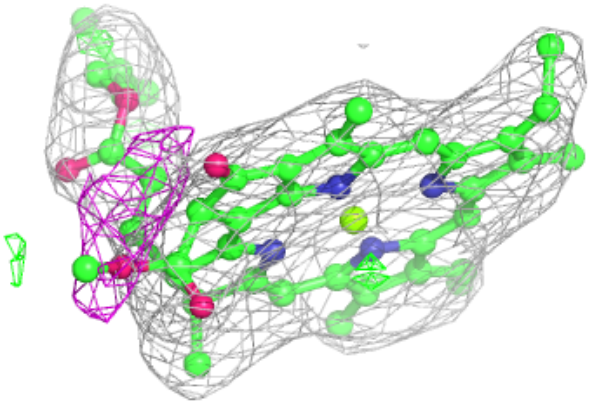


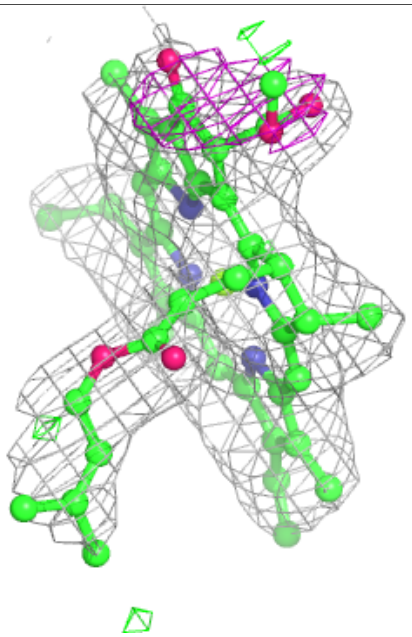


Electron density around CLA B 822:

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

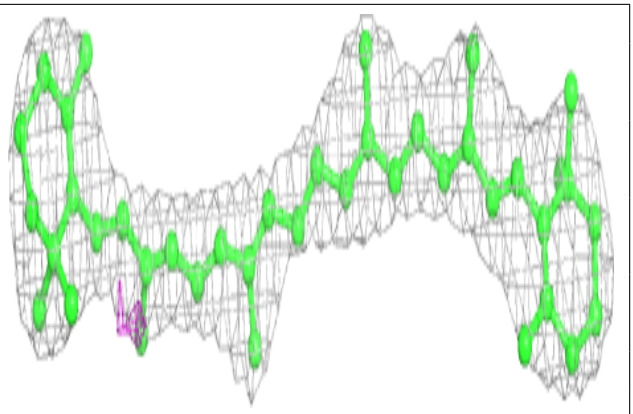


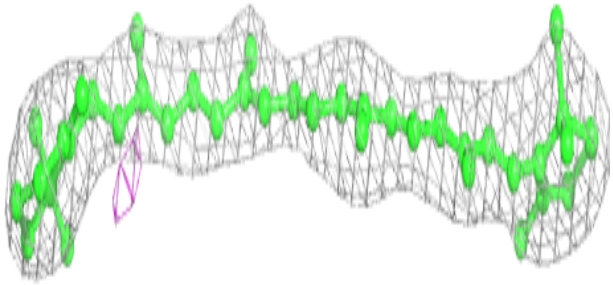




Electron density around BCR J 104:

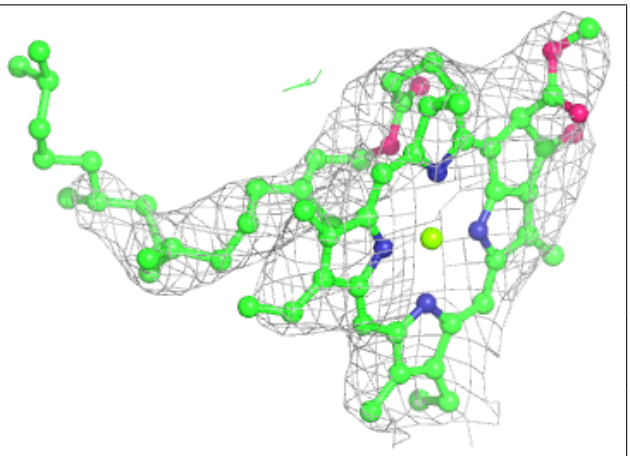
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

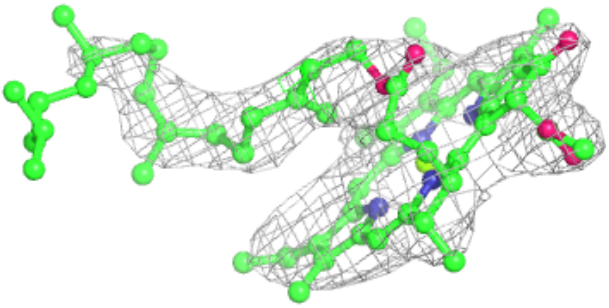


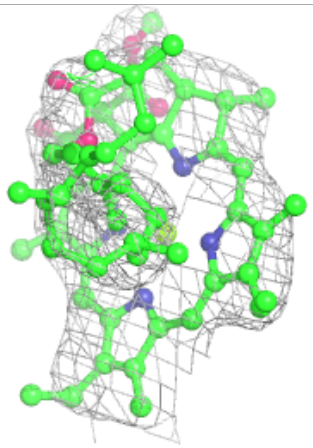


Electron density around CLA A 841:

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

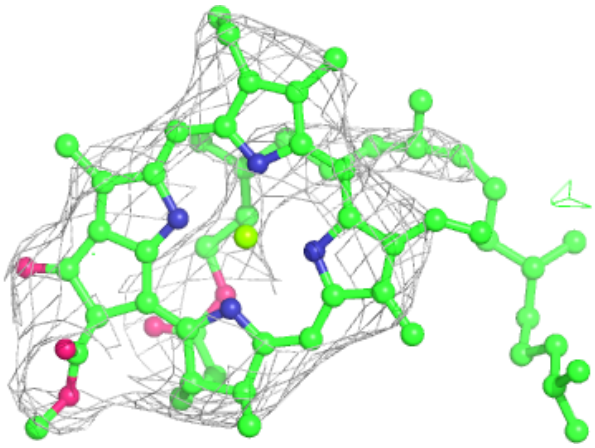


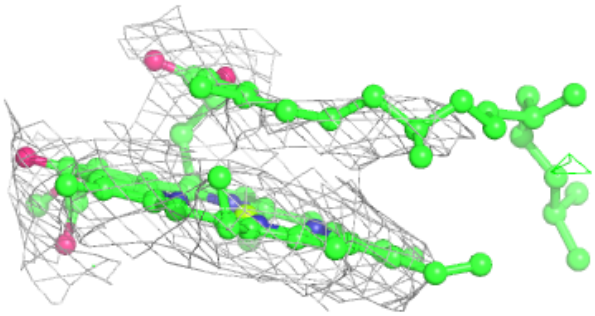


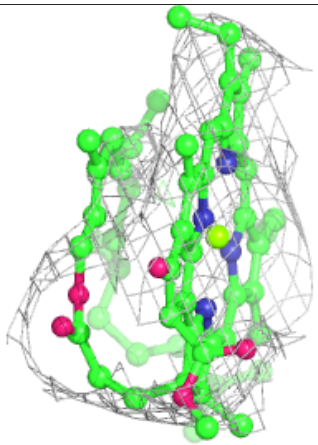


Electron density around CLA 2 311:

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

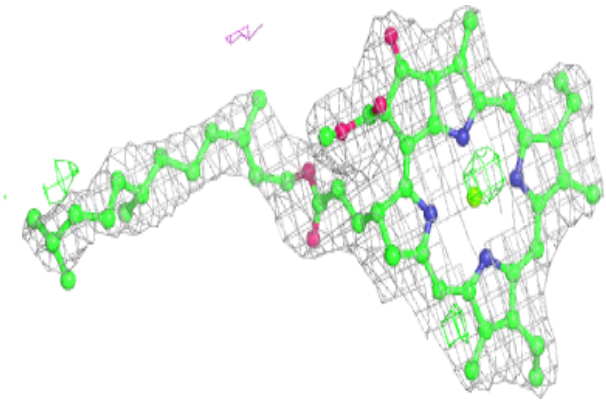


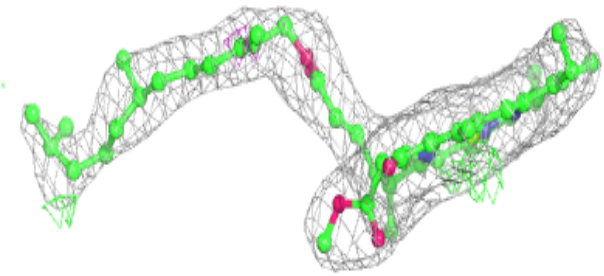


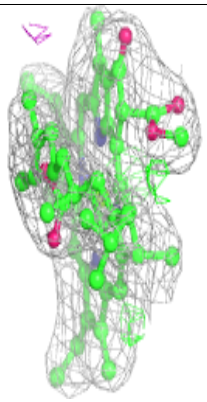


Electron density around CLA B 825:

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

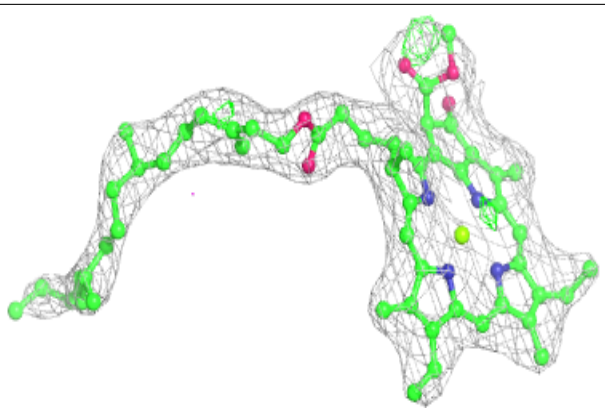


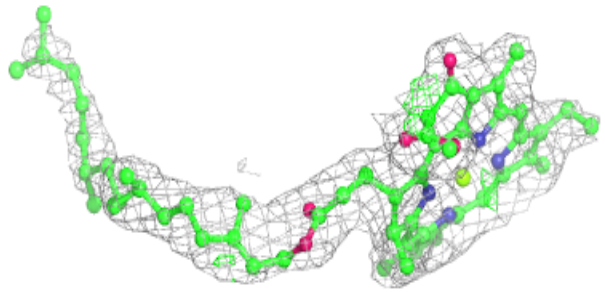


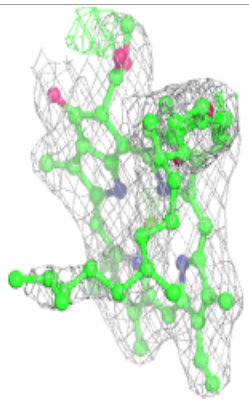


Electron density around CLA A 853:

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

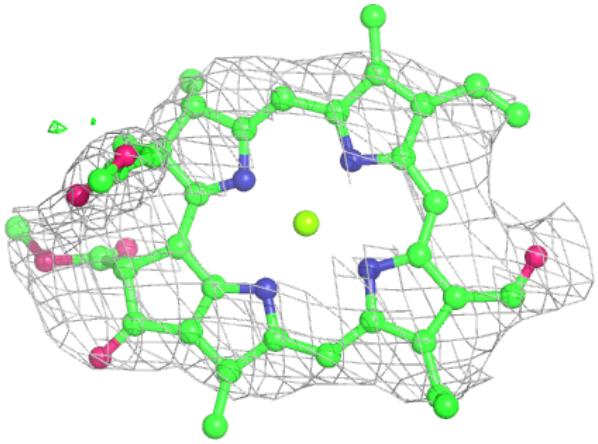


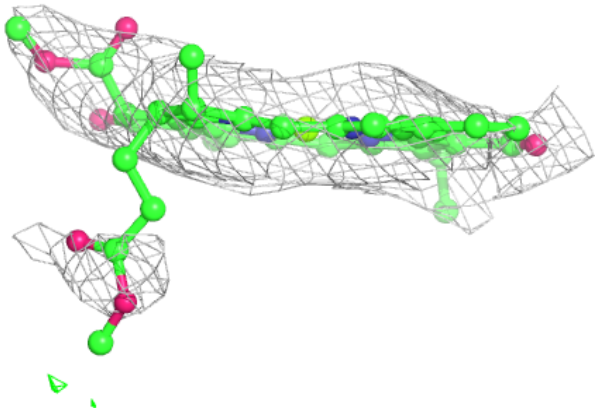


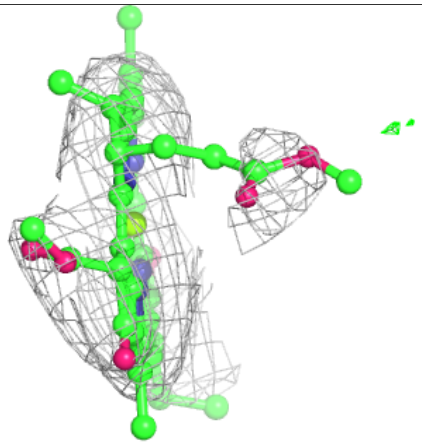


Electron density around CHL 3 607:

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

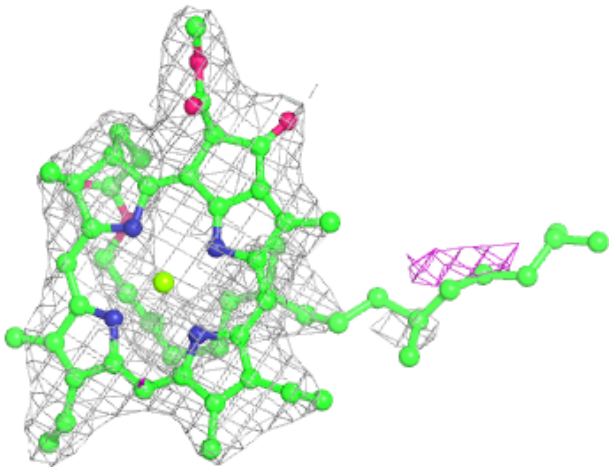


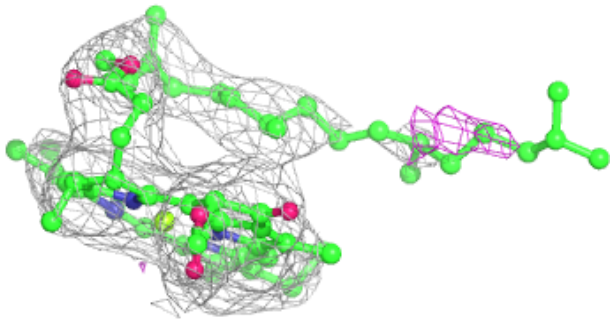


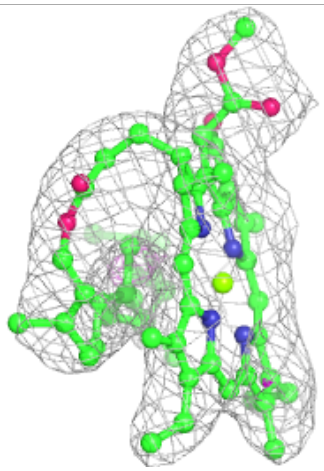


Electron density around CLA B 829:

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

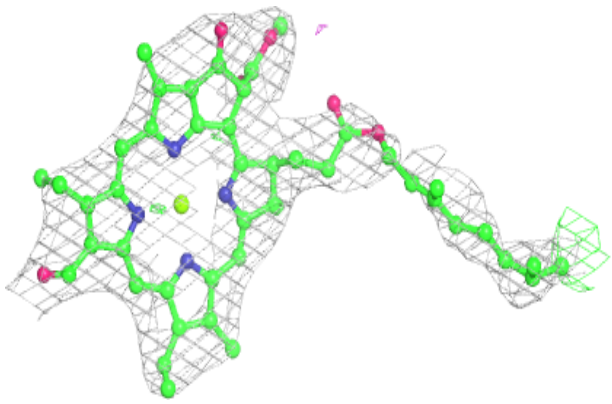


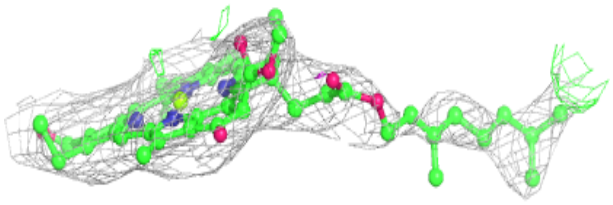


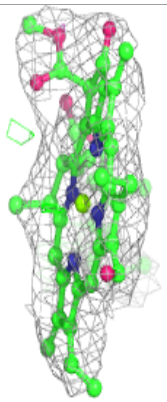


Electron density around CHL 4 305:

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

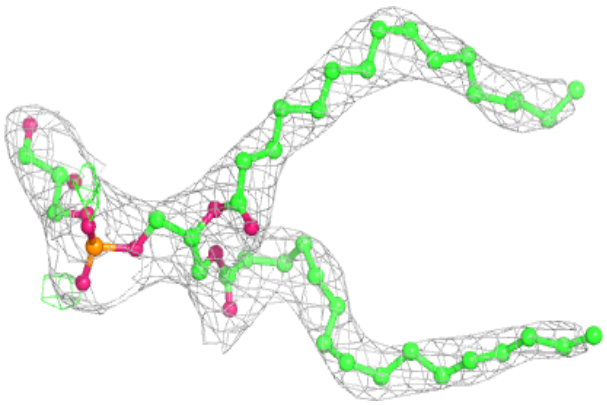


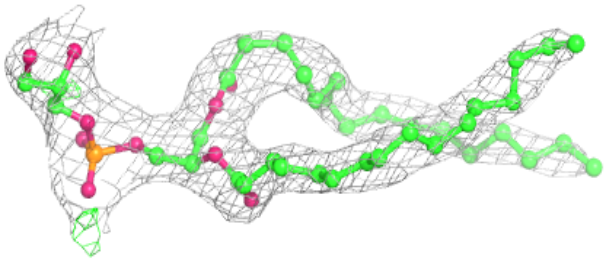


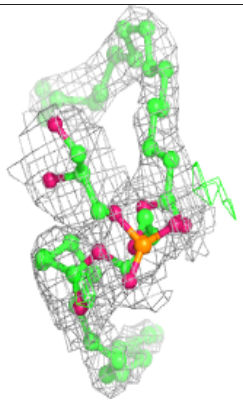


Electron density around LHG A 844:

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

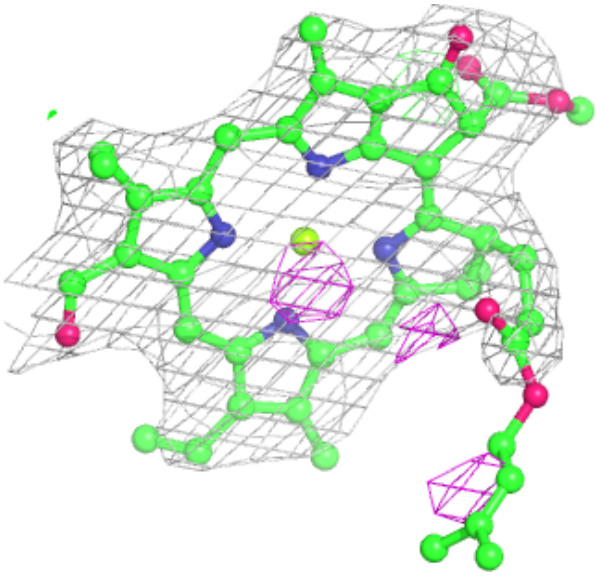


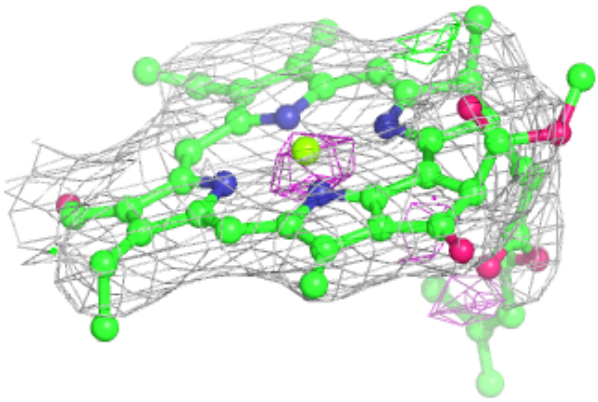


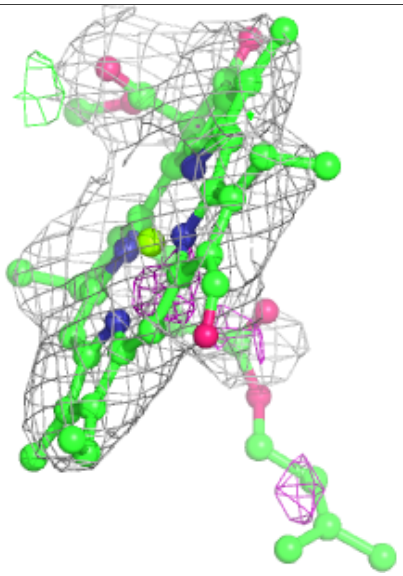


Electron density around CHL 4 306:

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

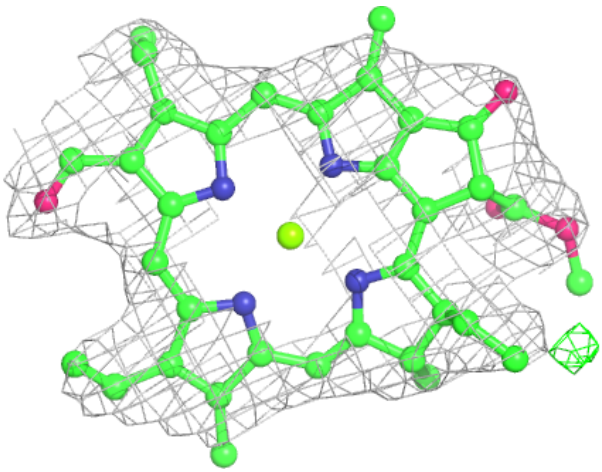


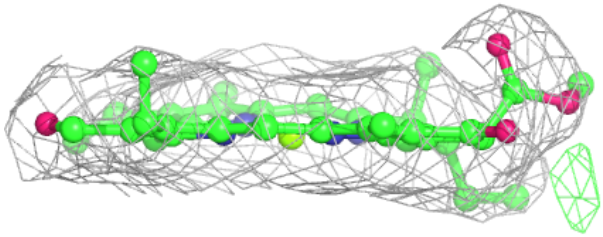


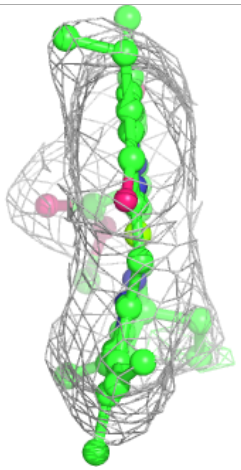


Electron density around CHL 4 315:

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

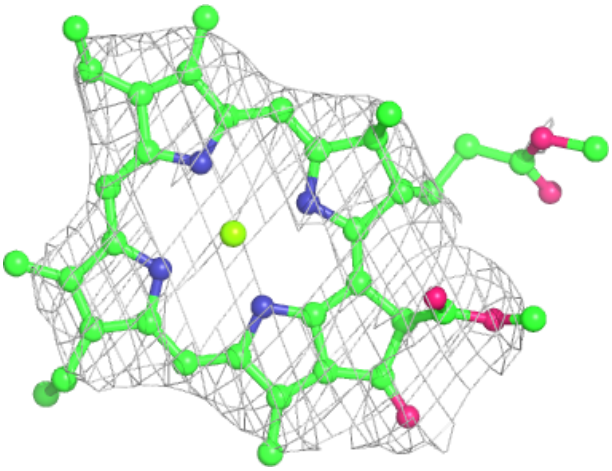


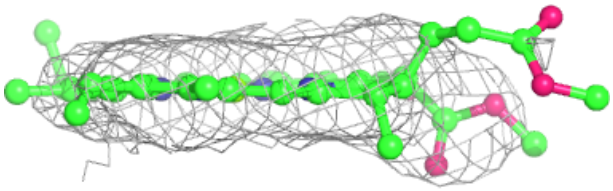


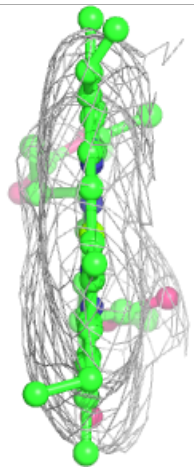


Electron density around CLA 3 613:

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

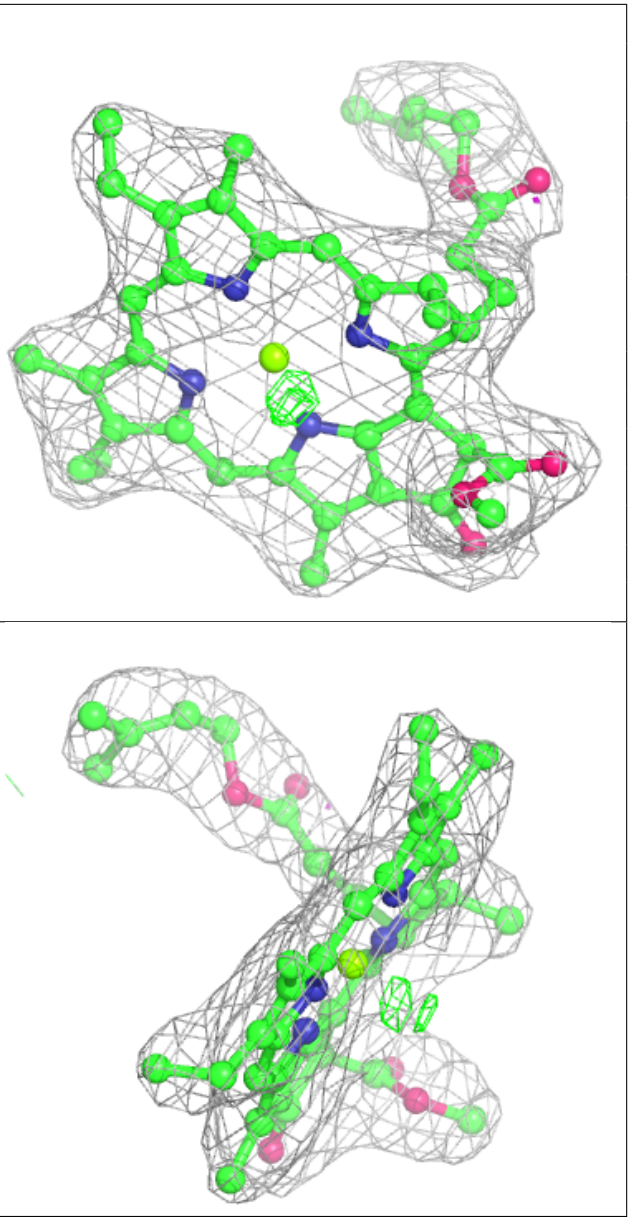






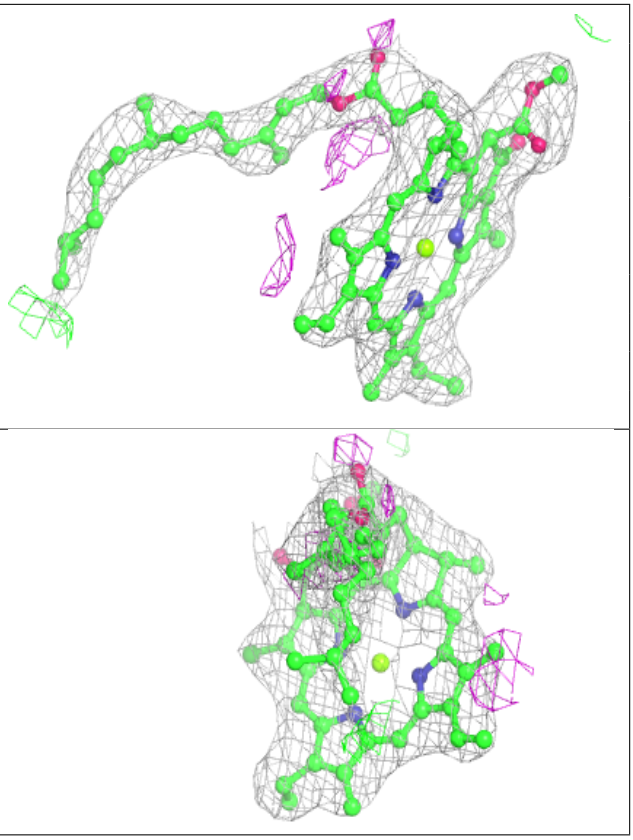
Electron density around CLA B 832:

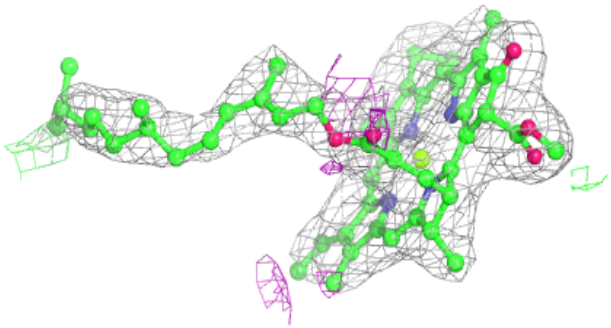
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 833:

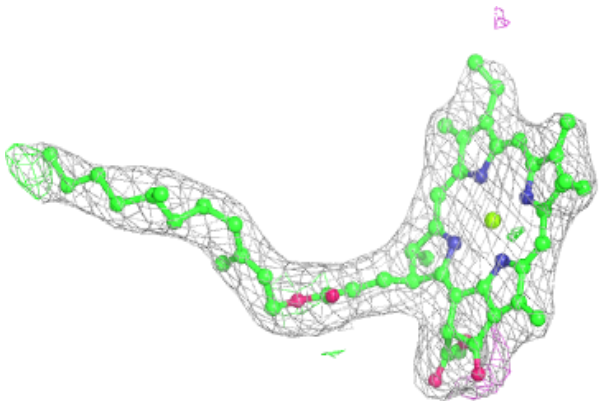
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

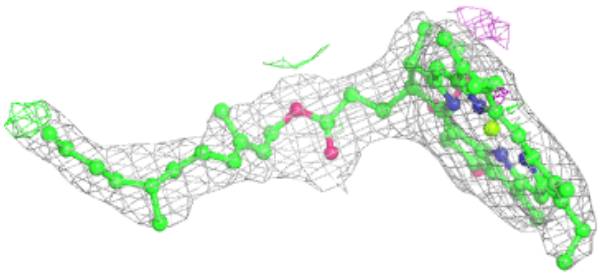


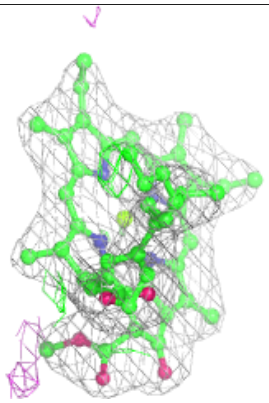


Electron density around CLA B 834:

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

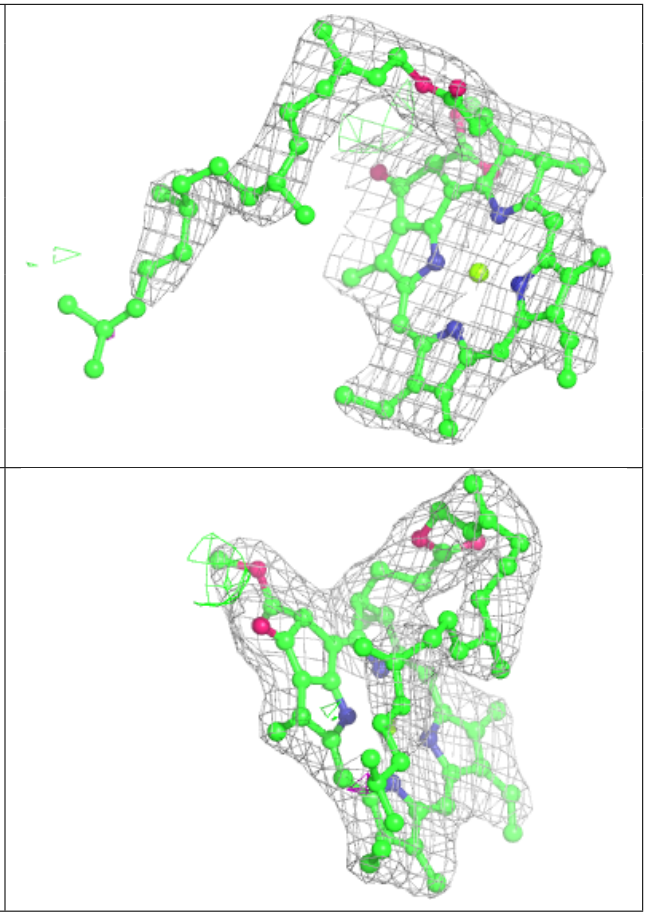






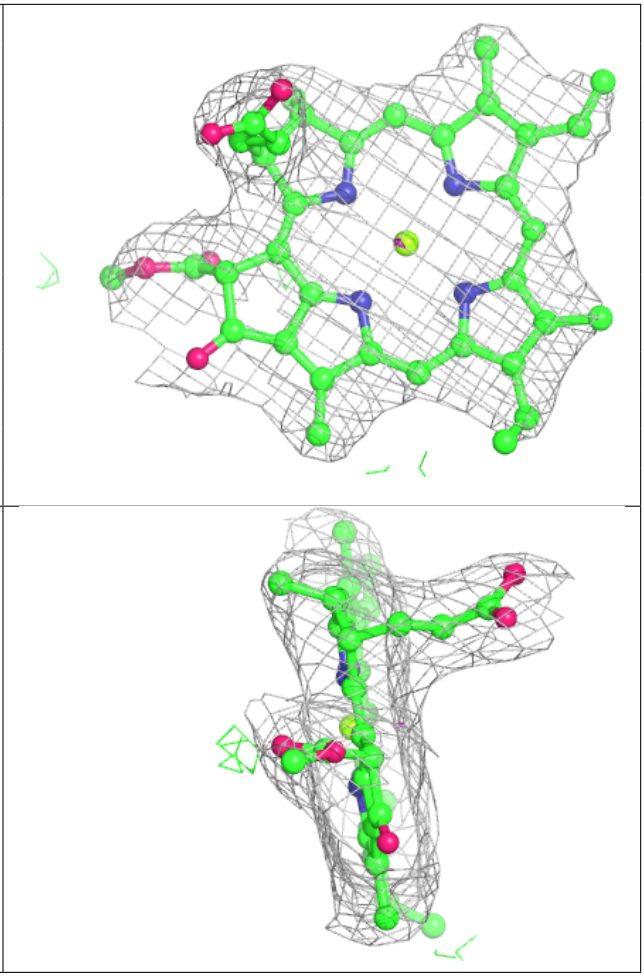
Electron density around CLA B 835:

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



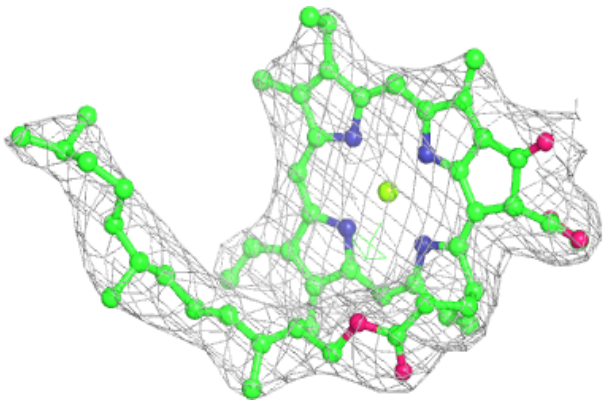
Electron density around CLA B 836:

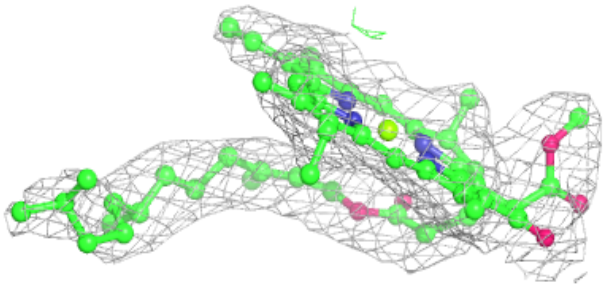
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

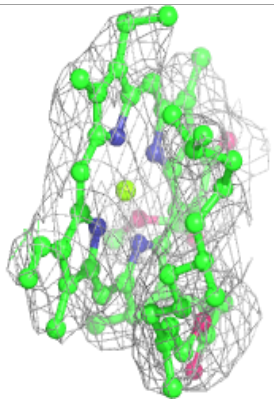


Electron density around CLA 4 302:

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

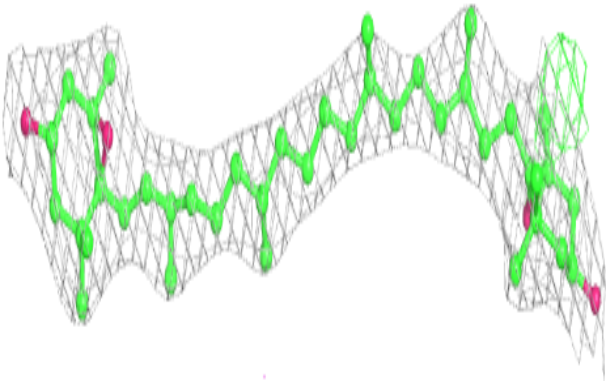


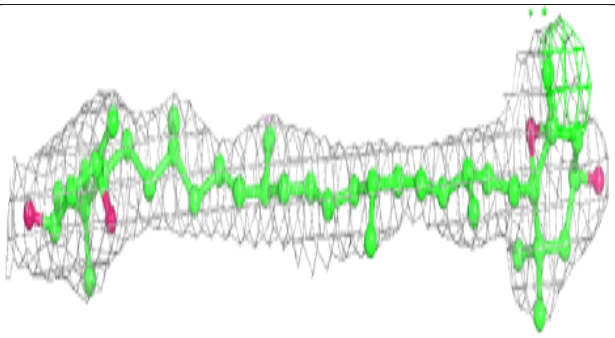


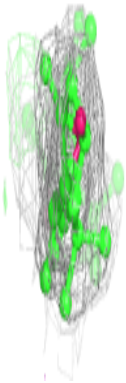


Electron density around XAT 4 317:

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

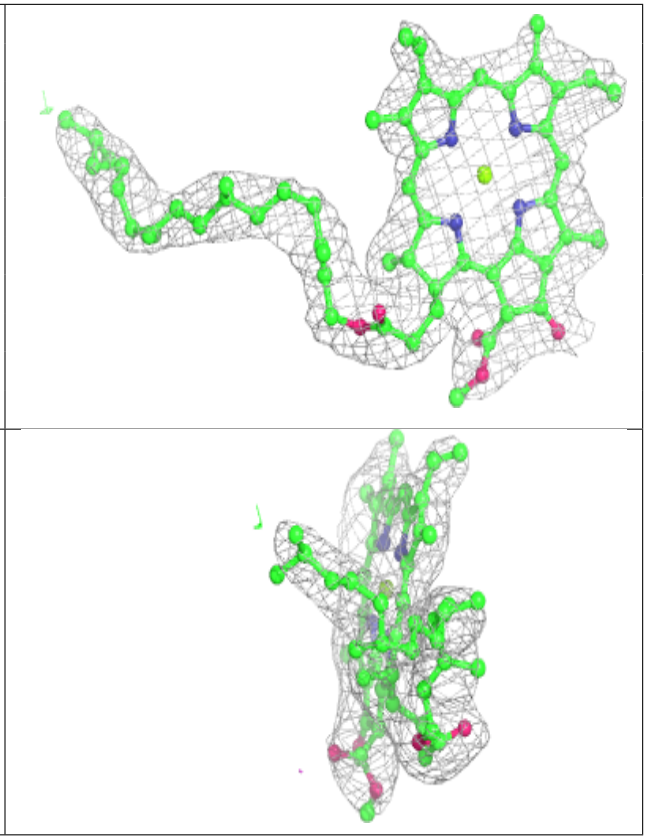






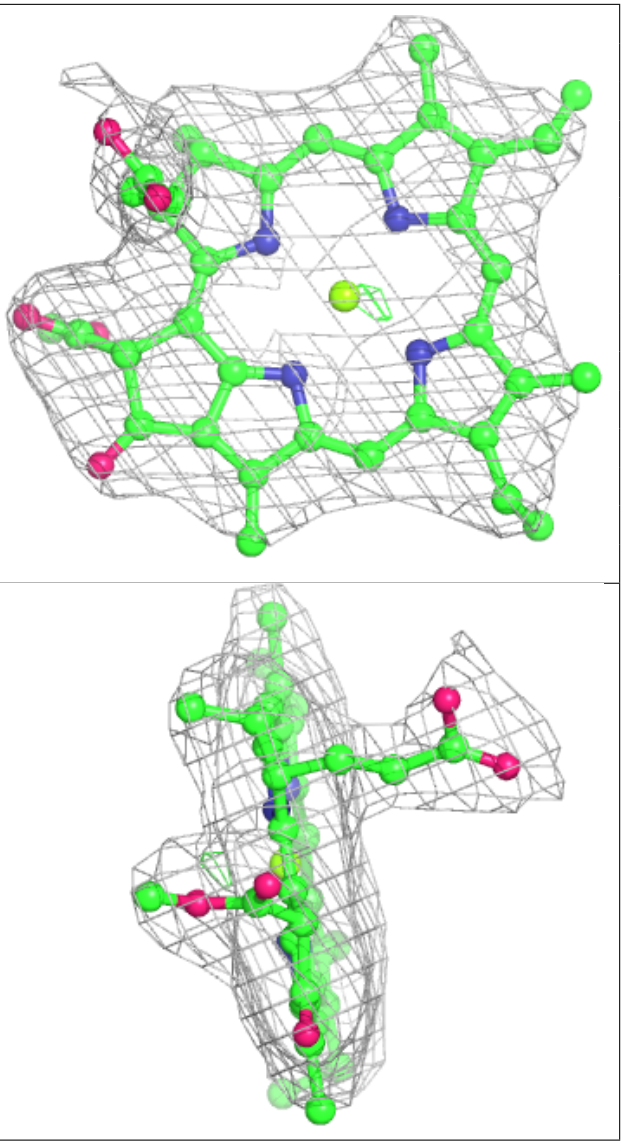
Electron density around CLA B 805:

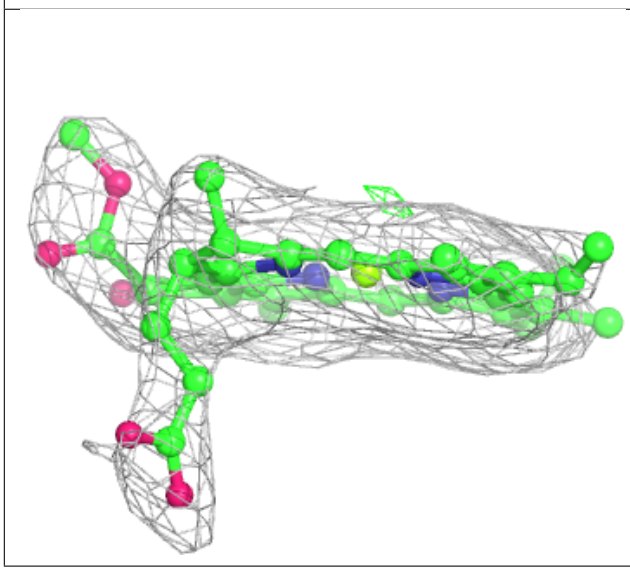
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 806:

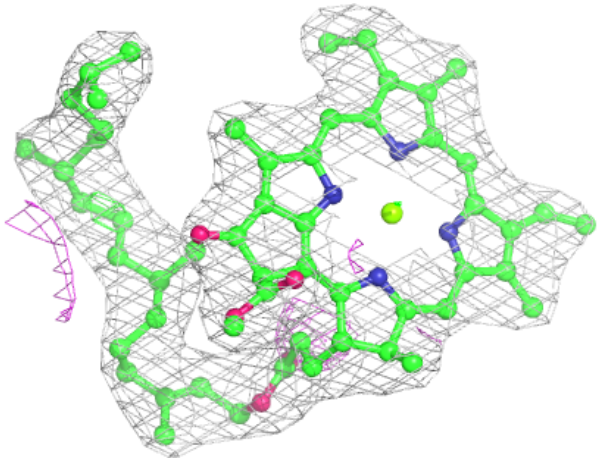
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

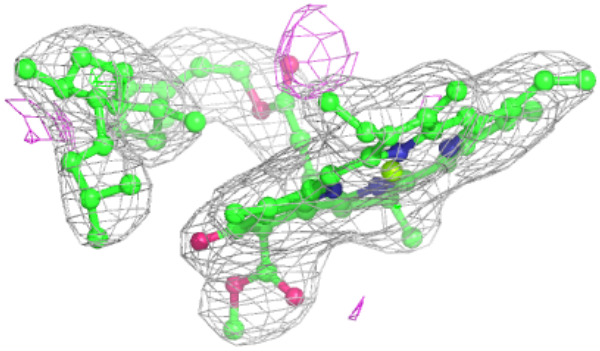


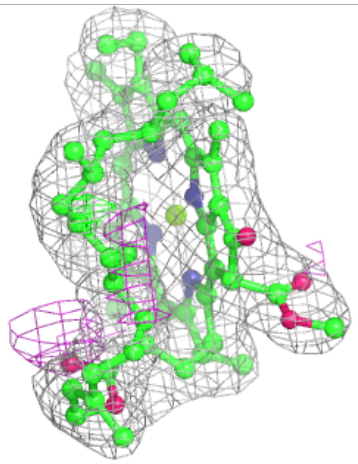


Electron density around CLA F 304:

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

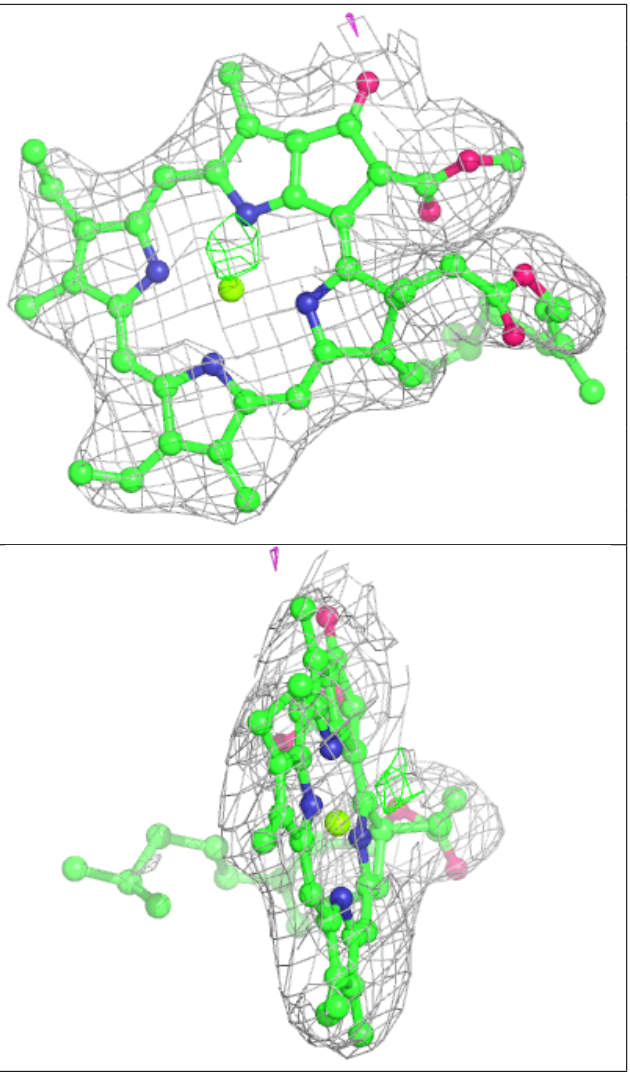






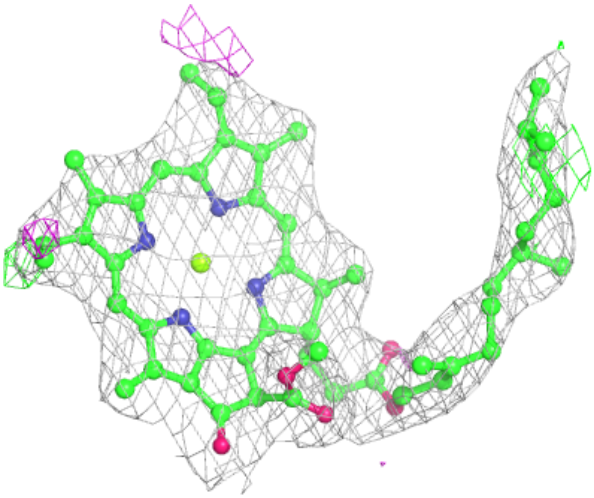
Electron density around CLA F 307:

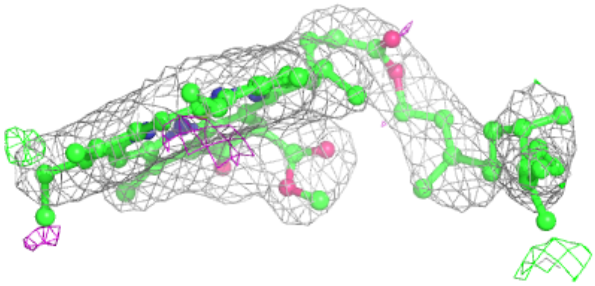
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA 4 303:

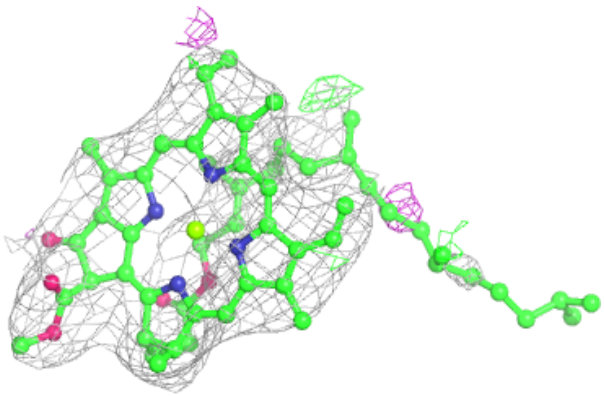
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

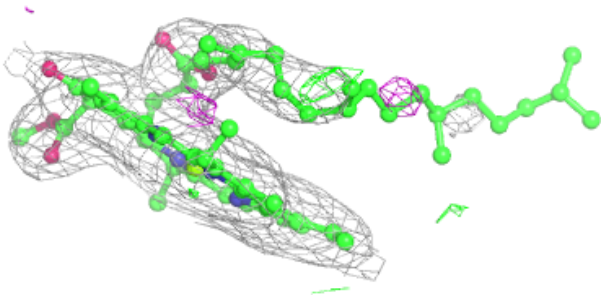


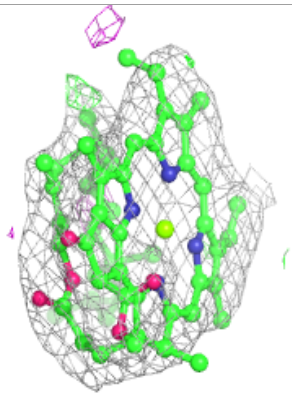


Electron density around CLA B 809:

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

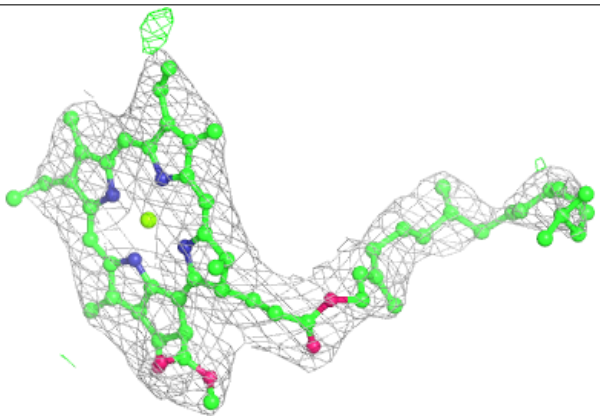


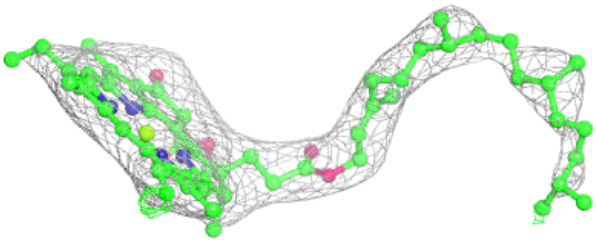


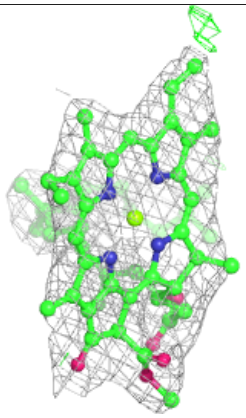


Electron density around CLA B 811:

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

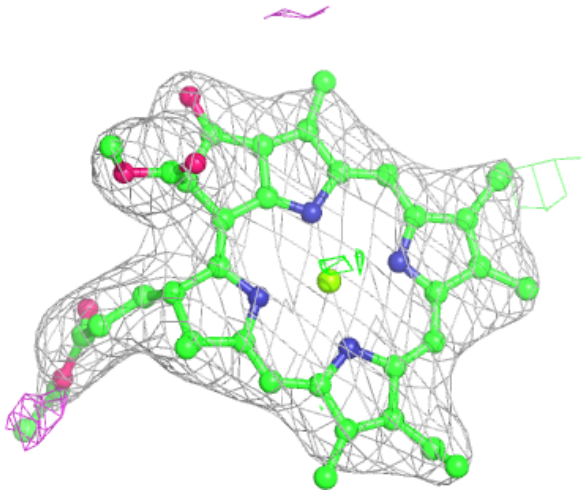


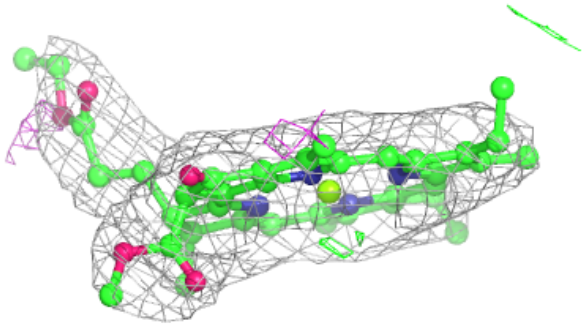


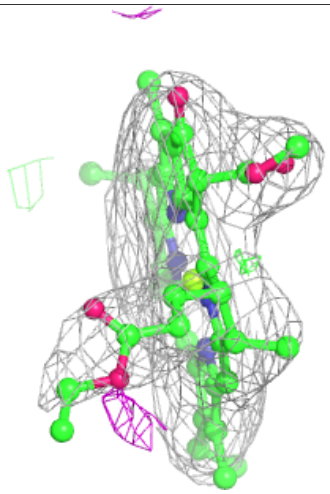


Electron density around CLA 4 314:

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

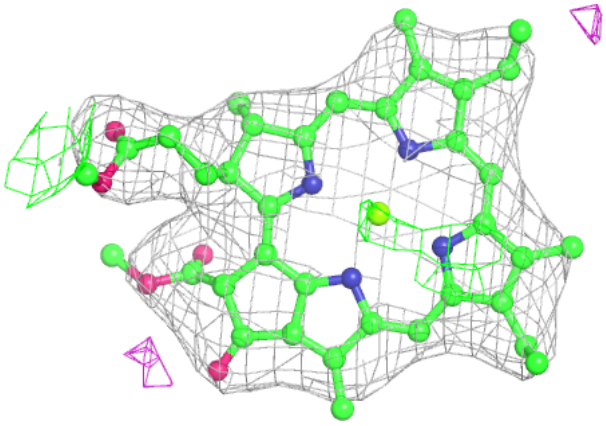


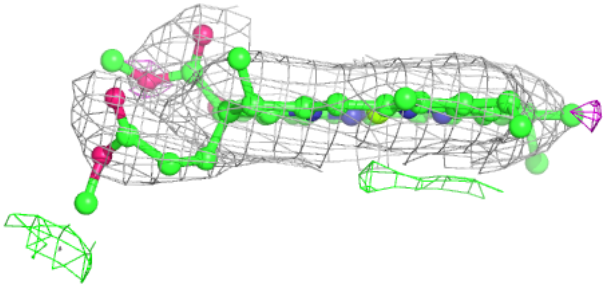


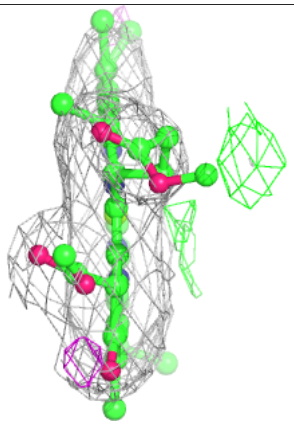


Electron density around CLA 1 313:

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

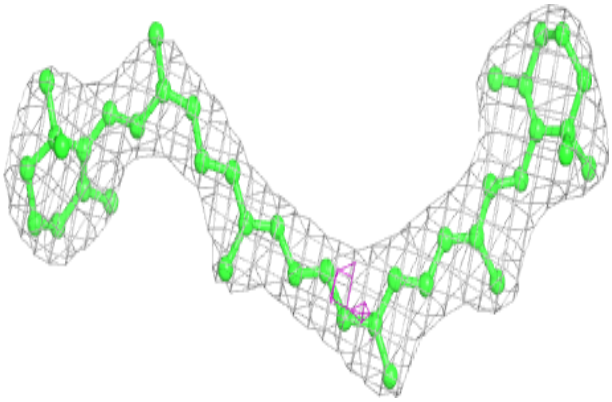


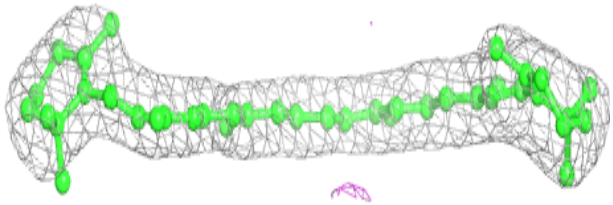


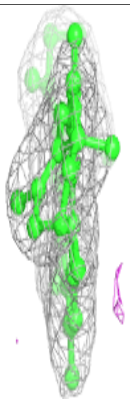


Electron density around BCR A 851:

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

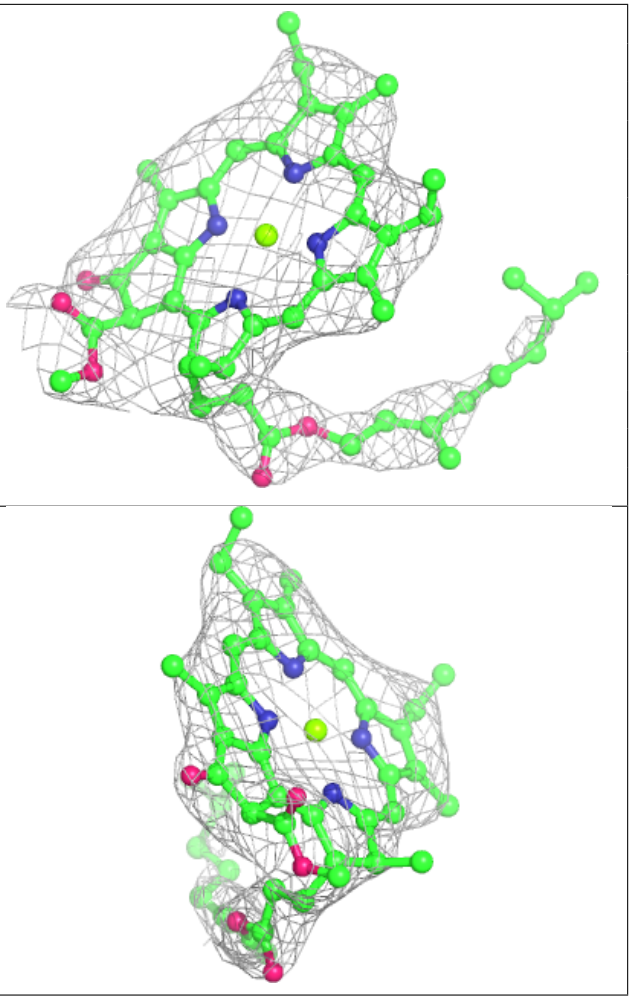






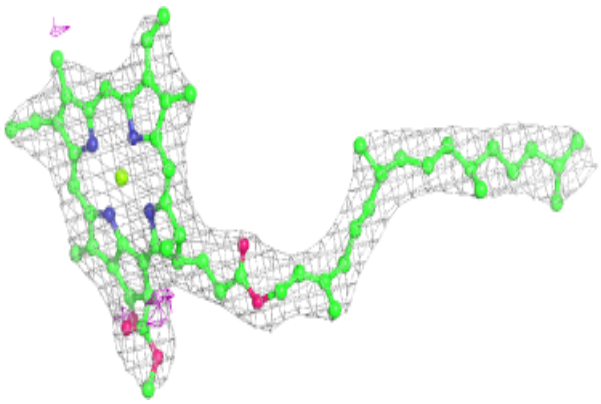
Electron density around CLA A 823:

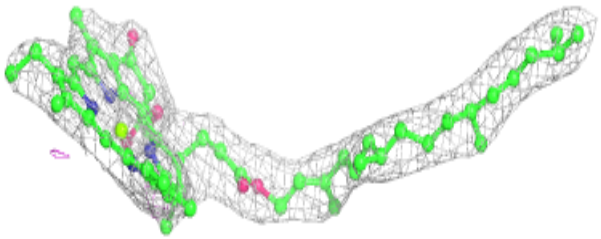
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

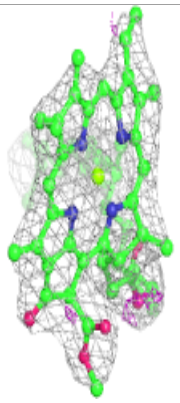


Electron density around CLA A 802:

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

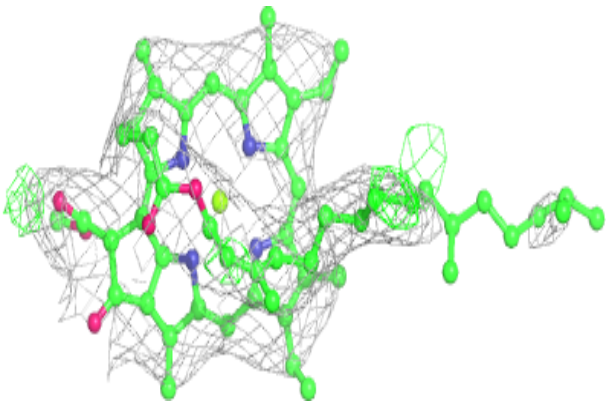


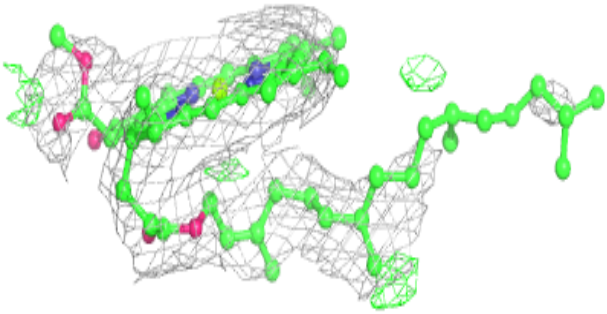


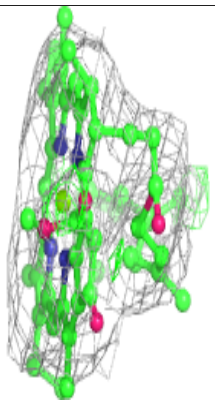


Electron density around CLA A 836:

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

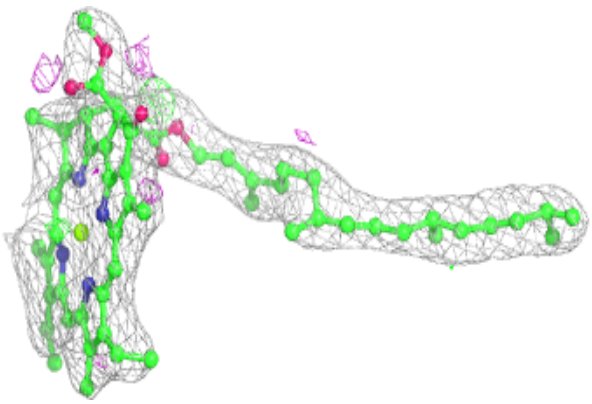


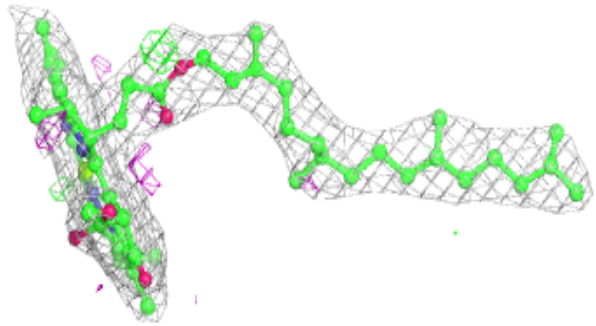


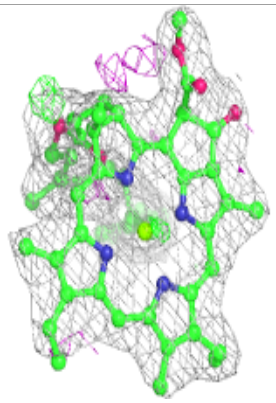


Electron density around CLA B 830:

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

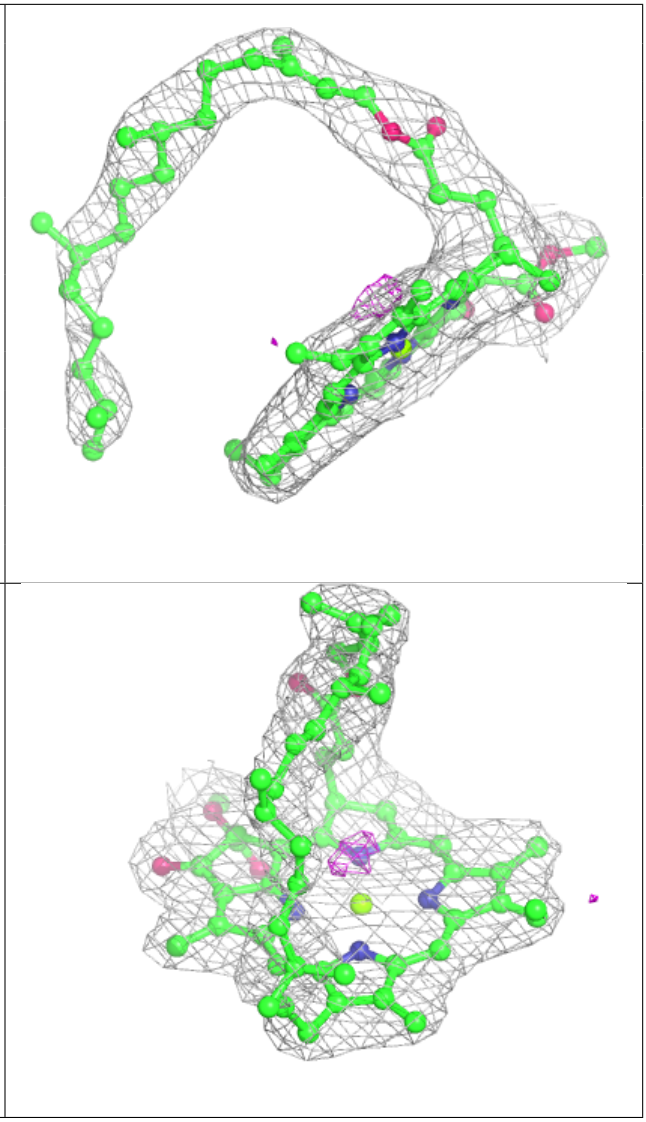






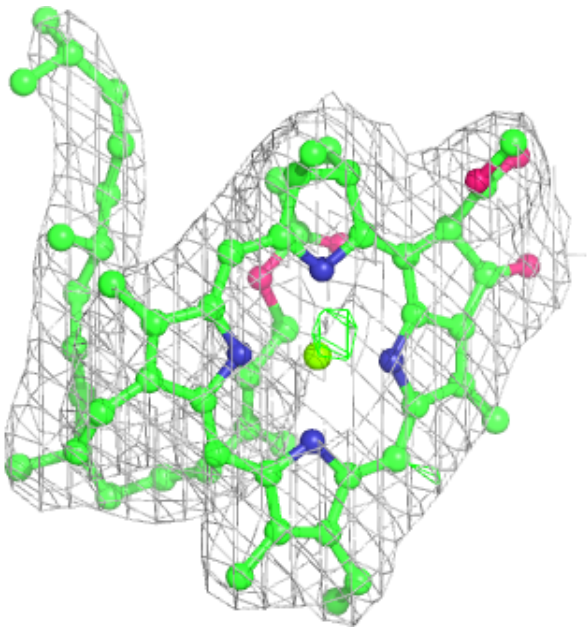
Electron density around CLA B 821:

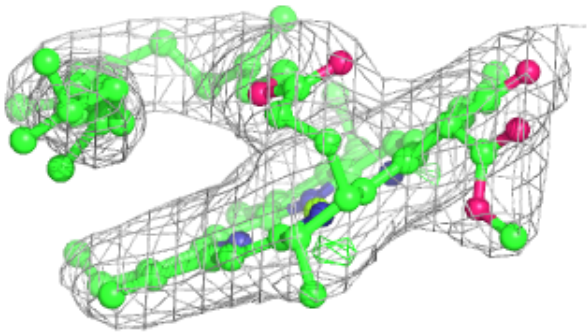
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

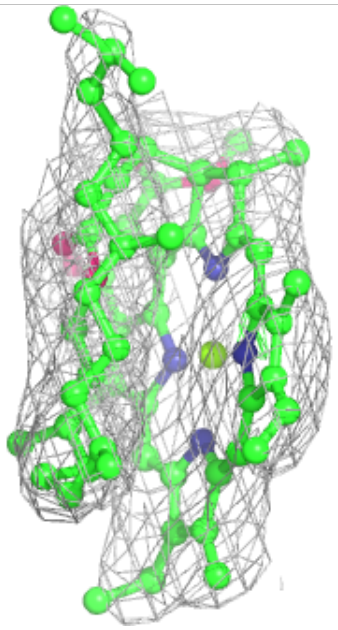


Electron density around CLA B 810:

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

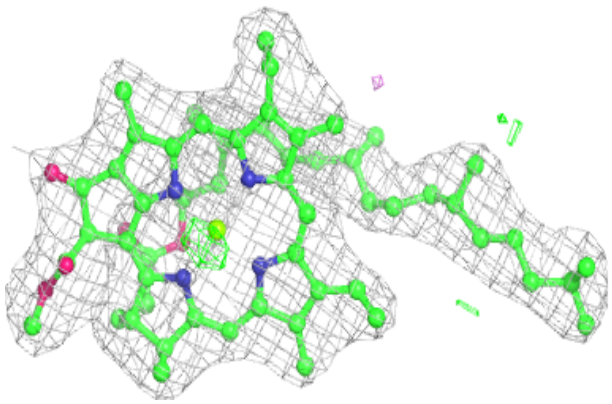


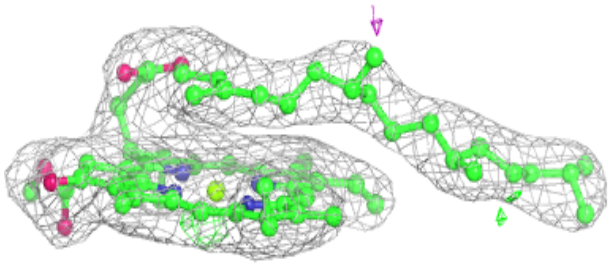


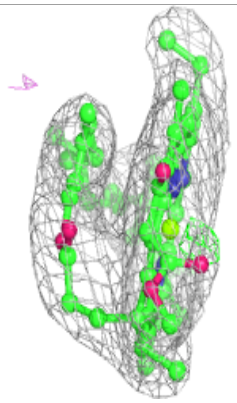


Electron density around CLA A 838:

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

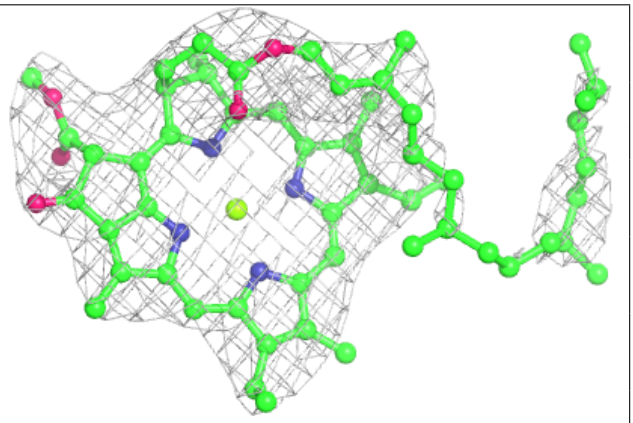


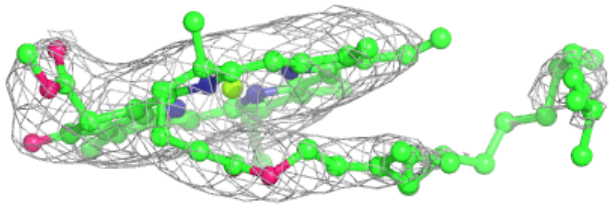


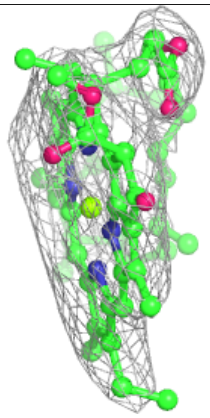


Electron density around CLA A 818:

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

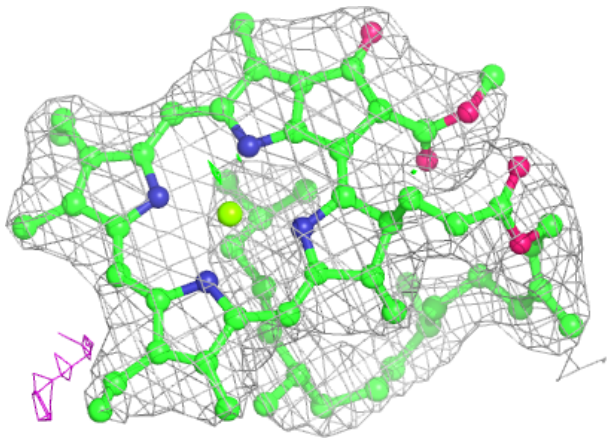


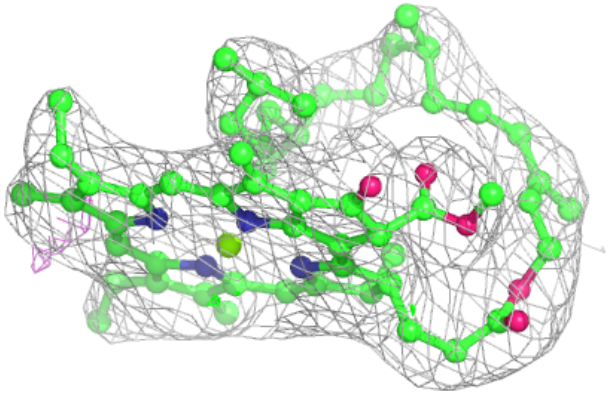


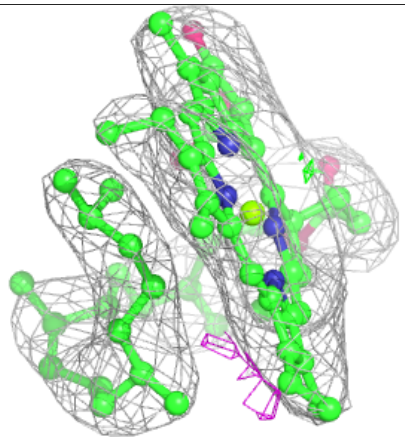


Electron density around CLA B 808:

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

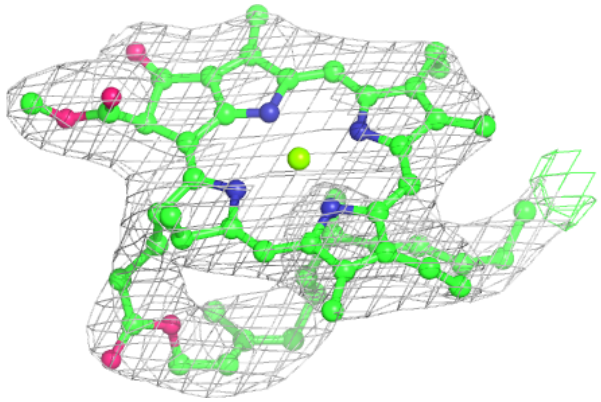


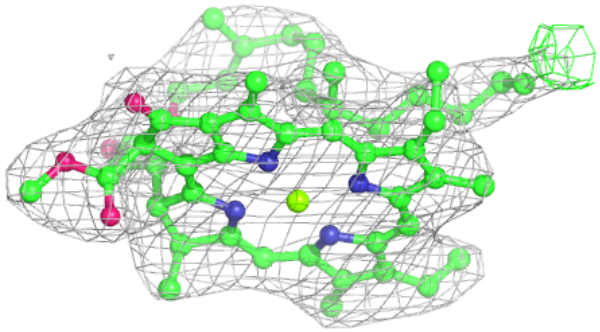


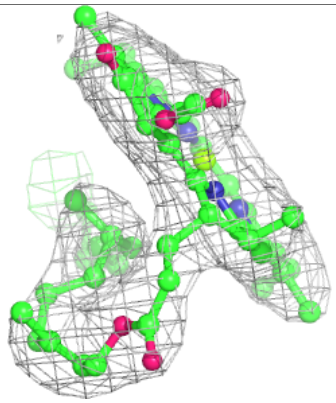


Electron density around CLA B 819:

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

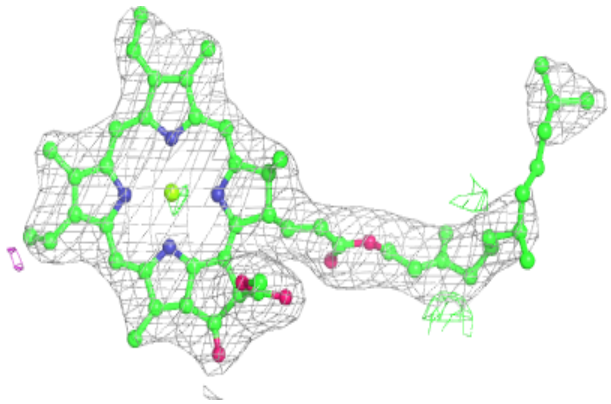


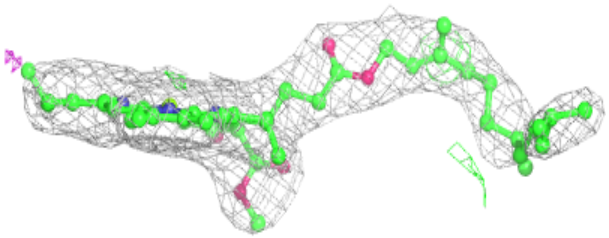


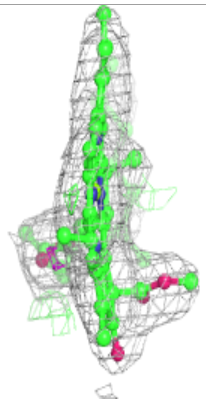


Electron density around CLA B 837:

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

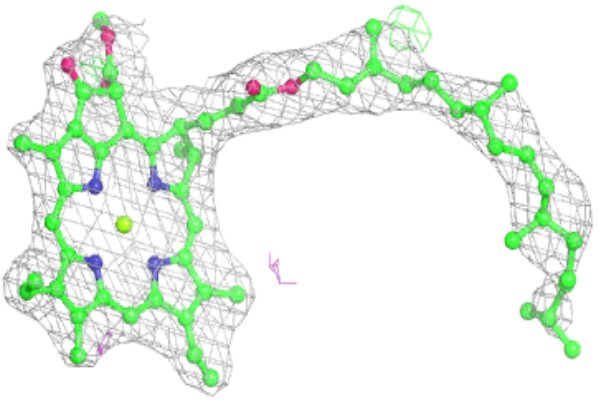


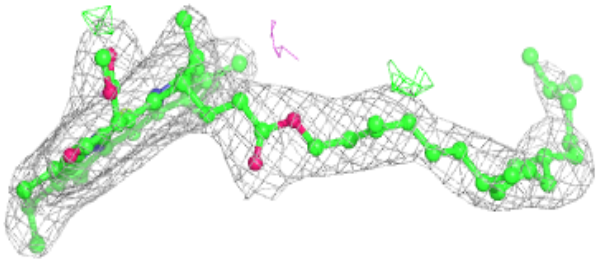


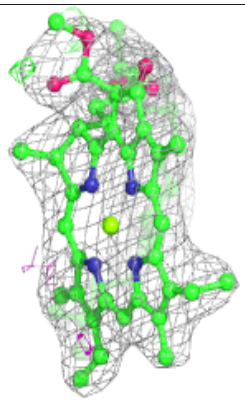


Electron density around CLA B 827:

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

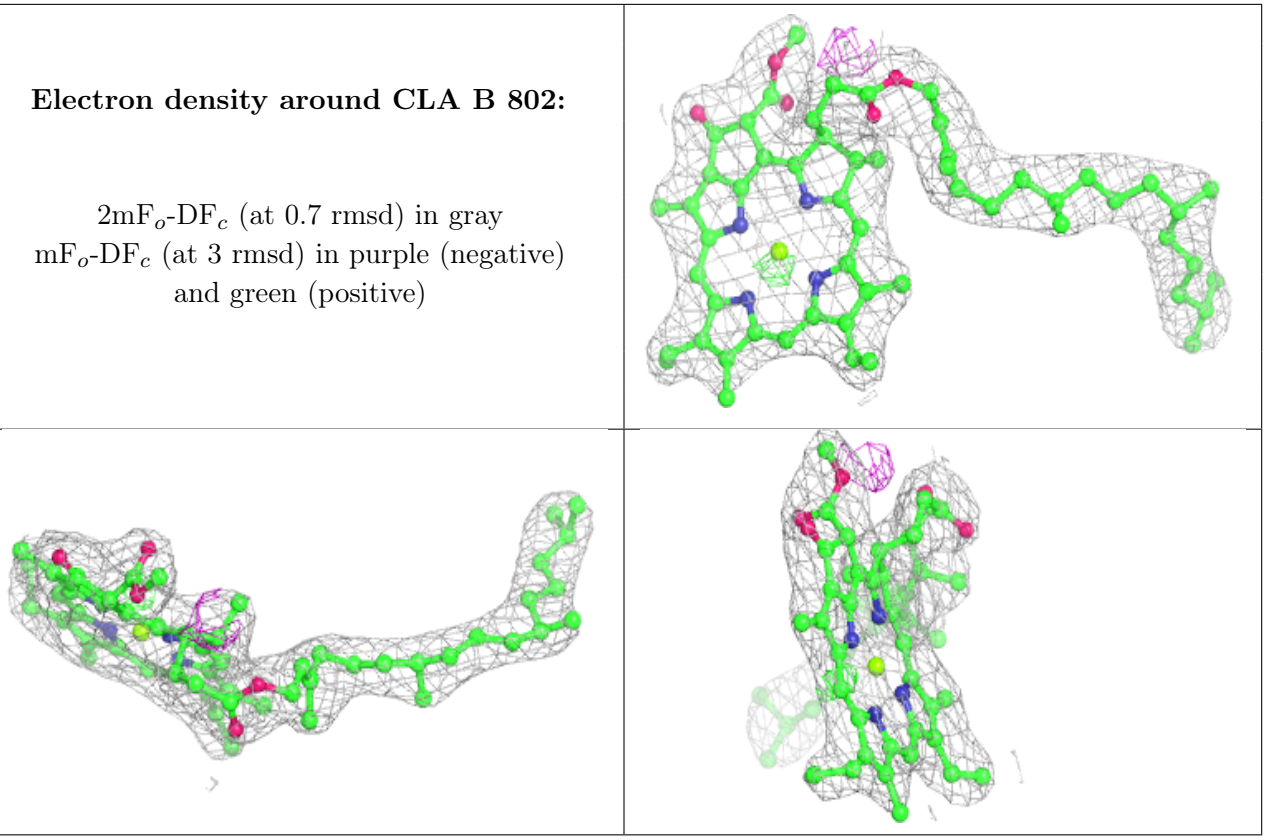






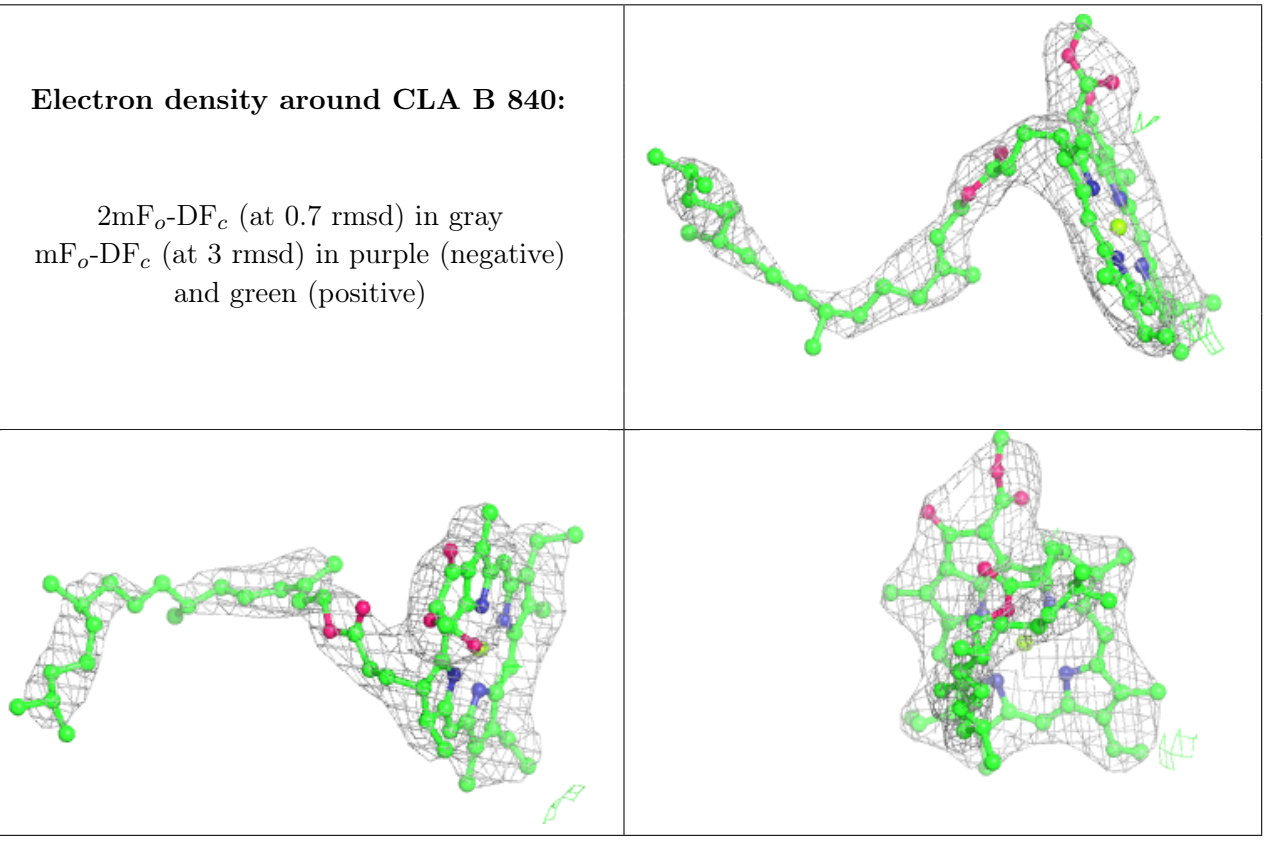
Electron density around CLA B 802:

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



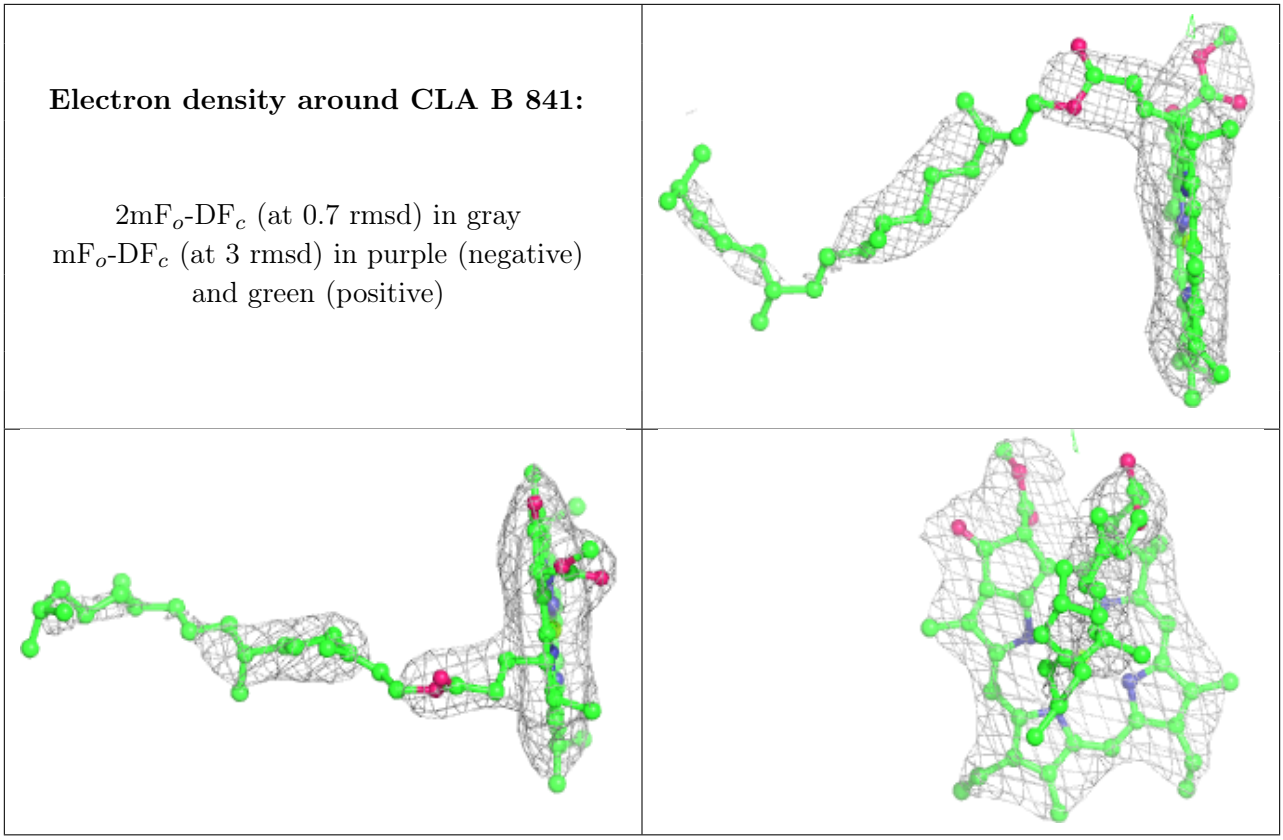
Electron density around CLA B 840:

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



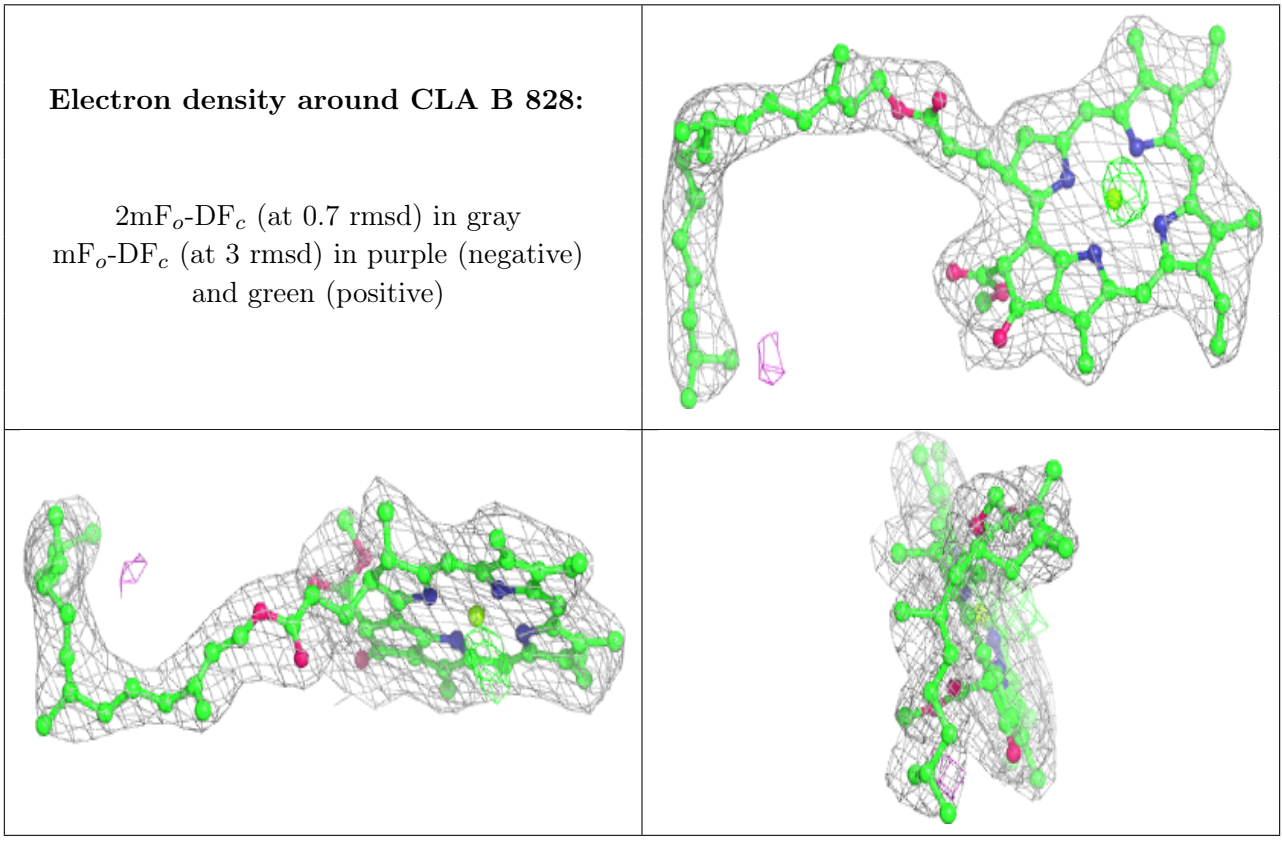
Electron density around CLA B 841:

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



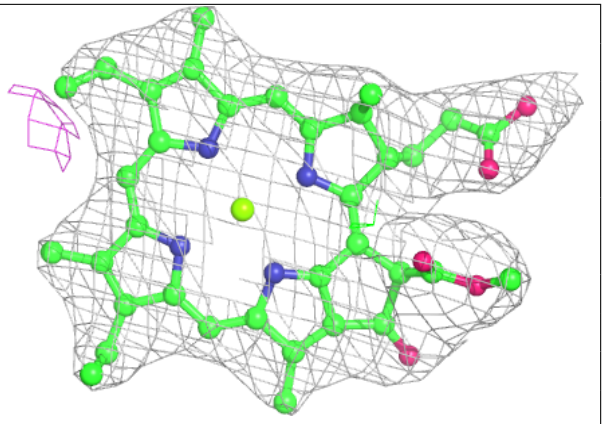
Electron density around CLA B 828:

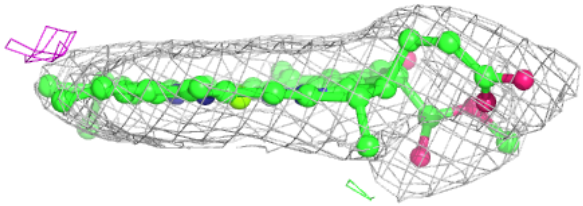
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

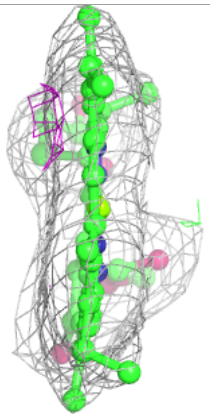


Electron density around CLA F 306:

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

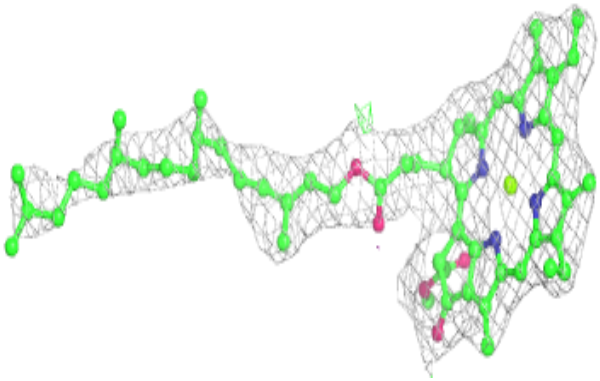


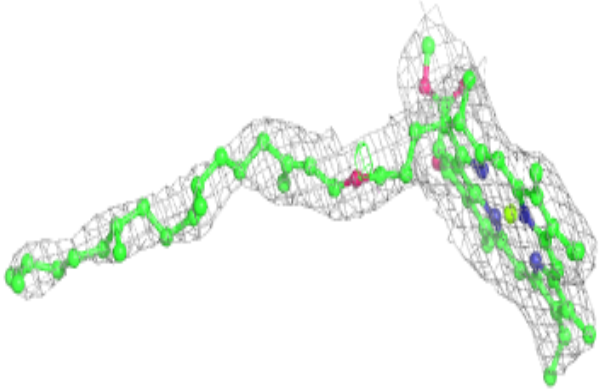


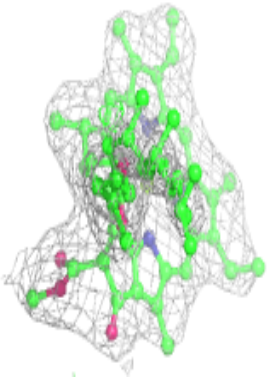


Electron density around CLA A 808:

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

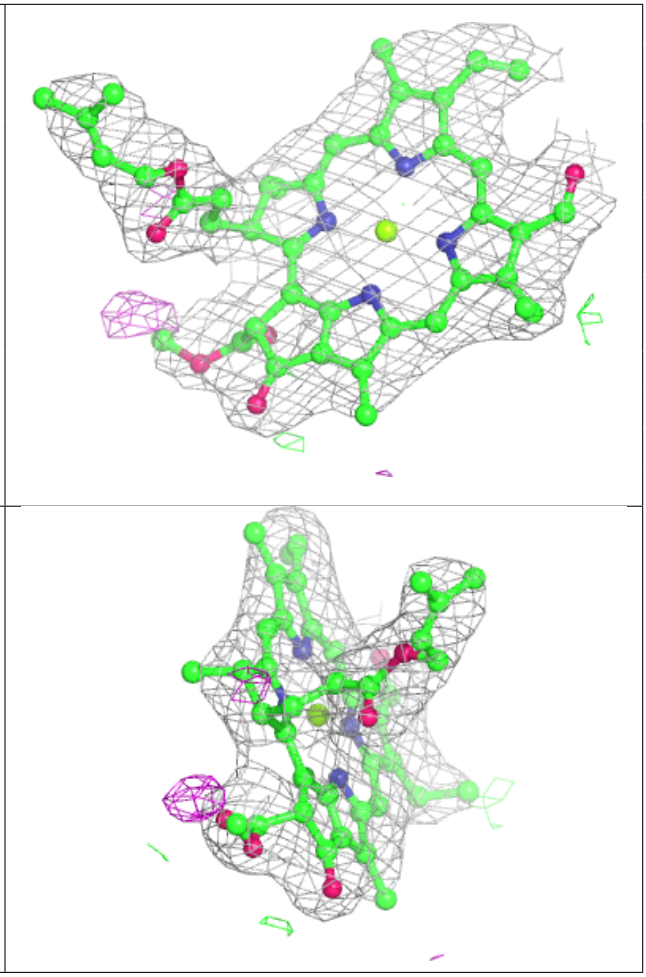






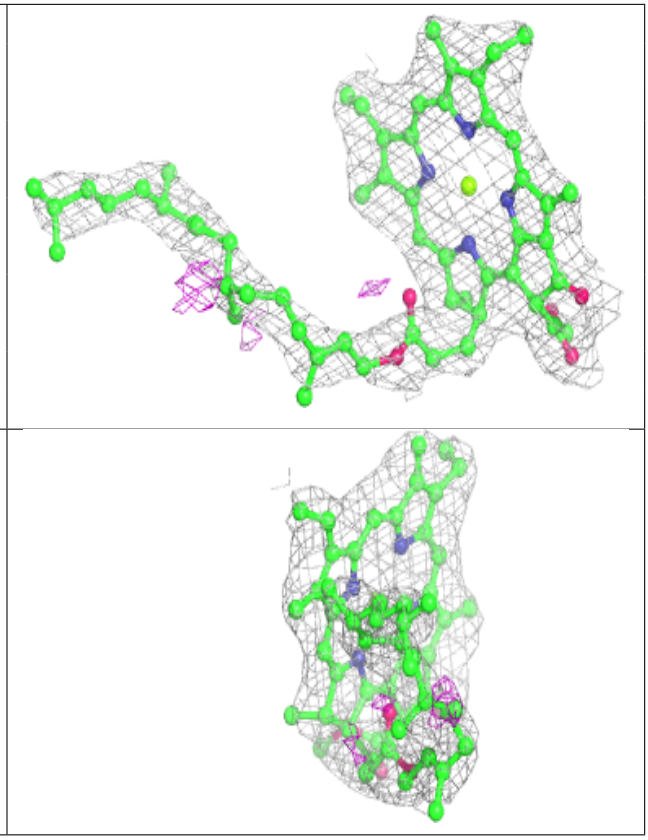
Electron density around CHL 4 307:

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



Electron density around CLA A 807:

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



6.5 Other polymers (i)

There are no such residues in this entry.